



Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 05:39 PM UTC

PDB ID : 7QJ2 / pdb_00007qj2
EMDB ID : EMD-14007
Title : Structure of recombinant human gamma-Tubulin Ring Complex 8-spoked assembly intermediate (spokes 5-12)
Authors : Zupa, E.; Pfeffer, S.
Deposited on : 2021-12-16
Resolution : 8.60 Å (reported)
Based on initial models : 6X0U, 6V6S, 7AS4, 6L81

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

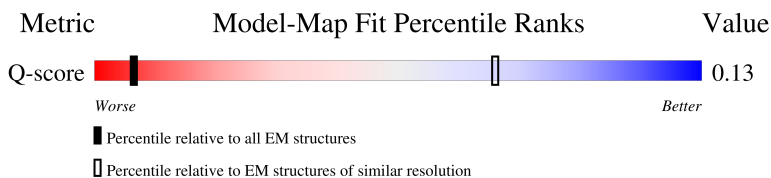
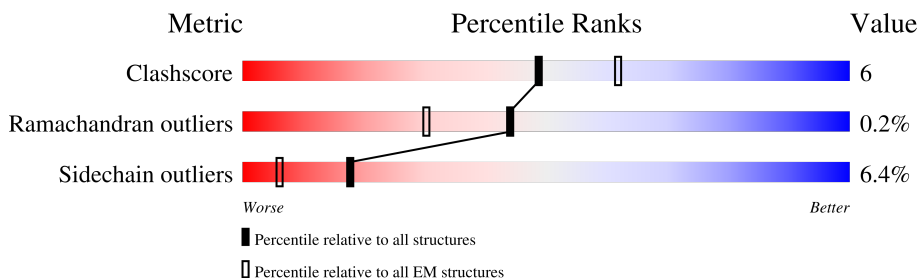
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

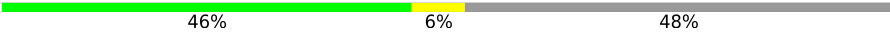
The reported resolution of this entry is 8.60 Å.

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.



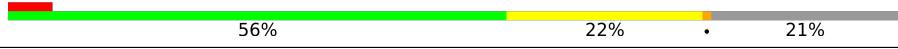
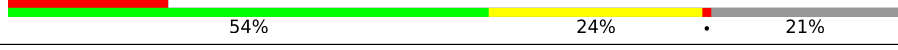
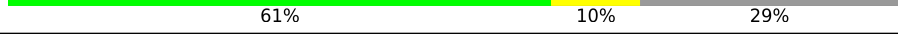
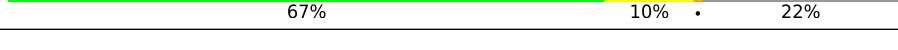
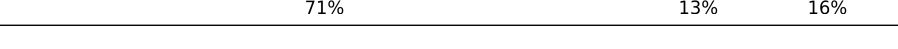
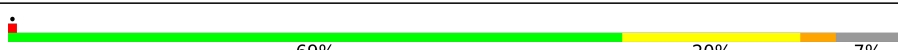
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	292 (8.10 - 9.10)

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	J	1024	 46% 6% 48%
1	l	1024	 9% 89%
2	F	907	 57% 9% 34%
2	H	907	 55% 10% 35%

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Mol	Chain	Length	Quality of chain
2	a	907	
2	j	907	
3	b	82	
3	k	82	
3	m	82	
4	E	902	
4	G	902	
5	I	667	
5	K	667	
6	L	1819	
7	S	451	
7	T	451	
7	U	451	
7	V	451	
7	W	451	
7	X	451	
7	Y	451	
7	Z	451	

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 69095 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

- Molecule 2 is a protein called Gamma-tubulin complex component 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	j	99	Total	C	N	O	S	0	0
			803	509	148	144	2		
2	F	599	Total	C	N	O	S	0	0
			4941	3151	871	894	25		
2	H	594	Total	C	N	O	S	0	0
			4907	3130	864	888	25		
2	a	116	Total	C	N	O	S	0	0
			933	591	171	169	2		

- Molecule 3 is a protein called Mitotic-spindle organizing protein 1.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	638	Total	C	N	O	S	0	0
			5202	3354	873	942	33		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	640	Total	C	N	O	S	0	0
			5206	3354	875	944	33		

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

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

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

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

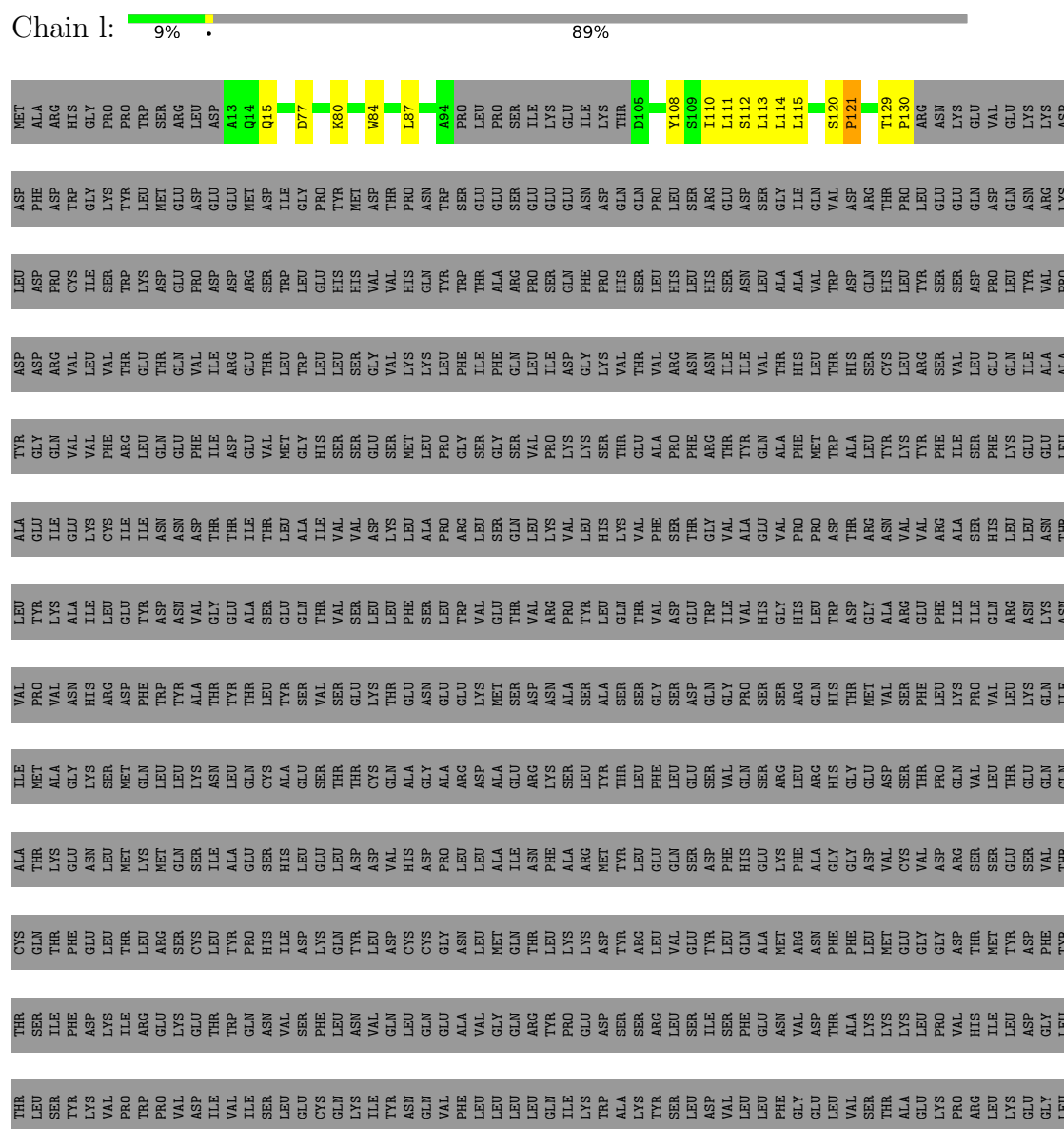
- Molecule 7 is a protein called Tubulin gamma-1 chain.

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

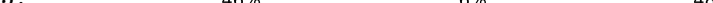
3 Residue-property plots [i](#)

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.

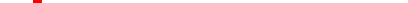
• Molecule 1: Gamma-tubulin complex component 5



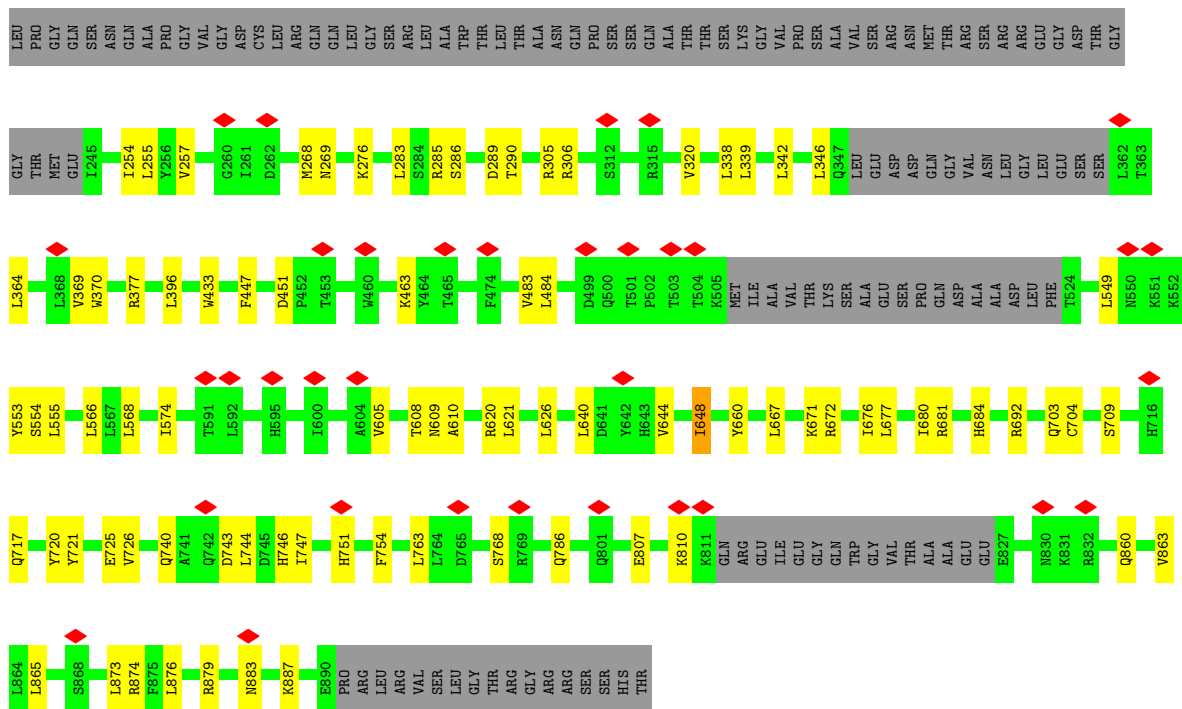
ILE	GLU	LYS	MET	GLU	ASP	SER	PHE	LYS	ASN	CYS	HIS	MET	PHE	LEU	VAL	THR	ILE	LEU	ASN	LYS	ALA	VAL	CYS	ARG	GLY	SER	PHE	PRO	HIS	LEU	GLU	SER	LEU	ALA	LEU	SER	LEU	ALA	GLY	GLU	GLN	SER
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----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

Chain J:  46% 6% 48%

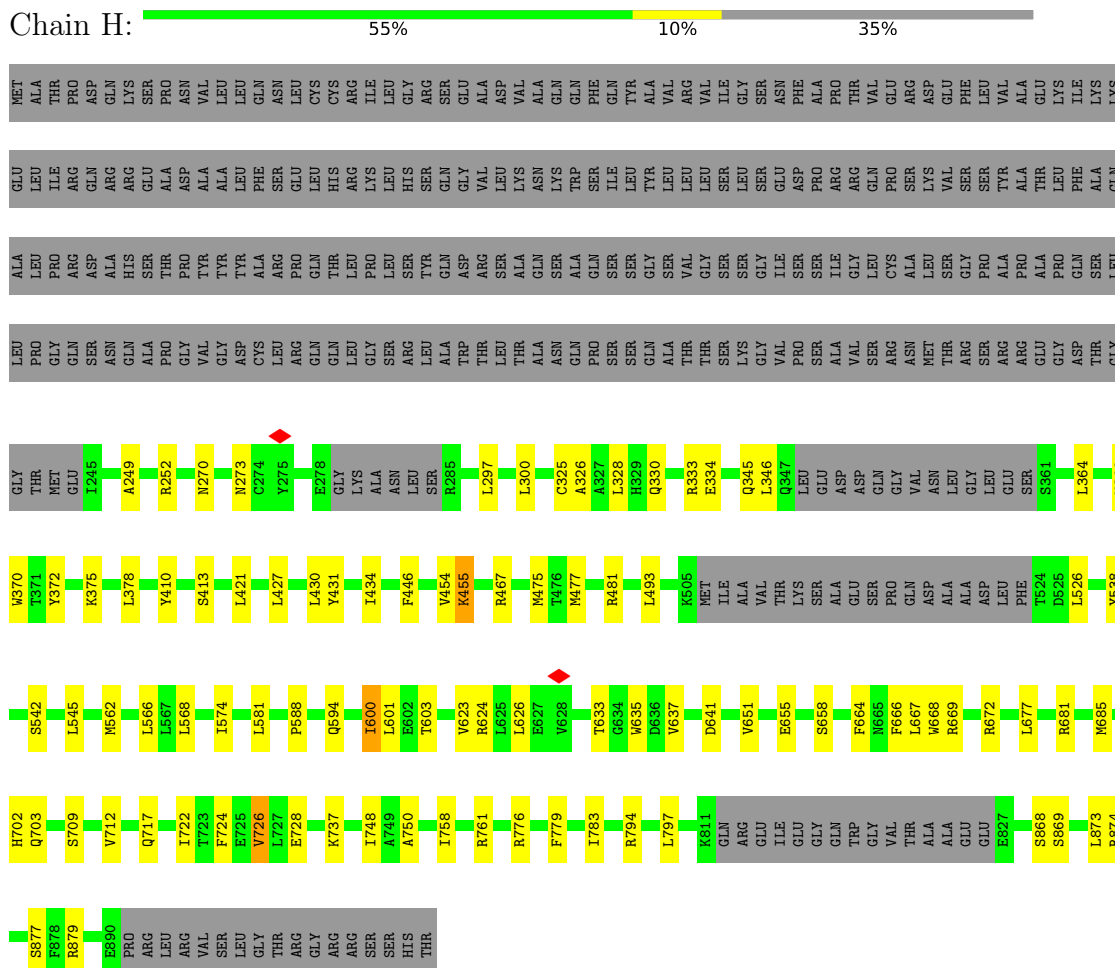
A953	L828	D713	THR	PRO	PRO	PRO	PRO	V294	ASP	PRO	ILE	MET
K956	L829	M723	LYS	SER	SER	ASP	ASP	T295	SER	SER	GLU	ALA
K968	Q830	M723	GLU	SER	GLU	T427	GLY	V296	GLY	ASN	THR	HIS
G968	I831	L728	ASN	ARG	ASN	T448	ILE	R297	ILE	SER	ILE	GLY
G968	K832	L728	LEU	GLN	GLN	D448	GLN		GLN	SER	TYR	PRO
K835			MET	MET		ASN	ASN	L305	VAL	ASP	GLY	TRP
			GLY	GLY	T647	VAL	VAL	T306	ASP	GLU	ILE	TRP
	L842	D733	MET	M548	GLY	GLY	GLY	H307	THR	THR	TYR	ARG
	PHE	D733	SER	SER	ALA	ALA	ALA	L310	PRO	PRO	GLU	ARG
THR	GLY		ILE	GLY	SER	SER	SER	R311	LEU	ARG	LYS	LEU
GLU	ALA	Y739	ALA	L572	E455	E455		S312	GLU	ASN	PHE	ASP
LEU	LEU		GLU	GLN				E315	GLN	GLU	VAL	ALA
VAL	VAL	D744	SER	CYS	LYS	I493	LYS		ASP	GLU	ILE	GLN
MET	GLU		HIS	ALA				G336	GLN	SER	VAL	SER
GLU	THR		LEU	GLU	THR	F496	THR		ASN	LYS	ASP	ARG
ALA	ALA		E637	SER	ASN	ASN	LYS	HIS	ASN	LYS	ASP	ARG
THR	GLU			THR	LYS	LYS	ASN	SER	ARG	LYS	LEU	ASP
GLU	LYS	Y641	THR	THR	ASN	ASN	ASN	SER	LYS	ASP	SER	VAL
PHO	PHO		CYS	CYS	VAL	VAL	VAL	GLU	LEU	LYS	LYS	ARG
ARG	ARG		GLN	GLN	PRO	PRO	PRO	SER	ASP	PHE	ALA	GLU
GLY	LEU	THR	ALA	ALA	VAL	VAL	VAL	MET	PRO	ASP	ALA	LEU
SER	LYS	D753	PHE	GLY	GLY	ASN	GLY	LEU	CYS	TRP	SER	VAL
GLU	GLY		ALA	ALA	ARG	HIS	PRO	PRO	ILE	ILE	GLY	ARG
F1007	F1007	E764	ARG	ARG	ALA	ARG	GLY	GLY	SER	SER	LYS	GLY
P1008	LEU		ALA	ASP	ASP	ASP	SER	SER	TRP	TRP	ARG	VAL
H1009	ILE		TYR	ALA	ALA	PHE	GLY	GLY	LYS	LYS	LEU	ALA
S1012	HIS		GLY	GLY	GLY	THR	SER	SER	ASP	MET	THR	GLY
L1013	GLN		GLN	ARG	LYS	ALA	ALA	VAL	GLU	GLU	GLU	LEU
	ASP		SER	LYS	SER	THR	THR	LYS	P210	ASP	GLU	GLN
S1016	LEU		THR	THR	THR	THR	THR	LYS		GLU	PHE	ASP
LEU	THR		ASP	LEU	LEU	TYR	TYR	LYS	R213	GLU	GLU	GLY
MET	VAL		PHE	SER	GLY	GLY	SER	SER	S214	ASN	LEU	GLY
ALA	ALA		HIS	THR	VAL	LEU	LEU	THR	W215	ASP	ALA	ALA
GLY	GLN		GLY	LEU	GLY	TYR	TYR	GLY		ILE	PRO	PRO
MET	PHE		LYS	PHE	LYS	SER	VAL	ALA	W225	GLY	LEU	ASN
GLU	GLY		PHE	LEU	LEU	VAL	VAL	P357		PRO	PRO	PHE
GLN	PHO		ALA	GLY	GLY	SER	GLY		S235	TYR	SER	GLN
SER	GLN		GLY	SER	SER	GLU	SER	Y369	L236	MET	ILE	LEU
	GLN		GLY	VAL	VAL	LYS	LYS		H237	ASP	LYS	ALA
	GLY		GLY	GLN	GLN	THR	THR	K376	L238	THR	GLY	LEU
	PRO		ASP	SER	SER	GLU	ASN		L242	PRO	ILE	ASN
VAL	VAL		CYS	ARG	ARG	ASN	ASN	E381		ASN	LYS	ASN
ARG	ARG		VAL	LEU	LEU	GLU	GLU	K384	W245	GLU	THR	PHE
GLN	GLN		ASP	ARG	HIS	LYS	LYS		W246	SER	ASP	ALA
			SER	GLY	GLY	MET	MET	R368		GLY	HIS	ASN
	Q879		SER	GLU	ASP	SER	ASP	ASN	P255	SER	TYR	PHE
I880	I880		ALA	LYS	ASP	ASN	ASN		L256	GLU	SER	ARG
			LYS	ASP	SER	ASN	ASN		L257	GLU	ILE	PHE
			LYS	THR	THR	ALA	ALA		V258	GLU	LEU	HIS
			LEU	PRO	SER	THR	SER		I393	ASN	SER	ASN
			CYS	GLN	ALA	ALA	ALA		I271	ASP	LEU	PHE
			VAL	VAL	VAL	SER	SER		L412	GLN	LEU	LEU
	I901		HIS	LEU	LEU	SER	SER		K283	GLN	LEU	LEU
			THR	THR	THR	GLY	GLY		V415	PRO	CYS	VAL
	L942		F684	GLN	GLN	SER	SER		F287	LEU	LEU	ASN
			L796	GLN	GLN	ASP	ASP		Q288	SER	SER	ASN
				GLN	GLN	THR	THR		E422	ARG	ASP	HIS
	V947		R825	GLN	GLN	LYS	LYS		V400	THR	THR	SER

Chain j:  10% 89%

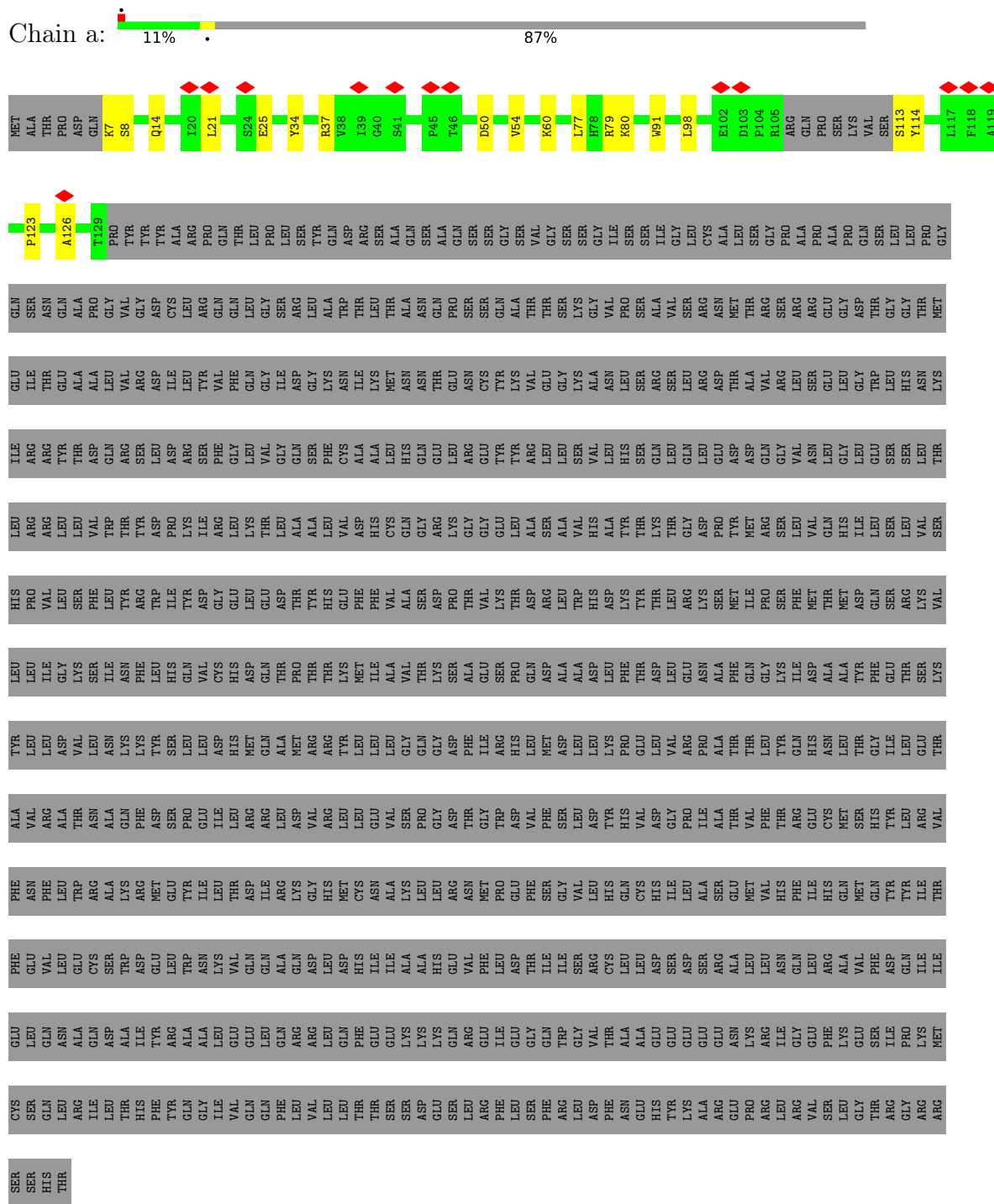




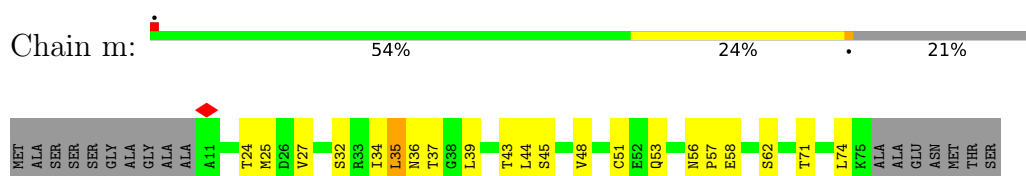
- Molecule 2: Gamma-tubulin complex component 3



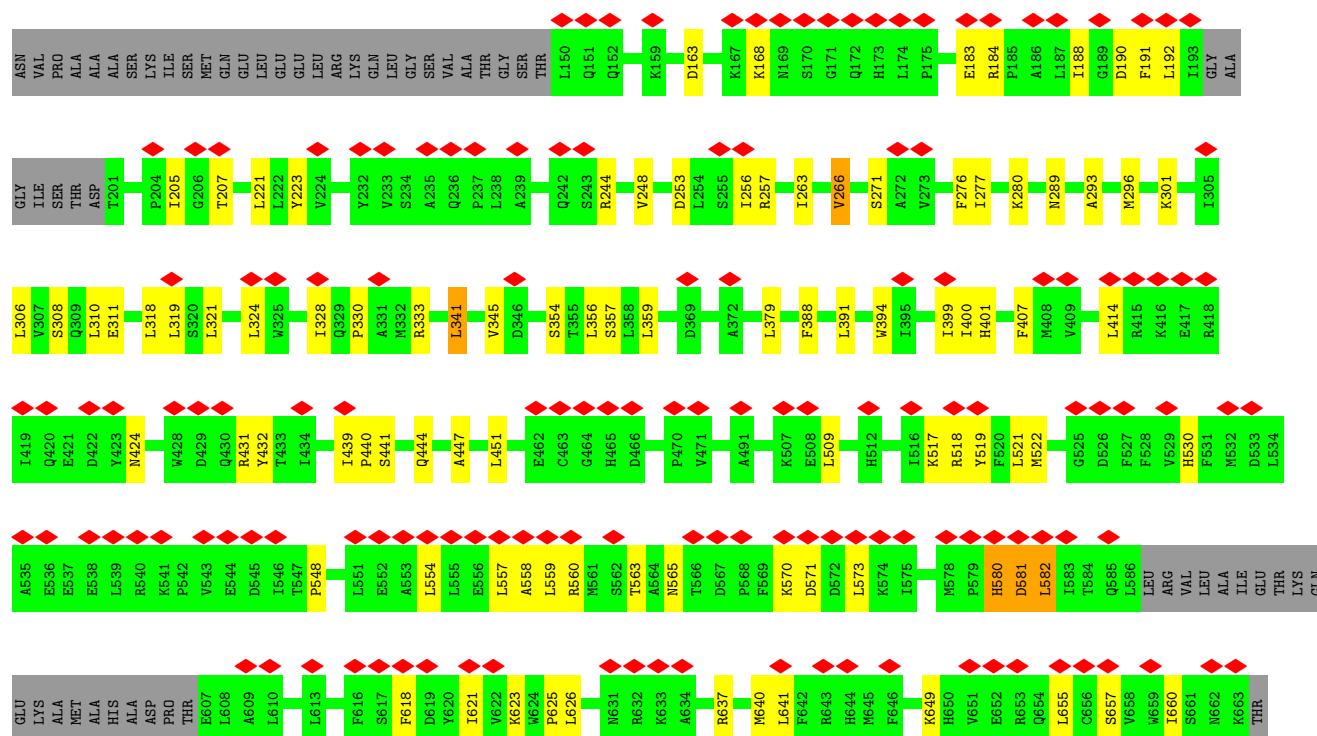
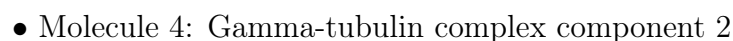
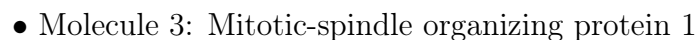
• Molecule 2: Gamma-tubulin complex component 3



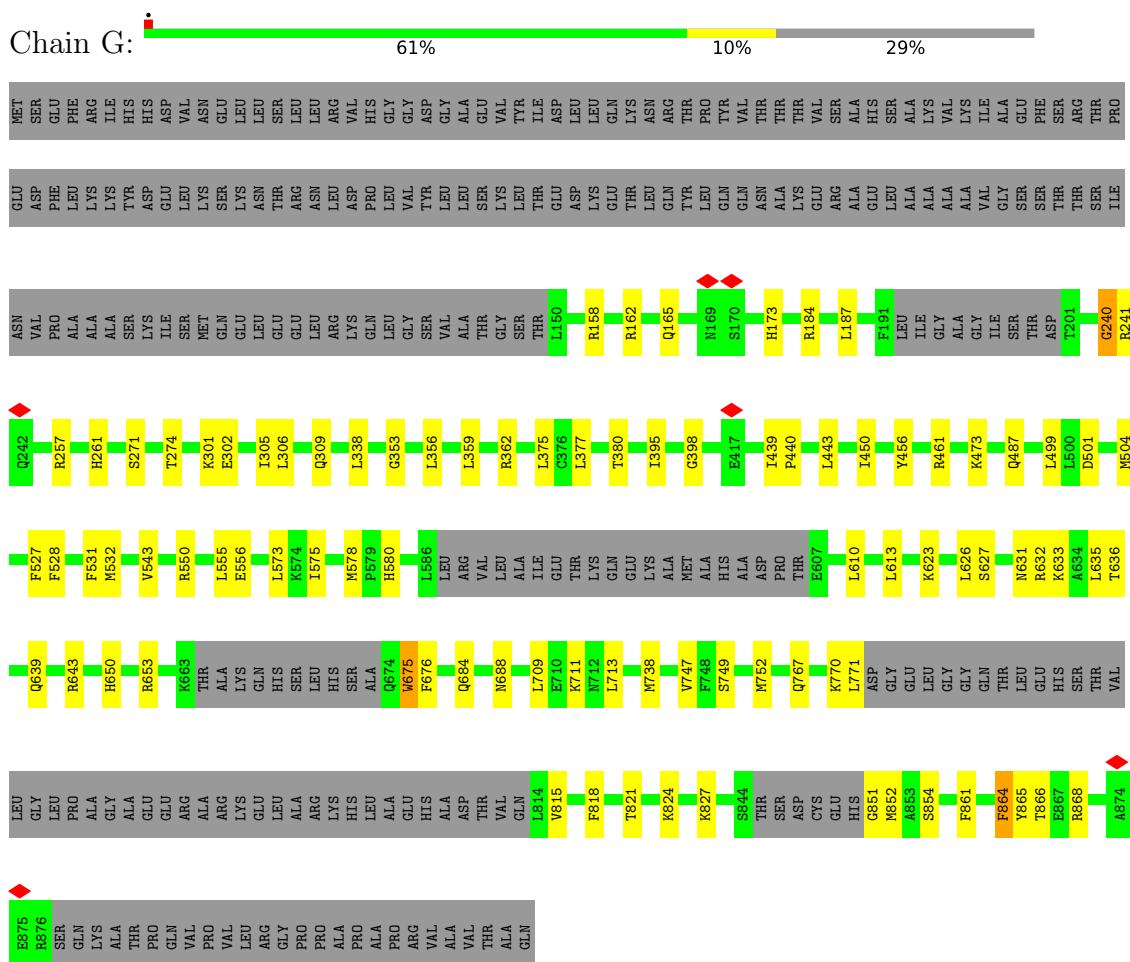
• Molecule 3: Mitotic-spindle organizing protein 1



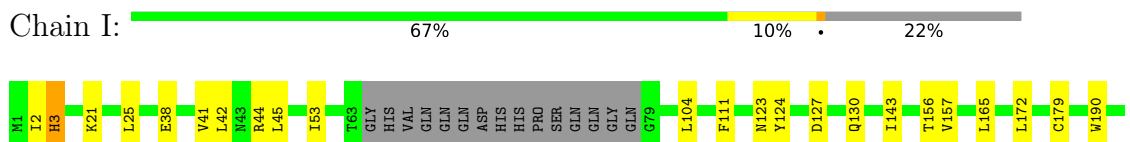
Chain k: 18% 54% 24% 21%



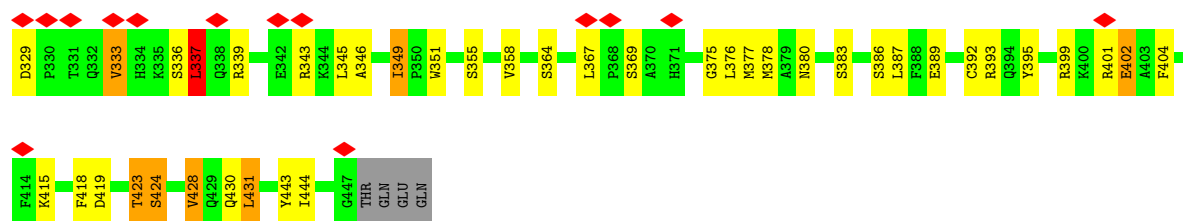
- Molecule 4: Gamma-tubulin complex component 2



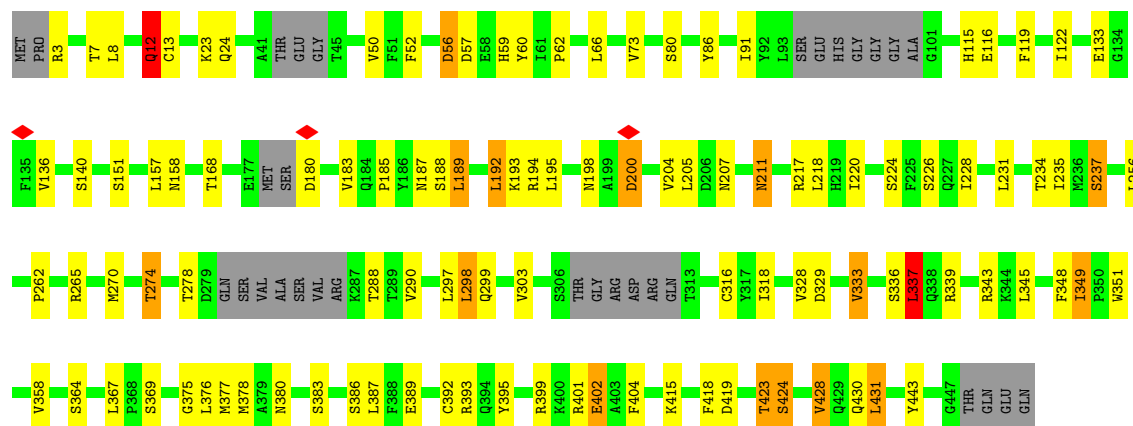
- Molecule 5: Gamma-tubulin complex component 4



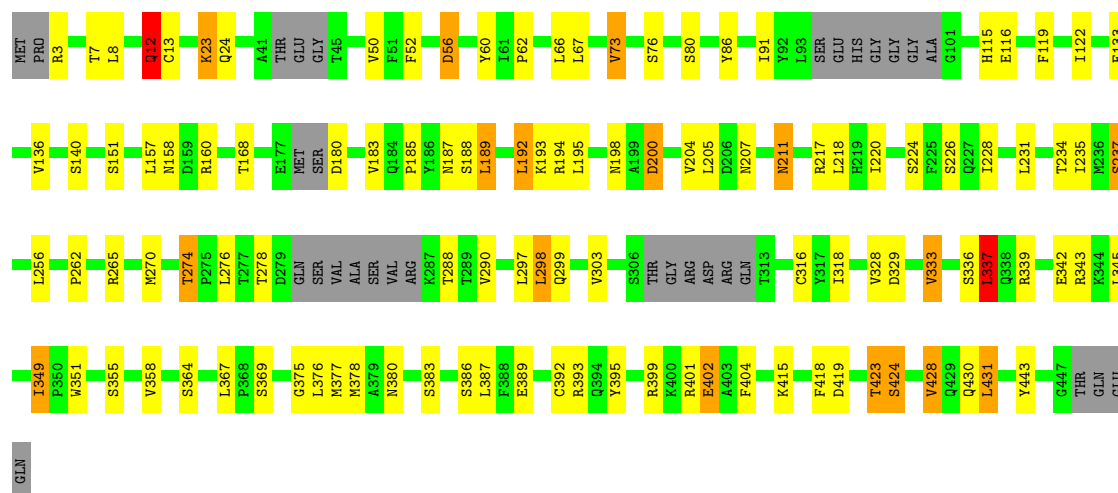




• Molecule 7: Tubulin gamma-1 chain

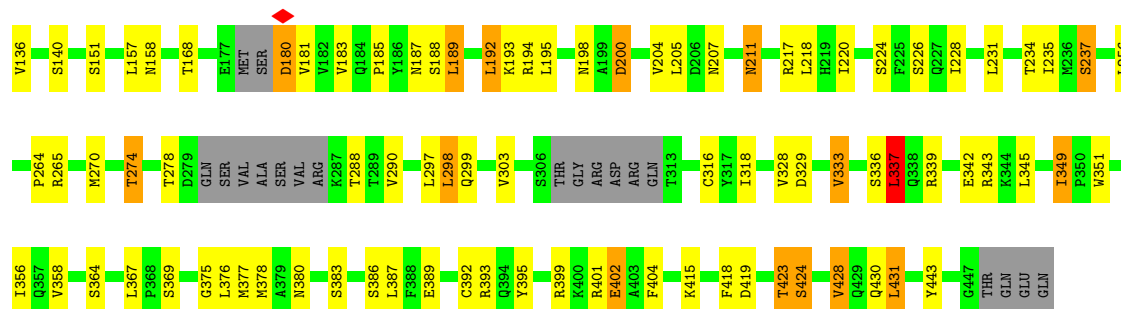


• Molecule 7: Tubulin gamma-1 chain

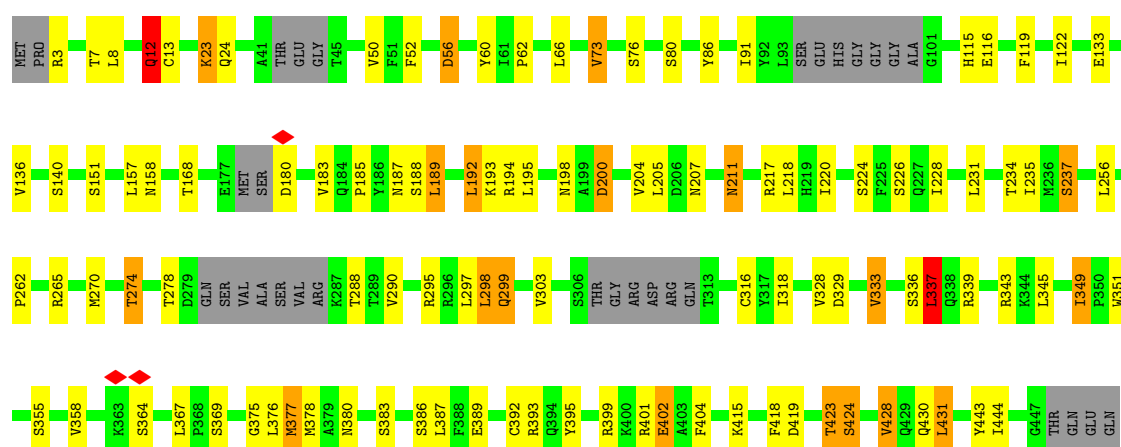


• Molecule 7: Tubulin gamma-1 chain

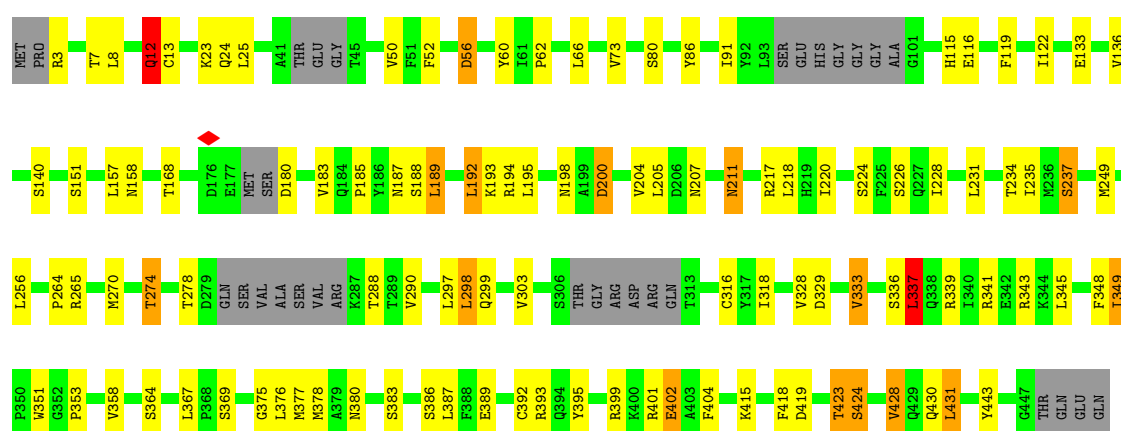




• Molecule 7: Tubulin gamma-1 chain

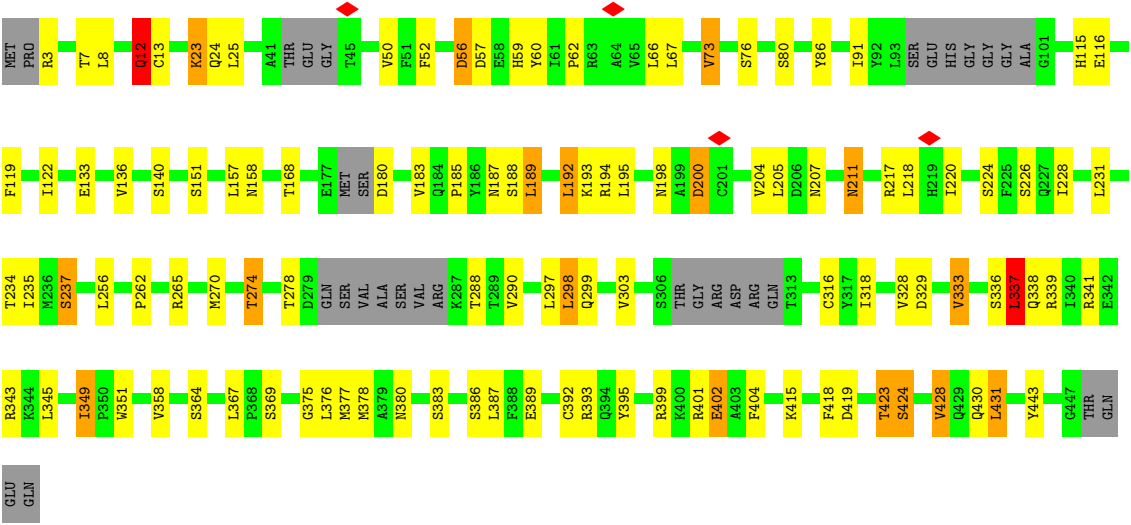


• Molecule 7: Tubulin gamma-1 chain



• Molecule 7: Tubulin gamma-1 chain





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	10965	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	0.239	Depositor
Minimum map value	-0.083	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.0287	Depositor
Map size ($\text{\AA}$)	532.0, 532.0, 532.0	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	2.66, 2.66, 2.66	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	J	0.41	3/4525 (0.1%)	0.78	9/6119 (0.1%)
1	l	0.29	0/863	0.80	2/1166 (0.2%)
2	F	0.33	0/5044	0.73	3/6809 (0.0%)
2	H	0.36	0/5009	0.73	3/6761 (0.0%)
2	a	0.29	0/948	0.66	0/1277
2	j	0.38	0/815	0.70	1/1096 (0.1%)
3	b	0.31	0/484	0.85	0/653
3	k	0.32	0/484	0.85	0/653
3	m	0.32	0/484	0.85	0/653
4	E	0.36	0/5311	0.73	2/7169 (0.0%)
4	G	0.32	0/5315	0.71	6/7175 (0.1%)
5	I	0.41	0/4322	0.80	9/5853 (0.2%)
5	K	0.41	1/4683 (0.0%)	0.77	9/6338 (0.1%)
6	L	0.36	0/4697	0.79	11/6348 (0.2%)
7	S	0.32	0/3441	0.74	4/4661 (0.1%)
7	T	0.32	0/3441	0.74	4/4661 (0.1%)
7	U	0.32	0/3441	0.74	4/4661 (0.1%)
7	V	0.32	0/3441	0.74	4/4661 (0.1%)
7	W	0.32	0/3441	0.74	4/4661 (0.1%)
7	X	0.32	0/3441	0.74	4/4661 (0.1%)
7	Y	0.32	0/3441	0.74	4/4661 (0.1%)
7	Z	0.32	0/3441	0.74	4/4661 (0.1%)
All	All	0.35	4/70512 (0.0%)	0.75	87/95358 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	J	0	3
2	F	0	1
2	H	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	b	0	1
3	k	0	1
3	m	0	1
4	E	0	3
4	G	0	3
5	I	0	3
5	K	0	2
6	L	0	1
All	All	0	20

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	225	TRP	CD2-CE2	6.90	1.53	1.41
5	K	35	HIS	N-CA	-5.71	1.38	1.45
1	J	225	TRP	CG-CD2	5.13	1.52	1.43
1	J	225	TRP	CZ3-CH2	5.11	1.53	1.40

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	l	121	PRO	N-CA-CB	7.96	111.61	103.25
7	T	337	LEU	CA-CB-CG	7.71	143.28	116.30
7	U	337	LEU	CA-CB-CG	7.70	143.26	116.30
7	V	337	LEU	CA-CB-CG	7.69	143.21	116.30
7	Y	337	LEU	CA-CB-CG	7.69	143.22	116.30
7	S	337	LEU	CA-CB-CG	7.69	143.21	116.30
7	W	337	LEU	CA-CB-CG	7.69	143.20	116.30
7	X	337	LEU	CA-CB-CG	7.68	143.19	116.30
7	Z	337	LEU	CA-CB-CG	7.68	143.19	116.30
1	J	237	HIS	CA-C-N	7.42	135.72	121.54
1	J	237	HIS	C-N-CA	7.42	135.72	121.54
2	H	726	VAL	N-CA-C	-7.38	105.94	113.10
5	I	3	HIS	N-CA-C	-7.32	104.96	114.04
2	F	726	VAL	N-CA-C	-6.91	106.76	113.53
1	l	130	PRO	N-CA-CB	6.83	110.51	103.00
5	I	503	LYS	N-CA-C	-6.46	104.08	114.09
2	F	269	ASN	CA-C-N	6.31	133.65	123.93
2	F	269	ASN	C-N-CA	6.31	133.65	123.93
5	K	651	TYR	CA-CB-CG	6.22	125.09	113.90
2	H	346	LEU	CA-C-N	6.21	132.88	121.70
2	H	346	LEU	C-N-CA	6.21	132.88	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	W	402	GLU	CA-CB-CG	6.13	126.36	114.10
7	X	402	GLU	CA-CB-CG	6.12	126.33	114.10
7	V	402	GLU	CA-CB-CG	6.11	126.32	114.10
7	S	402	GLU	CA-CB-CG	6.11	126.31	114.10
7	Y	402	GLU	CA-CB-CG	6.11	126.31	114.10
7	Z	402	GLU	CA-CB-CG	6.11	126.31	114.10
7	T	402	GLU	CA-CB-CG	6.10	126.30	114.10
7	U	402	GLU	CA-CB-CG	6.09	126.28	114.10
6	L	320	PHE	CA-CB-CG	6.07	119.87	113.80
6	L	340	GLN	CA-C-N	6.07	129.51	120.83
6	L	340	GLN	C-N-CA	6.07	129.51	120.83
5	K	574	ILE	N-CA-C	-6.07	107.95	113.71
6	L	317	ARG	N-CA-C	-5.98	107.80	114.62
4	G	864	PHE	CA-C-N	5.94	132.88	121.54
4	G	864	PHE	C-N-CA	5.94	132.88	121.54
7	W	12	GLN	CA-CB-CG	5.93	125.97	114.10
7	X	12	GLN	CA-CB-CG	5.93	125.96	114.10
7	Z	12	GLN	CA-CB-CG	5.93	125.96	114.10
7	S	12	GLN	CA-CB-CG	5.93	125.96	114.10
7	T	12	GLN	CA-CB-CG	5.92	125.94	114.10
7	V	12	GLN	CA-CB-CG	5.92	125.93	114.10
7	Y	12	GLN	CA-CB-CG	5.92	125.93	114.10
7	U	12	GLN	CA-CB-CG	5.91	125.93	114.10
1	J	713	ASP	CA-C-N	5.80	130.89	122.36
1	J	713	ASP	C-N-CA	5.80	130.89	122.36
5	I	475	TYR	CA-CB-CG	5.77	124.28	113.90
5	K	263	ILE	CA-C-N	5.68	128.96	120.83
5	K	263	ILE	C-N-CA	5.68	128.96	120.83
7	T	402	GLU	CB-CG-CD	5.61	122.14	112.60
7	Z	402	GLU	CB-CG-CD	5.61	122.13	112.60
7	Y	402	GLU	CB-CG-CD	5.60	122.11	112.60
7	S	402	GLU	CB-CG-CD	5.59	122.10	112.60
7	U	402	GLU	CB-CG-CD	5.58	122.09	112.60
7	X	402	GLU	CB-CG-CD	5.58	122.09	112.60
7	V	402	GLU	CB-CG-CD	5.58	122.08	112.60
1	J	256	LEU	CA-C-N	5.57	132.19	121.54
1	J	256	LEU	C-N-CA	5.57	132.19	121.54
7	W	402	GLU	CB-CG-CD	5.57	122.07	112.60
5	K	35	HIS	N-CA-CB	5.53	117.79	109.82
6	L	1689	ARG	N-CA-C	-5.47	107.86	114.75
6	L	568	TYR	CA-C-N	-5.43	115.06	122.93
6	L	568	TYR	C-N-CA	-5.43	115.06	122.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	580	HIS	CA-C-N	5.42	131.90	121.54
4	E	580	HIS	C-N-CA	5.42	131.90	121.54
5	I	407	ASP	CA-C-N	5.37	131.80	121.54
5	I	407	ASP	C-N-CA	5.37	131.80	121.54
2	j	45	PRO	N-CA-C	5.36	119.50	111.14
6	L	1688	PHE	N-CA-C	-5.34	105.56	113.40
5	I	508	ASN	N-CA-C	-5.31	99.48	110.80
1	J	238	LEU	N-CA-C	5.31	122.11	110.80
5	K	68	GLN	CA-C-N	5.31	131.25	121.70
5	K	68	GLN	C-N-CA	5.31	131.25	121.70
5	K	580	PHE	CA-C-N	5.29	129.06	120.60
5	K	580	PHE	C-N-CA	5.29	129.06	120.60
5	I	504	HIS	CA-C-N	5.25	131.58	121.54
5	I	504	HIS	C-N-CA	5.25	131.58	121.54
4	G	543	VAL	CA-C-N	5.25	131.56	121.54
4	G	543	VAL	C-N-CA	5.25	131.56	121.54
1	J	255	PRO	CA-C-N	5.24	131.14	121.70
1	J	255	PRO	C-N-CA	5.24	131.14	121.70
6	L	517	HIS	CA-C-N	5.09	126.45	120.09
6	L	517	HIS	C-N-CA	5.09	126.45	120.09
4	G	240	GLY	CA-C-N	5.08	131.25	121.54
4	G	240	GLY	C-N-CA	5.08	131.25	121.54
5	I	408	ASP	N-CA-C	5.05	121.57	110.80
6	L	1800	LEU	N-CA-CB	-5.01	102.23	110.40

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	E	318	LEU	Peptide
4	E	424	ASN	Peptide
4	E	580	HIS	Peptide
2	F	626	LEU	Peptide
4	G	240	GLY	Peptide
4	G	580	HIS	Peptide
4	G	866	THR	Peptide
2	H	454	VAL	Peptide
5	I	407	ASP	Peptide
5	I	507	SER	Peptide
5	I	508	ASN	Peptide
1	J	235	SER	Peptide
1	J	236	LEU	Mainchain

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Mol	Chain	Res	Type	Group
1	J	256	LEU	Peptide
5	K	406	ASP	Peptide
5	K	408	ASP	Peptide
6	L	346	LEU	Peptide
3	b	35	LEU	Peptide
3	k	35	LEU	Peptide
3	m	35	LEU	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J	4429	0	4482	34	0
1	l	847	0	789	8	0
2	F	4941	0	4935	55	0
2	H	4907	0	4896	58	0
2	a	933	0	953	12	0
2	j	803	0	831	12	0
3	b	484	0	512	5	0
3	k	484	0	512	11	0
3	m	484	0	512	7	0
4	E	5202	0	5241	71	0
4	G	5206	0	5230	53	0
5	I	4225	0	4259	38	0
5	K	4579	0	4586	53	0
6	L	4587	0	4636	52	0
7	S	3373	0	3325	52	0
7	T	3373	0	3325	50	0
7	U	3373	0	3325	45	0
7	V	3373	0	3325	50	0
7	W	3373	0	3325	52	0
7	X	3373	0	3325	51	0
7	Y	3373	0	3325	52	0
7	Z	3373	0	3325	48	0
All	All	69095	0	68974	798	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 (798) 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)
7:Z:207:ASN:O	7:Z:211:ASN:HB2	1.65	0.96
7:W:207:ASN:O	7:W:211:ASN:HB2	1.65	0.96
7:X:207:ASN:O	7:X:211:ASN:HB2	1.65	0.96
7:Y:207:ASN:O	7:Y:211:ASN:HB2	1.65	0.96
7:S:207:ASN:O	7:S:211:ASN:HB2	1.65	0.95
7:T:207:ASN:O	7:T:211:ASN:HB2	1.66	0.95
7:V:207:ASN:O	7:V:211:ASN:HB2	1.65	0.95
7:W:56:ASP:HB3	7:X:295:ARG:HG2	1.47	0.95
5:I:361:TYR:HE2	5:I:475:TYR:HB3	1.33	0.94
7:U:207:ASN:O	7:U:211:ASN:HB2	1.65	0.93
1:J:242:LEU:HD13	1:J:305:LEU:H	1.52	0.73
1:J:832:LYS:HA	1:J:835:LYS:HG2	1.69	0.73
2:F:879:ARG:O	7:T:355:SER:OG	2.08	0.71
7:W:56:ASP:HA	7:X:295:ARG:HD3	1.73	0.70
5:I:361:TYR:CE2	5:I:475:TYR:HB3	2.22	0.70
2:H:669:ARG:HA	2:H:672:ARG:HE	1.56	0.70
6:L:409:ARG:HD3	6:L:412:HIS:HE1	1.56	0.70
5:K:199:GLN:O	5:K:200:HIS:ND1	2.25	0.69
2:H:724:PHE:HA	2:H:728:GLU:HG2	1.75	0.69
5:K:255:LYS:HZ3	5:K:258:SER:HB3	1.59	0.67
1:J:892:HIS:HE1	7:X:355:SER:HB2	1.59	0.67
2:j:58:ILE:HD11	3:k:35:LEU:HD11	1.76	0.67
6:L:1738:LYS:O	6:L:1742:GLN:NE2	2.24	0.67
5:I:357:ILE:O	5:I:361:TYR:HB3	1.95	0.66
2:F:692:ARG:NH1	7:T:196:THR:O	2.29	0.66
2:H:372:TYR:HA	2:H:375:LYS:HE2	1.78	0.66
6:L:568:TYR:HB2	6:L:1602:TRP:HE1	1.59	0.66
7:T:158:ASN:HD21	7:T:198:ASN:HD22	1.44	0.66
5:K:500:MET:HG2	7:Y:264:PRO:HB3	1.78	0.65
5:K:653:LYS:HG2	7:Y:353:PRO:HG3	1.78	0.65
7:V:158:ASN:HD21	7:V:198:ASN:HD22	1.44	0.65
4:G:359:LEU:HB3	4:G:380:THR:HG22	1.76	0.65
7:X:158:ASN:HD21	7:X:198:ASN:HD22	1.44	0.65
5:K:48:LEU:HD21	5:K:130:GLN:HA	1.78	0.65
7:U:158:ASN:HD21	7:U:198:ASN:HD22	1.44	0.65
7:S:274:THR:HG1	7:S:375:GLY:H	1.43	0.64
6:L:1612:CYS:HG	6:L:1705:HIS:HE2	1.44	0.64
7:V:274:THR:HG1	7:V:375:GLY:H	1.44	0.64
4:E:570:LYS:HD2	4:E:571:ASP:HB2	1.80	0.64
7:Z:274:THR:HG1	7:Z:375:GLY:H	1.44	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:623:LYS:HG3	4:E:625:PRO:HD2	1.79	0.64
1:J:825:PHE:O	1:J:828:LEU:HB3	1.98	0.64
7:Z:158:ASN:HD21	7:Z:198:ASN:HD22	1.44	0.64
5:I:341:TRP:HD1	5:I:557:ILE:HD11	1.63	0.64
2:H:431:TYR:HA	2:H:434:ILE:HG22	1.80	0.63
5:K:649:LEU:HB3	7:Y:341:ARG:HH21	1.63	0.63
7:W:158:ASN:HD21	7:W:198:ASN:HD22	1.44	0.63
5:I:42:LEU:HA	5:I:45:LEU:HD12	1.79	0.63
2:j:65:GLN:HE21	2:j:104:PRO:HG2	1.61	0.63
4:E:660:ILE:HG23	7:S:254:ILE:HD12	1.80	0.63
4:E:559:LEU:HD21	4:E:570:LYS:HD3	1.79	0.63
7:Y:158:ASN:HD21	7:Y:198:ASN:HD22	1.44	0.63
7:S:158:ASN:HD21	7:S:198:ASN:HD22	1.44	0.63
5:K:590:CYS:SG	5:K:591:HIS:N	2.70	0.63
6:L:1800:LEU:HD13	7:Z:341:ARG:HG3	1.80	0.63
2:a:77:LEU:HA	2:a:80:LYS:HD2	1.80	0.63
6:L:350:CYS:SG	6:L:354:LYS:NZ	2.72	0.62
2:F:681:ARG:NH2	2:F:709:SER:OG	2.32	0.62
4:E:188:ILE:HG22	4:E:190:ASP:H	1.63	0.62
4:E:432:TYR:HB3	4:E:451:LEU:HD11	1.80	0.62
2:H:588:PRO:HA	2:H:633:THR:HA	1.81	0.62
7:X:274:THR:HG1	7:X:375:GLY:H	1.44	0.62
4:G:767:GLN:HA	4:G:770:LYS:HG2	1.80	0.62
7:T:274:THR:HG1	7:T:375:GLY:H	1.47	0.61
1:J:412:LEU:HA	1:J:415:VAL:HG22	1.82	0.61
7:S:298:LEU:HD13	7:S:345:LEU:HD23	1.83	0.61
7:W:298:LEU:HD13	7:W:345:LEU:HD23	1.83	0.61
2:H:651:VAL:HG23	2:H:748:ILE:HG12	1.83	0.61
7:U:298:LEU:HD13	7:U:345:LEU:HD23	1.82	0.61
2:F:721:TYR:O	2:F:725:GLU:HB2	2.01	0.61
5:I:41:VAL:HG13	5:I:44:ARG:HH22	1.65	0.61
7:Y:395:TYR:OH	7:Y:399:ARG:NH1	2.34	0.61
2:F:740:GLN:HE21	2:F:746:HIS:HE1	1.48	0.61
7:S:395:TYR:OH	7:S:399:ARG:NH1	2.34	0.61
2:F:763:LEU:HG	2:F:768:SER:HB2	1.82	0.60
7:V:298:LEU:HD13	7:V:345:LEU:HD23	1.82	0.60
4:G:770:LYS:HZ3	4:G:771:LEU:HD23	1.65	0.60
7:Y:274:THR:HG1	7:Y:375:GLY:H	1.44	0.60
7:Z:395:TYR:OH	7:Z:399:ARG:NH1	2.34	0.60
4:E:517:LYS:HG3	4:E:521:LEU:HD12	1.83	0.60
4:E:530:HIS:HB3	4:E:558:ALA:HB1	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:620:ARG:HH11	2:F:644:VAL:HA	1.67	0.60
7:V:395:TYR:OH	7:V:399:ARG:NH1	2.34	0.60
2:H:869:SER:HB3	2:H:873:LEU:HG	1.84	0.60
7:T:395:TYR:OH	7:T:399:ARG:NH1	2.34	0.60
5:K:392:VAL:O	5:K:396:PHE:HB2	2.02	0.60
7:U:395:TYR:OH	7:U:399:ARG:NH1	2.34	0.60
7:W:395:TYR:OH	7:W:399:ARG:NH1	2.34	0.60
6:L:1675:TYR:HB2	6:L:1801:ARG:HG3	1.83	0.60
7:T:298:LEU:HD13	7:T:345:LEU:HD23	1.82	0.60
7:Y:298:LEU:HD13	7:Y:345:LEU:HD23	1.82	0.60
6:L:1686:CYS:HA	6:L:1689:ARG:HH21	1.67	0.60
7:X:395:TYR:OH	7:X:399:ARG:NH1	2.34	0.60
7:Z:298:LEU:HD13	7:Z:345:LEU:HD23	1.83	0.60
1:l:15:GLN:HE21	3:m:53:GLN:HE22	1.50	0.59
4:E:319:LEU:HD21	4:E:324:LEU:HD13	1.84	0.59
2:H:562:MET:HA	2:H:566:LEU:HD13	1.83	0.59
7:W:274:THR:HG1	7:W:375:GLY:H	1.48	0.59
7:X:298:LEU:HD13	7:X:345:LEU:HD23	1.83	0.59
2:F:684:HIS:HE2	2:F:704:CYS:HG	1.50	0.59
4:G:865:TYR:H	4:G:868:ARG:HH12	1.50	0.59
5:I:499:GLN:HA	7:W:264:PRO:HB3	1.84	0.59
7:U:274:THR:HG1	7:U:375:GLY:H	1.49	0.59
5:I:143:ILE:HD11	5:I:156:THR:HG21	1.85	0.59
2:F:680:ILE:HD11	2:F:786:GLN:HE21	1.67	0.59
6:L:1801:ARG:HH22	7:Z:337:LEU:HD21	1.68	0.59
4:E:640:MET:HE2	4:E:734:LEU:HD11	1.85	0.58
7:S:217:ARG:HG3	7:S:218:LEU:HG	1.85	0.58
6:L:1732:ILE:HG23	6:L:1772:PHE:HE1	1.68	0.58
7:U:217:ARG:HG3	7:U:218:LEU:HG	1.85	0.58
7:W:217:ARG:HG3	7:W:218:LEU:HG	1.85	0.58
7:Z:217:ARG:HG3	7:Z:218:LEU:HG	1.85	0.58
7:V:217:ARG:HG3	7:V:218:LEU:HG	1.85	0.58
7:X:217:ARG:HG3	7:X:218:LEU:HG	1.85	0.58
7:T:217:ARG:HG3	7:T:218:LEU:HG	1.85	0.58
4:E:563:THR:OG1	7:S:45:THR:OG1	2.20	0.58
7:Y:217:ARG:HG3	7:Y:218:LEU:HG	1.85	0.58
7:V:185:PRO:O	7:V:189:LEU:HB2	2.05	0.57
7:X:185:PRO:O	7:X:189:LEU:HB2	2.05	0.57
7:Y:185:PRO:O	7:Y:189:LEU:HB2	2.05	0.57
2:H:600:ILE:HA	7:W:342:GLU:HG2	1.87	0.57
7:S:185:PRO:O	7:S:189:LEU:HB2	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:185:PRO:O	7:T:189:LEU:HB2	2.05	0.57
5:K:79:GLY:HA3	5:K:149:HIS:HA	1.86	0.57
7:Z:336:SER:HA	7:Z:339:ARG:HD2	1.87	0.57
5:I:586:ILE:HD13	5:I:622:GLN:HE21	1.70	0.57
7:U:185:PRO:O	7:U:189:LEU:HB2	2.05	0.57
1:J:493:ILE:HG12	1:J:548:MET:HA	1.87	0.56
2:F:364:LEU:HD22	2:F:370:TRP:HE1	1.70	0.56
5:K:197:LEU:HD13	6:L:510:LEU:HB3	1.86	0.56
4:G:527:PHE:O	4:G:531:PHE:HB2	2.05	0.56
7:W:185:PRO:O	7:W:189:LEU:HB2	2.05	0.56
7:W:336:SER:HA	7:W:339:ARG:HD2	1.87	0.56
7:X:336:SER:HA	7:X:339:ARG:HD2	1.87	0.56
4:E:655:LEU:HD22	4:E:687:LEU:HD13	1.87	0.56
4:G:528:PHE:HA	4:G:531:PHE:HB3	1.87	0.56
7:V:336:SER:HA	7:V:339:ARG:HD2	1.87	0.56
7:Z:185:PRO:O	7:Z:189:LEU:HB2	2.05	0.56
2:F:876:LEU:HD12	2:F:879:ARG:HD3	1.86	0.56
7:U:336:SER:HA	7:U:339:ARG:HD2	1.87	0.56
7:S:336:SER:HA	7:S:339:ARG:HD2	1.87	0.56
1:J:307:HIS:H	1:J:310:LEU:HD12	1.71	0.56
2:H:326:ALA:HB2	5:I:165:LEU:HG	1.89	0.55
4:E:356:LEU:HG	4:E:440:PRO:HB3	1.88	0.55
5:K:285:MET:HE1	5:K:465:ILE:HD12	1.88	0.55
5:K:283:VAL:O	5:K:287:GLU:HB2	2.07	0.55
5:K:301:LYS:HZ1	5:K:336:VAL:HG12	1.70	0.55
4:E:439:ILE:HG22	4:E:441:SER:H	1.71	0.55
7:Y:336:SER:HA	7:Y:339:ARG:HD2	1.87	0.55
5:K:530:TYR:CE2	7:Y:249:MET:HE3	2.42	0.55
7:T:336:SER:HA	7:T:339:ARG:HD2	1.87	0.55
2:H:635:TRP:HE3	2:H:672:ARG:HH11	1.55	0.55
4:E:530:HIS:CE1	7:S:47:ARG:HH21	2.25	0.55
5:I:38:GLU:O	5:I:41:VAL:HB	2.07	0.55
4:E:301:LYS:HG2	2:F:369:VAL:HG23	1.89	0.55
6:L:473:LEU:HA	6:L:476:LEU:HD13	1.89	0.54
4:G:527:PHE:O	4:G:531:PHE:CB	2.56	0.54
2:H:364:LEU:HB2	2:H:370:TRP:HE1	1.73	0.54
7:Z:183:VAL:HG13	7:Z:187:ASN:HD21	1.73	0.54
4:E:205:ILE:HG23	4:E:207:THR:H	1.72	0.54
2:F:751:HIS:O	2:F:754:PHE:HB3	2.07	0.54
4:G:353:GLY:HA2	4:G:356:LEU:HD12	1.89	0.54
3:k:32:SER:O	3:k:36:ASN:N	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:568:LEU:HD22	2:F:667:LEU:HG	1.89	0.54
5:I:555:GLU:HA	5:I:558:ARG:HD2	1.89	0.54
7:V:119:PHE:HA	7:V:122:ILE:HD12	1.90	0.54
7:Y:119:PHE:HA	7:Y:122:ILE:HD12	1.90	0.54
2:j:61:GLU:OE1	2:j:64:ARG:NH2	2.40	0.54
7:X:119:PHE:HA	7:X:122:ILE:HD12	1.90	0.54
7:Y:183:VAL:HG13	7:Y:187:ASN:HD21	1.73	0.54
4:G:550:ARG:NH2	7:V:342:GLU:OE2	2.40	0.54
5:K:143:ILE:HD12	5:K:153:ILE:HG23	1.90	0.54
7:S:119:PHE:HA	7:S:122:ILE:HD12	1.90	0.54
7:W:183:VAL:HG13	7:W:187:ASN:HD21	1.73	0.54
4:E:683:ARG:HA	4:E:686:MET:HE2	1.89	0.54
5:K:204:PHE:HA	5:K:260:ARG:HB2	1.90	0.54
3:b:32:SER:O	3:b:36:ASN:N	2.40	0.54
6:L:349:GLU:HG3	6:L:456:LEU:HG	1.90	0.53
7:T:183:VAL:HG13	7:T:187:ASN:HD21	1.73	0.53
4:G:302:GLU:HA	4:G:305:ILE:HD12	1.91	0.53
4:G:555:LEU:HD22	4:G:575:ILE:HD11	1.91	0.53
7:T:119:PHE:HA	7:T:122:ILE:HD12	1.90	0.53
7:X:183:VAL:HG13	7:X:187:ASN:HD21	1.73	0.53
6:L:1590:VAL:HG11	6:L:1733:PHE:HB3	1.90	0.53
7:V:3:ARG:HB2	7:V:133:GLU:HB2	1.91	0.53
7:V:183:VAL:HG13	7:V:187:ASN:HD21	1.73	0.53
7:S:3:ARG:HB2	7:S:133:GLU:HB2	1.91	0.53
7:U:183:VAL:HG13	7:U:187:ASN:HD21	1.73	0.53
2:H:325:CYS:HA	2:H:328:LEU:HD12	1.91	0.53
7:W:56:ASP:OD2	7:X:299:GLN:HG3	2.09	0.53
7:Z:3:ARG:HB2	7:Z:133:GLU:HB2	1.91	0.53
5:K:80:GLY:HA3	5:K:147:LYS:HA	1.90	0.53
4:E:253:ASP:HB3	4:E:256:ILE:HD12	1.91	0.53
6:L:507:GLN:O	6:L:511:HIS:HB2	2.08	0.53
7:T:3:ARG:HB2	7:T:133:GLU:HB2	1.91	0.53
2:H:297:LEU:HD21	2:H:375:LYS:HG2	1.91	0.53
5:K:486:ARG:NH1	7:Y:249:MET:HE1	2.24	0.53
6:L:409:ARG:HA	6:L:412:HIS:CE1	2.44	0.53
7:W:383:SER:O	7:W:386:SER:OG	2.27	0.53
4:E:183:GLU:OE2	4:E:184:ARG:NH1	2.42	0.53
7:S:183:VAL:HG13	7:S:187:ASN:HD21	1.73	0.53
7:T:12:GLN:OE1	7:T:13:CYS:N	2.42	0.53
2:j:96:LEU:HD11	3:k:60:LEU:HD12	1.90	0.52
4:G:301:LYS:NZ	2:H:369:VAL:O	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:359:LEU:HD21	4:E:379:LEU:HB3	1.91	0.52
7:U:119:PHE:HA	7:U:122:ILE:HD12	1.90	0.52
7:Z:119:PHE:HA	7:Z:122:ILE:HD12	1.90	0.52
7:Z:383:SER:O	7:Z:386:SER:OG	2.27	0.52
2:j:100:LEU:HB3	3:k:68:ARG:HH22	1.74	0.52
7:U:12:GLN:OE1	7:U:13:CYS:N	2.42	0.52
7:W:119:PHE:HA	7:W:122:ILE:HD12	1.90	0.52
1:J:210:PRO:HB2	1:J:213:ARG:HB3	1.91	0.52
7:S:383:SER:O	7:S:386:SER:OG	2.27	0.52
7:V:12:GLN:OE1	7:V:13:CYS:N	2.43	0.52
7:V:383:SER:O	7:V:386:SER:OG	2.27	0.52
7:Y:3:ARG:HB2	7:Y:133:GLU:HB2	1.91	0.52
4:E:684:GLN:NE2	7:S:259:SER:O	2.43	0.52
7:X:3:ARG:HB2	7:X:133:GLU:HB2	1.91	0.52
6:L:1597:ARG:O	6:L:1599:LYS:NZ	2.42	0.52
7:U:401:ARG:HD3	7:U:404:PHE:HE2	1.75	0.52
7:X:12:GLN:OE1	7:X:13:CYS:N	2.42	0.52
7:X:401:ARG:HD3	7:X:404:PHE:HE2	1.75	0.52
2:F:744:LEU:HD12	2:F:747:ILE:HD12	1.91	0.52
5:I:514:LYS:HG3	5:I:516:ARG:H	1.75	0.52
7:U:383:SER:O	7:U:386:SER:OG	2.27	0.52
7:V:401:ARG:HD3	7:V:404:PHE:HE2	1.75	0.52
7:W:3:ARG:HB2	7:W:133:GLU:HB2	1.91	0.52
2:F:883:ASN:ND2	7:T:346:ALA:O	2.43	0.52
5:K:651:TYR:CD2	7:Y:348:PHE:HB3	2.45	0.52
6:L:1612:CYS:SG	6:L:1705:HIS:NE2	2.77	0.52
7:S:401:ARG:HD3	7:S:404:PHE:HE2	1.75	0.52
7:Z:12:GLN:OE1	7:Z:13:CYS:N	2.42	0.52
7:S:12:GLN:OE1	7:S:13:CYS:N	2.42	0.51
7:T:401:ARG:HD3	7:T:404:PHE:HE2	1.75	0.51
7:Y:12:GLN:OE1	7:Y:13:CYS:N	2.43	0.51
2:F:283:LEU:HD21	2:F:286:SER:HB2	1.91	0.51
6:L:1724:PRO:HA	6:L:1727:ASN:HB3	1.91	0.51
7:V:13:CYS:HB2	7:V:140:SER:HB2	1.93	0.51
7:Y:401:ARG:HD3	7:Y:404:PHE:HE2	1.75	0.51
7:Z:13:CYS:HB2	7:Z:140:SER:HB2	1.93	0.51
1:J:381:GLU:HA	1:J:384:LYS:HD2	1.92	0.51
7:W:13:CYS:HB2	7:W:140:SER:HB2	1.93	0.51
7:W:401:ARG:HD3	7:W:404:PHE:HE2	1.75	0.51
2:j:97:LEU:HD21	3:k:32:SER:HA	1.93	0.51
4:G:306:LEU:HA	4:G:309:GLN:HE21	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:653:LYS:O	5:K:656:THR:OG1	2.28	0.51
7:Y:383:SER:O	7:Y:386:SER:OG	2.27	0.51
7:Z:401:ARG:HD3	7:Z:404:PHE:HE2	1.75	0.51
1:J:953:ALA:HA	1:J:956:LYS:HG2	1.93	0.51
5:K:418:ILE:HD13	5:K:453:LEU:HD23	1.93	0.51
7:U:3:ARG:HB2	7:U:133:GLU:HB2	1.91	0.51
7:U:13:CYS:HB2	7:U:140:SER:HB2	1.93	0.51
7:X:13:CYS:HB2	7:X:140:SER:HB2	1.93	0.51
2:H:655:GLU:O	2:H:658:SER:OG	2.28	0.51
7:W:12:GLN:OE1	7:W:13:CYS:N	2.42	0.51
6:L:1677:ALA:HA	6:L:1681:LEU:HD12	1.93	0.51
4:E:444:GLN:HA	4:E:447:ALA:HB2	1.92	0.50
4:E:522:MET:HB2	7:S:248:TYR:CE1	2.45	0.50
2:H:270:ASN:H	2:H:273:ASN:HB2	1.75	0.50
2:H:868:SER:HB3	2:H:873:LEU:HD12	1.92	0.50
3:m:32:SER:O	3:m:36:ASN:N	2.40	0.50
2:F:703:GLN:HE22	7:T:444:ILE:HG23	1.76	0.50
7:U:265:ARG:HH11	7:U:431:LEU:HD12	1.77	0.50
5:K:648:ARG:NH1	5:K:654:TYR:OH	2.43	0.50
2:F:860:GLN:HA	2:F:863:VAL:HG12	1.94	0.50
7:X:383:SER:O	7:X:386:SER:OG	2.27	0.50
1:l:87:LEU:HD22	3:m:27:VAL:HG13	1.92	0.50
5:K:344:MET:HE2	5:K:463:LEU:HA	1.94	0.50
5:K:380:LEU:HD22	5:K:453:LEU:HD21	1.94	0.50
7:X:265:ARG:HH11	7:X:431:LEU:HD12	1.77	0.50
2:F:717:GLN:HB3	2:F:879:ARG:HE	1.77	0.50
4:G:377:LEU:O	4:G:380:THR:OG1	2.30	0.50
7:V:265:ARG:HH11	7:V:431:LEU:HD12	1.77	0.50
7:Y:188:SER:O	7:Y:192:LEU:HB2	2.12	0.50
3:k:25:MET:HE1	3:k:48:VAL:HG11	1.93	0.50
7:S:13:CYS:HB2	7:S:140:SER:HB2	1.93	0.50
7:V:188:SER:O	7:V:192:LEU:HB2	2.12	0.50
3:m:25:MET:HE1	3:m:48:VAL:HG11	1.93	0.50
4:E:560:ARG:HA	4:E:565:ASN:HD22	1.77	0.50
2:H:477:MET:HG3	2:H:481:ARG:HE	1.77	0.50
2:H:666:PHE:HD2	2:H:667:LEU:HD12	1.76	0.50
5:I:553:ASP:O	5:I:556:SER:OG	2.27	0.50
1:J:829:LEU:HA	1:J:832:LYS:HG2	1.94	0.50
7:W:265:ARG:HH11	7:W:431:LEU:HD12	1.77	0.50
7:Y:13:CYS:HB2	7:Y:140:SER:HB2	1.93	0.50
4:G:709:LEU:HG	4:G:713:LEU:HD23	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:383:SER:O	7:T:386:SER:OG	2.27	0.50
7:Y:265:ARG:HH11	7:Y:431:LEU:HD12	1.77	0.50
1:J:1009:HIS:O	1:J:1012:SER:OG	2.24	0.49
4:G:456:TYR:HB3	4:G:499:LEU:HG	1.94	0.49
2:H:601:LEU:HD22	2:H:623:VAL:HG13	1.93	0.49
7:W:188:SER:O	7:W:192:LEU:HB2	2.12	0.49
4:G:824:LYS:HA	4:G:827:LYS:HE2	1.94	0.49
3:b:25:MET:HE1	3:b:48:VAL:HG11	1.93	0.49
2:a:14:GLN:NE2	2:a:25:GLU:OE1	2.44	0.49
7:S:265:ARG:HH11	7:S:431:LEU:HD12	1.77	0.49
7:T:13:CYS:HB2	7:T:140:SER:HB2	1.93	0.49
7:T:188:SER:O	7:T:192:LEU:HB2	2.12	0.49
7:V:428:VAL:HA	7:V:431:LEU:HB2	1.94	0.49
7:X:428:VAL:HA	7:X:431:LEU:HB2	1.95	0.49
4:E:763:GLN:HG2	4:E:767:GLN:HE21	1.77	0.49
7:S:151:SER:HB2	7:S:194:ARG:HG2	1.95	0.49
7:S:428:VAL:HA	7:S:431:LEU:HB2	1.95	0.49
7:T:265:ARG:HH11	7:T:431:LEU:HD12	1.77	0.49
4:E:191:PHE:HD2	2:F:289:ASP:HB3	1.77	0.49
2:F:621:LEU:HB2	2:F:640:LEU:HD12	1.94	0.49
5:I:354:LEU:HA	5:I:357:ILE:HD12	1.93	0.49
4:E:698:MET:HE1	7:S:249:MET:HG2	1.94	0.49
1:J:246:TRP:CD1	1:J:306:THR:HG1	2.29	0.49
7:S:389:GLU:O	7:S:393:ARG:N	2.45	0.49
7:T:428:VAL:HA	7:T:431:LEU:HB2	1.95	0.49
7:U:428:VAL:HA	7:U:431:LEU:HB2	1.95	0.49
7:V:151:SER:HB2	7:V:194:ARG:HG2	1.95	0.49
7:Z:265:ARG:HH11	7:Z:431:LEU:HD12	1.77	0.49
4:E:573:LEU:HD13	4:E:618:PHE:HB3	1.94	0.49
5:K:370:GLN:HB2	5:K:486:ARG:HE	1.78	0.49
6:L:1630:MET:SD	6:L:1630:MET:N	2.86	0.49
6:L:1680:ILE:HD11	6:L:1716:GLY:HA3	1.95	0.49
7:Z:151:SER:HB2	7:Z:194:ARG:HG2	1.95	0.49
7:T:389:GLU:O	7:T:393:ARG:N	2.45	0.49
7:Z:188:SER:O	7:Z:192:LEU:HB2	2.12	0.49
7:Z:389:GLU:O	7:Z:393:ARG:N	2.45	0.49
2:F:433:TRP:CD1	2:F:483:VAL:HG22	2.47	0.49
1:J:289:LEU:HA	1:J:294:VAL:HA	1.93	0.49
1:J:828:LEU:HG	1:J:832:LYS:HZ1	1.78	0.49
7:W:151:SER:HB2	7:W:194:ARG:HG2	1.95	0.49
4:E:682:LEU:HD21	4:E:826:ASP:HA	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:681:ARG:HG3	2:H:685:MET:HE2	1.95	0.49
2:H:702:HIS:HD2	2:H:703:GLN:HE22	1.60	0.49
7:X:188:SER:O	7:X:192:LEU:HB2	2.12	0.49
4:E:223:TYR:OH	2:F:285:ARG:O	2.24	0.48
2:H:333:ARG:HG2	5:I:124:TYR:CE1	2.48	0.48
2:H:410:TYR:O	2:H:413:SER:OG	2.29	0.48
7:W:428:VAL:HA	7:W:431:LEU:HB2	1.95	0.48
7:Y:151:SER:HB2	7:Y:194:ARG:HG2	1.95	0.48
7:Y:428:VAL:HA	7:Y:431:LEU:HB2	1.95	0.48
4:E:719:ILE:HA	4:E:722:VAL:HG22	1.95	0.48
4:G:738:MET:HE2	4:G:738:MET:HB2	1.67	0.48
1:J:942:LEU:HG	1:J:947:VAL:HG12	1.94	0.48
7:S:188:SER:O	7:S:192:LEU:HB2	2.12	0.48
7:X:151:SER:HB2	7:X:194:ARG:HG2	1.95	0.48
4:G:610:LEU:HB3	4:G:613:LEU:HD12	1.95	0.48
5:K:184:TYR:HB3	5:K:311:LEU:HD21	1.95	0.48
2:j:45:PRO:HA	3:k:56:ASN:HD21	1.78	0.48
4:E:276:PHE:CE1	4:E:280:LYS:HG3	2.48	0.48
4:E:276:PHE:HD2	4:E:296:MET:HE1	1.79	0.48
2:H:624:ARG:HB2	2:H:641:ASP:HB2	1.95	0.48
5:K:1:MET:SD	5:K:1:MET:N	2.86	0.48
4:G:338:LEU:HD21	4:G:375:LEU:HD21	1.94	0.48
2:H:345:GLN:HA	2:a:79:ARG:HH11	1.79	0.48
6:L:284:GLU:HA	6:L:287:LEU:HB2	1.95	0.48
2:F:608:THR:OG1	2:F:609:ASN:N	2.47	0.48
2:F:807:GLU:HA	2:F:810:LYS:HE3	1.96	0.48
5:I:190:TRP:CE2	5:I:280:GLY:HA3	2.49	0.48
6:L:1800:LEU:HD21	7:Z:338:GLN:HA	1.95	0.48
7:U:188:SER:O	7:U:192:LEU:HB2	2.12	0.48
7:X:200:ASP:OD1	7:X:200:ASP:N	2.47	0.48
7:S:200:ASP:N	7:S:200:ASP:OD1	2.47	0.48
7:Y:389:GLU:O	7:Y:393:ARG:N	2.45	0.48
2:F:684:HIS:NE2	2:F:704:CYS:SG	2.84	0.47
6:L:1503:LEU:HG	6:L:1604:LEU:HD21	1.96	0.47
2:a:54:VAL:HG13	2:a:98:LEU:HD12	1.95	0.47
7:Y:200:ASP:OD1	7:Y:200:ASP:N	2.47	0.47
7:Z:419:ASP:O	7:Z:423:THR:OG1	2.32	0.47
2:H:776:ARG:HE	2:H:779:PHE:HD2	1.62	0.47
5:I:526:ASP:OD2	5:I:529:GLN:NE2	2.47	0.47
6:L:409:ARG:HD3	6:L:412:HIS:CE1	2.43	0.47
7:V:200:ASP:OD1	7:V:200:ASP:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Z:428:VAL:HA	7:Z:431:LEU:HB2	1.95	0.47
5:K:651:TYR:CG	7:Y:348:PHE:HB3	2.50	0.47
1:l:108:TYR:HA	1:l:111:LEU:HD12	1.95	0.47
2:F:549:LEU:HB3	2:F:555:LEU:HD23	1.96	0.47
2:H:709:SER:HA	2:H:712:VAL:HG22	1.96	0.47
7:U:200:ASP:N	7:U:200:ASP:OD1	2.47	0.47
7:V:24:GLN:NE2	7:V:237:SER:OG	2.48	0.47
7:Y:24:GLN:NE2	7:Y:237:SER:OG	2.48	0.47
1:l:113:LEU:HB2	3:m:57:PRO:HB3	1.97	0.47
4:E:414:LEU:HD13	4:E:431:ARG:HA	1.97	0.47
5:K:358:LYS:NZ	5:K:359:ASP:OD1	2.47	0.47
6:L:284:GLU:H	3:b:49:ARG:NH2	2.13	0.47
7:U:151:SER:HB2	7:U:194:ARG:HG2	1.95	0.47
7:W:24:GLN:NE2	7:W:237:SER:OG	2.48	0.47
4:E:293:ALA:HA	4:E:296:MET:HE2	1.96	0.47
2:F:553:TYR:HB3	2:F:648:ILE:HD11	1.95	0.47
6:L:496:PRO:HB3	6:L:500:LYS:HG2	1.97	0.47
7:T:151:SER:HB2	7:T:194:ARG:HG2	1.95	0.47
7:W:200:ASP:N	7:W:200:ASP:OD1	2.47	0.47
7:W:419:ASP:O	7:W:423:THR:OG1	2.32	0.47
7:Z:24:GLN:NE2	7:Z:237:SER:OG	2.48	0.47
7:S:235:ILE:HA	7:S:376:LEU:HD21	1.97	0.47
7:V:235:ILE:HA	7:V:376:LEU:HD21	1.97	0.47
7:X:389:GLU:O	7:X:393:ARG:N	2.45	0.47
2:j:96:LEU:HD21	3:k:60:LEU:HB2	1.96	0.47
4:E:394:TRP:HB2	4:E:400:ILE:HG22	1.96	0.47
4:G:623:LYS:O	4:G:627:SER:N	2.48	0.47
5:I:2:ILE:HD12	5:I:111:PHE:HB3	1.96	0.47
5:I:498:LEU:HA	5:I:502:ARG:HB2	1.97	0.47
1:J:879:GLN:HG2	1:J:880:ILE:HD12	1.96	0.47
7:X:419:ASP:O	7:X:423:THR:OG1	2.32	0.47
7:Z:200:ASP:N	7:Z:200:ASP:OD1	2.47	0.47
2:H:568:LEU:HD23	2:H:574:ILE:HG21	1.97	0.47
7:S:419:ASP:O	7:S:423:THR:OG1	2.32	0.47
7:W:389:GLU:O	7:W:393:ARG:N	2.45	0.47
4:G:184:ARG:HD3	4:G:187:LEU:HD11	1.96	0.46
4:G:556:GLU:HB3	7:V:339:ARG:HE	1.80	0.46
4:G:815:VAL:HA	4:G:818:PHE:HB3	1.97	0.46
2:H:626:LEU:H	2:H:637:VAL:HG13	1.79	0.46
1:J:885:LEU:HD13	7:X:444:ILE:HG23	1.97	0.46
7:T:200:ASP:OD1	7:T:200:ASP:N	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:24:GLN:NE2	7:U:237:SER:OG	2.48	0.46
7:Y:419:ASP:O	7:Y:423:THR:OG1	2.32	0.46
1:I:112:SER:HA	1:I:115:LEU:HD12	1.96	0.46
4:G:158:ARG:HD2	4:G:162:ARG:HE	1.81	0.46
4:G:532:MET:HE3	4:G:532:MET:HB3	1.77	0.46
7:T:24:GLN:NE2	7:T:237:SER:OG	2.48	0.46
7:T:419:ASP:O	7:T:423:THR:OG1	2.32	0.46
7:X:24:GLN:NE2	7:X:237:SER:OG	2.48	0.46
2:j:97:LEU:HD12	2:j:97:LEU:HA	1.81	0.46
2:H:874:ARG:O	2:H:877:SER:OG	2.32	0.46
1:J:215:TRP:HE1	6:L:319:ALA:HB2	1.79	0.46
7:W:343:ARG:HA	7:W:343:ARG:HD2	1.67	0.46
7:X:235:ILE:HA	7:X:376:LEU:HD21	1.97	0.46
4:E:685:ARG:HE	7:S:353:PRO:HG2	1.80	0.46
7:S:24:GLN:NE2	7:S:237:SER:OG	2.48	0.46
7:T:193:LYS:HB2	7:T:424:SER:HB2	1.98	0.46
4:E:649:LYS:HD3	7:S:249:MET:HE1	1.97	0.46
2:F:717:GLN:HB3	2:F:879:ARG:HG3	1.98	0.46
4:G:578:MET:HG3	4:G:643:ARG:HD3	1.97	0.46
1:J:288:GLN:HE22	1:J:297:ARG:HB2	1.80	0.46
7:W:235:ILE:HA	7:W:376:LEU:HD21	1.97	0.46
7:U:193:LYS:HB2	7:U:424:SER:HB2	1.98	0.46
7:V:193:LYS:HB2	7:V:424:SER:HB2	1.98	0.46
7:V:343:ARG:HD2	7:V:343:ARG:HA	1.67	0.46
7:Y:235:ILE:HA	7:Y:376:LEU:HD21	1.97	0.46
4:E:266:VAL:HG21	4:E:328:ILE:HD13	1.97	0.46
7:V:389:GLU:O	7:V:393:ARG:N	2.45	0.46
7:W:351:TRP:CZ2	7:W:443:TYR:HB3	2.51	0.46
4:G:501:ASP:HA	4:G:504:MET:HE2	1.97	0.46
6:L:1653:VAL:HA	6:L:1656:ARG:NH1	2.31	0.46
4:G:165:GLN:HE22	4:G:173:HIS:H	1.64	0.46
5:I:45:LEU:HD21	5:I:123:ASN:HB2	1.98	0.46
5:I:366:GLY:HA2	5:I:486:ARG:HH22	1.80	0.46
5:K:647:LEU:HD11	7:Y:337:LEU:HD11	1.96	0.46
7:S:351:TRP:CZ2	7:S:443:TYR:HB3	2.51	0.46
7:T:235:ILE:HA	7:T:376:LEU:HD21	1.97	0.46
7:U:333:VAL:O	7:U:337:LEU:HB3	2.16	0.46
7:U:351:TRP:CZ2	7:U:443:TYR:HB3	2.51	0.46
7:Y:333:VAL:O	7:Y:337:LEU:HB3	2.16	0.46
7:Y:351:TRP:CZ2	7:Y:443:TYR:HB3	2.51	0.46
7:Z:343:ARG:HA	7:Z:343:ARG:HD2	1.67	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:351:TRP:CZ2	7:T:443:TYR:HB3	2.51	0.46
7:V:333:VAL:O	7:V:337:LEU:HB3	2.16	0.46
7:Z:193:LYS:HB2	7:Z:424:SER:HB2	1.98	0.46
4:E:341:LEU:O	4:E:345:VAL:HG22	2.16	0.45
4:E:657:SER:HA	4:E:660:ILE:HG12	1.98	0.45
5:K:496:TRP:O	5:K:500:MET:HB2	2.15	0.45
7:V:351:TRP:CZ2	7:V:443:TYR:HB3	2.51	0.45
7:W:333:VAL:O	7:W:337:LEU:HB3	2.16	0.45
7:X:351:TRP:CZ2	7:X:443:TYR:HB3	2.51	0.45
6:L:1626:LEU:HG	6:L:1630:MET:HE1	1.98	0.45
2:a:123:PRO:HG2	2:a:126:ALA:H	1.81	0.45
7:X:193:LYS:HB2	7:X:424:SER:HB2	1.98	0.45
7:X:343:ARG:HA	7:X:343:ARG:HD2	1.67	0.45
2:F:320:VAL:HG13	2:F:396:LEU:HD23	1.99	0.45
2:H:879:ARG:NH2	7:V:355:SER:OG	2.49	0.45
6:L:1615:LYS:HB2	6:L:1709:LEU:HD21	1.97	0.45
2:a:113:SER:OG	2:a:114:TYR:N	2.49	0.45
7:T:333:VAL:O	7:T:337:LEU:HB3	2.16	0.45
7:U:56:ASP:OD2	7:V:276:LEU:N	2.44	0.45
7:V:419:ASP:O	7:V:423:THR:OG1	2.32	0.45
7:Y:193:LYS:HB2	7:Y:424:SER:HB2	1.98	0.45
7:Z:333:VAL:O	7:Z:337:LEU:HB3	2.16	0.45
4:G:440:PRO:HD2	4:G:443:LEU:HD13	1.98	0.45
7:S:193:LYS:HB2	7:S:424:SER:HB2	1.98	0.45
7:Z:235:ILE:HA	7:Z:376:LEU:HD21	1.97	0.45
2:F:433:TRP:HD1	2:F:483:VAL:HG22	1.82	0.45
6:L:296:CYS:SG	6:L:297:TRP:N	2.89	0.45
7:S:333:VAL:O	7:S:337:LEU:HB3	2.16	0.45
7:Z:351:TRP:CZ2	7:Z:443:TYR:HB3	2.51	0.45
2:F:566:LEU:HD11	2:F:660:TYR:HB3	1.99	0.45
2:H:717:GLN:HE22	2:H:879:ARG:CZ	2.29	0.45
4:E:695:TYR:OH	7:S:250:ASN:ND2	2.50	0.45
2:F:447:PHE:HE2	2:F:484:LEU:HB2	1.82	0.45
5:K:92:GLY:HA3	5:K:175:ILE:HG23	1.97	0.45
4:E:834:LEU:HD21	4:E:868:ARG:HB3	1.99	0.45
4:G:852:MET:SD	4:G:852:MET:N	2.81	0.45
6:L:464:LYS:HZ1	6:L:468:ARG:HB3	1.81	0.45
7:S:67:LEU:HD23	7:S:67:LEU:HA	1.85	0.45
7:Z:67:LEU:HD23	7:Z:67:LEU:HA	1.85	0.45
4:G:821:THR:HA	4:G:824:LYS:HG2	1.98	0.45
2:H:249:ALA:HA	2:H:252:ARG:HH11	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:455:LYS:H	2:H:455:LYS:HG2	1.48	0.45
5:K:143:ILE:HD13	5:K:148:ILE:HD12	1.99	0.45
7:X:333:VAL:O	7:X:337:LEU:HB3	2.16	0.45
3:m:56:ASN:ND2	3:m:58:GLU:OE2	2.49	0.45
4:E:248:VAL:HG11	4:E:257:ARG:HG3	1.99	0.45
5:I:491:GLU:HA	5:I:494:HIS:CD2	2.52	0.45
7:U:62:PRO:HD2	7:U:86:TYR:HB3	1.99	0.45
7:U:235:ILE:HA	7:U:376:LEU:HD21	1.97	0.45
7:V:318:ILE:HB	7:V:380:ASN:HB3	1.99	0.45
7:Y:318:ILE:HB	7:Y:380:ASN:HB3	1.99	0.45
1:l:110:ILE:O	1:l:114:LEU:HG	2.17	0.44
2:F:672:ARG:O	2:F:676:ILE:HG12	2.16	0.44
4:G:632:ARG:O	4:G:636:THR:OG1	2.28	0.44
1:J:369:TYR:OH	5:K:127:ASP:O	2.34	0.44
7:T:318:ILE:HB	7:T:380:ASN:HB3	1.99	0.44
7:U:389:GLU:O	7:U:393:ARG:N	2.45	0.44
7:W:193:LYS:HB2	7:W:424:SER:HB2	1.98	0.44
7:Z:62:PRO:HD2	7:Z:86:TYR:HB3	2.00	0.44
1:l:84:TRP:CE3	3:m:34:ILE:HD11	2.52	0.44
5:I:484:SER:HB3	5:I:587:LEU:HD11	2.00	0.44
6:L:1502:GLU:HG2	6:L:1503:LEU:HD22	1.98	0.44
6:L:1522:GLU:H	6:L:1525:GLN:HG2	1.82	0.44
7:T:62:PRO:HD2	7:T:86:TYR:HB3	2.00	0.44
7:U:349:ILE:HD11	7:U:351:TRP:CE2	2.53	0.44
7:W:231:LEU:O	7:W:234:THR:OG1	2.32	0.44
2:F:268:MET:HG3	2:F:276:LYS:H	1.83	0.44
2:F:865:LEU:HD12	2:F:873:LEU:HD12	1.99	0.44
5:I:405:LEU:HD11	5:I:409:ASN:HB3	1.99	0.44
5:K:546:HIS:O	5:K:550:SER:OG	2.26	0.44
6:L:294:ARG:HH21	6:L:308:GLU:HA	1.83	0.44
7:W:62:PRO:HD2	7:W:86:TYR:HB3	1.99	0.44
4:E:388:PHE:HA	4:E:391:LEU:HD12	2.00	0.44
2:H:493:LEU:HD13	2:H:545:LEU:HD22	2.00	0.44
2:H:737:LYS:HG3	2:H:750:ALA:HB1	1.99	0.44
5:K:184:TYR:HD1	5:K:315:LYS:HG3	1.82	0.44
5:K:345:VAL:HG23	5:K:346:GLU:HG3	1.99	0.44
6:L:1632:ALA:HB1	6:L:1740:ARG:HD2	1.98	0.44
7:S:343:ARG:HA	7:S:343:ARG:HD2	1.67	0.44
7:U:318:ILE:HB	7:U:380:ASN:HB3	1.99	0.44
7:W:318:ILE:HB	7:W:380:ASN:HB3	2.00	0.44
7:Y:343:ARG:HD2	7:Y:343:ARG:HA	1.67	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:221:LEU:HD22	4:E:263:ILE:HD11	1.99	0.44
4:E:522:MET:SD	7:S:248:TYR:OH	2.68	0.44
5:I:3:HIS:HB2	6:L:297:TRP:CZ2	2.53	0.44
5:I:610:ALA:O	5:I:613:SER:OG	2.30	0.44
5:K:152:GLN:NE2	5:K:262:GLU:O	2.51	0.44
7:T:160:ARG:HE	7:T:160:ARG:HB3	1.59	0.44
7:T:343:ARG:HD2	7:T:343:ARG:HA	1.67	0.44
7:V:349:ILE:HD11	7:V:351:TRP:CE2	2.53	0.44
7:X:73:VAL:O	7:X:76:SER:OG	2.34	0.44
7:X:349:ILE:HD11	7:X:351:TRP:CE2	2.53	0.44
7:Z:23:LYS:HB3	7:Z:23:LYS:HE3	1.83	0.44
4:E:341:LEU:HD13	4:E:341:LEU:HA	1.79	0.44
2:H:668:TRP:O	2:H:672:ARG:HG3	2.17	0.44
5:I:340:LEU:O	5:I:344:MET:HB2	2.18	0.44
5:K:132:LEU:O	5:K:135:SER:OG	2.33	0.44
6:L:1786:LEU:O	6:L:1792:GLN:NE2	2.44	0.44
3:b:56:ASN:ND2	3:b:58:GLU:OE2	2.49	0.44
3:k:56:ASN:ND2	3:k:58:GLU:OE2	2.49	0.44
2:F:554:SER:O	2:F:554:SER:OG	2.29	0.44
4:G:711:LYS:HB3	4:G:711:LYS:HE3	1.81	0.44
2:F:254:ILE:HD12	2:F:257:VAL:HB	2.00	0.44
2:F:451:ASP:H	2:F:463:LYS:HA	1.82	0.44
5:I:279:VAL:HG13	5:I:336:VAL:HG11	1.99	0.44
7:W:349:ILE:HD11	7:W:351:TRP:CE2	2.53	0.44
7:Y:349:ILE:HD11	7:Y:351:TRP:CE2	2.53	0.44
2:F:692:ARG:NH1	7:T:265:ARG:HG2	2.33	0.44
5:I:498:LEU:HD21	7:W:264:PRO:HD3	1.99	0.44
1:J:242:LEU:HA	1:J:245:VAL:HG22	1.99	0.44
7:T:349:ILE:HD11	7:T:351:TRP:CE2	2.53	0.44
7:Z:349:ILE:HD11	7:Z:351:TRP:CE2	2.53	0.44
4:E:518:ARG:HG2	4:E:519:TYR:CD1	2.53	0.43
5:I:157:VAL:HG13	5:I:172:LEU:HG	2.00	0.43
7:S:349:ILE:HD11	7:S:351:TRP:CE2	2.53	0.43
7:T:23:LYS:HB3	7:T:23:LYS:HE3	1.83	0.43
7:Z:318:ILE:HB	7:Z:380:ASN:HB3	1.99	0.43
4:E:641:LEU:HD23	4:E:739:LEU:HD23	2.00	0.43
6:L:1687:GLU:OE1	6:L:1711:LYS:NZ	2.40	0.43
7:W:3:ARG:HE	7:W:3:ARG:HB3	1.73	0.43
7:X:318:ILE:HB	7:X:380:ASN:HB3	1.99	0.43
4:E:581:ASP:HB3	4:E:582:LEU:H	1.57	0.43
5:I:578:PRO:HA	5:I:581:HIS:CD2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:231:LEU:O	7:T:234:THR:OG1	2.32	0.43
7:U:3:ARG:HE	7:U:3:ARG:HB3	1.73	0.43
4:E:391:LEU:HG	4:E:407:PHE:HE1	1.84	0.43
2:F:339:LEU:HA	2:F:342:LEU:HD12	2.00	0.43
2:F:740:GLN:HE21	2:F:746:HIS:CE1	2.31	0.43
4:G:851:GLY:O	4:G:854:SER:OG	2.33	0.43
6:L:1607:VAL:HA	6:L:1702:GLN:HG2	2.00	0.43
7:S:318:ILE:HB	7:S:380:ASN:HB3	1.99	0.43
1:J:684:GLU:HG2	1:J:688:ARG:HB2	2.00	0.43
2:H:334:GLU:H	2:H:334:GLU:HG3	1.64	0.43
7:V:115:HIS:NE2	7:V:116:GLU:OE2	2.52	0.43
7:Z:265:ARG:HH12	7:Z:430:GLN:HB2	1.84	0.43
4:E:163:ASP:OD1	4:E:163:ASP:N	2.51	0.43
4:E:308:SER:O	4:E:311:GLU:HG2	2.18	0.43
2:F:876:LEU:O	2:F:879:ARG:HG2	2.19	0.43
4:G:271:SER:O	4:G:274:THR:HB	2.19	0.43
4:G:635:LEU:HG	4:G:639:GLN:HE21	1.84	0.43
7:X:62:PRO:HD2	7:X:86:TYR:HB3	2.00	0.43
7:Y:115:HIS:NE2	7:Y:116:GLU:OE2	2.52	0.43
2:F:338:LEU:HD11	2:F:377:ARG:HH22	1.83	0.43
5:K:646:LEU:HB3	7:Y:341:ARG:HD2	2.01	0.43
7:T:265:ARG:HH12	7:T:430:GLN:HB2	1.84	0.43
7:U:115:HIS:NE2	7:U:116:GLU:OE2	2.52	0.43
7:U:265:ARG:HH12	7:U:430:GLN:HB2	1.84	0.43
7:V:62:PRO:HD2	7:V:86:TYR:HB3	2.00	0.43
7:V:73:VAL:O	7:V:76:SER:OG	2.34	0.43
2:H:475:MET:HE2	2:H:475:MET:HB3	1.79	0.43
1:J:898:HIS:HA	1:J:901:ILE:HG12	2.00	0.43
5:K:17:PHE:HB3	5:K:25:LEU:HD22	2.01	0.43
5:K:191:MET:HE2	5:K:191:MET:HB3	1.91	0.43
6:L:1522:GLU:HA	6:L:1525:GLN:HB2	2.01	0.43
7:S:62:PRO:HD2	7:S:86:TYR:HB3	1.99	0.43
7:X:23:LYS:HB3	7:X:23:LYS:HE3	1.83	0.43
4:E:554:LEU:HD13	4:E:557:LEU:HD21	1.99	0.43
2:H:581:LEU:HD13	2:H:600:ILE:HD11	2.01	0.43
1:J:739:TYR:CG	1:J:832:LYS:HD3	2.54	0.43
7:W:265:ARG:HH12	7:W:430:GLN:HB2	1.84	0.43
2:F:433:TRP:HZ2	2:F:484:LEU:HD12	1.84	0.42
2:H:794:ARG:HH22	2:H:797:LEU:HD11	1.83	0.42
7:V:52:PHE:HB3	7:V:60:TYR:HB3	2.01	0.42
7:V:231:LEU:O	7:V:234:THR:OG1	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Z:52:PHE:HB3	7:Z:60:TYR:HB3	2.01	0.42
5:K:311:LEU:HA	5:K:314:LEU:HG	2.00	0.42
3:b:67:LEU:HD22	2:a:21:LEU:HD11	2.01	0.42
7:S:115:HIS:NE2	7:S:116:GLU:OE2	2.52	0.42
7:X:52:PHE:HB3	7:X:60:TYR:HB3	2.01	0.42
7:X:265:ARG:HH12	7:X:430:GLN:HB2	1.84	0.42
7:Z:231:LEU:O	7:Z:234:THR:OG1	2.32	0.42
1:J:312:SER:O	1:J:315:GLU:HG2	2.19	0.42
7:T:52:PHE:HB3	7:T:60:TYR:HB3	2.01	0.42
2:H:330:GLN:HE22	2:H:421:LEU:HD11	1.85	0.42
7:S:52:PHE:HB3	7:S:60:TYR:HB3	2.01	0.42
7:W:356:ILE:HD13	7:W:356:ILE:HA	1.83	0.42
7:Y:62:PRO:HD2	7:Y:86:TYR:HB3	2.00	0.42
5:I:21:LYS:HD3	5:I:21:LYS:HA	1.77	0.42
5:K:365:ARG:NH1	5:K:367:GLU:OE1	2.51	0.42
6:L:1555:SER:HA	6:L:1558:LEU:HD12	2.02	0.42
2:a:7:LYS:HG2	2:a:8:SER:H	1.84	0.42
2:a:34:TYR:HE1	2:a:37:ARG:HH11	1.68	0.42
2:a:50:ASP:H	2:a:91:TRP:CD1	2.38	0.42
7:S:274:THR:HG23	7:S:297:LEU:HB2	2.02	0.42
7:S:415:LYS:HG3	7:S:418:PHE:H	1.84	0.42
7:T:115:HIS:NE2	7:T:116:GLU:OE2	2.52	0.42
7:U:415:LYS:HG3	7:U:418:PHE:H	1.84	0.42
7:V:274:THR:HG23	7:V:297:LEU:HB2	2.02	0.42
7:V:415:LYS:HG3	7:V:418:PHE:H	1.84	0.42
7:X:115:HIS:NE2	7:X:116:GLU:OE2	2.52	0.42
7:Y:3:ARG:HE	7:Y:3:ARG:HB3	1.73	0.42
7:Y:265:ARG:HH12	7:Y:430:GLN:HB2	1.84	0.42
7:Z:274:THR:HG23	7:Z:297:LEU:HB2	2.02	0.42
7:Z:415:LYS:HG3	7:Z:418:PHE:H	1.84	0.42
4:E:548:PRO:HB2	2:F:874:ARG:HH22	1.85	0.42
4:G:675:TRP:HB2	4:G:676:PHE:H	1.65	0.42
4:G:684:GLN:HE21	4:G:688:ASN:HD21	1.68	0.42
2:H:635:TRP:CE3	2:H:672:ARG:HD3	2.54	0.42
7:U:351:TRP:H	7:U:351:TRP:CD1	2.38	0.42
7:U:419:ASP:O	7:U:423:THR:OG1	2.32	0.42
7:W:115:HIS:NE2	7:W:116:GLU:OE2	2.52	0.42
7:X:274:THR:HG23	7:X:297:LEU:HB2	2.02	0.42
7:X:415:LYS:HG3	7:X:418:PHE:H	1.84	0.42
4:E:637:ARG:HA	4:E:640:MET:HG2	2.02	0.42
4:G:439:ILE:HA	4:G:440:PRO:HD3	1.89	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:343:ARG:HD2	7:U:343:ARG:HA	1.67	0.42
7:V:67:LEU:HD23	7:V:67:LEU:HA	1.85	0.42
7:V:265:ARG:HH12	7:V:430:GLN:HB2	1.84	0.42
7:W:351:TRP:CD1	7:W:351:TRP:H	2.38	0.42
1:l:77:ASP:HB3	1:l:80:LYS:HE2	2.01	0.42
2:j:97:LEU:HD23	3:k:31:ILE:HG22	2.01	0.42
5:K:1:MET:N	6:L:320:PHE:HB2	2.35	0.42
7:Y:415:LYS:HG3	7:Y:418:PHE:H	1.85	0.42
7:Z:115:HIS:NE2	7:Z:116:GLU:OE2	2.52	0.42
4:E:509:LEU:HD13	4:E:626:LEU:HD22	2.02	0.42
6:L:1607:VAL:HG13	6:L:1702:GLN:HG2	2.00	0.42
6:L:1767:GLN:HE21	6:L:1771:THR:HG23	1.84	0.42
7:S:351:TRP:H	7:S:351:TRP:CD1	2.38	0.42
7:W:23:LYS:HB3	7:W:23:LYS:HE3	1.83	0.42
2:F:677:LEU:HD12	2:F:680:ILE:HD12	2.02	0.42
4:G:362:ARG:HD2	4:G:362:ARG:HA	1.85	0.42
4:G:473:LYS:HG3	4:G:487:GLN:NE2	2.35	0.42
2:H:603:THR:OG1	7:W:342:GLU:HB3	2.19	0.42
7:U:231:LEU:O	7:U:234:THR:OG1	2.32	0.42
2:F:255:LEU:HD22	2:F:346:LEU:HD13	2.02	0.41
2:F:743:ASP:N	2:F:743:ASP:OD1	2.53	0.41
1:J:376:LYS:HD3	5:K:124:TYR:HB2	2.02	0.41
6:L:428:VAL:HG12	6:L:531:PRO:HD2	2.02	0.41
7:S:265:ARG:HH12	7:S:430:GLN:HB2	1.84	0.41
7:T:415:LYS:HG3	7:T:418:PHE:H	1.84	0.41
7:U:274:THR:HG23	7:U:297:LEU:HB2	2.02	0.41
7:X:56:ASP:OD1	7:X:56:ASP:N	2.53	0.41
2:H:664:PHE:O	2:H:668:TRP:HB2	2.20	0.41
2:H:722:ILE:HA	2:H:726:VAL:HG22	2.02	0.41
1:J:723:MET:HE3	1:J:723:MET:HB3	1.94	0.41
7:S:73:VAL:O	7:S:76:SER:OG	2.34	0.41
4:E:306:LEU:O	4:E:310:LEU:HG	2.19	0.41
4:G:555:LEU:HD11	4:G:573:LEU:HD11	2.01	0.41
4:G:650:HIS:HD2	4:G:653:ARG:HH11	1.69	0.41
2:H:538:TYR:O	2:H:542:SER:OG	2.28	0.41
5:I:127:ASP:HA	5:I:130:GLN:HG3	2.02	0.41
1:J:287:PHE:H	1:J:296:VAL:HA	1.86	0.41
6:L:1476:MET:HE2	6:L:1476:MET:HB3	1.96	0.41
2:a:60:LYS:HE3	2:a:60:LYS:HB3	1.79	0.41
7:T:252:ASP:OD1	7:T:252:ASP:N	2.47	0.41
4:E:399:ILE:HD12	4:E:401:HIS:HE1	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:271:ILE:HD13	1:J:393:ILE:HG22	2.03	0.41
5:K:255:LYS:HG3	5:K:256:GLN:H	1.85	0.41
7:S:56:ASP:OD1	7:S:56:ASP:N	2.53	0.41
7:T:56:ASP:OD1	7:T:56:ASP:N	2.53	0.41
7:W:56:ASP:OD1	7:W:56:ASP:N	2.53	0.41
7:X:231:LEU:O	7:X:234:THR:OG1	2.32	0.41
4:E:168:LYS:HD2	4:E:168:LYS:HA	1.94	0.41
4:E:756:VAL:HA	4:E:759:THR:HG22	2.01	0.41
5:I:487:ARG:HE	5:I:488:VAL:HG13	1.85	0.41
5:K:48:LEU:HD13	5:K:126:LEU:HG	2.03	0.41
7:W:52:PHE:HB3	7:W:60:TYR:HB3	2.01	0.41
7:X:351:TRP:CD1	7:X:351:TRP:H	2.38	0.41
4:E:244:ARG:NH1	4:E:271:SER:OG	2.54	0.41
4:E:277:ILE:HG12	4:E:296:MET:HE3	2.03	0.41
4:E:280:LYS:HB3	4:E:289:ASN:ND2	2.35	0.41
2:F:305:ARG:NE	2:F:306:ARG:HH22	2.18	0.41
4:G:861:PHE:CD2	7:U:348:PHE:HD1	2.39	0.41
5:K:370:GLN:HB2	5:K:486:ARG:HH21	1.84	0.41
7:S:356:ILE:HD13	7:S:356:ILE:HA	1.83	0.41
7:U:52:PHE:HB3	7:U:60:TYR:HB3	2.01	0.41
7:W:274:THR:HG23	7:W:297:LEU:HB2	2.02	0.41
7:Y:56:ASP:OD1	7:Y:56:ASP:N	2.53	0.41
7:Y:274:THR:HG23	7:Y:297:LEU:HB2	2.02	0.41
2:j:51:GLU:HG3	2:j:91:TRP:HA	2.02	0.41
2:F:568:LEU:HG	2:F:574:ILE:HG13	2.03	0.41
4:G:257:ARG:O	4:G:261:HIS:ND1	2.48	0.41
4:G:623:LYS:H	4:G:626:LEU:HB2	1.86	0.41
4:G:749:SER:HA	4:G:752:MET:HE3	2.03	0.41
2:H:783:ILE:HD12	2:H:783:ILE:HA	1.92	0.41
5:I:25:LEU:HD11	5:I:53:ILE:HD12	2.02	0.41
5:I:582:CYS:O	5:I:586:ILE:HG12	2.21	0.41
1:J:892:HIS:CE1	7:X:355:SER:HB2	2.47	0.41
7:T:274:THR:HG23	7:T:297:LEU:HB2	2.02	0.41
7:X:377:MET:HE2	7:X:377:MET:HB2	1.91	0.41
7:Y:351:TRP:H	7:Y:351:TRP:CD1	2.38	0.41
7:Z:73:VAL:O	7:Z:76:SER:OG	2.34	0.41
2:H:526:LEU:HD23	2:H:526:LEU:HA	1.88	0.41
2:H:677:LEU:HG	2:H:712:VAL:HG12	2.02	0.41
5:I:345:VAL:HG23	5:I:346:GLU:HG3	2.03	0.41
7:V:262:PRO:HG3	7:V:318:ILE:HG21	2.03	0.41
7:W:57:ASP:HB3	7:W:59:HIS:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Y:399:ARG:HD2	7:Y:399:ARG:HA	1.91	0.41
4:E:354:SER:O	4:E:357:SER:OG	2.33	0.41
2:F:720:TYR:OH	7:T:250:ASN:ND2	2.54	0.41
2:F:887:LYS:HE2	2:F:887:LYS:HB3	1.60	0.41
4:G:631:ASN:HD21	4:G:633:LYS:HG2	1.86	0.41
2:H:726:VAL:HG12	2:H:761:ARG:HB3	2.03	0.41
5:K:530:TYR:O	5:K:534:VAL:HG23	2.21	0.41
6:L:434:SER:HB3	6:L:437:ARG:HH21	1.86	0.41
2:a:98:LEU:HD23	2:a:98:LEU:HA	1.96	0.41
7:S:424:SER:O	7:S:428:VAL:HG13	2.21	0.41
7:U:57:ASP:HB3	7:U:59:HIS:CE1	2.56	0.41
7:U:262:PRO:HG3	7:U:318:ILE:HG21	2.03	0.41
7:V:56:ASP:OD1	7:V:56:ASP:N	2.53	0.41
7:V:424:SER:O	7:V:428:VAL:HG13	2.21	0.41
7:X:424:SER:O	7:X:428:VAL:HG13	2.21	0.41
7:Y:231:LEU:O	7:Y:234:THR:OG1	2.32	0.41
7:Z:56:ASP:OD1	7:Z:56:ASP:N	2.53	0.41
7:Z:351:TRP:CD1	7:Z:351:TRP:H	2.38	0.41
4:E:330:PRO:HA	4:E:333:ARG:HE	1.85	0.41
4:G:395:ILE:HD11	4:G:450:ILE:HG23	2.03	0.41
2:H:758:ILE:HA	2:H:758:ILE:HD13	1.85	0.41
1:J:831:ILE:HG21	1:J:901:ILE:HD11	2.02	0.41
5:K:577:LYS:O	5:K:581:HIS:HB2	2.21	0.41
7:T:57:ASP:HB3	7:T:59:HIS:CE1	2.56	0.41
7:T:351:TRP:CD1	7:T:351:TRP:H	2.38	0.41
2:F:605:VAL:HG13	2:F:610:ALA:HB3	2.03	0.40
5:K:141:GLU:O	5:K:145:SER:OG	2.30	0.40
5:K:528:LEU:HD23	5:K:528:LEU:HA	1.80	0.40
7:W:180:ASP:HB3	7:W:181:VAL:H	1.74	0.40
7:Z:57:ASP:HB3	7:Z:59:HIS:CE1	2.56	0.40
7:Z:262:PRO:HG3	7:Z:318:ILE:HG21	2.03	0.40
4:G:398:GLY:HA3	4:G:461:ARG:HH22	1.85	0.40
2:H:594:GLN:HG3	2:H:623:VAL:HG23	2.03	0.40
1:J:283:LYS:HA	1:J:283:LYS:HD2	1.85	0.40
7:T:424:SER:O	7:T:428:VAL:HG13	2.21	0.40
7:W:424:SER:O	7:W:428:VAL:HG13	2.21	0.40
7:Y:24:GLN:HG2	7:Y:25:LEU:HD12	2.04	0.40
7:Y:52:PHE:HB3	7:Y:60:TYR:HB3	2.01	0.40
2:j:100:LEU:HA	3:k:65:LYS:HE3	2.03	0.40
2:H:300:LEU:HB2	2:H:378:LEU:HD21	2.04	0.40
2:H:427:LEU:HA	2:H:430:LEU:HG	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:554:ILE:HD13	6:L:596:TYR:HB2	2.04	0.40
7:V:23:LYS:HB3	7:V:23:LYS:HE3	1.83	0.40
7:V:351:TRP:CD1	7:V:351:TRP:H	2.38	0.40
7:W:415:LYS:HG3	7:W:418:PHE:H	1.85	0.40
7:X:3:ARG:HE	7:X:3:ARG:HB3	1.73	0.40
4:E:192:LEU:HA	4:E:192:LEU:HD13	1.91	0.40
4:G:747:VAL:H	4:G:747:VAL:HG22	1.69	0.40
2:H:446:PHE:O	2:H:467:ARG:NH1	2.54	0.40
7:U:56:ASP:OD1	7:U:56:ASP:N	2.53	0.40
7:U:424:SER:O	7:U:428:VAL:HG13	2.21	0.40
7:V:160:ARG:HE	7:V:160:ARG:HB3	1.59	0.40
7:V:395:TYR:O	7:V:399:ARG:N	2.52	0.40
7:Y:424:SER:O	7:Y:428:VAL:HG13	2.21	0.40
7:Z:24:GLN:HG2	7:Z:25:LEU:HD12	2.04	0.40
4:E:321:LEU:HD12	4:E:321:LEU:HA	1.91	0.40
4:E:655:LEU:HD11	4:E:686:MET:HG3	2.03	0.40
4:G:257:ARG:HG2	4:G:261:HIS:CE1	2.56	0.40
1:J:828:LEU:HG	1:J:832:LYS:NZ	2.35	0.40
6:L:1739:PHE:HA	6:L:1765:MET:SD	2.60	0.40
7:X:262:PRO:HG3	7:X:318:ILE:HG21	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	506/1024 (49%)	472 (93%)	30 (6%)	4 (1%)	16	54
1	l	104/1024 (10%)	94 (90%)	7 (7%)	3 (3%)	3	23
2	F	591/907 (65%)	555 (94%)	36 (6%)	0	100	100
2	H	584/907 (64%)	565 (97%)	18 (3%)	1 (0%)	43	78

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	a	112/907 (12%)	106 (95%)	6 (5%)	0	100	100
2	j	97/907 (11%)	95 (98%)	2 (2%)	0	100	100
3	b	63/82 (77%)	60 (95%)	3 (5%)	0	100	100
3	k	63/82 (77%)	60 (95%)	3 (5%)	0	100	100
3	m	63/82 (77%)	60 (95%)	3 (5%)	0	100	100
4	E	626/902 (69%)	590 (94%)	34 (5%)	2 (0%)	36	72
4	G	628/902 (70%)	593 (94%)	33 (5%)	2 (0%)	36	72
5	I	511/667 (77%)	481 (94%)	27 (5%)	3 (1%)	21	59
5	K	548/667 (82%)	536 (98%)	11 (2%)	1 (0%)	43	78
6	L	540/1819 (30%)	505 (94%)	33 (6%)	2 (0%)	30	67
7	S	408/451 (90%)	392 (96%)	16 (4%)	0	100	100
7	T	408/451 (90%)	392 (96%)	16 (4%)	0	100	100
7	U	408/451 (90%)	392 (96%)	16 (4%)	0	100	100
7	V	408/451 (90%)	392 (96%)	16 (4%)	0	100	100
7	W	408/451 (90%)	392 (96%)	16 (4%)	0	100	100
7	X	408/451 (90%)	392 (96%)	16 (4%)	0	100	100
7	Y	408/451 (90%)	392 (96%)	16 (4%)	0	100	100
7	Z	408/451 (90%)	392 (96%)	16 (4%)	0	100	100
All	All	8300/14487 (57%)	7908 (95%)	374 (4%)	18 (0%)	44	78

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	l	120	SER
1	l	121	PRO
4	E	581	ASP
2	H	455	LYS
5	I	408	ASP
5	I	508	ASN
1	J	236	LEU
1	J	238	LEU
1	J	257	TYR
5	K	409	ASN
6	L	308	GLU
4	G	241	ARG
5	I	405	LEU

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Mol	Chain	Res	Type
1	l	129	THR
4	E	582	LEU
4	G	864	PHE
6	L	307	ARG
1	J	258	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	498/933 (53%)	493 (99%)	5 (1%)	68	78
1	l	84/933 (9%)	84 (100%)	0	100	100
2	F	542/798 (68%)	539 (99%)	3 (1%)	78	83
2	H	539/798 (68%)	538 (100%)	1 (0%)	87	87
2	a	101/798 (13%)	101 (100%)	0	100	100
2	j	88/798 (11%)	88 (100%)	0	100	100
3	b	53/62 (86%)	42 (79%)	11 (21%)	1	6
3	k	53/62 (86%)	42 (79%)	11 (21%)	1	6
3	m	53/62 (86%)	42 (79%)	11 (21%)	1	6
4	E	574/791 (73%)	571 (100%)	3 (0%)	81	83
4	G	572/791 (72%)	571 (100%)	1 (0%)	87	87
5	I	472/594 (80%)	467 (99%)	5 (1%)	65	76
5	K	509/594 (86%)	505 (99%)	4 (1%)	73	80
6	L	501/1546 (32%)	498 (99%)	3 (1%)	78	83
7	S	376/400 (94%)	322 (86%)	54 (14%)	3	13
7	T	376/400 (94%)	322 (86%)	54 (14%)	3	13
7	U	376/400 (94%)	322 (86%)	54 (14%)	3	13
7	V	376/400 (94%)	322 (86%)	54 (14%)	3	13
7	W	376/400 (94%)	322 (86%)	54 (14%)	3	13
7	X	376/400 (94%)	322 (86%)	54 (14%)	3	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	Y	376/400 (94%)	322 (86%)	54 (14%)	3	13
7	Z	376/400 (94%)	322 (86%)	54 (14%)	3	13
All	All	7647/12760 (60%)	7157 (94%)	490 (6%)	18	37

All (490) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	m	24	THR
3	m	35	LEU
3	m	37	THR
3	m	39	LEU
3	m	43	THR
3	m	44	LEU
3	m	45	SER
3	m	51	CYS
3	m	62	SER
3	m	71	THR
3	m	74	LEU
3	k	24	THR
3	k	35	LEU
3	k	37	THR
3	k	39	LEU
3	k	43	THR
3	k	44	LEU
3	k	45	SER
3	k	51	CYS
3	k	62	SER
3	k	71	THR
3	k	74	LEU
4	E	266	VAL
4	E	341	LEU
4	E	621	ILE
2	F	290	THR
2	F	648	ILE
2	F	671	LYS
4	G	675	TRP
2	H	600	ILE
5	I	104	LEU
5	I	179	CYS
5	I	323	VAL
5	I	475	TYR

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Mol	Chain	Res	Type
5	I	498	LEU
1	J	236	LEU
1	J	238	LEU
1	J	560	ILE
1	J	641	VAL
1	J	1013	LEU
5	K	4	GLU
5	K	35	HIS
5	K	639	ASN
5	K	651	TYR
6	L	320	PHE
6	L	1553	VAL
6	L	1800	LEU
3	b	24	THR
3	b	35	LEU
3	b	37	THR
3	b	39	LEU
3	b	43	THR
3	b	44	LEU
3	b	45	SER
3	b	51	CYS
3	b	62	SER
3	b	71	THR
3	b	74	LEU
7	S	7	THR
7	S	8	LEU
7	S	12	GLN
7	S	23	LYS
7	S	50	VAL
7	S	56	ASP
7	S	66	LEU
7	S	73	VAL
7	S	80	SER
7	S	91	ILE
7	S	136	VAL
7	S	157	LEU
7	S	168	THR
7	S	180	ASP
7	S	189	LEU
7	S	192	LEU
7	S	195	LEU
7	S	200	ASP

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Mol	Chain	Res	Type
7	S	204	VAL
7	S	205	LEU
7	S	211	ASN
7	S	220	ILE
7	S	224	SER
7	S	226	SER
7	S	228	ILE
7	S	237	SER
7	S	256	LEU
7	S	270	MET
7	S	274	THR
7	S	278	THR
7	S	288	THR
7	S	290	VAL
7	S	298	LEU
7	S	299	GLN
7	S	303	VAL
7	S	316	CYS
7	S	328	VAL
7	S	329	ASP
7	S	333	VAL
7	S	337	LEU
7	S	349	ILE
7	S	358	VAL
7	S	364	SER
7	S	367	LEU
7	S	369	SER
7	S	377	MET
7	S	378	MET
7	S	387	LEU
7	S	392	CYS
7	S	402	GLU
7	S	423	THR
7	S	424	SER
7	S	428	VAL
7	S	431	LEU
7	T	7	THR
7	T	8	LEU
7	T	12	GLN
7	T	23	LYS
7	T	50	VAL
7	T	56	ASP

Continued on next page...

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Mol	Chain	Res	Type
7	T	66	LEU
7	T	73	VAL
7	T	80	SER
7	T	91	ILE
7	T	136	VAL
7	T	157	LEU
7	T	168	THR
7	T	180	ASP
7	T	189	LEU
7	T	192	LEU
7	T	195	LEU
7	T	200	ASP
7	T	204	VAL
7	T	205	LEU
7	T	211	ASN
7	T	220	ILE
7	T	224	SER
7	T	226	SER
7	T	228	ILE
7	T	237	SER
7	T	256	LEU
7	T	270	MET
7	T	274	THR
7	T	278	THR
7	T	288	THR
7	T	290	VAL
7	T	298	LEU
7	T	299	GLN
7	T	303	VAL
7	T	316	CYS
7	T	328	VAL
7	T	329	ASP
7	T	333	VAL
7	T	337	LEU
7	T	349	ILE
7	T	358	VAL
7	T	364	SER
7	T	367	LEU
7	T	369	SER
7	T	377	MET
7	T	378	MET
7	T	387	LEU

Continued on next page...

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Mol	Chain	Res	Type
7	T	392	CYS
7	T	402	GLU
7	T	423	THR
7	T	424	SER
7	T	428	VAL
7	T	431	LEU
7	U	7	THR
7	U	8	LEU
7	U	12	GLN
7	U	23	LYS
7	U	50	VAL
7	U	56	ASP
7	U	66	LEU
7	U	73	VAL
7	U	80	SER
7	U	91	ILE
7	U	136	VAL
7	U	157	LEU
7	U	168	THR
7	U	180	ASP
7	U	189	LEU
7	U	192	LEU
7	U	195	LEU
7	U	200	ASP
7	U	204	VAL
7	U	205	LEU
7	U	211	ASN
7	U	220	ILE
7	U	224	SER
7	U	226	SER
7	U	228	ILE
7	U	237	SER
7	U	256	LEU
7	U	270	MET
7	U	274	THR
7	U	278	THR
7	U	288	THR
7	U	290	VAL
7	U	298	LEU
7	U	299	GLN
7	U	303	VAL
7	U	316	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	U	328	VAL
7	U	329	ASP
7	U	333	VAL
7	U	337	LEU
7	U	349	ILE
7	U	358	VAL
7	U	364	SER
7	U	367	LEU
7	U	369	SER
7	U	377	MET
7	U	378	MET
7	U	387	LEU
7	U	392	CYS
7	U	402	GLU
7	U	423	THR
7	U	424	SER
7	U	428	VAL
7	U	431	LEU
7	V	7	THR
7	V	8	LEU
7	V	12	GLN
7	V	23	LYS
7	V	50	VAL
7	V	56	ASP
7	V	66	LEU
7	V	73	VAL
7	V	80	SER
7	V	91	ILE
7	V	136	VAL
7	V	157	LEU
7	V	168	THR
7	V	180	ASP
7	V	189	LEU
7	V	192	LEU
7	V	195	LEU
7	V	200	ASP
7	V	204	VAL
7	V	205	LEU
7	V	211	ASN
7	V	220	ILE
7	V	224	SER
7	V	226	SER

Continued on next page...

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Mol	Chain	Res	Type
7	V	228	ILE
7	V	237	SER
7	V	256	LEU
7	V	270	MET
7	V	274	THR
7	V	278	THR
7	V	288	THR
7	V	290	VAL
7	V	298	LEU
7	V	299	GLN
7	V	303	VAL
7	V	316	CYS
7	V	328	VAL
7	V	329	ASP
7	V	333	VAL
7	V	337	LEU
7	V	349	ILE
7	V	358	VAL
7	V	364	SER
7	V	367	LEU
7	V	369	SER
7	V	377	MET
7	V	378	MET
7	V	387	LEU
7	V	392	CYS
7	V	402	GLU
7	V	423	THR
7	V	424	SER
7	V	428	VAL
7	V	431	LEU
7	W	7	THR
7	W	8	LEU
7	W	12	GLN
7	W	23	LYS
7	W	50	VAL
7	W	56	ASP
7	W	66	LEU
7	W	73	VAL
7	W	80	SER
7	W	91	ILE
7	W	136	VAL
7	W	157	LEU

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Mol	Chain	Res	Type
7	W	168	THR
7	W	180	ASP
7	W	189	LEU
7	W	192	LEU
7	W	195	LEU
7	W	200	ASP
7	W	204	VAL
7	W	205	LEU
7	W	211	ASN
7	W	220	ILE
7	W	224	SER
7	W	226	SER
7	W	228	ILE
7	W	237	SER
7	W	256	LEU
7	W	270	MET
7	W	274	THR
7	W	278	THR
7	W	288	THR
7	W	290	VAL
7	W	298	LEU
7	W	299	GLN
7	W	303	VAL
7	W	316	CYS
7	W	328	VAL
7	W	329	ASP
7	W	333	VAL
7	W	337	LEU
7	W	349	ILE
7	W	358	VAL
7	W	364	SER
7	W	367	LEU
7	W	369	SER
7	W	377	MET
7	W	378	MET
7	W	387	LEU
7	W	392	CYS
7	W	402	GLU
7	W	423	THR
7	W	424	SER
7	W	428	VAL
7	W	431	LEU

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Mol	Chain	Res	Type
7	X	7	THR
7	X	8	LEU
7	X	12	GLN
7	X	23	LYS
7	X	50	VAL
7	X	56	ASP
7	X	66	LEU
7	X	73	VAL
7	X	80	SER
7	X	91	ILE
7	X	136	VAL
7	X	157	LEU
7	X	168	THR
7	X	180	ASP
7	X	189	LEU
7	X	192	LEU
7	X	195	LEU
7	X	200	ASP
7	X	204	VAL
7	X	205	LEU
7	X	211	ASN
7	X	220	ILE
7	X	224	SER
7	X	226	SER
7	X	228	ILE
7	X	237	SER
7	X	256	LEU
7	X	270	MET
7	X	274	THR
7	X	278	THR
7	X	288	THR
7	X	290	VAL
7	X	298	LEU
7	X	299	GLN
7	X	303	VAL
7	X	316	CYS
7	X	328	VAL
7	X	329	ASP
7	X	333	VAL
7	X	337	LEU
7	X	349	ILE
7	X	358	VAL

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Mol	Chain	Res	Type
7	X	364	SER
7	X	367	LEU
7	X	369	SER
7	X	377	MET
7	X	378	MET
7	X	387	LEU
7	X	392	CYS
7	X	402	GLU
7	X	423	THR
7	X	424	SER
7	X	428	VAL
7	X	431	LEU
7	Y	7	THR
7	Y	8	LEU
7	Y	12	GLN
7	Y	23	LYS
7	Y	50	VAL
7	Y	56	ASP
7	Y	66	LEU
7	Y	73	VAL
7	Y	80	SER
7	Y	91	ILE
7	Y	136	VAL
7	Y	157	LEU
7	Y	168	THR
7	Y	180	ASP
7	Y	189	LEU
7	Y	192	LEU
7	Y	195	LEU
7	Y	200	ASP
7	Y	204	VAL
7	Y	205	LEU
7	Y	211	ASN
7	Y	220	ILE
7	Y	224	SER
7	Y	226	SER
7	Y	228	ILE
7	Y	237	SER
7	Y	256	LEU
7	Y	270	MET
7	Y	274	THR
7	Y	278	THR

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Mol	Chain	Res	Type
7	Y	288	THR
7	Y	290	VAL
7	Y	298	LEU
7	Y	299	GLN
7	Y	303	VAL
7	Y	316	CYS
7	Y	328	VAL
7	Y	329	ASP
7	Y	333	VAL
7	Y	337	LEU
7	Y	349	ILE
7	Y	358	VAL
7	Y	364	SER
7	Y	367	LEU
7	Y	369	SER
7	Y	377	MET
7	Y	378	MET
7	Y	387	LEU
7	Y	392	CYS
7	Y	402	GLU
7	Y	423	THR
7	Y	424	SER
7	Y	428	VAL
7	Y	431	LEU
7	Z	7	THR
7	Z	8	LEU
7	Z	12	GLN
7	Z	23	LYS
7	Z	50	VAL
7	Z	56	ASP
7	Z	66	LEU
7	Z	73	VAL
7	Z	80	SER
7	Z	91	ILE
7	Z	136	VAL
7	Z	157	LEU
7	Z	168	THR
7	Z	180	ASP
7	Z	189	LEU
7	Z	192	LEU
7	Z	195	LEU
7	Z	200	ASP

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Mol	Chain	Res	Type
7	Z	204	VAL
7	Z	205	LEU
7	Z	211	ASN
7	Z	220	ILE
7	Z	224	SER
7	Z	226	SER
7	Z	228	ILE
7	Z	237	SER
7	Z	256	LEU
7	Z	270	MET
7	Z	274	THR
7	Z	278	THR
7	Z	288	THR
7	Z	290	VAL
7	Z	298	LEU
7	Z	299	GLN
7	Z	303	VAL
7	Z	316	CYS
7	Z	328	VAL
7	Z	329	ASP
7	Z	333	VAL
7	Z	337	LEU
7	Z	349	ILE
7	Z	358	VAL
7	Z	364	SER
7	Z	367	LEU
7	Z	369	SER
7	Z	377	MET
7	Z	378	MET
7	Z	387	LEU
7	Z	392	CYS
7	Z	402	GLU
7	Z	423	THR
7	Z	424	SER
7	Z	428	VAL
7	Z	431	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (239) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	30	GLN
1	1	57	ASN

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Mol	Chain	Res	Type
2	j	14	GLN
2	j	30	GLN
2	j	31	GLN
2	j	65	GLN
2	j	84	GLN
3	m	53	GLN
3	m	56	ASN
3	k	17	ASN
3	k	36	ASN
4	E	169	ASN
4	E	236	GLN
4	E	261	HIS
4	E	289	ASN
4	E	309	GLN
4	E	316	GLN
4	E	322	GLN
4	E	329	GLN
4	E	401	HIS
4	E	412	HIS
4	E	420	GLN
4	E	436	GLN
4	E	530	HIS
4	E	565	ASN
4	E	684	GLN
4	E	707	HIS
4	E	760	ASN
4	E	767	GLN
2	F	310	GLN
2	F	322	GLN
2	F	345	GLN
2	F	347	GLN
2	F	416	GLN
2	F	461	HIS
2	F	500	GLN
2	F	609	ASN
2	F	665	ASN
2	F	687	ASN
2	F	703	GLN
2	F	740	GLN
2	F	742	GLN
2	F	746	HIS
2	F	786	GLN

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Mol	Chain	Res	Type
2	F	830	ASN
4	G	165	GLN
4	G	169	ASN
4	G	172	GLN
4	G	236	GLN
4	G	303	HIS
4	G	309	GLN
4	G	312	GLN
4	G	314	HIS
4	G	360	HIS
4	G	412	HIS
4	G	436	GLN
4	G	438	GLN
4	G	444	GLN
4	G	487	GLN
4	G	512	HIS
4	G	565	ASN
4	G	585	GLN
4	G	639	GLN
4	G	650	HIS
4	G	684	GLN
4	G	691	GLN
4	G	694	GLN
2	H	330	GLN
2	H	401	HIS
2	H	479	GLN
2	H	702	HIS
2	H	703	GLN
2	H	717	GLN
2	H	719	GLN
2	H	736	ASN
2	H	740	GLN
2	H	805	GLN
2	H	859	GLN
2	H	885	HIS
5	I	20	ASN
5	I	26	GLN
5	I	29	GLN
5	I	35	HIS
5	I	82	HIS
5	I	109	GLN
5	I	123	ASN

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Mol	Chain	Res	Type
5	I	152	GLN
5	I	317	GLN
5	I	390	HIS
5	I	398	GLN
5	I	489	GLN
5	I	499	GLN
5	I	533	GLN
5	I	581	HIS
5	I	611	GLN
5	I	622	GLN
1	J	222	HIS
1	J	223	GLN
1	J	413	HIS
1	J	558	GLN
1	J	567	GLN
1	J	694	HIS
1	J	881	HIS
1	J	892	HIS
1	J	895	ASN
1	J	916	GLN
1	J	925	GLN
5	K	61	GLN
5	K	68	GLN
5	K	69	GLN
5	K	98	GLN
5	K	152	GLN
5	K	180	HIS
5	K	290	ASN
5	K	317	GLN
5	K	339	HIS
5	K	353	GLN
5	K	377	GLN
5	K	397	GLN
5	K	415	HIS
5	K	476	ASN
5	K	489	GLN
5	K	493	GLN
5	K	520	HIS
5	K	529	GLN
5	K	533	GLN
5	K	571	GLN
5	K	584	ASN

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Mol	Chain	Res	Type
5	K	600	ASN
6	L	332	GLN
6	L	343	GLN
6	L	412	HIS
6	L	571	HIS
6	L	1514	HIS
6	L	1657	GLN
6	L	1673	GLN
6	L	1678	ASN
6	L	1767	GLN
6	L	1788	ASN
6	L	1805	ASN
6	L	1806	ASN
3	b	56	ASN
2	a	14	GLN
2	a	30	GLN
2	a	31	GLN
2	a	82	HIS
2	a	84	GLN
7	S	15	ASN
7	S	54	GLN
7	S	59	HIS
7	S	187	ASN
7	S	197	GLN
7	S	198	ASN
7	S	221	GLN
7	S	250	ASN
7	S	251	ASN
7	S	347	ASN
7	S	357	GLN
7	T	24	GLN
7	T	54	GLN
7	T	59	HIS
7	T	187	ASN
7	T	197	GLN
7	T	198	ASN
7	T	221	GLN
7	T	250	ASN
7	T	251	ASN
7	T	338	GLN
7	T	347	ASN
7	T	357	GLN

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Mol	Chain	Res	Type
7	U	54	GLN
7	U	59	HIS
7	U	187	ASN
7	U	197	GLN
7	U	198	ASN
7	U	221	GLN
7	U	250	ASN
7	U	251	ASN
7	U	347	ASN
7	U	357	GLN
7	V	15	ASN
7	V	54	GLN
7	V	59	HIS
7	V	187	ASN
7	V	197	GLN
7	V	198	ASN
7	V	221	GLN
7	V	250	ASN
7	V	251	ASN
7	V	338	GLN
7	V	347	ASN
7	V	357	GLN
7	W	15	ASN
7	W	54	GLN
7	W	59	HIS
7	W	187	ASN
7	W	197	GLN
7	W	198	ASN
7	W	221	GLN
7	W	250	ASN
7	W	251	ASN
7	W	347	ASN
7	W	357	GLN
7	W	407	GLN
7	X	15	ASN
7	X	24	GLN
7	X	54	GLN
7	X	59	HIS
7	X	187	ASN
7	X	197	GLN
7	X	198	ASN
7	X	250	ASN

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Mol	Chain	Res	Type
7	X	251	ASN
7	X	338	GLN
7	X	347	ASN
7	X	357	GLN
7	Y	15	ASN
7	Y	54	GLN
7	Y	59	HIS
7	Y	187	ASN
7	Y	197	GLN
7	Y	198	ASN
7	Y	221	GLN
7	Y	250	ASN
7	Y	251	ASN
7	Y	347	ASN
7	Y	357	GLN
7	Z	15	ASN
7	Z	29	HIS
7	Z	54	GLN
7	Z	59	HIS
7	Z	187	ASN
7	Z	197	GLN
7	Z	198	ASN
7	Z	221	GLN
7	Z	250	ASN
7	Z	251	ASN
7	Z	347	ASN
7	Z	357	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 [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.

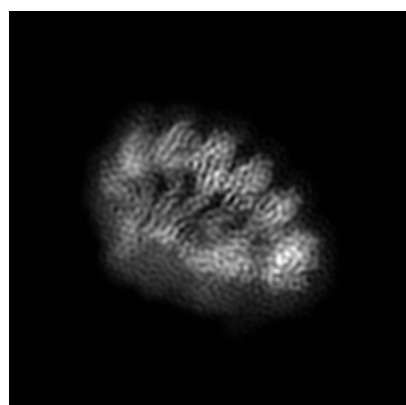
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14007. These allow visual inspection of the internal detail of the map and identification of artifacts.

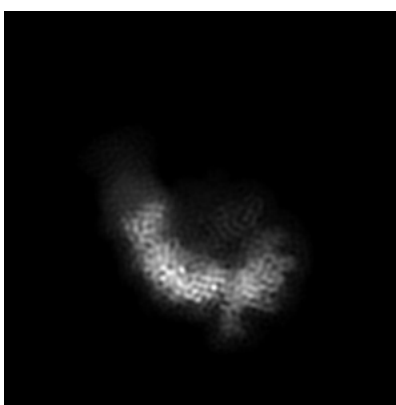
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

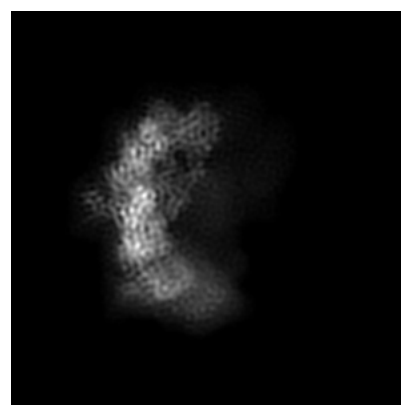
6.1.1 Primary map



X



Y

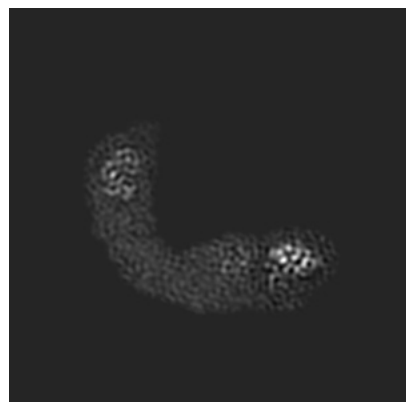


Z

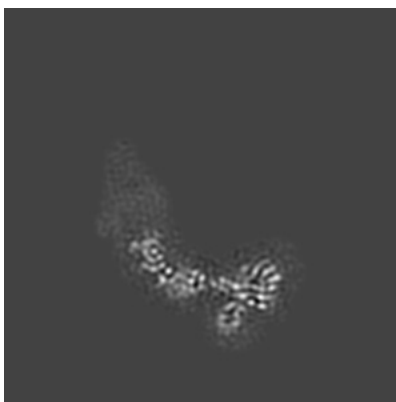
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

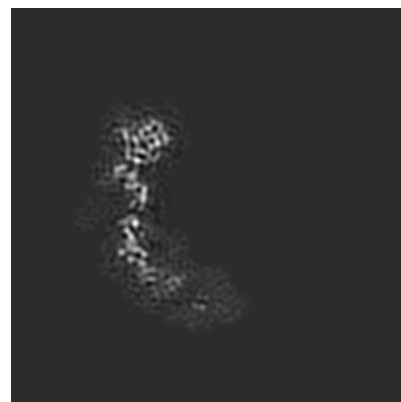
6.2.1 Primary map



X Index: 100



Y Index: 100



Z Index: 100

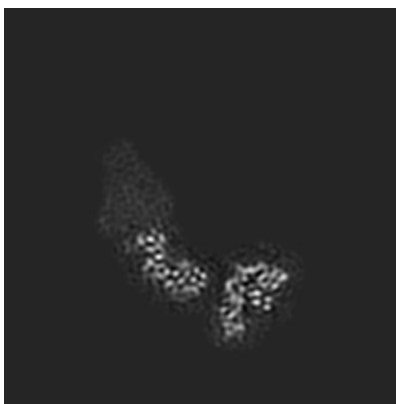
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 62



Y Index: 103



Z Index: 81

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

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

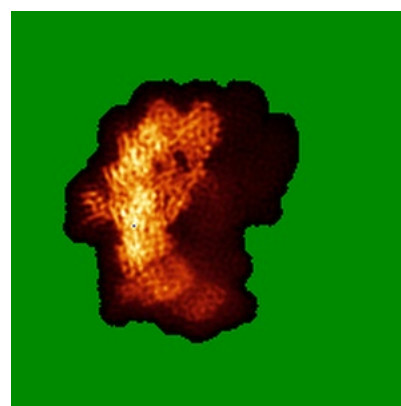
6.4.1 Primary map



X



Y

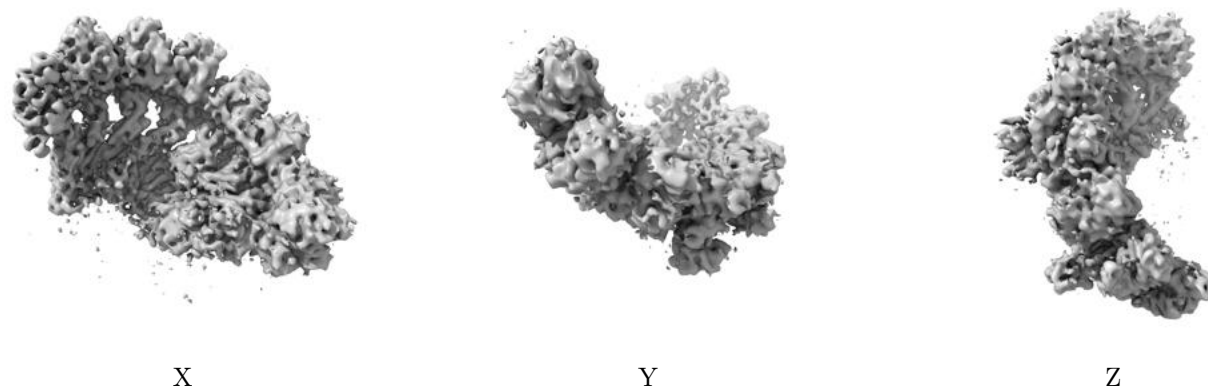


Z

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 0.0287. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

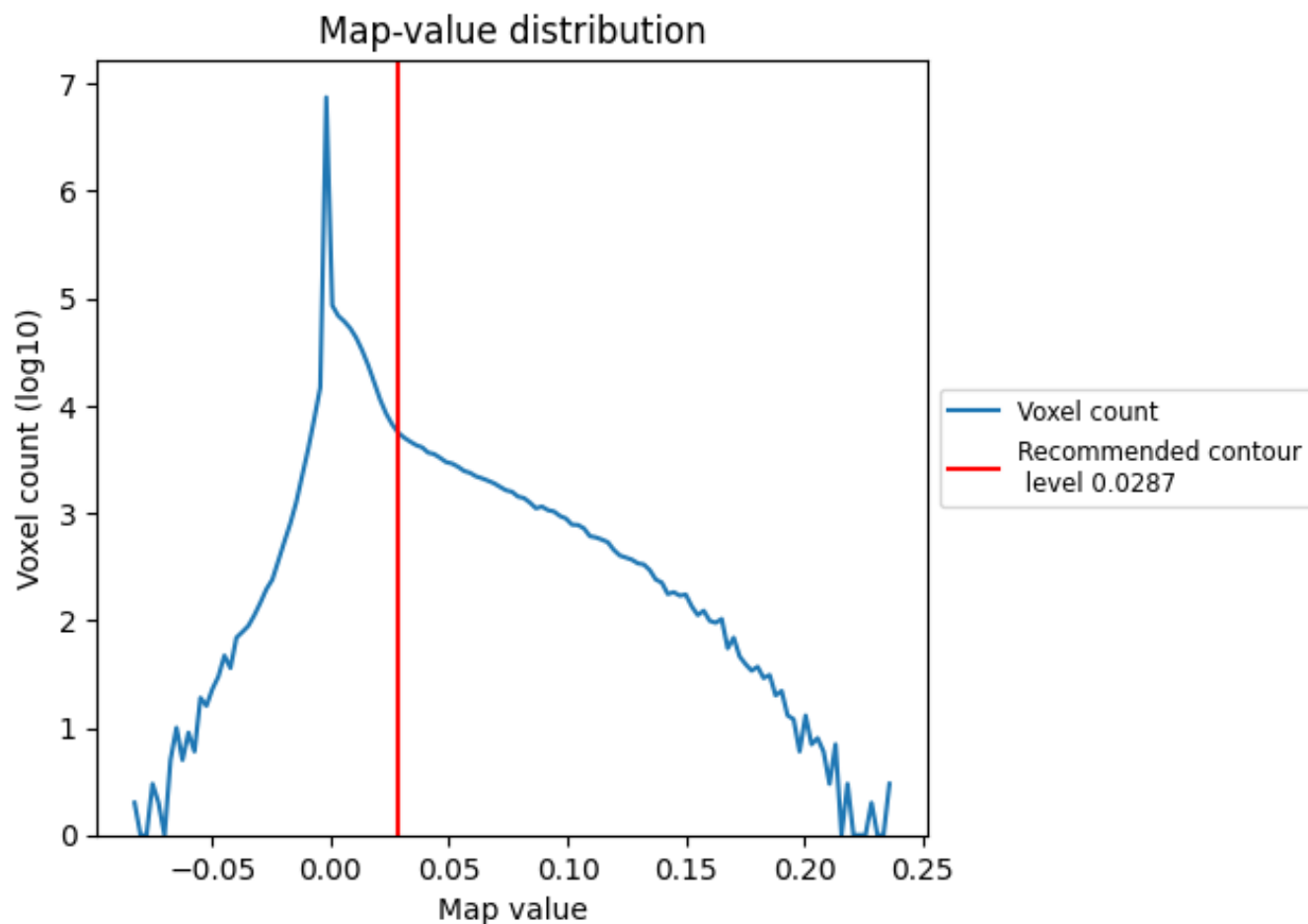
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

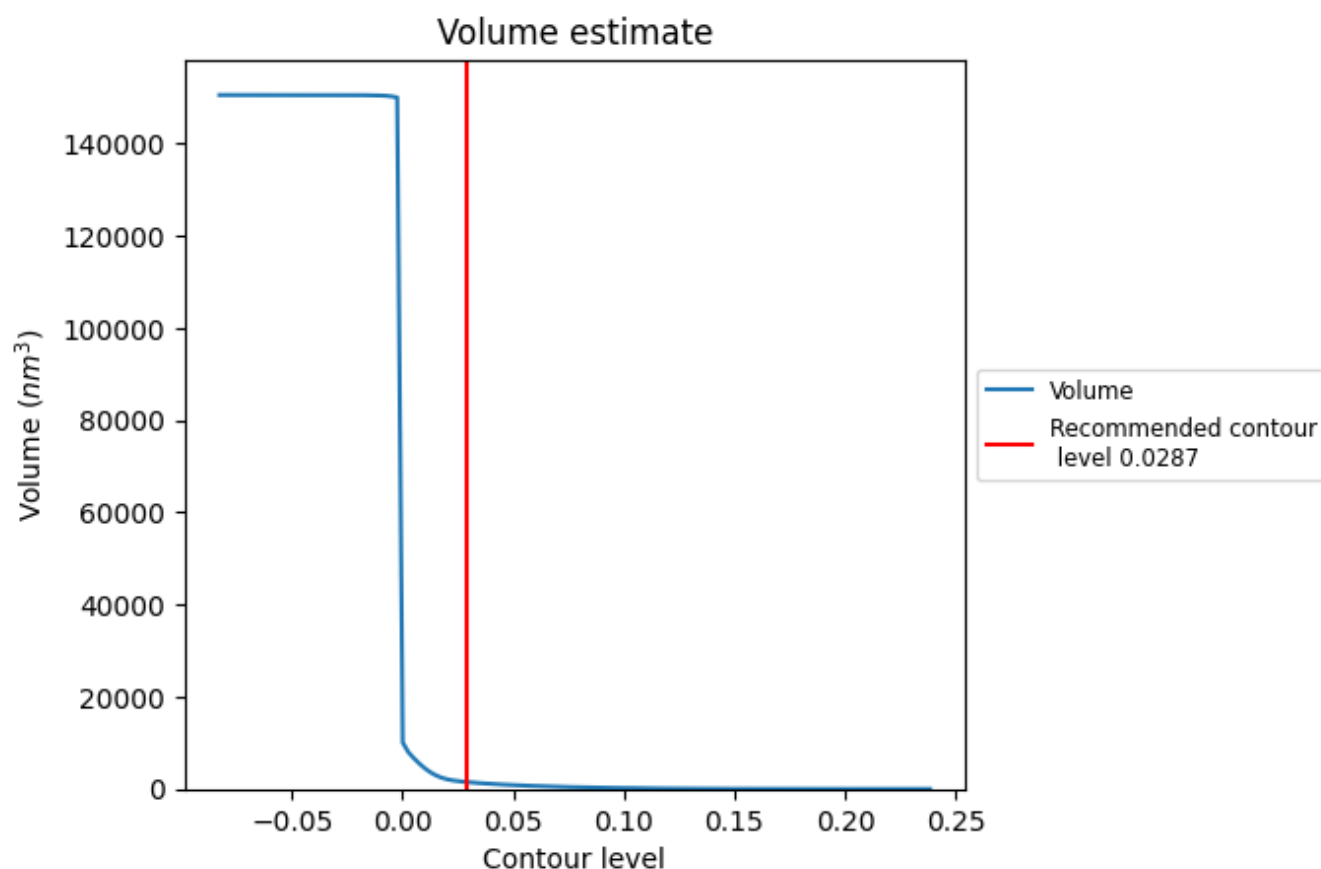
This section contains the results of statistical analysis of the map.

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.

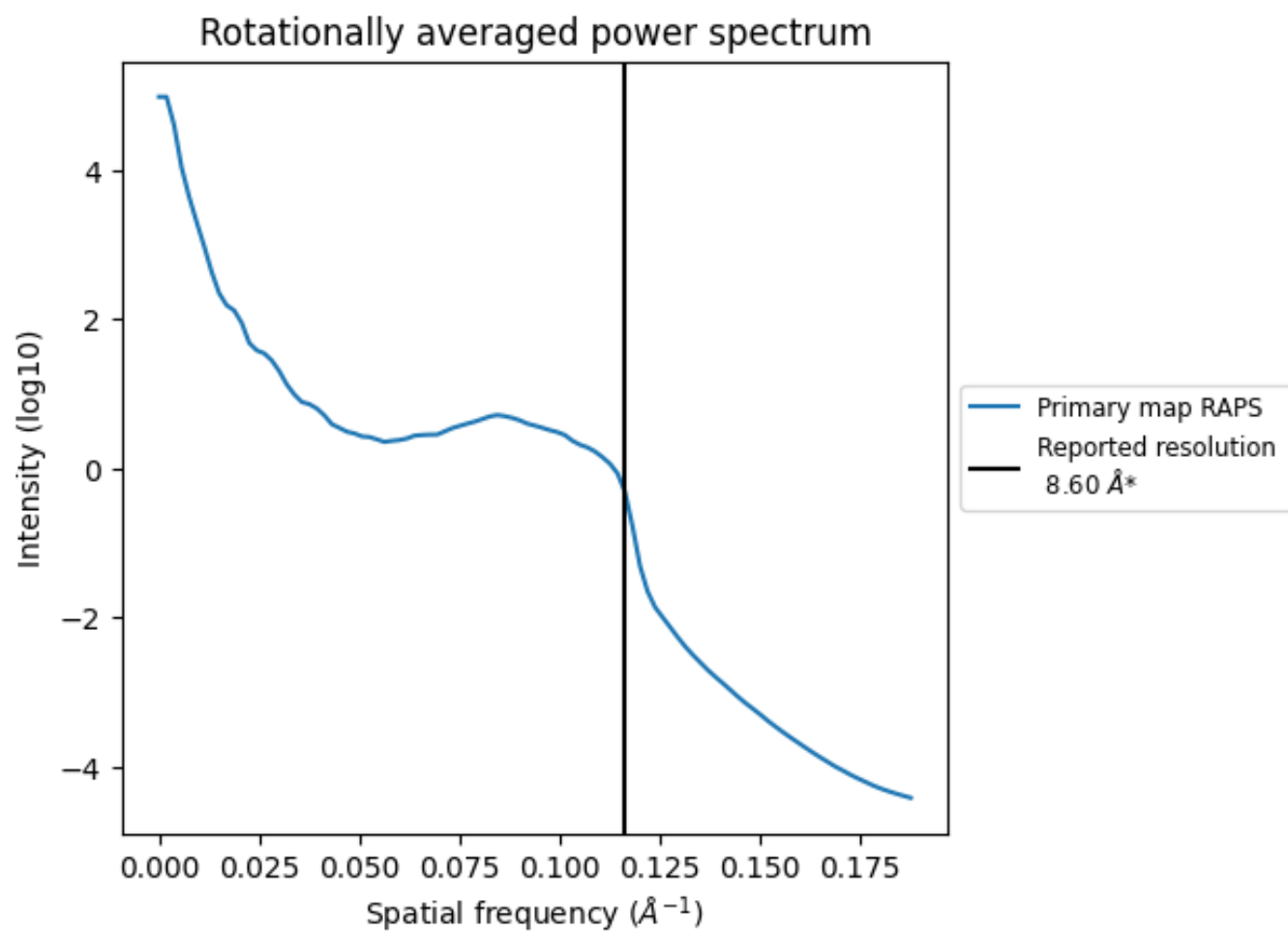
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1509 nm³; this corresponds to an approximate mass of 1363 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 0.116 Å⁻¹

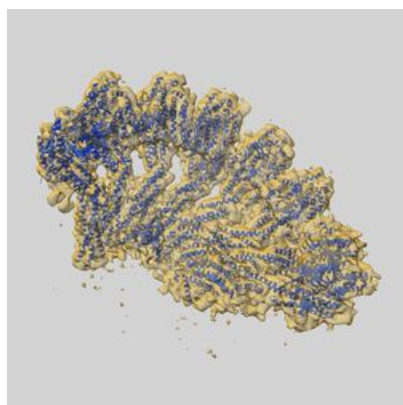
8 Fourier-Shell correlation

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

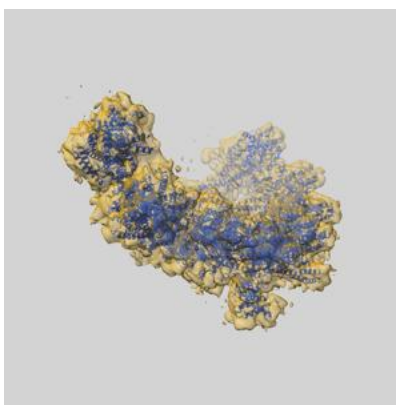
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-14007 and PDB model 7QJ2. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

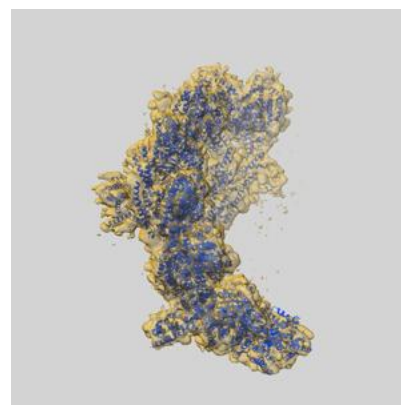
9.1 Map-model overlay [i](#)



X



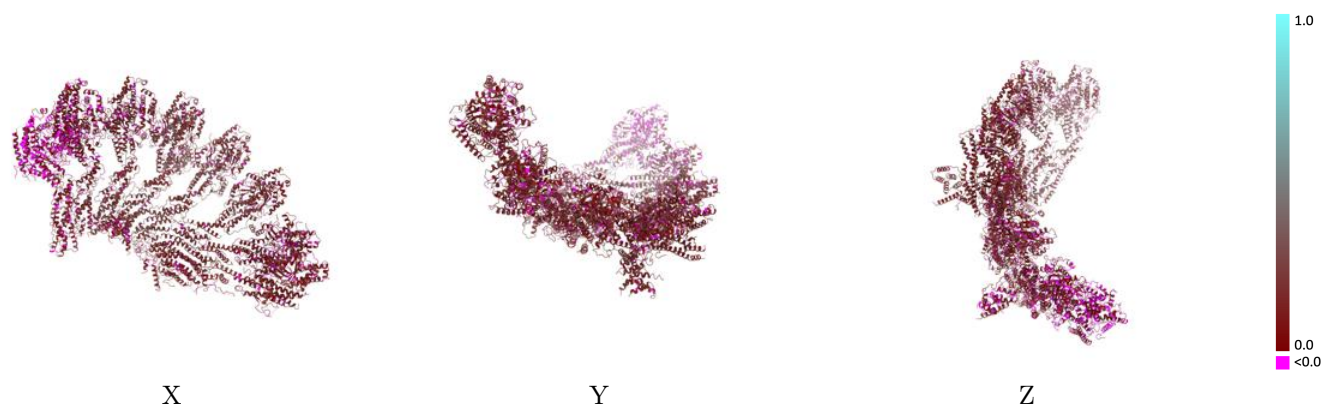
Y



Z

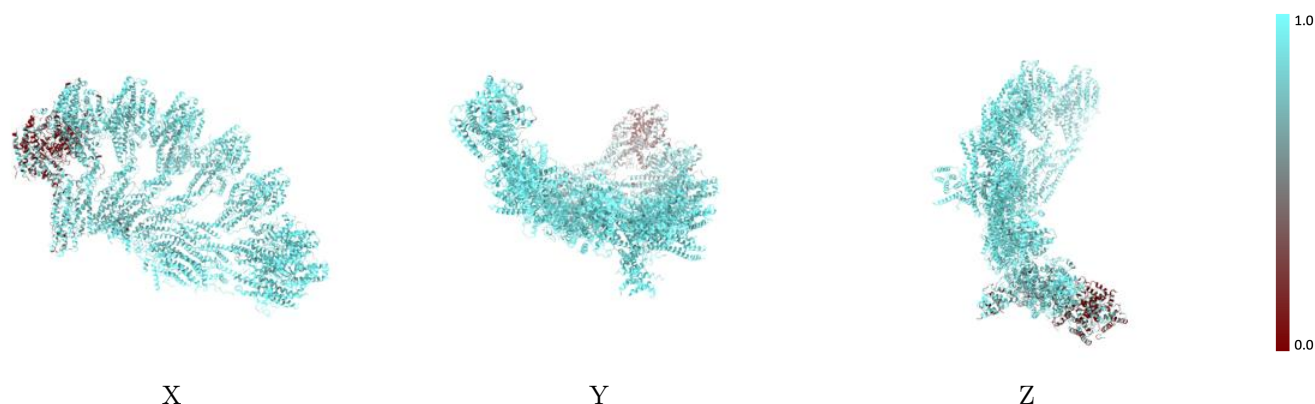
The images above show the 3D surface view of the map at the recommended contour level 0.0287 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



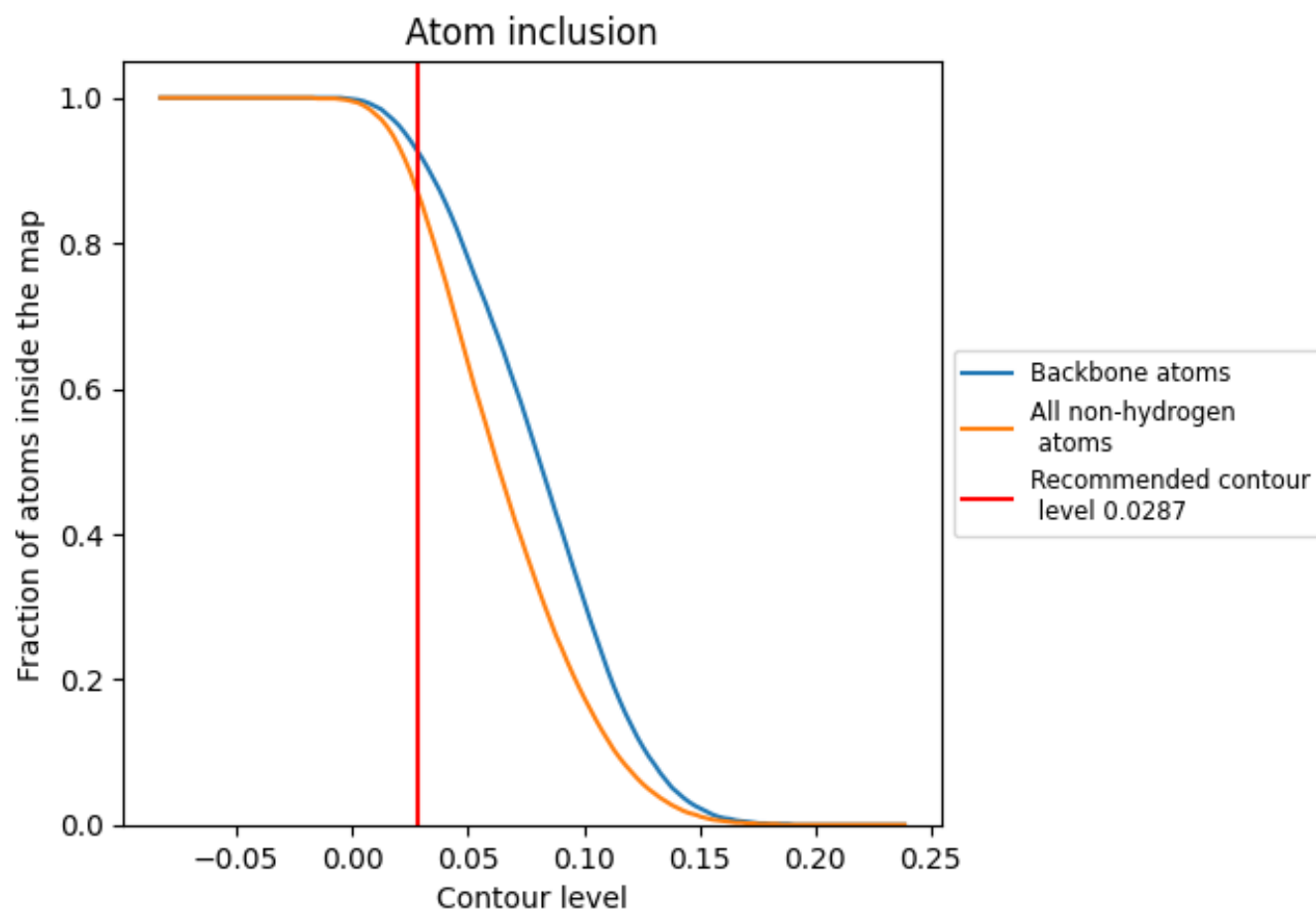
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0287).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 87% 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 (0.0287) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8660	 0.1300
E	 0.6140	 0.0890
F	 0.8370	 0.1210
G	 0.9270	 0.1450
H	 0.9320	 0.1530
I	 0.9340	 0.1610
J	 0.9510	 0.1610
K	 0.9520	 0.1500
L	 0.9450	 0.1520
S	 0.3440	 0.0050
T	 0.8210	 0.0870
U	 0.9240	 0.1350
V	 0.9490	 0.1520
W	 0.9500	 0.1410
X	 0.9490	 0.1410
Y	 0.9520	 0.1250
Z	 0.9180	 0.1290
a	 0.7920	 0.1130
b	 0.8000	 0.1340
j	 0.7650	 0.1090
k	 0.6910	 0.1050
l	 0.9460	 0.1660
m	 0.9350	 0.1730

