



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 06:11 PM UTC

PDB ID : 7QJA / pdb_00007qja
EMDB ID : EMD-14015
Title : Structure of recombinant human gamma-Tubulin Ring Complex 12-spoked assembly intermediate (spokes 1-12, homogeneous dataset)
Authors : Zupa, E.; Pfeffer, S.
Deposited on : 2021-12-16
Resolution : 9.20 Å (reported)
Based on initial models : 7AS4, 6L81, 6X0U, 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:

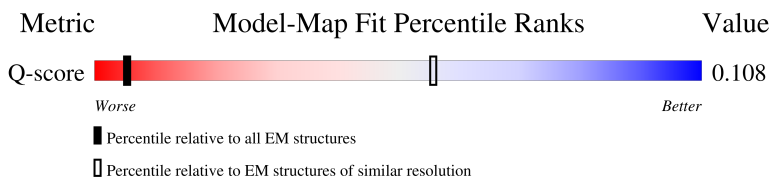
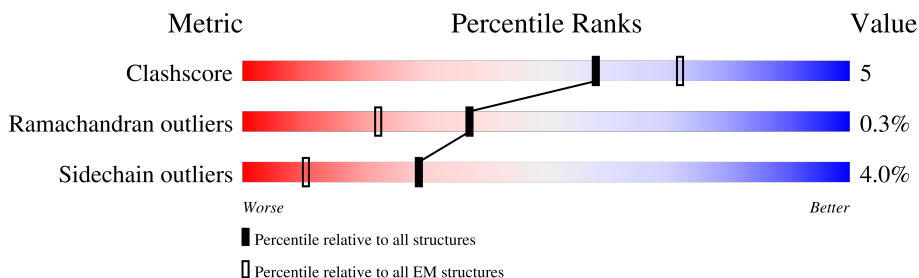
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

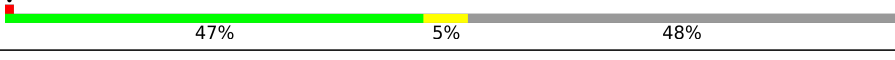
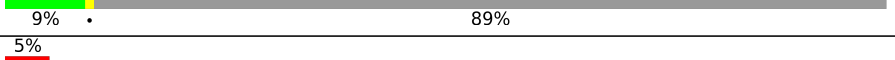
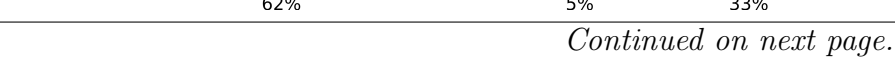
The reported resolution of this entry is 9.20 Å.

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



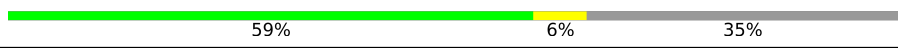
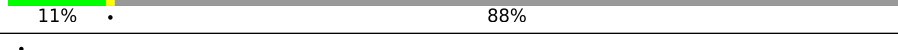
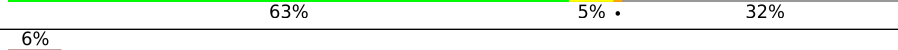
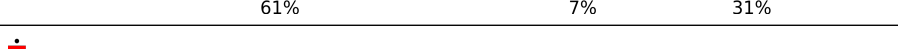
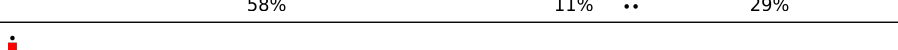
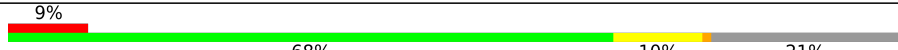
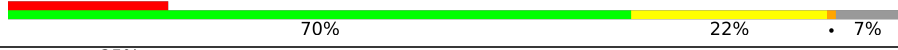
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	239 (8.70 - 9.70)

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

Mol	Chain	Length	Quality of chain
1	e	375	
2	J	1024	
2	l	1024	
3	B	907	

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Mol	Chain	Length	Quality of chain
3	D	907	
3	F	907	
3	H	907	
3	a	907	
3	f	907	
3	h	907	
3	j	907	
4	A	902	
4	C	902	
4	E	902	
4	G	902	
5	I	667	
5	K	667	
6	L	1819	
6	c	1819	
7	b	82	
7	d	82	
7	g	82	
7	i	82	
7	k	82	
7	m	82	
8	O	451	
8	P	451	
8	Q	451	
8	R	451	

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Mol	Chain	Length	Quality of chain
8	S	451	
8	T	451	
8	U	451	
8	V	451	
8	W	451	
8	X	451	
8	Y	451	
8	Z	451	

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 109569 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	610	Total	C	N	O	S	0	0
			5029	3203	888	913	25		
3	D	581	Total	C	N	O	S	0	0
			4796	3061	842	868	25		
3	F	599	Total	C	N	O	S	0	0
			4941	3151	871	894	25		
3	H	594	Total	C	N	O	S	0	0
			4907	3130	864	888	25		
3	a	116	Total	C	N	O	S	0	0
			933	591	171	169	2		
3	f	99	Total	C	N	O	S	0	0
			803	509	148	144	2		
3	h	99	Total	C	N	O	S	0	0
			803	509	148	144	2		
3	j	107	Total	C	N	O	S	0	0
			843	533	156	152	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	620	Total	C	N	O	S	0	0
			5044	3257	845	910	32		
4	E	638	Total	C	N	O	S	0	0
			5202	3354	873	942	33		
4	G	640	Total	C	N	O	S	0	0
			5206	3354	875	944	33		
4	A	613	Total	C	N	O	S	0	0
			4978	3212	831	903	32		

- 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		
6	c	158	Total	C	N	O	S	0	0
			1220	771	209	232	8		

- Molecule 7 is a protein called Mitotic-spindle organizing protein 1.

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

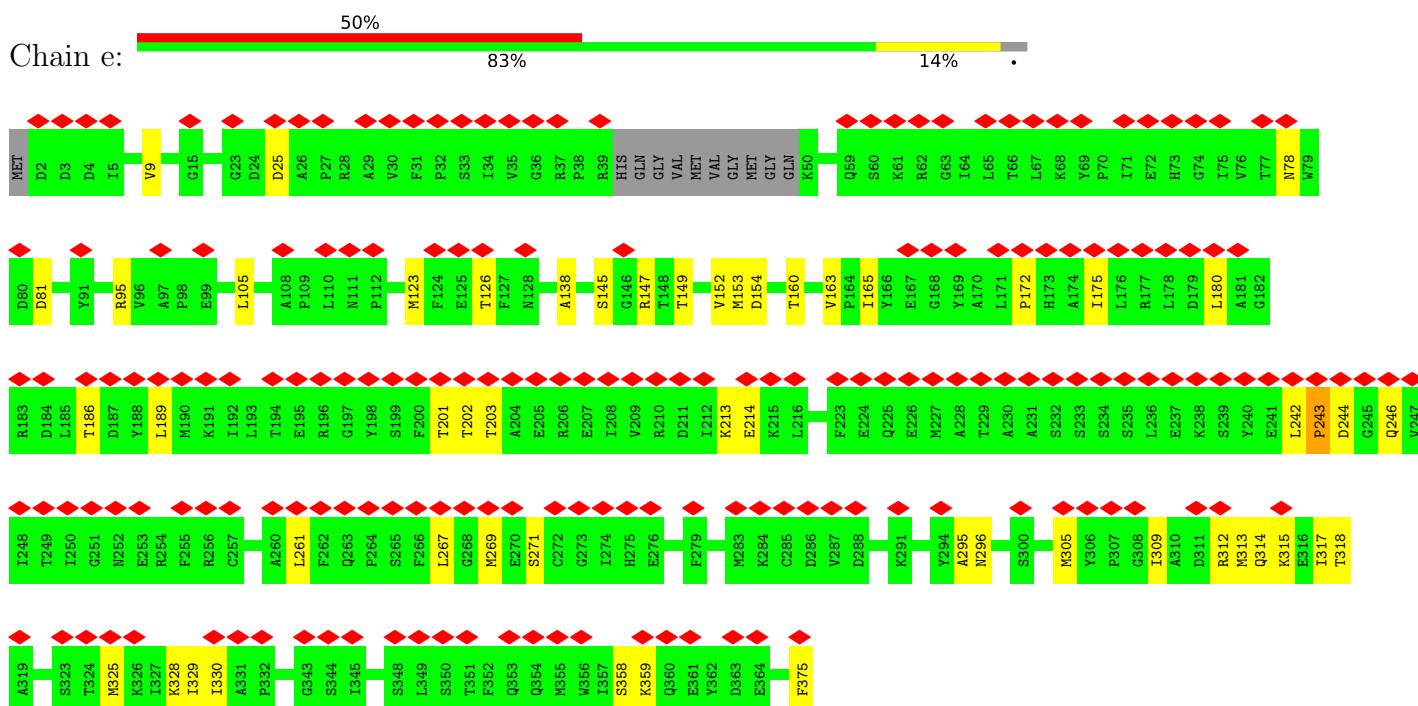
- Molecule 8 is a protein called Tubulin gamma-1 chain.

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

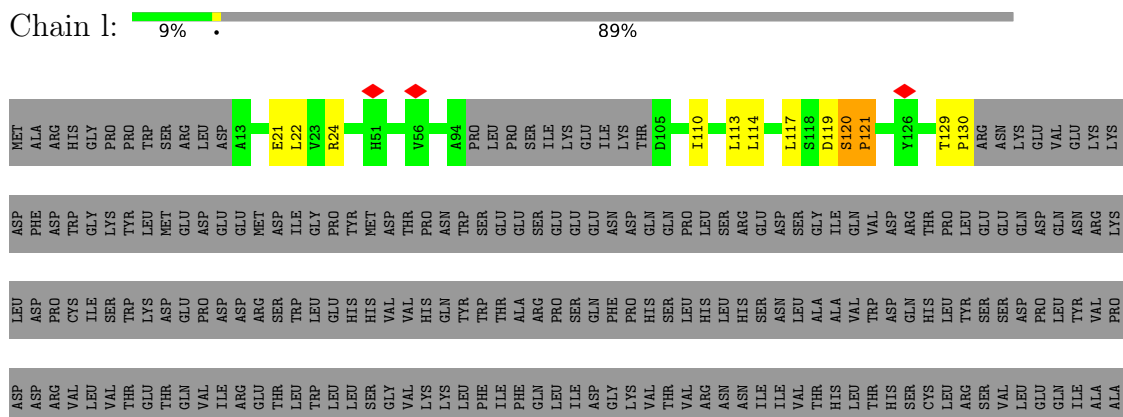
3 Residue-property plots

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

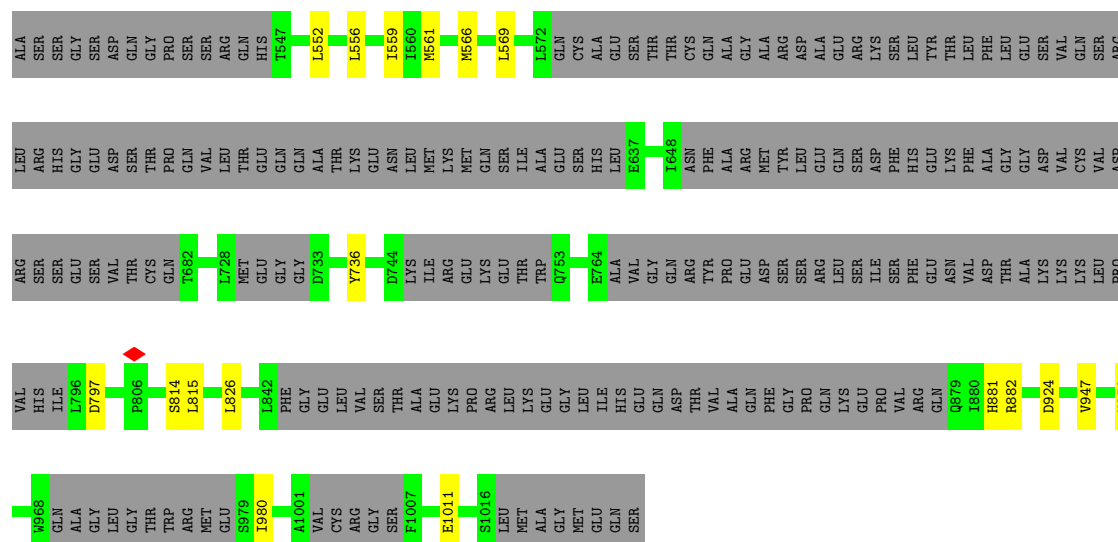
- Molecule 1: actin, cytoplasmic 1



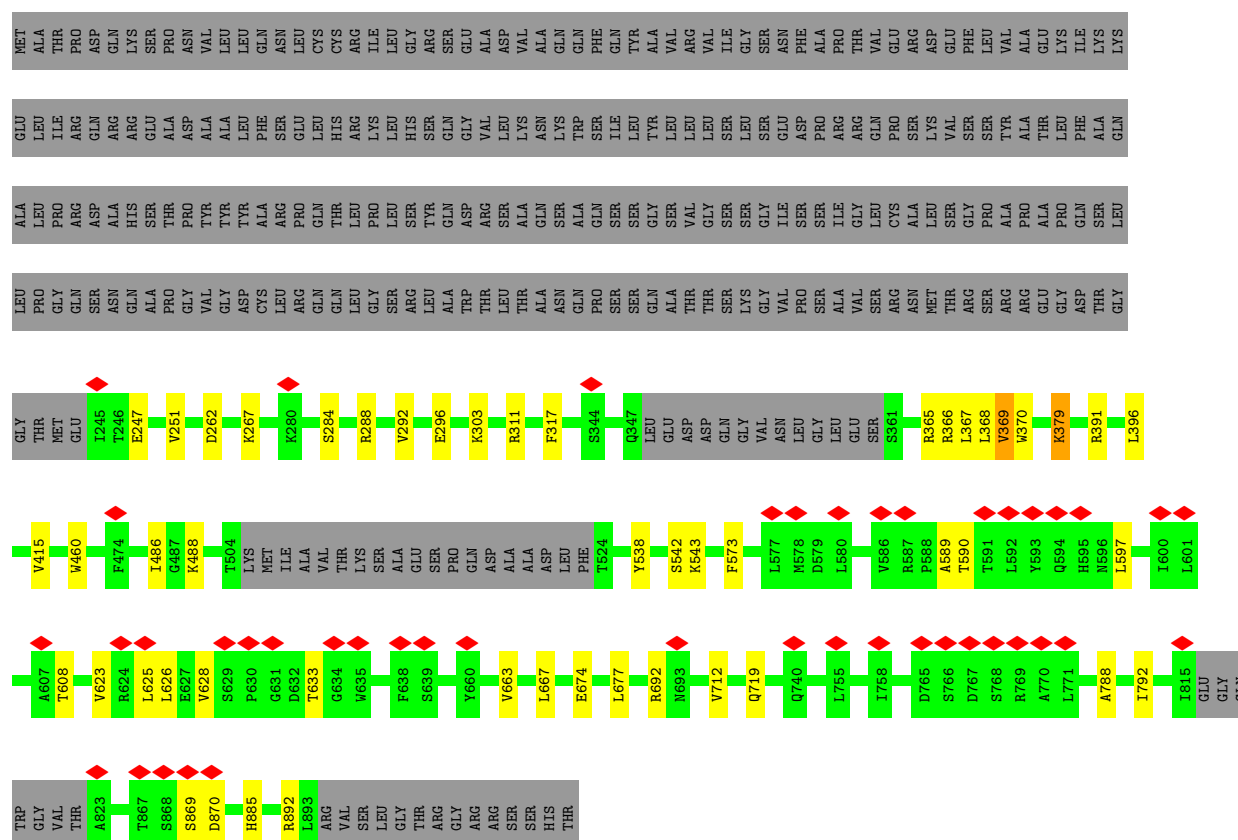
- Molecule 2: Gamma-tubulin complex component 5



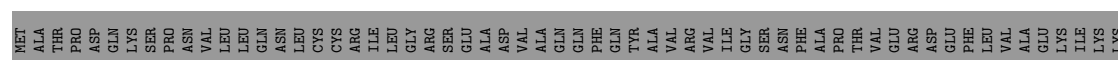


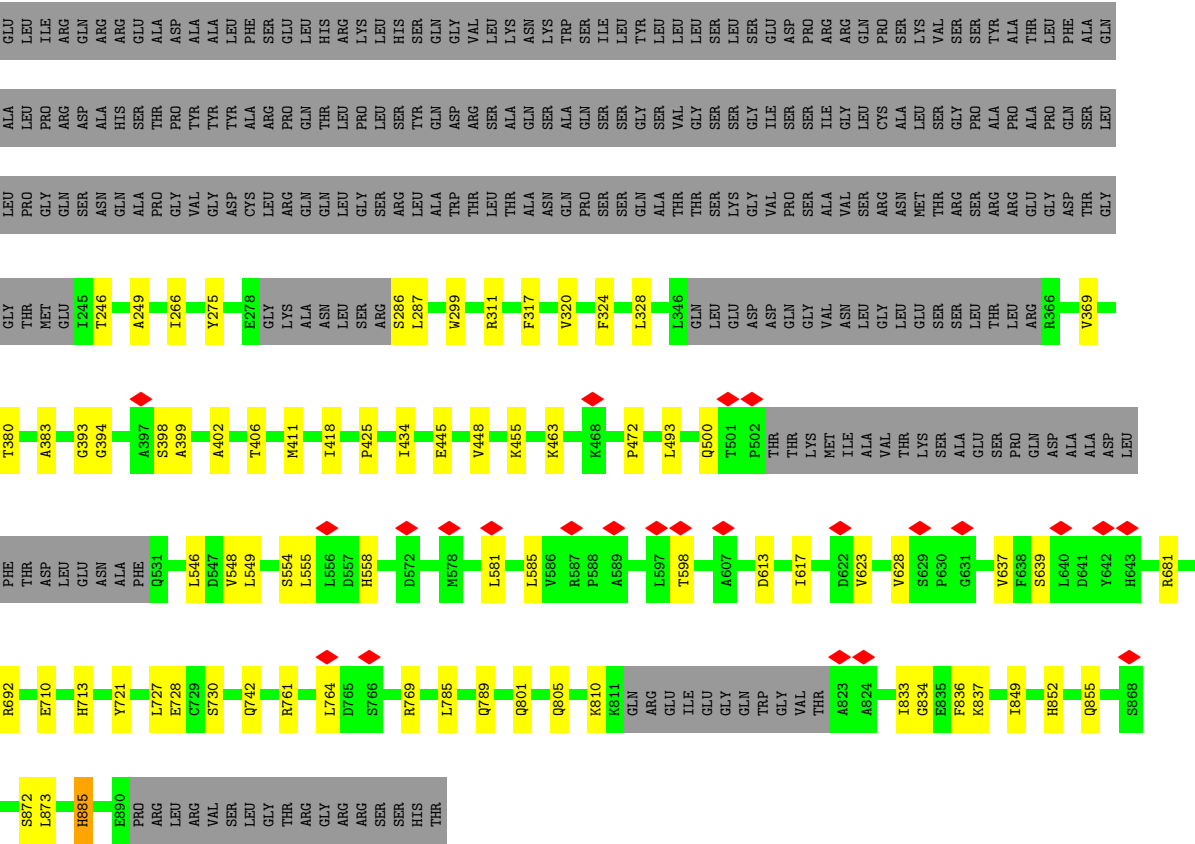


• Molecule 3: Gamma-tubulin complex component 3

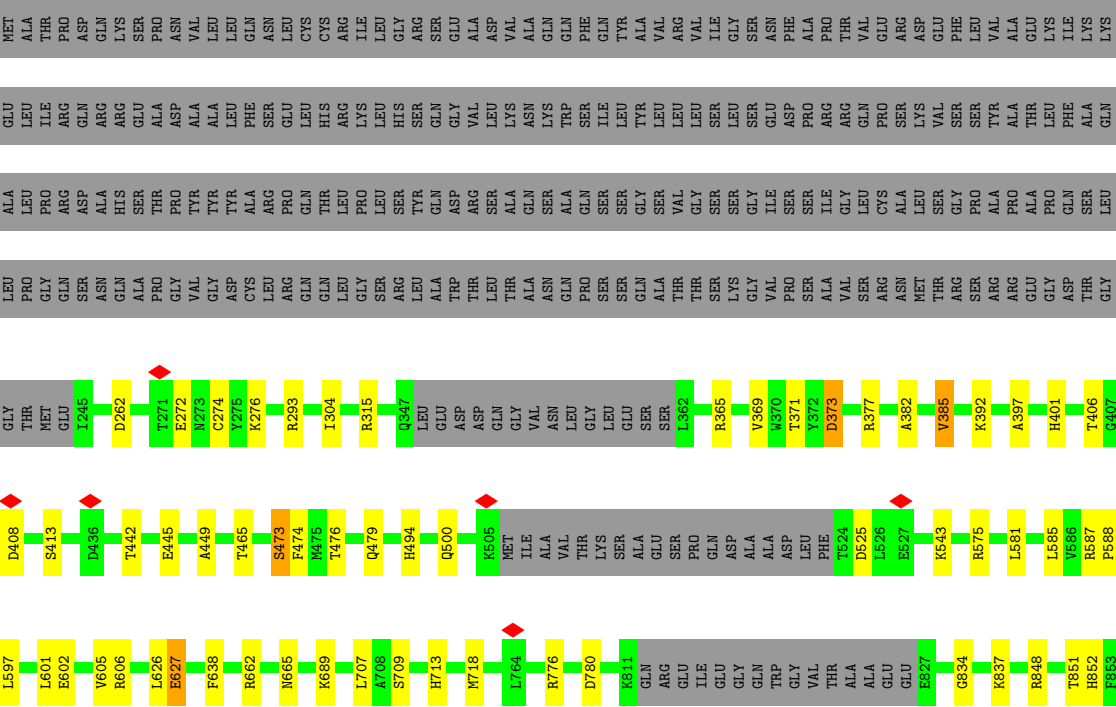


• Molecule 3: Gamma-tubulin complex component 3

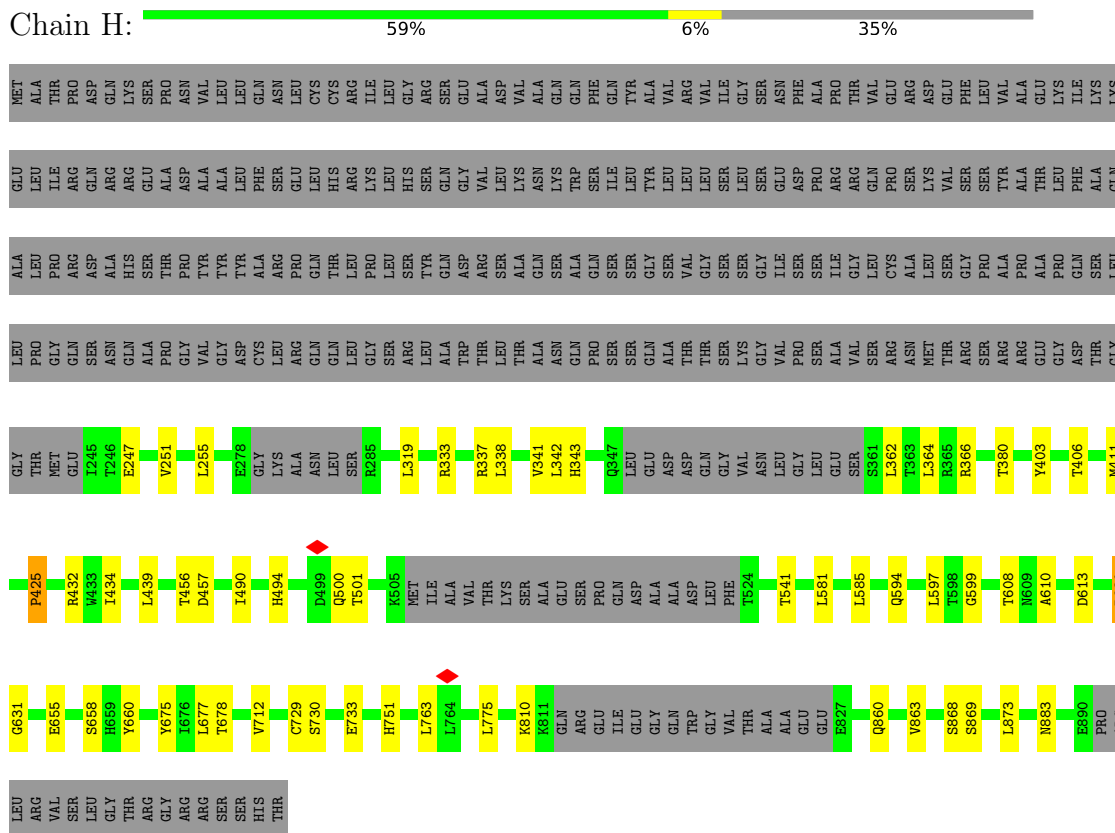




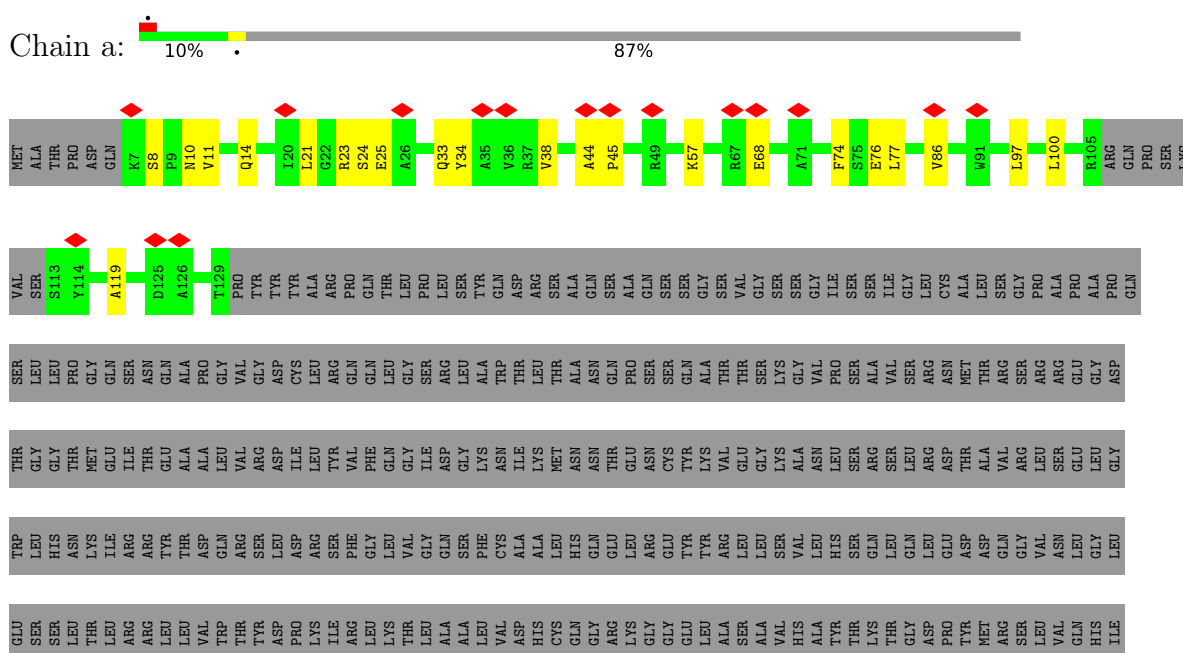
● Molecule 3: Gamma-tubulin complex component 3



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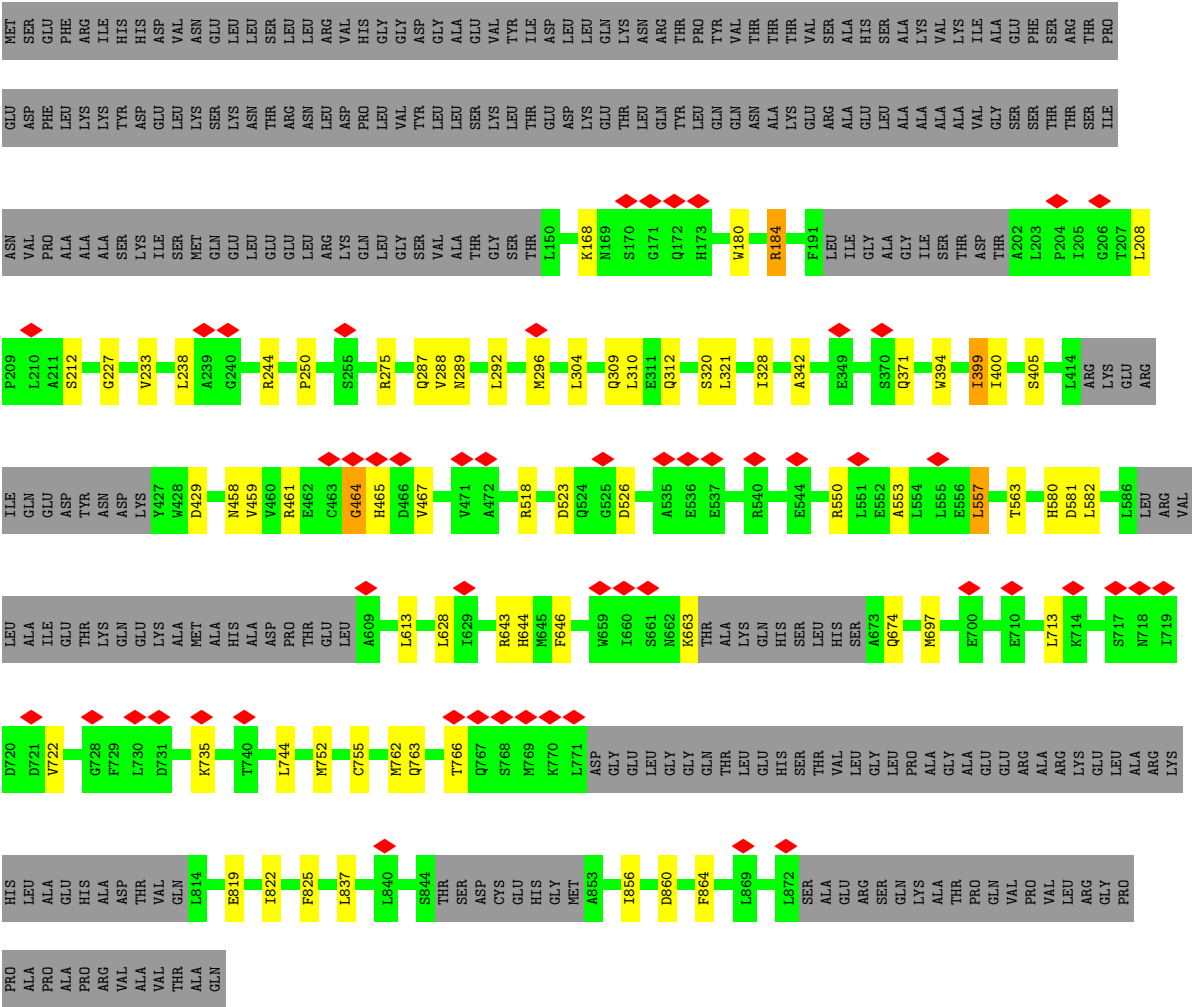
[illegible]

- Molecule 3: Gamma-tubulin complex component 3

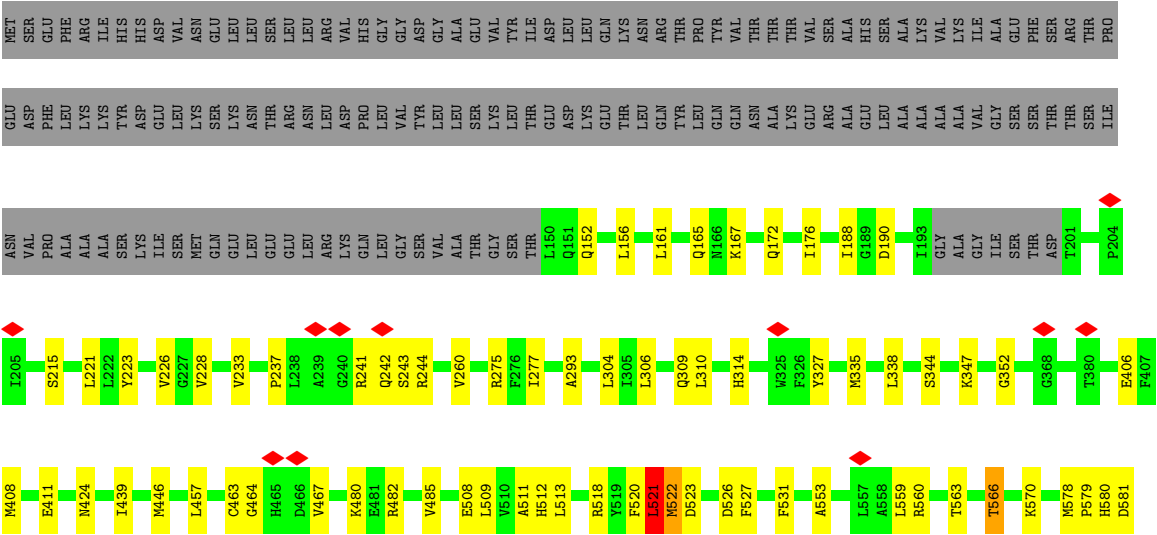
Chain f: 11% 89%

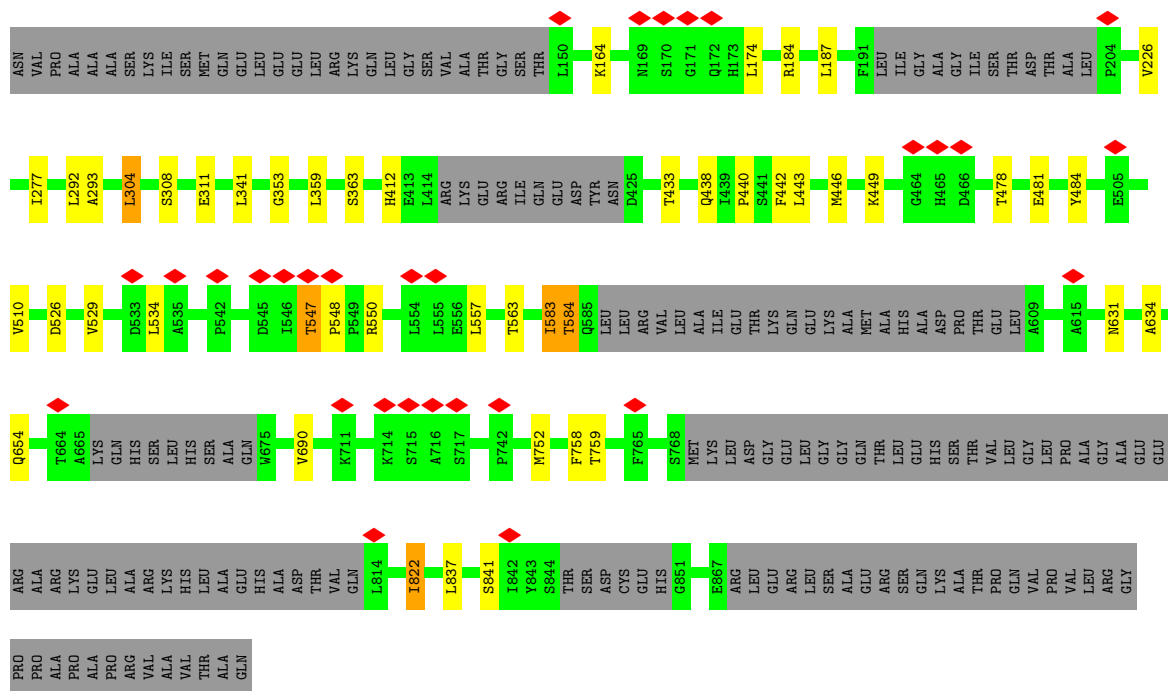
[illegible]





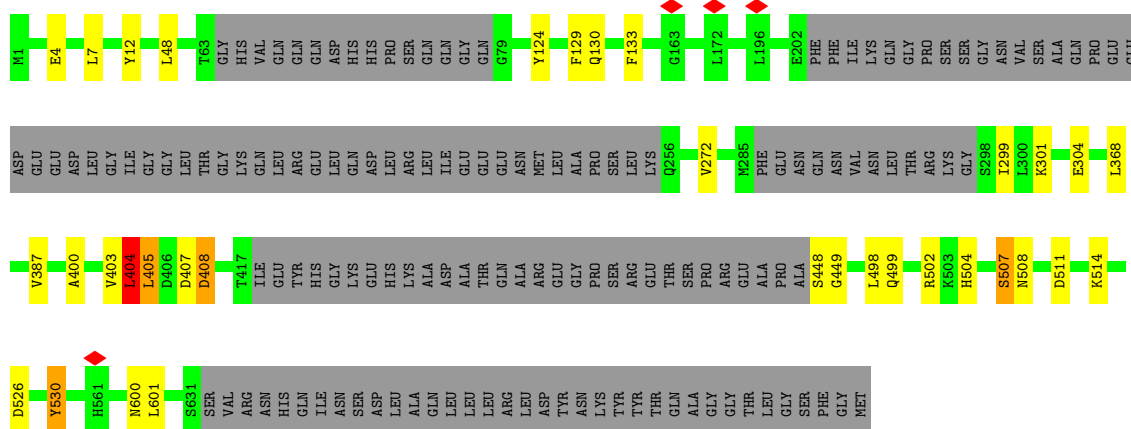
● Molecule 4: Gamma-tubulin complex component 2





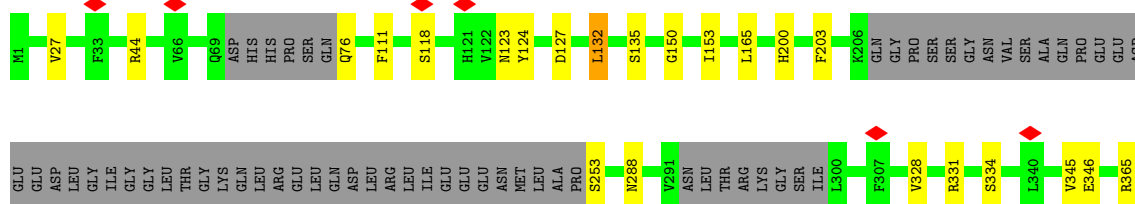
- Molecule 5: Gamma-tubulin complex component 4

Chain I: 73% 22%

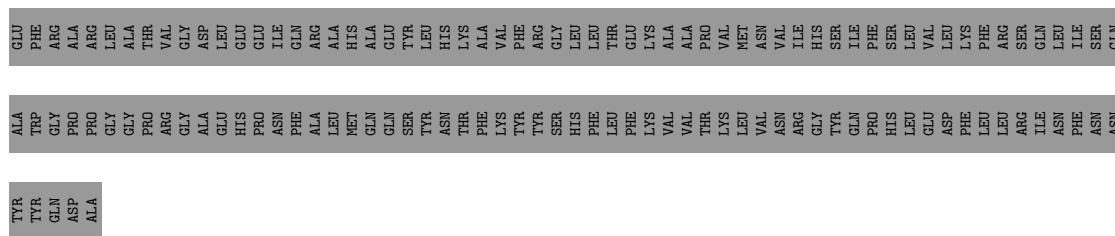


- Molecule 5: Gamma-tubulin complex component 4

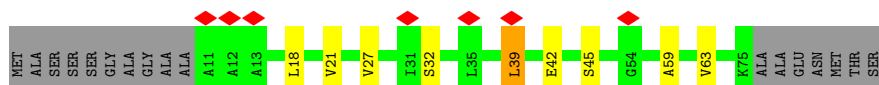
Chain K: 75% 8% 16%



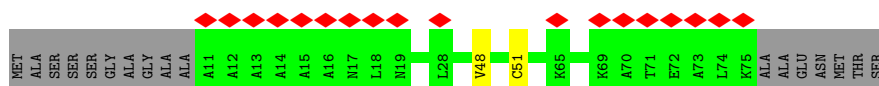
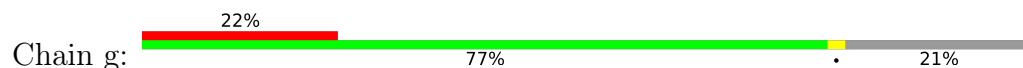




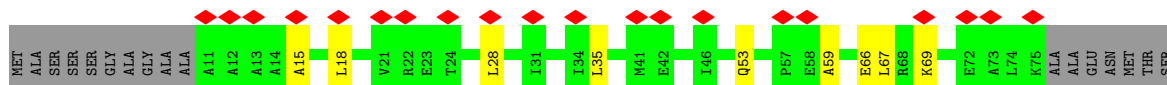
• Molecule 7: Mitotic-spindle organizing protein 1



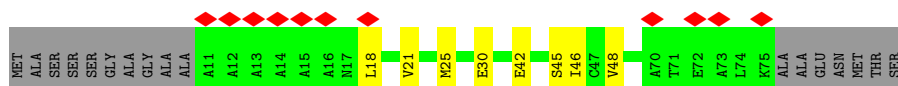
• Molecule 7: Mitotic-spindle organizing protein 1



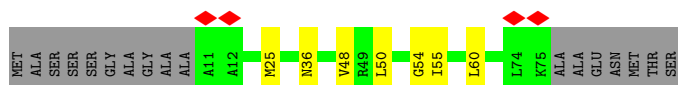
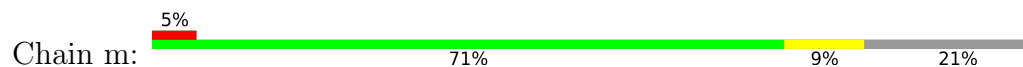
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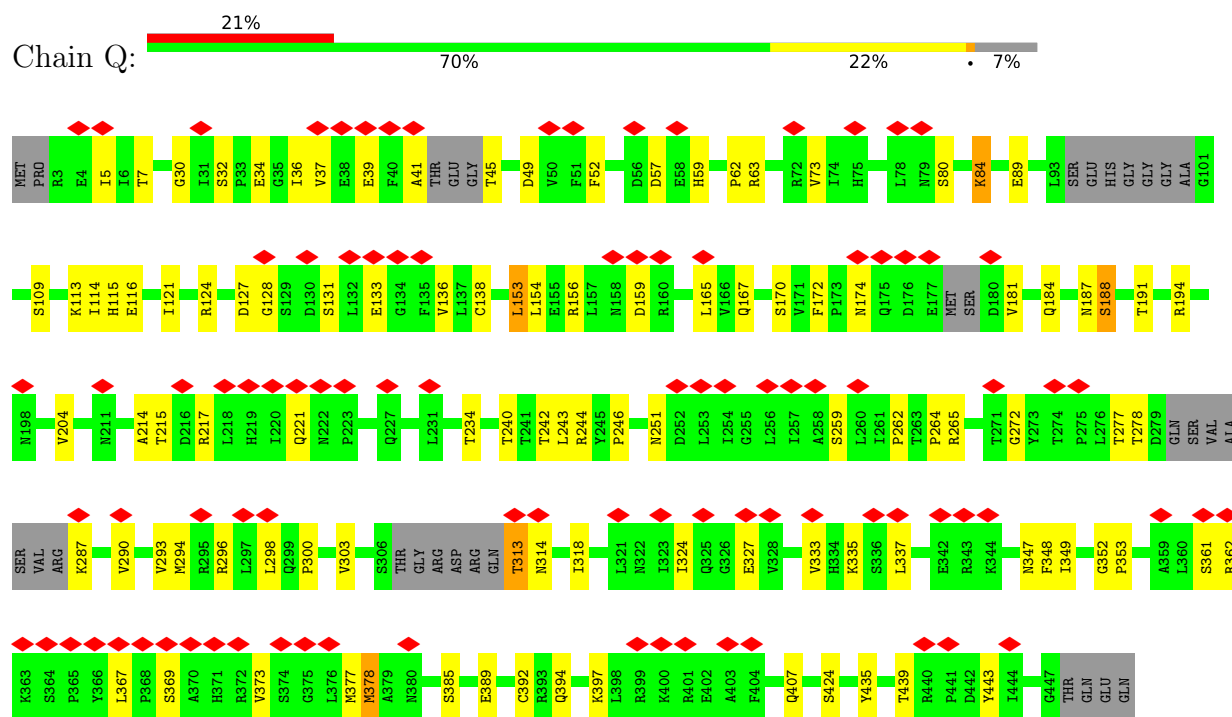
• Molecule 7: Mitotic-spindle organizing protein 1



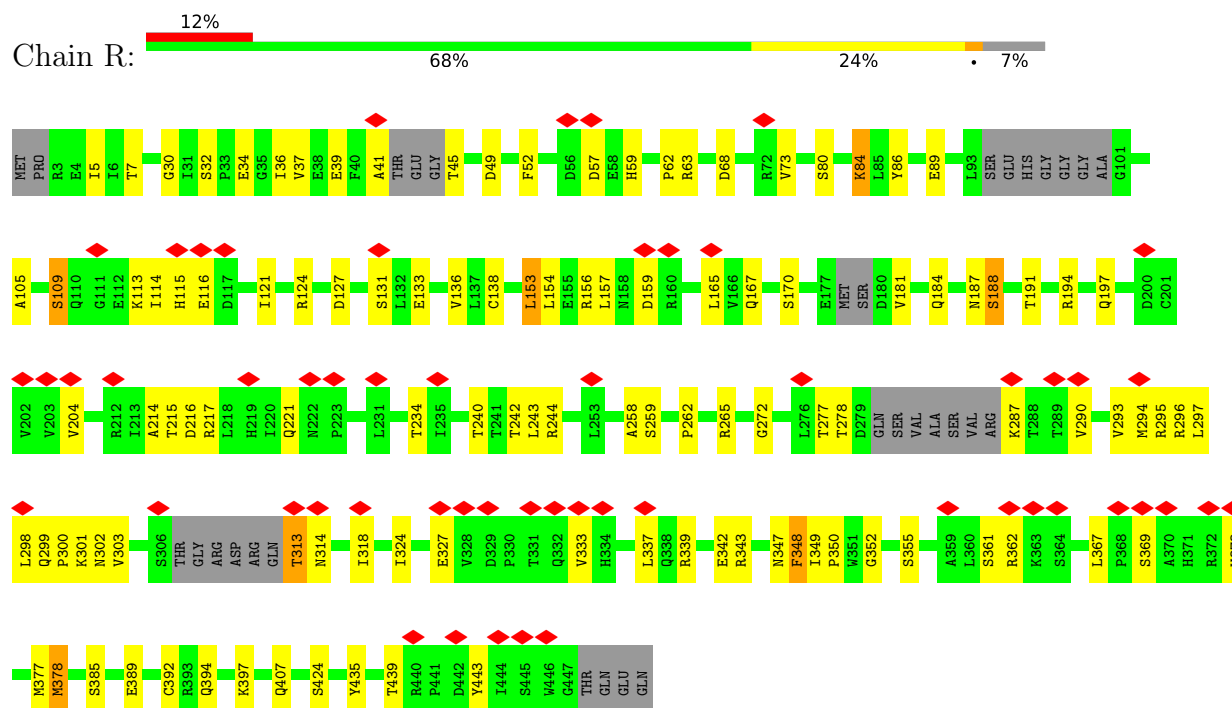
• Molecule 7: Mitotic-spindle organizing protein 1



- Molecule 8: Tubulin gamma-1 chain



- Molecule 8: Tubulin gamma-1 chain



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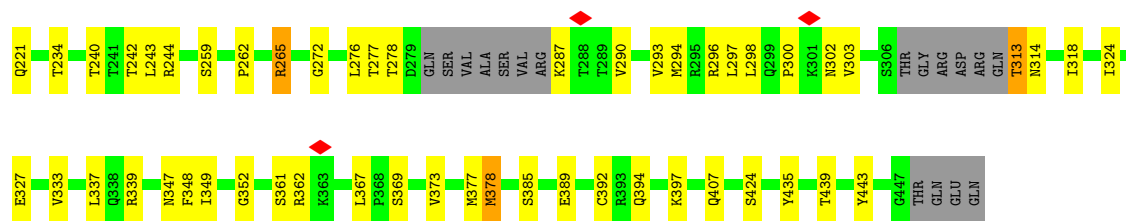




THR GLN GLU GLN	N314	H219	S109	MET
	H315	I220	K113	PRO
	I318	T234	I114	E4
		I324	T240	H115
E327	T241	I121	T7	
V333	L243	R124	G30	
H334	R244	D127	I31	
L337	N251	E133	S32	
Q338	D252	S131	E33	
R339	L253	I132	E34	
N347	S259	V136	G35	
F348	P262	L137	I36	
I349	R265	C138	V37	
G352	G272	L153	E38	
S355	L276	L154	E39	
L360	T277	L157	F40	
S361	T278	N158	A41	
R362	D279	L165	THR	
K363	GLN	V166	GLU	
S364	SER	Q167	GLY	
L367	ALA	S170	T45	
P368	SER	V171	D49	
S369	VAL	F172	F52	
V373	ARG	P173	D56	
M377	K287	N174	D57	
M378	V290	Q175	E58	
S385	D292	D176	H59	
E389	V293	E177	P62	
C392	M294	MET	R63	
R393	R295	SER	D68	
Q394	L297	D180	V73	
K397	L298	V181	S76	
Q407	Q299	Q184	S80	
S424	P300	S188	K84	
Y435	K301	R194	L85	
T439	N302	E89	Y86	
Y443	V303	D200	L93	
	S306	V204	SER	
	THR	GLY	GLU	
	ARG	A214	HIS	
	ASP	T215	GLY	
	ARG	D216	GLY	
	GLN	R217	ALA	
			G101	

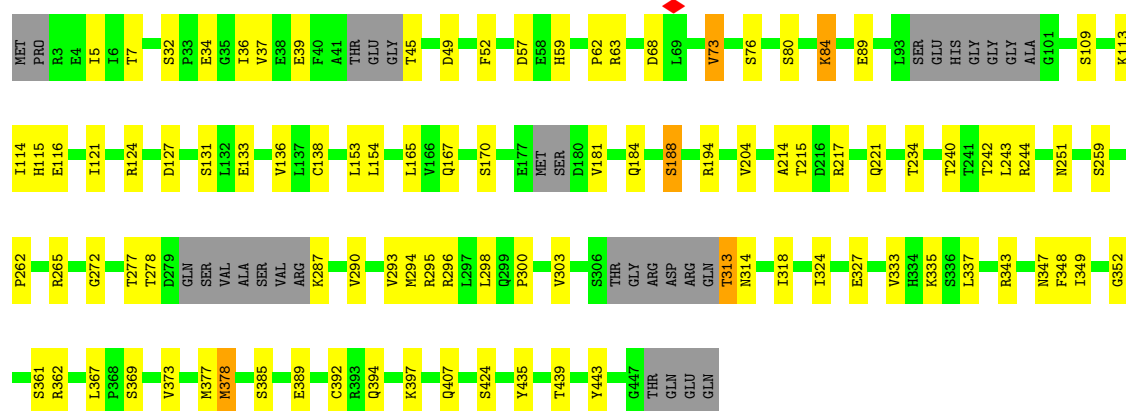
- Molecule 8: Tubulin gamma-1 chain

Met	Pro	R3	E4	I5	I6	T7	G30	I31	S32	P33	E34	G35	I36	V37	E38	E39	F40	A41	Thr	GLU	GLY	T45	D49	F52	D56	D57	E58	H59	P62	R63	D68	L69	V73	S80	K84	L85	Y86	E89	L83	SER	GLU	HIS	GLY	GLY	ALA	G101
A105	S109	K113	L114	H115	E116	I121	R124	D127	D130	I131	S132	E133	V136	L137	C138	L153	L154	L157	L165	V166	Q167	S170	E177	Met	SER	D180	V181	Q184	S188	R194	A199	D200	C201	V204	L210	A214	T215	D216	D217							



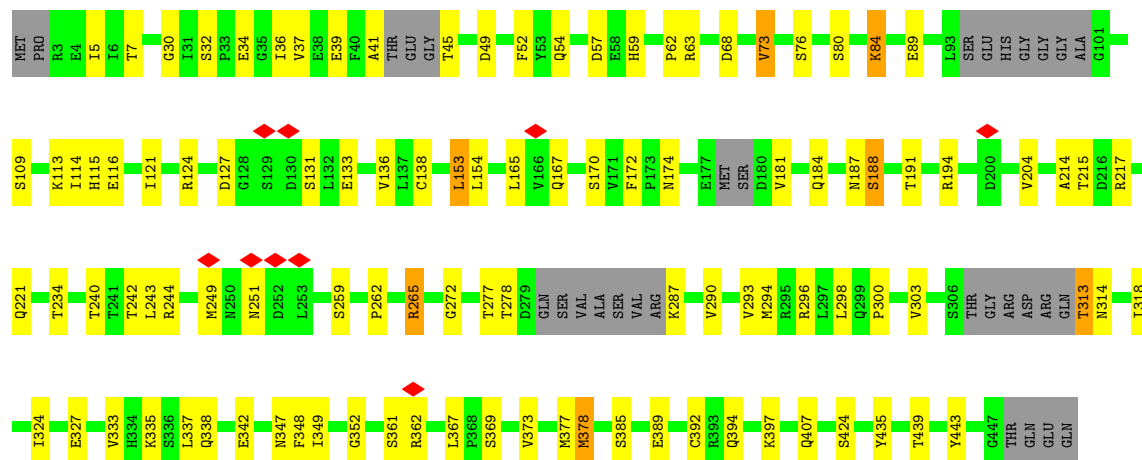
• Molecule 8: Tubulin gamma-1 chain

Chain V: 72% 20% 7%



• Molecule 8: Tubulin gamma-1 chain

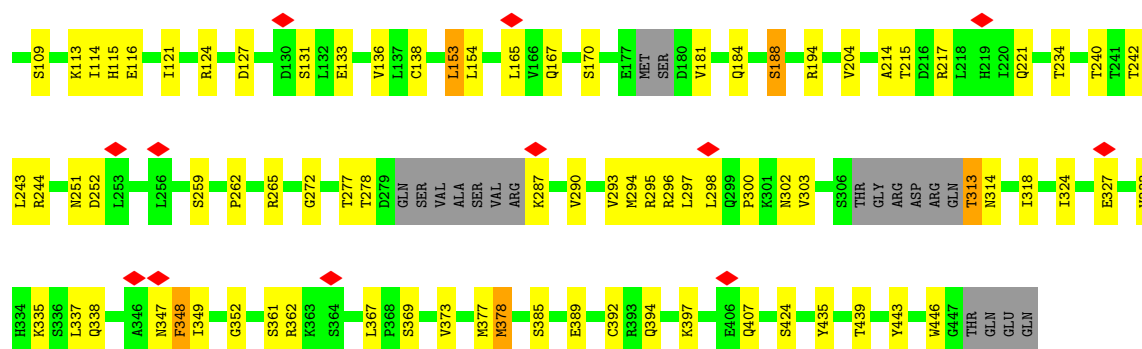
Chain W: 70% 22% 7%



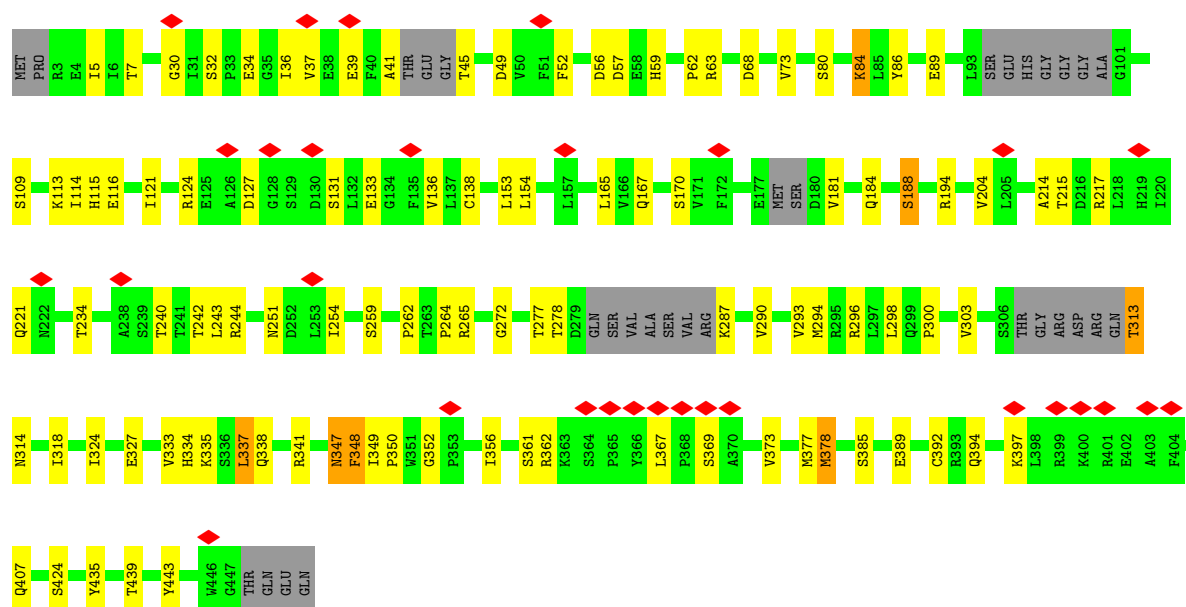
• Molecule 8: Tubulin gamma-1 chain

Chain X: 70% 22% 7%

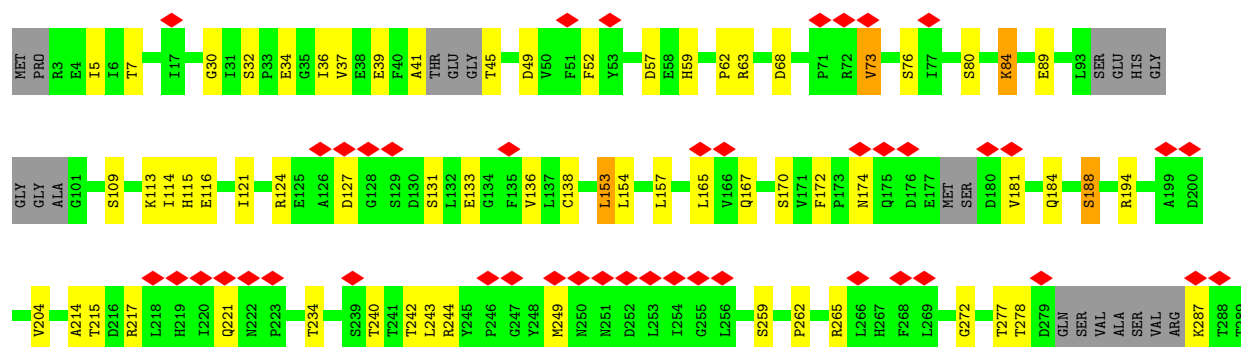


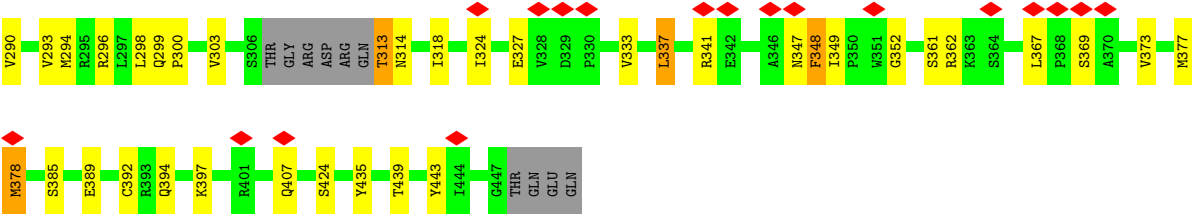


• Molecule 8: Tubulin gamma-1 chain



• Molecule 8: 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	5376	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	0.169	Depositor
Minimum map value	-0.027	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.0432	Depositor
Map size (Å)	532.0, 532.0, 532.0	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.66, 2.66, 2.66	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	e	0.60	1/2908 (0.0%)	0.72	2/3938 (0.1%)
2	J	0.37	0/4525	0.80	9/6119 (0.1%)
2	l	0.28	0/863	0.83	4/1166 (0.3%)
3	B	0.32	0/5133	0.70	2/6930 (0.0%)
3	D	0.33	0/4897	0.75	8/6610 (0.1%)
3	F	0.34	0/5044	0.75	6/6809 (0.1%)
3	H	0.33	1/5009 (0.0%)	0.73	4/6761 (0.1%)
3	a	0.31	0/948	0.70	0/1277
3	f	0.24	0/815	0.62	0/1096
3	h	0.23	0/815	0.63	2/1096 (0.2%)
3	j	0.24	0/855	0.92	8/1152 (0.7%)
4	A	0.27	0/5085	0.64	3/6866 (0.0%)
4	C	0.35	0/5151	0.77	6/6955 (0.1%)
4	E	0.41	0/5311	0.85	9/7169 (0.1%)
4	G	0.33	0/5315	0.76	11/7175 (0.2%)
5	I	0.34	0/4322	0.74	3/5853 (0.1%)
5	K	0.40	1/4683 (0.0%)	0.78	6/6338 (0.1%)
6	L	0.31	0/4697	0.72	3/6348 (0.0%)
6	c	0.26	0/1235	0.63	1/1664 (0.1%)
7	b	0.30	0/484	0.65	0/653
7	d	0.34	0/454	0.65	0/611
7	g	0.26	0/484	0.60	0/653
7	i	0.27	0/484	0.60	0/653
7	k	0.24	0/484	0.58	0/653
7	m	0.31	0/484	0.82	3/653 (0.5%)
8	O	0.28	0/3441	0.64	1/4661 (0.0%)
8	P	0.28	0/3441	0.64	1/4661 (0.0%)
8	Q	0.28	0/3441	0.64	1/4661 (0.0%)
8	R	0.28	0/3441	0.64	1/4661 (0.0%)
8	S	0.29	0/3441	0.64	1/4661 (0.0%)
8	T	0.28	0/3441	0.64	1/4661 (0.0%)
8	U	0.28	0/3441	0.64	1/4661 (0.0%)
8	V	0.28	0/3441	0.64	1/4661 (0.0%)
8	W	0.28	0/3441	0.64	1/4661 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
8	X	0.28	0/3441	0.64	1/4661 (0.0%)
8	Y	0.28	0/3441	0.64	1/4661 (0.0%)
8	Z	0.28	0/3441	0.63	1/4661 (0.0%)
All	All	0.33	3/111777 (0.0%)	0.71	102/151130 (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	J	0	2
3	B	0	1
3	D	0	1
3	F	0	1
3	h	0	2
3	j	0	1
4	A	0	2
4	C	0	2
4	E	0	3
4	G	0	5
5	I	0	6
5	K	0	3
6	L	0	3
8	O	0	1
8	P	0	1
8	Q	0	1
8	R	0	1
8	S	0	1
8	T	0	1
8	U	0	1
8	V	0	1
8	W	0	1
8	X	0	1
8	Y	0	1
8	Z	0	1
All	All	0	44

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	e	243	PRO	N-CD	28.16	1.87	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	K	646	LEU	CG-CD1	-7.78	1.26	1.52
3	H	630	PRO	CG-CD	-5.93	1.30	1.50

All (102) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	866	THR	N-CA-C	-12.51	98.02	113.28
4	E	704	PRO	N-CA-CB	-9.50	93.28	103.25
3	D	434	ILE	N-CA-C	-9.05	105.11	113.71
1	e	243	PRO	CA-N-CD	-8.78	99.71	112.00
2	l	121	PRO	N-CA-CB	8.47	112.14	103.25
3	j	108	PRO	N-CA-CB	7.82	111.46	103.25
4	E	684	GLN	CB-CA-C	-7.64	98.83	110.90
3	j	112	SER	CA-C-N	7.53	135.26	121.70
3	j	112	SER	C-N-CA	7.53	135.26	121.70
4	E	424	ASN	N-CA-C	-7.45	103.92	113.16
4	G	419	ILE	CA-C-N	7.30	135.49	121.54
4	G	419	ILE	C-N-CA	7.30	135.49	121.54
3	j	111	VAL	CA-C-N	7.30	135.49	121.54
3	j	111	VAL	C-N-CA	7.30	135.49	121.54
2	l	120	SER	CA-C-N	7.24	128.89	119.84
2	l	120	SER	C-N-CA	7.24	128.89	119.84
4	G	468	THR	CA-C-N	7.06	130.75	120.51
4	G	468	THR	C-N-CA	7.06	130.75	120.51
4	A	583	ILE	CA-C-N	6.96	134.83	121.54
4	A	583	ILE	C-N-CA	6.96	134.83	121.54
3	j	112	SER	N-CA-C	6.87	125.43	110.80
2	l	130	PRO	N-CA-CB	6.84	110.53	103.00
4	G	240	GLY	CA-C-N	6.83	134.58	121.54
4	G	240	GLY	C-N-CA	6.83	134.58	121.54
3	F	874	ARG	CA-C-N	6.65	129.85	120.28
3	F	874	ARG	C-N-CA	6.65	129.85	120.28
3	h	41	SER	N-CA-C	-6.62	107.07	114.62
4	C	464	GLY	CA-C-N	6.54	134.03	121.54
4	C	464	GLY	C-N-CA	6.54	134.03	121.54
5	I	299	ILE	N-CA-C	-6.51	104.98	111.88
5	I	387	VAL	N-CA-C	-6.40	106.57	111.62
7	m	54	GLY	CA-C-N	6.39	128.36	121.97
7	m	54	GLY	C-N-CA	6.39	128.36	121.97
4	C	557	LEU	CA-CB-CG	-6.37	94.02	116.30
4	C	288	VAL	N-CA-C	-6.27	106.69	112.96
6	L	1681	LEU	CB-CG-CD1	-6.26	91.93	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	241	ARG	O-C-N	-6.16	114.40	122.59
4	E	704	PRO	CA-N-CD	-6.14	103.40	112.00
4	G	442	PHE	N-CA-C	-6.14	105.49	114.39
4	E	521	LEU	CA-CB-CG	6.13	137.74	116.30
5	K	203	PHE	CA-C-N	6.06	132.06	122.61
5	K	203	PHE	C-N-CA	6.06	132.06	122.61
4	E	704	PRO	N-CA-C	6.05	124.93	112.47
3	j	104	PRO	CA-C-N	6.05	133.09	121.54
3	j	104	PRO	C-N-CA	6.05	133.09	121.54
3	F	272	GLU	CA-C-N	5.99	132.98	121.54
3	F	272	GLU	C-N-CA	5.99	132.98	121.54
3	B	415	VAL	N-CA-C	-5.95	106.70	112.29
3	H	631	GLY	N-CA-C	-5.90	99.19	113.18
2	J	950	VAL	N-CA-C	-5.90	107.17	112.12
2	J	235	SER	N-CA-C	-5.81	105.29	112.72
8	Q	378	MET	CB-CG-SD	5.76	129.98	112.70
8	V	378	MET	CB-CG-SD	5.76	129.97	112.70
8	R	378	MET	CB-CG-SD	5.75	129.97	112.70
8	Z	378	MET	CB-CG-SD	5.75	129.97	112.70
8	Y	378	MET	CB-CG-SD	5.75	129.96	112.70
8	P	378	MET	CB-CG-SD	5.75	129.95	112.70
8	T	378	MET	CB-CG-SD	5.75	129.94	112.70
8	O	378	MET	CB-CG-SD	5.75	129.94	112.70
8	U	378	MET	CB-CG-SD	5.75	129.93	112.70
8	S	378	MET	CB-CG-SD	5.74	129.93	112.70
8	W	378	MET	CB-CG-SD	5.74	129.91	112.70
3	D	418	ILE	N-CA-C	-5.73	107.31	112.12
8	X	378	MET	CB-CG-SD	5.73	129.89	112.70
5	K	650	ASP	CA-C-N	5.71	131.87	121.41
5	K	650	ASP	C-N-CA	5.71	131.87	121.41
1	e	243	PRO	N-CA-CB	5.64	109.17	103.25
3	D	402	ALA	N-CA-C	-5.58	105.43	114.09
3	H	434	ILE	N-CA-C	-5.51	107.44	111.90
4	G	581	ASP	N-CA-CB	-5.49	101.22	110.49
5	K	642	LEU	CA-C-N	-5.48	113.55	122.65
5	K	642	LEU	C-N-CA	-5.48	113.55	122.65
3	H	613	ASP	CA-C-N	5.44	128.40	120.51
3	H	613	ASP	C-N-CA	5.44	128.40	120.51
4	E	706	TRP	CA-C-O	-5.41	114.86	120.92
4	G	264	LEU	N-CA-C	5.39	121.73	109.81
6	c	82	LEU	CA-CB-CG	5.37	135.09	116.30
2	J	488	GLY	CA-C-N	5.36	131.77	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	488	GLY	C-N-CA	5.36	131.77	121.54
2	J	255	PRO	CA-C-N	5.35	131.33	121.70
2	J	255	PRO	C-N-CA	5.35	131.33	121.70
3	D	463	LYS	N-CA-C	-5.31	107.82	114.56
6	L	1800	LEU	CA-CB-CG	5.30	134.84	116.30
2	J	489	ALA	CA-C-N	5.26	131.59	121.54
2	J	489	ALA	C-N-CA	5.26	131.59	121.54
3	D	885	HIS	CA-CB-CG	-5.18	108.62	113.80
3	D	399	ALA	N-CA-C	-5.17	108.23	114.75
4	A	548	PRO	N-CA-C	5.15	116.99	110.70
4	C	227	GLY	CA-C-N	5.15	127.12	121.97
4	C	227	GLY	C-N-CA	5.15	127.12	121.97
3	h	27	ASP	N-CA-C	-5.13	106.15	112.72
3	F	888	ALA	CA-C-N	5.12	131.32	121.54
3	F	888	ALA	C-N-CA	5.12	131.32	121.54
3	D	500	GLN	N-CA-C	5.11	117.44	110.24
4	E	862	ASN	CB-CA-C	-5.10	100.27	110.42
4	G	565	ASN	N-CA-C	-5.09	106.19	114.09
3	D	637	VAL	N-CA-C	-5.08	108.33	113.20
7	m	55	ILE	N-CA-C	-5.07	101.52	107.70
3	B	692	ARG	N-CA-C	-5.07	106.24	114.09
6	L	1563	HIS	N-CA-C	-5.06	106.94	114.64
2	J	947	VAL	N-CA-C	-5.03	107.43	111.91
5	I	530	TYR	N-CA-CB	-5.01	102.79	110.26

There are no chirality outliers.

All (44) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	A	583	ILE	Peptide
4	A	584	THR	Mainchain
3	B	869	SER	Peptide
4	C	238	LEU	Peptide
4	C	464	GLY	Peptide
3	D	873	LEU	Peptide
4	E	520	PHE	Peptide
4	E	521	LEU	Peptide
4	E	580	HIS	Peptide
3	F	888	ALA	Peptide
4	G	189	GLY	Peptide
4	G	238	LEU	Peptide
4	G	240	GLY	Mainchain,Peptide

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Mol	Chain	Res	Type	Group
4	G	580	HIS	Peptide
5	I	403	VAL	Peptide
5	I	404	LEU	Mainchain
5	I	407	ASP	Peptide
5	I	408	ASP	Mainchain
5	I	507	SER	Peptide
5	I	600	ASN	Peptide
2	J	256	LEU	Peptide
2	J	489	ALA	Peptide
5	K	408	ASP	Peptide
5	K	409	ASN	Mainchain
5	K	651	TYR	Peptide
6	L	317	ARG	Peptide
6	L	346	LEU	Peptide
6	L	546	ARG	Peptide
8	O	348	PHE	Peptide
8	P	348	PHE	Peptide
8	Q	348	PHE	Peptide
8	R	348	PHE	Peptide
8	S	348	PHE	Peptide
8	T	348	PHE	Peptide
8	U	348	PHE	Peptide
8	V	348	PHE	Peptide
8	W	348	PHE	Peptide
8	X	348	PHE	Peptide
8	Y	348	PHE	Peptide
8	Z	348	PHE	Peptide
3	h	40	GLY	Peptide
3	h	49	ARG	Peptide
3	j	111	VAL	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	e	2847	0	2810	41	0
2	J	4429	0	4482	31	0
2	l	847	0	789	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	5029	0	5018	31	0
3	D	4796	0	4775	40	0
3	F	4941	0	4935	49	0
3	H	4907	0	4896	36	0
3	a	933	0	953	16	0
3	f	803	0	831	3	0
3	h	803	0	831	8	0
3	j	843	0	846	7	0
4	A	4978	0	4996	29	0
4	C	5044	0	5081	47	0
4	E	5202	0	5241	83	0
4	G	5206	0	5230	34	0
5	I	4225	0	4259	21	0
5	K	4579	0	4586	47	0
6	L	4587	0	4636	34	0
6	c	1220	0	1231	18	0
7	b	484	0	512	6	0
7	d	454	0	482	4	0
7	g	484	0	512	2	0
7	i	484	0	512	7	0
7	k	484	0	512	5	0
7	m	484	0	512	5	0
8	O	3373	0	3325	39	0
8	P	3373	0	3325	41	0
8	Q	3373	0	3325	46	0
8	R	3373	0	3325	52	0
8	S	3373	0	3325	62	0
8	T	3373	0	3325	54	0
8	U	3373	0	3325	45	0
8	V	3373	0	3325	41	0
8	W	3373	0	3325	46	0
8	X	3373	0	3325	45	0
8	Y	3373	0	3325	54	0
8	Z	3373	0	3325	41	0
All	All	109569	0	109368	1017	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (1017) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:e:243:PRO:CD	1:e:243:PRO:N	1.87	1.35
1:e:153:MET:CE	1:e:313:MET:HE3	1.55	1.35
1:e:153:MET:HE3	1:e:313:MET:CE	1.56	1.33
1:e:153:MET:CE	1:e:317:ILE:HD11	1.65	1.26
4:E:641:LEU:HD21	4:E:702:MET:CE	1.70	1.22
4:E:641:LEU:HD21	4:E:702:MET:HE3	1.34	1.09
1:e:153:MET:HE2	1:e:317:ILE:HD11	1.24	1.09
1:e:242:LEU:HD12	1:e:243:PRO:HD2	1.42	1.00
1:e:153:MET:HE1	1:e:317:ILE:HD11	1.45	0.98
4:E:641:LEU:HD21	4:E:702:MET:HE1	1.51	0.91
4:E:696:TYR:O	4:E:700:GLU:HB2	1.76	0.85
5:K:646:LEU:HD13	8:Y:341:ARG:HD2	1.62	0.82
1:e:153:MET:CE	1:e:317:ILE:CD1	2.57	0.79
4:C:553:ALA:HB3	8:R:342:GLU:HB2	1.64	0.79
1:e:242:LEU:HD12	1:e:243:PRO:CD	2.15	0.77
4:C:550:ARG:HA	8:R:342:GLU:HB3	1.67	0.76
1:e:153:MET:HE1	1:e:317:ILE:CD1	2.15	0.75
6:L:1800:LEU:HD13	8:Z:341:ARG:HD2	1.69	0.74
3:F:713:HIS:CE1	8:T:355:SER:HB2	2.22	0.73
4:E:704:PRO:HB3	8:S:331:THR:HA	1.72	0.71
5:K:643:ALA:HB3	8:Y:334:HIS:HB2	1.73	0.71
6:L:1800:LEU:HG	8:Z:337:LEU:HD23	1.72	0.71
5:K:516:ARG:HD2	8:Y:264:PRO:HD3	1.74	0.70
3:B:369:VAL:HG21	4:A:308:SER:HB2	1.73	0.70
4:C:663:LYS:HG2	8:Q:264:PRO:HG3	1.74	0.70
3:a:57:LYS:HD3	3:a:119:ALA:HB3	1.74	0.69
5:K:639:ASN:HB3	8:Y:334:HIS:CE1	2.27	0.69
5:K:653:LYS:NZ	8:Y:350:PRO:O	2.25	0.69
5:K:646:LEU:HD12	8:Y:338:GLN:HA	1.75	0.68
3:F:606:ARG:HG3	8:U:339:ARG:HG2	1.76	0.67
3:F:863:VAL:HG21	3:F:889:ARG:HH22	1.58	0.67
8:X:56:ASP:O	8:Y:287:LYS:N	2.27	0.66
1:e:269:MET:HG2	1:e:271:SER:H	1.60	0.66
4:E:700:GLU:HA	8:S:334:HIS:HB3	1.76	0.66
1:e:95:ARG:HH12	3:B:543:LYS:HB3	1.60	0.66
4:C:526:ASP:OD1	8:Q:251:ASN:ND2	2.29	0.66
4:G:443:LEU:HD22	4:G:450:ILE:HD11	1.78	0.66
4:C:518:ARG:HA	4:C:523:ASP:HB3	1.78	0.66
4:G:240:GLY:O	4:G:275:ARG:NH1	2.30	0.65
4:C:371:GLN:HE21	6:c:195:LEU:HB3	1.61	0.64
8:O:262:PRO:HG3	8:O:318:ILE:HG21	1.80	0.64
8:X:262:PRO:HG3	8:X:318:ILE:HG21	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:677:LEU:HD21	3:B:712:VAL:HA	1.81	0.63
4:C:304:LEU:HB3	3:D:369:VAL:HG13	1.80	0.63
4:E:241:ARG:HE	4:E:242:GLN:H	1.46	0.63
8:R:262:PRO:HG3	8:R:318:ILE:HG21	1.80	0.63
8:Z:262:PRO:HG3	8:Z:318:ILE:HG21	1.80	0.63
8:P:262:PRO:HG3	8:P:318:ILE:HG21	1.80	0.63
1:e:309:ILE:HD12	1:e:312:ARG:HD3	1.81	0.63
8:S:262:PRO:HG3	8:S:318:ILE:HG21	1.80	0.63
8:U:262:PRO:HG3	8:U:318:ILE:HG21	1.80	0.63
2:l:110:ILE:HA	2:l:113:LEU:HD12	1.81	0.63
8:W:262:PRO:HG3	8:W:318:ILE:HG21	1.80	0.63
3:a:21:LEU:HD11	3:a:23:ARG:HH21	1.64	0.63
4:E:653:ARG:NH1	8:S:252:ASP:OD2	2.32	0.62
3:B:365:ARG:NH1	4:A:311:GLU:OE2	2.32	0.62
2:J:1011:GLU:CD	8:X:338:GLN:HE22	2.07	0.62
5:K:393:ASN:OD1	5:K:397:GLN:NE2	2.32	0.62
4:C:563:THR:HG21	8:Q:246:PRO:HG3	1.80	0.62
8:V:262:PRO:HG3	8:V:318:ILE:HG21	1.80	0.62
1:e:154:ASP:O	1:e:160:THR:HG23	2.00	0.62
2:J:327:LEU:HD13	2:J:368:LEU:HD11	1.82	0.62
8:S:128:GLY:O	8:T:299:GLN:NE2	2.33	0.62
8:T:262:PRO:HG3	8:T:318:ILE:HG21	1.80	0.62
8:Y:262:PRO:HG3	8:Y:318:ILE:HG21	1.80	0.62
4:C:244:ARG:H	4:C:275:ARG:HH22	1.48	0.61
8:Q:262:PRO:HG3	8:Q:318:ILE:HG21	1.80	0.61
3:F:883:ASN:ND2	8:T:352:GLY:O	2.33	0.61
4:E:223:TYR:HA	3:F:365:ARG:HH22	1.64	0.61
4:E:641:LEU:CD2	4:E:702:MET:HE1	2.30	0.61
3:D:885:HIS:NE2	8:R:350:PRO:O	2.34	0.61
5:K:111:PHE:O	6:L:317:ARG:NH2	2.31	0.61
2:J:217:GLU:HG2	2:J:228:ARG:HH12	1.66	0.61
2:J:475:THR:HG21	2:J:491:GLU:HB3	1.83	0.60
8:T:56:ASP:HB3	8:U:296:ARG:NE	2.15	0.60
4:E:854:SER:O	4:E:858:ARG:HB2	2.01	0.60
4:C:180:TRP:HZ2	3:D:383:ALA:HA	1.65	0.60
3:F:377:ARG:HD3	6:c:145:TYR:HD1	1.67	0.60
8:X:184:GLN:O	8:X:188:SER:OG	2.20	0.60
8:V:184:GLN:O	8:V:188:SER:OG	2.20	0.59
8:Z:184:GLN:O	8:Z:188:SER:OG	2.20	0.59
6:c:111:LEU:HD13	6:c:114:LEU:HD12	1.84	0.59
8:W:184:GLN:O	8:W:188:SER:OG	2.20	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:R:184:GLN:O	8:R:188:SER:OG	2.20	0.59
8:O:184:GLN:O	8:O:188:SER:OG	2.20	0.59
2:J:369:TYR:OH	5:K:127:ASP:O	2.20	0.59
4:A:164:LYS:HE2	4:A:174:LEU:HD13	1.85	0.59
4:A:226:VAL:HG11	4:A:304:LEU:HG	1.84	0.59
1:e:295:ALA:HA	1:e:325:MET:HE1	1.85	0.59
5:K:651:TYR:HA	8:Y:347:ASN:HA	1.85	0.59
8:S:184:GLN:O	8:S:188:SER:OG	2.20	0.59
8:P:184:GLN:O	8:P:188:SER:OG	2.20	0.59
8:Q:184:GLN:O	8:Q:188:SER:OG	2.20	0.59
8:U:184:GLN:O	8:U:188:SER:OG	2.20	0.59
4:E:862:ASN:HB3	8:S:344:LYS:NZ	2.18	0.58
8:T:56:ASP:HB3	8:U:296:ARG:HE	1.68	0.58
7:d:18:LEU:HA	7:d:21:VAL:HG12	1.83	0.58
3:B:460:TRP:HA	3:B:488:LYS:HE2	1.85	0.58
4:A:359:LEU:O	4:A:363:SER:OG	2.22	0.58
1:e:214:GLU:HG2	1:e:305:MET:HG3	1.83	0.58
2:J:797:ASP:HA	2:J:826:LEU:HD11	1.84	0.58
5:K:551:THR:HG23	5:K:553:ASP:H	1.68	0.58
8:T:184:GLN:O	8:T:188:SER:OG	2.20	0.58
8:Y:184:GLN:O	8:Y:188:SER:OG	2.20	0.58
6:L:292:SER:O	6:L:295:ARG:NH1	2.36	0.58
5:K:518:ARG:HH12	5:K:619:PHE:HB2	1.68	0.58
4:C:459:VAL:HG11	4:C:628:LEU:HD11	1.86	0.58
4:G:426:LYS:HD2	4:G:431:ARG:HB2	1.86	0.58
5:K:345:VAL:HG23	5:K:346:GLU:HG3	1.86	0.58
4:C:309:GLN:HE21	6:c:184:ALA:HB3	1.69	0.57
5:I:499:GLN:HE22	8:W:265:ARG:HH11	1.52	0.57
1:e:180:LEU:HD13	1:e:261:LEU:HG	1.85	0.57
4:C:763:GLN:HG3	4:C:766:THR:H	1.68	0.57
5:I:502:ARG:HH21	5:I:601:LEU:HD13	1.69	0.57
4:A:440:PRO:HG2	4:A:443:LEU:HB2	1.86	0.57
4:E:641:LEU:CD2	4:E:702:MET:HE3	2.24	0.57
6:L:1615:LYS:HD2	6:L:1709:LEU:HD13	1.86	0.57
4:E:521:LEU:O	4:E:523:ASP:N	2.37	0.57
4:G:663:LYS:NZ	8:U:199:ALA:O	2.37	0.57
3:H:247:GLU:HG3	3:H:366:ARG:HH12	1.70	0.57
8:Q:113:LYS:HG3	8:Q:114:ILE:HG23	1.87	0.57
4:C:180:TRP:HD1	4:C:184:ARG:NH1	2.03	0.57
3:F:413:SER:OG	6:c:141:ARG:O	2.21	0.57
8:S:113:LYS:HG3	8:S:114:ILE:HG23	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Y:113:LYS:HG3	8:Y:114:ILE:HG23	1.87	0.57
3:H:883:ASN:ND2	8:V:352:GLY:O	2.38	0.57
5:K:118:SER:HA	6:L:314:GLU:HG2	1.87	0.57
8:R:113:LYS:HG3	8:R:114:ILE:HG23	1.87	0.57
8:Z:113:LYS:HG3	8:Z:114:ILE:HG23	1.87	0.57
4:E:699:PHE:CE2	8:S:333:VAL:HB	2.40	0.56
3:D:730:SER:OG	3:D:761:ARG:NH1	2.38	0.56
4:E:167:LYS:NZ	4:E:411:GLU:O	2.39	0.56
4:E:513:LEU:HD21	4:E:706:TRP:HE1	1.70	0.56
4:E:613:LEU:HG	4:E:614:GLU:HG3	1.86	0.56
3:F:377:ARG:HH22	6:c:137:LYS:HG2	1.71	0.56
8:T:113:LYS:HG3	8:T:114:ILE:HG23	1.87	0.56
8:X:113:LYS:HG3	8:X:114:ILE:HG23	1.87	0.56
3:H:380:THR:OG1	3:H:411:MET:SD	2.61	0.56
3:B:892:ARG:NH2	8:P:351:TRP:O	2.39	0.56
3:F:315:ARG:O	3:F:392:LYS:NZ	2.38	0.56
3:F:392:LYS:HG2	3:F:445:GLU:HG2	1.88	0.56
3:H:490:ILE:HD13	3:H:541:THR:HG22	1.86	0.56
8:O:293:VAL:HA	8:O:296:ARG:HD2	1.88	0.56
4:E:563:THR:OG1	8:S:45:THR:O	2.23	0.56
7:k:30:GLU:HB2	3:j:112:SER:H	1.71	0.56
4:C:296:MET:HE1	4:C:342:ALA:HB2	1.88	0.56
8:O:113:LYS:HG3	8:O:114:ILE:HG23	1.87	0.56
8:Y:293:VAL:HA	8:Y:296:ARG:HD2	1.88	0.56
4:E:699:PHE:CE2	8:S:358:VAL:HG21	2.41	0.56
8:W:293:VAL:HA	8:W:296:ARG:HD2	1.88	0.56
8:X:293:VAL:HA	8:X:296:ARG:HD2	1.88	0.56
4:G:581:ASP:H	4:G:607:GLU:HG2	1.71	0.56
3:H:869:SER:HB3	3:H:873:LEU:HG	1.87	0.56
5:K:649:LEU:HB3	8:Y:341:ARG:HE	1.70	0.56
6:L:1676:ILE:HG23	6:L:1680:ILE:HD12	1.88	0.56
8:Z:293:VAL:HA	8:Z:296:ARG:HD2	1.88	0.56
4:E:304:LEU:HB3	3:F:369:VAL:HG22	1.87	0.56
5:K:497:ALA:HB2	8:Y:254:ILE:HD11	1.88	0.56
4:E:518:ARG:O	4:E:523:ASP:N	2.38	0.55
3:F:602:GLU:OE1	3:F:606:ARG:NH2	2.39	0.55
2:J:566:MET:HA	2:J:569:LEU:HD12	1.87	0.55
8:U:113:LYS:HG3	8:U:114:ILE:HG23	1.87	0.55
1:e:153:MET:CE	1:e:313:MET:CE	2.43	0.55
1:e:186:THR:HA	1:e:189:LEU:HD12	1.88	0.55
8:W:113:LYS:HG3	8:W:114:ILE:HG23	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:e:267:LEU:HD22	1:e:269:MET:HB2	1.89	0.55
8:V:52:PHE:HA	8:V:62:PRO:HA	1.89	0.55
7:i:28:LEU:HD21	3:h:93:ILE:HG12	1.88	0.55
4:G:296:MET:HE3	4:G:338:LEU:HD12	1.89	0.55
8:P:52:PHE:HA	8:P:62:PRO:HA	1.89	0.55
8:W:52:PHE:HA	8:W:62:PRO:HA	1.89	0.55
4:E:277:ILE:HA	4:E:293:ALA:HB1	1.89	0.55
3:F:373:ASP:OD1	3:F:373:ASP:N	2.40	0.55
3:B:296:GLU:HB3	4:A:184:ARG:HH21	1.70	0.55
3:D:246:THR:HG23	3:D:249:ALA:H	1.71	0.55
6:L:1738:LYS:O	6:L:1742:GLN:NE2	2.40	0.55
8:T:293:VAL:HA	8:T:296:ARG:HD2	1.88	0.55
4:A:547:THR:HG23	4:A:550:ARG:HG3	1.89	0.55
8:U:52:PHE:HA	8:U:62:PRO:HA	1.89	0.55
8:V:293:VAL:HA	8:V:296:ARG:HD2	1.88	0.55
8:O:130:ASP:OD2	8:P:295:ARG:NH2	2.40	0.55
8:S:293:VAL:HA	8:S:296:ARG:HD2	1.88	0.55
8:P:293:VAL:HA	8:P:296:ARG:HD2	1.88	0.55
6:c:187:GLY:HA2	6:c:193:VAL:HG11	1.88	0.55
8:P:113:LYS:HG3	8:P:114:ILE:HG23	1.87	0.54
8:Q:293:VAL:HA	8:Q:296:ARG:HD2	1.88	0.54
8:U:293:VAL:HA	8:U:296:ARG:HD2	1.88	0.54
3:F:476:THR:HG22	3:F:479:GLN:HE21	1.72	0.54
8:V:49:ASP:OD1	8:V:63:ARG:NH2	2.41	0.54
3:F:397:ALA:O	3:F:473:SER:OG	2.25	0.54
7:b:32:SER:HA	3:a:97:LEU:HD21	1.89	0.54
8:V:113:LYS:HG3	8:V:114:ILE:HG23	1.87	0.54
3:H:599:GLY:HA2	8:W:338:GLN:HE21	1.72	0.54
8:X:49:ASP:OD1	8:X:63:ARG:NH2	2.41	0.54
8:Z:49:ASP:OD1	8:Z:63:ARG:NH2	2.41	0.54
7:m:25:MET:HE1	7:m:48:VAL:HG11	1.88	0.54
7:d:28:LEU:HD13	6:c:110:VAL:HG11	1.89	0.54
4:C:312:GLN:HG3	6:c:183:GLU:HG2	1.89	0.54
4:G:869:LEU:HG	4:G:871:ARG:H	1.73	0.54
5:I:511:ASP:H	5:I:514:LYS:HD2	1.73	0.54
8:O:52:PHE:HA	8:O:62:PRO:HA	1.89	0.54
8:R:293:VAL:HA	8:R:296:ARG:HD2	1.88	0.54
8:S:49:ASP:OD1	8:S:63:ARG:NH2	2.41	0.54
8:U:49:ASP:OD1	8:U:63:ARG:NH2	2.41	0.54
8:Y:49:ASP:OD1	8:Y:63:ARG:NH2	2.41	0.54
5:K:643:ALA:HA	5:K:646:LEU:HG	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:c:12:CYS:SG	6:c:34:LYS:NZ	2.81	0.54
4:C:461:ARG:HG3	4:C:467:VAL:HB	1.89	0.54
8:P:49:ASP:OD1	8:P:63:ARG:NH2	2.41	0.54
8:X:52:PHE:HA	8:X:62:PRO:HA	1.89	0.54
8:Z:52:PHE:HA	8:Z:62:PRO:HA	1.89	0.54
8:Z:115:HIS:NE2	8:Z:116:GLU:OE2	2.41	0.54
4:C:168:LYS:HG2	4:C:405:SER:HB2	1.90	0.54
3:D:598:THR:HG22	3:D:623:VAL:H	1.72	0.54
3:F:575:ARG:HH12	8:T:3:ARG:HG3	1.73	0.54
4:G:271:SER:OG	4:G:275:ARG:NH2	2.41	0.54
8:V:115:HIS:NE2	8:V:116:GLU:OE2	2.41	0.54
4:G:314:HIS:HB2	4:G:319:LEU:HD23	1.89	0.53
8:R:49:ASP:OD1	8:R:63:ARG:NH2	2.41	0.53
8:R:52:PHE:HA	8:R:62:PRO:HA	1.89	0.53
8:R:115:HIS:NE2	8:R:116:GLU:OE2	2.41	0.53
8:S:52:PHE:HA	8:S:62:PRO:HA	1.89	0.53
8:W:49:ASP:OD1	8:W:63:ARG:NH2	2.41	0.53
8:Y:52:PHE:HA	8:Y:62:PRO:HA	1.89	0.53
8:Y:115:HIS:NE2	8:Y:116:GLU:OE2	2.41	0.53
4:E:526:ASP:N	8:S:251:ASN:HD22	2.06	0.53
6:L:1513:ARG:HH12	6:L:1681:LEU:HB3	1.74	0.53
8:P:115:HIS:NE2	8:P:116:GLU:OE2	2.41	0.53
8:Q:52:PHE:HA	8:Q:62:PRO:HA	1.89	0.53
8:U:56:ASP:OD2	8:V:296:ARG:HG2	2.08	0.53
3:a:24:SER:OG	3:a:25:GLU:N	2.40	0.53
8:Q:49:ASP:OD1	8:Q:63:ARG:NH2	2.41	0.53
2:l:21:GLU:HA	2:l:24:ARG:HE	1.73	0.53
5:K:523:PHE:O	5:K:527:ASN:ND2	2.41	0.53
8:O:49:ASP:OD1	8:O:63:ARG:NH2	2.41	0.53
8:T:52:PHE:HA	8:T:62:PRO:HA	1.89	0.53
8:Y:56:ASP:OD1	8:Z:299:GLN:NE2	2.42	0.53
2:l:22:LEU:HD12	7:m:50:LEU:HD11	1.90	0.53
5:I:499:GLN:HE22	8:W:265:ARG:NH1	2.07	0.53
8:Q:115:HIS:NE2	8:Q:116:GLU:OE2	2.41	0.53
8:U:115:HIS:NE2	8:U:116:GLU:OE2	2.41	0.53
8:W:115:HIS:NE2	8:W:116:GLU:OE2	2.41	0.53
1:e:105:LEU:HD11	1:e:123:MET:HG3	1.90	0.53
8:T:49:ASP:OD1	8:T:63:ARG:NH2	2.41	0.53
6:c:70:ILE:HD11	6:c:111:LEU:HD12	1.91	0.53
8:S:115:HIS:NE2	8:S:116:GLU:OE2	2.41	0.53
8:T:115:HIS:NE2	8:T:116:GLU:OE2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:X:115:HIS:NE2	8:X:116:GLU:OE2	2.41	0.53
3:B:379:LYS:HD3	4:A:187:LEU:HD13	1.91	0.53
3:H:868:SER:HB2	3:H:873:LEU:HD12	1.89	0.53
8:U:181:VAL:HB	8:U:184:GLN:HB2	1.91	0.53
8:Q:181:VAL:HB	8:Q:184:GLN:HB2	1.91	0.53
4:A:353:GLY:H	4:A:438:GLN:HA	1.74	0.53
4:E:242:GLN:HE22	4:E:275:ARG:HE	1.56	0.52
4:G:521:LEU:HA	4:G:645:MET:HE1	1.90	0.52
8:O:115:HIS:NE2	8:O:116:GLU:OE2	2.41	0.52
8:P:181:VAL:HB	8:P:184:GLN:HB2	1.91	0.52
3:a:21:LEU:HG	3:a:23:ARG:H	1.74	0.52
5:K:651:TYR:HD2	8:Y:348:PHE:N	2.07	0.52
1:e:153:MET:HE3	1:e:313:MET:HE3	0.67	0.52
4:C:582:LEU:HD23	4:C:744:LEU:HD22	1.90	0.52
5:I:448:SER:OG	5:I:449:GLY:N	2.40	0.52
8:T:181:VAL:HB	8:T:184:GLN:HB2	1.91	0.52
4:E:221:LEU:HD11	4:E:260:VAL:HG12	1.91	0.52
3:F:406:THR:HG22	3:F:408:ASP:H	1.75	0.52
3:H:608:THR:HG23	3:H:610:ALA:H	1.75	0.52
5:K:393:ASN:O	5:K:397:GLN:NE2	2.43	0.52
8:W:181:VAL:HB	8:W:184:GLN:HB2	1.91	0.52
3:D:710:GLU:OE2	3:D:855:GLN:NE2	2.43	0.52
3:H:403:TYR:O	3:H:406:THR:OG1	2.24	0.52
3:D:713:HIS:CD2	8:R:355:SER:HB2	2.45	0.52
4:E:172:GLN:HE22	3:F:401:HIS:HB3	1.75	0.52
1:e:138:ALA:HB1	1:e:152:VAL:HG21	1.92	0.51
4:E:708:ILE:HA	4:E:711:LYS:HD2	1.92	0.51
3:F:713:HIS:NE2	8:T:355:SER:HB2	2.26	0.51
2:J:561:MET:HE3	2:J:924:ASP:HB3	1.92	0.51
6:L:1743:LEU:HB3	6:L:1760:PRO:HD3	1.92	0.51
8:O:181:VAL:HB	8:O:184:GLN:HB2	1.92	0.51
8:X:181:VAL:HB	8:X:184:GLN:HB2	1.91	0.51
8:Y:121:ILE:HG12	8:Y:124:ARG:HH22	1.76	0.51
8:R:181:VAL:HB	8:R:184:GLN:HB2	1.92	0.51
8:S:121:ILE:HG12	8:S:124:ARG:HH22	1.76	0.51
8:W:121:ILE:HG12	8:W:124:ARG:HH22	1.76	0.51
8:X:121:ILE:HG12	8:X:124:ARG:HH22	1.76	0.51
1:e:315:LYS:O	1:e:318:THR:OG1	2.28	0.51
3:F:860:GLN:O	3:F:864:LEU:HB2	2.11	0.51
8:S:181:VAL:HB	8:S:184:GLN:HB2	1.91	0.51
8:Z:290:VAL:HG21	8:Z:333:VAL:HG12	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:7:LEU:HD12	2:J:305:LEU:HD11	1.93	0.51
8:P:342:GLU:OE2	4:A:550:ARG:NE	2.44	0.51
8:T:287:LYS:NZ	8:T:327:GLU:O	2.44	0.51
8:X:287:LYS:NZ	8:X:327:GLU:O	2.44	0.51
8:Z:181:VAL:HB	8:Z:184:GLN:HB2	1.91	0.51
3:D:769:ARG:HH21	3:h:66:ARG:HG2	1.75	0.51
4:G:629:ILE:HG23	4:G:630:ILE:HD12	1.92	0.51
3:H:251:VAL:HG11	3:H:362:LEU:H	1.76	0.51
8:O:121:ILE:HG12	8:O:124:ARG:HH22	1.76	0.51
8:T:121:ILE:HG12	8:T:124:ARG:HH22	1.76	0.51
3:F:865:LEU:HD23	3:F:877:SER:HB3	1.93	0.51
4:A:758:PHE:HE1	4:A:822:ILE:HG23	1.74	0.51
3:F:834:GLY:HA2	3:F:837:LYS:HE2	1.93	0.51
8:Q:290:VAL:HG21	8:Q:333:VAL:HG12	1.93	0.51
8:W:290:VAL:HG21	8:W:333:VAL:HG12	1.93	0.51
8:Z:121:ILE:HG12	8:Z:124:ARG:HH22	1.76	0.51
3:F:879:ARG:HH12	8:T:334:HIS:HA	1.76	0.51
4:G:560:ARG:HD2	4:G:565:ASN:HD21	1.75	0.51
5:I:48:LEU:HD13	5:I:130:GLN:HG2	1.93	0.51
5:I:129:PHE:O	5:I:133:PHE:HB2	2.10	0.51
8:W:240:THR:OG1	8:W:244:ARG:NH1	2.45	0.51
8:X:290:VAL:HG21	8:X:333:VAL:HG12	1.93	0.51
8:Y:290:VAL:HG21	8:Y:333:VAL:HG12	1.93	0.51
8:O:240:THR:OG1	8:O:244:ARG:NH1	2.44	0.50
8:O:287:LYS:NZ	8:O:327:GLU:O	2.44	0.50
8:P:121:ILE:HG12	8:P:124:ARG:HH22	1.76	0.50
8:P:240:THR:OG1	8:P:244:ARG:NH1	2.45	0.50
8:S:240:THR:OG1	8:S:244:ARG:NH1	2.44	0.50
8:W:54:GLN:HG3	8:X:295:ARG:HH22	1.75	0.50
8:X:240:THR:OG1	8:X:244:ARG:NH1	2.44	0.50
8:Y:5:ILE:HG13	8:Y:133:GLU:HB3	1.94	0.50
4:C:399:ILE:HG23	4:C:461:ARG:NH1	2.26	0.50
4:E:699:PHE:CZ	8:S:358:VAL:HG21	2.46	0.50
2:J:408:GLN:HB3	2:J:460:LEU:HD13	1.94	0.50
8:Q:121:ILE:HG12	8:Q:124:ARG:HH22	1.76	0.50
8:U:121:ILE:HG12	8:U:124:ARG:HH22	1.76	0.50
8:V:121:ILE:HG12	8:V:124:ARG:HH22	1.76	0.50
8:Y:181:VAL:HB	8:Y:184:GLN:HB2	1.91	0.50
3:a:8:SER:OG	3:a:10:ASN:OD1	2.28	0.50
8:U:290:VAL:HG21	8:U:333:VAL:HG12	1.93	0.50
8:X:5:ILE:HG13	8:X:133:GLU:HB3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:P:290:VAL:HG21	8:P:333:VAL:HG12	1.93	0.50
8:T:240:THR:OG1	8:T:244:ARG:NH1	2.45	0.50
8:U:240:THR:OG1	8:U:244:ARG:NH1	2.44	0.50
8:V:181:VAL:HB	8:V:184:GLN:HB2	1.91	0.50
1:e:153:MET:HE2	1:e:317:ILE:CD1	2.18	0.50
3:F:709:SER:OG	8:T:262:PRO:O	2.25	0.50
3:H:677:LEU:HD13	3:H:712:VAL:HG22	1.94	0.50
8:O:290:VAL:HG21	8:O:333:VAL:HG12	1.93	0.50
8:U:287:LYS:NZ	8:U:327:GLU:O	2.44	0.50
8:W:5:ILE:HG13	8:W:133:GLU:HB3	1.94	0.50
8:Z:240:THR:OG1	8:Z:244:ARG:NH1	2.44	0.50
7:i:35:LEU:HD21	3:h:58:ILE:HG23	1.94	0.50
4:E:243:SER:OG	4:E:244:ARG:N	2.44	0.50
8:Q:287:LYS:NZ	8:Q:327:GLU:O	2.44	0.50
8:R:121:ILE:HG12	8:R:124:ARG:HH22	1.76	0.50
8:R:240:THR:OG1	8:R:244:ARG:NH1	2.45	0.50
8:R:290:VAL:HG21	8:R:333:VAL:HG12	1.93	0.50
8:S:290:VAL:HG21	8:S:333:VAL:HG12	1.93	0.50
8:T:5:ILE:HG13	8:T:133:GLU:HB3	1.94	0.50
8:Y:240:THR:OG1	8:Y:244:ARG:NH1	2.45	0.50
1:e:202:THR:OG1	1:e:203:THR:N	2.45	0.50
8:R:5:ILE:HG13	8:R:133:GLU:HB3	1.93	0.50
8:Q:240:THR:OG1	8:Q:244:ARG:NH1	2.44	0.50
8:T:290:VAL:HG21	8:T:333:VAL:HG12	1.93	0.50
8:V:290:VAL:HG21	8:V:333:VAL:HG12	1.93	0.50
8:X:80:SER:O	8:X:84:LYS:NZ	2.43	0.50
8:Y:80:SER:O	8:Y:84:LYS:NZ	2.43	0.50
4:E:408:MET:HE3	4:E:439:ILE:HG12	1.94	0.49
5:K:512:ALA:HA	5:K:515:TRP:CE3	2.47	0.49
1:e:145:SER:HB3	1:e:330:ILE:HD13	1.94	0.49
3:D:546:LEU:HD11	3:D:742:GLN:HA	1.94	0.49
8:P:5:ILE:HG13	8:P:133:GLU:HB3	1.94	0.49
8:Z:5:ILE:HG13	8:Z:133:GLU:HB3	1.94	0.49
5:K:132:LEU:O	5:K:135:SER:OG	2.30	0.49
6:L:1609:THR:HG23	6:L:1611:GLY:H	1.77	0.49
1:e:189:LEU:HD21	1:e:213:LYS:HB2	1.94	0.49
4:C:752:MET:O	4:C:755:CYS:HB3	2.11	0.49
3:H:319:LEU:HG	3:H:425:PRO:HB3	1.93	0.49
8:P:287:LYS:NZ	8:P:327:GLU:O	2.44	0.49
8:W:287:LYS:NZ	8:W:327:GLU:O	2.44	0.49
3:D:398:SER:HB3	3:D:472:PRO:HA	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:718:MET:HG3	3:F:880:LEU:HD21	1.92	0.49
4:G:557:LEU:HD21	8:V:343:ARG:HD3	1.94	0.49
8:Q:128:GLY:HA3	8:R:301:LYS:HE2	1.94	0.49
8:V:240:THR:OG1	8:V:244:ARG:NH1	2.45	0.49
4:A:631:ASN:H	4:A:634:ALA:HB3	1.77	0.49
1:e:358:SER:OG	1:e:359:LYS:N	2.45	0.49
7:g:51:CYS:SG	3:f:92:SER:OG	2.70	0.49
4:E:579:PRO:HA	4:E:608:LEU:HD13	1.94	0.49
6:L:294:ARG:HD2	6:L:307:ARG:HH11	1.78	0.49
7:g:48:VAL:HG13	3:f:87:LEU:HD11	1.92	0.49
3:B:573:PHE:HA	3:B:608:THR:HG21	1.94	0.49
8:S:5:ILE:HG13	8:S:133:GLU:HB3	1.94	0.49
8:U:5:ILE:HG13	8:U:133:GLU:HB3	1.94	0.49
8:Y:287:LYS:NZ	8:Y:327:GLU:O	2.44	0.49
8:Z:80:SER:O	8:Z:84:LYS:NZ	2.43	0.49
8:Q:5:ILE:HG13	8:Q:133:GLU:HB3	1.94	0.49
8:V:5:ILE:HG13	8:V:133:GLU:HB3	1.93	0.49
4:C:399:ILE:HG23	4:C:461:ARG:HH12	1.77	0.48
8:S:80:SER:O	8:S:84:LYS:NZ	2.44	0.48
8:Z:287:LYS:NZ	8:Z:327:GLU:O	2.44	0.48
2:l:114:LEU:HA	2:l:117:LEU:HD12	1.96	0.48
3:F:879:ARG:CZ	8:T:337:LEU:HD22	2.43	0.48
3:H:594:GLN:HA	3:H:597:LEU:HD13	1.95	0.48
3:H:660:TYR:OH	3:H:751:HIS:NE2	2.33	0.48
5:I:498:LEU:HA	5:I:502:ARG:HB2	1.95	0.48
6:L:332:GLN:HE22	6:L:340:GLN:HA	1.78	0.48
8:P:80:SER:O	8:P:84:LYS:NZ	2.43	0.48
4:A:534:LEU:HD21	4:A:557:LEU:HD23	1.96	0.48
4:E:857:SER:O	4:E:857:SER:OG	2.31	0.48
5:K:44:ARG:HE	5:K:123:ASN:HD21	1.59	0.48
4:C:557:LEU:HD13	8:R:343:ARG:HD3	1.96	0.48
4:C:613:LEU:HB2	4:C:646:PHE:HE2	1.77	0.48
2:J:413:HIS:O	2:J:417:SER:OG	2.30	0.48
2:J:882:ARG:HB3	2:J:980:ILE:HG21	1.96	0.48
8:O:5:ILE:HG13	8:O:133:GLU:HB3	1.94	0.48
4:E:560:ARG:NE	8:T:292:ASP:OD1	2.42	0.48
8:S:154:LEU:HD23	8:S:194:ARG:HB3	1.96	0.48
8:T:154:LEU:HD23	8:T:194:ARG:HB3	1.96	0.48
8:X:154:LEU:HD23	8:X:194:ARG:HB3	1.96	0.48
3:B:391:ARG:HB2	3:B:396:LEU:HD13	1.95	0.48
3:D:320:VAL:HG12	3:D:425:PRO:HG2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:663:LYS:HE3	8:U:265:ARG:HH12	1.78	0.48
4:G:824:LYS:HA	4:G:827:LYS:HE2	1.95	0.48
3:B:885:HIS:CE1	3:B:892:ARG:HB2	2.48	0.48
3:F:293:ARG:NH1	3:F:371:THR:OG1	2.42	0.48
8:P:154:LEU:HD23	8:P:194:ARG:HB3	1.96	0.48
8:R:80:SER:O	8:R:84:LYS:NZ	2.43	0.48
8:Y:154:LEU:HD23	8:Y:194:ARG:HB3	1.96	0.48
6:c:64:LEU:HD23	6:c:67:ARG:H	1.78	0.48
4:G:542:PRO:HA	4:G:610:LEU:HG	1.96	0.48
8:Q:154:LEU:HD23	8:Q:194:ARG:HB3	1.96	0.48
8:O:47:ARG:HA	4:A:563:THR:HG21	1.95	0.48
8:R:89:GLU:O	8:R:124:ARG:NH2	2.47	0.48
8:V:154:LEU:HD23	8:V:194:ARG:HB3	1.96	0.48
8:V:287:LYS:NZ	8:V:327:GLU:O	2.44	0.48
4:A:478:THR:OG1	4:A:481:GLU:O	2.29	0.48
2:l:21:GLU:HG2	2:l:24:ARG:HH21	1.79	0.47
5:K:649:LEU:HB3	8:Y:341:ARG:HH21	1.78	0.47
4:G:626:LEU:HA	4:G:629:ILE:HG22	1.96	0.47
3:H:494:HIS:CD2	3:H:500:GLN:HA	2.49	0.47
5:K:649:LEU:HD12	5:K:649:LEU:HA	1.64	0.47
8:R:154:LEU:HD23	8:R:194:ARG:HB3	1.96	0.47
8:Y:89:GLU:O	8:Y:124:ARG:NH2	2.47	0.47
8:Z:154:LEU:HD23	8:Z:194:ARG:HB3	1.96	0.47
8:Z:272:GLY:HA3	8:Z:377:MET:HG2	1.97	0.47
3:D:681:ARG:HG2	8:R:258:ALA:HB1	1.96	0.47
8:Q:80:SER:O	8:Q:84:LYS:NZ	2.44	0.47
8:Q:89:GLU:O	8:Q:124:ARG:NH2	2.47	0.47
4:E:674:GLN:HB2	4:E:675:TRP:CE3	2.49	0.47
3:H:677:LEU:HD22	3:H:712:VAL:HA	1.97	0.47
8:R:287:LYS:NZ	8:R:327:GLU:O	2.44	0.47
8:W:272:GLY:HA3	8:W:377:MET:HG2	1.97	0.47
4:C:458:ASN:OD1	4:C:461:ARG:NH2	2.48	0.47
8:X:272:GLY:HA3	8:X:377:MET:HG2	1.97	0.47
1:e:244:ASP:OD2	1:e:246:GLN:NE2	2.46	0.47
3:D:713:HIS:HD2	8:R:355:SER:HB2	1.80	0.47
5:K:512:ALA:HB1	5:K:516:ARG:HH12	1.78	0.47
8:R:272:GLY:HA3	8:R:377:MET:HG2	1.97	0.47
8:V:215:THR:HG22	8:V:221:GLN:HG3	1.97	0.47
8:Y:349:ILE:HG23	8:Y:352:GLY:H	1.80	0.47
3:B:597:LEU:HB3	3:B:623:VAL:HG11	1.96	0.47
4:E:699:PHE:CD2	8:S:358:VAL:HG11	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:848:ARG:HH21	3:F:852:HIS:CE1	2.33	0.47
8:O:80:SER:O	8:O:84:LYS:NZ	2.43	0.47
8:O:215:THR:HG22	8:O:221:GLN:HG3	1.97	0.47
8:O:272:GLY:HA3	8:O:377:MET:HG2	1.97	0.47
8:O:349:ILE:HG23	8:O:352:GLY:H	1.80	0.47
8:P:215:THR:HG22	8:P:221:GLN:HG3	1.97	0.47
8:S:215:THR:HG22	8:S:221:GLN:HG3	1.97	0.47
8:T:215:THR:HG22	8:T:221:GLN:HG3	1.97	0.47
8:U:154:LEU:HD23	8:U:194:ARG:HB3	1.96	0.47
8:U:272:GLY:HA3	8:U:377:MET:HG2	1.97	0.47
8:X:349:ILE:HG23	8:X:352:GLY:H	1.80	0.47
4:E:865:TYR:CE2	8:S:353:PRO:HB3	2.50	0.47
8:W:215:THR:HG22	8:W:221:GLN:HG3	1.97	0.47
8:Y:394:GLN:HA	8:Y:397:LYS:HE2	1.97	0.47
8:Z:300:PRO:HA	8:Z:303:VAL:HG23	1.97	0.47
4:C:394:TRP:HB2	4:C:400:ILE:HG12	1.97	0.47
2:J:814:SER:OG	2:J:815:LEU:N	2.48	0.47
8:R:394:GLN:HA	8:R:397:LYS:HE2	1.97	0.47
8:S:300:PRO:HA	8:S:303:VAL:HG23	1.97	0.47
8:V:272:GLY:HA3	8:V:377:MET:HG2	1.97	0.47
8:W:154:LEU:HD23	8:W:194:ARG:HB3	1.96	0.47
8:Z:349:ILE:HG23	8:Z:352:GLY:H	1.80	0.47
3:B:365:ARG:HB2	3:B:368:LEU:HB3	1.96	0.47
8:P:394:GLN:HA	8:P:397:LYS:HE2	1.97	0.47
8:U:394:GLN:HA	8:U:397:LYS:HE2	1.97	0.47
8:Y:272:GLY:HA3	8:Y:377:MET:HG2	1.97	0.47
3:B:262:ASP:HB2	3:B:267:LYS:HG2	1.96	0.46
4:C:581:ASP:HB2	4:C:643:ARG:HG2	1.98	0.46
3:F:377:ARG:HD3	6:c:145:TYR:CD1	2.49	0.46
2:J:552:LEU:HD13	2:J:559:ILE:HD12	1.97	0.46
8:S:394:GLN:HA	8:S:397:LYS:HE2	1.97	0.46
4:E:509:LEU:HD23	4:E:512:HIS:HD2	1.81	0.46
3:F:274:CYS:SG	3:F:276:LYS:NZ	2.77	0.46
5:K:328:VAL:HA	5:K:331:ARG:HE	1.80	0.46
8:O:154:LEU:HD23	8:O:194:ARG:HB3	1.96	0.46
8:Q:136:VAL:HG23	8:Q:167:GLN:HB3	1.98	0.46
8:Q:349:ILE:HG23	8:Q:352:GLY:H	1.80	0.46
8:S:89:GLU:O	8:S:124:ARG:NH2	2.47	0.46
8:S:272:GLY:HA3	8:S:377:MET:HG2	1.97	0.46
8:T:272:GLY:HA3	8:T:377:MET:HG2	1.97	0.46
8:U:136:VAL:HG23	8:U:167:GLN:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:349:ILE:HG23	8:V:352:GLY:H	1.80	0.46
8:X:136:VAL:HG23	8:X:167:GLN:HB3	1.98	0.46
8:Y:215:THR:HG22	8:Y:221:GLN:HG3	1.97	0.46
3:B:303:LYS:HE3	3:B:303:LYS:HB3	1.76	0.46
6:L:1742:GLN:HG2	6:L:1764:LEU:HG	1.97	0.46
8:T:300:PRO:HA	8:T:303:VAL:HG23	1.97	0.46
8:X:394:GLN:HA	8:X:397:LYS:HE2	1.97	0.46
8:Z:394:GLN:HA	8:Z:397:LYS:HE2	1.97	0.46
4:C:663:LYS:NZ	4:C:674:GLN:O	2.40	0.46
5:I:504:HIS:CD2	8:W:265:ARG:HH12	2.33	0.46
8:R:215:THR:HG22	8:R:221:GLN:HG3	1.97	0.46
8:U:130:ASP:OD2	8:V:295:ARG:NH2	2.48	0.46
8:V:394:GLN:HA	8:V:397:LYS:HE2	1.97	0.46
8:Q:394:GLN:HA	8:Q:397:LYS:HE2	1.97	0.46
8:R:349:ILE:HG23	8:R:352:GLY:H	1.80	0.46
8:S:349:ILE:HG23	8:S:352:GLY:H	1.80	0.46
8:V:80:SER:O	8:V:84:LYS:NZ	2.44	0.46
8:V:89:GLU:O	8:V:124:ARG:NH2	2.47	0.46
4:E:706:TRP:HA	4:E:706:TRP:CE3	2.51	0.46
3:F:474:PHE:HB2	3:F:525:ASP:HA	1.98	0.46
5:K:544:LEU:HD13	5:K:564:PHE:HB2	1.98	0.46
6:L:1575:ALA:HB3	6:L:1597:ARG:HH12	1.80	0.46
8:Q:215:THR:HG22	8:Q:221:GLN:HG3	1.97	0.46
8:Q:300:PRO:HA	8:Q:303:VAL:HG23	1.97	0.46
8:V:300:PRO:HA	8:V:303:VAL:HG23	1.97	0.46
8:Z:215:THR:HG22	8:Z:221:GLN:HG3	1.97	0.46
8:T:56:ASP:O	8:U:296:ARG:NH2	2.49	0.46
8:T:73:VAL:O	8:T:76:SER:OG	2.29	0.46
8:U:215:THR:HG22	8:U:221:GLN:HG3	1.97	0.46
8:U:300:PRO:HA	8:U:303:VAL:HG23	1.97	0.46
8:X:300:PRO:HA	8:X:303:VAL:HG23	1.97	0.46
3:H:456:THR:OG1	3:H:457:ASP:N	2.49	0.46
5:K:646:LEU:HD13	8:Y:341:ARG:CD	2.38	0.46
8:O:385:SER:HB2	8:O:435:TYR:CG	2.51	0.46
8:Q:214:ALA:HA	8:Q:217:ARG:HD3	1.98	0.46
8:S:214:ALA:HA	8:S:217:ARG:HD3	1.98	0.46
8:T:214:ALA:HA	8:T:217:ARG:HD3	1.98	0.46
8:X:385:SER:HB2	8:X:435:TYR:CG	2.51	0.46
4:A:690:VAL:HG12	4:A:752:MET:HE1	1.96	0.46
4:C:553:ALA:HB1	8:R:339:ARG:HA	1.98	0.46
4:C:837:LEU:HD22	4:C:856:ILE:HG13	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:699:PHE:CZ	8:S:333:VAL:HB	2.51	0.46
4:G:353:GLY:HA2	4:G:356:LEU:HD12	1.97	0.46
6:L:1670:LYS:HE3	8:Z:249:MET:HE1	1.98	0.46
8:O:300:PRO:HA	8:O:303:VAL:HG23	1.97	0.46
8:P:385:SER:HB2	8:P:435:TYR:CG	2.51	0.46
8:T:349:ILE:HG23	8:T:352:GLY:H	1.80	0.46
8:U:89:GLU:O	8:U:124:ARG:NH2	2.47	0.46
8:U:349:ILE:HG23	8:U:352:GLY:H	1.80	0.46
3:H:255:LEU:HB3	3:H:343:HIS:CE1	2.51	0.46
6:L:1784:THR:HG22	6:L:1799:LEU:HD22	1.98	0.46
8:P:136:VAL:HG23	8:P:167:GLN:HB3	1.98	0.46
8:R:300:PRO:HA	8:R:303:VAL:HG23	1.97	0.46
8:T:136:VAL:HG23	8:T:167:GLN:HB3	1.98	0.46
8:U:214:ALA:HA	8:U:217:ARG:HD3	1.98	0.46
8:W:349:ILE:HG23	8:W:352:GLY:H	1.80	0.46
6:L:1514:HIS:ND1	6:L:1520:ASP:OD1	2.48	0.45
8:W:385:SER:HB2	8:W:435:TYR:CG	2.51	0.45
8:X:214:ALA:HA	8:X:217:ARG:HD3	1.98	0.45
3:D:455:LYS:HA	3:D:455:LYS:HD2	1.84	0.45
4:E:684:GLN:HB2	8:S:262:PRO:HA	1.99	0.45
3:H:729:CYS:SG	3:H:730:SER:N	2.89	0.45
8:Q:385:SER:HB2	8:Q:435:TYR:CG	2.51	0.45
8:R:136:VAL:HG23	8:R:167:GLN:HB3	1.98	0.45
8:T:394:GLN:HA	8:T:397:LYS:HE2	1.97	0.45
8:W:394:GLN:HA	8:W:397:LYS:HE2	1.97	0.45
7:k:25:MET:HE1	7:k:48:VAL:HG11	1.98	0.45
4:G:537:GLU:HA	4:G:540:ARG:HH21	1.81	0.45
2:J:326:ARG:O	2:J:329:GLU:HG2	2.16	0.45
6:L:348:LYS:HG3	6:L:349:GLU:H	1.82	0.45
8:O:136:VAL:HG23	8:O:167:GLN:HB3	1.98	0.45
8:P:349:ILE:HG23	8:P:352:GLY:H	1.80	0.45
8:V:385:SER:HB2	8:V:435:TYR:CG	2.51	0.45
8:X:215:THR:HG22	8:X:221:GLN:HG3	1.97	0.45
8:Y:136:VAL:HG23	8:Y:167:GLN:HB3	1.98	0.45
8:Z:89:GLU:O	8:Z:124:ARG:NH2	2.47	0.45
4:E:680:PHE:CG	8:S:264:PRO:HD3	2.51	0.45
8:Y:385:SER:HB2	8:Y:435:TYR:CG	2.51	0.45
7:i:66:GLU:HA	7:i:69:LYS:HE2	1.99	0.45
3:H:432:ARG:HH21	3:H:439:LEU:HD12	1.82	0.45
5:K:533:GLN:HA	5:K:536:VAL:HG12	1.98	0.45
5:K:649:LEU:HD11	5:K:655:TYR:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:O:214:ALA:HA	8:O:217:ARG:HD3	1.98	0.45
8:P:272:GLY:HA3	8:P:377:MET:HG2	1.97	0.45
8:W:136:VAL:HG23	8:W:167:GLN:HB3	1.98	0.45
3:j:61:GLU:HG3	3:j:64:ARG:HH21	1.81	0.45
7:d:62:SER:OG	6:c:48:ASN:ND2	2.49	0.45
3:B:885:HIS:ND1	8:P:353:PRO:HB3	2.32	0.45
4:G:560:ARG:HD2	4:G:565:ASN:ND2	2.31	0.45
5:I:526:ASP:O	5:I:530:TYR:HB2	2.16	0.45
2:J:242:LEU:HB3	2:J:304:HIS:HA	1.97	0.45
8:S:56:ASP:HB2	8:T:276:LEU:HB2	1.98	0.45
8:W:187:ASN:O	8:W:191:THR:OG1	2.30	0.45
8:Z:136:VAL:HG23	8:Z:167:GLN:HB3	1.98	0.45
4:A:341:LEU:HD13	4:A:359:LEU:HD22	1.98	0.45
3:D:549:LEU:HD13	3:D:555:LEU:HD13	1.99	0.45
4:E:463:CYS:SG	4:E:464:GLY:N	2.90	0.45
3:H:675:TYR:HA	3:H:678:THR:HG22	1.99	0.45
2:J:881:HIS:CG	8:X:446:TRP:HE1	2.35	0.45
8:T:80:SER:O	8:T:84:LYS:NZ	2.43	0.45
8:X:89:GLU:O	8:X:124:ARG:NH2	2.47	0.45
8:Y:300:PRO:HA	8:Y:303:VAL:HG23	1.97	0.45
7:k:42:GLU:O	7:k:45:SER:OG	2.32	0.45
4:C:713:LEU:HD22	4:C:722:VAL:HG13	1.99	0.45
4:C:860:ASP:HA	4:C:864:PHE:HD2	1.82	0.45
4:G:302:GLU:HA	4:G:305:ILE:HD12	1.99	0.45
8:Q:272:GLY:HA3	8:Q:377:MET:HG2	1.97	0.45
8:S:136:VAL:HG23	8:S:167:GLN:HB3	1.98	0.45
8:V:136:VAL:HG23	8:V:167:GLN:HB3	1.98	0.45
8:Z:385:SER:HB2	8:Z:435:TYR:CG	2.51	0.45
3:H:599:GLY:C	8:W:342:GLU:HG3	2.42	0.45
5:K:646:LEU:HB2	8:Y:337:LEU:HD23	1.98	0.45
8:R:214:ALA:HA	8:R:217:ARG:HD3	1.98	0.45
8:S:385:SER:HB2	8:S:435:TYR:CG	2.51	0.45
8:W:214:ALA:HA	8:W:217:ARG:HD3	1.98	0.45
8:W:300:PRO:HA	8:W:303:VAL:HG23	1.97	0.45
8:Y:214:ALA:HA	8:Y:217:ARG:HD3	1.98	0.45
1:e:147:ARG:HD2	1:e:296:ASN:HB3	1.99	0.45
3:B:369:VAL:HG13	4:A:304:LEU:HB3	1.97	0.45
6:L:392:SER:O	6:L:395:SER:OG	2.35	0.45
8:O:394:GLN:HA	8:O:397:LYS:HE2	1.97	0.45
8:R:385:SER:HB2	8:R:435:TYR:CG	2.51	0.45
3:a:33:GLN:OE1	6:c:67:ARG:NH2	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:l:120:SER:HA	7:m:36:ASN:HD22	1.81	0.44
4:E:508:GLU:HG3	4:E:511:ALA:H	1.82	0.44
8:P:214:ALA:HA	8:P:217:ARG:HD3	1.98	0.44
8:T:385:SER:HB2	8:T:435:TYR:CG	2.51	0.44
4:E:833:LEU:HD21	8:S:353:PRO:HG3	2.00	0.44
5:I:7:LEU:HD23	5:I:7:LEU:HA	1.83	0.44
6:L:346:LEU:HD13	6:L:346:LEU:HA	1.84	0.44
6:L:568:TYR:CE2	6:L:600:LYS:HE2	2.52	0.44
8:P:300:PRO:HA	8:P:303:VAL:HG23	1.97	0.44
8:V:214:ALA:HA	8:V:217:ARG:HD3	1.98	0.44
4:A:654:GLN:HB3	4:A:759:THR:HG21	1.99	0.44
3:D:320:VAL:HG22	3:D:445:GLU:HG3	1.99	0.44
4:E:306:LEU:HD12	4:E:309:GLN:HE21	1.83	0.44
4:E:864:PHE:HB2	8:S:348:PHE:O	2.17	0.44
3:F:494:HIS:HD2	3:F:500:GLN:HG3	1.82	0.44
8:S:57:ASP:HB2	8:S:59:HIS:HB2	2.00	0.44
8:U:361:SER:OG	8:U:362:ARG:N	2.51	0.44
3:a:34:TYR:O	3:a:38:VAL:HG12	2.17	0.44
1:e:163:VAL:HG13	1:e:175:ILE:HG12	1.99	0.44
3:B:589:ALA:HB1	3:B:625:LEU:HD11	1.99	0.44
3:F:689:LYS:NZ	8:T:158:ASN:HD21	2.14	0.44
6:L:1483:PRO:O	6:L:1487:HIS:ND1	2.49	0.44
8:U:385:SER:HB2	8:U:435:TYR:CG	2.51	0.44
8:V:57:ASP:HB2	8:V:59:HIS:HB2	2.00	0.44
8:W:361:SER:OG	8:W:362:ARG:N	2.51	0.44
8:X:335:LYS:HD3	8:X:335:LYS:HA	1.79	0.44
8:Z:361:SER:OG	8:Z:362:ARG:N	2.51	0.44
4:C:864:PHE:CG	8:Q:353:PRO:HA	2.53	0.44
3:D:623:VAL:HG13	3:D:639:SER:H	1.83	0.44
8:Q:361:SER:OG	8:Q:362:ARG:N	2.51	0.44
8:T:57:ASP:HB2	8:T:59:HIS:HB2	2.00	0.44
8:V:361:SER:OG	8:V:362:ARG:N	2.51	0.44
4:E:566:THR:HG23	8:S:45:THR:HG23	1.99	0.44
3:H:810:LYS:HA	3:H:810:LYS:HD2	1.90	0.44
7:b:39:LEU:HD11	3:a:100:LEU:HD12	1.99	0.44
4:A:412:HIS:CE1	4:A:433:THR:HB	2.53	0.44
3:D:727:LEU:HD12	3:D:728:GLU:HG3	1.99	0.44
3:F:581:LEU:HG	3:F:585:LEU:HG	1.99	0.44
4:G:468:THR:OG1	4:G:469:CYS:N	2.50	0.44
8:P:73:VAL:O	8:P:76:SER:OG	2.29	0.44
8:Q:153:LEU:HD12	8:Q:153:LEU:HA	1.90	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Q:335:LYS:HD3	8:Q:335:LYS:HA	1.79	0.44
8:V:335:LYS:HD3	8:V:335:LYS:HA	1.79	0.44
8:X:57:ASP:HB2	8:X:59:HIS:HB2	2.00	0.44
3:D:801:GLN:O	3:D:805:GLN:NE2	2.51	0.44
2:J:736:TYR:HE2	8:X:3:ARG:HG3	1.83	0.44
8:R:187:ASN:O	8:R:191:THR:OG1	2.30	0.44
8:X:73:VAL:O	8:X:76:SER:OG	2.29	0.44
4:A:442:PHE:HB2	4:A:484:TYR:CZ	2.53	0.44
3:H:337:ARG:HB2	5:I:124:TYR:CZ	2.53	0.44
5:K:253:SER:OG	5:K:288:ASN:OD1	2.30	0.44
5:K:649:LEU:HD11	5:K:655:TYR:N	2.33	0.44
8:U:80:SER:O	8:U:84:LYS:NZ	2.43	0.44
8:X:361:SER:OG	8:X:362:ARG:N	2.51	0.44
8:Y:57:ASP:HB2	8:Y:59:HIS:HB2	2.00	0.44
8:Z:214:ALA:HA	8:Z:217:ARG:HD3	1.98	0.44
1:e:269:MET:HE2	1:e:269:MET:HB3	1.83	0.43
3:B:590:THR:HA	3:B:628:VAL:HG13	1.99	0.43
4:E:457:LEU:HD22	4:E:467:VAL:HB	2.00	0.43
4:G:201:THR:OG1	4:G:202:ALA:N	2.51	0.43
3:H:860:GLN:HA	3:H:863:VAL:HG12	2.00	0.43
8:P:361:SER:OG	8:P:362:ARG:N	2.51	0.43
4:E:344:SER:HA	4:E:347:LYS:HD3	2.00	0.43
4:E:685:ARG:HB3	4:E:829:PHE:CE2	2.53	0.43
3:H:341:VAL:HG22	3:a:76:GLU:HG2	2.00	0.43
8:R:57:ASP:HB2	8:R:59:HIS:HB2	2.00	0.43
1:e:314:GLN:HA	1:e:329:ILE:HD13	1.99	0.43
3:B:885:HIS:CG	8:P:353:PRO:HB3	2.53	0.43
4:E:684:GLN:CD	8:S:262:PRO:HB3	2.43	0.43
3:H:364:LEU:HD23	3:H:364:LEU:HA	1.90	0.43
2:J:490:ARG:HB3	2:J:492:PHE:H	1.83	0.43
5:K:654:TYR:HA	5:K:657:GLN:HE21	1.83	0.43
8:T:89:GLU:O	8:T:124:ARG:NH2	2.47	0.43
8:Z:389:GLU:HA	8:Z:392:CYS:HB2	2.01	0.43
7:i:67:LEU:HD23	3:h:31:GLN:HE21	1.83	0.43
3:B:379:LYS:HD2	3:B:379:LYS:HA	1.63	0.43
3:B:625:LEU:HD12	3:B:626:LEU:H	1.83	0.43
3:D:692:ARG:NH1	8:R:197:GLN:OE1	2.52	0.43
8:O:361:SER:OG	8:O:362:ARG:N	2.51	0.43
8:R:361:SER:OG	8:R:362:ARG:N	2.51	0.43
8:S:389:GLU:HA	8:S:392:CYS:HB2	2.01	0.43
8:Y:389:GLU:HA	8:Y:392:CYS:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Z:348:PHE:HD1	8:Z:348:PHE:HA	1.66	0.43
2:l:113:LEU:HD21	7:m:60:LEU:HB2	2.00	0.43
3:D:628:VAL:HG21	3:h:57:LYS:HB3	1.99	0.43
3:F:776:ARG:HH21	3:j:105:ARG:HH21	1.66	0.43
4:G:559:LEU:HD21	4:G:570:LYS:HB2	1.99	0.43
4:G:840:LEU:HD21	4:G:855:VAL:HG22	1.99	0.43
5:K:647:LEU:HD23	8:Y:356:ILE:O	2.19	0.43
8:P:89:GLU:O	8:P:124:ARG:NH2	2.47	0.43
8:Q:89:GLU:HB2	8:R:216:ASP:CG	2.44	0.43
8:R:313:THR:OG1	8:R:314:ASN:N	2.52	0.43
8:U:313:THR:OG1	8:U:314:ASN:N	2.52	0.43
8:Z:313:THR:OG1	8:Z:314:ASN:N	2.52	0.43
7:m:50:LEU:HD13	7:m:60:LEU:HD22	2.00	0.43
3:a:10:ASN:OD1	3:a:11:VAL:N	2.51	0.43
4:E:553:ALA:HB1	8:T:339:ARG:HA	2.01	0.43
3:F:707:LEU:HD13	3:F:851:THR:HG23	2.00	0.43
3:F:856:GLY:HA2	3:F:859:GLN:HE21	1.84	0.43
5:I:12:TYR:CG	2:J:313:VAL:HG22	2.53	0.43
6:L:1679:GLN:HA	6:L:1683:VAL:HG22	2.00	0.43
8:Q:57:ASP:HB2	8:Q:59:HIS:HB2	2.00	0.43
8:W:57:ASP:HB2	8:W:59:HIS:HB2	2.00	0.43
8:Y:361:SER:OG	8:Y:362:ARG:N	2.51	0.43
4:C:289:ASN:HA	4:C:292:LEU:HB3	2.00	0.43
3:D:394:GLY:O	3:D:398:SER:OG	2.32	0.43
4:E:215:SER:O	4:E:314:HIS:NE2	2.51	0.43
3:F:665:ASN:HB2	3:j:66:ARG:HD3	2.00	0.43
2:J:362:GLN:HE21	5:K:165:LEU:HG	1.83	0.43
8:O:389:GLU:HA	8:O:392:CYS:HB2	2.00	0.43
8:P:57:ASP:HB2	8:P:59:HIS:HB2	2.00	0.43
8:Q:187:ASN:O	8:Q:191:THR:OG1	2.30	0.43
8:S:361:SER:OG	8:S:362:ARG:N	2.51	0.43
8:T:313:THR:OG1	8:T:314:ASN:N	2.52	0.43
8:T:389:GLU:HA	8:T:392:CYS:HB2	2.01	0.43
8:U:57:ASP:HB2	8:U:59:HIS:HB2	2.00	0.43
8:Z:57:ASP:HB2	8:Z:59:HIS:HB2	2.00	0.43
4:E:635:LEU:HA	4:E:638:TYR:HB2	2.01	0.43
5:I:507:SER:O	5:I:507:SER:OG	2.30	0.43
5:K:76:GLN:O	5:K:200:HIS:ND1	2.51	0.43
8:W:313:THR:OG1	8:W:314:ASN:N	2.52	0.43
6:c:82:LEU:HD12	6:c:85:LYS:HD2	2.00	0.43
1:e:25:ASP:N	1:e:25:ASP:OD1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:l:119:ASP:H	3:H:630:PRO:HB3	1.84	0.43
4:E:482:ARG:HD3	4:E:485:VAL:HG21	2.01	0.43
3:F:262:ASP:O	4:G:255:SER:OG	2.34	0.43
4:G:538:GLU:HG3	4:G:546:ILE:HG22	2.01	0.43
5:I:368:LEU:HD11	5:I:400:ALA:HB2	1.99	0.43
7:b:42:GLU:O	7:b:45:SER:OG	2.30	0.43
8:P:68:ASP:OD1	8:P:68:ASP:N	2.52	0.43
8:T:361:SER:OG	8:T:362:ARG:N	2.51	0.43
8:V:313:THR:OG1	8:V:314:ASN:N	2.52	0.43
1:e:78:ASN:HB3	1:e:81:ASP:HB2	1.99	0.43
3:B:788:ALA:O	3:B:792:ILE:HG12	2.19	0.43
3:F:597:LEU:HD23	3:F:638:PHE:HD1	1.84	0.43
8:U:68:ASP:OD1	8:U:68:ASP:N	2.52	0.43
8:W:389:GLU:HA	8:W:392:CYS:HB2	2.00	0.43
4:C:429:ASP:OD1	4:C:429:ASP:N	2.49	0.42
4:C:557:LEU:HD11	8:R:295:ARG:CZ	2.48	0.42
3:H:581:LEU:HG	3:H:585:LEU:HG	2.01	0.42
8:Q:128:GLY:O	8:R:299:GLN:NE2	2.51	0.42
8:Q:156:ARG:NH2	8:Q:159:ASP:OD2	2.41	0.42
8:Q:313:THR:OG1	8:Q:314:ASN:N	2.52	0.42
8:R:389:GLU:HA	8:R:392:CYS:HB2	2.01	0.42
8:S:56:ASP:OD2	8:T:302:ASN:ND2	2.48	0.42
8:U:389:GLU:HA	8:U:392:CYS:HB2	2.01	0.42
3:j:72:ALA:O	3:j:75:SER:OG	2.37	0.42
4:C:762:MET:HG3	4:C:825:PHE:HE2	1.84	0.42
5:K:331:ARG:O	5:K:334:SER:OG	2.34	0.42
8:Q:389:GLU:HA	8:Q:392:CYS:HB2	2.01	0.42
8:S:313:THR:OG1	8:S:314:ASN:N	2.52	0.42
8:Y:56:ASP:CG	8:Z:299:GLN:NE2	2.78	0.42
6:c:45:LEU:O	6:c:48:ASN:ND2	2.52	0.42
3:D:721:TYR:OH	3:D:872:SER:O	2.33	0.42
4:E:241:ARG:HH21	4:E:242:GLN:HG2	1.83	0.42
5:I:301:LYS:O	5:I:304:GLU:HB3	2.20	0.42
5:K:639:ASN:HB3	8:Y:334:HIS:NE2	2.34	0.42
8:O:57:ASP:HB2	8:O:59:HIS:HB2	2.00	0.42
8:P:313:THR:OG1	8:P:314:ASN:N	2.52	0.42
8:Y:313:THR:OG1	8:Y:314:ASN:N	2.52	0.42
3:B:674:GLU:HB2	3:B:719:GLN:NE2	2.34	0.42
3:D:581:LEU:HG	3:D:585:LEU:HG	2.02	0.42
4:E:578:MET:HE2	4:E:643:ARG:HG3	2.01	0.42
4:G:164:LYS:HA	4:G:167:LYS:HG2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:b:27:VAL:HG13	3:a:77:LEU:HD22	2.01	0.42
8:O:73:VAL:O	8:O:76:SER:OG	2.30	0.42
8:P:389:GLU:HA	8:P:392:CYS:HB2	2.01	0.42
4:E:221:LEU:HD23	4:E:233:VAL:HG11	2.00	0.42
8:V:389:GLU:HA	8:V:392:CYS:HB2	2.01	0.42
3:a:57:LYS:NZ	3:a:119:ALA:H	2.18	0.42
4:A:446:MET:HG3	4:A:449:LYS:HD2	2.02	0.42
3:B:538:TYR:O	3:B:542:SER:OG	2.37	0.42
4:E:188:ILE:HG22	4:E:190:ASP:H	1.84	0.42
4:E:701:VAL:HG11	4:E:736:ASP:CB	2.50	0.42
4:E:702:MET:HB3	4:E:703:GLU:H	1.60	0.42
4:E:705:THR:O	4:E:706:TRP:C	2.63	0.42
3:F:662:ARG:HE	3:j:66:ARG:HH21	1.65	0.42
5:I:530:TYR:HE1	8:W:249:MET:SD	2.42	0.42
8:W:153:LEU:HD12	8:W:153:LEU:HA	1.90	0.42
8:X:389:GLU:HA	8:X:392:CYS:HB2	2.00	0.42
8:Z:73:VAL:O	8:Z:76:SER:OG	2.29	0.42
1:e:172:PRO:HB3	1:e:375:PHE:CZ	2.54	0.42
4:C:184:ARG:HE	4:C:184:ARG:HB2	1.24	0.42
3:D:286:SER:OG	3:D:287:LEU:N	2.51	0.42
4:E:152:GLN:HE22	4:E:156:LEU:HD21	1.84	0.42
5:K:499:GLN:HB3	5:K:516:ARG:HG3	2.01	0.42
8:O:89:GLU:O	8:O:124:ARG:NH2	2.47	0.42
8:W:80:SER:O	8:W:84:LYS:NZ	2.43	0.42
8:W:89:GLU:O	8:W:124:ARG:NH2	2.47	0.42
4:C:580:HIS:N	4:C:643:ARG:HH22	2.18	0.42
4:E:446:MET:SD	4:E:446:MET:N	2.92	0.42
5:I:404:LEU:HB3	5:I:405:LEU:H	1.52	0.42
8:R:68:ASP:OD1	8:R:68:ASP:N	2.52	0.42
8:R:242:THR:HG23	8:R:243:LEU:HD12	2.02	0.42
8:S:153:LEU:HD12	8:S:153:LEU:HA	1.90	0.42
8:U:242:THR:HG23	8:U:243:LEU:HD12	2.02	0.42
8:W:68:ASP:N	8:W:68:ASP:OD1	2.52	0.42
3:B:589:ALA:H	3:B:633:THR:HA	1.85	0.42
4:C:819:GLU:O	4:C:822:ILE:HB	2.20	0.42
3:D:324:PHE:O	3:D:328:LEU:HG	2.19	0.42
4:E:161:LEU:O	4:E:165:GLN:HG2	2.19	0.42
4:E:658:VAL:HG21	4:E:759:THR:HB	2.02	0.42
5:I:4:GLU:HB3	2:J:242:LEU:HD11	2.02	0.42
2:J:437:LEU:HD21	2:J:469:VAL:HG12	2.02	0.42
6:L:317:ARG:H	6:L:320:PHE:HB3	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:1534:LYS:HD3	6:L:1544:LEU:HD21	2.00	0.42
6:L:1638:PHE:HA	6:L:1641:LYS:HD2	2.02	0.42
8:O:313:THR:OG1	8:O:314:ASN:N	2.52	0.42
8:V:73:VAL:O	8:V:76:SER:OG	2.29	0.42
8:W:54:GLN:HE21	8:X:295:ARG:NH1	2.18	0.42
8:X:68:ASP:OD1	8:X:68:ASP:N	2.52	0.42
8:X:242:THR:HG23	8:X:243:LEU:HD12	2.02	0.42
8:Z:242:THR:HG23	8:Z:243:LEU:HD12	2.02	0.42
4:E:639:GLN:O	4:E:643:ARG:HG2	2.19	0.42
3:F:776:ARG:O	3:F:780:ASP:N	2.52	0.42
3:F:854:TYR:HA	3:F:857:ILE:HG22	2.01	0.42
2:J:254:ASP:OD1	2:J:256:LEU:HB2	2.20	0.42
7:b:18:LEU:HA	7:b:21:VAL:HG12	2.01	0.42
8:U:276:LEU:HD23	8:U:276:LEU:HA	1.93	0.42
8:X:153:LEU:HD12	8:X:153:LEU:HA	1.90	0.42
8:Y:36:ILE:HA	8:Y:59:HIS:HA	2.02	0.42
3:h:13:LEU:HD11	3:h:39:ILE:HG21	2.02	0.42
4:C:287:GLN:HE21	3:D:406:THR:C	2.28	0.41
4:C:735:LYS:HA	4:C:735:LYS:HD3	1.86	0.41
3:F:449:ALA:HB3	3:F:465:THR:HB	2.02	0.41
6:L:1550:LEU:HA	6:L:1553:VAL:HG22	2.02	0.41
8:O:242:THR:HG23	8:O:243:LEU:HD12	2.02	0.41
8:S:68:ASP:OD1	8:S:68:ASP:N	2.52	0.41
4:A:526:ASP:HA	4:A:529:VAL:HG12	2.02	0.41
6:c:16:LEU:HD12	6:c:17:PRO:HD2	2.01	0.41
1:e:147:ARG:CD	1:e:296:ASN:HB3	2.50	0.41
1:e:180:LEU:HD23	1:e:180:LEU:HA	1.85	0.41
3:B:247:GLU:HA	3:B:366:ARG:HE	1.85	0.41
8:R:348:PHE:HD1	8:R:348:PHE:HA	1.66	0.41
3:D:785:LEU:O	3:D:789:GLN:HG3	2.19	0.41
4:E:521:LEU:C	8:S:248:TYR:HE2	2.28	0.41
4:E:868:ARG:NH2	8:S:444:ILE:HG12	2.35	0.41
4:G:241:ARG:NE	4:G:243:SER:OG	2.53	0.41
3:H:763:LEU:HD23	3:H:775:LEU:HD22	2.01	0.41
2:J:309:CYS:O	2:J:313:VAL:HG23	2.20	0.41
6:L:1732:ILE:HG23	6:L:1772:PHE:HE1	1.85	0.41
8:T:36:ILE:HA	8:T:59:HIS:HA	2.02	0.41
8:W:242:THR:HG23	8:W:243:LEU:HD12	2.02	0.41
7:i:59:ALA:HB1	3:h:39:ILE:HD13	2.02	0.41
3:a:74:PHE:HA	3:a:77:LEU:HD12	2.02	0.41
4:A:446:MET:HE2	4:A:446:MET:HB2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:311:ARG:HB3	3:B:317:PHE:CD2	2.56	0.41
3:H:251:VAL:HG11	3:H:362:LEU:N	2.34	0.41
5:K:150:GLY:O	5:K:153:ILE:HD12	2.20	0.41
8:Q:243:LEU:HG	8:Q:251:ASN:HA	2.03	0.41
8:W:30:GLY:HA3	8:W:41:ALA:HA	2.03	0.41
8:X:313:THR:OG1	8:X:314:ASN:N	2.52	0.41
8:Y:68:ASP:N	8:Y:68:ASP:OD1	2.52	0.41
8:Y:242:THR:HG23	8:Y:243:LEU:HD12	2.02	0.41
8:Z:36:ILE:HA	8:Z:59:HIS:HA	2.02	0.41
7:i:53:GLN:HE21	3:h:9:PRO:HG3	1.84	0.41
4:A:277:ILE:HA	4:A:293:ALA:HB1	2.02	0.41
4:A:550:ARG:H	4:A:550:ARG:HG2	1.71	0.41
4:E:352:GLY:HA3	4:E:406:GLU:HB2	2.03	0.41
4:E:527:PHE:O	4:E:531:PHE:HB2	2.20	0.41
3:F:601:LEU:O	3:F:605:VAL:HG23	2.20	0.41
3:H:337:ARG:NH1	3:a:68:GLU:OE2	2.52	0.41
3:H:338:LEU:O	3:H:342:LEU:HG	2.20	0.41
8:Y:243:LEU:HG	8:Y:251:ASN:HA	2.03	0.41
8:Z:30:GLY:HA3	8:Z:41:ALA:HA	2.03	0.41
4:A:837:LEU:O	4:A:841:SER:OG	2.32	0.41
3:B:663:VAL:O	3:B:667:LEU:HG	2.20	0.41
3:D:810:LYS:HA	3:D:810:LYS:HD2	1.85	0.41
2:J:476:VAL:O	2:J:480:ILE:HG12	2.20	0.41
6:L:1677:ALA:HA	6:L:1681:LEU:HD12	2.03	0.41
8:O:243:LEU:HG	8:O:251:ASN:HA	2.03	0.41
8:P:276:LEU:HD23	8:P:276:LEU:HA	1.94	0.41
8:T:30:GLY:HA3	8:T:41:ALA:HA	2.03	0.41
8:U:30:GLY:HA3	8:U:41:ALA:HA	2.03	0.41
8:X:36:ILE:HA	8:X:59:HIS:HA	2.02	0.41
7:i:15:ALA:HA	7:i:18:LEU:HG	2.02	0.41
3:D:613:ASP:HB3	3:D:617:ILE:HD11	2.03	0.41
4:E:335:MET:HE3	4:E:338:LEU:HB2	2.01	0.41
4:E:700:GLU:CA	8:S:334:HIS:HB3	2.45	0.41
4:G:868:ARG:HH11	4:G:868:ARG:HD2	1.72	0.41
5:K:650:ASP:OD2	8:Y:341:ARG:HA	2.21	0.41
8:S:30:GLY:HA3	8:S:41:ALA:HA	2.03	0.41
8:Y:30:GLY:HA3	8:Y:41:ALA:HA	2.03	0.41
1:e:201:THR:HG23	1:e:202:THR:HG22	2.02	0.41
3:B:284:SER:HB3	3:B:288:ARG:HE	1.85	0.41
3:B:367:LEU:HA	3:B:370:TRP:CD1	2.56	0.41
3:D:380:THR:HG23	3:D:411:MET:HE2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:237:PRO:HA	4:E:244:ARG:NH1	2.36	0.41
3:F:382:ALA:HA	3:F:385:VAL:HG12	2.03	0.41
2:J:494:ILE:HG13	2:J:556:LEU:HD11	2.03	0.41
5:K:365:ARG:HB3	5:K:368:LEU:HG	2.02	0.41
8:O:30:GLY:HA3	8:O:41:ALA:HA	2.03	0.41
8:O:62:PRO:HD2	8:O:86:TYR:HB3	2.03	0.41
8:O:68:ASP:N	8:O:68:ASP:OD1	2.52	0.41
8:P:243:LEU:HG	8:P:251:ASN:HA	2.03	0.41
8:Q:30:GLY:HA3	8:Q:41:ALA:HA	2.03	0.41
8:R:105:ALA:O	8:R:109:SER:OG	2.38	0.41
8:R:156:ARG:NH2	8:R:159:ASP:OD2	2.41	0.41
8:S:242:THR:HG23	8:S:243:LEU:HD12	2.02	0.41
8:U:36:ILE:HA	8:U:59:HIS:HA	2.02	0.41
8:U:105:ALA:O	8:U:109:SER:OG	2.38	0.41
8:V:57:ASP:OD1	8:V:57:ASP:N	2.54	0.41
8:W:36:ILE:HA	8:W:59:HIS:HA	2.02	0.41
8:W:243:LEU:HG	8:W:251:ASN:HA	2.03	0.41
8:Y:62:PRO:HD2	8:Y:86:TYR:HB3	2.03	0.41
7:d:28:LEU:HD23	7:d:31:ILE:HD11	2.03	0.41
4:C:310:LEU:HD23	4:C:310:LEU:HA	1.83	0.41
4:E:522:MET:HB2	8:S:248:TYR:CZ	2.55	0.41
4:E:861:PHE:HE1	8:S:341:ARG:HA	1.86	0.41
3:H:333:ARG:HG2	5:I:124:TYR:CE1	2.56	0.41
3:H:730:SER:O	3:H:733:GLU:HG2	2.21	0.41
5:K:645:LEU:HB2	5:K:646:LEU:HD23	2.02	0.41
7:b:59:ALA:O	7:b:63:VAL:HG13	2.21	0.41
8:O:329:ASP:HA	8:O:330:PRO:HD3	1.90	0.41
8:P:153:LEU:HD12	8:P:153:LEU:HA	1.90	0.41
8:Q:242:THR:HG23	8:Q:243:LEU:HD12	2.02	0.41
8:R:30:GLY:HA3	8:R:41:ALA:HA	2.03	0.41
8:R:36:ILE:HA	8:R:59:HIS:HA	2.02	0.41
8:R:153:LEU:O	8:R:157:LEU:HG	2.21	0.41
8:S:36:ILE:HA	8:S:59:HIS:HA	2.03	0.41
8:S:335:LYS:HD3	8:S:335:LYS:HA	1.79	0.41
8:T:62:PRO:HD2	8:T:86:TYR:HB3	2.03	0.41
8:T:242:THR:HG23	8:T:243:LEU:HD12	2.02	0.41
8:U:62:PRO:HD2	8:U:86:TYR:HB3	2.03	0.41
8:V:243:LEU:HG	8:V:251:ASN:HA	2.03	0.41
8:W:335:LYS:HA	8:W:335:LYS:HD3	1.79	0.41
8:Y:335:LYS:HD3	8:Y:335:LYS:HA	1.79	0.41
8:Z:68:ASP:OD1	8:Z:68:ASP:N	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:292:LEU:HD13	4:A:359:LEU:HD11	2.02	0.41
4:C:208:LEU:HB3	4:C:212:SER:OG	2.21	0.41
3:D:849:ILE:HA	3:D:852:HIS:HB2	2.02	0.41
6:L:1685:TRP:HD1	6:L:1689:ARG:HH21	1.68	0.41
8:P:36:ILE:HA	8:P:59:HIS:HA	2.02	0.41
8:P:242:THR:HG23	8:P:243:LEU:HD12	2.02	0.41
8:Q:172:PHE:HE1	8:Q:174:ASN:HD22	1.69	0.41
8:T:243:LEU:HG	8:T:251:ASN:HA	2.03	0.41
8:W:73:VAL:O	8:W:76:SER:OG	2.29	0.41
8:X:30:GLY:HA3	8:X:41:ALA:HA	2.03	0.41
7:k:18:LEU:HA	7:k:21:VAL:HG12	2.03	0.41
3:D:266:ILE:HG22	3:D:275:TYR:HB3	2.02	0.40
3:D:393:GLY:HA2	3:D:445:GLU:HB3	2.03	0.40
4:E:310:LEU:HD11	4:E:327:TYR:CD2	2.56	0.40
4:E:663:LYS:HB3	4:E:675:TRP:HE1	1.86	0.40
4:E:824:LYS:HE2	4:E:824:LYS:HB2	1.98	0.40
4:G:557:LEU:HD22	8:V:343:ARG:HB2	2.03	0.40
8:O:36:ILE:HA	8:O:59:HIS:HA	2.02	0.40
8:V:36:ILE:HA	8:V:59:HIS:HA	2.02	0.40
1:e:296:ASN:HA	1:e:328:LYS:O	2.20	0.40
4:C:644:HIS:CD2	4:C:697:MET:HE1	2.56	0.40
3:D:554:SER:HB3	3:D:558:HIS:CE1	2.56	0.40
3:D:834:GLY:HA2	3:D:837:LYS:HG2	2.04	0.40
4:E:701:VAL:HG11	4:E:736:ASP:HB3	2.03	0.40
4:G:764:LYS:HG2	4:G:767:GLN:HE21	1.86	0.40
2:J:484:HIS:HA	2:J:496:ARG:HH12	1.85	0.40
8:P:335:LYS:HD3	8:P:335:LYS:HA	1.79	0.40
8:Q:36:ILE:HA	8:Q:59:HIS:HA	2.02	0.40
8:V:68:ASP:OD1	8:V:68:ASP:N	2.52	0.40
8:Z:153:LEU:O	8:Z:157:LEU:HG	2.21	0.40
3:D:311:ARG:HB3	3:D:317:PHE:CD2	2.56	0.40
3:D:833:ILE:O	3:D:836:PHE:HB2	2.21	0.40
4:E:226:VAL:HG23	4:E:228:VAL:HG23	2.04	0.40
3:F:494:HIS:CD2	3:F:500:GLN:HG3	2.56	0.40
4:G:716:ALA:HB2	4:G:725:HIS:HE1	1.86	0.40
2:J:283:LYS:HD2	2:J:283:LYS:HA	1.90	0.40
5:K:528:LEU:HD21	5:K:647:LEU:HD22	2.04	0.40
6:L:353:VAL:HA	6:L:356:VAL:HG12	2.03	0.40
8:Q:57:ASP:OD1	8:Q:57:ASP:N	2.54	0.40
8:R:62:PRO:HD2	8:R:86:TYR:HB3	2.03	0.40
8:R:297:LEU:HD12	8:R:302:ASN:HB3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:S:276:LEU:HD23	8:S:276:LEU:HA	1.94	0.40
8:T:172:PHE:HE1	8:T:174:ASN:HD22	1.69	0.40
8:T:297:LEU:HD12	8:T:302:ASN:HB3	2.04	0.40
8:U:297:LEU:HD12	8:U:302:ASN:HB3	2.04	0.40
8:V:242:THR:HG23	8:V:243:LEU:HD12	2.02	0.40
3:a:14:GLN:HG3	3:a:25:GLU:HG3	2.03	0.40
4:C:320:SER:OG	4:C:321:LEU:N	2.54	0.40
3:D:493:LEU:HD22	3:D:548:VAL:HG11	2.03	0.40
4:E:559:LEU:HD21	4:E:570:LYS:HD2	2.03	0.40
4:G:341:LEU:HD11	4:G:359:LEU:HD13	2.02	0.40
2:J:377:GLU:HB2	5:K:124:TYR:CE1	2.56	0.40
2:J:736:TYR:CZ	8:X:252:ASP:HB3	2.56	0.40
8:S:153:LEU:O	8:S:157:LEU:HG	2.21	0.40
8:T:68:ASP:N	8:T:68:ASP:OD1	2.52	0.40
8:T:153:LEU:O	8:T:157:LEU:HG	2.21	0.40
8:V:349:ILE:HD12	8:V:349:ILE:HA	2.01	0.40
8:X:243:LEU:HG	8:X:251:ASN:HA	2.03	0.40
8:X:348:PHE:HD1	8:X:348:PHE:HA	1.66	0.40
3:f:57:LYS:HB3	3:f:57:LYS:HE2	1.82	0.40
4:C:663:LYS:HG2	8:Q:264:PRO:CG	2.46	0.40
3:F:543:LYS:HD2	3:F:543:LYS:HA	1.76	0.40
3:F:587:ARG:NH1	3:F:588:PRO:O	2.54	0.40
3:H:655:GLU:O	3:H:658:SER:OG	2.40	0.40
6:L:393:ILE:O	6:L:397:LEU:HB2	2.21	0.40
6:L:1670:LYS:HB3	6:L:1670:LYS:HE2	1.95	0.40
8:O:297:LEU:HD12	8:O:302:ASN:HB3	2.04	0.40
8:S:243:LEU:HG	8:S:251:ASN:HA	2.03	0.40
8:U:153:LEU:O	8:U:157:LEU:HG	2.21	0.40
8:W:172:PHE:HE1	8:W:174:ASN:HD22	1.69	0.40
8:X:297:LEU:HD12	8:X:302:ASN:HB3	2.04	0.40
8:Z:172:PHE:HE1	8:Z:174:ASN:HD22	1.69	0.40
7:k:46:ILE:HG21	3:j:16:LEU:HB2	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	e	360/375 (96%)	341 (95%)	19 (5%)	0	100	100
2	J	506/1024 (49%)	465 (92%)	38 (8%)	3 (1%)	21	59
2	l	104/1024 (10%)	99 (95%)	3 (3%)	2 (2%)	6	32
3	B	602/907 (66%)	571 (95%)	30 (5%)	1 (0%)	43	78
3	D	571/907 (63%)	548 (96%)	23 (4%)	0	100	100
3	F	591/907 (65%)	559 (95%)	31 (5%)	1 (0%)	43	78
3	H	584/907 (64%)	562 (96%)	22 (4%)	0	100	100
3	a	112/907 (12%)	105 (94%)	5 (4%)	2 (2%)	6	34
3	f	97/907 (11%)	92 (95%)	5 (5%)	0	100	100
3	h	97/907 (11%)	95 (98%)	2 (2%)	0	100	100
3	j	105/907 (12%)	97 (92%)	5 (5%)	3 (3%)	3	23
4	A	599/902 (66%)	578 (96%)	20 (3%)	1 (0%)	43	78
4	C	606/902 (67%)	573 (95%)	31 (5%)	2 (0%)	36	72
4	E	626/902 (69%)	576 (92%)	43 (7%)	7 (1%)	11	46
4	G	628/902 (70%)	594 (95%)	31 (5%)	3 (0%)	24	63
5	I	511/667 (77%)	486 (95%)	21 (4%)	4 (1%)	16	54
5	K	548/667 (82%)	529 (96%)	17 (3%)	2 (0%)	30	67
6	L	540/1819 (30%)	512 (95%)	25 (5%)	3 (1%)	21	59
6	c	148/1819 (8%)	140 (95%)	8 (5%)	0	100	100
7	b	63/82 (77%)	62 (98%)	1 (2%)	0	100	100
7	d	57/82 (70%)	57 (100%)	0	0	100	100
7	g	63/82 (77%)	63 (100%)	0	0	100	100
7	i	63/82 (77%)	61 (97%)	2 (3%)	0	100	100
7	k	63/82 (77%)	62 (98%)	1 (2%)	0	100	100
7	m	63/82 (77%)	61 (97%)	2 (3%)	0	100	100
8	O	408/451 (90%)	387 (95%)	21 (5%)	0	100	100
8	P	408/451 (90%)	387 (95%)	21 (5%)	0	100	100
8	Q	408/451 (90%)	386 (95%)	22 (5%)	0	100	100
8	R	408/451 (90%)	386 (95%)	22 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	S	408/451 (90%)	386 (95%)	22 (5%)	0	100	100
8	T	408/451 (90%)	387 (95%)	21 (5%)	0	100	100
8	U	408/451 (90%)	387 (95%)	21 (5%)	0	100	100
8	V	408/451 (90%)	386 (95%)	22 (5%)	0	100	100
8	W	408/451 (90%)	386 (95%)	22 (5%)	0	100	100
8	X	408/451 (90%)	387 (95%)	21 (5%)	0	100	100
8	Y	408/451 (90%)	386 (95%)	22 (5%)	0	100	100
8	Z	408/451 (90%)	387 (95%)	21 (5%)	0	100	100
All	All	13203/24163 (55%)	12526 (95%)	643 (5%)	34 (0%)	37	72

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	I	121	PRO
3	B	870	ASP
4	C	465	HIS
4	E	522	MET
4	E	701	VAL
4	E	704	PRO
4	E	861	PHE
4	G	241	ARG
5	I	404	LEU
5	I	408	ASP
5	I	508	ASN
2	J	257	TYR
2	J	490	ARG
5	K	409	ASN
6	L	308	GLU
4	A	584	THR
3	j	108	PRO
3	j	111	VAL
3	j	112	SER
4	E	862	ASN
3	F	627	GLU
4	G	581	ASP
5	K	652	ASN
4	E	581	ASP
4	E	702	MET
4	G	239	ALA

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Mol	Chain	Res	Type
2	J	236	LEU
3	a	44	ALA
4	C	250	PRO
5	I	405	LEU
6	L	309	GLU
2	l	129	THR
6	L	307	ARG
3	a	45	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	e	310/318 (98%)	306 (99%)	4 (1%)	61	74
2	J	498/933 (53%)	497 (100%)	1 (0%)	87	87
2	l	84/933 (9%)	84 (100%)	0	100	100
3	B	551/798 (69%)	546 (99%)	5 (1%)	70	79
3	D	525/798 (66%)	522 (99%)	3 (1%)	78	83
3	F	542/798 (68%)	535 (99%)	7 (1%)	61	74
3	H	539/798 (68%)	537 (100%)	2 (0%)	84	84
3	a	101/798 (13%)	100 (99%)	1 (1%)	68	78
3	f	88/798 (11%)	88 (100%)	0	100	100
3	h	88/798 (11%)	88 (100%)	0	100	100
3	j	88/798 (11%)	88 (100%)	0	100	100
4	A	549/791 (69%)	545 (99%)	4 (1%)	76	81
4	C	556/791 (70%)	552 (99%)	4 (1%)	76	81
4	E	574/791 (73%)	562 (98%)	12 (2%)	47	65
4	G	572/791 (72%)	568 (99%)	4 (1%)	76	81
5	I	472/594 (80%)	471 (100%)	1 (0%)	87	87
5	K	509/594 (86%)	505 (99%)	4 (1%)	73	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	L	501/1546 (32%)	501 (100%)	0	100	100
6	c	135/1546 (9%)	135 (100%)	0	100	100
7	b	53/62 (86%)	52 (98%)	1 (2%)	50	67
7	d	53/62 (86%)	53 (100%)	0	100	100
7	g	53/62 (86%)	53 (100%)	0	100	100
7	i	53/62 (86%)	53 (100%)	0	100	100
7	k	53/62 (86%)	53 (100%)	0	100	100
7	m	53/62 (86%)	53 (100%)	0	100	100
8	O	376/400 (94%)	340 (90%)	36 (10%)	8	25
8	P	376/400 (94%)	340 (90%)	36 (10%)	8	25
8	Q	376/400 (94%)	340 (90%)	36 (10%)	8	25
8	R	376/400 (94%)	340 (90%)	36 (10%)	8	25
8	S	376/400 (94%)	340 (90%)	36 (10%)	8	25
8	T	376/400 (94%)	340 (90%)	36 (10%)	8	25
8	U	376/400 (94%)	340 (90%)	36 (10%)	8	25
8	V	376/400 (94%)	340 (90%)	36 (10%)	8	25
8	W	376/400 (94%)	340 (90%)	36 (10%)	8	25
8	X	376/400 (94%)	340 (90%)	36 (10%)	8	25
8	Y	376/400 (94%)	340 (90%)	36 (10%)	8	25
8	Z	376/400 (94%)	340 (90%)	36 (10%)	8	25
All	All	12112/21184 (57%)	11627 (96%)	485 (4%)	29	49

All (485) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	e	9	VAL
1	e	126	THR
1	e	149	THR
1	e	165	ILE
3	B	251	VAL
3	B	292	VAL
3	B	369	VAL
3	B	379	LYS
3	B	486	ILE
4	C	184	ARG

Continued on next page...

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Mol	Chain	Res	Type
4	C	233	VAL
4	C	328	ILE
4	C	399	ILE
3	D	299	TRP
3	D	448	VAL
3	D	764	LEU
4	E	176	ILE
4	E	480	LYS
4	E	566	THR
4	E	701	VAL
4	E	702	MET
4	E	703	GLU
4	E	704	PRO
4	E	705	THR
4	E	734	LEU
4	E	861	PHE
4	E	862	ASN
4	E	864	PHE
3	F	304	ILE
3	F	373	ASP
3	F	385	VAL
3	F	442	THR
3	F	473	SER
3	F	626	LEU
3	F	627	GLU
4	G	266	VAL
4	G	478	THR
4	G	546	ILE
4	G	660	ILE
3	H	425	PRO
3	H	501	THR
5	I	272	VAL
2	J	305	LEU
5	K	27	VAL
5	K	132	LEU
5	K	399	SER
5	K	646	LEU
7	b	39	LEU
8	O	7	THR
8	O	32	SER
8	O	34	GLU
8	O	37	VAL

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Mol	Chain	Res	Type
8	O	39	GLU
8	O	45	THR
8	O	73	VAL
8	O	84	LYS
8	O	109	SER
8	O	127	ASP
8	O	131	SER
8	O	138	CYS
8	O	153	LEU
8	O	165	LEU
8	O	170	SER
8	O	188	SER
8	O	204	VAL
8	O	234	THR
8	O	259	SER
8	O	265	ARG
8	O	277	THR
8	O	278	THR
8	O	294	MET
8	O	298	LEU
8	O	313	THR
8	O	324	ILE
8	O	337	LEU
8	O	347	ASN
8	O	367	LEU
8	O	369	SER
8	O	373	VAL
8	O	378	MET
8	O	407	GLN
8	O	424	SER
8	O	439	THR
8	O	443	TYR
8	P	7	THR
8	P	32	SER
8	P	34	GLU
8	P	37	VAL
8	P	39	GLU
8	P	45	THR
8	P	73	VAL
8	P	84	LYS
8	P	109	SER
8	P	127	ASP

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Mol	Chain	Res	Type
8	P	131	SER
8	P	138	CYS
8	P	153	LEU
8	P	165	LEU
8	P	170	SER
8	P	188	SER
8	P	204	VAL
8	P	234	THR
8	P	259	SER
8	P	265	ARG
8	P	277	THR
8	P	278	THR
8	P	294	MET
8	P	298	LEU
8	P	313	THR
8	P	324	ILE
8	P	337	LEU
8	P	347	ASN
8	P	367	LEU
8	P	369	SER
8	P	373	VAL
8	P	378	MET
8	P	407	GLN
8	P	424	SER
8	P	439	THR
8	P	443	TYR
8	Q	7	THR
8	Q	32	SER
8	Q	34	GLU
8	Q	37	VAL
8	Q	39	GLU
8	Q	45	THR
8	Q	73	VAL
8	Q	84	LYS
8	Q	109	SER
8	Q	127	ASP
8	Q	131	SER
8	Q	138	CYS
8	Q	153	LEU
8	Q	165	LEU
8	Q	170	SER
8	Q	188	SER

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Mol	Chain	Res	Type
8	Q	204	VAL
8	Q	234	THR
8	Q	259	SER
8	Q	265	ARG
8	Q	277	THR
8	Q	278	THR
8	Q	294	MET
8	Q	298	LEU
8	Q	313	THR
8	Q	324	ILE
8	Q	337	LEU
8	Q	347	ASN
8	Q	367	LEU
8	Q	369	SER
8	Q	373	VAL
8	Q	378	MET
8	Q	407	GLN
8	Q	424	SER
8	Q	439	THR
8	Q	443	TYR
8	R	7	THR
8	R	32	SER
8	R	34	GLU
8	R	37	VAL
8	R	39	GLU
8	R	45	THR
8	R	73	VAL
8	R	84	LYS
8	R	109	SER
8	R	127	ASP
8	R	131	SER
8	R	138	CYS
8	R	153	LEU
8	R	165	LEU
8	R	170	SER
8	R	188	SER
8	R	204	VAL
8	R	234	THR
8	R	259	SER
8	R	265	ARG
8	R	277	THR
8	R	278	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	R	294	MET
8	R	298	LEU
8	R	313	THR
8	R	324	ILE
8	R	337	LEU
8	R	347	ASN
8	R	367	LEU
8	R	369	SER
8	R	373	VAL
8	R	378	MET
8	R	407	GLN
8	R	424	SER
8	R	439	THR
8	R	443	TYR
8	S	7	THR
8	S	32	SER
8	S	34	GLU
8	S	37	VAL
8	S	39	GLU
8	S	45	THR
8	S	73	VAL
8	S	84	LYS
8	S	109	SER
8	S	127	ASP
8	S	131	SER
8	S	138	CYS
8	S	153	LEU
8	S	165	LEU
8	S	170	SER
8	S	188	SER
8	S	204	VAL
8	S	234	THR
8	S	259	SER
8	S	265	ARG
8	S	277	THR
8	S	278	THR
8	S	294	MET
8	S	298	LEU
8	S	313	THR
8	S	324	ILE
8	S	337	LEU
8	S	347	ASN

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Mol	Chain	Res	Type
8	S	367	LEU
8	S	369	SER
8	S	373	VAL
8	S	378	MET
8	S	407	GLN
8	S	424	SER
8	S	439	THR
8	S	443	TYR
8	T	7	THR
8	T	32	SER
8	T	34	GLU
8	T	37	VAL
8	T	39	GLU
8	T	45	THR
8	T	73	VAL
8	T	84	LYS
8	T	109	SER
8	T	127	ASP
8	T	131	SER
8	T	138	CYS
8	T	153	LEU
8	T	165	LEU
8	T	170	SER
8	T	188	SER
8	T	204	VAL
8	T	234	THR
8	T	259	SER
8	T	265	ARG
8	T	277	THR
8	T	278	THR
8	T	294	MET
8	T	298	LEU
8	T	313	THR
8	T	324	ILE
8	T	337	LEU
8	T	347	ASN
8	T	367	LEU
8	T	369	SER
8	T	373	VAL
8	T	378	MET
8	T	407	GLN
8	T	424	SER

Continued on next page...

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Mol	Chain	Res	Type
8	T	439	THR
8	T	443	TYR
8	U	7	THR
8	U	32	SER
8	U	34	GLU
8	U	37	VAL
8	U	39	GLU
8	U	45	THR
8	U	73	VAL
8	U	84	LYS
8	U	109	SER
8	U	127	ASP
8	U	131	SER
8	U	138	CYS
8	U	153	LEU
8	U	165	LEU
8	U	170	SER
8	U	188	SER
8	U	204	VAL
8	U	234	THR
8	U	259	SER
8	U	265	ARG
8	U	277	THR
8	U	278	THR
8	U	294	MET
8	U	298	LEU
8	U	313	THR
8	U	324	ILE
8	U	337	LEU
8	U	347	ASN
8	U	367	LEU
8	U	369	SER
8	U	373	VAL
8	U	378	MET
8	U	407	GLN
8	U	424	SER
8	U	439	THR
8	U	443	TYR
8	V	7	THR
8	V	32	SER
8	V	34	GLU
8	V	37	VAL

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Mol	Chain	Res	Type
8	V	39	GLU
8	V	45	THR
8	V	73	VAL
8	V	84	LYS
8	V	109	SER
8	V	127	ASP
8	V	131	SER
8	V	138	CYS
8	V	153	LEU
8	V	165	LEU
8	V	170	SER
8	V	188	SER
8	V	204	VAL
8	V	234	THR
8	V	259	SER
8	V	265	ARG
8	V	277	THR
8	V	278	THR
8	V	294	MET
8	V	298	LEU
8	V	313	THR
8	V	324	ILE
8	V	337	LEU
8	V	347	ASN
8	V	367	LEU
8	V	369	SER
8	V	373	VAL
8	V	378	MET
8	V	407	GLN
8	V	424	SER
8	V	439	THR
8	V	443	TYR
8	W	7	THR
8	W	32	SER
8	W	34	GLU
8	W	37	VAL
8	W	39	GLU
8	W	45	THR
8	W	73	VAL
8	W	84	LYS
8	W	109	SER
8	W	127	ASP

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Mol	Chain	Res	Type
8	W	131	SER
8	W	138	CYS
8	W	153	LEU
8	W	165	LEU
8	W	170	SER
8	W	188	SER
8	W	204	VAL
8	W	234	THR
8	W	259	SER
8	W	265	ARG
8	W	277	THR
8	W	278	THR
8	W	294	MET
8	W	298	LEU
8	W	313	THR
8	W	324	ILE
8	W	337	LEU
8	W	347	ASN
8	W	367	LEU
8	W	369	SER
8	W	373	VAL
8	W	378	MET
8	W	407	GLN
8	W	424	SER
8	W	439	THR
8	W	443	TYR
8	X	7	THR
8	X	32	SER
8	X	34	GLU
8	X	37	VAL
8	X	39	GLU
8	X	45	THR
8	X	73	VAL
8	X	84	LYS
8	X	109	SER
8	X	127	ASP
8	X	131	SER
8	X	138	CYS
8	X	153	LEU
8	X	165	LEU
8	X	170	SER
8	X	188	SER

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Mol	Chain	Res	Type
8	X	204	VAL
8	X	234	THR
8	X	259	SER
8	X	265	ARG
8	X	277	THR
8	X	278	THR
8	X	294	MET
8	X	298	LEU
8	X	313	THR
8	X	324	ILE
8	X	337	LEU
8	X	347	ASN
8	X	367	LEU
8	X	369	SER
8	X	373	VAL
8	X	378	MET
8	X	407	GLN
8	X	424	SER
8	X	439	THR
8	X	443	TYR
8	Y	7	THR
8	Y	32	SER
8	Y	34	GLU
8	Y	37	VAL
8	Y	39	GLU
8	Y	45	THR
8	Y	73	VAL
8	Y	84	LYS
8	Y	109	SER
8	Y	127	ASP
8	Y	131	SER
8	Y	138	CYS
8	Y	153	LEU
8	Y	165	LEU
8	Y	170	SER
8	Y	188	SER
8	Y	204	VAL
8	Y	234	THR
8	Y	259	SER
8	Y	265	ARG
8	Y	277	THR
8	Y	278	THR

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Mol	Chain	Res	Type
8	Y	294	MET
8	Y	298	LEU
8	Y	313	THR
8	Y	324	ILE
8	Y	337	LEU
8	Y	347	ASN
8	Y	367	LEU
8	Y	369	SER
8	Y	373	VAL
8	Y	378	MET
8	Y	407	GLN
8	Y	424	SER
8	Y	439	THR
8	Y	443	TYR
8	Z	7	THR
8	Z	32	SER
8	Z	34	GLU
8	Z	37	VAL
8	Z	39	GLU
8	Z	45	THR
8	Z	73	VAL
8	Z	84	LYS
8	Z	109	SER
8	Z	127	ASP
8	Z	131	SER
8	Z	138	CYS
8	Z	153	LEU
8	Z	165	LEU
8	Z	170	SER
8	Z	188	SER
8	Z	204	VAL
8	Z	234	THR
8	Z	259	SER
8	Z	265	ARG
8	Z	277	THR
8	Z	278	THR
8	Z	294	MET
8	Z	298	LEU
8	Z	313	THR
8	Z	324	ILE
8	Z	337	LEU
8	Z	347	ASN

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Mol	Chain	Res	Type
8	Z	367	LEU
8	Z	369	SER
8	Z	373	VAL
8	Z	378	MET
8	Z	407	GLN
8	Z	424	SER
8	Z	439	THR
8	Z	443	TYR
3	a	86	VAL
4	A	304	LEU
4	A	510	VAL
4	A	547	THR
4	A	822	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (317) such sidechains are listed below:

Mol	Chain	Res	Type
1	e	12	ASN
1	e	73	HIS
1	e	173	HIS
2	l	30	GLN
2	l	47	ASN
2	l	59	HIS
2	l	107	HIS
3	B	270	ASN
3	B	310	GLN
3	B	389	GLN
3	B	500	GLN
3	B	746	HIS
3	B	786	GLN
3	B	812	GLN
3	B	830	ASN
3	B	860	GLN
4	C	165	GLN
4	C	309	GLN
4	C	412	HIS
4	C	444	GLN
4	C	465	HIS
4	C	512	HIS
4	C	524	GLN
4	C	650	HIS
4	C	694	GLN

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Mol	Chain	Res	Type
4	C	862	ASN
3	D	259	GLN
3	D	265	ASN
3	D	273	ASN
3	D	310	GLN
3	D	322	GLN
3	D	345	GLN
3	D	416	GLN
3	D	444	HIS
3	D	479	GLN
3	D	491	ASN
3	D	498	HIS
3	D	570	GLN
3	D	595	HIS
3	D	596	ASN
3	D	705	HIS
3	D	716	HIS
3	D	736	ASN
3	D	746	HIS
3	D	773	ASN
3	D	774	GLN
3	D	801	GLN
3	D	805	GLN
3	D	855	GLN
4	E	152	GLN
4	E	165	GLN
4	E	172	GLN
4	E	236	GLN
4	E	242	GLN
4	E	309	GLN
4	E	312	GLN
4	E	360	HIS
4	E	424	ASN
4	E	436	GLN
4	E	530	HIS
4	E	565	ASN
4	E	644	HIS
4	E	712	ASN
3	F	269	ASN
3	F	322	GLN
3	F	330	GLN
3	F	461	HIS

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Mol	Chain	Res	Type
3	F	479	GLN
3	F	491	ASN
3	F	528	ASN
3	F	570	GLN
3	F	595	HIS
3	F	596	ASN
3	F	739	GLN
3	F	774	GLN
3	F	789	GLN
3	F	852	HIS
3	F	855	GLN
3	F	859	GLN
3	F	860	GLN
4	G	152	GLN
4	G	165	GLN
4	G	169	ASN
4	G	172	GLN
4	G	173	HIS
4	G	251	ASN
4	G	287	GLN
4	G	289	ASN
4	G	322	GLN
4	G	329	GLN
4	G	371	GLN
4	G	412	HIS
4	G	438	GLN
4	G	493	ASN
4	G	565	ASN
4	G	644	HIS
4	G	691	GLN
4	G	725	HIS
4	G	763	GLN
4	G	767	GLN
4	G	862	ASN
3	H	329	HIS
3	H	345	GLN
3	H	389	GLN
3	H	401	HIS
3	H	560	GLN
3	H	609	ASN
3	H	687	ASN
3	H	713	HIS

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Mol	Chain	Res	Type
3	H	719	GLN
3	H	736	ASN
3	H	746	HIS
3	H	786	GLN
3	H	805	GLN
5	I	35	HIS
5	I	102	GLN
5	I	256	GLN
5	I	303	GLN
5	I	317	GLN
5	I	327	GLN
5	I	377	GLN
5	I	397	GLN
5	I	460	GLN
5	I	464	HIS
5	I	499	GLN
5	I	527	ASN
5	I	533	GLN
5	I	543	GLN
5	I	547	GLN
5	I	622	GLN
2	J	237	HIS
2	J	248	GLN
2	J	269	GLN
2	J	299	ASN
2	J	322	GLN
2	J	435	HIS
2	J	456	GLN
2	J	495	GLN
2	J	558	GLN
2	J	567	GLN
2	J	721	GLN
2	J	898	HIS
2	J	938	HIS
5	K	29	GLN
5	K	43	ASN
5	K	67	GLN
5	K	98	GLN
5	K	116	HIS
5	K	123	ASN
5	K	284	GLN
5	K	289	GLN

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Mol	Chain	Res	Type
5	K	316	GLN
5	K	377	GLN
5	K	509	GLN
5	K	527	ASN
5	K	533	GLN
5	K	571	GLN
5	K	639	ASN
5	K	644	GLN
5	K	657	GLN
6	L	511	HIS
6	L	1563	HIS
6	L	1730	HIS
6	L	1761	ASN
6	L	1766	GLN
6	L	1770	ASN
6	L	1777	HIS
7	g	17	ASN
8	O	16	GLN
8	O	139	HIS
8	O	211	ASN
8	O	229	ASN
8	O	250	ASN
8	O	325	GLN
8	O	334	HIS
8	O	429	GLN
8	O	436	HIS
8	P	16	GLN
8	P	139	HIS
8	P	211	ASN
8	P	229	ASN
8	P	250	ASN
8	P	325	GLN
8	P	334	HIS
8	P	429	GLN
8	P	436	HIS
8	Q	16	GLN
8	Q	211	ASN
8	Q	229	ASN
8	Q	250	ASN
8	Q	325	GLN
8	Q	334	HIS
8	Q	357	GLN

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Mol	Chain	Res	Type
8	Q	429	GLN
8	Q	436	HIS
8	R	16	GLN
8	R	211	ASN
8	R	229	ASN
8	R	250	ASN
8	R	325	GLN
8	R	334	HIS
8	R	357	GLN
8	R	429	GLN
8	R	436	HIS
8	S	16	GLN
8	S	139	HIS
8	S	158	ASN
8	S	211	ASN
8	S	229	ASN
8	S	250	ASN
8	S	251	ASN
8	S	325	GLN
8	S	334	HIS
8	S	347	ASN
8	S	357	GLN
8	S	429	GLN
8	S	436	HIS
8	T	16	GLN
8	T	158	ASN
8	T	211	ASN
8	T	229	ASN
8	T	250	ASN
8	T	325	GLN
8	T	334	HIS
8	T	429	GLN
8	T	436	HIS
8	U	16	GLN
8	U	211	ASN
8	U	229	ASN
8	U	250	ASN
8	U	325	GLN
8	U	334	HIS
8	U	357	GLN
8	U	429	GLN
8	U	436	HIS

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Mol	Chain	Res	Type
8	V	16	GLN
8	V	211	ASN
8	V	229	ASN
8	V	250	ASN
8	V	325	GLN
8	V	334	HIS
8	V	357	GLN
8	V	429	GLN
8	V	436	HIS
8	W	16	GLN
8	W	54	GLN
8	W	158	ASN
8	W	211	ASN
8	W	229	ASN
8	W	250	ASN
8	W	325	GLN
8	W	334	HIS
8	W	338	GLN
8	W	357	GLN
8	W	429	GLN
8	W	436	HIS
8	X	16	GLN
8	X	211	ASN
8	X	229	ASN
8	X	250	ASN
8	X	325	GLN
8	X	334	HIS
8	X	429	GLN
8	X	436	HIS
8	Y	16	GLN
8	Y	139	HIS
8	Y	211	ASN
8	Y	229	ASN
8	Y	250	ASN
8	Y	325	GLN
8	Y	334	HIS
8	Y	357	GLN
8	Y	429	GLN
8	Y	436	HIS
8	Z	16	GLN
8	Z	211	ASN
8	Z	229	ASN

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Mol	Chain	Res	Type
8	Z	250	ASN
8	Z	325	GLN
8	Z	334	HIS
8	Z	357	GLN
8	Z	429	GLN
8	Z	436	HIS
7	i	53	GLN
7	k	17	ASN
7	k	53	GLN
7	m	36	ASN
7	m	53	GLN
3	a	14	GLN
3	a	15	ASN
3	a	31	GLN
3	f	14	GLN
3	h	15	ASN
3	h	30	GLN
3	h	31	GLN
3	h	82	HIS
4	A	169	ASN
4	A	236	GLN
4	A	251	ASN
4	A	371	GLN
4	A	412	HIS
4	A	487	GLN
4	A	639	GLN
4	A	644	HIS
4	A	662	ASN
4	A	688	ASN
4	A	718	ASN
4	A	763	GLN
4	A	767	GLN
4	A	828	ASN
3	j	30	GLN
3	j	65	GLN
3	j	84	GLN
6	c	48	ASN
6	c	136	ASN
6	c	138	HIS
6	c	180	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

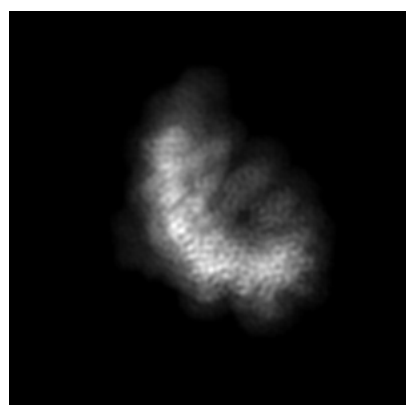
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14015. These allow visual inspection of the internal detail of the map and identification of artifacts.

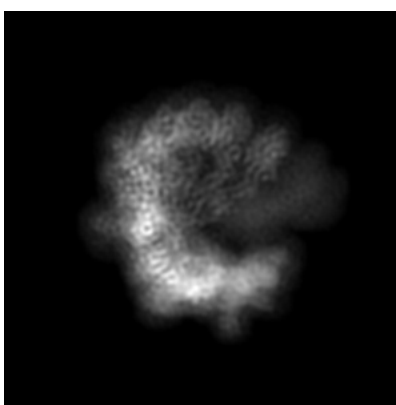
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

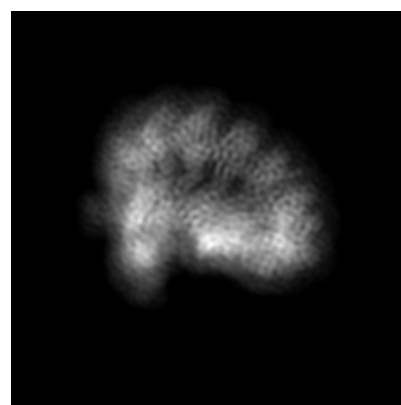
6.1.1 Primary map



X



Y



Z

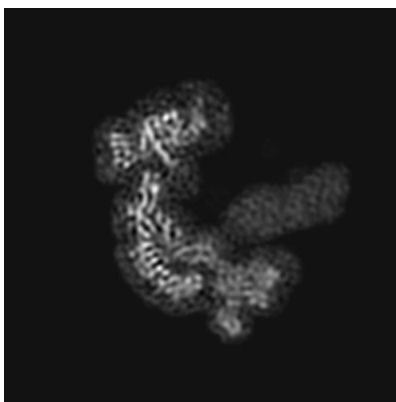
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 100



Y Index: 100

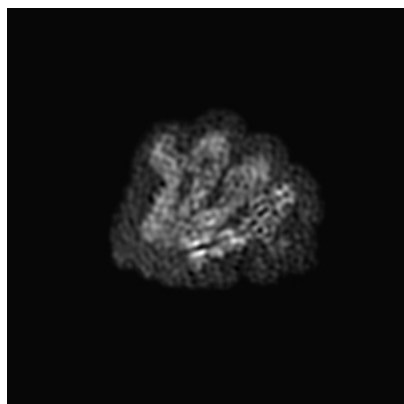


Z Index: 100

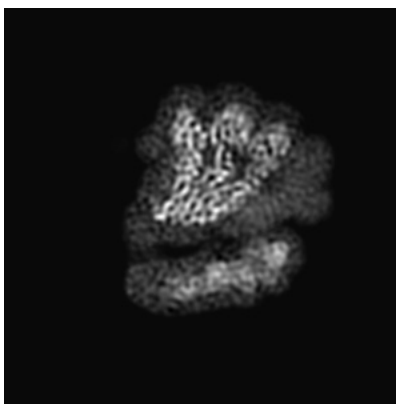
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

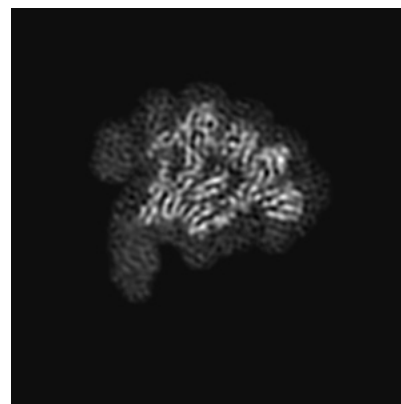
6.3.1 Primary map



X Index: 64



Y Index: 82

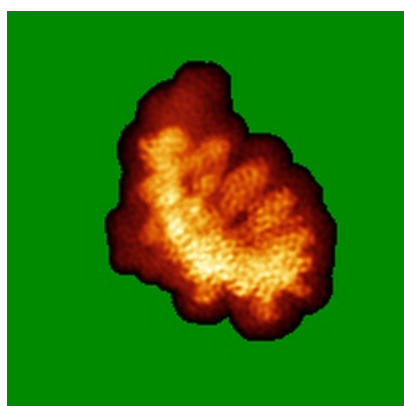


Z Index: 72

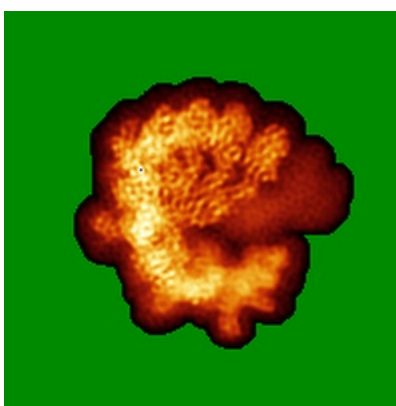
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X



Y

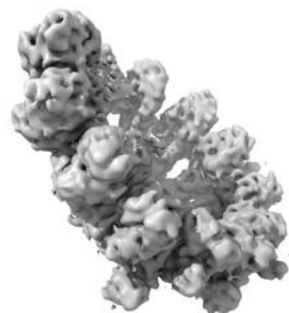


Z

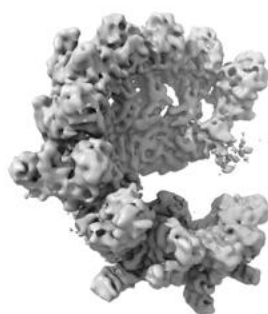
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

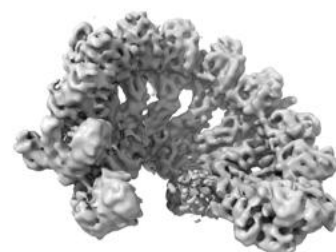
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0432. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

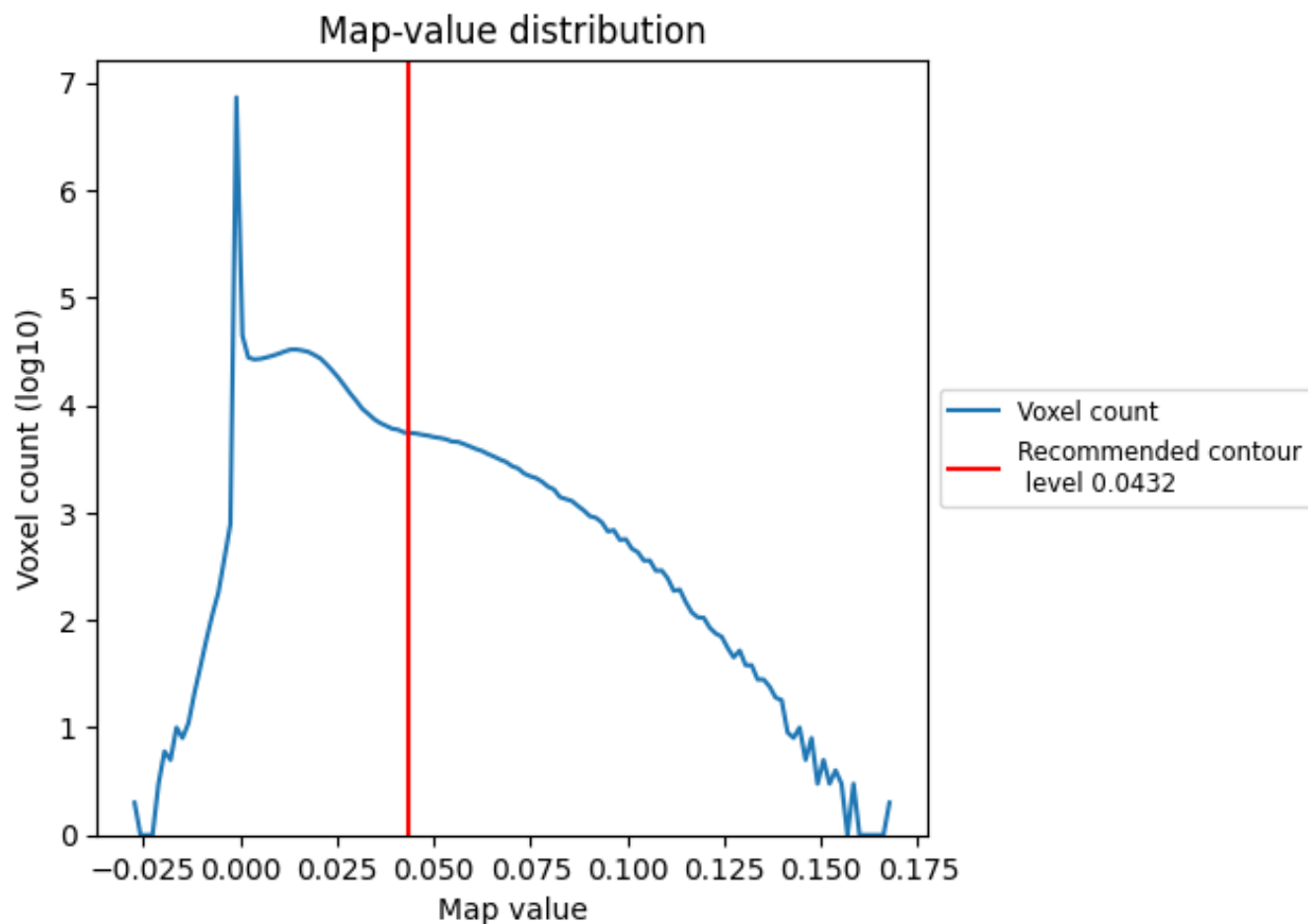
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

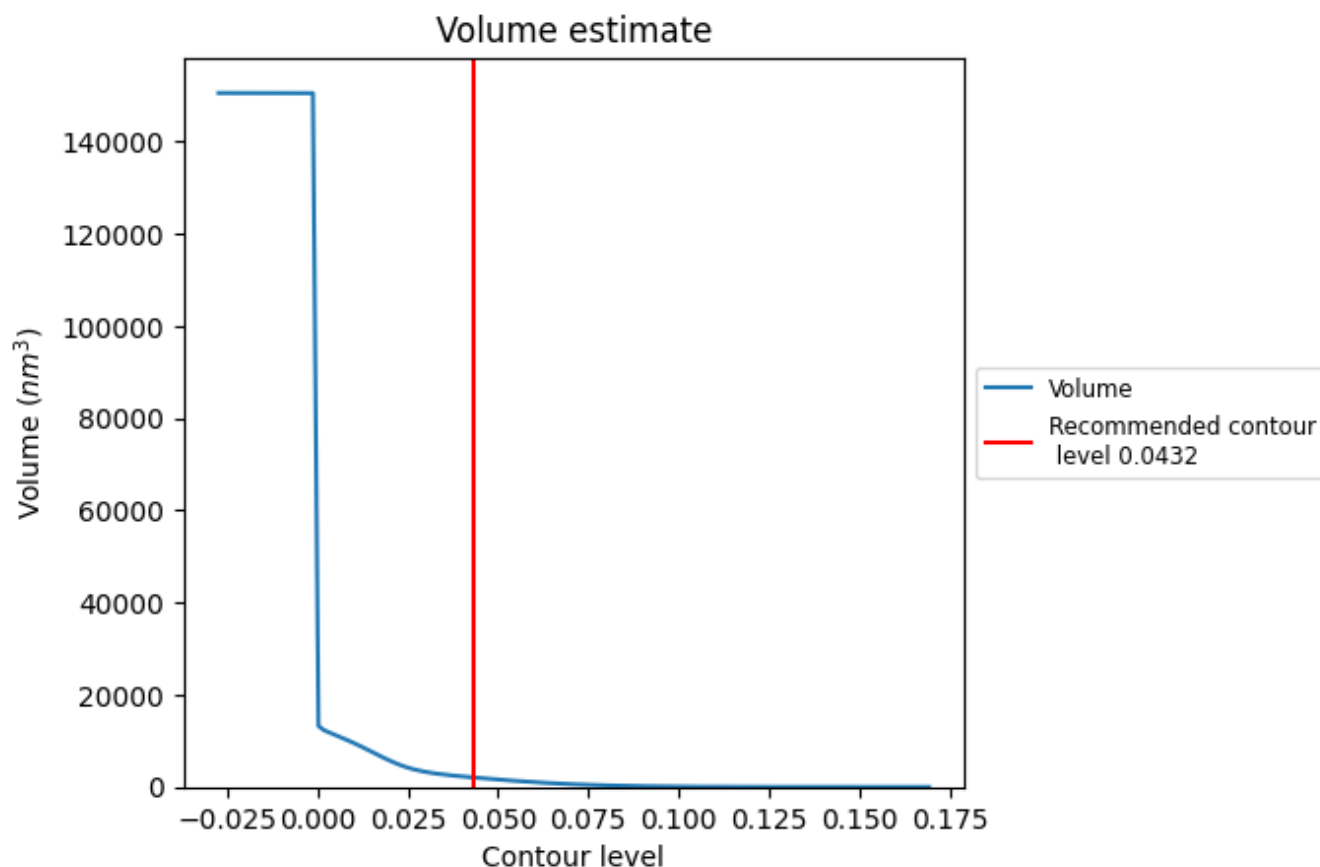
This section contains the results of statistical analysis of the map.

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.

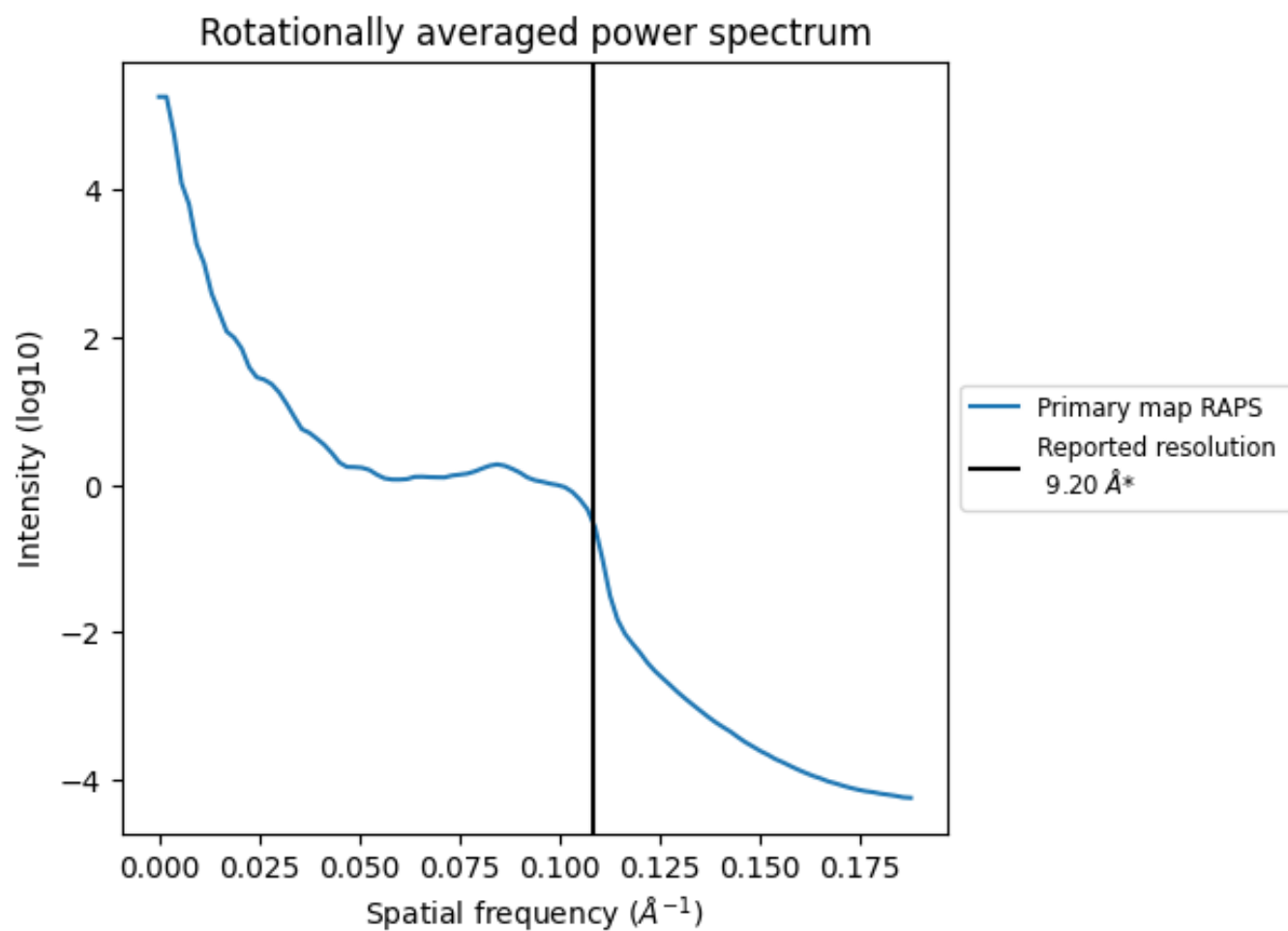
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2056 nm^3 ; this corresponds to an approximate mass of 1857 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



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

8 Fourier-Shell correlation

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

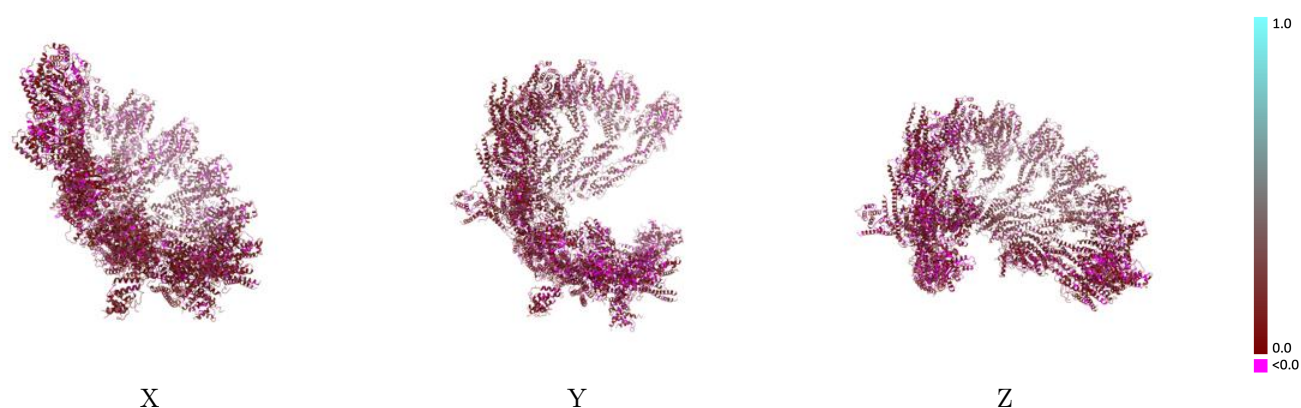
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-14015 and PDB model 7QJA. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)

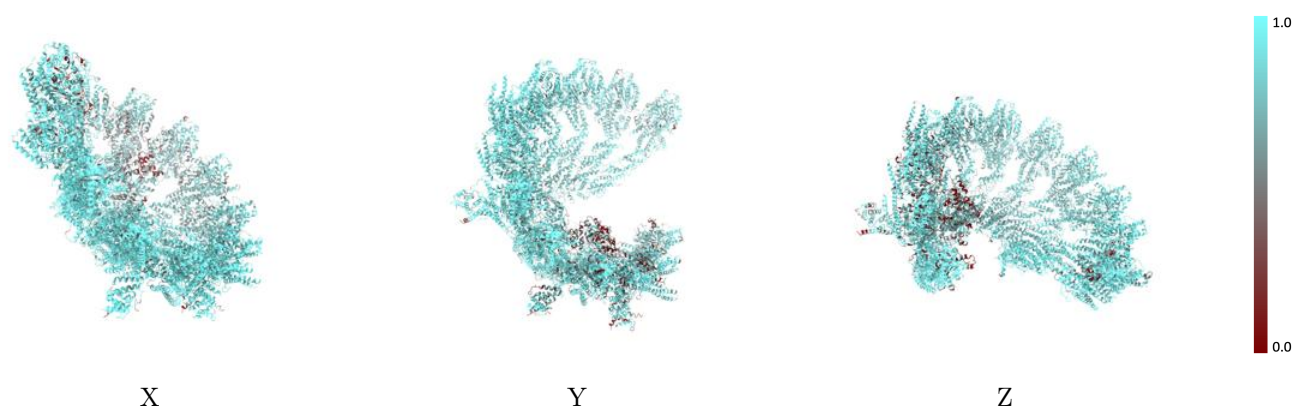
This section was not generated.

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



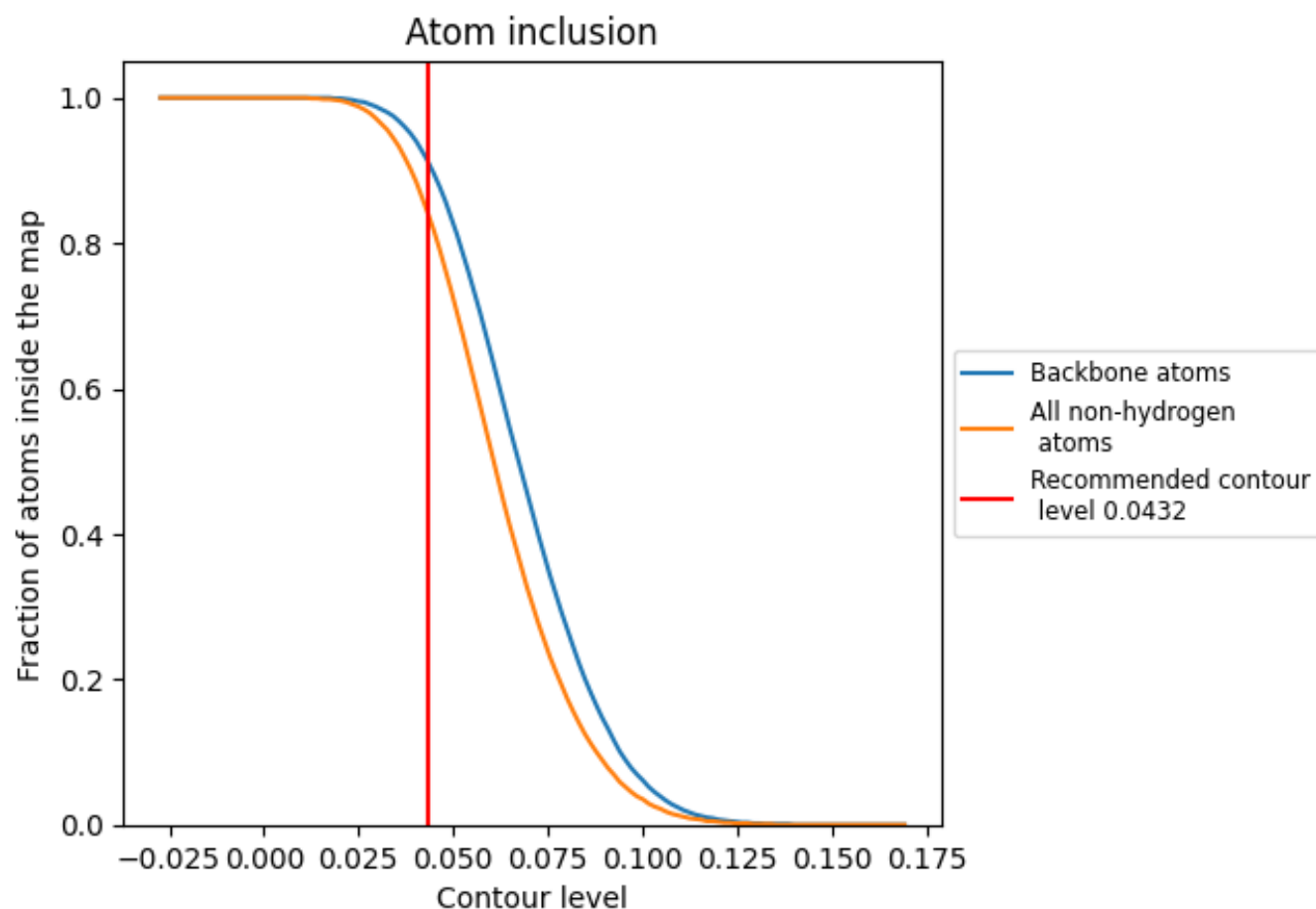
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0432).

9.4 Atom inclusion [i](#)



At the recommended contour level, 91% 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 (0.0432) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8430	 0.1080
A	 0.9090	 0.0920
B	 0.8520	 0.1050
C	 0.8690	 0.0910
D	 0.8560	 0.1250
E	 0.8820	 0.1250
F	 0.9140	 0.1250
G	 0.8990	 0.1340
H	 0.8980	 0.1350
I	 0.9110	 0.1380
J	 0.9280	 0.1290
K	 0.9010	 0.1300
L	 0.8950	 0.1230
O	 0.7640	 0.0690
P	 0.6720	 0.0580
Q	 0.7020	 0.0580
R	 0.7810	 0.0750
S	 0.8500	 0.0710
T	 0.9030	 0.1100
U	 0.8930	 0.1080
V	 0.9160	 0.1340
W	 0.9000	 0.1210
X	 0.8990	 0.1090
Y	 0.8500	 0.0810
Z	 0.7650	 0.0880
a	 0.7380	 0.1190
b	 0.7770	 0.1430
c	 0.6190	 0.1060
d	 0.5450	 0.1450
e	 0.4250	 0.0710
f	 0.7070	 0.0790
g	 0.6790	 0.1030
h	 0.6960	 0.0890
i	 0.6200	 0.0870
j	 0.8750	 0.1210



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Chain	Atom inclusion	Q-score
k	 0.8210	 0.1230
l	 0.9110	 0.1410
m	 0.8610	 0.1670