



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 07:06 PM UTC

PDB ID : 7QJ9 / pdb_00007qj9
EMDB ID : EMD-14014
Title : Structure of recombinant human gamma-Tubulin Ring Complex 10-spoked assembly intermediate (spokes 3-12, homogeneous dataset)
Authors : Zupa, E.; Pfeffer, S.
Deposited on : 2021-12-16
Resolution : 8.10 Å (reported)
Based on initial models : 6X0U, 7AS4, 6L81, 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:

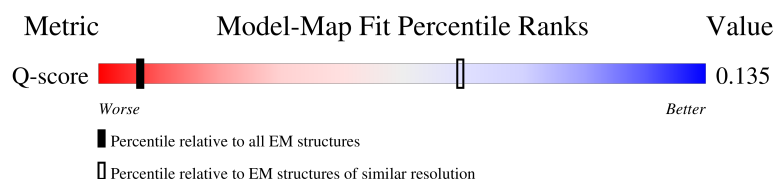
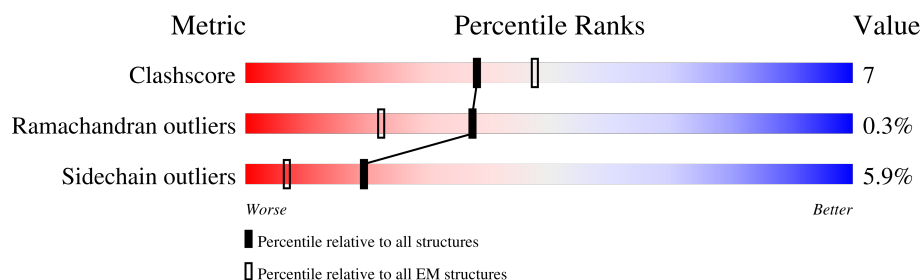
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 8.10 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	342 (7.60 - 8.60)

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

Mol	Chain	Length	Quality of chain
1	J	1024	
1	l	1024	
2	e	375	
3	b	82	

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

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

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 91535 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

- Molecule 2 is a protein called actin, cytoplasmic 1.

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

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

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

- Molecule 4 is a protein called Gamma-tubulin complex component 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	a	116	Total	C	N	O	S	0	0
			933	591	171	169	2		
4	D	581	Total	C	N	O	S	0	0
			4796	3061	842	868	25		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	599	Total	C	N	O	S	0	0
			4941	3151	871	894	25		
4	H	594	Total	C	N	O	S	0	0
			4907	3130	864	888	25		
4	h	99	Total	C	N	O	S	0	0
			803	509	148	144	2		
4	j	107	Total	C	N	O	S	0	0
			843	533	156	152	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	C	620	Total	C	N	O	S	0	0
			5044	3257	845	910	32		
5	E	638	Total	C	N	O	S	0	0
			5202	3354	873	942	33		
5	G	640	Total	C	N	O	S	0	0
			5206	3354	875	944	33		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	L	566	Total	C	N	O	S	0	0
			4587	3000	773	789	25		
7	c	158	Total	C	N	O	S	0	0
			1220	771	209	232	8		

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

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

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

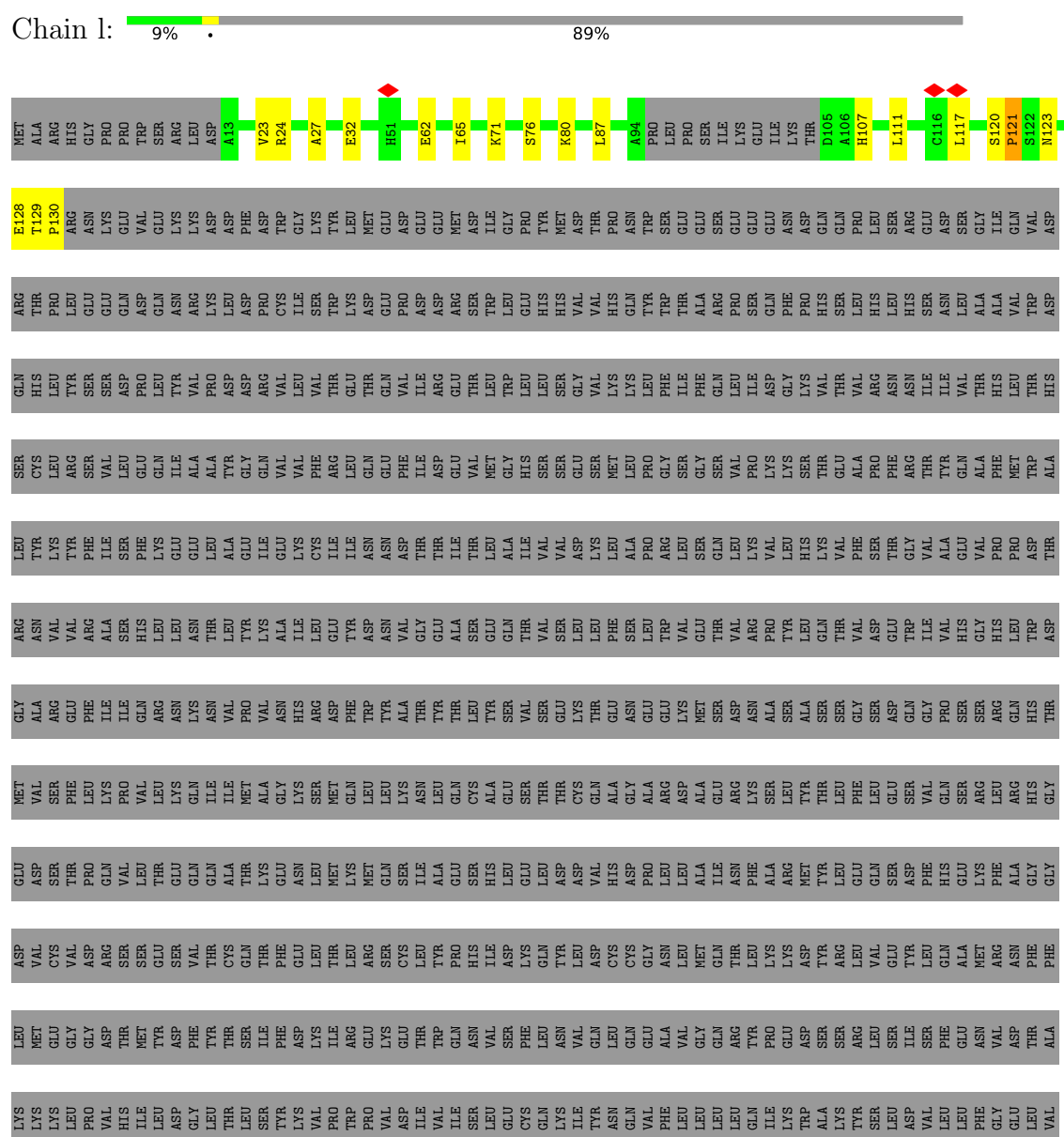
- Molecule 9 is water.

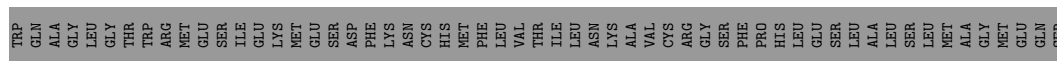
Mol	Chain	Residues	Atoms		AltConf
9	1	6	Total	O	0
			6	6	

3 Residue-property plots

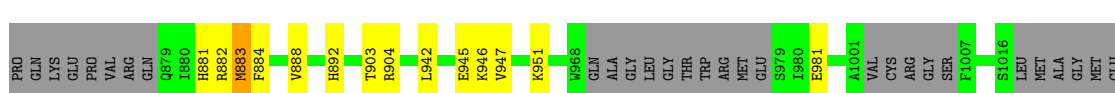
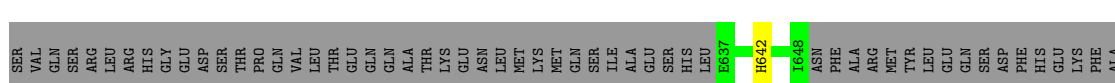
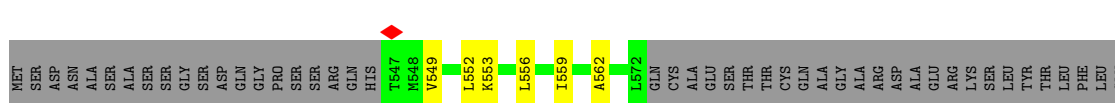
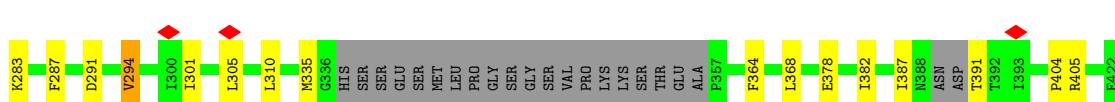
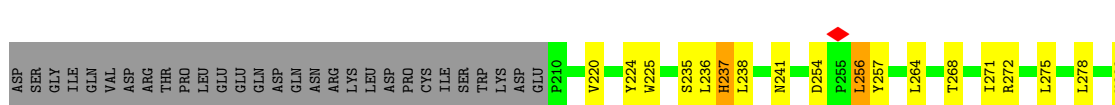
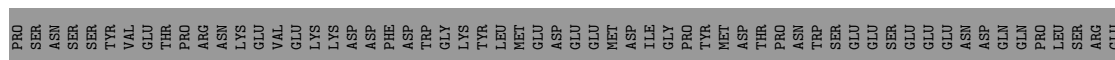
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Gamma-tubulin complex component 5

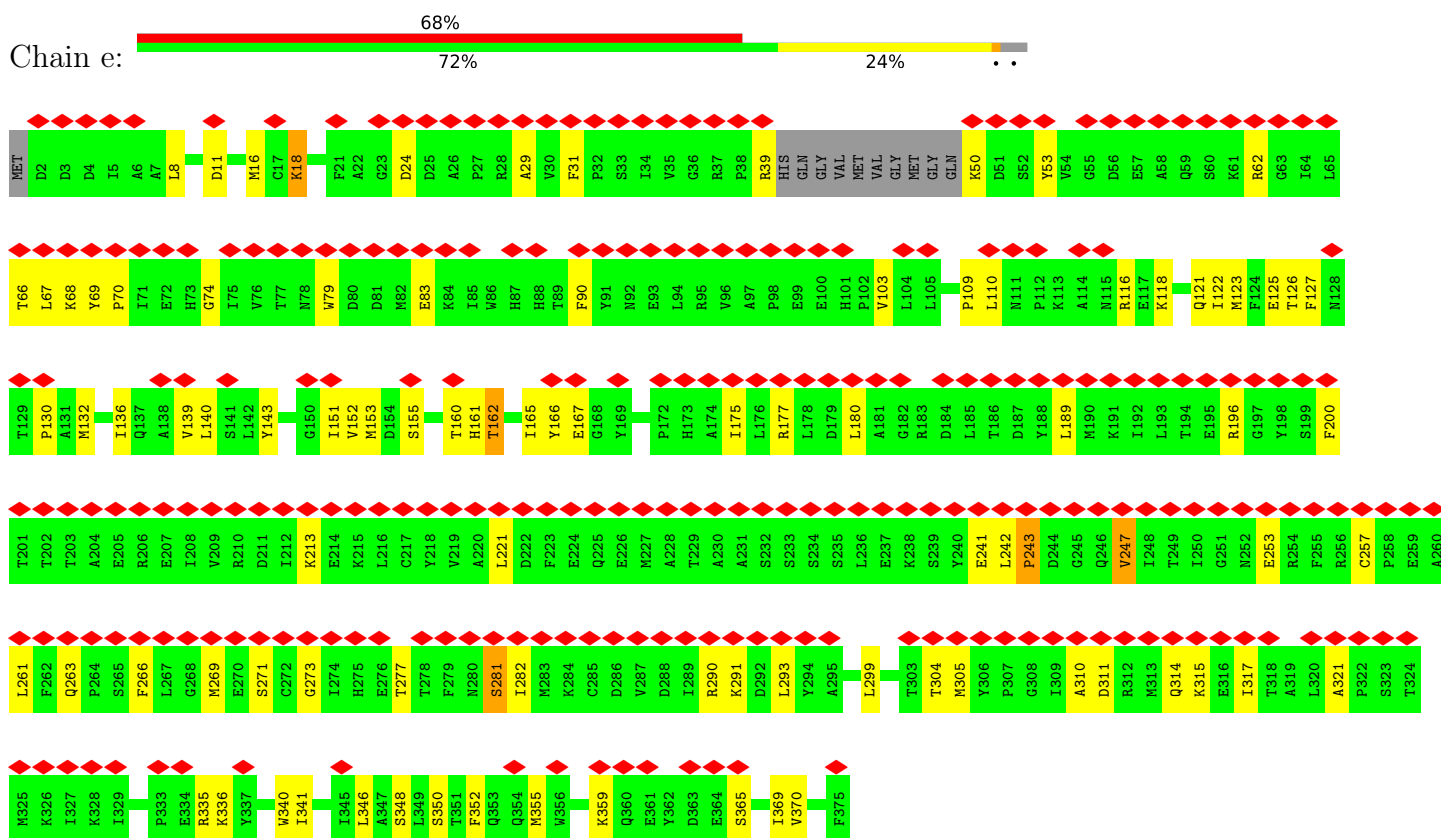




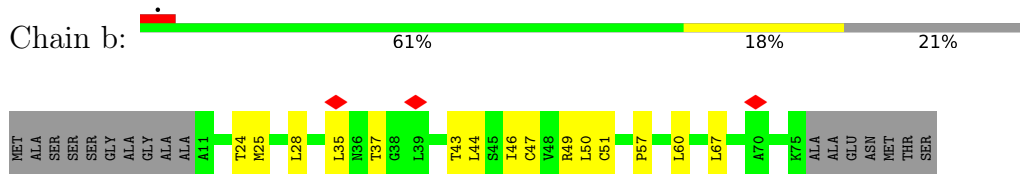
- Molecule 1: Gamma-tubulin complex component 5



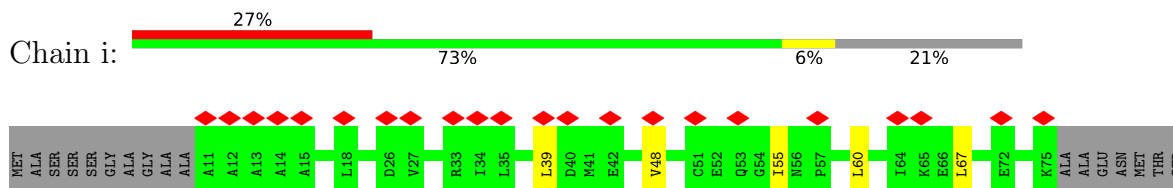
- Molecule 2: actin, cytoplasmic 1



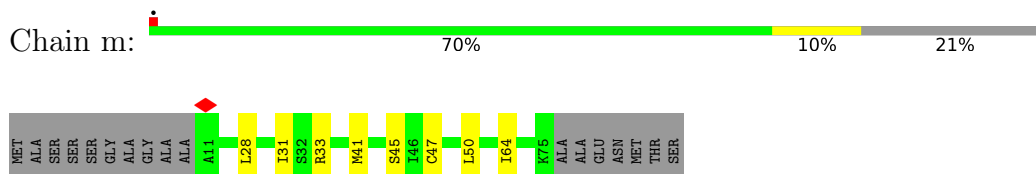
• Molecule 3: Mitotic-spindle organizing protein 1



• Molecule 3: Mitotic-spindle organizing protein 1



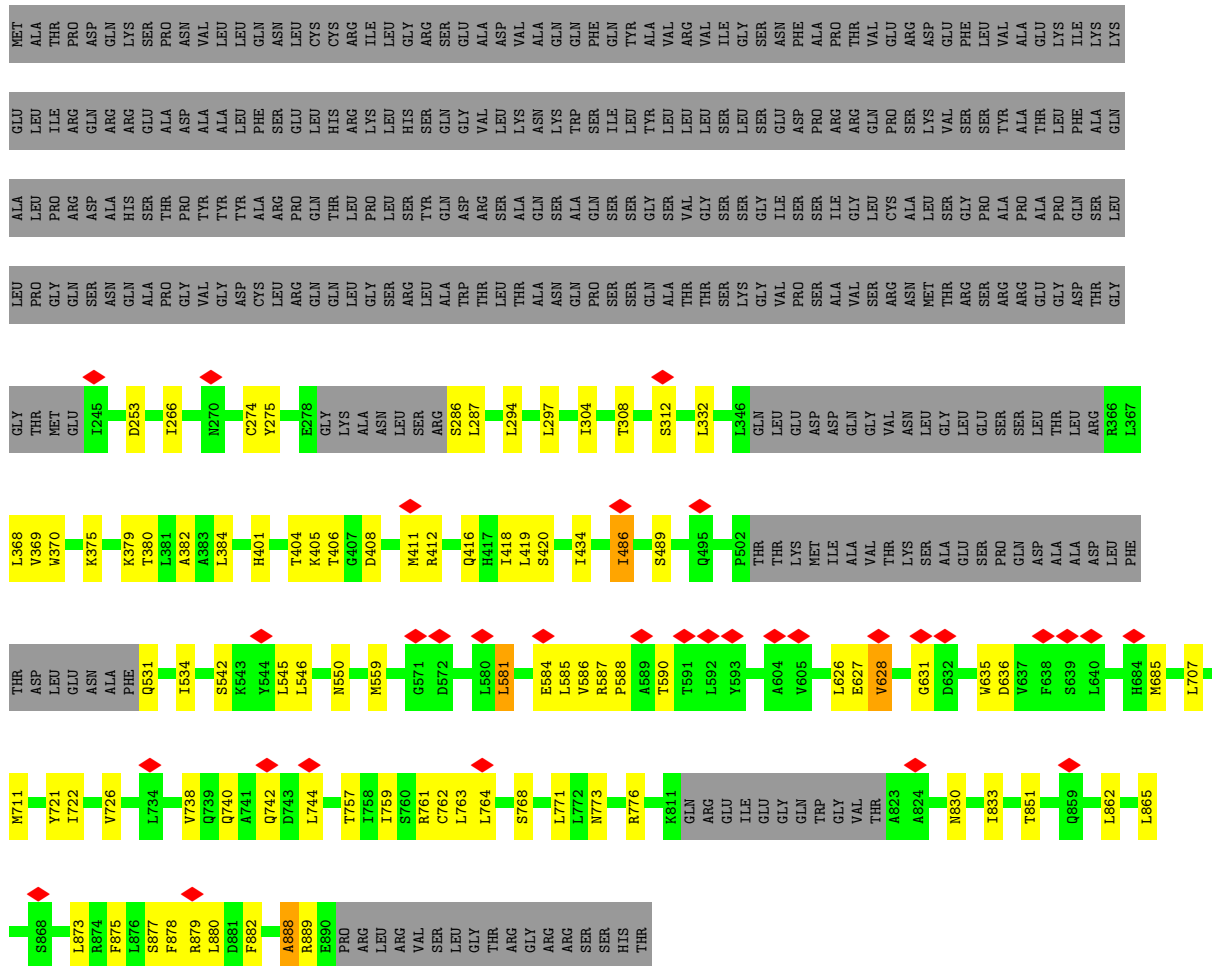
• Molecule 3: Mitotic-spindle organizing protein 1



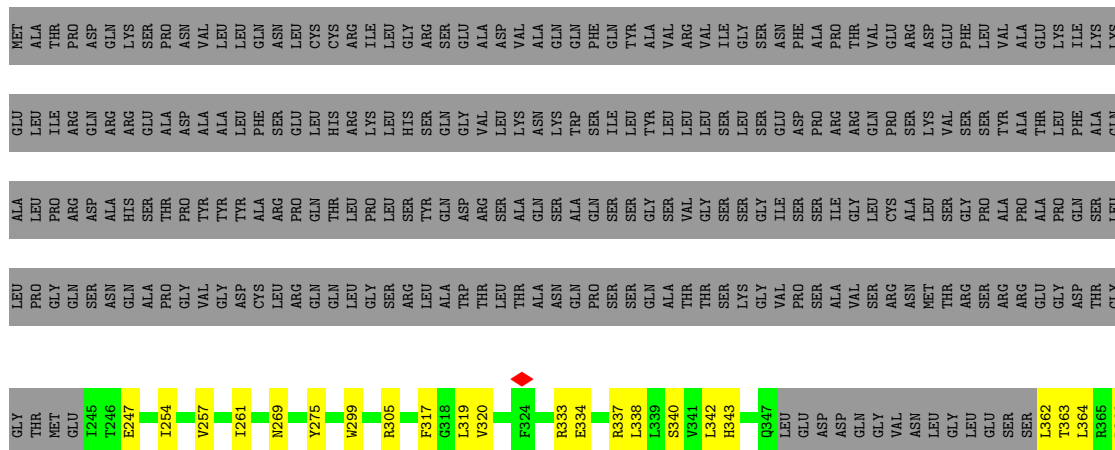
• Molecule 3: Mitotic-spindle organizing protein 1

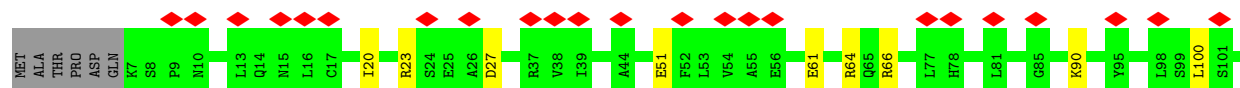


Chain D:

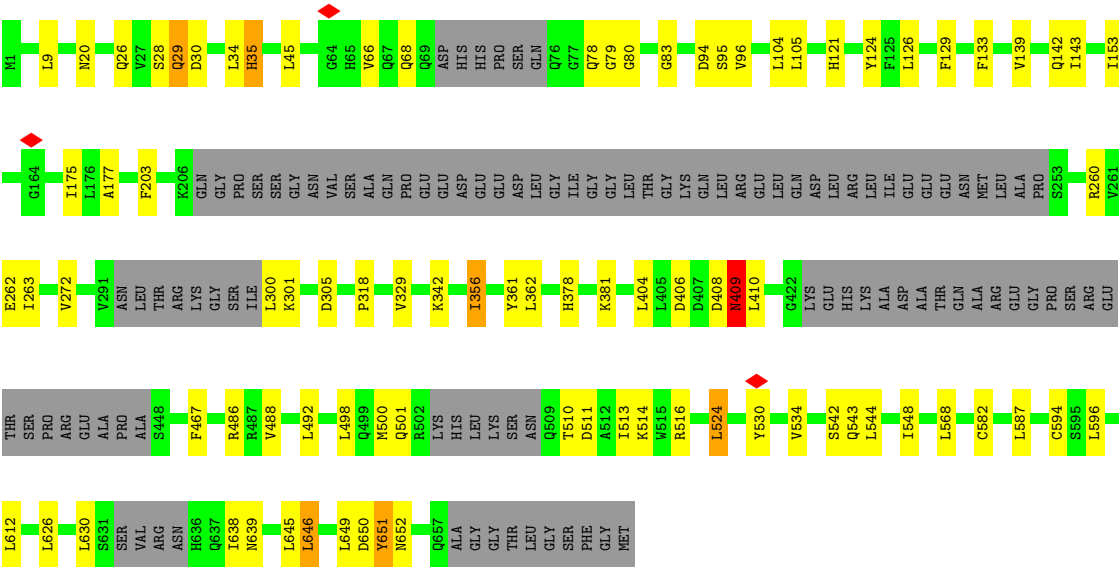


Chain F:

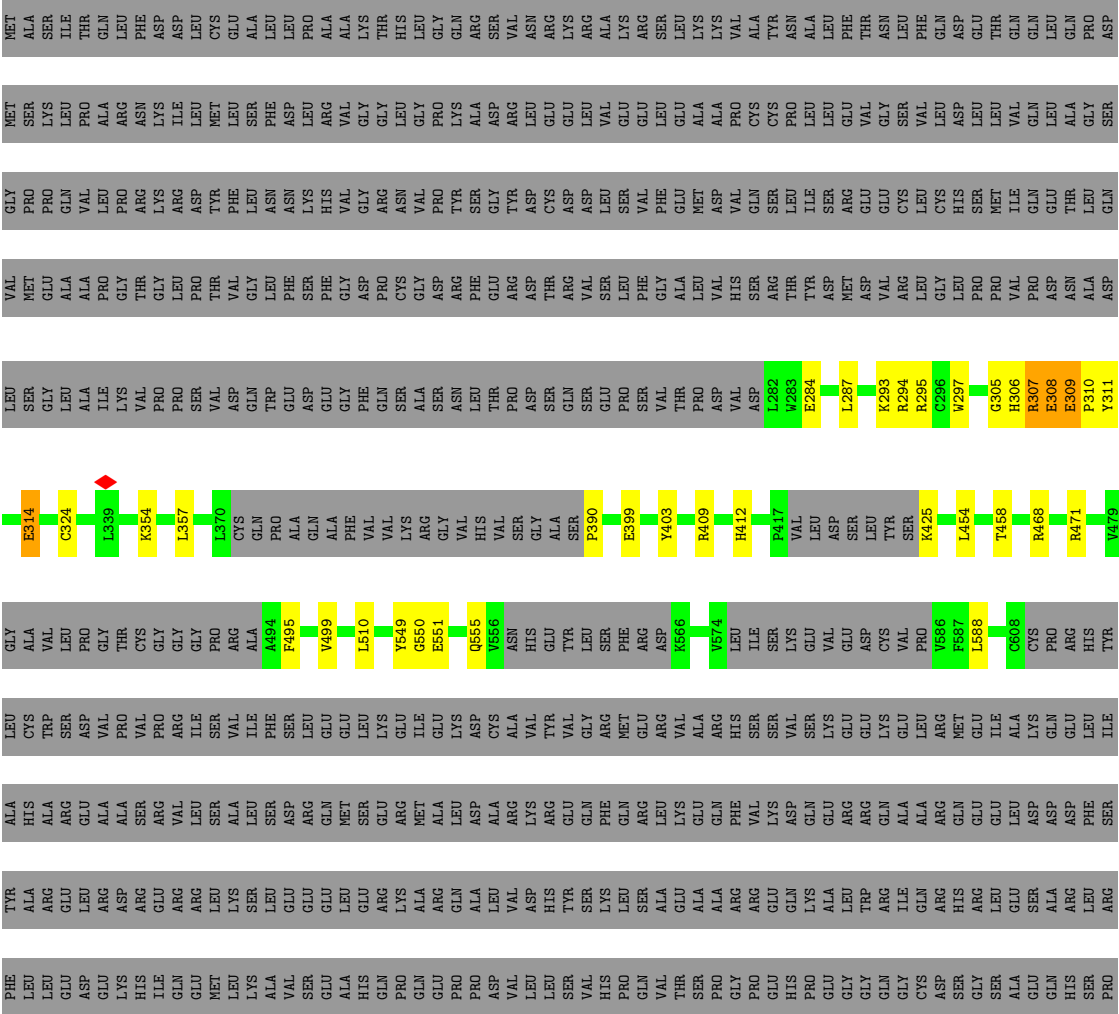








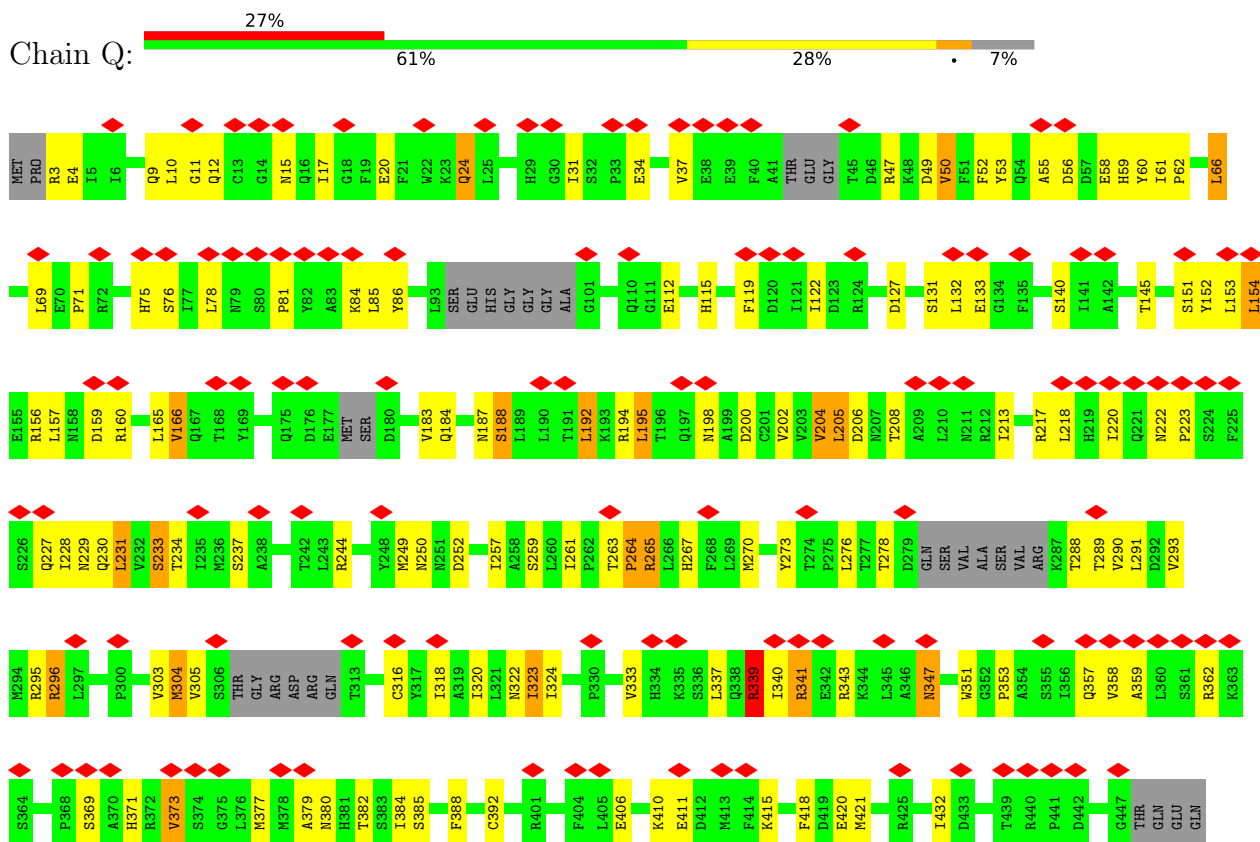
• Molecule 7: Gamma-tubulin complex component 6



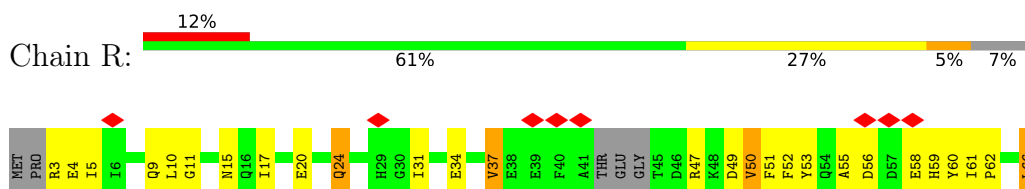


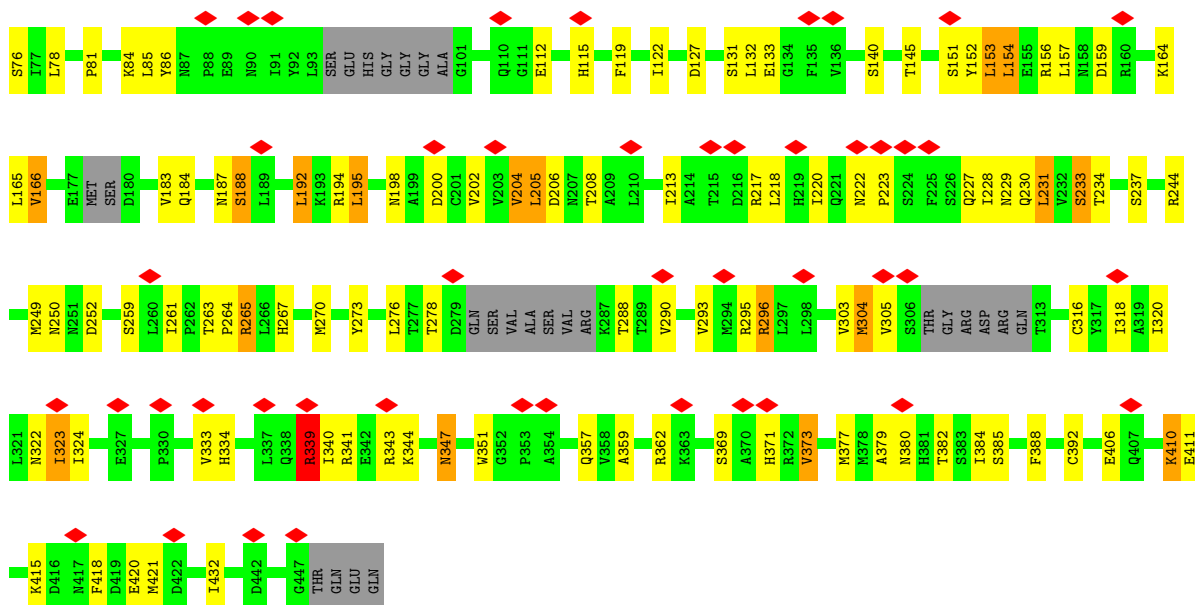
[illegible]

- Molecule 8: Tubulin gamma-1 chain



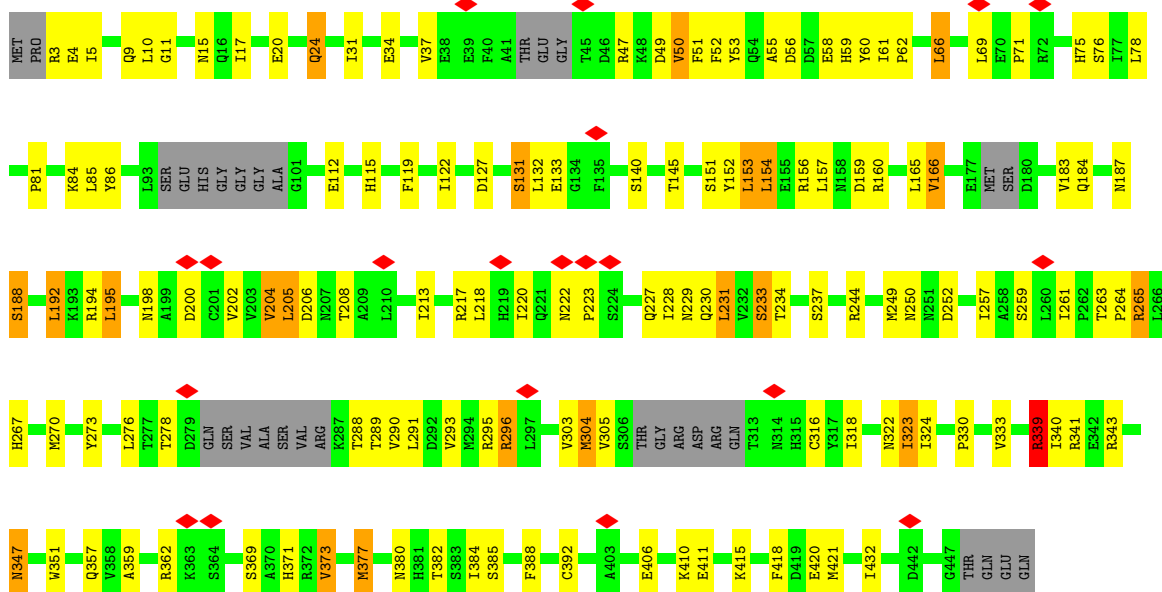
- Molecule 8: Tubulin gamma-1 chain





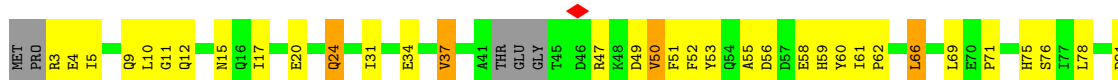
• Molecule 8: Tubulin gamma-1 chain

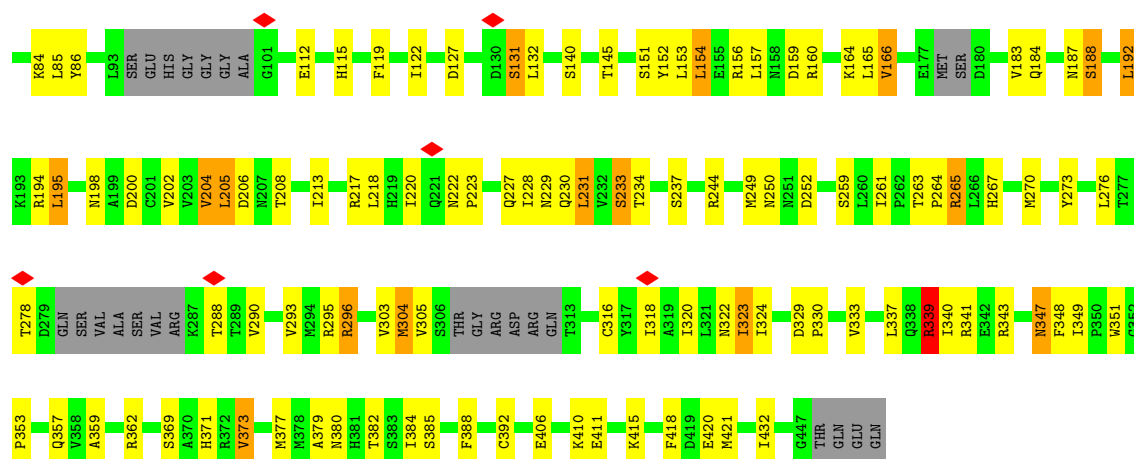
Chain S: 61% 27% 5% 7%



• Molecule 8: Tubulin gamma-1 chain

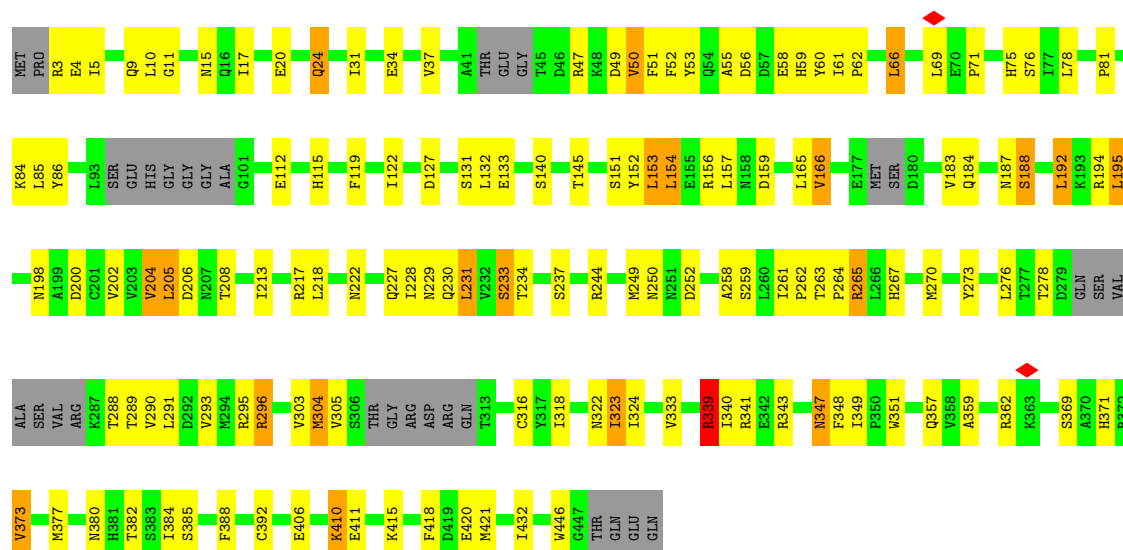
Chain T: 60% 28% 7%





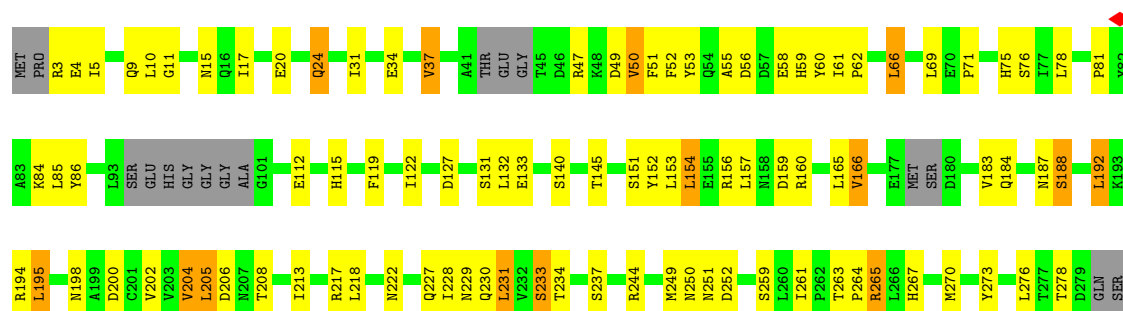
• Molecule 8: Tubulin gamma-1 chain

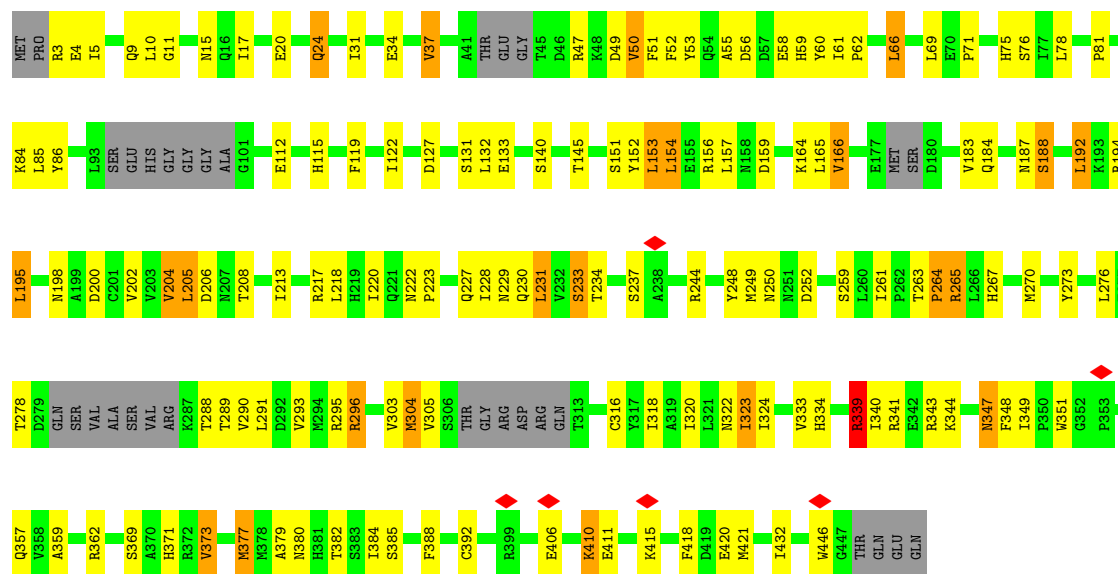
Chain U: 61% 27% 7%



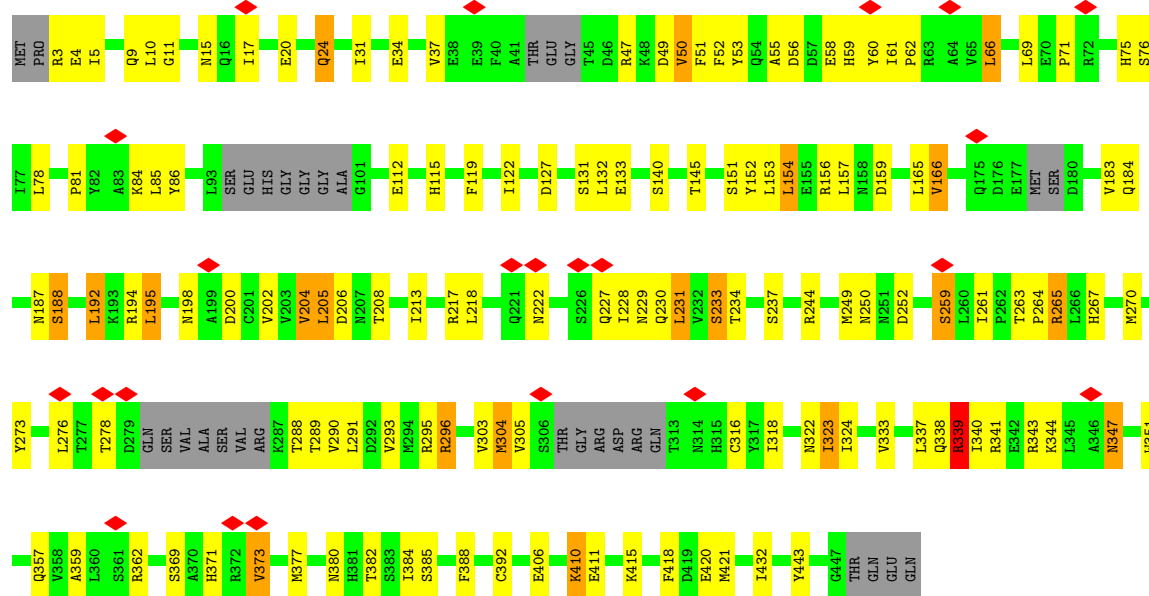
• Molecule 8: Tubulin gamma-1 chain

Chain V: 61% 27% 7%





• 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	21860	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	0.329	Depositor
Minimum map value	-0.148	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.0299	Depositor
Map size ($\text{\AA}$)	532.0, 532.0, 532.0	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	2.66, 2.66, 2.66	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	J	0.41	0/4525	0.82	3/6119 (0.0%)
1	l	0.35	0/863	0.84	2/1166 (0.2%)
2	e	0.51	1/2908 (0.0%)	0.79	0/3938
3	b	0.36	0/484	0.76	0/653
3	d	0.38	0/454	0.79	0/611
3	i	0.35	0/484	0.69	0/653
3	k	0.36	0/484	0.71	0/653
3	m	0.31	0/484	0.68	0/653
4	D	0.36	0/4897	0.77	4/6610 (0.1%)
4	F	0.35	0/5044	0.75	2/6809 (0.0%)
4	H	0.41	0/5009	0.80	4/6761 (0.1%)
4	a	0.41	0/948	0.81	1/1277 (0.1%)
4	h	0.33	0/815	0.71	0/1096
4	j	0.33	0/855	0.83	3/1152 (0.3%)
5	C	0.40	1/5151 (0.0%)	0.83	6/6955 (0.1%)
5	E	0.37	0/5311	0.78	5/7169 (0.1%)
5	G	0.38	0/5315	0.77	6/7175 (0.1%)
6	I	0.43	0/4322	0.80	8/5853 (0.1%)
6	K	0.43	1/4683 (0.0%)	0.83	10/6338 (0.2%)
7	L	0.36	0/4697	0.74	0/6348
7	c	0.36	0/1235	0.78	0/1664
8	Q	0.30	0/3441	0.72	1/4661 (0.0%)
8	R	0.30	0/3441	0.72	1/4661 (0.0%)
8	S	0.30	0/3441	0.72	1/4661 (0.0%)
8	T	0.30	0/3441	0.72	1/4661 (0.0%)
8	U	0.30	0/3441	0.72	1/4661 (0.0%)
8	V	0.30	0/3441	0.72	1/4661 (0.0%)
8	W	0.30	0/3441	0.72	1/4661 (0.0%)
8	X	0.30	0/3441	0.72	1/4661 (0.0%)
8	Y	0.30	0/3441	0.72	1/4661 (0.0%)
8	Z	0.30	0/3441	0.72	1/4661 (0.0%)
All	All	0.36	3/93378 (0.0%)	0.76	64/126263 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	J	0	4
2	e	0	1
4	D	0	1
4	F	0	1
4	H	0	5
5	C	0	1
5	E	0	1
5	G	0	3
6	I	0	2
6	K	0	4
8	Q	0	2
8	R	0	2
8	S	0	2
8	T	0	2
8	U	0	2
8	V	0	2
8	W	0	2
8	X	0	2
8	Y	0	2
8	Z	0	2
All	All	0	43

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	e	243	PRO	N-CD	18.08	1.73	1.47
5	C	236	GLN	C-N	6.29	1.41	1.33
6	K	651	TYR	CB-CG	-5.37	1.39	1.51

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	418	ILE	N-CA-C	-9.69	104.06	111.90
5	E	719	ILE	N-CA-C	-8.44	104.40	111.91
8	S	339	ARG	NE-CZ-NH2	7.88	126.29	119.20
8	V	339	ARG	NE-CZ-NH2	7.87	126.28	119.20
8	T	339	ARG	NE-CZ-NH2	7.87	126.28	119.20
8	W	339	ARG	NE-CZ-NH2	7.84	126.26	119.20
8	Z	339	ARG	NE-CZ-NH2	7.84	126.26	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	X	339	ARG	NE-CZ-NH2	7.84	126.25	119.20
8	U	339	ARG	NE-CZ-NH2	7.82	126.23	119.20
8	Y	339	ARG	NE-CZ-NH2	7.81	126.23	119.20
8	Q	339	ARG	NE-CZ-NH2	7.81	126.23	119.20
8	R	339	ARG	NE-CZ-NH2	7.81	126.23	119.20
5	C	464	GLY	CA-C-N	7.59	136.04	121.54
5	C	464	GLY	C-N-CA	7.59	136.04	121.54
4	j	104	PRO	CA-C-N	7.22	135.32	121.54
4	j	104	PRO	C-N-CA	7.22	135.32	121.54
5	E	424	ASN	N-CA-C	-6.94	104.32	114.39
1	l	121	PRO	N-CA-CB	6.90	110.50	103.25
1	l	130	PRO	N-CA-CB	6.89	110.58	103.00
6	K	651	TYR	CA-CB-CG	-6.84	101.59	113.90
6	I	475	TYR	CA-CB-CG	6.82	126.18	113.90
5	C	467	VAL	N-CA-C	-6.74	106.73	113.20
5	G	580	HIS	CA-C-N	6.66	134.26	121.54
5	G	580	HIS	C-N-CA	6.66	134.26	121.54
4	j	108	PRO	N-CA-CB	6.59	109.78	103.19
6	I	131	LEU	N-CA-C	-6.30	104.56	112.93
6	I	600	ASN	CA-C-N	6.26	133.50	121.54
6	I	600	ASN	C-N-CA	6.26	133.50	121.54
5	C	238	LEU	CA-C-N	6.21	133.39	121.54
5	C	238	LEU	C-N-CA	6.21	133.39	121.54
5	G	264	LEU	N-CA-C	6.13	122.03	113.57
4	H	692	ARG	N-CA-C	-6.05	106.51	114.31
5	C	237	PRO	N-CA-C	6.00	120.63	111.15
1	J	713	ASP	CA-C-N	5.98	132.97	121.54
1	J	713	ASP	C-N-CA	5.98	132.97	121.54
6	K	203	PHE	CA-C-N	5.92	132.86	121.54
6	K	203	PHE	C-N-CA	5.92	132.86	121.54
5	E	579	PRO	CA-C-N	5.85	132.71	121.54
5	E	579	PRO	C-N-CA	5.85	132.71	121.54
5	E	565	ASN	N-CA-C	-5.81	105.08	114.09
4	D	581	LEU	CA-CB-CG	5.76	136.46	116.30
4	F	879	ARG	CG-CD-NE	5.75	124.66	112.00
6	K	524	LEU	CB-CG-CD1	-5.64	93.79	110.70
4	H	455	LYS	CA-CB-CG	5.58	125.26	114.10
6	K	467	PHE	CA-C-N	5.48	128.99	120.60
6	K	467	PHE	C-N-CA	5.48	128.99	120.60
5	G	368	GLY	CA-C-N	5.46	131.98	121.54
5	G	368	GLY	C-N-CA	5.46	131.98	121.54
4	H	886	TYR	CA-C-N	5.45	131.96	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	886	TYR	C-N-CA	5.45	131.96	121.54
6	K	646	LEU	N-CA-CB	-5.45	101.25	110.41
4	D	888	ALA	CA-C-N	5.40	131.85	121.54
4	D	888	ALA	C-N-CA	5.40	131.85	121.54
4	F	317	PHE	N-CA-C	-5.34	104.48	112.54
6	I	162	CYS	CA-C-N	5.32	131.84	121.41
6	I	162	CYS	C-N-CA	5.32	131.84	121.41
6	I	503	LYS	N-CA-C	-5.31	105.08	112.30
6	K	29	GLN	N-CA-CB	5.31	119.46	110.49
6	K	409	ASN	CA-C-N	5.26	131.59	121.54
6	K	409	ASN	C-N-CA	5.26	131.59	121.54
6	I	386	ALA	N-CA-C	-5.13	108.04	114.56
5	G	862	ASN	N-CA-C	-5.09	106.89	114.64
1	J	224	TYR	OH-CZ-CE2	-5.06	104.71	119.90
4	a	50	ASP	N-CA-C	5.03	115.75	107.20

There are no chirality outliers.

All (43) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	C	464	GLY	Peptide
4	D	888	ALA	Peptide
5	E	370	SER	Peptide
4	F	269	ASN	Peptide
5	G	240	GLY	Peptide
5	G	580	HIS	Peptide
5	G	581	ASP	Mainchain
4	H	453	THR	Peptide
4	H	454	VAL	Mainchain,Peptide
4	H	637	VAL	Peptide
4	H	740	GLN	Peptide
6	I	600	ASN	Peptide
6	I	601	LEU	Peptide
1	J	235	SER	Peptide
1	J	237	HIS	Peptide
1	J	256	LEU	Peptide
1	J	726	PHE	Peptide
6	K	28	SER	Peptide
6	K	408	ASP	Peptide
6	K	409	ASN	Mainchain
6	K	638	ILE	Peptide
8	Q	264	PRO	Peptide

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Mol	Chain	Res	Type	Group
8	Q	406	GLU	Peptide
8	R	264	PRO	Peptide
8	R	406	GLU	Peptide
8	S	264	PRO	Peptide
8	S	406	GLU	Peptide
8	T	264	PRO	Peptide
8	T	406	GLU	Peptide
8	U	264	PRO	Peptide
8	U	406	GLU	Peptide
8	V	264	PRO	Peptide
8	V	406	GLU	Peptide
8	W	264	PRO	Peptide
8	W	406	GLU	Peptide
8	X	264	PRO	Peptide
8	X	406	GLU	Peptide
8	Y	264	PRO	Peptide
8	Y	406	GLU	Peptide
8	Z	264	PRO	Peptide
8	Z	406	GLU	Peptide
2	e	200	PHE	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J	4429	0	4482	44	0
1	l	847	0	789	11	0
2	e	2847	0	2810	63	0
3	b	484	0	512	11	0
3	d	454	0	482	10	0
3	i	484	0	512	3	0
3	k	484	0	512	6	0
3	m	484	0	512	8	0
4	D	4796	0	4775	54	0
4	F	4941	0	4935	50	0
4	H	4907	0	4896	61	0
4	a	933	0	953	12	0
4	h	803	0	831	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	j	843	0	846	8	0
5	C	5044	0	5081	72	0
5	E	5202	0	5241	59	0
5	G	5206	0	5230	63	0
6	I	4225	0	4259	51	0
6	K	4579	0	4586	52	0
7	L	4587	0	4636	50	0
7	c	1220	0	1231	22	0
8	Q	3373	0	3325	72	0
8	R	3373	0	3325	74	0
8	S	3373	0	3325	69	0
8	T	3373	0	3325	75	0
8	U	3373	0	3325	73	0
8	V	3373	0	3325	77	0
8	W	3373	0	3325	74	0
8	X	3373	0	3325	77	0
8	Y	3373	0	3325	79	0
8	Z	3373	0	3325	71	0
9	l	6	0	0	1	0
All	All	91535	0	91361	1357	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (1357) 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)
2:e:243:PRO:CD	2:e:243:PRO:N	1.73	1.43
2:e:242:LEU:HD12	2:e:243:PRO:CD	1.69	1.22
2:e:242:LEU:HD12	2:e:243:PRO:HD3	1.32	1.09
2:e:153:MET:SD	2:e:162:THR:HB	1.94	1.07
2:e:242:LEU:CD1	2:e:243:PRO:HD2	1.98	0.93
2:e:242:LEU:HD12	2:e:243:PRO:HD2	1.50	0.92
2:e:242:LEU:CD1	2:e:243:PRO:CD	2.50	0.89
4:F:879:ARG:HD2	8:T:337:LEU:HD23	1.58	0.83
8:W:56:ASP:HB2	8:X:296:ARG:HD2	1.62	0.81
5:E:578:MET:HE2	5:E:616:PHE:H	1.48	0.77
5:E:734:LEU:HB2	5:E:739:LEU:HD11	1.69	0.75
5:G:560:ARG:HB2	8:V:339:ARG:HE	1.52	0.74
2:e:155:SER:HA	2:e:160:THR:HG22	1.69	0.74
5:E:696:TYR:O	5:E:700:GLU:HB2	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:159:LYS:NZ	5:C:160:MET:SD	2.64	0.70
4:H:865:LEU:HD22	4:H:877:SER:HB3	1.72	0.70
2:e:269:MET:HE2	2:e:271:SER:OG	1.90	0.70
5:E:381:LYS:HG2	5:E:477:TYR:HB3	1.73	0.69
1:J:238:LEU:H	1:J:241:ASN:HB3	1.56	0.69
4:H:253:ASP:HB3	4:H:266:ILE:HG22	1.76	0.68
6:K:78:GLN:HE21	6:K:80:GLY:H	1.42	0.67
6:I:540:GLN:HG3	6:I:571:GLN:HE22	1.59	0.67
4:H:572:ASP:OD1	8:V:251:ASN:ND2	2.28	0.67
1:J:272:ARG:HH12	1:J:387:ILE:HG13	1.60	0.67
5:G:238:LEU:HG	5:G:240:GLY:H	1.60	0.67
4:D:862:LEU:HD21	4:D:880:LEU:HB3	1.77	0.67
8:S:347:ASN:OD1	8:S:347:ASN:N	2.29	0.66
8:T:347:ASN:OD1	8:T:347:ASN:N	2.29	0.66
8:W:347:ASN:OD1	8:W:347:ASN:N	2.29	0.66
2:e:269:MET:HG2	2:e:271:SER:OG	1.96	0.66
8:V:347:ASN:OD1	8:V:347:ASN:N	2.29	0.66
4:H:364:LEU:HD22	4:H:370:TRP:HE1	1.60	0.66
5:C:706:TRP:HA	5:C:709:LEU:HD12	1.77	0.66
5:G:370:SER:HA	5:G:373:GLN:HG2	1.78	0.66
8:X:47:ARG:HD3	8:X:50:VAL:HG13	1.79	0.65
8:Y:347:ASN:OD1	8:Y:347:ASN:N	2.29	0.65
8:Z:347:ASN:OD1	8:Z:347:ASN:N	2.29	0.65
8:R:347:ASN:OD1	8:R:347:ASN:N	2.29	0.65
8:U:47:ARG:HD3	8:U:50:VAL:HG13	1.79	0.65
7:c:70:ILE:HG21	7:c:93:VAL:HG11	1.77	0.65
8:W:47:ARG:HD3	8:W:50:VAL:HG13	1.79	0.65
4:F:840:ILE:HG13	4:F:841:PRO:HD3	1.79	0.65
5:G:222:LEU:HD11	4:H:365:ARG:HH12	1.60	0.65
8:U:347:ASN:OD1	8:U:347:ASN:N	2.29	0.65
8:Q:347:ASN:OD1	8:Q:347:ASN:N	2.29	0.65
8:Y:47:ARG:HD3	8:Y:50:VAL:HG13	1.79	0.65
6:I:361:TYR:CE2	6:I:475:TYR:HB3	2.31	0.64
8:S:47:ARG:HD3	8:S:50:VAL:HG13	1.79	0.64
8:V:295:ARG:HB3	8:V:296:ARG:HH21	1.63	0.64
8:X:295:ARG:HB3	8:X:296:ARG:HH21	1.63	0.64
2:e:213:LYS:NZ	2:e:257:CYS:SG	2.70	0.64
8:T:47:ARG:HD3	8:T:50:VAL:HG13	1.79	0.64
8:U:295:ARG:HB3	8:U:296:ARG:HH21	1.63	0.64
8:V:47:ARG:HD3	8:V:50:VAL:HG13	1.79	0.64
8:R:47:ARG:HD3	8:R:50:VAL:HG13	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Q:47:ARG:HD3	8:Q:50:VAL:HG13	1.79	0.64
8:Z:47:ARG:HD3	8:Z:50:VAL:HG13	1.79	0.64
4:F:343:HIS:HB3	5:G:323:LYS:HZ1	1.63	0.64
8:T:295:ARG:HB3	8:T:296:ARG:HH21	1.63	0.63
6:K:406:ASP:OD2	8:Z:339:ARG:NH1	2.30	0.63
8:W:263:THR:HG1	8:W:265:ARG:HH11	1.44	0.63
8:Z:295:ARG:HB3	8:Z:296:ARG:HH21	1.63	0.63
4:D:763:LEU:HD21	4:D:873:LEU:HD11	1.81	0.63
8:R:295:ARG:HB3	8:R:296:ARG:HH21	1.63	0.63
8:S:295:ARG:HB3	8:S:296:ARG:HH21	1.63	0.63
3:b:25:MET:HE1	3:b:44:LEU:HD22	1.79	0.63
5:C:527:PHE:O	5:C:531:PHE:HB2	1.98	0.63
5:C:862:ASN:HB2	5:C:864:PHE:HE2	1.64	0.63
1:J:467:GLU:HG3	1:J:470:ARG:HH22	1.63	0.63
8:W:295:ARG:HB3	8:W:296:ARG:HH21	1.63	0.63
8:X:347:ASN:N	8:X:347:ASN:OD1	2.29	0.63
6:I:367:GLU:OE1	8:W:251:ASN:ND2	2.28	0.62
5:G:359:LEU:HB3	5:G:380:THR:HG22	1.80	0.62
8:Q:295:ARG:HB3	8:Q:296:ARG:HH21	1.63	0.62
4:D:773:ASN:HA	4:D:776:ARG:HE	1.63	0.62
8:Y:343:ARG:O	8:Y:343:ARG:NH2	2.33	0.62
8:Y:295:ARG:HB3	8:Y:296:ARG:HH21	1.63	0.62
5:E:860:ASP:HB3	5:E:866:THR:HG22	1.82	0.62
8:R:343:ARG:NH2	8:R:343:ARG:O	2.33	0.62
4:D:759:ILE:HA	4:D:764:LEU:HD21	1.82	0.61
4:D:830:ASN:HA	4:D:833:ILE:HD12	1.81	0.61
6:I:540:GLN:OE1	6:I:543:GLN:NE2	2.33	0.61
8:V:343:ARG:O	8:V:343:ARG:NH2	2.33	0.61
8:X:343:ARG:O	8:X:343:ARG:NH2	2.33	0.61
6:I:504:HIS:CE1	8:W:158:ASN:HD21	2.18	0.61
8:W:343:ARG:NH2	8:W:343:ARG:O	2.33	0.61
8:Z:183:VAL:HG13	8:Z:187:ASN:HD21	1.66	0.61
8:U:343:ARG:NH2	8:U:343:ARG:O	2.33	0.60
7:L:1800:LEU:HD21	8:Z:337:LEU:HB3	1.83	0.60
8:U:183:VAL:HG13	8:U:187:ASN:HD21	1.66	0.60
7:L:1736:VAL:HG12	7:L:1740:ARG:HH11	1.67	0.60
7:L:1803:ASN:ND2	7:L:1806:ASN:O	2.34	0.60
8:V:183:VAL:HG13	8:V:187:ASN:HD21	1.66	0.60
5:C:862:ASN:HA	8:Q:341:ARG:HG2	1.83	0.60
8:R:183:VAL:HG13	8:R:187:ASN:HD21	1.66	0.60
8:Y:183:VAL:HG13	8:Y:187:ASN:HD21	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Q:411:GLU:HB3	8:Q:418:PHE:HE2	1.67	0.60
8:T:183:VAL:HG13	8:T:187:ASN:HD21	1.66	0.60
8:X:411:GLU:HB3	8:X:418:PHE:HE2	1.67	0.60
8:T:411:GLU:HB3	8:T:418:PHE:HE2	1.67	0.60
8:Y:411:GLU:HB3	8:Y:418:PHE:HE2	1.67	0.60
5:G:447:ALA:HA	5:G:450:ILE:HD12	1.82	0.60
8:Q:183:VAL:HG13	8:Q:187:ASN:HD21	1.67	0.60
8:Q:343:ARG:O	8:Q:343:ARG:NH2	2.33	0.60
4:a:35:ALA:HA	4:a:38:VAL:HG22	1.83	0.60
5:G:574:LYS:HG2	5:G:619:ASP:HB3	1.82	0.60
8:T:343:ARG:O	8:T:343:ARG:NH2	2.33	0.60
8:Z:343:ARG:NH2	8:Z:343:ARG:O	2.33	0.60
5:G:613:LEU:HD12	5:G:614:GLU:HG3	1.84	0.59
8:S:343:ARG:O	8:S:343:ARG:NH2	2.33	0.59
5:C:291:ALA:HA	5:C:294:ALA:HB3	1.84	0.59
5:C:560:ARG:HB2	8:R:339:ARG:HE	1.67	0.59
8:R:411:GLU:HB3	8:R:418:PHE:HE2	1.67	0.59
6:I:458:LYS:HE3	6:I:461:TRP:HZ2	1.68	0.59
6:I:486:ARG:NH1	8:W:248:TYR:O	2.33	0.59
8:W:183:VAL:HG13	8:W:187:ASN:HD21	1.67	0.59
8:X:183:VAL:HG13	8:X:187:ASN:HD21	1.67	0.59
8:Z:263:THR:OG1	8:Z:265:ARG:NH1	2.36	0.59
8:Z:411:GLU:HB3	8:Z:418:PHE:HE2	1.67	0.59
1:J:404:PRO:HB2	1:J:405:ARG:HH11	1.67	0.59
7:L:324:CYS:HG	7:L:390:PRO:N	2.01	0.59
8:W:263:THR:OG1	8:W:265:ARG:NH1	2.36	0.59
8:Q:263:THR:OG1	8:Q:265:ARG:NH1	2.36	0.59
8:R:263:THR:OG1	8:R:265:ARG:NH1	2.36	0.59
8:S:263:THR:OG1	8:S:265:ARG:NH1	2.36	0.59
2:e:348:SER:O	7:c:39:LYS:NZ	2.31	0.59
5:C:738:MET:SD	5:C:738:MET:N	2.75	0.59
5:E:205:ILE:HG23	5:E:207:THR:H	1.66	0.59
8:S:183:VAL:HG13	8:S:187:ASN:HD21	1.66	0.59
4:D:401:HIS:O	4:D:405:LYS:NZ	2.36	0.58
5:G:494:TYR:HA	5:G:497:LYS:HE2	1.85	0.58
8:W:411:GLU:HB3	8:W:418:PHE:HE2	1.67	0.58
5:G:159:LYS:HB2	5:G:160:MET:HE2	1.84	0.58
5:G:557:LEU:O	8:V:339:ARG:NH1	2.36	0.58
7:L:293:LYS:HZ3	7:L:295:ARG:HD3	1.68	0.58
2:e:153:MET:SD	2:e:162:THR:CB	2.83	0.58
4:F:337:ARG:HH21	7:c:148:TYR:HD1	1.50	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:433:TRP:HE1	4:H:484:LEU:HA	1.69	0.58
1:J:225:TRP:HE1	6:K:35:HIS:CG	2.20	0.58
8:S:411:GLU:HB3	8:S:418:PHE:HE2	1.67	0.58
8:T:263:THR:OG1	8:T:265:ARG:NH1	2.36	0.58
8:U:411:GLU:HB3	8:U:418:PHE:HE2	1.67	0.58
2:e:130:PRO:HA	2:e:359:LYS:HE2	1.85	0.58
4:F:454:VAL:HG12	4:F:459:LEU:HD22	1.86	0.58
5:G:688:ASN:HD21	8:U:357:GLN:HE22	1.51	0.58
3:m:47:CYS:HA	3:m:50:LEU:HD12	1.86	0.58
8:Z:166:VAL:HG13	8:Z:200:ASP:H	1.69	0.58
6:I:357:ILE:O	6:I:361:TYR:HB3	2.03	0.58
8:R:166:VAL:HG13	8:R:200:ASP:H	1.69	0.57
8:V:411:GLU:HB3	8:V:418:PHE:HE2	1.67	0.57
8:Y:166:VAL:HG13	8:Y:200:ASP:H	1.69	0.57
6:K:510:THR:HG1	8:Y:446:TRP:CD1	2.22	0.57
8:V:166:VAL:HG13	8:V:200:ASP:H	1.69	0.57
5:E:652:GLU:HA	5:E:655:LEU:HD12	1.84	0.57
8:U:166:VAL:HG13	8:U:200:ASP:H	1.69	0.57
8:S:166:VAL:HG13	8:S:200:ASP:H	1.69	0.57
5:C:448:ASP:N	5:C:448:ASP:OD1	2.37	0.57
8:T:227:GLN:HA	8:T:230:GLN:HG2	1.86	0.57
8:U:263:THR:OG1	8:U:265:ARG:NH1	2.36	0.57
8:U:323:ILE:HG13	8:U:359:ALA:HB3	1.87	0.57
8:V:227:GLN:HA	8:V:230:GLN:HG2	1.86	0.57
8:V:323:ILE:HG13	8:V:359:ALA:HB3	1.87	0.57
5:E:738:MET:SD	5:E:738:MET:N	2.78	0.57
4:F:677:LEU:HB2	4:F:782:ILE:HD11	1.85	0.57
4:H:737:LYS:NZ	4:H:750:ALA:O	2.36	0.57
8:U:227:GLN:HA	8:U:230:GLN:HG2	1.86	0.57
5:C:840:LEU:HB3	5:C:856:ILE:HD11	1.87	0.57
5:E:224:VAL:HG21	5:E:233:VAL:HG13	1.85	0.57
4:H:481:ARG:HB3	4:H:482:LYS:HZ2	1.69	0.57
8:R:229:ASN:O	8:R:233:SER:OG	2.23	0.57
4:D:542:SER:HA	4:D:545:LEU:HD12	1.86	0.57
6:K:650:ASP:HB3	6:K:651:TYR:CZ	2.40	0.57
8:X:166:VAL:HG13	8:X:200:ASP:H	1.69	0.57
8:X:263:THR:OG1	8:X:265:ARG:NH1	2.36	0.57
5:G:307:VAL:O	4:H:365:ARG:NH1	2.37	0.57
6:K:513:ILE:HA	6:K:516:ARG:HD2	1.86	0.57
8:Q:323:ILE:HG13	8:Q:359:ALA:HB3	1.87	0.57
8:S:227:GLN:HA	8:S:230:GLN:HG2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:k:63:VAL:HG12	4:j:38:VAL:HG11	1.86	0.57
6:I:129:PHE:HA	6:I:132:LEU:HB2	1.86	0.57
8:V:263:THR:OG1	8:V:265:ARG:NH1	2.36	0.57
8:W:166:VAL:HG13	8:W:200:ASP:H	1.69	0.57
2:e:263:GLN:HE21	2:e:266:PHE:HB2	1.70	0.56
4:D:865:LEU:HD11	4:D:873:LEU:HB3	1.86	0.56
4:h:51:GLU:HG2	4:h:90:LYS:HB2	1.86	0.56
8:Y:263:THR:OG1	8:Y:265:ARG:NH1	2.36	0.56
8:Z:323:ILE:HG13	8:Z:359:ALA:HB3	1.87	0.56
8:Q:227:GLN:HA	8:Q:230:GLN:HG2	1.86	0.56
8:W:56:ASP:HB2	8:X:296:ARG:CD	2.33	0.56
5:C:580:HIS:HB3	5:C:583:ILE:HG22	1.87	0.56
5:C:862:ASN:HB2	5:C:864:PHE:CE2	2.41	0.56
5:E:741:ASN:HD22	5:E:745:LEU:H	1.51	0.56
4:F:454:VAL:HB	4:F:463:LYS:HD2	1.87	0.56
8:Q:166:VAL:HG13	8:Q:200:ASP:H	1.69	0.56
8:R:227:GLN:HA	8:R:230:GLN:HG2	1.86	0.56
8:W:323:ILE:HG13	8:W:359:ALA:HB3	1.87	0.56
8:X:323:ILE:HG13	8:X:359:ALA:HB3	1.87	0.56
8:Y:323:ILE:HG13	8:Y:359:ALA:HB3	1.87	0.56
1:J:942:LEU:HB3	1:J:951:LYS:HD3	1.88	0.56
2:e:299:LEU:HD23	2:e:310:ALA:HB1	1.88	0.56
5:E:653:ARG:HH12	5:E:657:SER:HB3	1.69	0.56
5:G:687:LEU:HD11	8:U:258:ALA:HB1	1.88	0.56
8:S:323:ILE:HG13	8:S:359:ALA:HB3	1.87	0.56
4:F:860:GLN:HE21	4:F:864:LEU:HG	1.70	0.56
6:I:514:LYS:HG2	6:I:516:ARG:H	1.70	0.56
8:V:318:ILE:HD11	8:V:382:THR:HG23	1.88	0.56
8:W:227:GLN:HA	8:W:230:GLN:HG2	1.86	0.56
8:Y:53:TYR:O	8:Y:61:ILE:N	2.38	0.56
8:Y:227:GLN:HA	8:Y:230:GLN:HG2	1.86	0.56
4:F:333:ARG:HH21	4:F:334:GLU:HG3	1.69	0.56
8:Z:227:GLN:HA	8:Z:230:GLN:HG2	1.86	0.56
8:Z:229:ASN:O	8:Z:233:SER:OG	2.23	0.56
8:U:318:ILE:HD11	8:U:382:THR:HG23	1.88	0.56
8:Y:318:ILE:HD11	8:Y:382:THR:HG23	1.88	0.56
5:C:393:LYS:HD2	5:C:400:ILE:HD12	1.86	0.56
5:E:710:GLU:HB2	5:E:711:LYS:HZ2	1.71	0.55
8:R:323:ILE:HG13	8:R:359:ALA:HB3	1.87	0.55
8:T:323:ILE:HG13	8:T:359:ALA:HB3	1.87	0.55
8:W:4:GLU:OE2	8:W:47:ARG:NH2	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:d:67:LEU:HD11	7:c:12:CYS:HA	1.88	0.55
8:T:166:VAL:HG13	8:T:200:ASP:H	1.69	0.55
8:U:4:GLU:OE2	8:U:47:ARG:NH2	2.40	0.55
8:U:213:ILE:HD13	8:U:304:MET:HE3	1.89	0.55
8:X:227:GLN:HA	8:X:230:GLN:HG2	1.86	0.55
8:Z:213:ILE:HD13	8:Z:304:MET:HE3	1.89	0.55
4:H:720:TYR:HE2	8:V:357:GLN:HB3	1.71	0.55
8:X:4:GLU:OE2	8:X:47:ARG:NH2	2.40	0.55
8:Y:4:GLU:OE2	8:Y:47:ARG:NH2	2.40	0.55
8:Z:318:ILE:HB	8:Z:380:ASN:HB3	1.89	0.55
5:G:321:LEU:HA	5:G:324:LEU:HD12	1.88	0.55
4:H:589:ALA:HA	4:H:592:LEU:HG	1.88	0.55
8:R:318:ILE:HD11	8:R:382:THR:HG23	1.88	0.55
8:T:4:GLU:OE2	8:T:47:ARG:NH2	2.40	0.55
6:K:45:LEU:HD22	6:K:126:LEU:HD23	1.89	0.55
8:Q:213:ILE:HD13	8:Q:304:MET:HE3	1.89	0.55
8:V:4:GLU:OE2	8:V:47:ARG:NH2	2.40	0.55
8:X:318:ILE:HD11	8:X:382:THR:HG23	1.88	0.55
8:Z:4:GLU:OE2	8:Z:47:ARG:NH2	2.40	0.55
4:D:489:SER:HB2	4:D:545:LEU:HD21	1.88	0.55
8:R:4:GLU:OE2	8:R:47:ARG:NH2	2.40	0.55
8:S:4:GLU:OE2	8:S:47:ARG:NH2	2.40	0.55
8:T:318:ILE:HB	8:T:380:ASN:HB3	1.89	0.55
8:Y:213:ILE:HD13	8:Y:304:MET:HE3	1.89	0.55
8:Z:318:ILE:HD11	8:Z:382:THR:HG23	1.88	0.55
5:G:707:HIS:O	5:G:711:LYS:NZ	2.39	0.55
6:K:105:LEU:HD11	7:L:458:THR:HG22	1.87	0.55
8:W:213:ILE:HD13	8:W:304:MET:HE3	1.89	0.55
8:X:318:ILE:HB	8:X:380:ASN:HB3	1.89	0.55
6:K:514:LYS:HE3	6:K:612:LEU:HD21	1.88	0.55
8:S:318:ILE:HB	8:S:380:ASN:HB3	1.89	0.55
8:Y:318:ILE:HB	8:Y:380:ASN:HB3	1.89	0.55
1:I:62:GLU:HA	1:I:65:ILE:HD12	1.89	0.55
1:J:272:ARG:HE	7:L:308:GLU:HG3	1.72	0.55
1:J:881:HIS:CE1	8:X:446:TRP:HB3	2.42	0.55
7:L:1514:HIS:HA	7:L:1519:GLU:H	1.72	0.55
8:T:213:ILE:HD13	8:T:304:MET:HE3	1.89	0.55
8:W:318:ILE:HD11	8:W:382:THR:HG23	1.88	0.55
8:X:53:TYR:O	8:X:61:ILE:N	2.37	0.55
8:Y:229:ASN:O	8:Y:233:SER:OG	2.23	0.55
8:Z:47:ARG:HG2	8:Z:49:ASP:H	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:e:221:LEU:HD11	2:e:315:LYS:HG3	1.89	0.54
4:H:427:LEU:HA	4:H:430:LEU:HG	1.88	0.54
8:Q:4:GLU:OE2	8:Q:47:ARG:NH2	2.40	0.54
8:T:318:ILE:HD11	8:T:382:THR:HG23	1.88	0.54
8:V:47:ARG:HG2	8:V:49:ASP:H	1.73	0.54
8:W:47:ARG:HG2	8:W:49:ASP:H	1.72	0.54
6:K:356:ILE:HD11	6:K:410:LEU:HD13	1.88	0.54
8:R:53:TYR:O	8:R:61:ILE:N	2.37	0.54
8:X:213:ILE:HD13	8:X:304:MET:HE3	1.89	0.54
8:Y:47:ARG:HG2	8:Y:49:ASP:H	1.73	0.54
5:G:697:MET:HB3	5:G:702:MET:HE1	1.89	0.54
6:I:404:LEU:HD21	8:W:47:ARG:HG3	1.89	0.54
8:Q:47:ARG:HG2	8:Q:49:ASP:H	1.73	0.54
8:S:47:ARG:HG2	8:S:49:ASP:H	1.73	0.54
8:X:229:ASN:O	8:X:233:SER:OG	2.23	0.54
5:E:187:LEU:HD22	4:F:379:LYS:HD3	1.90	0.54
5:E:417:GLU:HG2	5:E:418:ARG:HG3	1.90	0.54
8:Q:318:ILE:HB	8:Q:380:ASN:HB3	1.89	0.54
8:R:318:ILE:HB	8:R:380:ASN:HB3	1.89	0.54
8:V:213:ILE:HD13	8:V:304:MET:HE3	1.89	0.54
8:R:47:ARG:HG2	8:R:49:ASP:H	1.73	0.54
8:S:318:ILE:HD11	8:S:382:THR:HG23	1.88	0.54
8:W:318:ILE:HB	8:W:380:ASN:HB3	1.89	0.54
5:C:334:THR:HG23	5:C:375:LEU:HD22	1.89	0.54
4:D:762:CYS:SG	4:D:763:LEU:N	2.81	0.54
5:G:301:LYS:NZ	4:H:373:ASP:OD1	2.40	0.54
7:c:10:ASP:HA	7:c:13:GLU:HG3	1.89	0.54
4:D:253:ASP:HB3	4:D:266:ILE:HG22	1.90	0.54
8:U:318:ILE:HB	8:U:380:ASN:HB3	1.89	0.54
8:T:47:ARG:HG2	8:T:49:ASP:H	1.72	0.54
2:e:50:LYS:HD3	2:e:53:TYR:HB2	1.90	0.54
5:E:249:ASP:HB2	5:E:252:LEU:HD23	1.89	0.54
5:E:557:LEU:HA	8:T:339:ARG:NH1	2.23	0.54
8:V:318:ILE:HB	8:V:380:ASN:HB3	1.89	0.54
2:e:189:LEU:HD13	2:e:213:LYS:HD2	1.90	0.53
2:e:242:LEU:CG	2:e:243:PRO:HD2	2.37	0.53
4:H:869:SER:HB3	4:H:873:LEU:HG	1.90	0.53
4:D:559:MET:HE1	4:D:738:VAL:HG21	1.90	0.53
5:G:180:TRP:HA	5:G:183:GLU:HG2	1.89	0.53
8:Q:252:ASP:OD1	8:Q:252:ASP:N	2.42	0.53
8:Q:318:ILE:HD11	8:Q:382:THR:HG23	1.88	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:R:213:ILE:HD13	8:R:304:MET:HE3	1.89	0.53
7:L:510:LEU:HG	7:L:1475:LEU:H	1.74	0.53
4:F:622:ASP:OD2	4:F:622:ASP:N	2.40	0.53
6:K:260:ARG:HB3	6:K:262:GLU:HG2	1.90	0.53
5:C:581:ASP:HB2	5:C:610:LEU:HD11	1.90	0.53
4:F:677:LEU:HD21	4:F:712:VAL:HG22	1.90	0.53
6:I:192:LEU:HD12	6:I:304:GLU:HG2	1.90	0.53
1:J:287:PHE:HB3	1:J:294:VAL:HG23	1.91	0.53
1:l:80:LYS:NZ	1:l:123:ASN:O	2.42	0.53
2:e:8:LEU:HD23	2:e:103:VAL:HG22	1.90	0.53
8:X:53:TYR:N	8:X:61:ILE:O	2.42	0.53
8:X:418:PHE:HB3	8:X:421:MET:HE2	1.91	0.53
8:Z:418:PHE:HB3	8:Z:421:MET:HE2	1.91	0.53
5:C:231:ARG:NH2	5:C:232:TYR:OH	2.38	0.53
8:Q:229:ASN:O	8:Q:233:SER:OG	2.23	0.53
8:W:418:PHE:HB3	8:W:421:MET:HE2	1.91	0.53
4:H:847:LEU:HA	4:H:850:LEU:HD12	1.91	0.53
6:K:582:CYS:HB3	6:K:626:LEU:HD12	1.90	0.53
8:Q:53:TYR:N	8:Q:61:ILE:O	2.42	0.53
8:S:184:GLN:O	8:S:188:SER:OG	2.27	0.53
8:W:184:GLN:O	8:W:188:SER:OG	2.27	0.53
7:L:311:TYR:H	7:L:314:GLU:HB2	1.74	0.53
8:U:53:TYR:O	8:U:61:ILE:N	2.37	0.53
8:X:47:ARG:HG2	8:X:49:ASP:H	1.73	0.53
3:k:28:LEU:HD21	4:j:81:LEU:HD21	1.90	0.53
5:C:641:LEU:HG	5:C:734:LEU:HD13	1.90	0.53
4:F:424:HIS:HA	4:F:427:LEU:HG	1.90	0.53
4:F:613:ASP:HB3	4:F:617:ILE:HD11	1.90	0.53
5:G:501:ASP:HA	5:G:504:MET:HE2	1.91	0.53
6:I:577:LYS:O	6:I:581:HIS:ND1	2.41	0.53
8:Q:184:GLN:O	8:Q:188:SER:OG	2.27	0.53
8:S:213:ILE:HD13	8:S:304:MET:HE3	1.89	0.53
8:W:53:TYR:N	8:W:61:ILE:O	2.42	0.53
8:Y:418:PHE:HB3	8:Y:421:MET:HE2	1.91	0.53
8:R:184:GLN:O	8:R:188:SER:OG	2.27	0.52
8:Z:184:GLN:O	8:Z:188:SER:OG	2.27	0.52
8:X:184:GLN:O	8:X:188:SER:OG	2.27	0.52
6:I:102:GLN:HE22	6:I:105:LEU:HD23	1.74	0.52
6:I:416:LEU:HG	6:I:452:ALA:HB1	1.91	0.52
8:Z:53:TYR:O	8:Z:61:ILE:N	2.38	0.52
8:S:229:ASN:O	8:S:233:SER:OG	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:U:47:ARG:HG2	8:U:49:ASP:H	1.72	0.52
8:U:184:GLN:O	8:U:188:SER:OG	2.27	0.52
8:W:81:PRO:HA	8:W:84:LYS:HE2	1.92	0.52
8:S:418:PHE:HB3	8:S:421:MET:HE2	1.91	0.52
7:L:294:ARG:HG2	7:L:305:GLY:HA3	1.92	0.52
7:L:1510:GLU:HA	7:L:1513:ARG:HD3	1.92	0.52
8:Q:278:THR:HA	8:Q:371:HIS:HE1	1.75	0.52
8:U:56:ASP:O	8:U:58:GLU:N	2.43	0.52
8:U:278:THR:HA	8:U:371:HIS:HE1	1.75	0.52
5:E:277:ILE:HA	5:E:293:ALA:HB1	1.92	0.52
4:H:448:VAL:HG22	4:H:484:LEU:HD12	1.91	0.52
4:H:878:PHE:HB2	4:H:879:ARG:HH22	1.75	0.52
7:L:1677:ALA:HA	7:L:1681:LEU:HD12	1.92	0.52
8:Q:62:PRO:HD2	8:Q:86:TYR:HB3	1.92	0.52
8:S:278:THR:HA	8:S:371:HIS:HE1	1.75	0.52
8:X:50:VAL:HG21	8:X:244:ARG:HG2	1.92	0.52
3:b:47:CYS:HA	3:b:50:LEU:HD12	1.92	0.52
5:C:319:LEU:HD21	5:C:324:LEU:HD13	1.91	0.52
5:C:526:ASP:N	5:C:526:ASP:OD1	2.40	0.52
6:I:268:ILE:HG12	6:I:322:LEU:HD11	1.91	0.52
6:I:403:VAL:HG22	6:I:404:LEU:HG	1.91	0.52
8:R:53:TYR:N	8:R:61:ILE:O	2.42	0.52
8:R:418:PHE:HB3	8:R:421:MET:HE2	1.91	0.52
8:T:62:PRO:HD2	8:T:86:TYR:HB3	1.92	0.52
8:T:184:GLN:O	8:T:188:SER:OG	2.27	0.52
8:U:50:VAL:HG21	8:U:244:ARG:HG2	1.92	0.52
8:V:184:GLN:O	8:V:188:SER:OG	2.27	0.52
8:Z:62:PRO:HD2	8:Z:86:TYR:HB3	1.92	0.52
5:C:623:LYS:HG3	5:C:625:PRO:HG2	1.92	0.52
8:S:53:TYR:O	8:S:61:ILE:N	2.38	0.52
8:U:249:MET:HE3	8:U:250:ASN:H	1.75	0.52
8:V:62:PRO:HD2	8:V:86:TYR:HB3	1.92	0.52
8:W:62:PRO:HD2	8:W:86:TYR:HB3	1.92	0.52
8:Y:278:THR:HA	8:Y:371:HIS:HE1	1.75	0.52
5:G:585:GLN:HE22	5:G:739:LEU:HD12	1.75	0.52
4:H:798:GLU:HA	4:H:801:GLN:HE21	1.75	0.52
8:Q:418:PHE:HB3	8:Q:421:MET:HE2	1.91	0.52
8:R:278:THR:HA	8:R:371:HIS:HE1	1.75	0.52
8:T:229:ASN:O	8:T:233:SER:OG	2.23	0.52
8:V:81:PRO:HA	8:V:84:LYS:HE2	1.92	0.52
8:W:50:VAL:HG21	8:W:244:ARG:HG2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Y:53:TYR:N	8:Y:61:ILE:O	2.42	0.52
7:c:165:SER:HA	7:c:168:GLU:HG2	1.92	0.52
4:H:419:LEU:HA	4:H:422:VAL:HG22	1.92	0.51
8:R:81:PRO:HA	8:R:84:LYS:HE2	1.92	0.51
8:S:50:VAL:HG21	8:S:244:ARG:HG2	1.92	0.51
8:S:81:PRO:HA	8:S:84:LYS:HE2	1.92	0.51
8:T:81:PRO:HA	8:T:84:LYS:HE2	1.92	0.51
8:V:418:PHE:HB3	8:V:421:MET:HE2	1.91	0.51
8:Z:53:TYR:N	8:Z:61:ILE:O	2.42	0.51
4:H:247:GLU:HG3	4:H:366:ARG:HH12	1.75	0.51
4:H:664:PHE:O	4:H:668:TRP:HB2	2.10	0.51
8:Q:81:PRO:HA	8:Q:84:LYS:HE2	1.92	0.51
5:C:674:GLN:O	8:Q:265:ARG:NH2	2.43	0.51
5:E:521:LEU:HD23	5:E:645:MET:HE1	1.92	0.51
4:F:562:MET:HA	4:F:642:TYR:HE1	1.75	0.51
8:R:62:PRO:HD2	8:R:86:TYR:HB3	1.92	0.51
8:Z:81:PRO:HA	8:Z:84:LYS:HE2	1.92	0.51
4:D:581:LEU:HG	4:D:585:LEU:HG	1.91	0.51
8:Q:53:TYR:O	8:Q:61:ILE:N	2.38	0.51
8:R:20:GLU:OE2	8:R:24:GLN:NE2	2.44	0.51
8:S:53:TYR:N	8:S:61:ILE:O	2.42	0.51
8:Z:249:MET:HE3	8:Z:250:ASN:H	1.75	0.51
4:H:694:MET:HG3	4:H:696:GLU:HG2	1.91	0.51
8:T:20:GLU:OE2	8:T:24:GLN:NE2	2.44	0.51
8:U:71:PRO:O	8:U:75:HIS:NE2	2.44	0.51
8:U:418:PHE:HB3	8:U:421:MET:HE2	1.91	0.51
8:V:53:TYR:O	8:V:61:ILE:N	2.37	0.51
8:V:71:PRO:O	8:V:75:HIS:NE2	2.44	0.51
8:X:20:GLU:OE2	8:X:24:GLN:NE2	2.44	0.51
8:Y:81:PRO:HA	8:Y:84:LYS:HE2	1.92	0.51
8:Z:388:PHE:HB2	8:Z:432:ILE:HD11	1.93	0.51
7:c:3:SER:OG	7:c:4:ILE:N	2.43	0.51
4:F:334:GLU:HB3	7:c:148:TYR:HE1	1.76	0.51
1:J:430:VAL:HG23	1:J:493:ILE:HA	1.93	0.51
8:Q:249:MET:HE3	8:Q:250:ASN:H	1.76	0.51
8:R:50:VAL:HG21	8:R:244:ARG:HG2	1.92	0.51
8:S:388:PHE:HB2	8:S:432:ILE:HD11	1.93	0.51
8:T:418:PHE:HB3	8:T:421:MET:HE2	1.91	0.51
8:U:81:PRO:HA	8:U:84:LYS:HE2	1.92	0.51
8:V:388:PHE:HB2	8:V:432:ILE:HD11	1.92	0.51
8:X:62:PRO:HD2	8:X:86:TYR:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:X:278:THR:HA	8:X:371:HIS:HE1	1.75	0.51
8:Y:20:GLU:OE2	8:Y:24:GLN:NE2	2.44	0.51
8:Y:249:MET:HE3	8:Y:250:ASN:H	1.75	0.51
4:H:778:VAL:HG23	4:H:854:TYR:HE1	1.75	0.51
6:K:404:LEU:HD22	8:Z:339:ARG:HH12	1.76	0.51
8:W:278:THR:HA	8:W:371:HIS:HE1	1.75	0.51
8:Q:388:PHE:HB2	8:Q:432:ILE:HD11	1.93	0.51
8:U:388:PHE:HB2	8:U:432:ILE:HD11	1.93	0.51
8:Y:71:PRO:O	8:Y:75:HIS:NE2	2.44	0.51
8:T:278:THR:HA	8:T:371:HIS:HE1	1.75	0.51
8:U:62:PRO:HD2	8:U:86:TYR:HB3	1.92	0.51
8:V:50:VAL:HG21	8:V:244:ARG:HG2	1.92	0.51
8:V:53:TYR:N	8:V:61:ILE:O	2.42	0.51
8:V:252:ASP:OD1	8:V:252:ASP:N	2.41	0.51
8:V:278:THR:HA	8:V:371:HIS:HE1	1.75	0.51
8:Z:278:THR:HA	8:Z:371:HIS:HE1	1.75	0.51
5:G:719:ILE:HA	5:G:722:VAL:HG22	1.93	0.51
1:J:728:LEU:HA	8:X:248:TYR:CE1	2.45	0.51
8:Q:20:GLU:OE2	8:Q:24:GLN:NE2	2.44	0.51
8:S:20:GLU:OE2	8:S:24:GLN:NE2	2.44	0.51
8:U:20:GLU:OE2	8:U:24:GLN:NE2	2.44	0.51
8:X:388:PHE:HB2	8:X:432:ILE:HD11	1.93	0.51
8:Y:388:PHE:HB2	8:Y:432:ILE:HD11	1.93	0.51
2:e:109:PRO:HG2	2:e:161:HIS:CE1	2.46	0.50
4:D:304:ILE:HD11	4:D:382:ALA:HA	1.91	0.50
5:G:840:LEU:HG	5:G:856:ILE:HD11	1.92	0.50
8:V:249:MET:HE3	8:V:250:ASN:H	1.75	0.50
8:Y:62:PRO:HD2	8:Y:86:TYR:HB3	1.92	0.50
1:J:831:ILE:HG22	1:J:835:LYS:HZ2	1.75	0.50
7:L:1514:HIS:CD2	7:L:1519:GLU:HB3	2.46	0.50
8:T:50:VAL:HG21	8:T:244:ARG:HG2	1.92	0.50
8:W:20:GLU:OE2	8:W:24:GLN:NE2	2.44	0.50
8:Z:20:GLU:OE2	8:Z:24:GLN:NE2	2.44	0.50
4:H:652:PHE:HB3	4:H:657:MET:HE3	1.94	0.50
6:K:305:ASP:N	6:K:305:ASP:OD1	2.44	0.50
6:K:639:ASN:HB2	8:Y:334:HIS:NE2	2.26	0.50
8:Q:50:VAL:HG21	8:Q:244:ARG:HG2	1.92	0.50
8:T:53:TYR:O	8:T:61:ILE:N	2.38	0.50
8:V:20:GLU:OE2	8:V:24:GLN:NE2	2.44	0.50
8:X:81:PRO:HA	8:X:84:LYS:HE2	1.92	0.50
8:Y:50:VAL:HG21	8:Y:244:ARG:HG2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:320:VAL:HG12	4:F:425:PRO:HB2	1.92	0.50
1:J:225:TRP:HE1	6:K:35:HIS:CD2	2.28	0.50
6:K:260:ARG:HB2	6:K:263:ILE:HG22	1.93	0.50
6:K:645:LEU:HB2	6:K:646:LEU:HD22	1.94	0.50
8:X:71:PRO:O	8:X:75:HIS:NE2	2.44	0.50
8:Y:184:GLN:O	8:Y:188:SER:OG	2.27	0.50
8:Z:156:ARG:NH2	8:Z:159:ASP:OD2	2.45	0.50
5:E:420:GLN:H	5:E:423:TYR:HB3	1.75	0.50
5:G:560:ARG:HB2	8:V:339:ARG:NE	2.23	0.50
8:Q:71:PRO:O	8:Q:75:HIS:NE2	2.44	0.50
8:Q:156:ARG:NH2	8:Q:159:ASP:OD2	2.45	0.50
8:S:62:PRO:HD2	8:S:86:TYR:HB3	1.92	0.50
8:S:156:ARG:NH2	8:S:159:ASP:OD2	2.45	0.50
8:S:249:MET:HE3	8:S:250:ASN:H	1.75	0.50
8:U:156:ARG:NH2	8:U:159:ASP:OD2	2.45	0.50
8:W:249:MET:HE3	8:W:250:ASN:H	1.75	0.50
8:X:322:ASN:ND2	8:X:357:GLN:O	2.45	0.50
8:Z:322:ASN:ND2	8:Z:357:GLN:O	2.45	0.50
1:I:71:LYS:NZ	9:I:1102:HOH:O	2.43	0.50
8:T:322:ASN:ND2	8:T:357:GLN:O	2.45	0.50
8:V:156:ARG:NH2	8:V:159:ASP:OD2	2.45	0.50
8:W:322:ASN:ND2	8:W:357:GLN:O	2.45	0.50
5:E:514:ARG:HG2	5:E:517:LYS:HE3	1.94	0.50
5:G:578:MET:HE3	5:G:580:HIS:H	1.76	0.50
6:I:504:HIS:HE1	8:W:158:ASN:HD21	1.60	0.50
1:J:882:ARG:HH21	1:J:981:GLU:HA	1.77	0.50
8:U:322:ASN:ND2	8:U:357:GLN:O	2.45	0.50
8:V:322:ASN:ND2	8:V:357:GLN:O	2.45	0.50
8:W:53:TYR:O	8:W:61:ILE:N	2.37	0.50
8:X:249:MET:HE3	8:X:250:ASN:H	1.75	0.50
8:X:415:LYS:HG3	8:X:418:PHE:H	1.77	0.50
8:Y:322:ASN:ND2	8:Y:357:GLN:O	2.45	0.50
8:Z:71:PRO:O	8:Z:75:HIS:NE2	2.44	0.50
5:C:861:PHE:CE1	8:Q:337:LEU:HG	2.47	0.50
8:Q:339:ARG:HG2	8:Q:339:ARG:HH21	1.77	0.50
8:W:252:ASP:OD1	8:W:252:ASP:N	2.41	0.50
8:W:388:PHE:HB2	8:W:432:ILE:HD11	1.93	0.50
8:Z:50:VAL:HG21	8:Z:244:ARG:HG2	1.92	0.50
1:I:76:SER:HB3	4:H:662:ARG:HH21	1.77	0.50
5:E:288:VAL:HG22	5:E:386:PRO:HG2	1.94	0.50
4:H:446:PHE:O	4:H:467:ARG:NH1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:R:156:ARG:NH2	8:R:159:ASP:OD2	2.45	0.50
8:R:322:ASN:ND2	8:R:357:GLN:O	2.45	0.50
8:S:322:ASN:ND2	8:S:357:GLN:O	2.45	0.50
1:J:305:LEU:HD22	1:J:310:LEU:HD13	1.94	0.49
8:S:71:PRO:O	8:S:75:HIS:NE2	2.44	0.49
8:S:339:ARG:HH21	8:S:339:ARG:HG2	1.77	0.49
8:S:415:LYS:HG3	8:S:418:PHE:H	1.77	0.49
8:T:71:PRO:O	8:T:75:HIS:NE2	2.44	0.49
8:T:249:MET:HE3	8:T:250:ASN:H	1.75	0.49
8:Y:415:LYS:HE3	8:Y:420:GLU:HG3	1.95	0.49
8:U:415:LYS:HG3	8:U:418:PHE:H	1.77	0.49
8:V:415:LYS:HG3	8:V:418:PHE:H	1.77	0.49
8:W:71:PRO:O	8:W:75:HIS:NE2	2.44	0.49
8:Z:415:LYS:HE3	8:Z:420:GLU:HG3	1.95	0.49
3:b:46:ILE:HA	3:b:49:ARG:HG3	1.93	0.49
8:R:56:ASP:O	8:R:58:GLU:N	2.43	0.49
8:R:71:PRO:O	8:R:75:HIS:NE2	2.44	0.49
8:T:156:ARG:NH2	8:T:159:ASP:OD2	2.45	0.49
8:T:388:PHE:HB2	8:T:432:ILE:HD11	1.92	0.49
8:V:339:ARG:HG2	8:V:339:ARG:HH21	1.77	0.49
8:W:156:ARG:NH2	8:W:159:ASP:OD2	2.45	0.49
8:Y:156:ARG:NH2	8:Y:159:ASP:OD2	2.45	0.49
4:D:297:LEU:HG	4:D:375:LYS:HE3	1.93	0.49
1:J:947:VAL:HA	1:J:951:LYS:HG2	1.93	0.49
8:V:47:ARG:HE	8:V:49:ASP:HB3	1.78	0.49
8:Y:415:LYS:HG3	8:Y:418:PHE:H	1.77	0.49
1:l:87:LEU:HD23	3:m:31:ILE:HG13	1.94	0.49
2:e:132:MET:N	2:e:132:MET:SD	2.86	0.49
3:b:43:THR:HG22	4:a:19:ARG:HE	1.77	0.49
4:D:721:TYR:HD1	4:D:875:PHE:HD2	1.59	0.49
4:F:655:GLU:O	4:F:659:HIS:ND1	2.46	0.49
8:Q:56:ASP:O	8:Q:58:GLU:N	2.43	0.49
8:Q:322:ASN:ND2	8:Q:357:GLN:O	2.45	0.49
8:Q:415:LYS:HG3	8:Q:418:PHE:H	1.77	0.49
8:R:249:MET:HE3	8:R:250:ASN:H	1.75	0.49
8:R:388:PHE:HB2	8:R:432:ILE:HD11	1.93	0.49
8:U:339:ARG:HH21	8:U:339:ARG:HG2	1.77	0.49
8:X:415:LYS:HE3	8:X:420:GLU:HG3	1.94	0.49
4:D:587:ARG:NH1	4:D:588:PRO:O	2.46	0.49
5:E:658:VAL:HG11	5:E:762:MET:HE3	1.94	0.49
6:I:184:TYR:O	6:I:188:SER:OG	2.25	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:272:ARG:NH1	1:J:387:ILE:HG13	2.27	0.49
8:R:339:ARG:HH21	8:R:339:ARG:HG2	1.77	0.49
8:V:229:ASN:O	8:V:233:SER:OG	2.23	0.49
2:e:39:ARG:HH11	2:e:66:THR:HA	1.78	0.49
5:G:263:ILE:HD12	5:G:328:ILE:HD11	1.94	0.49
5:G:561:MET:N	8:V:339:ARG:HH11	2.10	0.49
7:L:409:ARG:HA	7:L:412:HIS:CE1	2.48	0.49
4:h:61:GLU:OE1	4:h:64:ARG:NH1	2.37	0.49
8:R:47:ARG:HE	8:R:49:ASP:HB3	1.78	0.49
8:R:415:LYS:HE3	8:R:420:GLU:HG3	1.95	0.49
8:W:339:ARG:HG2	8:W:339:ARG:HH21	1.77	0.49
8:X:156:ARG:NH2	8:X:159:ASP:OD2	2.45	0.49
8:Y:56:ASP:O	8:Y:58:GLU:N	2.43	0.49
8:Y:252:ASP:OD1	8:Y:252:ASP:N	2.41	0.49
4:D:636:ASP:HA	4:h:66:ARG:HH12	1.78	0.49
4:F:397:ALA:HA	4:F:400:VAL:HG22	1.95	0.49
4:H:878:PHE:HB2	4:H:879:ARG:NH2	2.28	0.49
8:U:415:LYS:HE3	8:U:420:GLU:HG3	1.95	0.49
8:Z:56:ASP:O	8:Z:58:GLU:N	2.43	0.49
4:F:319:LEU:N	4:F:445:GLU:OE2	2.28	0.49
7:L:294:ARG:HE	7:L:306:HIS:N	2.11	0.49
8:T:339:ARG:HG2	8:T:339:ARG:HH21	1.77	0.49
8:T:415:LYS:HG3	8:T:418:PHE:H	1.77	0.49
8:W:415:LYS:HE3	8:W:420:GLU:HG3	1.95	0.49
8:X:339:ARG:HG2	8:X:339:ARG:HH21	1.77	0.49
2:e:290:ARG:HH11	2:e:321:ALA:HB2	1.78	0.49
5:C:282:SER:HB2	5:C:285:TYR:HD1	1.76	0.49
5:C:638:TYR:OH	5:C:726:HIS:NE2	2.46	0.49
8:R:415:LYS:HG3	8:R:418:PHE:H	1.77	0.49
8:W:47:ARG:HE	8:W:49:ASP:HB3	1.78	0.49
5:C:231:ARG:HH11	4:D:287:LEU:HB3	1.78	0.48
4:D:740:GLN:O	4:D:742:GLN:NE2	2.45	0.48
4:H:630:PRO:O	4:H:632:ASP:N	2.45	0.48
8:Q:47:ARG:HE	8:Q:49:ASP:HB3	1.78	0.48
8:V:56:ASP:O	8:V:58:GLU:N	2.43	0.48
8:V:415:LYS:HE3	8:V:420:GLU:HG3	1.95	0.48
8:Y:237:SER:O	8:Y:244:ARG:NH2	2.43	0.48
4:D:404:THR:HG21	4:D:419:LEU:HD13	1.95	0.48
4:D:531:GLN:HA	4:D:534:ILE:HG22	1.94	0.48
5:G:735:LYS:HA	5:G:740:THR:HB	1.94	0.48
8:S:56:ASP:O	8:S:58:GLU:N	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:S:415:LYS:HE3	8:S:420:GLU:HG3	1.94	0.48
8:T:47:ARG:HE	8:T:49:ASP:HB3	1.78	0.48
8:T:237:SER:O	8:T:244:ARG:NH2	2.43	0.48
8:Z:237:SER:O	8:Z:244:ARG:NH2	2.43	0.48
8:Z:324:ILE:HD11	8:Z:373:VAL:HG12	1.96	0.48
7:c:90:GLU:HA	7:c:93:VAL:HG22	1.95	0.48
2:e:109:PRO:HB2	2:e:177:ARG:HH22	1.78	0.48
4:F:247:GLU:OE1	4:F:366:ARG:NH2	2.42	0.48
1:J:562:ALA:HB2	1:J:699:TYR:HD1	1.78	0.48
8:T:53:TYR:N	8:T:61:ILE:O	2.42	0.48
8:W:415:LYS:HG3	8:W:418:PHE:H	1.77	0.48
8:Z:415:LYS:HG3	8:Z:418:PHE:H	1.77	0.48
5:C:253:ASP:OD2	5:C:255:SER:OG	2.28	0.48
5:E:719:ILE:HA	5:E:722:VAL:HG22	1.95	0.48
7:L:1533:GLU:HB2	7:L:1534:LYS:HZ2	1.79	0.48
3:i:39:LEU:HD11	4:h:100:LEU:HD12	1.94	0.48
8:Q:415:LYS:HE3	8:Q:420:GLU:HG3	1.95	0.48
8:U:324:ILE:HD11	8:U:373:VAL:HG12	1.96	0.48
8:V:237:SER:O	8:V:244:ARG:NH2	2.43	0.48
8:X:56:ASP:O	8:X:58:GLU:N	2.43	0.48
8:Y:324:ILE:HD11	8:Y:373:VAL:HG12	1.96	0.48
5:C:517:LYS:HA	5:C:521:LEU:HD13	1.96	0.48
5:G:688:ASN:ND2	8:U:357:GLN:HE22	2.11	0.48
7:L:354:LYS:HA	7:L:357:LEU:HD12	1.95	0.48
8:W:237:SER:O	8:W:244:ARG:NH2	2.43	0.48
8:Z:339:ARG:HH21	8:Z:339:ARG:HG2	1.77	0.48
3:d:67:LEU:HD13	7:c:15:LEU:HD22	1.95	0.48
1:l:23:VAL:O	1:l:27:ALA:HB3	2.13	0.48
4:D:721:TYR:CE1	4:D:875:PHE:HB3	2.49	0.48
4:D:721:TYR:HE1	4:D:875:PHE:HB3	1.78	0.48
4:H:733:GLU:O	4:H:737:LYS:HG2	2.13	0.48
8:U:47:ARG:HE	8:U:49:ASP:HB3	1.78	0.48
8:W:229:ASN:O	8:W:233:SER:OG	2.23	0.48
8:Z:47:ARG:HE	8:Z:49:ASP:HB3	1.78	0.48
4:D:586:VAL:HG12	4:D:635:TRP:HE1	1.77	0.48
7:L:1656:ARG:NH2	8:Z:443:TYR:OH	2.46	0.48
2:e:29:ALA:HB1	2:e:31:PHE:HE1	1.78	0.48
7:L:1800:LEU:HD22	8:Z:338:GLN:HG3	1.94	0.48
3:m:28:LEU:HA	3:m:31:ILE:HD12	1.95	0.48
8:Q:324:ILE:HD11	8:Q:373:VAL:HG12	1.96	0.48
8:T:56:ASP:O	8:T:58:GLU:N	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:U:237:SER:O	8:U:244:ARG:NH2	2.42	0.48
6:K:139:VAL:HA	6:K:142:GLN:HE21	1.79	0.48
7:L:1590:VAL:HG13	7:L:1737:LEU:HD23	1.96	0.48
8:W:324:ILE:HD11	8:W:373:VAL:HG12	1.96	0.48
2:e:277:THR:O	2:e:281:SER:OG	2.28	0.48
8:S:47:ARG:HE	8:S:49:ASP:HB3	1.78	0.48
8:T:415:LYS:HE3	8:T:420:GLU:HG3	1.95	0.48
8:U:53:TYR:N	8:U:61:ILE:O	2.42	0.48
8:X:47:ARG:HE	8:X:49:ASP:HB3	1.78	0.48
4:D:768:SER:HA	4:D:771:LEU:HD13	1.96	0.47
4:F:798:GLU:HA	4:F:801:GLN:HE21	1.79	0.47
1:J:553:LYS:HA	1:J:556:LEU:HD12	1.96	0.47
6:K:272:VAL:HG23	6:K:329:VAL:HG11	1.95	0.47
4:a:95:TYR:O	4:a:99:SER:OG	2.31	0.47
4:D:773:ASN:HD22	4:D:776:ARG:HE	1.61	0.47
6:K:488:VAL:HG21	6:K:587:LEU:HD22	1.96	0.47
7:L:499:VAL:HB	7:L:551:GLU:HG2	1.97	0.47
8:Y:47:ARG:HE	8:Y:49:ASP:HB3	1.78	0.47
6:I:518:ARG:HD2	6:I:619:PHE:HD1	1.79	0.47
7:L:425:LYS:HZ2	7:L:549:TYR:HE2	1.63	0.47
5:G:540:ARG:HA	5:G:613:LEU:HD23	1.97	0.47
6:I:343:LEU:HB2	6:I:344:MET:HE2	1.96	0.47
8:S:252:ASP:OD1	8:S:252:ASP:N	2.41	0.47
8:X:237:SER:O	8:X:244:ARG:NH2	2.43	0.47
7:c:190:LEU:HB3	7:c:192:THR:HG22	1.94	0.47
2:e:110:LEU:HD21	2:e:175:ILE:HB	1.97	0.47
5:C:762:MET:HB3	5:C:762:MET:HE3	1.77	0.47
4:D:406:THR:HG23	4:D:412:ARG:HG2	1.97	0.47
4:D:707:LEU:HD13	4:D:851:THR:HG22	1.95	0.47
5:E:341:LEU:HD21	5:E:362:ARG:HG3	1.97	0.47
4:F:426:VAL:HG22	4:F:430:LEU:HD13	1.96	0.47
8:Y:9:GLN:HG3	8:Y:66:LEU:HA	1.97	0.47
2:e:242:LEU:HG	2:e:243:PRO:HD2	1.97	0.47
5:C:611:SER:OG	5:C:612:GLY:N	2.47	0.47
4:H:361:SER:OG	4:H:362:LEU:N	2.46	0.47
1:J:268:THR:HA	1:J:271:ILE:HD12	1.96	0.47
1:J:391:THR:HA	7:L:293:LYS:HZ1	1.79	0.47
8:R:4:GLU:O	8:R:133:GLU:N	2.47	0.47
8:R:351:TRP:CD1	8:R:351:TRP:H	2.33	0.47
8:T:9:GLN:HG3	8:T:66:LEU:HA	1.97	0.47
8:T:324:ILE:HD11	8:T:373:VAL:HG12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:324:ILE:HD11	8:V:373:VAL:HG12	1.96	0.47
8:Y:351:TRP:CD1	8:Y:351:TRP:H	2.33	0.47
5:G:311:GLU:HB2	4:H:365:ARG:HH11	1.80	0.47
5:G:512:HIS:HE1	5:G:630:ILE:HD12	1.79	0.47
5:G:693:ILE:HA	5:G:696:TYR:CE1	2.50	0.47
7:L:550:GLY:HA2	7:L:555:GLN:HE21	1.79	0.47
7:L:1664:GLU:HG3	7:L:1772:PHE:HE2	1.80	0.47
3:i:55:ILE:HD13	3:i:60:LEU:HD22	1.97	0.47
8:T:231:LEU:O	8:T:234:THR:OG1	2.30	0.47
8:U:119:PHE:HA	8:U:122:ILE:HD12	1.97	0.47
2:e:350:SER:OG	7:c:43:ASN:ND2	2.48	0.47
5:C:187:LEU:HD21	4:D:379:LYS:HD3	1.96	0.47
5:C:814:LEU:HD22	5:C:818:PHE:HD1	1.80	0.47
5:G:241:ARG:HG3	5:G:242:GLN:H	1.79	0.47
8:Q:9:GLN:HG3	8:Q:66:LEU:HA	1.97	0.47
8:R:324:ILE:HD11	8:R:373:VAL:HG12	1.96	0.47
4:j:34:TYR:O	4:j:38:VAL:HG12	2.15	0.47
2:e:11:ASP:HB3	2:e:18:LYS:HE2	1.96	0.47
5:C:649:LYS:HE2	5:C:649:LYS:HB3	1.63	0.47
4:D:369:VAL:HG23	4:D:370:TRP:HD1	1.80	0.47
4:H:447:PHE:O	4:H:467:ARG:N	2.44	0.47
6:I:59:ILE:HD11	6:I:93:LEU:HG	1.97	0.47
6:K:20:ASN:HD22	6:K:26:GLN:HE22	1.62	0.47
8:W:9:GLN:HG3	8:W:66:LEU:HA	1.97	0.47
8:W:119:PHE:HA	8:W:122:ILE:HD12	1.97	0.47
8:Y:339:ARG:HG2	8:Y:339:ARG:HH21	1.77	0.47
8:Z:351:TRP:H	8:Z:351:TRP:CD1	2.33	0.47
6:K:498:LEU:HD12	6:K:501:GLN:HE21	1.81	0.46
8:U:9:GLN:HG3	8:U:66:LEU:HA	1.97	0.46
8:V:410:LYS:H	8:V:410:LYS:HG2	1.51	0.46
8:X:119:PHE:HA	8:X:122:ILE:HD12	1.97	0.46
8:X:324:ILE:HD11	8:X:373:VAL:HG12	1.96	0.46
5:E:507:LYS:HZ2	5:E:623:LYS:HE3	1.80	0.46
8:Q:119:PHE:HA	8:Q:122:ILE:HD12	1.97	0.46
8:S:324:ILE:HD11	8:S:373:VAL:HG12	1.96	0.46
8:S:351:TRP:H	8:S:351:TRP:CD1	2.33	0.46
8:W:351:TRP:H	8:W:351:TRP:CD1	2.33	0.46
4:D:590:THR:HG21	4:D:631:GLY:HA2	1.96	0.46
4:D:757:THR:O	4:D:761:ARG:HG2	2.16	0.46
1:J:883:MET:SD	1:J:883:MET:N	2.88	0.46
8:Q:237:SER:O	8:Q:244:ARG:NH2	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Q:351:TRP:CD1	8:Q:351:TRP:H	2.33	0.46
8:U:231:LEU:O	8:U:234:THR:OG1	2.30	0.46
5:G:561:MET:HB2	8:V:339:ARG:HH12	1.81	0.46
6:I:19:TRP:HA	6:I:25:LEU:H	1.81	0.46
3:m:41:MET:O	3:m:45:SER:OG	2.31	0.46
8:R:270:MET:HE1	8:R:384:ILE:HD13	1.98	0.46
2:e:304:THR:HG21	2:e:335:ARG:HG3	1.97	0.46
5:G:637:ARG:HB3	5:G:734:LEU:HD11	1.97	0.46
6:I:357:ILE:O	6:I:361:TYR:CB	2.64	0.46
1:J:556:LEU:HA	1:J:559:ILE:HD12	1.96	0.46
6:K:630:LEU:HG	6:K:645:LEU:HD21	1.96	0.46
7:L:1513:ARG:HG3	7:L:1514:HIS:CD2	2.51	0.46
8:Q:270:MET:HE1	8:Q:384:ILE:HD13	1.98	0.46
8:R:119:PHE:HA	8:R:122:ILE:HD12	1.97	0.46
8:U:229:ASN:O	8:U:233:SER:OG	2.23	0.46
8:U:410:LYS:H	8:U:410:LYS:HG2	1.51	0.46
8:V:119:PHE:HA	8:V:122:ILE:HD12	1.97	0.46
8:W:270:MET:HE1	8:W:384:ILE:HD13	1.98	0.46
8:Z:52:PHE:HB3	8:Z:60:TYR:HB3	1.98	0.46
3:i:67:LEU:HB3	4:h:20:ILE:HG21	1.97	0.46
8:R:9:GLN:HG3	8:R:66:LEU:HA	1.97	0.46
8:S:119:PHE:HA	8:S:122:ILE:HD12	1.97	0.46
8:V:351:TRP:CD1	8:V:351:TRP:H	2.33	0.46
8:Y:52:PHE:HB3	8:Y:60:TYR:HB3	1.98	0.46
2:e:83:GLU:HG2	2:e:126:THR:HG21	1.97	0.46
4:F:433:TRP:CD1	4:F:483:VAL:HG22	2.51	0.46
5:G:693:ILE:HD12	5:G:696:TYR:HE1	1.81	0.46
6:K:121:HIS:HA	6:K:124:TYR:CE1	2.51	0.46
7:L:1669:VAL:HA	7:L:1672:ILE:HG22	1.96	0.46
8:Q:205:LEU:HA	8:Q:305:VAL:HG22	1.98	0.46
8:U:252:ASP:OD1	8:U:252:ASP:N	2.42	0.46
8:Z:231:LEU:O	8:Z:234:THR:OG1	2.30	0.46
3:d:21:VAL:HA	3:d:24:THR:HG22	1.97	0.46
5:C:231:ARG:HG2	4:D:286:SER:HB3	1.98	0.46
1:J:552:LEU:HG	1:J:556:LEU:HG	1.98	0.46
6:K:378:HIS:HA	6:K:381:LYS:HG2	1.97	0.46
6:K:542:SER:OG	6:K:543:GLN:NE2	2.48	0.46
8:Q:3:ARG:HH11	8:Q:132:LEU:H	1.64	0.46
8:X:9:GLN:HG3	8:X:66:LEU:HA	1.97	0.46
8:X:270:MET:HE1	8:X:384:ILE:HD13	1.98	0.46
8:Y:270:MET:HE1	8:Y:384:ILE:HD13	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Z:119:PHE:HA	8:Z:122:ILE:HD12	1.97	0.46
2:e:121:GLN:HE21	2:e:125:GLU:HG2	1.81	0.46
4:D:434:ILE:HG22	4:D:486:ILE:HD11	1.98	0.46
5:E:746:LYS:O	5:E:749:SER:OG	2.29	0.46
4:H:578:MET:SD	4:H:671:LYS:HD3	2.56	0.46
4:H:580:LEU:HB3	4:H:600:ILE:HD11	1.97	0.46
1:J:282:LYS:HG3	1:J:283:LYS:HG2	1.98	0.46
1:J:884:PHE:O	1:J:888:VAL:HG23	2.16	0.46
8:T:52:PHE:HB3	8:T:60:TYR:HB3	1.98	0.46
8:U:192:LEU:HA	8:U:195:LEU:HB2	1.98	0.46
8:U:202:VAL:HG12	8:U:204:VAL:HG12	1.98	0.46
8:V:205:LEU:HA	8:V:305:VAL:HG22	1.98	0.46
8:Z:55:ALA:N	8:Z:59:HIS:O	2.49	0.46
8:Z:202:VAL:HG12	8:Z:204:VAL:HG12	1.98	0.46
5:C:183:GLU:HB3	5:C:184:ARG:HH11	1.81	0.46
5:E:478:THR:OG1	5:E:482:ARG:HA	2.16	0.46
5:E:727:THR:HA	5:E:730:LEU:HG	1.98	0.46
4:F:571:GLY:H	4:F:574:ILE:HD12	1.80	0.46
4:H:430:LEU:HD23	4:H:446:PHE:HE1	1.81	0.46
1:J:707:MET:HA	1:J:710:LEU:HG	1.98	0.46
8:R:252:ASP:OD1	8:R:252:ASP:N	2.41	0.46
8:S:3:ARG:HH11	8:S:132:LEU:H	1.64	0.46
8:W:52:PHE:HB3	8:W:60:TYR:HB3	1.98	0.46
8:W:192:LEU:HA	8:W:195:LEU:HB2	1.98	0.46
8:X:3:ARG:HH11	8:X:132:LEU:H	1.64	0.46
8:X:4:GLU:O	8:X:133:GLU:N	2.47	0.46
8:Z:4:GLU:O	8:Z:133:GLU:N	2.47	0.46
2:e:314:GLN:HA	2:e:317:ILE:HG12	1.97	0.45
5:E:159:LYS:HB2	5:E:160:MET:HE2	1.97	0.45
4:F:538:TYR:O	4:F:542:SER:OG	2.27	0.45
4:F:848:ARG:HH21	4:F:852:HIS:CE1	2.34	0.45
5:G:694:GLN:HE22	8:U:249:MET:HG2	1.81	0.45
4:H:655:GLU:O	4:H:658:SER:OG	2.33	0.45
4:H:697:PHE:HB3	4:H:701:LEU:HD23	1.97	0.45
6:I:345:VAL:HG23	6:I:346:GLU:HG3	1.98	0.45
1:J:892:HIS:CD2	8:X:353:PRO:HB2	2.51	0.45
1:J:903:THR:OG1	1:J:904:ARG:N	2.49	0.45
7:L:1666:GLN:HE22	8:Z:259:SER:HA	1.81	0.45
8:S:9:GLN:HG3	8:S:66:LEU:HA	1.97	0.45
8:S:52:PHE:HB3	8:S:60:TYR:HB3	1.98	0.45
8:U:270:MET:HE1	8:U:384:ILE:HD13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:W:3:ARG:HH11	8:W:132:LEU:H	1.64	0.45
8:Z:3:ARG:HH11	8:Z:132:LEU:H	1.64	0.45
8:Z:270:MET:HE1	8:Z:384:ILE:HD13	1.98	0.45
2:e:116:ARG:HG2	2:e:370:VAL:HG23	1.98	0.45
2:e:196:ARG:NH2	2:e:253:GLU:OE2	2.49	0.45
2:e:241:GLU:HG3	2:e:247:VAL:HG22	1.98	0.45
4:a:113:SER:OG	4:a:114:TYR:N	2.44	0.45
6:K:511:ASP:HA	6:K:514:LYS:HE2	1.98	0.45
8:S:205:LEU:HA	8:S:305:VAL:HG22	1.98	0.45
8:U:153:LEU:HD13	8:U:153:LEU:HA	1.82	0.45
8:V:9:GLN:HG3	8:V:66:LEU:HA	1.97	0.45
8:V:202:VAL:HG12	8:V:204:VAL:HG12	1.98	0.45
8:V:231:LEU:O	8:V:234:THR:OG1	2.30	0.45
8:W:56:ASP:O	8:W:58:GLU:N	2.43	0.45
8:X:52:PHE:HB3	8:X:60:TYR:HB3	1.98	0.45
8:Y:202:VAL:HG12	8:Y:204:VAL:HG12	1.98	0.45
7:c:70:ILE:HD11	7:c:111:LEU:HD12	1.98	0.45
5:E:632:ARG:CZ	5:E:633:LYS:HG2	2.46	0.45
6:K:409:ASN:O	6:K:410:LEU:HG	2.16	0.45
6:K:649:LEU:HD13	6:K:652:ASN:HA	1.98	0.45
8:R:303:VAL:HG12	8:R:305:VAL:H	1.82	0.45
8:S:4:GLU:O	8:S:133:GLU:N	2.47	0.45
8:S:69:LEU:HD23	8:S:145:THR:HB	1.98	0.45
8:S:303:VAL:HG12	8:S:305:VAL:H	1.82	0.45
8:T:252:ASP:OD1	8:T:252:ASP:N	2.41	0.45
8:U:205:LEU:HA	8:U:305:VAL:HG22	1.98	0.45
8:Y:55:ALA:N	8:Y:59:HIS:O	2.49	0.45
8:Z:9:GLN:HG3	8:Z:66:LEU:HA	1.97	0.45
2:e:74:GLY:HA3	2:e:177:ARG:HH11	1.81	0.45
4:F:568:LEU:HD13	4:F:667:LEU:HB3	1.98	0.45
6:I:31:PHE:HB2	6:I:34:LEU:HG	1.98	0.45
1:J:466:VAL:HG13	1:J:642:HIS:HE1	1.81	0.45
7:L:293:LYS:HA	7:L:293:LYS:HD2	1.74	0.45
8:Q:55:ALA:N	8:Q:59:HIS:O	2.49	0.45
8:Q:303:VAL:HG12	8:Q:305:VAL:H	1.82	0.45
8:T:351:TRP:CD1	8:T:351:TRP:H	2.33	0.45
8:V:270:MET:HE1	8:V:384:ILE:HD13	1.98	0.45
8:Y:192:LEU:HA	8:Y:195:LEU:HB2	1.98	0.45
1:l:24:ARG:NH1	1:l:32:GLU:OE2	2.48	0.45
4:D:581:LEU:HD12	4:D:584:GLU:HB2	1.99	0.45
5:G:576:ASP:OD1	5:G:576:ASP:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:350:LEU:HD13	6:I:464:HIS:CE1	2.52	0.45
1:J:721:GLN:HA	1:J:724:ARG:HE	1.81	0.45
1:J:832:LYS:HD2	1:J:835:LYS:NZ	2.31	0.45
1:J:835:LYS:HE2	1:J:835:LYS:HB2	1.67	0.45
8:Q:202:VAL:HG12	8:Q:204:VAL:HG12	1.98	0.45
8:R:3:ARG:HH11	8:R:132:LEU:H	1.64	0.45
8:R:69:LEU:HD23	8:R:145:THR:HB	1.98	0.45
8:T:119:PHE:HA	8:T:122:ILE:HD12	1.97	0.45
8:U:351:TRP:CD1	8:U:351:TRP:H	2.33	0.45
8:Y:119:PHE:HA	8:Y:122:ILE:HD12	1.97	0.45
2:e:180:LEU:HD13	2:e:261:LEU:HA	1.98	0.45
3:b:51:CYS:SG	4:a:93:ILE:HB	2.57	0.45
5:C:299:LEU:HD22	5:C:338:LEU:HD11	1.98	0.45
5:C:697:MET:HE3	5:C:701:VAL:HG21	1.98	0.45
8:U:303:VAL:HG12	8:U:305:VAL:H	1.82	0.45
3:d:28:LEU:HD12	3:d:31:ILE:HD11	1.99	0.45
4:D:707:LEU:HG	4:D:711:MET:HE1	1.99	0.45
6:K:544:LEU:O	6:K:548:ILE:HG12	2.17	0.45
8:R:205:LEU:HA	8:R:305:VAL:HG22	1.98	0.45
8:W:69:LEU:HD23	8:W:145:THR:HB	1.98	0.45
8:Y:4:GLU:O	8:Y:133:GLU:N	2.47	0.45
8:Z:3:ARG:HB3	8:Z:4:GLU:H	1.51	0.45
5:C:519:TYR:HB3	5:C:618:PHE:HE1	1.82	0.45
5:E:695:TYR:HD1	5:E:698:MET:HE3	1.82	0.45
4:H:621:LEU:HD11	4:H:640:LEU:HD21	1.98	0.45
6:I:477:VAL:HA	6:I:480:LYS:HD2	1.98	0.45
8:S:273:TYR:N	8:S:304:MET:SD	2.90	0.45
8:T:202:VAL:HG12	8:T:204:VAL:HG12	1.98	0.45
8:T:303:VAL:HG12	8:T:305:VAL:H	1.82	0.45
8:W:303:VAL:HG12	8:W:305:VAL:H	1.82	0.45
3:b:35:LEU:HD21	4:a:97:LEU:HB3	1.98	0.45
5:C:501:ASP:HA	5:C:504:MET:HG2	1.98	0.45
6:I:298:SER:OG	6:I:299:ILE:N	2.50	0.45
6:K:143:ILE:HD12	6:K:153:ILE:HG12	1.98	0.45
8:R:231:LEU:O	8:R:234:THR:OG1	2.30	0.45
8:U:3:ARG:HH11	8:U:132:LEU:H	1.64	0.45
8:Y:273:TYR:N	8:Y:304:MET:SD	2.90	0.45
8:Z:303:VAL:HG12	8:Z:305:VAL:H	1.82	0.45
3:d:48:VAL:HG22	7:c:110:VAL:HG21	1.99	0.45
5:E:473:LYS:HZ1	5:E:487:GLN:HA	1.82	0.45
5:E:556:GLU:O	5:E:560:ARG:NH1	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:K:500:MET:HA	8:Y:264:PRO:HG3	1.97	0.45
8:Q:192:LEU:HA	8:Q:195:LEU:HB2	1.98	0.45
8:V:4:GLU:O	8:V:133:GLU:N	2.47	0.45
8:X:351:TRP:H	8:X:351:TRP:CD1	2.33	0.45
8:Y:69:LEU:HD23	8:Y:145:THR:HB	1.98	0.45
8:Y:303:VAL:HG12	8:Y:305:VAL:H	1.82	0.45
8:Z:69:LEU:HD23	8:Z:145:THR:HB	1.98	0.45
3:d:47:CYS:HA	3:d:50:LEU:HD12	1.98	0.45
2:e:62:ARG:HE	2:e:67:LEU:HB2	1.82	0.44
5:E:707:HIS:O	5:E:711:LYS:NZ	2.45	0.44
8:Q:34:GLU:HG3	8:Q:84:LYS:HE3	1.99	0.44
8:Q:52:PHE:HB3	8:Q:60:TYR:HB3	1.98	0.44
8:T:3:ARG:HH11	8:T:132:LEU:H	1.64	0.44
8:V:3:ARG:HH11	8:V:132:LEU:H	1.64	0.44
8:V:34:GLU:HG3	8:V:84:LYS:HE3	1.99	0.44
8:V:52:PHE:HB3	8:V:60:TYR:HB3	1.98	0.44
8:W:34:GLU:HG3	8:W:84:LYS:HE3	1.99	0.44
8:W:202:VAL:HG12	8:W:204:VAL:HG12	1.98	0.44
8:X:192:LEU:HA	8:X:195:LEU:HB2	1.98	0.44
8:X:202:VAL:HG12	8:X:204:VAL:HG12	1.98	0.44
8:X:273:TYR:N	8:X:304:MET:SD	2.90	0.44
2:e:16:MET:SD	2:e:16:MET:N	2.91	0.44
5:C:663:LYS:NZ	8:Q:264:PRO:HB3	2.33	0.44
4:F:860:GLN:HA	4:F:863:VAL:HG12	1.99	0.44
5:G:356:LEU:HG	5:G:440:PRO:HB3	1.99	0.44
5:G:376:CYS:SG	5:G:377:LEU:N	2.90	0.44
4:H:875:PHE:O	4:H:879:ARG:NH2	2.50	0.44
6:I:20:ASN:H	6:I:24:GLY:HA2	1.82	0.44
8:R:192:LEU:HA	8:R:195:LEU:HB2	1.98	0.44
8:S:192:LEU:HA	8:S:195:LEU:HB2	1.98	0.44
8:S:270:MET:HE1	8:S:384:ILE:HD13	1.98	0.44
8:W:205:LEU:HA	8:W:305:VAL:HG22	1.98	0.44
8:Z:34:GLU:HG3	8:Z:84:LYS:HE3	1.99	0.44
2:e:151:ILE:HB	2:e:293:LEU:HD21	2.00	0.44
5:E:188:ILE:HG22	5:E:190:ASP:H	1.82	0.44
5:E:659:TRP:HA	5:E:662:ASN:HD21	1.82	0.44
4:F:563:ARG:HA	4:F:567:LEU:HD13	1.99	0.44
4:H:308:THR:HG21	4:H:328:LEU:HD22	1.99	0.44
4:h:23:ARG:HB3	4:h:27:ASP:HB3	1.99	0.44
8:Q:69:LEU:HD23	8:Q:145:THR:HB	1.98	0.44
8:V:303:VAL:HG12	8:V:305:VAL:H	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Y:3:ARG:HH11	8:Y:132:LEU:H	1.64	0.44
8:Y:34:GLU:HG3	8:Y:84:LYS:HE3	1.99	0.44
8:Y:205:LEU:HA	8:Y:305:VAL:HG22	1.98	0.44
4:F:605:VAL:HG13	4:F:610:ALA:HB3	2.00	0.44
8:R:52:PHE:HB3	8:R:60:TYR:HB3	1.98	0.44
8:S:202:VAL:HG12	8:S:204:VAL:HG12	1.98	0.44
8:T:270:MET:HE1	8:T:384:ILE:HD13	1.98	0.44
8:U:273:TYR:N	8:U:304:MET:SD	2.90	0.44
8:W:4:GLU:O	8:W:133:GLU:N	2.47	0.44
8:X:69:LEU:HD23	8:X:145:THR:HB	1.98	0.44
8:Z:273:TYR:N	8:Z:304:MET:SD	2.90	0.44
2:e:352:PHE:HD1	2:e:355:MET:HE2	1.83	0.44
5:C:469:CYS:HB3	5:C:471:VAL:HG12	2.00	0.44
5:C:690:VAL:HA	5:C:693:ILE:HG22	1.98	0.44
4:D:332:LEU:HD23	4:D:332:LEU:HA	1.68	0.44
5:E:313:LEU:HD22	7:c:164:ILE:HD11	2.00	0.44
8:R:273:TYR:N	8:R:304:MET:SD	2.90	0.44
8:T:205:LEU:HA	8:T:305:VAL:HG22	1.98	0.44
8:V:69:LEU:HD23	8:V:145:THR:HB	1.98	0.44
8:V:192:LEU:HA	8:V:195:LEU:HB2	1.98	0.44
8:V:273:TYR:N	8:V:304:MET:SD	2.90	0.44
8:X:34:GLU:HG3	8:X:84:LYS:HE3	1.99	0.44
8:X:205:LEU:HA	8:X:305:VAL:HG22	1.98	0.44
8:X:252:ASP:OD1	8:X:252:ASP:N	2.41	0.44
4:a:93:ILE:O	4:a:97:LEU:HG	2.17	0.44
5:C:461:ARG:HD3	5:C:467:VAL:HG21	2.00	0.44
5:C:766:THR:HG23	5:C:769:MET:H	1.82	0.44
4:F:419:LEU:O	4:F:423:SER:OG	2.23	0.44
8:T:192:LEU:HA	8:T:195:LEU:HB2	1.98	0.44
8:T:273:TYR:N	8:T:304:MET:SD	2.90	0.44
8:V:160:ARG:HD2	8:V:160:ARG:HA	1.82	0.44
8:W:273:TYR:N	8:W:304:MET:SD	2.90	0.44
8:X:303:VAL:HG12	8:X:305:VAL:H	1.82	0.44
8:Z:192:LEU:HA	8:Z:195:LEU:HB2	1.98	0.44
2:e:305:MET:HE2	2:e:336:LYS:HE2	2.00	0.44
5:C:217:VAL:HG23	5:C:321:LEU:HD21	2.00	0.44
4:D:726:VAL:HA	4:D:761:ARG:HD3	1.98	0.44
8:Q:273:TYR:N	8:Q:304:MET:SD	2.90	0.44
8:R:202:VAL:HG12	8:R:204:VAL:HG12	1.98	0.44
8:U:52:PHE:HB3	8:U:60:TYR:HB3	1.98	0.44
3:d:25:MET:O	3:d:29:LEU:HG	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:280:LYS:HE3	5:C:289:ASN:HB3	2.00	0.44
6:K:129:PHE:HB3	6:K:133:PHE:CE2	2.53	0.44
8:U:34:GLU:HG3	8:U:84:LYS:HE3	1.99	0.44
8:X:55:ALA:N	8:X:59:HIS:O	2.49	0.44
7:c:89:LEU:HD13	7:c:89:LEU:HA	1.90	0.44
4:D:546:LEU:HD23	4:D:744:LEU:HD23	1.98	0.44
4:F:589:ALA:HA	4:F:592:LEU:HG	2.00	0.44
4:H:589:ALA:HB2	4:H:637:VAL:HG21	1.99	0.44
6:K:486:ARG:HB2	6:K:530:TYR:HE2	1.83	0.44
8:S:154:LEU:HD23	8:S:198:ASN:HB2	2.00	0.44
8:T:34:GLU:HG3	8:T:84:LYS:HE3	1.99	0.44
8:U:69:LEU:HD23	8:U:145:THR:HB	1.98	0.44
8:X:160:ARG:HD2	8:X:160:ARG:HA	1.83	0.44
8:Z:205:LEU:HA	8:Z:305:VAL:HG22	1.98	0.44
5:C:555:LEU:HD21	5:C:573:LEU:HG	1.99	0.43
5:C:865:TYR:HE1	8:Q:353:PRO:HG3	1.83	0.43
4:H:595:HIS:HA	4:H:598:THR:HG22	1.99	0.43
6:K:534:VAL:HG21	8:Y:248:TYR:HE2	1.83	0.43
8:Q:4:GLU:O	8:Q:133:GLU:N	2.47	0.43
8:R:261:ILE:HG12	8:R:267:HIS:HA	2.00	0.43
8:X:410:LYS:H	8:X:410:LYS:HG2	1.51	0.43
5:C:527:PHE:O	5:C:531:PHE:CB	2.66	0.43
4:D:546:LEU:O	4:D:550:ASN:ND2	2.51	0.43
4:F:337:ARG:O	4:F:340:SER:OG	2.29	0.43
4:F:364:LEU:HB2	4:F:367:LEU:HD12	1.98	0.43
5:G:709:LEU:HD13	5:G:729:PHE:HB2	1.99	0.43
7:L:468:ARG:HA	7:L:471:ARG:HD3	2.00	0.43
8:T:69:LEU:HD23	8:T:145:THR:HB	1.98	0.43
8:X:154:LEU:HD23	8:X:198:ASN:HB2	2.00	0.43
8:X:261:ILE:HG12	8:X:267:HIS:HA	2.00	0.43
8:Y:261:ILE:HG12	8:Y:267:HIS:HA	2.00	0.43
8:Z:252:ASP:OD1	8:Z:252:ASP:N	2.41	0.43
3:k:47:CYS:HA	3:k:50:LEU:HD12	2.00	0.43
2:e:24:ASP:OD1	2:e:24:ASP:N	2.47	0.43
5:C:209:PRO:O	5:C:212:SER:OG	2.26	0.43
6:I:116:HIS:HE1	1:J:237:HIS:CD2	2.36	0.43
8:R:55:ALA:N	8:R:59:HIS:O	2.49	0.43
8:U:4:GLU:O	8:U:133:GLU:N	2.47	0.43
8:V:344:LYS:HD3	8:V:344:LYS:HA	1.82	0.43
8:W:261:ILE:HG12	8:W:267:HIS:HA	2.01	0.43
2:e:68:LYS:HZ3	2:e:70:PRO:HA	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:560:ARG:HB2	8:R:339:ARG:HH11	1.82	0.43
5:E:507:LYS:NZ	5:E:623:LYS:HE3	2.32	0.43
7:L:1625:GLN:HA	7:L:1628:LEU:HD12	2.00	0.43
8:S:34:GLU:HG3	8:S:84:LYS:HE3	1.99	0.43
5:C:518:ARG:HA	5:C:523:ASP:HB3	2.01	0.43
5:C:554:LEU:HA	5:C:557:LEU:HG	2.00	0.43
8:S:151:SER:HB2	8:S:194:ARG:HG2	2.01	0.43
8:T:261:ILE:HG12	8:T:267:HIS:HA	2.00	0.43
3:k:21:VAL:HG13	3:k:25:MET:HE3	2.01	0.43
5:C:296:MET:HE2	5:C:338:LEU:HB3	2.01	0.43
4:H:574:ILE:O	4:H:578:MET:HG2	2.17	0.43
6:I:165:LEU:HA	6:I:166:PRO:HD3	1.80	0.43
8:T:154:LEU:HD23	8:T:198:ASN:HB2	2.00	0.43
8:T:348:PHE:HB3	8:T:349:ILE:H	1.69	0.43
8:U:3:ARG:HB3	8:U:4:GLU:H	1.51	0.43
8:W:151:SER:HB2	8:W:194:ARG:HG2	2.01	0.43
3:d:37:THR:HB	3:d:39:LEU:HD12	2.00	0.43
5:C:460:VAL:HG12	5:C:499:LEU:HD13	1.99	0.43
5:C:623:LYS:HE2	5:C:626:LEU:HG	2.01	0.43
4:D:875:PHE:HA	4:D:878:PHE:HB3	1.99	0.43
1:J:335:MET:HE2	1:J:335:MET:HB2	1.88	0.43
8:R:34:GLU:HG3	8:R:84:LYS:HE3	1.99	0.43
8:R:37:VAL:N	8:R:58:GLU:O	2.49	0.43
8:R:154:LEU:HD23	8:R:198:ASN:HB2	2.00	0.43
8:R:344:LYS:HD3	8:R:344:LYS:HA	1.82	0.43
8:W:160:ARG:HA	8:W:160:ARG:HD2	1.83	0.43
8:X:12:GLN:H	8:X:12:GLN:HG2	1.68	0.43
2:e:18:LYS:HD2	2:e:340:TRP:HE3	1.84	0.43
2:e:350:SER:H	7:c:43:ASN:HD21	1.67	0.43
4:a:98:LEU:HD12	4:a:98:LEU:HA	1.85	0.43
4:D:308:THR:O	4:D:312:SER:OG	2.37	0.43
4:D:380:THR:O	4:D:384:LEU:HG	2.19	0.43
4:F:616:GLU:O	4:F:620:ARG:HG2	2.18	0.43
4:F:843:MET:O	4:F:847:LEU:HG	2.19	0.43
4:H:883:ASN:ND2	8:V:352:GLY:O	2.52	0.43
6:K:96:VAL:HG21	6:K:175:ILE:HG13	2.01	0.43
7:L:1594:LEU:HD23	7:L:1594:LEU:HA	1.89	0.43
8:Q:154:LEU:HD23	8:Q:198:ASN:HB2	2.00	0.43
8:U:348:PHE:HB3	8:U:349:ILE:H	1.70	0.43
8:X:151:SER:HB2	8:X:194:ARG:HG2	2.01	0.43
3:b:57:PRO:HA	3:b:60:LEU:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:a:78:HIS:HA	4:a:81:LEU:HD12	2.00	0.43
5:E:741:ASN:HD22	5:E:745:LEU:N	2.16	0.43
4:F:362:LEU:HB3	4:F:363:THR:H	1.61	0.43
4:H:447:PHE:HA	4:H:467:ARG:HB3	2.01	0.43
7:L:284:GLU:HA	7:L:287:LEU:HD12	2.01	0.43
7:L:1665:MET:HE3	7:L:1736:VAL:HG22	2.00	0.43
8:X:37:VAL:N	8:X:58:GLU:O	2.49	0.43
5:G:155:GLU:O	5:G:159:LYS:HG2	2.18	0.43
6:I:509:GLN:HB3	6:I:510:THR:H	1.67	0.43
1:J:364:PHE:O	1:J:368:LEU:HG	2.19	0.43
8:R:237:SER:O	8:R:244:ARG:NH2	2.43	0.43
8:Y:154:LEU:HD23	8:Y:198:ASN:HB2	2.00	0.43
7:c:114:LEU:HD23	7:c:114:LEU:HA	1.85	0.43
4:j:61:GLU:HG2	4:j:64:ARG:HH21	1.84	0.43
5:C:266:VAL:HG21	5:C:328:ILE:HD13	2.00	0.42
4:D:722:ILE:HD13	4:D:726:VAL:HG21	2.00	0.42
5:E:557:LEU:HD13	8:T:339:ARG:CZ	2.49	0.42
5:E:560:ARG:HB2	8:T:339:ARG:HH11	1.83	0.42
5:G:696:TYR:CE2	5:G:697:MET:HG3	2.54	0.42
7:L:399:GLU:OE2	7:L:403:TYR:OH	2.34	0.42
7:L:1518:MET:HB2	7:L:1623:LEU:HD21	2.00	0.42
8:R:278:THR:HG23	8:R:371:HIS:ND1	2.34	0.42
8:S:231:LEU:O	8:S:234:THR:OG1	2.30	0.42
8:T:12:GLN:H	8:T:12:GLN:HG2	1.68	0.42
8:V:151:SER:HB2	8:V:194:ARG:HG2	2.01	0.42
8:V:154:LEU:HD23	8:V:198:ASN:HB2	2.00	0.42
8:W:154:LEU:HD23	8:W:198:ASN:HB2	2.00	0.42
8:Z:151:SER:HB2	8:Z:194:ARG:HG2	2.01	0.42
1:l:117:LEU:HD21	3:m:64:ILE:HB	2.01	0.42
5:E:547:THR:HA	5:E:548:PRO:HD3	1.93	0.42
5:G:692:ASN:HA	5:G:858:ARG:HH22	1.85	0.42
4:H:388:CYS:HB3	4:H:396:LEU:HG	2.01	0.42
6:I:3:HIS:CG	7:L:297:TRP:HE1	2.37	0.42
8:Q:278:THR:HG23	8:Q:371:HIS:ND1	2.34	0.42
8:S:115:HIS:HB3	8:S:152:TYR:HE2	1.85	0.42
8:U:278:THR:HG23	8:U:371:HIS:ND1	2.34	0.42
8:V:3:ARG:HB3	8:V:4:GLU:H	1.51	0.42
8:V:261:ILE:HG12	8:V:267:HIS:HA	2.00	0.42
8:Y:348:PHE:HB3	8:Y:349:ILE:H	1.70	0.42
8:Z:261:ILE:HG12	8:Z:267:HIS:HA	2.00	0.42
4:H:549:LEU:HD12	4:H:555:LEU:HD21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:722:ILE:O	4:H:727:LEU:HG	2.19	0.42
8:X:278:THR:HG23	8:X:371:HIS:ND1	2.34	0.42
8:Y:37:VAL:N	8:Y:58:GLU:O	2.49	0.42
3:d:21:VAL:HG22	3:d:25:MET:HE2	2.00	0.42
5:C:305:ILE:HG22	7:c:190:LEU:HD21	2.00	0.42
4:F:686:CYS:HA	4:F:689:LYS:HD3	2.01	0.42
5:G:536:GLU:HA	5:G:539:LEU:HB2	2.01	0.42
4:H:716:HIS:HA	4:H:719:GLN:HE21	1.83	0.42
6:I:524:LEU:HD22	8:W:353:PRO:HB2	2.01	0.42
7:L:284:GLU:HA	7:L:287:LEU:HB2	2.02	0.42
8:Q:231:LEU:O	8:Q:234:THR:OG1	2.30	0.42
8:T:278:THR:HG23	8:T:371:HIS:ND1	2.34	0.42
8:W:278:THR:HG23	8:W:371:HIS:ND1	2.34	0.42
4:H:616:GLU:HG2	4:H:619:ARG:HH11	1.83	0.42
6:K:651:TYR:CE1	8:Y:348:PHE:HB2	2.54	0.42
8:Q:11:GLY:O	8:Q:15:ASN:ND2	2.52	0.42
8:R:151:SER:HB2	8:R:194:ARG:HG2	2.01	0.42
8:U:154:LEU:HD23	8:U:198:ASN:HB2	2.00	0.42
8:U:261:ILE:HG12	8:U:267:HIS:HA	2.00	0.42
8:V:11:GLY:O	8:V:15:ASN:ND2	2.52	0.42
8:V:278:THR:HG23	8:V:371:HIS:ND1	2.34	0.42
8:W:115:HIS:HB3	8:W:152:TYR:HE2	1.85	0.42
8:Z:154:LEU:HD23	8:Z:198:ASN:HB2	2.00	0.42
2:e:273:GLY:O	2:e:277:THR:OG1	2.34	0.42
5:G:312:GLN:NE2	5:G:316:GLN:HE21	2.17	0.42
8:Q:151:SER:HB2	8:Q:194:ARG:HG2	2.01	0.42
8:Q:261:ILE:HG12	8:Q:267:HIS:HA	2.00	0.42
8:R:11:GLY:O	8:R:15:ASN:ND2	2.52	0.42
8:T:151:SER:HB2	8:T:194:ARG:HG2	2.01	0.42
8:W:11:GLY:O	8:W:15:ASN:ND2	2.52	0.42
3:d:32:SER:OG	3:d:37:THR:OG1	2.36	0.42
5:C:540:ARG:HA	5:C:613:LEU:HD11	2.02	0.42
5:E:695:TYR:CD1	5:E:698:MET:HE3	2.54	0.42
5:G:302:GLU:HA	5:G:305:ILE:HD12	2.01	0.42
5:G:311:GLU:HB2	4:H:365:ARG:NH1	2.34	0.42
7:L:1783:VAL:HG21	7:L:1798:PHE:CD1	2.54	0.42
8:S:11:GLY:O	8:S:15:ASN:ND2	2.52	0.42
8:T:115:HIS:HB3	8:T:152:TYR:HE2	1.85	0.42
8:Z:11:GLY:O	8:Z:15:ASN:ND2	2.52	0.42
4:j:51:GLU:HA	4:j:54:VAL:HG22	2.01	0.42
1:J:275:LEU:HA	1:J:278:LEU:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:K:524:LEU:HA	6:K:524:LEU:HD12	1.83	0.42
8:R:115:HIS:HB3	8:R:152:TYR:HE2	1.85	0.42
8:R:164:LYS:HD3	8:R:164:LYS:HA	1.84	0.42
8:S:55:ALA:N	8:S:59:HIS:O	2.49	0.42
8:S:237:SER:O	8:S:244:ARG:NH2	2.43	0.42
8:S:261:ILE:HG12	8:S:267:HIS:HA	2.00	0.42
8:T:3:ARG:HB3	8:T:4:GLU:H	1.51	0.42
8:V:55:ALA:N	8:V:59:HIS:O	2.49	0.42
8:X:11:GLY:O	8:X:15:ASN:ND2	2.52	0.42
2:e:67:LEU:HD11	2:e:69:TYR:CZ	2.55	0.42
2:e:365:SER:O	2:e:365:SER:OG	2.34	0.42
5:C:436:GLN:CD	5:C:436:GLN:H	2.28	0.42
5:E:411:GLU:HG2	5:E:432:TYR:HE1	1.85	0.42
5:G:186:ALA:HB1	4:H:293:ARG:HA	2.01	0.42
6:K:639:ASN:HB2	8:Y:334:HIS:CE1	2.54	0.42
8:Q:12:GLN:H	8:Q:12:GLN:HG2	1.68	0.42
8:Q:115:HIS:HB3	8:Q:152:TYR:HE2	1.85	0.42
8:T:5:ILE:HB	8:T:51:PHE:HE1	1.85	0.42
8:T:329:ASP:HA	8:T:330:PRO:HD3	1.91	0.42
8:U:55:ALA:N	8:U:59:HIS:O	2.49	0.42
8:Y:11:GLY:O	8:Y:15:ASN:ND2	2.52	0.42
8:Y:278:THR:HG23	8:Y:371:HIS:ND1	2.34	0.42
8:Z:344:LYS:HA	8:Z:344:LYS:HD3	1.82	0.42
3:b:24:THR:O	3:b:28:LEU:HG	2.20	0.42
5:C:526:ASP:HA	5:C:529:VAL:HG22	2.02	0.42
4:D:294:LEU:HD23	4:D:294:LEU:HA	1.83	0.42
4:F:305:ARG:HH22	5:G:262:ARG:HD3	1.85	0.42
5:G:578:MET:H	5:G:615:ALA:HB1	1.85	0.42
1:J:291:ASP:N	1:J:291:ASP:OD1	2.51	0.42
6:K:66:VAL:HG13	6:K:68:GLN:H	1.84	0.42
7:L:1530:LEU:HD23	7:L:1530:LEU:HA	1.94	0.42
8:S:5:ILE:HB	8:S:51:PHE:HE1	1.85	0.42
8:U:5:ILE:HB	8:U:51:PHE:HE1	1.85	0.42
8:Y:151:SER:HB2	8:Y:194:ARG:HG2	2.01	0.42
4:a:93:ILE:HG23	4:a:94:LEU:HD22	2.02	0.41
5:C:188:ILE:HG21	5:C:275:ARG:HG2	2.03	0.41
5:C:353:GLY:HA3	5:C:440:PRO:HD3	2.02	0.41
4:D:685:MET:HE2	4:D:685:MET:HB3	1.95	0.41
5:E:752:MET:HE2	5:E:752:MET:HB3	1.86	0.41
5:E:861:PHE:CD2	5:E:862:ASN:HB2	2.55	0.41
4:F:707:LEU:HD22	4:F:851:THR:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:504:HIS:C	6:I:506:LYS:H	2.28	0.41
6:I:565:LEU:O	6:I:569:LEU:HG	2.20	0.41
6:I:568:LEU:O	6:I:572:SER:OG	2.21	0.41
6:K:9:LEU:HD23	6:K:104:LEU:HD22	2.01	0.41
6:K:177:ALA:HB2	6:K:318:PRO:HA	2.02	0.41
8:Q:160:ARG:HD2	8:Q:160:ARG:HA	1.82	0.41
8:R:5:ILE:HB	8:R:51:PHE:HE1	1.85	0.41
8:S:278:THR:HG23	8:S:371:HIS:ND1	2.34	0.41
8:U:151:SER:HB2	8:U:194:ARG:HG2	2.01	0.41
8:Z:115:HIS:HB3	8:Z:152:TYR:HE2	1.85	0.41
8:Z:278:THR:HG23	8:Z:371:HIS:ND1	2.34	0.41
1:l:129:THR:H	3:m:33:ARG:NH1	2.18	0.41
3:b:67:LEU:HD12	3:b:67:LEU:HA	1.90	0.41
5:E:642:PHE:HA	5:E:645:MET:HE3	2.02	0.41
4:F:275:TYR:HE1	4:F:299:TRP:HB2	1.84	0.41
6:K:94:ASP:OD1	6:K:95:SER:N	2.53	0.41
3:m:28:LEU:HD23	3:m:31:ILE:HD12	2.02	0.41
8:S:289:THR:HG23	8:S:291:LEU:HB3	2.03	0.41
8:T:11:GLY:O	8:T:15:ASN:ND2	2.52	0.41
8:T:55:ALA:N	8:T:59:HIS:O	2.49	0.41
8:V:115:HIS:HB3	8:V:152:TYR:HE2	1.85	0.41
8:V:289:THR:HG23	8:V:291:LEU:HB3	2.02	0.41
1:l:107:HIS:O	1:l:111:LEU:HG	2.20	0.41
3:b:49:ARG:CZ	7:L:284:GLU:HB2	2.51	0.41
5:C:557:LEU:HA	8:R:339:ARG:NE	2.35	0.41
4:D:416:GLN:HE22	4:D:420:SER:HB3	1.85	0.41
5:G:499:LEU:HD23	5:G:719:ILE:HG13	2.01	0.41
5:G:709:LEU:HD22	5:G:729:PHE:CG	2.55	0.41
6:I:132:LEU:HA	6:I:132:LEU:HD23	1.83	0.41
1:J:254:ASP:HA	1:J:256:LEU:HD13	2.01	0.41
1:J:264:LEU:HD13	1:J:301:ILE:HG23	2.02	0.41
8:T:164:LYS:HD3	8:T:164:LYS:HA	1.84	0.41
8:U:289:THR:HG23	8:U:291:LEU:HB3	2.03	0.41
8:W:348:PHE:HB3	8:W:349:ILE:H	1.70	0.41
7:c:111:LEU:HA	7:c:114:LEU:HB2	2.01	0.41
5:C:858:ARG:HH11	8:Q:358:VAL:HG11	1.85	0.41
5:E:284:GLU:H	5:E:284:GLU:CD	2.24	0.41
6:I:131:LEU:HD22	6:I:167:PRO:HB2	2.02	0.41
6:I:515:TRP:CE2	6:I:517:LEU:HA	2.55	0.41
8:Y:5:ILE:HB	8:Y:51:PHE:HE1	1.85	0.41
4:j:50:ASP:N	4:j:50:ASP:OD1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:356:LEU:HB2	5:C:440:PRO:HB3	2.02	0.41
5:G:259:LEU:O	5:G:263:ILE:HG12	2.21	0.41
5:G:304:LEU:HA	5:G:307:VAL:HG22	2.03	0.41
4:H:578:MET:HG2	4:H:578:MET:H	1.62	0.41
4:H:675:TYR:HA	4:H:678:THR:HG22	2.03	0.41
8:R:410:LYS:H	8:R:410:LYS:HG2	1.51	0.41
8:S:153:LEU:HD13	8:S:153:LEU:HA	1.82	0.41
8:U:11:GLY:O	8:U:15:ASN:ND2	2.52	0.41
8:X:3:ARG:HB3	8:X:4:GLU:H	1.51	0.41
8:X:115:HIS:HB3	8:X:152:TYR:HE2	1.85	0.41
8:Z:5:ILE:HB	8:Z:51:PHE:HE1	1.85	0.41
7:c:179:LEU:HD23	7:c:182:MET:HG2	2.03	0.41
2:e:143:TYR:HD2	2:e:346:LEU:HD11	1.85	0.41
2:e:341:ILE:HD13	2:e:341:ILE:HG21	1.89	0.41
5:E:473:LYS:HE3	5:E:487:GLN:HB3	2.03	0.41
4:F:261:ILE:HG13	5:G:262:ARG:HH22	1.85	0.41
4:F:735:TRP:O	4:F:739:GLN:HG2	2.21	0.41
1:J:437:LEU:HD22	1:J:549:VAL:HG11	2.03	0.41
6:K:300:LEU:HB3	6:K:301:LYS:H	1.61	0.41
7:L:1524:ALA:HA	7:L:1527:LEU:HG	2.03	0.41
8:S:160:ARG:HD2	8:S:160:ARG:HA	1.83	0.41
8:W:55:ALA:N	8:W:59:HIS:O	2.49	0.41
8:X:5:ILE:HB	8:X:51:PHE:HE1	1.85	0.41
8:Y:344:LYS:HA	8:Y:344:LYS:HD3	1.82	0.41
3:k:63:VAL:O	3:k:67:LEU:HG	2.20	0.41
1:l:128:GLU:HA	3:m:33:ARG:HH12	1.86	0.41
4:D:865:LEU:HG	4:D:877:SER:HB2	2.02	0.41
5:E:653:ARG:NH1	5:E:657:SER:HB3	2.36	0.41
7:L:307:ARG:O	7:L:309:GLU:HG3	2.20	0.41
8:R:320:ILE:HG23	8:R:379:ALA:HB2	2.03	0.41
8:W:5:ILE:HB	8:W:51:PHE:HE1	1.85	0.41
8:X:263:THR:HG1	8:X:265:ARG:HH11	1.64	0.41
8:Y:231:LEU:O	8:Y:234:THR:OG1	2.30	0.41
8:Y:320:ILE:HG23	8:Y:379:ALA:HB2	2.03	0.41
8:Y:410:LYS:H	8:Y:410:LYS:HG2	1.51	0.41
5:G:683:ARG:NH2	8:U:262:PRO:O	2.53	0.41
7:L:454:LEU:HD22	7:L:458:THR:HG21	2.02	0.41
7:L:1574:LEU:HD12	7:L:1574:LEU:HA	1.95	0.41
8:R:3:ARG:HB3	8:R:4:GLU:H	1.51	0.41
8:S:377:MET:HE3	8:S:377:MET:HB2	2.01	0.41
8:T:320:ILE:HG23	8:T:379:ALA:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:5:ILE:HB	8:V:51:PHE:HE1	1.85	0.41
2:e:166:TYR:CZ	2:e:167:GLU:HG2	2.56	0.41
2:e:311:ASP:O	2:e:315:LYS:HG2	2.20	0.41
5:C:439:ILE:HD11	5:C:444:GLN:HA	2.03	0.41
5:C:652:GLU:O	5:C:655:LEU:HG	2.21	0.41
4:D:274:CYS:SG	4:D:275:TYR:N	2.92	0.41
4:F:543:LYS:HD2	4:F:543:LYS:HA	1.91	0.41
4:F:754:PHE:O	4:F:758:ILE:HG12	2.21	0.41
5:G:184:ARG:NH1	4:H:273:ASN:OD1	2.53	0.41
4:H:369:VAL:HG13	4:H:370:TRP:CD1	2.56	0.41
4:H:475:MET:HB3	4:H:475:MET:HE3	1.80	0.41
4:H:562:MET:HG3	4:H:566:LEU:HD12	2.02	0.41
6:I:148:ILE:HG23	6:I:152:GLN:HB2	2.03	0.41
6:I:568:LEU:HA	6:I:571:GLN:NE2	2.36	0.41
6:I:583:LEU:O	6:I:587:LEU:HG	2.21	0.41
6:K:361:TYR:HB2	6:K:362:LEU:HD12	2.01	0.41
7:L:588:LEU:HA	7:L:588:LEU:HD12	1.85	0.41
7:L:1736:VAL:O	7:L:1740:ARG:HD3	2.21	0.41
8:Q:257:ILE:HD13	8:Q:257:ILE:HA	1.93	0.41
8:Q:320:ILE:HG23	8:Q:379:ALA:HB2	2.03	0.41
8:S:257:ILE:HD13	8:S:257:ILE:HA	1.93	0.41
8:T:3:ARG:HH11	8:T:131:SER:HA	1.86	0.41
8:T:37:VAL:N	8:T:58:GLU:O	2.49	0.41
8:V:320:ILE:HG23	8:V:379:ALA:HB2	2.03	0.41
8:Y:3:ARG:HB3	8:Y:4:GLU:H	1.51	0.41
8:Y:115:HIS:HB3	8:Y:152:TYR:HE2	1.85	0.41
3:k:59:ALA:O	3:k:63:VAL:HG13	2.21	0.41
3:b:57:PRO:HB3	4:a:96:LEU:HD22	2.03	0.41
5:C:303:HIS:O	5:C:307:VAL:HG23	2.20	0.41
5:C:381:LYS:HG3	5:C:477:TYR:HB3	2.03	0.41
4:D:368:LEU:HA	4:D:368:LEU:HD13	1.74	0.41
5:E:252:LEU:HD11	5:E:257:ARG:HB3	2.03	0.41
5:E:415:ARG:HD2	5:E:415:ARG:HA	1.92	0.41
5:E:426:LYS:HE2	5:E:428:TRP:CZ3	2.56	0.41
5:E:745:LEU:HD12	5:E:745:LEU:HA	1.96	0.41
5:E:829:PHE:O	5:E:833:LEU:HG	2.21	0.41
6:I:579:VAL:O	6:I:583:LEU:HG	2.21	0.41
6:K:650:ASP:HB3	6:K:651:TYR:CE2	2.55	0.41
7:L:1671:VAL:HG23	7:L:1801:ARG:HH21	1.86	0.41
8:R:153:LEU:HD13	8:R:153:LEU:HA	1.82	0.41
8:S:220:ILE:HB	8:S:223:PRO:HD2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:T:160:ARG:HD2	8:T:160:ARG:HA	1.82	0.41
8:Y:164:LYS:HA	8:Y:164:LYS:HD3	1.84	0.41
8:Y:192:LEU:HA	8:Y:192:LEU:HD13	1.96	0.41
8:Y:220:ILE:HB	8:Y:223:PRO:HD2	2.03	0.41
8:Z:410:LYS:H	8:Z:410:LYS:HG2	1.51	0.41
4:F:254:ILE:HD12	4:F:257:VAL:HB	2.03	0.40
5:G:168:LYS:HG2	5:G:171:GLY:H	1.85	0.40
4:H:865:LEU:HD21	4:H:873:LEU:O	2.21	0.40
6:I:363:LEU:HD12	6:I:482:LEU:HG	2.03	0.40
1:J:283:LYS:HA	1:J:283:LYS:HD2	1.96	0.40
8:Q:220:ILE:HB	8:Q:223:PRO:HD2	2.03	0.40
8:V:352:GLY:HA2	8:V:353:PRO:HD3	1.94	0.40
8:X:377:MET:HE3	8:X:377:MET:HB2	2.01	0.40
4:j:19:ARG:HA	4:j:19:ARG:HD2	1.92	0.40
2:e:79:TRP:CZ2	2:e:118:LYS:HB3	2.57	0.40
2:e:123:MET:HA	2:e:127:PHE:HB3	2.03	0.40
5:E:479:LEU:HD12	5:E:479:LEU:HA	1.94	0.40
4:F:338:LEU:O	4:F:342:LEU:HG	2.22	0.40
4:F:878:PHE:HB3	4:F:879:ARG:HE	1.86	0.40
6:I:305:ASP:OD1	6:I:305:ASP:N	2.55	0.40
1:J:378:GLU:O	1:J:382:ILE:HG12	2.21	0.40
6:K:30:ASP:HA	6:K:34:LEU:HD11	2.03	0.40
6:K:79:GLY:HA2	6:K:83:GLY:HA3	2.04	0.40
8:V:37:VAL:N	8:V:58:GLU:O	2.49	0.40
8:X:220:ILE:HB	8:X:223:PRO:HD2	2.03	0.40
8:X:320:ILE:HG23	8:X:379:ALA:HB2	2.03	0.40
8:Y:377:MET:HE3	8:Y:377:MET:HB2	2.01	0.40
2:e:291:LYS:HE3	2:e:291:LYS:HB3	1.90	0.40
5:C:238:LEU:HD23	5:C:239:ALA:H	1.85	0.40
5:C:408:MET:HG2	5:C:439:ILE:HA	2.03	0.40
4:D:875:PHE:CE1	8:R:334:HIS:HB2	2.56	0.40
5:E:283:PHE:HA	5:E:290:HIS:NE2	2.36	0.40
5:E:635:LEU:HA	5:E:638:TYR:HB2	2.04	0.40
5:E:707:HIS:CG	8:S:330:PRO:HG2	2.56	0.40
4:H:837:LYS:HD2	4:H:837:LYS:HA	1.81	0.40
8:R:220:ILE:HB	8:R:223:PRO:HD2	2.03	0.40
2:e:90:PHE:HB2	2:e:127:PHE:CE1	2.55	0.40
4:D:408:ASP:HB3	4:D:411:MET:HE2	2.04	0.40
4:D:879:ARG:HH12	4:D:882:PHE:HD2	1.68	0.40
4:F:713:HIS:CG	8:T:353:PRO:HB2	2.57	0.40
5:G:530:HIS:HE1	8:U:3:ARG:HG2	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:658:SER:O	4:H:662:ARG:HG3	2.21	0.40
6:I:343:LEU:O	6:I:347:GLU:HG3	2.22	0.40
6:I:530:TYR:HE2	8:W:249:MET:HB2	1.87	0.40
1:J:721:GLN:HA	1:J:724:ARG:NE	2.36	0.40
6:K:492:LEU:HD22	6:K:594:CYS:SG	2.62	0.40
7:L:1778:PHE:HA	7:L:1781:LYS:HE2	2.03	0.40
8:R:295:ARG:HB3	8:R:296:ARG:NH2	2.35	0.40
8:U:115:HIS:HB3	8:U:152:TYR:HE2	1.85	0.40
8:W:289:THR:HG23	8:W:291:LEU:HB3	2.03	0.40
8:X:231:LEU:O	8:X:234:THR:OG1	2.30	0.40
8:X:289:THR:HG23	8:X:291:LEU:HB3	2.03	0.40
8:Y:153:LEU:HD13	8:Y:153:LEU:HA	1.82	0.40
8:Z:289:THR:HG23	8:Z:291:LEU:HB3	2.03	0.40
4:j:23:ARG:NE	4:j:28:VAL:HB	2.35	0.40
2:e:136:ILE:HG23	2:e:139:VAL:HB	2.04	0.40
2:e:282:ILE:HD13	2:e:282:ILE:HA	1.91	0.40
4:a:94:LEU:HA	4:a:94:LEU:HD13	1.88	0.40
5:C:289:ASN:HA	5:C:292:LEU:HB2	2.04	0.40
5:G:680:PHE:HA	5:G:683:ARG:HE	1.87	0.40
6:I:108:GLU:H	6:I:108:GLU:HG3	1.69	0.40
6:I:314:LEU:HD13	6:I:314:LEU:HA	1.88	0.40
6:K:342:LYS:HE2	6:K:342:LYS:HB2	1.90	0.40
6:K:500:MET:H	6:K:500:MET:HG3	1.73	0.40
8:Q:289:THR:HG23	8:Q:291:LEU:HB3	2.03	0.40
8:S:3:ARG:HH11	8:S:131:SER:HA	1.87	0.40
8:T:220:ILE:HB	8:T:223:PRO:HD2	2.03	0.40
8:U:446:TRP:CD1	8:U:446:TRP:H	2.40	0.40
8:W:320:ILE:HG23	8:W:379:ALA:HB2	2.03	0.40
8:X:160:ARG:HD2	8:X:160:ARG:HH11	1.77	0.40
8:Y:289:THR:HG23	8:Y:291:LEU:HB3	2.03	0.40
7:c:137:LYS:HA	7:c:137:LYS:HD3	1.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	506/1024 (49%)	464 (92%)	38 (8%)	4 (1%)	16	54
1	l	104/1024 (10%)	97 (93%)	5 (5%)	2 (2%)	6	32
2	e	360/375 (96%)	345 (96%)	15 (4%)	0	100	100
3	b	63/82 (77%)	61 (97%)	2 (3%)	0	100	100
3	d	57/82 (70%)	56 (98%)	1 (2%)	0	100	100
3	i	63/82 (77%)	63 (100%)	0	0	100	100
3	k	63/82 (77%)	61 (97%)	2 (3%)	0	100	100
3	m	63/82 (77%)	63 (100%)	0	0	100	100
4	D	571/907 (63%)	552 (97%)	17 (3%)	2 (0%)	30	67
4	F	591/907 (65%)	561 (95%)	30 (5%)	0	100	100
4	H	584/907 (64%)	557 (95%)	23 (4%)	4 (1%)	18	56
4	a	112/907 (12%)	109 (97%)	3 (3%)	0	100	100
4	h	97/907 (11%)	94 (97%)	3 (3%)	0	100	100
4	j	105/907 (12%)	99 (94%)	6 (6%)	0	100	100
5	C	606/902 (67%)	575 (95%)	28 (5%)	3 (0%)	24	63
5	E	626/902 (69%)	587 (94%)	38 (6%)	1 (0%)	43	78
5	G	628/902 (70%)	596 (95%)	29 (5%)	3 (0%)	24	63
6	I	511/667 (77%)	484 (95%)	25 (5%)	2 (0%)	30	67
6	K	548/667 (82%)	530 (97%)	16 (3%)	2 (0%)	30	67
7	L	540/1819 (30%)	495 (92%)	38 (7%)	7 (1%)	9	42
7	c	148/1819 (8%)	142 (96%)	6 (4%)	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
8	S	408/451 (90%)	386 (95%)	22 (5%)	0	100	100
8	T	408/451 (90%)	386 (95%)	22 (5%)	0	100	100
8	U	408/451 (90%)	386 (95%)	22 (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%)	386 (95%)	22 (5%)	0	100	100
8	Y	408/451 (90%)	386 (95%)	22 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	Z	408/451 (90%)	386 (95%)	22 (5%)	0	100	100
All	All	11026/20463 (54%)	10451 (95%)	545 (5%)	30 (0%)	37	72

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	121	PRO
5	C	465	HIS
5	G	581	ASP
4	H	454	VAL
4	H	632	ASP
6	I	601	LEU
1	J	236	LEU
6	K	29	GLN
6	K	409	ASN
7	L	308	GLU
5	G	582	LEU
5	G	675	TRP
4	H	631	GLY
4	H	633	THR
6	I	600	ASN
4	D	628	VAL
4	D	889	ARG
5	E	581	ASP
1	I	120	SER
1	J	257	TYR
1	J	946	LYS
7	L	307	ARG
7	L	309	GLU
5	C	861	PHE
1	J	945	GLU
7	L	314	GLU
7	L	495	PHE
7	L	1760	PRO
7	L	310	PRO
5	C	240	GLY

5.3.2 Protein sidechains ⓘ

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

entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	498/933 (53%)	492 (99%)	6 (1%)	63	75
1	l	84/933 (9%)	84 (100%)	0	100	100
2	e	310/318 (98%)	301 (97%)	9 (3%)	37	58
3	b	53/62 (86%)	52 (98%)	1 (2%)	50	67
3	d	53/62 (86%)	52 (98%)	1 (2%)	50	67
3	i	53/62 (86%)	52 (98%)	1 (2%)	50	67
3	k	53/62 (86%)	50 (94%)	3 (6%)	18	40
3	m	53/62 (86%)	53 (100%)	0	100	100
4	D	525/798 (66%)	521 (99%)	4 (1%)	73	80
4	F	542/798 (68%)	540 (100%)	2 (0%)	84	84
4	H	539/798 (68%)	536 (99%)	3 (1%)	78	83
4	a	101/798 (13%)	98 (97%)	3 (3%)	36	57
4	h	88/798 (11%)	88 (100%)	0	100	100
4	j	88/798 (11%)	87 (99%)	1 (1%)	65	76
5	C	556/791 (70%)	554 (100%)	2 (0%)	84	84
5	E	574/791 (73%)	572 (100%)	2 (0%)	86	86
5	G	572/791 (72%)	567 (99%)	5 (1%)	70	79
6	I	472/594 (80%)	467 (99%)	5 (1%)	65	76
6	K	509/594 (86%)	505 (99%)	4 (1%)	73	80
7	L	501/1546 (32%)	501 (100%)	0	100	100
7	c	135/1546 (9%)	134 (99%)	1 (1%)	76	81
8	Q	376/400 (94%)	322 (86%)	54 (14%)	3	13
8	R	376/400 (94%)	322 (86%)	54 (14%)	3	13
8	S	376/400 (94%)	322 (86%)	54 (14%)	3	13
8	T	376/400 (94%)	322 (86%)	54 (14%)	3	13
8	U	376/400 (94%)	322 (86%)	54 (14%)	3	13
8	V	376/400 (94%)	322 (86%)	54 (14%)	3	13
8	W	376/400 (94%)	322 (86%)	54 (14%)	3	13
8	X	376/400 (94%)	322 (86%)	54 (14%)	3	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	Y	376/400 (94%)	322 (86%)	54 (14%)	3	13
8	Z	376/400 (94%)	322 (86%)	54 (14%)	3	13
All	All	10119/17935 (56%)	9526 (94%)	593 (6%)	19	39

All (593) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	e	18	LYS
2	e	122	ILE
2	e	140	LEU
2	e	152	VAL
2	e	162	THR
2	e	165	ILE
2	e	247	VAL
2	e	281	SER
2	e	369	ILE
3	b	37	THR
4	a	8	SER
4	a	50	ASP
4	a	96	LEU
5	C	328	ILE
5	C	526	ASP
4	D	486	ILE
4	D	626	LEU
4	D	627	GLU
4	D	628	VAL
5	E	305	ILE
5	E	328	ILE
4	F	426	VAL
4	F	887	LYS
5	G	190	ASP
5	G	233	VAL
5	G	310	LEU
5	G	641	LEU
5	G	693	ILE
4	H	617	ILE
4	H	627	GLU
4	H	628	VAL
6	I	45	LEU
6	I	263	ILE
6	I	314	LEU

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Mol	Chain	Res	Type
6	I	506	LYS
6	I	507	SER
1	J	220	VAL
1	J	294	VAL
1	J	463	SER
1	J	473	LEU
1	J	809	VAL
1	J	883	MET
6	K	35	HIS
6	K	356	ILE
6	K	568	LEU
6	K	596	LEU
3	i	48	VAL
8	Q	10	LEU
8	Q	17	ILE
8	Q	24	GLN
8	Q	31	ILE
8	Q	37	VAL
8	Q	50	VAL
8	Q	66	LEU
8	Q	76	SER
8	Q	78	LEU
8	Q	85	LEU
8	Q	112	GLU
8	Q	127	ASP
8	Q	131	SER
8	Q	140	SER
8	Q	153	LEU
8	Q	154	LEU
8	Q	157	LEU
8	Q	165	LEU
8	Q	166	VAL
8	Q	188	SER
8	Q	192	LEU
8	Q	195	LEU
8	Q	204	VAL
8	Q	205	LEU
8	Q	206	ASP
8	Q	208	THR
8	Q	217	ARG
8	Q	218	LEU
8	Q	222	ASN

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Mol	Chain	Res	Type
8	Q	228	ILE
8	Q	231	LEU
8	Q	233	SER
8	Q	259	SER
8	Q	265	ARG
8	Q	276	LEU
8	Q	288	THR
8	Q	290	VAL
8	Q	293	VAL
8	Q	296	ARG
8	Q	304	MET
8	Q	316	CYS
8	Q	323	ILE
8	Q	333	VAL
8	Q	339	ARG
8	Q	340	ILE
8	Q	341	ARG
8	Q	347	ASN
8	Q	362	ARG
8	Q	369	SER
8	Q	373	VAL
8	Q	377	MET
8	Q	385	SER
8	Q	392	CYS
8	Q	410	LYS
8	R	10	LEU
8	R	17	ILE
8	R	24	GLN
8	R	31	ILE
8	R	37	VAL
8	R	50	VAL
8	R	66	LEU
8	R	76	SER
8	R	78	LEU
8	R	85	LEU
8	R	112	GLU
8	R	127	ASP
8	R	131	SER
8	R	140	SER
8	R	153	LEU
8	R	154	LEU
8	R	157	LEU

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Mol	Chain	Res	Type
8	R	165	LEU
8	R	166	VAL
8	R	188	SER
8	R	192	LEU
8	R	195	LEU
8	R	204	VAL
8	R	205	LEU
8	R	206	ASP
8	R	208	THR
8	R	217	ARG
8	R	218	LEU
8	R	222	ASN
8	R	228	ILE
8	R	231	LEU
8	R	233	SER
8	R	259	SER
8	R	265	ARG
8	R	276	LEU
8	R	288	THR
8	R	290	VAL
8	R	293	VAL
8	R	296	ARG
8	R	304	MET
8	R	316	CYS
8	R	323	ILE
8	R	333	VAL
8	R	339	ARG
8	R	340	ILE
8	R	341	ARG
8	R	347	ASN
8	R	362	ARG
8	R	369	SER
8	R	373	VAL
8	R	377	MET
8	R	385	SER
8	R	392	CYS
8	R	410	LYS
8	S	10	LEU
8	S	17	ILE
8	S	24	GLN
8	S	31	ILE
8	S	37	VAL

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Mol	Chain	Res	Type
8	S	50	VAL
8	S	66	LEU
8	S	76	SER
8	S	78	LEU
8	S	85	LEU
8	S	112	GLU
8	S	127	ASP
8	S	131	SER
8	S	140	SER
8	S	153	LEU
8	S	154	LEU
8	S	157	LEU
8	S	165	LEU
8	S	166	VAL
8	S	188	SER
8	S	192	LEU
8	S	195	LEU
8	S	204	VAL
8	S	205	LEU
8	S	206	ASP
8	S	208	THR
8	S	217	ARG
8	S	218	LEU
8	S	222	ASN
8	S	228	ILE
8	S	231	LEU
8	S	233	SER
8	S	259	SER
8	S	265	ARG
8	S	276	LEU
8	S	288	THR
8	S	290	VAL
8	S	293	VAL
8	S	296	ARG
8	S	304	MET
8	S	316	CYS
8	S	323	ILE
8	S	333	VAL
8	S	339	ARG
8	S	340	ILE
8	S	341	ARG
8	S	347	ASN

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Mol	Chain	Res	Type
8	S	362	ARG
8	S	369	SER
8	S	373	VAL
8	S	377	MET
8	S	385	SER
8	S	392	CYS
8	S	410	LYS
8	T	10	LEU
8	T	17	ILE
8	T	24	GLN
8	T	31	ILE
8	T	37	VAL
8	T	50	VAL
8	T	66	LEU
8	T	76	SER
8	T	78	LEU
8	T	85	LEU
8	T	112	GLU
8	T	127	ASP
8	T	131	SER
8	T	140	SER
8	T	153	LEU
8	T	154	LEU
8	T	157	LEU
8	T	165	LEU
8	T	166	VAL
8	T	188	SER
8	T	192	LEU
8	T	195	LEU
8	T	204	VAL
8	T	205	LEU
8	T	206	ASP
8	T	208	THR
8	T	217	ARG
8	T	218	LEU
8	T	222	ASN
8	T	228	ILE
8	T	231	LEU
8	T	233	SER
8	T	259	SER
8	T	265	ARG
8	T	276	LEU

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Mol	Chain	Res	Type
8	T	288	THR
8	T	290	VAL
8	T	293	VAL
8	T	296	ARG
8	T	304	MET
8	T	316	CYS
8	T	323	ILE
8	T	333	VAL
8	T	339	ARG
8	T	340	ILE
8	T	341	ARG
8	T	347	ASN
8	T	362	ARG
8	T	369	SER
8	T	373	VAL
8	T	377	MET
8	T	385	SER
8	T	392	CYS
8	T	410	LYS
8	U	10	LEU
8	U	17	ILE
8	U	24	GLN
8	U	31	ILE
8	U	37	VAL
8	U	50	VAL
8	U	66	LEU
8	U	76	SER
8	U	78	LEU
8	U	85	LEU
8	U	112	GLU
8	U	127	ASP
8	U	131	SER
8	U	140	SER
8	U	153	LEU
8	U	154	LEU
8	U	157	LEU
8	U	165	LEU
8	U	166	VAL
8	U	188	SER
8	U	192	LEU
8	U	195	LEU
8	U	204	VAL

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Mol	Chain	Res	Type
8	U	205	LEU
8	U	206	ASP
8	U	208	THR
8	U	217	ARG
8	U	218	LEU
8	U	222	ASN
8	U	228	ILE
8	U	231	LEU
8	U	233	SER
8	U	259	SER
8	U	265	ARG
8	U	276	LEU
8	U	288	THR
8	U	290	VAL
8	U	293	VAL
8	U	296	ARG
8	U	304	MET
8	U	316	CYS
8	U	323	ILE
8	U	333	VAL
8	U	339	ARG
8	U	340	ILE
8	U	341	ARG
8	U	347	ASN
8	U	362	ARG
8	U	369	SER
8	U	373	VAL
8	U	377	MET
8	U	385	SER
8	U	392	CYS
8	U	410	LYS
8	V	10	LEU
8	V	17	ILE
8	V	24	GLN
8	V	31	ILE
8	V	37	VAL
8	V	50	VAL
8	V	66	LEU
8	V	76	SER
8	V	78	LEU
8	V	85	LEU
8	V	112	GLU

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Mol	Chain	Res	Type
8	V	127	ASP
8	V	131	SER
8	V	140	SER
8	V	153	LEU
8	V	154	LEU
8	V	157	LEU
8	V	165	LEU
8	V	166	VAL
8	V	188	SER
8	V	192	LEU
8	V	195	LEU
8	V	204	VAL
8	V	205	LEU
8	V	206	ASP
8	V	208	THR
8	V	217	ARG
8	V	218	LEU
8	V	222	ASN
8	V	228	ILE
8	V	231	LEU
8	V	233	SER
8	V	259	SER
8	V	265	ARG
8	V	276	LEU
8	V	288	THR
8	V	290	VAL
8	V	293	VAL
8	V	296	ARG
8	V	304	MET
8	V	316	CYS
8	V	323	ILE
8	V	333	VAL
8	V	339	ARG
8	V	340	ILE
8	V	341	ARG
8	V	347	ASN
8	V	362	ARG
8	V	369	SER
8	V	373	VAL
8	V	377	MET
8	V	385	SER
8	V	392	CYS

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Mol	Chain	Res	Type
8	V	410	LYS
8	W	10	LEU
8	W	17	ILE
8	W	24	GLN
8	W	31	ILE
8	W	37	VAL
8	W	50	VAL
8	W	66	LEU
8	W	76	SER
8	W	78	LEU
8	W	85	LEU
8	W	112	GLU
8	W	127	ASP
8	W	131	SER
8	W	140	SER
8	W	153	LEU
8	W	154	LEU
8	W	157	LEU
8	W	165	LEU
8	W	166	VAL
8	W	188	SER
8	W	192	LEU
8	W	195	LEU
8	W	204	VAL
8	W	205	LEU
8	W	206	ASP
8	W	208	THR
8	W	217	ARG
8	W	218	LEU
8	W	222	ASN
8	W	228	ILE
8	W	231	LEU
8	W	233	SER
8	W	259	SER
8	W	265	ARG
8	W	276	LEU
8	W	288	THR
8	W	290	VAL
8	W	293	VAL
8	W	296	ARG
8	W	304	MET
8	W	316	CYS

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Mol	Chain	Res	Type
8	W	323	ILE
8	W	333	VAL
8	W	339	ARG
8	W	340	ILE
8	W	341	ARG
8	W	347	ASN
8	W	362	ARG
8	W	369	SER
8	W	373	VAL
8	W	377	MET
8	W	385	SER
8	W	392	CYS
8	W	410	LYS
8	X	10	LEU
8	X	17	ILE
8	X	24	GLN
8	X	31	ILE
8	X	37	VAL
8	X	50	VAL
8	X	66	LEU
8	X	76	SER
8	X	78	LEU
8	X	85	LEU
8	X	112	GLU
8	X	127	ASP
8	X	131	SER
8	X	140	SER
8	X	153	LEU
8	X	154	LEU
8	X	157	LEU
8	X	165	LEU
8	X	166	VAL
8	X	188	SER
8	X	192	LEU
8	X	195	LEU
8	X	204	VAL
8	X	205	LEU
8	X	206	ASP
8	X	208	THR
8	X	217	ARG
8	X	218	LEU
8	X	222	ASN

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Mol	Chain	Res	Type
8	X	228	ILE
8	X	231	LEU
8	X	233	SER
8	X	259	SER
8	X	265	ARG
8	X	276	LEU
8	X	288	THR
8	X	290	VAL
8	X	293	VAL
8	X	296	ARG
8	X	304	MET
8	X	316	CYS
8	X	323	ILE
8	X	333	VAL
8	X	339	ARG
8	X	340	ILE
8	X	341	ARG
8	X	347	ASN
8	X	362	ARG
8	X	369	SER
8	X	373	VAL
8	X	377	MET
8	X	385	SER
8	X	392	CYS
8	X	410	LYS
8	Y	10	LEU
8	Y	17	ILE
8	Y	24	GLN
8	Y	31	ILE
8	Y	37	VAL
8	Y	50	VAL
8	Y	66	LEU
8	Y	76	SER
8	Y	78	LEU
8	Y	85	LEU
8	Y	112	GLU
8	Y	127	ASP
8	Y	131	SER
8	Y	140	SER
8	Y	153	LEU
8	Y	154	LEU
8	Y	157	LEU

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Mol	Chain	Res	Type
8	Y	165	LEU
8	Y	166	VAL
8	Y	188	SER
8	Y	192	LEU
8	Y	195	LEU
8	Y	204	VAL
8	Y	205	LEU
8	Y	206	ASP
8	Y	208	THR
8	Y	217	ARG
8	Y	218	LEU
8	Y	222	ASN
8	Y	228	ILE
8	Y	231	LEU
8	Y	233	SER
8	Y	259	SER
8	Y	265	ARG
8	Y	276	LEU
8	Y	288	THR
8	Y	290	VAL
8	Y	293	VAL
8	Y	296	ARG
8	Y	304	MET
8	Y	316	CYS
8	Y	323	ILE
8	Y	333	VAL
8	Y	339	ARG
8	Y	340	ILE
8	Y	341	ARG
8	Y	347	ASN
8	Y	362	ARG
8	Y	369	SER
8	Y	373	VAL
8	Y	377	MET
8	Y	385	SER
8	Y	392	CYS
8	Y	410	LYS
8	Z	10	LEU
8	Z	17	ILE
8	Z	24	GLN
8	Z	31	ILE
8	Z	37	VAL

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Mol	Chain	Res	Type
8	Z	50	VAL
8	Z	66	LEU
8	Z	76	SER
8	Z	78	LEU
8	Z	85	LEU
8	Z	112	GLU
8	Z	127	ASP
8	Z	131	SER
8	Z	140	SER
8	Z	153	LEU
8	Z	154	LEU
8	Z	157	LEU
8	Z	165	LEU
8	Z	166	VAL
8	Z	188	SER
8	Z	192	LEU
8	Z	195	LEU
8	Z	204	VAL
8	Z	205	LEU
8	Z	206	ASP
8	Z	208	THR
8	Z	217	ARG
8	Z	218	LEU
8	Z	222	ASN
8	Z	228	ILE
8	Z	231	LEU
8	Z	233	SER
8	Z	259	SER
8	Z	265	ARG
8	Z	276	LEU
8	Z	288	THR
8	Z	290	VAL
8	Z	293	VAL
8	Z	296	ARG
8	Z	304	MET
8	Z	316	CYS
8	Z	323	ILE
8	Z	333	VAL
8	Z	339	ARG
8	Z	340	ILE
8	Z	341	ARG
8	Z	347	ASN

Continued on next page...

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Mol	Chain	Res	Type
8	Z	362	ARG
8	Z	369	SER
8	Z	373	VAL
8	Z	377	MET
8	Z	385	SER
8	Z	392	CYS
8	Z	410	LYS
3	k	34	ILE
3	k	39	LEU
3	k	63	VAL
3	d	31	ILE
7	c	89	LEU
4	j	38	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (279) such sidechains are listed below:

Mol	Chain	Res	Type
1	l	107	HIS
2	e	263	GLN
3	b	36	ASN
4	a	30	GLN
4	a	82	HIS
4	a	120	GLN
5	C	165	GLN
5	C	169	ASN
5	C	172	GLN
5	C	373	GLN
5	C	493	ASN
5	C	524	GLN
5	C	644	HIS
5	C	654	GLN
5	C	674	GLN
5	C	688	ASN
5	C	691	GLN
5	C	707	HIS
5	C	718	ASN
5	C	741	ASN
5	C	823	ASN
4	D	269	ASN
4	D	387	HIS
4	D	416	GLN
4	D	491	ASN

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Mol	Chain	Res	Type
4	D	595	HIS
4	D	596	ASN
4	D	702	HIS
4	D	703	GLN
4	D	705	HIS
4	D	716	HIS
4	D	773	ASN
4	D	787	ASN
4	D	801	GLN
4	D	860	GLN
5	E	236	GLN
5	E	261	HIS
5	E	329	GLN
5	E	420	GLN
5	E	430	GLN
5	E	436	GLN
5	E	458	ASN
5	E	580	HIS
5	E	654	GLN
5	E	662	ASN
5	E	684	GLN
5	E	691	GLN
5	E	741	ASN
4	F	558	HIS
4	F	570	GLN
4	F	596	ASN
4	F	609	ASN
4	F	684	HIS
4	F	702	HIS
4	F	705	HIS
4	F	719	GLN
4	F	746	HIS
4	F	773	ASN
4	F	774	GLN
4	F	786	GLN
4	F	801	GLN
4	F	852	HIS
4	F	860	GLN
5	G	152	GLN
5	G	236	GLN
5	G	287	GLN
5	G	316	GLN

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Mol	Chain	Res	Type
5	G	412	HIS
5	G	487	GLN
5	G	512	HIS
5	G	580	HIS
5	G	585	GLN
5	G	631	ASN
5	G	644	HIS
5	G	674	GLN
5	G	688	ASN
5	G	694	GLN
5	G	707	HIS
5	G	726	HIS
5	G	862	ASN
4	H	265	ASN
4	H	347	GLN
4	H	389	GLN
4	H	401	HIS
4	H	461	HIS
4	H	479	GLN
4	H	491	ASN
4	H	560	GLN
4	H	570	GLN
4	H	611	GLN
4	H	717	GLN
4	H	719	GLN
4	H	739	GLN
4	H	774	GLN
4	H	801	GLN
4	H	852	HIS
6	I	26	GLN
6	I	43	ASN
6	I	102	GLN
6	I	116	HIS
6	I	128	GLN
6	I	130	GLN
6	I	186	GLN
6	I	199	GLN
6	I	317	GLN
6	I	378	HIS
6	I	397	GLN
6	I	527	ASN
6	I	547	GLN

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Mol	Chain	Res	Type
6	I	563	HIS
6	I	571	GLN
6	I	591	HIS
6	I	611	GLN
6	I	622	GLN
1	J	237	HIS
1	J	239	HIS
1	J	248	GLN
1	J	316	GLN
1	J	642	HIS
1	J	705	ASN
1	J	818	GLN
1	J	892	HIS
1	J	898	HIS
1	J	930	HIS
6	K	26	GLN
6	K	35	HIS
6	K	67	GLN
6	K	78	GLN
6	K	98	GLN
6	K	128	GLN
6	K	142	GLN
6	K	160	HIS
6	K	180	HIS
6	K	316	GLN
6	K	370	GLN
6	K	377	GLN
6	K	415	HIS
6	K	489	GLN
6	K	501	GLN
6	K	509	GLN
6	K	519	ASN
6	K	529	GLN
6	K	543	GLN
6	K	567	ASN
6	K	591	HIS
6	K	637	GLN
7	L	327	HIS
7	L	507	GLN
7	L	515	ASN
7	L	603	ASN
7	L	1514	HIS

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Mol	Chain	Res	Type
7	L	1525	GLN
7	L	1563	HIS
7	L	1605	ASN
7	L	1625	GLN
7	L	1666	GLN
7	L	1679	GLN
7	L	1702	GLN
7	L	1742	GLN
7	L	1770	ASN
7	L	1805	ASN
3	i	19	ASN
8	Q	9	GLN
8	Q	15	ASN
8	Q	87	ASN
8	Q	110	GLN
8	Q	174	ASN
8	Q	187	ASN
8	Q	229	ASN
8	Q	251	ASN
8	Q	299	GLN
8	Q	314	ASN
8	Q	322	ASN
8	Q	332	GLN
8	R	9	GLN
8	R	15	ASN
8	R	87	ASN
8	R	110	GLN
8	R	174	ASN
8	R	187	ASN
8	R	229	ASN
8	R	251	ASN
8	R	314	ASN
8	R	322	ASN
8	R	332	GLN
8	S	9	GLN
8	S	15	ASN
8	S	87	ASN
8	S	110	GLN
8	S	174	ASN
8	S	187	ASN
8	S	251	ASN
8	S	299	GLN

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Mol	Chain	Res	Type
8	S	314	ASN
8	S	322	ASN
8	T	9	GLN
8	T	15	ASN
8	T	87	ASN
8	T	110	GLN
8	T	174	ASN
8	T	187	ASN
8	T	229	ASN
8	T	251	ASN
8	T	299	GLN
8	T	314	ASN
8	T	322	ASN
8	U	9	GLN
8	U	15	ASN
8	U	87	ASN
8	U	110	GLN
8	U	174	ASN
8	U	187	ASN
8	U	229	ASN
8	U	251	ASN
8	U	299	GLN
8	U	314	ASN
8	U	322	ASN
8	U	407	GLN
8	V	9	GLN
8	V	15	ASN
8	V	87	ASN
8	V	110	GLN
8	V	174	ASN
8	V	187	ASN
8	V	314	ASN
8	V	322	ASN
8	V	357	GLN
8	W	9	GLN
8	W	15	ASN
8	W	87	ASN
8	W	110	GLN
8	W	158	ASN
8	W	174	ASN
8	W	187	ASN
8	W	299	GLN

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Mol	Chain	Res	Type
8	W	314	ASN
8	W	322	ASN
8	W	357	GLN
8	X	9	GLN
8	X	15	ASN
8	X	87	ASN
8	X	110	GLN
8	X	174	ASN
8	X	187	ASN
8	X	251	ASN
8	X	299	GLN
8	X	314	ASN
8	X	322	ASN
8	Y	9	GLN
8	Y	15	ASN
8	Y	87	ASN
8	Y	110	GLN
8	Y	174	ASN
8	Y	187	ASN
8	Y	229	ASN
8	Y	251	ASN
8	Y	299	GLN
8	Y	314	ASN
8	Y	322	ASN
8	Z	9	GLN
8	Z	15	ASN
8	Z	24	GLN
8	Z	87	ASN
8	Z	110	GLN
8	Z	174	ASN
8	Z	187	ASN
8	Z	251	ASN
8	Z	299	GLN
8	Z	314	ASN
8	Z	322	ASN
8	Z	357	GLN
3	d	36	ASN
7	c	43	ASN
7	c	48	ASN
7	c	161	GLN
4	j	14	GLN
4	j	30	GLN

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Mol	Chain	Res	Type
4	j	42	ASN
4	j	78	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

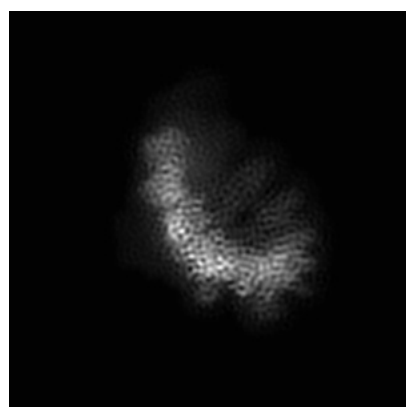
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14014. These allow visual inspection of the internal detail of the map and identification of artifacts.

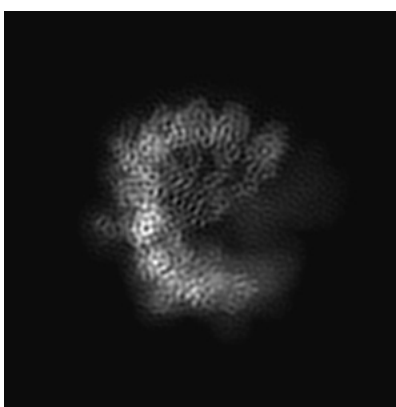
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

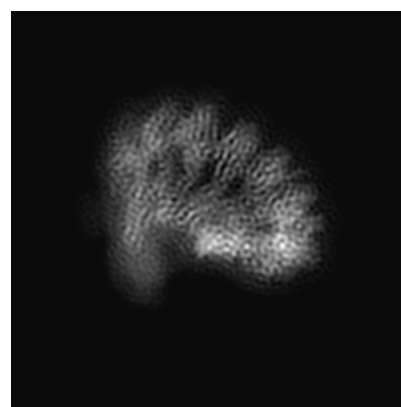
6.1.1 Primary map



X



Y



Z

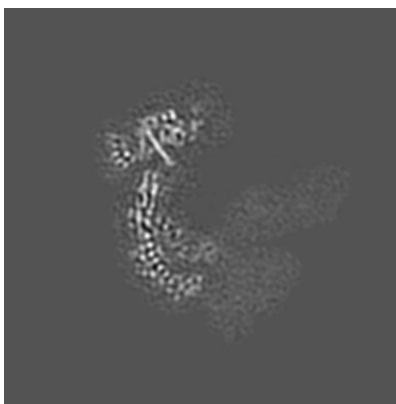
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 100



Y Index: 100



Z Index: 100

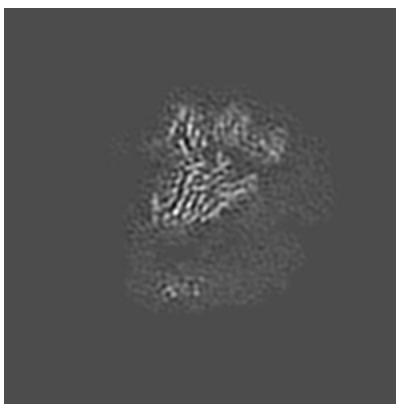
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

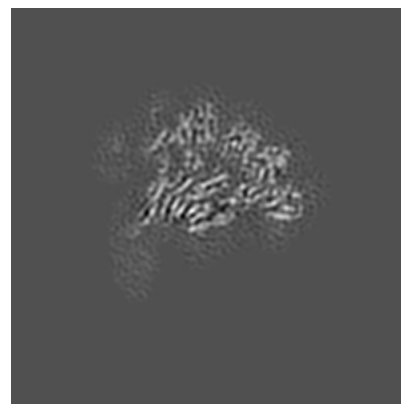
6.3.1 Primary map



X Index: 134



Y Index: 84

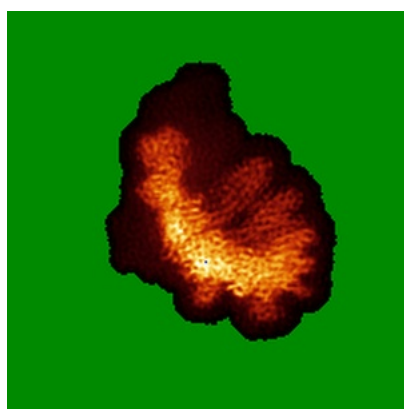


Z Index: 72

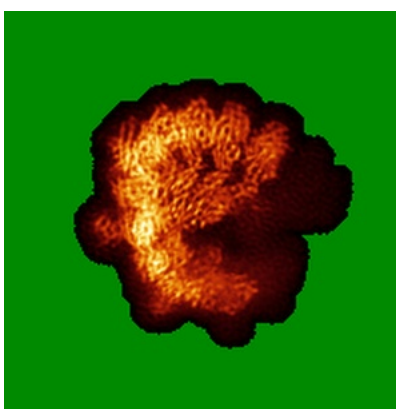
The images above show the largest variance slices of the map in three orthogonal directions.

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

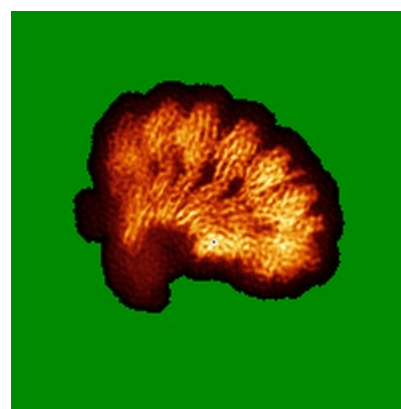
6.4.1 Primary map



X



Y

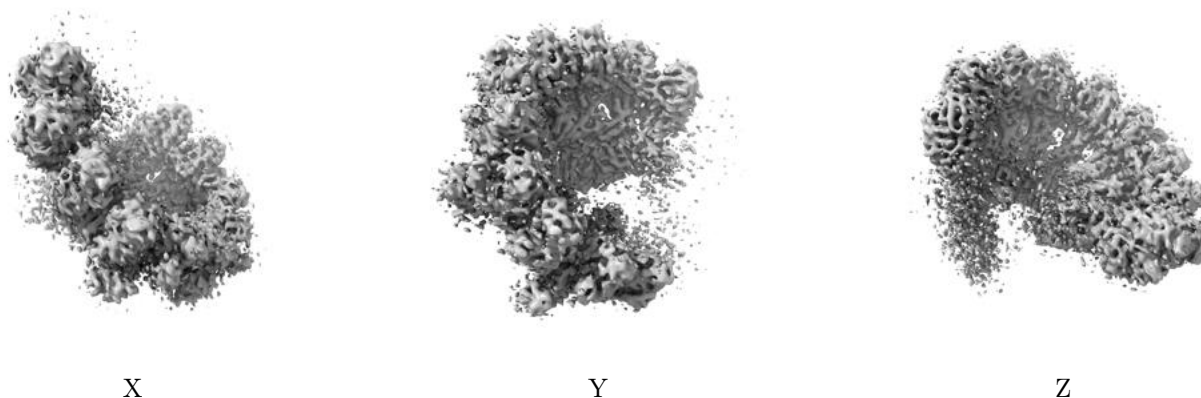


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0299. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

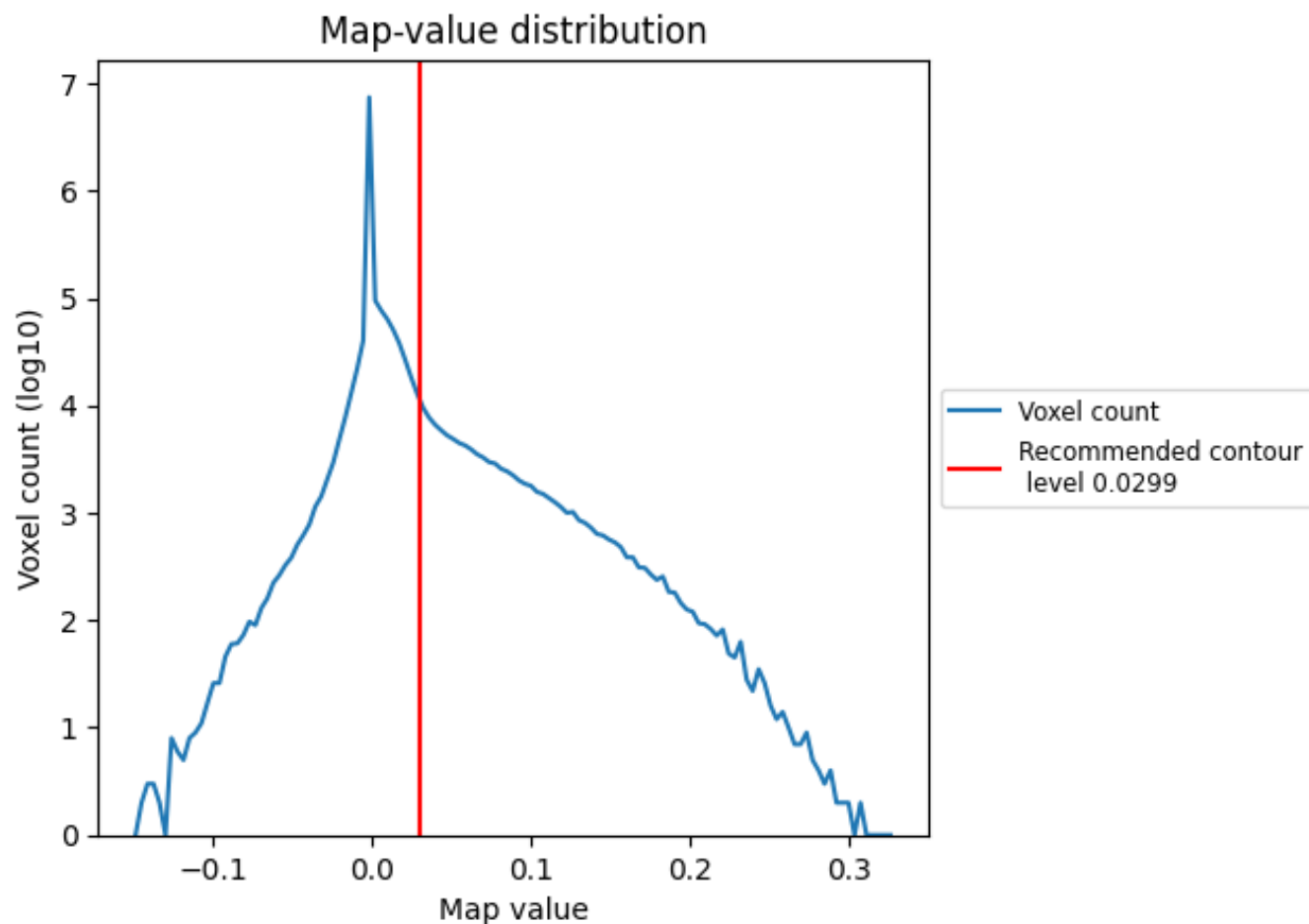
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

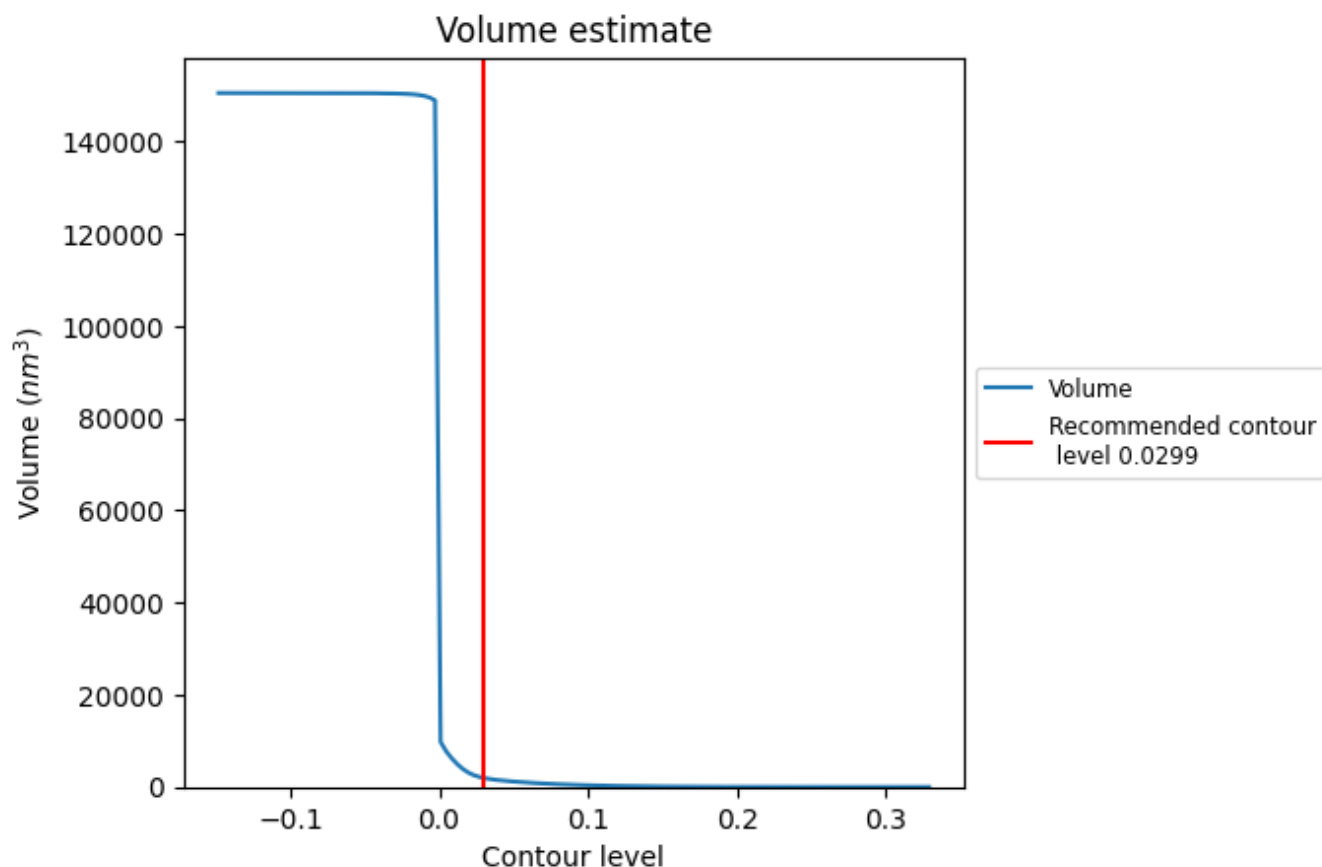
This section contains the results of statistical analysis of the map.

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.

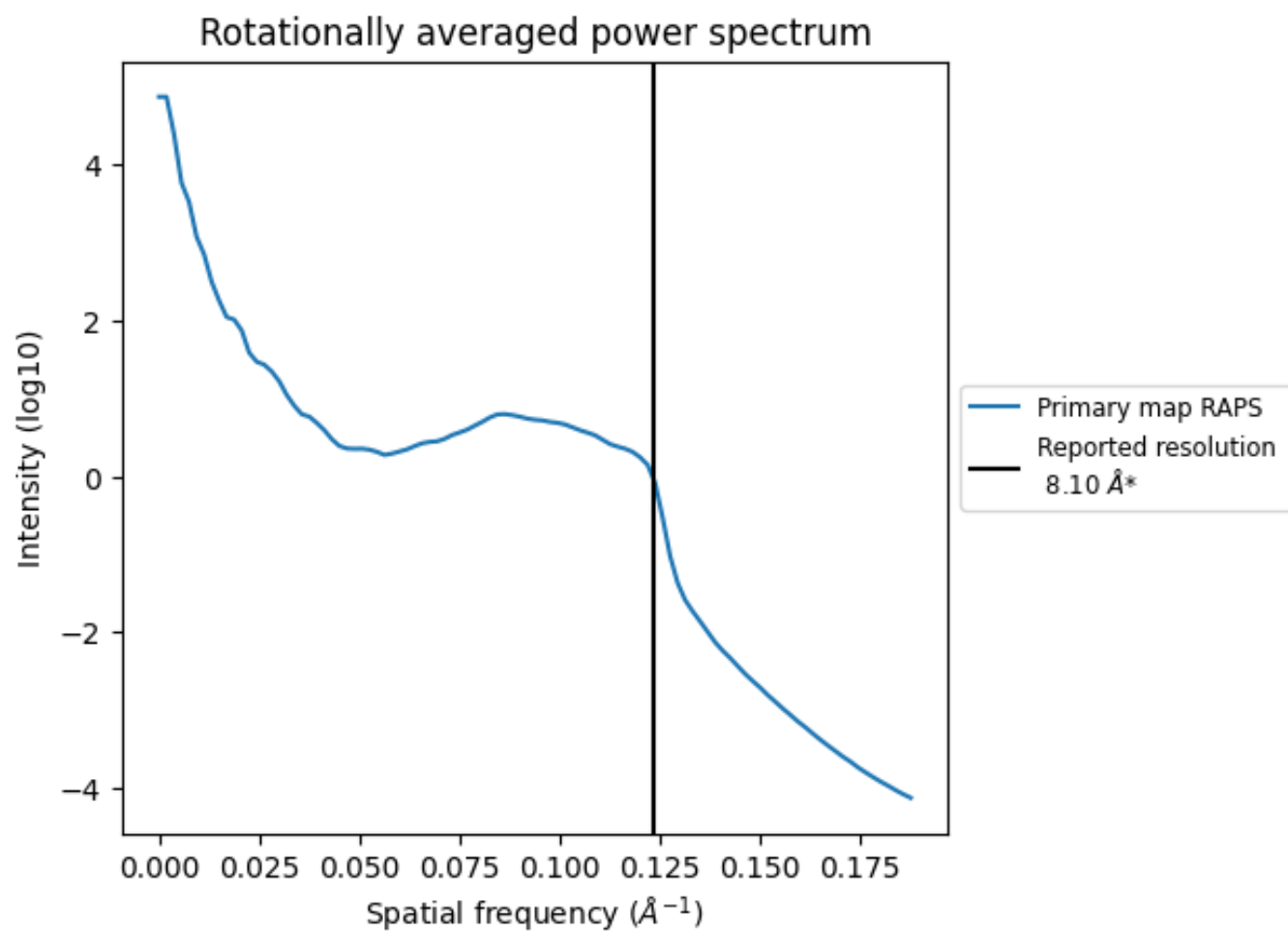
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1956 nm³; this corresponds to an approximate mass of 1767 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 0.123 Å⁻¹

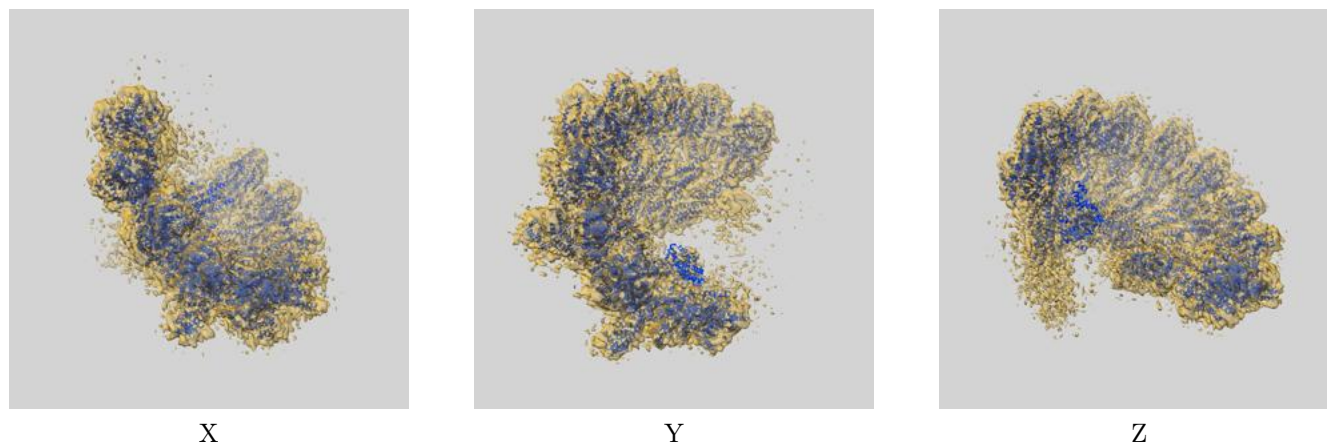
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

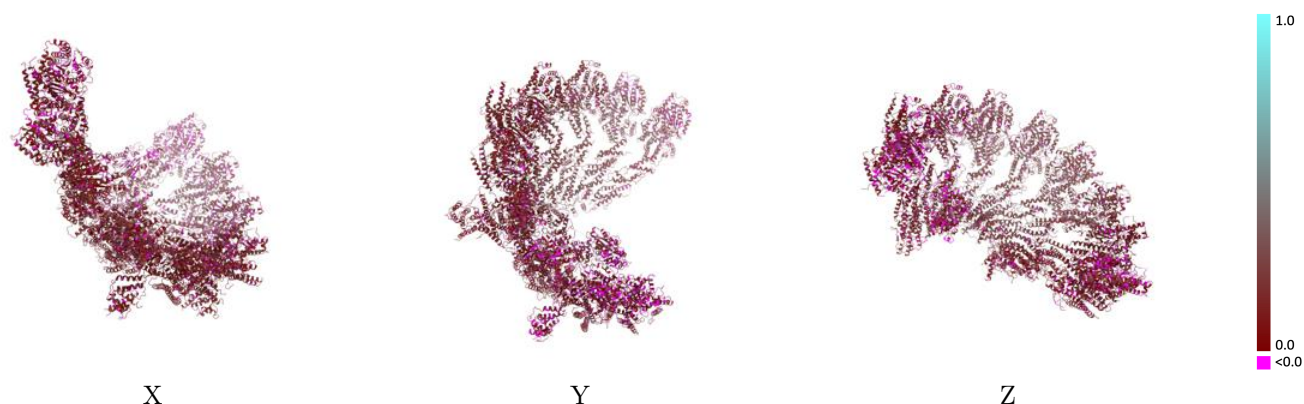
This section contains information regarding the fit between EMDB map EMD-14014 and PDB model 7QJ9. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.0299 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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

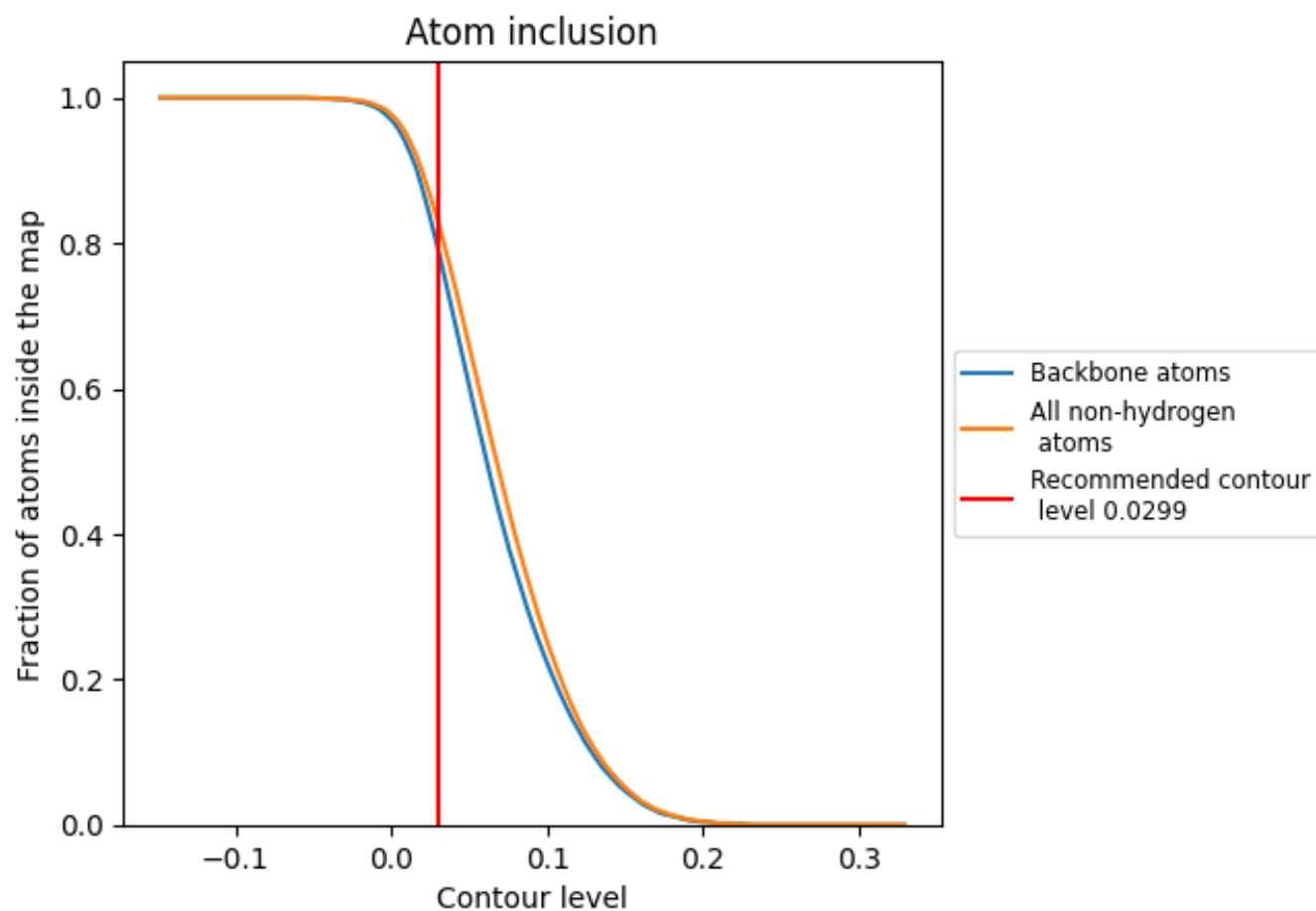


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 83% 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 (0.0299) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8290	 0.1350
C	 0.7880	 0.1240
D	 0.8150	 0.1370
E	 0.8830	 0.1430
F	 0.8900	 0.1520
G	 0.8940	 0.1650
H	 0.8920	 0.1560
I	 0.8980	 0.1660
J	 0.8940	 0.1610
K	 0.8950	 0.1550
L	 0.8970	 0.1460
Q	 0.6110	 0.0570
R	 0.7460	 0.0890
S	 0.8370	 0.1150
T	 0.8850	 0.1250
U	 0.8950	 0.1410
V	 0.9040	 0.1540
W	 0.9090	 0.1490
X	 0.9000	 0.1380
Y	 0.8990	 0.1160
Z	 0.8400	 0.1040
a	 0.7910	 0.1470
b	 0.8130	 0.1740
c	 0.6150	 0.1270
d	 0.5430	 0.1340
e	 0.2650	 0.0730
h	 0.6910	 0.1030
i	 0.6220	 0.0620
j	 0.8710	 0.1380
k	 0.8930	 0.1590
l	 0.8770	 0.1570
m	 0.8760	 0.1450

