



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 03:26 PM UTC

PDB ID : 7QJ7 / pdb_00007qj7
EMDB ID : EMD-14012
Title : Structure of recombinant human gamma-Tubulin Ring Complex 12-spoked assembly intermediate (spokes 1-12 substoichiometric spokes 13-14)
Authors : Zupa, E.; Pfeffer, S.
Deposited on : 2021-12-16
Resolution : 8.70 Å (reported)
Based on initial models : 7AS4, 6X0U, 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:

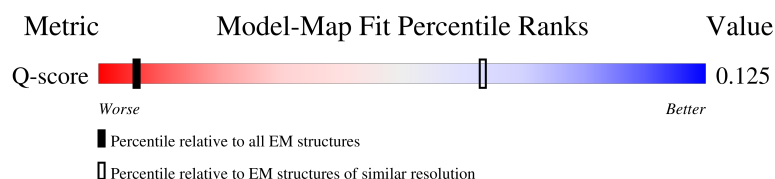
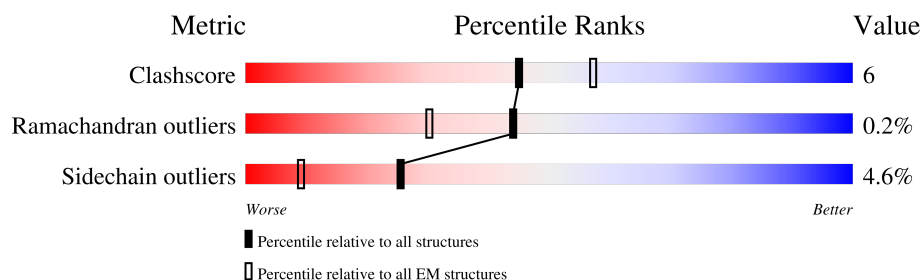
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 8.70 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.



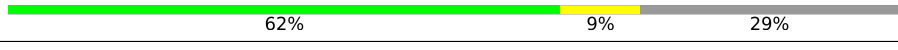
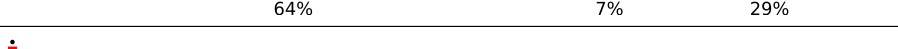
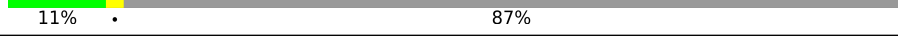
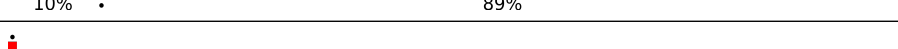
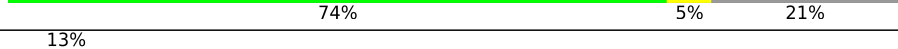
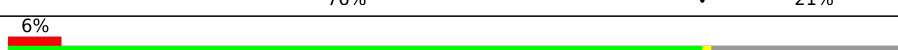
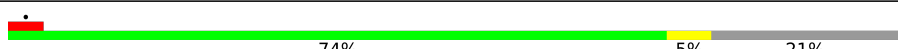
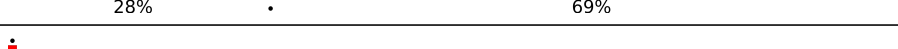
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	282 (8.20 - 9.20)

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	A	902	

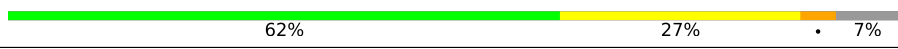
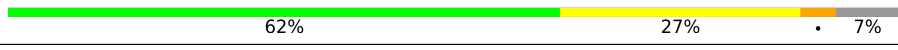
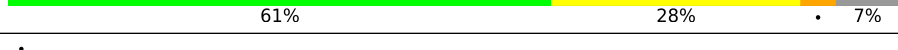
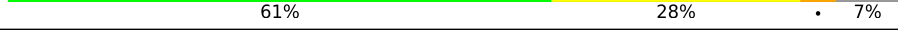
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Mol	Chain	Length	Quality of chain
3	C	902	
3	E	902	
3	G	902	
4	B	907	
4	D	907	
4	F	907	
4	H	907	
4	a	907	
4	f	907	
4	h	907	
4	j	907	
5	b	82	
5	d	82	
5	g	82	
5	i	82	
5	k	82	
5	m	82	
6	I	667	
6	K	667	
7	L	1819	
7	c	1819	
8	O	451	
8	P	451	
8	Q	451	
8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

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Mol	Chain	Length	Quality of chain
8	S	451	 63%27%7%
8	T	451	 62%27%7%
8	U	451	 62%27%7%
8	V	451	 62%27%7%
8	W	451	 62%27%7%
8	X	451	 61%28%7%
8	Y	451	 61%28%7%
8	Z	451	 61%28%7%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 109579 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	I	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 Gamma-tubulin complex component 2.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	610	Total	C	N	O	S	0	0
			5029	3203	888	913	25		
4	D	581	Total	C	N	O	S	0	0
			4796	3061	842	868	25		
4	F	599	Total	C	N	O	S	0	0
			4941	3151	871	894	25		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	594	Total	C	N	O	S	0	0
			4907	3130	864	888	25		
4	a	116	Total	C	N	O	S	0	0
			933	591	171	169	2		
4	f	99	Total	C	N	O	S	0	0
			803	509	148	144	2		
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 Mitotic-spindle organizing protein 1.

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

- 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		

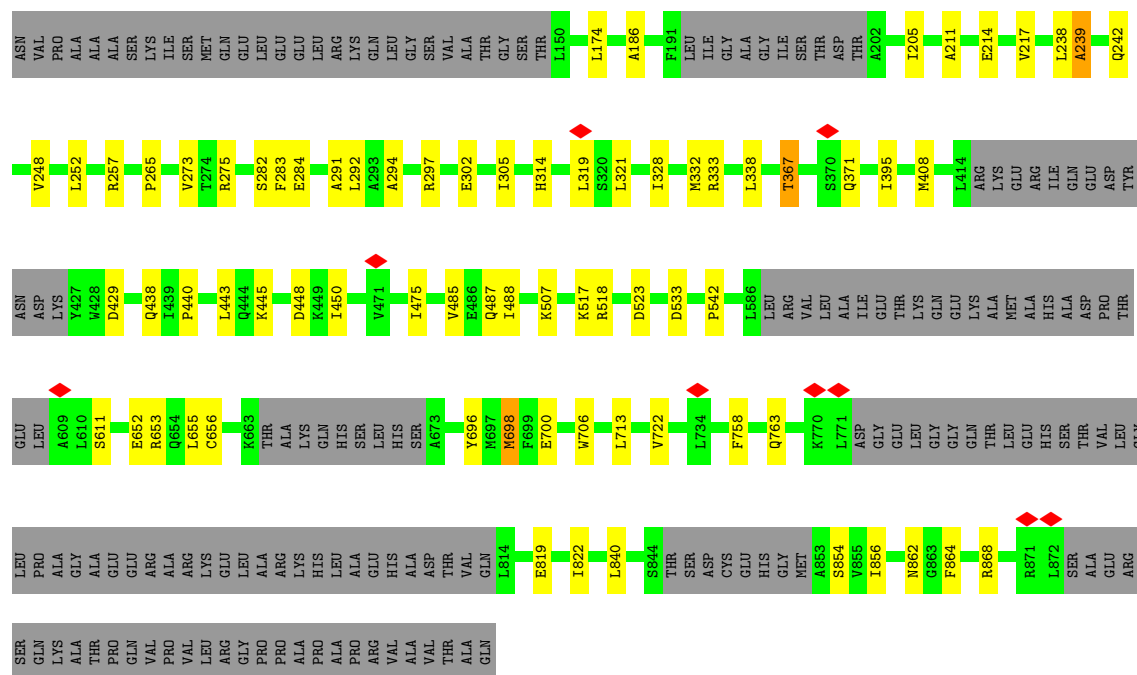
- Molecule 8 is a protein called Tubulin gamma-1 chain.

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

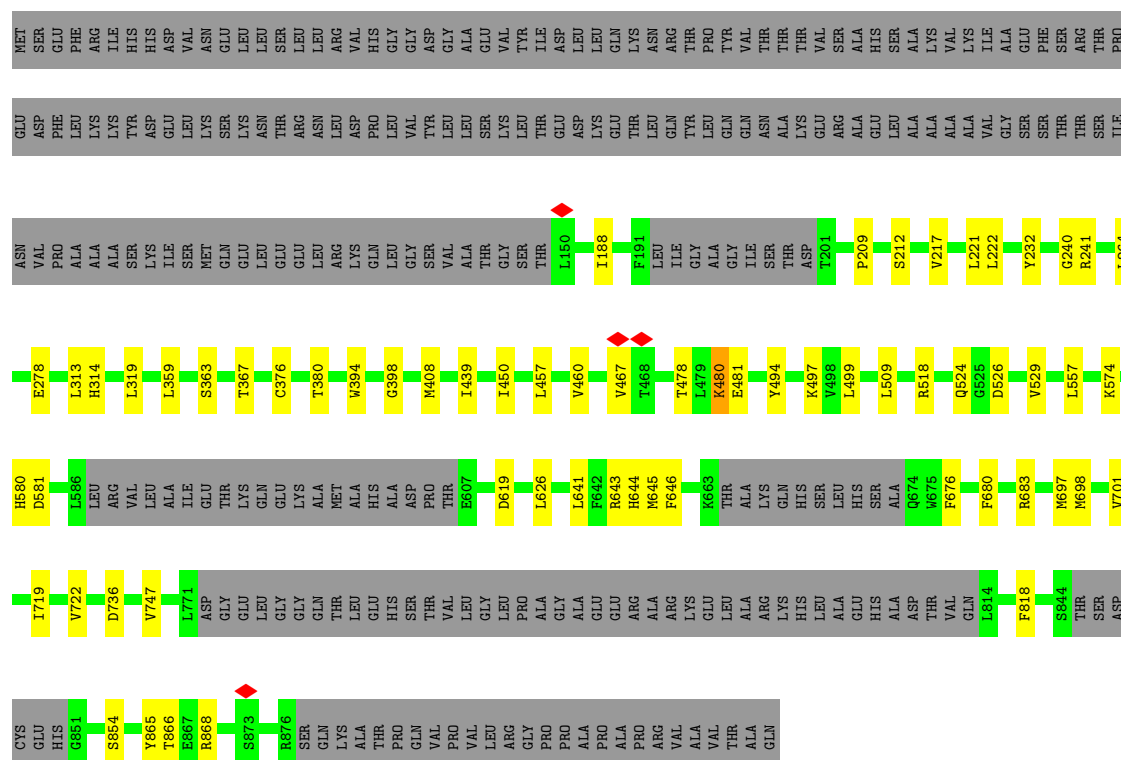
Mol	Chain	Residues	Atoms		AltConf
9	l	6	Total	O	0
			6	6	





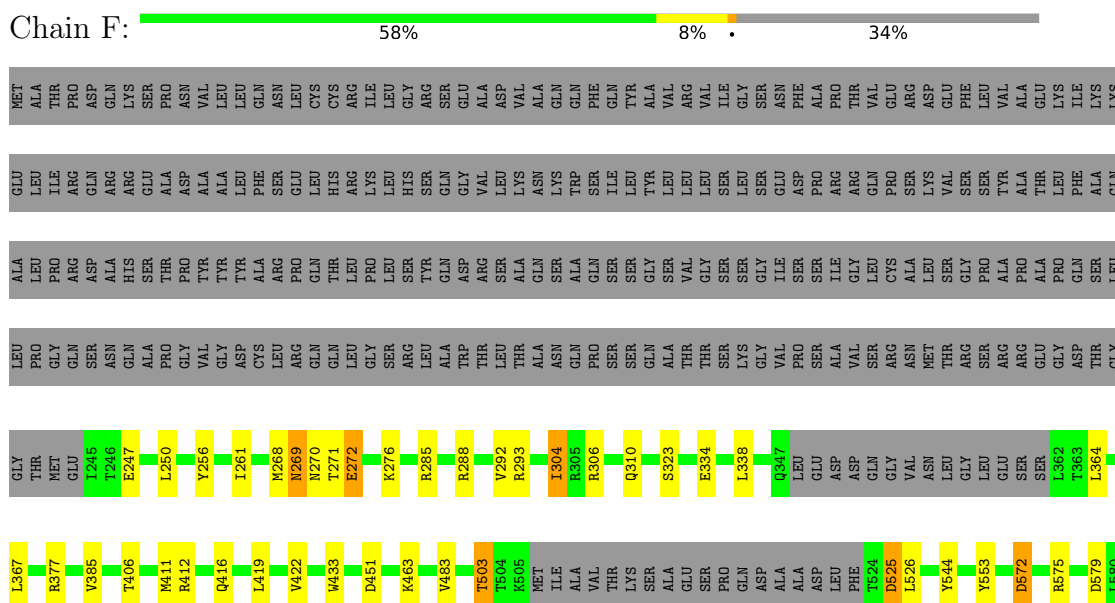
• Molecule 3: Gamma-tubulin complex component 2

Chain G: 64% 7% 29%



• Molecule 3: Gamma-tubulin complex component 2

Chain E: 62% 9% 29%



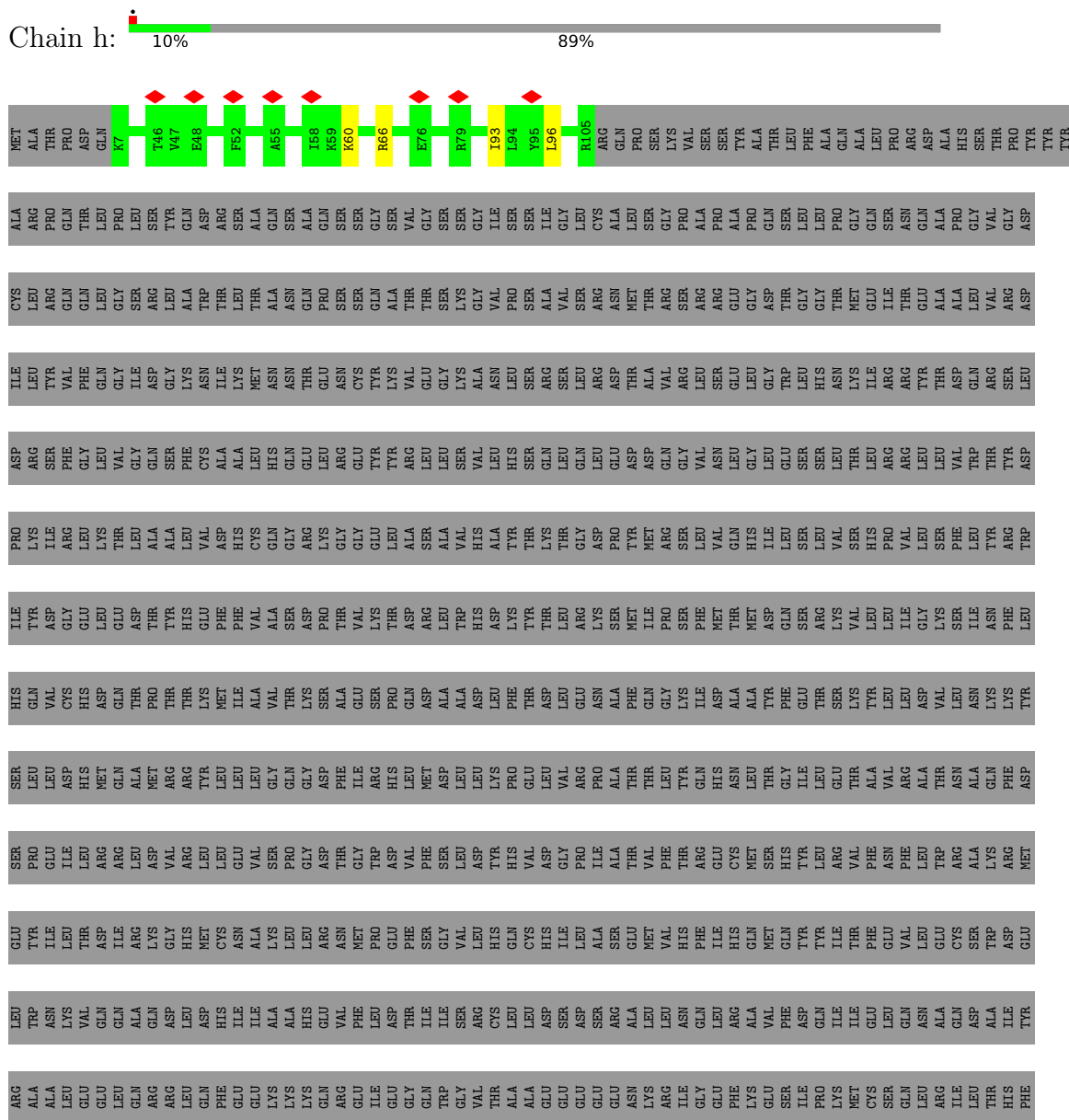
[illegible]

- Molecule 4: Gamma-tubulin complex component 3

Chain f: 10% : 89%

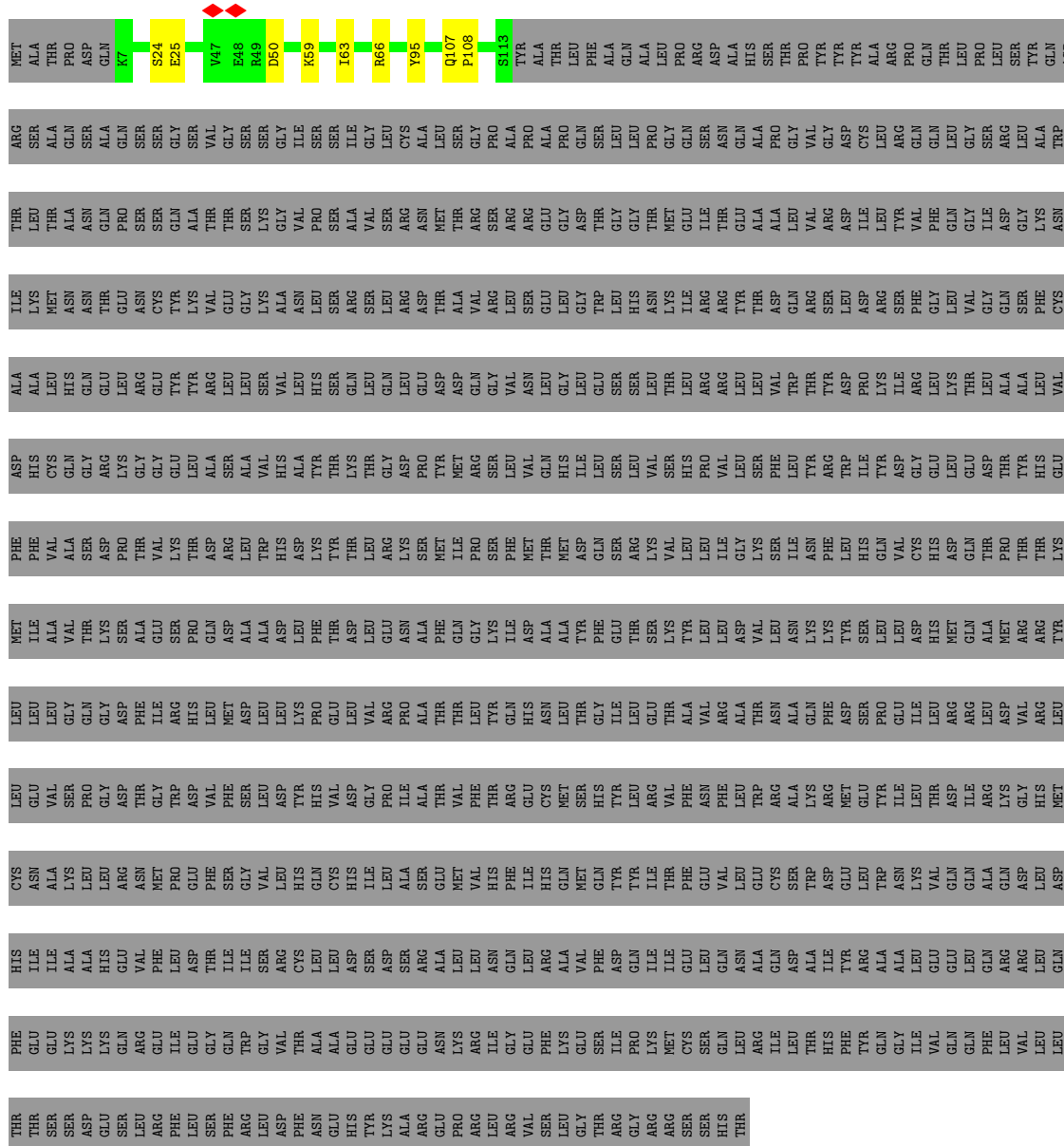
LEU	ASP	VAL	ASP	TLE	SER	TTR	ARG	PRO	MET
HIS	GLU	CYS	GLY	ARG	PHE	VAL	GLN	GLN	ALA
MET	LEU	HIS	GLU	LEU	GLY	PHE	GLN	THR	ALA
GLN	GLU	ASP	THR	THR	VAL	GLN	GLY	LEU	PRO
ALA	ASP	THR	ASP	LEU	GLY	ILE	SER	LEU	GLN
MET	THR	PRO	THR	ALA	GLN	ASP	ARG	SER	K7
ARG	THR	THR	TTR	ALA	SER	GLY	LEU	TTR	
THR	HIS	THR	HIS	LEU	PHE	GLY	ALA	GLN	S41
TYR	GLU	THR	VAL	VAL	LYS	ASN	TRP	ASP	
LEU	PHE	MET	ASP	ASP	ALA	ILE	THR	ARG	I58
LEU	PHE	ILE	THR	HIS	ALA	LYS	LEU	SER	
LEU	VAL	ALA	CYS	VAL	LEU	MET	THR	ALA	R66
GLY	ALA	VAL	ALA	GLN	HIS	ASN	ALA	SER	R67
GLN	SER	THR	SER	GLY	GLN	ASN	ASN	GLN	E68
GLY	ASP	LYS	ASP	ARG	GLU	THR	GLN	ALA	A69
ASP	PRO	SER	PRO	LYS	LEU	GLU	PRO	GLN	
PHE	THR	ALA	THR	GLY	GLY	ASN	SER	SER	A72
ARG	VAL	GLU	VAL	GLY	GLU	TYR	GLN	GLY	
HIS	LYS	SER	LYS	LEU	TTR	TTR	ALA	GLY	S75
PRO	THR	PRO	THR	ALA	ARG	VAL	THR	VAL	
GLU	ASP	GLN	ASP	ALA	THR	LYS	THR	GLY	L61
THR	ARG	LEU	LEU	ALA	LEU	GLY	SER	SER	
LEU	ASP	ALA	LEU	ALA	LEU	LYS	LYS	SER	V86
LEU	ALA	ALA	HIS	HIS	VAL	ALA	GLY	GLY	
LYS	ASP	THR	ASP	TTR	LEU	ASN	VAL	ILE	K90
PHE	LYS	LEU	LYS	TYR	HIS	LEU	PRO	SER	
LEU	THR	GLN	TYR	THR	GLU	LEU	ASP	SER	L100
GLU	TYR	ASP	TYR	LYS	SER	SER	PRO	SER	
LEU	THR	LEU	THR	LYS	GLN	ARG	ALA	ILE	
VAL	LEU	ASP	LEU	THR	LEU	ARG	VAL	GLY	R105
ARG	GLU	GLU	ARG	GLY	GLN	LEU	SER	LEU	ARG
PRO	LYS	ASN	LYS	ASP	LEU	ARG	ARG	CYS	
ALA	SER	ALA	SER	PRO	GLU	ASP	ASN	ALA	GLN
THR	MET	PHE	MET	TYR	ASP	THR	MET	LEU	PRO
THR	ILE	GLN	ILE	TYR	ASP	ALA	THR	LEU	SER
LEU	PRO	GLY	PRO	ARG	GLN	VAL	ARG	GLY	LYS
TYR	SER	LYS	SER	SER	GLY	ARG	SER	PRO	SER
GLN	PHE	ILE	THR	LEU	VAL	LEU	ARG	ALA	SER
HIS	MET	ASP	THR	VAL	ASN	SER	ARG	PRO	TTR
ASN	THR	ALA	THR	GLN	LEU	GLU	GLU	ALA	ALA
LEU	MET	ALA	MET	HIS	GLY	LEU	ASP	PRO	THR
THR	ASP	TTR	ASP	ILE	LEU	GLY	GLY	GLN	LEU
VAL	LEU	LEU	LEU	VAL	GLU	TRP	THR	LEU	PHE
ARG	ILE	GLU	SER	SER	SER	LEU	GLY	LEU	ALA
THR	LYS	THR	ARG	VAL	LEU	HIS	THR	PRO	ALA
GLU	VAL	SER	LYS	SER	LEU	ASN	THR	GLY	LEU
THR	VAL	SER	VAL	SER	THR	LYS	MET	GLY	ALA
ALA	LEU	TYR	LEU	HIS	LEU	ILE	GLU	GLN	PRO
VAL	LEU	LEU	LEU	VAL	ARG	ARG	ILE	SER	ARG
ARG	ILE	LEU	ILE	VAL	THR	TYR	GLU	ASN	ALA
THR	GLY	ASP	GLY	LEU	LEU	TYR	THR	GLN	ASP
ASN	LYS	VAL	LYS	SER	VAL	ASP	ALA	ALA	HIS
ALA	ILE	THR	ILE	PHE	THR	TRP	LEU	PRO	SER
ASN	ILE	LEU	SER	THR	VAL	GLN	LEU	GLY	THR
GLN	ASP	ASN	GLY	LEU	THR	ARG	VAL	VAL	THR
LYS	ASN	LYS	ASN	TYR	THR	SER	ARG	VAL	GLY
PHE	THR	LYS	THR	TYR	THR	SER	ARG	GLY	PRO
GLN	THR	THR	ASP	ARG	GLY	GLY	THR	THR	THR
ASP	THR	THR	THR	THR	GLY	GLY	THR	THR	THR
THR	THR	THR	THR	THR	GLY	GLY	THR	THR	THR
THR	THR	THR	THR	THR	GLY	GLY	THR	THR	THR

- Molecule 4: Gamma-tubulin complex component 3

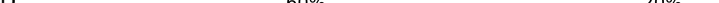


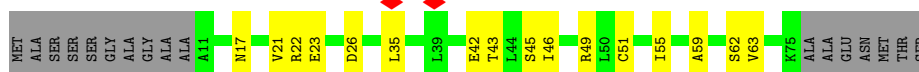
- Molecule 4: Gamma-tubulin complex component 3

Chain j: 11% . 88%

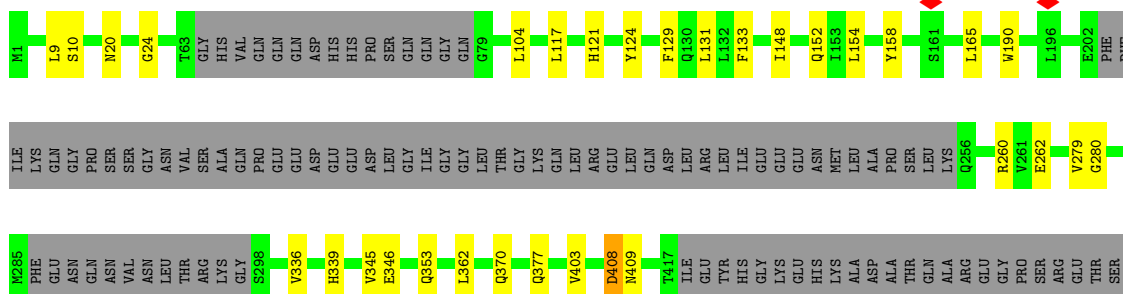
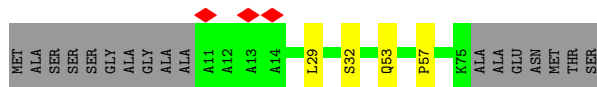
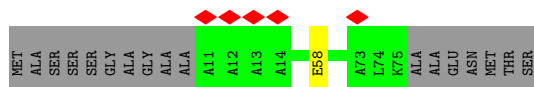
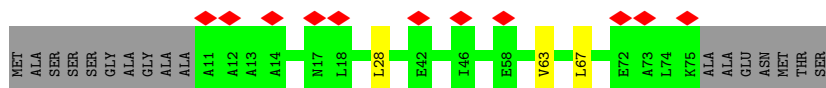
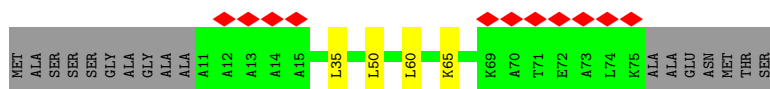


- Molecule 5: Mitotic-spindle organizing protein 1

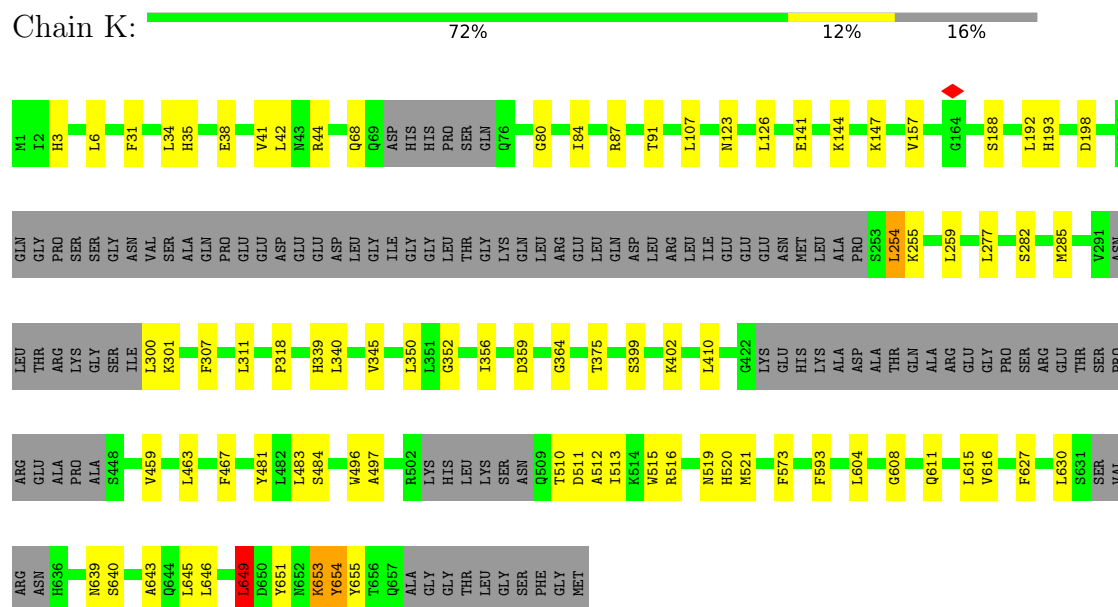
Chain b: 



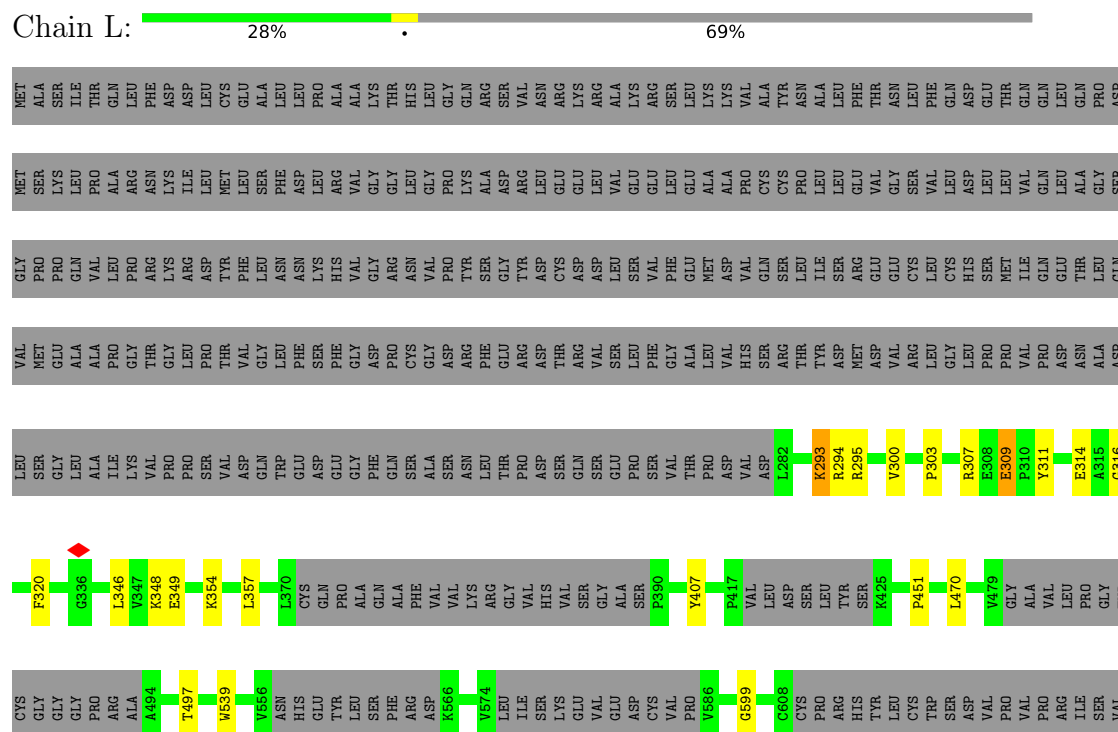
- Molecule 5: Mitotic-spindle organizing protein 1



- Molecule 6: Gamma-tubulin complex component 4



- Molecule 7: Gamma-tubulin complex component 6



- Molecule 7: Gamma-tubulin complex component 6

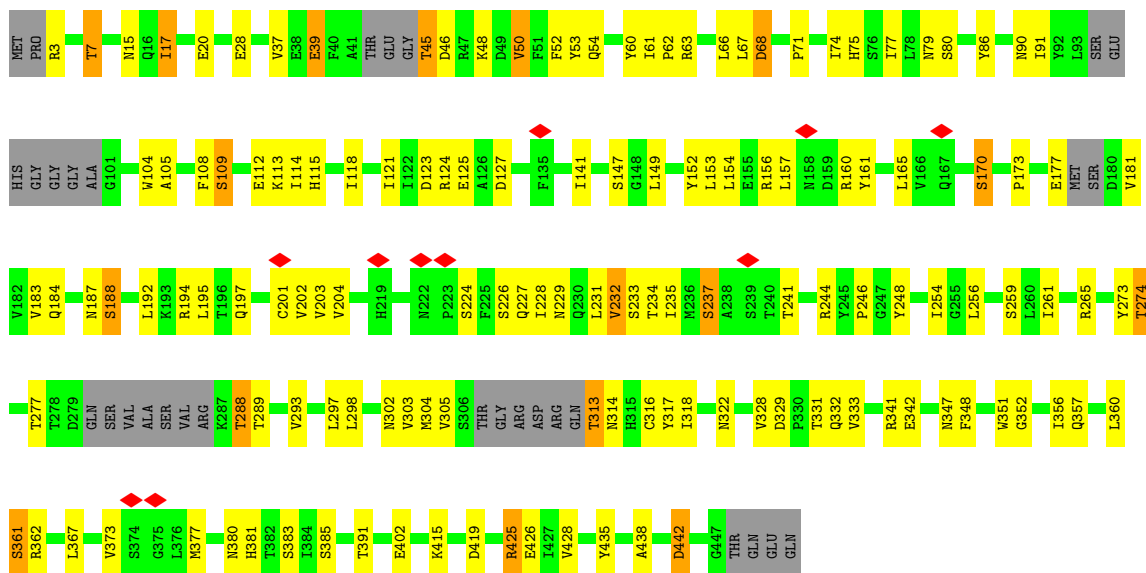




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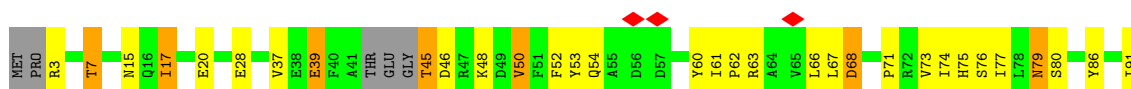
- Molecule 8: Tubulin gamma-1 chain

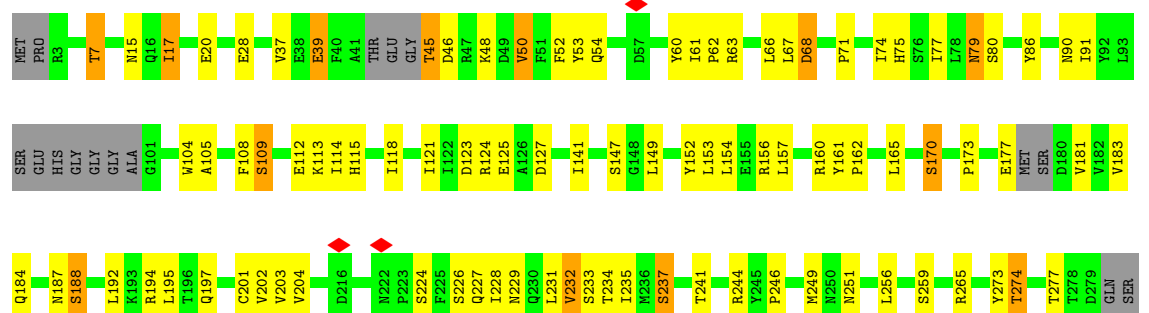
Chain 0:  61% 28% 7%



- Molecule 8: Tubulin gamma-1 chain

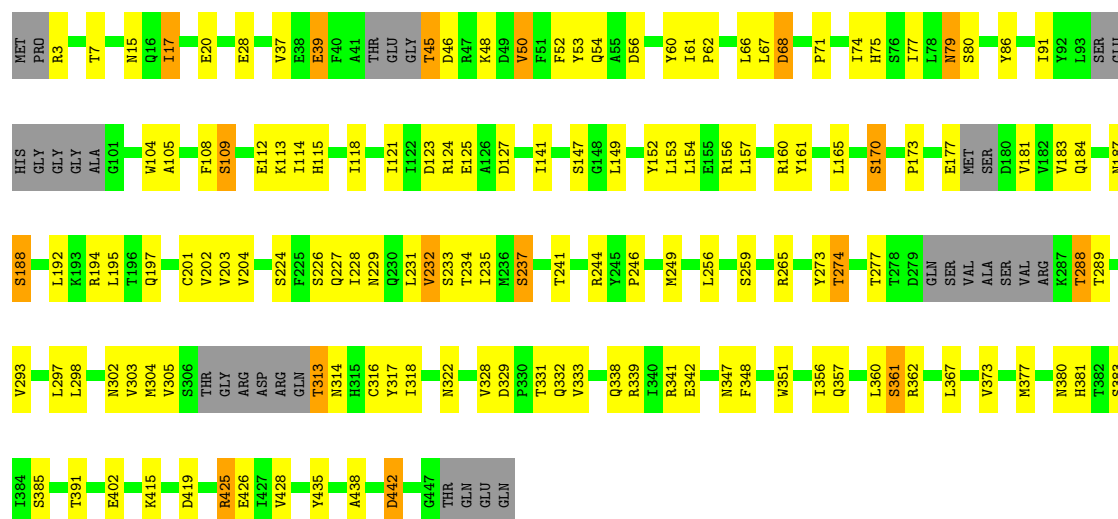
Chain P: 61% 29% 7%





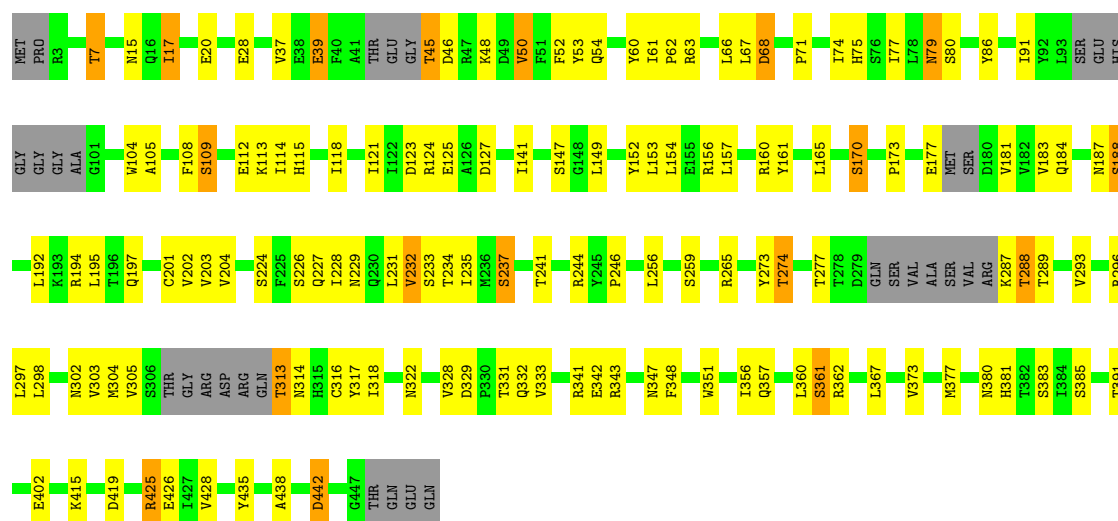


Chain U:  62% 27% 7%



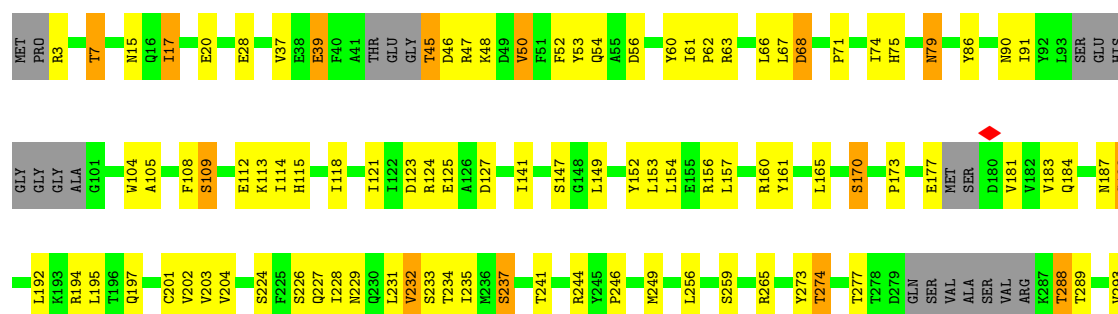
• Molecule 8: Tubulin gamma-1 chain

Chain V:  62% 27% 7%



• Molecule 8: Tubulin gamma-1 chain

Chain W:  62% 27% 7%

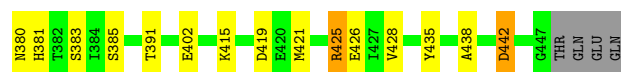




Chain X: 61% 28% 7%

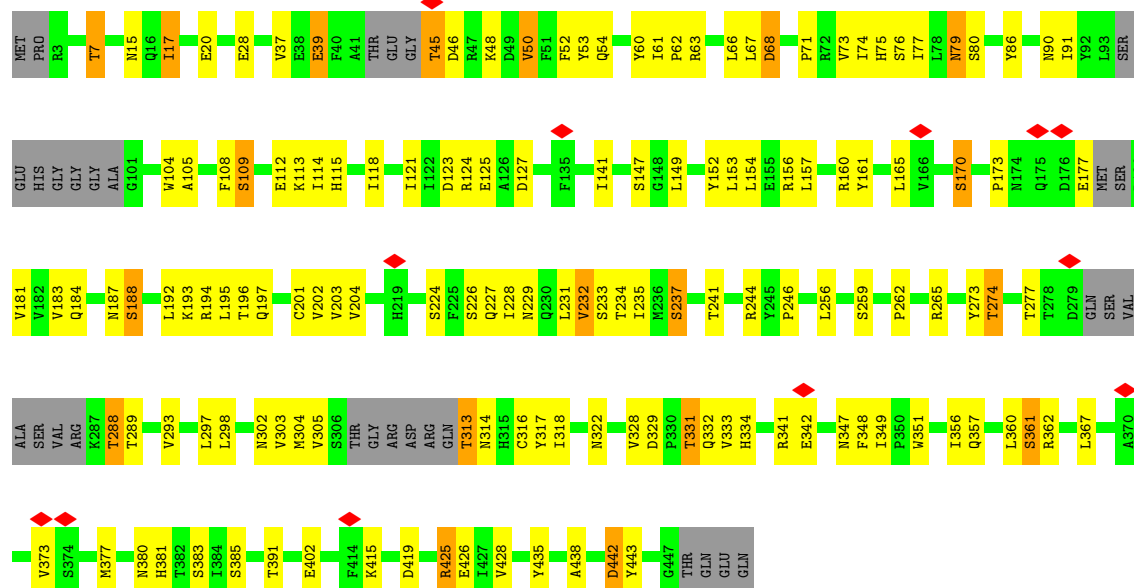


Chain Y: 61% 28% 7%



WORLDWIDE
PDB
PROTEIN DATA BANK

Chain Z:  61% 28% 7%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	8270	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	0.184	Depositor
Minimum map value	-0.046	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.0368	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	0.35	0/4525	0.81	12/6119 (0.2%)
1	l	0.29	0/863	0.77	2/1166 (0.2%)
2	e	0.51	2/2908 (0.1%)	0.75	2/3938 (0.1%)
3	A	0.34	0/5085	0.70	3/6866 (0.0%)
3	C	0.32	0/5151	0.75	6/6955 (0.1%)
3	E	0.33	0/5315	0.76	4/7175 (0.1%)
3	G	0.34	0/5315	0.76	5/7175 (0.1%)
4	B	0.33	0/5133	0.76	5/6930 (0.1%)
4	D	0.33	1/4897 (0.0%)	0.70	6/6610 (0.1%)
4	F	0.32	0/5044	0.72	5/6809 (0.1%)
4	H	0.35	0/5009	0.73	5/6761 (0.1%)
4	a	0.31	0/948	0.67	0/1277
4	f	0.24	0/815	0.60	0/1096
4	h	0.26	0/815	0.65	0/1096
4	j	0.32	0/855	0.82	3/1152 (0.3%)
5	b	0.29	0/484	0.70	0/653
5	d	0.29	0/454	0.65	0/611
5	g	0.25	0/484	0.63	0/653
5	i	0.28	0/484	0.64	0/653
5	k	0.30	0/484	0.68	0/653
5	m	0.28	0/484	0.71	0/653
6	I	0.35	0/4322	0.77	8/5853 (0.1%)
6	K	0.41	1/4683 (0.0%)	0.77	4/6338 (0.1%)
7	L	0.32	0/4697	0.73	4/6348 (0.1%)
7	c	0.24	0/1235	0.59	0/1664
8	O	0.27	0/3441	0.64	0/4661
8	P	0.27	0/3441	0.64	0/4661
8	Q	0.27	0/3441	0.64	0/4661
8	R	0.27	0/3441	0.64	0/4661
8	S	0.27	0/3441	0.64	0/4661
8	T	0.27	0/3441	0.64	0/4661
8	U	0.27	0/3441	0.64	0/4661
8	V	0.27	0/3441	0.64	0/4661
8	W	0.27	0/3441	0.64	0/4661

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
8	X	0.27	0/3441	0.64	0/4661
8	Y	0.27	0/3441	0.64	0/4661
8	Z	0.27	0/3441	0.64	0/4661
All	All	0.32	4/111781 (0.0%)	0.70	74/151136 (0.0%)

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	5
1	l	0	1
2	e	0	1
3	A	0	1
3	C	0	2
3	E	0	4
3	G	0	2
4	B	0	2
4	D	0	1
4	F	0	1
4	H	0	3
6	I	0	6
6	K	0	3
7	L	0	3
8	O	0	1
8	P	0	1
8	Q	0	1
8	R	0	1
8	S	0	1
8	T	0	1
8	U	0	1
8	V	0	1
8	W	0	1
8	X	0	1
8	Y	0	1
8	Z	0	1
All	All	0	47

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	e	243	PRO	N-CD	19.95	1.75	1.47
6	K	653	LYS	CD-CE	-7.08	1.31	1.52
2	e	108	ALA	C-N	5.33	1.39	1.33
4	D	692	ARG	CB-CG	-5.32	1.36	1.52

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	248	VAL	CA-C-N	8.98	132.70	120.67
3	C	248	VAL	C-N-CA	8.98	132.70	120.67
1	J	237	HIS	CA-C-N	8.72	138.20	121.54
1	J	237	HIS	C-N-CA	8.72	138.20	121.54
1	l	121	PRO	N-CA-CB	8.38	112.05	103.25
2	e	64	ILE	N-CA-C	-8.12	105.40	113.20
1	J	420	VAL	N-CA-C	-7.27	106.22	113.20
4	D	400	VAL	N-CA-C	-7.07	106.60	113.53
4	j	107	GLN	CA-C-N	7.07	128.67	119.84
4	j	107	GLN	C-N-CA	7.07	128.67	119.84
7	L	300	VAL	N-CA-C	-7.00	105.96	112.96
1	J	238	LEU	CA-CB-CG	6.98	140.73	116.30
1	l	130	PRO	N-CA-CB	6.83	110.52	103.00
3	G	232	TYR	N-CA-C	-6.66	106.11	114.56
6	K	649	LEU	CA-CB-CG	6.62	139.47	116.30
6	K	654	TYR	N-CA-C	-6.50	104.98	113.17
3	E	264	LEU	N-CA-C	6.42	122.43	113.57
4	B	868	SER	CA-C-N	6.34	133.66	121.54
4	B	868	SER	C-N-CA	6.34	133.66	121.54
6	I	600	ASN	CA-C-N	6.34	133.65	121.54
6	I	600	ASN	C-N-CA	6.34	133.65	121.54
7	L	1478	ARG	N-CA-C	-6.33	106.78	114.75
4	D	418	ILE	N-CA-C	-6.30	106.80	111.90
4	D	886	TYR	N-CA-C	-6.25	99.73	109.72
3	G	480	LYS	CA-C-N	6.21	133.41	121.54
3	G	480	LYS	C-N-CA	6.21	133.41	121.54
3	G	264	LEU	N-CA-C	6.18	123.47	109.81
4	F	883	ASN	N-CA-C	-6.09	107.07	114.75
3	A	479	LEU	CA-C-N	6.05	133.09	121.54
3	A	479	LEU	C-N-CA	6.05	133.09	121.54
1	J	224	TYR	N-CA-C	-6.00	107.18	114.75
4	F	269	ASN	CA-C-N	5.99	131.25	122.63
4	F	269	ASN	C-N-CA	5.99	131.25	122.63
6	I	377	GLN	N-CA-C	-5.95	105.60	114.64
6	K	573	PHE	N-CA-C	5.94	117.86	110.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	I	507	SER	CA-C-N	5.90	132.82	121.54
6	I	507	SER	C-N-CA	5.90	132.82	121.54
4	F	272	GLU	CA-C-N	5.88	132.77	121.54
4	F	272	GLU	C-N-CA	5.88	132.77	121.54
6	I	131	LEU	N-CA-C	-5.86	106.78	114.04
4	B	869	SER	N-CA-C	-5.85	98.33	110.80
3	C	367	THR	N-CA-C	-5.85	105.74	114.64
4	j	108	PRO	N-CA-CB	5.83	109.38	103.25
1	J	223	GLN	N-CA-C	-5.70	105.97	114.64
4	H	362	LEU	N-CA-C	-5.70	107.57	114.75
4	H	365	ARG	CG-CD-NE	-5.66	99.54	112.00
4	D	872	SER	N-CA-C	-5.66	107.38	114.56
1	J	238	LEU	N-CA-C	5.59	122.70	110.80
4	D	495	GLN	CA-C-N	-5.47	117.03	122.77
4	D	495	GLN	C-N-CA	-5.47	117.03	122.77
3	G	367	THR	N-CA-C	-5.45	106.36	114.64
1	J	255	PRO	CA-C-N	5.45	131.50	121.70
1	J	255	PRO	C-N-CA	5.45	131.50	121.70
1	J	238	LEU	CB-CG-CD1	-5.40	94.51	110.70
3	A	548	PRO	N-CA-C	5.36	117.24	110.70
4	H	365	ARG	NE-CZ-NH1	-5.36	116.14	121.50
7	L	316	GLY	CA-C-N	5.30	131.67	121.54
7	L	316	GLY	C-N-CA	5.30	131.67	121.54
4	B	372	TYR	CA-C-N	5.28	126.69	120.09
4	B	372	TYR	C-N-CA	5.28	126.69	120.09
3	E	155	GLU	CA-C-N	5.20	127.51	120.38
3	E	155	GLU	C-N-CA	5.20	127.51	120.38
3	C	507	LYS	CA-C-N	5.19	128.47	121.05
3	C	507	LYS	C-N-CA	5.19	128.47	121.05
2	e	243	PRO	CA-N-CD	-5.18	104.75	112.00
3	C	868	ARG	N-CA-C	-5.17	108.72	114.62
3	E	170	SER	N-CA-C	-5.17	107.99	114.56
1	J	256	LEU	CA-C-N	5.14	131.35	121.54
1	J	256	LEU	C-N-CA	5.14	131.35	121.54
4	H	613	ASP	CA-C-N	5.12	127.94	120.51
4	H	613	ASP	C-N-CA	5.12	127.94	120.51
6	I	408	ASP	CA-C-N	5.07	131.23	121.54
6	I	408	ASP	C-N-CA	5.07	131.23	121.54
6	K	193	HIS	N-CA-C	-5.03	108.41	114.75

There are no chirality outliers.

All (47) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	583	ILE	Peptide
4	B	868	SER	Peptide
4	B	889	ARG	Peptide
3	C	238	LEU	Peptide
3	C	239	ALA	Peptide
4	D	626	LEU	Peptide
3	E	240	GLY	Peptide
3	E	474	GLU	Peptide
3	E	580	HIS	Peptide
3	E	674	GLN	Peptide
4	F	525	ASP	Peptide
3	G	240	GLY	Peptide
3	G	580	HIS	Peptide
4	H	321	GLY	Peptide
4	H	626	LEU	Peptide
4	H	632	ASP	Peptide
6	I	507	SER	Peptide
6	I	508	ASN	Mainchain
6	I	511	ASP	Peptide
6	I	516	ARG	Peptide
6	I	600	ASN	Peptide
6	I	601	LEU	Peptide
1	J	210	PRO	Peptide
1	J	235	SER	Peptide
1	J	237	HIS	Peptide
1	J	256	LEU	Peptide
1	J	726	PHE	Peptide
6	K	254	LEU	Peptide
6	K	318	PRO	Peptide
6	K	410	LEU	Peptide
7	L	1688	PHE	Peptide
7	L	293	LYS	Peptide
7	L	346	LEU	Peptide
8	O	347	ASN	Peptide
8	P	347	ASN	Peptide
8	Q	347	ASN	Peptide
8	R	347	ASN	Peptide
8	S	347	ASN	Peptide
8	T	347	ASN	Peptide
8	U	347	ASN	Peptide
8	V	347	ASN	Peptide
8	W	347	ASN	Peptide
8	X	347	ASN	Peptide

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Mol	Chain	Res	Type	Group
8	Y	347	ASN	Peptide
8	Z	347	ASN	Peptide
2	e	249	THR	Peptide
1	l	121	PRO	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	38	0
1	l	847	0	789	8	0
2	e	2847	0	2810	34	0
3	A	4978	0	4996	34	0
3	C	5044	0	5081	44	0
3	E	5206	0	5230	46	0
3	G	5206	0	5230	35	0
4	B	5029	0	5018	50	0
4	D	4796	0	4775	46	0
4	F	4941	0	4935	51	0
4	H	4907	0	4896	36	0
4	a	933	0	953	9	0
4	f	803	0	831	5	0
4	h	803	0	831	4	0
4	j	843	0	846	7	0
5	b	484	0	512	8	0
5	d	454	0	482	9	0
5	g	484	0	512	3	0
5	i	484	0	512	2	0
5	k	484	0	512	1	0
5	m	484	0	512	3	0
6	I	4225	0	4259	31	0
6	K	4579	0	4586	61	0
7	L	4587	0	4636	26	0
7	c	1220	0	1231	10	0
8	O	3373	0	3325	75	0
8	P	3373	0	3325	78	0
8	Q	3373	0	3325	72	0
8	R	3373	0	3325	75	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	S	3373	0	3325	73	0
8	T	3373	0	3325	72	0
8	U	3373	0	3325	72	0
8	V	3373	0	3325	71	0
8	W	3373	0	3325	72	0
8	X	3373	0	3325	73	0
8	Y	3373	0	3325	84	0
8	Z	3373	0	3325	76	0
9	l	6	0	0	1	0
All	All	109579	0	109357	1375	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (1375) 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	1.75	1.34
2:e:5:ILE:HG21	2:e:100:GLU:O	1.58	1.04
2:e:5:ILE:CG2	2:e:100:GLU:O	2.11	0.98
2:e:242:LEU:HD22	2:e:243:PRO:HD2	1.52	0.88
6:K:653:LYS:NZ	8:Y:349:ILE:O	2.13	0.80
3:G:222:LEU:HG	4:H:365:ARG:HH12	1.46	0.80
2:e:79:TRP:HE1	2:e:122:ILE:HG13	1.47	0.77
3:C:696:TYR:O	3:C:700:GLU:HB2	1.85	0.76
6:K:497:ALA:HB2	8:Y:254:ILE:HD11	1.68	0.76
4:F:572:ASP:OD1	8:T:251:ASN:ND2	2.21	0.74
4:B:799:GLU:OE2	4:B:803:ARG:NH1	2.22	0.73
8:S:3:ARG:HH12	3:E:533:ASP:HB3	1.55	0.72
4:F:692:ARG:HD3	8:T:265:ARG:HD2	1.72	0.72
8:O:328:VAL:HG21	8:O:360:LEU:HD11	1.74	0.70
8:Z:328:VAL:HG21	8:Z:360:LEU:HD11	1.74	0.70
8:U:328:VAL:HG21	8:U:360:LEU:HD11	1.74	0.70
8:S:328:VAL:HG21	8:S:360:LEU:HD11	1.74	0.70
8:W:328:VAL:HG21	8:W:360:LEU:HD11	1.74	0.70
8:R:328:VAL:HG21	8:R:360:LEU:HD11	1.74	0.69
8:V:328:VAL:HG21	8:V:360:LEU:HD11	1.74	0.69
2:e:242:LEU:CD2	2:e:243:PRO:HD2	2.22	0.69
8:Q:328:VAL:HG21	8:Q:360:LEU:HD11	1.74	0.69
4:B:364:LEU:H	4:B:370:TRP:HE1	1.39	0.69
8:P:328:VAL:HG21	8:P:360:LEU:HD11	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:154:LEU:O	6:I:158:TYR:HB2	1.93	0.68
3:A:529:VAL:HG22	8:O:3:ARG:HH11	1.57	0.68
8:X:328:VAL:HG21	8:X:360:LEU:HD11	1.74	0.68
8:Y:328:VAL:HG21	8:Y:360:LEU:HD11	1.74	0.68
3:A:698:MET:SD	8:O:248:TYR:OH	2.47	0.68
6:K:375:THR:OG1	6:K:402:LYS:NZ	2.26	0.68
6:K:646:LEU:HB3	8:Y:341:ARG:HD2	1.75	0.68
2:e:5:ILE:HG21	2:e:100:GLU:C	2.18	0.67
8:T:328:VAL:HG21	8:T:360:LEU:HD11	1.74	0.67
3:G:313:LEU:HD22	4:a:122:LEU:HD21	1.75	0.67
6:I:362:LEU:HB3	6:I:537:LEU:HD13	1.76	0.67
6:K:651:TYR:CZ	8:Y:354:ALA:HB3	2.30	0.67
3:C:533:ASP:OD2	8:Q:3:ARG:NH1	2.26	0.66
4:B:579:ASP:OD2	8:P:3:ARG:NH1	2.30	0.65
8:Q:48:LYS:O	8:Q:54:GLN:NE2	2.30	0.65
3:E:578:MET:H	3:E:615:ALA:HB1	1.61	0.65
4:H:560:GLN:OE1	4:H:563:ARG:NH1	2.30	0.65
8:Z:48:LYS:O	8:Z:54:GLN:NE2	2.30	0.65
4:B:609:ASN:ND2	8:P:46:ASP:O	2.30	0.64
3:G:854:SER:OG	8:U:338:GLN:NE2	2.29	0.64
8:S:48:LYS:O	8:S:54:GLN:NE2	2.30	0.64
3:E:293:ALA:HA	3:E:296:MET:HE2	1.78	0.64
3:G:408:MET:HE3	3:G:439:ILE:HG12	1.80	0.64
8:P:48:LYS:O	8:P:54:GLN:NE2	2.30	0.64
8:U:48:LYS:O	8:U:54:GLN:NE2	2.30	0.64
2:e:186:THR:HG22	2:e:210:ARG:HG3	1.77	0.64
4:B:319:LEU:HD21	3:C:367:THR:HB	1.80	0.64
6:I:345:VAL:HG13	6:I:346:GLU:HG3	1.80	0.64
8:O:273:TYR:HB2	8:O:304:MET:HE2	1.80	0.64
8:R:273:TYR:HB2	8:R:304:MET:HE2	1.80	0.64
8:X:273:TYR:HB2	8:X:304:MET:HE2	1.80	0.64
8:S:273:TYR:HB2	8:S:304:MET:HE2	1.80	0.64
8:T:273:TYR:HB2	8:T:304:MET:HE2	1.80	0.64
8:W:48:LYS:O	8:W:54:GLN:NE2	2.30	0.64
8:T:48:LYS:O	8:T:54:GLN:NE2	2.30	0.64
8:X:48:LYS:O	8:X:54:GLN:NE2	2.30	0.64
4:F:306:ARG:HH11	4:F:310:GLN:HE22	1.46	0.64
8:V:48:LYS:O	8:V:54:GLN:NE2	2.30	0.64
3:E:685:ARG:HE	3:E:865:TYR:HE2	1.46	0.64
6:K:649:LEU:HB3	6:K:655:TYR:HB2	1.80	0.63
6:K:649:LEU:HB2	8:Y:341:ARG:HH21	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Y:48:LYS:O	8:Y:54:GLN:NE2	2.30	0.63
4:H:599:GLY:HA3	8:W:342:GLU:HG3	1.80	0.63
8:R:48:LYS:O	8:R:54:GLN:NE2	2.30	0.63
8:V:273:TYR:HB2	8:V:304:MET:HE2	1.80	0.63
8:W:273:TYR:HB2	8:W:304:MET:HE2	1.80	0.63
8:O:66:LEU:HD21	8:O:74:ILE:HG12	1.81	0.63
8:Y:273:TYR:HB2	8:Y:304:MET:HE2	1.80	0.63
8:O:48:LYS:O	8:O:54:GLN:NE2	2.30	0.63
8:Z:66:LEU:HD21	8:Z:74:ILE:HG12	1.81	0.63
3:G:698:MET:HE1	8:U:249:MET:HE2	1.79	0.63
8:S:45:THR:HG23	3:E:566:THR:HG21	1.81	0.63
8:U:273:TYR:HB2	8:U:304:MET:HE2	1.80	0.63
1:J:266:THR:OG1	1:J:269:GLN:NE2	2.32	0.63
6:K:516:ARG:HD2	8:Y:264:PRO:HD3	1.81	0.63
8:P:66:LEU:HD21	8:P:74:ILE:HG12	1.81	0.63
8:T:442:ASP:OD1	8:T:442:ASP:N	2.32	0.63
8:V:66:LEU:HD21	8:V:74:ILE:HG12	1.81	0.63
4:D:454:VAL:H	4:D:463:LYS:HE3	1.63	0.62
8:W:66:LEU:HD21	8:W:74:ILE:HG12	1.81	0.62
4:D:686:CYS:O	4:D:689:LYS:NZ	2.31	0.62
8:Q:273:TYR:HB2	8:Q:304:MET:HE2	1.80	0.62
8:Z:273:TYR:HB2	8:Z:304:MET:HE2	1.80	0.62
4:F:694:MET:HE3	4:F:695:PRO:HD2	1.80	0.62
8:P:273:TYR:HB2	8:P:304:MET:HE2	1.80	0.62
8:W:442:ASP:OD1	8:W:442:ASP:N	2.32	0.62
8:Z:442:ASP:OD1	8:Z:442:ASP:N	2.32	0.62
8:Q:442:ASP:N	8:Q:442:ASP:OD1	2.32	0.62
8:S:233:SER:O	8:S:237:SER:OG	2.18	0.62
8:X:442:ASP:N	8:X:442:ASP:OD1	2.32	0.62
8:Y:66:LEU:HD21	8:Y:74:ILE:HG12	1.81	0.62
8:R:442:ASP:OD1	8:R:442:ASP:N	2.32	0.62
8:U:66:LEU:HD21	8:U:74:ILE:HG12	1.81	0.62
8:U:233:SER:O	8:U:237:SER:OG	2.18	0.62
8:W:233:SER:O	8:W:237:SER:OG	2.18	0.62
8:X:66:LEU:HD21	8:X:74:ILE:HG12	1.81	0.62
8:Y:233:SER:O	8:Y:237:SER:OG	2.18	0.62
3:E:359:LEU:HB3	3:E:380:THR:HG22	1.82	0.62
4:F:338:LEU:HD21	7:c:148:TYR:HB2	1.82	0.62
8:S:442:ASP:OD1	8:S:442:ASP:N	2.32	0.62
8:Z:233:SER:O	8:Z:237:SER:OG	2.18	0.62
4:B:681:ARG:NH1	8:P:261:ILE:O	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:529:VAL:O	8:U:3:ARG:NH1	2.33	0.61
6:I:148:ILE:HG23	6:I:152:GLN:HG2	1.81	0.61
8:Q:66:LEU:HD21	8:Q:74:ILE:HG12	1.81	0.61
4:f:81:LEU:HD21	4:f:90:LYS:HB3	1.80	0.61
6:K:649:LEU:HB2	8:Y:341:ARG:NH2	2.16	0.61
8:T:66:LEU:HD21	8:T:74:ILE:HG12	1.81	0.61
4:H:593:TYR:H	4:H:596:ASN:HD22	1.48	0.61
8:Y:442:ASP:OD1	8:Y:442:ASP:N	2.32	0.61
8:Q:233:SER:O	8:Q:237:SER:OG	2.18	0.61
8:R:66:LEU:HD21	8:R:74:ILE:HG12	1.81	0.61
8:X:233:SER:O	8:X:237:SER:OG	2.18	0.61
3:C:698:MET:HE1	8:Q:249:MET:HE2	1.82	0.61
8:S:66:LEU:HD21	8:S:74:ILE:HG12	1.81	0.61
8:V:351:TRP:NE1	8:V:438:ALA:O	2.31	0.61
8:P:351:TRP:NE1	8:P:438:ALA:O	2.31	0.61
8:P:442:ASP:OD1	8:P:442:ASP:N	2.32	0.61
8:R:351:TRP:NE1	8:R:438:ALA:O	2.31	0.61
8:V:233:SER:O	8:V:237:SER:OG	2.18	0.61
8:V:442:ASP:N	8:V:442:ASP:OD1	2.32	0.61
4:F:665:ASN:HB3	4:j:66:ARG:HE	1.66	0.61
6:K:259:LEU:HG	6:K:277:LEU:HD22	1.81	0.60
8:P:233:SER:O	8:P:237:SER:OG	2.18	0.60
8:Z:313:THR:OG1	8:Z:314:ASN:N	2.34	0.60
4:H:430:LEU:HD23	4:H:446:PHE:HE1	1.66	0.60
8:T:313:THR:OG1	8:T:314:ASN:N	2.34	0.60
8:V:313:THR:OG1	8:V:314:ASN:N	2.34	0.60
3:C:475:ILE:HG12	3:C:487:GLN:HE21	1.67	0.60
8:O:351:TRP:NE1	8:O:438:ALA:O	2.31	0.60
8:U:313:THR:OG1	8:U:314:ASN:N	2.34	0.60
8:W:313:THR:OG1	8:W:314:ASN:N	2.34	0.60
8:T:233:SER:O	8:T:237:SER:OG	2.18	0.60
8:P:313:THR:OG1	8:P:314:ASN:N	2.34	0.60
8:Y:313:THR:OG1	8:Y:314:ASN:N	2.34	0.60
8:S:313:THR:OG1	8:S:314:ASN:N	2.34	0.60
3:A:554:LEU:HA	3:A:557:LEU:HD12	1.84	0.60
3:C:314:HIS:HB2	3:C:319:LEU:HD12	1.84	0.59
4:D:319:LEU:N	4:D:445:GLU:OE2	2.35	0.59
8:Q:313:THR:OG1	8:Q:314:ASN:N	2.34	0.59
7:L:1683:VAL:HG12	8:Z:331:THR:HA	1.84	0.59
8:O:233:SER:O	8:O:237:SER:OG	2.18	0.59
8:U:442:ASP:OD1	8:U:442:ASP:N	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:e:242:LEU:CD2	2:e:243:PRO:CD	2.80	0.59
8:R:313:THR:OG1	8:R:314:ASN:N	2.34	0.59
4:B:561:ALA:HA	4:B:564:ARG:HE	1.68	0.59
6:K:31:PHE:HB2	6:K:34:LEU:HG	1.84	0.59
6:K:399:SER:HA	6:K:402:LYS:HE2	1.83	0.59
6:K:646:LEU:O	8:Y:341:ARG:NE	2.35	0.59
8:O:442:ASP:N	8:O:442:ASP:OD1	2.32	0.59
2:e:153:MET:HE3	2:e:278:THR:OG1	2.03	0.59
8:X:351:TRP:NE1	8:X:438:ALA:O	2.31	0.59
8:Y:351:TRP:NE1	8:Y:438:ALA:O	2.31	0.59
3:C:371:GLN:HE21	7:c:195:LEU:HB3	1.67	0.58
4:F:406:THR:HG21	4:F:411:MET:HB2	1.85	0.58
3:G:641:LEU:HG	3:G:645:MET:HE1	1.85	0.58
8:X:313:THR:OG1	8:X:314:ASN:N	2.34	0.58
3:E:719:ILE:HA	3:E:722:VAL:HG22	1.85	0.58
4:D:572:ASP:OD1	8:R:251:ASN:ND2	2.36	0.58
6:I:511:ASP:H	6:I:514:LYS:HD2	1.67	0.58
3:A:533:ASP:HB2	8:O:3:ARG:HH12	1.69	0.58
6:K:188:SER:HA	6:K:311:LEU:HD13	1.85	0.58
7:c:29:ASN:HD21	7:c:32:ARG:HB2	1.68	0.58
8:O:141:ILE:HB	8:O:173:PRO:HD3	1.86	0.58
8:O:303:VAL:HG12	8:O:305:VAL:H	1.69	0.58
8:S:303:VAL:HG12	8:S:305:VAL:H	1.69	0.58
8:Y:226:SER:OG	8:Y:227:GLN:NE2	2.37	0.58
8:Z:303:VAL:HG12	8:Z:305:VAL:H	1.69	0.58
4:B:737:LYS:HE3	4:B:746:HIS:HB3	1.85	0.58
8:Q:226:SER:OG	8:Q:227:GLN:NE2	2.37	0.58
8:V:141:ILE:HB	8:V:173:PRO:HD3	1.86	0.58
8:O:226:SER:OG	8:O:227:GLN:NE2	2.37	0.58
8:R:141:ILE:HB	8:R:173:PRO:HD3	1.86	0.58
4:H:589:ALA:HA	4:H:592:LEU:HG	1.86	0.58
8:P:226:SER:OG	8:P:227:GLN:NE2	2.37	0.58
8:S:141:ILE:HB	8:S:173:PRO:HD3	1.86	0.58
8:T:303:VAL:HG12	8:T:305:VAL:H	1.69	0.58
8:U:351:TRP:NE1	8:U:438:ALA:O	2.31	0.58
8:W:303:VAL:HG12	8:W:305:VAL:H	1.69	0.58
8:Y:303:VAL:HG12	8:Y:305:VAL:H	1.69	0.58
4:B:886:TYR:CE2	8:P:353:PRO:HG3	2.39	0.58
8:W:226:SER:OG	8:W:227:GLN:NE2	2.37	0.58
4:F:419:LEU:HA	4:F:422:VAL:HG22	1.86	0.57
1:J:724:ARG:HH12	1:J:914:GLN:HB3	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:R:226:SER:OG	8:R:227:GLN:NE2	2.37	0.57
8:S:226:SER:OG	8:S:227:GLN:NE2	2.37	0.57
8:U:303:VAL:HG12	8:U:305:VAL:H	1.69	0.57
8:X:141:ILE:HB	8:X:173:PRO:HD3	1.86	0.57
4:H:599:GLY:HA2	4:H:602:GLU:HG3	1.85	0.57
8:R:233:SER:O	8:R:237:SER:OG	2.18	0.57
8:R:303:VAL:HG12	8:R:305:VAL:H	1.69	0.57
8:X:303:VAL:HG12	8:X:305:VAL:H	1.69	0.57
1:I:71:LYS:NZ	9:I:1102:HOH:O	2.36	0.57
8:O:313:THR:OG1	8:O:314:ASN:N	2.34	0.57
3:E:154:LEU:HA	3:E:157:LYS:HD2	1.87	0.57
8:V:226:SER:OG	8:V:227:GLN:NE2	2.37	0.57
8:Z:141:ILE:HB	8:Z:173:PRO:HD3	1.86	0.57
4:B:284:SER:OG	4:B:285:ARG:NH2	2.36	0.57
4:D:494:HIS:HD2	4:D:500:GLN:HG3	1.70	0.57
1:J:885:LEU:HD11	8:X:444:ILE:HA	1.86	0.57
8:T:141:ILE:HB	8:T:173:PRO:HD3	1.86	0.57
6:I:353:GLN:NE2	6:I:457:TYR:OH	2.37	0.57
8:Z:226:SER:OG	8:Z:227:GLN:NE2	2.37	0.57
3:A:160:MET:HE1	3:A:351:LEU:HD13	1.86	0.57
8:Q:303:VAL:HG12	8:Q:305:VAL:H	1.69	0.57
8:Y:141:ILE:HB	8:Y:173:PRO:HD3	1.86	0.57
4:F:645:ASP:HA	4:F:649:ALA:HB2	1.87	0.57
7:L:1677:ALA:HA	7:L:1681:LEU:HD12	1.86	0.57
8:T:226:SER:OG	8:T:227:GLN:NE2	2.37	0.57
8:W:141:ILE:HB	8:W:173:PRO:HD3	1.86	0.57
8:X:226:SER:OG	8:X:227:GLN:NE2	2.37	0.57
3:E:518:ARG:HA	3:E:523:ASP:H	1.69	0.57
8:S:258:ALA:HB1	3:E:687:LEU:HD21	1.87	0.57
8:U:141:ILE:HB	8:U:173:PRO:HD3	1.86	0.57
8:U:226:SER:OG	8:U:227:GLN:NE2	2.37	0.57
3:C:297:ARG:HH12	4:D:410:TYR:HB2	1.70	0.57
4:B:764:LEU:HG	4:f:66:ARG:HH12	1.69	0.56
7:c:8:PHE:HA	7:c:11:LEU:HD12	1.87	0.56
8:V:303:VAL:HG12	8:V:305:VAL:H	1.69	0.56
8:P:303:VAL:HG12	8:P:305:VAL:H	1.69	0.56
2:e:39:ARG:HG3	2:e:66:THR:HG23	1.88	0.56
3:C:864:PHE:HB3	8:Q:353:PRO:HA	1.88	0.56
8:T:351:TRP:NE1	8:T:438:ALA:O	2.31	0.56
4:D:560:GLN:HE21	4:D:564:ARG:HE	1.54	0.56
4:D:594:GLN:NE2	4:D:623:VAL:O	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:b:22:ARG:NH2	5:b:26:ASP:OD1	2.39	0.56
4:H:563:ARG:HH21	4:H:569:GLY:HA3	1.71	0.56
2:e:242:LEU:HD22	2:e:243:PRO:CD	2.32	0.56
8:U:177:GLU:OE2	8:U:184:GLN:NE2	2.39	0.56
8:X:177:GLU:OE2	8:X:184:GLN:NE2	2.39	0.56
8:P:141:ILE:HB	8:P:173:PRO:HD3	1.86	0.56
8:Q:351:TRP:NE1	8:Q:438:ALA:O	2.31	0.56
3:A:237:PRO:HA	3:A:244:ARG:HE	1.71	0.56
8:Q:141:ILE:HB	8:Q:173:PRO:HD3	1.86	0.56
8:R:177:GLU:OE2	8:R:184:GLN:NE2	2.39	0.56
8:W:177:GLU:OE2	8:W:184:GLN:NE2	2.39	0.56
8:S:112:GLU:O	8:S:115:HIS:ND1	2.39	0.56
8:S:177:GLU:OE2	8:S:184:GLN:NE2	2.39	0.56
8:Y:177:GLU:OE2	8:Y:184:GLN:NE2	2.39	0.56
5:d:21:VAL:HA	5:d:24:THR:HG22	1.87	0.56
5:d:48:VAL:HG12	7:c:110:VAL:HG21	1.87	0.56
1:J:1015:LEU:HD13	8:X:341:ARG:HG3	1.89	0.55
8:R:112:GLU:O	8:R:115:HIS:ND1	2.39	0.55
8:T:177:GLU:OE2	8:T:184:GLN:NE2	2.39	0.55
8:Z:177:GLU:OE2	8:Z:184:GLN:NE2	2.39	0.55
3:C:518:ARG:HA	3:C:523:ASP:HB3	1.87	0.55
8:O:177:GLU:OE2	8:O:184:GLN:NE2	2.39	0.55
8:P:177:GLU:OE2	8:P:184:GLN:NE2	2.39	0.55
8:Z:124:ARG:NH1	8:Z:125:GLU:OE2	2.40	0.55
1:J:278:LEU:HD23	1:J:379:LEU:HD11	1.89	0.55
8:X:121:ILE:HG23	8:X:124:ARG:HH21	1.72	0.55
8:Y:112:GLU:O	8:Y:115:HIS:ND1	2.39	0.55
8:Z:351:TRP:NE1	8:Z:438:ALA:O	2.31	0.55
8:O:124:ARG:NH1	8:O:125:GLU:OE2	2.40	0.55
8:W:124:ARG:NH1	8:W:125:GLU:OE2	2.40	0.55
8:O:62:PRO:HD2	8:O:86:TYR:HB3	1.89	0.55
4:H:633:THR:OG1	4:H:634:GLY:N	2.40	0.55
6:I:528:LEU:HD13	6:I:531:TYR:HD2	1.70	0.55
8:O:112:GLU:O	8:O:115:HIS:ND1	2.39	0.55
8:Q:112:GLU:O	8:Q:115:HIS:ND1	2.39	0.55
8:R:62:PRO:HD2	8:R:86:TYR:HB3	1.89	0.55
8:S:121:ILE:HG23	8:S:124:ARG:HH21	1.72	0.55
8:S:229:ASN:O	8:S:233:SER:OG	2.22	0.55
8:Y:62:PRO:HD2	8:Y:86:TYR:HB3	1.89	0.55
8:Y:121:ILE:HG23	8:Y:124:ARG:HH21	1.72	0.55
8:Q:124:ARG:NH1	8:Q:125:GLU:OE2	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Q:177:GLU:OE2	8:Q:184:GLN:NE2	2.39	0.55
8:V:62:PRO:HD2	8:V:86:TYR:HB3	1.89	0.55
8:V:177:GLU:OE2	8:V:184:GLN:NE2	2.39	0.55
8:X:62:PRO:HD2	8:X:86:TYR:HB3	1.89	0.55
7:L:311:TYR:HD2	7:L:314:GLU:HG3	1.71	0.55
8:P:112:GLU:O	8:P:115:HIS:ND1	2.39	0.55
8:R:124:ARG:NH1	8:R:125:GLU:OE2	2.40	0.55
8:S:351:TRP:NE1	8:S:438:ALA:O	2.31	0.55
8:V:121:ILE:HG23	8:V:124:ARG:HH21	1.72	0.55
8:X:124:ARG:NH1	8:X:125:GLU:OE2	2.40	0.55
3:C:696:TYR:HE1	3:C:854:SER:HB2	1.71	0.55
3:G:359:LEU:HB3	3:G:380:THR:HG22	1.89	0.55
8:W:62:PRO:HD2	8:W:86:TYR:HB3	1.89	0.55
8:R:121:ILE:HG23	8:R:124:ARG:HH21	1.72	0.54
8:U:124:ARG:NH1	8:U:125:GLU:OE2	2.40	0.54
8:V:112:GLU:O	8:V:115:HIS:ND1	2.39	0.54
8:V:124:ARG:NH1	8:V:125:GLU:OE2	2.40	0.54
8:W:112:GLU:O	8:W:115:HIS:ND1	2.39	0.54
8:W:121:ILE:HG23	8:W:124:ARG:HH21	1.72	0.54
2:e:305:MET:HE2	2:e:336:LYS:HE2	1.89	0.54
8:O:121:ILE:HG23	8:O:124:ARG:HH21	1.72	0.54
8:S:124:ARG:NH1	8:S:125:GLU:OE2	2.40	0.54
4:B:550:ASN:HB3	4:B:551:LYS:HZ3	1.71	0.54
4:D:699:GLY:HA2	8:R:446:TRP:HE1	1.73	0.54
4:F:451:ASP:H	4:F:463:LYS:HA	1.72	0.54
8:T:121:ILE:HG23	8:T:124:ARG:HH21	1.72	0.54
8:W:351:TRP:NE1	8:W:438:ALA:O	2.31	0.54
8:Z:62:PRO:HD2	8:Z:86:TYR:HB3	1.89	0.54
3:C:440:PRO:HD2	3:C:443:LEU:HD11	1.90	0.54
6:K:68:GLN:NE2	6:K:198:ASP:OD2	2.40	0.54
8:W:184:GLN:O	8:W:188:SER:OG	2.26	0.54
8:Z:121:ILE:HG23	8:Z:124:ARG:HH21	1.72	0.54
8:Z:184:GLN:O	8:Z:188:SER:OG	2.26	0.54
8:R:184:GLN:O	8:R:188:SER:OG	2.26	0.54
8:T:112:GLU:O	8:T:115:HIS:ND1	2.39	0.54
8:Y:124:ARG:NH1	8:Y:125:GLU:OE2	2.40	0.54
8:Z:112:GLU:O	8:Z:115:HIS:ND1	2.39	0.54
4:B:566:LEU:HG	4:B:640:LEU:HD21	1.89	0.54
8:Q:62:PRO:HD2	8:Q:86:TYR:HB3	1.89	0.54
8:T:124:ARG:NH1	8:T:125:GLU:OE2	2.40	0.54
8:U:62:PRO:HD2	8:U:86:TYR:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:W:361:SER:OG	8:W:362:ARG:N	2.41	0.54
8:X:184:GLN:O	8:X:188:SER:OG	2.26	0.54
8:Z:20:GLU:HG2	8:Z:229:ASN:HB3	1.90	0.54
8:U:112:GLU:O	8:U:115:HIS:ND1	2.39	0.54
8:X:112:GLU:O	8:X:115:HIS:ND1	2.39	0.54
8:V:20:GLU:HG2	8:V:229:ASN:HB3	1.90	0.54
3:E:356:LEU:HG	3:E:440:PRO:HB3	1.89	0.54
2:e:153:MET:CE	2:e:278:THR:OG1	2.56	0.54
4:H:627:GLU:HG2	4:H:628:VAL:H	1.73	0.54
8:P:121:ILE:HG23	8:P:124:ARG:HH21	1.72	0.54
8:Q:121:ILE:HG23	8:Q:124:ARG:HH21	1.72	0.54
8:U:20:GLU:HG2	8:U:229:ASN:HB3	1.90	0.54
8:Y:184:GLN:O	8:Y:188:SER:OG	2.26	0.54
4:B:866:THR:HA	4:B:874:ARG:HE	1.71	0.53
8:R:20:GLU:HG2	8:R:229:ASN:HB3	1.90	0.53
8:T:62:PRO:HD2	8:T:86:TYR:HB3	1.89	0.53
8:Z:231:LEU:O	8:Z:234:THR:OG1	2.24	0.53
6:I:515:TRP:HE1	6:I:519:ASN:H	1.55	0.53
8:O:20:GLU:HG2	8:O:229:ASN:HB3	1.90	0.53
8:S:62:PRO:HD2	8:S:86:TYR:HB3	1.89	0.53
8:V:184:GLN:O	8:V:188:SER:OG	2.26	0.53
8:Y:20:GLU:HG2	8:Y:229:ASN:HB3	1.90	0.53
5:i:28:LEU:HD21	4:h:93:ILE:HG12	1.91	0.53
8:P:62:PRO:HD2	8:P:86:TYR:HB3	1.89	0.53
8:S:20:GLU:HG2	8:S:229:ASN:HB3	1.90	0.53
8:T:184:GLN:O	8:T:188:SER:OG	2.26	0.53
3:E:764:LYS:HG2	3:E:767:GLN:HE21	1.73	0.53
2:e:216:LEU:HD21	2:e:238:LYS:HE2	1.90	0.53
8:O:184:GLN:O	8:O:188:SER:OG	2.26	0.53
8:P:124:ARG:NH1	8:P:125:GLU:OE2	2.40	0.53
8:Q:361:SER:OG	8:Q:362:ARG:N	2.41	0.53
3:E:242:GLN:NE2	3:E:272:ALA:O	2.42	0.53
4:H:433:TRP:HD1	4:H:483:VAL:HG22	1.74	0.53
3:E:578:MET:HE2	3:E:584:THR:HG21	1.90	0.53
3:C:485:VAL:HA	3:C:488:ILE:HD12	1.89	0.53
6:I:370:GLN:HE22	8:W:3:ARG:NH1	2.07	0.53
8:Q:184:GLN:O	8:Q:188:SER:OG	2.26	0.53
8:S:67:LEU:HD13	8:S:118:ILE:HB	1.91	0.53
8:W:67:LEU:HD13	8:W:118:ILE:HB	1.91	0.53
8:Y:231:LEU:O	8:Y:234:THR:OG1	2.24	0.53
8:S:53:TYR:HB3	8:S:61:ILE:HB	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Q:20:GLU:HG2	8:Q:229:ASN:HB3	1.90	0.53
8:S:184:GLN:O	8:S:188:SER:OG	2.26	0.53
3:E:223:TYR:HB3	3:E:228:VAL:HG13	1.89	0.53
8:S:353:PRO:HG3	3:E:865:TYR:CD2	2.44	0.53
8:U:184:GLN:O	8:U:188:SER:OG	2.26	0.53
8:U:231:LEU:O	8:U:234:THR:OG1	2.24	0.53
3:E:698:MET:HA	3:E:702:MET:HE2	1.91	0.53
4:D:885:HIS:NE2	4:D:890:GLU:HG3	2.24	0.53
8:O:53:TYR:HB3	8:O:61:ILE:HB	1.91	0.53
8:Q:67:LEU:HD13	8:Q:118:ILE:HB	1.91	0.53
8:S:231:LEU:O	8:S:234:THR:OG1	2.24	0.53
8:T:67:LEU:HD13	8:T:118:ILE:HB	1.91	0.53
8:U:52:PHE:HB3	8:U:60:TYR:HB3	1.92	0.53
8:U:121:ILE:HG23	8:U:124:ARG:HH21	1.72	0.53
8:W:20:GLU:HG2	8:W:229:ASN:HB3	1.90	0.53
8:W:52:PHE:HB3	8:W:60:TYR:HB3	1.92	0.53
3:G:529:VAL:HG22	8:U:3:ARG:HH11	1.73	0.52
8:P:20:GLU:HG2	8:P:229:ASN:HB3	1.90	0.52
8:Q:53:TYR:HB3	8:Q:61:ILE:HB	1.91	0.52
8:R:67:LEU:HD13	8:R:118:ILE:HB	1.91	0.52
8:S:361:SER:OG	8:S:362:ARG:N	2.41	0.52
8:T:361:SER:OG	8:T:362:ARG:N	2.41	0.52
8:X:53:TYR:HB3	8:X:61:ILE:HB	1.91	0.52
8:P:361:SER:OG	8:P:362:ARG:N	2.40	0.52
8:R:381:HIS:HD1	8:R:383:SER:HG	1.54	0.52
8:T:20:GLU:HG2	8:T:229:ASN:HB3	1.90	0.52
8:X:46:ASP:OD1	8:X:46:ASP:N	2.42	0.52
8:X:67:LEU:HD13	8:X:118:ILE:HB	1.91	0.52
2:e:250:ILE:HG23	2:e:253:GLU:H	1.73	0.52
4:H:427:LEU:HD12	4:H:430:LEU:HD12	1.90	0.52
8:O:46:ASP:OD1	8:O:46:ASP:N	2.42	0.52
8:P:53:TYR:HB3	8:P:61:ILE:HB	1.91	0.52
8:Y:415:LYS:HZ2	8:Y:419:ASP:H	1.58	0.52
8:O:67:LEU:HD13	8:O:118:ILE:HB	1.91	0.52
8:P:184:GLN:O	8:P:188:SER:OG	2.26	0.52
8:S:353:PRO:HA	3:E:862:ASN:ND2	2.24	0.52
8:X:20:GLU:HG2	8:X:229:ASN:HB3	1.90	0.52
8:X:231:LEU:O	8:X:234:THR:OG1	2.24	0.52
4:B:336:TYR:HA	4:B:339:LEU:HD12	1.92	0.52
8:X:52:PHE:HB3	8:X:60:TYR:HB3	1.91	0.52
3:C:217:VAL:HG23	3:C:321:LEU:HD21	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:K:520:HIS:NE2	8:Y:259:SER:O	2.39	0.52
8:P:46:ASP:OD1	8:P:46:ASP:N	2.42	0.52
8:T:52:PHE:HB3	8:T:60:TYR:HB3	1.91	0.52
8:V:361:SER:OG	8:V:362:ARG:N	2.41	0.52
8:Z:67:LEU:HD13	8:Z:118:ILE:HB	1.91	0.52
3:E:546:ILE:HD11	3:E:551:LEU:HD21	1.92	0.52
6:K:651:TYR:HB3	6:K:653:LYS:NZ	2.25	0.52
8:P:67:LEU:HD13	8:P:118:ILE:HB	1.91	0.52
8:R:46:ASP:OD1	8:R:46:ASP:N	2.42	0.52
8:U:67:LEU:HD13	8:U:118:ILE:HB	1.91	0.52
4:D:627:GLU:HB3	4:h:60:LYS:HG2	1.92	0.52
4:H:626:LEU:HG	4:H:637:VAL:HA	1.92	0.52
8:Q:52:PHE:HB3	8:Q:60:TYR:HB3	1.92	0.52
8:Q:415:LYS:HZ2	8:Q:419:ASP:H	1.58	0.52
8:T:53:TYR:HB3	8:T:61:ILE:HB	1.91	0.52
8:W:415:LYS:HZ2	8:W:419:ASP:H	1.58	0.52
8:P:415:LYS:HZ2	8:P:419:ASP:H	1.58	0.52
8:R:52:PHE:HB3	8:R:60:TYR:HB3	1.91	0.52
8:Y:67:LEU:HD13	8:Y:118:ILE:HB	1.91	0.52
8:Y:361:SER:OG	8:Y:362:ARG:N	2.41	0.52
3:C:395:ILE:HD11	3:C:450:ILE:HG23	1.91	0.52
6:I:117:LEU:HD22	6:I:121:HIS:HB2	1.92	0.52
1:J:273:GLU:OE2	1:J:284:LEU:HB3	2.10	0.52
8:P:229:ASN:O	8:P:233:SER:OG	2.22	0.52
8:V:381:HIS:HD1	8:V:383:SER:HG	1.52	0.52
8:Y:46:ASP:N	8:Y:46:ASP:OD1	2.42	0.52
8:Y:53:TYR:HB3	8:Y:61:ILE:HB	1.91	0.52
8:P:52:PHE:HB3	8:P:60:TYR:HB3	1.92	0.51
8:Q:46:ASP:OD1	8:Q:46:ASP:N	2.42	0.51
8:T:46:ASP:N	8:T:46:ASP:OD1	2.42	0.51
8:W:46:ASP:N	8:W:46:ASP:OD1	2.42	0.51
8:Z:46:ASP:OD1	8:Z:46:ASP:N	2.42	0.51
4:H:874:ARG:HH21	4:H:875:PHE:HB2	1.74	0.51
8:O:231:LEU:O	8:O:234:THR:OG1	2.24	0.51
8:R:415:LYS:HZ2	8:R:419:ASP:H	1.59	0.51
8:T:231:LEU:O	8:T:234:THR:OG1	2.24	0.51
8:V:53:TYR:HB3	8:V:61:ILE:HB	1.91	0.51
5:d:24:THR:HA	5:d:27:VAL:HG12	1.92	0.51
3:C:186:ALA:HB1	4:D:293:ARG:HA	1.92	0.51
1:J:320:TYR:HD1	1:J:409:LEU:HD23	1.75	0.51
8:O:317:TYR:HB2	8:O:348:PHE:HE1	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:P:231:LEU:O	8:P:234:THR:OG1	2.24	0.51
8:Q:231:LEU:O	8:Q:234:THR:OG1	2.24	0.51
8:V:67:LEU:HD13	8:V:118:ILE:HB	1.91	0.51
8:V:317:TYR:HB2	8:V:348:PHE:HE1	1.76	0.51
8:Z:53:TYR:HB3	8:Z:61:ILE:HB	1.91	0.51
8:Z:317:TYR:HB2	8:Z:348:PHE:HE1	1.76	0.51
8:Z:361:SER:OG	8:Z:362:ARG:N	2.41	0.51
4:F:694:MET:HG3	4:F:696:GLU:HG2	1.92	0.51
4:H:707:LEU:HD21	4:H:850:LEU:HD22	1.92	0.51
5:g:35:LEU:HD21	4:f:58:ILE:HG23	1.93	0.51
3:G:314:HIS:HB2	3:G:319:LEU:HD12	1.93	0.51
8:O:52:PHE:HB3	8:O:60:TYR:HB3	1.91	0.51
8:X:15:ASN:ND2	8:X:68:ASP:OD1	2.40	0.51
4:D:729:CYS:SG	4:D:730:SER:N	2.83	0.51
6:K:649:LEU:HD22	8:Y:341:ARG:HH22	1.74	0.51
8:O:361:SER:OG	8:O:362:ARG:N	2.40	0.51
8:P:317:TYR:HB2	8:P:348:PHE:HE1	1.76	0.51
8:S:52:PHE:HB3	8:S:60:TYR:HB3	1.92	0.51
8:T:317:TYR:HB2	8:T:348:PHE:HE1	1.76	0.51
8:W:381:HIS:HD1	8:W:383:SER:HG	1.51	0.51
8:S:415:LYS:HZ2	8:S:419:ASP:H	1.59	0.51
8:U:317:TYR:HB2	8:U:348:PHE:HE1	1.76	0.51
8:U:361:SER:OG	8:U:362:ARG:N	2.41	0.51
8:W:53:TYR:HB3	8:W:61:ILE:HB	1.91	0.51
8:W:231:LEU:O	8:W:234:THR:OG1	2.24	0.51
8:W:274:THR:HA	8:W:302:ASN:HD22	1.76	0.51
8:X:415:LYS:HZ2	8:X:419:ASP:H	1.58	0.51
3:A:427:TYR:OH	3:A:462:GLU:OE1	2.29	0.51
8:P:156:ARG:O	8:P:160:ARG:HB2	2.11	0.51
8:R:53:TYR:HB3	8:R:61:ILE:HB	1.91	0.51
8:T:415:LYS:HZ2	8:T:419:ASP:H	1.58	0.51
8:U:156:ARG:O	8:U:160:ARG:HB2	2.11	0.51
8:Y:156:ARG:O	8:Y:160:ARG:HB2	2.11	0.51
8:U:46:ASP:OD1	8:U:46:ASP:N	2.42	0.51
8:U:274:THR:HA	8:U:302:ASN:HD22	1.76	0.51
8:V:46:ASP:OD1	8:V:46:ASP:N	2.42	0.51
8:Z:52:PHE:HB3	8:Z:60:TYR:HB3	1.92	0.51
8:Z:156:ARG:O	8:Z:160:ARG:HB2	2.11	0.51
4:h:93:ILE:HA	4:h:96:LEU:HD12	1.92	0.51
3:C:273:VAL:HG22	3:C:338:LEU:HD22	1.93	0.51
3:G:557:LEU:HD13	8:V:343:ARG:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:P:15:ASN:ND2	8:P:68:ASP:OD1	2.40	0.51
8:S:46:ASP:OD1	8:S:46:ASP:N	2.42	0.51
8:S:274:THR:HA	8:S:302:ASN:HD22	1.76	0.51
8:U:53:TYR:HB3	8:U:61:ILE:HB	1.91	0.51
8:V:52:PHE:HB3	8:V:60:TYR:HB3	1.92	0.51
8:V:274:THR:HA	8:V:302:ASN:HD22	1.76	0.51
8:V:415:LYS:HZ2	8:V:419:ASP:H	1.58	0.51
8:X:274:THR:HA	8:X:302:ASN:HD22	1.76	0.51
8:Y:274:THR:HA	8:Y:302:ASN:HD22	1.76	0.51
8:T:156:ARG:O	8:T:160:ARG:HB2	2.11	0.50
8:V:156:ARG:O	8:V:160:ARG:HB2	2.11	0.50
3:A:290:HIS:ND1	4:B:406:THR:O	2.39	0.50
3:A:862:ASN:ND2	8:O:352:GLY:O	2.39	0.50
4:H:317:PHE:HE2	4:H:321:GLY:HA3	1.75	0.50
8:R:231:LEU:O	8:R:234:THR:OG1	2.24	0.50
8:R:274:THR:HA	8:R:302:ASN:HD22	1.76	0.50
8:R:361:SER:OG	8:R:362:ARG:N	2.41	0.50
8:X:361:SER:OG	8:X:362:ARG:N	2.41	0.50
8:Y:317:TYR:HB2	8:Y:348:PHE:HE1	1.76	0.50
8:Q:274:THR:HA	8:Q:302:ASN:HD22	1.76	0.50
8:W:317:TYR:HB2	8:W:348:PHE:HE1	1.76	0.50
8:Y:15:ASN:ND2	8:Y:68:ASP:OD1	2.40	0.50
3:E:214:GLU:OE2	3:E:321:LEU:N	2.45	0.50
5:b:51:CYS:HA	5:b:55:ILE:HG22	1.93	0.50
4:H:367:LEU:HA	4:H:370:TRP:HD1	1.77	0.50
6:K:630:LEU:HD13	6:K:645:LEU:HD21	1.93	0.50
8:O:415:LYS:HZ2	8:O:419:ASP:H	1.58	0.50
8:P:160:ARG:O	8:P:160:ARG:NH1	2.45	0.50
8:Q:317:TYR:HB2	8:Q:348:PHE:HE1	1.76	0.50
8:S:317:TYR:HB2	8:S:348:PHE:HE1	1.76	0.50
8:W:156:ARG:O	8:W:160:ARG:HB2	2.11	0.50
8:X:317:TYR:HB2	8:X:348:PHE:HE1	1.76	0.50
8:Y:52:PHE:HB3	8:Y:60:TYR:HB3	1.92	0.50
8:Z:274:THR:HA	8:Z:302:ASN:HD22	1.76	0.50
3:C:302:GLU:HA	3:C:305:ILE:HD12	1.93	0.50
4:F:247:GLU:HA	4:F:250:LEU:HD12	1.93	0.50
4:H:597:LEU:HD12	4:H:600:ILE:HD11	1.94	0.50
6:K:510:THR:OG1	6:K:511:ASP:N	2.45	0.50
8:P:274:THR:HA	8:P:302:ASN:HD22	1.76	0.50
8:Q:160:ARG:O	8:Q:160:ARG:NH1	2.45	0.50
8:R:317:TYR:HB2	8:R:348:PHE:HE1	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:S:156:ARG:O	8:S:160:ARG:HB2	2.11	0.50
8:U:415:LYS:HZ2	8:U:419:ASP:H	1.58	0.50
8:X:156:ARG:O	8:X:160:ARG:HB2	2.11	0.50
3:C:265:PRO:HB3	3:C:332:MET:HE2	1.94	0.50
3:C:542:PRO:HA	3:C:611:SER:HA	1.92	0.50
4:F:606:ARG:HE	8:U:339:ARG:NE	2.10	0.50
8:O:160:ARG:NH1	8:O:160:ARG:O	2.45	0.50
8:T:160:ARG:O	8:T:160:ARG:NH1	2.45	0.50
8:Z:160:ARG:O	8:Z:160:ARG:NH1	2.45	0.50
8:Z:415:LYS:HZ2	8:Z:419:ASP:H	1.58	0.50
5:d:28:LEU:HD21	7:c:110:VAL:HG11	1.93	0.50
5:b:42:GLU:O	5:b:45:SER:OG	2.29	0.50
4:H:585:LEU:HD22	4:H:635:TRP:HA	1.92	0.50
8:Q:156:ARG:O	8:Q:160:ARG:HB2	2.11	0.50
8:R:156:ARG:O	8:R:160:ARG:HB2	2.11	0.50
4:D:462:ASP:OD2	4:D:462:ASP:N	2.43	0.50
7:L:1761:ASN:OD1	7:L:1761:ASN:N	2.44	0.50
8:R:160:ARG:O	8:R:160:ARG:NH1	2.45	0.50
3:A:152:GLN:HE22	3:A:241:ARG:HB2	1.76	0.50
8:Q:183:VAL:HG13	8:Q:187:ASN:HD21	1.77	0.50
8:S:160:ARG:O	8:S:160:ARG:NH1	2.45	0.50
8:U:160:ARG:O	8:U:160:ARG:NH1	2.45	0.50
3:E:276:PHE:HD2	3:E:296:MET:HE1	1.76	0.50
8:V:183:VAL:HG13	8:V:187:ASN:HD21	1.77	0.49
8:W:160:ARG:O	8:W:160:ARG:NH1	2.45	0.49
8:W:195:LEU:HB3	8:W:202:VAL:HG21	1.94	0.49
6:I:553:ASP:O	6:I:556:SER:OG	2.30	0.49
1:J:556:LEU:HA	1:J:559:ILE:HD12	1.93	0.49
8:Q:195:LEU:HB3	8:Q:202:VAL:HG21	1.94	0.49
8:T:195:LEU:HB3	8:T:202:VAL:HG21	1.94	0.49
8:Y:183:VAL:HG13	8:Y:187:ASN:HD21	1.77	0.49
8:Z:229:ASN:O	8:Z:233:SER:OG	2.22	0.49
4:F:553:TYR:HB3	4:F:648:ILE:HD11	1.94	0.49
8:S:183:VAL:HG13	8:S:187:ASN:HD21	1.77	0.49
8:T:274:THR:HA	8:T:302:ASN:HD22	1.76	0.49
8:U:113:LYS:HG3	8:U:114:ILE:HG23	1.95	0.49
8:Z:381:HIS:HD1	8:Z:383:SER:HG	1.53	0.49
4:B:319:LEU:HD11	3:C:367:THR:H	1.77	0.49
4:D:651:VAL:HG22	4:D:744:LEU:HD11	1.94	0.49
1:J:487:ASP:OD1	1:J:487:ASP:N	2.44	0.49
8:O:156:ARG:O	8:O:160:ARG:HB2	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:T:183:VAL:HG13	8:T:187:ASN:HD21	1.77	0.49
8:V:113:LYS:HG3	8:V:114:ILE:HG23	1.95	0.49
8:W:183:VAL:HG13	8:W:187:ASN:HD21	1.77	0.49
8:X:183:VAL:HG13	8:X:187:ASN:HD21	1.77	0.49
8:Y:160:ARG:O	8:Y:160:ARG:NH1	2.45	0.49
3:A:224:VAL:HG21	3:A:233:VAL:HG13	1.92	0.49
4:D:490:ILE:HG13	4:D:494:HIS:CE1	2.48	0.49
4:F:433:TRP:HD1	4:F:483:VAL:HG22	1.77	0.49
8:O:183:VAL:HG13	8:O:187:ASN:HD21	1.77	0.49
8:O:274:THR:HA	8:O:302:ASN:HD22	1.76	0.49
8:P:79:ASN:OD1	8:P:79:ASN:N	2.46	0.49
8:S:56:ASP:HA	8:T:296:ARG:HH21	1.78	0.49
8:T:113:LYS:HG3	8:T:114:ILE:HG23	1.95	0.49
8:W:79:ASN:OD1	8:W:79:ASN:N	2.46	0.49
4:B:886:TYR:HE2	8:P:353:PRO:HG3	1.76	0.49
4:F:660:TYR:HA	4:F:663:VAL:HG12	1.94	0.49
6:I:260:ARG:HG2	6:I:262:GLU:H	1.77	0.49
8:S:188:SER:O	8:S:192:LEU:HB2	2.13	0.49
8:U:79:ASN:OD1	8:U:79:ASN:N	2.46	0.49
8:W:113:LYS:HG3	8:W:114:ILE:HG23	1.95	0.49
8:X:160:ARG:O	8:X:160:ARG:NH1	2.45	0.49
8:X:188:SER:O	8:X:192:LEU:HB2	2.13	0.49
4:a:51:GLU:HA	4:a:54:VAL:HG22	1.95	0.49
3:A:307:VAL:HA	3:A:310:LEU:HD12	1.95	0.49
4:H:308:THR:O	4:H:312:SER:OG	2.26	0.49
6:K:254:LEU:HD23	6:K:285:MET:HE3	1.95	0.49
8:P:183:VAL:HG13	8:P:187:ASN:HD21	1.77	0.49
8:R:183:VAL:HG13	8:R:187:ASN:HD21	1.77	0.49
8:V:160:ARG:O	8:V:160:ARG:NH1	2.45	0.49
8:Z:79:ASN:OD1	8:Z:79:ASN:N	2.46	0.49
8:Z:188:SER:O	8:Z:192:LEU:HB2	2.13	0.49
1:l:15:GLN:HA	5:m:53:GLN:HE22	1.78	0.49
8:O:188:SER:O	8:O:192:LEU:HB2	2.13	0.49
8:U:195:LEU:HB3	8:U:202:VAL:HG21	1.94	0.49
8:Y:195:LEU:HB3	8:Y:202:VAL:HG21	1.94	0.49
2:e:133:TYR:OH	2:e:355:MET:SD	2.63	0.49
4:D:688:ALA:HB1	4:D:692:ARG:NH1	2.28	0.49
4:F:412:ARG:O	4:F:416:GLN:HB2	2.12	0.49
1:J:221:VAL:HG22	6:K:35:HIS:CE1	2.48	0.49
8:O:195:LEU:HB3	8:O:202:VAL:HG21	1.94	0.49
8:P:188:SER:O	8:P:192:LEU:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:R:79:ASN:OD1	8:R:79:ASN:N	2.46	0.49
8:R:188:SER:O	8:R:192:LEU:HB2	2.13	0.49
8:T:15:ASN:ND2	8:T:68:ASP:OD1	2.40	0.49
8:U:183:VAL:HG13	8:U:187:ASN:HD21	1.77	0.49
8:W:188:SER:O	8:W:192:LEU:HB2	2.13	0.49
8:X:113:LYS:HG3	8:X:114:ILE:HG23	1.95	0.49
8:Z:183:VAL:HG13	8:Z:187:ASN:HD21	1.77	0.49
4:B:330:GLN:HB2	3:C:333:ARG:HH12	1.78	0.49
4:F:712:VAL:O	4:F:716:HIS:HB2	2.12	0.49
1:J:886:LEU:HD21	1:J:984:GLU:HB3	1.95	0.49
8:S:7:THR:OG1	8:S:63:ARG:O	2.28	0.49
8:V:231:LEU:O	8:V:234:THR:OG1	2.24	0.49
8:Z:15:ASN:ND2	8:Z:68:ASP:OD1	2.40	0.49
8:Z:113:LYS:HG3	8:Z:114:ILE:HG23	1.95	0.49
8:Z:195:LEU:HB3	8:Z:202:VAL:HG21	1.94	0.49
1:l:118:SER:OG	4:H:629:SER:O	2.30	0.48
2:e:208:ILE:HG21	2:e:242:LEU:HD11	1.95	0.48
5:b:23:GLU:HG3	4:a:84:GLN:HG2	1.94	0.48
6:K:627:PHE:CE1	6:K:645:LEU:HB3	2.48	0.48
8:P:113:LYS:HG3	8:P:114:ILE:HG23	1.95	0.48
8:S:195:LEU:HB3	8:S:202:VAL:HG21	1.94	0.48
8:U:188:SER:O	8:U:192:LEU:HB2	2.13	0.48
3:C:653:ARG:NH1	3:C:656:CYS:SG	2.86	0.48
6:I:531:TYR:CD1	8:W:249:MET:HE1	2.49	0.48
8:P:381:HIS:HD1	8:P:383:SER:HG	1.54	0.48
8:Q:113:LYS:HG3	8:Q:114:ILE:HG23	1.95	0.48
8:R:195:LEU:HB3	8:R:202:VAL:HG21	1.94	0.48
8:S:113:LYS:HG3	8:S:114:ILE:HG23	1.95	0.48
8:T:17:ILE:HD13	8:T:232:VAL:HB	1.95	0.48
8:T:188:SER:O	8:T:192:LEU:HB2	2.13	0.48
7:L:1571:ASN:HB3	7:L:1599:LYS:HG2	1.95	0.48
8:P:195:LEU:HB3	8:P:202:VAL:HG21	1.95	0.48
8:S:17:ILE:HD13	8:S:232:VAL:HB	1.95	0.48
8:S:341:ARG:HD2	3:E:857:SER:HB2	1.95	0.48
8:T:237:SER:O	8:T:244:ARG:NH2	2.44	0.48
8:V:195:LEU:HB3	8:V:202:VAL:HG21	1.94	0.48
8:V:329:ASP:HB3	8:V:332:GLN:HB2	1.96	0.48
8:X:123:ASP:OD1	8:X:161:TYR:OH	2.32	0.48
4:a:48:GLU:HB2	4:a:122:LEU:HB3	1.95	0.48
2:e:54:VAL:HG11	2:e:85:ILE:HG13	1.94	0.48
4:F:364:LEU:HB2	4:F:367:LEU:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:P:17:ILE:HD13	8:P:232:VAL:HB	1.95	0.48
8:Q:123:ASP:OD1	8:Q:161:TYR:OH	2.32	0.48
8:R:17:ILE:HD13	8:R:232:VAL:HB	1.95	0.48
8:U:56:ASP:HA	8:V:296:ARG:HH21	1.78	0.48
8:V:188:SER:O	8:V:192:LEU:HB2	2.13	0.48
3:G:557:LEU:HD22	8:V:343:ARG:HD3	1.94	0.48
4:H:655:GLU:O	4:H:658:SER:OG	2.31	0.48
8:Q:329:ASP:HB3	8:Q:332:GLN:HB2	1.96	0.48
8:X:229:ASN:O	8:X:233:SER:OG	2.22	0.48
8:Y:381:HIS:CG	8:Y:383:SER:HG	2.31	0.48
8:Z:329:ASP:HB3	8:Z:332:GLN:HB2	1.96	0.48
4:B:795:ALA:O	4:B:799:GLU:HB2	2.13	0.48
3:G:188:ILE:HG22	3:G:278:GLU:HG3	1.94	0.48
6:I:370:GLN:HE22	8:W:3:ARG:HH11	1.60	0.48
7:L:1797:ASP:HB2	8:Z:334:HIS:CE1	2.48	0.48
8:R:329:ASP:HB3	8:R:332:GLN:HB2	1.96	0.48
8:T:329:ASP:HB3	8:T:332:GLN:HB2	1.96	0.48
8:X:17:ILE:HD13	8:X:232:VAL:HB	1.95	0.48
8:X:197:GLN:HA	8:X:265:ARG:HH22	1.79	0.48
8:Y:113:LYS:HG3	8:Y:114:ILE:HG23	1.95	0.48
8:Y:329:ASP:HB3	8:Y:332:GLN:HB2	1.96	0.48
3:E:435:VAL:HG12	3:E:437:GLN:H	1.79	0.48
1:l:24:ARG:NH1	1:l:32:GLU:OE2	2.44	0.48
2:e:242:LEU:HD23	2:e:243:PRO:CD	2.44	0.48
4:B:794:ARG:HH11	4:B:798:GLU:HG2	1.78	0.48
4:D:436:ASP:HB2	4:D:490:ILE:HG23	1.96	0.48
4:H:555:LEU:HD11	4:H:651:VAL:HG21	1.96	0.48
8:O:7:THR:OG1	8:O:63:ARG:O	2.28	0.48
8:Q:197:GLN:HA	8:Q:265:ARG:HH22	1.79	0.48
8:R:123:ASP:OD1	8:R:161:TYR:OH	2.32	0.48
8:V:17:ILE:HD13	8:V:232:VAL:HB	1.95	0.48
8:X:195:LEU:HB3	8:X:202:VAL:HG21	1.94	0.48
8:X:329:ASP:HB3	8:X:332:GLN:HB2	1.96	0.48
8:Y:188:SER:O	8:Y:192:LEU:HB2	2.13	0.48
8:Y:197:GLN:HA	8:Y:265:ARG:HH22	1.79	0.48
2:e:18:LYS:HG3	2:e:30:VAL:HG22	1.94	0.48
2:e:237:GLU:HG2	2:e:251:GLY:H	1.78	0.48
3:C:862:ASN:HA	8:Q:344:LYS:HZ3	1.79	0.48
8:O:197:GLN:HA	8:O:265:ARG:HH22	1.79	0.48
8:Q:17:ILE:HD13	8:Q:232:VAL:HB	1.95	0.48
8:W:197:GLN:HA	8:W:265:ARG:HH22	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:279:VAL:HG13	6:I:336:VAL:HG11	1.96	0.48
8:T:197:GLN:HA	8:T:265:ARG:HH22	1.79	0.48
8:O:15:ASN:ND2	8:O:68:ASP:OD1	2.40	0.48
8:O:17:ILE:HD13	8:O:232:VAL:HB	1.95	0.48
8:S:123:ASP:OD1	8:S:161:TYR:OH	2.32	0.48
8:U:232:VAL:HA	8:U:235:ILE:HD12	1.96	0.48
8:X:141:ILE:HG12	8:X:170:SER:HB2	1.96	0.48
4:B:253:ASP:HB3	4:B:266:ILE:HG22	1.96	0.47
5:g:50:LEU:HD13	5:g:60:LEU:HD21	1.96	0.47
8:O:113:LYS:HG3	8:O:114:ILE:HG23	1.95	0.47
8:O:318:ILE:HB	8:O:380:ASN:HB3	1.96	0.47
8:P:197:GLN:HA	8:P:265:ARG:HH22	1.79	0.47
8:R:318:ILE:HB	8:R:380:ASN:HB3	1.96	0.47
8:S:232:VAL:HA	8:S:235:ILE:HD12	1.96	0.47
8:S:329:ASP:HB3	8:S:332:GLN:HB2	1.96	0.47
8:T:7:THR:OG1	8:T:63:ARG:O	2.28	0.47
8:T:123:ASP:OD1	8:T:161:TYR:OH	2.32	0.47
8:U:318:ILE:HB	8:U:380:ASN:HB3	1.96	0.47
8:V:197:GLN:HA	8:V:265:ARG:HH22	1.79	0.47
8:W:237:SER:O	8:W:244:ARG:NH2	2.43	0.47
8:W:329:ASP:HB3	8:W:332:GLN:HB2	1.96	0.47
4:F:575:ARG:NH1	8:T:252:ASP:OD1	2.48	0.47
1:J:334:VAL:HG21	1:J:365:MET:HG2	1.95	0.47
6:K:107:LEU:HD11	6:K:126:LEU:HD21	1.95	0.47
8:R:66:LEU:HD22	8:R:91:ILE:HG23	1.96	0.47
8:S:197:GLN:HA	8:S:265:ARG:HH22	1.79	0.47
8:S:318:ILE:HB	8:S:380:ASN:HB3	1.96	0.47
8:Y:17:ILE:HD13	8:Y:232:VAL:HB	1.95	0.47
8:Z:7:THR:OG1	8:Z:63:ARG:O	2.28	0.47
8:Z:66:LEU:HD22	8:Z:91:ILE:HG23	1.96	0.47
2:e:79:TRP:NE1	2:e:122:ILE:HG13	2.21	0.47
4:B:327:ALA:HB2	4:B:421:LEU:HD12	1.96	0.47
3:C:291:ALA:HA	3:C:294:ALA:HB3	1.96	0.47
8:O:123:ASP:OD1	8:O:161:TYR:OH	2.32	0.47
8:R:113:LYS:HG3	8:R:114:ILE:HG23	1.95	0.47
8:U:197:GLN:HA	8:U:265:ARG:HH22	1.79	0.47
8:W:141:ILE:HG12	8:W:170:SER:HB2	1.96	0.47
8:Y:123:ASP:OD1	8:Y:161:TYR:OH	2.32	0.47
8:Z:17:ILE:HD13	8:Z:232:VAL:HB	1.95	0.47
8:T:66:LEU:HD22	8:T:91:ILE:HG23	1.96	0.47
8:W:15:ASN:ND2	8:W:68:ASP:OD1	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:W:232:VAL:HA	8:W:235:ILE:HD12	1.96	0.47
8:X:66:LEU:HD22	8:X:91:ILE:HG23	1.96	0.47
8:Y:66:LEU:HD22	8:Y:91:ILE:HG23	1.96	0.47
8:Y:232:VAL:HA	8:Y:235:ILE:HD12	1.96	0.47
3:A:533:ASP:CB	8:O:3:ARG:HH12	2.26	0.47
4:B:885:HIS:CD2	4:B:893:LEU:HB2	2.50	0.47
6:I:515:TRP:CD1	6:I:516:ARG:H	2.31	0.47
6:K:649:LEU:HG	6:K:654:TYR:C	2.39	0.47
8:Q:188:SER:O	8:Q:192:LEU:HB2	2.13	0.47
8:T:232:VAL:HA	8:T:235:ILE:HD12	1.96	0.47
8:U:123:ASP:OD1	8:U:161:TYR:OH	2.32	0.47
8:Z:141:ILE:HG12	8:Z:170:SER:HB2	1.97	0.47
8:Z:232:VAL:HA	8:Z:235:ILE:HD12	1.96	0.47
4:B:674:GLU:O	4:B:678:THR:OG1	2.27	0.47
1:J:707:MET:HE2	1:J:921:LYS:HA	1.97	0.47
6:K:80:GLY:HA3	6:K:147:LYS:HA	1.97	0.47
8:O:329:ASP:HB3	8:O:332:GLN:HB2	1.96	0.47
8:P:232:VAL:HA	8:P:235:ILE:HD12	1.96	0.47
8:W:17:ILE:HD13	8:W:232:VAL:HB	1.95	0.47
8:W:66:LEU:HD22	8:W:91:ILE:HG23	1.96	0.47
4:D:656:CYS:SG	4:D:657:MET:N	2.87	0.47
4:D:711:MET:HG2	4:D:854:TYR:CZ	2.50	0.47
5:b:59:ALA:O	5:b:62:SER:OG	2.31	0.47
4:F:665:ASN:HB3	4:j:66:ARG:HH11	1.79	0.47
6:I:545:LEU:HD12	6:I:548:ILE:HD11	1.97	0.47
6:K:141:GLU:OE2	6:K:144:LYS:NZ	2.46	0.47
6:K:496:TRP:HZ2	8:Y:261:ILE:HB	1.79	0.47
8:O:66:LEU:HD22	8:O:91:ILE:HG23	1.96	0.47
8:O:141:ILE:HG12	8:O:170:SER:HB2	1.97	0.47
8:O:229:ASN:O	8:O:233:SER:OG	2.22	0.47
8:P:123:ASP:OD1	8:P:161:TYR:OH	2.32	0.47
8:R:15:ASN:ND2	8:R:68:ASP:OD1	2.40	0.47
8:R:232:VAL:HA	8:R:235:ILE:HD12	1.96	0.47
8:S:248:TYR:HE1	3:E:522:MET:HB3	1.80	0.47
8:T:318:ILE:HB	8:T:380:ASN:HB3	1.96	0.47
8:U:141:ILE:HG12	8:U:170:SER:HB2	1.96	0.47
8:X:237:SER:O	8:X:244:ARG:NH2	2.44	0.47
8:Y:237:SER:O	8:Y:244:ARG:NH2	2.43	0.47
3:A:737:CYS:HB2	3:A:739:LEU:HD23	1.96	0.47
4:B:874:ARG:O	4:B:877:SER:OG	2.33	0.47
3:C:282:SER:OG	3:C:284:GLU:OE1	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:293:LYS:HA	7:L:295:ARG:HH11	1.80	0.47
8:Q:66:LEU:HD22	8:Q:91:ILE:HG23	1.96	0.47
8:S:15:ASN:ND2	8:S:68:ASP:OD1	2.40	0.47
8:Z:197:GLN:HA	8:Z:265:ARG:HH22	1.79	0.47
3:A:310:LEU:HD13	3:A:324:LEU:HD13	1.96	0.47
4:D:677:LEU:HD21	4:D:782:ILE:HD12	1.97	0.47
1:J:223:GLN:HB2	1:J:230:SER:HB2	1.96	0.47
8:Q:318:ILE:HB	8:Q:380:ASN:HB3	1.96	0.47
8:S:66:LEU:HD22	8:S:91:ILE:HG23	1.96	0.47
8:U:329:ASP:HB3	8:U:332:GLN:HB2	1.96	0.47
8:V:66:LEU:HD22	8:V:91:ILE:HG23	1.96	0.47
4:D:401:HIS:HA	4:D:404:THR:HG23	1.97	0.47
8:U:66:LEU:HD22	8:U:91:ILE:HG23	1.96	0.47
8:V:232:VAL:HA	8:V:235:ILE:HD12	1.96	0.47
4:a:113:SER:OG	4:a:114:TYR:N	2.45	0.47
4:j:24:SER:OG	4:j:25:GLU:N	2.48	0.47
3:E:581:ASP:OD2	3:E:647:TYR:OH	2.33	0.47
3:C:242:GLN:O	3:C:275:ARG:NH1	2.48	0.46
4:F:575:ARG:NH2	8:T:249:MET:HA	2.29	0.46
5:g:65:LYS:HE2	4:f:100:LEU:HD13	1.97	0.46
8:R:229:ASN:O	8:R:233:SER:OG	2.22	0.46
8:V:7:THR:OG1	8:V:63:ARG:O	2.28	0.46
8:Z:322:ASN:ND2	8:Z:357:GLN:O	2.49	0.46
4:D:885:HIS:CE1	4:D:890:GLU:HA	2.50	0.46
4:H:312:SER:HB3	6:I:165:LEU:HD11	1.97	0.46
8:Q:232:VAL:HA	8:Q:235:ILE:HD12	1.96	0.46
3:C:713:LEU:HD22	3:C:722:VAL:HG13	1.96	0.46
1:J:953:ALA:HA	1:J:956:LYS:HG2	1.97	0.46
8:P:318:ILE:HB	8:P:380:ASN:HB3	1.96	0.46
8:Q:381:HIS:HD1	8:Q:383:SER:HG	1.57	0.46
8:R:7:THR:OG1	8:R:63:ARG:O	2.28	0.46
8:T:141:ILE:HG12	8:T:170:SER:HB2	1.96	0.46
8:W:7:THR:OG1	8:W:63:ARG:O	2.28	0.46
8:X:232:VAL:HA	8:X:235:ILE:HD12	1.96	0.46
4:a:79:ARG:O	4:a:83:SER:OG	2.31	0.46
4:B:284:SER:HB2	4:B:288:ARG:HE	1.80	0.46
4:B:308:THR:O	4:B:312:SER:OG	2.23	0.46
4:D:308:THR:O	4:D:312:SER:OG	2.24	0.46
8:P:141:ILE:HG12	8:P:170:SER:HB2	1.96	0.46
8:U:17:ILE:HD13	8:U:232:VAL:HB	1.95	0.46
8:U:322:ASN:ND2	8:U:357:GLN:O	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:123:ASP:OD1	8:V:161:TYR:OH	2.32	0.46
8:V:322:ASN:ND2	8:V:357:GLN:O	2.49	0.46
8:X:322:ASN:ND2	8:X:357:GLN:O	2.49	0.46
3:A:287:GLN:N	3:A:406:GLU:OE2	2.49	0.46
6:K:3:HIS:HB2	7:L:320:PHE:CZ	2.51	0.46
7:L:354:LYS:HA	7:L:357:LEU:HD12	1.98	0.46
8:R:197:GLN:HA	8:R:265:ARG:HH22	1.79	0.46
8:Z:123:ASP:OD1	8:Z:161:TYR:OH	2.32	0.46
8:Z:318:ILE:HB	8:Z:380:ASN:HB3	1.96	0.46
3:G:581:ASP:OD1	3:G:643:ARG:NH2	2.48	0.46
6:K:627:PHE:HE1	6:K:645:LEU:HB3	1.81	0.46
8:P:66:LEU:HD22	8:P:91:ILE:HG23	1.96	0.46
8:P:329:ASP:HB3	8:P:332:GLN:HB2	1.96	0.46
8:Q:141:ILE:HG12	8:Q:170:SER:HB2	1.96	0.46
8:R:322:ASN:ND2	8:R:357:GLN:O	2.49	0.46
8:S:141:ILE:HG12	8:S:170:SER:HB2	1.96	0.46
8:V:237:SER:O	8:V:244:ARG:NH2	2.43	0.46
3:A:283:PHE:HA	3:A:290:HIS:CE1	2.51	0.46
3:G:457:LEU:HD21	3:G:467:VAL:HG23	1.97	0.46
4:H:648:ILE:HD12	4:H:652:PHE:HE2	1.79	0.46
8:W:318:ILE:HB	8:W:380:ASN:HB3	1.96	0.46
8:Y:141:ILE:HG12	8:Y:170:SER:HB2	1.96	0.46
8:Y:322:ASN:ND2	8:Y:357:GLN:O	2.49	0.46
6:K:496:TRP:HB2	6:K:519:ASN:ND2	2.31	0.46
8:V:141:ILE:HG12	8:V:170:SER:HB2	1.97	0.46
3:E:517:LYS:HD2	3:E:523:ASP:HB2	1.97	0.46
8:P:322:ASN:ND2	8:P:357:GLN:O	2.49	0.46
8:R:141:ILE:HG12	8:R:170:SER:HB2	1.96	0.46
8:T:154:LEU:HD23	8:T:194:ARG:HB3	1.98	0.46
8:U:15:ASN:ND2	8:U:68:ASP:OD1	2.40	0.46
4:D:785:LEU:HD23	4:D:789:GLN:HB2	1.97	0.46
7:L:1656:ARG:NH2	8:Z:443:TYR:OH	2.49	0.46
8:Q:154:LEU:HD23	8:Q:194:ARG:HB3	1.98	0.46
8:V:79:ASN:OD1	8:V:79:ASN:N	2.46	0.46
8:X:318:ILE:HB	8:X:380:ASN:HB3	1.96	0.46
8:Y:318:ILE:HB	8:Y:380:ASN:HB3	1.96	0.46
8:Z:154:LEU:HD23	8:Z:194:ARG:HB3	1.98	0.46
3:A:734:LEU:HD13	3:A:740:THR:HG21	1.97	0.45
3:C:819:GLU:HA	3:C:822:ILE:HD12	1.97	0.45
4:D:493:LEU:O	4:D:497:CYS:HB3	2.17	0.45
4:D:662:ARG:HA	4:h:66:ARG:HH11	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:712:LYS:HA	1:J:715:ARG:HE	1.80	0.45
8:T:50:VAL:HG21	8:T:244:ARG:HG2	1.99	0.45
8:W:123:ASP:OD1	8:W:161:TYR:OH	2.32	0.45
2:e:50:LYS:HB3	2:e:51:ASP:H	1.57	0.45
5:b:46:ILE:HD13	5:b:49:ARG:HH21	1.80	0.45
6:K:87:ARG:O	6:K:91:THR:HG23	2.16	0.45
6:K:611:GLN:O	6:K:615:LEU:HG	2.16	0.45
8:O:232:VAL:HA	8:O:235:ILE:HD12	1.96	0.45
8:O:381:HIS:CG	8:O:383:SER:HG	2.33	0.45
8:Q:322:ASN:ND2	8:Q:357:GLN:O	2.49	0.45
8:Y:50:VAL:HG21	8:Y:244:ARG:HG2	1.98	0.45
3:E:277:ILE:HG12	3:E:296:MET:HE3	1.98	0.45
7:L:1728:VAL:O	7:L:1731:SER:OG	2.33	0.45
8:O:322:ASN:ND2	8:O:357:GLN:O	2.49	0.45
8:R:237:SER:O	8:R:244:ARG:NH2	2.43	0.45
8:V:318:ILE:HB	8:V:380:ASN:HB3	1.96	0.45
8:W:154:LEU:HD23	8:W:194:ARG:HB3	1.98	0.45
8:W:322:ASN:ND2	8:W:357:GLN:O	2.49	0.45
4:B:587:ARG:HD3	4:B:591:THR:OG1	2.16	0.45
4:D:490:ILE:HG13	4:D:494:HIS:HE1	1.82	0.45
8:P:50:VAL:HG21	8:P:244:ARG:HG2	1.98	0.45
8:Q:56:ASP:HA	8:R:296:ARG:HH21	1.82	0.45
8:Q:237:SER:O	8:Q:244:ARG:NH2	2.44	0.45
8:S:322:ASN:ND2	8:S:357:GLN:O	2.49	0.45
4:F:268:MET:HB2	4:F:276:LYS:H	1.81	0.45
1:J:331:ILE:HG23	1:J:365:MET:HE2	1.98	0.45
1:J:895:ASN:OD1	8:X:357:GLN:NE2	2.49	0.45
6:K:646:LEU:HD22	8:Y:341:ARG:NH1	2.32	0.45
8:P:154:LEU:HD23	8:P:194:ARG:HB3	1.98	0.45
8:R:50:VAL:HG21	8:R:244:ARG:HG2	1.98	0.45
8:R:108:PHE:CD1	8:R:152:TYR:HB2	2.52	0.45
8:U:105:ALA:O	8:U:109:SER:OG	2.34	0.45
8:V:154:LEU:HD23	8:V:194:ARG:HB3	1.98	0.45
8:W:105:ALA:O	8:W:109:SER:OG	2.34	0.45
4:F:581:LEU:HG	4:F:585:LEU:HG	1.97	0.45
8:O:50:VAL:HG21	8:O:244:ARG:HG2	1.98	0.45
8:O:154:LEU:HD23	8:O:194:ARG:HB3	1.98	0.45
8:Q:108:PHE:CD1	8:Q:152:TYR:HB2	2.52	0.45
8:R:154:LEU:HD23	8:R:194:ARG:HB3	1.98	0.45
8:S:108:PHE:CD1	8:S:152:TYR:HB2	2.52	0.45
8:T:322:ASN:ND2	8:T:357:GLN:O	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:U:154:LEU:HD23	8:U:194:ARG:HB3	1.98	0.45
8:V:50:VAL:HG21	8:V:244:ARG:HG2	1.98	0.45
2:e:152:VAL:HG13	2:e:163:VAL:HB	1.99	0.45
8:T:381:HIS:CG	8:T:383:SER:HG	2.33	0.45
8:U:50:VAL:HG21	8:U:244:ARG:HG2	1.99	0.45
8:Z:193:LYS:O	8:Z:196:THR:OG1	2.32	0.45
1:J:265:VAL:HB	1:J:300:ILE:HD11	1.98	0.45
5:i:63:VAL:O	5:i:67:LEU:HG	2.17	0.45
8:Q:50:VAL:HG21	8:Q:244:ARG:HG2	1.99	0.45
8:U:108:PHE:CD1	8:U:152:TYR:HB2	2.52	0.45
8:X:108:PHE:CD1	8:X:152:TYR:HB2	2.52	0.45
8:X:154:LEU:HD23	8:X:194:ARG:HB3	1.98	0.45
8:Z:50:VAL:HG21	8:Z:244:ARG:HG2	1.98	0.45
8:P:7:THR:OG1	8:P:63:ARG:O	2.28	0.45
8:W:50:VAL:HG21	8:W:244:ARG:HG2	1.98	0.45
8:Y:7:THR:OG1	8:Y:63:ARG:O	2.28	0.45
8:Y:108:PHE:CD1	8:Y:152:TYR:HB2	2.52	0.45
4:B:419:LEU:HA	4:B:422:VAL:HG22	1.99	0.45
3:G:526:ASP:HA	3:G:529:VAL:HG12	1.99	0.45
8:P:108:PHE:CD1	8:P:152:TYR:HB2	2.52	0.45
8:Q:229:ASN:O	8:Q:233:SER:OG	2.22	0.45
8:W:104:TRP:O	8:W:108:PHE:HB2	2.17	0.45
6:K:653:LYS:HD2	6:K:653:LYS:N	2.33	0.44
8:Q:105:ALA:O	8:Q:109:SER:OG	2.34	0.44
8:S:104:TRP:O	8:S:108:PHE:HB2	2.17	0.44
8:T:108:PHE:CD1	8:T:152:TYR:HB2	2.52	0.44
8:Y:154:LEU:HD23	8:Y:194:ARG:HB3	1.98	0.44
3:E:258:GLU:HA	3:E:261:HIS:CD2	2.52	0.44
1:l:109:SER:HA	5:m:57:PRO:HG3	2.00	0.44
4:D:833:ILE:HA	4:D:836:PHE:HD2	1.81	0.44
4:F:364:LEU:H	4:F:367:LEU:H	1.66	0.44
1:J:271:ILE:HD13	1:J:393:ILE:HG22	1.99	0.44
8:S:154:LEU:HD23	8:S:194:ARG:HB3	1.98	0.44
8:V:108:PHE:CD1	8:V:152:TYR:HB2	2.52	0.44
8:W:108:PHE:CD1	8:W:152:TYR:HB2	2.52	0.44
2:e:139:VAL:HG22	2:e:165:ILE:HD12	2.00	0.44
4:B:658:SER:HA	4:B:661:LEU:HD12	1.98	0.44
3:C:840:LEU:HB3	3:C:856:ILE:HD11	1.98	0.44
4:F:572:ASP:OD1	4:F:572:ASP:N	2.50	0.44
6:K:639:ASN:OD1	6:K:640:SER:N	2.51	0.44
6:K:643:ALA:HA	6:K:646:LEU:HD12	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:O:104:TRP:O	8:O:108:PHE:HB2	2.18	0.44
8:P:104:TRP:O	8:P:108:PHE:HB2	2.17	0.44
8:S:381:HIS:CE1	8:S:383:SER:HG	2.32	0.44
8:X:77:ILE:O	8:X:80:SER:OG	2.31	0.44
5:k:58:GLU:HG2	4:j:95:TYR:CE2	2.53	0.44
5:d:67:LEU:HD11	7:c:12:CYS:HA	2.00	0.44
3:E:285:TYR:HB3	3:E:289:ASN:HD22	1.82	0.44
3:E:504:MET:HE1	3:E:509:LEU:HB3	2.00	0.44
1:l:108:TYR:HA	1:l:111:LEU:HD12	1.99	0.44
2:e:38:PRO:HA	2:e:65:LEU:HA	2.00	0.44
4:B:686:CYS:HA	4:B:689:LYS:HZ3	1.82	0.44
4:F:666:PHE:HA	4:F:669:ARG:HE	1.82	0.44
1:J:806:PRO:O	1:J:810:ASP:N	2.50	0.44
1:J:892:HIS:HB2	8:X:353:PRO:O	2.18	0.44
8:V:77:ILE:O	8:V:80:SER:OG	2.31	0.44
8:Z:108:PHE:CD1	8:Z:152:TYR:HB2	2.52	0.44
8:V:45:THR:OG1	8:V:46:ASP:N	2.50	0.44
3:A:427:TYR:H	3:A:624:TRP:HZ3	1.65	0.44
4:F:269:ASN:O	4:F:270:ASN:ND2	2.51	0.44
4:H:730:SER:HB3	4:H:754:PHE:HE1	1.82	0.44
8:S:45:THR:OG1	8:S:46:ASP:N	2.50	0.44
8:V:104:TRP:O	8:V:108:PHE:HB2	2.17	0.44
8:W:56:ASP:OD2	8:X:296:ARG:NE	2.51	0.44
8:X:50:VAL:HG21	8:X:244:ARG:HG2	1.99	0.44
6:I:20:ASN:H	6:I:24:GLY:HA3	1.82	0.44
8:Q:104:TRP:O	8:Q:108:PHE:HB2	2.17	0.44
4:j:50:ASP:OD1	4:j:50:ASP:N	2.50	0.44
3:E:517:LYS:O	3:E:522:MET:N	2.51	0.44
3:G:574:LYS:HB2	3:G:619:ASP:HB3	1.99	0.44
4:a:24:SER:OG	4:a:25:GLU:N	2.51	0.44
5:d:57:PRO:HA	5:d:60:LEU:HD12	2.00	0.44
3:A:659:TRP:CZ2	8:O:261:ILE:HG21	2.53	0.44
4:B:257:VAL:HG21	4:B:266:ILE:HD13	1.99	0.44
4:D:720:TYR:CE1	8:R:249:MET:HE1	2.53	0.44
4:F:433:TRP:CD1	4:F:483:VAL:HG22	2.53	0.44
4:H:275:TYR:CD2	4:H:295:SER:HB2	2.52	0.44
4:H:535:ASP:OD1	4:H:535:ASP:N	2.50	0.44
1:J:212:ASP:OD1	1:J:212:ASP:N	2.51	0.44
6:K:68:GLN:NE2	6:K:84:ILE:HB	2.32	0.44
6:K:192:LEU:HD21	6:K:307:PHE:HB2	2.00	0.44
8:R:104:TRP:O	8:R:108:PHE:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:S:237:SER:O	8:S:244:ARG:NH2	2.43	0.44
4:D:367:LEU:HD23	7:c:182:MET:HE2	2.00	0.43
8:O:45:THR:OG1	8:O:46:ASP:N	2.50	0.43
8:O:77:ILE:O	8:O:80:SER:OG	2.31	0.43
8:O:108:PHE:CD1	8:O:152:TYR:HB2	2.52	0.43
8:O:381:HIS:HD1	8:O:383:SER:HG	1.59	0.43
8:U:104:TRP:O	8:U:108:PHE:HB2	2.17	0.43
3:C:696:TYR:CE1	3:C:854:SER:HB2	2.51	0.43
4:F:285:ARG:NH1	3:E:220:ASP:OD1	2.51	0.43
3:G:865:TYR:H	3:G:868:ARG:NH1	2.16	0.43
4:H:456:THR:OG1	4:H:457:ASP:N	2.50	0.43
6:K:459:VAL:HG21	6:K:467:PHE:HB2	1.99	0.43
8:P:77:ILE:O	8:P:80:SER:OG	2.31	0.43
8:U:77:ILE:O	8:U:80:SER:OG	2.31	0.43
8:X:104:TRP:O	8:X:108:PHE:HB2	2.17	0.43
6:I:121:HIS:HA	6:I:124:TYR:CE1	2.52	0.43
7:L:1657:GLN:HA	7:L:1660:LEU:HG	2.01	0.43
8:O:297:LEU:HD21	8:O:377:MET:HB3	2.01	0.43
8:S:39:GLU:CD	8:S:39:GLU:H	2.27	0.43
8:Y:297:LEU:HD21	8:Y:377:MET:HB3	2.01	0.43
5:d:24:THR:O	5:d:28:LEU:HB2	2.18	0.43
3:A:351:LEU:HG	3:A:438:GLN:HE22	1.83	0.43
3:G:644:HIS:HE1	3:G:697:MET:HE1	1.83	0.43
6:K:300:LEU:HB3	6:K:301:LYS:H	1.67	0.43
8:O:39:GLU:H	8:O:39:GLU:CD	2.27	0.43
8:R:297:LEU:HD21	8:R:377:MET:HB3	2.01	0.43
8:S:425:ARG:HA	8:S:428:VAL:HG12	2.01	0.43
8:T:104:TRP:O	8:T:108:PHE:HB2	2.17	0.43
8:W:39:GLU:H	8:W:39:GLU:CD	2.26	0.43
8:Z:105:ALA:O	8:Z:109:SER:OG	2.34	0.43
3:A:183:GLU:HG2	3:A:184:ARG:HD2	2.01	0.43
4:B:304:ILE:HD12	4:B:381:LEU:HB3	2.01	0.43
3:C:294:ALA:HA	3:C:297:ARG:HE	1.84	0.43
4:F:878:PHE:HE2	8:T:338:GLN:HE22	1.66	0.43
6:I:190:TRP:CE2	6:I:280:GLY:HA3	2.53	0.43
1:J:904:ARG:HH11	1:J:1012:SER:HB3	1.84	0.43
6:K:44:ARG:NE	6:K:123:ASN:HD21	2.16	0.43
8:R:45:THR:OG1	8:R:46:ASP:N	2.50	0.43
8:S:105:ALA:O	8:S:109:SER:OG	2.34	0.43
8:T:297:LEU:HD21	8:T:377:MET:HB3	2.01	0.43
8:X:297:LEU:HD21	8:X:377:MET:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:X:381:HIS:CE1	8:X:383:SER:HG	2.33	0.43
8:X:425:ARG:HA	8:X:428:VAL:HG12	2.01	0.43
8:Y:39:GLU:H	8:Y:39:GLU:CD	2.27	0.43
8:Y:104:TRP:O	8:Y:108:PHE:HB2	2.17	0.43
8:Z:104:TRP:O	8:Z:108:PHE:HB2	2.17	0.43
3:E:303:HIS:O	3:E:307:VAL:HG22	2.18	0.43
4:B:803:ARG:HH12	4:B:833:ILE:HD11	1.84	0.43
4:H:681:ARG:HG3	4:H:685:MET:HE2	2.00	0.43
8:P:341:ARG:NH1	8:P:342:GLU:OE2	2.46	0.43
8:U:425:ARG:HA	8:U:428:VAL:HG12	2.01	0.43
8:W:297:LEU:HD21	8:W:377:MET:HB3	2.01	0.43
3:E:306:LEU:O	3:E:310:LEU:HG	2.19	0.43
3:G:518:ARG:HG2	3:G:524:GLN:HG2	2.01	0.43
8:O:425:ARG:HA	8:O:428:VAL:HG12	2.01	0.43
8:V:39:GLU:CD	8:V:39:GLU:H	2.27	0.43
8:Z:297:LEU:HD21	8:Z:377:MET:HB3	2.01	0.43
4:F:526:LEU:HA	4:F:526:LEU:HD12	1.80	0.43
8:P:425:ARG:HA	8:P:428:VAL:HG12	2.01	0.43
8:S:50:VAL:HG21	8:S:244:ARG:HG2	1.99	0.43
8:U:45:THR:OG1	8:U:46:ASP:N	2.50	0.43
8:Y:421:MET:H	8:Y:421:MET:HG3	1.69	0.43
5:d:28:LEU:HD12	5:d:31:ILE:HD11	2.00	0.43
4:B:855:GLN:HA	4:B:858:VAL:HG22	2.01	0.43
3:G:217:VAL:O	3:G:221:LEU:HG	2.19	0.43
6:I:403:VAL:HG11	8:W:47:ARG:NH1	2.34	0.43
8:O:425:ARG:HH21	8:O:426:GLU:HA	1.84	0.43
8:Q:45:THR:OG1	8:Q:46:ASP:N	2.50	0.43
8:V:297:LEU:HD21	8:V:377:MET:HB3	2.01	0.43
8:X:105:ALA:O	8:X:109:SER:OG	2.34	0.43
8:X:425:ARG:HH21	8:X:426:GLU:HA	1.84	0.43
8:Z:39:GLU:CD	8:Z:39:GLU:H	2.27	0.43
8:Z:425:ARG:HA	8:Z:428:VAL:HG12	2.01	0.43
2:e:82:MET:HA	2:e:85:ILE:HG22	2.01	0.43
2:e:242:LEU:HD23	2:e:243:PRO:HD3	2.00	0.43
4:B:692:ARG:HH22	4:B:698:SER:HA	1.84	0.43
1:J:889:LYS:HA	8:X:353:PRO:HG2	2.00	0.43
6:K:481:TYR:O	6:K:484:SER:OG	2.33	0.43
6:K:639:ASN:HB2	8:Y:334:HIS:NE2	2.34	0.43
8:P:45:THR:OG1	8:P:46:ASP:N	2.50	0.43
8:S:425:ARG:HH21	8:S:426:GLU:HA	1.84	0.43
8:U:297:LEU:HD21	8:U:377:MET:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:X:39:GLU:CD	8:X:39:GLU:H	2.26	0.43
3:E:150:LEU:HB2	3:E:152:GLN:HE22	1.83	0.43
3:A:557:LEU:HD13	8:P:343:ARG:HD3	2.00	0.42
4:F:256:TYR:HB3	4:F:261:ILE:HB	2.00	0.42
3:G:494:TYR:HA	3:G:497:LYS:HE2	2.01	0.42
4:H:675:TYR:HA	4:H:678:THR:HG22	2.00	0.42
6:K:345:VAL:HG23	6:K:350:LEU:HB3	2.00	0.42
6:K:651:TYR:HB3	6:K:653:LYS:HZ2	1.83	0.42
8:R:425:ARG:HH21	8:R:426:GLU:HA	1.84	0.42
8:Y:45:THR:OG1	8:Y:46:ASP:N	2.50	0.42
3:C:758:PHE:O	3:C:763:GLN:HG2	2.19	0.42
4:F:616:GLU:O	4:F:620:ARG:HG2	2.18	0.42
6:K:282:SER:HB2	6:K:340:LEU:HD11	2.01	0.42
8:T:39:GLU:H	8:T:39:GLU:CD	2.27	0.42
8:V:105:ALA:O	8:V:109:SER:OG	2.34	0.42
8:V:425:ARG:HA	8:V:428:VAL:HG12	2.01	0.42
8:W:45:THR:OG1	8:W:46:ASP:N	2.50	0.42
3:E:408:MET:O	3:E:435:VAL:N	2.49	0.42
3:A:510:VAL:HG12	3:A:713:LEU:HD13	2.02	0.42
4:B:459:LEU:HA	4:B:463:LYS:HB2	2.02	0.42
3:C:445:LYS:H	3:C:445:LYS:HG3	1.62	0.42
4:H:275:TYR:HD2	4:H:295:SER:HB2	1.84	0.42
6:I:621:ARG:O	6:I:624:SER:OG	2.33	0.42
1:J:230:SER:HB3	1:J:264:LEU:O	2.19	0.42
6:K:352:GLY:O	6:K:356:ILE:HG12	2.18	0.42
6:K:604:LEU:HD13	6:K:608:GLY:HA3	2.02	0.42
8:P:39:GLU:H	8:P:39:GLU:CD	2.27	0.42
8:P:237:SER:O	8:P:244:ARG:NH2	2.43	0.42
8:R:105:ALA:O	8:R:109:SER:OG	2.34	0.42
8:U:39:GLU:CD	8:U:39:GLU:H	2.27	0.42
8:W:90:ASN:OD1	8:W:90:ASN:N	2.53	0.42
3:E:837:LEU:HD21	3:E:859:LEU:HD23	2.01	0.42
4:B:294:LEU:HD11	4:B:368:LEU:HD22	2.01	0.42
4:D:611:GLN:H	4:D:611:GLN:HG2	1.63	0.42
6:I:477:VAL:HA	6:I:480:LYS:HE2	2.02	0.42
6:I:601:LEU:HD23	6:I:601:LEU:HA	1.67	0.42
7:L:348:LYS:HG3	7:L:349:GLU:H	1.85	0.42
8:W:425:ARG:HH21	8:W:426:GLU:HA	1.84	0.42
8:X:193:LYS:O	8:X:196:THR:OG1	2.32	0.42
8:Y:79:ASN:OD1	8:Y:79:ASN:N	2.46	0.42
8:Y:425:ARG:HH21	8:Y:426:GLU:HA	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Z:90:ASN:OD1	8:Z:90:ASN:N	2.53	0.42
8:Z:341:ARG:NH1	8:Z:342:GLU:OE2	2.46	0.42
4:D:427:LEU:HD13	4:D:427:LEU:HA	1.94	0.42
3:G:363:SER:HA	3:G:376:CYS:SG	2.60	0.42
1:J:386:ILE:O	7:L:294:ARG:NH1	2.52	0.42
8:P:28:GLU:HG3	8:P:367:LEU:HD11	2.02	0.42
8:P:425:ARG:HH21	8:P:426:GLU:HA	1.84	0.42
8:Q:288:THR:OG1	8:Q:289:THR:N	2.53	0.42
8:R:425:ARG:HA	8:R:428:VAL:HG12	2.01	0.42
4:B:769:ARG:O	4:B:772:LEU:HG	2.19	0.42
4:F:674:GLU:O	4:F:678:THR:OG1	2.28	0.42
4:F:677:LEU:HD13	4:F:712:VAL:HG22	2.02	0.42
3:G:460:VAL:HB	3:G:499:LEU:HD13	2.02	0.42
3:G:680:PHE:HA	3:G:683:ARG:HG2	2.01	0.42
6:K:521:MET:HE1	6:K:616:VAL:HG22	2.01	0.42
7:L:1663:HIS:CD2	8:Z:262:PRO:HB3	2.54	0.42
8:P:297:LEU:HD21	8:P:377:MET:HB3	2.01	0.42
8:P:421:MET:H	8:P:421:MET:HG3	1.69	0.42
8:R:90:ASN:OD1	8:R:90:ASN:N	2.53	0.42
8:U:425:ARG:HH21	8:U:426:GLU:HA	1.84	0.42
8:V:341:ARG:NH1	8:V:342:GLU:OE2	2.46	0.42
8:Y:288:THR:OG1	8:Y:289:THR:N	2.53	0.42
8:Y:381:HIS:ND1	8:Y:383:SER:OG	2.44	0.42
8:Z:73:VAL:O	8:Z:76:SER:OG	2.31	0.42
3:A:547:THR:HA	3:A:548:PRO:HD3	1.94	0.42
4:B:802:ARG:HH22	4:B:836:PHE:HE2	1.65	0.42
4:D:713:HIS:NE2	8:R:355:SER:OG	2.48	0.42
4:F:334:GLU:HB2	4:F:377:ARG:HH22	1.84	0.42
3:G:644:HIS:CE1	3:G:697:MET:HE1	2.55	0.42
1:J:222:HIS:CG	1:J:225:TRP:HB2	2.55	0.42
8:Q:39:GLU:CD	8:Q:39:GLU:H	2.27	0.42
8:Q:297:LEU:HD21	8:Q:377:MET:HB3	2.01	0.42
8:R:39:GLU:H	8:R:39:GLU:CD	2.27	0.42
8:R:46:ASP:HA	8:R:246:PRO:HD3	2.02	0.42
8:R:288:THR:OG1	8:R:289:THR:N	2.53	0.42
8:W:425:ARG:HA	8:W:428:VAL:HG12	2.01	0.42
8:X:7:THR:OG1	8:X:63:ARG:O	2.28	0.42
8:Z:45:THR:OG1	8:Z:46:ASP:N	2.50	0.42
5:m:29:LEU:O	5:m:32:SER:OG	2.34	0.42
1:l:71:LYS:O	1:l:75:HIS:ND1	2.53	0.42
2:e:5:ILE:HD13	2:e:100:GLU:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:e:242:LEU:HB2	2:e:246:GLN:HB3	2.02	0.42
4:D:685:MET:HE3	4:D:685:MET:HB3	1.98	0.42
4:F:726:VAL:O	4:F:730:SER:OG	2.30	0.42
3:G:701:VAL:HG13	3:G:736:ASP:HB3	2.01	0.42
3:G:719:ILE:HA	3:G:722:VAL:HG22	2.01	0.42
4:H:887:LYS:HA	4:H:887:LYS:HD3	1.80	0.42
7:L:1680:ILE:HD11	7:L:1716:GLY:HA3	2.02	0.42
8:O:90:ASN:OD1	8:O:90:ASN:N	2.53	0.42
8:T:288:THR:OG1	8:T:289:THR:N	2.53	0.42
8:V:425:ARG:HH21	8:V:426:GLU:HA	1.84	0.42
8:Y:425:ARG:HA	8:Y:428:VAL:HG12	2.01	0.42
8:Z:288:THR:OG1	8:Z:289:THR:N	2.53	0.42
3:A:219:GLU:HB2	3:A:314:HIS:CE1	2.55	0.42
4:B:589:ALA:HB3	4:B:632:ASP:HB3	2.02	0.42
4:F:848:ARG:HD2	4:F:848:ARG:HA	1.86	0.42
6:I:9:LEU:HD22	6:I:104:LEU:HD13	2.01	0.42
6:K:593:PHE:HB2	6:K:615:LEU:HD13	2.00	0.42
7:L:1803:ASN:HD22	8:Z:341:ARG:NH2	2.17	0.42
8:O:288:THR:OG1	8:O:289:THR:N	2.53	0.42
8:R:77:ILE:O	8:R:80:SER:OG	2.31	0.42
8:Y:90:ASN:OD1	8:Y:90:ASN:N	2.53	0.42
8:Z:46:ASP:HA	8:Z:246:PRO:HD3	2.02	0.42
8:Z:425:ARG:HH21	8:Z:426:GLU:HA	1.84	0.42
3:E:257:ARG:HG2	3:E:261:HIS:CE1	2.55	0.42
4:B:577:LEU:HD12	4:B:578:MET:HG3	2.02	0.42
4:F:293:ARG:HA	3:E:186:ALA:HB1	2.01	0.42
4:F:606:ARG:HH21	8:U:339:ARG:HE	1.68	0.42
8:O:105:ALA:O	8:O:109:SER:OG	2.34	0.42
8:Q:153:LEU:HD12	8:Q:153:LEU:HA	1.95	0.42
8:Q:425:ARG:HA	8:Q:428:VAL:HG12	2.01	0.42
8:Q:425:ARG:HH21	8:Q:426:GLU:HA	1.84	0.42
8:R:381:HIS:CG	8:R:383:SER:HG	2.36	0.42
8:T:28:GLU:HG3	8:T:367:LEU:HD11	2.02	0.42
8:T:425:ARG:HA	8:T:428:VAL:HG12	2.01	0.42
8:T:425:ARG:HH21	8:T:426:GLU:HA	1.84	0.42
8:V:381:HIS:CE1	8:V:383:SER:HG	2.35	0.42
8:V:385:SER:HB2	8:V:435:TYR:CD2	2.55	0.42
8:W:46:ASP:HA	8:W:246:PRO:HD3	2.02	0.42
8:X:28:GLU:HG3	8:X:367:LEU:HD11	2.02	0.42
8:Z:28:GLU:HG3	8:Z:367:LEU:HD11	2.02	0.42
5:d:59:ALA:HB2	7:c:48:ASN:HD21	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:720:TYR:HA	8:P:249:MET:HE1	2.02	0.41
3:C:429:ASP:N	3:C:429:ASP:OD1	2.53	0.41
6:K:651:TYR:HH	8:Y:318:ILE:C	2.23	0.41
8:P:228:ILE:O	8:P:232:VAL:HG23	2.20	0.41
8:S:46:ASP:HA	8:S:246:PRO:HD3	2.02	0.41
8:Z:348:PHE:HB3	8:Z:349:ILE:H	1.76	0.41
4:B:497:CYS:SG	4:B:552:LYS:NZ	2.93	0.41
4:D:433:TRP:HZ2	4:D:484:LEU:HD12	1.85	0.41
6:I:515:TRP:HE1	6:I:519:ASN:N	2.18	0.41
6:I:533:GLN:O	6:I:537:LEU:HG	2.20	0.41
8:P:288:THR:OG1	8:P:289:THR:N	2.53	0.41
8:Q:28:GLU:HG3	8:Q:367:LEU:HD11	2.02	0.41
8:Q:77:ILE:O	8:Q:80:SER:OG	2.31	0.41
8:Q:385:SER:HB2	8:Q:435:TYR:CD2	2.55	0.41
8:R:28:GLU:HG3	8:R:367:LEU:HD11	2.02	0.41
8:T:45:THR:OG1	8:T:46:ASP:N	2.50	0.41
8:U:228:ILE:O	8:U:232:VAL:HG23	2.20	0.41
8:V:287:LYS:HB3	8:V:288:THR:H	1.74	0.41
8:W:385:SER:HB2	8:W:435:TYR:CD2	2.55	0.41
8:X:45:THR:OG1	8:X:46:ASP:N	2.50	0.41
8:Z:77:ILE:O	8:Z:80:SER:OG	2.31	0.41
8:Z:385:SER:HB2	8:Z:435:TYR:CD2	2.55	0.41
3:A:679:ALA:HB1	3:A:762:MET:HE3	2.02	0.41
3:C:652:GLU:O	3:C:655:LEU:HG	2.21	0.41
4:F:594:GLN:HA	4:F:597:LEU:HD13	2.02	0.41
1:J:723:MET:HE3	1:J:723:MET:HB3	1.93	0.41
6:K:646:LEU:HB3	8:Y:341:ARG:CD	2.48	0.41
8:P:46:ASP:HA	8:P:246:PRO:HD3	2.02	0.41
8:P:381:HIS:CG	8:P:383:SER:HG	2.36	0.41
8:S:349:ILE:HD12	8:S:349:ILE:HA	1.98	0.41
8:T:228:ILE:O	8:T:232:VAL:HG23	2.21	0.41
8:T:385:SER:HB2	8:T:435:TYR:CD2	2.55	0.41
8:X:228:ILE:O	8:X:232:VAL:HG23	2.21	0.41
8:X:385:SER:HB2	8:X:435:TYR:CD2	2.55	0.41
8:Y:385:SER:HB2	8:Y:435:TYR:CD2	2.55	0.41
3:E:526:ASP:HA	3:E:529:VAL:HG12	2.02	0.41
3:C:408:MET:HA	3:C:438:GLN:HB2	2.03	0.41
3:C:448:ASP:OD1	3:C:448:ASP:N	2.54	0.41
4:F:288:ARG:O	4:F:292:VAL:HG22	2.20	0.41
4:F:665:ASN:HB3	4:j:66:ARG:NE	2.33	0.41
1:J:272:ARG:HH12	7:L:311:TYR:HB2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:691:LEU:HD12	1:J:694:HIS:HD2	1.85	0.41
7:L:1595:GLU:OE1	7:L:1597:ARG:NH2	2.53	0.41
8:S:288:THR:OG1	8:S:289:THR:N	2.53	0.41
8:U:46:ASP:HA	8:U:246:PRO:HD3	2.02	0.41
8:U:288:THR:OG1	8:U:289:THR:N	2.53	0.41
8:X:341:ARG:NH1	8:X:342:GLU:OE2	2.46	0.41
3:A:243:SER:HA	3:A:275:ARG:HH22	1.86	0.41
4:B:290:THR:HB	4:B:368:LEU:HD21	2.03	0.41
1:J:475:THR:HA	1:J:478:GLU:HG3	2.02	0.41
8:T:193:LYS:O	8:T:196:THR:OG1	2.32	0.41
8:X:71:PRO:O	8:X:75:HIS:NE2	2.54	0.41
8:Y:46:ASP:HA	8:Y:246:PRO:HD3	2.02	0.41
8:Y:71:PRO:O	8:Y:75:HIS:NE2	2.54	0.41
2:e:109:PRO:HA	2:e:136:ILE:HG13	2.01	0.41
3:A:743:GLU:HG3	3:A:745:LEU:H	1.86	0.41
4:B:859:GLN:NE2	4:B:890:GLU:OE2	2.53	0.41
3:C:211:ALA:O	3:C:214:GLU:HG2	2.20	0.41
3:C:698:MET:HB3	3:C:698:MET:HE3	1.45	0.41
1:J:221:VAL:HG22	6:K:35:HIS:HE1	1.86	0.41
8:P:73:VAL:O	8:P:76:SER:OG	2.31	0.41
8:S:297:LEU:HD21	8:S:377:MET:HB3	2.01	0.41
8:U:385:SER:HB2	8:U:435:TYR:CD2	2.55	0.41
8:W:28:GLU:HG3	8:W:367:LEU:HD11	2.02	0.41
8:Y:132:LEU:HD12	8:Y:132:LEU:HA	1.95	0.41
3:E:443:LEU:HG	3:E:450:ILE:HD11	2.02	0.41
2:e:248:ILE:HD12	2:e:248:ILE:HA	1.96	0.41
4:B:406:THR:HG21	4:B:411:MET:HB2	2.01	0.41
4:D:548:VAL:HA	4:D:552:LYS:HE2	2.02	0.41
4:D:887:LYS:HD2	4:D:887:LYS:HA	1.92	0.41
4:F:304:ILE:HG13	4:F:385:VAL:HG21	2.02	0.41
3:G:676:PHE:HB2	3:G:818:PHE:CE2	2.56	0.41
6:K:300:LEU:HD12	6:K:339:HIS:HE1	1.86	0.41
8:O:28:GLU:HG3	8:O:367:LEU:HD11	2.02	0.41
8:Q:15:ASN:ND2	8:Q:68:ASP:OD1	2.40	0.41
8:S:28:GLU:HG3	8:S:367:LEU:HD11	2.02	0.41
8:S:79:ASN:OD1	8:S:79:ASN:N	2.46	0.41
8:U:28:GLU:HG3	8:U:367:LEU:HD11	2.02	0.41
8:V:288:THR:OG1	8:V:289:THR:N	2.53	0.41
8:W:71:PRO:O	8:W:75:HIS:NE2	2.54	0.41
8:Y:193:LYS:O	8:Y:196:THR:OG1	2.32	0.41
7:c:30:ARG:HD2	7:c:30:ARG:HA	1.97	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:843:MET:O	4:D:847:LEU:HG	2.21	0.41
4:F:779:PHE:HA	4:F:782:ILE:HD12	2.03	0.41
3:G:643:ARG:HA	3:G:646:PHE:HB3	2.03	0.41
1:J:221:VAL:HG12	7:L:309:GLU:HB3	2.02	0.41
1:J:979:SER:OG	1:J:980:ILE:N	2.53	0.41
8:O:228:ILE:O	8:O:232:VAL:HG23	2.20	0.41
8:O:385:SER:HB2	8:O:435:TYR:CD2	2.55	0.41
8:Q:71:PRO:O	8:Q:75:HIS:NE2	2.54	0.41
8:T:46:ASP:HA	8:T:246:PRO:HD3	2.02	0.41
8:U:71:PRO:O	8:U:75:HIS:NE2	2.54	0.41
8:Y:28:GLU:HG3	8:Y:367:LEU:HD11	2.02	0.41
8:Y:228:ILE:O	8:Y:232:VAL:HG23	2.20	0.41
4:j:59:LYS:O	4:j:63:ILE:HG12	2.21	0.41
3:A:393:LYS:HD2	3:A:397:ARG:HE	1.86	0.41
3:A:431:ARG:HH11	3:A:458:ASN:HD21	1.68	0.41
3:C:174:LEU:HD13	3:C:283:PHE:HB2	2.03	0.41
3:C:252:LEU:HB2	3:C:257:ARG:HE	1.85	0.41
4:D:558:HIS:CD2	4:D:617:ILE:HD11	2.56	0.41
4:D:653:THR:O	4:D:657:MET:HG2	2.20	0.41
4:F:268:MET:HG3	4:F:276:LYS:HB2	2.03	0.41
4:F:503:THR:HG21	4:F:544:TYR:CD2	2.56	0.41
4:H:433:TRP:HE1	4:H:484:LEU:HA	1.86	0.41
6:I:129:PHE:O	6:I:133:PHE:HB2	2.20	0.41
6:I:336:VAL:HA	6:I:339:HIS:HD1	1.86	0.41
1:J:456:GLN:O	1:J:459:SER:OG	2.36	0.41
6:K:359:ASP:HA	6:K:364:GLY:HA3	2.02	0.41
7:L:1658:LEU:HG	7:L:1762:PHE:HE1	1.84	0.41
7:L:1678:ASN:OD1	7:L:1679:GLN:NE2	2.54	0.41
8:P:385:SER:HB2	8:P:435:TYR:CD2	2.55	0.41
8:V:15:ASN:ND2	8:V:68:ASP:OD1	2.40	0.41
8:W:228:ILE:O	8:W:232:VAL:HG23	2.20	0.41
8:W:421:MET:H	8:W:421:MET:HG3	1.69	0.41
8:X:46:ASP:HA	8:X:246:PRO:HD3	2.02	0.41
8:X:288:THR:OG1	8:X:289:THR:N	2.53	0.41
4:a:9:PRO:O	4:a:13:LEU:HG	2.20	0.41
4:f:72:ALA:O	4:f:75:SER:OG	2.35	0.41
3:E:244:ARG:HD3	3:E:244:ARG:HA	1.89	0.41
3:E:276:PHE:CD2	3:E:296:MET:HE1	2.54	0.41
1:l:23:VAL:O	1:l:27:ALA:HB3	2.21	0.41
3:A:824:LYS:HA	3:A:827:LYS:HD2	2.03	0.41
3:C:517:LYS:HB2	3:C:706:TRP:CZ2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:b:17:ASN:O	5:b:21:VAL:HG22	2.21	0.41
4:F:579:ASP:OD2	8:T:3:ARG:NH1	2.48	0.41
3:G:509:LEU:HD13	3:G:626:LEU:HD22	2.02	0.41
6:K:38:GLU:O	6:K:42:LEU:HG	2.20	0.41
8:O:71:PRO:O	8:O:75:HIS:NE2	2.54	0.41
8:S:28:GLU:CD	8:S:244:ARG:HH12	2.30	0.41
1:J:296:VAL:HG23	1:J:314:LEU:HB2	2.04	0.40
7:L:1485:ALA:HA	7:L:1488:ILE:HD12	2.02	0.40
7:L:1574:LEU:HD23	7:L:1574:LEU:HA	1.91	0.40
8:P:289:THR:OG1	8:P:332:GLN:NE2	2.55	0.40
8:R:385:SER:HB2	8:R:435:TYR:CD2	2.55	0.40
8:S:228:ILE:O	8:S:232:VAL:HG23	2.20	0.40
3:A:282:SER:O	3:A:290:HIS:NE2	2.54	0.40
3:C:292:LEU:HD23	3:C:292:LEU:HA	1.93	0.40
3:G:209:PRO:O	3:G:212:SER:OG	2.36	0.40
3:G:319:LEU:HD23	3:G:319:LEU:HA	1.73	0.40
6:K:512:ALA:HA	6:K:515:TRP:CE3	2.55	0.40
6:K:513:ILE:HG13	8:Y:263:THR:HG23	2.02	0.40
8:P:252:ASP:OD1	8:P:252:ASP:N	2.51	0.40
8:R:71:PRO:O	8:R:75:HIS:NE2	2.54	0.40
8:T:71:PRO:O	8:T:75:HIS:NE2	2.54	0.40
8:V:228:ILE:O	8:V:232:VAL:HG23	2.20	0.40
8:V:289:THR:OG1	8:V:332:GLN:NE2	2.55	0.40
8:Z:28:GLU:CD	8:Z:244:ARG:HH12	2.29	0.40
8:Z:71:PRO:O	8:Z:75:HIS:NE2	2.54	0.40
8:Z:228:ILE:O	8:Z:232:VAL:HG23	2.20	0.40
4:D:324:PHE:O	4:D:328:LEU:HG	2.21	0.40
1:J:281:VAL:HG11	6:K:41:VAL:HG22	2.03	0.40
8:O:289:THR:OG1	8:O:332:GLN:NE2	2.55	0.40
8:Q:320:ILE:HB	8:Q:356:ILE:HG13	2.04	0.40
8:R:28:GLU:CD	8:R:244:ARG:HH12	2.30	0.40
8:S:71:PRO:O	8:S:75:HIS:NE2	2.54	0.40
8:T:105:ALA:O	8:T:109:SER:OG	2.34	0.40
8:T:320:ILE:HB	8:T:356:ILE:HG13	2.04	0.40
8:U:28:GLU:CD	8:U:244:ARG:HH12	2.30	0.40
8:V:71:PRO:O	8:V:75:HIS:NE2	2.54	0.40
3:E:301:LYS:O	3:E:305:ILE:HG12	2.21	0.40
4:B:872:SER:HA	4:B:875:PHE:CE2	2.56	0.40
4:D:401:HIS:CE1	4:D:474:PHE:HB3	2.57	0.40
4:D:689:LYS:HE3	8:R:162:PRO:HB2	2.03	0.40
4:D:791:ALA:HA	4:D:794:ARG:HH21	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:b:35:LEU:HD23	4:a:97:LEU:HG	2.04	0.40
4:F:889:ARG:HD3	4:F:889:ARG:HA	1.82	0.40
3:G:394:TRP:NE1	3:G:450:ILE:O	2.51	0.40
3:G:676:PHE:HB2	3:G:818:PHE:CZ	2.57	0.40
4:H:419:LEU:HA	4:H:422:VAL:HG22	2.04	0.40
6:K:483:LEU:HD12	6:K:483:LEU:HA	1.89	0.40
8:O:341:ARG:NH1	8:O:342:GLU:OE2	2.46	0.40
8:P:193:LYS:O	8:P:196:THR:OG1	2.32	0.40
8:Q:46:ASP:HA	8:Q:246:PRO:HD3	2.02	0.40
8:Q:73:VAL:O	8:Q:76:SER:OG	2.31	0.40
8:Q:193:LYS:O	8:Q:196:THR:OG1	2.32	0.40
8:R:228:ILE:O	8:R:232:VAL:HG23	2.20	0.40
8:U:237:SER:O	8:U:244:ARG:NH2	2.43	0.40
8:U:341:ARG:NH1	8:U:342:GLU:OE2	2.46	0.40
8:V:46:ASP:HA	8:V:246:PRO:HD3	2.02	0.40
8:W:28:GLU:CD	8:W:244:ARG:HH12	2.30	0.40
8:W:288:THR:OG1	8:W:289:THR:N	2.53	0.40
8:Z:237:SER:O	8:Z:244:ARG:NH2	2.43	0.40
3:E:637:ARG:HA	3:E:637:ARG:HD3	1.88	0.40
3:E:712:ASN:HB3	3:E:725:HIS:CG	2.56	0.40
2:e:221:LEU:N	2:e:226:GLU:OE2	2.51	0.40
3:A:660:ILE:HD11	8:O:254:ILE:HD12	2.03	0.40
4:B:245:ILE:HG22	4:B:282:ASN:HB3	2.04	0.40
4:D:720:TYR:HA	4:D:723:THR:HG22	2.02	0.40
4:F:271:THR:OG1	4:F:272:GLU:N	2.55	0.40
4:H:433:TRP:CD1	4:H:483:VAL:HG22	2.54	0.40
6:I:148:ILE:HA	6:I:152:GLN:HE21	1.85	0.40
7:L:407:TYR:HB2	7:L:470:LEU:HD21	2.03	0.40
7:L:539:TRP:CE2	7:L:599:GLY:HA3	2.57	0.40
8:O:28:GLU:CD	8:O:244:ARG:HH12	2.30	0.40
8:O:46:ASP:HA	8:O:246:PRO:HD3	2.02	0.40
8:P:71:PRO:O	8:P:75:HIS:NE2	2.54	0.40
8:Q:381:HIS:CG	8:Q:383:SER:HG	2.34	0.40
8:R:341:ARG:NH1	8:R:342:GLU:OE2	2.46	0.40
8:T:28:GLU:CD	8:T:244:ARG:HH12	2.29	0.40
8:U:381:HIS:CE1	8:U:383:SER:HG	2.33	0.40
8:V:28:GLU:HG3	8:V:367:LEU:HD11	2.02	0.40
8:X:421:MET:H	8:X:421:MET:HG3	1.69	0.40
8:Y:289:THR:OG1	8:Y:332:GLN:NE2	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	506/1024 (49%)	465 (92%)	38 (8%)	3 (1%)	21	59
1	l	104/1024 (10%)	96 (92%)	4 (4%)	4 (4%)	2	19
2	e	360/375 (96%)	339 (94%)	21 (6%)	0	100	100
3	A	599/902 (66%)	576 (96%)	22 (4%)	1 (0%)	43	78
3	C	606/902 (67%)	568 (94%)	37 (6%)	1 (0%)	43	78
3	E	628/902 (70%)	594 (95%)	32 (5%)	2 (0%)	36	72
3	G	628/902 (70%)	587 (94%)	37 (6%)	4 (1%)	21	59
4	B	602/907 (66%)	573 (95%)	27 (4%)	2 (0%)	36	72
4	D	571/907 (63%)	547 (96%)	21 (4%)	3 (0%)	24	63
4	F	591/907 (65%)	555 (94%)	35 (6%)	1 (0%)	43	78
4	H	584/907 (64%)	559 (96%)	23 (4%)	2 (0%)	36	72
4	a	112/907 (12%)	107 (96%)	5 (4%)	0	100	100
4	f	97/907 (11%)	92 (95%)	5 (5%)	0	100	100
4	h	97/907 (11%)	93 (96%)	4 (4%)	0	100	100
4	j	105/907 (12%)	98 (93%)	7 (7%)	0	100	100
5	b	63/82 (77%)	62 (98%)	1 (2%)	0	100	100
5	d	57/82 (70%)	55 (96%)	2 (4%)	0	100	100
5	g	63/82 (77%)	62 (98%)	1 (2%)	0	100	100
5	i	63/82 (77%)	60 (95%)	3 (5%)	0	100	100
5	k	63/82 (77%)	61 (97%)	2 (3%)	0	100	100
5	m	63/82 (77%)	62 (98%)	1 (2%)	0	100	100
6	I	511/667 (77%)	482 (94%)	24 (5%)	5 (1%)	12	49
6	K	548/667 (82%)	528 (96%)	19 (4%)	1 (0%)	43	78
7	L	540/1819 (30%)	493 (91%)	43 (8%)	4 (1%)	18	56
7	c	148/1819 (8%)	142 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	O	408/451 (90%)	390 (96%)	18 (4%)	0	100	100
8	P	408/451 (90%)	390 (96%)	18 (4%)	0	100	100
8	Q	408/451 (90%)	390 (96%)	18 (4%)	0	100	100
8	R	408/451 (90%)	390 (96%)	18 (4%)	0	100	100
8	S	408/451 (90%)	390 (96%)	18 (4%)	0	100	100
8	T	408/451 (90%)	390 (96%)	18 (4%)	0	100	100
8	U	408/451 (90%)	390 (96%)	18 (4%)	0	100	100
8	V	408/451 (90%)	390 (96%)	18 (4%)	0	100	100
8	W	408/451 (90%)	390 (96%)	18 (4%)	0	100	100
8	X	408/451 (90%)	390 (96%)	18 (4%)	0	100	100
8	Y	408/451 (90%)	390 (96%)	18 (4%)	0	100	100
8	Z	408/451 (90%)	390 (96%)	18 (4%)	0	100	100
All	All	13205/24163 (55%)	12536 (95%)	636 (5%)	33 (0%)	44	78

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	121	PRO
3	A	584	THR
3	C	239	ALA
4	D	627	GLU
4	D	884	GLU
3	G	241	ARG
6	I	508	ASN
6	I	601	LEU
1	J	236	LEU
1	J	238	LEU
1	J	257	TYR
6	K	255	LYS
3	E	675	TRP
1	I	116	CYS
4	B	871	GLU
4	H	633	THR
6	I	600	ASN
3	E	581	ASP
3	G	481	GLU
7	L	451	PRO
1	I	115	LEU

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Mol	Chain	Res	Type
1	I	118	SER
4	D	883	ASN
6	I	408	ASP
6	I	409	ASN
4	B	870	ASP
4	F	525	ASP
3	G	480	LYS
4	H	627	GLU
7	L	307	ARG
7	L	303	PRO
7	L	309	GLU
3	G	398	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%)	497 (100%)	1 (0%)	87	87
1	I	84/933 (9%)	84 (100%)	0	100	100
2	e	310/318 (98%)	305 (98%)	5 (2%)	55	70
3	A	549/791 (69%)	548 (100%)	1 (0%)	87	87
3	C	556/791 (70%)	553 (100%)	3 (0%)	81	83
3	E	572/791 (72%)	570 (100%)	2 (0%)	86	86
3	G	572/791 (72%)	569 (100%)	3 (0%)	81	83
4	B	551/798 (69%)	549 (100%)	2 (0%)	84	84
4	D	525/798 (66%)	524 (100%)	1 (0%)	87	87
4	F	542/798 (68%)	537 (99%)	5 (1%)	70	79
4	H	539/798 (68%)	535 (99%)	4 (1%)	76	81
4	a	101/798 (13%)	100 (99%)	1 (1%)	68	78
4	f	88/798 (11%)	87 (99%)	1 (1%)	65	76
4	h	88/798 (11%)	88 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	j	88/798 (11%)	88 (100%)	0	100	100
5	b	53/62 (86%)	51 (96%)	2 (4%)	29	50
5	d	53/62 (86%)	53 (100%)	0	100	100
5	g	53/62 (86%)	53 (100%)	0	100	100
5	i	53/62 (86%)	53 (100%)	0	100	100
5	k	53/62 (86%)	53 (100%)	0	100	100
5	m	53/62 (86%)	53 (100%)	0	100	100
6	I	472/594 (80%)	471 (100%)	1 (0%)	87	87
6	K	509/594 (86%)	505 (99%)	4 (1%)	73	80
7	L	501/1546 (32%)	500 (100%)	1 (0%)	87	87
7	c	135/1546 (9%)	135 (100%)	0	100	100
8	O	376/400 (94%)	333 (89%)	43 (11%)	5	18
8	P	376/400 (94%)	333 (89%)	43 (11%)	5	18
8	Q	376/400 (94%)	333 (89%)	43 (11%)	5	18
8	R	376/400 (94%)	333 (89%)	43 (11%)	5	18
8	S	376/400 (94%)	333 (89%)	43 (11%)	5	18
8	T	376/400 (94%)	333 (89%)	43 (11%)	5	18
8	U	376/400 (94%)	333 (89%)	43 (11%)	5	18
8	V	376/400 (94%)	333 (89%)	43 (11%)	5	18
8	W	376/400 (94%)	333 (89%)	43 (11%)	5	18
8	X	376/400 (94%)	333 (89%)	43 (11%)	5	18
8	Y	376/400 (94%)	333 (89%)	43 (11%)	5	18
8	Z	376/400 (94%)	333 (89%)	43 (11%)	5	18
All	All	12110/21184 (57%)	11557 (95%)	553 (5%)	25	45

All (553) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	e	66	THR
2	e	152	VAL
2	e	165	ILE
2	e	247	VAL
2	e	298	VAL
3	A	762	MET

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Mol	Chain	Res	Type
4	B	406	THR
4	B	552	LYS
3	C	205	ILE
3	C	328	ILE
3	C	698	MET
4	D	572	ASP
5	b	43	THR
5	b	63	VAL
4	F	304	ILE
4	F	323	SER
4	F	503	THR
4	F	572	ASP
4	F	719	GLN
3	G	478	THR
3	G	747	VAL
3	G	866	THR
4	H	598	THR
4	H	600	ILE
4	H	626	LEU
4	H	651	VAL
6	I	10	SER
1	J	220	VAL
6	K	6	LEU
6	K	157	VAL
6	K	463	LEU
6	K	649	LEU
7	L	497	THR
8	O	7	THR
8	O	17	ILE
8	O	37	VAL
8	O	39	GLU
8	O	45	THR
8	O	50	VAL
8	O	68	ASP
8	O	79	ASN
8	O	109	SER
8	O	127	ASP
8	O	147	SER
8	O	149	LEU
8	O	153	LEU
8	O	157	LEU
8	O	165	LEU

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Mol	Chain	Res	Type
8	O	170	SER
8	O	181	VAL
8	O	188	SER
8	O	201	CYS
8	O	203	VAL
8	O	204	VAL
8	O	224	SER
8	O	232	VAL
8	O	237	SER
8	O	241	THR
8	O	256	LEU
8	O	259	SER
8	O	274	THR
8	O	277	THR
8	O	288	THR
8	O	293	VAL
8	O	298	LEU
8	O	313	THR
8	O	316	CYS
8	O	331	THR
8	O	333	VAL
8	O	356	ILE
8	O	361	SER
8	O	373	VAL
8	O	391	THR
8	O	402	GLU
8	O	425	ARG
8	O	442	ASP
8	P	7	THR
8	P	17	ILE
8	P	37	VAL
8	P	39	GLU
8	P	45	THR
8	P	50	VAL
8	P	68	ASP
8	P	79	ASN
8	P	109	SER
8	P	127	ASP
8	P	147	SER
8	P	149	LEU
8	P	153	LEU
8	P	157	LEU

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Mol	Chain	Res	Type
8	P	165	LEU
8	P	170	SER
8	P	181	VAL
8	P	188	SER
8	P	201	CYS
8	P	203	VAL
8	P	204	VAL
8	P	224	SER
8	P	232	VAL
8	P	237	SER
8	P	241	THR
8	P	256	LEU
8	P	259	SER
8	P	274	THR
8	P	277	THR
8	P	288	THR
8	P	293	VAL
8	P	298	LEU
8	P	313	THR
8	P	316	CYS
8	P	331	THR
8	P	333	VAL
8	P	356	ILE
8	P	361	SER
8	P	373	VAL
8	P	391	THR
8	P	402	GLU
8	P	425	ARG
8	P	442	ASP
8	Q	7	THR
8	Q	17	ILE
8	Q	37	VAL
8	Q	39	GLU
8	Q	45	THR
8	Q	50	VAL
8	Q	68	ASP
8	Q	79	ASN
8	Q	109	SER
8	Q	127	ASP
8	Q	147	SER
8	Q	149	LEU
8	Q	153	LEU

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Mol	Chain	Res	Type
8	Q	157	LEU
8	Q	165	LEU
8	Q	170	SER
8	Q	181	VAL
8	Q	188	SER
8	Q	201	CYS
8	Q	203	VAL
8	Q	204	VAL
8	Q	224	SER
8	Q	232	VAL
8	Q	237	SER
8	Q	241	THR
8	Q	256	LEU
8	Q	259	SER
8	Q	274	THR
8	Q	277	THR
8	Q	288	THR
8	Q	293	VAL
8	Q	298	LEU
8	Q	313	THR
8	Q	316	CYS
8	Q	331	THR
8	Q	333	VAL
8	Q	356	ILE
8	Q	361	SER
8	Q	373	VAL
8	Q	391	THR
8	Q	402	GLU
8	Q	425	ARG
8	Q	442	ASP
8	R	7	THR
8	R	17	ILE
8	R	37	VAL
8	R	39	GLU
8	R	45	THR
8	R	50	VAL
8	R	68	ASP
8	R	79	ASN
8	R	109	SER
8	R	127	ASP
8	R	147	SER
8	R	149	LEU

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Mol	Chain	Res	Type
8	R	153	LEU
8	R	157	LEU
8	R	165	LEU
8	R	170	SER
8	R	181	VAL
8	R	188	SER
8	R	201	CYS
8	R	203	VAL
8	R	204	VAL
8	R	224	SER
8	R	232	VAL
8	R	237	SER
8	R	241	THR
8	R	256	LEU
8	R	259	SER
8	R	274	THR
8	R	277	THR
8	R	288	THR
8	R	293	VAL
8	R	298	LEU
8	R	313	THR
8	R	316	CYS
8	R	331	THR
8	R	333	VAL
8	R	356	ILE
8	R	361	SER
8	R	373	VAL
8	R	391	THR
8	R	402	GLU
8	R	425	ARG
8	R	442	ASP
8	S	7	THR
8	S	17	ILE
8	S	37	VAL
8	S	39	GLU
8	S	45	THR
8	S	50	VAL
8	S	68	ASP
8	S	79	ASN
8	S	109	SER
8	S	127	ASP
8	S	147	SER

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Mol	Chain	Res	Type
8	S	149	LEU
8	S	153	LEU
8	S	157	LEU
8	S	165	LEU
8	S	170	SER
8	S	181	VAL
8	S	188	SER
8	S	201	CYS
8	S	203	VAL
8	S	204	VAL
8	S	224	SER
8	S	232	VAL
8	S	237	SER
8	S	241	THR
8	S	256	LEU
8	S	259	SER
8	S	274	THR
8	S	277	THR
8	S	288	THR
8	S	293	VAL
8	S	298	LEU
8	S	313	THR
8	S	316	CYS
8	S	331	THR
8	S	333	VAL
8	S	356	ILE
8	S	361	SER
8	S	373	VAL
8	S	391	THR
8	S	402	GLU
8	S	425	ARG
8	S	442	ASP
8	T	7	THR
8	T	17	ILE
8	T	37	VAL
8	T	39	GLU
8	T	45	THR
8	T	50	VAL
8	T	68	ASP
8	T	79	ASN
8	T	109	SER
8	T	127	ASP

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Mol	Chain	Res	Type
8	T	147	SER
8	T	149	LEU
8	T	153	LEU
8	T	157	LEU
8	T	165	LEU
8	T	170	SER
8	T	181	VAL
8	T	188	SER
8	T	201	CYS
8	T	203	VAL
8	T	204	VAL
8	T	224	SER
8	T	232	VAL
8	T	237	SER
8	T	241	THR
8	T	256	LEU
8	T	259	SER
8	T	274	THR
8	T	277	THR
8	T	288	THR
8	T	293	VAL
8	T	298	LEU
8	T	313	THR
8	T	316	CYS
8	T	331	THR
8	T	333	VAL
8	T	356	ILE
8	T	361	SER
8	T	373	VAL
8	T	391	THR
8	T	402	GLU
8	T	425	ARG
8	T	442	ASP
8	U	7	THR
8	U	17	ILE
8	U	37	VAL
8	U	39	GLU
8	U	45	THR
8	U	50	VAL
8	U	68	ASP
8	U	79	ASN
8	U	109	SER

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Mol	Chain	Res	Type
8	U	127	ASP
8	U	147	SER
8	U	149	LEU
8	U	153	LEU
8	U	157	LEU
8	U	165	LEU
8	U	170	SER
8	U	181	VAL
8	U	188	SER
8	U	201	CYS
8	U	203	VAL
8	U	204	VAL
8	U	224	SER
8	U	232	VAL
8	U	237	SER
8	U	241	THR
8	U	256	LEU
8	U	259	SER
8	U	274	THR
8	U	277	THR
8	U	288	THR
8	U	293	VAL
8	U	298	LEU
8	U	313	THR
8	U	316	CYS
8	U	331	THR
8	U	333	VAL
8	U	356	ILE
8	U	361	SER
8	U	373	VAL
8	U	391	THR
8	U	402	GLU
8	U	425	ARG
8	U	442	ASP
8	V	7	THR
8	V	17	ILE
8	V	37	VAL
8	V	39	GLU
8	V	45	THR
8	V	50	VAL
8	V	68	ASP
8	V	79	ASN

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Mol	Chain	Res	Type
8	V	109	SER
8	V	127	ASP
8	V	147	SER
8	V	149	LEU
8	V	153	LEU
8	V	157	LEU
8	V	165	LEU
8	V	170	SER
8	V	181	VAL
8	V	188	SER
8	V	201	CYS
8	V	203	VAL
8	V	204	VAL
8	V	224	SER
8	V	232	VAL
8	V	237	SER
8	V	241	THR
8	V	256	LEU
8	V	259	SER
8	V	274	THR
8	V	277	THR
8	V	288	THR
8	V	293	VAL
8	V	298	LEU
8	V	313	THR
8	V	316	CYS
8	V	331	THR
8	V	333	VAL
8	V	356	ILE
8	V	361	SER
8	V	373	VAL
8	V	391	THR
8	V	402	GLU
8	V	425	ARG
8	V	442	ASP
8	W	7	THR
8	W	17	ILE
8	W	37	VAL
8	W	39	GLU
8	W	45	THR
8	W	50	VAL
8	W	68	ASP

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Mol	Chain	Res	Type
8	W	79	ASN
8	W	109	SER
8	W	127	ASP
8	W	147	SER
8	W	149	LEU
8	W	153	LEU
8	W	157	LEU
8	W	165	LEU
8	W	170	SER
8	W	181	VAL
8	W	188	SER
8	W	201	CYS
8	W	203	VAL
8	W	204	VAL
8	W	224	SER
8	W	232	VAL
8	W	237	SER
8	W	241	THR
8	W	256	LEU
8	W	259	SER
8	W	274	THR
8	W	277	THR
8	W	288	THR
8	W	293	VAL
8	W	298	LEU
8	W	313	THR
8	W	316	CYS
8	W	331	THR
8	W	333	VAL
8	W	356	ILE
8	W	361	SER
8	W	373	VAL
8	W	391	THR
8	W	402	GLU
8	W	425	ARG
8	W	442	ASP
8	X	7	THR
8	X	17	ILE
8	X	37	VAL
8	X	39	GLU
8	X	45	THR
8	X	50	VAL

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Mol	Chain	Res	Type
8	X	68	ASP
8	X	79	ASN
8	X	109	SER
8	X	127	ASP
8	X	147	SER
8	X	149	LEU
8	X	153	LEU
8	X	157	LEU
8	X	165	LEU
8	X	170	SER
8	X	181	VAL
8	X	188	SER
8	X	201	CYS
8	X	203	VAL
8	X	204	VAL
8	X	224	SER
8	X	232	VAL
8	X	237	SER
8	X	241	THR
8	X	256	LEU
8	X	259	SER
8	X	274	THR
8	X	277	THR
8	X	288	THR
8	X	293	VAL
8	X	298	LEU
8	X	313	THR
8	X	316	CYS
8	X	331	THR
8	X	333	VAL
8	X	356	ILE
8	X	361	SER
8	X	373	VAL
8	X	391	THR
8	X	402	GLU
8	X	425	ARG
8	X	442	ASP
8	Y	7	THR
8	Y	17	ILE
8	Y	37	VAL
8	Y	39	GLU
8	Y	45	THR

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Mol	Chain	Res	Type
8	Y	50	VAL
8	Y	68	ASP
8	Y	79	ASN
8	Y	109	SER
8	Y	127	ASP
8	Y	147	SER
8	Y	149	LEU
8	Y	153	LEU
8	Y	157	LEU
8	Y	165	LEU
8	Y	170	SER
8	Y	181	VAL
8	Y	188	SER
8	Y	201	CYS
8	Y	203	VAL
8	Y	204	VAL
8	Y	224	SER
8	Y	232	VAL
8	Y	237	SER
8	Y	241	THR
8	Y	256	LEU
8	Y	259	SER
8	Y	274	THR
8	Y	277	THR
8	Y	288	THR
8	Y	293	VAL
8	Y	298	LEU
8	Y	313	THR
8	Y	316	CYS
8	Y	331	THR
8	Y	333	VAL
8	Y	356	ILE
8	Y	361	SER
8	Y	373	VAL
8	Y	391	THR
8	Y	402	GLU
8	Y	425	ARG
8	Y	442	ASP
8	Z	7	THR
8	Z	17	ILE
8	Z	37	VAL
8	Z	39	GLU

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Mol	Chain	Res	Type
8	Z	45	THR
8	Z	50	VAL
8	Z	68	ASP
8	Z	79	ASN
8	Z	109	SER
8	Z	127	ASP
8	Z	147	SER
8	Z	149	LEU
8	Z	153	LEU
8	Z	157	LEU
8	Z	165	LEU
8	Z	170	SER
8	Z	181	VAL
8	Z	188	SER
8	Z	201	CYS
8	Z	203	VAL
8	Z	204	VAL
8	Z	224	SER
8	Z	232	VAL
8	Z	237	SER
8	Z	241	THR
8	Z	256	LEU
8	Z	259	SER
8	Z	274	THR
8	Z	277	THR
8	Z	288	THR
8	Z	293	VAL
8	Z	298	LEU
8	Z	313	THR
8	Z	316	CYS
8	Z	331	THR
8	Z	333	VAL
8	Z	356	ILE
8	Z	361	SER
8	Z	373	VAL
8	Z	391	THR
8	Z	402	GLU
8	Z	425	ARG
8	Z	442	ASP
4	a	60	LYS
4	f	86	VAL
3	E	233	VAL

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Mol	Chain	Res	Type
3	E	549	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (389) such sidechains are listed below:

Mol	Chain	Res	Type
1	l	107	HIS
2	e	78	ASN
2	e	101	HIS
2	e	137	GLN
2	e	161	HIS
2	e	173	HIS
2	e	280	ASN
3	A	152	GLN
3	A	242	GLN
3	A	314	HIS
3	A	329	GLN
3	A	360	HIS
3	A	438	GLN
3	A	458	ASN
3	A	631	ASN
3	A	684	GLN
3	A	688	ASN
3	A	692	ASN
3	A	694	GLN
3	A	828	ASN
4	B	330	GLN
4	B	444	HIS
4	B	500	GLN
4	B	550	ASN
4	B	596	ASN
4	B	693	ASN
4	B	702	HIS
4	B	703	GLN
4	B	773	ASN
4	B	781	GLN
4	B	812	GLN
4	B	830	ASN
4	B	860	GLN
4	B	883	ASN
4	B	885	HIS
3	C	166	ASN
3	C	173	HIS

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Mol	Chain	Res	Type
3	C	287	GLN
3	C	329	GLN
3	C	371	GLN
3	C	512	HIS
3	C	530	HIS
3	C	639	GLN
3	C	674	GLN
3	C	684	GLN
3	C	691	GLN
4	D	259	GLN
4	D	389	GLN
4	D	401	HIS
4	D	500	GLN
4	D	531	GLN
4	D	558	HIS
4	D	560	GLN
4	D	596	ASN
4	D	609	ASN
4	D	665	ASN
4	D	705	HIS
4	D	740	GLN
4	D	742	GLN
4	D	773	ASN
4	D	781	GLN
4	D	789	GLN
4	D	801	GLN
4	D	859	GLN
4	D	860	GLN
4	F	265	ASN
4	F	310	GLN
4	F	329	HIS
4	F	387	HIS
4	F	416	GLN
4	F	491	ASN
4	F	495	GLN
4	F	500	GLN
4	F	595	HIS
4	F	702	HIS
4	F	716	HIS
4	F	773	ASN
4	F	774	GLN
4	F	855	GLN

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Mol	Chain	Res	Type
4	F	860	GLN
4	F	885	HIS
3	G	172	GLN
3	G	236	GLN
3	G	287	GLN
3	G	289	ASN
3	G	322	GLN
3	G	329	GLN
3	G	424	ASN
3	G	458	ASN
3	G	644	HIS
3	G	662	ASN
3	G	691	GLN
3	G	726	HIS
3	G	741	ASN
3	G	763	GLN
3	G	828	ASN
4	H	322	GLN
4	H	329	HIS
4	H	387	HIS
4	H	389	GLN
4	H	416	GLN
4	H	479	GLN
4	H	596	ASN
4	H	693	ASN
4	H	703	GLN
4	H	717	GLN
4	H	719	GLN
4	H	736	ASN
4	H	739	GLN
4	H	883	ASN
6	I	284	GLN
6	I	353	GLN
6	I	370	GLN
6	I	390	HIS
6	I	397	GLN
6	I	398	GLN
6	I	401	HIS
6	I	504	HIS
6	I	547	GLN
6	I	561	HIS
1	J	231	GLN

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Mol	Chain	Res	Type
1	J	269	GLN
1	J	304	HIS
1	J	328	GLN
1	J	408	GLN
1	J	495	GLN
1	J	694	HIS
1	J	698	GLN
1	J	705	ASN
1	J	721	GLN
1	J	754	ASN
1	J	822	ASN
1	J	892	HIS
1	J	895	ASN
1	J	915	HIS
1	J	925	GLN
1	J	938	HIS
6	K	35	HIS
6	K	43	ASN
6	K	61	GLN
6	K	67	GLN
6	K	69	GLN
6	K	123	ASN
6	K	152	GLN
6	K	186	GLN
6	K	193	HIS
6	K	290	ASN
6	K	302	ASN
6	K	339	HIS
6	K	390	HIS
6	K	499	GLN
6	K	509	GLN
6	K	533	GLN
6	K	543	GLN
6	K	547	GLN
7	L	328	GLN
7	L	469	GLN
7	L	603	ASN
7	L	1492	ASN
7	L	1508	HIS
7	L	1625	GLN
7	L	1654	GLN
7	L	1673	GLN

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Mol	Chain	Res	Type
7	L	1679	GLN
7	L	1759	HIS
7	L	1770	ASN
8	O	54	GLN
8	O	110	GLN
8	O	167	GLN
8	O	174	ASN
8	O	175	GLN
8	O	184	GLN
8	O	187	ASN
8	O	207	ASN
8	O	227	GLN
8	O	229	ASN
8	O	302	ASN
8	O	332	GLN
8	O	357	GLN
8	O	407	GLN
8	O	429	GLN
8	O	430	GLN
8	P	54	GLN
8	P	110	GLN
8	P	167	GLN
8	P	174	ASN
8	P	175	GLN
8	P	184	GLN
8	P	187	ASN
8	P	207	ASN
8	P	227	GLN
8	P	229	ASN
8	P	250	ASN
8	P	302	ASN
8	P	332	GLN
8	P	407	GLN
8	P	429	GLN
8	P	430	GLN
8	Q	54	GLN
8	Q	110	GLN
8	Q	167	GLN
8	Q	174	ASN
8	Q	175	GLN
8	Q	184	GLN
8	Q	187	ASN

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Mol	Chain	Res	Type
8	Q	207	ASN
8	Q	227	GLN
8	Q	229	ASN
8	Q	302	ASN
8	Q	332	GLN
8	Q	407	GLN
8	Q	429	GLN
8	Q	430	GLN
8	R	54	GLN
8	R	110	GLN
8	R	167	GLN
8	R	174	ASN
8	R	175	GLN
8	R	184	GLN
8	R	187	ASN
8	R	207	ASN
8	R	227	GLN
8	R	229	ASN
8	R	302	ASN
8	R	332	GLN
8	R	357	GLN
8	R	407	GLN
8	R	429	GLN
8	R	430	GLN
8	S	54	GLN
8	S	110	GLN
8	S	167	GLN
8	S	174	ASN
8	S	175	GLN
8	S	187	ASN
8	S	207	ASN
8	S	227	GLN
8	S	229	ASN
8	S	302	ASN
8	S	332	GLN
8	S	334	HIS
8	S	407	GLN
8	S	429	GLN
8	S	430	GLN
8	T	54	GLN
8	T	110	GLN
8	T	167	GLN

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Mol	Chain	Res	Type
8	T	174	ASN
8	T	175	GLN
8	T	184	GLN
8	T	187	ASN
8	T	207	ASN
8	T	227	GLN
8	T	229	ASN
8	T	250	ASN
8	T	302	ASN
8	T	332	GLN
8	T	334	HIS
8	T	357	GLN
8	T	407	GLN
8	T	429	GLN
8	T	430	GLN
8	U	54	GLN
8	U	110	GLN
8	U	167	GLN
8	U	174	ASN
8	U	175	GLN
8	U	184	GLN
8	U	187	ASN
8	U	207	ASN
8	U	227	GLN
8	U	229	ASN
8	U	302	ASN
8	U	332	GLN
8	U	334	HIS
8	U	338	GLN
8	U	407	GLN
8	U	429	GLN
8	U	430	GLN
8	V	54	GLN
8	V	110	GLN
8	V	167	GLN
8	V	174	ASN
8	V	175	GLN
8	V	184	GLN
8	V	187	ASN
8	V	207	ASN
8	V	227	GLN
8	V	229	ASN

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Mol	Chain	Res	Type
8	V	302	ASN
8	V	332	GLN
8	V	407	GLN
8	V	429	GLN
8	V	430	GLN
8	W	54	GLN
8	W	110	GLN
8	W	167	GLN
8	W	174	ASN
8	W	175	GLN
8	W	184	GLN
8	W	187	ASN
8	W	207	ASN
8	W	227	GLN
8	W	229	ASN
8	W	302	ASN
8	W	332	GLN
8	W	407	GLN
8	W	429	GLN
8	W	430	GLN
8	X	54	GLN
8	X	110	GLN
8	X	167	GLN
8	X	174	ASN
8	X	175	GLN
8	X	184	GLN
8	X	187	ASN
8	X	207	ASN
8	X	227	GLN
8	X	229	ASN
8	X	302	ASN
8	X	332	GLN
8	X	334	HIS
8	X	357	GLN
8	X	407	GLN
8	X	429	GLN
8	X	430	GLN
8	Y	54	GLN
8	Y	110	GLN
8	Y	167	GLN
8	Y	174	ASN
8	Y	175	GLN

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Mol	Chain	Res	Type
8	Y	184	GLN
8	Y	187	ASN
8	Y	207	ASN
8	Y	227	GLN
8	Y	229	ASN
8	Y	302	ASN
8	Y	332	GLN
8	Y	357	GLN
8	Y	407	GLN
8	Y	429	GLN
8	Y	430	GLN
8	Z	54	GLN
8	Z	110	GLN
8	Z	167	GLN
8	Z	174	ASN
8	Z	175	GLN
8	Z	184	GLN
8	Z	187	ASN
8	Z	207	ASN
8	Z	227	GLN
8	Z	229	ASN
8	Z	302	ASN
8	Z	332	GLN
8	Z	407	GLN
8	Z	429	GLN
8	Z	430	GLN
4	a	14	GLN
4	a	30	GLN
4	a	31	GLN
4	a	33	GLN
4	a	65	GLN
4	a	78	HIS
4	f	14	GLN
4	f	30	GLN
4	f	33	GLN
4	h	78	HIS
5	d	17	ASN
7	c	29	ASN
7	c	48	ASN
7	c	161	GLN
7	c	176	GLN
7	c	180	GLN

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Mol	Chain	Res	Type
4	j	14	GLN
4	j	31	GLN
3	E	152	GLN
3	E	261	HIS
3	E	289	ASN
3	E	316	GLN
3	E	412	HIS
3	E	430	GLN
3	E	438	GLN
3	E	465	HIS
3	E	585	GLN
3	E	644	HIS
3	E	694	GLN
3	E	741	ASN
3	E	763	GLN
3	E	767	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

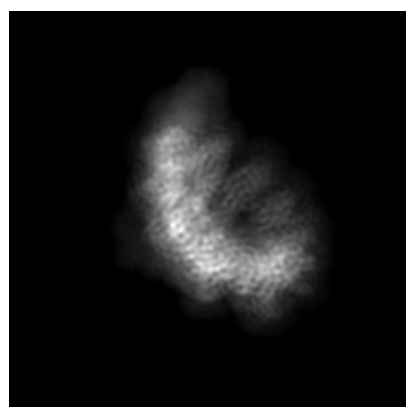
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14012. These allow visual inspection of the internal detail of the map and identification of artifacts.

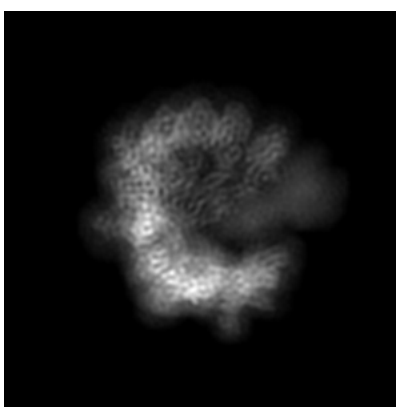
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

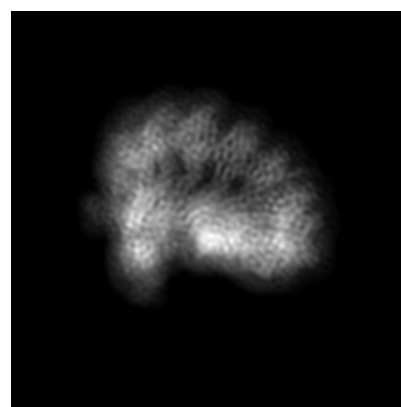
6.1.1 Primary map



X



Y



Z

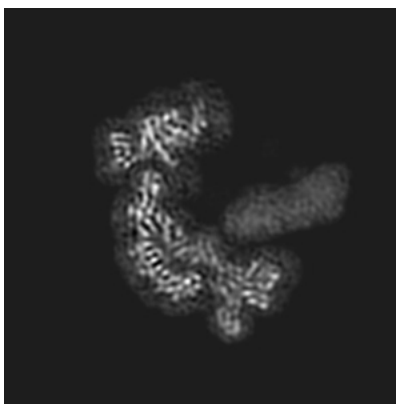
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

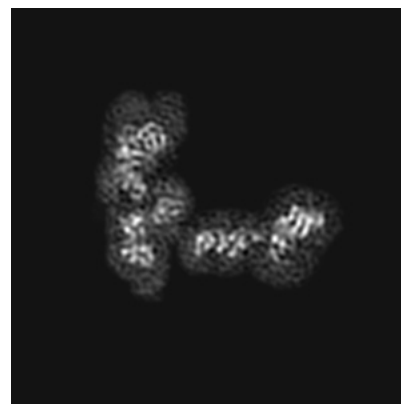
6.2.1 Primary map



X Index: 100



Y Index: 100

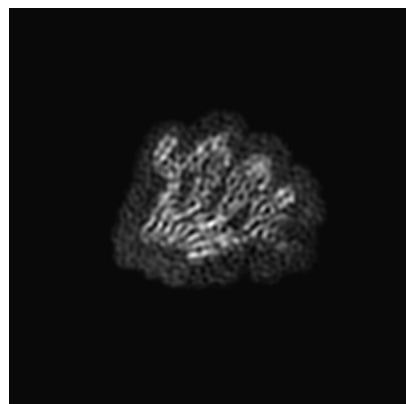


Z Index: 100

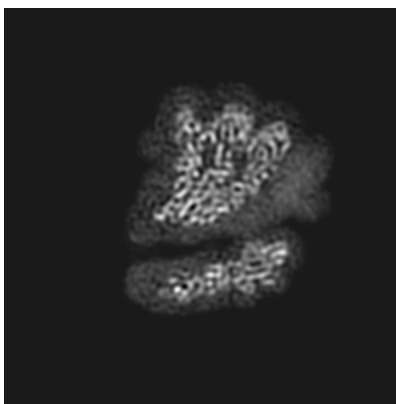
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

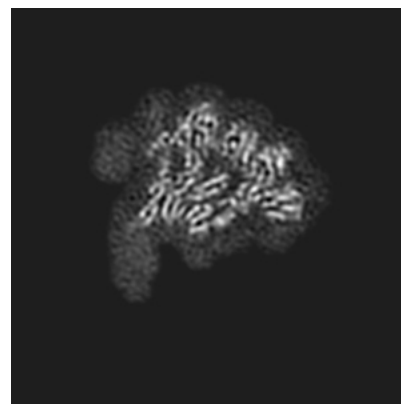
6.3.1 Primary map



X Index: 63



Y Index: 81



Z Index: 72

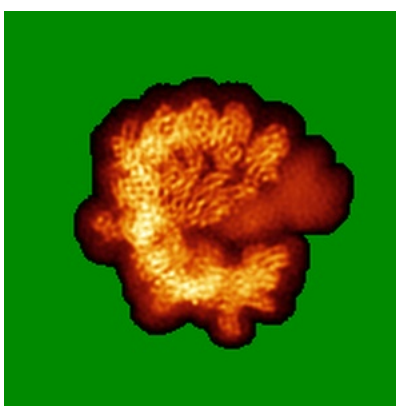
The images above show the largest variance slices of the map in three orthogonal directions.

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 0.0368. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

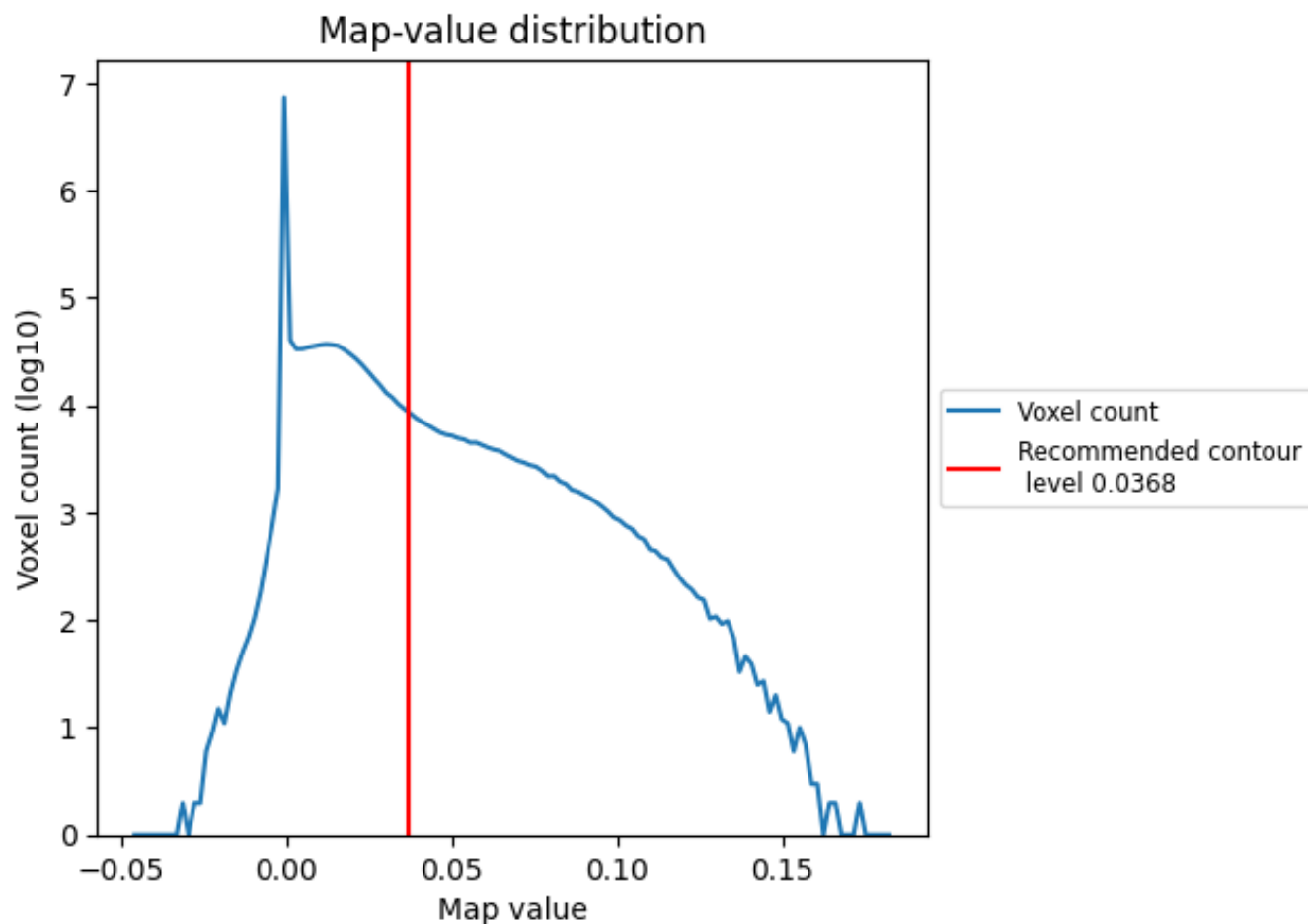
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

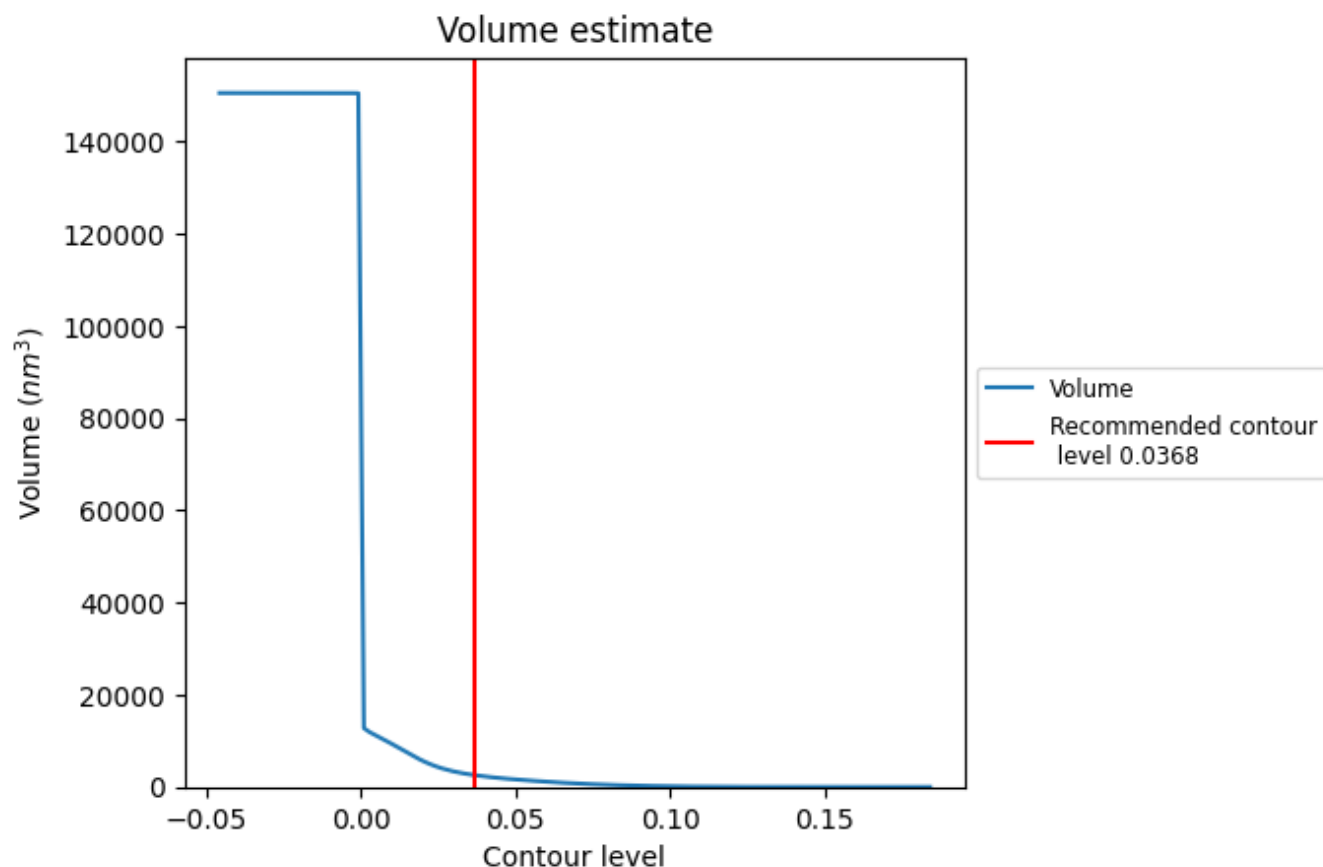
This section contains the results of statistical analysis of the map.

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.

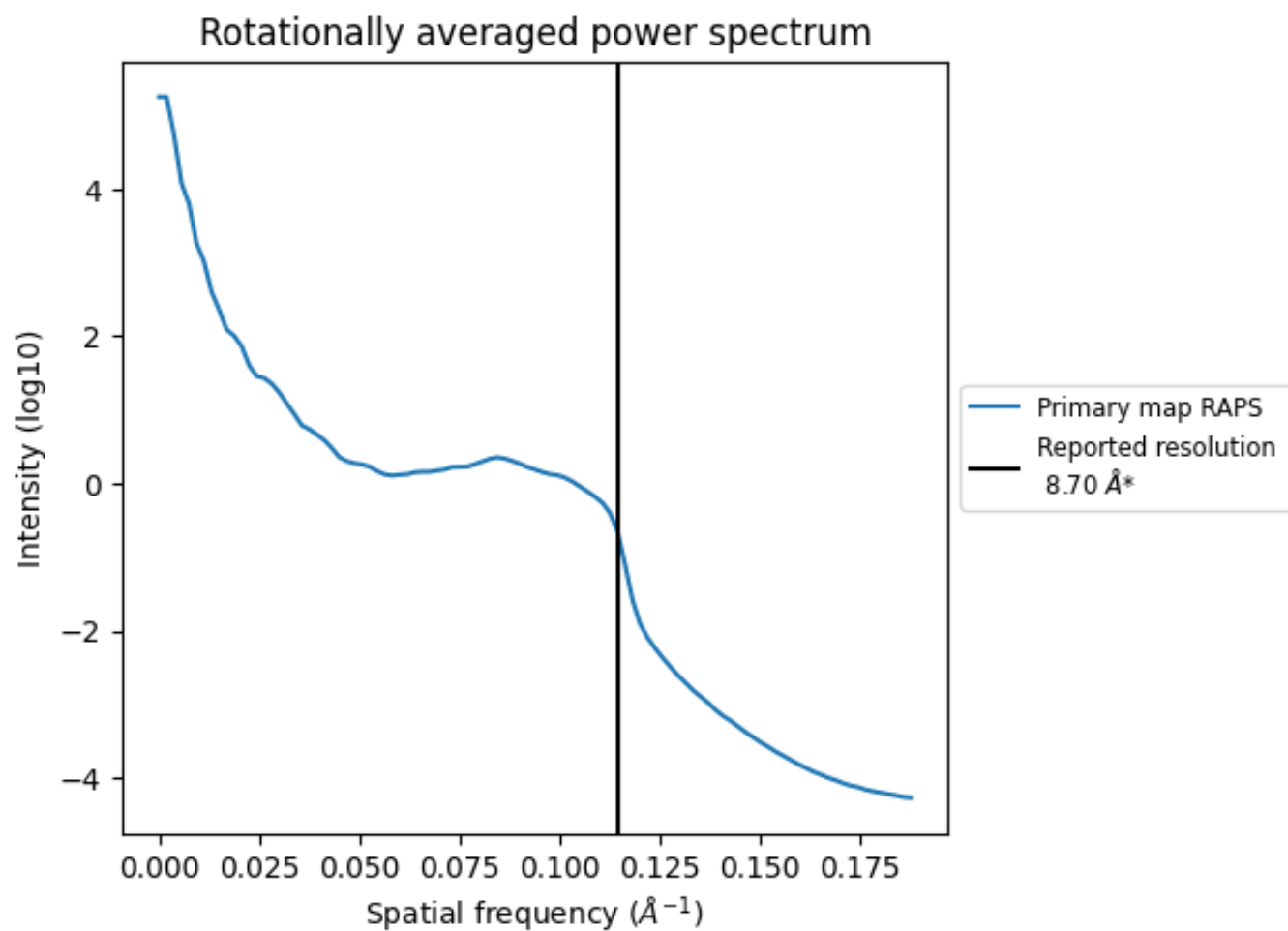
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2556 nm^3 ; this corresponds to an approximate mass of 2308 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 0.115 Å⁻¹

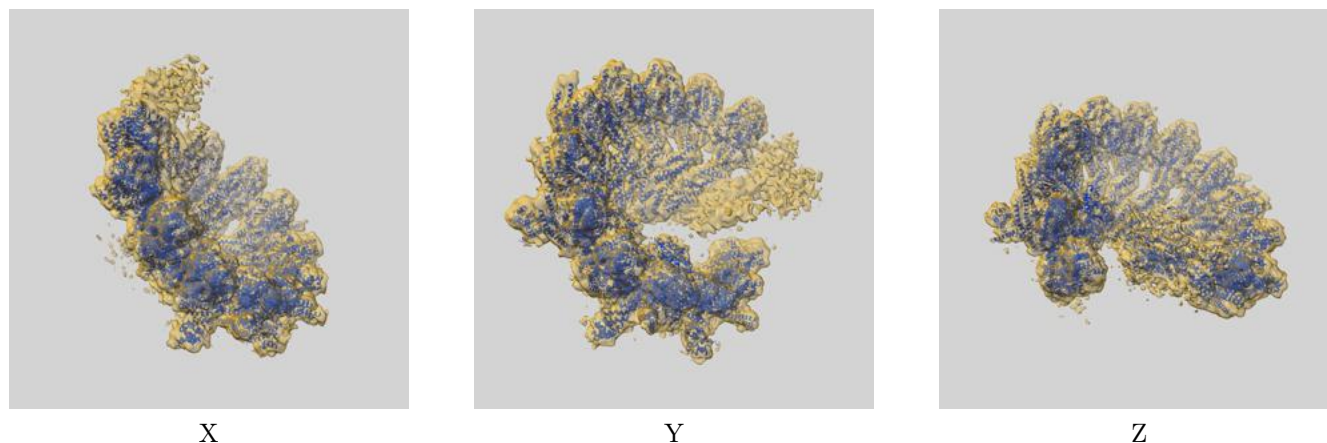
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

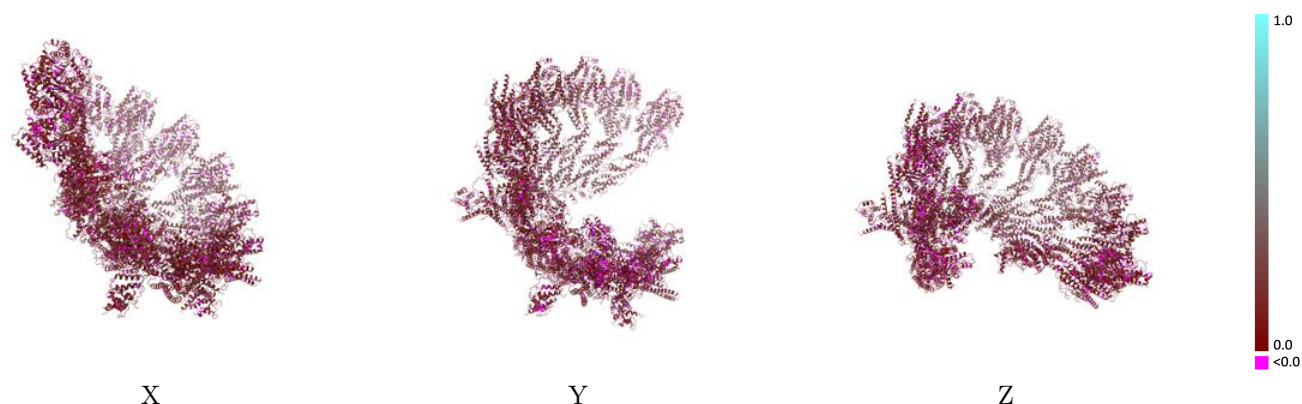
This section contains information regarding the fit between EMDB map EMD-14012 and PDB model 7QJ7. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



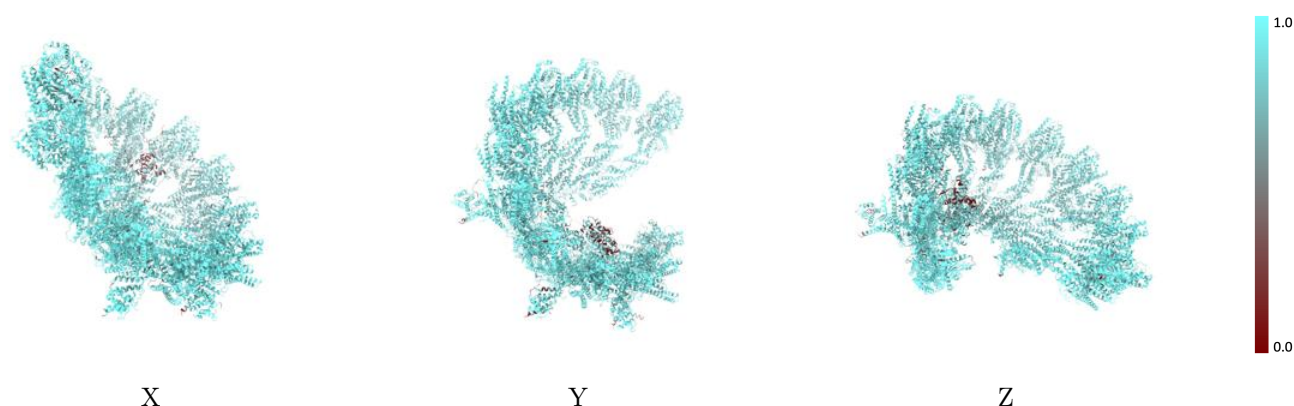
The images above show the 3D surface view of the map at the recommended contour level 0.0368 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



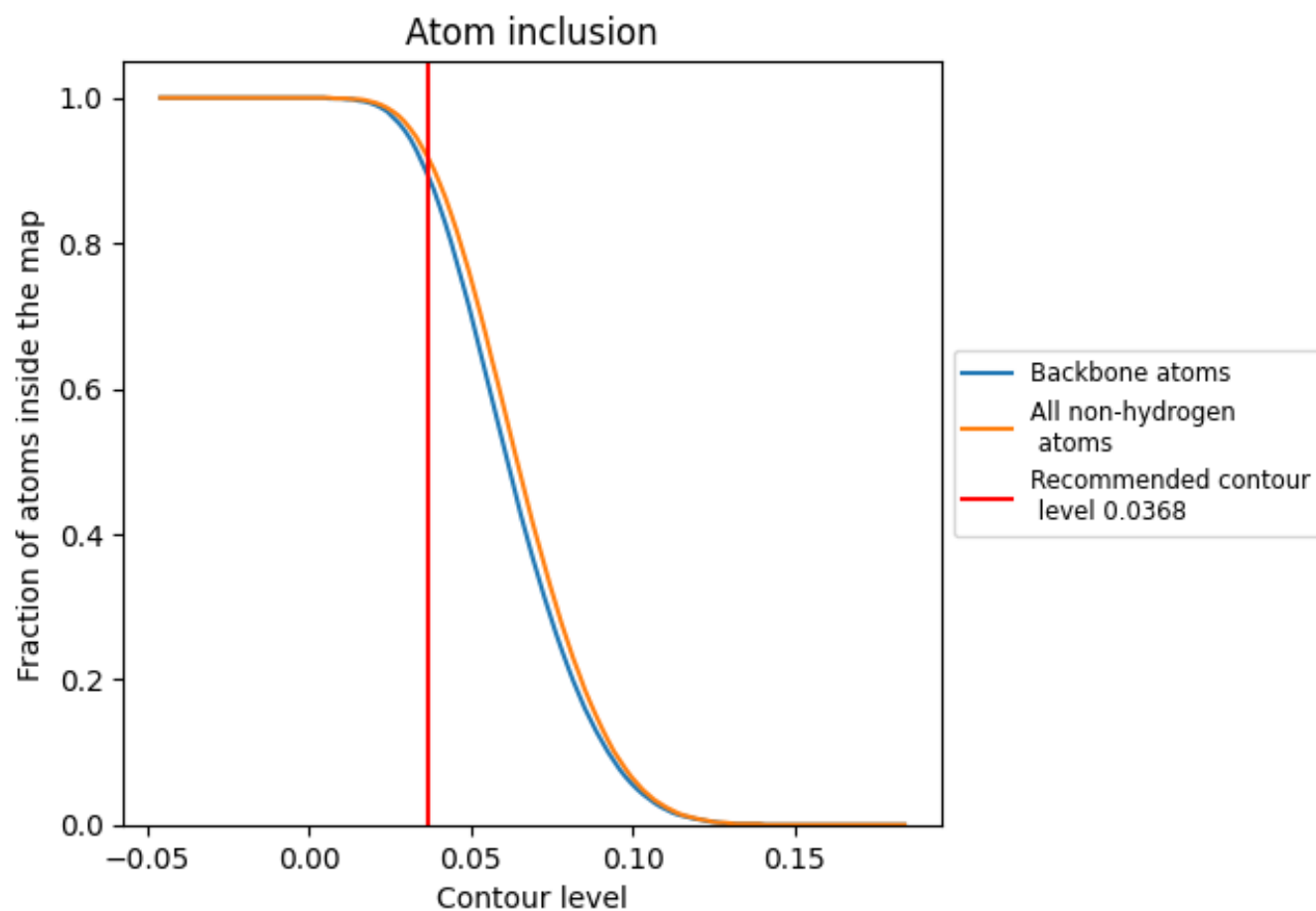
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0368).

9.4 Atom inclusion ⓘ



At the recommended contour level, 89% of all backbone atoms, 92% 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 (0.0368) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9180	 0.1250
A	 0.9460	 0.1230
B	 0.9210	 0.1280
C	 0.9400	 0.1260
D	 0.9330	 0.1350
E	 0.9360	 0.1360
F	 0.9430	 0.1320
G	 0.9420	 0.1440
H	 0.9390	 0.1410
I	 0.9430	 0.1480
J	 0.9500	 0.1390
K	 0.9470	 0.1370
L	 0.9550	 0.1330
O	 0.9340	 0.0950
P	 0.8950	 0.1120
Q	 0.8780	 0.0970
R	 0.9080	 0.1030
S	 0.9300	 0.1010
T	 0.9440	 0.1230
U	 0.9450	 0.1250
V	 0.9530	 0.1420
W	 0.9530	 0.1300
X	 0.9600	 0.1240
Y	 0.9380	 0.1020
Z	 0.8930	 0.1080
a	 0.8410	 0.1240
b	 0.8700	 0.1620
c	 0.8360	 0.1090
d	 0.8360	 0.1670
e	 0.6190	 0.0790
f	 0.9030	 0.1040
g	 0.8070	 0.1270
h	 0.8360	 0.1190
i	 0.7580	 0.0870
j	 0.9330	 0.1090



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Chain	Atom inclusion	Q-score
k	 0.8870	 0.1210
l	 0.9300	 0.1370
m	 0.9180	 0.1680