



Full wwPDB EM Validation Report ⓘ

Mar 4, 2026 – 08:07 PM UTC

PDB ID : 7QJ4 / pdb_00007qj4
EMDB ID : EMD-14009
Title : Structure of recombinant human gamma-Tubulin Ring Complex 10-spoked assembly intermediate (spokes 5-14)
Authors : Zupa, E.; Pfeffer, S.
Deposited on : 2021-12-16
Resolution : 9.00 Å (reported)
Based on initial models : 6V6S, 6L81, 6X0U, 7AS4

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

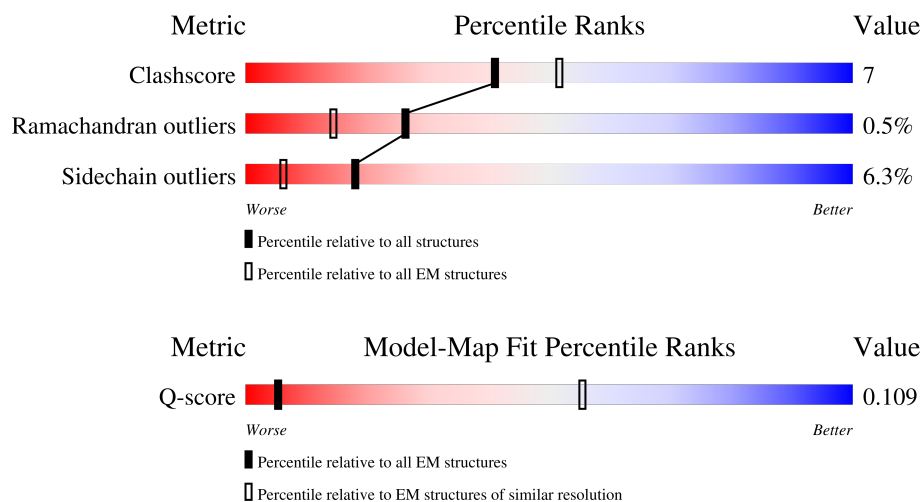
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 9.00 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	257 (8.50 - 9.50)

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

Mol	Chain	Length	Quality of chain
1	1	451	64% 64% 23% 6% 7%
1	2	451	80% 64% 23% 6% 7%
1	S	451	85% 64% 23% 6% 7%
1	T	451	53% 64% 23% 6% 7%

Continued on next page...

Continued from previous page...

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

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 87259 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	n	99	Total	C	N	O	S	0	0
			803	509	148	144	2		

Continued on next page...

Continued from previous page...

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

- Molecule 4 is a protein called Mitotic-spindle organizing protein 1.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	638	Total	C	N	O	S	0	0
			5202	3354	873	942	33		
5	G	640	Total	C	N	O	S	0	0
			5216	3359	878	946	33		
5	M	636	Total	C	N	O	S	0	0
			5186	3342	871	940	33		

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

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

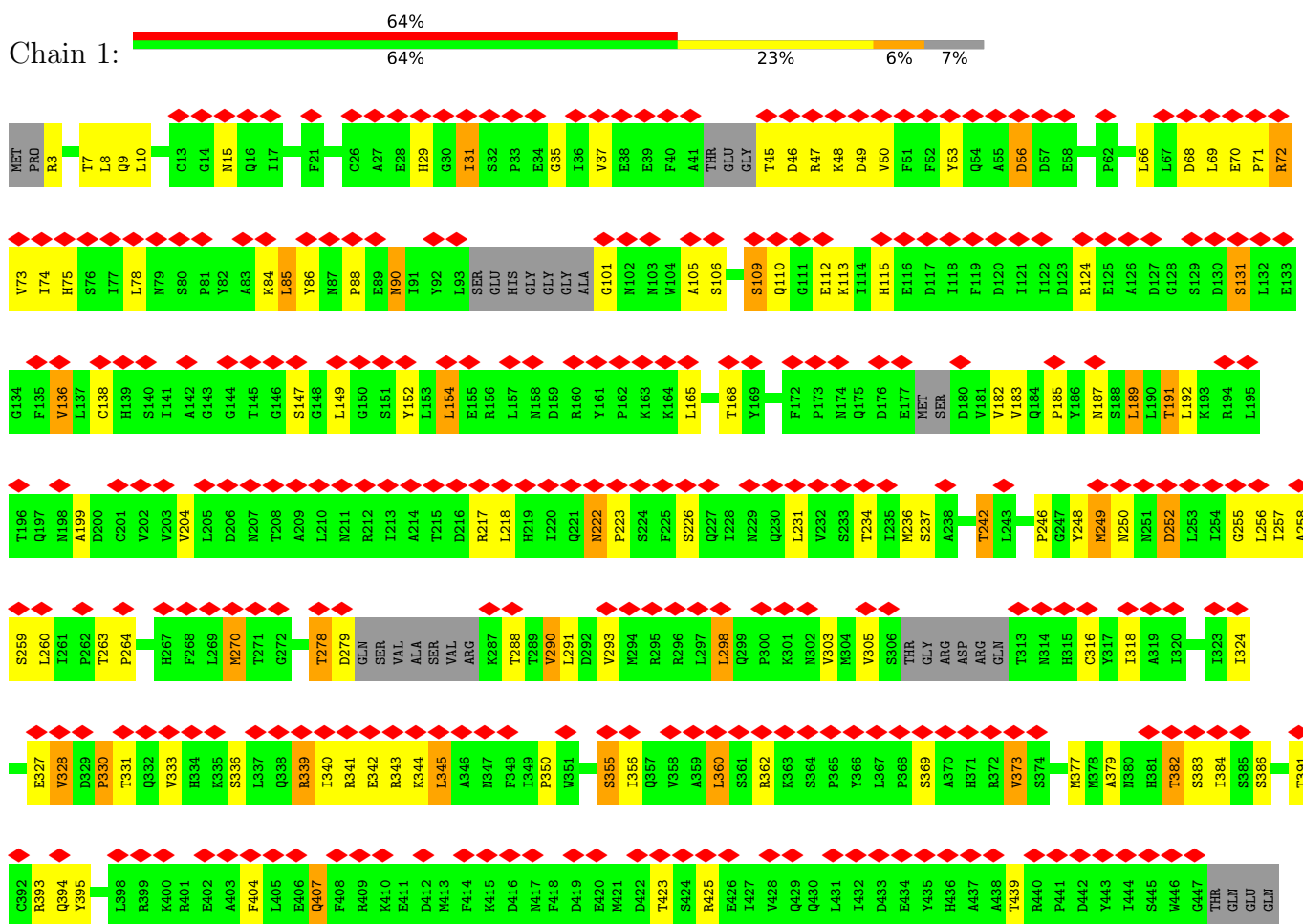
- Molecule 7 is a protein called Gamma-tubulin complex component 6.

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

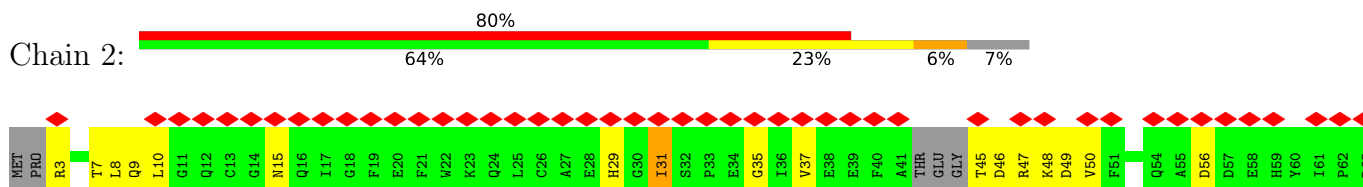
3 Residue-property plots

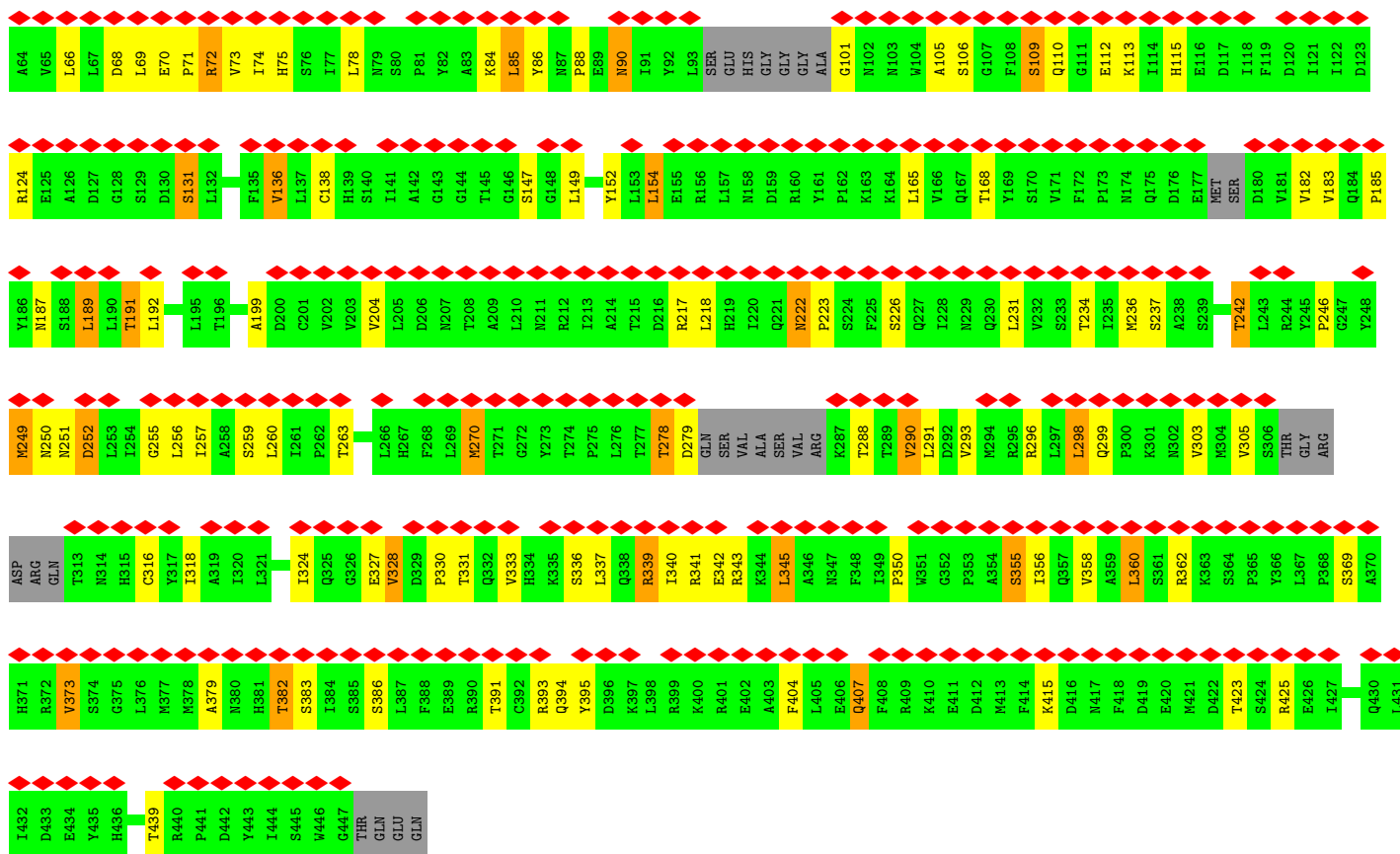
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Tubulin gamma-1 chain

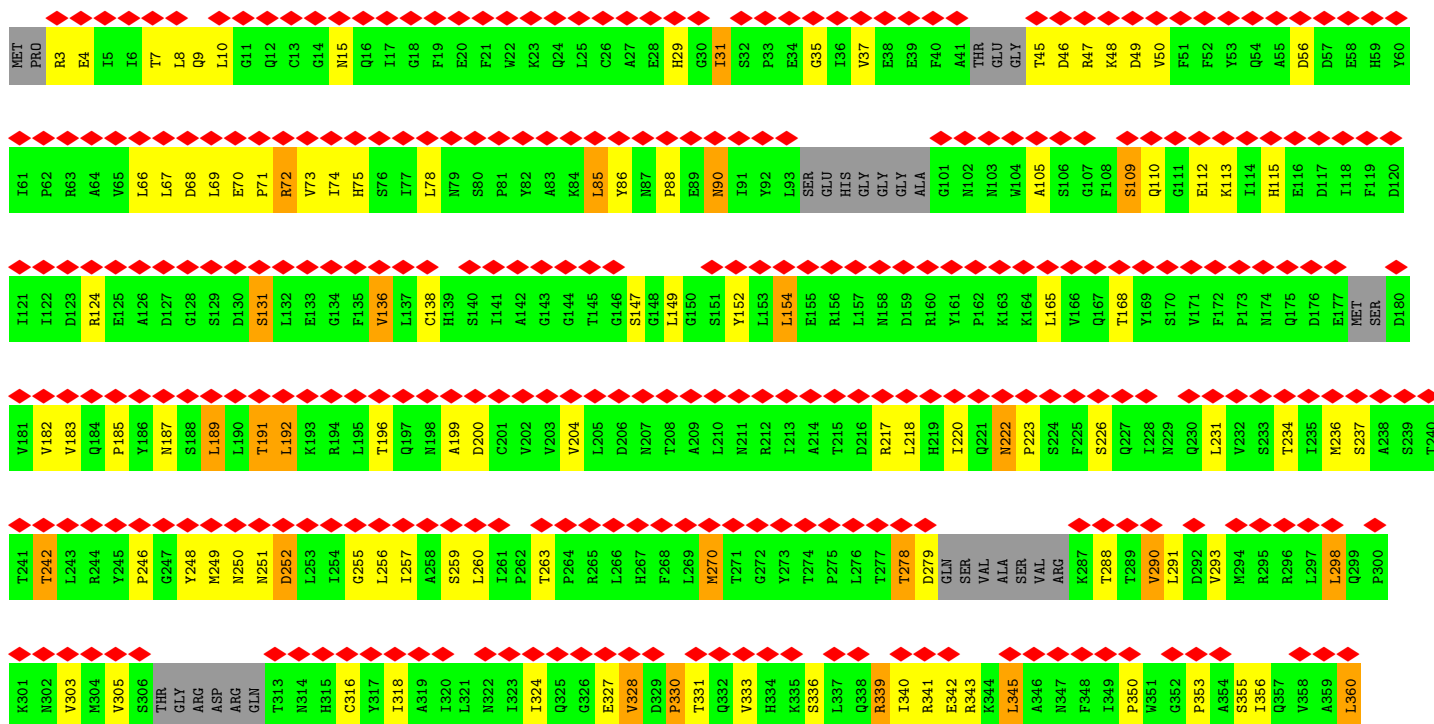
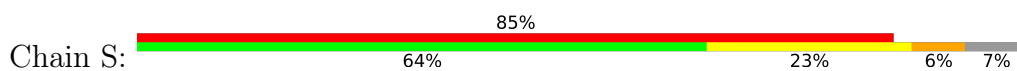


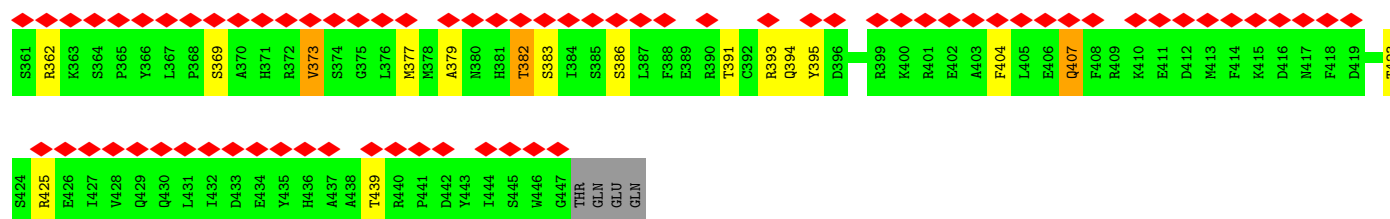
- Molecule 1: Tubulin gamma-1 chain



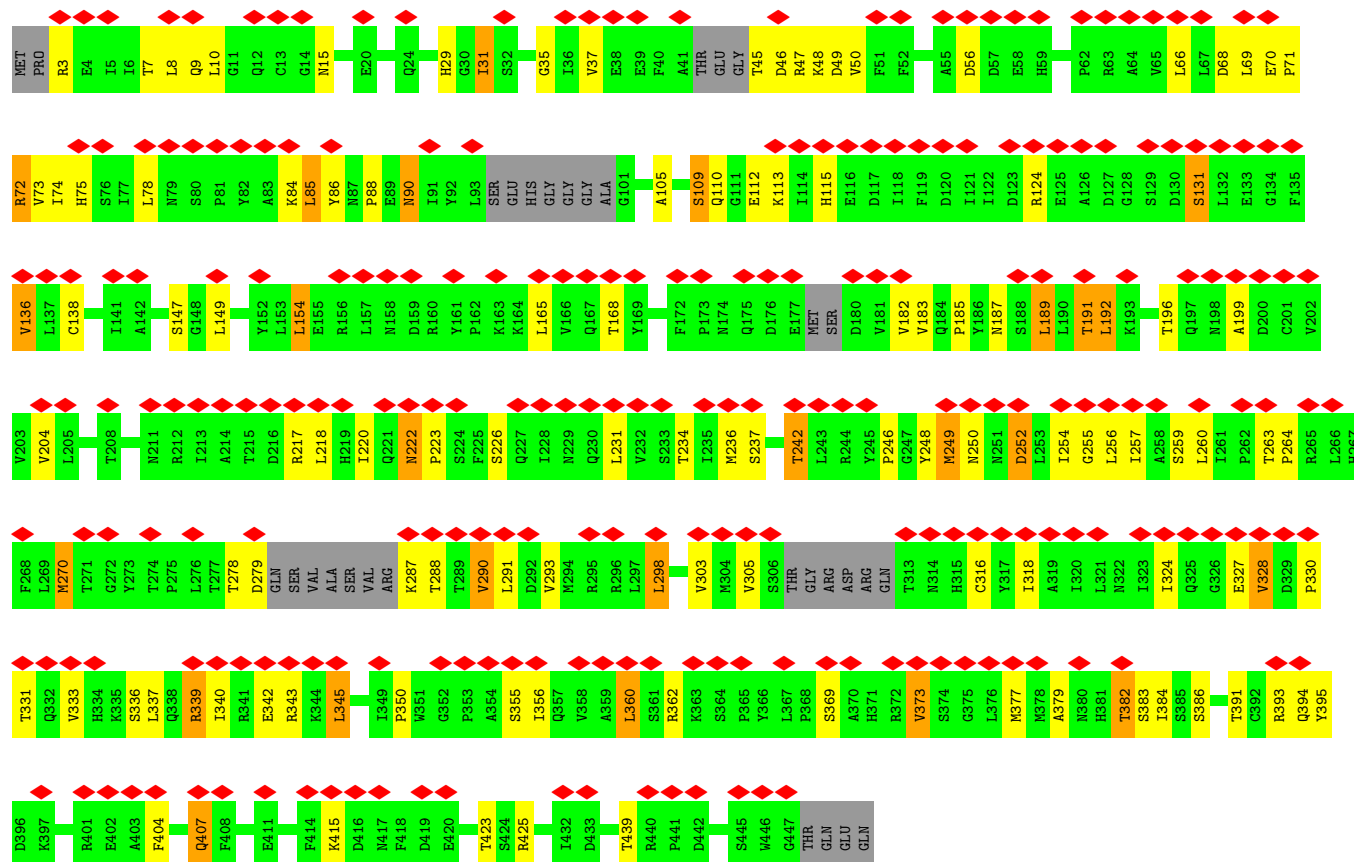


• Molecule 1: Tubulin gamma-1 chain

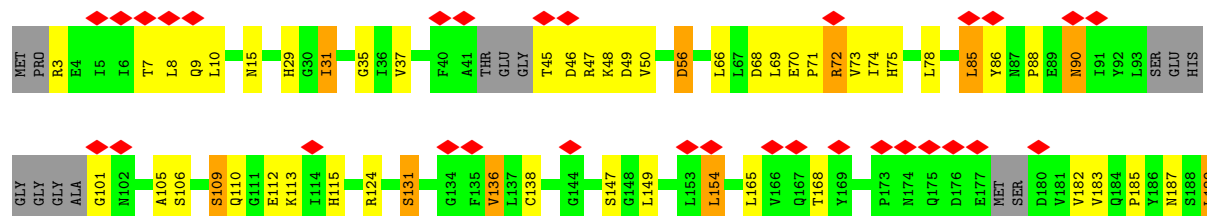


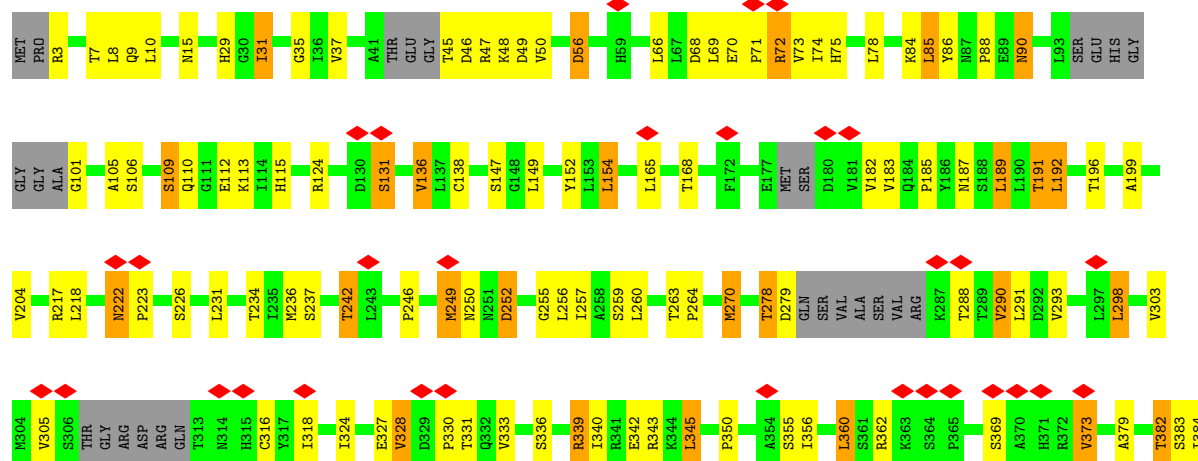


• Molecule 1: Tubulin gamma-1 chain

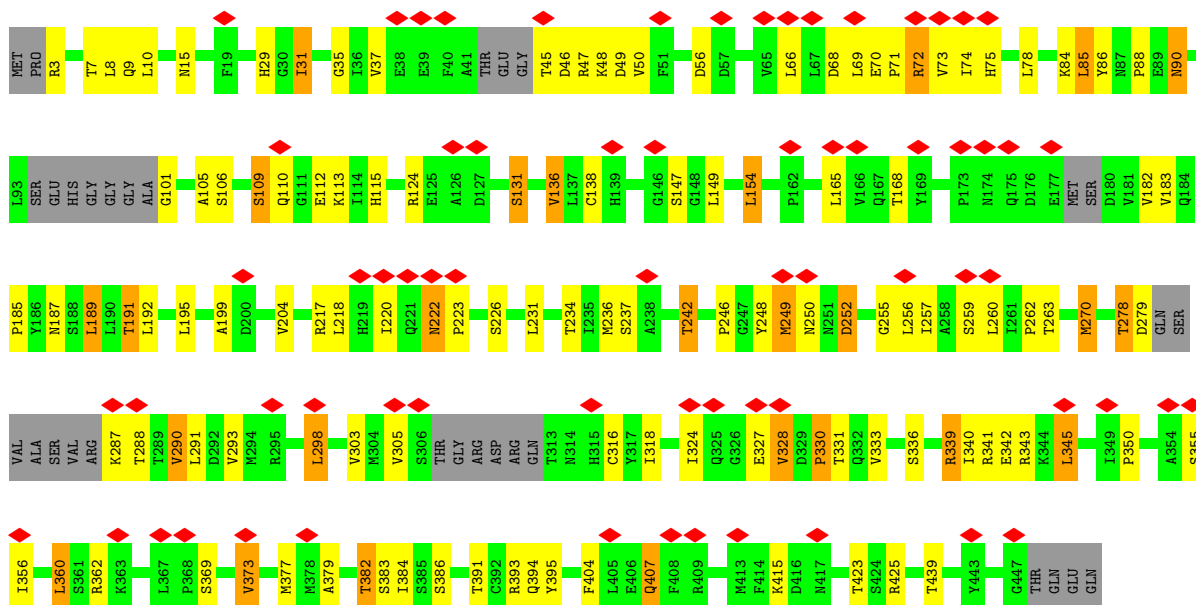


• Molecule 1: Tubulin gamma-1 chain



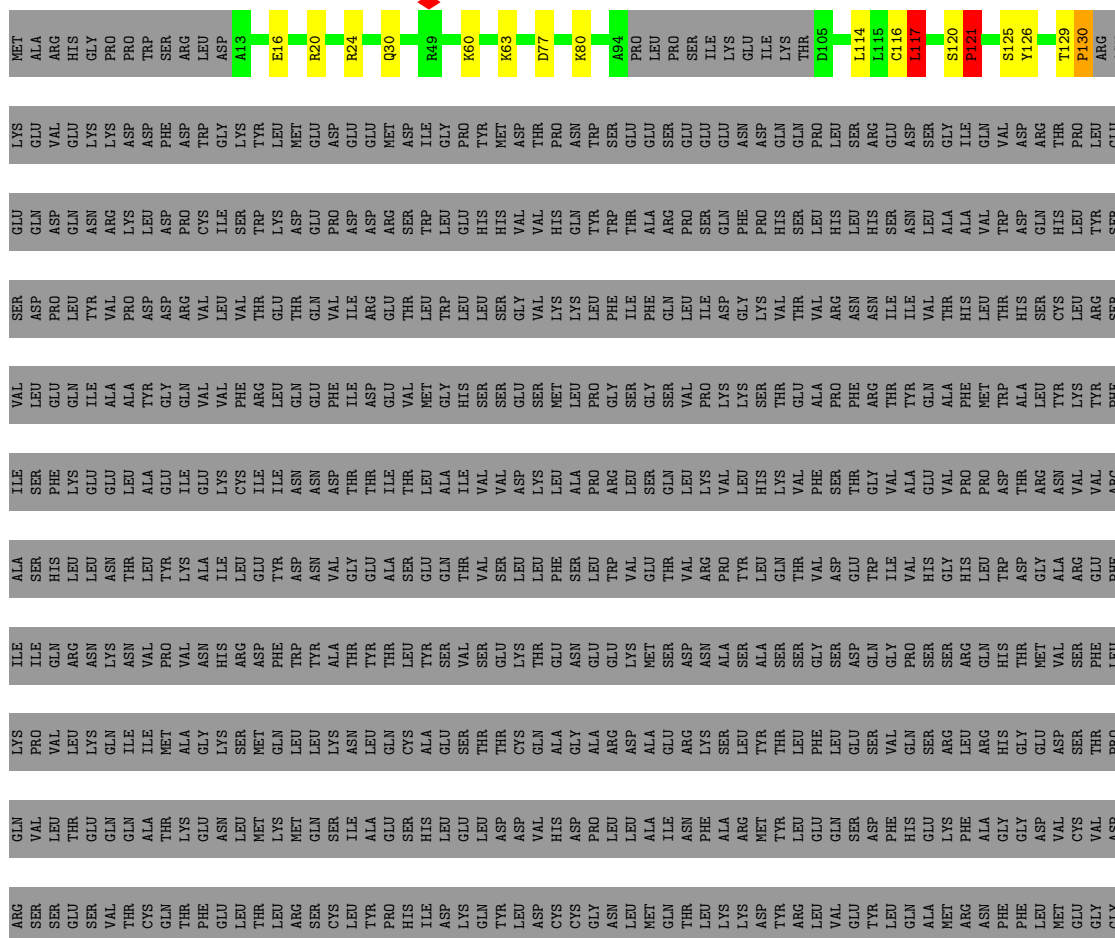




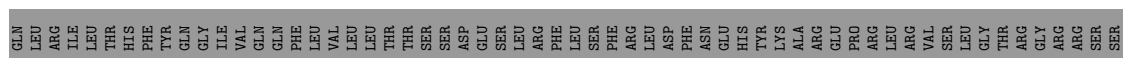


• Molecule 2: Gamma-tubulin complex component 5

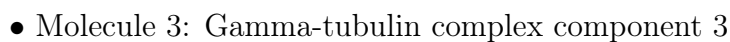
Chain 1: 9% . 89%

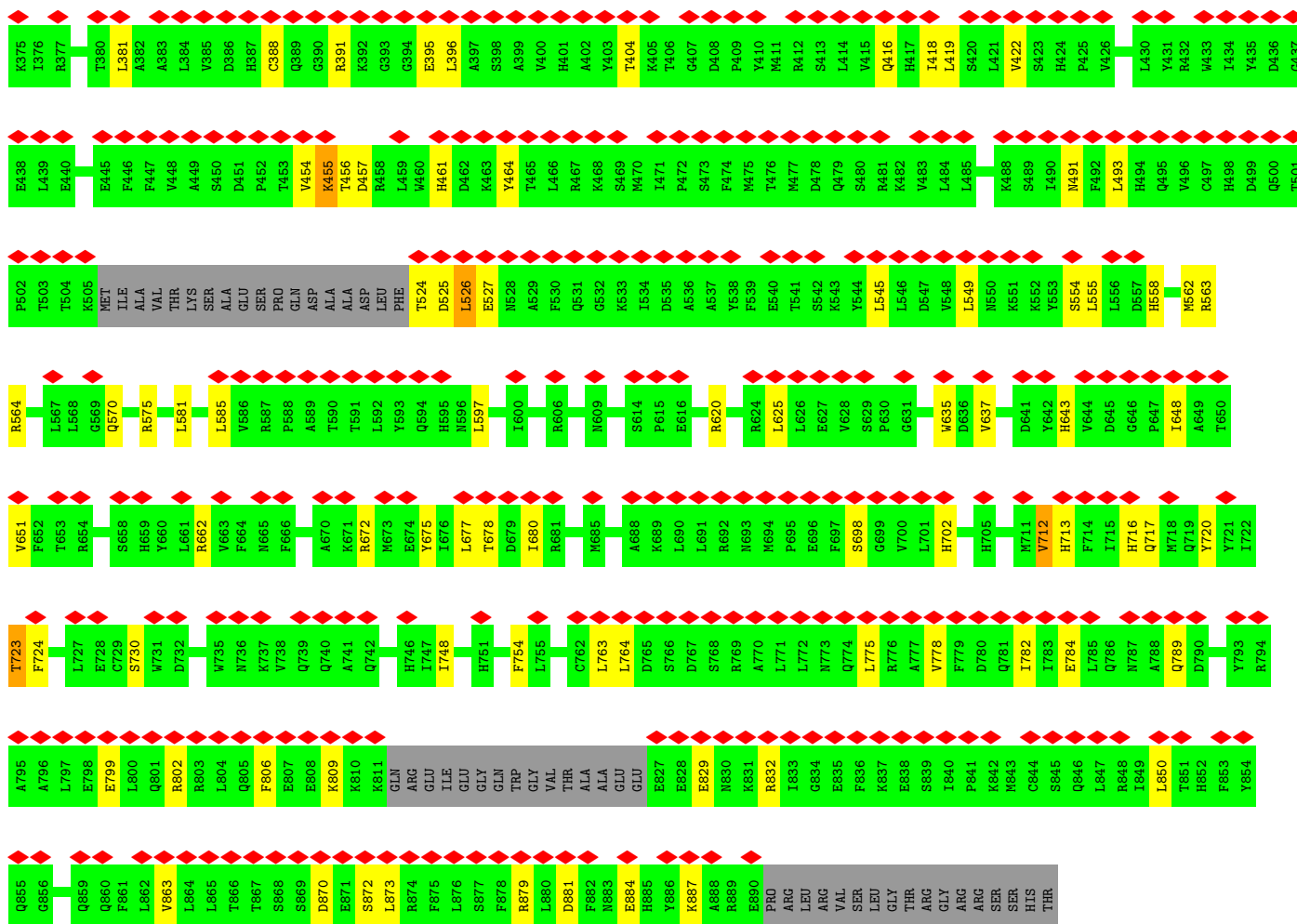




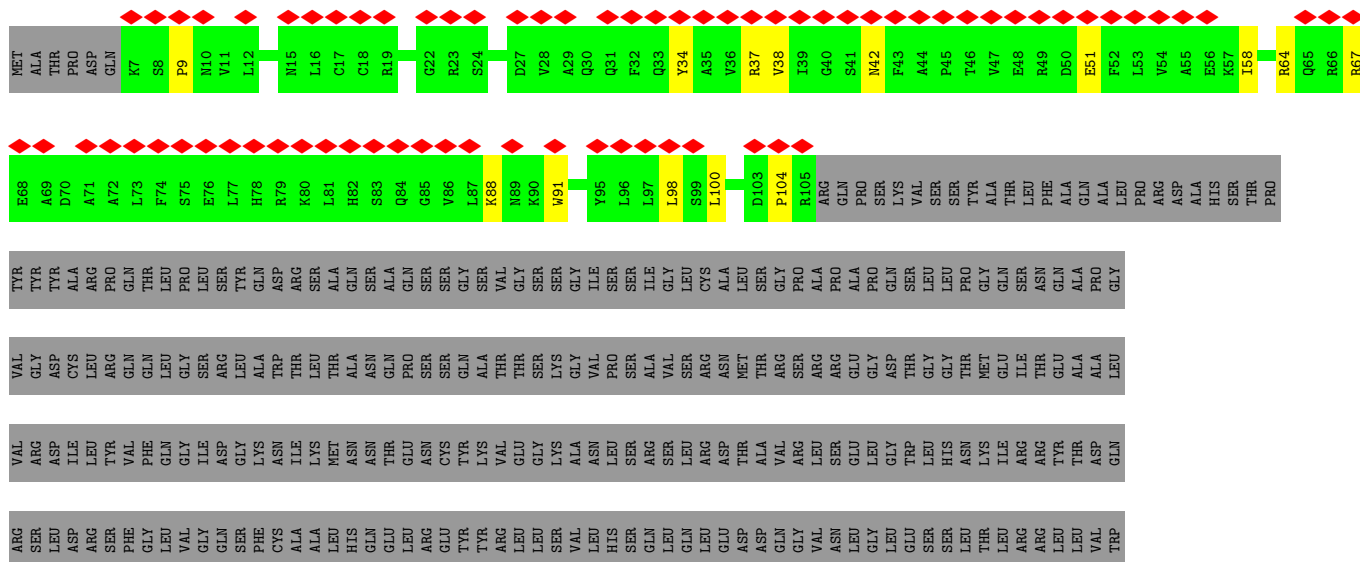


- Molecule 3: Gamma-tubulin complex component 3

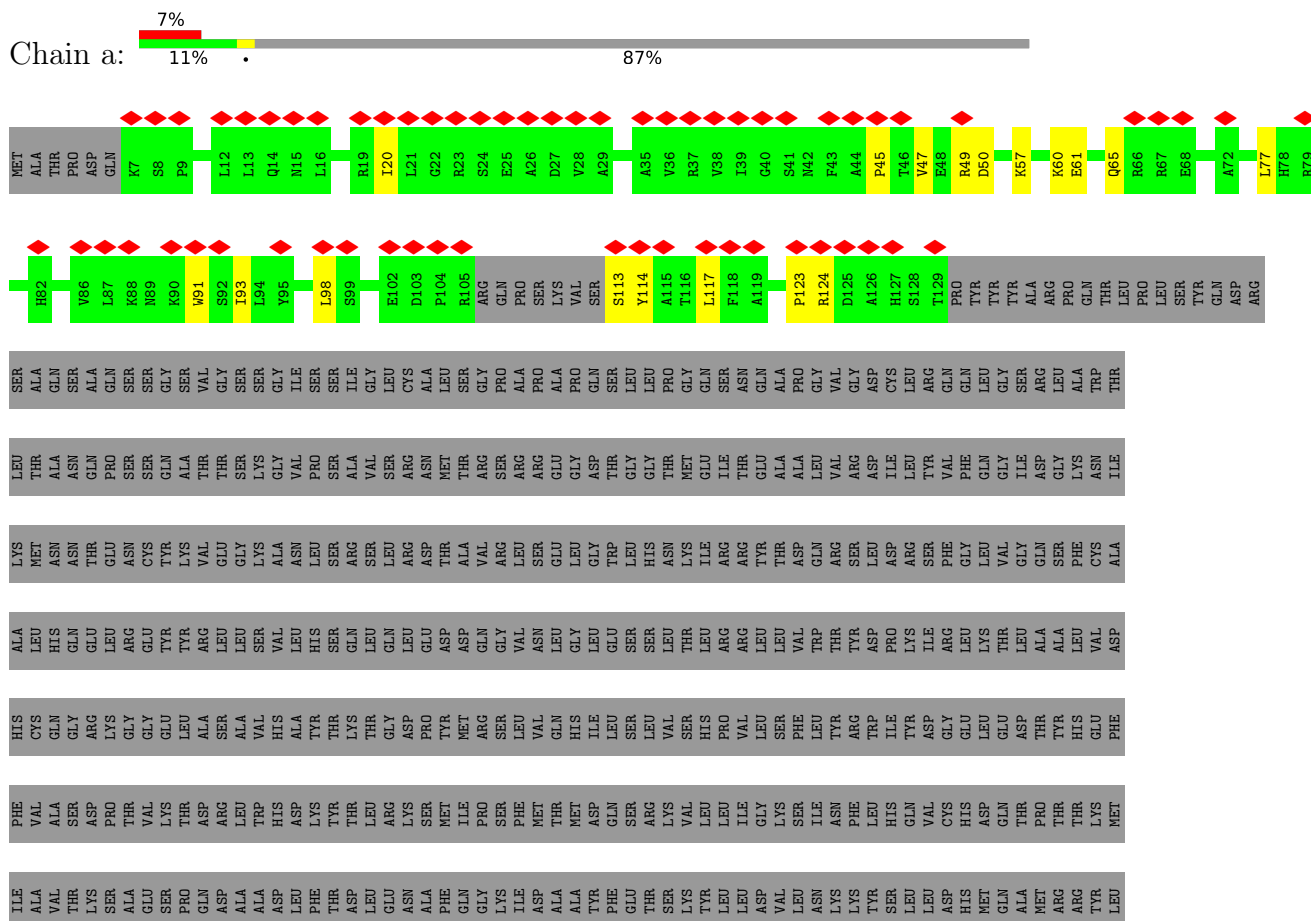


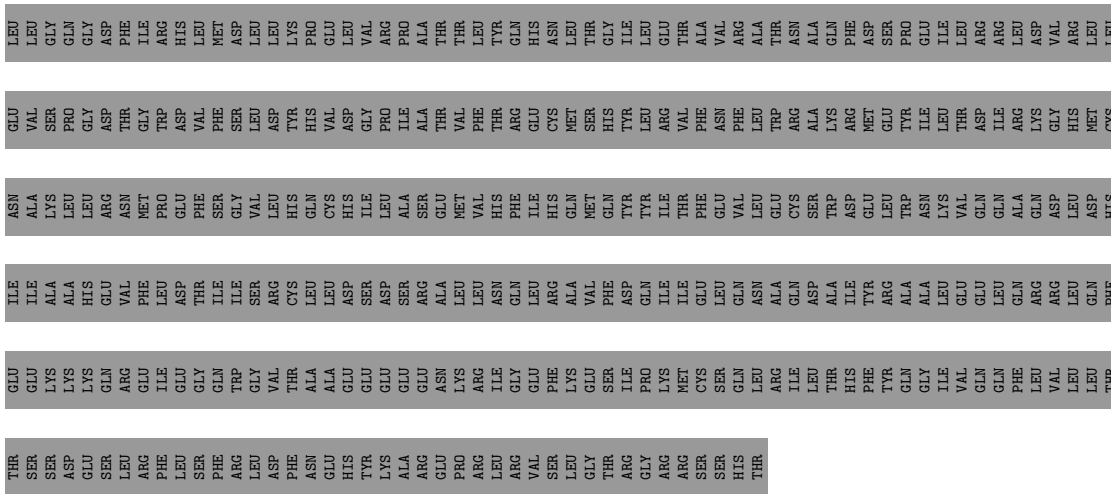


• Molecule 3: Gamma-tubulin complex component 3

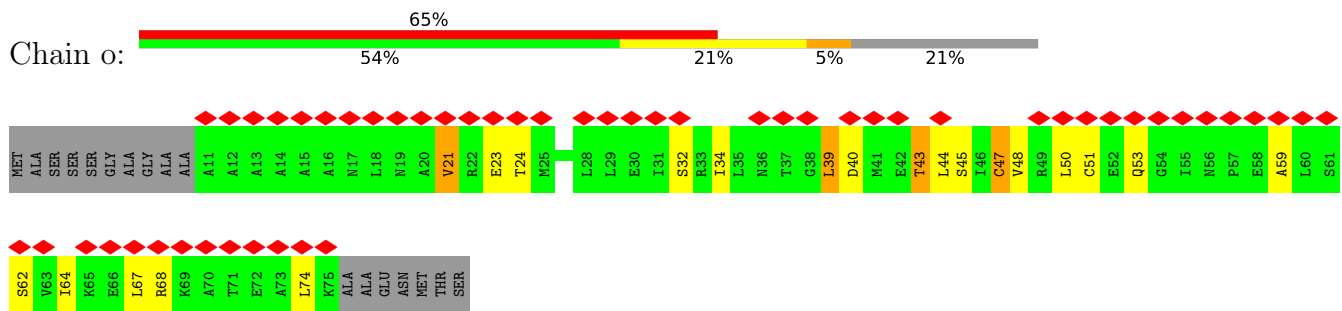


- Molecule 3: Gamma-tubulin complex component 3

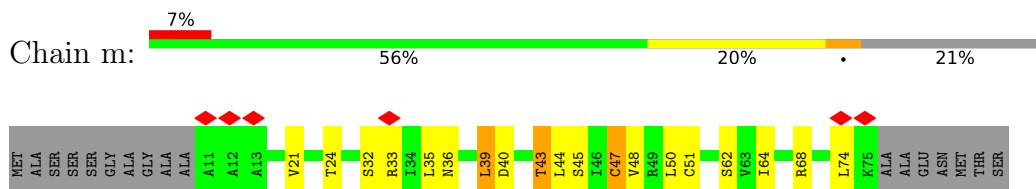




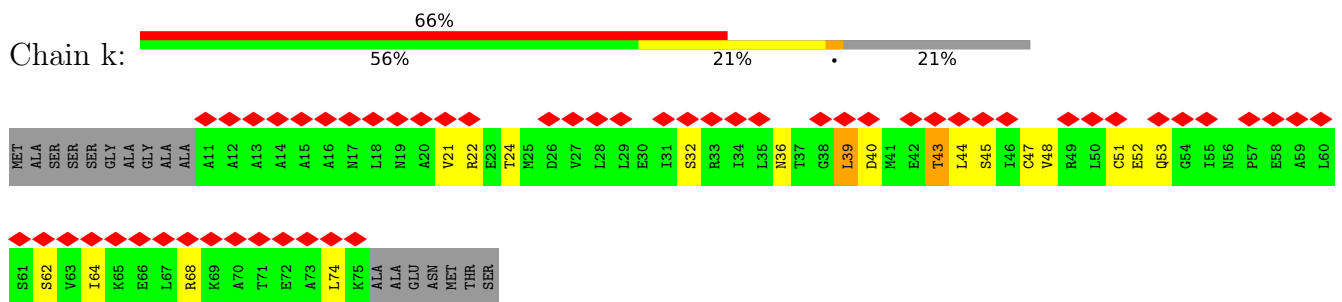
- Molecule 4: Mitotic-spindle organizing protein 1



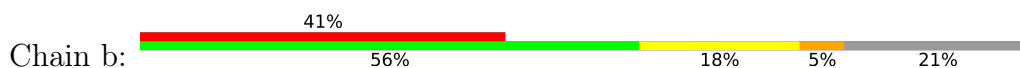
- Molecule 4: Mitotic-spindle organizing protein 1

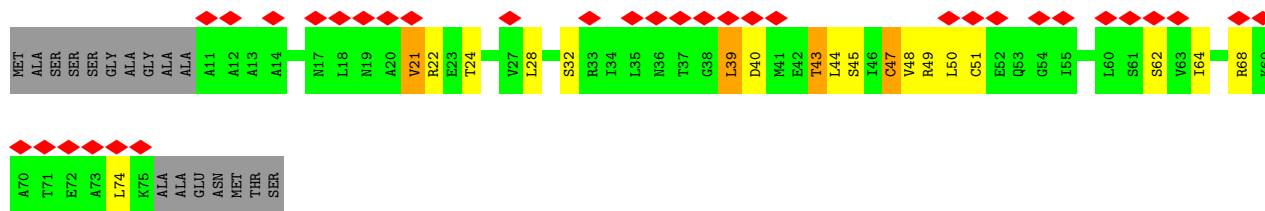


- Molecule 4: Mitotic-spindle organizing protein 1

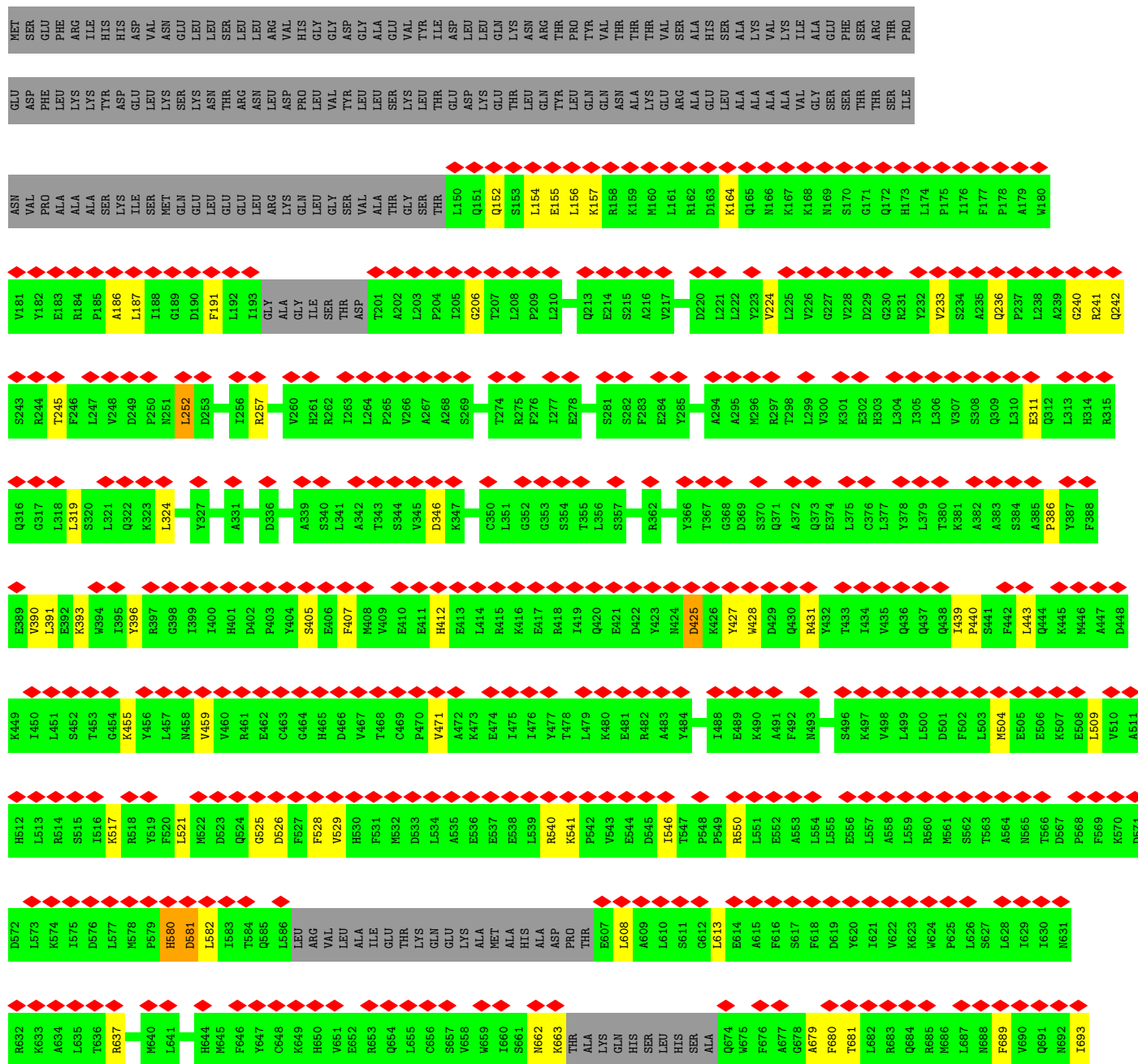


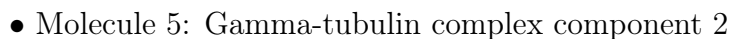
- Molecule 4: Mitotic-spindle organizing protein 1





• Molecule 5: Gamma-tubulin complex component 2











4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	6097	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	0.272	Depositor
Minimum map value	-0.099	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.0514	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	1	0.33	0/3441	0.70	1/4661 (0.0%)
1	2	0.33	0/3441	0.70	1/4661 (0.0%)
1	S	0.33	0/3441	0.70	1/4661 (0.0%)
1	T	0.33	0/3441	0.70	1/4661 (0.0%)
1	U	0.33	0/3441	0.70	1/4661 (0.0%)
1	V	0.33	0/3441	0.70	1/4661 (0.0%)
1	W	0.33	0/3441	0.70	1/4661 (0.0%)
1	X	0.33	0/3441	0.70	1/4661 (0.0%)
1	Y	0.33	0/3441	0.70	1/4661 (0.0%)
1	Z	0.33	0/3441	0.70	1/4661 (0.0%)
2	J	0.41	1/4525 (0.0%)	0.82	10/6119 (0.2%)
2	l	0.39	0/894	0.82	2/1209 (0.2%)
3	F	0.34	0/5044	0.75	7/6809 (0.1%)
3	H	0.45	1/5009 (0.0%)	0.80	10/6761 (0.1%)
3	N	0.39	0/5009	0.75	2/6761 (0.0%)
3	a	0.37	0/948	0.78	1/1277 (0.1%)
3	j	0.36	0/815	0.74	0/1096
3	n	0.37	0/815	0.76	0/1096
4	b	0.32	0/484	0.77	0/653
4	k	0.32	0/484	0.77	0/653
4	m	0.32	0/484	0.77	0/653
4	o	0.32	0/484	0.77	0/653
5	E	0.39	1/5311 (0.0%)	0.75	7/7169 (0.1%)
5	G	0.37	0/5325	0.75	2/7187 (0.0%)
5	M	0.41	0/5295	0.87	20/7147 (0.3%)
6	I	0.41	0/4322	0.81	5/5853 (0.1%)
6	K	0.37	0/4683	0.77	12/6338 (0.2%)
7	L	0.34	0/4697	0.74	3/6348 (0.0%)
All	All	0.37	3/89038 (0.0%)	0.75	91/120392 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1	0	2
1	2	0	2
1	S	0	2
1	T	0	2
1	U	0	2
1	V	0	2
1	W	0	2
1	X	0	2
1	Y	0	2
1	Z	0	2
2	J	0	2
3	H	0	5
3	N	0	2
5	E	0	2
5	G	0	2
5	M	0	5
6	I	0	4
7	L	0	3
All	All	0	45

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	703	GLU	C-N	7.40	1.43	1.34
3	H	603	THR	CB-CG2	6.69	1.74	1.52
2	J	403	ALA	C-N	5.40	1.39	1.34

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	705	THR	N-CA-C	-13.99	95.54	112.89
6	K	651	TYR	CA-CB-CG	9.28	130.61	113.90
2	J	235	SER	N-CA-C	-8.81	103.65	114.75
2	l	121	PRO	CA-N-CD	-8.43	100.20	112.00
2	l	130	PRO	CA-N-CD	-8.41	100.22	112.00
7	L	1787	VAL	N-CA-C	-7.57	106.11	113.53
5	M	703	GLU	CB-CA-C	7.36	124.67	110.17
5	E	439	ILE	N-CA-C	-7.14	102.49	108.63
2	J	950	VAL	N-CA-C	-7.11	106.15	112.12
5	M	241	ARG	O-C-N	-7.05	113.21	122.59
3	H	362	LEU	N-CA-C	-6.83	106.15	114.75
3	F	269	ASN	CA-C-N	6.81	134.55	121.54
3	F	269	ASN	C-N-CA	6.81	134.55	121.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	240	GLY	CA-C-N	6.77	134.48	121.54
5	G	240	GLY	C-N-CA	6.77	134.48	121.54
5	M	240	GLY	CA-C-N	6.74	134.42	121.54
5	M	240	GLY	C-N-CA	6.74	134.42	121.54
5	E	580	HIS	CA-C-N	6.62	134.19	121.54
5	E	580	HIS	C-N-CA	6.62	134.19	121.54
3	a	77	LEU	CB-CG-CD2	-6.60	90.90	110.70
3	F	500	GLN	CA-C-N	6.45	128.97	122.00
3	F	500	GLN	C-N-CA	6.45	128.97	122.00
6	K	651	TYR	CB-CG-CD1	6.43	130.44	120.80
2	J	555	VAL	N-CA-C	-6.32	107.13	113.20
3	H	888	ALA	N-CA-C	-6.32	104.30	114.09
2	J	225	TRP	N-CA-C	-6.25	106.63	114.56
5	E	206	GLY	CA-C-N	6.23	133.43	121.54
5	E	206	GLY	C-N-CA	6.23	133.43	121.54
1	2	407	GLN	CB-CG-CD	6.20	123.14	112.60
1	X	407	GLN	CB-CG-CD	6.20	123.14	112.60
1	Z	407	GLN	CB-CG-CD	6.20	123.13	112.60
1	V	407	GLN	CB-CG-CD	6.19	123.13	112.60
1	W	407	GLN	CB-CG-CD	6.19	123.12	112.60
1	S	407	GLN	CB-CG-CD	6.18	123.11	112.60
6	K	68	GLN	CA-C-N	6.18	132.82	121.70
6	K	68	GLN	C-N-CA	6.18	132.82	121.70
1	U	407	GLN	CB-CG-CD	6.18	123.10	112.60
1	T	407	GLN	CB-CG-CD	6.18	123.10	112.60
1	Y	407	GLN	CB-CG-CD	6.17	123.09	112.60
1	1	407	GLN	CB-CG-CD	6.17	123.09	112.60
5	M	580	HIS	CA-C-N	6.15	133.29	121.54
5	M	580	HIS	C-N-CA	6.15	133.29	121.54
5	M	581	ASP	N-CA-CB	-6.14	100.11	110.49
6	K	409	ASN	CA-C-N	6.10	136.94	126.32
6	K	409	ASN	C-N-CA	6.10	136.94	126.32
5	M	419	ILE	CA-C-N	6.00	132.99	121.54
5	M	419	ILE	C-N-CA	6.00	132.99	121.54
5	M	704	PRO	N-CD-CG	-5.97	94.25	103.20
6	K	203	PHE	CA-C-N	5.93	130.80	122.08
6	K	203	PHE	C-N-CA	5.93	130.80	122.08
5	M	702	MET	O-C-N	5.87	125.18	120.83
2	J	255	PRO	CA-C-N	5.85	132.23	121.70
2	J	255	PRO	C-N-CA	5.85	132.23	121.70
3	H	270	ASN	CA-C-N	-5.84	112.15	122.26
3	H	270	ASN	C-N-CA	-5.84	112.15	122.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	854	SER	CA-CB-OG	-5.84	99.42	111.10
5	E	866	THR	N-CA-C	-5.83	105.78	114.64
3	F	372	TYR	N-CA-C	-5.83	107.97	114.62
6	K	574	ILE	N-CA-C	-5.82	107.14	112.96
6	I	507	SER	CA-C-N	5.80	132.62	121.54
6	I	507	SER	C-N-CA	5.80	132.62	121.54
5	M	176	ILE	CA-C-N	5.76	135.79	122.31
5	M	176	ILE	C-N-CA	5.76	135.79	122.31
3	F	272	GLU	CA-C-N	5.68	132.40	121.54
3	F	272	GLU	C-N-CA	5.68	132.40	121.54
3	H	568	LEU	CA-CB-CG	5.61	135.93	116.30
5	M	702	MET	CA-C-O	-5.58	116.59	119.77
3	N	723	THR	N-CA-C	-5.55	107.15	114.31
5	M	563	THR	OG1-CB-CG2	5.50	120.29	109.30
2	J	216	LEU	CA-C-N	5.49	127.89	120.38
2	J	216	LEU	C-N-CA	5.49	127.89	120.38
3	H	603	THR	N-CA-C	-5.46	105.74	112.72
3	H	603	THR	CA-CB-CG2	5.45	119.77	110.50
3	H	603	THR	N-CA-CB	-5.45	100.95	110.44
6	K	255	LYS	CA-C-N	5.44	131.94	121.54
6	K	255	LYS	C-N-CA	5.44	131.94	121.54
6	I	404	LEU	CA-C-N	5.36	131.77	121.54
6	I	404	LEU	C-N-CA	5.36	131.77	121.54
5	M	155	GLU	CA-C-N	5.34	127.70	120.38
5	M	155	GLU	C-N-CA	5.34	127.70	120.38
3	H	613	ASP	CA-C-N	5.23	128.31	120.83
3	H	613	ASP	C-N-CA	5.23	128.31	120.83
6	I	451	ALA	N-CA-C	-5.18	105.70	113.89
2	J	713	ASP	CA-C-N	5.15	131.37	121.54
2	J	713	ASP	C-N-CA	5.15	131.37	121.54
5	E	252	LEU	CA-CB-CG	5.12	134.21	116.30
7	L	288	THR	CA-C-N	5.11	129.51	120.87
7	L	288	THR	C-N-CA	5.11	129.51	120.87
6	K	290	ASN	N-CA-C	-5.09	106.90	114.64
5	M	406	GLU	N-CA-C	-5.03	108.17	114.56
3	N	455	LYS	N-CA-C	5.03	121.51	110.80

There are no chirality outliers.

All (45) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	327	GLU	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	1	56	ASP	Peptide
1	2	327	GLU	Peptide
1	2	56	ASP	Peptide
5	E	580	HIS	Peptide
5	E	861	PHE	Mainchain
5	G	355	THR	Peptide
5	G	580	HIS	Peptide
3	H	269	ASN	Peptide
3	H	270	ASN	Peptide
3	H	501	THR	Peptide
3	H	602	GLU	Peptide
3	H	603	THR	Mainchain
6	I	407	ASP	Peptide
6	I	502	ARG	Peptide
6	I	507	SER	Peptide
6	I	508	ASN	Mainchain
2	J	256	LEU	Peptide
2	J	760	VAL	Peptide
7	L	311	TYR	Peptide
7	L	342	PRO	Peptide
7	L	346	LEU	Peptide
5	M	240	GLY	Peptide
5	M	241	ARG	Mainchain
5	M	525	GLY	Peptide
5	M	581	ASP	Mainchain
5	M	674	GLN	Peptide
3	N	454	VAL	Peptide
3	N	526	LEU	Peptide
1	S	327	GLU	Peptide
1	S	56	ASP	Peptide
1	T	327	GLU	Peptide
1	T	56	ASP	Peptide
1	U	327	GLU	Peptide
1	U	56	ASP	Peptide
1	V	327	GLU	Peptide
1	V	56	ASP	Peptide
1	W	327	GLU	Peptide
1	W	56	ASP	Peptide
1	X	327	GLU	Peptide
1	X	56	ASP	Peptide
1	Y	327	GLU	Peptide
1	Y	56	ASP	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	Z	327	GLU	Peptide
1	Z	56	ASP	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	1	3373	0	3325	81	0
1	2	3373	0	3325	73	0
1	S	3373	0	3325	66	0
1	T	3373	0	3325	68	0
1	U	3373	0	3325	61	0
1	V	3373	0	3325	75	0
1	W	3373	0	3325	62	0
1	X	3373	0	3325	58	0
1	Y	3373	0	3325	74	0
1	Z	3373	0	3325	68	0
2	J	4429	0	4482	39	0
2	l	875	0	842	28	0
3	F	4941	0	4935	43	0
3	H	4907	0	4896	64	0
3	N	4907	0	4896	63	0
3	a	933	0	953	10	0
3	j	803	0	831	23	0
3	n	803	0	831	16	0
4	b	484	0	512	9	0
4	k	484	0	512	8	0
4	m	484	0	512	15	0
4	o	484	0	512	12	0
5	E	5202	0	5241	45	0
5	G	5216	0	5246	82	0
5	M	5186	0	5219	72	0
6	I	4225	0	4259	52	0
6	K	4579	0	4586	44	0
7	L	4587	0	4636	41	0
All	All	87259	0	87151	1210	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 7.

All (1210) 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)
3:H:603:THR:CB	3:H:603:THR:CG2	1.74	1.62
5:G:876:ARG:HH22	3:j:37:ARG:CA	1.39	1.35
5:G:876:ARG:NH2	3:j:37:ARG:CB	1.95	1.29
5:G:876:ARG:HH22	3:j:37:ARG:CB	1.49	1.25
5:G:876:ARG:NH2	3:j:37:ARG:HB3	1.47	1.24
5:G:876:ARG:HH22	3:j:37:ARG:C	1.36	1.10
5:G:876:ARG:NH2	3:j:37:ARG:C	1.95	0.97
2:l:80:LYS:NZ	2:l:126:TYR:CE2	2.34	0.95
2:l:121:PRO:HG3	4:m:35:LEU:C	1.96	0.90
6:I:357:ILE:O	6:I:361:TYR:HB3	1.71	0.90
2:l:80:LYS:NZ	2:l:126:TYR:CZ	2.41	0.89
3:H:603:THR:CG2	3:H:603:THR:HB	2.04	0.86
5:M:703:GLU:HB3	5:M:704:PRO:HD3	1.56	0.85
2:l:129:THR:HG21	4:m:33:ARG:HD2	1.59	0.83
5:G:280:LYS:HB3	5:G:289:ASN:HD21	1.44	0.81
5:G:557:LEU:HB2	1:V:339:ARG:HH11	1.46	0.81
2:l:77:ASP:OD2	2:l:126:TYR:CZ	2.35	0.80
5:E:581:ASP:H	5:E:608:LEU:HD21	1.47	0.79
1:l:47:ARG:HB2	5:M:563:THR:HB	1.64	0.78
1:U:56:ASP:HB3	1:V:296:ARG:NE	1.99	0.78
1:l:341:ARG:NH1	5:M:857:SER:O	2.17	0.77
5:G:876:ARG:HH21	3:j:37:ARG:CB	1.97	0.77
2:l:121:PRO:HG3	4:m:35:LEU:O	1.85	0.75
6:I:527:ASN:O	6:I:530:TYR:HB3	1.88	0.74
6:K:63:THR:HG22	7:L:468:ARG:HH21	1.52	0.74
1:2:250:ASN:HD21	3:N:716:HIS:HD2	1.35	0.72
1:2:355:SER:OG	3:N:879:ARG:O	2.08	0.72
2:l:129:THR:CG2	4:m:33:ARG:HD2	2.20	0.71
3:F:294:LEU:HD11	3:F:371:THR:HG21	1.72	0.71
6:I:361:TYR:HE2	6:I:475:TYR:HB3	1.55	0.71
3:F:594:GLN:HB2	3:F:625:LEU:HD23	1.74	0.70
3:F:597:LEU:HB2	3:F:623:VAL:HG21	1.73	0.70
5:M:698:MET:HE3	5:M:703:GLU:H	1.57	0.69
3:H:883:ASN:HB2	1:V:353:PRO:HA	1.75	0.69
2:l:121:PRO:HD3	4:m:35:LEU:HA	1.75	0.69
6:I:555:GLU:HA	6:I:558:ARG:HE	1.58	0.68
1:T:270:MET:N	1:T:270:MET:SD	2.67	0.68
1:l:270:MET:HE1	1:l:379:ALA:HB3	1.76	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:270:MET:SD	1:1:270:MET:N	2.67	0.68
5:G:876:ARG:HH21	3:j:37:ARG:HB3	1.55	0.68
1:S:270:MET:SD	1:S:270:MET:N	2.67	0.68
1:V:270:MET:SD	1:V:270:MET:N	2.67	0.68
1:V:270:MET:HE1	1:V:379:ALA:HB3	1.76	0.68
1:1:47:ARG:HB2	5:M:563:THR:CB	2.24	0.68
1:S:270:MET:HE1	1:S:379:ALA:HB3	1.76	0.67
1:T:270:MET:HE1	1:T:379:ALA:HB3	1.76	0.67
1:U:270:MET:SD	1:U:270:MET:N	2.67	0.67
5:G:876:ARG:NH2	3:j:37:ARG:HB2	2.06	0.67
2:l:77:ASP:OD2	2:l:126:TYR:CE2	2.47	0.67
3:H:608:THR:HG23	3:H:610:ALA:H	1.59	0.67
1:U:47:ARG:HE	1:U:49:ASP:HB3	1.60	0.67
1:S:47:ARG:HE	1:S:49:ASP:HB3	1.60	0.67
1:Y:47:ARG:HE	1:Y:49:ASP:HB3	1.60	0.67
1:2:47:ARG:HE	1:2:49:ASP:HB3	1.60	0.67
1:X:47:ARG:HE	1:X:49:ASP:HB3	1.60	0.67
1:Z:270:MET:SD	1:Z:270:MET:N	2.67	0.67
1:T:47:ARG:HE	1:T:49:ASP:HB3	1.60	0.67
1:U:270:MET:HE1	1:U:379:ALA:HB3	1.76	0.67
1:W:270:MET:HE1	1:W:379:ALA:HB3	1.76	0.67
1:Z:270:MET:HE1	1:Z:379:ALA:HB3	1.76	0.66
1:X:270:MET:SD	1:X:270:MET:N	2.67	0.66
1:2:270:MET:HE1	1:2:379:ALA:HB3	1.76	0.66
3:n:87:LEU:HD21	3:n:93:ILE:HG13	1.76	0.66
2:l:80:LYS:NZ	2:l:126:TYR:CD2	2.57	0.66
1:Y:270:MET:HE1	1:Y:379:ALA:HB3	1.76	0.66
5:G:876:ARG:NH2	3:j:37:ARG:CA	2.24	0.66
3:N:698:SER:O	3:N:702:HIS:HB2	1.96	0.66
1:Z:101:GLY:N	1:Z:106:SER:HG	1.94	0.66
1:X:270:MET:HE1	1:X:379:ALA:HB3	1.76	0.65
1:1:47:ARG:HE	1:1:49:ASP:HB3	1.60	0.65
1:Z:47:ARG:HE	1:Z:49:ASP:HB3	1.60	0.65
1:1:339:ARG:HH22	1:1:342:GLU:HB2	1.61	0.65
1:2:270:MET:SD	1:2:270:MET:N	2.67	0.65
1:U:339:ARG:HH22	1:U:342:GLU:HB2	1.61	0.65
1:2:339:ARG:HH22	1:2:342:GLU:HB2	1.61	0.65
1:T:339:ARG:HH22	1:T:342:GLU:HB2	1.61	0.65
1:W:47:ARG:HE	1:W:49:ASP:HB3	1.60	0.65
1:Y:339:ARG:HH22	1:Y:342:GLU:HB2	1.61	0.65
6:K:653:LYS:HA	6:K:657:GLN:HG3	1.78	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:339:ARG:HH22	1:S:342:GLU:HB2	1.61	0.65
5:G:557:LEU:CB	1:V:339:ARG:HH11	2.10	0.65
1:Z:339:ARG:HH22	1:Z:342:GLU:HB2	1.61	0.65
1:2:185:PRO:O	1:2:189:LEU:HB3	1.97	0.64
3:n:7:LYS:O	4:o:53:GLN:NE2	2.30	0.64
5:E:241:ARG:NH2	5:E:346:ASP:OD1	2.31	0.64
1:U:185:PRO:O	1:U:189:LEU:HB3	1.98	0.64
1:V:339:ARG:HH22	1:V:342:GLU:HB2	1.62	0.64
1:2:290:VAL:HG21	1:2:333:VAL:HG12	1.80	0.64
1:T:185:PRO:O	1:T:189:LEU:HB3	1.97	0.64
1:X:290:VAL:HG21	1:X:333:VAL:HG12	1.80	0.64
3:N:799:GLU:HA	3:N:802:ARG:HE	1.63	0.64
1:W:270:MET:SD	1:W:270:MET:N	2.67	0.64
1:W:339:ARG:HH22	1:W:342:GLU:HB2	1.61	0.64
1:T:290:VAL:HG21	1:T:333:VAL:HG12	1.80	0.64
1:V:47:ARG:HE	1:V:49:ASP:HB3	1.60	0.64
1:X:339:ARG:HH22	1:X:342:GLU:HB2	1.61	0.64
6:I:471:VAL:O	6:I:475:TYR:HB2	1.97	0.64
2:l:77:ASP:OD2	2:l:126:TYR:CE1	2.51	0.64
5:M:510:VAL:HG12	5:M:514:ARG:HE	1.63	0.64
1:V:185:PRO:O	1:V:189:LEU:HB3	1.97	0.64
1:W:185:PRO:O	1:W:189:LEU:HB3	1.97	0.64
1:X:101:GLY:N	1:X:106:SER:HG	1.96	0.64
1:W:290:VAL:HG21	1:W:333:VAL:HG12	1.80	0.64
1:Y:185:PRO:O	1:Y:189:LEU:HB3	1.97	0.64
1:Z:290:VAL:HG21	1:Z:333:VAL:HG12	1.80	0.64
1:1:185:PRO:O	1:1:189:LEU:HB3	1.97	0.63
1:S:185:PRO:O	1:S:189:LEU:HB3	1.97	0.63
1:X:185:PRO:O	1:X:189:LEU:HB3	1.98	0.63
1:Z:185:PRO:O	1:Z:189:LEU:HB3	1.97	0.63
6:I:361:TYR:CE2	6:I:475:TYR:HB3	2.34	0.63
1:1:3:ARG:HA	5:M:530:HIS:HE1	1.64	0.63
1:U:290:VAL:HG21	1:U:333:VAL:HG12	1.80	0.63
1:V:290:VAL:HG21	1:V:333:VAL:HG12	1.80	0.63
1:X:222:ASN:OD1	1:X:222:ASN:N	2.32	0.63
1:Y:222:ASN:OD1	1:Y:222:ASN:N	2.32	0.63
3:H:733:GLU:HG3	3:H:737:LYS:HE2	1.80	0.62
1:1:222:ASN:OD1	1:1:222:ASN:N	2.32	0.62
2:l:121:PRO:HG2	2:l:125:SER:OG	1.99	0.62
1:W:222:ASN:OD1	1:W:222:ASN:N	2.32	0.62
1:Y:270:MET:SD	1:Y:270:MET:N	2.67	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:222:ASN:OD1	1:V:222:ASN:N	2.32	0.62
2:J:697:LYS:HA	2:J:700:LEU:HD12	1.82	0.62
1:1:290:VAL:HG21	1:1:333:VAL:HG12	1.80	0.62
1:1:298:LEU:HD21	1:1:340:ILE:HD12	1.82	0.62
1:S:290:VAL:HG21	1:S:333:VAL:HG12	1.80	0.62
1:U:298:LEU:HD21	1:U:340:ILE:HD12	1.82	0.62
1:Y:290:VAL:HG21	1:Y:333:VAL:HG12	1.80	0.62
1:2:298:LEU:HD21	1:2:340:ILE:HD12	1.82	0.62
2:I:60:LYS:HA	2:I:63:LYS:HD2	1.81	0.62
6:K:513:ILE:HA	6:K:516:ARG:HD2	1.82	0.62
3:N:464:TYR:OH	3:N:491:ASN:ND2	2.33	0.62
1:V:298:LEU:HD21	1:V:340:ILE:HD12	1.82	0.62
1:Y:298:LEU:HD21	1:Y:340:ILE:HD12	1.82	0.62
5:G:852:MET:SD	5:G:852:MET:N	2.72	0.61
3:F:261:ILE:HG12	5:G:262:ARG:HH22	1.65	0.61
1:2:337:LEU:HD21	3:N:879:ARG:HG3	1.83	0.61
3:F:526:LEU:HB3	3:F:529:ALA:HB3	1.82	0.61
1:T:298:LEU:HD21	1:T:340:ILE:HD12	1.82	0.61
7:L:332:GLN:HG2	7:L:337:GLY:HA2	1.81	0.61
1:S:222:ASN:OD1	1:S:222:ASN:N	2.32	0.61
3:F:555:LEU:HD13	3:F:648:ILE:HG23	1.81	0.61
6:I:392:VAL:HG22	6:I:414:LEU:HD13	1.81	0.61
1:S:298:LEU:HD21	1:S:340:ILE:HD12	1.82	0.61
1:U:222:ASN:OD1	1:U:222:ASN:N	2.32	0.60
2:J:945:GLU:HG3	2:J:946:LYS:HD2	1.82	0.60
1:2:355:SER:HB2	3:N:713:HIS:NE2	2.16	0.60
1:Z:298:LEU:HD21	1:Z:340:ILE:HD12	1.82	0.60
3:F:806:PHE:HA	3:F:809:LYS:HD2	1.82	0.60
3:H:689:LYS:NZ	1:V:158:ASN:OD1	2.33	0.60
1:T:90:ASN:N	1:T:90:ASN:OD1	2.35	0.60
1:X:298:LEU:HD21	1:X:340:ILE:HD12	1.82	0.60
1:W:298:LEU:HD21	1:W:340:ILE:HD12	1.82	0.60
1:X:90:ASN:OD1	1:X:90:ASN:N	2.35	0.60
2:J:221:VAL:O	2:J:228:ARG:NH2	2.35	0.60
1:U:90:ASN:OD1	1:U:90:ASN:N	2.35	0.60
1:Y:101:GLY:N	1:Y:106:SER:HG	2.00	0.60
2:I:129:THR:HG22	4:m:33:ARG:NE	2.16	0.59
3:n:86:VAL:O	3:n:90:LYS:NZ	2.33	0.59
1:U:101:GLY:N	1:U:106:SER:HG	2.00	0.59
1:S:90:ASN:OD1	1:S:90:ASN:N	2.35	0.59
6:K:509:GLN:HG3	6:K:511:ASP:H	1.67	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:101:GLY:N	1:V:106:SER:HG	2.00	0.59
1:X:56:ASP:HB3	1:Y:287:LYS:HD2	1.85	0.59
1:1:341:ARG:NH1	5:M:860:ASP:O	2.35	0.59
5:G:485:VAL:HA	5:G:488:ILE:HD12	1.85	0.59
6:K:27:VAL:HG13	6:K:29:GLN:HG2	1.85	0.59
1:2:222:ASN:OD1	1:2:222:ASN:N	2.32	0.59
5:G:876:ARG:NH2	3:j:34:TYR:O	2.36	0.59
6:K:407:ASP:HB3	6:K:411:LEU:HD13	1.84	0.59
3:H:274:CYS:SG	3:H:275:TYR:N	2.76	0.58
6:I:96:VAL:HG12	6:I:174:LYS:HD2	1.85	0.58
1:W:90:ASN:N	1:W:90:ASN:OD1	2.35	0.58
5:G:415:ARG:HB2	5:G:431:ARG:HH22	1.68	0.58
6:K:509:GLN:HG2	6:K:603:PRO:HB3	1.85	0.58
6:K:639:ASN:HB3	1:Y:334:HIS:NE2	2.18	0.58
1:Z:90:ASN:OD1	1:Z:90:ASN:N	2.35	0.58
1:1:90:ASN:OD1	1:1:90:ASN:N	2.35	0.58
3:H:680:ILE:HD11	3:H:786:GLN:HE21	1.68	0.58
1:Y:90:ASN:N	1:Y:90:ASN:OD1	2.35	0.58
1:2:339:ARG:HH12	5:M:554:LEU:HD22	1.68	0.58
1:1:101:GLY:N	1:1:106:SER:HG	2.02	0.58
3:N:339:LEU:O	3:N:343:HIS:ND1	2.35	0.58
1:1:246:PRO:HA	5:M:563:THR:HG21	1.86	0.58
3:H:253:ASP:HB3	3:H:266:ILE:HG22	1.86	0.58
3:H:388:CYS:HA	3:H:391:ARG:HE	1.67	0.58
1:1:355:SER:OG	5:M:858:ARG:O	2.22	0.58
5:G:313:LEU:HD23	5:G:319:LEU:HD13	1.85	0.58
1:V:90:ASN:OD1	1:V:90:ASN:N	2.35	0.58
2:J:829:LEU:HA	2:J:832:LYS:HE3	1.86	0.58
1:W:56:ASP:OD2	1:X:296:ARG:HG3	2.04	0.58
5:G:578:MET:H	5:G:615:ALA:HB1	1.68	0.57
5:M:221:LEU:HD11	5:M:260:VAL:HG22	1.86	0.57
1:2:90:ASN:N	1:2:90:ASN:OD1	2.35	0.57
5:M:236:GLN:O	5:M:244:ARG:NH1	2.36	0.57
1:X:343:ARG:HB3	1:X:345:LEU:HD12	1.86	0.57
6:I:569:LEU:HD21	6:I:575:LEU:HD13	1.86	0.57
6:K:646:LEU:O	1:Y:341:ARG:NH1	2.32	0.57
1:V:343:ARG:HB3	1:V:345:LEU:HD12	1.86	0.57
1:W:101:GLY:N	1:W:106:SER:HG	2.02	0.57
5:G:241:ARG:O	5:G:275:ARG:NH1	2.37	0.57
1:X:383:SER:O	1:X:386:SER:OG	2.22	0.57
5:M:398:GLY:H	5:M:457:LEU:HD22	1.69	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:651:VAL:HG23	3:N:748:ILE:HG12	1.86	0.57
1:X:56:ASP:OD1	1:Y:288:THR:OG1	2.22	0.57
2:I:80:LYS:CB	2:I:126:TYR:CE1	2.64	0.57
3:N:555:LEU:HD11	3:N:651:VAL:HG11	1.86	0.57
1:U:343:ARG:HB3	1:U:345:LEU:HD12	1.86	0.57
1:I:47:ARG:CB	5:M:563:THR:HB	2.33	0.57
6:I:477:VAL:HA	6:I:480:LYS:HE2	1.87	0.57
1:Z:343:ARG:HB3	1:Z:345:LEU:HD12	1.86	0.57
3:j:58:ILE:HG12	3:j:98:LEU:HD13	1.85	0.57
1:T:383:SER:O	1:T:386:SER:OG	2.22	0.57
1:Y:343:ARG:HB3	1:Y:345:LEU:HD12	1.87	0.57
1:I:264:PRO:O	5:M:663:LYS:NZ	2.38	0.57
1:I:343:ARG:HB3	1:I:345:LEU:HD12	1.86	0.56
1:2:101:GLY:N	1:2:106:SER:HG	2.03	0.56
1:T:222:ASN:OD1	1:T:222:ASN:N	2.32	0.56
3:F:553:TYR:HB3	3:F:648:ILE:HD11	1.87	0.56
6:K:149:HIS:NE2	6:K:202:GLU:OE1	2.35	0.56
1:S:343:ARG:HB3	1:S:345:LEU:HD12	1.86	0.56
5:E:311:GLU:OE2	3:F:366:ARG:NH2	2.37	0.56
1:2:343:ARG:HB3	1:2:345:LEU:HD12	1.86	0.56
3:n:55:ALA:HA	3:n:58:ILE:HD12	1.87	0.56
2:J:827:LEU:HG	2:J:943:LEU:HD11	1.86	0.56
1:W:343:ARG:HB3	1:W:345:LEU:HD12	1.86	0.56
5:G:334:THR:HG23	5:G:375:LEU:HD22	1.88	0.56
2:J:828:LEU:HG	2:J:832:LYS:HE2	1.88	0.56
6:K:131:LEU:HD13	6:K:165:LEU:HD21	1.88	0.56
1:T:343:ARG:HB3	1:T:345:LEU:HD12	1.86	0.56
1:2:182:VAL:HB	1:2:404:PHE:HD1	1.71	0.56
5:M:613:LEU:HD12	5:M:614:GLU:HG3	1.88	0.56
5:E:517:LYS:HG3	5:E:521:LEU:HD12	1.87	0.55
5:E:637:ARG:HG2	5:E:734:LEU:HD22	1.88	0.55
3:N:784:GLU:HG2	3:N:850:LEU:HD11	1.88	0.55
6:I:154:LEU:HD11	6:I:179:CYS:HB2	1.88	0.55
6:I:357:ILE:O	6:I:361:TYR:CB	2.50	0.55
3:j:67:ARG:HH12	3:j:104:PRO:HG2	1.71	0.55
3:F:579:ASP:HA	3:F:582:LYS:HE3	1.86	0.55
3:H:466:LEU:HD11	3:H:471:ILE:HD11	1.88	0.55
2:J:286:ILE:HG23	2:J:297:ARG:H	1.70	0.55
3:a:61:GLU:HG3	3:a:98:LEU:HD11	1.88	0.55
1:U:56:ASP:HB3	1:V:296:ARG:HE	1.69	0.55
1:V:182:VAL:HB	1:V:404:PHE:HD1	1.72	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:152:GLN:NE2	5:E:240:GLY:O	2.39	0.55
6:I:411:LEU:HD23	6:I:458:LYS:HE2	1.87	0.55
1:Y:383:SER:O	1:Y:386:SER:OG	2.22	0.55
5:G:434:ILE:HD11	5:G:439:ILE:HD11	1.88	0.55
1:U:395:TYR:OH	1:U:425:ARG:NH2	2.40	0.55
1:Z:182:VAL:HB	1:Z:404:PHE:HD1	1.72	0.55
5:E:662:ASN:HD22	5:E:680:PHE:HE2	1.52	0.55
1:S:182:VAL:HB	1:S:404:PHE:HD1	1.72	0.55
1:2:290:VAL:HA	1:2:293:VAL:HG22	1.89	0.55
1:X:182:VAL:HB	1:X:404:PHE:HD1	1.72	0.55
6:K:337:ALA:HB1	6:K:554:PHE:H	1.72	0.55
3:H:332:LEU:HA	3:H:335:TYR:HD2	1.72	0.55
3:F:406:THR:HG21	3:F:411:MET:HB2	1.89	0.54
5:G:557:LEU:HB2	1:V:339:ARG:NH1	2.18	0.54
5:M:558:ALA:O	5:M:562:SER:HB3	2.07	0.54
1:T:182:VAL:HB	1:T:404:PHE:HD1	1.72	0.54
1:U:182:VAL:HB	1:U:404:PHE:HD1	1.72	0.54
1:1:182:VAL:HB	1:1:404:PHE:HD1	1.72	0.54
3:N:829:GLU:HA	3:N:832:ARG:HD2	1.89	0.54
1:W:395:TYR:OH	1:W:425:ARG:NH2	2.40	0.54
1:Z:290:VAL:HA	1:Z:293:VAL:HG22	1.89	0.54
1:2:250:ASN:ND2	3:N:720:TYR:OH	2.39	0.54
3:H:400:VAL:HG11	3:H:422:VAL:HG21	1.89	0.54
7:L:1732:ILE:HG23	7:L:1772:PHE:HE1	1.71	0.54
1:W:182:VAL:HB	1:W:404:PHE:HD1	1.72	0.54
1:X:395:TYR:OH	1:X:425:ARG:NH2	2.40	0.54
1:Y:395:TYR:OH	1:Y:425:ARG:NH2	2.40	0.54
1:Z:395:TYR:OH	1:Z:425:ARG:NH2	2.40	0.54
1:1:290:VAL:HA	1:1:293:VAL:HG22	1.89	0.54
1:U:88:PRO:O	1:U:124:ARG:NH2	2.39	0.54
1:U:290:VAL:HA	1:U:293:VAL:HG22	1.89	0.54
1:1:395:TYR:OH	1:1:425:ARG:NH2	2.40	0.54
1:2:395:TYR:OH	1:2:425:ARG:NH2	2.40	0.54
1:W:290:VAL:HA	1:W:293:VAL:HG22	1.89	0.54
1:X:88:PRO:O	1:X:124:ARG:NH2	2.39	0.54
1:Y:290:VAL:HA	1:Y:293:VAL:HG22	1.89	0.54
6:I:540:GLN:HA	6:I:543:GLN:HE21	1.73	0.54
1:Y:182:VAL:HB	1:Y:404:PHE:HD1	1.72	0.54
5:G:876:ARG:HG3	3:j:34:TYR:OH	2.08	0.54
7:L:287:LEU:HG	4:b:22:ARG:HD3	1.89	0.54
7:L:348:LYS:HG3	7:L:349:GLU:H	1.73	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:395:TYR:OH	1:V:425:ARG:NH2	2.40	0.54
1:1:328:VAL:HG21	1:1:360:LEU:HD11	1.90	0.54
1:T:290:VAL:HA	1:T:293:VAL:HG22	1.89	0.54
1:X:328:VAL:HG21	1:X:360:LEU:HD11	1.90	0.54
1:Y:154:LEU:HD11	1:Y:199:ALA:HB2	1.90	0.54
1:2:341:ARG:NH2	3:N:884:GLU:OE2	2.41	0.53
3:H:277:VAL:HG21	3:H:288:ARG:HA	1.90	0.53
5:M:699:PHE:HE1	5:M:703:GLU:HG3	1.73	0.53
1:Z:154:LEU:HD11	1:Z:199:ALA:HB2	1.90	0.53
5:E:504:MET:HE1	5:E:509:LEU:HD23	1.90	0.53
3:F:346:LEU:HD13	3:F:362:LEU:HD22	1.91	0.53
3:N:625:LEU:HD22	3:N:637:VAL:HG12	1.90	0.53
3:H:728:GLU:HG3	1:V:330:PRO:HG3	1.89	0.53
4:b:28:LEU:HD22	3:a:93:ILE:HG12	1.90	0.53
1:S:328:VAL:HG21	1:S:360:LEU:HD11	1.90	0.53
1:S:395:TYR:OH	1:S:425:ARG:NH2	2.40	0.53
1:T:395:TYR:OH	1:T:425:ARG:NH2	2.40	0.53
3:n:94:LEU:HD23	3:n:97:LEU:HD21	1.90	0.53
3:H:432:ARG:HH22	3:H:439:LEU:HA	1.73	0.53
6:K:29:GLN:HA	6:K:34:LEU:HD11	1.90	0.53
3:N:416:GLN:O	3:N:416:GLN:NE2	2.41	0.53
3:N:872:SER:OG	3:N:873:LEU:N	2.41	0.53
1:T:88:PRO:O	1:T:124:ARG:NH2	2.39	0.53
1:U:154:LEU:HD11	1:U:199:ALA:HB2	1.90	0.53
1:U:328:VAL:HG21	1:U:360:LEU:HD11	1.90	0.53
3:H:709:SER:HA	3:H:712:VAL:HG22	1.90	0.53
6:K:499:GLN:HB3	6:K:516:ARG:HE	1.73	0.53
1:T:328:VAL:HG21	1:T:360:LEU:HD11	1.90	0.53
1:V:88:PRO:O	1:V:124:ARG:NH2	2.39	0.53
1:W:291:LEU:HG	1:W:336:SER:HA	1.91	0.53
3:F:629:SER:OG	3:j:64:ARG:NH2	2.42	0.53
1:V:290:VAL:HA	1:V:293:VAL:HG22	1.89	0.53
1:Y:291:LEU:HG	1:Y:336:SER:HA	1.91	0.53
1:Z:88:PRO:O	1:Z:124:ARG:NH2	2.39	0.53
1:1:154:LEU:HD11	1:1:199:ALA:HB2	1.90	0.53
3:F:466:LEU:HD22	3:F:481:ARG:HH12	1.74	0.53
1:T:291:LEU:HG	1:T:336:SER:HA	1.91	0.53
1:U:291:LEU:HG	1:U:336:SER:HA	1.91	0.53
1:2:250:ASN:ND2	3:N:716:HIS:HD2	2.05	0.53
3:F:879:ARG:CZ	3:F:879:ARG:HA	2.39	0.53
6:I:89:PHE:HZ	6:I:140:VAL:HG22	1.74	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:886:LEU:HD11	2:J:980:ILE:HG23	1.91	0.53
5:M:356:LEU:HB3	5:M:440:PRO:HB3	1.90	0.53
1:Z:222:ASN:OD1	1:Z:222:ASN:N	2.32	0.53
1:1:340:ILE:HG22	5:M:861:PHE:HZ	1.74	0.53
1:2:328:VAL:HG21	1:2:360:LEU:HD11	1.91	0.53
6:I:279:VAL:HG13	6:I:336:VAL:HG11	1.91	0.53
2:J:557:LYS:O	2:J:557:LYS:NZ	2.41	0.53
5:M:518:ARG:HA	5:M:523:ASP:HB2	1.91	0.53
1:S:383:SER:O	1:S:386:SER:OG	2.22	0.53
1:V:328:VAL:HG21	1:V:360:LEU:HD11	1.90	0.53
1:X:154:LEU:HD11	1:X:199:ALA:HB2	1.90	0.53
1:X:290:VAL:HA	1:X:293:VAL:HG22	1.89	0.53
1:X:291:LEU:HG	1:X:336:SER:HA	1.91	0.53
2:J:1009:HIS:O	2:J:1012:SER:OG	2.23	0.53
1:Z:291:LEU:HG	1:Z:336:SER:HA	1.91	0.53
6:K:370:GLN:HB2	6:K:486:ARG:HH21	1.74	0.52
1:V:252:ASP:OD1	1:V:252:ASP:N	2.42	0.52
1:W:154:LEU:HD11	1:W:199:ALA:HB2	1.90	0.52
1:W:252:ASP:OD1	1:W:252:ASP:N	2.42	0.52
1:Y:328:VAL:HG21	1:Y:360:LEU:HD11	1.90	0.52
1:1:252:ASP:OD1	1:1:252:ASP:N	2.42	0.52
3:N:575:ARG:NE	3:N:675:TYR:OH	2.42	0.52
1:S:154:LEU:HD11	1:S:199:ALA:HB2	1.90	0.52
1:S:290:VAL:HA	1:S:293:VAL:HG22	1.89	0.52
1:T:231:LEU:O	1:T:234:THR:OG1	2.26	0.52
1:1:88:PRO:O	1:1:124:ARG:NH2	2.39	0.52
1:2:291:LEU:HG	1:2:336:SER:HA	1.91	0.52
1:U:69:LEU:HB2	1:U:149:LEU:HD13	1.92	0.52
1:2:252:ASP:OD1	1:2:252:ASP:N	2.42	0.52
3:F:878:PHE:O	3:F:879:ARG:NH2	2.42	0.52
6:K:544:LEU:HD13	6:K:564:PHE:HB2	1.92	0.52
1:S:69:LEU:HB2	1:S:149:LEU:HD13	1.92	0.52
1:S:88:PRO:O	1:S:124:ARG:NH2	2.39	0.52
1:S:252:ASP:OD1	1:S:252:ASP:N	2.42	0.52
3:F:568:LEU:HD23	3:F:574:ILE:HG21	1.92	0.52
5:M:530:HIS:CD2	5:M:561:MET:HG3	2.44	0.52
1:T:154:LEU:HD11	1:T:199:ALA:HB2	1.90	0.52
1:1:242:THR:HA	1:1:362:ARG:HH11	1.75	0.52
6:K:365:ARG:HB3	6:K:368:LEU:HD13	1.90	0.52
3:N:456:THR:OG1	3:N:457:ASP:N	2.42	0.52
1:W:328:VAL:HG21	1:W:360:LEU:HD11	1.90	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:154:LEU:HD11	1:2:199:ALA:HB2	1.90	0.52
3:N:806:PHE:HA	3:N:809:LYS:HD3	1.90	0.52
1:U:242:THR:HA	1:U:362:ARG:HH11	1.75	0.52
1:V:69:LEU:HB2	1:V:149:LEU:HD13	1.92	0.52
1:V:154:LEU:HD11	1:V:199:ALA:HB2	1.90	0.52
1:V:291:LEU:HG	1:V:336:SER:HA	1.91	0.52
1:Y:242:THR:HA	1:Y:362:ARG:HH11	1.75	0.52
5:E:732:THR:HA	5:E:735:LYS:HG2	1.91	0.52
3:a:45:PRO:O	3:a:124:ARG:NH2	2.43	0.52
1:T:242:THR:HA	1:T:362:ARG:HH11	1.75	0.52
1:X:242:THR:HA	1:X:362:ARG:HH11	1.75	0.52
1:Z:252:ASP:OD1	1:Z:252:ASP:N	2.42	0.52
1:Z:328:VAL:HG21	1:Z:360:LEU:HD11	1.90	0.52
1:2:358:VAL:O	3:N:879:ARG:NH1	2.43	0.51
5:G:408:MET:HE2	5:G:439:ILE:HA	1.92	0.51
3:H:879:ARG:HH12	1:V:341:ARG:HB2	1.75	0.51
7:L:1513:ARG:NH1	7:L:1681:LEU:O	2.43	0.51
3:N:763:LEU:HD22	3:N:775:LEU:HD22	1.92	0.51
1:S:70:GLU:HB3	1:S:72:ARG:HH21	1.75	0.51
1:S:242:THR:HA	1:S:362:ARG:HH11	1.75	0.51
1:S:291:LEU:HG	1:S:336:SER:HA	1.91	0.51
1:U:70:GLU:HB3	1:U:72:ARG:HH21	1.75	0.51
1:V:242:THR:HA	1:V:362:ARG:HH11	1.75	0.51
1:W:242:THR:HA	1:W:362:ARG:HH11	1.75	0.51
1:X:69:LEU:HB2	1:X:149:LEU:HD13	1.92	0.51
1:1:258:ALA:HB1	5:M:687:LEU:HD13	1.93	0.51
3:n:13:LEU:HD21	3:n:39:ILE:HG21	1.91	0.51
3:N:416:GLN:NE2	3:N:526:LEU:HD21	2.25	0.51
1:U:187:ASN:O	1:U:191:THR:OG1	2.28	0.51
1:Y:70:GLU:HB3	1:Y:72:ARG:HH21	1.75	0.51
1:Z:69:LEU:HB2	1:Z:149:LEU:HD13	1.92	0.51
1:1:69:LEU:HB2	1:1:149:LEU:HD13	1.92	0.51
1:2:242:THR:HA	1:2:362:ARG:HH11	1.75	0.51
3:F:716:HIS:CE1	1:T:250:ASN:HD21	2.27	0.51
5:G:446:MET:SD	5:G:446:MET:N	2.83	0.51
1:U:252:ASP:OD1	1:U:252:ASP:N	2.43	0.51
3:H:706:ILE:O	3:H:709:SER:OG	2.24	0.51
3:H:716:HIS:CE1	1:V:250:ASN:HD21	2.29	0.51
1:W:69:LEU:HB2	1:W:149:LEU:HD13	1.92	0.51
1:X:70:GLU:HB3	1:X:72:ARG:HH21	1.75	0.51
5:G:341:LEU:HD21	5:G:362:ARG:HG3	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:289:LEU:HA	2:J:294:VAL:HA	1.93	0.51
1:V:187:ASN:O	1:V:191:THR:OG1	2.28	0.51
1:2:383:SER:O	1:2:386:SER:OG	2.22	0.51
5:M:373:GLN:HE22	5:M:377:LEU:HD22	1.76	0.51
5:M:679:ALA:HB2	5:M:822:ILE:HG13	1.92	0.51
1:V:70:GLU:HB3	1:V:72:ARG:HH21	1.75	0.51
1:X:187:ASN:O	1:X:191:THR:OG1	2.28	0.51
1:X:231:LEU:O	1:X:234:THR:OG1	2.26	0.51
2:l:24:ARG:HG2	2:l:30:GLN:HA	1.92	0.51
5:M:506:GLU:HG3	5:M:507:LYS:HD2	1.91	0.51
1:T:70:GLU:HB3	1:T:72:ARG:HH21	1.75	0.51
1:T:252:ASP:OD1	1:T:252:ASP:N	2.42	0.51
1:Y:88:PRO:O	1:Y:124:ARG:NH2	2.39	0.51
5:E:390:VAL:HA	5:E:393:LYS:HE3	1.92	0.51
5:G:168:LYS:HG2	5:G:171:GLY:H	1.75	0.51
1:S:231:LEU:O	1:S:234:THR:OG1	2.26	0.51
1:V:383:SER:O	1:V:386:SER:OG	2.22	0.51
1:Y:252:ASP:OD1	1:Y:252:ASP:N	2.42	0.51
3:n:86:VAL:HG21	4:o:21:VAL:HG13	1.93	0.51
7:L:1485:ALA:HA	7:L:1488:ILE:HD12	1.93	0.51
1:Y:69:LEU:HB2	1:Y:149:LEU:HD13	1.92	0.51
1:l:291:LEU:HG	1:l:336:SER:HA	1.91	0.51
1:l:340:ILE:HG22	5:M:861:PHE:CZ	2.46	0.51
3:H:587:ARG:HD2	3:H:588:PRO:HD2	1.92	0.51
3:N:662:ARG:HB3	3:N:764:LEU:HD13	1.92	0.51
4:k:53:GLN:HE21	3:j:9:PRO:HD3	1.76	0.51
1:Z:242:THR:HA	1:Z:362:ARG:HH11	1.75	0.51
1:U:383:SER:O	1:U:386:SER:OG	2.22	0.50
6:K:565:LEU:O	6:K:569:LEU:HB2	2.11	0.50
1:W:70:GLU:HB3	1:W:72:ARG:HH21	1.75	0.50
1:Z:70:GLU:HB3	1:Z:72:ARG:HH21	1.75	0.50
1:2:69:LEU:HB2	1:2:149:LEU:HD13	1.92	0.50
3:H:659:HIS:HB3	3:H:759:ILE:HD11	1.94	0.50
6:I:164:GLY:H	6:I:169:ARG:HE	1.58	0.50
1:T:46:ASP:N	1:T:46:ASP:OD1	2.45	0.50
1:V:46:ASP:OD1	1:V:46:ASP:N	2.45	0.50
1:W:88:PRO:O	1:W:124:ARG:NH2	2.39	0.50
1:l:187:ASN:O	1:l:191:THR:OG1	2.28	0.50
1:l:70:GLU:HB3	1:l:72:ARG:HH21	1.75	0.50
2:l:80:LYS:CE	2:l:126:TYR:CZ	2.63	0.50
6:I:1:MET:HB2	2:J:242:LEU:HD13	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:1549:VAL:HG13	7:L:1550:LEU:HD12	1.92	0.50
7:L:1555:SER:HA	7:L:1558:LEU:HD12	1.92	0.50
5:M:555:LEU:HD21	5:M:573:LEU:HD22	1.93	0.50
1:X:252:ASP:OD1	1:X:252:ASP:N	2.42	0.50
1:1:383:SER:O	1:1:386:SER:OG	2.22	0.50
6:K:344:MET:HG3	6:K:463:LEU:HD12	1.93	0.50
1:T:187:ASN:O	1:T:191:THR:OG1	2.28	0.50
1:V:68:ASP:N	1:V:68:ASP:OD1	2.45	0.50
5:M:704:PRO:C	5:M:707:HIS:H	2.20	0.50
1:T:69:LEU:HB2	1:T:149:LEU:HD13	1.92	0.50
1:W:187:ASN:O	1:W:191:THR:OG1	2.28	0.50
1:2:187:ASN:O	1:2:191:THR:OG1	2.28	0.50
3:H:380:THR:OG1	3:H:411:MET:SD	2.68	0.50
2:J:473:LEU:HA	2:J:476:VAL:HG12	1.93	0.50
5:E:525:GLY:HA2	5:E:528:PHE:HD2	1.77	0.50
1:1:46:ASP:OD1	1:1:46:ASP:N	2.45	0.49
1:2:70:GLU:HB3	1:2:72:ARG:HH21	1.75	0.49
3:F:682:LYS:HE3	1:T:254:ILE:HD12	1.92	0.49
6:I:154:LEU:O	6:I:158:TYR:HB2	2.12	0.49
6:I:496:TRP:CH2	6:I:499:GLN:HB3	2.47	0.49
7:L:1664:GLU:HG2	7:L:1769:TYR:HE1	1.77	0.49
1:U:71:PRO:O	1:U:75:HIS:NE2	2.45	0.49
2:l:121:PRO:HD2	2:l:121:PRO:O	2.11	0.49
5:E:540:ARG:HH11	5:E:613:LEU:HD11	1.76	0.49
5:M:233:VAL:HG22	5:M:248:VAL:HG13	1.94	0.49
1:S:187:ASN:O	1:S:191:THR:OG1	2.28	0.49
1:U:68:ASP:OD1	1:U:68:ASP:N	2.45	0.49
1:W:68:ASP:OD1	1:W:68:ASP:N	2.45	0.49
5:G:307:VAL:O	3:H:365:ARG:NH2	2.45	0.49
5:G:482:ARG:HD3	5:G:485:VAL:HG21	1.94	0.49
3:N:328:LEU:HD22	3:N:381:LEU:HD11	1.94	0.49
1:1:330:PRO:HG2	5:M:705:THR:HG23	1.95	0.49
2:l:16:GLU:OE2	2:l:20:ARG:NH2	2.45	0.49
2:l:129:THR:CG2	4:m:33:ARG:CD	2.88	0.49
5:G:319:LEU:HD21	5:G:324:LEU:HD21	1.95	0.49
2:J:437:LEU:HD22	2:J:549:VAL:HG21	1.95	0.49
5:M:526:ASP:HA	5:M:529:VAL:HG12	1.95	0.49
1:W:46:ASP:N	1:W:46:ASP:OD1	2.45	0.49
1:Z:46:ASP:OD1	1:Z:46:ASP:N	2.45	0.49
1:Z:383:SER:O	1:Z:386:SER:OG	2.22	0.49
3:H:656:CYS:HB2	3:H:657:MET:HE2	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:419:LEU:HA	3:H:422:VAL:HG22	1.95	0.49
2:J:922:ASP:HB3	2:J:925:GLN:HG2	1.94	0.49
3:a:61:GLU:O	3:a:65:GLN:NE2	2.44	0.49
3:a:113:SER:OG	3:a:114:TYR:N	2.46	0.49
1:S:71:PRO:O	1:S:75:HIS:NE2	2.45	0.49
1:2:88:PRO:O	1:2:124:ARG:NH2	2.39	0.49
6:I:151:CYS:HB3	6:I:263:ILE:HB	1.95	0.49
2:J:938:HIS:HB3	2:J:944:ARG:HH21	1.77	0.49
7:L:1800:LEU:HD11	1:Z:341:ARG:HG2	1.95	0.49
1:T:45:THR:HB	1:T:246:PRO:HD2	1.95	0.49
1:V:71:PRO:O	1:V:75:HIS:NE2	2.45	0.49
1:2:71:PRO:O	1:2:75:HIS:NE2	2.45	0.49
1:U:46:ASP:OD1	1:U:46:ASP:N	2.45	0.49
3:N:564:ARG:HB3	3:N:570:GLN:HB2	1.95	0.49
3:N:677:LEU:HD21	3:N:782:ILE:HG12	1.95	0.49
1:U:45:THR:HB	1:U:246:PRO:HD2	1.95	0.49
1:X:217:ARG:HB2	1:X:279:ASP:HB2	1.95	0.49
1:2:45:THR:HB	1:2:246:PRO:HD2	1.95	0.49
1:X:45:THR:HB	1:X:246:PRO:HD2	1.95	0.49
1:Y:68:ASP:OD1	1:Y:68:ASP:N	2.45	0.49
3:H:603:THR:HG23	1:W:339:ARG:HH12	1.78	0.48
6:K:646:LEU:HB3	1:Y:341:ARG:NH1	2.28	0.48
3:N:404:THR:HG21	3:N:419:LEU:HD22	1.95	0.48
3:N:554:SER:O	3:N:558:HIS:ND1	2.36	0.48
1:X:46:ASP:OD1	1:X:46:ASP:N	2.45	0.48
1:1:45:THR:HB	1:1:246:PRO:HD2	1.95	0.48
1:2:46:ASP:N	1:2:46:ASP:OD1	2.45	0.48
2:J:396:ALA:HA	2:J:399:VAL:HG22	1.94	0.48
6:K:368:LEU:HD21	6:K:405:LEU:HD23	1.95	0.48
3:N:720:TYR:HD2	3:N:879:ARG:HH12	1.60	0.48
1:S:46:ASP:OD1	1:S:46:ASP:N	2.45	0.48
1:Z:68:ASP:OD1	1:Z:68:ASP:N	2.45	0.48
6:I:20:ASN:H	6:I:24:GLY:HA2	1.78	0.48
2:J:277:LEU:HD11	2:J:294:VAL:HG21	1.94	0.48
1:S:45:THR:HB	1:S:246:PRO:HD2	1.95	0.48
1:Z:231:LEU:O	1:Z:234:THR:OG1	2.26	0.48
1:2:68:ASP:OD1	1:2:68:ASP:N	2.45	0.48
3:H:433:TRP:CE2	3:H:487:GLY:HA3	2.48	0.48
6:K:118:SER:OG	6:K:119:ILE:N	2.44	0.48
1:U:3:ARG:HH11	1:U:131:SER:HA	1.79	0.48
1:X:71:PRO:O	1:X:75:HIS:NE2	2.45	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:341:ARG:NH1	3:N:881:ASP:O	2.46	0.48
3:n:12:LEU:HG	4:o:50:LEU:HG	1.96	0.48
4:m:40:ASP:OD1	4:m:43:THR:OG1	2.32	0.48
3:F:451:ASP:H	3:F:463:LYS:HA	1.78	0.48
6:K:651:TYR:CE2	1:Y:354:ALA:HB3	2.47	0.48
3:N:717:GLN:HE22	3:N:879:ARG:HG2	1.79	0.48
1:1:3:ARG:HH11	1:1:131:SER:HA	1.79	0.48
5:E:428:TRP:CD1	5:E:455:LYS:HZ2	2.31	0.48
2:J:466:VAL:HG13	2:J:642:HIS:HE1	1.78	0.48
5:G:864:PHE:HB3	1:U:353:PRO:HB3	1.95	0.48
7:L:1732:ILE:HG23	7:L:1772:PHE:CE1	2.48	0.48
3:a:50:ASP:OD1	3:a:50:ASP:N	2.45	0.48
1:T:217:ARG:HB2	1:T:279:ASP:HB2	1.95	0.48
1:Y:46:ASP:N	1:Y:46:ASP:OD1	2.45	0.48
1:Z:3:ARG:HH11	1:Z:131:SER:HA	1.79	0.48
1:1:68:ASP:N	1:1:68:ASP:OD1	2.45	0.48
1:1:217:ARG:HB2	1:1:279:ASP:HB2	1.95	0.48
3:F:382:ALA:HA	3:F:385:VAL:HB	1.95	0.48
3:H:567:LEU:HD21	3:H:660:TYR:HD1	1.78	0.48
1:V:3:ARG:HH11	1:V:131:SER:HA	1.79	0.48
1:Y:45:THR:HB	1:Y:246:PRO:HD2	1.95	0.48
1:2:217:ARG:HB2	1:2:279:ASP:HB2	1.95	0.48
1:S:3:ARG:HH11	1:S:131:SER:HA	1.79	0.48
1:T:68:ASP:OD1	1:T:68:ASP:N	2.45	0.48
1:W:217:ARG:HB2	1:W:279:ASP:HB2	1.95	0.48
4:o:40:ASP:OD1	4:o:43:THR:OG1	2.32	0.48
5:M:702:MET:O	5:M:703:GLU:C	2.56	0.48
3:N:620:ARG:HA	3:N:643:HIS:CE1	2.49	0.48
1:S:217:ARG:HB2	1:S:279:ASP:HB2	1.95	0.48
1:U:217:ARG:HB2	1:U:279:ASP:HB2	1.95	0.48
1:W:3:ARG:HH11	1:W:131:SER:HA	1.79	0.48
1:Y:217:ARG:HB2	1:Y:279:ASP:HB2	1.95	0.48
5:G:578:MET:HE1	5:G:640:MET:HG2	1.95	0.47
6:I:59:ILE:HD11	6:I:93:LEU:HG	1.96	0.47
6:I:526:ASP:HA	6:I:529:GLN:HE21	1.78	0.47
5:M:536:GLU:HA	5:M:539:LEU:HB2	1.96	0.47
5:M:682:LEU:HG	5:M:686:MET:HE3	1.96	0.47
4:k:36:ASN:HD22	3:j:104:PRO:HA	1.78	0.47
4:k:40:ASP:OD1	4:k:43:THR:OG1	2.32	0.47
3:F:409:PRO:HA	3:F:412:ARG:HG2	1.95	0.47
6:I:575:LEU:HD12	6:I:576:LEU:H	1.78	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:314:HIS:HB2	5:M:319:LEU:HD12	1.96	0.47
3:N:416:GLN:HE22	3:N:526:LEU:HD21	1.79	0.47
3:N:461:HIS:HE1	3:N:748:ILE:HG21	1.79	0.47
3:N:712:VAL:O	3:N:716:HIS:ND1	2.48	0.47
1:W:45:THR:HB	1:W:246:PRO:HD2	1.95	0.47
5:G:531:PHE:HB2	5:G:558:ALA:HB1	1.96	0.47
1:X:3:ARG:HH11	1:X:131:SER:HA	1.79	0.47
1:1:339:ARG:HA	1:1:339:ARG:NH2	2.30	0.47
2:l:121:PRO:HG3	4:m:36:ASN:HB2	1.96	0.47
6:I:299:ILE:HG22	6:I:303:GLN:HE21	1.78	0.47
5:M:519:TYR:HE1	5:M:524:GLN:HE22	1.63	0.47
3:N:346:LEU:HD13	3:N:362:LEU:H	1.79	0.47
3:N:581:LEU:HG	3:N:585:LEU:HG	1.97	0.47
1:S:339:ARG:HA	1:S:339:ARG:NH2	2.30	0.47
1:V:45:THR:HB	1:V:246:PRO:HD2	1.95	0.47
1:Z:217:ARG:HB2	1:Z:279:ASP:HB2	1.95	0.47
6:I:369:PHE:HA	6:I:372:PHE:HB3	1.96	0.47
7:L:288:THR:HA	4:b:22:ARG:HE	1.79	0.47
1:V:217:ARG:HB2	1:V:279:ASP:HB2	1.95	0.47
1:W:339:ARG:NH2	1:W:339:ARG:HA	2.30	0.47
1:1:35:GLY:HA2	1:1:85:LEU:HD12	1.97	0.47
1:2:251:ASN:HD21	3:N:575:ARG:HG3	1.79	0.47
7:L:1664:GLU:OE2	7:L:1773:LYS:NZ	2.35	0.47
1:S:35:GLY:HA2	1:S:85:LEU:HD12	1.97	0.47
1:T:35:GLY:HA2	1:T:85:LEU:HD12	1.97	0.47
1:T:339:ARG:HA	1:T:339:ARG:NH2	2.30	0.47
1:U:339:ARG:HA	1:U:339:ARG:NH2	2.30	0.47
1:V:35:GLY:HA2	1:V:85:LEU:HD12	1.97	0.47
1:Z:187:ASN:O	1:Z:191:THR:OG1	2.28	0.47
1:1:231:LEU:O	1:1:234:THR:OG1	2.26	0.47
2:l:80:LYS:HB3	2:l:126:TYR:CE1	2.48	0.47
5:E:525:GLY:H	1:S:248:TYR:HB3	1.79	0.47
3:F:879:ARG:CZ	1:T:337:LEU:HD21	2.45	0.47
5:G:557:LEU:HD11	1:V:295:ARG:HH22	1.78	0.47
5:G:557:LEU:HD22	5:G:561:MET:HB2	1.97	0.47
2:J:444:ILE:HG12	2:J:461:LEU:HG	1.95	0.47
6:K:651:TYR:CE1	1:Y:348:PHE:HE2	2.32	0.47
6:K:651:TYR:CZ	1:Y:354:ALA:HB3	2.50	0.47
7:L:346:LEU:HA	7:L:347:VAL:HA	1.75	0.47
1:U:231:LEU:O	1:U:234:THR:OG1	2.26	0.47
1:W:223:PRO:O	1:W:226:SER:OG	2.33	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:339:ARG:HA	1:X:339:ARG:NH2	2.30	0.47
1:Y:183:VAL:HG13	1:Y:187:ASN:HD21	1.80	0.47
1:Z:45:THR:HB	1:Z:246:PRO:HD2	1.95	0.47
1:2:35:GLY:HA2	1:2:85:LEU:HD12	1.97	0.47
7:L:287:LEU:HD11	4:b:21:VAL:HB	1.97	0.47
3:N:558:HIS:O	3:N:562:MET:N	2.48	0.47
4:b:40:ASP:OD1	4:b:43:THR:OG1	2.32	0.47
1:T:3:ARG:HH11	1:T:131:SER:HA	1.79	0.47
1:1:71:PRO:O	1:1:75:HIS:NE2	2.45	0.47
3:F:712:VAL:O	3:F:716:HIS:HB2	2.15	0.47
5:G:168:LYS:HE3	5:G:170:SER:HB2	1.97	0.47
7:L:1505:LEU:HD22	7:L:1604:LEU:HG	1.96	0.47
5:M:719:ILE:HA	5:M:722:VAL:HG22	1.96	0.47
1:X:68:ASP:N	1:X:68:ASP:OD1	2.45	0.47
1:Z:339:ARG:HA	1:Z:339:ARG:NH2	2.30	0.47
5:G:222:LEU:HG	3:H:365:ARG:HH22	1.80	0.47
5:G:517:LYS:HG3	5:G:521:LEU:HD12	1.95	0.47
3:j:51:GLU:HB3	3:j:91:TRP:HB2	1.97	0.47
1:V:223:PRO:O	1:V:226:SER:OG	2.33	0.47
1:Y:339:ARG:HA	1:Y:339:ARG:NH2	2.30	0.47
1:Z:105:ALA:O	1:Z:109:SER:OG	2.33	0.47
1:1:105:ALA:O	1:1:109:SER:OG	2.33	0.46
1:2:105:ALA:O	1:2:109:SER:OG	2.33	0.46
5:E:154:LEU:HA	5:E:157:LYS:HE2	1.97	0.46
2:J:557:LYS:HE3	2:J:561:MET:HE3	1.97	0.46
1:U:35:GLY:HA2	1:U:85:LEU:HD12	1.97	0.46
1:U:223:PRO:O	1:U:226:SER:OG	2.33	0.46
1:W:35:GLY:HA2	1:W:85:LEU:HD12	1.97	0.46
1:W:105:ALA:O	1:W:109:SER:OG	2.33	0.46
1:2:3:ARG:HH11	1:2:131:SER:HA	1.79	0.46
6:I:499:GLN:HA	1:W:264:PRO:HB3	1.97	0.46
3:N:563:ARG:HH11	3:N:564:ARG:HG2	1.79	0.46
1:X:183:VAL:HG13	1:X:187:ASN:HD21	1.80	0.46
1:Y:3:ARG:HH11	1:Y:131:SER:HA	1.79	0.46
1:1:56:ASP:OD1	1:2:296:ARG:HD3	2.16	0.46
1:2:339:ARG:HA	1:2:339:ARG:NH2	2.30	0.46
2:J:221:VAL:HG12	2:J:228:ARG:HH22	1.80	0.46
6:K:64:GLY:HA3	7:L:468:ARG:HH22	1.81	0.46
6:K:646:LEU:C	1:Y:341:ARG:HH12	2.22	0.46
1:S:105:ALA:O	1:S:109:SER:OG	2.33	0.46
1:T:183:VAL:HG13	1:T:187:ASN:HD21	1.80	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:105:ALA:O	1:U:109:SER:OG	2.33	0.46
1:V:183:VAL:HG13	1:V:187:ASN:HD21	1.80	0.46
1:V:339:ARG:HA	1:V:339:ARG:NH2	2.30	0.46
1:Y:231:LEU:O	1:Y:234:THR:OG1	2.26	0.46
1:1:183:VAL:HG13	1:1:187:ASN:HD21	1.80	0.46
1:1:223:PRO:O	1:1:226:SER:OG	2.33	0.46
3:F:571:GLY:HA3	1:T:248:TYR:HB3	1.98	0.46
3:F:865:LEU:HB3	3:F:873:LEU:HD21	1.98	0.46
5:M:698:MET:HE3	5:M:703:GLU:N	2.27	0.46
1:S:183:VAL:HG13	1:S:187:ASN:HD21	1.80	0.46
1:2:360:LEU:HB2	3:N:724:PHE:CE2	2.50	0.46
5:G:443:LEU:HD12	5:G:450:ILE:HD11	1.98	0.46
3:H:635:TRP:CD2	3:H:672:ARG:HD3	2.50	0.46
2:J:279:SER:HB3	2:J:379:LEU:HD22	1.97	0.46
7:L:588:LEU:HD21	7:L:590:HIS:HB2	1.98	0.46
5:M:157:LYS:HB3	5:M:284:GLU:HG3	1.97	0.46
3:N:635:TRP:CG	3:N:672:ARG:HE	2.34	0.46
1:T:223:PRO:O	1:T:226:SER:OG	2.33	0.46
1:X:223:PRO:O	1:X:226:SER:OG	2.33	0.46
3:F:845:SER:HA	3:F:848:ARG:HE	1.79	0.46
5:G:370:SER:HA	5:G:373:GLN:HB3	1.97	0.46
1:S:223:PRO:O	1:S:226:SER:OG	2.33	0.46
1:X:7:THR:HA	1:X:136:VAL:HG13	1.98	0.46
1:Z:35:GLY:HA2	1:Z:85:LEU:HD12	1.97	0.46
1:2:223:PRO:O	1:2:226:SER:OG	2.33	0.46
5:E:526:ASP:HA	5:E:529:VAL:HG12	1.98	0.46
2:J:925:GLN:HA	2:J:928:LYS:HD3	1.98	0.46
6:K:368:LEU:HG	6:K:403:VAL:HG21	1.97	0.46
1:T:7:THR:HA	1:T:136:VAL:HG13	1.98	0.46
1:Y:71:PRO:O	1:Y:75:HIS:NE2	2.45	0.46
1:Y:105:ALA:O	1:Y:109:SER:OG	2.33	0.46
5:G:577:LEU:HD11	5:G:608:LEU:HD12	1.97	0.46
3:H:493:LEU:HD13	3:H:545:LEU:HD13	1.97	0.46
1:S:68:ASP:N	1:S:68:ASP:OD1	2.45	0.46
1:S:278:THR:O	1:S:278:THR:OG1	2.34	0.46
1:W:71:PRO:O	1:W:75:HIS:NE2	2.45	0.46
1:W:183:VAL:HG13	1:W:187:ASN:HD21	1.80	0.46
1:X:105:ALA:O	1:X:109:SER:OG	2.33	0.46
1:Z:183:VAL:HG13	1:Z:187:ASN:HD21	1.80	0.46
1:1:3:ARG:HA	5:M:530:HIS:CE1	2.46	0.46
1:1:7:THR:HA	1:1:136:VAL:HG13	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:490:ILE:HG12	3:F:494:HIS:CE1	2.51	0.46
5:G:557:LEU:O	5:G:558:ALA:C	2.58	0.46
3:N:555:LEU:HD13	3:N:648:ILE:HB	1.97	0.46
1:T:105:ALA:O	1:T:109:SER:OG	2.33	0.46
1:Y:7:THR:HA	1:Y:136:VAL:HG13	1.98	0.46
5:E:663:LYS:NZ	1:S:200:ASP:OD2	2.49	0.46
3:H:666:PHE:HE1	3:H:772:LEU:HD13	1.81	0.46
6:K:11:GLY:HA2	6:K:53:ILE:HG12	1.97	0.46
6:K:59:ILE:HG23	6:K:90:CYS:HB3	1.98	0.46
5:M:732:THR:HA	5:M:735:LYS:HG2	1.97	0.46
1:U:7:THR:HA	1:U:136:VAL:HG13	1.98	0.46
1:U:183:VAL:HG13	1:U:187:ASN:HD21	1.80	0.46
1:W:278:THR:O	1:W:278:THR:OG1	2.34	0.46
1:Y:223:PRO:O	1:Y:226:SER:OG	2.33	0.46
1:Y:250:ASN:ND2	1:Y:255:GLY:O	2.50	0.46
5:G:288:VAL:HG23	5:G:383:ALA:HB1	1.96	0.45
5:G:363:SER:HA	5:G:376:CYS:SG	2.56	0.45
5:G:439:ILE:HG22	5:G:441:SER:H	1.81	0.45
6:I:401:HIS:O	1:X:339:ARG:NH1	2.46	0.45
6:I:565:LEU:HA	6:I:568:LEU:HD12	1.98	0.45
1:U:250:ASN:ND2	1:U:255:GLY:O	2.50	0.45
1:V:47:ARG:HG2	1:V:49:ASP:H	1.81	0.45
1:2:231:LEU:O	1:2:234:THR:OG1	2.26	0.45
5:G:532:MET:HE1	5:G:646:PHE:HE1	1.81	0.45
3:N:549:LEU:HD23	3:N:549:LEU:HA	1.80	0.45
1:T:250:ASN:ND2	1:T:255:GLY:O	2.50	0.45
1:U:47:ARG:HG2	1:U:49:ASP:H	1.81	0.45
1:W:29:HIS:HB3	1:W:48:LYS:HD3	1.98	0.45
1:W:383:SER:O	1:W:386:SER:OG	2.22	0.45
1:Y:35:GLY:HA2	1:Y:85:LEU:HD12	1.97	0.45
1:2:7:THR:HA	1:2:136:VAL:HG13	1.98	0.45
1:2:47:ARG:HG2	1:2:49:ASP:H	1.81	0.45
6:K:204:PHE:HB2	6:K:259:LEU:HD12	1.98	0.45
1:U:29:HIS:HB3	1:U:48:LYS:HD3	1.98	0.45
1:V:29:HIS:HB3	1:V:48:LYS:HD3	1.98	0.45
1:X:35:GLY:HA2	1:X:85:LEU:HD12	1.97	0.45
1:Z:7:THR:HA	1:Z:136:VAL:HG13	1.98	0.45
5:E:861:PHE:HA	1:S:341:ARG:NH1	2.30	0.45
6:I:345:VAL:HG23	6:I:346:GLU:HG3	1.98	0.45
6:K:653:LYS:HG3	6:K:657:GLN:HG3	1.98	0.45
3:a:47:VAL:HA	3:a:123:PRO:HA	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:303:VAL:HG12	1:S:305:VAL:H	1.82	0.45
1:T:47:ARG:HG2	1:T:49:ASP:H	1.81	0.45
1:T:303:VAL:HG12	1:T:305:VAL:H	1.82	0.45
1:U:278:THR:O	1:U:278:THR:OG1	2.34	0.45
1:W:47:ARG:HG2	1:W:49:ASP:H	1.81	0.45
1:Z:71:PRO:O	1:Z:75:HIS:NE2	2.45	0.45
1:Z:223:PRO:O	1:Z:226:SER:OG	2.33	0.45
1:Z:278:THR:O	1:Z:278:THR:OG1	2.34	0.45
3:F:526:LEU:HD12	3:F:526:LEU:HA	1.80	0.45
2:J:406:LEU:HA	2:J:409:LEU:HD12	1.99	0.45
6:K:651:TYR:CE1	1:Y:348:PHE:CE2	3.04	0.45
3:a:57:LYS:O	3:a:61:GLU:HG2	2.17	0.45
1:S:7:THR:HA	1:S:136:VAL:HG13	1.98	0.45
1:T:71:PRO:O	1:T:75:HIS:NE2	2.45	0.45
1:1:29:HIS:HB3	1:1:48:LYS:HD3	1.98	0.45
1:2:183:VAL:HG13	1:2:187:ASN:HD21	1.80	0.45
3:H:601:LEU:C	3:H:603:THR:H	2.24	0.45
3:H:803:ARG:HH22	3:H:833:ILE:HD11	1.81	0.45
3:N:680:ILE:HD12	3:N:789:GLN:HG2	1.98	0.45
1:V:303:VAL:HG12	1:V:305:VAL:H	1.82	0.45
1:W:250:ASN:ND2	1:W:255:GLY:O	2.50	0.45
2:J:720:LEU:HG	2:J:724:ARG:HH21	1.82	0.45
1:U:303:VAL:HG12	1:U:305:VAL:H	1.82	0.45
4:o:68:ARG:HA	4:o:68:ARG:HD3	1.70	0.45
6:I:344:MET:HE1	6:I:463:LEU:HA	1.99	0.45
3:j:100:LEU:HD23	3:j:100:LEU:HA	1.57	0.45
1:W:7:THR:HA	1:W:136:VAL:HG13	1.98	0.45
1:2:250:ASN:ND2	1:2:255:GLY:O	2.50	0.45
1:S:29:HIS:HB3	1:S:48:LYS:HD3	1.98	0.45
1:Y:278:THR:O	1:Y:278:THR:OG1	2.34	0.45
1:Y:303:VAL:HG12	1:Y:305:VAL:H	1.82	0.45
1:1:377:MET:HE3	1:1:377:MET:HB2	1.88	0.45
3:H:294:LEU:HD21	3:H:368:LEU:HD22	1.97	0.45
6:I:190:TRP:CE2	6:I:280:GLY:HA3	2.52	0.45
7:L:1803:ASN:O	1:Z:341:ARG:NH1	2.45	0.45
4:k:68:ARG:HA	4:k:68:ARG:HD3	1.70	0.45
1:V:105:ALA:O	1:V:109:SER:OG	2.33	0.45
1:V:250:ASN:ND2	1:V:255:GLY:O	2.50	0.45
1:X:303:VAL:HG12	1:X:305:VAL:H	1.82	0.45
1:Y:47:ARG:HG2	1:Y:49:ASP:H	1.81	0.45
1:Z:69:LEU:HG	1:Z:70:GLU:HG3	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:250:ASN:ND2	1:Z:255:GLY:O	2.50	0.45
1:1:250:ASN:ND2	1:1:255:GLY:O	2.50	0.44
1:1:330:PRO:HD3	5:M:704:PRO:C	2.42	0.44
3:n:45:PRO:HG3	3:n:89:ASN:HD21	1.83	0.44
1:X:250:ASN:ND2	1:X:255:GLY:O	2.50	0.44
3:H:397:ALA:HB1	3:H:474:PHE:HE2	1.83	0.44
3:N:730:SER:C	3:N:754:PHE:HE1	2.24	0.44
1:V:69:LEU:HG	1:V:70:GLU:HG3	1.99	0.44
1:X:29:HIS:HB3	1:X:48:LYS:HD3	1.98	0.44
1:Y:69:LEU:HG	1:Y:70:GLU:HG3	1.99	0.44
1:2:303:VAL:HG12	1:2:305:VAL:H	1.82	0.44
3:H:603:THR:HG21	1:W:342:GLU:HG3	1.98	0.44
5:M:559:LEU:HD21	5:M:570:LYS:HG2	2.00	0.44
3:N:391:ARG:HD3	3:N:395:GLU:HG2	2.00	0.44
1:S:47:ARG:HG2	1:S:49:ASP:H	1.81	0.44
1:U:377:MET:HE3	1:U:377:MET:HB2	1.88	0.44
1:X:47:ARG:HG2	1:X:49:ASP:H	1.81	0.44
1:1:47:ARG:HG2	1:1:49:ASP:H	1.81	0.44
1:2:29:HIS:HB3	1:2:48:LYS:HD3	1.98	0.44
1:2:69:LEU:HG	1:2:70:GLU:HG3	1.99	0.44
1:2:260:LEU:HD22	1:2:379:ALA:HA	2.00	0.44
3:H:625:LEU:HD12	3:H:637:VAL:HG12	1.99	0.44
6:I:569:LEU:HG	6:I:575:LEU:HB2	1.99	0.44
6:I:610:ALA:O	6:I:613:SER:OG	2.30	0.44
6:K:544:LEU:HD12	6:K:560:ALA:HB1	2.00	0.44
7:L:1670:LYS:NZ	1:Z:250:ASN:HD21	2.16	0.44
3:N:419:LEU:HA	3:N:422:VAL:HG22	1.99	0.44
3:N:717:GLN:NE2	3:N:879:ARG:HH21	2.16	0.44
1:Y:29:HIS:HB3	1:Y:48:LYS:HD3	1.98	0.44
1:Z:29:HIS:HB3	1:Z:48:LYS:HD3	1.98	0.44
6:I:97:LEU:HB2	6:I:101:ARG:HH21	1.82	0.44
7:L:601:THR:HG21	7:L:1495:ALA:HB2	2.00	0.44
7:L:1663:HIS:CG	1:Z:262:PRO:HA	2.53	0.44
5:M:527:PHE:HZ	5:M:555:LEU:HG	1.82	0.44
1:W:231:LEU:O	1:W:234:THR:OG1	2.26	0.44
1:Z:47:ARG:HG2	1:Z:49:ASP:H	1.81	0.44
1:Z:303:VAL:HG12	1:Z:305:VAL:H	1.82	0.44
1:1:278:THR:O	1:1:278:THR:OG1	2.34	0.44
5:G:861:PHE:HA	1:U:341:ARG:HH12	1.81	0.44
2:J:212:ASP:HB3	7:L:325:ARG:HH12	1.82	0.44
5:M:695:TYR:HD2	5:M:858:ARG:HH12	1.64	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:250:ASN:ND2	1:S:255:GLY:O	2.50	0.44
1:Y:187:ASN:O	1:Y:191:THR:OG1	2.28	0.44
1:1:264:PRO:HB3	5:M:663:LYS:HG3	1.99	0.44
5:E:427:TYR:HE2	5:E:455:LYS:HD3	1.83	0.44
3:F:836:PHE:O	3:F:840:ILE:HG12	2.18	0.44
5:M:354:SER:OG	5:M:437:GLN:NE2	2.50	0.44
5:M:518:ARG:C	5:M:523:ASP:H	2.25	0.44
1:S:69:LEU:HG	1:S:70:GLU:HG3	1.99	0.44
1:V:7:THR:HA	1:V:136:VAL:HG13	1.98	0.44
1:Z:260:LEU:HD22	1:Z:379:ALA:HA	2.00	0.44
1:1:339:ARG:NH2	1:1:342:GLU:HB2	2.32	0.44
5:E:224:VAL:HB	5:E:233:VAL:HG21	2.00	0.44
3:F:249:ALA:HB1	3:F:252:ARG:HH21	1.83	0.44
6:K:653:LYS:H	1:Y:353:PRO:HB3	1.82	0.44
1:T:29:HIS:HB3	1:T:48:LYS:HD3	1.98	0.44
1:U:69:LEU:HG	1:U:70:GLU:HG3	1.99	0.44
1:X:69:LEU:HG	1:X:70:GLU:HG3	1.99	0.44
1:1:303:VAL:HG12	1:1:305:VAL:H	1.82	0.44
6:I:460:GLN:O	6:I:464:HIS:N	2.51	0.44
5:M:518:ARG:O	5:M:523:ASP:N	2.50	0.44
1:Z:339:ARG:NH2	1:Z:342:GLU:HB2	2.31	0.44
1:2:415:LYS:HD2	1:2:415:LYS:HA	1.88	0.43
5:G:286:GLY:O	5:G:290:HIS:ND1	2.50	0.43
1:S:260:LEU:HD22	1:S:379:ALA:HA	2.00	0.43
1:T:69:LEU:HG	1:T:70:GLU:HG3	1.99	0.43
1:W:303:VAL:HG12	1:W:305:VAL:H	1.82	0.43
1:Z:84:LYS:H	1:Z:84:LYS:HG2	1.50	0.43
1:1:260:LEU:HD22	1:1:379:ALA:HA	2.00	0.43
5:E:152:GLN:HA	5:E:155:GLU:HG2	1.99	0.43
5:E:689:PHE:CZ	5:E:693:ILE:HD11	2.53	0.43
5:G:350:CYS:HB3	5:G:355:THR:HB	1.99	0.43
5:G:445:LYS:HE2	5:G:446:MET:HE1	1.99	0.43
3:a:49:ARG:HG3	3:a:91:TRP:CD2	2.53	0.43
1:U:324:ILE:HD11	1:U:373:VAL:HG12	2.01	0.43
1:W:260:LEU:HD22	1:W:379:ALA:HA	2.00	0.43
1:1:318:ILE:HD11	1:1:382:THR:HG23	2.01	0.43
4:m:39:LEU:HD13	4:m:44:LEU:HB2	2.00	0.43
3:F:582:LYS:HG3	3:F:583:PRO:HD3	2.00	0.43
6:I:363:LEU:HD23	6:I:363:LEU:HA	1.82	0.43
3:N:850:LEU:HD13	3:N:850:LEU:HA	1.80	0.43
1:T:260:LEU:HD22	1:T:379:ALA:HA	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:318:ILE:HD11	1:T:382:THR:HG23	2.01	0.43
1:V:260:LEU:HD22	1:V:379:ALA:HA	2.00	0.43
1:X:260:LEU:HD22	1:X:379:ALA:HA	2.00	0.43
1:1:344:LYS:HE2	1:1:344:LYS:HB3	1.92	0.43
3:n:84:GLN:NE2	4:o:23:GLU:OE1	2.51	0.43
7:L:1679:GLN:HA	7:L:1683:VAL:HG22	2.00	0.43
5:M:468:THR:OG1	5:M:469:CYS:N	2.48	0.43
1:2:9:GLN:HA	1:2:138:CYS:HB2	2.01	0.43
1:2:249:MET:HG2	3:N:723:THR:HG21	2.00	0.43
3:F:688:ALA:HB3	1:T:264:PRO:HG2	2.00	0.43
5:G:559:LEU:HD12	5:G:559:LEU:HA	1.82	0.43
5:G:865:TYR:HA	5:G:868:ARG:HE	1.83	0.43
3:H:593:TYR:HB2	3:H:595:HIS:CD2	2.52	0.43
3:H:799:GLU:HG2	3:H:836:PHE:CZ	2.53	0.43
2:J:291:ASP:N	2:J:291:ASP:OD1	2.49	0.43
5:M:408:MET:HE2	5:M:408:MET:HB3	1.92	0.43
3:N:806:PHE:HE2	3:N:832:ARG:HH12	1.66	0.43
1:T:9:GLN:HA	1:T:138:CYS:HB2	2.01	0.43
1:W:9:GLN:HA	1:W:138:CYS:HB2	2.01	0.43
1:1:69:LEU:HG	1:1:70:GLU:HG3	1.99	0.43
5:E:386:PRO:HB3	3:F:412:ARG:HH22	1.84	0.43
5:G:306:LEU:O	5:G:310:LEU:HG	2.18	0.43
2:J:377:GLU:HB2	6:K:124:TYR:CE1	2.53	0.43
3:N:863:VAL:HG12	3:N:887:LYS:HD3	1.99	0.43
1:T:324:ILE:HD11	1:T:373:VAL:HG12	2.01	0.43
1:T:377:MET:HE3	1:T:377:MET:HB2	1.88	0.43
1:V:324:ILE:HD11	1:V:373:VAL:HG12	2.01	0.43
1:Z:318:ILE:HD11	1:Z:382:THR:HG23	2.01	0.43
1:U:339:ARG:NH2	1:U:342:GLU:HB2	2.31	0.43
1:V:231:LEU:O	1:V:234:THR:OG1	2.26	0.43
1:W:69:LEU:HG	1:W:70:GLU:HG3	1.99	0.43
1:X:278:THR:O	1:X:278:THR:OG1	2.34	0.43
1:1:53:TYR:OH	1:2:299:GLN:OE1	2.16	0.43
1:1:249:MET:HB3	5:M:695:TYR:HE1	1.83	0.43
4:b:39:LEU:HD13	4:b:44:LEU:HB2	2.01	0.43
1:U:260:LEU:HD22	1:U:379:ALA:HA	2.00	0.43
1:X:324:ILE:HD11	1:X:373:VAL:HG12	2.00	0.43
1:Y:318:ILE:HD11	1:Y:382:THR:HG23	2.01	0.43
1:1:9:GLN:HA	1:1:138:CYS:HB2	2.01	0.43
1:1:110:GLN:HA	1:1:113:LYS:HE3	2.01	0.43
5:E:236:GLN:HG3	5:E:245:THR:HG23	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:241:ARG:HE	5:E:242:GLN:H	1.67	0.43
3:F:620:ARG:HA	3:F:643:HIS:CE1	2.53	0.43
5:G:341:LEU:HD23	5:G:341:LEU:HA	1.89	0.43
5:G:446:MET:HG3	5:G:449:LYS:HD2	2.00	0.43
5:G:827:LYS:HD2	5:G:827:LYS:HA	1.83	0.43
3:H:704:CYS:SG	3:H:705:HIS:N	2.92	0.43
5:M:206:GLY:H	5:M:251:ASN:ND2	2.17	0.43
4:b:68:ARG:HA	4:b:68:ARG:HD3	1.70	0.43
1:S:9:GLN:HA	1:S:138:CYS:HB2	2.01	0.43
1:S:31:ILE:HG23	1:S:37:VAL:HA	2.01	0.43
1:T:84:LYS:H	1:T:84:LYS:HG2	1.50	0.43
1:Y:260:LEU:HD22	1:Y:379:ALA:HA	2.00	0.43
1:Z:31:ILE:HG23	1:Z:37:VAL:HA	2.01	0.43
5:E:252:LEU:HG	5:E:257:ARG:HB2	2.00	0.43
5:E:704:PRO:HG3	1:S:330:PRO:HG2	2.00	0.43
5:G:691:GLN:HE21	5:G:691:GLN:HB2	1.62	0.43
6:I:578:PRO:HA	6:I:581:HIS:HD2	1.84	0.43
6:K:653:LYS:HD3	1:Y:353:PRO:HD3	2.00	0.43
1:S:339:ARG:NH2	1:S:342:GLU:HB2	2.32	0.43
1:T:31:ILE:HG23	1:T:37:VAL:HA	2.01	0.43
1:T:110:GLN:HA	1:T:113:LYS:HE3	2.01	0.43
1:T:339:ARG:NH2	1:T:342:GLU:HB2	2.32	0.43
1:V:9:GLN:HA	1:V:138:CYS:HB2	2.01	0.43
1:Y:110:GLN:HA	1:Y:113:LYS:HE3	2.01	0.43
5:E:164:LYS:HD2	5:E:405:SER:H	1.84	0.42
5:G:256:ILE:O	5:G:260:VAL:HG12	2.19	0.42
3:H:669:ARG:HG2	3:H:672:ARG:HH22	1.84	0.42
6:K:191:MET:HE3	6:K:276:ILE:HA	2.01	0.42
3:j:38:VAL:O	3:j:42:ASN:ND2	2.41	0.42
1:U:318:ILE:HD11	1:U:382:THR:HG23	2.01	0.42
1:2:31:ILE:HG23	1:2:37:VAL:HA	2.01	0.42
2:l:121:PRO:CG	4:m:36:ASN:HB2	2.49	0.42
5:E:187:LEU:HD21	3:F:379:LYS:HE2	2.01	0.42
5:E:814:LEU:HB3	5:E:815:VAL:H	1.69	0.42
3:H:878:PHE:O	1:V:341:ARG:NH1	2.44	0.42
6:I:539:SER:O	6:I:542:SER:OG	2.31	0.42
2:J:938:HIS:CD2	2:J:944:ARG:HB3	2.54	0.42
5:M:164:LYS:HG2	5:M:404:TYR:HA	2.01	0.42
1:V:318:ILE:HD11	1:V:382:THR:HG23	2.01	0.42
1:W:318:ILE:HD11	1:W:382:THR:HG23	2.01	0.42
1:W:324:ILE:HD11	1:W:373:VAL:HG12	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:318:ILE:HD11	1:X:382:THR:HG23	2.01	0.42
1:Z:9:GLN:HA	1:Z:138:CYS:HB2	2.01	0.42
1:1:15:ASN:HD22	1:1:74:ILE:HG12	1.85	0.42
1:1:31:ILE:HG23	1:1:37:VAL:HA	2.01	0.42
1:2:324:ILE:HD11	1:2:373:VAL:HG12	2.01	0.42
5:G:388:PHE:O	5:G:392:GLU:HB2	2.19	0.42
3:H:734:LEU:HB2	3:H:754:PHE:CD1	2.54	0.42
2:J:358:PHE:CD1	2:J:429:ASN:HB2	2.54	0.42
3:N:327:ALA:HB1	3:N:418:ILE:HG13	2.00	0.42
4:k:39:LEU:HD13	4:k:44:LEU:HB2	2.00	0.42
1:S:318:ILE:HD11	1:S:382:THR:HG23	2.01	0.42
1:V:31:ILE:HG23	1:V:37:VAL:HA	2.01	0.42
1:W:110:GLN:HA	1:W:113:LYS:HE3	2.01	0.42
1:X:9:GLN:HA	1:X:138:CYS:HB2	2.01	0.42
1:X:110:GLN:HA	1:X:113:LYS:HE3	2.01	0.42
1:Y:393:ARG:HE	1:Y:394:GLN:HG3	1.85	0.42
1:2:15:ASN:HD22	1:2:74:ILE:HG12	1.85	0.42
3:F:568:LEU:HD13	3:F:667:LEU:HB2	2.02	0.42
3:H:716:HIS:HE1	1:V:250:ASN:HD21	1.67	0.42
5:M:241:ARG:O	5:M:275:ARG:NH1	2.53	0.42
1:T:393:ARG:HE	1:T:394:GLN:HG3	1.85	0.42
1:U:15:ASN:HD22	1:U:74:ILE:HG12	1.85	0.42
1:1:324:ILE:HD11	1:1:373:VAL:HG12	2.00	0.42
4:o:39:LEU:HD13	4:o:44:LEU:HB2	2.01	0.42
5:G:415:ARG:N	5:G:431:ARG:HH12	2.17	0.42
3:H:336:TYR:HB2	6:I:124:TYR:CD1	2.55	0.42
2:J:392:THR:HG21	7:L:295:ARG:HB2	2.02	0.42
5:M:702:MET:HB3	5:M:703:GLU:H	1.62	0.42
1:S:377:MET:HE3	1:S:377:MET:HB2	1.88	0.42
1:S:393:ARG:HE	1:S:394:GLN:HG3	1.85	0.42
1:U:393:ARG:HE	1:U:394:GLN:HG3	1.85	0.42
1:Y:9:GLN:HA	1:Y:138:CYS:HB2	2.01	0.42
1:Y:15:ASN:HD22	1:Y:74:ILE:HG12	1.85	0.42
1:Z:110:GLN:HA	1:Z:113:LYS:HE3	2.01	0.42
1:2:318:ILE:HD11	1:2:382:THR:HG23	2.01	0.42
2:l:129:THR:N	2:l:130:PRO:CD	2.83	0.42
5:G:329:GLN:H	5:G:329:GLN:HG2	1.73	0.42
7:L:1661:PHE:O	7:L:1664:GLU:HB3	2.20	0.42
5:M:343:THR:O	5:M:347:LYS:HB2	2.20	0.42
3:n:97:LEU:O	3:n:101:SER:OG	2.37	0.42
4:m:68:ARG:HA	4:m:68:ARG:HD3	1.70	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:156:LEU:HD12	5:E:156:LEU:HA	1.80	0.42
5:G:637:ARG:O	5:G:641:LEU:HG	2.20	0.42
3:H:389:GLN:O	3:H:391:ARG:NH1	2.53	0.42
3:H:597:LEU:HG	3:H:623:VAL:HG21	2.01	0.42
3:H:837:LYS:HA	3:H:837:LYS:HD2	1.80	0.42
6:I:530:TYR:CE1	1:W:249:MET:HG2	2.53	0.42
7:L:416:GLN:HG3	7:L:433:THR:HG21	2.01	0.42
3:N:597:LEU:HA	3:N:597:LEU:HD13	1.81	0.42
1:T:384:ILE:HD12	1:T:384:ILE:HA	1.92	0.42
1:Y:377:MET:HE3	1:Y:377:MET:HB2	1.88	0.42
3:F:557:ASP:HA	3:F:560:GLN:HB3	2.01	0.42
3:F:879:ARG:HA	3:F:879:ARG:NE	2.34	0.42
5:G:532:MET:HE3	5:G:532:MET:HB3	1.82	0.42
6:I:143:ILE:HG23	6:I:148:ILE:HB	2.00	0.42
7:L:1728:VAL:HG11	7:L:1779:LEU:HB3	2.01	0.42
1:S:3:ARG:HB2	1:S:4:GLU:H	1.73	0.42
1:S:15:ASN:HD22	1:S:74:ILE:HG12	1.85	0.42
1:Z:15:ASN:HD22	1:Z:74:ILE:HG12	1.85	0.42
1:Z:324:ILE:HD11	1:Z:373:VAL:HG12	2.01	0.42
1:2:84:LYS:H	1:2:84:LYS:HG2	1.50	0.42
2:l:116:CYS:O	2:l:117:LEU:C	2.62	0.42
2:l:129:THR:CG2	4:m:33:ARG:NE	2.81	0.42
3:F:489:SER:HB2	3:F:545:LEU:HD11	2.01	0.42
5:G:222:LEU:HD21	5:G:310:LEU:HB2	2.01	0.42
5:G:259:LEU:HA	5:G:262:ARG:HE	1.84	0.42
3:H:448:VAL:HG22	3:H:484:LEU:HD12	2.02	0.42
2:J:707:MET:HE3	2:J:707:MET:HB3	1.83	0.42
4:k:52:GLU:OE2	3:j:88:LYS:HD3	2.20	0.42
1:S:110:GLN:HA	1:S:113:LYS:HE3	2.01	0.42
1:V:15:ASN:HD22	1:V:74:ILE:HG12	1.85	0.42
1:V:85:LEU:HD23	1:V:86:TYR:HD1	1.85	0.42
1:V:110:GLN:HA	1:V:113:LYS:HE3	2.01	0.42
1:V:393:ARG:HE	1:V:394:GLN:HG3	1.85	0.42
1:X:31:ILE:HG23	1:X:37:VAL:HA	2.01	0.42
1:2:393:ARG:HE	1:2:394:GLN:HG3	1.85	0.42
5:G:332:MET:HE3	5:G:333:ARG:HH12	1.85	0.42
5:G:356:LEU:HD13	5:G:440:PRO:HB3	2.02	0.42
5:G:446:MET:HE2	5:G:446:MET:HB2	1.84	0.42
5:M:659:TRP:HD1	5:M:683:ARG:HE	1.66	0.42
4:k:22:ARG:HA	4:k:22:ARG:HD2	1.80	0.42
3:a:60:LYS:HE3	3:a:60:LYS:HB3	1.89	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:15:ASN:HD22	1:T:74:ILE:HG12	1.85	0.42
1:T:287:LYS:HA	1:T:287:LYS:HD2	1.94	0.42
1:Y:324:ILE:HD11	1:Y:373:VAL:HG12	2.01	0.42
1:1:112:GLU:O	1:1:115:HIS:ND1	2.53	0.41
3:n:21:LEU:HB3	3:n:23:ARG:HG2	2.02	0.41
5:E:391:LEU:HG	5:E:407:PHE:HE1	1.85	0.41
5:G:470:PRO:HD3	5:G:494:TYR:CZ	2.55	0.41
2:J:267:GLU:HB3	7:L:298:GLU:OE2	2.20	0.41
5:M:329:GLN:HB3	5:M:333:ARG:HH12	1.85	0.41
1:S:112:GLU:O	1:S:115:HIS:ND1	2.53	0.41
1:S:324:ILE:HD11	1:S:373:VAL:HG12	2.01	0.41
1:W:31:ILE:HG23	1:W:37:VAL:HA	2.01	0.41
1:W:84:LYS:H	1:W:84:LYS:HG2	1.50	0.41
1:W:393:ARG:HE	1:W:394:GLN:HG3	1.85	0.41
1:X:112:GLU:O	1:X:115:HIS:ND1	2.53	0.41
1:Y:339:ARG:NH2	1:Y:342:GLU:HB2	2.32	0.41
1:2:339:ARG:NH2	1:2:342:GLU:HB2	2.32	0.41
3:F:490:ILE:HG12	3:F:494:HIS:HE1	1.85	0.41
3:H:277:VAL:HB	3:H:288:ARG:HG3	2.02	0.41
3:H:291:ALA:HA	3:H:366:ARG:HH22	1.85	0.41
7:L:1512:LEU:O	7:L:1516:LEU:HB2	2.20	0.41
5:M:154:LEU:HA	5:M:157:LYS:HD2	2.02	0.41
5:M:659:TRP:CD1	5:M:683:ARG:HE	2.37	0.41
1:S:339:ARG:HH21	1:S:339:ARG:HD2	1.73	0.41
1:U:9:GLN:HA	1:U:138:CYS:HB2	2.01	0.41
1:U:31:ILE:HG23	1:U:37:VAL:HA	2.01	0.41
1:X:393:ARG:HE	1:X:394:GLN:HG3	1.85	0.41
1:Y:85:LEU:HD23	1:Y:86:TYR:HD1	1.85	0.41
1:Z:377:MET:HE3	1:Z:377:MET:HB2	1.88	0.41
1:1:84:LYS:H	1:1:84:LYS:HG2	1.50	0.41
5:E:319:LEU:HD21	5:E:324:LEU:HD13	2.01	0.41
5:E:396:TYR:CE2	5:E:471:VAL:HG13	2.55	0.41
3:F:719:GLN:HE22	1:T:249:MET:HG2	1.84	0.41
5:G:280:LYS:O	5:G:289:ASN:ND2	2.54	0.41
5:M:311:GLU:HG3	3:N:365:ARG:HH11	1.86	0.41
5:M:499:LEU:HD23	5:M:719:ILE:HG13	2.01	0.41
5:M:504:MET:SD	5:M:714:LYS:NZ	2.85	0.41
5:M:551:LEU:HD13	5:M:575:ILE:HG21	2.02	0.41
1:U:85:LEU:HD23	1:U:86:TYR:HD1	1.85	0.41
1:U:110:GLN:HA	1:U:113:LYS:HE3	2.01	0.41
1:W:305:VAL:HG11	1:W:384:ILE:HD13	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:110:GLN:HA	1:2:113:LYS:HE3	2.01	0.41
5:G:422:ASP:HB2	5:G:627:SER:HB2	2.02	0.41
5:G:574:LYS:HB2	5:G:619:ASP:HB3	2.03	0.41
3:H:576:HIS:O	3:H:580:LEU:HG	2.20	0.41
6:I:263:ILE:H	6:I:263:ILE:HG13	1.74	0.41
6:I:403:VAL:HG22	6:I:404:LEU:HD12	2.01	0.41
6:K:381:LYS:HA	6:K:381:LYS:HD3	1.95	0.41
1:S:67:LEU:HD23	1:S:67:LEU:HA	1.96	0.41
1:T:85:LEU:HD23	1:T:86:TYR:HD1	1.85	0.41
1:T:112:GLU:O	1:T:115:HIS:ND1	2.53	0.41
1:T:415:LYS:HD2	1:T:415:LYS:HA	1.88	0.41
1:W:15:ASN:HD22	1:W:74:ILE:HG12	1.85	0.41
1:Y:112:GLU:O	1:Y:115:HIS:ND1	2.53	0.41
1:1:393:ARG:HE	1:1:394:GLN:HG3	1.85	0.41
5:E:186:ALA:HA	5:E:191:PHE:CE2	2.54	0.41
5:E:716:ALA:HB2	5:E:725:HIS:HE1	1.85	0.41
5:E:868:ARG:HE	5:E:868:ARG:HB3	1.71	0.41
3:H:398:SER:HA	3:H:473:SER:OG	2.21	0.41
3:H:885:HIS:HB3	1:V:353:PRO:HB3	2.03	0.41
2:J:797:ASP:OD2	2:J:797:ASP:N	2.53	0.41
2:J:938:HIS:CE1	2:J:943:LEU:HB2	2.55	0.41
1:V:287:LYS:HA	1:V:287:LYS:HD2	1.94	0.41
2:1:129:THR:HG22	4:m:33:ARG:CZ	2.50	0.41
5:E:679:ALA:HB1	5:E:762:MET:SD	2.60	0.41
5:E:738:MET:N	5:E:738:MET:SD	2.93	0.41
3:H:600:ILE:O	3:H:603:THR:HB	2.20	0.41
2:J:370:LYS:HE3	2:J:370:LYS:HB2	1.88	0.41
5:M:739:LEU:HD13	5:M:739:LEU:HA	1.77	0.41
3:N:388:CYS:HB3	3:N:396:LEU:HG	2.02	0.41
1:S:85:LEU:HD23	1:S:86:TYR:HD1	1.85	0.41
1:V:3:ARG:HB2	1:V:4:GLU:H	1.73	0.41
1:V:112:GLU:O	1:V:115:HIS:ND1	2.53	0.41
1:Z:195:LEU:HD23	1:Z:195:LEU:HA	1.97	0.41
1:1:85:LEU:HD23	1:1:86:TYR:HD1	1.85	0.41
1:1:112:GLU:HA	1:1:152:TYR:CE2	2.56	0.41
5:G:623:LYS:O	5:G:627:SER:OG	2.33	0.41
5:G:693:ILE:HD13	5:G:859:LEU:HD11	2.02	0.41
3:H:409:PRO:HA	3:H:412:ARG:HG2	2.02	0.41
7:L:283:TRP:CD1	4:b:49:ARG:HE	2.38	0.41
7:L:392:SER:O	7:L:395:SER:OG	2.35	0.41
7:L:1683:VAL:HG12	1:Z:330:PRO:HG2	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:395:TYR:HE2	1:T:425:ARG:HE	1.69	0.41
1:V:112:GLU:HA	1:V:152:TYR:CE2	2.56	0.41
1:V:305:VAL:HG11	1:V:384:ILE:HD13	2.03	0.41
1:Z:85:LEU:HD23	1:Z:86:TYR:HD1	1.85	0.41
1:Z:305:VAL:HG11	1:Z:384:ILE:HD13	2.03	0.41
1:2:85:LEU:HD23	1:2:86:TYR:HD1	1.85	0.41
5:M:356:LEU:HD12	5:M:356:LEU:HA	1.95	0.41
1:V:195:LEU:HD23	1:V:195:LEU:HA	1.96	0.41
1:X:15:ASN:HD22	1:X:74:ILE:HG12	1.85	0.41
1:Y:31:ILE:HG23	1:Y:37:VAL:HA	2.01	0.41
1:Y:305:VAL:HG11	1:Y:384:ILE:HD13	2.03	0.41
1:Z:112:GLU:O	1:Z:115:HIS:ND1	2.53	0.41
1:Z:415:LYS:HD2	1:Z:415:LYS:HA	1.88	0.41
1:1:395:TYR:HE2	1:1:425:ARG:HE	1.69	0.41
2:l:77:ASP:OD2	2:l:126:TYR:CD2	2.73	0.41
3:n:73:LEU:HD23	4:o:34:ILE:HG21	2.02	0.41
5:E:550:ARG:NH2	1:T:342:GLU:OE2	2.54	0.41
5:G:876:ARG:HH21	3:j:37:ARG:HB2	1.76	0.41
2:J:234:HIS:ND1	2:J:236:LEU:HG	2.36	0.41
2:J:327:LEU:HD13	2:J:372:PHE:CE1	2.55	0.41
6:K:81:LEU:HG	6:K:147:LYS:HZ1	1.85	0.41
6:K:105:LEU:HA	6:K:105:LEU:HD23	1.87	0.41
6:K:253:SER:HB2	6:K:288:ASN:HD21	1.86	0.41
7:L:1588:PRO:HB2	7:L:1737:LEU:HD13	2.02	0.41
5:M:408:MET:HG2	5:M:434:ILE:HG13	2.03	0.41
3:N:524:THR:OG1	3:N:525:ASP:N	2.54	0.41
1:S:220:ILE:HD12	1:S:223:PRO:HG2	2.03	0.41
1:U:220:ILE:HD12	1:U:223:PRO:HG2	2.03	0.41
1:V:339:ARG:NH2	1:V:342:GLU:HB2	2.32	0.41
1:W:112:GLU:O	1:W:115:HIS:ND1	2.53	0.41
1:Y:220:ILE:HD12	1:Y:223:PRO:HG2	2.03	0.41
1:Z:287:LYS:HA	1:Z:287:LYS:HD2	1.94	0.41
3:n:31:GLN:OE1	4:o:67:LEU:HD22	2.21	0.41
4:o:47:CYS:HA	4:o:50:LEU:HB2	2.03	0.41
5:E:440:PRO:HD2	5:E:443:LEU:HD13	2.02	0.41
5:G:150:LEU:O	5:G:153:SER:OG	2.34	0.41
6:I:315:LYS:HB3	6:I:315:LYS:HE3	1.80	0.41
7:L:588:LEU:HD23	7:L:591:ILE:HG12	2.03	0.41
7:L:1608:ILE:HG12	7:L:1705:HIS:CE1	2.56	0.41
1:T:305:VAL:HG11	1:T:384:ILE:HD13	2.03	0.41
1:1:339:ARG:HH21	1:1:339:ARG:HD2	1.72	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:384:ILE:HD12	1:1:384:ILE:HA	1.92	0.40
3:H:664:PHE:HA	3:H:667:LEU:HG	2.02	0.40
3:H:862:LEU:HD11	3:H:887:LYS:HE2	2.02	0.40
7:L:357:LEU:HD21	7:L:448:LEU:HD21	2.03	0.40
3:N:493:LEU:HD13	3:N:545:LEU:HD22	2.01	0.40
4:k:36:ASN:ND2	3:j:104:PRO:HA	2.36	0.40
1:U:112:GLU:O	1:U:115:HIS:ND1	2.53	0.40
1:X:112:GLU:HA	1:X:152:TYR:CE2	2.56	0.40
1:Z:220:ILE:HD12	1:Z:223:PRO:HG2	2.03	0.40
1:Z:384:ILE:HD12	1:Z:384:ILE:HA	1.92	0.40
1:Z:393:ARG:HE	1:Z:394:GLN:HG3	1.85	0.40
1:2:278:THR:O	1:2:278:THR:OG1	2.34	0.40
5:E:864:PHE:CD2	1:S:353:PRO:HA	2.57	0.40
3:H:568:LEU:HD12	3:H:571:GLY:HA2	2.02	0.40
3:H:717:GLN:OE1	3:H:879:ARG:HB2	2.21	0.40
6:I:367:GLU:OE2	6:I:367:GLU:N	2.54	0.40
6:K:350:LEU:HD13	6:K:463:LEU:HG	2.03	0.40
1:V:278:THR:O	1:V:278:THR:OG1	2.34	0.40
1:X:85:LEU:HD23	1:X:86:TYR:HD1	1.85	0.40
1:Y:112:GLU:HA	1:Y:152:TYR:CE2	2.56	0.40
1:Y:195:LEU:HD23	1:Y:195:LEU:HA	1.96	0.40
1:2:112:GLU:O	1:2:115:HIS:ND1	2.53	0.40
3:n:31:GLN:CD	4:o:67:LEU:HD22	2.46	0.40
4:m:47:CYS:HA	4:m:50:LEU:HB2	2.03	0.40
5:E:412:HIS:HB2	5:E:431:ARG:HA	2.02	0.40
3:F:657:MET:HA	3:F:660:TYR:HB2	2.03	0.40
5:G:741:ASN:HD22	5:G:745:LEU:HG	1.87	0.40
3:H:303:LYS:H	3:H:303:LYS:HG2	1.62	0.40
3:H:857:ILE:HD12	3:H:857:ILE:HA	1.95	0.40
6:I:42:LEU:O	6:I:45:LEU:HB2	2.21	0.40
6:K:260:ARG:HE	6:K:260:ARG:HB3	1.68	0.40
7:L:1668:PHE:CE2	7:L:1732:ILE:HG21	2.56	0.40
1:S:112:GLU:HA	1:S:152:TYR:CE2	2.56	0.40
1:W:85:LEU:HD23	1:W:86:TYR:HD1	1.85	0.40
1:Y:395:TYR:HE2	1:Y:425:ARG:HE	1.69	0.40
1:Z:248:TYR:CZ	1:Z:249:MET:HE2	2.57	0.40
1:1:248:TYR:CZ	1:1:249:MET:HE2	2.57	0.40
1:2:112:GLU:HA	1:2:152:TYR:CE2	2.56	0.40
5:G:292:LEU:HA	5:G:292:LEU:HD23	1.88	0.40
6:I:259:LEU:HB3	6:I:277:LEU:HD21	2.04	0.40
6:I:270:VAL:HG22	6:I:271:ARG:HH11	1.86	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:548:ILE:HG22	6:I:557:ILE:HD12	2.04	0.40
5:M:517:LYS:O	5:M:523:ASP:N	2.54	0.40
5:M:855:VAL:O	5:M:859:LEU:HG	2.21	0.40
1:T:220:ILE:HD12	1:T:223:PRO:HG2	2.03	0.40
1:V:395:TYR:HE2	1:V:425:ARG:HE	1.69	0.40
1:W:112:GLU:HA	1:W:152:TYR:CE2	2.56	0.40
1:Y:248:TYR:CZ	1:Y:249:MET:HE2	2.57	0.40
1:2:358:VAL:HG23	3:N:879:ARG:HH11	1.86	0.40
3:n:39:ILE:HD13	4:o:59:ALA:HB1	2.04	0.40
5:E:529:VAL:HG11	1:S:251:ASN:HD21	1.87	0.40
5:E:541:LYS:O	5:E:546:ILE:HD11	2.20	0.40
5:G:408:MET:O	5:G:435:VAL:N	2.54	0.40
5:G:578:MET:HG2	5:G:581:ASP:HA	2.04	0.40
6:I:196:LEU:HD23	6:I:196:LEU:HA	1.98	0.40
7:L:467:GLY:O	7:L:470:LEU:HG	2.22	0.40
7:L:1522:GLU:HA	7:L:1525:GLN:HB2	2.03	0.40
3:N:870:ASP:OD2	3:N:870:ASP:N	2.53	0.40
4:b:47:CYS:HA	4:b:50:LEU:HB2	2.03	0.40
1:S:192:LEU:O	1:S:196:THR:HG23	2.22	0.40
1:T:192:LEU:O	1:T:196:THR:HG23	2.22	0.40
1:U:248:TYR:CZ	1:U:249:MET:HE2	2.57	0.40
1:V:192:LEU:O	1:V:196:THR:HG23	2.22	0.40
1:W:192:LEU:O	1:W:196:THR:HG23	2.22	0.40
1:Y:192:LEU:O	1:Y:196:THR:HG23	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	1	408/451 (90%)	391 (96%)	15 (4%)	2 (0%)	24 63

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	2	408/451 (90%)	391 (96%)	15 (4%)	2 (0%)	24	63
1	S	408/451 (90%)	391 (96%)	15 (4%)	2 (0%)	24	63
1	T	408/451 (90%)	391 (96%)	15 (4%)	2 (0%)	24	63
1	U	408/451 (90%)	391 (96%)	15 (4%)	2 (0%)	24	63
1	V	408/451 (90%)	391 (96%)	15 (4%)	2 (0%)	24	63
1	W	408/451 (90%)	391 (96%)	15 (4%)	2 (0%)	24	63
1	X	408/451 (90%)	391 (96%)	15 (4%)	2 (0%)	24	63
1	Y	408/451 (90%)	391 (96%)	15 (4%)	2 (0%)	24	63
1	Z	408/451 (90%)	391 (96%)	15 (4%)	2 (0%)	24	63
2	J	506/1024 (49%)	470 (93%)	33 (6%)	3 (1%)	21	59
2	l	104/1024 (10%)	94 (90%)	7 (7%)	3 (3%)	3	23
3	F	591/907 (65%)	559 (95%)	32 (5%)	0	100	100
3	H	584/907 (64%)	560 (96%)	22 (4%)	2 (0%)	36	72
3	N	584/907 (64%)	556 (95%)	26 (4%)	2 (0%)	36	72
3	a	112/907 (12%)	106 (95%)	6 (5%)	0	100	100
3	j	97/907 (11%)	96 (99%)	1 (1%)	0	100	100
3	n	97/907 (11%)	91 (94%)	6 (6%)	0	100	100
4	b	63/82 (77%)	62 (98%)	1 (2%)	0	100	100
4	k	63/82 (77%)	62 (98%)	1 (2%)	0	100	100
4	m	63/82 (77%)	62 (98%)	1 (2%)	0	100	100
4	o	63/82 (77%)	62 (98%)	1 (2%)	0	100	100
5	E	626/902 (69%)	590 (94%)	33 (5%)	3 (0%)	24	63
5	G	628/902 (70%)	590 (94%)	35 (6%)	3 (0%)	24	63
5	M	624/902 (69%)	581 (93%)	38 (6%)	5 (1%)	16	54
6	I	511/667 (77%)	477 (93%)	30 (6%)	4 (1%)	16	54
6	K	548/667 (82%)	528 (96%)	19 (4%)	1 (0%)	43	78
7	L	540/1819 (30%)	505 (94%)	30 (6%)	5 (1%)	14	51
All	All	10484/18187 (58%)	9961 (95%)	472 (4%)	51 (0%)	26	63

All (51) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	l	117	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	E	581	ASP
5	G	241	ARG
3	H	270	ASN
6	I	408	ASP
6	I	508	ASN
5	M	241	ARG
5	M	703	GLU
3	N	527	GLU
1	1	350	PRO
1	2	350	PRO
3	H	602	GLU
7	L	308	GLU
3	N	455	LYS
1	S	350	PRO
1	T	350	PRO
1	U	350	PRO
1	V	350	PRO
1	W	350	PRO
1	X	350	PRO
1	Y	350	PRO
1	Z	350	PRO
1	1	330	PRO
1	2	330	PRO
5	E	425	ASP
6	I	405	LEU
7	L	310	PRO
7	L	311	TYR
5	M	675	TRP
1	S	330	PRO
1	T	330	PRO
1	U	330	PRO
1	V	330	PRO
1	W	330	PRO
1	X	330	PRO
1	Y	330	PRO
1	Z	330	PRO
2	J	238	LEU
2	J	714	TYR
6	K	409	ASN
7	L	309	GLU
2	l	120	SER
5	E	582	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	I	404	LEU
2	J	257	TYR
7	L	346	LEU
5	G	558	ALA
5	G	581	ASP
5	M	704	PRO
5	M	701	VAL
2	l	121	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	376/400 (94%)	324 (86%)	52 (14%)	3	14
1	2	376/400 (94%)	324 (86%)	52 (14%)	3	14
1	S	376/400 (94%)	324 (86%)	52 (14%)	3	14
1	T	376/400 (94%)	324 (86%)	52 (14%)	3	14
1	U	376/400 (94%)	324 (86%)	52 (14%)	3	14
1	V	376/400 (94%)	324 (86%)	52 (14%)	3	14
1	W	376/400 (94%)	324 (86%)	52 (14%)	3	14
1	X	376/400 (94%)	324 (86%)	52 (14%)	3	14
1	Y	376/400 (94%)	324 (86%)	52 (14%)	3	14
1	Z	376/400 (94%)	324 (86%)	52 (14%)	3	14
2	J	498/933 (53%)	494 (99%)	4 (1%)	73	80
2	l	96/933 (10%)	94 (98%)	2 (2%)	47	65
3	F	542/798 (68%)	539 (99%)	3 (1%)	78	83
3	H	539/798 (68%)	537 (100%)	2 (0%)	84	84
3	N	539/798 (68%)	536 (99%)	3 (1%)	78	83
3	a	101/798 (13%)	99 (98%)	2 (2%)	48	66
3	j	88/798 (11%)	88 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	n	88/798 (11%)	88 (100%)	0	100	100
4	b	53/62 (86%)	41 (77%)	12 (23%)	1	6
4	k	53/62 (86%)	41 (77%)	12 (23%)	1	6
4	m	53/62 (86%)	41 (77%)	12 (23%)	1	6
4	o	53/62 (86%)	41 (77%)	12 (23%)	1	6
5	E	574/791 (73%)	571 (100%)	3 (0%)	81	83
5	G	575/791 (73%)	570 (99%)	5 (1%)	70	79
5	M	572/791 (72%)	563 (98%)	9 (2%)	55	70
6	I	472/594 (80%)	467 (99%)	5 (1%)	65	76
6	K	509/594 (86%)	506 (99%)	3 (1%)	78	83
7	L	501/1546 (32%)	497 (99%)	4 (1%)	73	80
All	All	9666/16009 (60%)	9053 (94%)	613 (6%)	18	37

All (613) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	8	LEU
1	1	10	LEU
1	1	31	ILE
1	1	50	VAL
1	1	66	LEU
1	1	72	ARG
1	1	73	VAL
1	1	78	LEU
1	1	85	LEU
1	1	90	ASN
1	1	109	SER
1	1	131	SER
1	1	136	VAL
1	1	147	SER
1	1	154	LEU
1	1	165	LEU
1	1	168	THR
1	1	189	LEU
1	1	191	THR
1	1	192	LEU
1	1	204	VAL
1	1	218	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	222	ASN
1	1	236	MET
1	1	237	SER
1	1	242	THR
1	1	249	MET
1	1	252	ASP
1	1	256	LEU
1	1	257	ILE
1	1	259	SER
1	1	263	THR
1	1	270	MET
1	1	278	THR
1	1	288	THR
1	1	290	VAL
1	1	298	LEU
1	1	316	CYS
1	1	328	VAL
1	1	331	THR
1	1	339	ARG
1	1	345	LEU
1	1	355	SER
1	1	356	ILE
1	1	360	LEU
1	1	369	SER
1	1	373	VAL
1	1	382	THR
1	1	391	THR
1	1	407	GLN
1	1	423	THR
1	1	439	THR
1	2	8	LEU
1	2	10	LEU
1	2	31	ILE
1	2	50	VAL
1	2	66	LEU
1	2	72	ARG
1	2	73	VAL
1	2	78	LEU
1	2	85	LEU
1	2	90	ASN
1	2	109	SER
1	2	131	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2	136	VAL
1	2	147	SER
1	2	154	LEU
1	2	165	LEU
1	2	168	THR
1	2	189	LEU
1	2	191	THR
1	2	192	LEU
1	2	204	VAL
1	2	218	LEU
1	2	222	ASN
1	2	236	MET
1	2	237	SER
1	2	242	THR
1	2	249	MET
1	2	252	ASP
1	2	256	LEU
1	2	257	ILE
1	2	259	SER
1	2	263	THR
1	2	270	MET
1	2	278	THR
1	2	288	THR
1	2	290	VAL
1	2	298	LEU
1	2	316	CYS
1	2	328	VAL
1	2	331	THR
1	2	339	ARG
1	2	345	LEU
1	2	355	SER
1	2	356	ILE
1	2	360	LEU
1	2	369	SER
1	2	373	VAL
1	2	382	THR
1	2	391	THR
1	2	407	GLN
1	2	423	THR
1	2	439	THR
2	1	114	LEU
2	1	117	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	o	21	VAL
4	o	24	THR
4	o	32	SER
4	o	39	LEU
4	o	43	THR
4	o	45	SER
4	o	47	CYS
4	o	48	VAL
4	o	51	CYS
4	o	62	SER
4	o	64	ILE
4	o	74	LEU
4	m	21	VAL
4	m	24	THR
4	m	32	SER
4	m	39	LEU
4	m	43	THR
4	m	45	SER
4	m	47	CYS
4	m	48	VAL
4	m	51	CYS
4	m	62	SER
4	m	64	ILE
4	m	74	LEU
5	E	425	ASP
5	E	459	VAL
5	E	681	THR
3	F	371	THR
3	F	648	ILE
3	F	873	LEU
5	G	248	VAL
5	G	328	ILE
5	G	379	LEU
5	G	551	LEU
5	G	557	LEU
3	H	266	ILE
3	H	603	THR
6	I	263	ILE
6	I	282	SER
6	I	475	TYR
6	I	600	ASN
6	I	601	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	J	238	LEU
2	J	473	LEU
2	J	559	ILE
2	J	569	LEU
6	K	86	LEU
6	K	647	LEU
6	K	651	TYR
7	L	338	VAL
7	L	414	SER
7	L	458	THR
7	L	588	LEU
5	M	266	VAL
5	M	400	ILE
5	M	433	THR
5	M	562	SER
5	M	563	THR
5	M	701	VAL
5	M	703	GLU
5	M	705	THR
5	M	759	THR
3	N	678	THR
3	N	712	VAL
3	N	778	VAL
4	k	21	VAL
4	k	24	THR
4	k	32	SER
4	k	39	LEU
4	k	43	THR
4	k	45	SER
4	k	47	CYS
4	k	48	VAL
4	k	51	CYS
4	k	62	SER
4	k	64	ILE
4	k	74	LEU
4	b	21	VAL
4	b	24	THR
4	b	32	SER
4	b	39	LEU
4	b	43	THR
4	b	45	SER
4	b	47	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	b	48	VAL
4	b	51	CYS
4	b	62	SER
4	b	64	ILE
4	b	74	LEU
3	a	20	ILE
3	a	117	LEU
1	S	8	LEU
1	S	10	LEU
1	S	31	ILE
1	S	50	VAL
1	S	66	LEU
1	S	72	ARG
1	S	73	VAL
1	S	78	LEU
1	S	85	LEU
1	S	90	ASN
1	S	109	SER
1	S	131	SER
1	S	136	VAL
1	S	147	SER
1	S	154	LEU
1	S	165	LEU
1	S	168	THR
1	S	189	LEU
1	S	191	THR
1	S	192	LEU
1	S	204	VAL
1	S	218	LEU
1	S	222	ASN
1	S	236	MET
1	S	237	SER
1	S	242	THR
1	S	249	MET
1	S	252	ASP
1	S	256	LEU
1	S	257	ILE
1	S	259	SER
1	S	263	THR
1	S	270	MET
1	S	278	THR
1	S	288	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	S	290	VAL
1	S	298	LEU
1	S	316	CYS
1	S	328	VAL
1	S	331	THR
1	S	339	ARG
1	S	345	LEU
1	S	355	SER
1	S	356	ILE
1	S	360	LEU
1	S	369	SER
1	S	373	VAL
1	S	382	THR
1	S	391	THR
1	S	407	GLN
1	S	423	THR
1	S	439	THR
1	T	8	LEU
1	T	10	LEU
1	T	31	ILE
1	T	50	VAL
1	T	66	LEU
1	T	72	ARG
1	T	73	VAL
1	T	78	LEU
1	T	85	LEU
1	T	90	ASN
1	T	109	SER
1	T	131	SER
1	T	136	VAL
1	T	147	SER
1	T	154	LEU
1	T	165	LEU
1	T	168	THR
1	T	189	LEU
1	T	191	THR
1	T	192	LEU
1	T	204	VAL
1	T	218	LEU
1	T	222	ASN
1	T	236	MET
1	T	237	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	T	242	THR
1	T	249	MET
1	T	252	ASP
1	T	256	LEU
1	T	257	ILE
1	T	259	SER
1	T	263	THR
1	T	270	MET
1	T	278	THR
1	T	288	THR
1	T	290	VAL
1	T	298	LEU
1	T	316	CYS
1	T	328	VAL
1	T	331	THR
1	T	339	ARG
1	T	345	LEU
1	T	355	SER
1	T	356	ILE
1	T	360	LEU
1	T	369	SER
1	T	373	VAL
1	T	382	THR
1	T	391	THR
1	T	407	GLN
1	T	423	THR
1	T	439	THR
1	U	8	LEU
1	U	10	LEU
1	U	31	ILE
1	U	50	VAL
1	U	66	LEU
1	U	72	ARG
1	U	73	VAL
1	U	78	LEU
1	U	85	LEU
1	U	90	ASN
1	U	109	SER
1	U	131	SER
1	U	136	VAL
1	U	147	SER
1	U	154	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	U	165	LEU
1	U	168	THR
1	U	189	LEU
1	U	191	THR
1	U	192	LEU
1	U	204	VAL
1	U	218	LEU
1	U	222	ASN
1	U	236	MET
1	U	237	SER
1	U	242	THR
1	U	249	MET
1	U	252	ASP
1	U	256	LEU
1	U	257	ILE
1	U	259	SER
1	U	263	THR
1	U	270	MET
1	U	278	THR
1	U	288	THR
1	U	290	VAL
1	U	298	LEU
1	U	316	CYS
1	U	328	VAL
1	U	331	THR
1	U	339	ARG
1	U	345	LEU
1	U	355	SER
1	U	356	ILE
1	U	360	LEU
1	U	369	SER
1	U	373	VAL
1	U	382	THR
1	U	391	THR
1	U	407	GLN
1	U	423	THR
1	U	439	THR
1	V	8	LEU
1	V	10	LEU
1	V	31	ILE
1	V	50	VAL
1	V	66	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	V	72	ARG
1	V	73	VAL
1	V	78	LEU
1	V	85	LEU
1	V	90	ASN
1	V	109	SER
1	V	131	SER
1	V	136	VAL
1	V	147	SER
1	V	154	LEU
1	V	165	LEU
1	V	168	THR
1	V	189	LEU
1	V	191	THR
1	V	192	LEU
1	V	204	VAL
1	V	218	LEU
1	V	222	ASN
1	V	236	MET
1	V	237	SER
1	V	242	THR
1	V	249	MET
1	V	252	ASP
1	V	256	LEU
1	V	257	ILE
1	V	259	SER
1	V	263	THR
1	V	270	MET
1	V	278	THR
1	V	288	THR
1	V	290	VAL
1	V	298	LEU
1	V	316	CYS
1	V	328	VAL
1	V	331	THR
1	V	339	ARG
1	V	345	LEU
1	V	355	SER
1	V	356	ILE
1	V	360	LEU
1	V	369	SER
1	V	373	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	V	382	THR
1	V	391	THR
1	V	407	GLN
1	V	423	THR
1	V	439	THR
1	W	8	LEU
1	W	10	LEU
1	W	31	ILE
1	W	50	VAL
1	W	66	LEU
1	W	72	ARG
1	W	73	VAL
1	W	78	LEU
1	W	85	LEU
1	W	90	ASN
1	W	109	SER
1	W	131	SER
1	W	136	VAL
1	W	147	SER
1	W	154	LEU
1	W	165	LEU
1	W	168	THR
1	W	189	LEU
1	W	191	THR
1	W	192	LEU
1	W	204	VAL
1	W	218	LEU
1	W	222	ASN
1	W	236	MET
1	W	237	SER
1	W	242	THR
1	W	249	MET
1	W	252	ASP
1	W	256	LEU
1	W	257	ILE
1	W	259	SER
1	W	263	THR
1	W	270	MET
1	W	278	THR
1	W	288	THR
1	W	290	VAL
1	W	298	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	W	316	CYS
1	W	328	VAL
1	W	331	THR
1	W	339	ARG
1	W	345	LEU
1	W	355	SER
1	W	356	ILE
1	W	360	LEU
1	W	369	SER
1	W	373	VAL
1	W	382	THR
1	W	391	THR
1	W	407	GLN
1	W	423	THR
1	W	439	THR
1	X	8	LEU
1	X	10	LEU
1	X	31	ILE
1	X	50	VAL
1	X	66	LEU
1	X	72	ARG
1	X	73	VAL
1	X	78	LEU
1	X	85	LEU
1	X	90	ASN
1	X	109	SER
1	X	131	SER
1	X	136	VAL
1	X	147	SER
1	X	154	LEU
1	X	165	LEU
1	X	168	THR
1	X	189	LEU
1	X	191	THR
1	X	192	LEU
1	X	204	VAL
1	X	218	LEU
1	X	222	ASN
1	X	236	MET
1	X	237	SER
1	X	242	THR
1	X	249	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	X	252	ASP
1	X	256	LEU
1	X	257	ILE
1	X	259	SER
1	X	263	THR
1	X	270	MET
1	X	278	THR
1	X	288	THR
1	X	290	VAL
1	X	298	LEU
1	X	316	CYS
1	X	328	VAL
1	X	331	THR
1	X	339	ARG
1	X	345	LEU
1	X	355	SER
1	X	356	ILE
1	X	360	LEU
1	X	369	SER
1	X	373	VAL
1	X	382	THR
1	X	391	THR
1	X	407	GLN
1	X	423	THR
1	X	439	THR
1	Y	8	LEU
1	Y	10	LEU
1	Y	31	ILE
1	Y	50	VAL
1	Y	66	LEU
1	Y	72	ARG
1	Y	73	VAL
1	Y	78	LEU
1	Y	85	LEU
1	Y	90	ASN
1	Y	109	SER
1	Y	131	SER
1	Y	136	VAL
1	Y	147	SER
1	Y	154	LEU
1	Y	165	LEU
1	Y	168	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	Y	189	LEU
1	Y	191	THR
1	Y	192	LEU
1	Y	204	VAL
1	Y	218	LEU
1	Y	222	ASN
1	Y	236	MET
1	Y	237	SER
1	Y	242	THR
1	Y	249	MET
1	Y	252	ASP
1	Y	256	LEU
1	Y	257	ILE
1	Y	259	SER
1	Y	263	THR
1	Y	270	MET
1	Y	278	THR
1	Y	288	THR
1	Y	290	VAL
1	Y	298	LEU
1	Y	316	CYS
1	Y	328	VAL
1	Y	331	THR
1	Y	339	ARG
1	Y	345	LEU
1	Y	355	SER
1	Y	356	ILE
1	Y	360	LEU
1	Y	369	SER
1	Y	373	VAL
1	Y	382	THR
1	Y	391	THR
1	Y	407	GLN
1	Y	423	THR
1	Y	439	THR
1	Z	8	LEU
1	Z	10	LEU
1	Z	31	ILE
1	Z	50	VAL
1	Z	66	LEU
1	Z	72	ARG
1	Z	73	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	Z	78	LEU
1	Z	85	LEU
1	Z	90	ASN
1	Z	109	SER
1	Z	131	SER
1	Z	136	VAL
1	Z	147	SER
1	Z	154	LEU
1	Z	165	LEU
1	Z	168	THR
1	Z	189	LEU
1	Z	191	THR
1	Z	192	LEU
1	Z	204	VAL
1	Z	218	LEU
1	Z	222	ASN
1	Z	236	MET
1	Z	237	SER
1	Z	242	THR
1	Z	249	MET
1	Z	252	ASP
1	Z	256	LEU
1	Z	257	ILE
1	Z	259	SER
1	Z	263	THR
1	Z	270	MET
1	Z	278	THR
1	Z	288	THR
1	Z	290	VAL
1	Z	298	LEU
1	Z	316	CYS
1	Z	328	VAL
1	Z	331	THR
1	Z	339	ARG
1	Z	345	LEU
1	Z	355	SER
1	Z	356	ILE
1	Z	360	LEU
1	Z	369	SER
1	Z	373	VAL
1	Z	382	THR
1	Z	391	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	Z	407	GLN
1	Z	423	THR
1	Z	439	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (263) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	15	ASN
1	1	16	GLN
1	1	24	GLN
1	1	59	HIS
1	1	103	ASN
1	1	110	GLN
1	1	187	ASN
1	1	229	ASN
1	1	267	HIS
1	1	315	HIS
1	1	334	HIS
1	1	338	GLN
1	1	394	GLN
1	2	15	ASN
1	2	16	GLN
1	2	24	GLN
1	2	103	ASN
1	2	110	GLN
1	2	229	ASN
1	2	250	ASN
1	2	267	HIS
1	2	315	HIS
1	2	338	GLN
1	2	394	GLN
2	1	42	ASN
2	1	47	ASN
2	1	57	ASN
3	n	42	ASN
4	o	17	ASN
4	o	53	GLN
4	m	17	ASN
4	m	53	GLN
5	E	213	GLN
5	E	314	HIS
5	E	412	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	E	424	ASN
5	E	644	HIS
5	E	691	GLN
5	E	725	HIS
5	E	862	ASN
3	F	302	ASN
3	F	345	GLN
3	F	387	HIS
3	F	424	HIS
3	F	500	GLN
3	F	550	ASN
3	F	594	GLN
3	F	643	HIS
3	F	687	ASN
3	F	693	ASN
3	F	719	GLN
3	F	773	ASN
3	F	781	GLN
5	G	166	ASN
5	G	169	ASN
5	G	173	HIS
5	G	242	GLN
5	G	289	ASN
5	G	444	GLN
5	G	465	HIS
5	G	639	GLN
5	G	644	HIS
5	G	691	GLN
5	G	763	GLN
5	G	862	ASN
3	H	322	GLN
3	H	345	GLN
3	H	401	HIS
3	H	417	HIS
3	H	558	HIS
3	H	576	HIS
3	H	716	HIS
3	H	719	GLN
3	H	736	ASN
3	H	739	GLN
3	H	751	HIS
3	H	855	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	H	883	ASN
6	I	26	GLN
6	I	29	GLN
6	I	102	GLN
6	I	121	HIS
6	I	130	GLN
6	I	152	GLN
6	I	284	GLN
6	I	303	GLN
6	I	508	ASN
6	I	519	ASN
6	I	529	GLN
6	I	533	GLN
6	I	543	GLN
6	I	581	HIS
2	J	237	HIS
2	J	248	GLN
2	J	269	GLN
2	J	288	GLN
2	J	299	ASN
2	J	642	HIS
2	J	705	ASN
2	J	721	GLN
2	J	753	GLN
2	J	754	ASN
2	J	830	GLN
2	J	895	ASN
2	J	930	HIS
2	J	938	HIS
6	K	78	GLN
6	K	98	GLN
6	K	109	GLN
6	K	288	ASN
6	K	290	ASN
6	K	316	GLN
6	K	327	GLN
6	K	339	HIS
6	K	353	GLN
6	K	370	GLN
6	K	377	GLN
6	K	393	ASN
6	K	489	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	K	519	ASN
6	K	520	HIS
6	K	529	GLN
6	K	540	GLN
6	K	567	ASN
7	L	430	GLN
7	L	1487	HIS
7	L	1568	HIS
7	L	1663	HIS
7	L	1666	GLN
7	L	1759	HIS
7	L	1766	GLN
7	L	1770	ASN
7	L	1792	GLN
5	M	173	HIS
5	M	213	GLN
5	M	242	GLN
5	M	261	HIS
5	M	316	GLN
5	M	373	GLN
5	M	437	GLN
5	M	512	HIS
5	M	530	HIS
5	M	639	GLN
5	M	674	GLN
5	M	694	GLN
5	M	712	ASN
3	N	265	ASN
3	N	329	HIS
3	N	389	GLN
3	N	416	GLN
3	N	461	HIS
3	N	479	GLN
3	N	491	ASN
3	N	494	HIS
3	N	643	HIS
3	N	716	HIS
3	N	717	GLN
3	N	719	GLN
3	N	736	ASN
3	N	742	GLN
3	N	830	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	k	17	ASN
4	k	53	GLN
4	b	17	ASN
4	b	53	GLN
3	j	15	ASN
3	a	30	GLN
3	a	42	ASN
3	a	84	GLN
1	S	15	ASN
1	S	16	GLN
1	S	24	GLN
1	S	103	ASN
1	S	110	GLN
1	S	229	ASN
1	S	251	ASN
1	S	267	HIS
1	S	315	HIS
1	S	334	HIS
1	S	338	GLN
1	S	394	GLN
1	T	15	ASN
1	T	16	GLN
1	T	24	GLN
1	T	103	ASN
1	T	110	GLN
1	T	158	ASN
1	T	229	ASN
1	T	250	ASN
1	T	251	ASN
1	T	267	HIS
1	T	315	HIS
1	T	334	HIS
1	T	338	GLN
1	T	371	HIS
1	T	394	GLN
1	U	15	ASN
1	U	16	GLN
1	U	24	GLN
1	U	103	ASN
1	U	110	GLN
1	U	187	ASN
1	U	229	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	U	267	HIS
1	U	315	HIS
1	U	334	HIS
1	U	338	GLN
1	U	394	GLN
1	V	15	ASN
1	V	16	GLN
1	V	24	GLN
1	V	103	ASN
1	V	110	GLN
1	V	229	ASN
1	V	267	HIS
1	V	315	HIS
1	V	338	GLN
1	V	394	GLN
1	W	15	ASN
1	W	16	GLN
1	W	24	GLN
1	W	103	ASN
1	W	110	GLN
1	W	229	ASN
1	W	315	HIS
1	W	334	HIS
1	W	338	GLN
1	W	394	GLN
1	X	15	ASN
1	X	16	GLN
1	X	24	GLN
1	X	103	ASN
1	X	110	GLN
1	X	229	ASN
1	X	267	HIS
1	X	315	HIS
1	X	334	HIS
1	X	338	GLN
1	X	394	GLN
1	Y	15	ASN
1	Y	16	GLN
1	Y	24	GLN
1	Y	103	ASN
1	Y	110	GLN
1	Y	229	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	Y	251	ASN
1	Y	267	HIS
1	Y	315	HIS
1	Y	338	GLN
1	Y	394	GLN
1	Z	15	ASN
1	Z	16	GLN
1	Z	24	GLN
1	Z	103	ASN
1	Z	110	GLN
1	Z	187	ASN
1	Z	229	ASN
1	Z	250	ASN
1	Z	267	HIS
1	Z	315	HIS
1	Z	334	HIS
1	Z	338	GLN
1	Z	394	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.

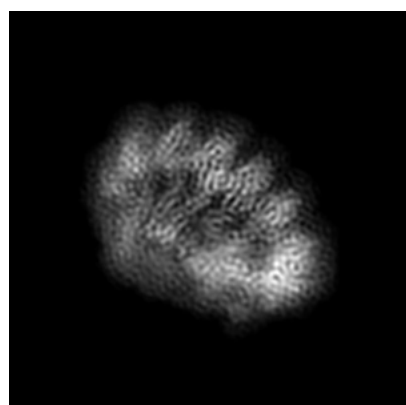
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14009. These allow visual inspection of the internal detail of the map and identification of artifacts.

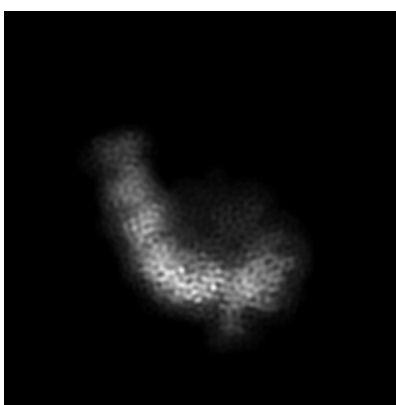
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

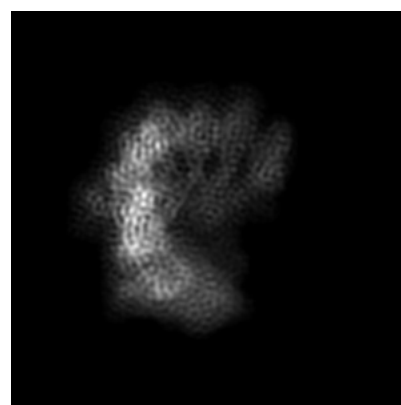
6.1.1 Primary map



X



Y



Z

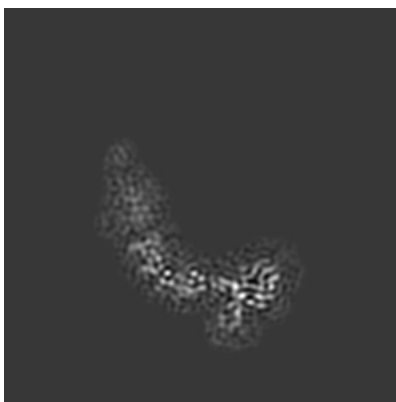
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 100



Y Index: 100

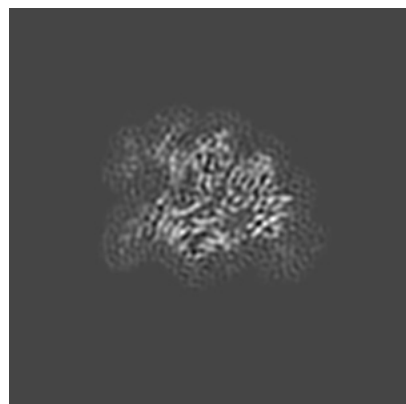


Z Index: 100

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

6.3 Largest variance slices [i](#)

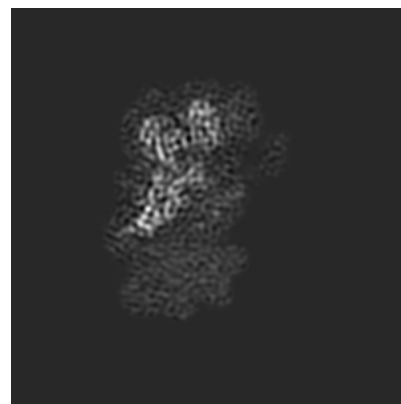
6.3.1 Primary map



X Index: 62



Y Index: 98



Z Index: 74

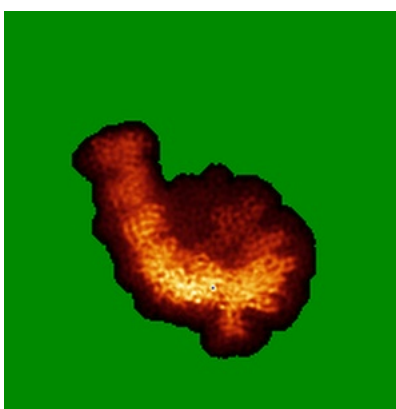
The images above show the largest variance slices of the map in three orthogonal directions.

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

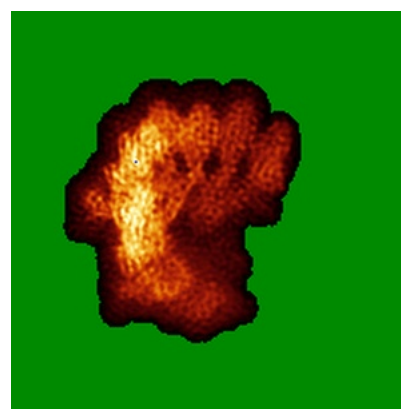
6.4.1 Primary map



X



Y

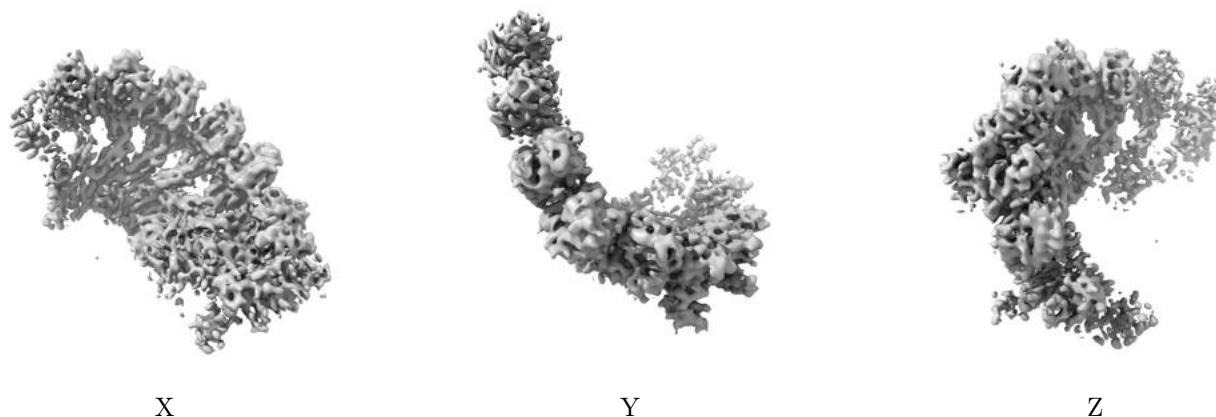


Z

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 0.0514. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

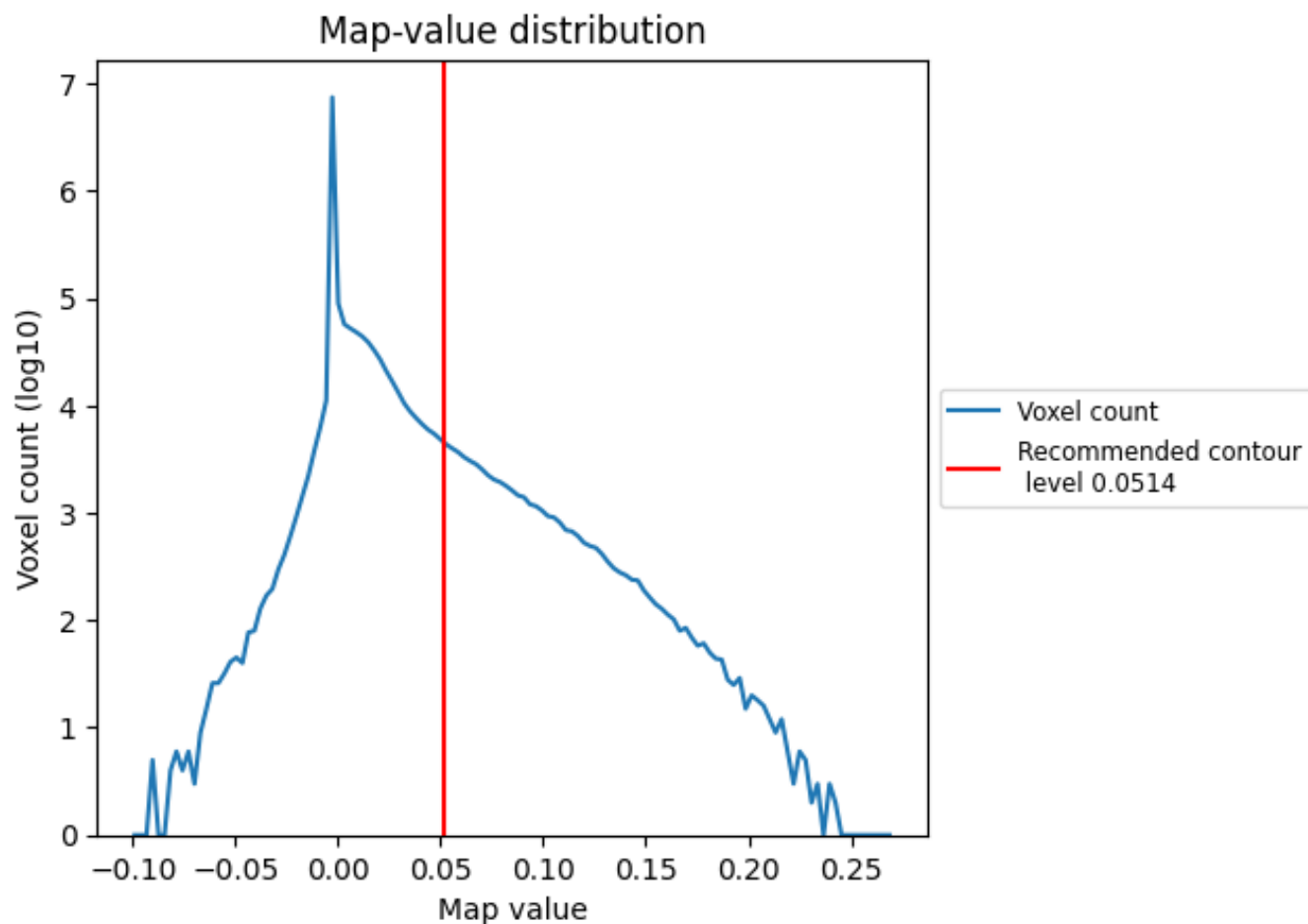
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

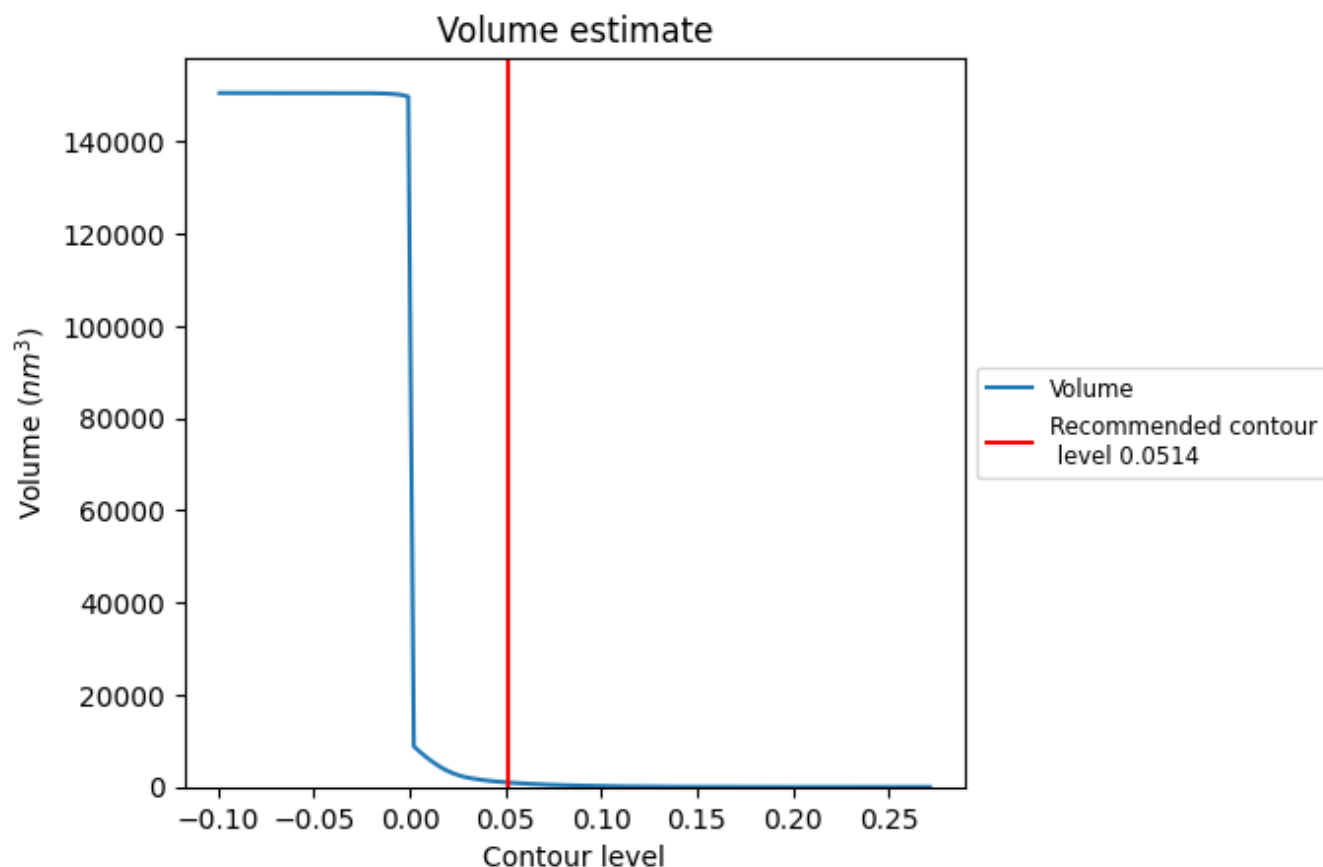
This section contains the results of statistical analysis of the map.

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.

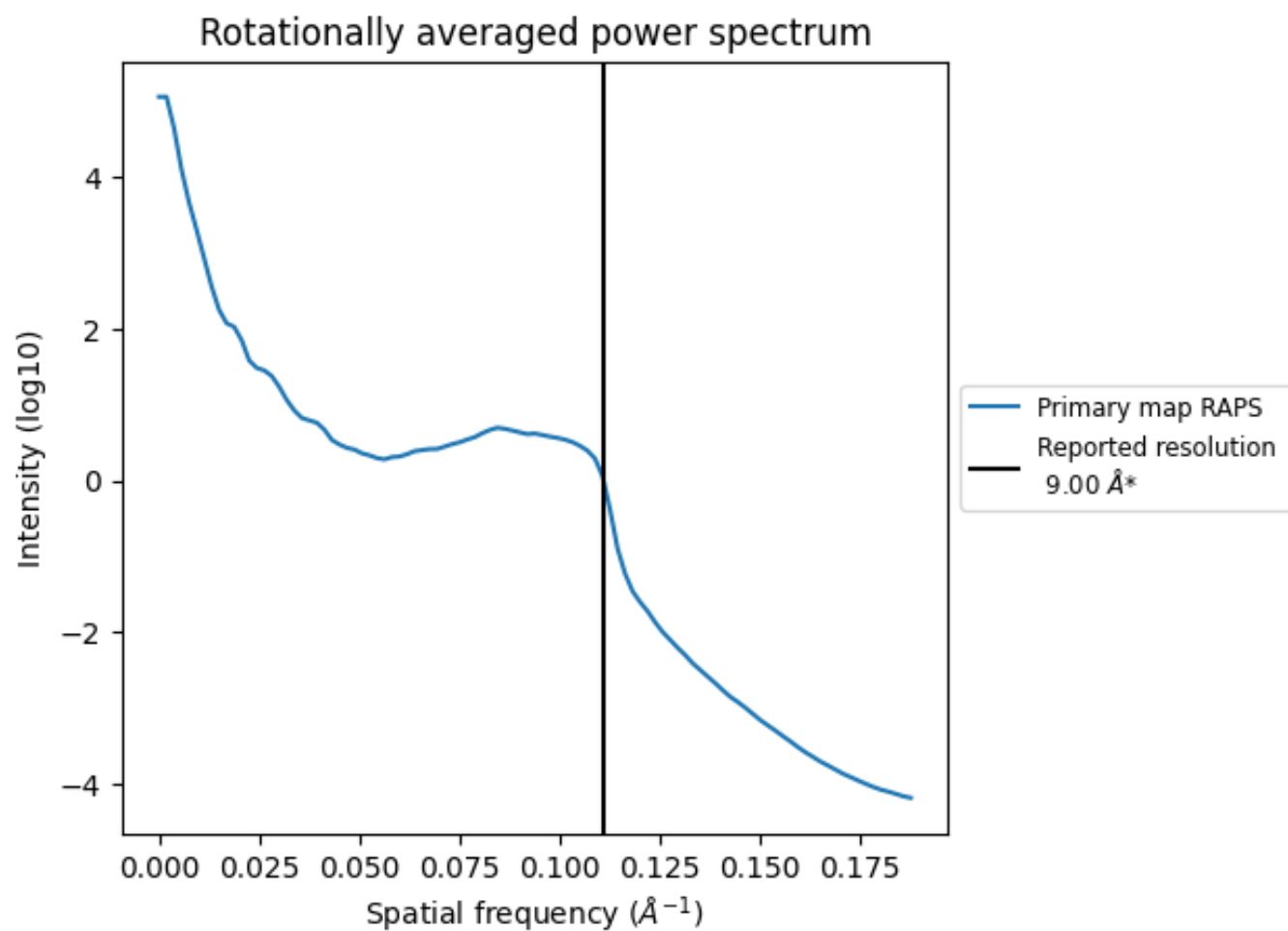
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 970 nm³; this corresponds to an approximate mass of 876 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 0.111 Å⁻¹

8 Fourier-Shell correlation ⓘ

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

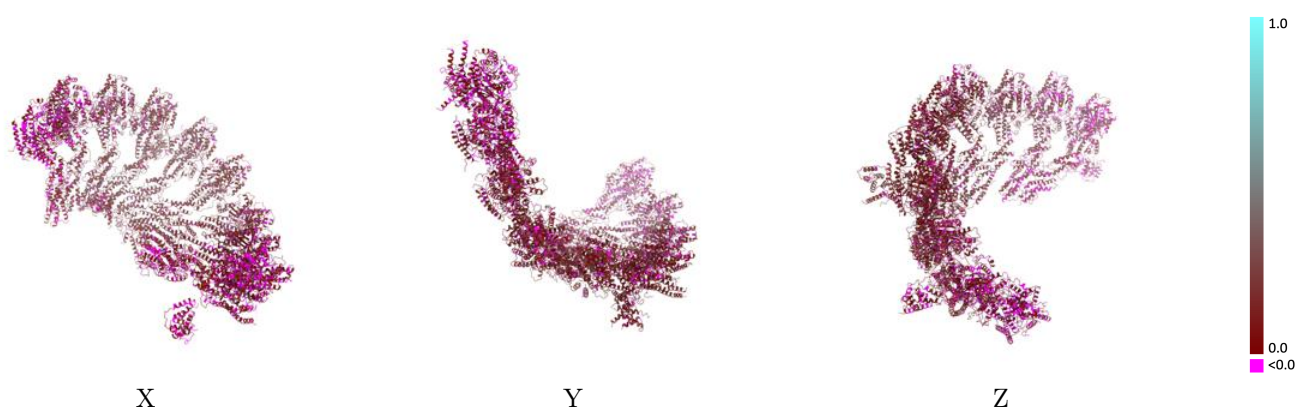
9 Map-model fit [i](#)

This section contains information regarding the fit between EMD map EMD-14009 and PDB model 7QJ4. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)

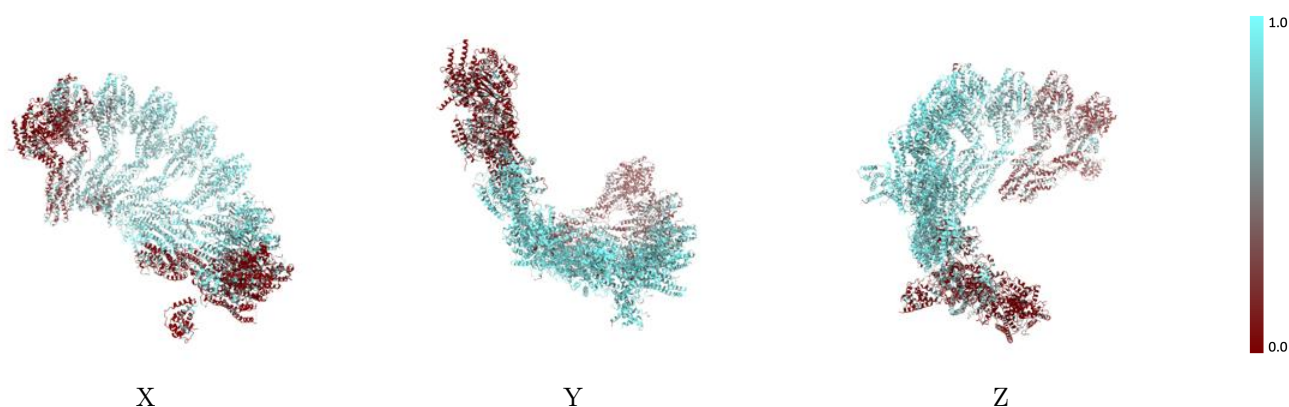
This section was not generated.

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



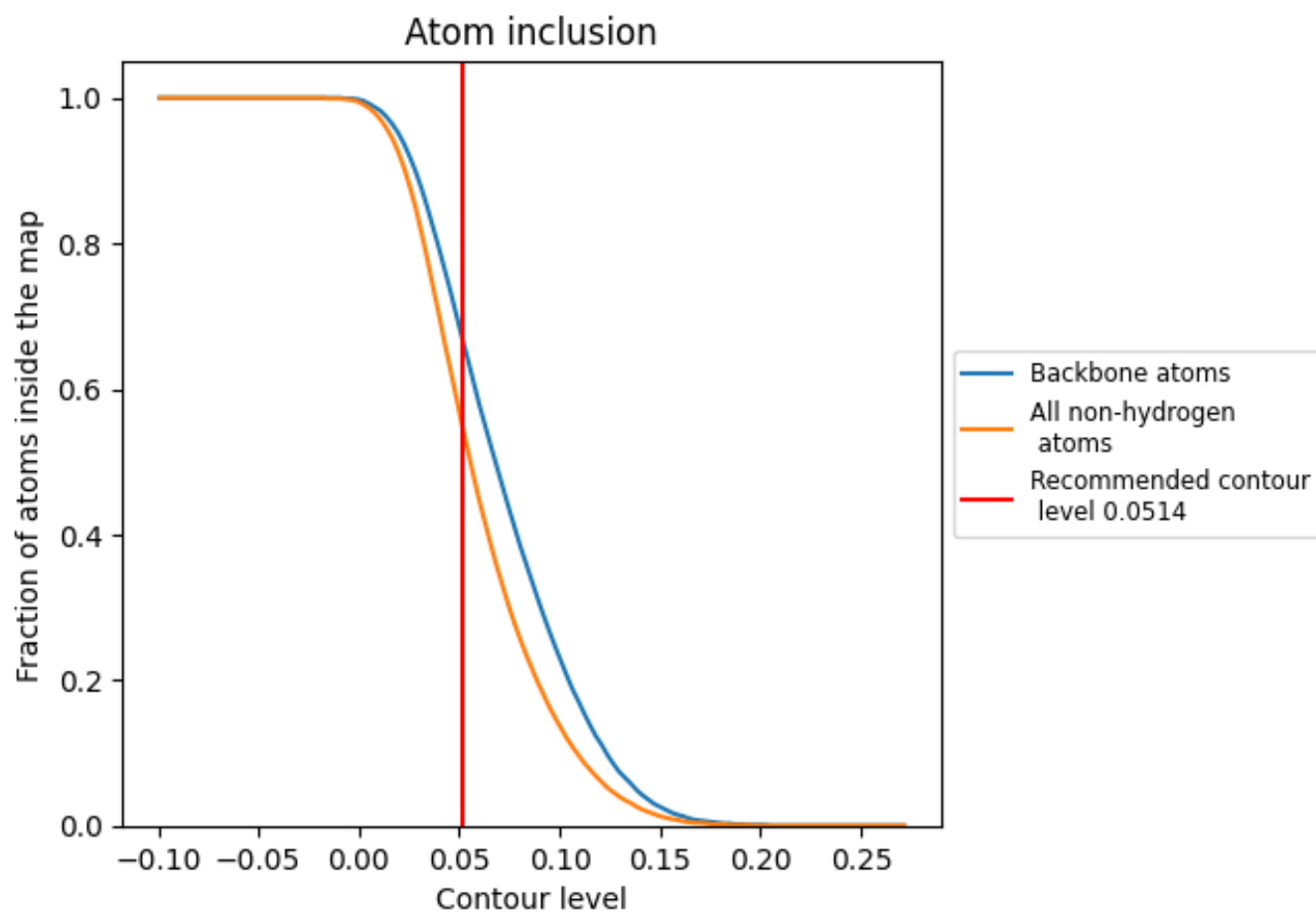
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0514).

9.4 Atom inclusion [i](#)



At the recommended contour level, 67% of all backbone atoms, 55% 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 (0.0514) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5510	 0.1090
1	 0.2640	 0.0620
2	 0.1360	 0.0390
E	 0.1810	 0.0680
F	 0.4140	 0.1160
G	 0.7340	 0.1390
H	 0.7970	 0.1480
I	 0.7980	 0.1570
J	 0.8170	 0.1580
K	 0.7930	 0.1380
L	 0.7720	 0.1310
M	 0.2980	 0.0810
N	 0.2730	 0.0760
S	 0.0880	 0.0420
T	 0.3620	 0.0720
U	 0.6790	 0.1040
V	 0.7740	 0.1270
W	 0.7930	 0.1320
X	 0.8320	 0.1400
Y	 0.7740	 0.1070
Z	 0.6950	 0.1160
a	 0.3940	 0.1220
b	 0.3970	 0.1150
j	 0.2400	 0.1020
k	 0.1680	 0.0770
l	 0.7840	 0.1480
m	 0.7650	 0.1600
n	 0.1470	 0.0420
o	 0.1850	 0.0310

