



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 10:29 AM UTC

PDB ID : 7QJD / pdb_00007qjd
EMDB ID : EMD-14018
Title : Structure of recombinant human gamma-Tubulin Ring Complex without actin
Authors : Zupa, E.; Pfeffer, S.
Deposited on : 2021-12-16
Resolution : 7.10 Å (reported)
Based on initial models : 6X0U, 6L81, 6V6S, 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:

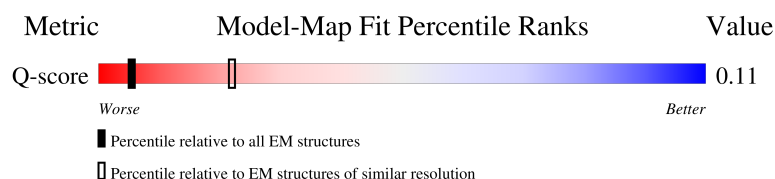
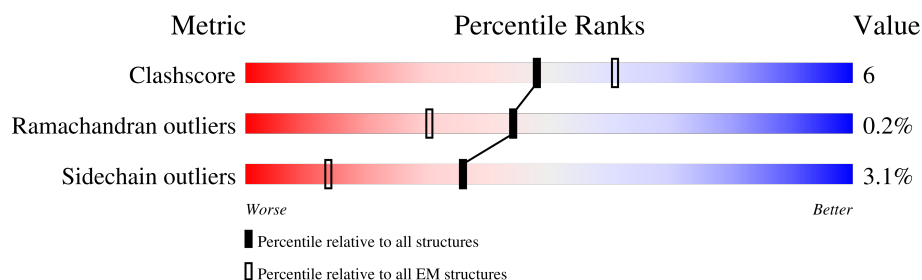
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

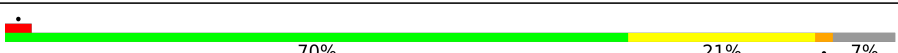
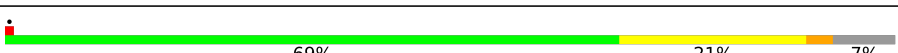
The reported resolution of this entry is 7.10 Å.

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



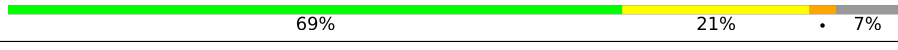
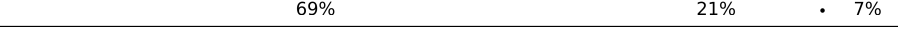
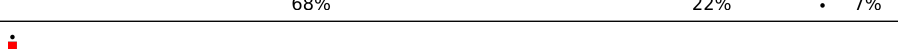
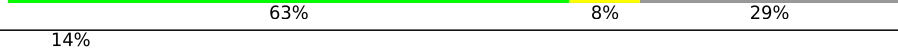
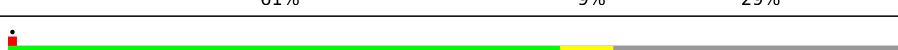
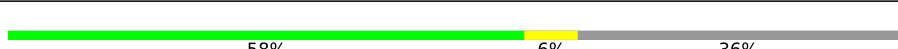
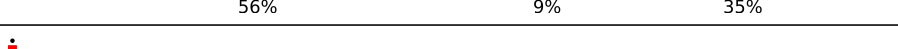
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	464 (6.60 - 7.60)

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

Mol	Chain	Length	Quality of chain
1	1	451	
1	2	451	
1	O	451	
1	P	451	

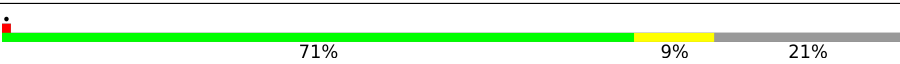
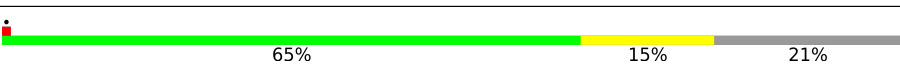
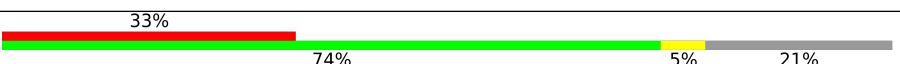
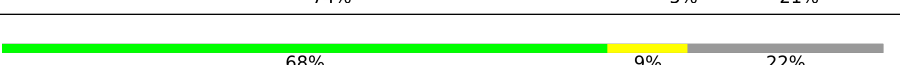
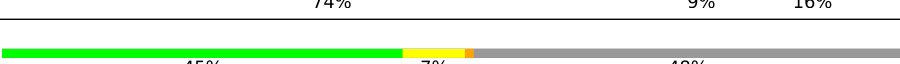
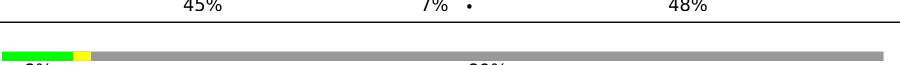
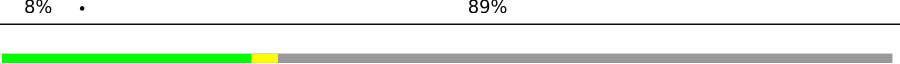
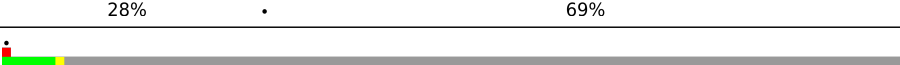
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	Q	451	
1	R	451	
1	S	451	
1	T	451	
1	U	451	
1	V	451	
1	W	451	
1	X	451	
1	Y	451	
1	Z	451	
2	A	902	
2	C	902	
2	E	902	
2	G	902	
2	M	902	
3	B	907	
3	D	907	
3	F	907	
3	H	907	
3	N	907	
3	a	907	
3	f	907	
3	h	907	
3	j	907	
3	n	907	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	b	82	
4	d	82	
4	g	82	
4	i	82	
4	k	82	
4	m	82	
4	o	82	
5	I	667	
5	K	667	
6	J	1024	
6	l	1024	
7	L	1819	
7	c	1819	

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 124666 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	O	420	Total	C	N	O	S	0	0
			3373	2134	586	638	15		
1	P	420	Total	C	N	O	S	0	0
			3373	2134	586	638	15		
1	Q	420	Total	C	N	O	S	0	0
			3373	2134	586	638	15		
1	R	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 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	613	Total	C	N	O	S	0	0
			4978	3212	831	903	32		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	620	Total	C	N	O	S	0	0
			5044	3257	845	910	32		
2	G	640	Total	C	N	O	S	0	0
			5216	3359	878	946	33		
2	M	636	Total	C	N	O	S	0	0
			5186	3342	871	940	33		
2	E	640	Total	C	N	O	S	0	0
			5216	3359	878	946	33		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	610	Total	C	N	O	S	0	0
			5029	3203	888	913	25		
3	D	581	Total	C	N	O	S	0	0
			4796	3061	842	868	25		
3	F	599	Total	C	N	O	S	0	0
			4941	3151	871	894	25		
3	H	594	Total	C	N	O	S	0	0
			4907	3130	864	888	25		
3	N	594	Total	C	N	O	S	0	0
			4907	3130	864	888	25		
3	n	99	Total	C	N	O	S	0	0
			803	509	148	144	2		
3	f	99	Total	C	N	O	S	0	0
			803	509	148	144	2		
3	j	107	Total	C	N	O	S	0	0
			863	545	161	155	2		
3	a	116	Total	C	N	O	S	0	0
			933	591	171	169	2		
3	h	107	Total	C	N	O	S	0	0
			863	545	161	155	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	k	65	Total	C	N	O	S	0	0
			484	299	85	96	4		
4	i	65	Total	C	N	O	S	0	0
			484	299	85	96	4		

Continued on next page...

Continued from previous page...

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

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

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

- Molecule 6 is a protein called Gamma-tubulin complex component 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	534	Total	C	N	O	S	0	0
			4429	2893	737	776	23		
6	l	108	Total	C	N	O	S	0	0
			876	556	151	168	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	L	566	Total	C	N	O	S	0	0
			4587	3000	773	789	25		
7	c	118	Total	C	N	O	S	0	0
			899	565	151	176	7		

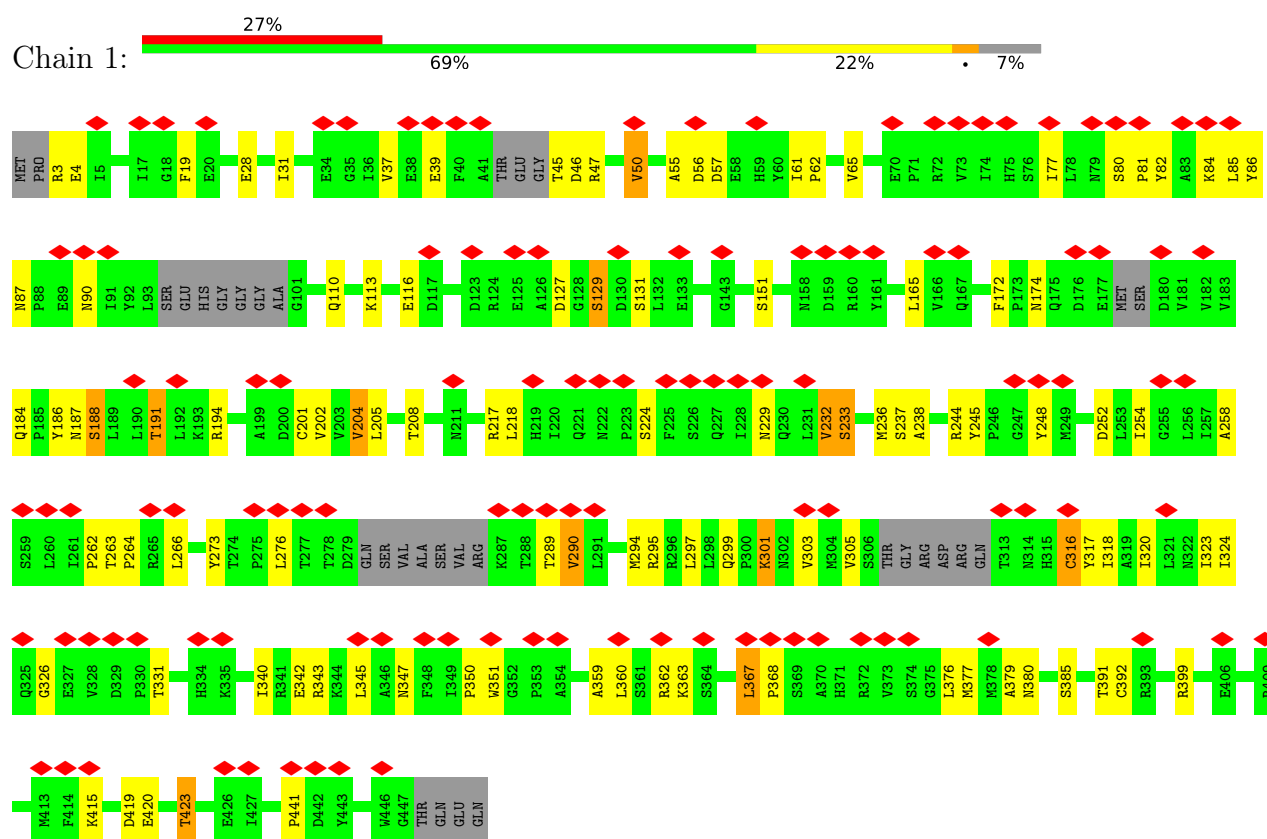
- Molecule 8 is water.

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

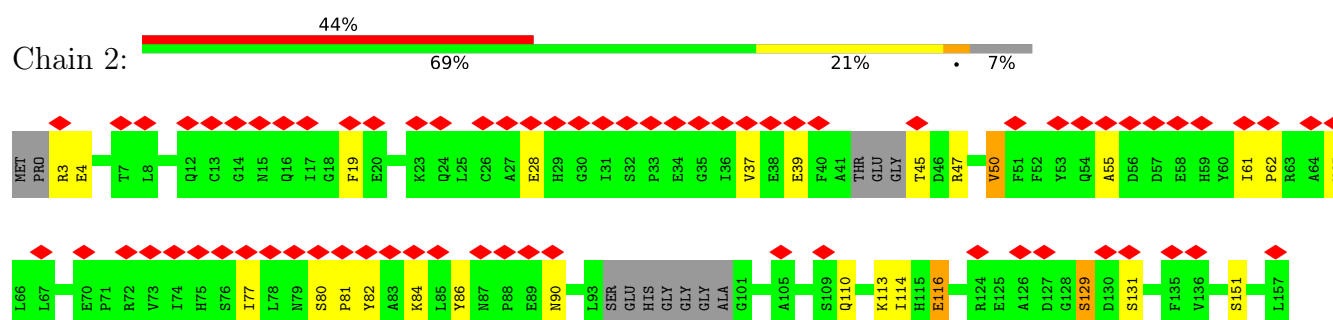
3 Residue-property plots

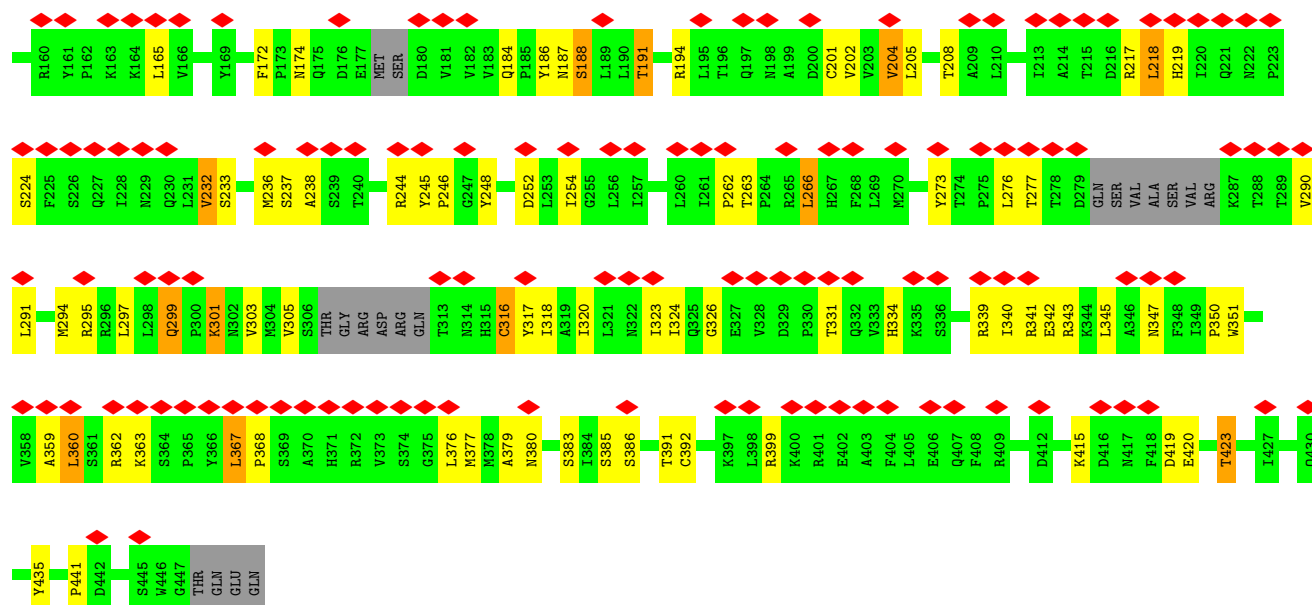
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Tubulin gamma-1 chain

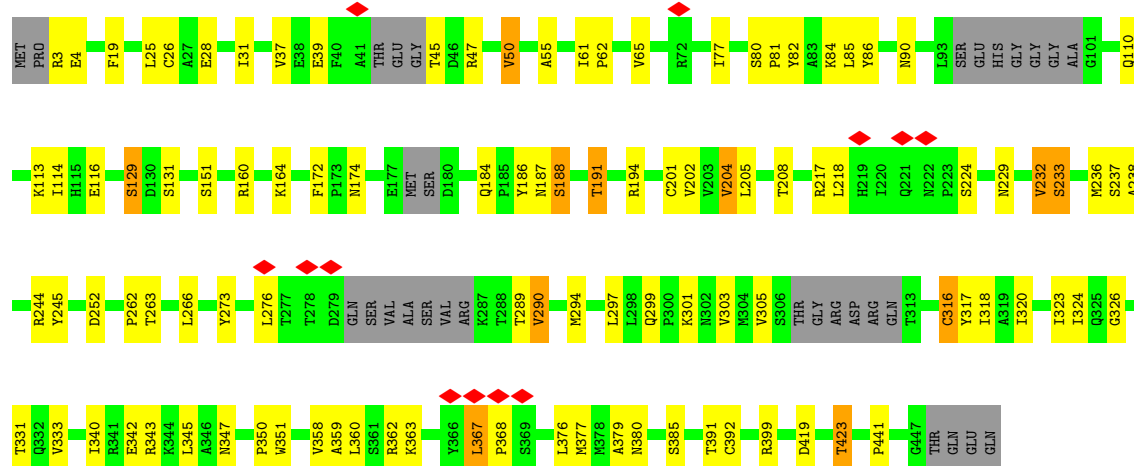


- Molecule 1: Tubulin gamma-1 chain

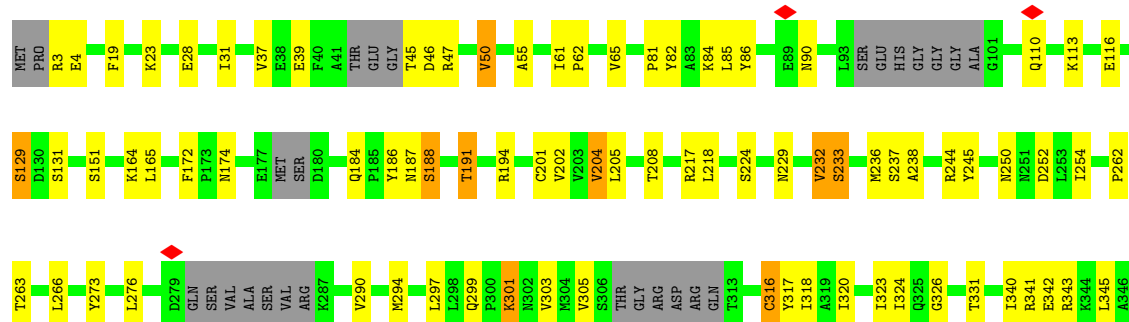




• Molecule 1: Tubulin gamma-1 chain



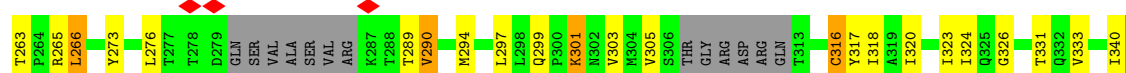
• Molecule 1: Tubulin gamma-1 chain





• Molecule 1: Tubulin gamma-1 chain

Chain Q: 69% 21% 7%



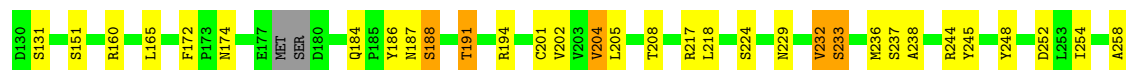
• Molecule 1: Tubulin gamma-1 chain

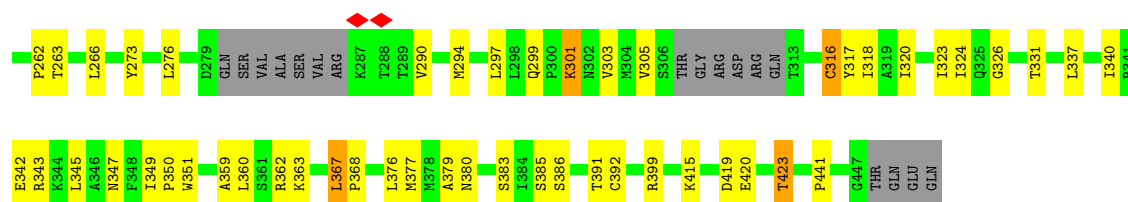
Chain R: 69% 21% 7%



• Molecule 1: Tubulin gamma-1 chain

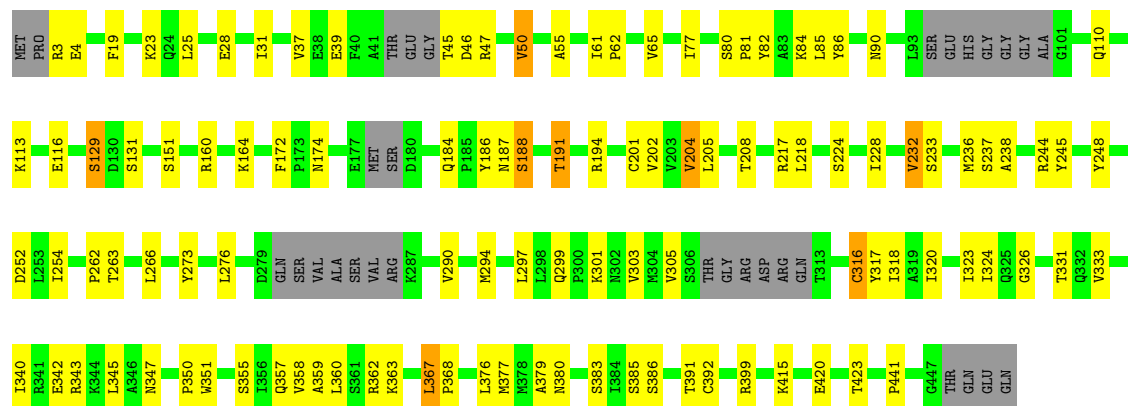
Chain S: 69% 21% 7%





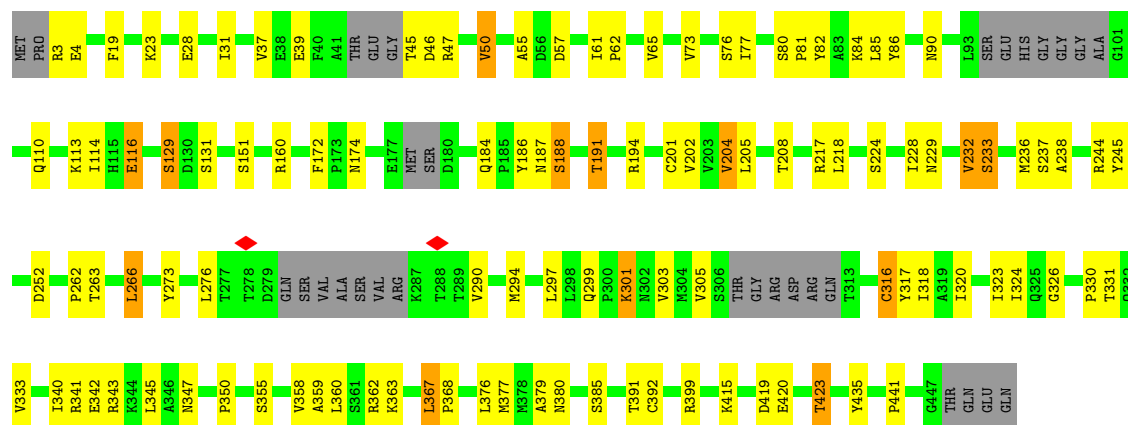
• Molecule 1: Tubulin gamma-1 chain

Chain T: 69% 23% 7%



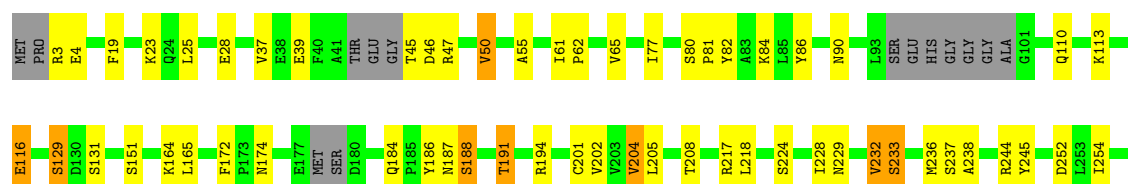
• Molecule 1: Tubulin gamma-1 chain

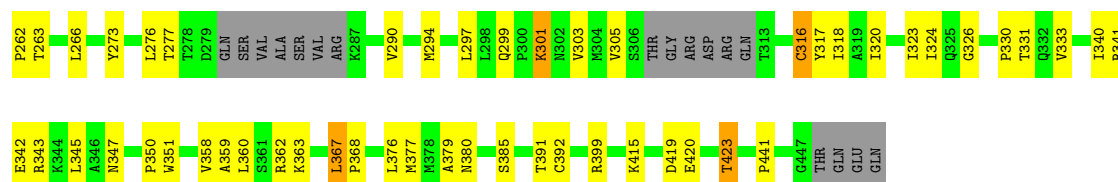
Chain U: 68% 22% 7%



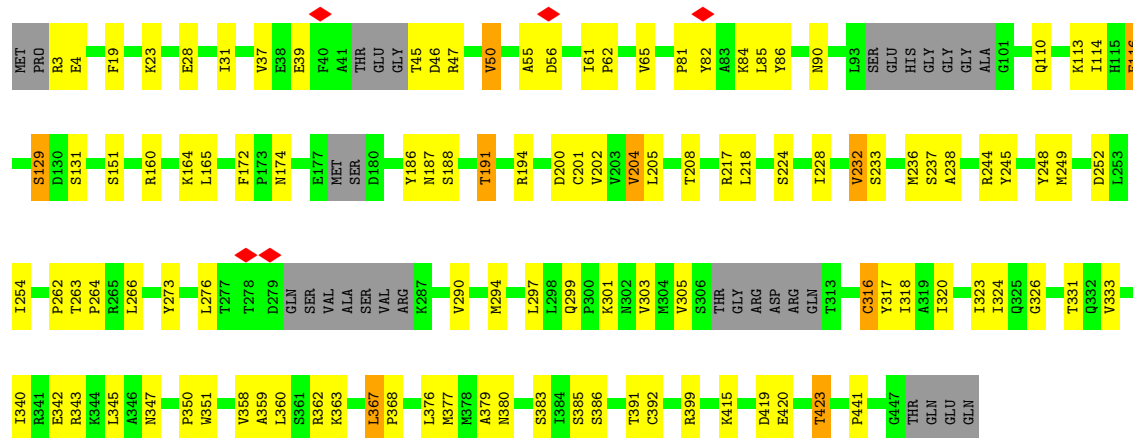
• Molecule 1: Tubulin gamma-1 chain

Chain V: 69% 22% 7%

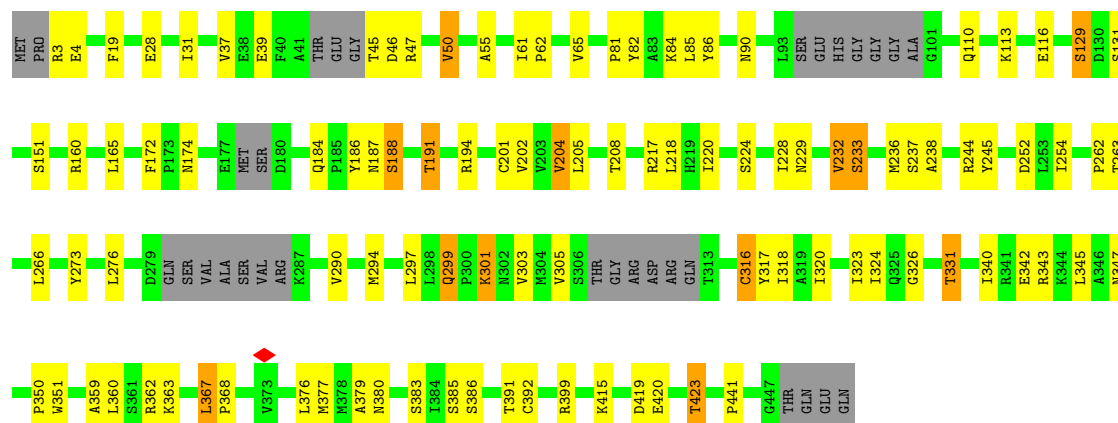




• Molecule 1: Tubulin gamma-1 chain

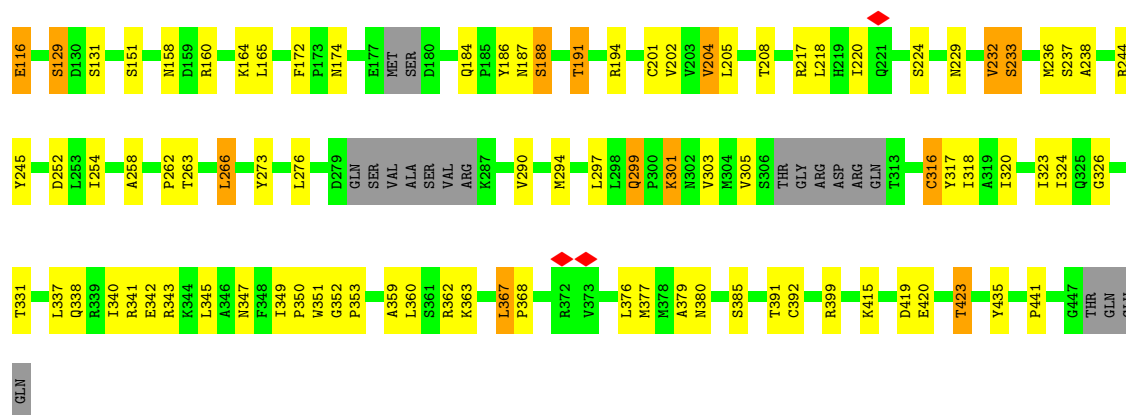


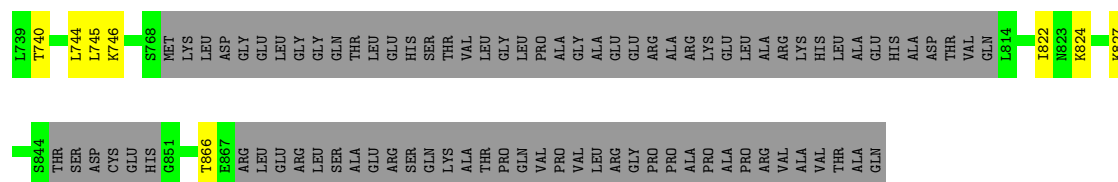
• Molecule 1: Tubulin gamma-1 chain



• Molecule 1: Tubulin gamma-1 chain

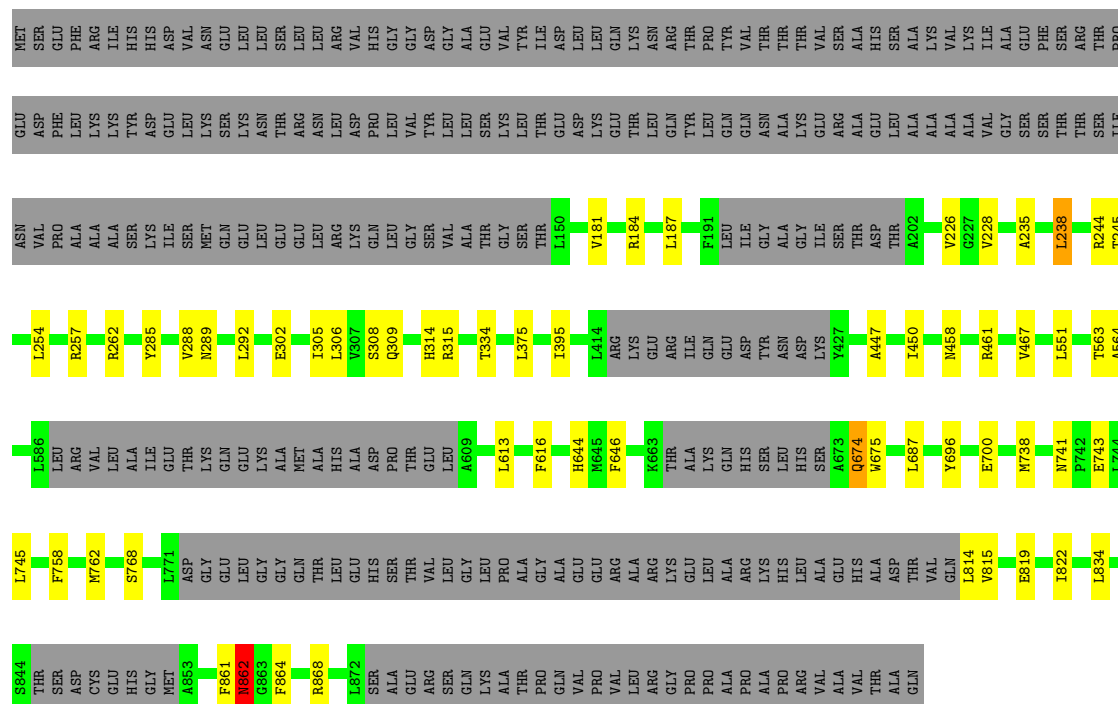






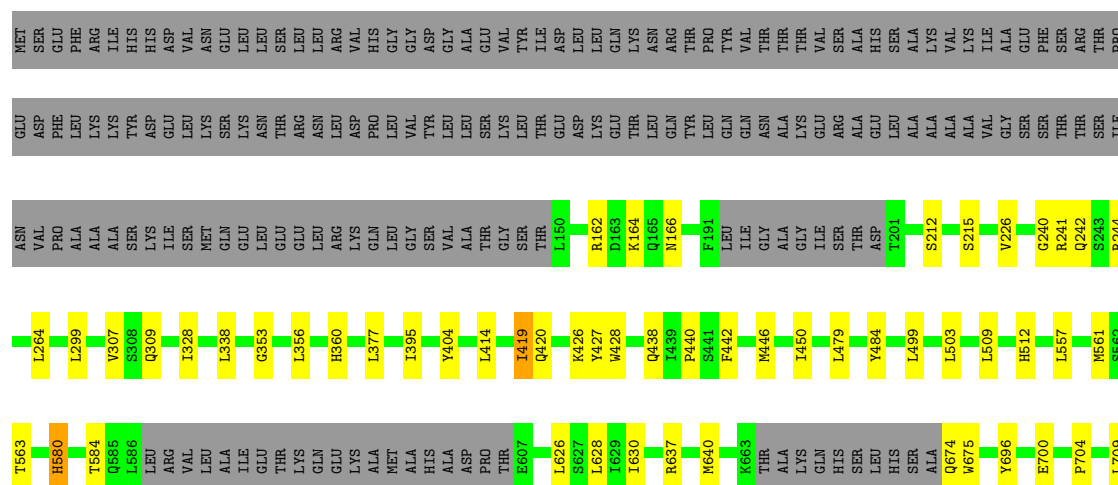
• Molecule 2: Gamma-tubulin complex component 2

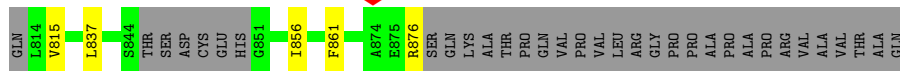
Chain C: 62% 6% 31%



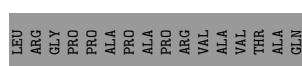
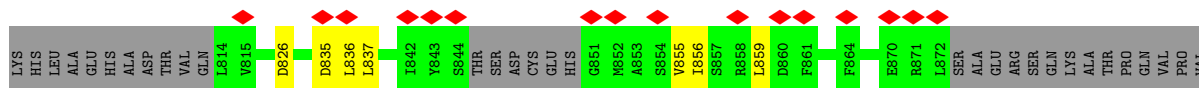
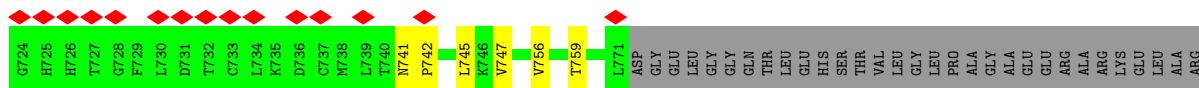
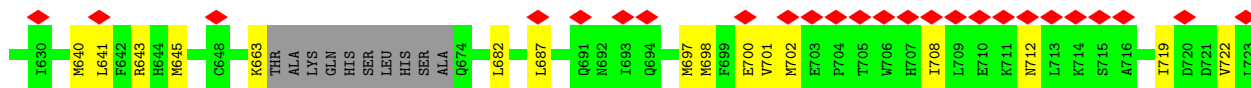
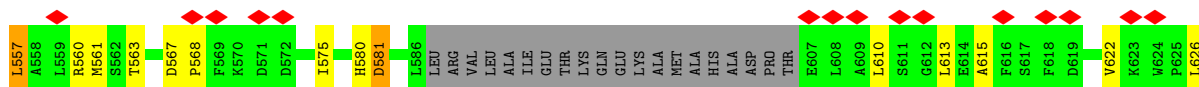
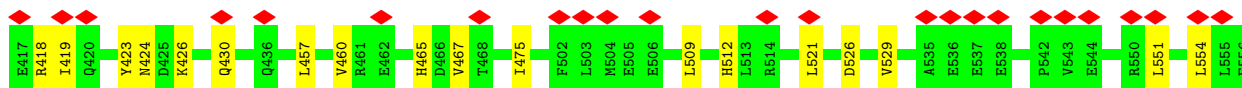
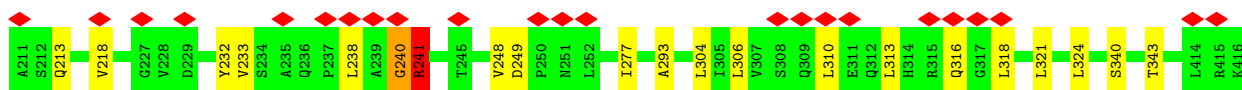
• Molecule 2: Gamma-tubulin complex component 2

Chain G: 63% 8% 29%

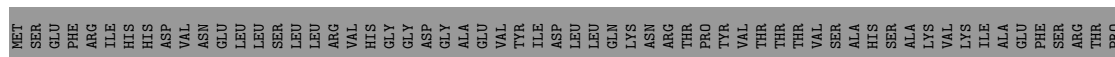


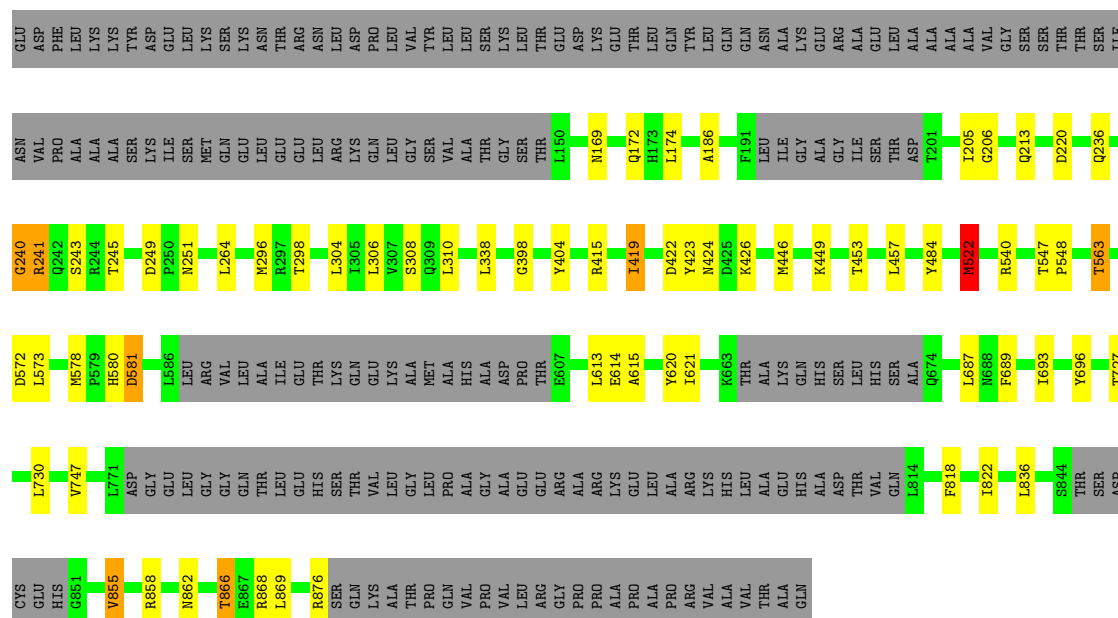


- Molecule 2: Gamma-tubulin complex component 2



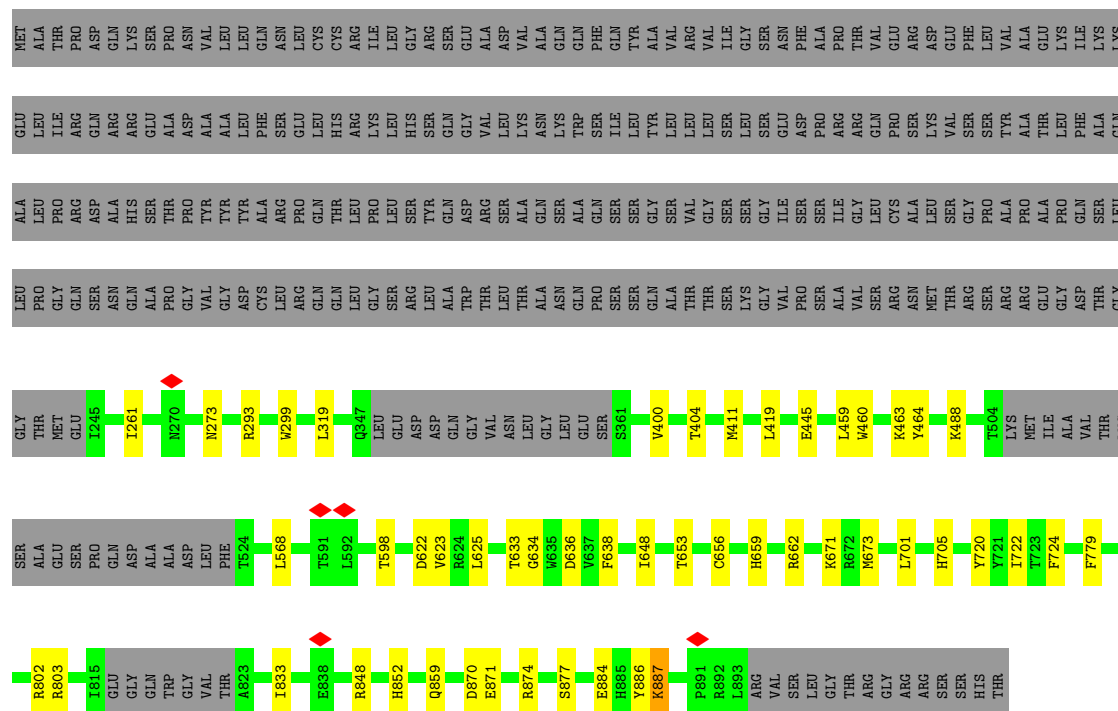
- Molecule 2: Gamma-tubulin complex component 2





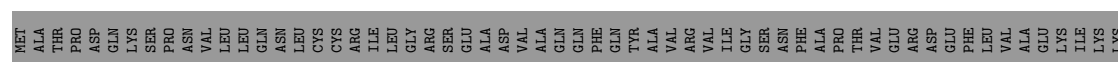
• Molecule 3: Gamma-tubulin complex component 3

Chain B: 62% 6% 33%



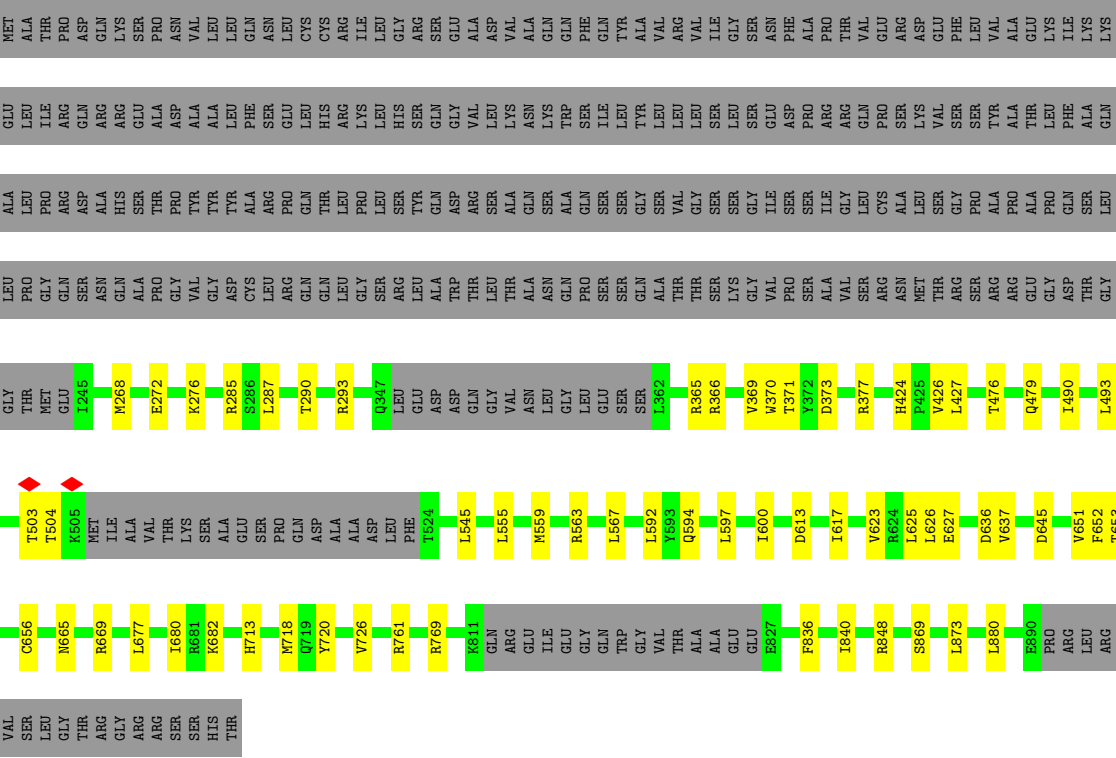
• Molecule 3: Gamma-tubulin complex component 3

Chain D: 58% 6% 36%



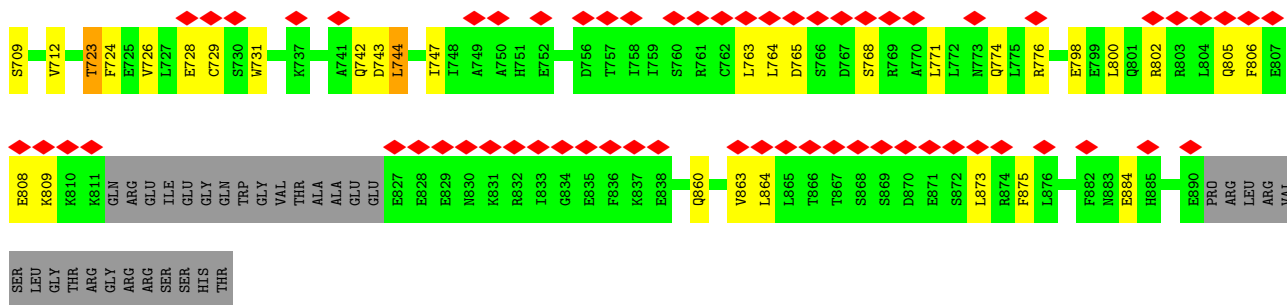


• Molecule 3: Gamma-tubulin complex component 3

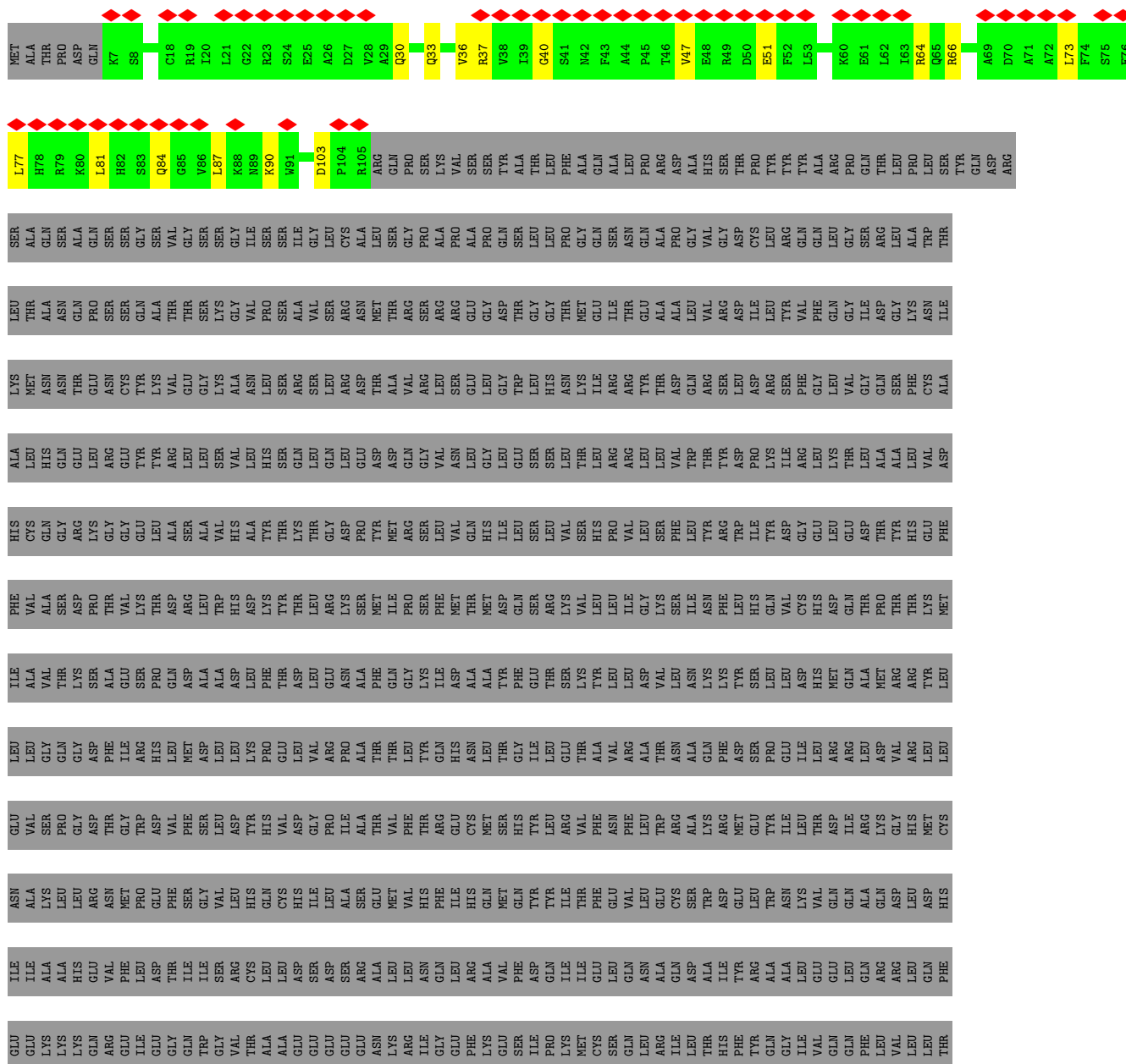


• Molecule 3: Gamma-tubulin complex component 3

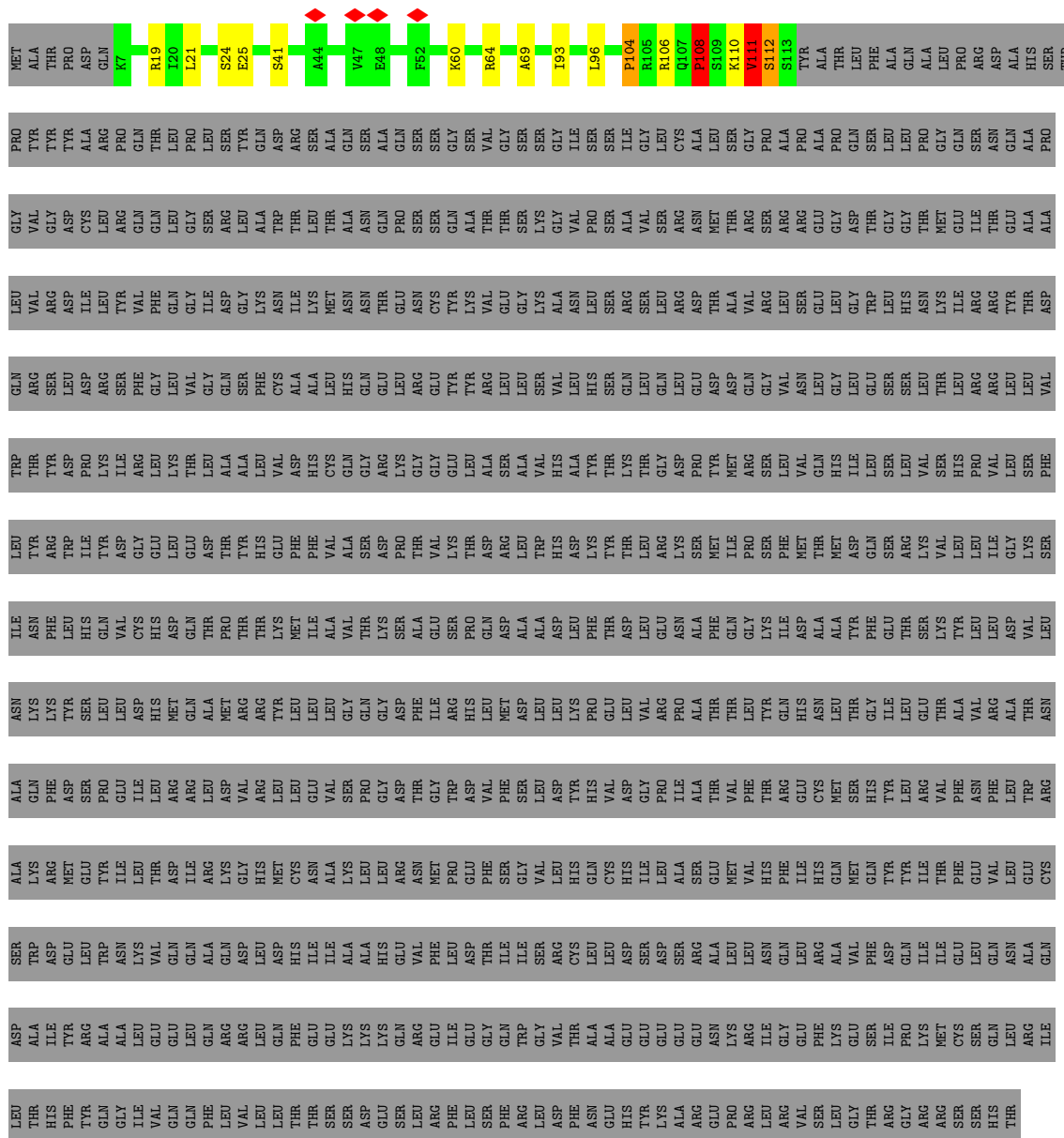




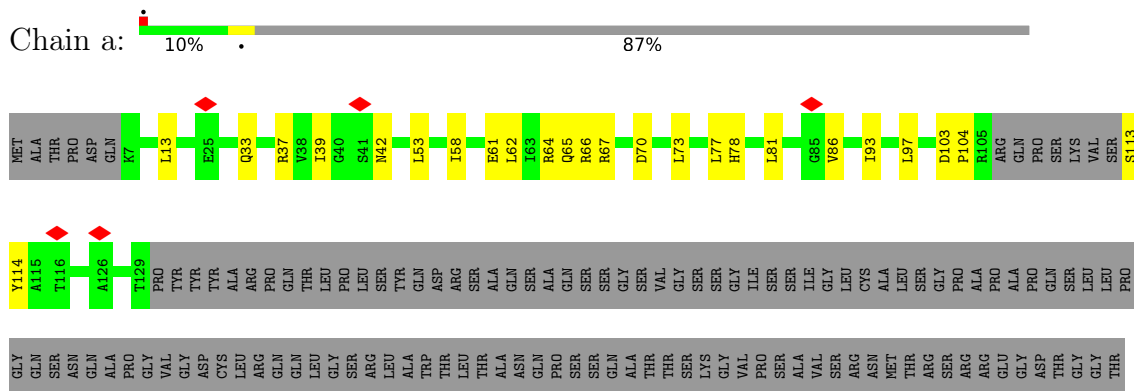
• Molecule 3: Gamma-tubulin complex component 3



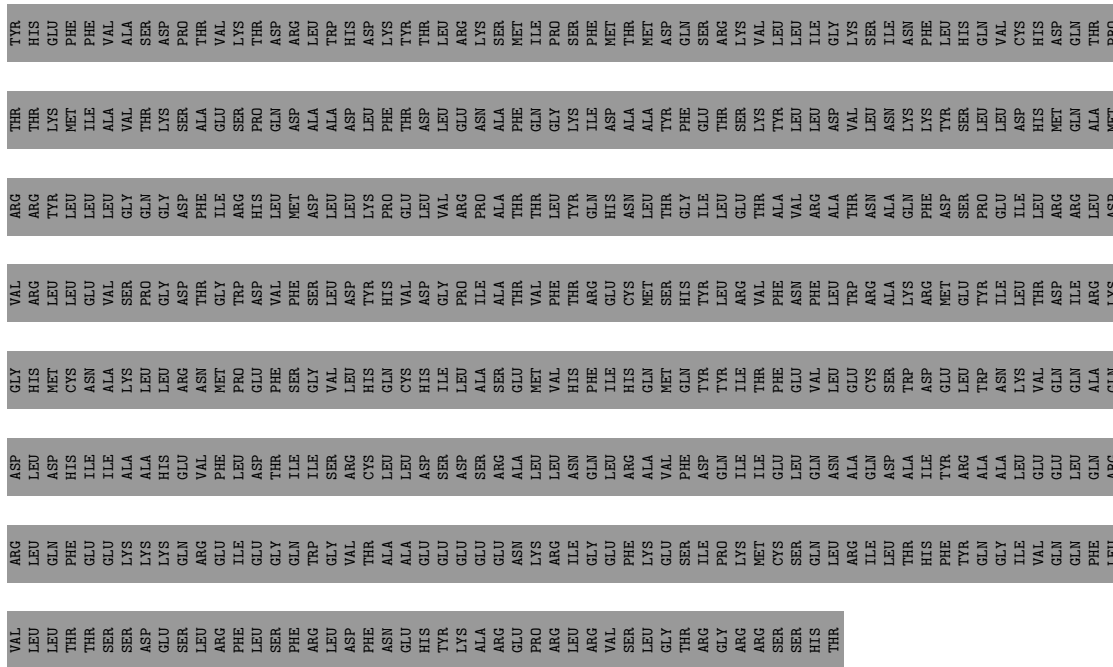
Chain j:  10% . 88%



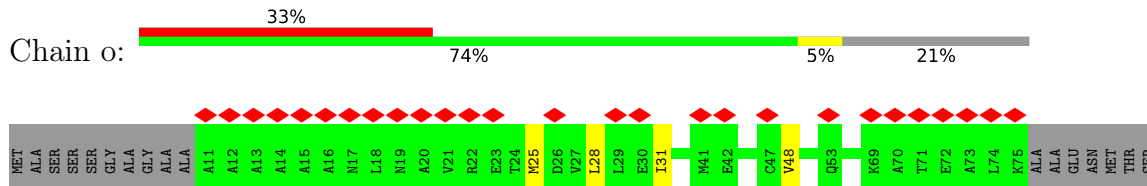
- Molecule 3: Gamma-tubulin complex component 3



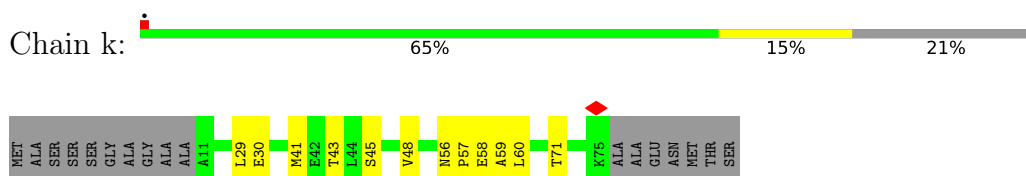




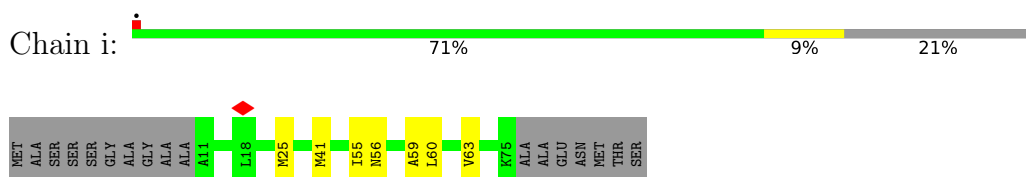
- Molecule 4: Mitotic-spindle organizing protein 1



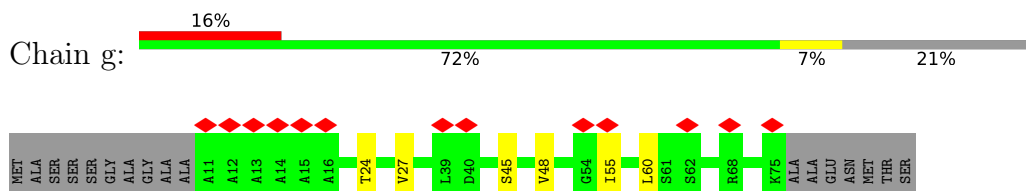
- Molecule 4: Mitotic-spindle organizing protein 1



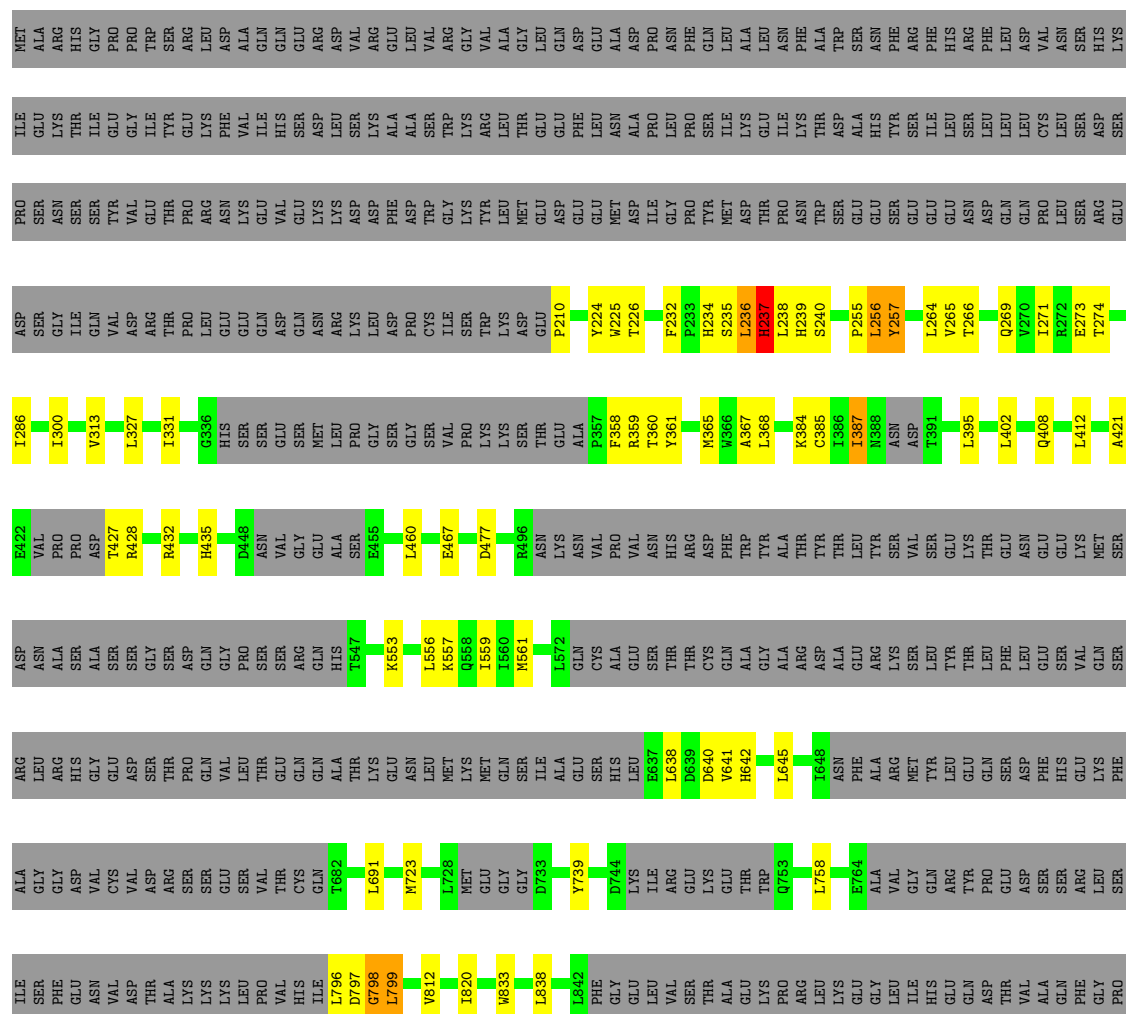
- Molecule 4: Mitotic-spindle organizing protein 1

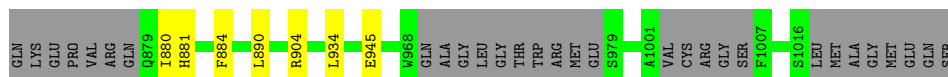


- Molecule 4: Mitotic-spindle organizing protein 1



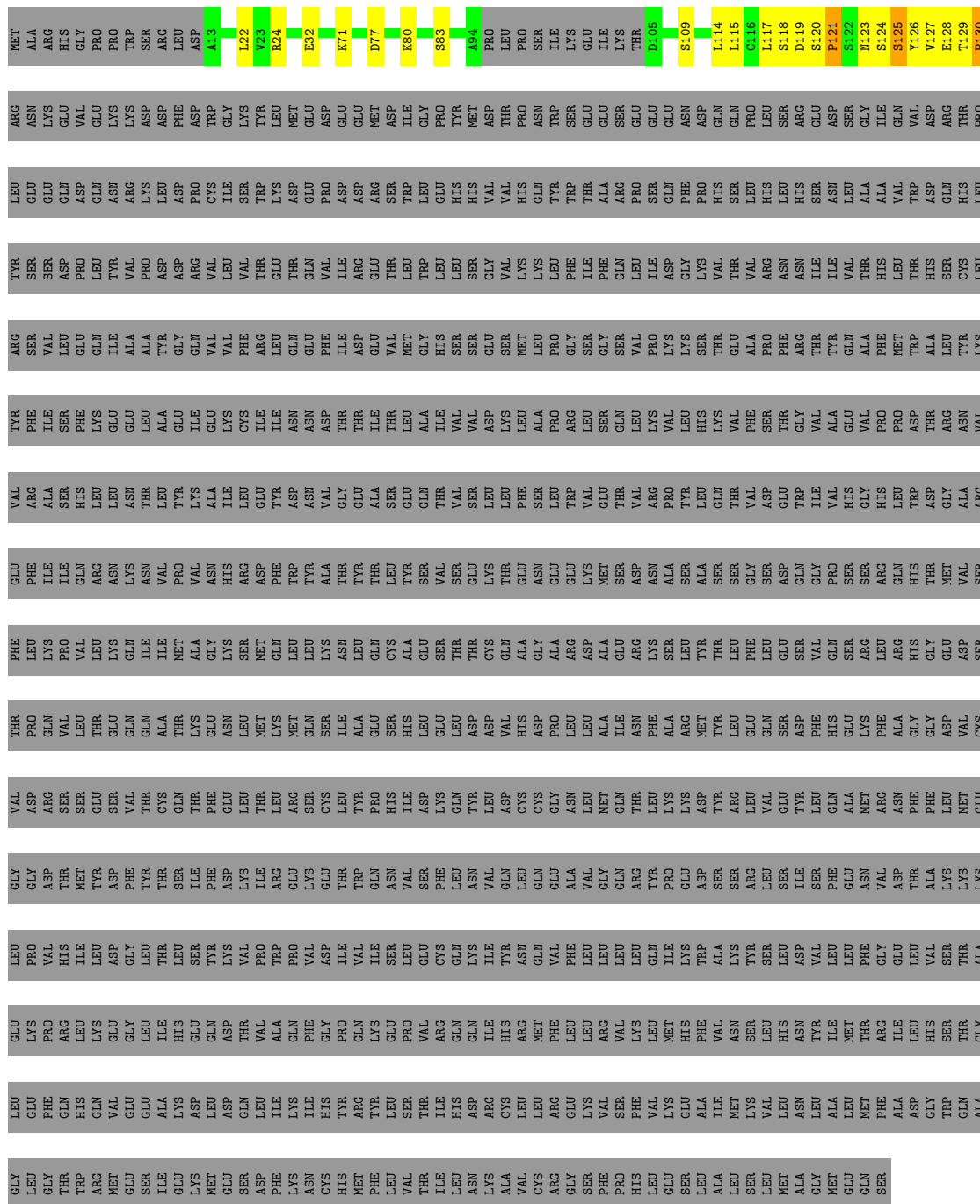
- Molecule 6: Gamma-tubulin complex component 5





• Molecule 6: Gamma-tubulin complex component 5

Chain 1: 8% . 89%



• Molecule 7: Gamma-tubulin complex component 6

Chain L: 28% . 69%





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	40115	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 ($e^-/\text{\AA}^2$)	42.6	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	0.203	Depositor
Minimum map value	-0.030	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.0274	Depositor
Map size (Å)	532.0, 532.0, 532.0	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.66, 2.66, 2.66	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	1	0.26	0/3441	0.60	0/4661
1	2	0.26	0/3441	0.60	0/4661
1	O	0.26	0/3441	0.60	0/4661
1	P	0.26	0/3441	0.60	0/4661
1	Q	0.26	0/3441	0.60	0/4661
1	R	0.26	0/3441	0.60	0/4661
1	S	0.26	0/3441	0.60	0/4661
1	T	0.26	0/3441	0.60	0/4661
1	U	0.26	0/3441	0.60	0/4661
1	V	0.26	0/3441	0.60	0/4661
1	W	0.26	0/3441	0.60	0/4661
1	X	0.26	0/3441	0.60	0/4661
1	Y	0.26	0/3441	0.60	0/4661
1	Z	0.26	0/3441	0.60	0/4661
2	A	0.34	0/5085	0.72	2/6866 (0.0%)
2	C	0.38	1/5151 (0.0%)	0.78	5/6955 (0.1%)
2	E	0.36	1/5325 (0.0%)	0.78	10/7187 (0.1%)
2	G	0.35	0/5325	0.75	4/7187 (0.1%)
2	M	0.38	0/5295	0.82	10/7147 (0.1%)
3	B	0.34	0/5133	0.75	4/6930 (0.1%)
3	D	0.36	0/4897	0.74	4/6610 (0.1%)
3	F	0.32	0/5044	0.72	5/6809 (0.1%)
3	H	0.36	0/5009	0.76	7/6761 (0.1%)
3	N	0.43	1/5009 (0.0%)	0.82	6/6761 (0.1%)
3	a	0.34	0/948	0.77	2/1277 (0.2%)
3	f	0.42	0/815	0.73	0/1096
3	h	0.29	0/876	0.82	4/1178 (0.3%)
3	j	0.29	0/876	0.73	2/1178 (0.2%)
3	n	0.34	0/815	0.77	1/1096 (0.1%)
4	b	0.35	0/484	0.77	0/653
4	d	0.33	0/454	0.72	0/611
4	g	0.34	0/484	0.67	0/653
4	i	0.34	0/484	0.77	0/653
4	k	0.28	0/484	0.65	0/653

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
4	m	0.26	0/484	0.65	0/653
4	o	0.36	0/484	0.73	0/653
5	I	0.39	0/4322	0.77	4/5853 (0.1%)
5	K	0.42	0/4683	0.82	12/6338 (0.2%)
6	J	0.40	0/4525	0.86	16/6119 (0.3%)
6	l	0.33	0/895	0.81	2/1210 (0.2%)
7	L	0.34	0/4697	0.73	2/6348 (0.0%)
7	c	0.35	0/911	0.74	1/1231 (0.1%)
All	All	0.33	3/127168 (0.0%)	0.71	103/171920 (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	1
1	2	0	1
1	O	0	1
1	P	0	1
1	Q	0	1
1	R	0	1
1	S	0	1
1	T	0	1
1	U	0	1
1	V	0	1
1	W	0	1
1	X	0	1
1	Y	0	1
1	Z	0	1
2	A	0	2
2	C	0	3
2	E	0	5
2	G	0	3
2	M	0	4
3	B	0	1
3	F	0	1
3	H	0	2
3	N	0	2
3	f	0	1
3	h	0	1
3	j	0	2

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
5	I	0	7
5	K	0	2
6	J	0	4
7	L	0	2
All	All	0	56

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	862	ASN	CB-CG	-6.93	1.34	1.52
3	N	723	THR	CB-CG2	-5.90	1.33	1.52
2	E	563	THR	CB-CG2	-5.71	1.33	1.52

All (103) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	557	LEU	CB-CG-CD2	-11.26	76.91	110.70
6	l	121	PRO	CA-N-CD	-8.76	99.73	112.00
3	h	108	PRO	CA-N-CD	-8.71	99.81	112.00
6	l	130	PRO	CA-N-CD	-8.68	99.86	112.00
3	j	108	PRO	CA-N-CD	-8.62	99.94	112.00
2	M	240	GLY	CA-C-N	7.25	135.38	121.54
2	M	240	GLY	C-N-CA	7.25	135.38	121.54
2	C	862	ASN	N-CA-C	7.22	120.38	110.06
6	J	237	HIS	CA-C-N	7.20	135.29	121.54
6	J	237	HIS	C-N-CA	7.20	135.29	121.54
3	H	868	SER	N-CA-C	-7.14	105.75	114.75
5	K	409	ASN	CA-C-N	7.13	135.17	121.54
5	K	409	ASN	C-N-CA	7.13	135.17	121.54
2	G	815	VAL	N-CA-C	-7.13	106.27	113.47
6	J	255	PRO	CA-C-N	6.94	134.19	121.70
6	J	255	PRO	C-N-CA	6.94	134.19	121.70
6	J	798	GLY	CA-C-N	6.91	134.74	121.54
6	J	798	GLY	C-N-CA	6.91	134.74	121.54
5	I	512	ALA	N-CA-C	-6.79	96.34	110.80
3	B	636	ASP	N-CA-C	-6.75	106.24	114.75
2	C	564	ALA	N-CA-C	-6.75	103.13	112.30
5	I	511	ASP	CA-C-N	6.68	134.31	121.54
5	I	511	ASP	C-N-CA	6.68	134.31	121.54
3	H	366	ARG	NE-CZ-NH1	-6.65	114.85	121.50
5	K	16	ILE	N-CA-C	-6.61	106.35	112.96
2	E	522	MET	CA-C-N	-6.54	112.07	122.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	522	MET	C-N-CA	-6.54	112.07	122.08
3	F	371	THR	CA-C-N	6.49	133.93	121.54
3	F	371	THR	C-N-CA	6.49	133.93	121.54
3	D	882	PHE	CA-C-N	6.43	131.26	122.19
3	D	882	PHE	C-N-CA	6.43	131.26	122.19
2	G	419	ILE	CA-C-N	6.41	133.78	121.54
2	G	419	ILE	C-N-CA	6.41	133.78	121.54
7	c	148	TYR	CA-CB-CG	6.41	125.43	113.90
2	C	288	VAL	N-CA-C	-6.39	106.57	112.96
3	N	455	LYS	CA-C-N	-6.36	113.02	122.56
3	N	455	LYS	C-N-CA	-6.36	113.02	122.56
2	C	862	ASN	CB-CA-C	-6.28	99.48	111.97
2	E	264	LEU	N-CA-C	6.25	123.61	109.81
7	L	1689	ARG	N-CA-C	-6.09	105.38	114.64
5	I	84	ILE	N-CA-C	-6.07	106.58	112.29
2	E	240	GLY	N-CA-C	-6.01	103.90	112.55
3	n	40	GLY	N-CA-C	6.00	118.93	112.33
2	M	719	ILE	N-CA-C	-5.89	107.00	112.83
3	j	41	SER	N-CA-C	-5.89	107.90	114.62
3	H	882	PHE	CB-CA-C	5.82	121.36	111.35
3	h	112	SER	CA-C-N	5.76	132.06	121.70
3	h	112	SER	C-N-CA	5.76	132.06	121.70
2	E	419	ILE	CA-C-N	5.74	132.51	121.54
2	E	419	ILE	C-N-CA	5.74	132.51	121.54
6	J	387	ILE	N-CA-C	-5.70	107.26	112.96
3	F	287	LEU	N-CA-C	-5.69	107.33	114.56
3	h	107	GLN	N-CA-C	5.64	122.27	109.81
2	M	580	HIS	CA-C-N	5.53	132.10	121.54
2	M	580	HIS	C-N-CA	5.53	132.10	121.54
2	E	240	GLY	CA-C-N	5.49	132.02	121.54
2	E	240	GLY	C-N-CA	5.49	132.02	121.54
2	G	264	LEU	N-CA-C	5.48	121.93	109.81
3	N	726	VAL	N-CA-C	-5.47	107.02	113.42
2	M	241	ARG	O-C-N	-5.44	115.36	122.59
6	J	880	ILE	N-CA-C	-5.43	98.04	109.34
5	K	203	PHE	CA-C-N	5.39	131.84	121.54
5	K	203	PHE	C-N-CA	5.39	131.84	121.54
6	J	359	ARG	N-CA-C	5.38	119.12	112.24
2	A	557	LEU	CA-CB-CG	5.37	135.11	116.30
3	N	454	VAL	CA-C-N	5.34	131.74	121.54
3	N	454	VAL	C-N-CA	5.34	131.74	121.54
3	B	722	ILE	CA-C-N	5.32	127.67	120.65

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	722	ILE	C-N-CA	5.32	127.67	120.65
3	D	882	PHE	N-CA-C	-5.29	100.41	109.24
3	D	883	ASN	N-CA-C	5.29	118.88	111.74
5	K	403	VAL	CA-C-N	5.27	130.05	122.35
5	K	403	VAL	C-N-CA	5.27	130.05	122.35
2	M	836	LEU	CA-CB-CG	5.26	134.72	116.30
3	H	677	LEU	CA-C-N	-5.26	111.33	121.58
3	H	677	LEU	C-N-CA	-5.26	111.33	121.58
3	a	86	VAL	N-CA-C	-5.25	108.16	113.20
2	A	427	TYR	CA-CB-CG	5.24	123.33	113.90
5	K	288	ASN	CA-C-N	5.22	131.50	121.54
5	K	288	ASN	C-N-CA	5.22	131.50	121.54
3	N	455	LYS	N-CA-C	-5.21	99.70	110.80
6	J	421	ALA	CA-C-N	5.18	131.03	121.70
6	J	421	ALA	C-N-CA	5.18	131.03	121.70
6	J	210	PRO	CA-C-N	5.15	131.37	121.54
6	J	210	PRO	C-N-CA	5.15	131.37	121.54
2	E	581	ASP	N-CA-CB	-5.15	101.79	110.49
2	M	419	ILE	CA-C-N	5.14	131.36	121.54
2	M	419	ILE	C-N-CA	5.14	131.36	121.54
6	J	945	GLU	CA-C-N	5.13	129.90	122.36
6	J	945	GLU	C-N-CA	5.13	129.90	122.36
7	L	1563	HIS	N-CA-C	-5.13	106.14	114.09
5	K	651	TYR	OH-CZ-CE2	-5.12	104.52	119.90
3	H	495	GLN	CA-C-N	-5.11	117.97	122.97
3	H	495	GLN	C-N-CA	-5.11	117.97	122.97
5	K	653	LYS	CA-C-N	-5.11	113.96	122.08
5	K	653	LYS	C-N-CA	-5.11	113.96	122.08
3	F	272	GLU	CA-C-N	5.08	131.24	121.54
3	F	272	GLU	C-N-CA	5.08	131.24	121.54
2	E	423	TYR	CA-CB-CG	5.08	123.04	113.90
3	B	411	MET	N-CA-C	-5.04	106.27	114.09
6	J	812	VAL	N-CA-C	-5.03	108.60	113.53
3	a	42	ASN	N-CA-C	-5.02	104.98	111.71
2	C	675	TRP	N-CA-C	-5.01	108.44	114.75

There are no chirality outliers.

All (56) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	55	ALA	Peptide
1	2	55	ALA	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
2	A	583	ILE	Peptide
2	A	584	THR	Mainchain
3	B	887	LYS	Peptide
2	C	238	LEU	Peptide
2	C	674	GLN	Peptide
2	C	862	ASN	Sidechain
2	E	240	GLY	Peptide
2	E	522	MET	Mainchain
2	E	563	THR	Peptide
2	E	580	HIS	Peptide
2	E	866	THR	Peptide
3	F	373	ASP	Peptide
2	G	240	GLY	Peptide
2	G	580	HIS	Peptide
2	G	674	GLN	Peptide
3	H	627	GLU	Peptide
3	H	867	THR	Peptide
5	I	403	VAL	Peptide
5	I	404	LEU	Mainchain
5	I	407	ASP	Peptide
5	I	408	ASP	Mainchain
5	I	507	SER	Peptide
5	I	508	ASN	Mainchain
5	I	600	ASN	Peptide
6	J	235	SER	Peptide
6	J	237	HIS	Peptide
6	J	256	LEU	Peptide
6	J	798	GLY	Peptide
5	K	653	LYS	Peptide
5	K	67	GLN	Peptide
7	L	1805	ASN	Peptide
7	L	346	LEU	Peptide
2	M	240	GLY	Peptide
2	M	241	ARG	Mainchain
2	M	430	GLN	Peptide
2	M	581	ASP	Mainchain
3	N	454	VAL	Peptide
3	N	501	THR	Peptide
1	O	55	ALA	Peptide
1	P	55	ALA	Peptide
1	Q	55	ALA	Peptide
1	R	55	ALA	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	S	55	ALA	Peptide
1	T	55	ALA	Peptide
1	U	55	ALA	Peptide
1	V	55	ALA	Peptide
1	W	55	ALA	Peptide
1	X	55	ALA	Peptide
1	Y	55	ALA	Peptide
1	Z	55	ALA	Peptide
3	f	49	ARG	Peptide
3	h	106	ARG	Peptide
3	j	104	PRO	Peptide
3	j	111	VAL	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	66	0
1	2	3373	0	3325	73	0
1	O	3373	0	3325	52	0
1	P	3373	0	3325	55	0
1	Q	3373	0	3325	57	0
1	R	3373	0	3325	60	0
1	S	3373	0	3325	56	0
1	T	3373	0	3325	56	0
1	U	3373	0	3325	59	0
1	V	3373	0	3325	56	0
1	W	3373	0	3325	58	0
1	X	3373	0	3325	54	0
1	Y	3373	0	3325	64	0
1	Z	3373	0	3325	62	0
2	A	4978	0	4996	25	0
2	C	5044	0	5081	35	0
2	E	5216	0	5247	72	0
2	G	5216	0	5245	64	0
2	M	5186	0	5219	47	0
3	B	5029	0	5018	30	0
3	D	4796	0	4775	38	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	4941	0	4934	45	0
3	H	4907	0	4896	37	0
3	N	4907	0	4896	54	0
3	a	933	0	953	15	0
3	f	803	0	831	1	0
3	h	863	0	896	30	0
3	j	863	0	896	25	0
3	n	803	0	831	12	0
4	b	484	0	512	7	0
4	d	454	0	482	3	0
4	g	484	0	512	3	0
4	i	484	0	512	21	0
4	k	484	0	511	35	0
4	m	484	0	512	21	0
4	o	484	0	512	3	0
5	I	4225	0	4259	36	0
5	K	4579	0	4586	40	0
6	J	4429	0	4482	40	0
6	l	876	0	842	67	0
7	L	4587	0	4636	34	0
7	c	899	0	895	8	0
8	l	6	0	0	1	0
All	All	124666	0	124517	1467	0

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

All (1467) 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)
6:l:80:LYS:HD2	6:l:126:TYR:CD1	1.36	1.57
6:l:80:LYS:CD	6:l:126:TYR:CE1	1.90	1.55
6:l:80:LYS:HD2	6:l:126:TYR:CE1	0.96	1.47
2:E:876:ARG:CZ	3:h:42:ASN:CB	1.90	1.45
4:i:56:ASN:ND2	2:E:876:ARG:HD3	1.30	1.38
6:l:80:LYS:CD	6:l:126:TYR:CD1	2.03	1.38
2:G:876:ARG:CD	4:k:59:ALA:HB2	1.48	1.34
2:G:876:ARG:CD	4:k:59:ALA:CB	2.06	1.23
4:i:56:ASN:ND2	2:E:876:ARG:CD	2.00	1.22
4:i:56:ASN:HD22	2:E:876:ARG:CD	1.51	1.21
2:E:876:ARG:NH1	3:h:42:ASN:HB3	1.60	1.16

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:i:59:ALA:HB2	2:E:876:ARG:NE	1.58	1.16
3:F:769:ARG:NH2	3:j:108:PRO:HG3	1.57	1.16
4:m:30:GLU:OE2	6:l:130:PRO:CD	1.95	1.14
2:E:876:ARG:CZ	3:h:42:ASN:HB3	1.57	1.14
4:m:30:GLU:CD	6:l:130:PRO:CD	2.22	1.13
2:E:876:ARG:CZ	3:h:42:ASN:HB2	1.63	1.11
2:G:876:ARG:NH1	4:k:60:LEU:N	2.01	1.08
6:l:80:LYS:CE	6:l:126:TYR:CD1	2.37	1.08
3:F:769:ARG:HH21	3:j:108:PRO:CG	1.68	1.06
2:G:876:ARG:HG2	4:k:56:ASN:ND2	1.70	1.06
2:G:876:ARG:HD3	4:k:59:ALA:HB2	1.26	1.06
2:G:876:ARG:CZ	4:k:60:LEU:H	1.70	1.05
4:m:30:GLU:OE2	6:l:130:PRO:HD3	1.57	1.04
2:E:876:ARG:NE	3:h:42:ASN:CB	2.20	1.03
6:l:77:ASP:OD2	6:l:126:TYR:CZ	2.12	1.02
2:E:876:ARG:NE	3:h:42:ASN:HB2	1.73	1.02
4:m:30:GLU:CD	6:l:130:PRO:CG	2.32	1.02
2:G:876:ARG:NH2	4:k:60:LEU:H	1.56	1.02
4:m:30:GLU:OE1	6:l:130:PRO:CG	2.09	0.99
6:l:119:ASP:C	6:l:121:PRO:HD3	1.87	0.99
6:l:119:ASP:O	6:l:121:PRO:HD3	1.63	0.98
4:m:30:GLU:CD	6:l:130:PRO:HG2	1.87	0.98
6:l:124:SER:O	6:l:126:TYR:CD2	2.17	0.97
6:l:77:ASP:OD2	6:l:126:TYR:CE1	2.19	0.96
6:l:83:SER:OG	6:l:128:GLU:OE1	1.82	0.96
2:G:876:ARG:HD2	4:k:59:ALA:CB	1.61	0.95
2:G:876:ARG:NH2	4:k:57:PRO:C	2.24	0.95
4:m:30:GLU:OE1	6:l:130:PRO:HG2	1.65	0.95
3:F:669:ARG:HG3	3:j:106:ARG:HH22	1.30	0.95
4:m:30:GLU:OE2	6:l:130:PRO:HD2	1.69	0.93
3:F:669:ARG:HG3	3:j:106:ARG:NH2	1.80	0.92
2:G:876:ARG:HD2	4:k:59:ALA:HB2	1.16	0.92
6:l:80:LYS:CD	6:l:126:TYR:HD1	1.78	0.92
3:D:776:ARG:NH1	3:h:106:ARG:HG2	1.86	0.91
2:G:876:ARG:CZ	4:k:60:LEU:N	2.33	0.90
3:h:73:LEU:CD2	3:h:111:VAL:HG22	2.02	0.90
6:l:80:LYS:HE3	6:l:126:TYR:CD1	2.07	0.89
2:E:876:ARG:NH2	3:h:42:ASN:HB2	1.89	0.87
6:l:80:LYS:CD	6:l:126:TYR:HE1	1.52	0.87
2:G:876:ARG:HH12	4:k:60:LEU:N	1.72	0.86
4:m:30:GLU:CD	6:l:130:PRO:HD2	2.01	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:876:ARG:NH2	4:k:57:PRO:CA	2.33	0.86
4:i:56:ASN:HD22	2:E:876:ARG:HD2	1.39	0.85
6:l:124:SER:O	6:l:126:TYR:CE2	2.30	0.85
3:F:669:ARG:CG	3:j:106:ARG:NH2	2.31	0.84
3:h:73:LEU:HD22	3:h:111:VAL:HG22	1.60	0.83
2:E:876:ARG:NE	3:h:42:ASN:HB3	1.91	0.83
5:K:651:TYR:HD2	1:Y:349:ILE:HG22	1.44	0.83
2:E:876:ARG:HH12	3:h:42:ASN:C	1.84	0.81
6:l:124:SER:HA	6:l:126:TYR:CE2	2.16	0.81
6:l:127:VAL:HG12	6:l:127:VAL:O	1.81	0.80
1:l:56:ASP:HB2	1:2:217:ARG:HB3	1.64	0.78
6:l:115:LEU:HA	6:l:119:ASP:OD1	1.83	0.77
4:i:56:ASN:ND2	2:E:876:ARG:HD2	1.98	0.76
2:E:876:ARG:NH1	3:h:42:ASN:C	2.29	0.76
2:E:876:ARG:NH2	3:h:42:ASN:CB	2.42	0.74
2:E:424:ASN:HD21	2:E:426:LYS:HB3	1.52	0.74
4:i:59:ALA:CB	2:E:876:ARG:NE	2.47	0.73
2:G:876:ARG:HG3	4:k:58:GLU:CB	2.17	0.73
5:K:649:LEU:HD11	5:K:654:TYR:HB2	1.70	0.73
4:i:59:ALA:HB2	2:E:876:ARG:CZ	2.19	0.72
3:H:587:ARG:HG3	3:H:592:LEU:HD21	1.71	0.72
3:H:728:GLU:HG3	1:V:330:PRO:HB3	1.69	0.72
2:E:876:ARG:NH1	3:h:42:ASN:CB	2.33	0.72
1:U:57:ASP:OD1	1:V:277:THR:OG1	2.06	0.71
3:h:73:LEU:HD22	3:h:111:VAL:CG2	2.20	0.71
7:c:74:SER:HB3	7:c:89:LEU:HD22	1.73	0.71
4:i:59:ALA:HB2	2:E:876:ARG:HE	1.51	0.71
7:L:1800:LEU:HD22	1:Z:338:GLN:HE21	1.54	0.71
2:G:861:PHE:HE1	1:U:341:ARG:HA	1.56	0.70
6:l:124:SER:C	6:l:126:TYR:CD2	2.70	0.70
4:m:34:ILE:CG2	6:l:128:GLU:HG2	2.22	0.70
2:G:876:ARG:HD3	4:k:59:ALA:CB	2.00	0.69
6:l:80:LYS:HD2	6:l:126:TYR:HE1	0.87	0.69
6:l:80:LYS:CG	6:l:126:TYR:HD1	2.06	0.69
5:K:646:LEU:HD22	1:Y:338:GLN:NE2	2.08	0.69
1:S:258:ALA:HB1	2:E:687:LEU:HD21	1.73	0.69
6:l:123:ASN:O	6:l:126:TYR:HE2	1.76	0.69
7:L:1663:HIS:HE1	1:Z:259:SER:HA	1.58	0.68
3:j:110:LYS:O	3:j:111:VAL:HG23	1.92	0.68
4:i:56:ASN:HB2	2:E:876:ARG:NH1	2.09	0.68
4:m:34:ILE:HG21	6:l:128:GLU:HG2	1.75	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:313:VAL:HG21	6:J:395:LEU:HD12	1.76	0.68
7:L:328:GLN:NE2	7:L:341:ALA:O	2.26	0.68
7:L:294:ARG:HH11	7:L:306:HIS:H	1.41	0.67
6:l:80:LYS:CG	6:l:126:TYR:CD1	2.75	0.67
6:l:124:SER:HA	6:l:126:TYR:HE2	1.55	0.67
3:D:885:HIS:CD2	1:R:353:PRO:HD3	2.30	0.67
6:J:884:PHE:HB3	1:X:262:PRO:O	1.95	0.67
6:l:115:LEU:O	6:l:119:ASP:CG	2.39	0.66
5:I:501:GLN:HG3	5:I:502:ARG:HG3	1.77	0.66
1:S:349:ILE:O	2:E:862:ASN:ND2	2.28	0.66
2:G:309:GLN:HG2	3:a:53:LEU:HD21	1.76	0.66
3:B:799:GLU:HG2	3:B:802:ARG:HH11	1.61	0.66
2:C:334:THR:HA	2:C:375:LEU:HD11	1.77	0.66
3:B:884:GLU:OE2	1:P:341:ARG:NH2	2.29	0.66
5:I:555:GLU:HA	5:I:558:ARG:HE	1.61	0.65
3:h:107:GLN:HB3	3:h:108:PRO:CD	2.26	0.65
5:K:646:LEU:HD22	1:Y:338:GLN:HE22	1.62	0.65
6:J:387:ILE:O	7:L:307:ARG:NH2	2.30	0.65
3:F:377:ARG:NH1	7:c:145:TYR:OH	2.30	0.64
6:J:232:PHE:O	6:J:234:HIS:ND1	2.25	0.64
3:D:883:ASN:ND2	1:R:355:SER:OG	2.30	0.64
2:C:235:ALA:HB1	2:C:244:ARG:HH21	1.61	0.64
3:F:769:ARG:HH21	3:j:108:PRO:HG3	0.72	0.64
1:W:297:LEU:HD21	1:W:377:MET:HB3	1.80	0.64
3:N:798:GLU:OE2	3:N:802:ARG:NH2	2.30	0.64
1:X:297:LEU:HD21	1:X:377:MET:HB3	1.80	0.64
4:i:56:ASN:CG	2:E:876:ARG:HD3	2.16	0.64
6:l:115:LEU:O	6:l:119:ASP:OD2	2.15	0.64
5:K:647:LEU:HG	1:Y:337:LEU:HD21	1.79	0.64
1:l:297:LEU:HD21	1:l:377:MET:HB3	1.80	0.64
5:I:530:TYR:CE2	1:W:249:MET:HB2	2.32	0.64
4:i:56:ASN:HD22	2:E:876:ARG:HH11	1.45	0.64
3:F:594:GLN:HB2	3:F:625:LEU:HD23	1.79	0.64
2:G:876:ARG:NH1	4:k:60:LEU:H	1.74	0.64
5:I:362:LEU:HD23	5:I:537:LEU:HD22	1.78	0.64
1:O:62:PRO:HD2	1:O:86:TYR:HB3	1.81	0.63
1:W:62:PRO:HD2	1:W:86:TYR:HB3	1.81	0.63
2:C:563:THR:OG1	1:Q:46:ASP:O	2.16	0.63
5:K:631:SER:HA	5:K:645:LEU:HD21	1.80	0.63
1:O:297:LEU:HD21	1:O:377:MET:HB3	1.80	0.63
1:S:297:LEU:HD21	1:S:377:MET:HB3	1.80	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:297:LEU:HD21	1:Y:377:MET:HB3	1.80	0.63
3:N:543:LYS:HD3	3:N:742:GLN:HG3	1.80	0.63
1:P:297:LEU:HD21	1:P:377:MET:HB3	1.80	0.63
1:Q:62:PRO:HD2	1:Q:86:TYR:HB3	1.81	0.63
1:R:297:LEU:HD21	1:R:377:MET:HB3	1.80	0.63
1:1:62:PRO:HD2	1:1:86:TYR:HB3	1.81	0.63
3:D:586:VAL:HG12	3:D:635:TRP:HE1	1.63	0.63
1:V:297:LEU:HD21	1:V:377:MET:HB3	1.80	0.63
1:S:62:PRO:HD2	1:S:86:TYR:HB3	1.81	0.63
1:T:297:LEU:HD21	1:T:377:MET:HB3	1.80	0.63
1:V:62:PRO:HD2	1:V:86:TYR:HB3	1.80	0.63
1:P:62:PRO:HD2	1:P:86:TYR:HB3	1.81	0.62
1:V:50:VAL:HG21	1:V:244:ARG:HA	1.81	0.62
1:Q:297:LEU:HD21	1:Q:377:MET:HB3	1.79	0.62
1:U:50:VAL:HG21	1:U:244:ARG:HA	1.81	0.62
6:J:358:PHE:HE2	6:J:361:TYR:H	1.47	0.62
1:O:50:VAL:HG21	1:O:244:ARG:HA	1.81	0.62
1:Q:50:VAL:HG21	1:Q:244:ARG:HA	1.81	0.62
1:U:62:PRO:HD2	1:U:86:TYR:HB3	1.81	0.62
1:2:297:LEU:HD21	1:2:377:MET:HB3	1.80	0.62
2:E:446:MET:HE3	2:E:484:TYR:HE2	1.65	0.62
1:2:62:PRO:HD2	1:2:86:TYR:HB3	1.81	0.62
1:R:50:VAL:HG21	1:R:244:ARG:HA	1.81	0.62
1:S:50:VAL:HG21	1:S:244:ARG:HA	1.81	0.62
1:Y:50:VAL:HG21	1:Y:244:ARG:HA	1.81	0.62
1:Y:62:PRO:HD2	1:Y:86:TYR:HB3	1.81	0.62
1:U:297:LEU:HD21	1:U:377:MET:HB3	1.80	0.62
7:L:1677:ALA:HA	7:L:1681:LEU:HD12	1.80	0.62
1:Z:297:LEU:HD21	1:Z:377:MET:HB3	1.80	0.62
6:l:123:ASN:O	6:l:126:TYR:CE2	2.53	0.62
5:I:131:LEU:HD11	5:I:165:LEU:HD13	1.81	0.61
4:i:56:ASN:CB	2:E:876:ARG:NH1	2.63	0.61
2:E:540:ARG:HA	2:E:613:LEU:HD23	1.81	0.61
1:1:50:VAL:HG21	1:1:244:ARG:HA	1.81	0.61
3:N:546:LEU:HD21	3:N:744:LEU:H	1.65	0.61
3:N:774:GLN:HG3	3:N:864:LEU:HD21	1.82	0.61
1:Z:62:PRO:HD2	1:Z:86:TYR:HB3	1.81	0.61
1:T:62:PRO:HD2	1:T:86:TYR:HB3	1.81	0.61
1:2:317:TYR:HD2	1:2:347:ASN:HB2	1.66	0.61
1:O:317:TYR:HD2	1:O:347:ASN:HB2	1.66	0.61
1:Y:317:TYR:HD2	1:Y:347:ASN:HB2	1.66	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:720:TYR:HE2	1:T:357:GLN:HB3	1.66	0.61
5:I:345:VAL:HA	5:I:350:LEU:HB2	1.83	0.61
1:P:317:TYR:HD2	1:P:347:ASN:HB2	1.66	0.61
1:R:62:PRO:HD2	1:R:86:TYR:HB3	1.81	0.61
1:R:317:TYR:HD2	1:R:347:ASN:HB2	1.66	0.61
1:X:50:VAL:HG21	1:X:244:ARG:HA	1.81	0.61
1:Q:317:TYR:HD2	1:Q:347:ASN:HB2	1.66	0.61
1:T:317:TYR:HD2	1:T:347:ASN:HB2	1.66	0.61
1:1:317:TYR:HD2	1:1:347:ASN:HB2	1.66	0.61
3:F:555:LEU:HG	3:F:559:MET:HE2	1.83	0.61
1:T:50:VAL:HG21	1:T:244:ARG:HA	1.81	0.61
1:U:317:TYR:HD2	1:U:347:ASN:HB2	1.66	0.61
3:H:589:ALA:HA	3:H:592:LEU:HD23	1.82	0.60
1:S:317:TYR:HD2	1:S:347:ASN:HB2	1.66	0.60
1:V:317:TYR:HD2	1:V:347:ASN:HB2	1.66	0.60
1:Z:50:VAL:HG21	1:Z:244:ARG:HA	1.81	0.60
1:X:62:PRO:HD2	1:X:86:TYR:HB3	1.81	0.60
1:X:317:TYR:HD2	1:X:347:ASN:HB2	1.66	0.60
1:2:50:VAL:HG21	1:2:244:ARG:HA	1.81	0.60
1:P:50:VAL:HG21	1:P:244:ARG:HA	1.81	0.60
1:W:50:VAL:HG21	1:W:244:ARG:HA	1.81	0.60
1:1:258:ALA:HB1	2:M:687:LEU:HD21	1.83	0.60
2:G:876:ARG:HE	4:k:58:GLU:N	1.96	0.60
1:W:317:TYR:HD2	1:W:347:ASN:HB2	1.66	0.60
3:B:460:TRP:HA	3:B:488:LYS:HE2	1.83	0.60
1:Z:317:TYR:HD2	1:Z:347:ASN:HB2	1.66	0.60
2:E:236:GLN:HB2	2:E:245:THR:HG23	1.83	0.60
3:F:268:MET:HG3	3:F:276:LYS:H	1.67	0.60
3:F:365:ARG:HE	2:E:308:SER:HB3	1.68	0.59
3:B:568:LEU:HD22	3:B:671:LYS:HZ1	1.66	0.59
2:G:356:LEU:HG	2:G:440:PRO:HB3	1.84	0.59
4:m:30:GLU:OE1	6:l:130:PRO:HG3	2.01	0.59
2:E:169:ASN:HA	2:E:172:GLN:HE21	1.68	0.59
2:G:876:ARG:HG3	4:k:58:GLU:HB3	1.84	0.59
2:M:581:ASP:O	2:M:643:ARG:NH1	2.35	0.59
1:U:262:PRO:HG2	1:U:263:THR:HG22	1.85	0.59
1:X:262:PRO:HG2	1:X:263:THR:HG22	1.85	0.59
3:B:459:LEU:HG	3:B:463:LYS:HD3	1.85	0.59
1:P:28:GLU:OE2	1:P:244:ARG:NH1	2.36	0.59
1:Y:262:PRO:HG2	1:Y:263:THR:HG22	1.85	0.59
1:Q:262:PRO:HG2	1:Q:263:THR:HG22	1.85	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:28:GLU:OE2	1:U:244:ARG:NH1	2.36	0.59
2:A:554:LEU:HA	2:A:557:LEU:HD13	1.85	0.58
3:H:555:LEU:HD11	3:H:651:VAL:HG11	1.85	0.58
1:R:28:GLU:OE2	1:R:244:ARG:NH1	2.36	0.58
1:W:262:PRO:HG2	1:W:263:THR:HG22	1.85	0.58
1:Z:262:PRO:HG2	1:Z:263:THR:HG22	1.85	0.58
1:2:262:PRO:HG2	1:2:263:THR:HG22	1.85	0.58
3:B:720:TYR:OH	1:P:250:ASN:ND2	2.36	0.58
2:G:446:MET:HE3	2:G:484:TYR:HE2	1.68	0.58
1:T:262:PRO:HG2	1:T:263:THR:HG22	1.85	0.58
4:i:59:ALA:CB	2:E:876:ARG:CZ	2.81	0.58
7:c:70:ILE:HG22	7:c:89:LEU:HD21	1.84	0.58
1:W:28:GLU:OE2	1:W:244:ARG:NH1	2.36	0.58
4:i:55:ILE:HG12	4:i:60:LEU:HD12	1.83	0.58
4:d:24:THR:HA	4:d:27:VAL:HG12	1.85	0.58
1:2:28:GLU:OE2	1:2:244:ARG:NH1	2.36	0.58
2:G:876:ARG:NE	4:k:56:ASN:HB3	2.17	0.58
5:I:355:LYS:NZ	5:I:359:ASP:OD1	2.37	0.58
1:T:28:GLU:OE2	1:T:244:ARG:NH1	2.36	0.58
1:1:28:GLU:OE2	1:1:244:ARG:NH1	2.36	0.58
1:1:56:ASP:HA	1:2:277:THR:OG1	2.04	0.58
6:J:273:GLU:HG3	6:J:286:ILE:HD12	1.86	0.58
1:Q:28:GLU:OE2	1:Q:244:ARG:NH1	2.36	0.58
1:V:232:VAL:HG22	1:V:236:MET:HE2	1.86	0.58
1:O:232:VAL:HG22	1:O:236:MET:HE2	1.86	0.58
5:K:192:LEU:HB3	5:K:304:GLU:HG3	1.86	0.58
1:O:262:PRO:HG2	1:O:263:THR:HG22	1.85	0.58
1:Y:28:GLU:OE2	1:Y:244:ARG:NH1	2.36	0.58
2:M:741:ASN:HD22	2:M:745:LEU:HG	1.68	0.58
1:Q:232:VAL:HG22	1:Q:236:MET:HE2	1.86	0.58
1:S:28:GLU:OE2	1:S:244:ARG:NH1	2.36	0.58
1:U:232:VAL:HG22	1:U:236:MET:HE2	1.86	0.58
1:2:339:ARG:NH2	2:M:557:LEU:HA	2.19	0.58
1:Z:232:VAL:HG22	1:Z:236:MET:HE2	1.86	0.58
1:R:262:PRO:HG2	1:R:263:THR:HG22	1.85	0.57
2:G:876:ARG:HG3	4:k:58:GLU:HB2	1.86	0.57
5:K:340:LEU:HA	5:K:343:LEU:HD12	1.85	0.57
1:P:237:SER:O	1:P:244:ARG:NH2	2.37	0.57
1:S:237:SER:O	1:S:244:ARG:NH2	2.37	0.57
1:T:232:VAL:HG22	1:T:236:MET:HE2	1.86	0.57
1:W:237:SER:O	1:W:244:ARG:NH2	2.37	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:232:VAL:HG22	1:Y:236:MET:HE2	1.86	0.57
1:1:232:VAL:HG22	1:1:236:MET:HE2	1.86	0.57
1:O:28:GLU:OE2	1:O:244:ARG:NH1	2.36	0.57
1:U:237:SER:O	1:U:244:ARG:NH2	2.37	0.57
1:W:232:VAL:HG22	1:W:236:MET:HE2	1.86	0.57
1:X:28:GLU:OE2	1:X:244:ARG:NH1	2.36	0.57
1:Z:28:GLU:OE2	1:Z:244:ARG:NH1	2.36	0.57
1:1:262:PRO:HG2	1:1:263:THR:HG22	1.85	0.57
1:S:262:PRO:HG2	1:S:263:THR:HG22	1.85	0.57
1:X:237:SER:O	1:X:244:ARG:NH2	2.37	0.57
3:H:608:THR:HG23	3:H:610:ALA:H	1.69	0.57
3:N:471:ILE:HD12	3:N:472:PRO:HD2	1.86	0.57
1:R:232:VAL:HG22	1:R:236:MET:HE2	1.86	0.57
1:R:237:SER:O	1:R:244:ARG:NH2	2.37	0.57
1:V:28:GLU:OE2	1:V:244:ARG:NH1	2.36	0.57
1:X:232:VAL:HG22	1:X:236:MET:HE2	1.86	0.57
1:S:232:VAL:HG22	1:S:236:MET:HE2	1.86	0.57
5:I:328:VAL:HG12	5:I:331:ARG:HH22	1.69	0.57
2:M:316:GLN:HG3	2:M:318:LEU:HG	1.87	0.57
4:k:30:GLU:OE1	3:j:112:SER:OG	2.21	0.57
2:E:876:ARG:CD	3:h:42:ASN:HB3	2.34	0.57
1:2:237:SER:O	1:2:244:ARG:NH2	2.37	0.57
2:C:613:LEU:HB2	2:C:646:PHE:HE2	1.68	0.57
6:J:477:ASP:HB2	6:J:638:LEU:HG	1.86	0.57
2:M:610:LEU:HD21	2:M:613:LEU:HB2	1.87	0.57
1:2:232:VAL:HG22	1:2:236:MET:HE2	1.86	0.57
7:L:1766:GLN:NE2	7:L:1770:ASN:OD1	2.38	0.57
1:O:237:SER:O	1:O:244:ARG:NH2	2.37	0.57
4:d:38:GLY:H	7:c:117:LEU:HD13	1.70	0.57
1:V:262:PRO:HG2	1:V:263:THR:HG22	1.85	0.56
3:a:39:ILE:HG23	7:c:75:PHE:HE2	1.70	0.56
3:B:848:ARG:O	3:B:852:HIS:ND1	2.34	0.56
1:P:232:VAL:HG22	1:P:236:MET:HE2	1.86	0.56
1:Q:237:SER:O	1:Q:244:ARG:NH2	2.37	0.56
1:V:237:SER:O	1:V:244:ARG:NH2	2.37	0.56
4:i:59:ALA:HB2	2:E:876:ARG:CD	2.35	0.56
3:B:464:TYR:H	3:B:488:LYS:HZ1	1.51	0.56
6:J:408:GLN:HB3	6:J:460:LEU:HD22	1.87	0.56
7:L:1800:LEU:HD22	1:Z:338:GLN:NE2	2.20	0.56
1:P:262:PRO:HG2	1:P:263:THR:HG22	1.85	0.56
3:D:776:ARG:HH12	3:h:106:ARG:HG2	1.70	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:681:ARG:HH11	3:N:685:MET:HE3	1.70	0.56
1:Y:237:SER:O	1:Y:244:ARG:NH2	2.37	0.56
5:I:399:SER:HA	5:I:402:LYS:HE2	1.86	0.56
3:a:62:LEU:HD11	3:a:67:ARG:HE	1.69	0.56
1:1:264:PRO:HG3	2:M:663:LYS:HB2	1.86	0.56
3:F:597:LEU:HB2	3:F:623:VAL:HG11	1.86	0.56
5:I:530:TYR:OH	1:W:248:TYR:O	2.19	0.56
4:k:30:GLU:CD	3:j:112:SER:HG	2.14	0.55
1:1:237:SER:O	1:1:244:ARG:NH2	2.37	0.55
2:G:704:PRO:HG3	1:U:330:PRO:HB2	1.88	0.55
3:N:318:GLY:HA3	3:N:392:LYS:HD2	1.87	0.55
1:P:350:PRO:HB2	1:P:441:PRO:HA	1.89	0.55
1:Z:237:SER:O	1:Z:244:ARG:NH2	2.37	0.55
3:F:613:ASP:HB3	3:F:617:ILE:HD11	1.87	0.55
2:G:360:HIS:CE1	2:G:442:PHE:HB3	2.41	0.55
2:G:696:TYR:O	2:G:700:GLU:HB3	2.05	0.55
1:T:237:SER:O	1:T:244:ARG:NH2	2.37	0.55
2:C:834:LEU:HD22	2:C:868:ARG:HB2	1.89	0.55
1:T:350:PRO:HB2	1:T:441:PRO:HA	1.89	0.55
2:C:814:LEU:HG	2:C:815:VAL:HG22	1.88	0.55
7:L:287:LEU:HD11	4:b:25:MET:HG2	1.89	0.55
2:M:521:LEU:HA	2:M:645:MET:HE1	1.88	0.55
5:K:330:ASP:HA	5:K:333:ARG:HB2	1.89	0.55
4:b:39:LEU:HD21	4:b:44:LEU:HB3	1.89	0.55
1:1:87:ASN:HB3	1:2:219:HIS:ND1	2.21	0.55
3:H:614:SER:OG	3:H:616:GLU:OE1	2.24	0.55
1:S:350:PRO:HB2	1:S:441:PRO:HA	1.89	0.55
1:2:350:PRO:HB2	1:2:441:PRO:HA	1.89	0.55
3:H:573:PHE:HA	3:H:608:THR:HG21	1.88	0.55
1:R:65:VAL:HA	1:R:90:ASN:HD21	1.72	0.55
1:T:65:VAL:HA	1:T:90:ASN:HD21	1.72	0.55
3:n:51:GLU:HG2	3:n:90:LYS:HB2	1.89	0.55
3:F:636:ASP:OD1	3:F:669:ARG:NH1	2.39	0.55
3:N:768:SER:HA	3:N:771:LEU:HD13	1.89	0.55
1:Y:65:VAL:HA	1:Y:90:ASN:HD21	1.72	0.55
4:k:43:THR:HG22	3:j:19:ARG:HE	1.72	0.55
3:H:455:LYS:HA	3:H:458:ARG:HH21	1.71	0.54
1:Z:350:PRO:HB2	1:Z:441:PRO:HA	1.89	0.54
1:1:65:VAL:HA	1:1:90:ASN:HD21	1.72	0.54
1:1:350:PRO:HB2	1:1:441:PRO:HA	1.89	0.54
3:N:388:CYS:HB3	3:N:396:LEU:HG	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:174:ASN:O	1:Q:208:THR:OG1	2.25	0.54
1:V:65:VAL:HA	1:V:90:ASN:HD21	1.72	0.54
1:2:291:LEU:HD22	2:M:560:ARG:HD2	1.89	0.54
6:l:130:PRO:HD2	6:l:130:PRO:O	2.06	0.54
3:H:829:GLU:OE1	3:H:832:ARG:NH1	2.41	0.54
7:L:1676:ILE:HG23	7:L:1680:ILE:HD12	1.88	0.54
1:W:174:ASN:O	1:W:208:THR:OG1	2.25	0.54
1:Y:350:PRO:HB2	1:Y:441:PRO:HA	1.89	0.54
2:A:526:ASP:HA	2:A:529:VAL:HG12	1.90	0.54
3:F:285:ARG:NH1	2:E:220:ASP:OD1	2.40	0.54
1:P:65:VAL:HA	1:P:90:ASN:HD21	1.72	0.54
1:U:174:ASN:O	1:U:208:THR:OG1	2.25	0.54
1:U:350:PRO:HB2	1:U:441:PRO:HA	1.89	0.54
1:V:350:PRO:HB2	1:V:441:PRO:HA	1.89	0.54
2:G:299:LEU:HD22	2:G:338:LEU:HD11	1.88	0.54
5:K:653:LYS:HD2	1:Y:352:GLY:HA2	1.88	0.54
1:R:174:ASN:O	1:R:208:THR:OG1	2.25	0.54
1:U:65:VAL:HA	1:U:90:ASN:HD21	1.72	0.54
1:W:65:VAL:HA	1:W:90:ASN:HD21	1.72	0.54
1:W:350:PRO:HB2	1:W:441:PRO:HA	1.89	0.54
6:l:80:LYS:HD3	6:l:126:TYR:HE1	1.61	0.54
2:G:876:ARG:NH2	4:k:57:PRO:HA	2.20	0.54
6:J:904:ARG:HH22	1:X:331:THR:HG23	1.73	0.54
2:M:551:LEU:HB3	2:M:575:ILE:HD12	1.89	0.54
1:Z:65:VAL:HA	1:Z:90:ASN:HD21	1.72	0.54
1:P:174:ASN:O	1:P:208:THR:OG1	2.25	0.54
1:Q:65:VAL:HA	1:Q:90:ASN:HD21	1.72	0.54
6:J:427:THR:OG1	6:J:428:ARG:N	2.38	0.53
1:O:350:PRO:HB2	1:O:441:PRO:HA	1.89	0.53
1:X:65:VAL:HA	1:X:90:ASN:HD21	1.72	0.53
1:1:187:ASN:O	1:1:191:THR:OG1	2.26	0.53
1:2:343:ARG:HD3	2:M:557:LEU:HD21	1.88	0.53
6:J:331:ILE:HG23	6:J:365:MET:HE2	1.90	0.53
4:k:71:THR:HG23	3:j:21:LEU:HG	1.89	0.53
1:1:367:LEU:HD12	1:1:368:PRO:HD2	1.91	0.53
1:S:65:VAL:HA	1:S:90:ASN:HD21	1.72	0.53
1:T:174:ASN:O	1:T:208:THR:OG1	2.25	0.53
1:W:187:ASN:O	1:W:191:THR:OG1	2.26	0.53
1:Y:174:ASN:O	1:Y:208:THR:OG1	2.25	0.53
4:b:50:LEU:O	4:b:53:GLN:NE2	2.41	0.53
3:a:113:SER:OG	3:a:114:TYR:N	2.42	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:367:LEU:HD12	1:2:368:PRO:HD2	1.91	0.53
7:L:1682:HIS:HB3	1:Z:330:PRO:HB3	1.89	0.53
2:M:218:VAL:HG23	2:M:324:LEU:HD13	1.91	0.53
1:X:350:PRO:HB2	1:X:441:PRO:HA	1.89	0.53
1:2:174:ASN:O	1:2:208:THR:OG1	2.25	0.53
3:H:712:VAL:O	3:H:716:HIS:ND1	2.29	0.53
1:Y:367:LEU:HD12	1:Y:368:PRO:HD2	1.91	0.53
2:E:415:ARG:HE	2:E:419:ILE:HA	1.73	0.53
3:D:885:HIS:CE1	3:D:890:GLU:HG3	2.44	0.53
3:F:626:LEU:HB3	3:j:64:ARG:HE	1.73	0.53
1:X:367:LEU:HD12	1:X:368:PRO:HD2	1.91	0.53
3:n:33:GLN:HG2	3:n:37:ARG:HH11	1.72	0.53
1:2:129:SER:OG	1:2:131:SER:O	2.27	0.53
1:2:360:LEU:HB2	3:N:724:PHE:CE1	2.44	0.53
3:D:266:ILE:HG12	3:D:277:VAL:HG22	1.91	0.53
3:D:337:ARG:O	3:D:340:SER:OG	2.27	0.53
3:D:585:LEU:HD22	3:D:635:TRP:HA	1.91	0.53
3:F:563:ARG:NH2	1:T:248:TYR:OH	2.41	0.53
2:G:637:ARG:NH2	2:G:640:MET:SD	2.82	0.53
2:M:232:TYR:HB3	2:M:249:ASP:HB2	1.90	0.53
3:N:433:TRP:HE1	3:N:484:LEU:HA	1.74	0.53
1:Q:367:LEU:HD12	1:Q:368:PRO:HD2	1.91	0.53
1:R:350:PRO:HB2	1:R:441:PRO:HA	1.89	0.53
1:V:367:LEU:HD12	1:V:368:PRO:HD2	1.91	0.53
1:1:129:SER:OG	1:1:131:SER:O	2.27	0.53
1:2:65:VAL:HA	1:2:90:ASN:HD21	1.72	0.53
7:L:1566:THR:HG23	7:L:1569:ALA:H	1.73	0.53
1:Y:129:SER:OG	1:Y:131:SER:O	2.27	0.53
7:c:130:ARG:HH22	2:E:298:THR:HG22	1.73	0.53
2:E:876:ARG:NH1	3:h:42:ASN:CA	2.71	0.53
1:O:65:VAL:HA	1:O:90:ASN:HD21	1.72	0.53
1:O:367:LEU:HD12	1:O:368:PRO:HD2	1.91	0.53
1:W:129:SER:OG	1:W:131:SER:O	2.27	0.53
3:a:65:GLN:NE2	3:a:103:ASP:OD1	2.42	0.53
2:C:674:GLN:HB3	1:Q:265:ARG:HH22	1.74	0.53
1:V:187:ASN:O	1:V:191:THR:OG1	2.26	0.53
3:h:73:LEU:CD2	3:h:111:VAL:CG2	2.79	0.53
6:J:224:TYR:OH	6:J:269:GLN:HG2	2.09	0.52
2:M:509:LEU:HD13	2:M:626:LEU:HD22	1.91	0.52
3:N:776:ARG:HH11	3:n:66:ARG:HH11	1.57	0.52
1:P:367:LEU:HD12	1:P:368:PRO:HD2	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:350:PRO:HB2	1:Q:441:PRO:HA	1.89	0.52
1:W:294:MET:HE3	1:W:340:ILE:HG13	1.91	0.52
1:Z:129:SER:OG	1:Z:131:SER:O	2.27	0.52
6:l:127:VAL:O	6:l:127:VAL:CG1	2.54	0.52
2:A:437:GLN:HG3	2:A:438:GLN:HE21	1.74	0.52
3:B:464:TYR:H	3:B:488:LYS:NZ	2.07	0.52
7:L:1513:ARG:NH1	1:Z:248:TYR:OH	2.43	0.52
1:T:187:ASN:O	1:T:191:THR:OG1	2.26	0.52
3:H:627:GLU:O	3:H:630:PRO:HD3	2.09	0.52
1:T:367:LEU:HD12	1:T:368:PRO:HD2	1.91	0.52
2:M:835:ASP:OD2	2:M:835:ASP:N	2.40	0.52
1:P:294:MET:HE3	1:P:340:ILE:HG13	1.91	0.52
1:R:294:MET:HE3	1:R:340:ILE:HG13	1.92	0.52
1:R:367:LEU:HD12	1:R:368:PRO:HD2	1.91	0.52
1:1:294:MET:HE3	1:1:340:ILE:HG13	1.91	0.52
1:2:294:MET:HE3	1:2:340:ILE:HG13	1.92	0.52
2:G:509:LEU:HD13	2:G:626:LEU:HD22	1.91	0.52
5:I:499:GLN:OE1	5:I:504:HIS:NE2	2.40	0.52
5:I:553:ASP:O	5:I:556:SER:OG	2.23	0.52
1:1:57:ASP:OD1	1:2:217:ARG:NE	2.43	0.52
3:j:110:LYS:O	3:j:111:VAL:CG2	2.57	0.52
3:B:803:ARG:HD3	3:B:833:ILE:HD11	1.91	0.52
1:U:367:LEU:HD12	1:U:368:PRO:HD2	1.91	0.52
6:l:80:LYS:HD3	6:l:126:TYR:CE1	2.26	0.52
2:A:408:MET:HA	2:A:438:GLN:HB2	1.92	0.52
2:C:238:LEU:HB3	2:C:244:ARG:NH1	2.25	0.52
3:H:546:LEU:O	3:H:550:ASN:ND2	2.43	0.52
2:M:837:LEU:HD22	2:M:856:ILE:HG23	1.92	0.52
1:S:129:SER:OG	1:S:131:SER:O	2.27	0.52
1:S:337:LEU:HD21	2:E:858:ARG:HG3	1.92	0.52
2:C:254:LEU:HD13	2:C:257:ARG:HD2	1.91	0.52
1:S:367:LEU:HD12	1:S:368:PRO:HD2	1.91	0.52
1:T:129:SER:OG	1:T:131:SER:O	2.27	0.52
1:V:294:MET:HE3	1:V:340:ILE:HG13	1.92	0.52
2:C:285:TYR:O	2:C:289:ASN:ND2	2.37	0.51
2:G:580:HIS:HB2	2:G:584:THR:HG23	1.91	0.51
1:Q:129:SER:OG	1:Q:131:SER:O	2.27	0.51
1:Z:174:ASN:O	1:Z:208:THR:OG1	2.25	0.51
1:Z:367:LEU:HD12	1:Z:368:PRO:HD2	1.91	0.51
3:h:8:SER:OG	3:h:10:ASN:OD1	2.26	0.51
2:A:353:GLY:H	2:A:438:GLN:HA	1.74	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:796:LEU:HG	6:J:797:ASP:H	1.75	0.51
5:K:279:VAL:HG23	5:K:333:ARG:HD2	1.92	0.51
1:U:294:MET:HE3	1:U:340:ILE:HG13	1.92	0.51
1:X:294:MET:HE3	1:X:340:ILE:HG13	1.92	0.51
1:1:56:ASP:HB3	1:2:276:LEU:HB2	1.91	0.51
3:F:563:ARG:HA	3:F:567:LEU:HD12	1.90	0.51
2:G:876:ARG:CG	4:k:58:GLU:HB2	2.39	0.51
1:O:294:MET:HE3	1:O:340:ILE:HG13	1.92	0.51
2:M:457:LEU:HB3	2:M:467:VAL:HG11	1.92	0.51
1:R:187:ASN:O	1:R:191:THR:OG1	2.26	0.51
3:B:404:THR:HG21	3:B:419:LEU:HD22	1.90	0.51
1:Q:294:MET:HE3	1:Q:340:ILE:HG13	1.91	0.51
1:W:367:LEU:HD12	1:W:368:PRO:HD2	1.91	0.51
3:N:608:THR:HG23	3:N:610:ALA:H	1.75	0.51
3:j:108:PRO:HD2	3:j:108:PRO:O	2.10	0.51
3:a:64:ARG:O	3:a:66:ARG:NH2	2.43	0.51
2:E:422:ASP:OD2	2:E:426:LYS:NZ	2.44	0.51
1:T:294:MET:HE3	1:T:340:ILE:HG13	1.91	0.51
1:P:187:ASN:O	1:P:191:THR:OG1	2.27	0.51
1:Q:187:ASN:O	1:Q:191:THR:OG1	2.26	0.51
1:S:294:MET:HE3	1:S:340:ILE:HG13	1.91	0.51
4:m:30:GLU:CG	6:l:130:PRO:HG2	2.40	0.51
2:G:837:LEU:HD22	2:G:856:ILE:HG12	1.92	0.51
3:H:315:ARG:NH1	3:H:322:GLN:OE1	2.44	0.51
1:Y:273:TYR:HA	1:Y:376:LEU:HA	1.93	0.51
1:1:174:ASN:O	1:1:208:THR:OG1	2.25	0.51
1:2:295:ARG:NH1	2:M:561:MET:HB2	2.26	0.51
5:K:516:ARG:NH1	5:K:519:ASN:OD1	2.44	0.51
3:N:694:MET:HE1	3:N:800:LEU:HD22	1.92	0.51
1:U:187:ASN:O	1:U:191:THR:OG1	2.27	0.51
1:Y:294:MET:HE3	1:Y:340:ILE:HG13	1.91	0.51
1:Z:294:MET:HE3	1:Z:340:ILE:HG13	1.91	0.51
3:B:673:MET:HE3	3:B:779:PHE:HB3	1.94	0.50
3:a:65:GLN:HE21	3:a:104:PRO:HD2	1.76	0.50
2:E:205:ILE:HG13	2:E:213:GLN:HG2	1.93	0.50
2:E:727:THR:HA	2:E:730:LEU:HD12	1.93	0.50
6:J:820:ILE:HD13	6:J:934:LEU:HD13	1.93	0.50
1:O:187:ASN:O	1:O:191:THR:OG1	2.27	0.50
6:l:71:LYS:NZ	8:l:1102:HOH:O	2.43	0.50
1:1:273:TYR:HA	1:1:376:LEU:HA	1.94	0.50
3:B:319:LEU:N	3:B:445:GLU:OE2	2.44	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:427:TYR:HB2	2:G:628:LEU:HD21	1.94	0.50
3:H:400:VAL:HG21	3:H:422:VAL:HG21	1.93	0.50
3:N:765:ASP:HB2	3:N:768:SER:H	1.77	0.50
3:D:738:VAL:HG12	3:D:747:ILE:HG23	1.94	0.50
1:P:273:TYR:HA	1:P:376:LEU:HA	1.93	0.50
1:R:129:SER:OG	1:R:131:SER:O	2.27	0.50
1:Y:187:ASN:O	1:Y:191:THR:OG1	2.26	0.50
3:a:65:GLN:HB3	3:a:67:ARG:HG3	1.94	0.50
6:l:124:SER:CA	6:l:126:TYR:CE2	2.90	0.50
1:2:273:TYR:HA	1:2:376:LEU:HA	1.93	0.50
1:V:273:TYR:HA	1:V:376:LEU:HA	1.93	0.50
1:X:174:ASN:O	1:X:208:THR:OG1	2.25	0.50
4:g:45:SER:HA	4:g:48:VAL:HG22	1.93	0.50
4:g:55:ILE:HD13	4:g:60:LEU:HD12	1.92	0.50
6:J:758:LEU:HD13	6:J:799:LEU:HD13	1.93	0.50
7:c:113:LEU:HG	7:c:116:GLN:HE21	1.76	0.50
2:E:296:MET:HG3	2:E:338:LEU:HD22	1.93	0.50
2:A:161:LEU:HD12	2:A:162:ARG:HG2	1.94	0.50
2:G:876:ARG:NH2	4:k:60:LEU:N	2.40	0.50
5:I:7:LEU:HD11	6:J:395:LEU:HD21	1.93	0.50
5:I:548:ILE:HD12	5:I:557:ILE:HG23	1.94	0.50
3:N:644:VAL:O	3:N:654:ARG:NH1	2.45	0.50
1:O:129:SER:OG	1:O:131:SER:O	2.27	0.50
1:O:273:TYR:HA	1:O:376:LEU:HA	1.93	0.50
1:S:187:ASN:O	1:S:191:THR:OG1	2.27	0.50
3:n:87:LEU:HD23	3:n:90:LYS:HD3	1.94	0.50
3:F:726:VAL:HG13	3:F:761:ARG:HB2	1.93	0.50
2:G:162:ARG:O	2:G:166:ASN:ND2	2.44	0.50
2:G:712:ASN:HB3	2:G:725:HIS:CG	2.47	0.50
1:O:174:ASN:O	1:O:208:THR:OG1	2.25	0.50
1:T:4:GLU:HG2	1:T:47:ARG:HH22	1.77	0.50
1:2:4:GLU:HG2	1:2:47:ARG:HH22	1.77	0.50
3:B:598:THR:HG22	3:B:623:VAL:HB	1.94	0.50
2:C:244:ARG:NH2	2:C:245:THR:O	2.45	0.50
5:I:8:ALA:HA	5:I:13:PRO:HA	1.94	0.50
1:P:129:SER:OG	1:P:131:SER:O	2.27	0.50
1:1:4:GLU:HG2	1:1:47:ARG:HH22	1.77	0.49
5:K:501:GLN:NE2	1:Y:158:ASN:O	2.44	0.49
2:M:210:LEU:HA	2:M:213:GLN:HE21	1.77	0.49
3:N:539:PHE:O	3:N:543:LYS:HG2	2.12	0.49
1:2:334:HIS:HE1	3:N:875:PHE:CG	2.30	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:367:ALA:HB2	6:J:467:GLU:HB2	1.94	0.49
2:M:708:ILE:HG22	2:M:712:ASN:HD21	1.76	0.49
1:W:238:ALA:HB1	1:W:376:LEU:HD22	1.94	0.49
1:Z:4:GLU:HG2	1:Z:47:ARG:HH22	1.77	0.49
6:l:119:ASP:C	6:l:121:PRO:CD	2.76	0.49
1:1:238:ALA:HB1	1:1:376:LEU:HD22	1.94	0.49
2:M:460:VAL:HG22	2:M:465:HIS:HB3	1.93	0.49
1:P:238:ALA:HB1	1:P:376:LEU:HD22	1.94	0.49
1:Q:4:GLU:HG2	1:Q:47:ARG:HH22	1.77	0.49
1:Q:229:ASN:O	1:Q:233:SER:OG	2.29	0.49
1:R:4:GLU:HG2	1:R:47:ARG:HH22	1.77	0.49
1:S:4:GLU:HG2	1:S:47:ARG:HH22	1.77	0.49
1:V:4:GLU:HG2	1:V:47:ARG:HH22	1.77	0.49
1:V:238:ALA:HB1	1:V:376:LEU:HD22	1.94	0.49
1:W:4:GLU:HG2	1:W:47:ARG:HH22	1.77	0.49
1:Z:273:TYR:HA	1:Z:376:LEU:HA	1.93	0.49
3:F:559:MET:HG2	3:F:652:PHE:HZ	1.77	0.49
3:F:626:LEU:HB3	3:j:64:ARG:NE	2.28	0.49
1:Q:238:ALA:HB1	1:Q:376:LEU:HD22	1.94	0.49
1:S:238:ALA:HB1	1:S:376:LEU:HD22	1.94	0.49
1:X:129:SER:OG	1:X:131:SER:O	2.27	0.49
1:Y:4:GLU:HG2	1:Y:47:ARG:HH22	1.77	0.49
6:l:124:SER:HA	6:l:126:TYR:CD2	2.47	0.49
1:2:238:ALA:HB1	1:2:376:LEU:HD22	1.94	0.49
2:A:429:ASP:N	2:A:429:ASP:OD1	2.45	0.49
6:J:265:VAL:HG11	6:J:300:ILE:HD12	1.95	0.49
1:P:4:GLU:HG2	1:P:47:ARG:HH22	1.77	0.49
1:Q:273:TYR:HA	1:Q:376:LEU:HA	1.93	0.49
1:R:238:ALA:HB1	1:R:376:LEU:HD22	1.94	0.49
1:S:273:TYR:HA	1:S:376:LEU:HA	1.93	0.49
3:H:675:TYR:HA	3:H:678:THR:HG22	1.94	0.49
1:U:238:ALA:HB1	1:U:376:LEU:HD22	1.94	0.49
1:X:187:ASN:O	1:X:191:THR:OG1	2.27	0.49
1:X:303:VAL:HG12	1:X:305:VAL:H	1.78	0.49
2:A:613:LEU:HD11	2:A:650:HIS:HB2	1.94	0.49
2:A:744:LEU:HD22	2:A:746:LYS:HD3	1.95	0.49
3:F:503:THR:HG23	3:F:504:THR:HG23	1.93	0.49
3:H:336:TYR:HA	3:H:339:LEU:HG	1.94	0.49
5:I:151:CYS:H	5:I:202:GLU:HG2	1.78	0.49
2:M:640:MET:SD	2:M:643:ARG:NH1	2.85	0.49
1:O:303:VAL:HG12	1:O:305:VAL:H	1.78	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:303:VAL:HG12	1:P:305:VAL:H	1.78	0.49
1:W:303:VAL:HG12	1:W:305:VAL:H	1.78	0.49
4:m:24:THR:HA	4:m:27:VAL:HG12	1.95	0.49
4:b:47:CYS:HA	4:b:50:LEU:HD12	1.94	0.49
5:I:345:VAL:HG13	5:I:346:GLU:HG3	1.95	0.49
1:T:273:TYR:HA	1:T:376:LEU:HA	1.93	0.49
1:V:174:ASN:O	1:V:208:THR:OG1	2.25	0.49
1:R:273:TYR:HA	1:R:376:LEU:HA	1.93	0.49
1:R:303:VAL:HG12	1:R:305:VAL:H	1.78	0.49
1:U:273:TYR:HA	1:U:376:LEU:HA	1.93	0.49
1:Z:303:VAL:HG12	1:Z:305:VAL:H	1.78	0.49
2:A:268:ALA:O	2:A:271:SER:OG	2.31	0.49
2:C:447:ALA:HA	2:C:450:ILE:HD12	1.94	0.49
3:D:712:VAL:O	3:D:716:HIS:HB2	2.13	0.49
2:M:313:LEU:HA	2:M:316:GLN:HE21	1.77	0.49
1:Q:184:GLN:O	1:Q:188:SER:OG	2.31	0.49
1:S:303:VAL:HG12	1:S:305:VAL:H	1.78	0.49
1:T:238:ALA:HB1	1:T:376:LEU:HD22	1.94	0.49
1:U:129:SER:OG	1:U:131:SER:O	2.27	0.49
1:O:238:ALA:HB1	1:O:376:LEU:HD22	1.94	0.48
1:T:184:GLN:O	1:T:188:SER:OG	2.31	0.48
1:T:303:VAL:HG12	1:T:305:VAL:H	1.78	0.48
1:U:4:GLU:HG2	1:U:47:ARG:HH22	1.77	0.48
1:W:273:TYR:HA	1:W:376:LEU:HA	1.93	0.48
6:l:24:ARG:NH1	6:l:32:GLU:OE2	2.45	0.48
3:F:718:MET:HB3	3:F:880:LEU:HD21	1.95	0.48
7:L:1637:CYS:SG	7:L:1641:LYS:NZ	2.86	0.48
1:Z:238:ALA:HB1	1:Z:376:LEU:HD22	1.94	0.48
3:j:69:ALA:HB3	3:j:110:LYS:NZ	2.28	0.48
3:B:273:ASN:HB3	3:B:299:TRP:CE2	2.48	0.48
5:I:358:LYS:HA	5:I:362:LEU:HD13	1.95	0.48
1:X:4:GLU:HG2	1:X:47:ARG:HH22	1.77	0.48
1:Y:238:ALA:HB1	1:Y:376:LEU:HD22	1.94	0.48
1:Y:303:VAL:HG12	1:Y:305:VAL:H	1.78	0.48
2:C:181:VAL:HG13	2:C:187:LEU:HD23	1.95	0.48
3:F:665:ASN:OD1	3:j:106:ARG:NH2	2.45	0.48
5:K:518:ARG:HH11	5:K:615:LEU:HB3	1.77	0.48
1:Q:303:VAL:HG12	1:Q:305:VAL:H	1.78	0.48
1:X:184:GLN:O	1:X:188:SER:OG	2.31	0.48
1:X:238:ALA:HB1	1:X:376:LEU:HD22	1.94	0.48
3:B:633:THR:OG1	3:B:634:GLY:N	2.45	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:701:LEU:HG	3:B:705:HIS:CE1	2.48	0.48
4:i:25:MET:HG3	4:i:41:MET:HE1	1.94	0.48
2:E:578:MET:H	2:E:615:ALA:HB1	1.78	0.48
3:H:677:LEU:HD13	3:H:712:VAL:HG22	1.94	0.48
1:U:303:VAL:HG12	1:U:305:VAL:H	1.78	0.48
2:C:395:ILE:HD11	2:C:450:ILE:HG23	1.95	0.48
2:G:226:VAL:HG11	2:G:307:VAL:HG21	1.94	0.48
2:M:554:LEU:HA	2:M:557:LEU:HD23	1.95	0.48
2:M:581:ASP:HB2	2:M:615:ALA:HB2	1.95	0.48
1:R:262:PRO:HG3	1:R:318:ILE:HG21	1.96	0.48
1:S:174:ASN:O	1:S:208:THR:OG1	2.25	0.48
1:T:262:PRO:HG3	1:T:318:ILE:HG21	1.96	0.48
1:X:273:TYR:HA	1:X:376:LEU:HA	1.93	0.48
3:j:60:LYS:HB3	3:j:64:ARG:HH12	1.78	0.48
1:2:303:VAL:HG12	1:2:305:VAL:H	1.78	0.48
3:D:774:GLN:HG3	3:D:864:LEU:HD12	1.95	0.48
7:L:294:ARG:NH1	7:L:306:HIS:H	2.10	0.48
3:N:433:TRP:HB2	3:N:439:LEU:HD23	1.96	0.48
1:O:4:GLU:HG2	1:O:47:ARG:HH22	1.77	0.48
1:Q:262:PRO:HG3	1:Q:318:ILE:HG21	1.96	0.48
1:1:262:PRO:HG3	1:1:318:ILE:HG21	1.96	0.48
1:1:303:VAL:HG12	1:1:305:VAL:H	1.78	0.48
1:V:129:SER:OG	1:V:131:SER:O	2.27	0.48
6:l:115:LEU:HA	6:l:119:ASP:CG	2.37	0.48
1:1:56:ASP:CG	1:2:276:LEU:HB2	2.39	0.48
3:N:563:ARG:HD2	3:N:731:TRP:CD2	2.48	0.48
1:1:84:LYS:HA	1:2:219:HIS:CD2	2.49	0.47
1:1:248:TYR:HB2	2:M:698:MET:HE3	1.95	0.47
1:P:262:PRO:HG3	1:P:318:ILE:HG21	1.96	0.47
1:R:217:ARG:NH1	1:R:276:LEU:O	2.47	0.47
1:Y:262:PRO:HG3	1:Y:318:ILE:HG21	1.96	0.47
1:Z:262:PRO:HG3	1:Z:318:ILE:HG21	1.96	0.47
3:h:107:GLN:HB3	3:h:108:PRO:HD3	1.95	0.47
6:l:80:LYS:CE	6:l:126:TYR:CE1	2.75	0.47
5:K:132:LEU:O	5:K:135:SER:OG	2.30	0.47
5:K:579:VAL:HB	5:K:629:ILE:HG21	1.96	0.47
1:O:217:ARG:NH1	1:O:276:LEU:O	2.47	0.47
1:Y:217:ARG:NH1	1:Y:276:LEU:O	2.47	0.47
2:C:819:GLU:HA	2:C:822:ILE:HD12	1.96	0.47
2:G:395:ILE:HD11	2:G:450:ILE:HG23	1.97	0.47
2:M:756:VAL:HA	2:M:759:THR:HG22	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:398:SER:HB3	3:N:472:PRO:HA	1.96	0.47
1:O:262:PRO:HG3	1:O:318:ILE:HG21	1.96	0.47
3:h:73:LEU:HD21	3:h:111:VAL:HG22	1.94	0.47
1:1:57:ASP:OD2	1:2:218:LEU:HG	2.14	0.47
5:I:498:LEU:HD21	5:I:517:LEU:HD13	1.95	0.47
1:S:262:PRO:HG3	1:S:318:ILE:HG21	1.96	0.47
2:G:876:ARG:HG2	4:k:56:ASN:HD21	1.70	0.47
2:G:876:ARG:CZ	4:k:56:ASN:HB3	2.45	0.47
3:N:546:LEU:HD21	3:N:744:LEU:N	2.28	0.47
1:P:217:ARG:NH1	1:P:276:LEU:O	2.47	0.47
1:V:184:GLN:O	1:V:188:SER:OG	2.31	0.47
1:V:303:VAL:HG12	1:V:305:VAL:H	1.78	0.47
1:W:217:ARG:NH1	1:W:276:LEU:O	2.47	0.47
1:2:187:ASN:O	1:2:191:THR:OG1	2.27	0.47
3:H:308:THR:O	3:H:312:SER:OG	2.27	0.47
5:K:6:LEU:O	5:K:10:SER:OG	2.26	0.47
1:2:262:PRO:HG3	1:2:318:ILE:HG21	1.96	0.47
1:2:341:ARG:NH2	3:N:884:GLU:OE2	2.46	0.47
3:H:285:ARG:HE	3:H:288:ARG:HH22	1.61	0.47
7:L:1618:GLY:O	7:L:1621:SER:OG	2.32	0.47
3:N:334:GLU:OE1	3:N:377:ARG:NH1	2.47	0.47
1:Q:217:ARG:NH1	1:Q:276:LEU:O	2.47	0.47
1:S:217:ARG:NH1	1:S:276:LEU:O	2.47	0.47
1:W:252:ASP:OD1	1:W:252:ASP:N	2.48	0.47
1:X:217:ARG:NH1	1:X:276:LEU:O	2.47	0.47
1:X:252:ASP:N	1:X:252:ASP:OD1	2.48	0.47
1:2:217:ARG:NH1	1:2:276:LEU:O	2.47	0.47
2:C:758:PHE:HD1	2:C:762:MET:HE3	1.79	0.47
3:F:677:LEU:HA	3:F:680:ILE:HD12	1.97	0.47
3:F:869:SER:H	3:F:873:LEU:HD12	1.79	0.47
5:I:42:LEU:HA	5:I:42:LEU:HD23	1.80	0.47
1:S:252:ASP:OD1	1:S:252:ASP:N	2.48	0.47
1:U:217:ARG:NH1	1:U:276:LEU:O	2.47	0.47
1:V:229:ASN:O	1:V:233:SER:OG	2.29	0.47
1:Z:187:ASN:O	1:Z:191:THR:OG1	2.27	0.47
3:a:58:ILE:O	3:a:61:GLU:HG3	2.15	0.47
1:1:217:ARG:NH1	1:1:276:LEU:O	2.47	0.47
1:2:252:ASP:OD1	1:2:252:ASP:N	2.48	0.47
1:Q:252:ASP:OD1	1:Q:252:ASP:N	2.48	0.47
1:U:262:PRO:HG3	1:U:318:ILE:HG21	1.96	0.47
1:V:217:ARG:NH1	1:V:276:LEU:O	2.47	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:184:GLN:O	1:Z:188:SER:OG	2.31	0.47
4:m:34:ILE:HG22	6:l:128:GLU:HG2	1.95	0.47
3:a:70:ASP:HA	3:a:73:LEU:HG	1.97	0.47
6:J:904:ARG:HD2	6:J:904:ARG:HA	1.60	0.47
1:R:301:LYS:H	1:R:301:LYS:HG3	1.65	0.47
1:Z:217:ARG:NH1	1:Z:276:LEU:O	2.47	0.47
3:f:14:GLN:NE2	3:f:25:GLU:O	2.48	0.47
2:A:402:ASP:OD1	2:A:402:ASP:N	2.48	0.46
2:G:767:GLN:NE2	2:G:768:SER:OG	2.48	0.46
3:N:805:GLN:HA	3:N:808:GLU:HG2	1.96	0.46
1:X:262:PRO:HG3	1:X:318:ILE:HG21	1.96	0.46
2:E:876:ARG:HD2	3:h:42:ASN:HB3	1.97	0.46
2:A:738:MET:HG3	2:A:745:LEU:HD12	1.96	0.46
3:F:476:THR:HG22	3:F:479:GLN:HG3	1.98	0.46
5:I:333:ARG:HA	5:I:336:VAL:HG12	1.97	0.46
3:N:860:GLN:HA	3:N:863:VAL:HG22	1.98	0.46
1:O:252:ASP:OD1	1:O:252:ASP:N	2.48	0.46
1:P:316:CYS:HA	1:P:347:ASN:HB3	1.98	0.46
1:V:23:LYS:HE3	1:V:23:LYS:HB3	1.83	0.46
1:W:160:ARG:HA	1:W:160:ARG:HD2	1.74	0.46
4:k:29:LEU:HD13	4:k:41:MET:HG3	1.97	0.46
4:m:30:GLU:CD	6:l:130:PRO:HD3	2.17	0.46
6:l:124:SER:C	6:l:126:TYR:CE2	2.92	0.46
1:1:252:ASP:N	1:1:252:ASP:OD1	2.48	0.46
2:A:478:THR:OG1	2:A:481:GLU:O	2.33	0.46
3:D:886:TYR:HE2	1:R:353:PRO:HG3	1.81	0.46
3:a:78:HIS:HD2	3:a:81:LEU:HD12	1.78	0.46
1:1:184:GLN:O	1:1:188:SER:OG	2.31	0.46
3:B:886:TYR:CE2	1:P:353:PRO:HD3	2.50	0.46
5:K:410:LEU:HD13	5:K:413:LEU:HD22	1.96	0.46
3:N:477:MET:SD	3:N:477:MET:N	2.89	0.46
1:R:316:CYS:HA	1:R:347:ASN:HB3	1.98	0.46
1:S:160:ARG:HD2	1:S:160:ARG:HA	1.74	0.46
1:T:217:ARG:NH1	1:T:276:LEU:O	2.47	0.46
1:2:248:TYR:OH	3:N:728:GLU:OE1	2.29	0.46
3:B:874:ARG:O	3:B:877:SER:OG	2.32	0.46
3:D:628:VAL:H	3:h:60:LYS:HE2	1.81	0.46
5:I:361:TYR:HB2	5:I:362:LEU:HD12	1.97	0.46
6:J:239:HIS:HB2	7:L:300:VAL:HG11	1.97	0.46
1:S:229:ASN:O	1:S:233:SER:OG	2.29	0.46
1:V:262:PRO:HG3	1:V:318:ILE:HG21	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:262:PRO:HG3	1:W:318:ILE:HG21	1.96	0.46
1:Y:316:CYS:HA	1:Y:347:ASN:HB3	1.98	0.46
1:Z:23:LYS:HE3	1:Z:23:LYS:HB3	1.83	0.46
1:2:316:CYS:HA	1:2:347:ASN:HB3	1.98	0.46
2:A:655:LEU:HD12	2:A:683:ARG:HG3	1.97	0.46
3:B:653:THR:OG1	3:B:656:CYS:SG	2.64	0.46
5:I:499:GLN:HA	1:W:264:PRO:HG3	1.98	0.46
6:J:240:SER:OG	7:L:297:TRP:O	2.28	0.46
1:T:252:ASP:OD1	1:T:252:ASP:N	2.48	0.46
1:Z:252:ASP:N	1:Z:252:ASP:OD1	2.48	0.46
1:1:56:ASP:OD1	1:2:276:LEU:HB2	2.16	0.46
1:1:316:CYS:HA	1:1:347:ASN:HB3	1.98	0.46
3:D:885:HIS:CE1	3:D:890:GLU:HA	2.51	0.46
2:G:241:ARG:HG2	2:G:242:GLN:H	1.80	0.46
1:V:252:ASP:OD1	1:V:252:ASP:N	2.48	0.46
1:W:316:CYS:HA	1:W:347:ASN:HB3	1.98	0.46
3:j:24:SER:OG	3:j:25:GLU:N	2.48	0.46
2:C:738:MET:HA	2:C:741:ASN:ND2	2.30	0.46
5:K:654:TYR:CE2	1:Y:353:PRO:HG3	2.51	0.46
1:Z:110:GLN:HA	1:Z:113:LYS:HE3	1.98	0.46
1:Z:316:CYS:HA	1:Z:347:ASN:HB3	1.98	0.46
3:n:30:GLN:NE2	3:n:37:ARG:HH12	2.14	0.46
2:C:458:ASN:OD1	2:C:461:ARG:NH2	2.48	0.46
5:K:520:HIS:HD2	1:Y:258:ALA:O	1.99	0.46
7:L:1590:VAL:HA	7:L:1628:LEU:HD13	1.98	0.46
1:P:252:ASP:OD1	1:P:252:ASP:N	2.48	0.46
1:R:110:GLN:HA	1:R:113:LYS:HE3	1.98	0.46
1:R:252:ASP:OD1	1:R:252:ASP:N	2.48	0.46
1:Z:229:ASN:O	1:Z:233:SER:OG	2.29	0.46
4:m:64:ILE:HB	6:l:117:LEU:HD21	1.97	0.46
1:2:248:TYR:CD1	3:N:723:THR:HG23	2.51	0.46
2:G:709:LEU:HD13	2:G:729:PHE:HB2	1.97	0.46
3:N:763:LEU:HD11	3:N:873:LEU:HD11	1.98	0.46
1:Q:318:ILE:HB	1:Q:380:ASN:HB3	1.98	0.46
1:R:318:ILE:HB	1:R:380:ASN:HB3	1.98	0.46
1:W:110:GLN:HA	1:W:113:LYS:HE3	1.98	0.46
1:X:316:CYS:HA	1:X:347:ASN:HB3	1.98	0.46
3:D:433:TRP:HZ2	3:D:484:LEU:HD23	1.81	0.45
3:F:293:ARG:HA	2:E:186:ALA:HB1	1.98	0.45
1:U:318:ILE:HB	1:U:380:ASN:HB3	1.98	0.45
1:X:318:ILE:HB	1:X:380:ASN:HB3	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:a:13:LEU:HD11	3:a:39:ILE:HG21	1.98	0.45
2:G:876:ARG:CG	4:k:56:ASN:ND2	2.60	0.45
1:P:3:ARG:HB2	1:P:4:GLU:H	1.63	0.45
1:U:73:VAL:O	1:U:76:SER:OG	2.30	0.45
1:U:252:ASP:OD1	1:U:252:ASP:N	2.48	0.45
1:Z:301:LYS:H	1:Z:301:LYS:HG3	1.65	0.45
3:H:550:ASN:OD1	3:H:551:LYS:NZ	2.38	0.45
5:I:148:ILE:HG22	5:I:153:ILE:HG12	1.99	0.45
1:R:383:SER:O	1:R:386:SER:OG	2.28	0.45
1:S:316:CYS:HA	1:S:347:ASN:HB3	1.98	0.45
1:U:110:GLN:HA	1:U:113:LYS:HE3	1.98	0.45
1:X:151:SER:HB2	1:X:194:ARG:HG2	1.99	0.45
1:Z:151:SER:HB2	1:Z:194:ARG:HG2	1.99	0.45
2:C:861:PHE:HZ	1:Q:340:ILE:HG22	1.81	0.45
7:L:365:SER:OG	7:L:366:ALA:N	2.49	0.45
3:N:657:MET:O	3:N:661:LEU:HG	2.17	0.45
1:Q:110:GLN:HA	1:Q:113:LYS:HE3	1.98	0.45
1:Q:172:PHE:N	1:Q:205:LEU:O	2.50	0.45
1:S:172:PHE:N	1:S:205:LEU:O	2.50	0.45
1:U:151:SER:HB2	1:U:194:ARG:HG2	1.98	0.45
1:V:316:CYS:HA	1:V:347:ASN:HB3	1.98	0.45
1:W:318:ILE:HB	1:W:380:ASN:HB3	1.98	0.45
4:d:21:VAL:HA	4:d:24:THR:HG22	1.98	0.45
1:1:151:SER:HB2	1:1:194:ARG:HG2	1.99	0.45
1:2:318:ILE:HB	1:2:380:ASN:HB3	1.98	0.45
1:S:301:LYS:H	1:S:301:LYS:HG3	1.65	0.45
1:U:160:ARG:HA	1:U:160:ARG:HD2	1.74	0.45
1:V:110:GLN:HA	1:V:113:LYS:HE3	1.98	0.45
1:W:172:PHE:N	1:W:205:LEU:O	2.50	0.45
1:Y:151:SER:HB2	1:Y:194:ARG:HG2	1.99	0.45
1:Z:172:PHE:N	1:Z:205:LEU:O	2.50	0.45
3:n:81:LEU:O	3:n:84:GLN:NE2	2.50	0.45
1:1:318:ILE:HB	1:1:380:ASN:HB3	1.98	0.45
1:2:172:PHE:N	1:2:205:LEU:O	2.50	0.45
1:P:151:SER:HB2	1:P:194:ARG:HG2	1.98	0.45
1:R:151:SER:HB2	1:R:194:ARG:HG2	1.99	0.45
1:S:110:GLN:HA	1:S:113:LYS:HE3	1.98	0.45
1:T:172:PHE:N	1:T:205:LEU:O	2.50	0.45
1:U:229:ASN:O	1:U:233:SER:OG	2.29	0.45
1:Y:184:GLN:O	1:Y:188:SER:OG	2.31	0.45
3:D:563:ARG:NH2	1:R:248:TYR:OH	2.49	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:172:PHE:N	1:U:205:LEU:O	2.50	0.45
4:g:24:THR:HA	4:g:27:VAL:HG22	1.98	0.45
1:1:46:ASP:O	2:M:563:THR:HG21	2.17	0.45
1:1:110:GLN:HA	1:1:113:LYS:HE3	1.98	0.45
1:2:151:SER:HB2	1:2:194:ARG:HG2	1.99	0.45
2:A:679:ALA:HB2	2:A:822:ILE:HG21	1.99	0.45
3:B:622:ASP:N	3:B:622:ASP:OD2	2.49	0.45
5:I:610:ALA:O	5:I:613:SER:OG	2.30	0.45
1:O:172:PHE:N	1:O:205:LEU:O	2.50	0.45
1:R:184:GLN:O	1:R:188:SER:OG	2.31	0.45
1:V:172:PHE:N	1:V:205:LEU:O	2.50	0.45
1:X:229:ASN:O	1:X:233:SER:OG	2.29	0.45
1:Y:110:GLN:HA	1:Y:113:LYS:HE3	1.98	0.45
1:Y:318:ILE:HB	1:Y:380:ASN:HB3	1.98	0.45
1:Z:160:ARG:HD2	1:Z:160:ARG:HA	1.74	0.45
3:D:388:CYS:HA	3:D:391:ARG:HE	1.82	0.45
3:F:369:VAL:HB	3:F:370:TRP:CE2	2.52	0.45
5:I:503:LYS:NZ	5:I:507:SER:O	2.40	0.45
6:J:358:PHE:HD2	6:J:360:THR:H	1.65	0.45
1:O:110:GLN:HA	1:O:113:LYS:HE3	1.98	0.45
1:O:151:SER:HB2	1:O:194:ARG:HG2	1.98	0.45
1:Q:316:CYS:HA	1:Q:347:ASN:HB3	1.98	0.45
1:T:23:LYS:HE3	1:T:23:LYS:HB3	1.83	0.45
1:W:383:SER:O	1:W:386:SER:OG	2.28	0.45
1:X:172:PHE:N	1:X:205:LEU:O	2.50	0.45
1:Y:172:PHE:N	1:Y:205:LEU:O	2.50	0.45
3:n:33:GLN:HA	3:n:36:VAL:HG22	1.99	0.45
2:E:206:GLY:H	2:E:251:ASN:ND2	2.15	0.45
2:A:279:GLU:O	2:A:282:SER:OG	2.29	0.45
2:C:768:SER:O	2:C:768:SER:OG	2.33	0.45
1:S:116:GLU:H	1:S:116:GLU:HG2	1.45	0.45
1:V:320:ILE:HG23	1:V:379:ALA:HB2	1.99	0.45
1:Y:252:ASP:OD1	1:Y:252:ASP:N	2.48	0.45
1:Z:383:SER:O	1:Z:386:SER:OG	2.28	0.45
4:k:30:GLU:CD	3:j:112:SER:OG	2.60	0.45
3:j:60:LYS:O	3:j:64:ARG:NH1	2.48	0.45
1:1:320:ILE:HG23	1:1:379:ALA:HB2	1.99	0.44
1:2:320:ILE:HG23	1:2:379:ALA:HB2	1.99	0.44
3:F:645:ASP:OD1	3:F:645:ASP:N	2.50	0.44
3:N:597:LEU:H	3:N:597:LEU:HD12	1.82	0.44
1:P:110:GLN:HA	1:P:113:LYS:HE3	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:318:ILE:HB	1:S:380:ASN:HB3	1.98	0.44
1:S:320:ILE:HG23	1:S:379:ALA:HB2	1.99	0.44
1:T:110:GLN:HA	1:T:113:LYS:HE3	1.98	0.44
1:T:151:SER:HB2	1:T:194:ARG:HG2	1.99	0.44
1:T:316:CYS:HA	1:T:347:ASN:HB3	1.98	0.44
1:V:151:SER:HB2	1:V:194:ARG:HG2	1.99	0.44
1:V:318:ILE:HB	1:V:380:ASN:HB3	1.98	0.44
1:W:323:ILE:HG12	1:W:359:ALA:HB3	1.99	0.44
1:Y:160:ARG:HD2	1:Y:160:ARG:HA	1.74	0.44
1:1:229:ASN:O	1:1:233:SER:OG	2.29	0.44
1:1:323:ILE:HG12	1:1:359:ALA:HB3	2.00	0.44
1:2:116:GLU:H	1:2:116:GLU:HG2	1.45	0.44
6:J:556:LEU:HA	6:J:559:ILE:HD12	2.00	0.44
1:O:316:CYS:HA	1:O:347:ASN:HB3	1.98	0.44
1:P:318:ILE:HB	1:P:380:ASN:HB3	1.98	0.44
1:Q:151:SER:HB2	1:Q:194:ARG:HG2	1.99	0.44
1:T:318:ILE:HB	1:T:380:ASN:HB3	1.98	0.44
1:T:320:ILE:HG23	1:T:379:ALA:HB2	1.99	0.44
1:W:56:ASP:HB3	1:X:299:GLN:NE2	2.32	0.44
1:W:320:ILE:HG23	1:W:379:ALA:HB2	1.99	0.44
1:Z:318:ILE:HB	1:Z:380:ASN:HB3	1.98	0.44
3:j:93:ILE:HA	3:j:96:LEU:HD12	1.99	0.44
1:2:110:GLN:HA	1:2:113:LYS:HE3	1.98	0.44
3:D:404:THR:HG22	3:D:415:VAL:HG11	1.98	0.44
3:D:691:LEU:HD13	3:D:800:LEU:HD11	1.99	0.44
5:I:502:ARG:O	5:I:508:ASN:ND2	2.50	0.44
1:O:318:ILE:HB	1:O:380:ASN:HB3	1.98	0.44
1:Q:320:ILE:HG23	1:Q:379:ALA:HB2	1.99	0.44
1:S:151:SER:HB2	1:S:194:ARG:HG2	1.99	0.44
1:U:184:GLN:O	1:U:188:SER:OG	2.31	0.44
1:W:151:SER:HB2	1:W:194:ARG:HG2	1.99	0.44
1:X:301:LYS:H	1:X:301:LYS:HG3	1.65	0.44
4:b:56:ASN:HB3	4:b:58:GLU:CD	2.43	0.44
3:n:81:LEU:HA	3:n:84:GLN:HE21	1.81	0.44
5:K:540:GLN:NE2	5:K:543:GLN:OE1	2.49	0.44
2:M:418:ARG:HD2	2:M:423:TYR:H	1.83	0.44
3:N:597:LEU:HB3	3:N:623:VAL:HG21	1.98	0.44
1:P:323:ILE:HG12	1:P:359:ALA:HB3	2.00	0.44
1:X:110:GLN:HA	1:X:113:LYS:HE3	1.98	0.44
2:C:461:ARG:HG3	2:C:467:VAL:HB	1.99	0.44
2:G:557:LEU:O	2:G:561:MET:HB3	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:229:ASN:O	1:O:233:SER:OG	2.29	0.44
1:R:229:ASN:O	1:R:233:SER:OG	2.29	0.44
2:E:206:GLY:H	2:E:251:ASN:HD22	1.65	0.44
1:1:172:PHE:N	1:1:205:LEU:O	2.50	0.44
3:B:659:HIS:CD2	3:B:662:ARG:HH21	2.35	0.44
2:C:314:HIS:CE1	2:C:315:ARG:HG3	2.52	0.44
2:G:861:PHE:CE1	1:U:341:ARG:HA	2.43	0.44
6:J:838:LEU:HD11	6:J:890:LEU:HD23	1.99	0.44
5:K:115:PRO:HA	7:L:317:ARG:NH2	2.32	0.44
5:K:529:GLN:HE22	5:K:586:ILE:HG21	1.82	0.44
3:N:406:THR:HG23	3:N:412:ARG:HB2	2.00	0.44
1:P:172:PHE:N	1:P:205:LEU:O	2.50	0.44
1:T:323:ILE:HG12	1:T:359:ALA:HB3	2.00	0.44
1:R:323:ILE:HG12	1:R:359:ALA:HB3	2.00	0.44
1:Y:320:ILE:HG23	1:Y:379:ALA:HB2	1.99	0.44
3:a:93:ILE:O	3:a:97:LEU:HG	2.17	0.44
2:E:449:LYS:O	2:E:453:THR:OG1	2.29	0.44
6:J:384:LYS:NZ	6:J:385:CYS:SG	2.78	0.44
3:N:774:GLN:HE22	3:N:860:GLN:CD	2.25	0.44
1:U:316:CYS:HA	1:U:347:ASN:HB3	1.98	0.44
1:V:323:ILE:HG12	1:V:359:ALA:HB3	2.00	0.44
1:X:343:ARG:HB3	1:X:345:LEU:HG	2.00	0.44
4:b:27:VAL:HG13	3:a:77:LEU:HD22	1.98	0.44
1:1:245:TYR:O	1:1:362:ARG:NH1	2.51	0.44
3:D:878:PHE:CE1	1:R:341:ARG:HD3	2.53	0.44
5:I:158:TYR:HB3	5:I:159:LYS:NZ	2.32	0.44
1:O:323:ILE:HG12	1:O:359:ALA:HB3	2.00	0.44
1:W:343:ARG:HB3	1:W:345:LEU:HG	2.00	0.44
1:X:320:ILE:HG23	1:X:379:ALA:HB2	1.99	0.44
3:H:630:PRO:HD2	3:H:637:VAL:HG13	1.99	0.43
6:J:723:MET:HE3	6:J:723:MET:HB3	1.93	0.43
1:Q:323:ILE:HG12	1:Q:359:ALA:HB3	2.00	0.43
1:V:61:ILE:HG23	1:V:86:TYR:HA	2.00	0.43
1:V:116:GLU:H	1:V:116:GLU:HG2	1.45	0.43
1:X:323:ILE:HG12	1:X:359:ALA:HB3	2.00	0.43
1:Y:343:ARG:HB3	1:Y:345:LEU:HG	2.00	0.43
6:l:118:SER:OG	6:l:119:ASP:N	2.51	0.43
2:C:184:ARG:NH2	3:D:273:ASN:OD1	2.44	0.43
3:F:424:HIS:HA	3:F:427:LEU:HG	1.99	0.43
3:F:682:LYS:HE3	1:T:254:ILE:HD12	1.99	0.43
6:J:412:LEU:HD11	6:J:460:LEU:HD11	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:646:LEU:HD23	1:Y:341:ARG:HD3	2.00	0.43
7:L:1773:LYS:HD2	7:L:1773:LYS:HA	1.86	0.43
3:N:419:LEU:HA	3:N:422:VAL:HG22	2.00	0.43
1:P:343:ARG:HB3	1:P:345:LEU:HG	2.00	0.43
1:R:172:PHE:N	1:R:205:LEU:O	2.50	0.43
1:S:383:SER:O	1:S:386:SER:OG	2.28	0.43
1:T:61:ILE:HG23	1:T:86:TYR:HA	2.00	0.43
1:V:19:PHE:HE1	1:V:82:TYR:HB2	1.84	0.43
1:Y:229:ASN:O	1:Y:233:SER:OG	2.29	0.43
4:m:57:PRO:HG3	6:l:109:SER:HA	2.00	0.43
2:G:428:TRP:HE1	2:G:723:LEU:HD22	1.84	0.43
2:M:697:MET:HG2	2:M:702:MET:HE2	2.01	0.43
1:O:61:ILE:HG23	1:O:86:TYR:HA	2.00	0.43
1:Q:61:ILE:HG23	1:Q:86:TYR:HA	2.00	0.43
1:R:320:ILE:HG23	1:R:379:ALA:HB2	1.99	0.43
1:V:343:ARG:HB3	1:V:345:LEU:HG	2.00	0.43
1:l:61:ILE:HG23	1:l:86:TYR:HA	2.00	0.43
1:l:81:PRO:HA	1:l:84:LYS:HE2	2.01	0.43
1:2:299:GLN:H	1:2:299:GLN:HG2	1.67	0.43
3:D:887:LYS:HA	3:D:887:LYS:HD3	1.76	0.43
5:I:481:TYR:O	5:I:484:SER:OG	2.35	0.43
6:J:234:HIS:CD2	6:J:236:LEU:HG	2.53	0.43
5:K:518:ARG:HH12	5:K:589:LEU:HD13	1.83	0.43
7:L:328:GLN:HG3	7:L:332:GLN:HE22	1.83	0.43
2:M:340:SER:O	2:M:343:THR:OG1	2.37	0.43
3:N:248:ALA:O	3:N:252:ARG:HG2	2.19	0.43
1:Q:245:TYR:O	1:Q:362:ARG:NH1	2.51	0.43
1:U:202:VAL:HG12	1:U:204:VAL:HG22	2.01	0.43
1:U:245:TYR:O	1:U:362:ARG:NH1	2.51	0.43
1:Z:61:ILE:HG23	1:Z:86:TYR:HA	2.00	0.43
1:Z:343:ARG:HB3	1:Z:345:LEU:HG	2.00	0.43
6:l:121:PRO:HD2	6:l:121:PRO:O	2.18	0.43
1:2:323:ILE:HG12	1:2:359:ALA:HB3	2.00	0.43
2:A:186:ALA:HB1	3:B:293:ARG:HA	2.01	0.43
2:G:713:LEU:HD11	2:G:722:VAL:HG13	2.00	0.43
3:H:554:SER:HB3	3:H:557:ASP:HB2	2.00	0.43
3:H:689:LYS:HB2	3:H:692:ARG:NH2	2.33	0.43
6:J:271:ILE:HA	6:J:274:THR:HG22	1.99	0.43
1:O:19:PHE:HE1	1:O:82:TYR:HB2	1.84	0.43
1:R:81:PRO:HA	1:R:84:LYS:HE2	2.01	0.43
1:R:245:TYR:O	1:R:362:ARG:NH1	2.51	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:245:TYR:O	1:V:362:ARG:NH1	2.51	0.43
1:W:19:PHE:HE1	1:W:82:TYR:HB2	1.84	0.43
1:W:245:TYR:O	1:W:362:ARG:NH1	2.51	0.43
1:Z:19:PHE:HE1	1:Z:82:TYR:HB2	1.84	0.43
1:Z:320:ILE:HG23	1:Z:379:ALA:HB2	1.99	0.43
1:Z:323:ILE:HG12	1:Z:359:ALA:HB3	2.00	0.43
1:2:295:ARG:HH11	2:M:561:MET:HB2	1.81	0.43
5:I:197:LEU:HD11	5:I:200:HIS:HA	2.01	0.43
2:M:306:LEU:O	2:M:310:LEU:HG	2.19	0.43
3:N:706:ILE:O	3:N:709:SER:OG	2.36	0.43
1:O:202:VAL:HG12	1:O:204:VAL:HG22	2.01	0.43
1:P:61:ILE:HG23	1:P:86:TYR:HA	2.01	0.43
1:S:323:ILE:HG12	1:S:359:ALA:HB3	1.99	0.43
1:T:245:TYR:O	1:T:362:ARG:NH1	2.51	0.43
1:T:326:GLY:HA2	1:T:363:LYS:HD3	2.01	0.43
1:U:301:LYS:H	1:U:301:LYS:HG3	1.65	0.43
1:U:320:ILE:HG23	1:U:379:ALA:HB2	1.99	0.43
1:U:323:ILE:HG12	1:U:359:ALA:HB3	2.00	0.43
2:E:747:VAL:HG13	2:E:836:LEU:HD12	2.00	0.43
2:E:869:LEU:HD23	2:E:869:LEU:HA	1.91	0.43
6:I:114:LEU:HA	6:I:117:LEU:HD12	2.00	0.43
1:2:3:ARG:HB2	1:2:4:GLU:H	1.62	0.43
1:2:61:ILE:HG23	1:2:86:TYR:HA	2.00	0.43
2:C:289:ASN:HA	2:C:292:LEU:HB2	2.01	0.43
2:G:244:ARG:HA	2:G:244:ARG:HD3	1.88	0.43
5:I:333:ARG:NH2	5:I:553:ASP:OD1	2.47	0.43
7:L:346:LEU:HA	7:L:347:VAL:HA	1.67	0.43
3:N:312:SER:HB3	3:N:325:CYS:SG	2.58	0.43
3:N:563:ARG:NH1	3:N:728:GLU:OE1	2.51	0.43
1:P:81:PRO:HA	1:P:84:LYS:HE2	2.01	0.43
1:Q:160:ARG:HD2	1:Q:160:ARG:HA	1.74	0.43
1:Q:326:GLY:HA2	1:Q:363:LYS:HD3	2.01	0.43
1:R:326:GLY:HA2	1:R:363:LYS:HD3	2.01	0.43
1:W:81:PRO:HA	1:W:84:LYS:HE2	2.01	0.43
1:Y:245:TYR:O	1:Y:362:ARG:NH1	2.51	0.43
4:i:56:ASN:ND2	2:E:876:ARG:HH11	2.12	0.43
2:G:861:PHE:CD2	1:U:355:SER:HB3	2.54	0.43
3:H:419:LEU:HA	3:H:422:VAL:HG22	2.01	0.43
3:H:882:PHE:CE1	1:V:341:ARG:HA	2.54	0.43
7:L:427:LEU:HA	7:L:430:GLN:HE21	1.84	0.43
2:M:641:LEU:HG	2:M:645:MET:HE2	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:320:ILE:HG23	1:P:379:ALA:HB2	1.99	0.43
1:R:116:GLU:H	1:R:116:GLU:HG2	1.45	0.43
1:S:245:TYR:O	1:S:362:ARG:NH1	2.51	0.43
1:T:343:ARG:HB3	1:T:345:LEU:HG	2.00	0.43
1:U:19:PHE:HE1	1:U:82:TYR:HB2	1.84	0.43
1:W:326:GLY:HA2	1:W:363:LYS:HD3	2.01	0.43
1:X:61:ILE:HG23	1:X:86:TYR:HA	2.00	0.43
1:X:81:PRO:HA	1:X:84:LYS:HE2	2.01	0.43
1:Y:23:LYS:HE3	1:Y:23:LYS:HB3	1.83	0.43
1:2:343:ARG:HB3	1:2:345:LEU:HG	2.00	0.43
3:F:493:LEU:HB2	3:F:545:LEU:HD13	2.01	0.43
5:K:2:ILE:HG21	7:L:317:ARG:HH12	1.84	0.43
3:N:641:ASP:N	3:N:641:ASP:OD2	2.52	0.43
1:O:245:TYR:O	1:O:362:ARG:NH1	2.51	0.43
1:O:343:ARG:HB3	1:O:345:LEU:HG	2.00	0.43
1:P:301:LYS:H	1:P:301:LYS:HG3	1.65	0.43
1:S:184:GLN:O	1:S:188:SER:OG	2.31	0.43
1:V:301:LYS:H	1:V:301:LYS:HG3	1.65	0.43
1:X:3:ARG:HB2	1:X:4:GLU:H	1.62	0.43
1:Y:323:ILE:HG12	1:Y:359:ALA:HB3	1.99	0.43
1:2:19:PHE:HE1	1:2:82:TYR:HB2	1.84	0.43
2:C:551:LEU:HD21	2:C:616:PHE:HD1	1.84	0.43
3:H:545:LEU:O	3:H:549:LEU:HG	2.19	0.43
6:J:225:TRP:HE1	5:K:35:HIS:CE1	2.37	0.43
6:J:642:HIS:HB3	6:J:691:LEU:HD13	2.01	0.43
2:M:526:ASP:HA	2:M:529:VAL:HG12	2.01	0.43
3:N:392:LYS:NZ	3:N:443:TYR:HB3	2.33	0.43
1:O:77:ILE:O	1:O:80:SER:OG	2.35	0.43
1:O:81:PRO:HA	1:O:84:LYS:HE2	2.01	0.43
1:R:343:ARG:HB3	1:R:345:LEU:HG	2.00	0.43
1:S:61:ILE:HG23	1:S:86:TYR:HA	2.00	0.43
1:U:419:ASP:O	1:U:423:THR:OG1	2.37	0.43
1:V:419:ASP:O	1:V:423:THR:OG1	2.37	0.43
1:X:19:PHE:HE1	1:X:82:TYR:HB2	1.84	0.43
1:X:326:GLY:HA2	1:X:363:LYS:HD3	2.01	0.43
1:Y:164:LYS:HA	1:Y:164:LYS:HD3	1.85	0.43
1:Z:202:VAL:HG12	1:Z:204:VAL:HG22	2.01	0.43
1:Z:326:GLY:HA2	1:Z:363:LYS:HD3	2.01	0.43
1:1:202:VAL:HG12	1:1:204:VAL:HG22	2.01	0.42
2:C:862:ASN:HD21	1:Q:344:LYS:NZ	2.17	0.42
3:D:609:ASN:HD21	1:R:49:ASP:HB2	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:713:HIS:CE1	1:T:355:SER:H	2.36	0.42
3:H:655:GLU:O	3:H:658:SER:OG	2.32	0.42
3:H:730:SER:HB3	3:H:754:PHE:CE1	2.53	0.42
6:J:256:LEU:HG	6:J:257:TYR:H	1.84	0.42
5:K:29:GLN:HA	5:K:34:LEU:HD21	2.00	0.42
5:K:275:LYS:HB3	5:K:333:ARG:HG3	1.99	0.42
2:M:682:LEU:HD22	2:M:826:ASP:HB2	2.00	0.42
3:N:245:ILE:HG21	3:N:288:ARG:HH22	1.83	0.42
3:N:262:ASP:OD1	3:N:267:LYS:HG2	2.19	0.42
1:R:19:PHE:HE1	1:R:82:TYR:HB2	1.84	0.42
1:S:81:PRO:HA	1:S:84:LYS:HE2	2.01	0.42
1:S:326:GLY:HA2	1:S:363:LYS:HD3	2.01	0.42
1:S:343:ARG:HB3	1:S:345:LEU:HG	2.00	0.42
1:T:81:PRO:HA	1:T:84:LYS:HE2	2.01	0.42
1:U:23:LYS:HE3	1:U:23:LYS:HB3	1.83	0.42
1:U:343:ARG:HB3	1:U:345:LEU:HG	2.00	0.42
1:V:202:VAL:HG12	1:V:204:VAL:HG22	2.01	0.42
2:E:398:GLY:N	2:E:457:LEU:HD22	2.34	0.42
1:1:326:GLY:HA2	1:1:363:LYS:HD3	2.01	0.42
1:1:419:ASP:O	1:1:423:THR:OG1	2.37	0.42
1:2:81:PRO:HA	1:2:84:LYS:HE2	2.01	0.42
2:C:696:TYR:O	2:C:700:GLU:HB2	2.20	0.42
2:C:743:GLU:HB2	2:C:745:LEU:HD23	2.01	0.42
3:D:431:TYR:HA	3:D:434:ILE:HG22	2.01	0.42
3:D:568:LEU:HD23	3:D:574:ILE:HG21	2.01	0.42
4:o:25:MET:HE1	4:o:48:VAL:HB	2.01	0.42
3:F:836:PHE:O	3:F:840:ILE:HG12	2.20	0.42
3:N:806:PHE:HA	3:N:809:LYS:HD2	2.02	0.42
1:O:25:LEU:HD23	1:O:25:LEU:HA	1.90	0.42
1:O:184:GLN:O	1:O:188:SER:OG	2.31	0.42
1:P:229:ASN:O	1:P:233:SER:OG	2.29	0.42
1:R:3:ARG:HB2	1:R:4:GLU:H	1.62	0.42
1:R:202:VAL:HG12	1:R:204:VAL:HG22	2.01	0.42
1:U:326:GLY:HA2	1:U:363:LYS:HD3	2.01	0.42
1:V:3:ARG:HD2	1:V:131:SER:HB2	2.02	0.42
1:W:61:ILE:HG23	1:W:86:TYR:HA	2.00	0.42
1:Y:61:ILE:HG23	1:Y:86:TYR:HA	2.01	0.42
1:Z:116:GLU:H	1:Z:116:GLU:HG2	1.45	0.42
1:Z:245:TYR:O	1:Z:362:ARG:NH1	2.51	0.42
3:j:60:LYS:HB3	3:j:64:ARG:NH1	2.33	0.42
6:l:80:LYS:HG3	6:l:126:TYR:HD1	1.78	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:3:ARG:HD2	1:2:131:SER:HB2	2.02	0.42
1:2:77:ILE:O	1:2:80:SER:OG	2.35	0.42
2:G:746:LYS:O	2:G:749:SER:OG	2.33	0.42
5:K:111:PHE:O	7:L:317:ARG:NH2	2.50	0.42
7:L:1731:SER:O	7:L:1735:LEU:HG	2.19	0.42
1:O:320:ILE:HG23	1:O:379:ALA:HB2	1.99	0.42
1:S:419:ASP:O	1:S:423:THR:OG1	2.37	0.42
1:U:116:GLU:H	1:U:116:GLU:HG2	1.45	0.42
1:W:202:VAL:HG12	1:W:204:VAL:HG22	2.01	0.42
1:Y:19:PHE:HE1	1:Y:82:TYR:HB2	1.84	0.42
1:Z:419:ASP:O	1:Z:423:THR:OG1	2.37	0.42
2:E:547:THR:HA	2:E:548:PRO:HD3	1.88	0.42
1:1:19:PHE:HE1	1:1:82:TYR:HB2	1.84	0.42
1:2:326:GLY:HA2	1:2:363:LYS:HD3	2.01	0.42
1:2:351:TRP:CD1	1:2:351:TRP:H	2.38	0.42
1:2:383:SER:O	1:2:386:SER:OG	2.28	0.42
2:C:302:GLU:HA	2:C:305:ILE:HD12	2.01	0.42
3:D:776:ARG:NH1	3:h:106:ARG:CG	2.69	0.42
3:H:459:LEU:HD21	3:H:492:PHE:HA	2.01	0.42
5:I:504:HIS:HE1	1:W:200:ASP:OD1	2.02	0.42
5:K:94:ASP:OD1	5:K:95:SER:N	2.52	0.42
1:P:245:TYR:O	1:P:362:ARG:NH1	2.51	0.42
1:R:419:ASP:O	1:R:423:THR:OG1	2.37	0.42
1:S:19:PHE:HE1	1:S:82:TYR:HB2	1.83	0.42
1:S:248:TYR:HE2	2:E:522:MET:O	2.02	0.42
1:Z:81:PRO:HA	1:Z:84:LYS:HE2	2.01	0.42
4:k:45:SER:HA	4:k:48:VAL:HG12	2.01	0.42
6:l:115:LEU:HD23	6:l:119:ASP:OD2	2.19	0.42
1:1:3:ARG:HD2	1:1:131:SER:HB2	2.02	0.42
1:2:186:TYR:HE1	1:2:399:ARG:HD3	1.85	0.42
3:B:653:THR:HG1	3:B:656:CYS:HG	1.58	0.42
3:B:724:PHE:CE1	1:P:360:LEU:HB2	2.54	0.42
3:H:601:LEU:HD22	3:H:623:VAL:HG13	2.02	0.42
6:J:641:VAL:O	6:J:645:LEU:HG	2.19	0.42
1:P:3:ARG:HD2	1:P:131:SER:HB2	2.02	0.42
1:P:19:PHE:HE1	1:P:82:TYR:HB2	1.84	0.42
1:Q:343:ARG:HB3	1:Q:345:LEU:HG	2.00	0.42
1:R:160:ARG:HA	1:R:160:ARG:HD2	1.74	0.42
1:V:326:GLY:HA2	1:V:363:LYS:HD3	2.01	0.42
1:W:46:ASP:OD1	1:W:46:ASP:N	2.53	0.42
1:X:46:ASP:OD1	1:X:46:ASP:N	2.53	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:i:59:ALA:CB	2:E:876:ARG:HE	2.25	0.42
3:h:111:VAL:O	3:h:111:VAL:HG12	2.19	0.42
1:2:202:VAL:HG12	1:2:204:VAL:HG22	2.01	0.42
3:D:457:ASP:OD1	3:D:457:ASP:N	2.51	0.42
4:o:48:VAL:HG13	3:n:87:LEU:HD13	2.01	0.42
2:M:567:ASP:HA	2:M:568:PRO:HD3	1.95	0.42
1:P:46:ASP:OD1	1:P:46:ASP:N	2.53	0.42
1:Q:19:PHE:HE1	1:Q:82:TYR:HB2	1.84	0.42
1:Q:186:TYR:HE1	1:Q:399:ARG:HD3	1.85	0.42
1:R:351:TRP:CD1	1:R:351:TRP:H	2.38	0.42
1:U:77:ILE:O	1:U:80:SER:OG	2.35	0.42
1:W:56:ASP:HB3	1:X:299:GLN:CD	2.45	0.42
1:X:160:ARG:HD2	1:X:160:ARG:HA	1.74	0.42
1:X:186:TYR:HE1	1:X:399:ARG:HD3	1.85	0.42
1:X:202:VAL:HG12	1:X:204:VAL:HG22	2.01	0.42
2:G:499:LEU:O	2:G:503:LEU:HG	2.20	0.42
1:P:326:GLY:HA2	1:P:363:LYS:HD3	2.01	0.42
1:P:419:ASP:O	1:P:423:THR:OG1	2.37	0.42
1:Q:301:LYS:H	1:Q:301:LYS:HG3	1.65	0.42
1:V:46:ASP:OD1	1:V:46:ASP:N	2.53	0.42
1:X:245:TYR:O	1:X:362:ARG:NH1	2.51	0.42
1:X:383:SER:O	1:X:386:SER:OG	2.28	0.42
1:Y:301:LYS:H	1:Y:301:LYS:HG3	1.65	0.42
2:E:241:ARG:O	2:E:243:SER:N	2.51	0.42
2:E:573:LEU:HG	2:E:620:TYR:HD1	1.84	0.42
2:E:696:TYR:CZ	2:E:855:VAL:HB	2.55	0.42
3:F:555:LEU:HD11	3:F:651:VAL:HG21	2.02	0.42
2:G:414:LEU:HB2	2:G:426:LYS:HD3	2.00	0.42
2:M:512:HIS:CE1	2:M:622:VAL:HG13	2.55	0.42
1:Q:351:TRP:CD1	1:Q:351:TRP:H	2.38	0.42
1:R:3:ARG:HD2	1:R:131:SER:HB2	2.02	0.42
1:R:186:TYR:HE1	1:R:399:ARG:HD3	1.85	0.42
1:S:202:VAL:HG12	1:S:204:VAL:HG22	2.01	0.42
1:T:3:ARG:HD2	1:T:131:SER:HB2	2.02	0.42
1:T:46:ASP:OD1	1:T:46:ASP:N	2.53	0.42
1:U:3:ARG:HD2	1:U:131:SER:HB2	2.02	0.42
1:W:186:TYR:HE1	1:W:399:ARG:HD3	1.85	0.42
1:Z:77:ILE:O	1:Z:80:SER:OG	2.35	0.42
4:b:53:GLN:HE22	4:b:55:ILE:HD12	1.85	0.42
3:n:64:ARG:NH2	3:n:103:ASP:OD1	2.53	0.42
1:1:343:ARG:HB3	1:1:345:LEU:HG	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:866:THR:O	2:A:866:THR:OG1	2.31	0.42
3:B:261:ILE:HD11	2:C:262:ARG:HH11	1.84	0.42
3:F:592:LEU:HD11	3:F:597:LEU:HD21	2.01	0.42
5:I:544:LEU:O	5:I:548:ILE:HG12	2.19	0.42
5:K:318:PRO:HA	5:K:319:LEU:HA	1.86	0.42
5:K:639:ASN:O	5:K:642:LEU:N	2.50	0.42
2:M:855:VAL:O	2:M:859:LEU:HG	2.19	0.42
1:O:3:ARG:HD2	1:O:131:SER:HB2	2.02	0.42
1:O:186:TYR:HE1	1:O:399:ARG:HD3	1.85	0.42
1:P:202:VAL:HG12	1:P:204:VAL:HG22	2.01	0.42
1:Q:3:ARG:HD2	1:Q:131:SER:HB2	2.02	0.42
1:W:419:ASP:O	1:W:423:THR:OG1	2.37	0.42
1:X:415:LYS:HG2	1:X:420:GLU:HG2	2.02	0.42
2:E:249:ASP:HB3	2:E:251:ASN:OD1	2.20	0.42
1:1:186:TYR:HE1	1:1:399:ARG:HD3	1.85	0.42
1:1:351:TRP:CD1	1:1:351:TRP:H	2.38	0.42
2:A:734:LEU:HB3	2:A:740:THR:HG22	2.02	0.42
3:N:546:LEU:HD13	3:N:546:LEU:HA	1.77	0.42
3:N:666:PHE:HB2	3:N:764:LEU:HD21	2.02	0.42
1:Q:81:PRO:HA	1:Q:84:LYS:HE2	2.01	0.42
1:R:46:ASP:N	1:R:46:ASP:OD1	2.53	0.42
1:S:3:ARG:HD2	1:S:131:SER:HB2	2.02	0.42
1:V:81:PRO:HA	1:V:84:LYS:HE2	2.01	0.42
1:W:351:TRP:H	1:W:351:TRP:CD1	2.38	0.42
1:X:419:ASP:O	1:X:423:THR:OG1	2.37	0.42
1:Y:3:ARG:HD2	1:Y:131:SER:HB2	2.02	0.42
1:Y:202:VAL:HG12	1:Y:204:VAL:HG22	2.01	0.42
1:1:127:ASP:O	1:2:301:LYS:HG2	2.20	0.41
1:2:415:LYS:HG2	1:2:420:GLU:HG2	2.02	0.41
2:G:212:SER:O	2:G:215:SER:OG	2.35	0.41
2:G:876:ARG:HG3	4:k:58:GLU:C	2.45	0.41
3:H:700:VAL:HB	3:H:844:CYS:SG	2.60	0.41
2:M:175:PRO:HG3	3:N:402:ALA:HB1	2.02	0.41
2:M:277:ILE:HG12	2:M:293:ALA:HB1	2.01	0.41
1:P:23:LYS:HE3	1:P:23:LYS:HB3	1.83	0.41
1:R:61:ILE:HG23	1:R:86:TYR:HA	2.01	0.41
1:V:415:LYS:HG2	1:V:420:GLU:HG2	2.02	0.41
1:Y:186:TYR:HE1	1:Y:399:ARG:HD3	1.85	0.41
1:Y:419:ASP:O	1:Y:423:THR:OG1	2.37	0.41
1:Z:46:ASP:OD1	1:Z:46:ASP:N	2.53	0.41
1:Z:415:LYS:HG2	1:Z:420:GLU:HG2	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:613:LEU:HD12	2:E:614:GLU:HG2	2.01	0.41
6:l:124:SER:OG	6:l:125:SER:N	2.53	0.41
1:1:3:ARG:HB2	1:1:4:GLU:H	1.62	0.41
3:D:685:MET:HE3	3:D:685:MET:HB3	1.98	0.41
3:F:597:LEU:HA	3:F:600:ILE:HG22	2.01	0.41
2:G:353:GLY:H	2:G:438:GLN:NE2	2.17	0.41
5:K:96:VAL:HG21	5:K:175:ILE:HG13	2.02	0.41
2:M:238:LEU:HD11	2:M:241:ARG:HH21	1.85	0.41
2:M:304:LEU:HB3	3:N:369:VAL:HG13	2.02	0.41
1:T:19:PHE:HE1	1:T:82:TYR:HB2	1.84	0.41
1:U:81:PRO:HA	1:U:84:LYS:HE2	2.01	0.41
1:U:415:LYS:HG2	1:U:420:GLU:HG2	2.02	0.41
1:V:351:TRP:H	1:V:351:TRP:CD1	2.38	0.41
1:W:164:LYS:HD3	1:W:164:LYS:HA	1.85	0.41
1:W:415:LYS:HG2	1:W:420:GLU:HG2	2.02	0.41
1:Y:46:ASP:OD1	1:Y:46:ASP:N	2.53	0.41
1:Y:81:PRO:HA	1:Y:84:LYS:HE2	2.01	0.41
1:Y:299:GLN:H	1:Y:299:GLN:HG2	1.67	0.41
2:E:876:ARG:CD	3:h:42:ASN:CB	2.94	0.41
1:2:245:TYR:O	1:2:362:ARG:NH1	2.51	0.41
6:J:432:ARG:HA	6:J:435:HIS:CD2	2.56	0.41
5:K:533:GLN:O	5:K:537:LEU:HG	2.20	0.41
1:P:186:TYR:HE1	1:P:399:ARG:HD3	1.85	0.41
1:Q:31:ILE:HD12	1:Q:85:LEU:HD11	2.02	0.41
1:U:31:ILE:HD12	1:U:85:LEU:HD11	2.02	0.41
1:V:164:LYS:HA	1:V:164:LYS:HD3	1.85	0.41
1:V:186:TYR:HE1	1:V:399:ARG:HD3	1.85	0.41
1:Y:116:GLU:H	1:Y:116:GLU:HG2	1.45	0.41
1:Y:351:TRP:CD1	1:Y:351:TRP:H	2.38	0.41
1:Z:3:ARG:HD2	1:Z:131:SER:HB2	2.02	0.41
4:m:46:ILE:HG21	6:l:22:LEU:HB2	2.02	0.41
1:2:423:THR:H	1:2:423:THR:HG1	1.55	0.41
2:A:824:LYS:HA	2:A:827:LYS:HD3	2.03	0.41
3:D:563:ARG:NH2	3:D:728:GLU:OE1	2.43	0.41
3:F:365:ARG:NH1	2:E:304:LEU:HB3	2.34	0.41
3:H:287:LEU:HB3	3:H:366:ARG:HH12	1.85	0.41
7:L:1630:MET:HB3	7:L:1630:MET:HE2	1.73	0.41
1:Q:202:VAL:HG12	1:Q:204:VAL:HG22	2.01	0.41
1:T:77:ILE:O	1:T:80:SER:OG	2.35	0.41
1:T:202:VAL:HG12	1:T:204:VAL:HG22	2.01	0.41
1:T:415:LYS:HG2	1:T:420:GLU:HG2	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:116:GLU:H	1:W:116:GLU:HG2	1.45	0.41
1:X:31:ILE:HD12	1:X:85:LEU:HD11	2.02	0.41
1:Z:3:ARG:HB2	1:Z:4:GLU:H	1.62	0.41
1:2:184:GLN:O	1:2:188:SER:OG	2.31	0.41
3:D:300:LEU:HD22	3:D:379:LYS:HA	2.02	0.41
3:D:672:ARG:O	3:D:676:ILE:HG12	2.21	0.41
7:L:1595:GLU:OE2	7:L:1617:SER:OG	2.39	0.41
1:Q:164:LYS:HD3	1:Q:164:LYS:HA	1.85	0.41
1:U:61:ILE:HG23	1:U:86:TYR:HA	2.01	0.41
1:Y:326:GLY:HA2	1:Y:363:LYS:HD3	2.01	0.41
1:1:77:ILE:O	1:1:80:SER:OG	2.35	0.41
1:1:301:LYS:H	1:1:301:LYS:HG3	1.65	0.41
2:A:409:VAL:HG22	2:A:451:LEU:HD12	2.03	0.41
3:B:625:LEU:HD12	3:B:638:PHE:HA	2.03	0.41
3:F:626:LEU:HB2	3:F:637:VAL:HG12	2.02	0.41
3:H:626:LEU:HD12	6:I:71:LYS:HG3	2.01	0.41
5:I:20:ASN:H	5:I:24:GLY:HA2	1.85	0.41
6:J:327:LEU:HD22	6:J:368:LEU:HD21	2.03	0.41
6:J:402:LEU:HD13	6:J:402:LEU:HA	1.79	0.41
6:J:640:ASP:OD1	6:J:640:ASP:N	2.53	0.41
5:K:492:LEU:HB2	5:K:590:CYS:SG	2.61	0.41
1:O:351:TRP:CD1	1:O:351:TRP:H	2.38	0.41
1:P:164:LYS:HA	1:P:164:LYS:HD3	1.85	0.41
1:P:351:TRP:H	1:P:351:TRP:CD1	2.38	0.41
1:P:415:LYS:HG2	1:P:420:GLU:HG2	2.02	0.41
1:R:25:LEU:HD23	1:R:25:LEU:HA	1.90	0.41
1:S:23:LYS:HB3	1:S:23:LYS:HE3	1.83	0.41
1:W:31:ILE:HD12	1:W:85:LEU:HD11	2.02	0.41
1:1:31:ILE:HD12	1:1:85:LEU:HD11	2.02	0.41
1:1:56:ASP:HB3	1:2:276:LEU:CB	2.50	0.41
1:1:165:LEU:HD11	1:1:254:ILE:HB	2.03	0.41
2:A:282:SER:O	2:A:290:HIS:NE2	2.51	0.41
2:C:306:LEU:HA	2:C:309:GLN:HE21	1.85	0.41
4:o:28:LEU:HD23	4:o:31:ILE:HD12	2.03	0.41
5:I:147:LYS:HD2	5:I:147:LYS:HA	1.86	0.41
7:L:1681:LEU:HD13	1:Z:248:TYR:CE2	2.56	0.41
7:L:1805:ASN:O	7:L:1805:ASN:ND2	2.54	0.41
2:M:233:VAL:HG22	2:M:248:VAL:HG23	2.02	0.41
1:O:326:GLY:HA2	1:O:363:LYS:HD3	2.01	0.41
1:P:31:ILE:HD12	1:P:85:LEU:HD11	2.02	0.41
1:P:383:SER:O	1:P:386:SER:OG	2.28	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:186:TYR:HE1	1:S:399:ARG:HD3	1.85	0.41
1:Y:31:ILE:HD12	1:Y:85:LEU:HD11	2.02	0.41
3:n:87:LEU:HB3	3:n:90:LYS:HZ2	1.85	0.41
3:j:69:ALA:HB3	3:j:110:LYS:HZ1	1.85	0.41
3:a:33:GLN:HE22	3:a:37:ARG:HH11	1.66	0.41
2:E:866:THR:HB	2:E:868:ARG:HH12	1.86	0.41
6:l:124:SER:CA	6:l:126:TYR:CD2	3.03	0.41
1:1:295:ARG:NH2	1:Z:53:TYR:OH	2.54	0.41
1:2:165:LEU:HD11	1:2:254:ILE:HB	2.03	0.41
3:B:859:GLN:HE22	3:B:887:LYS:H	1.68	0.41
2:C:226:VAL:HG23	2:C:228:VAL:HG12	2.01	0.41
3:D:468:LYS:HZ3	3:D:481:ARG:HH21	1.68	0.41
3:H:338:LEU:O	3:H:342:LEU:HG	2.20	0.41
7:L:299:ARG:HH22	7:L:305:GLY:HA2	1.85	0.41
2:M:554:LEU:O	2:M:557:LEU:HB3	2.21	0.41
3:N:454:VAL:HG13	3:N:455:LYS:H	1.86	0.41
3:N:624:ARG:HB2	3:N:641:ASP:CG	2.46	0.41
1:O:160:ARG:HA	1:O:160:ARG:HD2	1.74	0.41
1:O:419:ASP:O	1:O:423:THR:OG1	2.37	0.41
1:T:186:TYR:HE1	1:T:399:ARG:HD3	1.85	0.41
1:T:351:TRP:CD1	1:T:351:TRP:H	2.38	0.41
1:U:333:VAL:HB	1:U:358:VAL:HG11	2.03	0.41
1:V:25:LEU:HD23	1:V:25:LEU:HA	1.90	0.41
1:V:77:ILE:O	1:V:80:SER:OG	2.35	0.41
1:W:23:LYS:HE3	1:W:23:LYS:HB3	1.83	0.41
1:Z:164:LYS:HA	1:Z:164:LYS:HD3	1.85	0.41
4:i:56:ASN:HD22	2:E:876:ARG:NH1	2.13	0.41
2:E:818:PHE:O	2:E:822:ILE:HG12	2.21	0.41
2:C:687:LEU:HD21	1:Q:258:ALA:HB1	2.02	0.41
3:D:667:LEU:O	3:D:671:LYS:HG2	2.21	0.41
3:F:653:THR:OG1	3:F:656:CYS:SG	2.73	0.41
2:G:377:LEU:HD13	2:G:479:LEU:HB2	2.03	0.41
2:G:512:HIS:CE1	2:G:630:ILE:HD13	2.56	0.41
3:H:737:LYS:HE3	3:H:750:ALA:HB1	2.02	0.41
6:J:557:LYS:HE3	6:J:561:MET:HE3	2.03	0.41
6:J:739:TYR:HE2	6:J:833:TRP:HB2	1.85	0.41
5:K:410:LEU:HA	5:K:413:LEU:HD13	2.03	0.41
5:K:466:LEU:HD21	5:K:561:HIS:CE1	2.56	0.41
3:N:324:PHE:O	3:N:328:LEU:HG	2.20	0.41
1:O:113:LYS:HG3	1:O:114:ILE:HG23	2.03	0.41
1:O:164:LYS:HA	1:O:164:LYS:HD3	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:419:ASP:O	1:Q:423:THR:OG1	2.37	0.41
1:S:165:LEU:HD11	1:S:254:ILE:HB	2.03	0.41
1:T:25:LEU:HD23	1:T:25:LEU:HA	1.90	0.41
1:U:46:ASP:OD1	1:U:46:ASP:N	2.53	0.41
1:V:165:LEU:HD11	1:V:254:ILE:HB	2.03	0.41
1:W:3:ARG:HD2	1:W:131:SER:HB2	2.02	0.41
1:W:113:LYS:HG3	1:W:114:ILE:HG23	2.03	0.41
1:W:165:LEU:HD11	1:W:254:ILE:HB	2.03	0.41
1:X:165:LEU:HD11	1:X:254:ILE:HB	2.03	0.41
1:X:351:TRP:H	1:X:351:TRP:CD1	2.38	0.41
1:Z:186:TYR:HE1	1:Z:399:ARG:HD3	1.85	0.41
1:Z:351:TRP:H	1:Z:351:TRP:CD1	2.38	0.41
4:i:59:ALA:O	4:i:63:VAL:HG23	2.21	0.41
2:A:333:ARG:HH21	2:A:372:ALA:HB2	1.85	0.41
3:B:273:ASN:HB3	3:B:299:TRP:NE1	2.36	0.41
3:B:400:VAL:O	3:B:404:THR:HG23	2.21	0.41
3:D:855:GLN:HA	3:D:858:VAL:HG12	2.03	0.41
5:I:48:LEU:HD11	5:I:129:PHE:HB2	2.03	0.41
2:M:424:ASN:HD21	2:M:426:LYS:HB3	1.86	0.41
1:P:184:GLN:O	1:P:188:SER:OG	2.31	0.41
1:R:31:ILE:HD12	1:R:85:LEU:HD11	2.02	0.41
1:R:289:THR:OG1	1:R:290:VAL:N	2.55	0.41
1:S:363:LYS:HD2	1:S:363:LYS:HA	1.97	0.41
1:T:31:ILE:HD12	1:T:85:LEU:HD11	2.02	0.41
1:Y:415:LYS:HG2	1:Y:420:GLU:HG2	2.02	0.41
1:Z:228:ILE:O	1:Z:232:VAL:HG12	2.21	0.41
3:n:73:LEU:O	3:n:77:LEU:HG	2.21	0.41
1:l:415:LYS:HG2	1:l:420:GLU:HG2	2.02	0.40
3:D:762:CYS:SG	3:D:763:LEU:N	2.93	0.40
2:G:419:ILE:O	2:G:420:GLN:HG3	2.21	0.40
3:H:482:LYS:NZ	3:H:534:ILE:HG22	2.36	0.40
2:M:321:LEU:HD12	2:M:324:LEU:HD22	2.03	0.40
1:Q:228:ILE:O	1:Q:232:VAL:HG12	2.21	0.40
1:R:333:VAL:HB	1:R:358:VAL:HG11	2.03	0.40
1:T:164:LYS:HA	1:T:164:LYS:HD3	1.85	0.40
1:T:333:VAL:HB	1:T:358:VAL:HG11	2.03	0.40
1:X:228:ILE:O	1:X:232:VAL:HG12	2.21	0.40
7:c:88:ARG:HH11	7:c:91:GLU:HB2	1.85	0.40
2:E:306:LEU:O	2:E:310:LEU:HG	2.21	0.40
2:A:337:ILE:HG23	2:A:362:ARG:HH21	1.87	0.40
2:C:305:ILE:O	2:C:308:SER:OG	2.39	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:164:LYS:HG2	2:G:404:TYR:HA	2.04	0.40
2:G:696:TYR:O	2:G:700:GLU:CB	2.69	0.40
3:H:615:PRO:HA	3:H:618:LEU:HD12	2.04	0.40
3:N:677:LEU:HD21	3:N:712:VAL:HA	2.02	0.40
1:Q:289:THR:OG1	1:Q:290:VAL:N	2.55	0.40
1:Q:333:VAL:HB	1:Q:358:VAL:HG11	2.03	0.40
1:S:415:LYS:HG2	1:S:420:GLU:HG2	2.02	0.40
1:U:228:ILE:O	1:U:232:VAL:HG12	2.21	0.40
1:Y:25:LEU:HD23	1:Y:25:LEU:HA	1.90	0.40
1:Y:165:LEU:HD11	1:Y:254:ILE:HB	2.03	0.40
1:Z:113:LYS:HG3	1:Z:114:ILE:HG23	2.03	0.40
4:m:25:MET:HE1	4:m:48:VAL:HG21	2.03	0.40
4:m:33:ARG:HH21	6:l:127:VAL:HB	1.86	0.40
2:E:689:PHE:O	2:E:693:ILE:HG12	2.21	0.40
6:l:129:THR:OG1	6:l:130:PRO:HD3	2.21	0.40
3:D:885:HIS:CE1	1:R:352:GLY:HA2	2.56	0.40
3:F:290:THR:HG21	3:F:366:ARG:HG3	2.02	0.40
6:J:553:LYS:HD3	6:J:553:LYS:HA	1.89	0.40
7:L:465:LYS:HE3	7:L:465:LYS:HB3	1.93	0.40
1:O:333:VAL:HB	1:O:358:VAL:HG11	2.03	0.40
1:Q:46:ASP:OD1	1:Q:46:ASP:N	2.53	0.40
1:Q:266:LEU:HD22	1:Q:435:TYR:CD1	2.57	0.40
1:U:113:LYS:HG3	1:U:114:ILE:HG23	2.03	0.40
1:U:186:TYR:HE1	1:U:399:ARG:HD3	1.85	0.40
1:V:333:VAL:HB	1:V:358:VAL:HG11	2.03	0.40
1:W:228:ILE:O	1:W:232:VAL:HG12	2.21	0.40
1:Y:56:ASP:HB2	1:Z:301:LYS:HE2	2.03	0.40
2:E:572:ASP:HB3	2:E:621:ILE:HG12	2.03	0.40
1:1:46:ASP:OD1	1:1:46:ASP:N	2.53	0.40
1:2:245:TYR:HA	1:2:246:PRO:HD3	1.97	0.40
1:2:266:LEU:HD22	1:2:435:TYR:CD1	2.57	0.40
1:2:419:ASP:O	1:2:423:THR:OG1	2.37	0.40
2:A:319:LEU:HD21	2:A:324:LEU:HD12	2.02	0.40
2:C:644:HIS:CE1	2:C:738:MET:HB2	2.56	0.40
3:F:627:GLU:H	3:j:64:ARG:HH21	1.70	0.40
3:N:447:PHE:O	3:N:467:ARG:N	2.54	0.40
1:O:363:LYS:HD2	1:O:363:LYS:HA	1.97	0.40
1:Q:113:LYS:HG3	1:Q:114:ILE:HG23	2.03	0.40
1:S:31:ILE:HD12	1:S:85:LEU:HD11	2.02	0.40
1:S:46:ASP:OD1	1:S:46:ASP:N	2.53	0.40
1:S:351:TRP:CD1	1:S:351:TRP:H	2.38	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:383:SER:O	1:T:386:SER:OG	2.28	0.40
1:Y:266:LEU:HD22	1:Y:435:TYR:CD1	2.57	0.40
3:h:10:ASN:OD1	3:h:11:VAL:N	2.54	0.40
1:1:289:THR:OG1	1:1:290:VAL:N	2.55	0.40
1:2:113:LYS:HG3	1:2:114:ILE:HG23	2.03	0.40
3:D:724:PHE:CE1	1:R:360:LEU:HB2	2.57	0.40
3:F:848:ARG:HD2	3:F:848:ARG:HA	1.89	0.40
2:G:876:ARG:CD	4:k:56:ASN:HB3	2.51	0.40
5:K:300:LEU:HD23	5:K:339:HIS:HE1	1.86	0.40
5:K:381:LYS:HD2	5:K:381:LYS:HA	1.94	0.40
1:O:26:CYS:HA	1:O:31:ILE:HD11	2.04	0.40
1:O:31:ILE:HD12	1:O:85:LEU:HD11	2.02	0.40
1:O:289:THR:OG1	1:O:290:VAL:N	2.55	0.40
1:P:165:LEU:HD11	1:P:254:ILE:HB	2.03	0.40
1:T:3:ARG:HB2	1:T:4:GLU:H	1.62	0.40
1:T:160:ARG:HD2	1:T:160:ARG:HA	1.74	0.40
1:T:228:ILE:O	1:T:232:VAL:HG12	2.21	0.40
1:U:266:LEU:HD22	1:U:435:TYR:CD1	2.57	0.40
1:V:228:ILE:O	1:V:232:VAL:HG12	2.21	0.40
1:W:333:VAL:HB	1:W:358:VAL:HG11	2.03	0.40
2:E:174:LEU:HB3	2:E:404:TYR:OH	2.21	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%)	17 (4%)	0	100	100
1	2	408/451 (90%)	391 (96%)	17 (4%)	0	100	100
1	O	408/451 (90%)	391 (96%)	17 (4%)	0	100	100
1	P	408/451 (90%)	391 (96%)	17 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Q	408/451 (90%)	391 (96%)	17 (4%)	0	100	100
1	R	408/451 (90%)	391 (96%)	17 (4%)	0	100	100
1	S	408/451 (90%)	391 (96%)	17 (4%)	0	100	100
1	T	408/451 (90%)	391 (96%)	17 (4%)	0	100	100
1	U	408/451 (90%)	391 (96%)	17 (4%)	0	100	100
1	V	408/451 (90%)	391 (96%)	17 (4%)	0	100	100
1	W	408/451 (90%)	391 (96%)	17 (4%)	0	100	100
1	X	408/451 (90%)	391 (96%)	17 (4%)	0	100	100
1	Y	408/451 (90%)	391 (96%)	17 (4%)	0	100	100
1	Z	408/451 (90%)	391 (96%)	17 (4%)	0	100	100
2	A	599/902 (66%)	567 (95%)	31 (5%)	1 (0%)	43	78
2	C	606/902 (67%)	579 (96%)	27 (4%)	0	100	100
2	E	628/902 (70%)	589 (94%)	36 (6%)	3 (0%)	24	63
2	G	628/902 (70%)	600 (96%)	27 (4%)	1 (0%)	43	78
2	M	624/902 (69%)	585 (94%)	38 (6%)	1 (0%)	43	78
3	B	602/907 (66%)	580 (96%)	20 (3%)	2 (0%)	36	72
3	D	571/907 (63%)	540 (95%)	31 (5%)	0	100	100
3	F	591/907 (65%)	567 (96%)	24 (4%)	0	100	100
3	H	584/907 (64%)	560 (96%)	23 (4%)	1 (0%)	43	78
3	N	584/907 (64%)	556 (95%)	25 (4%)	3 (0%)	24	63
3	a	112/907 (12%)	107 (96%)	5 (4%)	0	100	100
3	f	97/907 (11%)	92 (95%)	5 (5%)	0	100	100
3	h	105/907 (12%)	102 (97%)	2 (2%)	1 (1%)	12	48
3	j	105/907 (12%)	96 (91%)	5 (5%)	4 (4%)	2	19
3	n	97/907 (11%)	93 (96%)	4 (4%)	0	100	100
4	b	63/82 (77%)	63 (100%)	0	0	100	100
4	d	57/82 (70%)	55 (96%)	2 (4%)	0	100	100
4	g	63/82 (77%)	62 (98%)	1 (2%)	0	100	100
4	i	63/82 (77%)	63 (100%)	0	0	100	100
4	k	63/82 (77%)	62 (98%)	1 (2%)	0	100	100
4	m	63/82 (77%)	63 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	o	63/82 (77%)	62 (98%)	1 (2%)	0	100	100
5	I	511/667 (77%)	483 (94%)	23 (4%)	5 (1%)	12	48
5	K	548/667 (82%)	532 (97%)	15 (3%)	1 (0%)	43	78
6	J	506/1024 (49%)	470 (93%)	29 (6%)	7 (1%)	9	40
6	l	104/1024 (10%)	92 (88%)	10 (10%)	2 (2%)	6	32
7	L	540/1819 (30%)	500 (93%)	35 (6%)	5 (1%)	14	51
7	c	112/1819 (6%)	108 (96%)	4 (4%)	0	100	100
All	All	15001/27488 (55%)	14302 (95%)	662 (4%)	37 (0%)	44	78

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	584	THR
2	G	675	TRP
5	I	404	LEU
5	I	408	ASP
5	I	508	ASN
6	J	236	LEU
6	J	238	LEU
6	J	799	LEU
2	M	241	ARG
3	N	455	LYS
2	E	241	ARG
3	B	871	GLU
3	H	628	VAL
7	L	308	GLU
3	j	104	PRO
3	j	108	PRO
3	j	112	SER
5	I	601	LEU
5	K	409	ASN
7	L	303	PRO
2	E	581	ASP
5	I	509	GLN
6	J	257	TYR
6	J	881	HIS
7	L	309	GLU
3	N	743	ASP
3	N	744	LEU
3	h	107	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	I	120	SER
3	B	870	ASP
6	J	264	LEU
2	E	522	MET
6	I	125	SER
6	J	237	HIS
7	L	310	PRO
3	j	111	VAL
7	L	343	GLN

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%)	348 (93%)	28 (7%)	13	33
1	2	376/400 (94%)	348 (93%)	28 (7%)	13	33
1	O	376/400 (94%)	348 (93%)	28 (7%)	13	33
1	P	376/400 (94%)	348 (93%)	28 (7%)	13	33
1	Q	376/400 (94%)	347 (92%)	29 (8%)	12	32
1	R	376/400 (94%)	348 (93%)	28 (7%)	13	33
1	S	376/400 (94%)	348 (93%)	28 (7%)	13	33
1	T	376/400 (94%)	348 (93%)	28 (7%)	13	33
1	U	376/400 (94%)	348 (93%)	28 (7%)	13	33
1	V	376/400 (94%)	348 (93%)	28 (7%)	13	33
1	W	376/400 (94%)	348 (93%)	28 (7%)	13	33
1	X	376/400 (94%)	347 (92%)	29 (8%)	12	32
1	Y	376/400 (94%)	347 (92%)	29 (8%)	12	32
1	Z	376/400 (94%)	348 (93%)	28 (7%)	13	33
2	A	549/791 (69%)	546 (100%)	3 (0%)	81	83
2	C	556/791 (70%)	555 (100%)	1 (0%)	87	87
2	E	575/791 (73%)	574 (100%)	1 (0%)	87	87

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	G	575/791 (73%)	573 (100%)	2 (0%)	86	86
2	M	572/791 (72%)	564 (99%)	8 (1%)	59	72
3	B	551/798 (69%)	550 (100%)	1 (0%)	87	87
3	D	525/798 (66%)	524 (100%)	1 (0%)	87	87
3	F	542/798 (68%)	540 (100%)	2 (0%)	84	84
3	H	539/798 (68%)	537 (100%)	2 (0%)	84	84
3	N	539/798 (68%)	535 (99%)	4 (1%)	76	81
3	a	101/798 (13%)	101 (100%)	0	100	100
3	f	88/798 (11%)	88 (100%)	0	100	100
3	h	96/798 (12%)	96 (100%)	0	100	100
3	j	96/798 (12%)	96 (100%)	0	100	100
3	n	88/798 (11%)	87 (99%)	1 (1%)	65	76
4	b	53/62 (86%)	52 (98%)	1 (2%)	50	67
4	d	53/62 (86%)	53 (100%)	0	100	100
4	g	53/62 (86%)	53 (100%)	0	100	100
4	i	53/62 (86%)	53 (100%)	0	100	100
4	k	53/62 (86%)	53 (100%)	0	100	100
4	m	53/62 (86%)	53 (100%)	0	100	100
4	o	53/62 (86%)	53 (100%)	0	100	100
5	I	472/594 (80%)	471 (100%)	1 (0%)	87	87
5	K	509/594 (86%)	506 (99%)	3 (1%)	78	83
6	J	498/933 (53%)	496 (100%)	2 (0%)	84	84
6	l	96/933 (10%)	96 (100%)	0	100	100
7	L	501/1546 (32%)	501 (100%)	0	100	100
7	c	101/1546 (6%)	101 (100%)	0	100	100
All	All	13804/24115 (57%)	13376 (97%)	428 (3%)	36	56

All (428) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	37	VAL
1	1	39	GLU
1	1	45	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	50	VAL
1	1	116	GLU
1	1	129	SER
1	1	188	SER
1	1	191	THR
1	1	201	CYS
1	1	204	VAL
1	1	218	LEU
1	1	224	SER
1	1	232	VAL
1	1	233	SER
1	1	266	LEU
1	1	290	VAL
1	1	299	GLN
1	1	301	LYS
1	1	316	CYS
1	1	324	ILE
1	1	331	THR
1	1	342	GLU
1	1	360	LEU
1	1	367	LEU
1	1	385	SER
1	1	391	THR
1	1	392	CYS
1	1	423	THR
1	2	37	VAL
1	2	39	GLU
1	2	45	THR
1	2	50	VAL
1	2	116	GLU
1	2	129	SER
1	2	188	SER
1	2	191	THR
1	2	201	CYS
1	2	204	VAL
1	2	218	LEU
1	2	224	SER
1	2	232	VAL
1	2	233	SER
1	2	266	LEU
1	2	290	VAL
1	2	299	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2	301	LYS
1	2	316	CYS
1	2	324	ILE
1	2	331	THR
1	2	342	GLU
1	2	360	LEU
1	2	367	LEU
1	2	385	SER
1	2	391	THR
1	2	392	CYS
1	2	423	THR
2	A	265	PRO
2	A	534	LEU
2	A	563	THR
3	B	648	ILE
2	C	864	PHE
3	D	592	LEU
3	F	426	VAL
3	F	490	ILE
2	G	328	ILE
2	G	563	THR
3	H	459	LEU
3	H	637	VAL
5	I	282	SER
6	J	226	THR
6	J	266	THR
5	K	140	VAL
5	K	469	PRO
5	K	645	LEU
2	M	176	ILE
2	M	181	VAL
2	M	475	ILE
2	M	700	GLU
2	M	701	VAL
2	M	722	VAL
2	M	742	PRO
2	M	747	VAL
3	N	271	THR
3	N	339	LEU
3	N	729	CYS
3	N	747	ILE
1	O	37	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	O	39	GLU
1	O	45	THR
1	O	50	VAL
1	O	116	GLU
1	O	129	SER
1	O	188	SER
1	O	191	THR
1	O	201	CYS
1	O	204	VAL
1	O	218	LEU
1	O	224	SER
1	O	232	VAL
1	O	233	SER
1	O	266	LEU
1	O	290	VAL
1	O	299	GLN
1	O	301	LYS
1	O	316	CYS
1	O	324	ILE
1	O	331	THR
1	O	342	GLU
1	O	360	LEU
1	O	367	LEU
1	O	385	SER
1	O	391	THR
1	O	392	CYS
1	O	423	THR
1	P	37	VAL
1	P	39	GLU
1	P	45	THR
1	P	50	VAL
1	P	116	GLU
1	P	129	SER
1	P	188	SER
1	P	191	THR
1	P	201	CYS
1	P	204	VAL
1	P	218	LEU
1	P	224	SER
1	P	232	VAL
1	P	233	SER
1	P	266	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	P	290	VAL
1	P	299	GLN
1	P	301	LYS
1	P	316	CYS
1	P	324	ILE
1	P	331	THR
1	P	342	GLU
1	P	360	LEU
1	P	367	LEU
1	P	385	SER
1	P	391	THR
1	P	392	CYS
1	P	423	THR
1	Q	37	VAL
1	Q	39	GLU
1	Q	45	THR
1	Q	50	VAL
1	Q	116	GLU
1	Q	129	SER
1	Q	188	SER
1	Q	191	THR
1	Q	201	CYS
1	Q	204	VAL
1	Q	218	LEU
1	Q	220	ILE
1	Q	224	SER
1	Q	232	VAL
1	Q	233	SER
1	Q	266	LEU
1	Q	290	VAL
1	Q	299	GLN
1	Q	301	LYS
1	Q	316	CYS
1	Q	324	ILE
1	Q	331	THR
1	Q	342	GLU
1	Q	360	LEU
1	Q	367	LEU
1	Q	385	SER
1	Q	391	THR
1	Q	392	CYS
1	Q	423	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	R	37	VAL
1	R	39	GLU
1	R	45	THR
1	R	50	VAL
1	R	116	GLU
1	R	129	SER
1	R	188	SER
1	R	191	THR
1	R	201	CYS
1	R	204	VAL
1	R	218	LEU
1	R	224	SER
1	R	232	VAL
1	R	233	SER
1	R	266	LEU
1	R	290	VAL
1	R	299	GLN
1	R	301	LYS
1	R	316	CYS
1	R	324	ILE
1	R	331	THR
1	R	342	GLU
1	R	360	LEU
1	R	367	LEU
1	R	385	SER
1	R	391	THR
1	R	392	CYS
1	R	423	THR
1	S	37	VAL
1	S	39	GLU
1	S	45	THR
1	S	50	VAL
1	S	116	GLU
1	S	129	SER
1	S	188	SER
1	S	191	THR
1	S	201	CYS
1	S	204	VAL
1	S	218	LEU
1	S	224	SER
1	S	232	VAL
1	S	233	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	S	266	LEU
1	S	290	VAL
1	S	299	GLN
1	S	301	LYS
1	S	316	CYS
1	S	324	ILE
1	S	331	THR
1	S	342	GLU
1	S	360	LEU
1	S	367	LEU
1	S	385	SER
1	S	391	THR
1	S	392	CYS
1	S	423	THR
1	T	37	VAL
1	T	39	GLU
1	T	45	THR
1	T	50	VAL
1	T	116	GLU
1	T	129	SER
1	T	188	SER
1	T	191	THR
1	T	201	CYS
1	T	204	VAL
1	T	218	LEU
1	T	224	SER
1	T	232	VAL
1	T	233	SER
1	T	266	LEU
1	T	290	VAL
1	T	299	GLN
1	T	301	LYS
1	T	316	CYS
1	T	324	ILE
1	T	331	THR
1	T	342	GLU
1	T	360	LEU
1	T	367	LEU
1	T	385	SER
1	T	391	THR
1	T	392	CYS
1	T	423	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	U	37	VAL
1	U	39	GLU
1	U	45	THR
1	U	50	VAL
1	U	116	GLU
1	U	129	SER
1	U	188	SER
1	U	191	THR
1	U	201	CYS
1	U	204	VAL
1	U	218	LEU
1	U	224	SER
1	U	232	VAL
1	U	233	SER
1	U	266	LEU
1	U	290	VAL
1	U	299	GLN
1	U	301	LYS
1	U	316	CYS
1	U	324	ILE
1	U	331	THR
1	U	342	GLU
1	U	360	LEU
1	U	367	LEU
1	U	385	SER
1	U	391	THR
1	U	392	CYS
1	U	423	THR
1	V	37	VAL
1	V	39	GLU
1	V	45	THR
1	V	50	VAL
1	V	116	GLU
1	V	129	SER
1	V	188	SER
1	V	191	THR
1	V	201	CYS
1	V	204	VAL
1	V	218	LEU
1	V	224	SER
1	V	232	VAL
1	V	233	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	V	266	LEU
1	V	290	VAL
1	V	299	GLN
1	V	301	LYS
1	V	316	CYS
1	V	324	ILE
1	V	331	THR
1	V	342	GLU
1	V	360	LEU
1	V	367	LEU
1	V	385	SER
1	V	391	THR
1	V	392	CYS
1	V	423	THR
1	W	37	VAL
1	W	39	GLU
1	W	45	THR
1	W	50	VAL
1	W	116	GLU
1	W	129	SER
1	W	188	SER
1	W	191	THR
1	W	201	CYS
1	W	204	VAL
1	W	218	LEU
1	W	224	SER
1	W	232	VAL
1	W	233	SER
1	W	266	LEU
1	W	290	VAL
1	W	299	GLN
1	W	301	LYS
1	W	316	CYS
1	W	324	ILE
1	W	331	THR
1	W	342	GLU
1	W	360	LEU
1	W	367	LEU
1	W	385	SER
1	W	391	THR
1	W	392	CYS
1	W	423	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	X	37	VAL
1	X	39	GLU
1	X	45	THR
1	X	50	VAL
1	X	116	GLU
1	X	129	SER
1	X	188	SER
1	X	191	THR
1	X	201	CYS
1	X	204	VAL
1	X	218	LEU
1	X	220	ILE
1	X	224	SER
1	X	232	VAL
1	X	233	SER
1	X	266	LEU
1	X	290	VAL
1	X	299	GLN
1	X	301	LYS
1	X	316	CYS
1	X	324	ILE
1	X	331	THR
1	X	342	GLU
1	X	360	LEU
1	X	367	LEU
1	X	385	SER
1	X	391	THR
1	X	392	CYS
1	X	423	THR
1	Y	37	VAL
1	Y	39	GLU
1	Y	45	THR
1	Y	50	VAL
1	Y	116	GLU
1	Y	129	SER
1	Y	188	SER
1	Y	191	THR
1	Y	201	CYS
1	Y	204	VAL
1	Y	218	LEU
1	Y	220	ILE
1	Y	224	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	Y	232	VAL
1	Y	233	SER
1	Y	266	LEU
1	Y	290	VAL
1	Y	299	GLN
1	Y	301	LYS
1	Y	316	CYS
1	Y	324	ILE
1	Y	331	THR
1	Y	342	GLU
1	Y	360	LEU
1	Y	367	LEU
1	Y	385	SER
1	Y	391	THR
1	Y	392	CYS
1	Y	423	THR
1	Z	37	VAL
1	Z	39	GLU
1	Z	45	THR
1	Z	50	VAL
1	Z	116	GLU
1	Z	129	SER
1	Z	188	SER
1	Z	191	THR
1	Z	201	CYS
1	Z	204	VAL
1	Z	218	LEU
1	Z	224	SER
1	Z	232	VAL
1	Z	233	SER
1	Z	266	LEU
1	Z	290	VAL
1	Z	299	GLN
1	Z	301	LYS
1	Z	316	CYS
1	Z	324	ILE
1	Z	331	THR
1	Z	342	GLU
1	Z	360	LEU
1	Z	367	LEU
1	Z	385	SER
1	Z	391	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	Z	392	CYS
1	Z	423	THR
4	b	39	LEU
3	n	47	VAL
2	E	855	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (383) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	15	ASN
1	1	29	HIS
1	1	54	GLN
1	1	103	ASN
1	1	175	GLN
1	1	184	GLN
1	1	219	HIS
1	1	250	ASN
1	1	314	ASN
1	1	322	ASN
1	1	429	GLN
1	1	436	HIS
1	2	12	GLN
1	2	15	ASN
1	2	29	HIS
1	2	54	GLN
1	2	103	ASN
1	2	184	GLN
1	2	250	ASN
1	2	314	ASN
1	2	334	HIS
1	2	357	GLN
1	2	429	GLN
1	2	436	HIS
2	A	165	GLN
2	A	172	GLN
2	A	213	GLN
2	A	261	HIS
2	A	303	HIS
2	A	438	GLN
2	A	644	HIS
2	A	662	ASN
2	A	688	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A	691	GLN
2	A	694	GLN
2	A	763	GLN
3	B	259	GLN
3	B	273	ASN
3	B	301	HIS
3	B	329	HIS
3	B	461	HIS
3	B	491	ASN
3	B	498	HIS
3	B	705	HIS
3	B	717	GLN
3	B	739	GLN
3	B	740	GLN
3	B	786	GLN
3	B	859	GLN
3	B	860	GLN
2	C	309	GLN
2	C	322	GLN
2	C	373	GLN
2	C	401	HIS
2	C	430	GLN
2	C	465	HIS
2	C	639	GLN
2	C	692	ASN
2	C	862	ASN
3	D	265	ASN
3	D	330	GLN
3	D	345	GLN
3	D	479	GLN
3	D	491	ASN
3	D	609	ASN
3	D	665	ASN
3	D	684	HIS
3	D	719	GLN
3	D	751	HIS
3	D	773	ASN
3	D	781	GLN
3	D	789	GLN
3	D	883	ASN
3	D	885	HIS
4	o	17	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	F	310	GLN
3	F	347	GLN
3	F	389	GLN
3	F	444	HIS
3	F	479	GLN
3	F	495	GLN
3	F	595	HIS
3	F	596	ASN
3	F	684	HIS
3	F	705	HIS
3	F	717	GLN
3	F	781	GLN
3	F	787	ASN
3	F	859	GLN
2	G	166	ASN
2	G	169	ASN
2	G	289	ASN
2	G	303	HIS
2	G	312	GLN
2	G	360	HIS
2	G	401	HIS
2	G	436	GLN
2	G	438	GLN
2	G	465	HIS
2	G	524	GLN
2	G	530	HIS
2	G	565	ASN
2	G	650	HIS
2	G	674	GLN
2	G	688	ASN
2	G	691	GLN
2	G	767	GLN
3	H	273	ASN
3	H	343	HIS
3	H	345	GLN
3	H	416	GLN
3	H	479	GLN
3	H	491	ASN
3	H	495	GLN
3	H	531	GLN
3	H	560	GLN
3	H	609	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	H	717	GLN
3	H	742	GLN
3	H	751	HIS
3	H	786	GLN
3	H	883	ASN
3	H	885	HIS
5	I	61	GLN
5	I	82	HIS
5	I	199	GLN
5	I	200	HIS
5	I	312	HIS
5	I	316	GLN
5	I	393	ASN
5	I	476	ASN
5	I	543	GLN
5	I	599	GLN
6	J	223	GLN
6	J	435	HIS
6	J	823	GLN
6	J	879	GLN
6	J	895	ASN
6	J	914	GLN
6	J	938	HIS
6	J	1009	HIS
5	K	3	HIS
5	K	43	ASN
5	K	61	GLN
5	K	67	GLN
5	K	76	GLN
5	K	98	GLN
5	K	116	HIS
5	K	123	ASN
5	K	152	GLN
5	K	160	HIS
5	K	290	ASN
5	K	316	GLN
5	K	327	GLN
5	K	353	GLN
5	K	398	GLN
5	K	493	GLN
5	K	547	GLN
5	K	561	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	K	567	ASN
5	K	599	GLN
5	K	657	GLN
7	L	430	GLN
7	L	469	GLN
7	L	507	GLN
7	L	603	ASN
7	L	1492	ASN
7	L	1654	GLN
7	L	1663	HIS
7	L	1666	GLN
7	L	1682	HIS
7	L	1742	GLN
7	L	1766	GLN
7	L	1767	GLN
7	L	1770	ASN
7	L	1792	GLN
7	L	1805	ASN
7	L	1806	ASN
2	M	213	GLN
2	M	261	HIS
2	M	287	GLN
2	M	289	ASN
2	M	314	HIS
2	M	316	GLN
2	M	329	GLN
2	M	465	HIS
2	M	493	ASN
2	M	530	HIS
2	M	585	GLN
2	M	654	GLN
2	M	694	GLN
2	M	712	ASN
2	M	718	ASN
2	M	726	HIS
2	M	760	ASN
2	M	862	ASN
3	N	269	ASN
3	N	302	ASN
3	N	416	GLN
3	N	461	HIS
3	N	494	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	N	495	GLN
3	N	643	HIS
3	N	665	ASN
3	N	716	HIS
3	N	719	GLN
3	N	736	ASN
3	N	739	GLN
3	N	742	GLN
3	N	751	HIS
3	N	774	GLN
3	N	781	GLN
3	N	885	HIS
1	O	12	GLN
1	O	15	ASN
1	O	29	HIS
1	O	54	GLN
1	O	103	ASN
1	O	110	GLN
1	O	184	GLN
1	O	219	HIS
1	O	250	ASN
1	O	314	ASN
1	O	322	ASN
1	O	429	GLN
1	O	436	HIS
1	P	15	ASN
1	P	29	HIS
1	P	54	GLN
1	P	103	ASN
1	P	110	GLN
1	P	184	GLN
1	P	219	HIS
1	P	250	ASN
1	P	322	ASN
1	P	334	HIS
1	P	429	GLN
1	P	436	HIS
1	Q	12	GLN
1	Q	15	ASN
1	Q	29	HIS
1	Q	54	GLN
1	Q	103	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	Q	184	GLN
1	Q	219	HIS
1	Q	250	ASN
1	Q	314	ASN
1	Q	322	ASN
1	Q	429	GLN
1	R	12	GLN
1	R	15	ASN
1	R	29	HIS
1	R	54	GLN
1	R	102	ASN
1	R	103	ASN
1	R	184	GLN
1	R	219	HIS
1	R	250	ASN
1	R	314	ASN
1	R	322	ASN
1	R	429	GLN
1	S	12	GLN
1	S	15	ASN
1	S	29	HIS
1	S	54	GLN
1	S	103	ASN
1	S	158	ASN
1	S	184	GLN
1	S	219	HIS
1	S	250	ASN
1	S	322	ASN
1	S	429	GLN
1	T	12	GLN
1	T	15	ASN
1	T	29	HIS
1	T	54	GLN
1	T	103	ASN
1	T	184	GLN
1	T	219	HIS
1	T	250	ASN
1	T	314	ASN
1	T	322	ASN
1	T	429	GLN
1	U	12	GLN
1	U	15	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	U	29	HIS
1	U	54	GLN
1	U	103	ASN
1	U	175	GLN
1	U	184	GLN
1	U	219	HIS
1	U	250	ASN
1	U	314	ASN
1	U	322	ASN
1	U	429	GLN
1	U	436	HIS
1	V	15	ASN
1	V	29	HIS
1	V	54	GLN
1	V	103	ASN
1	V	175	GLN
1	V	184	GLN
1	V	219	HIS
1	V	250	ASN
1	V	314	ASN
1	V	322	ASN
1	V	338	GLN
1	V	357	GLN
1	V	429	GLN
1	W	15	ASN
1	W	29	HIS
1	W	54	GLN
1	W	103	ASN
1	W	184	GLN
1	W	219	HIS
1	W	314	ASN
1	W	322	ASN
1	X	12	GLN
1	X	15	ASN
1	X	29	HIS
1	X	54	GLN
1	X	103	ASN
1	X	184	GLN
1	X	219	HIS
1	X	250	ASN
1	X	314	ASN
1	X	322	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	X	429	GLN
1	Y	15	ASN
1	Y	29	HIS
1	Y	54	GLN
1	Y	103	ASN
1	Y	184	GLN
1	Y	219	HIS
1	Y	250	ASN
1	Y	314	ASN
1	Y	322	ASN
1	Y	334	HIS
1	Y	338	GLN
1	Y	429	GLN
1	Z	12	GLN
1	Z	15	ASN
1	Z	29	HIS
1	Z	54	GLN
1	Z	103	ASN
1	Z	184	GLN
1	Z	219	HIS
1	Z	250	ASN
1	Z	314	ASN
1	Z	322	ASN
1	Z	338	GLN
1	Z	429	GLN
4	i	56	ASN
4	b	17	ASN
4	b	53	GLN
3	n	30	GLN
3	n	33	GLN
3	j	14	GLN
3	j	30	GLN
3	j	78	HIS
3	a	31	GLN
3	a	65	GLN
3	a	78	HIS
7	c	138	HIS
7	c	142	ASN
2	E	169	ASN
2	E	172	GLN
2	E	287	GLN
2	E	303	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	373	GLN
2	E	420	GLN
2	E	424	ASN
2	E	438	GLN
2	E	487	GLN
2	E	512	HIS
2	E	585	GLN
2	E	631	ASN
2	E	650	HIS
2	E	691	GLN
2	E	741	ASN
6	1	38	GLN
6	1	42	ASN
6	1	107	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

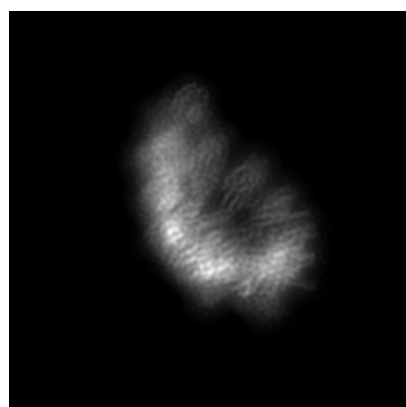
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14018. These allow visual inspection of the internal detail of the map and identification of artifacts.

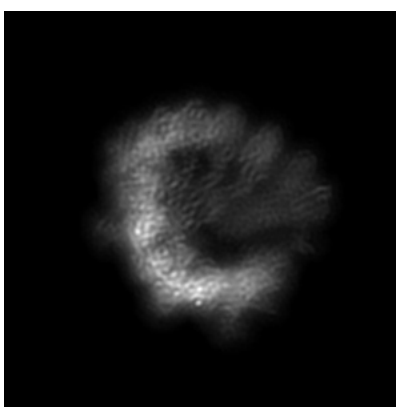
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

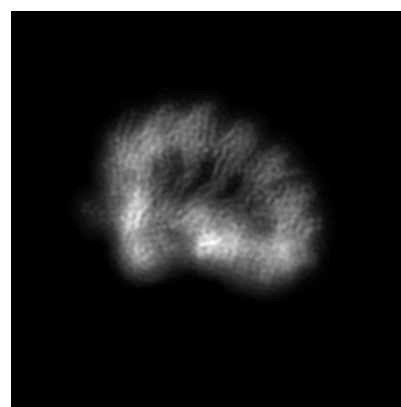
6.1.1 Primary map



X



Y



Z

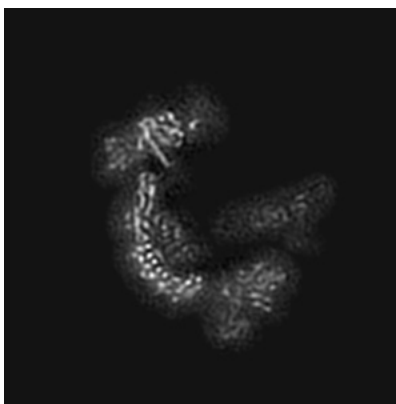
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

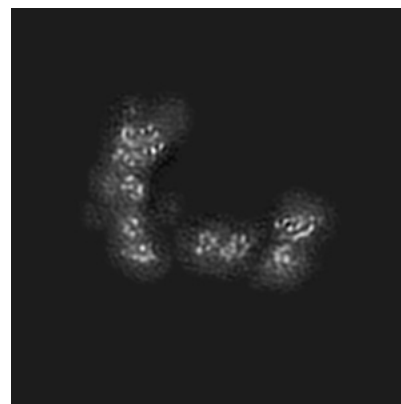
6.2.1 Primary map



X Index: 100



Y Index: 100

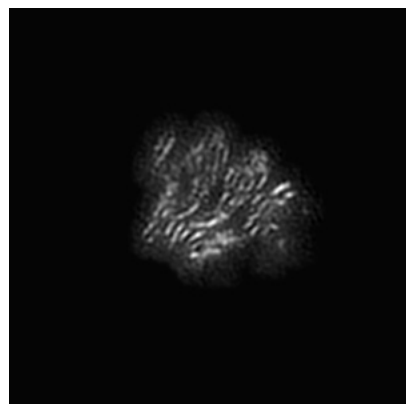


Z Index: 100

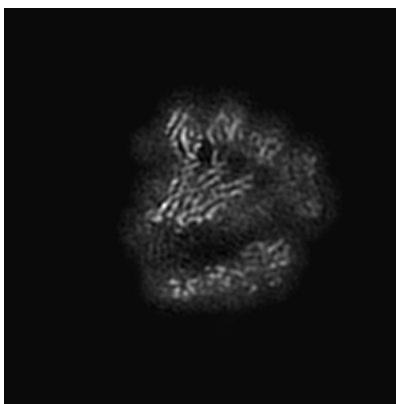
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

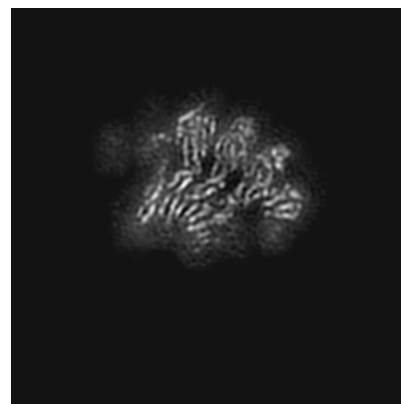
6.3.1 Primary map



X Index: 62



Y Index: 82

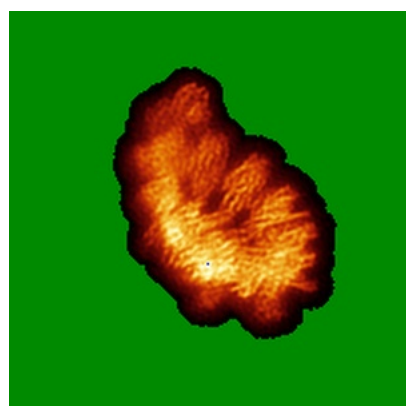


Z Index: 71

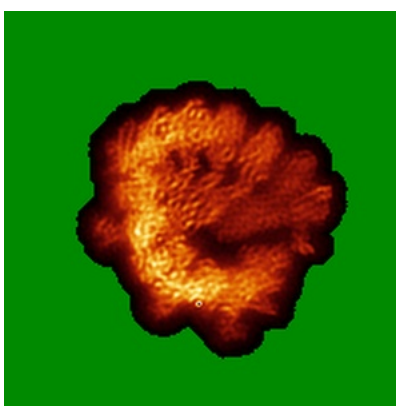
The images above show the largest variance slices of the map in three orthogonal directions.

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

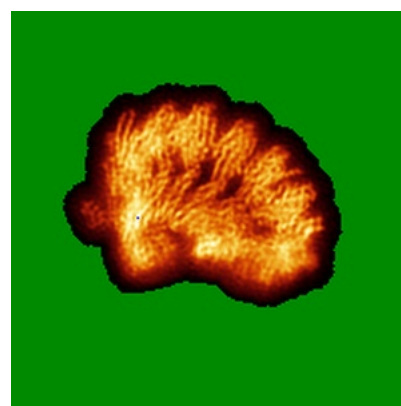
6.4.1 Primary map



X



Y



Z

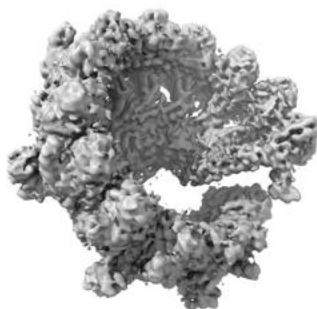
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

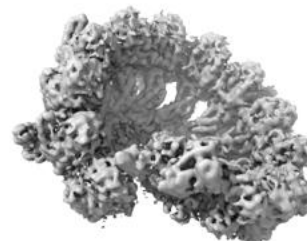
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0274. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

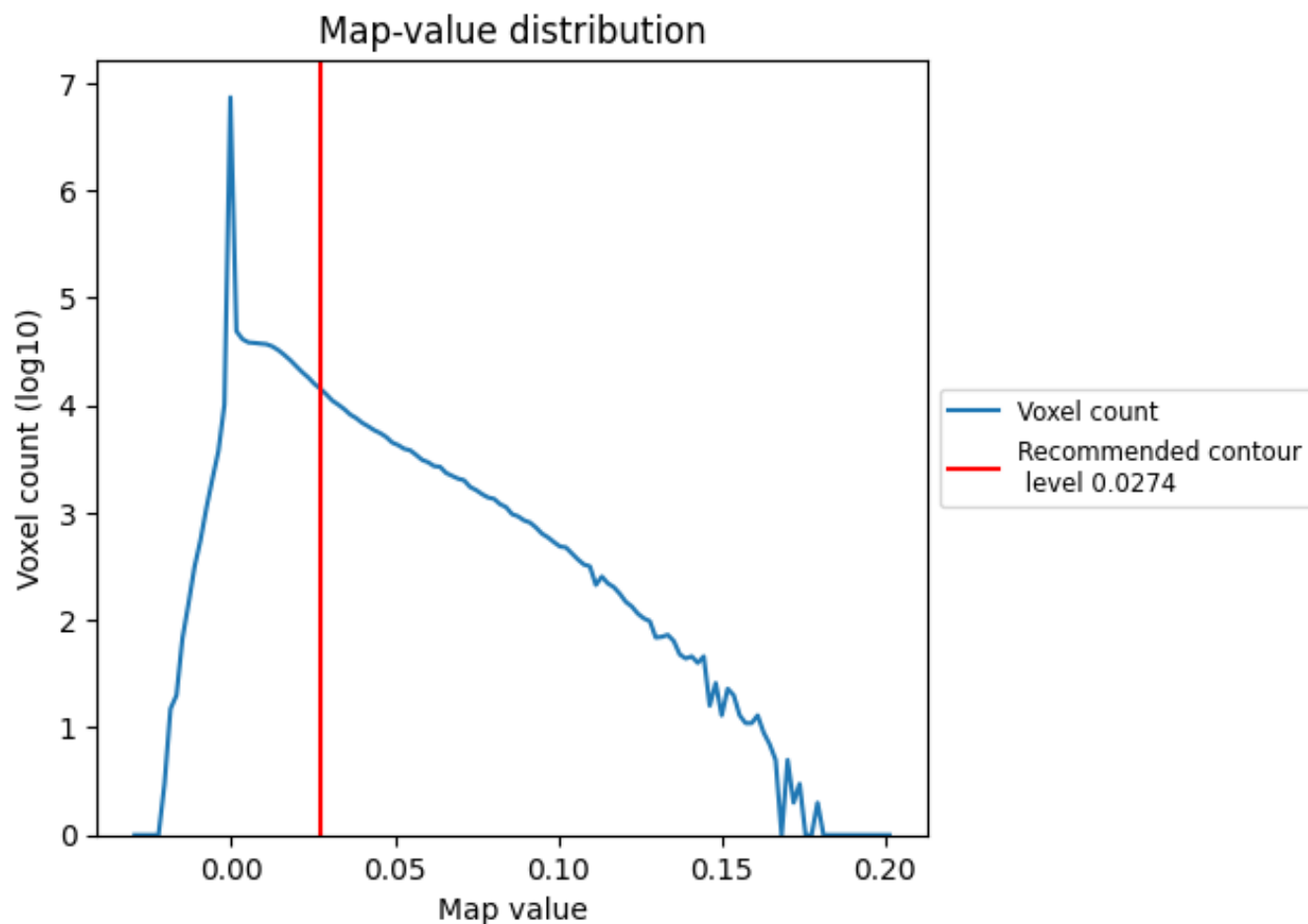
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

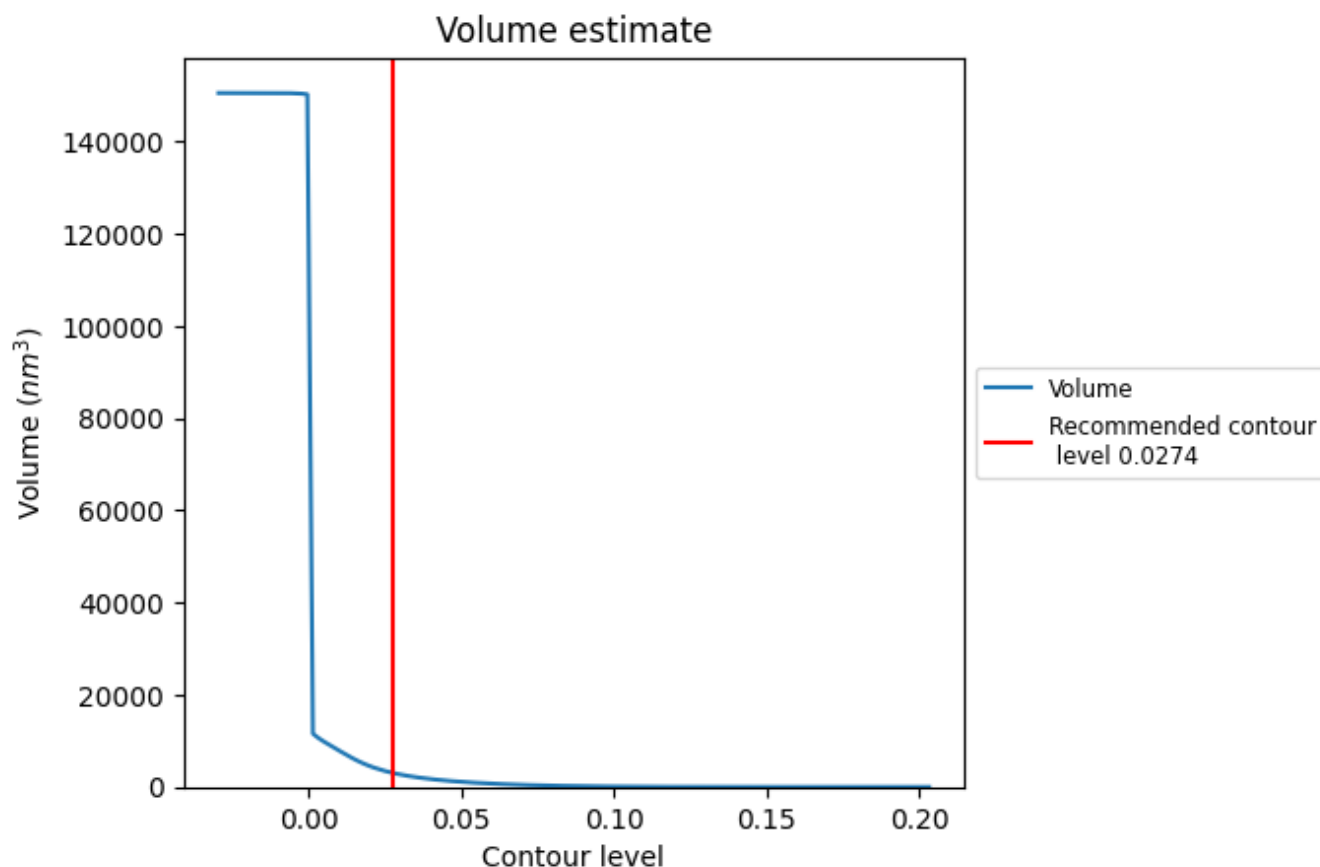
This section contains the results of statistical analysis of the map.

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.

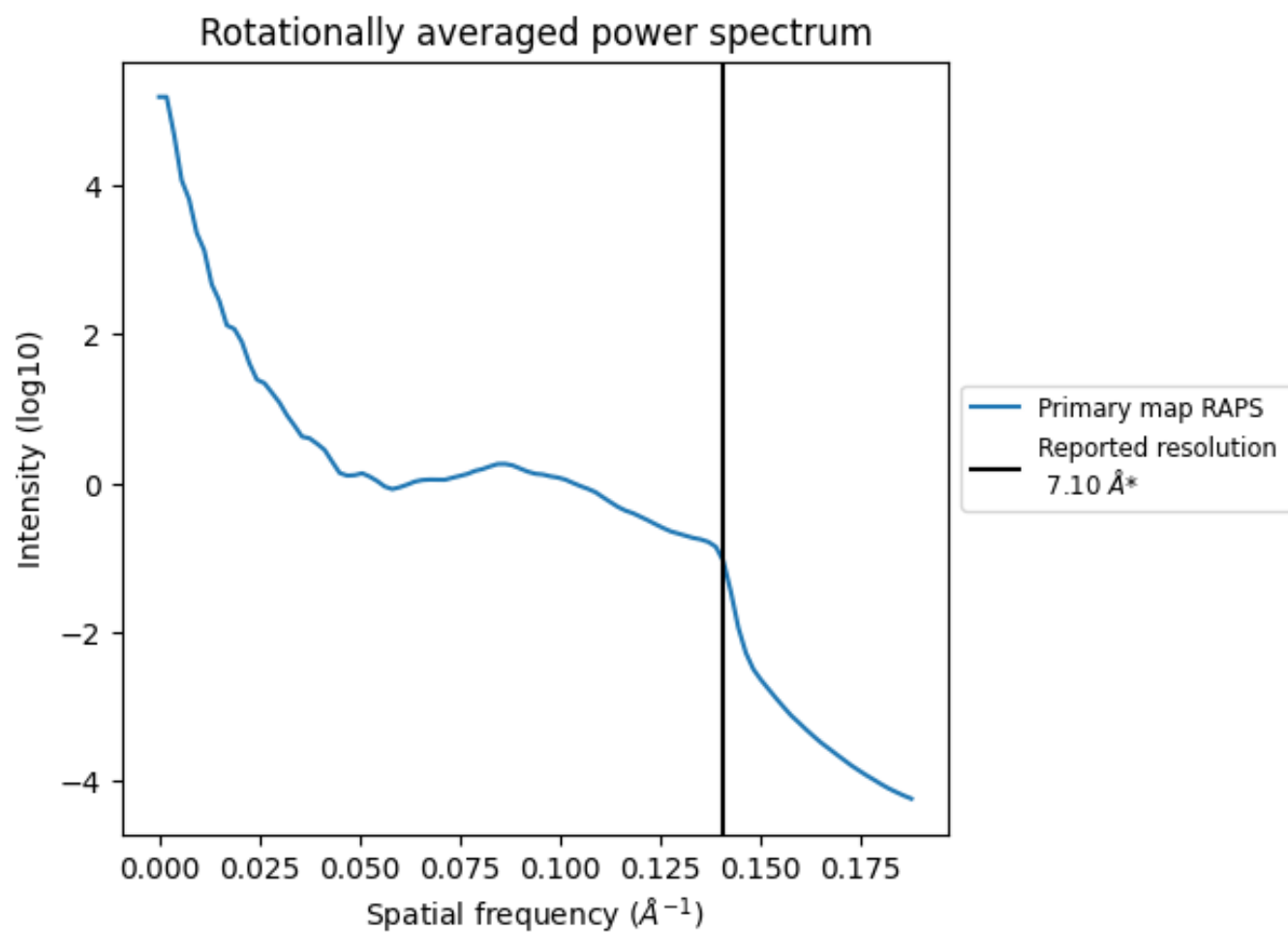
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3057 nm^3 ; this corresponds to an approximate mass of 2762 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 0.141 Å⁻¹

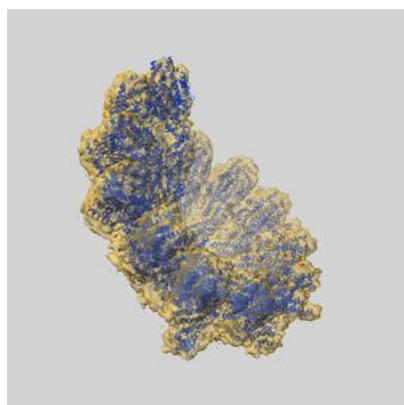
8 Fourier-Shell correlation

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

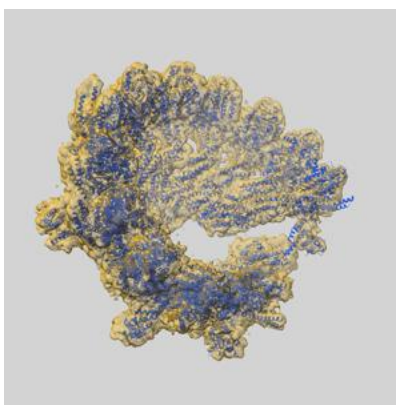
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-14018 and PDB model 7QJD. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

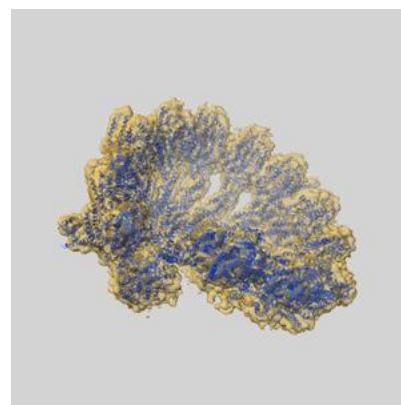
9.1 Map-model overlay [i](#)



X



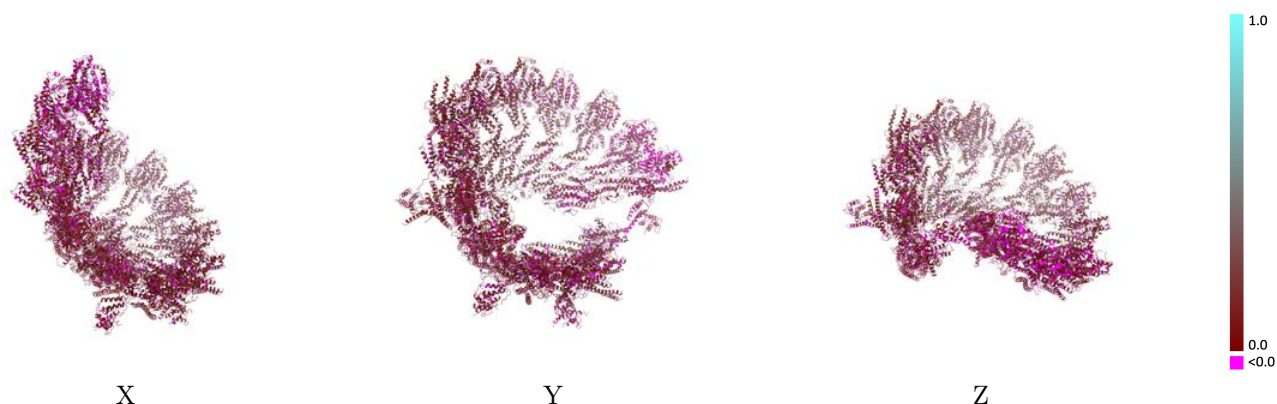
Y



Z

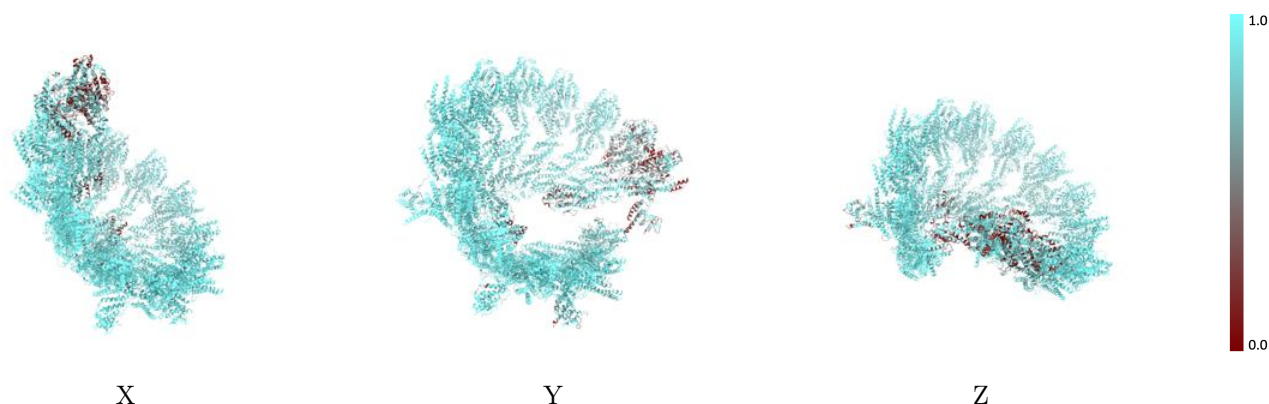
The images above show the 3D surface view of the map at the recommended contour level 0.0274 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



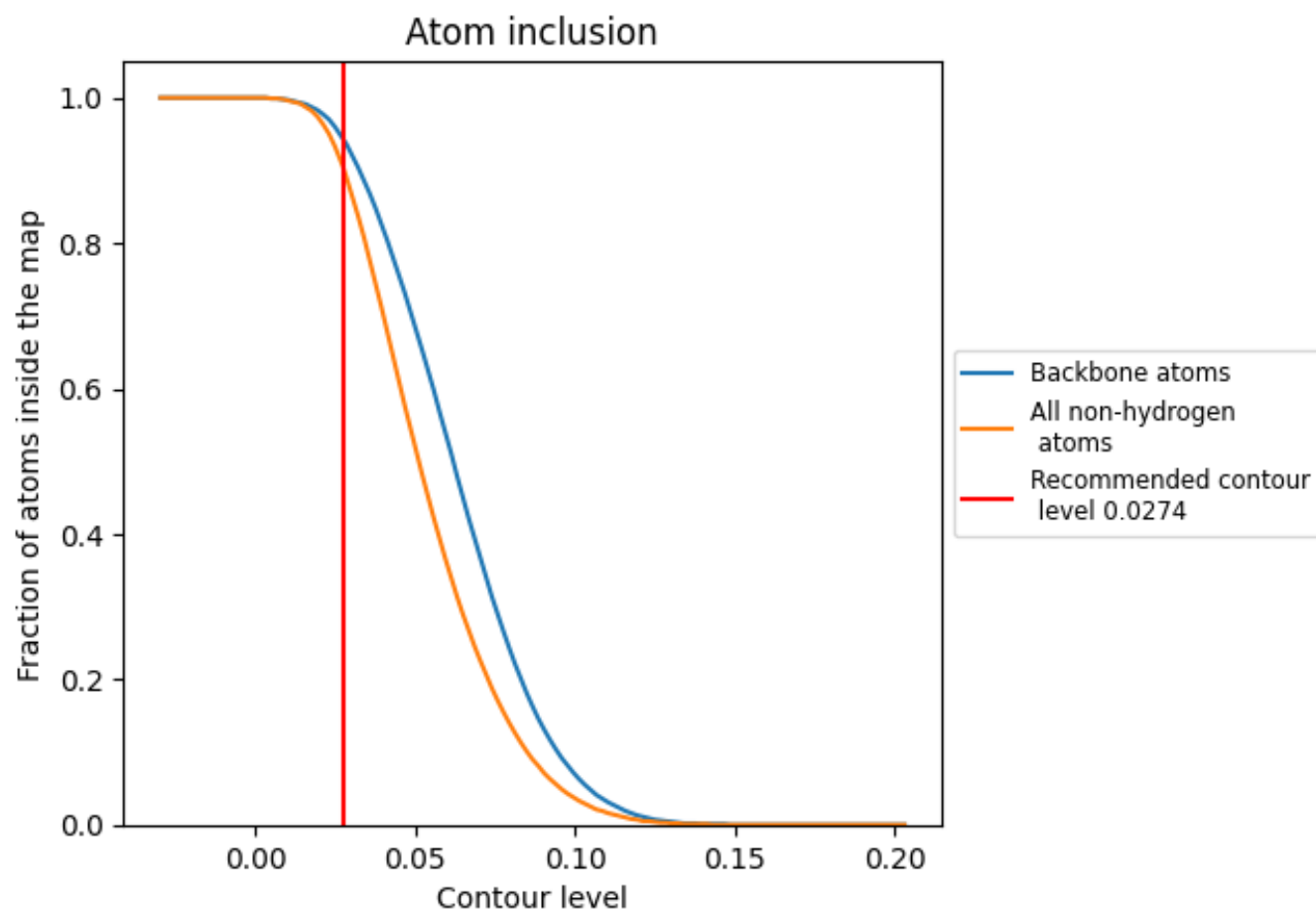
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0274).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 91% 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 (0.0274) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9060	 0.1100
1	 0.6200	 0.0410
2	 0.4660	 0.0060
A	 0.9530	 0.1130
B	 0.9430	 0.1190
C	 0.9840	 0.1270
D	 0.9790	 0.1300
E	 0.9820	 0.1300
F	 0.9690	 0.1280
G	 0.9610	 0.1340
H	 0.9610	 0.1380
I	 0.9430	 0.1440
J	 0.9680	 0.1380
K	 0.9530	 0.1210
L	 0.9600	 0.1160
M	 0.7100	 0.0800
N	 0.7020	 0.0790
O	 0.9080	 0.0810
P	 0.9410	 0.0990
Q	 0.9560	 0.1120
R	 0.9730	 0.1140
S	 0.9730	 0.1140
T	 0.9790	 0.1310
U	 0.9720	 0.1210
V	 0.9710	 0.1220
W	 0.9620	 0.1140
X	 0.9770	 0.1190
Y	 0.9720	 0.0760
Z	 0.9580	 0.0800
a	 0.8160	 0.1300
b	 0.8490	 0.1630
c	 0.7680	 0.1160
d	 0.4130	 0.1250
f	 0.7210	 0.0840
g	 0.7460	 0.1280



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
h	 0.9040	 0.1040
i	 0.9310	 0.1110
j	 0.9190	 0.0920
k	 0.9240	 0.1570
l	 0.9430	 0.1030
m	 0.9450	 0.1230
n	 0.4260	 0.0490
o	 0.5610	 0.0750