



## Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 02:10 PM EST

PDB ID : 3B63  
EMDB ID : EMD-1088  
Title : Actin filament model in the extended form of acromsomal bundle in the Limulus sperm  
Authors : Cong, Y.; Topf, M.; Sali, A.; Matsudaira, P.; Dougherty, M.; Chiu, W.; Schmid, M.F.  
Deposited on : 2007-10-26  
Resolution : 9.50 Å (reported)  
Based on initial models : 1HIV, 1HLU, 1YAG, 1ATN, 1YVN, 1MDU, 1ESV, 1T44, 1NWK

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.dev43  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.3

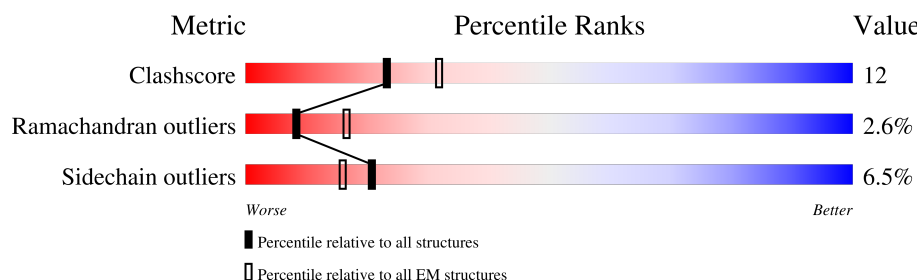
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 9.50 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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  $\geq 3$ , 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	A	365	<div> <div>92%</div> <div>66% 29% 5%</div> </div>
1	G	365	<div> <div>93%</div> <div>70% 27% .</div> </div>
2	B	364	<div> <div>90%</div> <div>63% 31% 5% .</div> </div>
3	C	365	<div> <div>90%</div> <div>68% 30% ..</div> </div>
3	I	365	<div> <div>99%</div> <div>67% 30% .</div> </div>
4	D	357	<div> <div>92%</div> <div>63% 31% 6%</div> </div>
5	E	365	<div> <div>92%</div> <div>62% 33% 5% .</div> </div>
5	H	365	<div> <div>97%</div> <div>66% 30% . .</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	J	365	<div><div>97%</div><div><div></div><div></div><div></div></div><div>64%30%5%•</div></div>
5	K	365	<div><div>96%</div><div><div></div><div></div><div></div></div><div>63%33%••</div></div>
5	N	365	<div><div>93%</div><div><div></div><div></div><div></div></div><div>58%36%5%•</div></div>
6	F	357	<div><div>90%</div><div><div></div><div></div><div></div></div><div>57%37%5%•</div></div>
7	L	365	<div><div>95%</div><div><div></div><div></div><div></div></div><div>60%35%••</div></div>
7	M	365	<div><div>92%</div><div><div></div><div></div><div></div></div><div>64%32%•</div></div>

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 39685 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Actin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	365	Total	C	N	O	S	0	0
			2843	1800	480	545	18		
1	G	365	Total	C	N	O	S	0	0
			2843	1800	480	545	18		

- Molecule 2 is a protein called Actin.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	364	Total	C	N	O	S	0	0
			2835	1796	474	545	20		

- Molecule 3 is a protein called Actin.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	365	Total	C	N	O	S	0	0
			2842	1801	479	544	18		
3	I	365	Total	C	N	O	S	0	0
			2842	1801	479	544	18		

- Molecule 4 is a protein called Actin.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	357	Total	C	N	O	S	0	0
			2791	1768	467	536	20		

- Molecule 5 is a protein called Actin.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	365	Total	C	N	O	S	0	0
			2845	1802	477	546	20		
5	H	365	Total	C	N	O	S	0	0
			2845	1802	477	546	20		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf	Trace
5	J	365	Total	C	N	O	S	0	0
			2845	1802	477	546	20		
5	K	365	Total	C	N	O	S	0	0
			2845	1802	477	546	20		
5	N	365	Total	C	N	O	S	0	0
			2845	1802	477	546	20		

- Molecule 6 is a protein called Actin.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	357	Total	C	N	O	S	0	0
			2788	1767	467	534	20		

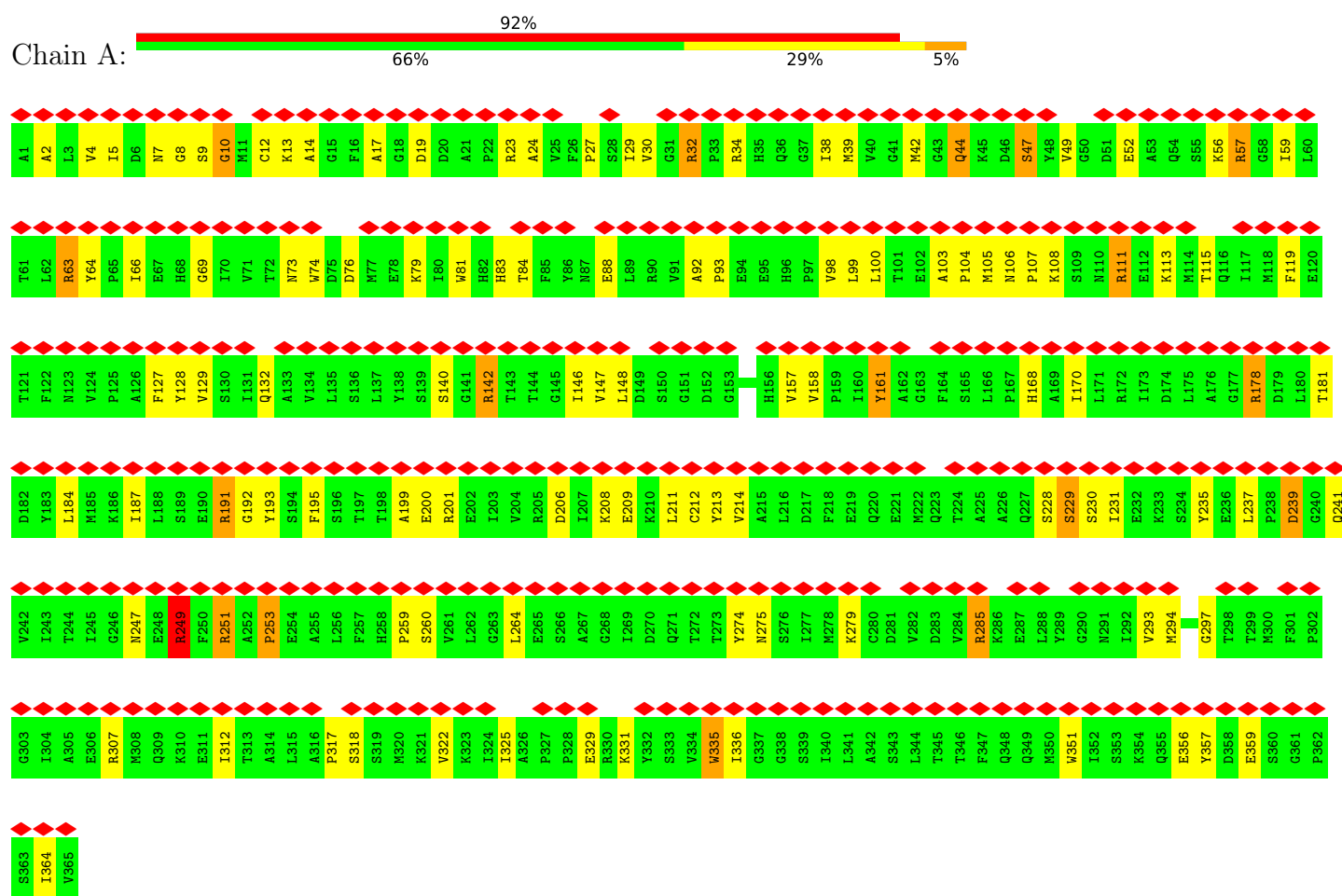
- Molecule 7 is a protein called Actin.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	L	365	Total	C	N	O	S	0	0
			2838	1797	475	545	21		
7	M	365	Total	C	N	O	S	0	0
			2838	1797	475	545	21		

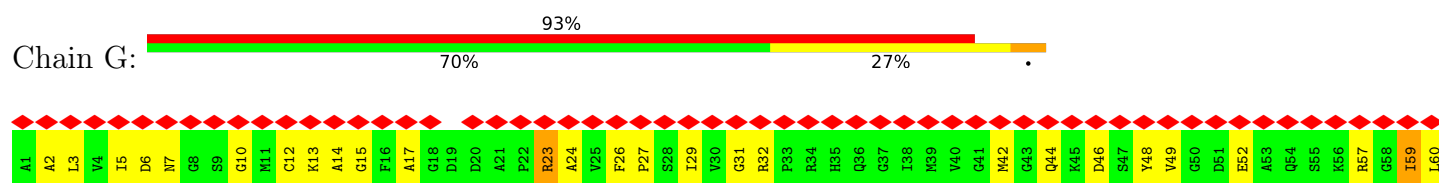
### 3 Residue-property plots

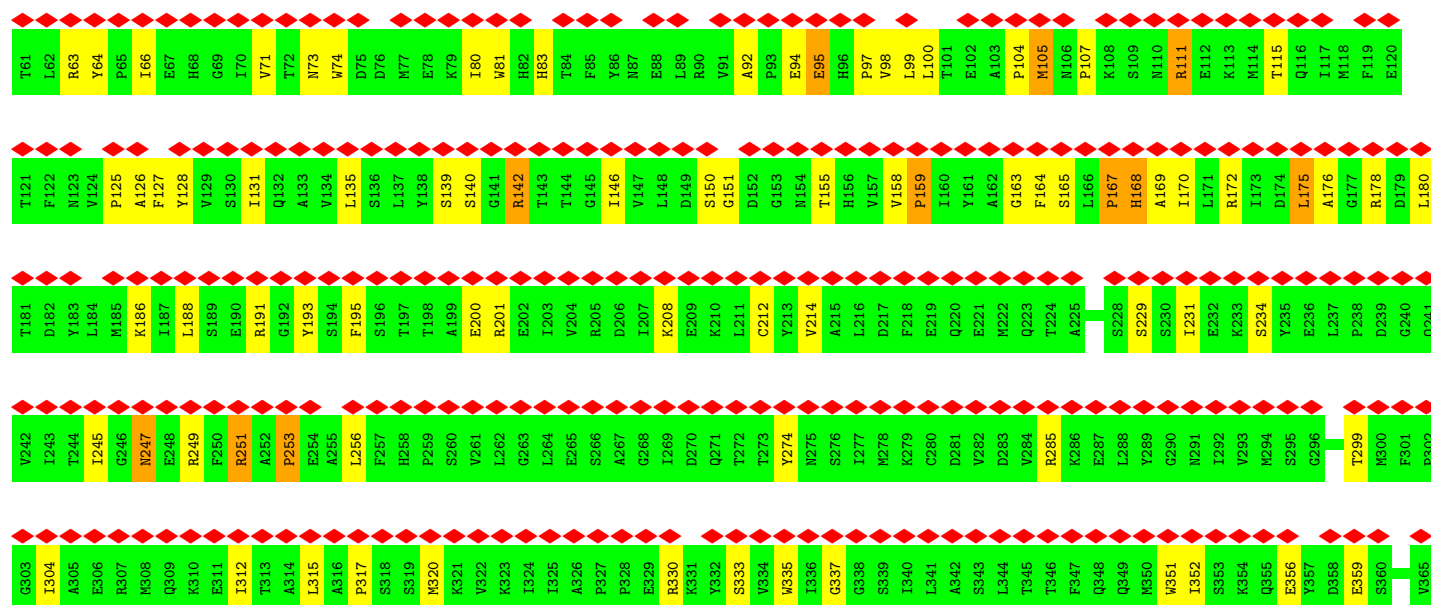
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

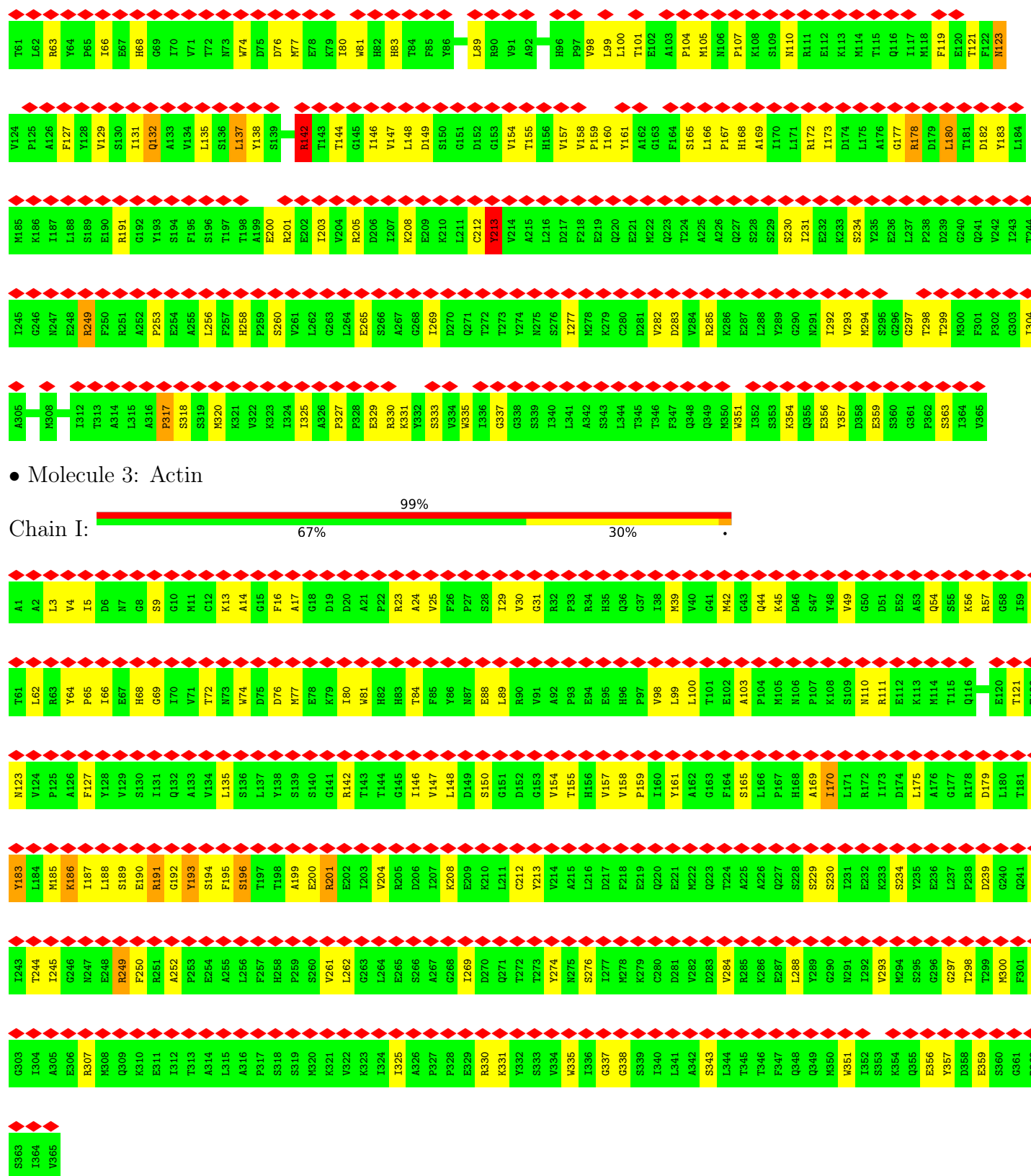
#### • Molecule 1: Actin



#### • Molecule 1: Actin



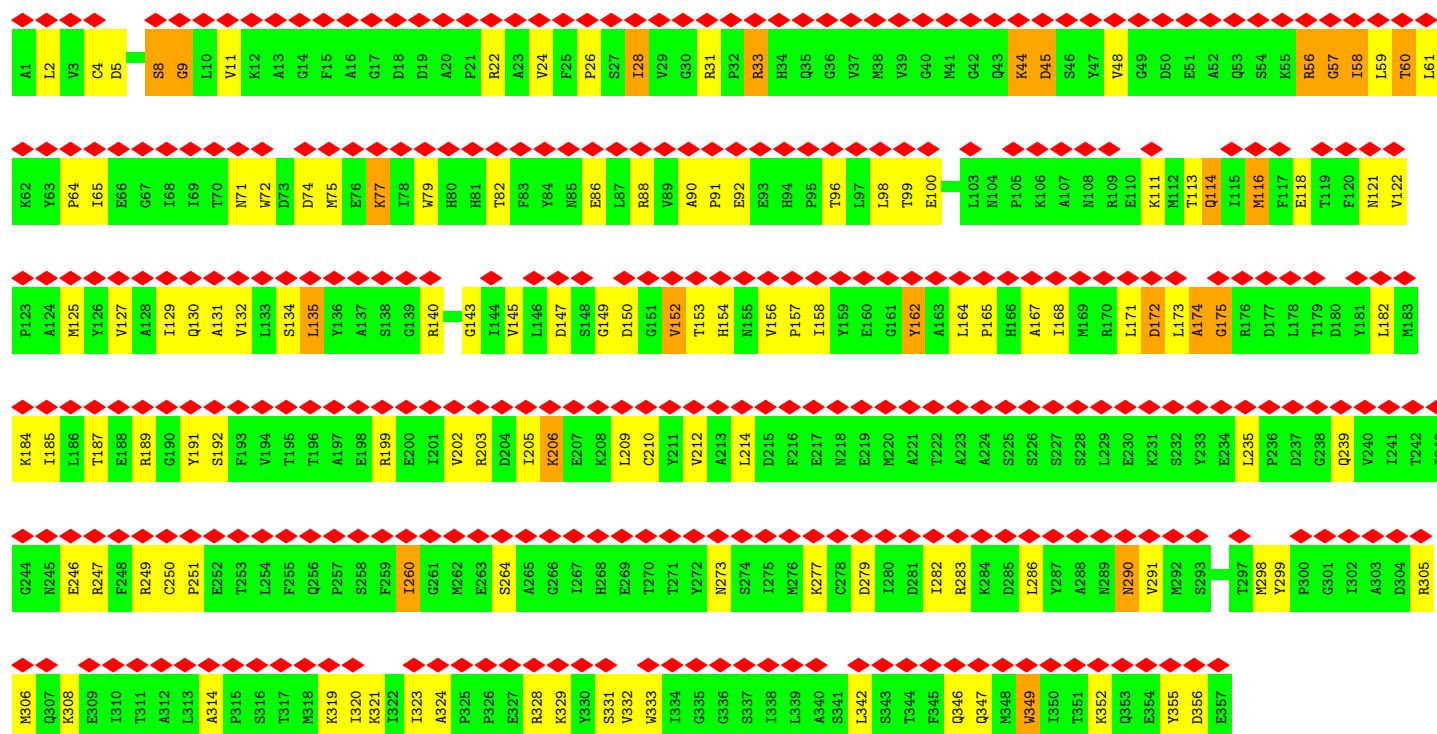




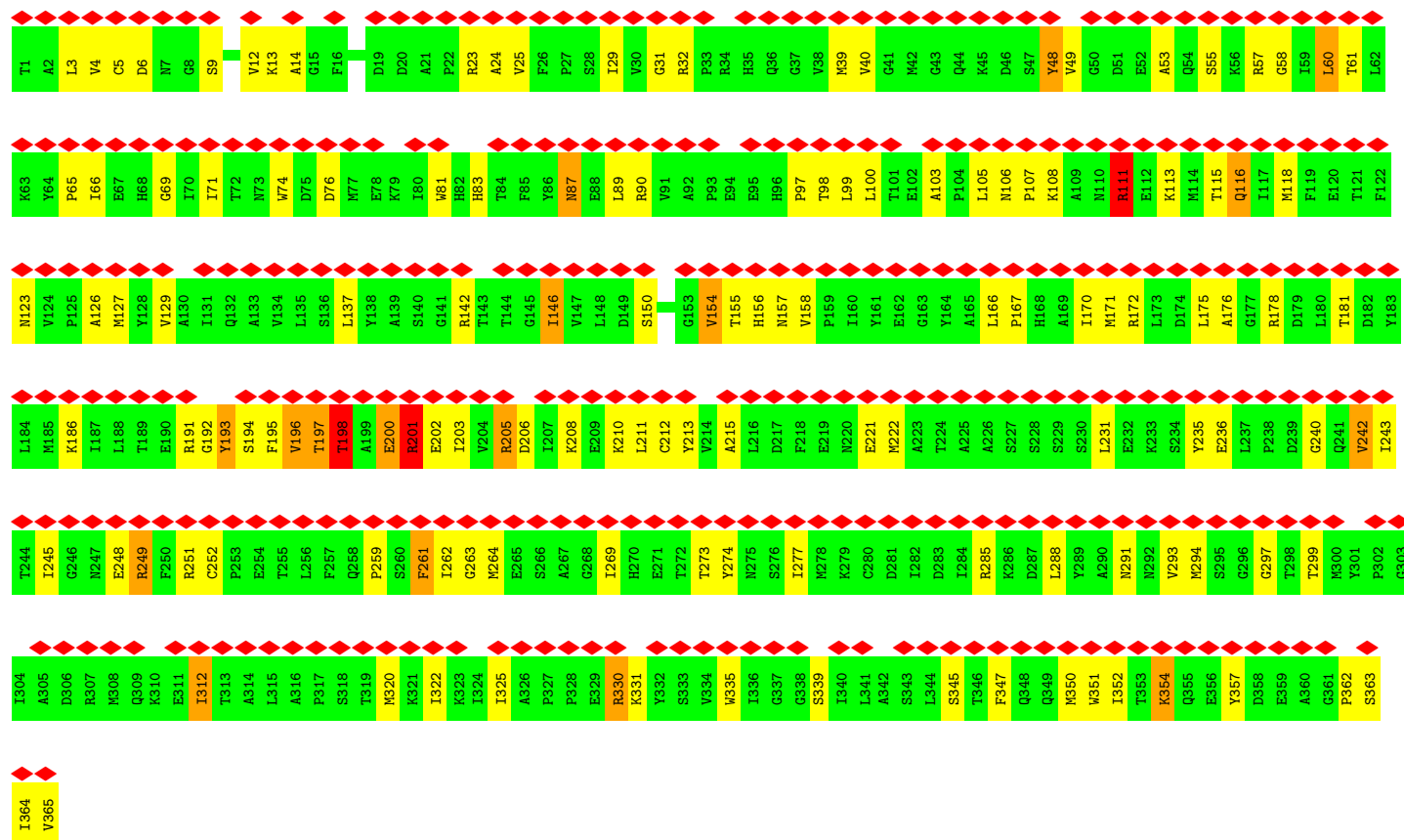
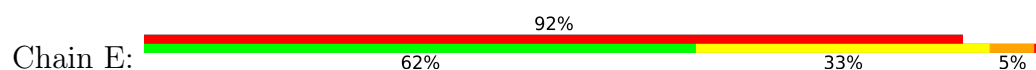
• Molecule 4: Actin



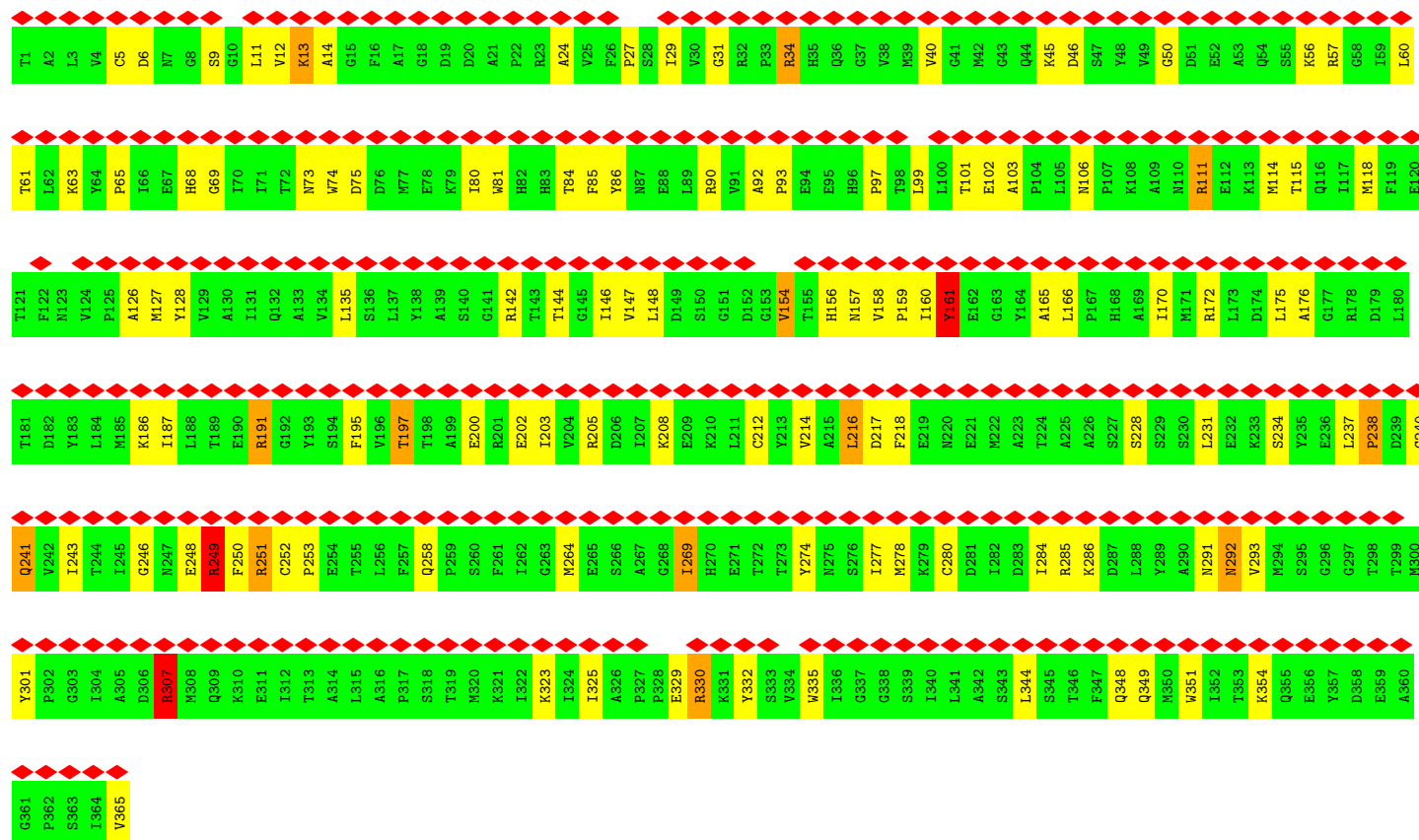




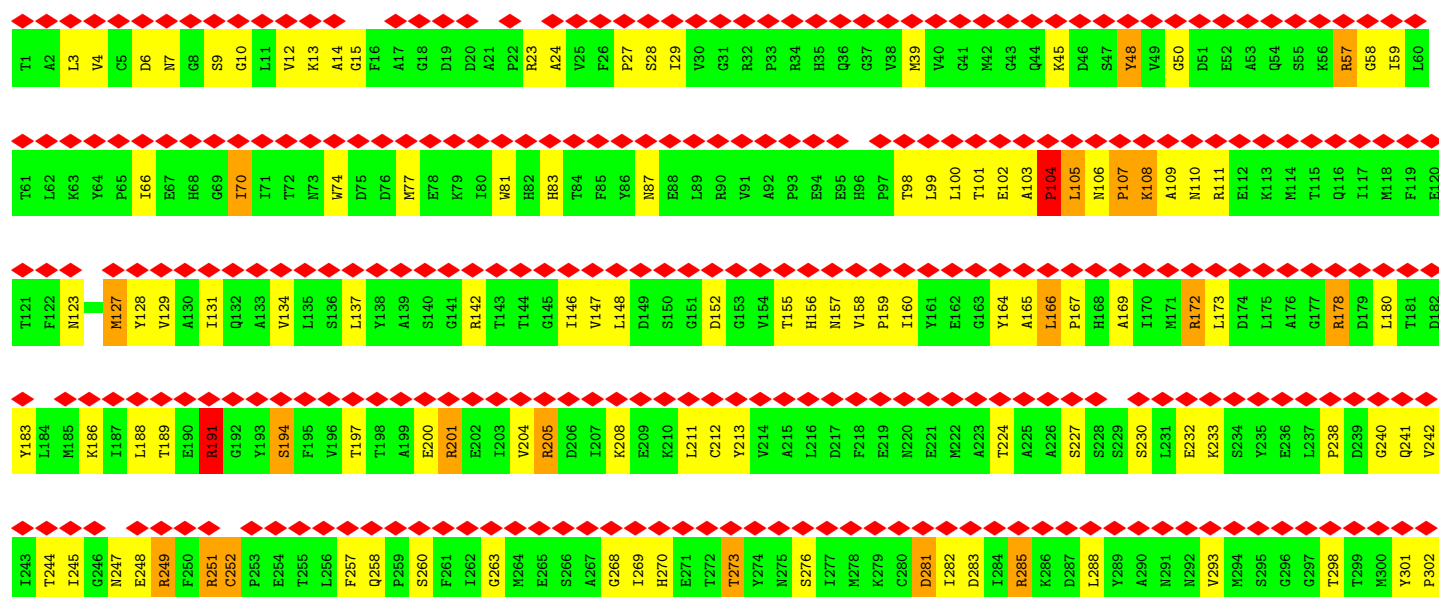
## ● Molecule 5: Actin



## ● Molecule 5: Actin

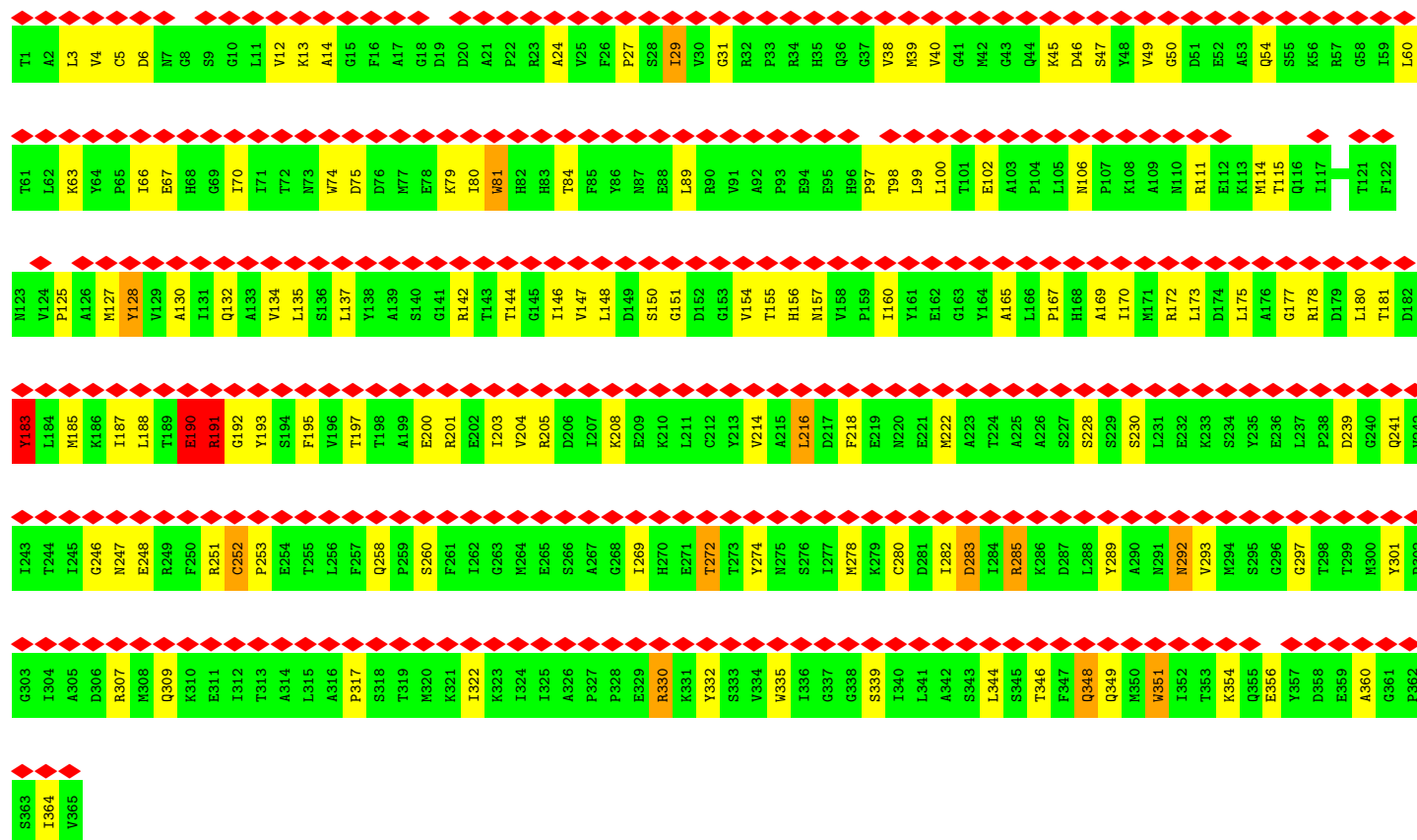


## ● Molecule 5: Actin



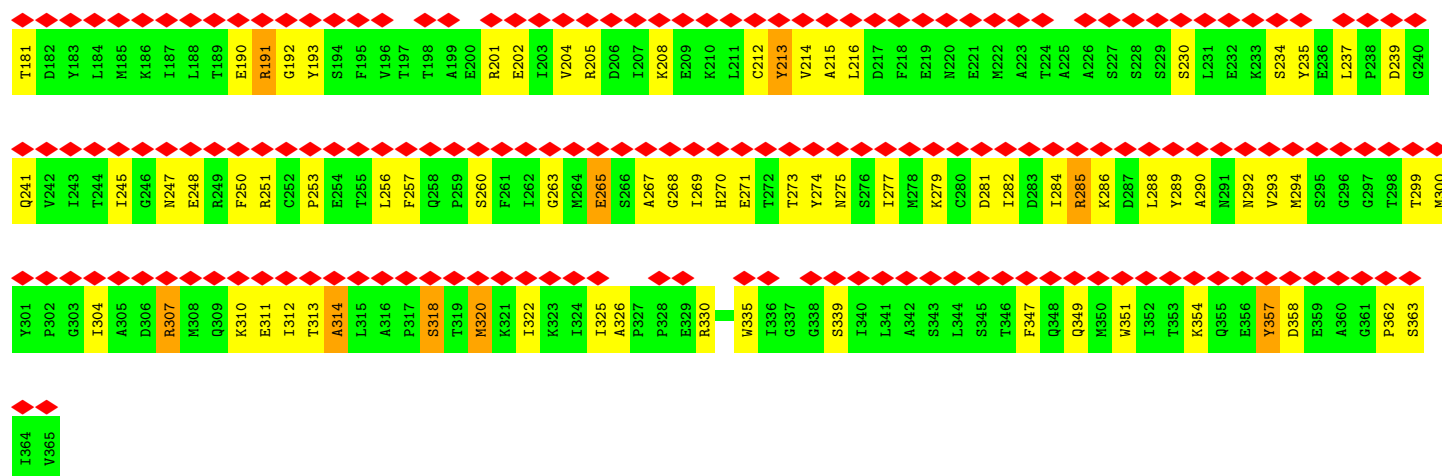


• Molecule 5: Actin

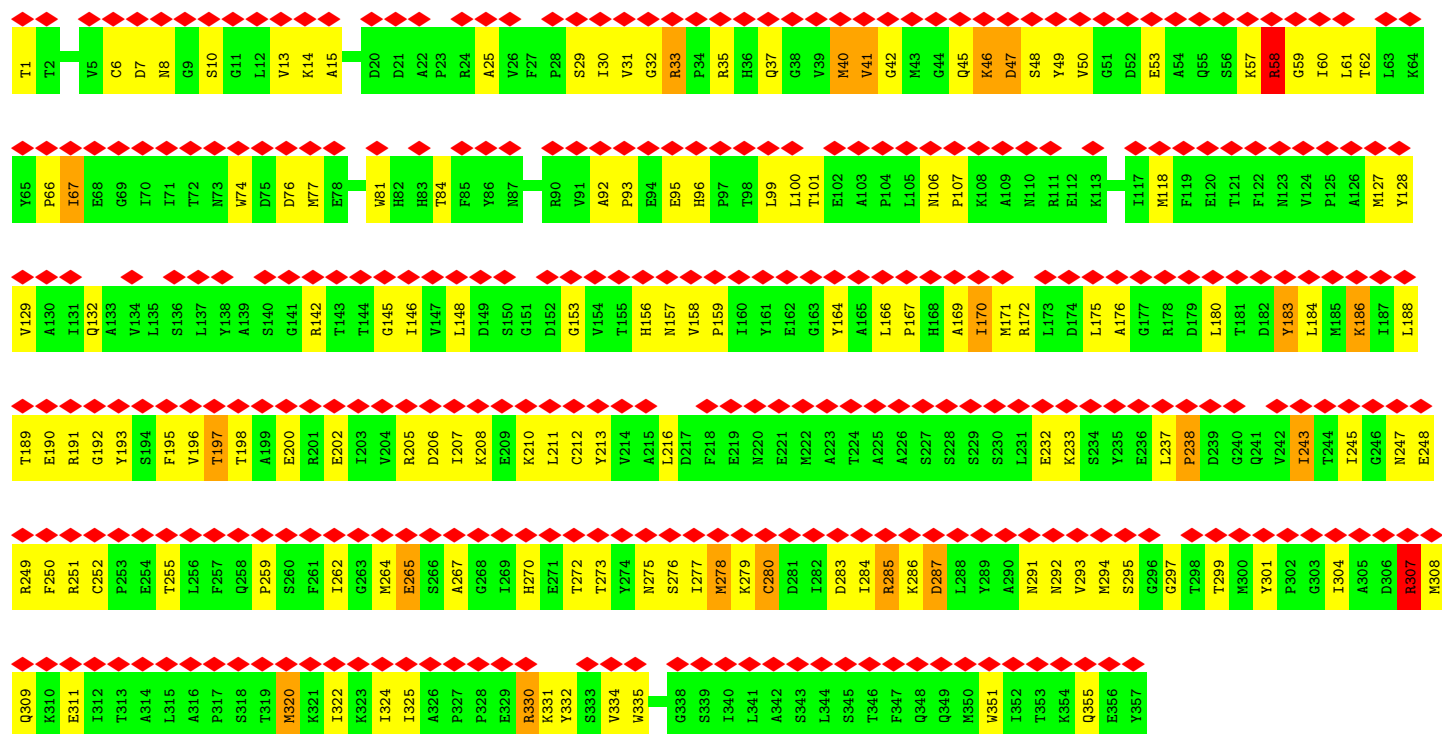


• Molecule 5: Actin



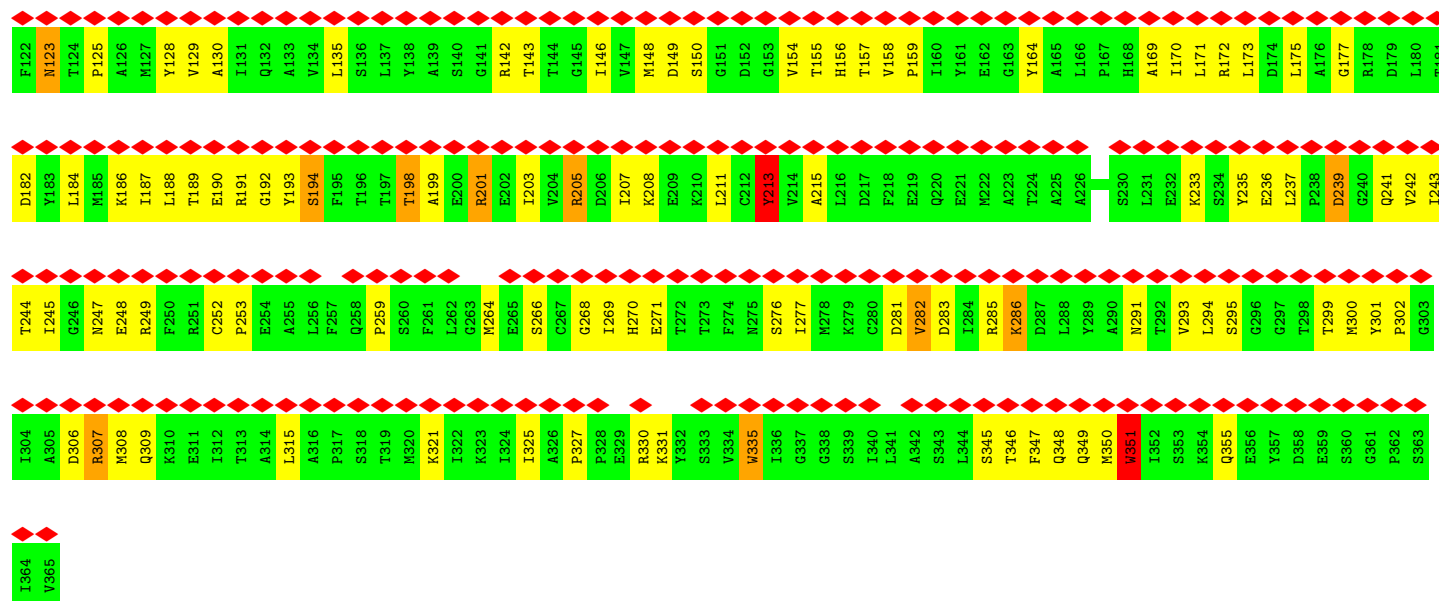


• Molecule 6: Actin

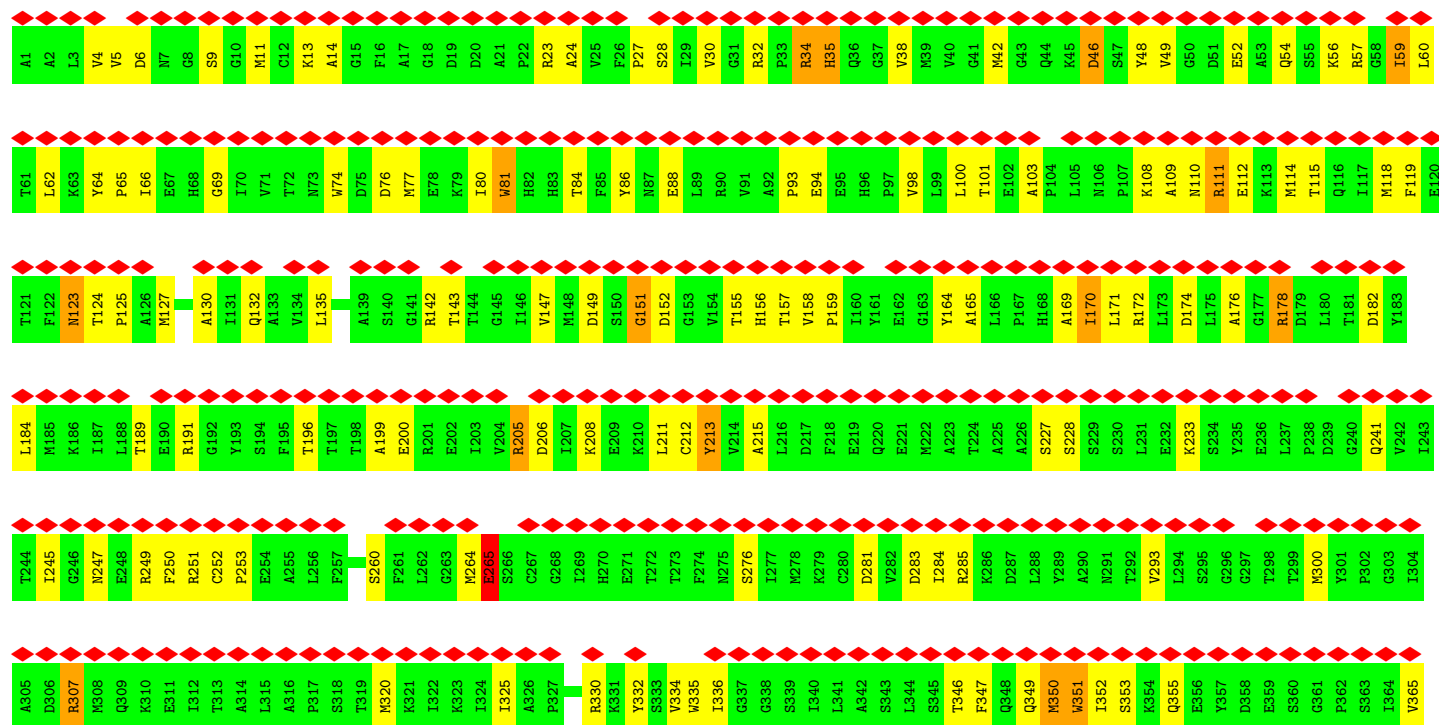


• Molecule 7: Actin





• Molecule 7: Actin



## 4 Experimental information

Property	Value	Source
EM reconstruction method	CRYSTALLOGRAPHY	Depositor
Imposed symmetry	3D CRYSTAL, $a$ =Not provided Å, $b$ =Not provided Å, $c$ =Not provided Å, $\alpha$ =Not provided°, $\beta$ =Not provided°, $\gamma$ =Not provided°, space group=Not provided	Depositor
Number of images used	Not provided	
Resolution determination method	Not provided	
CTF correction method	Not provided	
Microscope	JEOL 4000EX	Depositor
Voltage (kV)	400	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	15	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	40000	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	977.199	Depositor
Minimum map value	-974.403	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	215.097	Depositor
Recommended contour level	430.0	Depositor
Map size (Å)	255.99936, 148.00015, 765.7977	wwPDB
Map dimensions	576, 192, 112	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.33333, 1.32143, 1.32951	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	A	0.64	0/2904	1.31	30/3931 (0.8%)
1	G	0.64	0/2904	1.25	25/3931 (0.6%)
2	B	0.64	0/2895	1.37	29/3923 (0.7%)
3	C	0.64	0/2903	1.29	26/3930 (0.7%)
3	I	0.64	0/2903	1.28	26/3930 (0.7%)
4	D	0.64	0/2850	1.29	18/3860 (0.5%)
5	E	0.64	0/2906	1.31	27/3938 (0.7%)
5	H	0.63	0/2906	1.32	26/3938 (0.7%)
5	J	0.65	0/2906	1.35	32/3938 (0.8%)
5	K	0.64	0/2906	1.34	29/3938 (0.7%)
5	N	0.65	0/2906	1.29	24/3938 (0.6%)
6	F	0.63	0/2847	1.32	19/3857 (0.5%)
7	L	0.64	0/2899	1.34	22/3927 (0.6%)
7	M	0.64	0/2899	1.28	18/3927 (0.5%)
All	All	0.64	0/40534	1.31	351/54906 (0.6%)

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	A	0	12
1	G	0	7
2	B	0	9
3	C	0	6
3	I	0	9
4	D	0	5
5	E	0	8
5	H	0	7
5	J	0	6
5	K	0	9
5	N	0	8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	#Chirality outliers	#Planarity outliers
6	F	0	7
7	L	0	5
7	M	0	6
All	All	0	104

There are no bond length outliers.

All (351) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	204	ARG	NE-CZ-NH2	-13.13	113.74	120.30
2	B	204	ARG	NE-CZ-NH1	10.70	125.65	120.30
6	F	58	ARG	NE-CZ-NH2	-10.32	115.14	120.30
5	N	32	ARG	NE-CZ-NH2	-10.25	115.18	120.30
5	K	191	ARG	NE-CZ-NH1	10.18	125.39	120.30
6	F	285	ARG	NE-CZ-NH2	-9.74	115.43	120.30
4	D	22	ARG	NE-CZ-NH2	-9.51	115.54	120.30
5	J	142	ARG	NE-CZ-NH2	-9.28	115.66	120.30
5	J	205	ARG	NE-CZ-NH2	-9.25	115.67	120.30
1	A	142	ARG	NE-CZ-NH2	-9.13	115.73	120.30
3	I	351	TRP	CD1-CG-CD2	9.04	113.53	106.30
5	J	335	TRP	CD1-CG-CD2	9.01	113.51	106.30
3	C	74	TRP	CD1-CG-CD2	9.00	113.50	106.30
5	K	191	ARG	NE-CZ-NH2	-8.90	115.85	120.30
3	C	351	TRP	CD1-CG-CD2	8.87	113.40	106.30
1	A	111	ARG	NE-CZ-NH2	-8.86	115.87	120.30
2	B	350	TRP	CD1-CG-CD2	8.83	113.36	106.30
5	J	351	TRP	CD1-CG-CD2	8.82	113.35	106.30
5	K	351	TRP	CD1-CG-CD2	8.79	113.33	106.30
3	I	249	ARG	NE-CZ-NH2	-8.78	115.91	120.30
5	N	307	ARG	NE-CZ-NH1	8.70	124.65	120.30
5	N	335	TRP	CD1-CG-CD2	8.70	113.26	106.30
3	I	74	TRP	CD1-CG-CD2	8.68	113.25	106.30
5	H	351	TRP	CD1-CG-CD2	8.63	113.20	106.30
2	B	73	TRP	CD1-CG-CD2	8.60	113.18	106.30
7	M	74	TRP	CD1-CG-CD2	8.54	113.13	106.30
5	N	351	TRP	CD1-CG-CD2	8.54	113.13	106.30
5	N	81	TRP	CD1-CG-CD2	8.50	113.10	106.30
3	C	81	TRP	CD1-CG-CD2	8.48	113.08	106.30
5	E	74	TRP	CD1-CG-CD2	8.47	113.07	106.30
5	J	74	TRP	CD1-CG-CD2	8.44	113.05	106.30
1	A	32	ARG	NE-CZ-NH1	8.42	124.51	120.30
5	H	81	TRP	CD1-CG-CD2	8.38	113.00	106.30

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	334	TRP	CD1-CG-CD2	8.38	113.00	106.30
4	D	349	TRP	CD1-CG-CD2	8.34	112.97	106.30
7	L	74	TRP	CD1-CG-CD2	8.31	112.95	106.30
5	J	335	TRP	CE2-CD2-CG	-8.29	100.66	107.30
3	C	74	TRP	CE2-CD2-CG	-8.28	100.68	107.30
5	H	335	TRP	CD1-CG-CD2	8.27	112.92	106.30
5	H	74	TRP	CD1-CG-CD2	8.27	112.92	106.30
4	D	189	ARG	NE-CZ-NH2	-8.26	116.17	120.30
5	H	172	ARG	NE-CZ-NH2	-8.25	116.17	120.30
1	G	81	TRP	CD1-CG-CD2	8.24	112.89	106.30
5	H	161	TYR	CB-CG-CD1	-8.23	116.06	121.00
4	D	189	ARG	NE-CZ-NH1	8.22	124.41	120.30
7	M	81	TRP	CD1-CG-CD2	8.22	112.87	106.30
1	A	335	TRP	CD1-CG-CD2	8.21	112.87	106.30
6	F	351	TRP	CD1-CG-CD2	8.19	112.86	106.30
1	A	23	ARG	NE-CZ-NH2	-8.18	116.21	120.30
5	E	81	TRP	CD1-CG-CD2	8.18	112.84	106.30
3	I	335	TRP	CD1-CG-CD2	8.15	112.82	106.30
6	F	74	TRP	CD1-CG-CD2	8.14	112.81	106.30
6	F	335	TRP	CD1-CG-CD2	8.14	112.81	106.30
5	K	351	TRP	CE2-CD2-CG	-8.12	100.80	107.30
1	G	74	TRP	CD1-CG-CD2	8.11	112.78	106.30
3	I	81	TRP	CD1-CG-CD2	8.05	112.74	106.30
4	D	72	TRP	CD1-CG-CD2	8.04	112.73	106.30
3	I	74	TRP	CE2-CD2-CG	-8.02	100.88	107.30
3	C	351	TRP	CE2-CD2-CG	-8.01	100.89	107.30
1	G	142	ARG	NE-CZ-NH2	-7.99	116.31	120.30
5	K	335	TRP	CD1-CG-CD2	7.97	112.68	106.30
5	E	335	TRP	CD1-CG-CD2	7.96	112.67	106.30
5	E	74	TRP	CE2-CD2-CG	-7.96	100.93	107.30
7	M	74	TRP	CE2-CD2-CG	-7.93	100.95	107.30
1	A	74	TRP	CD1-CG-CD2	7.93	112.64	106.30
4	D	333	TRP	CD1-CG-CD2	7.93	112.64	106.30
5	J	205	ARG	NE-CZ-NH1	7.92	124.26	120.30
1	G	111	ARG	NE-CZ-NH2	-7.92	116.34	120.30
3	I	351	TRP	CE2-CD2-CG	-7.91	100.97	107.30
2	B	73	TRP	CE2-CD2-CG	-7.88	101.00	107.30
5	K	111	ARG	NE-CZ-NH2	-7.84	116.38	120.30
7	L	81	TRP	CD1-CG-CD2	7.83	112.57	106.30
6	F	172	ARG	NE-CZ-NH2	-7.82	116.39	120.30
6	F	335	TRP	CE2-CD2-CG	-7.82	101.05	107.30
5	N	351	TRP	CE2-CD2-CG	-7.81	101.05	107.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	L	351	TRP	CD1-CG-CD2	7.79	112.53	106.30
5	J	172	ARG	NE-CZ-NH2	-7.79	116.41	120.30
2	B	350	TRP	CE2-CD2-CG	-7.78	101.08	107.30
7	L	335	TRP	CD1-CG-CD2	7.77	112.52	106.30
1	A	351	TRP	CD1-CG-CD2	7.77	112.51	106.30
5	N	81	TRP	CE2-CD2-CG	-7.76	101.09	107.30
5	J	81	TRP	CD1-CG-CD2	7.76	112.51	106.30
5	K	74	TRP	CD1-CG-CD2	7.76	112.50	106.30
5	H	351	TRP	CE2-CD2-CG	-7.75	101.10	107.30
5	E	351	TRP	CD1-CG-CD2	7.74	112.50	106.30
5	K	285	ARG	NE-CZ-NH1	7.74	124.17	120.30
1	A	74	TRP	CE2-CD2-CG	-7.73	101.11	107.30
6	F	58	ARG	NE-CZ-NH1	7.72	124.16	120.30
5	J	74	TRP	CE2-CD2-CG	-7.71	101.14	107.30
5	E	81	TRP	CE2-CD2-CG	-7.70	101.14	107.30
1	G	351	TRP	CD1-CG-CD2	7.69	112.45	106.30
6	F	81	TRP	CD1-CG-CD2	7.69	112.45	106.30
6	F	351	TRP	CE2-CD2-CG	-7.69	101.15	107.30
5	N	335	TRP	CE2-CD2-CG	-7.69	101.15	107.30
1	G	351	TRP	CE2-CD2-CG	-7.67	101.16	107.30
1	G	74	TRP	CE2-CD2-CG	-7.66	101.18	107.30
3	I	335	TRP	CE2-CD2-CG	-7.66	101.17	107.30
3	C	191	ARG	NE-CZ-NH2	-7.65	116.48	120.30
5	H	335	TRP	CE2-CD2-CG	-7.64	101.19	107.30
5	N	191	ARG	NE-CZ-NH2	-7.63	116.49	120.30
3	C	178	ARG	NE-CZ-NH1	7.62	124.11	120.30
7	M	351	TRP	CD1-CG-CD2	7.62	112.39	106.30
3	C	81	TRP	CE2-CD2-CG	-7.61	101.21	107.30
5	N	74	TRP	CD1-CG-CD2	7.61	112.39	106.30
5	H	74	TRP	CE2-CD2-CG	-7.60	101.22	107.30
2	B	334	TRP	CE2-CD2-CG	-7.59	101.22	107.30
5	J	351	TRP	CE2-CD2-CG	-7.59	101.23	107.30
1	A	335	TRP	CE2-CD2-CG	-7.59	101.23	107.30
5	K	81	TRP	CD1-CG-CD2	7.58	112.36	106.30
7	M	335	TRP	CD1-CG-CD2	7.55	112.34	106.30
1	G	335	TRP	CD1-CG-CD2	7.55	112.34	106.30
5	K	335	TRP	CE2-CD2-CG	-7.55	101.26	107.30
5	H	81	TRP	CE2-CD2-CG	-7.54	101.27	107.30
5	H	307	ARG	NE-CZ-NH2	7.53	124.07	120.30
1	G	81	TRP	CE2-CD2-CG	-7.53	101.27	107.30
6	F	74	TRP	CE2-CD2-CG	-7.53	101.28	107.30
7	M	81	TRP	CE2-CD2-CG	-7.51	101.29	107.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	142	ARG	NE-CZ-NH2	-7.51	116.55	120.30
1	A	81	TRP	CD1-CG-CD2	7.51	112.31	106.30
5	E	335	TRP	CE2-CD2-CG	-7.50	101.30	107.30
4	D	79	TRP	CD1-CG-CD2	7.50	112.30	106.30
2	B	110	ARG	NE-CZ-NH1	7.50	124.05	120.30
2	B	248	ARG	NE-CZ-NH2	-7.49	116.56	120.30
7	L	74	TRP	CE2-CD2-CG	-7.49	101.31	107.30
2	B	80	TRP	CD1-CG-CD2	7.47	112.28	106.30
7	L	81	TRP	CE2-CD2-CG	-7.47	101.32	107.30
5	K	142	ARG	NE-CZ-NH2	-7.47	116.56	120.30
5	J	81	TRP	CE2-CD2-CG	-7.46	101.33	107.30
5	H	330	ARG	NE-CZ-NH2	-7.46	116.57	120.30
5	K	74	TRP	CE2-CD2-CG	-7.45	101.34	107.30
6	F	307	ARG	NE-CZ-NH2	-7.43	116.59	120.30
1	G	172	ARG	NE-CZ-NH2	-7.39	116.61	120.30
5	N	74	TRP	CE2-CD2-CG	-7.37	101.40	107.30
4	D	333	TRP	CE2-CD2-CG	-7.37	101.40	107.30
5	K	111	ARG	NE-CZ-NH1	7.34	123.97	120.30
7	L	57	ARG	NE-CZ-NH2	-7.33	116.63	120.30
3	I	81	TRP	CE2-CD2-CG	-7.32	101.45	107.30
6	F	33	ARG	NE-CZ-NH2	-7.31	116.64	120.30
4	D	349	TRP	CE2-CD2-CG	-7.30	101.46	107.30
4	D	72	TRP	CE2-CD2-CG	-7.29	101.47	107.30
5	K	330	ARG	NE-CZ-NH2	-7.27	116.67	120.30
5	J	57	ARG	NE-CZ-NH2	-7.26	116.67	120.30
7	M	335	TRP	CE2-CD2-CG	-7.24	101.51	107.30
7	L	335	TRP	CE2-CD2-CG	-7.24	101.51	107.30
2	B	80	TRP	CE2-CD2-CG	-7.23	101.52	107.30
7	L	194	SER	N-CA-C	7.20	130.44	111.00
3	C	335	TRP	CD1-CG-CD2	7.20	112.06	106.30
3	C	335	TRP	CE2-CD2-CG	-7.19	101.54	107.30
1	A	351	TRP	CE2-CD2-CG	-7.18	101.56	107.30
1	A	191	ARG	NE-CZ-NH2	-7.16	116.72	120.30
1	G	335	TRP	CE2-CD2-CG	-7.16	101.57	107.30
6	F	81	TRP	CE2-CD2-CG	-7.15	101.58	107.30
6	F	33	ARG	NE-CZ-NH1	7.14	123.87	120.30
5	K	81	TRP	CE2-CD2-CG	-7.14	101.59	107.30
7	L	198	THR	O-C-N	-7.12	111.31	122.70
2	B	177	ARG	NE-CZ-NH2	-7.11	116.74	120.30
1	A	178	ARG	NE-CZ-NH2	-7.08	116.76	120.30
5	E	351	TRP	CE2-CD2-CG	-7.07	101.64	107.30
7	L	351	TRP	CE2-CD2-CG	-7.06	101.66	107.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	K	178	ARG	NE-CZ-NH2	-7.02	116.79	120.30
1	A	178	ARG	NE-CZ-NH1	7.01	123.81	120.30
1	G	23	ARG	NE-CZ-NH2	-6.98	116.81	120.30
7	M	265	GLU	CA-CB-CG	6.97	128.74	113.40
5	J	191	ARG	NE-CZ-NH2	-6.91	116.85	120.30
5	J	172	ARG	NE-CZ-NH1	6.86	123.73	120.30
7	M	351	TRP	CE2-CD2-CG	-6.85	101.82	107.30
5	J	251	ARG	NE-CZ-NH1	6.78	123.69	120.30
1	G	201	ARG	NE-CZ-NH2	-6.77	116.91	120.30
1	A	81	TRP	CE2-CD2-CG	-6.76	101.89	107.30
5	K	172	ARG	NE-CZ-NH2	-6.71	116.94	120.30
4	D	79	TRP	CE2-CD2-CG	-6.71	101.93	107.30
2	B	190	ARG	NE-CZ-NH2	-6.69	116.95	120.30
7	L	172	ARG	NE-CZ-NH1	6.69	123.64	120.30
1	A	34	ARG	NE-CZ-NH1	6.66	123.63	120.30
5	J	191	ARG	NE-CZ-NH1	6.66	123.63	120.30
5	E	205	ARG	NE-CZ-NH2	-6.63	116.98	120.30
3	C	32	ARG	NE-CZ-NH2	-6.60	117.00	120.30
3	I	23	ARG	NE-CZ-NH1	6.57	123.58	120.30
7	M	307	ARG	NE-CZ-NH1	6.57	123.58	120.30
3	C	205	ARG	NE-CZ-NH2	-6.56	117.02	120.30
3	I	142	ARG	NE-CZ-NH2	-6.53	117.03	120.30
5	H	172	ARG	NE-CZ-NH1	6.52	123.56	120.30
2	B	284	ARG	NE-CZ-NH2	-6.51	117.04	120.30
7	M	142	ARG	NE-CZ-NH2	-6.51	117.05	120.30
7	M	285	ARG	NE-CZ-NH2	-6.50	117.05	120.30
5	H	161	TYR	CA-CB-CG	6.45	125.66	113.40
5	E	201	ARG	NE-CZ-NH2	-6.44	117.08	120.30
5	E	197	THR	CA-CB-CG2	6.44	121.42	112.40
5	N	52	GLU	CA-CB-CG	6.40	127.49	113.40
1	A	34	ARG	NE-CZ-NH2	-6.40	117.10	120.30
5	J	249	ARG	NE-CZ-NH2	-6.36	117.12	120.30
5	J	307	ARG	NE-CZ-NH1	-6.35	117.12	120.30
3	I	201	ARG	NE-CZ-NH1	6.26	123.43	120.30
5	H	249	ARG	NE-CZ-NH2	-6.25	117.18	120.30
5	E	32	ARG	NE-CZ-NH1	6.23	123.42	120.30
1	A	251	ARG	NE-CZ-NH2	-6.17	117.21	120.30
5	J	201	ARG	NE-CZ-NH1	6.11	123.35	120.30
3	C	351	TRP	CB-CG-CD1	-6.05	119.13	127.00
5	H	251	ARG	NE-CZ-NH1	6.01	123.31	120.30
5	K	142	ARG	NE-CZ-NH1	6.01	123.31	120.30
7	L	198	THR	CA-C-N	6.00	130.40	117.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	305	ARG	NE-CZ-NH1	5.99	123.30	120.30
1	G	351	TRP	CG-CD2-CE3	5.95	139.26	133.90
3	C	63	ARG	NE-CZ-NH1	5.93	123.27	120.30
2	B	329	ARG	N-CA-C	5.88	126.88	111.00
1	A	249	ARG	NE-CZ-NH1	5.88	123.24	120.30
2	B	248	ARG	NE-CZ-NH1	5.87	123.24	120.30
5	K	351	TRP	CG-CD2-CE3	5.87	139.18	133.90
3	C	260	SER	N-CA-CB	-5.86	101.71	110.50
1	A	285	ARG	NE-CZ-NH2	-5.85	117.37	120.30
5	J	48	TYR	CB-CG-CD2	-5.84	117.50	121.00
6	F	335	TRP	CG-CD2-CE3	5.82	139.14	133.90
5	N	285	ARG	NE-CZ-NH2	-5.82	117.39	120.30
5	J	191	ARG	CA-CB-CG	5.76	126.08	113.40
5	E	249	ARG	NE-CZ-NH2	-5.75	117.42	120.30
7	M	34	ARG	NE-CZ-NH2	-5.75	117.43	120.30
7	M	307	ARG	NE-CZ-NH2	-5.74	117.43	120.30
3	I	351	TRP	CB-CG-CD1	-5.71	119.58	127.00
1	G	32	ARG	NE-CZ-NH1	5.70	123.15	120.30
5	J	335	TRP	CB-CG-CD1	-5.68	119.61	127.00
7	L	107	PRO	O-C-N	-5.68	113.61	122.70
1	A	74	TRP	CG-CD2-CE3	5.68	139.01	133.90
5	J	178	ARG	NE-CZ-NH2	-5.64	117.48	120.30
2	B	340	LEU	CA-CB-CG	5.64	128.27	115.30
6	F	335	TRP	CB-CG-CD1	-5.63	119.68	127.00
2	B	215	LEU	CA-CB-CG	5.63	128.25	115.30
3	C	74	TRP	CG-CD2-CE3	5.63	138.97	133.90
5	N	289	TYR	CB-CG-CD2	-5.59	117.64	121.00
3	I	111	ARG	NE-CZ-NH1	5.59	123.10	120.30
7	L	107	PRO	CA-C-N	5.58	129.48	117.20
4	D	22	ARG	NE-CZ-NH1	5.57	123.08	120.30
5	H	335	TRP	CB-CG-CD1	-5.56	119.77	127.00
3	I	335	TRP	CB-CG-CD1	-5.56	119.78	127.00
5	E	111	ARG	NE-CZ-NH2	-5.55	117.53	120.30
5	E	285	ARG	NE-CZ-NH2	-5.54	117.53	120.30
5	E	116	GLN	CA-CB-CG	5.53	125.56	113.40
5	N	318	SER	N-CA-C	5.53	125.92	111.00
5	J	201	ARG	CA-CB-CG	5.52	125.54	113.40
5	K	330	ARG	N-CA-C	5.51	125.87	111.00
2	B	250	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	G	285	ARG	NE-CZ-NH2	-5.50	117.55	120.30
5	H	34	ARG	NE-CZ-NH1	5.50	123.05	120.30
5	E	74	TRP	CG-CD2-CE3	5.49	138.84	133.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	335	TRP	CB-CG-CD1	-5.49	119.87	127.00
4	D	333	TRP	CB-CG-CD1	-5.49	119.87	127.00
6	F	49	TYR	CB-CG-CD2	-5.48	117.71	121.00
3	I	351	TRP	CG-CD1-NE1	-5.47	104.63	110.10
2	B	141	ARG	NE-CZ-NH2	-5.47	117.57	120.30
5	J	285	ARG	NE-CZ-NH1	5.47	123.03	120.30
5	N	335	TRP	CG-CD1-NE1	-5.46	104.64	110.10
1	G	95	GLU	CA-CB-CG	5.44	125.37	113.40
3	I	74	TRP	CG-CD2-CE3	5.44	138.79	133.90
1	A	63	ARG	NE-CZ-NH2	-5.43	117.58	120.30
3	I	111	ARG	NE-CZ-NH2	-5.43	117.58	120.30
3	C	74	TRP	CG-CD1-NE1	-5.42	104.68	110.10
7	L	142	ARG	NE-CZ-NH2	-5.42	117.59	120.30
2	B	334	TRP	CB-CG-CD1	-5.42	119.96	127.00
5	J	335	TRP	CG-CD2-CE3	5.42	138.77	133.90
5	K	272	THR	CA-CB-CG2	5.41	119.98	112.40
1	A	142	ARG	NE-CZ-NH1	5.41	123.00	120.30
5	N	175	LEU	CA-CB-CG	5.40	127.72	115.30
5	E	205	ARG	NE-CZ-NH1	5.39	123.00	120.30
7	L	307	ARG	NE-CZ-NH1	5.39	123.00	120.30
5	J	335	TRP	CG-CD1-NE1	-5.39	104.71	110.10
5	E	335	TRP	CB-CG-CD1	-5.38	120.01	127.00
5	H	111	ARG	NE-CZ-NH1	5.37	122.99	120.30
1	A	201	ARG	NE-CZ-NH1	5.36	122.98	120.30
5	E	330	ARG	NE-CZ-NH2	-5.36	117.62	120.30
5	J	81	TRP	CG-CD2-CE3	5.35	138.71	133.90
1	G	32	ARG	NE-CZ-NH2	-5.34	117.63	120.30
5	N	351	TRP	CB-CG-CD1	-5.34	120.06	127.00
5	J	351	TRP	CG-CD1-NE1	-5.33	104.77	110.10
2	B	334	TRP	CG-CD2-CE3	5.32	138.69	133.90
3	I	335	TRP	CG-CD2-CE3	5.32	138.69	133.90
7	L	307	ARG	NE-CZ-NH2	-5.32	117.64	120.30
2	B	334	TRP	CG-CD1-NE1	-5.32	104.78	110.10
7	M	74	TRP	CG-CD1-NE1	-5.32	104.78	110.10
7	L	191	ARG	CA-C-N	5.31	126.83	116.20
7	M	74	TRP	CG-CD2-CE3	5.30	138.67	133.90
5	K	190	GLU	CA-C-N	5.30	128.86	117.20
5	H	351	TRP	CG-CD1-NE1	-5.28	104.82	110.10
1	G	330	ARG	NE-CZ-NH2	-5.28	117.66	120.30
5	J	104	PRO	N-CA-C	5.28	125.82	112.10
5	K	351	TRP	CG-CD1-NE1	-5.28	104.82	110.10
5	E	330	ARG	N-CA-C	5.27	125.24	111.00

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	11	LEU	CA-CB-CG	5.26	127.40	115.30
1	A	161	TYR	CB-CG-CD1	-5.26	117.84	121.00
3	I	23	ARG	NE-CZ-NH2	-5.26	117.67	120.30
5	N	154	VAL	CA-C-N	-5.26	105.64	117.20
5	N	81	TRP	CG-CD1-NE1	-5.25	104.85	110.10
2	B	114	THR	CA-CB-OG1	-5.25	97.98	109.00
7	M	191	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	G	172	ARG	NE-CZ-NH1	5.23	122.92	120.30
5	K	180	LEU	CA-C-N	5.23	128.71	117.20
3	I	74	TRP	CG-CD1-NE1	-5.21	104.89	110.10
5	N	351	TRP	CG-CD2-CE3	5.21	138.59	133.90
5	E	81	TRP	CG-CD2-CE3	5.21	138.59	133.90
5	N	335	TRP	CB-CG-CD1	-5.20	120.24	127.00
4	D	31	ARG	NE-CZ-NH1	5.20	122.90	120.30
4	D	349	TRP	CG-CD1-NE1	-5.20	104.90	110.10
7	L	201	ARG	NE-CZ-NH2	-5.20	117.70	120.30
3	C	351	TRP	CG-CD1-NE1	-5.20	104.90	110.10
5	N	32	ARG	NE-CZ-NH1	5.19	122.90	120.30
1	A	57	ARG	NE-CZ-NH2	-5.19	117.71	120.30
2	B	280	ASP	N-CA-C	5.17	124.97	111.00
1	A	23	ARG	NE-CZ-NH1	5.17	122.88	120.30
5	J	23	ARG	NE-CZ-NH2	-5.17	117.72	120.30
5	N	201	ARG	NE-CZ-NH2	-5.17	117.72	120.30
7	L	285	ARG	CA-C-N	5.16	128.54	117.20
3	C	191	ARG	NE-CZ-NH1	5.14	122.87	120.30
3	C	81	TRP	CG-CD1-NE1	-5.14	104.96	110.10
2	B	350	TRP	CG-CD1-NE1	-5.13	104.97	110.10
5	H	330	ARG	N-CA-C	5.12	124.84	111.00
4	D	135	LEU	CA-CB-CG	5.12	127.08	115.30
5	E	197	THR	N-CA-C	5.12	124.82	111.00
5	K	283	ASP	CB-CG-OD2	-5.12	113.69	118.30
5	K	301	TYR	CB-CG-CD2	-5.12	117.93	121.00
1	A	307	ARG	NE-CZ-NH1	5.12	122.86	120.30
2	B	300	TYR	CB-CG-CD2	-5.11	117.93	121.00
5	K	183	TYR	CB-CG-CD2	-5.11	117.93	121.00
3	I	335	TRP	CG-CD1-NE1	-5.11	104.99	110.10
1	A	351	TRP	CB-CG-CD1	-5.11	120.36	127.00
1	G	48	TYR	CB-CG-CD2	-5.10	117.94	121.00
5	H	81	TRP	CG-CD1-NE1	-5.10	105.00	110.10
3	C	351	TRP	CG-CD2-CE3	5.10	138.49	133.90
5	E	335	TRP	CG-CD2-CE3	5.10	138.49	133.90
1	G	191	ARG	NE-CZ-NH2	-5.09	117.75	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	335	TRP	CB-CG-CD1	-5.09	120.38	127.00
5	K	74	TRP	CG-CD2-CE3	5.09	138.48	133.90
5	K	335	TRP	CB-CG-CD1	-5.08	120.39	127.00
1	G	81	TRP	CG-CD1-NE1	-5.08	105.02	110.10
3	I	351	TRP	CG-CD2-CE3	5.08	138.47	133.90
2	B	73	TRP	CG-CD1-NE1	-5.07	105.03	110.10
1	G	74	TRP	CG-CD2-CE3	5.06	138.46	133.90
3	I	81	TRP	CG-CD1-NE1	-5.06	105.04	110.10
3	I	155	THR	N-CA-CB	-5.05	100.70	110.30
3	C	249	ARG	NE-CZ-NH2	-5.05	117.78	120.30
4	D	77	LYS	CA-CB-CG	-5.04	102.30	113.40
3	C	63	ARG	NE-CZ-NH2	-5.03	117.79	120.30
5	E	198	THR	N-CA-C	5.02	124.56	111.00
6	F	335	TRP	CG-CD1-NE1	-5.02	105.08	110.10
5	H	74	TRP	CG-CD1-NE1	-5.02	105.08	110.10
3	I	74	TRP	CB-CG-CD1	-5.02	120.47	127.00
7	L	74	TRP	CG-CD1-NE1	-5.02	105.08	110.10
3	C	76	ASP	CB-CG-OD2	5.02	122.81	118.30
5	E	74	TRP	CG-CD1-NE1	-5.02	105.08	110.10
7	M	335	TRP	CG-CD2-CE3	5.01	138.41	133.90
3	C	178	ARG	NE-CZ-NH2	-5.01	117.79	120.30
5	H	351	TRP	CG-CD2-CE3	5.01	138.41	133.90
5	E	48	TYR	CB-CG-CD2	-5.00	118.00	121.00
5	H	74	TRP	CG-CD2-CE3	5.00	138.40	133.90

There are no chirality outliers.

All (104) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	111	ARG	Sidechain
1	A	142	ARG	Sidechain
1	A	161	TYR	Sidechain
1	A	191	ARG	Sidechain
1	A	193	TYR	Sidechain
1	A	249	ARG	Sidechain
1	A	251	ARG	Sidechain
1	A	274	TYR	Sidechain
1	A	285	ARG	Sidechain
1	A	357	TYR	Sidechain
1	A	57	ARG	Sidechain
1	A	64	TYR	Sidechain
2	B	177	ARG	Sidechain

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Group
2	B	190	ARG	Sidechain
2	B	212	TYR	Sidechain
2	B	273	TYR	Sidechain
2	B	284	ARG	Sidechain
2	B	329	ARG	Sidechain
2	B	34	ARG	Sidechain
2	B	48	TYR	Sidechain
2	B	64	TYR	Sidechain
3	C	138	TYR	Sidechain
3	C	142	ARG	Peptide
3	C	161	TYR	Sidechain
3	C	183	TYR	Sidechain
3	C	213	TYR	Sidechain
3	C	357	TYR	Sidechain
4	D	140	ARG	Sidechain
4	D	199	ARG	Sidechain
4	D	33	ARG	Sidechain,Peptide
4	D	57	GLY	Peptide
5	E	111	ARG	Sidechain
5	E	193	TYR	Sidechain
5	E	196	VAL	Peptide
5	E	201	ARG	Sidechain
5	E	274	TYR	Sidechain
5	E	357	TYR	Sidechain
5	E	57	ARG	Sidechain
5	E	90	ARG	Sidechain
6	F	164	TYR	Sidechain
6	F	183	TYR	Sidechain
6	F	193	TYR	Sidechain
6	F	301	TYR	Sidechain
6	F	307	ARG	Sidechain
6	F	33	ARG	Sidechain
6	F	332	TYR	Sidechain
1	G	111	ARG	Sidechain
1	G	142	ARG	Sidechain
1	G	167	PRO	Peptide
1	G	193	TYR	Sidechain
1	G	251	ARG	Sidechain
1	G	274	TYR	Sidechain
1	G	64	TYR	Sidechain
5	H	161	TYR	Sidechain
5	H	191	ARG	Sidechain

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
5	H	205	ARG	Sidechain
5	H	249	ARG	Sidechain
5	H	274	TYR	Sidechain
5	H	332	TYR	Sidechain
5	H	57	ARG	Sidechain
3	I	161	TYR	Sidechain
3	I	183	TYR	Sidechain
3	I	186	LYS	Peptide
3	I	191	ARG	Sidechain
3	I	193	TYR	Sidechain
3	I	274	TYR	Sidechain
3	I	307	ARG	Sidechain
3	I	357	TYR	Sidechain
3	I	64	TYR	Sidechain
5	J	164	TYR	Sidechain
5	J	166	LEU	Peptide
5	J	191	ARG	Sidechain
5	J	281	ASP	Peptide
5	J	307	ARG	Sidechain
5	J	48	TYR	Sidechain
5	K	128	TYR	Sidechain
5	K	183	TYR	Sidechain
5	K	191	ARG	Sidechain
5	K	193	TYR	Sidechain
5	K	201	ARG	Sidechain
5	K	205	ARG	Sidechain
5	K	274	TYR	Sidechain
5	K	317	PRO	Peptide
5	K	332	TYR	Sidechain
7	L	128	TYR	Sidechain
7	L	164	TYR	Sidechain
7	L	213	TYR	Sidechain
7	L	64	TYR	Sidechain
7	L	86	TYR	Sidechain
7	M	111	ARG	Sidechain
7	M	164	TYR	Sidechain
7	M	213	TYR	Sidechain
7	M	227	SER	Peptide
7	M	64	TYR	Sidechain
7	M	86	TYR	Sidechain
5	N	190	GLU	Peptide
5	N	191	ARG	Sidechain

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
5	N	193	TYR	Sidechain
5	N	213	TYR	Sidechain
5	N	274	TYR	Sidechain
5	N	357	TYR	Sidechain
5	N	60	LEU	Peptide
5	N	64	TYR	Sidechain

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2843	0	2818	55	0
1	G	2843	0	2818	57	0
2	B	2835	0	2813	80	0
3	C	2842	0	2821	69	0
3	I	2842	0	2821	81	0
4	D	2791	0	2766	75	0
5	E	2845	0	2820	78	0
5	H	2845	0	2820	66	0
5	J	2845	0	2820	80	0
5	K	2845	0	2820	69	0
5	N	2845	0	2820	85	0
6	F	2788	0	2770	108	0
7	L	2838	0	2812	78	0
7	M	2838	0	2812	66	0
All	All	39685	0	39351	972	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 12.

All (972) 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)
5:E:198:THR:HA	6:F:265:GLU:HG3	1.51	0.91
5:E:248:GLU:HA	5:E:251:ARG:HB3	1.54	0.88
7:L:159:PRO:HG3	7:L:169:ALA:HB3	1.56	0.86

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:317:PRO:HG2	1:G:320:MET:HB2	1.58	0.85
7:L:259:PRO:HG2	7:L:266:SER:HB2	1.58	0.84
7:M:159:PRO:HG3	7:M:169:ALA:HB3	1.58	0.84
6:F:190:GLU:HG2	1:G:167:PRO:HB2	1.60	0.83
2:B:154:THR:HB	2:B:172:LEU:HB3	1.59	0.81
4:D:185:ILE:HD13	4:D:246:GLU:HB3	1.62	0.81
1:G:14:ALA:HB3	1:G:24:ALA:HB3	1.61	0.81
3:I:14:ALA:HB3	3:I:24:ALA:HB3	1.62	0.81
5:H:280:CYS:HB3	5:H:284:ILE:HD11	1.62	0.81
5:E:197:THR:HA	6:F:264:MET:HA	1.64	0.79
4:D:64:PRO:HB3	4:D:74:ASP:HB2	1.63	0.79
6:F:259:PRO:HB2	6:F:264:MET:HB2	1.64	0.79
3:I:84:THR:HA	3:I:88:GLU:HG2	1.64	0.78
5:H:200:GLU:HA	5:H:203:ILE:HB	1.65	0.78
6:F:66:PRO:HG3	6:F:76:ASP:HB3	1.64	0.77
4:D:157:PRO:HG3	4:D:167:ALA:HB3	1.68	0.76
5:H:159:PRO:HB2	5:H:166:LEU:HD12	1.65	0.76
3:I:195:PHE:HA	3:I:200:GLU:HB3	1.68	0.76
5:J:159:PRO:HG3	5:J:169:ALA:HB3	1.67	0.76
4:D:279:ASP:HB3	4:D:282:ILE:HG12	1.67	0.75
5:N:14:ALA:HB3	5:N:24:ALA:HB3	1.67	0.75
2:B:131:GLN:HG2	2:B:333:VAL:HG21	1.68	0.75
7:M:48:TYR:HB2	7:M:60:LEU:HD21	1.67	0.75
1:G:208:LYS:HA	1:G:212:CYS:SG	2.27	0.75
5:K:191:ARG:HA	7:L:109:ALA:HB3	1.68	0.75
6:F:132:GLN:HG2	6:F:334:VAL:HG11	1.69	0.75
5:K:222:MET:SD	5:K:251:ARG:HD3	2.26	0.74
4:D:57:GLY:HA2	6:F:283:ASP:HB2	1.68	0.74
5:N:215:ALA:HB2	5:N:250:PHE:HB2	1.70	0.74
5:N:6:ASP:HA	5:N:101:THR:HB	1.68	0.74
5:J:263:GLY:HA3	5:K:167:PRO:HD2	1.71	0.73
5:J:200:GLU:HG2	7:L:283:ASP:HB2	1.70	0.72
7:M:132:GLN:HG2	7:M:334:VAL:HG11	1.71	0.72
5:K:248:GLU:HA	5:K:251:ARG:HB2	1.70	0.72
5:J:240:GLY:HA3	7:L:286:LYS:HB3	1.72	0.72
1:A:297:GLY:HA2	1:A:331:LYS:HG2	1.72	0.72
2:B:65:PRO:HG2	2:B:79:ILE:HD12	1.71	0.72
7:L:14:ALA:HB3	7:L:24:ALA:HB3	1.71	0.72
4:D:5:ASP:HA	4:D:99:THR:OG1	1.90	0.71
1:A:239:ASP:HA	3:C:317:PRO:HB3	1.72	0.71
5:K:218:PHE:HD2	5:K:307:ARG:HH21	1.36	0.71

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:31:GLY:HA3	7:L:60:LEU:HD23	1.72	0.71
3:C:148:LEU:HD13	3:C:157:VAL:HG22	1.73	0.71
3:C:208:LYS:HA	3:C:212:CYS:SG	2.32	0.70
3:I:297:GLY:HA2	3:I:331:LYS:HG2	1.74	0.70
1:A:184:LEU:HA	1:A:187:ILE:HG12	1.74	0.69
3:C:14:ALA:HB3	3:C:24:ALA:HB3	1.73	0.69
6:F:186:LYS:HD2	1:G:168:HIS:HA	1.72	0.69
5:E:186:LYS:HZ1	6:F:272:THR:HG22	1.58	0.69
2:B:194:PHE:HA	2:B:199:GLU:HB3	1.74	0.69
1:A:208:LYS:HA	1:A:212:CYS:SG	2.33	0.69
3:C:159:PRO:HG3	3:C:169:ALA:HB3	1.75	0.69
5:E:196:VAL:HB	6:F:264:MET:SD	2.32	0.68
3:C:178:ARG:HB3	3:C:178:ARG:NH1	2.08	0.68
1:G:167:PRO:HA	1:G:170:ILE:HG13	1.73	0.68
5:H:14:ALA:HB3	5:H:24:ALA:HB3	1.75	0.68
7:M:252:CYS:SG	7:M:253:PRO:HD3	2.34	0.68
6:F:15:ALA:HB3	6:F:25:ALA:HB3	1.76	0.68
1:G:104:PRO:HG3	1:G:131:ILE:HG23	1.76	0.68
5:K:14:ALA:HB3	5:K:24:ALA:HB3	1.76	0.67
7:M:6:ASP:HB3	7:M:13:LYS:HB2	1.74	0.67
3:I:191:ARG:HG2	5:J:110:ASN:HB2	1.77	0.67
3:C:178:ARG:HB3	3:C:178:ARG:HH11	1.60	0.67
1:A:14:ALA:HB3	1:A:24:ALA:HB3	1.76	0.67
4:D:113:THR:HA	4:D:125:MET:SD	2.35	0.67
5:J:3:LEU:HB2	5:J:98:THR:HG22	1.77	0.66
6:F:273:THR:O	6:F:277:ILE:HG12	1.95	0.66
4:D:64:PRO:HG2	4:D:65:ILE:HG13	1.78	0.66
5:N:31:GLY:HA3	5:N:60:LEU:HD13	1.78	0.66
3:C:135:LEU:HB3	3:C:337:GLY:HA3	1.78	0.66
5:H:248:GLU:HA	5:H:251:ARG:HB2	1.77	0.65
7:L:327:PRO:HG2	7:L:330:ARG:HB3	1.77	0.65
1:A:214:VAL:HG22	1:A:253:PRO:HB3	1.78	0.65
1:A:148:LEU:HD13	1:A:157:VAL:HG22	1.77	0.65
5:K:200:GLU:HA	5:K:203:ILE:HG22	1.76	0.65
1:G:195:PHE:HA	1:G:200:GLU:HB3	1.78	0.65
3:I:175:LEU:HD13	3:I:262:LEU:HG	1.78	0.65
7:L:252:CYS:SG	7:L:253:PRO:HD3	2.36	0.65
5:N:214:VAL:HG22	5:N:253:PRO:HB2	1.78	0.65
5:N:10:GLY:O	5:N:27:PRO:HA	1.97	0.65
5:E:236:GLU:HG2	5:E:242:VAL:HG22	1.78	0.65
3:I:234:SER:HA	3:I:244:THR:HA	1.78	0.64

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:184:MET:HB2	2:B:203:VAL:HG11	1.78	0.64
6:F:175:LEU:HD11	6:F:255:THR:HG22	1.80	0.64
3:I:30:VAL:HG21	3:I:76:ASP:HB3	1.80	0.64
3:I:190:GLU:HB3	5:J:102:GLU:HB2	1.78	0.64
3:I:192:GLY:HA3	5:J:70:ILE:HG23	1.80	0.64
7:L:150:SER:HA	7:L:154:VAL:O	1.97	0.64
7:M:14:ALA:HB3	7:M:24:ALA:HB3	1.79	0.64
5:H:208:LYS:HA	5:H:212:CYS:SG	2.38	0.64
7:M:247:ASN:HB3	7:M:251:ARG:HH21	1.62	0.64
1:A:237:LEU:HD12	1:A:241:GLN:HG3	1.78	0.63
2:B:191:GLY:HA3	3:C:107:PRO:HA	1.80	0.63
2:B:195:VAL:HG22	3:C:172:ARG:NH1	2.14	0.63
3:I:57:ARG:HG2	3:I:62:LEU:HD11	1.79	0.63
5:N:277:ILE:HG22	5:N:285:ARG:HG2	1.81	0.63
1:A:147:VAL:HA	1:A:293:VAL:O	1.98	0.63
5:H:68:HIS:HB3	5:H:154:VAL:HG13	1.79	0.63
5:E:48:TYR:HB3	5:E:53:ALA:HB2	1.80	0.63
3:I:159:PRO:HG3	3:I:169:ALA:HB3	1.80	0.63
7:L:148:MET:HA	7:L:156:HIS:O	1.98	0.63
2:B:147:LEU:HA	2:B:155:HIS:O	1.99	0.62
5:H:218:PHE:HD2	5:H:307:ARG:HH21	1.46	0.62
4:D:145:VAL:HA	4:D:291:VAL:O	1.99	0.62
7:M:98:VAL:O	7:M:127:MET:HA	1.99	0.62
5:N:115:THR:HA	5:N:127:MET:SD	2.40	0.62
5:K:137:LEU:HD22	5:K:160:ILE:HD13	1.81	0.62
5:N:97:PRO:HB3	5:N:126:ALA:HB3	1.80	0.62
2:B:193:SER:HB3	3:C:172:ARG:NH2	2.14	0.62
3:C:66:ILE:HD11	3:C:77:MET:SD	2.39	0.62
6:F:237:LEU:HG	6:F:243:ILE:HD12	1.80	0.62
5:N:83:HIS:HA	5:N:87:ASN:HD22	1.66	0.61
3:C:327:PRO:HB2	3:C:330:ARG:HB3	1.82	0.61
5:E:9:SER:HA	5:E:66:ILE:HB	1.81	0.61
1:G:247:ASN:ND2	1:G:251:ARG:HH21	1.98	0.61
2:B:14:ALA:HB3	2:B:24:ALA:HB3	1.81	0.61
5:E:312:ILE:HB	5:E:322:ILE:HG13	1.81	0.61
5:J:127:MET:SD	5:J:129:VAL:HG23	2.40	0.61
1:A:10:GLY:O	1:A:27:PRO:HA	2.00	0.60
2:B:29:ILE:HD11	2:B:62:LEU:HB3	1.83	0.60
3:C:49:VAL:HG21	3:C:80:ILE:HA	1.83	0.60
3:I:183:TYR:HD2	3:I:252:ALA:HA	1.65	0.60
7:L:70:ILE:HG13	7:L:106:ASN:HD21	1.66	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:GLU:HA	1:A:359:GLU:HG2	1.83	0.60
5:E:297:GLY:HA2	5:E:331:LYS:HG3	1.84	0.60
2:B:34:ARG:HG2	2:B:34:ARG:HH21	1.66	0.60
5:J:146:ILE:HD11	5:J:157:ASN:HB3	1.83	0.60
7:M:147:VAL:O	7:M:157:THR:HA	2.02	0.60
5:N:277:ILE:HD12	5:N:288:LEU:HD23	1.82	0.60
3:I:186:LYS:HE2	5:J:167:PRO:HD2	1.84	0.60
6:F:277:ILE:HG22	6:F:285:ARG:HG2	1.83	0.60
7:L:104:PRO:HB2	7:L:156:HIS:CD2	2.37	0.60
5:E:14:ALA:HB3	5:E:24:ALA:HB3	1.84	0.60
5:E:195:PHE:HZ	5:E:243:ILE:HG12	1.67	0.60
6:F:32:GLY:O	6:F:48:SER:HA	2.02	0.60
5:N:281:ASP:O	5:N:285:ARG:HG3	2.02	0.60
6:F:171:MET:HG2	6:F:276:SER:HB3	1.84	0.59
6:F:248:GLU:HA	6:F:251:ARG:HB3	1.83	0.59
5:J:6:ASP:HA	5:J:101:THR:HG22	1.84	0.59
3:I:148:LEU:HD13	3:I:157:VAL:HG22	1.83	0.59
3:I:39:MET:SD	5:K:346:THR:HB	2.43	0.59
3:I:245:ILE:HG22	3:I:249:ARG:HG3	1.84	0.59
5:J:99:LEU:HA	5:J:128:TYR:O	2.03	0.59
7:L:31:GLY:HA2	7:L:61:THR:O	2.03	0.59
5:J:131:ILE:HB	5:J:134:VAL:HB	1.84	0.59
7:L:300:MET:SD	7:L:331:LYS:HG3	2.43	0.59
2:B:190:ARG:NH2	2:B:246:ASN:HB3	2.18	0.59
5:J:330:ARG:HA	5:J:333:SER:OG	2.03	0.59
2:B:97:THR:O	2:B:126:MET:HA	2.03	0.58
3:I:188:LEU:HA	5:J:107:PRO:HG3	1.84	0.58
6:F:211:LEU:HD12	6:F:233:LYS:HB3	1.85	0.58
3:I:183:TYR:CD2	3:I:252:ALA:HA	2.38	0.58
5:K:4:VAL:HG21	5:K:339:SER:HA	1.85	0.58
5:N:256:LEU:HB3	5:N:269:ILE:HD12	1.84	0.58
7:L:6:ASP:HB3	7:L:13:LYS:HB2	1.84	0.58
7:M:62:LEU:HB2	5:N:265:GLU:HG2	1.84	0.58
1:G:97:PRO:HA	1:G:126:ALA:O	2.03	0.58
5:N:146:ILE:HD12	5:N:277:ILE:HD11	1.84	0.58
5:N:281:ASP:HB3	5:N:284:ILE:HG12	1.84	0.58
2:B:3:LEU:HB3	2:B:97:THR:HA	1.85	0.58
6:F:46:LYS:HZ1	6:F:61:LEU:HD21	1.68	0.58
5:K:183:TYR:HE2	5:K:252:CYS:HA	1.68	0.57
5:K:148:LEU:HA	5:K:156:HIS:O	2.03	0.57
5:J:147:VAL:HA	5:J:293:VAL:O	2.04	0.57

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:98:VAL:O	3:C:127:PHE:HA	2.04	0.57
6:F:6:CYS:HA	6:F:14:LYS:O	2.05	0.57
3:I:31:GLY:HA3	3:I:60:LEU:HD13	1.86	0.57
7:L:155:THR:OG1	7:L:173:LEU:HB3	2.05	0.57
7:M:184:LEU:HD13	7:M:252:CYS:SG	2.44	0.57
4:D:5:ASP:O	4:D:11:VAL:HA	2.04	0.57
6:F:45:GLN:HE22	6:F:60:ILE:HB	1.70	0.57
5:N:140:SER:HB2	5:N:142:ARG:HH21	1.69	0.57
2:B:190:ARG:HH21	2:B:246:ASN:HB3	1.69	0.57
5:J:14:ALA:HB3	5:J:24:ALA:HB3	1.84	0.57
2:B:29:ILE:HG23	2:B:50:GLY:HA2	1.87	0.57
4:D:152:VAL:HG12	4:D:172:ASP:HA	1.85	0.57
5:E:113:LYS:HA	5:E:116:GLN:NE2	2.20	0.57
1:G:159:PRO:HG2	1:G:169:ALA:HB3	1.87	0.57
5:H:203:ILE:HD12	5:H:238:PRO:HD3	1.87	0.57
2:B:146:VAL:HA	2:B:292:VAL:O	2.05	0.56
4:D:203:ARG:O	4:D:206:LYS:HG2	2.05	0.56
5:H:148:LEU:HA	5:H:156:HIS:O	2.04	0.56
5:H:234:SER:HA	5:H:243:ILE:O	2.06	0.56
3:C:149:ASP:O	3:C:155:THR:HA	2.05	0.56
5:H:157:ASN:O	5:H:170:ILE:HA	2.05	0.56
5:K:102:GLU:HB2	5:K:106:ASN:ND2	2.18	0.56
5:J:6:ASP:O	5:J:12:VAL:HA	2.05	0.56
2:B:200:ARG:HA	2:B:203:VAL:HG12	1.87	0.56
5:E:158:VAL:HG22	5:E:170:ILE:HG23	1.88	0.56
7:L:158:VAL:HG22	7:L:170:ILE:HG23	1.88	0.56
1:A:7:ASN:HA	1:A:12:CYS:SG	2.46	0.56
2:B:30:VAL:HG12	2:B:49:VAL:HG23	1.87	0.56
5:K:98:THR:O	5:K:127:MET:HA	2.06	0.56
7:M:94:GLU:HA	7:M:123:ASN:O	2.06	0.56
6:F:37:GLN:OE1	6:F:37:GLN:HA	2.06	0.56
5:N:267:ALA:HB1	5:N:271:GLU:HB2	1.88	0.56
5:E:6:ASP:O	5:E:12:VAL:HA	2.06	0.55
5:H:65:PRO:HG2	5:H:80:ILE:HD11	1.89	0.55
3:C:33:PRO:HG2	3:C:36:GLN:HG2	1.88	0.55
4:D:9:GLY:O	4:D:26:PRO:HA	2.05	0.55
6:F:192:GLY:HA2	1:G:105:MET:HA	1.88	0.55
5:N:257:PHE:O	5:N:268:GLY:HA3	2.05	0.55
6:F:286:LYS:HD3	6:F:320:MET:HG3	1.87	0.55
7:L:293:VAL:HA	7:L:325:ILE:O	2.06	0.55
7:M:6:ASP:HA	7:M:101:THR:HG22	1.89	0.55

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:146:ILE:HB	5:E:288:LEU:HG	1.88	0.55
5:E:197:THR:OG1	6:F:264:MET:SD	2.64	0.55
7:L:188:LEU:HD23	7:L:193:TYR:HB2	1.89	0.55
7:L:192:GLY:O	7:M:109:ALA:HB2	2.06	0.55
2:B:174:LEU:HD12	2:B:263:MET:SD	2.46	0.55
7:M:293:VAL:HA	7:M:325:ILE:O	2.07	0.55
2:B:186:ILE:HA	2:B:189:GLU:HG2	1.89	0.55
4:D:153:THR:OG1	4:D:171:LEU:HB3	2.07	0.55
6:F:7:ASP:HA	6:F:101:THR:OG1	2.06	0.55
3:I:190:GLU:HB2	5:J:106:ASN:CG	2.27	0.55
7:M:30:VAL:HG21	7:M:76:ASP:O	2.07	0.55
1:G:356:GLU:HA	1:G:359:GLU:HG2	1.89	0.55
6:F:148:LEU:HA	6:F:156:HIS:O	2.07	0.55
5:E:196:VAL:HG12	6:F:264:MET:HB3	1.88	0.54
5:E:3:LEU:HD22	5:E:89:LEU:HD13	1.89	0.54
5:E:40:VAL:HB	1:G:163:GLY:HA3	1.89	0.54
5:E:4:VAL:HG21	5:E:339:SER:HA	1.89	0.54
3:I:54:GLN:O	3:I:57:ARG:HG3	2.06	0.54
5:J:10:GLY:O	5:J:27:PRO:HA	2.07	0.54
7:M:157:THR:O	7:M:170:ILE:HA	2.08	0.54
1:G:5:ILE:HB	1:G:100:LEU:HD23	1.89	0.54
5:H:31:GLY:HA3	5:H:60:LEU:HD13	1.88	0.54
5:H:146:ILE:O	5:H:292:ASN:HA	2.08	0.54
6:F:259:PRO:CB	6:F:264:MET:HB2	2.35	0.54
5:K:239:ASP:HB3	7:M:283:ASP:HA	1.90	0.54
5:N:152:ASP:HA	5:N:177:GLY:HA3	1.90	0.54
5:J:201:ARG:HG3	5:J:201:ARG:HH11	1.71	0.54
7:L:130:ALA:HB1	7:L:135:LEU:HD11	1.90	0.54
5:N:286:LYS:HD2	5:N:320:MET:HA	1.90	0.54
2:B:202:ILE:HD12	2:B:237:PRO:HD2	1.90	0.54
4:D:98:LEU:HD11	4:D:116:MET:SD	2.48	0.54
6:F:210:LYS:HB2	6:F:211:LEU:HD22	1.88	0.54
7:L:293:VAL:HG22	7:L:325:ILE:HB	1.90	0.54
6:F:146:ILE:HD11	6:F:157:ASN:HB3	1.88	0.54
3:I:44:GLN:HG3	3:I:45:LYS:HG3	1.88	0.54
3:I:175:LEU:HD12	3:I:179:ASP:HB2	1.89	0.54
3:I:300:MET:HA	3:I:330:ARG:NH2	2.23	0.54
5:K:146:ILE:O	5:K:292:ASN:HA	2.07	0.54
2:B:155:HIS:HA	2:B:170:MET:O	2.08	0.54
4:D:130:GLN:HG2	4:D:332:VAL:HG11	1.90	0.54
5:E:150:SER:HA	5:E:155:THR:HA	1.89	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:157:ASN:HB2	5:E:171:MET:HB2	1.90	0.54
5:E:200:GLU:HA	5:E:203:ILE:HB	1.89	0.54
1:G:146:ILE:HA	1:G:158:VAL:O	2.07	0.54
3:I:68:HIS:HA	3:I:154:VAL:HB	1.89	0.54
5:J:208:LYS:HA	5:J:212:CYS:SG	2.47	0.54
7:M:151:GLY:O	7:M:176:ALA:HB1	2.08	0.54
4:D:156:VAL:HG22	4:D:168:ILE:HG23	1.91	0.53
3:I:148:LEU:HD21	3:I:269:ILE:HB	1.90	0.53
2:B:4:VAL:HG12	2:B:98:LEU:HB3	1.90	0.53
5:N:4:VAL:HG21	5:N:339:SER:HA	1.90	0.53
2:B:207:LYS:HA	2:B:211:CYS:SG	2.48	0.53
5:E:293:VAL:HG22	5:E:325:ILE:HB	1.91	0.53
7:L:186:LYS:O	7:L:189:THR:HG22	2.09	0.53
2:B:6:ASP:O	2:B:12:VAL:HA	2.09	0.53
5:H:27:PRO:HB2	5:H:29:ILE:HG12	1.90	0.53
1:A:30:VAL:HB	1:A:76:ASP:OD2	2.09	0.53
1:A:84:THR:HA	1:A:88:GLU:HB2	1.91	0.53
3:I:356:GLU:HA	3:I:359:GLU:HG2	1.90	0.53
5:K:102:GLU:HB2	5:K:106:ASN:HD22	1.74	0.53
5:J:148:LEU:HA	5:J:156:HIS:O	2.08	0.53
7:M:52:GLU:O	7:M:56:LYS:HG2	2.09	0.53
5:H:86:TYR:O	5:H:90:ARG:HA	2.08	0.53
3:I:3:LEU:HD22	3:I:89:LEU:HD13	1.91	0.53
5:K:188:LEU:HA	5:K:191:ARG:HB2	1.91	0.53
5:N:146:ILE:O	5:N:292:ASN:HA	2.09	0.53
3:C:180:LEU:HB3	3:C:208:LYS:HD2	1.91	0.53
7:L:58:GLY:O	7:M:265:GLU:HB2	2.09	0.53
7:L:205:ARG:O	7:L:208:LYS:HB3	2.09	0.53
3:C:142:ARG:HG2	3:C:144:THR:O	2.09	0.53
6:F:208:LYS:HA	6:F:212:CYS:SG	2.49	0.53
5:E:69:GLY:O	5:E:103:ALA:HB2	2.08	0.52
6:F:95:GLU:HB2	6:F:96:HIS:ND1	2.24	0.52
7:M:59:ILE:HG23	7:M:60:LEU:HD13	1.91	0.52
4:D:91:PRO:O	4:D:122:VAL:HA	2.10	0.52
4:D:210:CYS:HB3	4:D:251:PRO:HD3	1.90	0.52
4:D:214:LEU:O	4:D:308:LYS:HE2	2.08	0.52
5:H:69:GLY:O	5:H:103:ALA:HB2	2.09	0.52
5:K:289:TYR:O	5:K:322:ILE:HA	2.10	0.52
7:L:294:LEU:HD23	7:L:299:THR:HB	1.89	0.52
5:N:27:PRO:O	5:N:50:GLY:HA2	2.10	0.52
2:B:308:GLN:HG3	2:B:321:ILE:HG21	1.91	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:5:ILE:HB	3:C:100:LEU:HD23	1.91	0.52
4:D:57:GLY:CA	6:F:283:ASP:HB2	2.37	0.52
5:J:27:PRO:O	5:J:50:GLY:HA2	2.09	0.52
7:L:184:LEU:HD13	7:L:252:CYS:SG	2.49	0.52
7:L:236:GLU:HG3	7:L:242:VAL:HG22	1.91	0.52
2:B:34:ARG:NH1	3:C:258:HIS:HB3	2.25	0.52
4:D:28:ILE:O	4:D:48:VAL:HA	2.09	0.52
1:G:180:LEU:HD21	1:G:256:LEU:HG	1.90	0.52
3:I:98:VAL:O	3:I:127:PHE:HA	2.09	0.52
7:L:70:ILE:HG13	7:L:106:ASN:ND2	2.24	0.52
5:N:98:THR:O	5:N:127:MET:HA	2.08	0.52
5:E:108:LYS:HA	5:E:111:ARG:HG2	1.92	0.52
6:F:67:ILE:HG13	6:F:77:MET:SD	2.50	0.52
5:H:45:LYS:HD3	5:H:46:ASP:H	1.74	0.52
3:I:4:VAL:HG11	3:I:338:GLY:HA3	1.90	0.52
5:J:197:THR:OG1	5:J:200:GLU:HG3	2.09	0.52
7:L:270:HIS:HD2	7:L:315:LEU:HD11	1.74	0.52
7:M:189:THR:HG21	5:N:107:PRO:HB3	1.91	0.52
1:A:113:LYS:NZ	1:A:113:LYS:HA	2.25	0.52
3:I:49:VAL:HG21	3:I:80:ILE:HA	1.91	0.52
7:M:211:LEU:O	7:M:249:ARG:HD2	2.10	0.52
1:G:2:ALA:HB3	1:G:17:ALA:HB2	1.92	0.52
1:G:92:ALA:O	1:G:95:GLU:HB3	2.10	0.52
3:I:147:VAL:O	3:I:157:VAL:HA	2.10	0.52
3:I:186:LYS:HZ1	3:I:262:LEU:HA	1.74	0.52
5:J:312:ILE:HG22	5:J:322:ILE:HD13	1.91	0.52
2:B:209:LYS:HB2	2:B:210:LEU:HD22	1.92	0.52
3:C:294:MET:O	3:C:327:PRO:HD2	2.09	0.52
5:J:3:LEU:HA	5:J:15:GLY:O	2.10	0.52
5:J:4:VAL:O	5:J:14:ALA:HA	2.10	0.52
5:N:7:ASN:HA	5:N:12:VAL:HA	1.91	0.52
2:B:5:CYS:HA	2:B:13:LYS:O	2.09	0.52
3:C:297:GLY:HA2	3:C:331:LYS:HG2	1.91	0.52
5:K:5:CYS:O	5:K:100:LEU:HA	2.10	0.52
1:G:98:VAL:O	1:G:127:PHE:HA	2.10	0.51
7:L:235:TYR:O	7:L:243:ILE:HG12	2.10	0.51
7:M:11:MET:O	7:M:13:LYS:NZ	2.43	0.51
5:J:160:ILE:HA	5:J:165:ALA:HA	1.92	0.51
7:L:149:ASP:HB3	7:L:156:HIS:HB2	1.92	0.51
4:D:111:LYS:HA	4:D:114:GLN:HG3	1.92	0.51
5:H:148:LEU:HD11	5:H:269:ILE:HG23	1.92	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:208:LYS:HA	7:M:212:CYS:SG	2.50	0.51
5:N:5:CYS:HB3	5:N:100:LEU:HD23	1.92	0.51
4:D:33:ARG:HG2	4:D:58:ILE:HA	1.93	0.51
3:I:192:GLY:O	5:J:70:ILE:HD12	2.10	0.51
7:L:155:THR:HG23	7:L:175:LEU:O	2.10	0.51
3:I:3:LEU:HA	3:I:16:PHE:HA	1.92	0.51
2:B:183:LEU:HD23	2:B:203:VAL:HG22	1.92	0.51
2:B:274:ASN:HA	2:B:277:MET:HB2	1.92	0.51
4:D:246:GLU:HG3	4:D:249:ARG:HH11	1.76	0.51
5:E:347:PHE:HA	5:E:350:MET:HB2	1.93	0.51
7:L:187:ILE:HG22	7:L:248:GLU:HG3	1.92	0.51
2:B:180:THR:OG1	2:B:204:ARG:HA	2.11	0.51
5:E:98:THR:O	5:E:127:MET:HA	2.10	0.51
5:H:187:ILE:HD11	5:H:252:CYS:HB2	1.93	0.51
5:N:248:GLU:HA	5:N:251:ARG:HB2	1.92	0.51
3:C:107:PRO:HB2	3:C:110:ASN:HB2	1.92	0.51
4:D:135:LEU:HD11	4:D:158:ILE:HG13	1.93	0.51
7:M:34:ARG:HD2	5:N:260:SER:O	2.11	0.51
5:E:97:PRO:HB3	5:E:126:ALA:HB3	1.93	0.51
6:F:189:THR:O	1:G:105:MET:HG3	2.11	0.51
6:F:207:ILE:HG23	6:F:211:LEU:HD23	1.93	0.51
3:I:186:LYS:NZ	3:I:261:VAL:O	2.44	0.51
5:J:361:GLY:O	5:J:364:ILE:HG13	2.10	0.51
3:I:190:GLU:HG2	5:J:103:ALA:C	2.32	0.51
5:E:181:THR:HG22	5:E:208:LYS:HE2	1.92	0.50
6:F:293:VAL:HA	6:F:325:ILE:O	2.11	0.50
3:I:4:VAL:O	3:I:14:ALA:HA	2.11	0.50
3:I:135:LEU:HB3	3:I:337:GLY:HA3	1.93	0.50
7:L:48:TYR:HB2	7:L:60:LEU:HD21	1.93	0.50
2:B:183:LEU:HD22	2:B:207:LYS:HB2	1.93	0.50
5:E:261:PHE:HD1	6:F:279:LYS:HE2	1.77	0.50
6:F:14:LYS:N	6:F:14:LYS:HD2	2.26	0.50
6:F:233:LYS:HB2	6:F:249:ARG:HD2	1.93	0.50
5:J:7:ASN:HA	5:J:12:VAL:HG22	1.92	0.50
5:J:188:LEU:HA	5:J:191:ARG:HB3	1.93	0.50
7:M:211:LEU:HD23	7:M:233:LYS:HB3	1.94	0.50
5:K:31:GLY:HA3	5:K:60:LEU:HD13	1.94	0.50
5:N:3:LEU:HB2	5:N:98:THR:HA	1.93	0.50
1:A:5:ILE:HB	1:A:100:LEU:HD23	1.92	0.50
3:C:104:PRO:HD3	3:C:132:GLN:HB2	1.93	0.50
3:C:146:ILE:O	3:C:292:ILE:HA	2.12	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:153:THR:HG23	4:D:173:LEU:O	2.11	0.50
4:D:210:CYS:HA	4:D:247:ARG:O	2.11	0.50
5:E:175:LEU:HD13	5:E:262:ILE:HG21	1.94	0.50
7:L:29:ILE:HD11	7:L:54:GLN:HG2	1.93	0.50
7:L:268:GLY:HA3	7:L:270:HIS:CE1	2.47	0.50
3:C:5:ILE:HA	3:C:13:LYS:O	2.12	0.50
5:K:165:ALA:HB1	5:K:170:ILE:HD11	1.92	0.50
7:M:281:ASP:HB3	7:M:284:ILE:HG12	1.92	0.50
5:N:66:ILE:HG12	5:N:71:ILE:HG12	1.93	0.50
5:N:294:MET:SD	5:N:326:ALA:HB2	2.52	0.50
1:A:5:ILE:HA	1:A:13:LYS:O	2.11	0.50
3:I:208:LYS:HA	3:I:212:CYS:SG	2.51	0.50
7:L:94:GLU:HA	7:L:123:ASN:O	2.12	0.50
7:L:345:SER:O	7:L:348:GLN:HB2	2.11	0.50
7:M:34:ARG:O	7:M:35:HIS:HB2	2.12	0.50
1:A:4:VAL:O	1:A:14:ALA:HA	2.12	0.50
2:B:185:LYS:HD2	3:C:168:HIS:HB3	1.94	0.50
4:D:132:VAL:HG22	4:D:158:ILE:HD12	1.94	0.50
1:G:150:SER:HA	1:G:155:THR:HA	1.92	0.50
1:A:98:VAL:O	1:A:127:PHE:HA	2.12	0.49
2:B:289:ALA:O	2:B:322:LYS:NZ	2.42	0.49
6:F:186:LYS:O	6:F:190:GLU:HG3	2.12	0.49
5:J:104:PRO:HG2	5:J:158:VAL:HG21	1.94	0.49
5:J:240:GLY:HA2	7:L:286:LYS:NZ	2.27	0.49
7:M:93:PRO:O	7:M:125:PRO:HD3	2.12	0.49
7:M:215:ALA:O	7:M:307:ARG:HD3	2.12	0.49
1:A:206:ASP:HA	1:A:209:GLU:HB2	1.93	0.49
3:C:148:LEU:HD21	3:C:269:ILE:HB	1.94	0.49
5:E:83:HIS:HA	5:E:87:ASN:HB2	1.93	0.49
5:N:202:GLU:HA	5:N:205:ARG:HG2	1.92	0.49
1:A:9:SER:HA	1:A:66:ILE:HB	1.94	0.49
1:A:157:VAL:O	1:A:170:ILE:HA	2.12	0.49
5:E:9:SER:HB3	5:E:178:ARG:NH2	2.27	0.49
1:G:66:ILE:HG12	1:G:71:VAL:HG22	1.92	0.49
5:N:299:THR:O	5:N:304:ILE:HG21	2.12	0.49
3:I:186:LYS:NZ	3:I:262:LEU:HA	2.27	0.49
5:K:66:ILE:HA	5:K:70:ILE:O	2.12	0.49
7:M:205:ARG:O	7:M:208:LYS:HB3	2.12	0.49
5:N:4:VAL:O	5:N:14:ALA:HA	2.12	0.49
5:N:175:LEU:HD11	5:N:256:LEU:HA	1.95	0.49
3:C:4:VAL:HA	3:C:99:LEU:O	2.11	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:298:MET:SD	4:D:329:LYS:HD2	2.53	0.49
6:F:184:LEU:HB2	6:F:252:CYS:SG	2.53	0.49
1:A:279:LYS:HB3	1:A:279:LYS:HZ2	1.77	0.49
6:F:157:ASN:O	6:F:170:ILE:HA	2.12	0.49
6:F:192:GLY:HA2	1:G:105:MET:CA	2.42	0.49
5:N:151:GLY:O	5:N:176:ALA:HB1	2.12	0.49
3:I:5:ILE:HB	3:I:100:LEU:HD23	1.95	0.49
1:A:2:ALA:HB3	1:A:17:ALA:HB2	1.95	0.49
2:B:156:ASN:O	2:B:169:ILE:HA	2.13	0.49
4:D:45:ASP:HA	4:D:77:LYS:HD3	1.95	0.49
4:D:235:LEU:HD12	4:D:239:GLN:HB2	1.94	0.49
1:G:247:ASN:HD21	1:G:251:ARG:NH2	2.11	0.49
5:J:317:PRO:O	5:J:320:MET:HB2	2.12	0.49
7:L:28:SER:HB3	7:L:80:ILE:HD13	1.94	0.49
2:B:10:GLY:O	2:B:27:PRO:HA	2.13	0.49
5:H:240:GLY:HA3	5:J:317:PRO:HB3	1.94	0.49
5:K:185:MET:HA	5:K:204:VAL:HG21	1.95	0.49
2:B:107:LYS:N	2:B:107:LYS:HD3	2.28	0.49
3:C:177:GLY:O	3:C:208:LYS:NZ	2.44	0.49
5:H:214:VAL:HG23	5:H:301:TYR:HB3	1.95	0.49
7:L:11:MET:O	7:L:13:LYS:NZ	2.46	0.49
7:L:93:PRO:O	7:L:125:PRO:HD3	2.12	0.49
5:N:118:MET:HB3	5:N:127:MET:SD	2.53	0.49
2:B:210:LEU:HB3	2:B:248:ARG:HD2	1.94	0.48
4:D:182:LEU:HD12	4:D:185:ILE:HD11	1.95	0.48
6:F:211:LEU:HG	6:F:245:ILE:HD11	1.95	0.48
5:K:27:PRO:HB2	5:K:29:ILE:HD11	1.95	0.48
5:J:189:THR:HG22	5:J:194:SER:HA	1.94	0.48
2:B:45:LYS:HB2	2:B:48:TYR:CE1	2.48	0.48
2:B:247:GLU:HA	2:B:250:ARG:HB3	1.94	0.48
5:E:5:CYS:HA	5:E:13:LYS:O	2.13	0.48
3:C:146:ILE:HG21	3:C:277:ILE:HD11	1.94	0.48
6:F:206:ASP:O	6:F:210:LYS:HG2	2.13	0.48
1:G:7:ASN:HD21	1:G:100:LEU:HD22	1.79	0.48
3:I:150:SER:HB3	3:I:298:THR:HB	1.95	0.48
5:K:187:ILE:HD11	5:K:252:CYS:HB2	1.95	0.48
5:N:107:PRO:O	5:N:111:ARG:HG3	2.13	0.48
7:L:19:ASP:HB2	7:L:335:TRP:CH2	2.48	0.48
5:N:119:PHE:O	5:N:123:ASN:HA	2.14	0.48
3:C:56:LYS:HD3	3:C:59:ILE:HD11	1.96	0.48
3:C:155:THR:O	3:C:172:ARG:HA	2.13	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:98:LEU:O	4:D:127:VAL:HA	2.13	0.48
7:L:239:ASP:HA	5:N:313:THR:HG23	1.95	0.48
7:M:112:GLU:HA	7:M:365:VAL:HG21	1.95	0.48
1:A:211:LEU:HD11	1:A:235:TYR:HB2	1.96	0.48
2:B:186:ILE:O	2:B:189:GLU:HG2	2.14	0.48
7:L:348:GLN:NE2	7:L:351:TRP:HE1	2.11	0.48
5:E:146:ILE:HD11	5:E:157:ASN:HB3	1.95	0.48
3:I:239:ASP:HB3	5:K:285:ARG:HE	1.79	0.48
5:E:4:VAL:HG13	5:E:99:LEU:HD22	1.95	0.48
3:I:191:ARG:NH2	5:J:109:ALA:HB3	2.29	0.48
5:J:146:ILE:HA	5:J:158:VAL:O	2.14	0.48
5:J:155:THR:HG21	5:J:269:ILE:HD11	1.96	0.48
7:M:84:THR:HA	7:M:88:GLU:HB2	1.96	0.48
2:B:236:LEU:HG	2:B:238:ASP:OD1	2.14	0.48
1:G:214:VAL:HG22	1:G:253:PRO:HB3	1.95	0.48
1:A:49:VAL:HB	1:A:83:HIS:CD2	2.49	0.47
3:C:330:ARG:HA	3:C:333:SER:OG	2.14	0.47
6:F:297:GLY:HA2	6:F:331:LYS:HG2	1.96	0.47
7:L:110:ASN:O	7:L:114:MET:HB2	2.14	0.47
7:L:301:TYR:HA	7:L:302:PRO:HD3	1.76	0.47
7:M:101:THR:HA	7:M:130:ALA:O	2.14	0.47
7:M:347:PHE:HA	7:M:350:MET:HB3	1.95	0.47
1:A:38:ILE:HG13	1:A:39:MET:HG3	1.96	0.47
2:B:9:SER:HB3	2:B:66:ILE:O	2.14	0.47
5:J:6:ASP:HB3	5:J:13:LYS:HD3	1.95	0.47
1:A:104:PRO:HD3	1:A:132:GLN:HB2	1.96	0.47
3:C:104:PRO:HA	3:C:131:ILE:HG23	1.96	0.47
6:F:41:VAL:HB	5:H:280:CYS:HA	1.95	0.47
1:G:10:GLY:O	1:G:27:PRO:HA	2.14	0.47
3:I:158:VAL:HG22	3:I:170:ILE:HG23	1.97	0.47
4:D:260:ILE:HD13	4:D:260:ILE:H	1.79	0.47
3:I:188:LEU:HD23	5:J:107:PRO:HG3	1.96	0.47
5:N:29:ILE:HG21	5:N:62:LEU:HB3	1.94	0.47
1:G:312:ILE:HD13	1:G:315:LEU:HD12	1.97	0.47
5:H:6:ASP:O	5:H:12:VAL:HA	2.14	0.47
5:H:34:ARG:HD3	5:H:61:THR:HG23	1.95	0.47
3:I:158:VAL:HG13	3:I:170:ILE:HG12	1.96	0.47
5:K:3:LEU:HD22	5:K:89:LEU:HD13	1.96	0.47
7:L:156:HIS:HA	7:L:171:LEU:O	2.15	0.47
7:M:32:ARG:HD2	7:M:46:ASP:O	2.15	0.47
7:M:130:ALA:HB3	7:M:135:LEU:HD11	1.97	0.47

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:N:208:LYS:HA	5:N:212:CYS:SG	2.54	0.47
1:A:147:VAL:O	1:A:157:VAL:HA	2.14	0.47
7:M:65:PRO:HG2	7:M:80:ILE:HD11	1.96	0.47
5:N:216:LEU:O	5:N:310:LYS:NZ	2.43	0.47
1:A:47:SER:OG	1:A:79:LYS:HG2	2.15	0.47
3:C:159:PRO:HG2	3:C:166:LEU:HB2	1.97	0.47
5:E:362:PRO:O	5:E:365:VAL:HG12	2.14	0.47
5:H:280:CYS:O	5:H:285:ARG:NH1	2.48	0.47
3:I:157:VAL:O	3:I:170:ILE:HA	2.15	0.47
3:I:284:VAL:O	3:I:288:LEU:HG	2.15	0.47
5:K:134:VAL:HG13	5:K:160:ILE:HG12	1.97	0.47
7:L:159:PRO:HD3	7:L:276:SER:HB3	1.96	0.47
5:N:181:THR:HG23	5:N:204:VAL:HG23	1.95	0.47
2:B:230:LEU:HB3	2:B:246:ASN:H	1.80	0.47
3:C:137:LEU:HD22	3:C:160:ILE:HG21	1.96	0.47
4:D:65:ILE:HD11	4:D:75:MET:SD	2.55	0.47
6:F:42:GLY:O	5:H:161:TYR:HB3	2.15	0.47
5:H:142:ARG:HD3	5:H:291:ASN:OD1	2.15	0.47
3:I:165:SER:HB2	3:I:170:ILE:HD11	1.97	0.47
5:K:147:VAL:HA	5:K:293:VAL:O	2.14	0.47
5:N:147:VAL:HA	5:N:293:VAL:O	2.15	0.47
1:A:113:LYS:HA	1:A:113:LYS:HZ3	1.79	0.47
5:H:195:PHE:HA	5:H:200:GLU:HG3	1.97	0.47
7:M:100:LEU:HD11	7:M:118:MET:HE2	1.97	0.47
7:M:158:VAL:HA	7:M:170:ILE:HG12	1.97	0.47
4:D:150:ASP:HA	4:D:175:GLY:HA3	1.97	0.47
6:F:309:GLN:HE22	6:F:322:ILE:HB	1.79	0.47
5:K:150:SER:HA	5:K:155:THR:HA	1.97	0.47
3:C:256:LEU:HD11	3:C:298:THR:HG22	1.96	0.46
6:F:213:TYR:O	6:F:250:PHE:HA	2.14	0.46
5:H:214:VAL:HG12	5:H:307:ARG:HG3	1.96	0.46
5:K:75:ASP:CG	5:K:79:LYS:HZ1	2.18	0.46
2:B:6:ASP:HB3	2:B:13:LYS:HD3	1.96	0.46
5:K:169:ALA:HB2	5:K:280:CYS:SG	2.55	0.46
7:L:286:LYS:HD2	7:L:321:LYS:H	1.79	0.46
7:M:62:LEU:O	5:N:265:GLU:HB3	2.15	0.46
5:E:49:VAL:HB	5:E:83:HIS:CD2	2.50	0.46
5:E:215:ALA:HB1	5:E:221:GLU:HG3	1.97	0.46
5:E:263:GLY:HA3	6:F:278:MET:HB3	1.97	0.46
5:H:216:LEU:HD23	5:H:216:LEU:H	1.80	0.46
3:I:5:ILE:HB	3:I:100:LEU:CD2	2.45	0.46

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:332:SER:HA	2:B:335:ILE:HG12	1.97	0.46
3:C:299:THR:O	3:C:304:ILE:HG21	2.15	0.46
4:D:291:VAL:HG22	4:D:323:ILE:HB	1.97	0.46
5:K:183:TYR:CE2	5:K:252:CYS:HA	2.47	0.46
5:K:282:ILE:HA	5:K:285:ARG:HG3	1.96	0.46
2:B:291:ASN:O	2:B:323:ILE:HA	2.16	0.46
4:D:246:GLU:HA	4:D:249:ARG:HD3	1.97	0.46
5:E:123:ASN:HD22	5:E:354:LYS:HD3	1.79	0.46
3:I:190:GLU:HG3	5:J:105:LEU:C	2.36	0.46
7:L:149:ASP:HA	7:L:295:SER:O	2.16	0.46
5:N:69:GLY:O	5:N:103:ALA:HB2	2.15	0.46
1:A:99:LEU:HD13	1:A:128:TYR:HB3	1.98	0.46
6:F:42:GLY:C	5:H:161:TYR:HB3	2.35	0.46
3:I:13:LYS:HG3	3:I:25:VAL:HG13	1.97	0.46
3:I:56:LYS:O	3:I:60:LEU:HG	2.16	0.46
3:I:66:ILE:HD11	3:I:77:MET:SD	2.56	0.46
7:L:146:ILE:HG21	7:L:277:ILE:HD11	1.98	0.46
5:N:109:ALA:HA	5:N:112:GLU:HG2	1.98	0.46
5:N:157:ASN:O	5:N:170:ILE:HA	2.15	0.46
5:N:286:LYS:HZ1	5:N:290:ALA:HB2	1.80	0.46
2:B:286:ASP:HB2	2:B:289:ALA:HB3	1.96	0.46
7:L:19:ASP:HB2	7:L:335:TRP:HH2	1.79	0.46
7:M:30:VAL:HG22	7:M:49:VAL:HG23	1.97	0.46
1:A:168:HIS:O	1:A:279:LYS:NZ	2.49	0.46
5:E:155:THR:HG21	5:E:269:ILE:HG22	1.98	0.46
6:F:175:LEU:HD12	6:F:264:MET:HG3	1.98	0.46
6:F:212:CYS:HA	6:F:249:ARG:O	2.16	0.46
5:J:224:THR:HA	5:J:227:SER:OG	2.16	0.46
5:N:52:GLU:HG3	5:N:83:HIS:HE1	1.80	0.46
1:A:5:ILE:HB	1:A:100:LEU:CD2	2.46	0.46
2:B:4:VAL:O	2:B:14:ALA:HA	2.16	0.46
2:B:11:LEU:HB2	2:B:13:LYS:HE3	1.98	0.46
5:E:210:LYS:HB2	5:E:211:LEU:HD22	1.97	0.46
5:N:54:GLN:OE1	5:N:57:ARG:HD2	2.16	0.46
2:B:12:VAL:HG23	2:B:28:SER:HB2	1.98	0.46
2:B:190:ARG:O	3:C:107:PRO:HA	2.16	0.46
4:D:58:ILE:HD12	6:F:284:ILE:H	1.81	0.46
5:E:100:LEU:O	5:E:129:VAL:HA	2.16	0.46
1:G:165:SER:O	1:G:167:PRO:HD3	2.15	0.46
5:K:348:GLN:HA	5:K:351:TRP:HD1	1.81	0.46
1:A:69:GLY:HA3	1:A:103:ALA:HB2	1.98	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:39:MET:HA	1:G:164:PHE:HE1	1.81	0.45
6:F:46:LYS:NZ	6:F:61:LEU:HD21	2.31	0.45
5:K:185:MET:SD	5:K:195:PHE:HB2	2.56	0.45
7:L:215:ALA:O	7:L:307:ARG:HD3	2.16	0.45
7:M:4:VAL:O	7:M:14:ALA:HA	2.16	0.45
2:B:186:ILE:HG23	2:B:189:GLU:OE2	2.16	0.45
5:E:245:ILE:HG12	5:E:249:ARG:HG3	1.98	0.45
5:H:73:ASN:HD21	5:H:75:ASP:HB3	1.81	0.45
5:N:148:LEU:O	5:N:294:MET:HA	2.16	0.45
1:A:199:ALA:HB3	3:C:282:VAL:HB	1.98	0.45
3:C:147:VAL:HG22	3:C:293:VAL:HB	1.98	0.45
4:D:2:LEU:HB2	4:D:96:THR:HA	1.96	0.45
5:E:123:ASN:ND2	5:E:354:LYS:HD3	2.30	0.45
5:E:240:GLY:HA3	1:G:317:PRO:HB3	1.98	0.45
6:F:291:ASN:HA	6:F:325:ILE:HD13	1.99	0.45
2:B:188:THR:O	3:C:105:MET:HB3	2.16	0.45
3:C:356:GLU:HA	3:C:359:GLU:HG2	1.98	0.45
1:G:299:THR:HA	1:G:304:ILE:HD13	1.98	0.45
5:H:323:LYS:HE3	5:H:325:ILE:HG13	1.99	0.45
3:I:69:GLY:HA3	3:I:103:ALA:HB2	1.99	0.45
5:J:169:ALA:HB1	5:J:276:SER:HB2	1.97	0.45
5:K:195:PHE:HD1	5:K:200:GLU:HB3	1.81	0.45
7:L:213:TYR:O	7:L:253:PRO:HG2	2.15	0.45
7:M:81:TRP:CH2	7:M:114:MET:HG3	2.51	0.45
5:E:156:HIS:NE2	5:E:172:ARG:HG3	2.31	0.45
5:H:101:THR:HG22	5:H:135:LEU:HD12	1.99	0.45
5:H:158:VAL:HG22	5:H:170:ILE:HG12	1.98	0.45
5:H:237:LEU:HD22	5:H:241:GLN:HB3	1.98	0.45
7:L:203:ILE:O	7:L:207:ILE:HG13	2.17	0.45
7:L:259:PRO:CG	7:L:266:SER:HB2	2.39	0.45
4:D:33:ARG:NH2	4:D:60:THR:OG1	2.49	0.45
6:F:66:PRO:CG	6:F:76:ASP:HB3	2.42	0.45
5:H:56:LYS:O	5:H:60:LEU:HG	2.16	0.45
5:J:98:THR:O	5:J:127:MET:HA	2.16	0.45
5:J:200:GLU:O	5:J:204:VAL:HG23	2.16	0.45
3:C:119:PHE:O	3:C:123:ASN:HA	2.17	0.45
4:D:114:GLN:HB2	4:D:118:GLU:OE2	2.17	0.45
4:D:156:VAL:HG13	4:D:168:ILE:HG12	1.97	0.45
5:H:118:MET:HG3	5:H:127:MET:HE2	1.99	0.45
3:I:9:SER:HA	3:I:66:ILE:HB	1.99	0.45
5:N:237:LEU:HD12	5:N:241:GLN:HG3	1.98	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:N:293:VAL:HA	5:N:325:ILE:O	2.17	0.45
2:B:282:ASP:O	2:B:285:LYS:HG2	2.17	0.45
2:B:286:ASP:HA	2:B:289:ALA:H	1.81	0.45
6:F:183:TYR:O	6:F:186:LYS:HG3	2.17	0.45
6:F:247:ASN:HA	6:F:250:PHE:CE2	2.51	0.45
3:I:199:ALA:HB1	5:K:283:ASP:H	1.82	0.45
7:L:3:LEU:HB2	7:L:98:VAL:HG23	1.97	0.45
7:M:23:ARG:HA	7:M:23:ARG:HD3	1.81	0.45
1:A:181:THR:OG1	1:A:208:LYS:NZ	2.46	0.45
2:B:103:PRO:HD3	2:B:131:GLN:HB2	1.98	0.45
3:C:6:ASP:HA	3:C:101:THR:OG1	2.16	0.45
4:D:4:CYS:HB3	4:D:98:LEU:HD23	1.99	0.45
5:E:186:LYS:NZ	6:F:272:THR:HG22	2.28	0.45
6:F:32:GLY:HA2	6:F:62:THR:O	2.16	0.45
7:M:165:ALA:HB1	7:M:170:ILE:HD11	1.97	0.45
4:D:212:VAL:HG23	4:D:299:TYR:HB3	1.99	0.45
5:H:175:LEU:HD23	5:H:264:MET:SD	2.57	0.45
7:M:300:MET:HA	7:M:330:ARG:NH1	2.32	0.45
5:N:5:CYS:HA	5:N:13:LYS:O	2.17	0.45
5:N:300:MET:HA	5:N:330:ARG:HH11	1.82	0.45
3:C:14:ALA:HB1	3:C:89:LEU:HD11	1.99	0.44
1:G:231:ILE:O	1:G:249:ARG:NH1	2.50	0.44
5:J:83:HIS:O	5:J:87:ASN:HB2	2.16	0.44
5:K:4:VAL:HG13	5:K:99:LEU:HD22	1.99	0.44
2:B:224:ALA:HA	2:B:230:LEU:HG	1.98	0.44
2:B:329:ARG:HA	2:B:332:SER:OG	2.18	0.44
3:C:3:LEU:HD22	3:C:89:LEU:HD13	1.98	0.44
6:F:10:SER:HA	6:F:67:ILE:O	2.17	0.44
5:H:147:VAL:HA	5:H:293:VAL:O	2.17	0.44
5:J:111:ARG:HH12	5:J:365:VAL:HG22	1.82	0.44
5:E:352:ILE:HG23	5:E:364:ILE:HD13	1.99	0.44
3:I:293:VAL:HA	3:I:325:ILE:O	2.17	0.44
7:L:198:THR:N	7:L:199:ALA:HA	2.31	0.44
7:M:152:ASP:O	7:M:178:ARG:HG3	2.17	0.44
2:B:149:SER:HA	2:B:154:THR:HA	2.00	0.44
2:B:188:THR:HA	2:B:192:TYR:O	2.16	0.44
4:D:149:GLY:O	4:D:174:ALA:HB1	2.18	0.44
5:H:5:CYS:SG	5:H:84:THR:HG21	2.56	0.44
5:H:147:VAL:HG22	5:H:293:VAL:HB	1.99	0.44
3:I:213:TYR:O	3:I:250:PHE:HA	2.17	0.44
1:A:146:ILE:HA	1:A:158:VAL:O	2.17	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:155:THR:O	5:E:172:ARG:HA	2.17	0.44
6:F:92:ALA:HA	6:F:93:PRO:HD3	1.89	0.44
5:K:214:VAL:HG22	5:K:253:PRO:HB3	2.00	0.44
7:L:56:LYS:O	7:L:59:ILE:HG22	2.17	0.44
7:M:5:VAL:HA	7:M:13:LYS:O	2.17	0.44
5:N:123:ASN:ND2	5:N:354:LYS:HE3	2.32	0.44
2:B:30:VAL:HG11	2:B:78:LYS:HB3	2.00	0.44
3:C:317:PRO:HB2	3:C:320:MET:HB2	2.00	0.44
4:D:273:ASN:O	4:D:277:LYS:HG2	2.17	0.44
6:F:40:MET:O	5:H:166:LEU:HD22	2.17	0.44
5:K:29:ILE:HG13	5:K:54:GLN:HE21	1.83	0.44
5:K:157:ASN:OD1	5:K:272:THR:HG22	2.18	0.44
5:K:177:GLY:O	5:K:208:LYS:NZ	2.51	0.44
7:L:199:ALA:HB3	5:N:282:ILE:HG21	1.99	0.44
3:C:146:ILE:HA	3:C:158:VAL:O	2.18	0.44
5:E:31:GLY:HA3	5:E:60:LEU:HD12	2.00	0.44
5:H:27:PRO:O	5:H:50:GLY:HA2	2.18	0.44
7:L:211:LEU:O	7:L:249:ARG:HD2	2.17	0.44
7:M:9:SER:HA	7:M:66:ILE:HB	1.99	0.44
5:N:277:ILE:CG2	5:N:285:ARG:HG2	2.47	0.44
3:C:80:ILE:O	3:C:83:HIS:HB3	2.17	0.44
5:E:29:ILE:O	5:E:49:VAL:HA	2.18	0.44
5:E:157:ASN:O	5:E:170:ILE:HA	2.18	0.44
6:F:202:GLU:HG3	6:F:205:ARG:HH12	1.82	0.44
6:F:308:MET:HA	6:F:311:GLU:HB2	2.00	0.44
6:F:309:GLN:NE2	6:F:322:ILE:HB	2.33	0.44
5:H:111:ARG:O	5:H:114:MET:HG2	2.17	0.44
3:I:4:VAL:HA	3:I:99:LEU:O	2.17	0.44
7:L:175:LEU:HD13	7:L:264:MET:SD	2.58	0.44
5:N:3:LEU:HA	5:N:15:GLY:O	2.17	0.44
6:F:60:ILE:HG13	6:F:61:LEU:HG	2.00	0.44
6:F:99:LEU:HA	6:F:128:TYR:O	2.18	0.44
1:G:247:ASN:ND2	1:G:251:ARG:NH2	2.66	0.44
5:H:218:PHE:HE1	5:H:250:PHE:HB2	1.82	0.44
5:J:9:SER:HA	5:J:66:ILE:HB	1.99	0.44
7:M:6:ASP:N	7:M:13:LYS:O	2.51	0.44
1:A:195:PHE:HA	1:A:200:GLU:HB3	2.00	0.43
4:D:57:GLY:HA3	4:D:59:LEU:N	2.33	0.43
5:J:194:SER:O	7:L:282:VAL:HG11	2.18	0.43
7:L:149:ASP:O	7:L:155:THR:HA	2.18	0.43
7:L:299:THR:OG1	7:L:330:ARG:NH1	2.51	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:111:ARG:O	7:M:114:MET:HB3	2.17	0.43
4:D:100:GLU:O	4:D:129:ILE:HA	2.18	0.43
5:J:285:ARG:HA	5:J:288:LEU:HD22	2.00	0.43
5:K:130:ALA:HB3	5:K:135:LEU:HD11	2.00	0.43
5:K:151:GLY:HA2	5:K:297:GLY:H	1.83	0.43
5:N:270:HIS:CD2	5:N:271:GLU:HG3	2.53	0.43
5:E:208:LYS:HA	5:E:212:CYS:SG	2.58	0.43
5:E:294:MET:HB3	5:E:299:THR:HG21	2.00	0.43
5:K:45:LYS:HD3	5:K:46:ASP:H	1.84	0.43
7:L:291:ASN:HA	7:L:325:ILE:HD12	1.99	0.43
1:A:148:LEU:HD23	1:A:294:MET:SD	2.58	0.43
3:C:10:GLY:O	3:C:27:PRO:HA	2.19	0.43
3:C:68:HIS:HA	3:C:154:VAL:HB	2.00	0.43
4:D:4:CYS:SG	4:D:82:THR:HG21	2.58	0.43
4:D:205:ILE:HG23	4:D:209:LEU:HD23	2.00	0.43
5:E:65:PRO:HG3	5:E:76:ASP:HB3	2.00	0.43
6:F:100:LEU:O	6:F:129:VAL:HA	2.18	0.43
3:I:194:SER:HA	5:J:172:ARG:NE	2.33	0.43
7:M:115:THR:HG23	7:M:127:MET:SD	2.59	0.43
7:M:119:PHE:HZ	7:M:352:ILE:O	2.01	0.43
5:N:357:TYR:HE1	5:N:362:PRO:HG3	1.82	0.43
6:F:67:ILE:HD11	6:F:77:MET:HE1	2.00	0.43
6:F:95:GLU:HB2	6:F:96:HIS:HD1	1.82	0.43
5:K:4:VAL:O	5:K:14:ALA:HA	2.17	0.43
5:K:252:CYS:HB3	5:K:253:PRO:HD3	1.99	0.43
2:B:102:ALA:HA	2:B:131:GLN:OE1	2.18	0.43
2:B:138:ALA:HB1	2:B:335:ILE:HG13	2.00	0.43
3:C:7:ASN:HD21	3:C:100:LEU:HD22	1.84	0.43
3:C:155:THR:HB	3:C:173:ILE:O	2.19	0.43
1:G:247:ASN:HD21	1:G:251:ARG:HH21	1.66	0.43
5:J:273:THR:HG21	5:J:312:ILE:HD13	2.00	0.43
1:A:231:ILE:O	1:A:249:ARG:NH1	2.50	0.43
1:A:259:PRO:HB2	1:A:264:LEU:O	2.19	0.43
3:C:165:SER:O	3:C:167:PRO:HD3	2.18	0.43
4:D:184:LYS:O	4:D:187:THR:HB	2.18	0.43
5:E:235:TYR:O	5:E:243:ILE:HG13	2.19	0.43
6:F:7:ASP:O	6:F:13:VAL:HA	2.19	0.43
6:F:35:ARG:HD3	6:F:59:GLY:O	2.19	0.43
5:H:5:CYS:HA	5:H:13:LYS:O	2.19	0.43
7:M:149:ASP:O	7:M:155:THR:HA	2.19	0.43
7:M:169:ALA:HB1	7:M:276:SER:O	2.17	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:105:LEU:HD12	5:E:172:ARG:HD3	2.01	0.43
6:F:295:SER:HA	6:F:330:ARG:HB2	2.01	0.43
1:G:115:THR:HA	1:G:127:PHE:HE2	1.83	0.43
5:K:5:CYS:HB3	5:K:100:LEU:HD23	2.00	0.43
5:K:155:THR:HB	5:K:173:LEU:HB3	2.00	0.43
7:M:69:GLY:HA3	7:M:103:ALA:HB2	2.00	0.43
5:N:7:ASN:ND2	5:N:12:VAL:HG13	2.34	0.43
2:B:145:ILE:HG23	2:B:291:ASN:ND2	2.34	0.43
1:G:15:GLY:HA2	1:G:23:ARG:HB2	2.01	0.43
5:N:150:SER:HA	5:N:154:VAL:O	2.19	0.43
2:B:57:ARG:HE	2:B:62:LEU:HD11	1.83	0.43
2:B:148:ASP:O	2:B:154:THR:HA	2.19	0.43
4:D:164:LEU:HA	4:D:165:PRO:HD2	1.83	0.43
4:D:290:ASN:O	4:D:323:ILE:N	2.52	0.43
6:F:142:ARG:HD3	6:F:291:ASN:OD1	2.18	0.43
6:F:216:LEU:HD12	6:F:307:ARG:HA	2.01	0.43
5:H:85:PHE:HB3	5:H:93:PRO:HD3	2.01	0.43
1:A:92:ALA:HA	1:A:93:PRO:HD2	1.89	0.42
5:E:142:ARG:NH1	5:E:291:ASN:OD1	2.51	0.42
6:F:46:LYS:NZ	6:F:46:LYS:O	2.48	0.42
6:F:157:ASN:OD1	6:F:272:THR:HB	2.19	0.42
6:F:166:LEU:HA	6:F:167:PRO:HD3	1.85	0.42
5:H:197:THR:HB	5:J:283:ASP:HB2	2.01	0.42
5:H:277:ILE:HG22	5:H:285:ARG:HD3	2.00	0.42
3:I:186:LYS:HB3	5:J:167:PRO:HB2	2.00	0.42
5:K:216:LEU:HD23	5:K:216:LEU:H	1.84	0.42
4:D:167:ALA:HB2	4:D:277:LYS:HB2	2.01	0.42
5:E:31:GLY:HA3	5:E:48:TYR:HB2	2.00	0.42
1:G:5:ILE:HA	1:G:13:LYS:O	2.19	0.42
1:G:31:GLY:HA3	1:G:60:LEU:HD13	2.01	0.42
5:H:97:PRO:HA	5:H:126:ALA:O	2.19	0.42
5:H:115:THR:HG21	5:H:365:VAL:HG21	2.00	0.42
5:J:100:LEU:O	5:J:129:VAL:HA	2.19	0.42
6:F:30:ILE:O	6:F:50:VAL:HA	2.19	0.42
1:G:175:LEU:HD11	1:G:256:LEU:HA	2.01	0.42
5:H:61:THR:O	5:H:63:LYS:NZ	2.52	0.42
5:K:115:THR:HG23	5:K:127:MET:SD	2.60	0.42
5:N:119:PHE:O	5:N:354:LYS:HE2	2.19	0.42
1:A:119:PHE:CZ	1:A:127:PHE:HB3	2.55	0.42
2:B:2:ALA:HB3	2:B:17:ALA:HB2	2.00	0.42
2:B:145:ILE:O	2:B:291:ASN:HA	2.19	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:144:THR:HA	3:C:160:ILE:O	2.20	0.42
3:C:282:VAL:HG22	3:C:285:ARG:NH1	2.34	0.42
4:D:86:GLU:O	4:D:88:ARG:NH1	2.52	0.42
6:F:40:MET:SD	6:F:41:VAL:N	2.92	0.42
6:F:106:ASN:HA	6:F:107:PRO:HD3	1.91	0.42
1:G:26:PHE:HE2	1:G:80:ILE:HG23	1.84	0.42
1:G:151:GLY:O	1:G:176:ALA:HB1	2.18	0.42
3:I:17:ALA:HB1	3:I:343:SER:OG	2.19	0.42
1:A:105:MET:HG3	1:A:170:ILE:HD12	2.01	0.42
2:B:289:ALA:O	2:B:322:LYS:HB3	2.20	0.42
3:C:6:ASP:O	3:C:12:CYS:HA	2.19	0.42
3:C:182:ASP:CG	3:C:201:ARG:HH21	2.23	0.42
3:C:325:ILE:O	3:C:327:PRO:HD3	2.19	0.42
5:E:106:ASN:HA	5:E:107:PRO:HD3	1.81	0.42
5:E:154:VAL:HG21	5:E:156:HIS:CE1	2.54	0.42
5:E:231:LEU:O	5:E:249:ARG:NH1	2.52	0.42
6:F:31:VAL:HG22	6:F:50:VAL:HG22	2.02	0.42
6:F:145:GLY:HA2	6:F:287:ASP:O	2.19	0.42
5:H:6:ASP:OD2	5:H:13:LYS:NZ	2.50	0.42
5:N:354:LYS:NZ	5:N:358:ASP:OD1	2.52	0.42
1:A:99:LEU:HA	1:A:128:TYR:O	2.20	0.42
1:A:312:ILE:HB	1:A:322:VAL:HG11	2.01	0.42
5:E:97:PRO:HA	5:E:126:ALA:O	2.20	0.42
6:F:192:GLY:O	1:G:107:PRO:HG3	2.19	0.42
6:F:275:ASN:O	6:F:279:LYS:HB2	2.19	0.42
1:G:27:PRO:HB2	1:G:29:ILE:HG13	2.02	0.42
3:I:191:ARG:HD2	5:J:108:LYS:H	1.83	0.42
3:I:213:TYR:HB2	3:I:302:PRO:O	2.20	0.42
5:N:85:PHE:HD1	5:N:89:LEU:HD12	1.84	0.42
5:N:96:HIS:HA	5:N:97:PRO:HD2	1.92	0.42
5:N:108:LYS:HA	5:N:108:LYS:HD3	1.84	0.42
2:B:29:ILE:CG2	2:B:50:GLY:HA2	2.50	0.42
5:N:54:GLN:O	5:N:57:ARG:HG3	2.19	0.42
3:C:34:ARG:NH2	3:C:60:LEU:O	2.52	0.42
4:D:11:VAL:O	4:D:24:VAL:HA	2.20	0.42
5:J:258:GLN:HB3	5:J:260:SER:OG	2.20	0.42
5:K:144:THR:HA	5:K:160:ILE:O	2.19	0.42
5:E:146:ILE:HG21	5:E:277:ILE:HD11	2.01	0.42
6:F:188:LEU:HA	6:F:191:ARG:HD3	2.01	0.42
3:I:179:ASP:HA	3:I:182:ASP:HB2	2.01	0.42
5:K:49:VAL:HG13	5:K:80:ILE:HG12	2.02	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:148:LEU:HD21	5:K:269:ILE:HG23	2.02	0.42
5:K:356:GLU:HB3	5:K:364:ILE:HG12	2.01	0.42
7:L:182:ASP:CG	7:L:201:ARG:HH21	2.23	0.42
7:M:172:ARG:HH12	7:M:174:ASP:CG	2.23	0.42
1:A:115:THR:HA	1:A:127:PHE:HE2	1.85	0.42
2:B:186:ILE:HD13	2:B:250:ARG:HD3	2.02	0.42
3:C:119:PHE:HB3	3:C:354:LYS:HE2	2.02	0.42
4:D:131:ALA:O	4:D:134:SER:HB2	2.20	0.42
4:D:158:ILE:HA	4:D:162:TYR:O	2.20	0.42
4:D:352:LYS:HE3	4:D:356:ASP:OD2	2.20	0.42
6:F:183:TYR:CD1	6:F:262:ILE:HG22	2.54	0.42
6:F:245:ILE:HB	6:F:248:GLU:HG2	2.02	0.42
1:G:6:ASP:O	1:G:12:CYS:HA	2.20	0.42
1:G:188:LEU:HD22	1:G:245:ILE:HD12	2.01	0.42
5:H:144:THR:OG1	5:H:161:TYR:HA	2.20	0.42
5:H:246:GLY:O	5:H:249:ARG:HB3	2.19	0.42
3:I:169:ALA:HB1	3:I:276:SER:HA	2.01	0.42
5:K:360:ALA:HB3	5:K:364:ILE:HB	2.01	0.42
7:L:110:ASN:O	7:L:114:MET:N	2.52	0.42
5:N:215:ALA:O	5:N:307:ARG:HD3	2.20	0.42
1:A:19:ASP:HB2	1:A:335:TRP:HH2	1.86	0.41
2:B:6:ASP:HA	2:B:100:THR:OG1	2.20	0.41
4:D:185:ILE:HD11	4:D:250:CYS:SG	2.60	0.41
4:D:314:ALA:HB3	4:D:320:ILE:HD11	2.01	0.41
5:E:115:THR:HA	5:E:127:MET:SD	2.60	0.41
5:E:259:PRO:HB3	5:E:264:MET:HB2	2.02	0.41
1:G:49:VAL:HB	1:G:83:HIS:CD2	2.55	0.41
1:G:146:ILE:HA	1:G:159:PRO:HA	2.02	0.41
5:J:247:ASN:OD1	5:J:251:ARG:NH1	2.53	0.41
5:K:157:ASN:O	5:K:170:ILE:HA	2.19	0.41
5:K:160:ILE:HA	5:K:165:ALA:HA	2.02	0.41
5:K:173:LEU:HG	5:K:175:LEU:HG	2.02	0.41
5:N:27:PRO:HB2	5:N:29:ILE:HD11	2.02	0.41
5:H:103:ALA:HB3	5:H:106:ASN:HB2	2.03	0.41
5:K:63:LYS:HB2	5:K:63:LYS:HE2	1.76	0.41
7:L:106:ASN:N	7:L:107:PRO:HD3	2.35	0.41
7:L:270:HIS:CD2	7:L:271:GLU:HG3	2.54	0.41
2:B:133:VAL:HA	2:B:159:ILE:HD13	2.02	0.41
2:B:316:PRO:O	2:B:319:MET:SD	2.79	0.41
5:H:214:VAL:HG22	5:H:253:PRO:HB3	2.02	0.41
5:K:190:GLU:HG2	7:L:110:ASN:HB2	2.02	0.41

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:90:ALA:HA	4:D:91:PRO:HD2	1.94	0.41
4:D:202:VAL:HA	4:D:205:ILE:HD12	2.01	0.41
4:D:324:ALA:HB1	4:D:328:ARG:HD3	2.02	0.41
5:E:158:VAL:HG13	5:E:170:ILE:HG12	2.03	0.41
6:F:159:PRO:HG3	6:F:280:CYS:SG	2.60	0.41
3:I:188:LEU:HA	5:J:107:PRO:CG	2.49	0.41
5:J:178:ARG:HG3	5:J:201:ARG:HH22	1.84	0.41
3:C:231:ILE:O	3:C:249:ARG:NH1	2.53	0.41
5:E:13:LYS:HG3	5:E:25:VAL:HG13	2.02	0.41
5:E:66:ILE:HG12	5:E:71:ILE:HG12	2.02	0.41
6:F:46:LYS:HE3	6:F:57:LYS:HE3	2.02	0.41
6:F:208:LYS:O	6:F:212:CYS:HB2	2.21	0.41
6:F:267:ALA:O	6:F:272:THR:HG23	2.21	0.41
1:G:94:GLU:O	1:G:125:PRO:HD3	2.21	0.41
3:I:187:ILE:HA	5:J:105:LEU:HB3	2.02	0.41
5:J:232:GLU:HA	5:J:245:ILE:O	2.20	0.41
5:K:6:ASP:O	5:K:12:VAL:HA	2.20	0.41
2:B:184:MET:HG3	2:B:194:PHE:O	2.19	0.41
3:C:212:CYS:HB3	3:C:253:PRO:HG3	2.02	0.41
4:D:92:GLU:HA	4:D:121:ASN:O	2.21	0.41
3:I:191:ARG:NH1	3:I:244:THR:O	2.52	0.41
5:N:65:PRO:HB3	5:N:76:ASP:CB	2.51	0.41
5:N:312:ILE:O	5:N:314:ALA:N	2.54	0.41
3:C:213:TYR:OH	3:C:231:ILE:HG23	2.21	0.41
4:D:147:ASP:O	4:D:154:HIS:N	2.53	0.41
4:D:182:LEU:HD13	4:D:250:CYS:SG	2.61	0.41
7:L:102:GLU:HB3	7:L:129:VAL:HG12	2.03	0.41
7:L:237:LEU:HG	7:L:241:GLN:O	2.21	0.41
1:G:135:LEU:O	1:G:337:GLY:HA3	2.21	0.41
1:A:293:VAL:HA	1:A:325:ILE:O	2.21	0.41
3:C:5:ILE:HB	3:C:100:LEU:CD2	2.51	0.41
4:D:44:LYS:H	4:D:44:LYS:HD2	1.85	0.41
4:D:279:ASP:O	4:D:283:ARG:HG3	2.21	0.41
5:E:39:MET:HA	1:G:164:PHE:CE1	2.55	0.41
5:E:202:GLU:HA	5:E:205:ARG:HG2	2.03	0.41
6:F:118:MET:HB3	6:F:127:MET:SD	2.61	0.41
5:H:99:LEU:HG	5:H:128:TYR:HB3	2.03	0.41
3:I:193:TYR:HB3	3:I:195:PHE:CE2	2.55	0.41
5:J:9:SER:HB2	5:J:152:ASP:HB3	2.02	0.41
5:K:27:PRO:O	5:K:50:GLY:HA2	2.20	0.41
7:M:81:TRP:HH2	7:M:114:MET:HG3	1.86	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:159:PRO:HG3	7:M:169:ALA:CB	2.38	0.41
7:M:332:TYR:O	7:M:336:ILE:HG12	2.20	0.41
5:N:160:ILE:HA	5:N:164:TYR:O	2.21	0.41
3:C:200:GLU:HG2	3:C:203:ILE:HD12	2.02	0.41
6:F:308:MET:HB3	6:F:324:ILE:HG12	2.03	0.41
1:G:99:LEU:HA	1:G:128:TYR:O	2.21	0.41
7:M:156:HIS:HA	7:M:171:LEU:O	2.21	0.41
5:N:2:ALA:O	5:N:16:PHE:HA	2.20	0.41
5:N:235:TYR:CE2	5:N:237:LEU:HD23	2.56	0.41
4:D:143:GLY:HA2	4:D:286:LEU:HA	2.01	0.40
6:F:158:VAL:HG12	6:F:170:ILE:HG23	2.03	0.40
6:F:294:MET:HB3	6:F:299:THR:HB	2.03	0.40
5:H:160:ILE:HG13	5:H:165:ALA:HA	2.03	0.40
3:I:146:ILE:HB	3:I:288:LEU:HD22	2.02	0.40
3:I:201:ARG:O	3:I:204:VAL:HG12	2.21	0.40
5:J:233:LYS:HD3	5:J:233:LYS:HA	1.95	0.40
5:N:6:ASP:HB3	5:N:13:LYS:HB2	2.02	0.40
5:N:97:PRO:HA	5:N:126:ALA:O	2.20	0.40
1:A:8:GLY:H	1:A:12:CYS:HA	1.86	0.40
2:B:72:ASN:O	2:B:76:MET:HB2	2.21	0.40
6:F:47:ASP:HB3	6:F:48:SER:H	1.69	0.40
6:F:190:GLU:CG	1:G:167:PRO:HB2	2.41	0.40
6:F:195:PHE:HD1	6:F:200:GLU:HB3	1.85	0.40
1:G:3:LEU:HD12	1:G:98:VAL:HG22	2.02	0.40
1:G:59:ILE:HD13	1:G:59:ILE:H	1.86	0.40
3:I:65:PRO:HG2	3:I:66:ILE:HG13	2.03	0.40
3:I:185:MET:HB2	3:I:204:VAL:HG11	2.03	0.40
5:J:12:VAL:HG23	5:J:28:SER:OG	2.21	0.40
5:J:301:TYR:HA	5:J:302:PRO:HD3	1.82	0.40
7:L:249:ARG:HD2	7:L:249:ARG:HH11	1.77	0.40
4:D:321:LYS:NZ	4:D:323:ILE:HD13	2.36	0.40
5:E:166:LEU:HA	5:E:167:PRO:HD3	1.87	0.40
6:F:40:MET:HG2	6:F:57:LYS:HD2	2.04	0.40
1:G:13:LYS:HB2	1:G:13:LYS:HE2	1.95	0.40
5:H:92:ALA:HA	5:H:93:PRO:HD2	1.90	0.40
5:H:102:GLU:HB2	5:H:106:ASN:ND2	2.37	0.40
3:I:196:SER:HB3	5:J:172:ARG:HB3	2.04	0.40
5:J:248:GLU:HA	5:J:251:ARG:HB2	2.03	0.40
5:J:269:ILE:HD13	5:J:269:ILE:HA	1.98	0.40
5:K:97:PRO:HG3	5:K:125:PRO:HG2	2.02	0.40
7:L:146:ILE:HD11	7:L:157:THR:HB	2.03	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:N:65:PRO:HG3	5:N:80:ILE:HD12	2.02	0.40
5:N:275:ASN:HD22	5:N:275:ASN:HA	1.77	0.40
1:A:44:GLN:H	1:A:44:GLN:NE2	2.19	0.40
4:D:56:ARG:HB3	4:D:61:LEU:HD11	2.03	0.40
4:D:157:PRO:HG2	4:D:164:LEU:HB2	2.02	0.40
5:E:206:ASP:O	5:E:210:LYS:HG2	2.22	0.40
6:F:58:ARG:HD2	6:F:198:THR:HB	2.03	0.40
6:F:169:ALA:HA	6:F:279:LYS:HG2	2.03	0.40
5:H:166:LEU:O	5:H:170:ILE:HG13	2.21	0.40
3:I:189:SER:HB2	5:J:104:PRO:O	2.20	0.40
5:J:180:LEU:O	5:J:252:CYS:SG	2.79	0.40
5:J:183:TYR:HD2	5:J:252:CYS:HA	1.86	0.40
5:J:257:PHE:O	5:J:268:GLY:HA3	2.22	0.40
5:K:99:LEU:HG	5:K:128:TYR:HB3	2.04	0.40
5:K:165:ALA:O	5:K:167:PRO:HD3	2.22	0.40
7:M:215:ALA:HB2	7:M:250:PHE:HB2	2.04	0.40
5:N:273:THR:O	5:N:277:ILE:HG12	2.22	0.40
1:A:52:GLU:HG2	1:A:56:LYS:NZ	2.36	0.40
1:A:106:ASN:HA	1:A:107:PRO:HD3	1.90	0.40
1:A:329:GLU:HG3	1:A:336:ILE:HD12	2.03	0.40
5:H:31:GLY:HA2	5:H:61:THR:O	2.22	0.40
3:I:29:ILE:O	3:I:49:VAL:HA	2.22	0.40
5:J:57:ARG:HG3	5:J:58:GLY:N	2.36	0.40
5:J:211:LEU:HB3	5:J:249:ARG:HD2	2.02	0.40
5:K:81:TRP:HA	5:K:84:THR:OG1	2.21	0.40
7:M:330:ARG:HH11	7:M:330:ARG:HD2	1.76	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	A	363/365 (100%)	319 (88%)	36 (10%)	8 (2%)	6	35
1	G	363/365 (100%)	333 (92%)	25 (7%)	5 (1%)	11	46
2	B	362/364 (100%)	317 (88%)	33 (9%)	12 (3%)	4	26
3	C	363/365 (100%)	328 (90%)	33 (9%)	2 (1%)	25	66
3	I	363/365 (100%)	328 (90%)	30 (8%)	5 (1%)	11	46
4	D	355/357 (99%)	307 (86%)	36 (10%)	12 (3%)	3	26
5	E	363/365 (100%)	314 (86%)	36 (10%)	13 (4%)	3	25
5	H	363/365 (100%)	319 (88%)	36 (10%)	8 (2%)	6	35
5	J	363/365 (100%)	309 (85%)	44 (12%)	10 (3%)	5	30
5	K	363/365 (100%)	315 (87%)	38 (10%)	10 (3%)	5	30
5	N	363/365 (100%)	322 (89%)	32 (9%)	9 (2%)	5	32
6	F	355/357 (99%)	295 (83%)	47 (13%)	13 (4%)	3	24
7	L	363/365 (100%)	305 (84%)	48 (13%)	10 (3%)	5	30
7	M	363/365 (100%)	307 (85%)	42 (12%)	14 (4%)	3	23
All	All	5065/5093 (100%)	4418 (87%)	516 (10%)	131 (3%)	8	31

All (131) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	40	VAL
2	B	280	ASP
2	B	329	ARG
2	B	362	SER
3	C	265	GLU
4	D	8	SER
4	D	175	GLY
4	D	346	GLN
5	E	198	THR
5	E	345	SER
6	F	58	ARG
6	F	197	THR
6	F	330	ARG
1	G	168	HIS
5	J	104	PRO
5	J	107	PRO
5	J	166	LEU
5	J	241	GLN
5	K	132	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
5	K	330	ARG
7	L	57	ARG
7	L	59	ILE
7	L	123	ASN
7	L	177	GLY
7	L	194	SER
7	L	239	ASP
7	M	35	HIS
7	M	57	ARG
7	M	59	ILE
7	M	196	THR
7	M	199	ALA
5	N	57	ARG
5	N	314	ALA
5	N	318	SER
1	A	192	GLY
2	B	52	GLU
2	B	317	SER
4	D	56	ARG
4	D	58	ILE
4	D	174	ALA
4	D	192	SER
4	D	331	SER
4	D	355	TYR
5	E	58	GLY
5	E	191	ARG
5	E	200	GLU
5	E	330	ARG
5	E	363	SER
6	F	232	GLU
6	F	280	CYS
1	G	57	ARG
5	H	40	VAL
5	H	191	ARG
5	H	228	SER
5	H	330	ARG
5	J	45	LYS
5	J	230	SER
5	K	38	VAL
5	K	228	SER
7	M	123	ASN
7	M	350	MET

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
5	N	84	THR
5	N	192	GLY
5	N	230	SER
1	A	229	SER
1	A	318	SER
3	C	132	GLN
4	D	9	GLY
5	E	55	SER
5	E	194	SER
6	F	84	THR
6	F	355	GLN
1	G	229	SER
5	J	105	LEU
5	J	242	VAL
7	L	281	ASP
7	M	108	LYS
7	M	151	GLY
7	M	200	GLU
5	N	263	GLY
5	N	347	PHE
1	A	42	MET
1	A	260	SER
1	A	317	PRO
1	A	364	ILE
2	B	237	PRO
4	D	349	TRP
5	E	252	CYS
6	F	47	ASP
5	H	176	ALA
3	I	42	MET
3	I	196	SER
3	I	229	SER
3	I	242	VAL
5	K	40	VAL
5	K	230	SER
7	L	45	LYS
7	L	346	THR
7	L	350	MET
7	M	38	VAL
7	M	228	SER
1	A	10	GLY
4	D	342	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
5	E	176	ALA
6	F	176	ALA
6	F	238	PRO
5	H	217	ASP
5	H	249	ARG
5	J	252	CYS
5	K	39	MET
7	M	170	ILE
2	B	228	SER
2	B	251	CYS
2	B	281	ILE
2	B	316	PRO
5	H	269	ILE
5	K	192	GLY
7	M	28	SER
5	E	242	VAL
6	F	170	ILE
1	G	159	PRO
1	G	352	ILE
5	J	59	ILE
5	K	246	GLY
5	N	65	PRO
5	E	192	GLY
6	F	196	VAL
6	F	153	GLY
2	B	241	VAL
3	I	170	ILE
5	K	252	CYS

### 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	A	310/310 (100%)	291 (94%)	19 (6%)	18	44
1	G	310/310 (100%)	293 (94%)	17 (6%)	21	47
2	B	307/307 (100%)	284 (92%)	23 (8%)	13	38

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	310/310 (100%)	297 (96%)	13 (4%)	30	54
3	I	310/310 (100%)	305 (98%)	5 (2%)	62	79
4	D	302/302 (100%)	283 (94%)	19 (6%)	18	43
5	E	308/308 (100%)	290 (94%)	18 (6%)	20	45
5	H	308/308 (100%)	287 (93%)	21 (7%)	16	41
5	J	308/308 (100%)	283 (92%)	25 (8%)	11	35
5	K	308/308 (100%)	286 (93%)	22 (7%)	14	39
5	N	308/308 (100%)	284 (92%)	24 (8%)	12	36
6	F	302/302 (100%)	282 (93%)	20 (7%)	16	41
7	L	308/308 (100%)	280 (91%)	28 (9%)	9	29
7	M	308/308 (100%)	284 (92%)	24 (8%)	12	36
All	All	4307/4307 (100%)	4029 (94%)	278 (6%)	21	42

All (278) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	ILE
1	A	32	ARG
1	A	44	GLN
1	A	47	SER
1	A	59	ILE
1	A	63	ARG
1	A	73	ASN
1	A	108	LYS
1	A	129	VAL
1	A	140	SER
1	A	178	ARG
1	A	213	TYR
1	A	228	SER
1	A	229	SER
1	A	230	SER
1	A	239	ASP
1	A	247	ASN
1	A	253	PRO
1	A	275	ASN
2	B	3	LEU
2	B	34	ARG
2	B	55	SER

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
2	B	60	LEU
2	B	74	ASP
2	B	76	MET
2	B	89	ARG
2	B	107	LYS
2	B	139	SER
2	B	173	ASP
2	B	180	THR
2	B	188	THR
2	B	215	LEU
2	B	236	LEU
2	B	246	ASN
2	B	280	ASP
2	B	286	ASP
2	B	291	ASN
2	B	294	SER
2	B	312	THR
2	B	319	MET
2	B	348	GLN
2	B	362	SER
3	C	121	THR
3	C	123	ASN
3	C	129	VAL
3	C	137	LEU
3	C	180	LEU
3	C	213	TYR
3	C	230	SER
3	C	234	SER
3	C	283	ASP
3	C	317	PRO
3	C	318	SER
3	C	329	GLU
3	C	363	SER
4	D	8	SER
4	D	28	ILE
4	D	44	LYS
4	D	45	ASP
4	D	60	THR
4	D	71	ASN
4	D	114	GLN
4	D	116	MET
4	D	152	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
4	D	162	TYR
4	D	172	ASP
4	D	191	TYR
4	D	206	LYS
4	D	260	ILE
4	D	264	SER
4	D	290	ASN
4	D	306	MET
4	D	319	LYS
4	D	347	GLN
5	E	23	ARG
5	E	60	LEU
5	E	61	THR
5	E	87	ASN
5	E	118	MET
5	E	137	LEU
5	E	146	ILE
5	E	154	VAL
5	E	193	TYR
5	E	198	THR
5	E	201	ARG
5	E	213	TYR
5	E	222	MET
5	E	261	PHE
5	E	273	THR
5	E	312	ILE
5	E	320	MET
5	E	354	LYS
6	F	1	THR
6	F	8	ASN
6	F	29	SER
6	F	40	MET
6	F	41	VAL
6	F	46	LYS
6	F	53	GLU
6	F	67	ILE
6	F	180	LEU
6	F	186	LYS
6	F	197	THR
6	F	238	PRO
6	F	243	ILE
6	F	265	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
6	F	270	HIS
6	F	278	MET
6	F	287	ASP
6	F	292	ASN
6	F	304	ILE
6	F	320	MET
1	G	42	MET
1	G	44	GLN
1	G	46	ASP
1	G	52	GLU
1	G	59	ILE
1	G	63	ARG
1	G	73	ASN
1	G	105	MET
1	G	139	SER
1	G	140	SER
1	G	175	LEU
1	G	178	ARG
1	G	186	LYS
1	G	234	SER
1	G	247	ASN
1	G	253	PRO
1	G	333	SER
5	H	9	SER
5	H	13	LYS
5	H	154	VAL
5	H	161	TYR
5	H	186	LYS
5	H	197	THR
5	H	202	GLU
5	H	216	LEU
5	H	231	LEU
5	H	238	PRO
5	H	241	GLN
5	H	258	GLN
5	H	278	MET
5	H	286	LYS
5	H	292	ASN
5	H	307	ARG
5	H	329	GLU
5	H	344	LEU
5	H	348	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
5	H	349	GLN
5	H	354	LYS
3	I	72	THR
3	I	110	ASN
3	I	121	THR
3	I	123	ASN
3	I	230	SER
5	J	29	ILE
5	J	39	MET
5	J	70	ILE
5	J	77	MET
5	J	104	PRO
5	J	108	LYS
5	J	123	ASN
5	J	127	MET
5	J	137	LEU
5	J	173	LEU
5	J	186	LYS
5	J	194	SER
5	J	205	ARG
5	J	213	TYR
5	J	238	PRO
5	J	244	THR
5	J	270	HIS
5	J	273	THR
5	J	281	ASP
5	J	282	ILE
5	J	298	THR
5	J	307	ARG
5	J	310	LYS
5	J	317	PRO
5	J	363	SER
5	K	13	LYS
5	K	29	ILE
5	K	47	SER
5	K	67	GLU
5	K	114	MET
5	K	154	VAL
5	K	181	THR
5	K	190	GLU
5	K	191	ARG
5	K	197	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
5	K	216	LEU
5	K	241	GLN
5	K	247	ASN
5	K	258	GLN
5	K	260	SER
5	K	278	MET
5	K	292	ASN
5	K	309	GLN
5	K	344	LEU
5	K	348	GLN
5	K	349	GLN
5	K	354	LYS
7	L	34	ARG
7	L	42	MET
7	L	47	SER
7	L	51	ASP
7	L	54	GLN
7	L	55	SER
7	L	75	ASP
7	L	77	MET
7	L	84	THR
7	L	106	ASN
7	L	143	THR
7	L	190	GLU
7	L	205	ARG
7	L	213	TYR
7	L	233	LYS
7	L	244	THR
7	L	245	ILE
7	L	247	ASN
7	L	269	ILE
7	L	282	VAL
7	L	286	LYS
7	L	306	ASP
7	L	308	MET
7	L	309	GLN
7	L	347	PHE
7	L	349	GLN
7	L	351	TRP
7	L	355	GLN
7	M	27	PRO
7	M	42	MET

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
7	M	46	ASP
7	M	54	GLN
7	M	77	MET
7	M	110	ASN
7	M	124	THR
7	M	143	THR
7	M	178	ARG
7	M	182	ASP
7	M	205	ARG
7	M	206	ASP
7	M	213	TYR
7	M	241	GLN
7	M	245	ILE
7	M	260	SER
7	M	264	MET
7	M	265	GLU
7	M	320	MET
7	M	346	THR
7	M	349	GLN
7	M	351	TRP
7	M	353	SER
7	M	355	GLN
5	N	13	LYS
5	N	29	ILE
5	N	49	VAL
5	N	59	ILE
5	N	75	ASP
5	N	94	GLU
5	N	101	THR
5	N	107	PRO
5	N	123	ASN
5	N	154	VAL
5	N	175	LEU
5	N	178	ARG
5	N	213	TYR
5	N	234	SER
5	N	239	ASP
5	N	245	ILE
5	N	247	ASN
5	N	265	GLU
5	N	279	LYS
5	N	311	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
5	N	320	MET
5	N	322	ILE
5	N	349	GLN
5	N	363	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	GLN
1	A	73	ASN
1	A	83	HIS
1	A	271	GLN
1	A	275	ASN
2	B	122	ASN
2	B	219	ASN
2	B	348	GLN
3	C	44	GLN
3	C	275	ASN
4	D	121	ASN
4	D	239	GLN
4	D	245	ASN
4	D	290	ASN
5	E	7	ASN
5	E	116	GLN
5	E	123	ASN
5	E	292	ASN
6	F	309	GLN
1	G	7	ASN
1	G	36	GLN
1	G	73	ASN
1	G	247	ASN
1	G	275	ASN
5	H	54	GLN
5	H	106	ASN
5	H	168	HIS
5	H	258	GLN
5	H	275	ASN
5	J	157	ASN
5	J	241	GLN
5	K	87	ASN
5	K	106	ASN
5	K	309	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
7	L	241	GLN
7	L	270	HIS
7	L	348	GLN
7	M	275	ASN
5	N	87	ASN
5	N	123	ASN
5	N	156	HIS
5	N	275	ASN

### 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 monosaccharides 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.



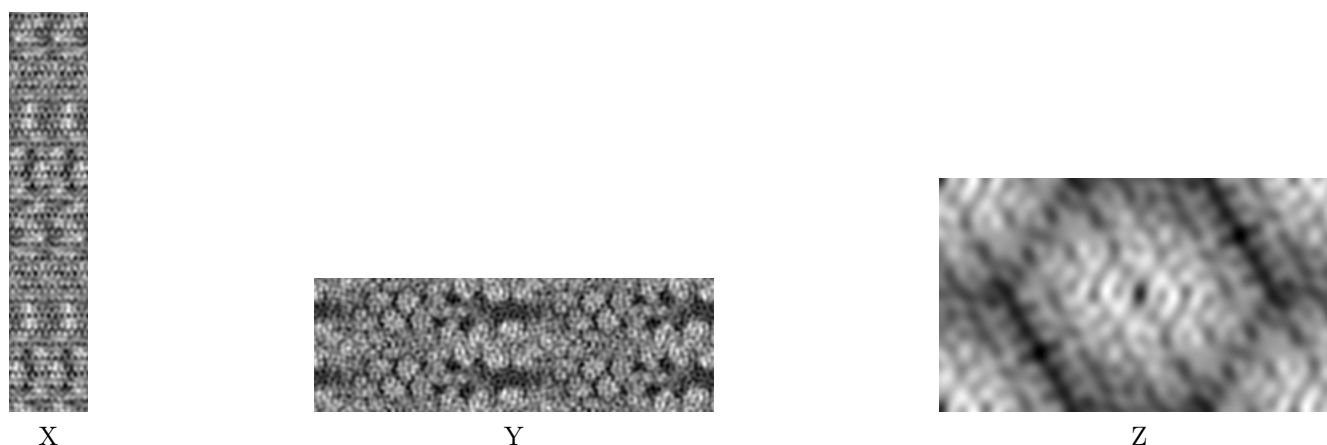
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-1088. 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](#)

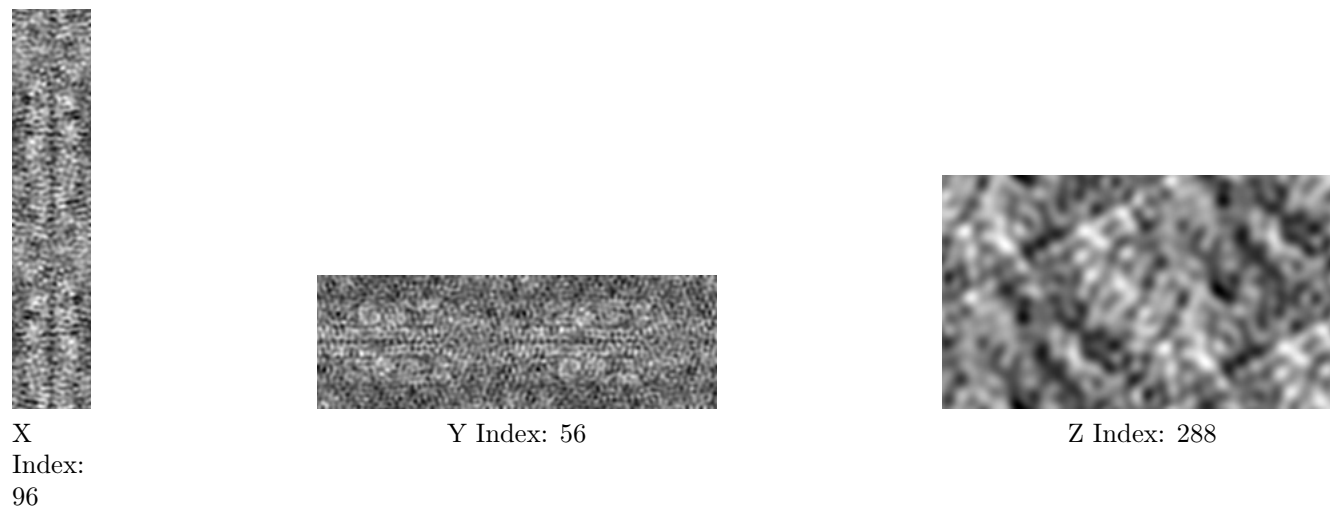
#### 6.1.1 Primary map



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

### 6.2 Central slices [i](#)

#### 6.2.1 Primary map



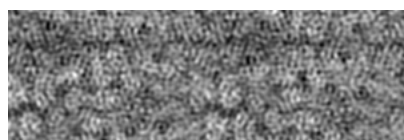
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

### 6.3.1 Primary map



X  
Index:  
123



Y Index: 84



Z Index: 413

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

## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 430.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

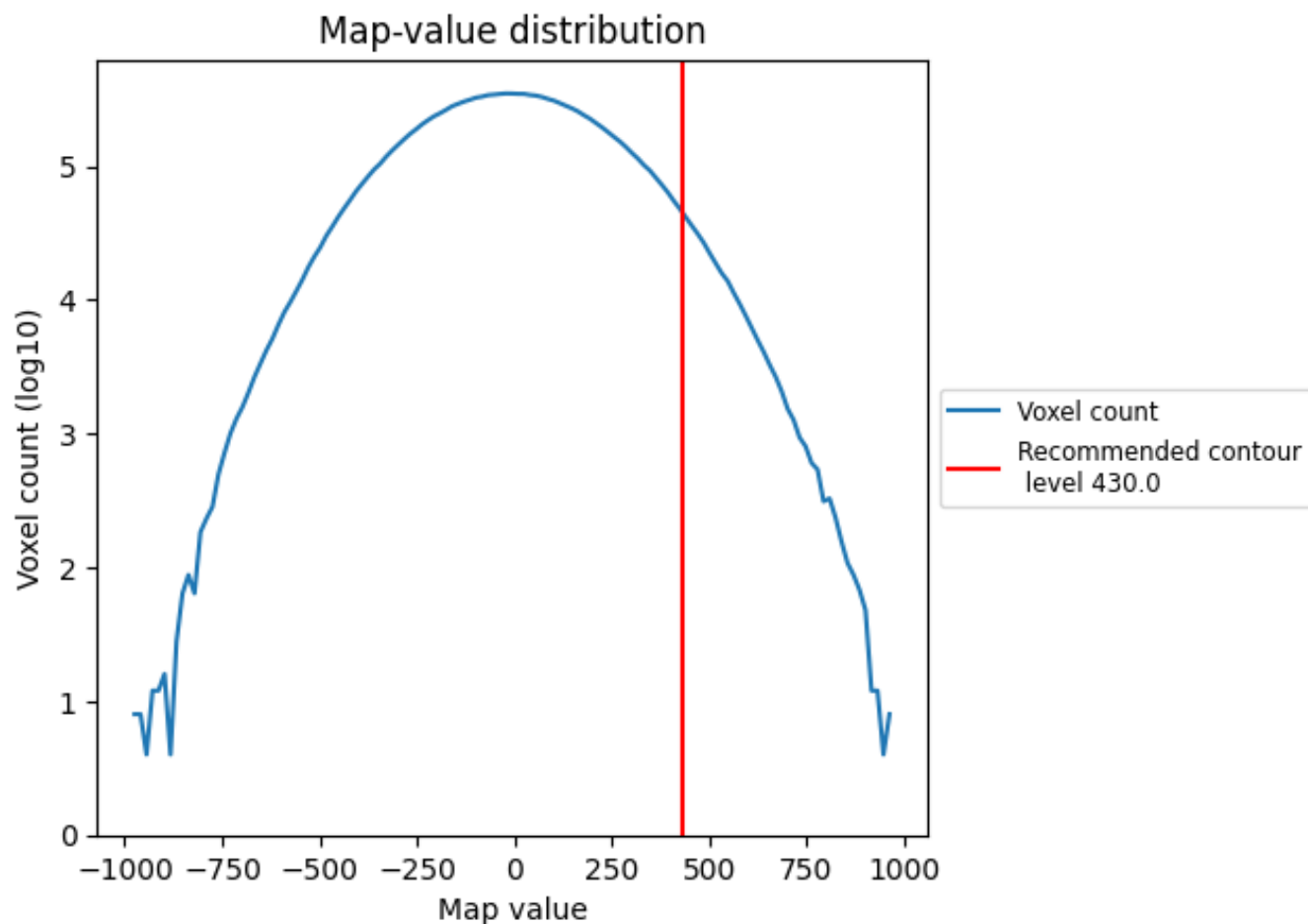
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

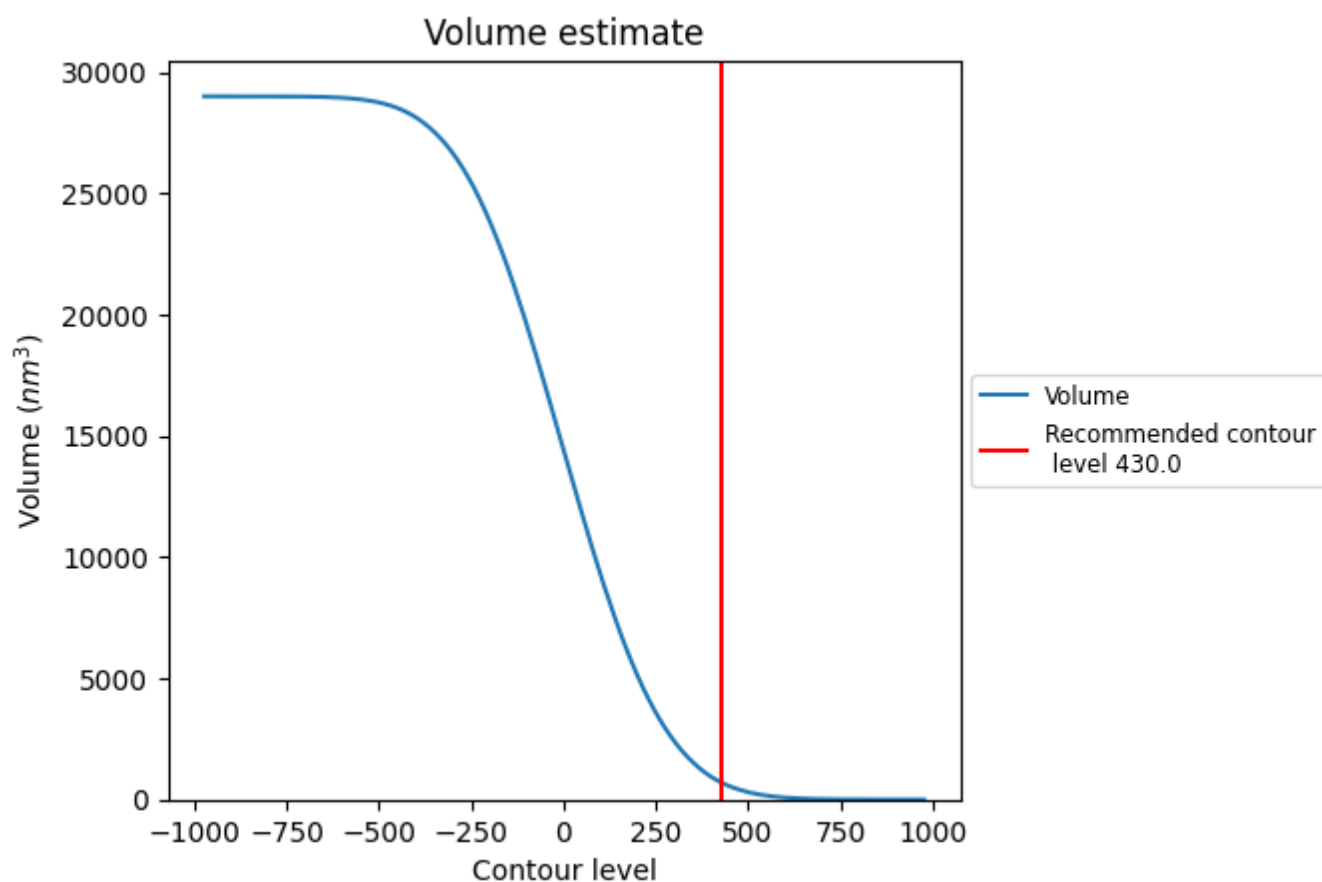
This section contains the results of statistical analysis of the map.

### 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 687 nm<sup>3</sup>; this corresponds to an approximate mass of 621 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 [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

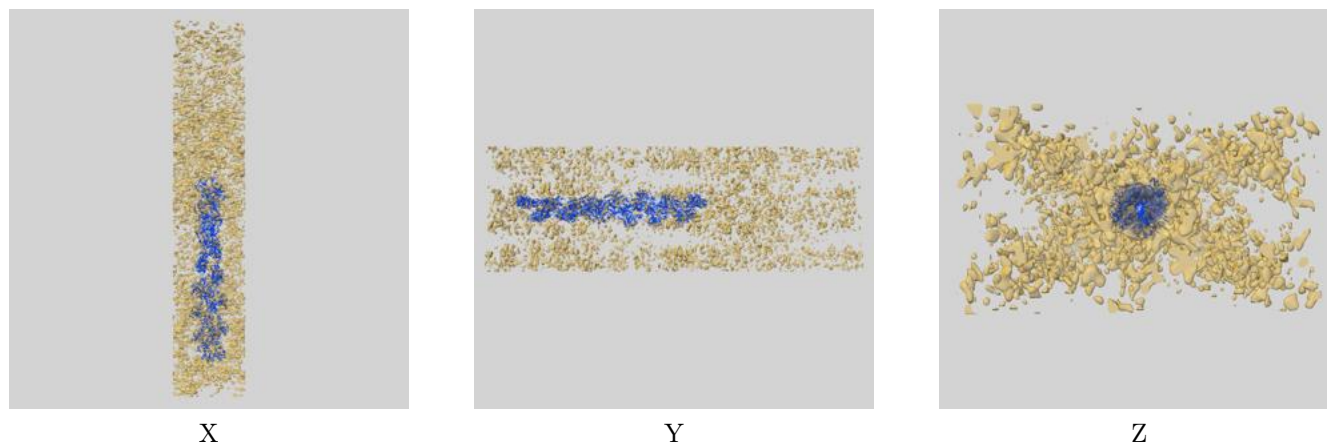
## 8 Fourier-Shell correlation

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

## 9 Map-model fit [i](#)

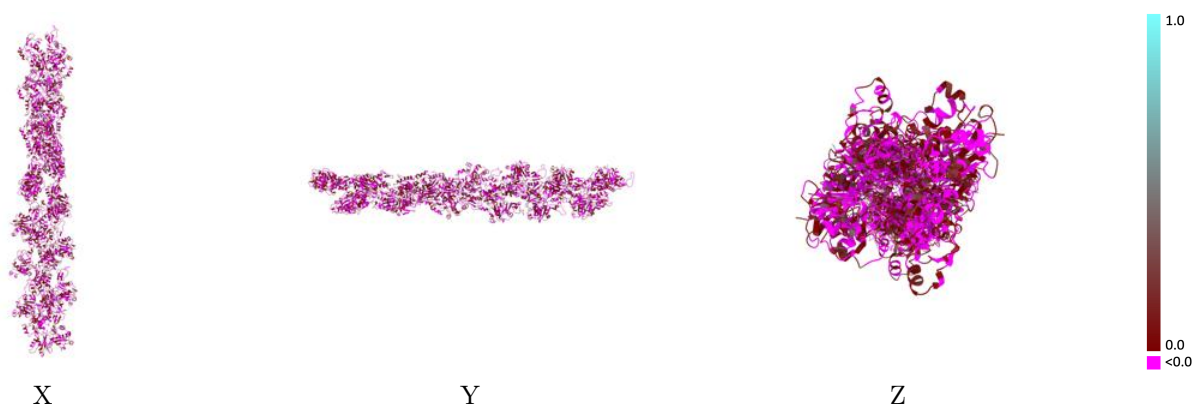
This section contains information regarding the fit between EMDB map EMD-1088 and PDB model 3B63. Per-residue inclusion information can be found in section [3](#) on page [6](#).

### 9.1 Map-model overlay [i](#)



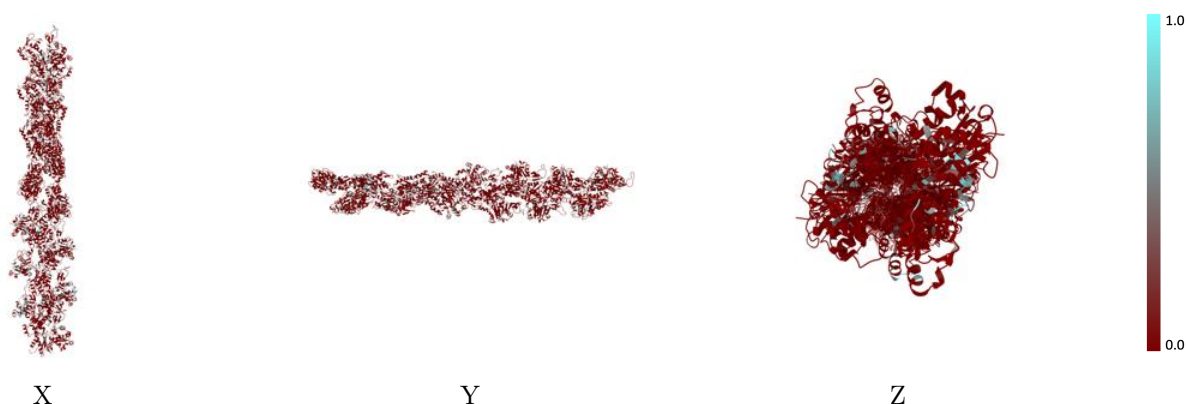
The images above show the 3D surface view of the map at the recommended contour level 430.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



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

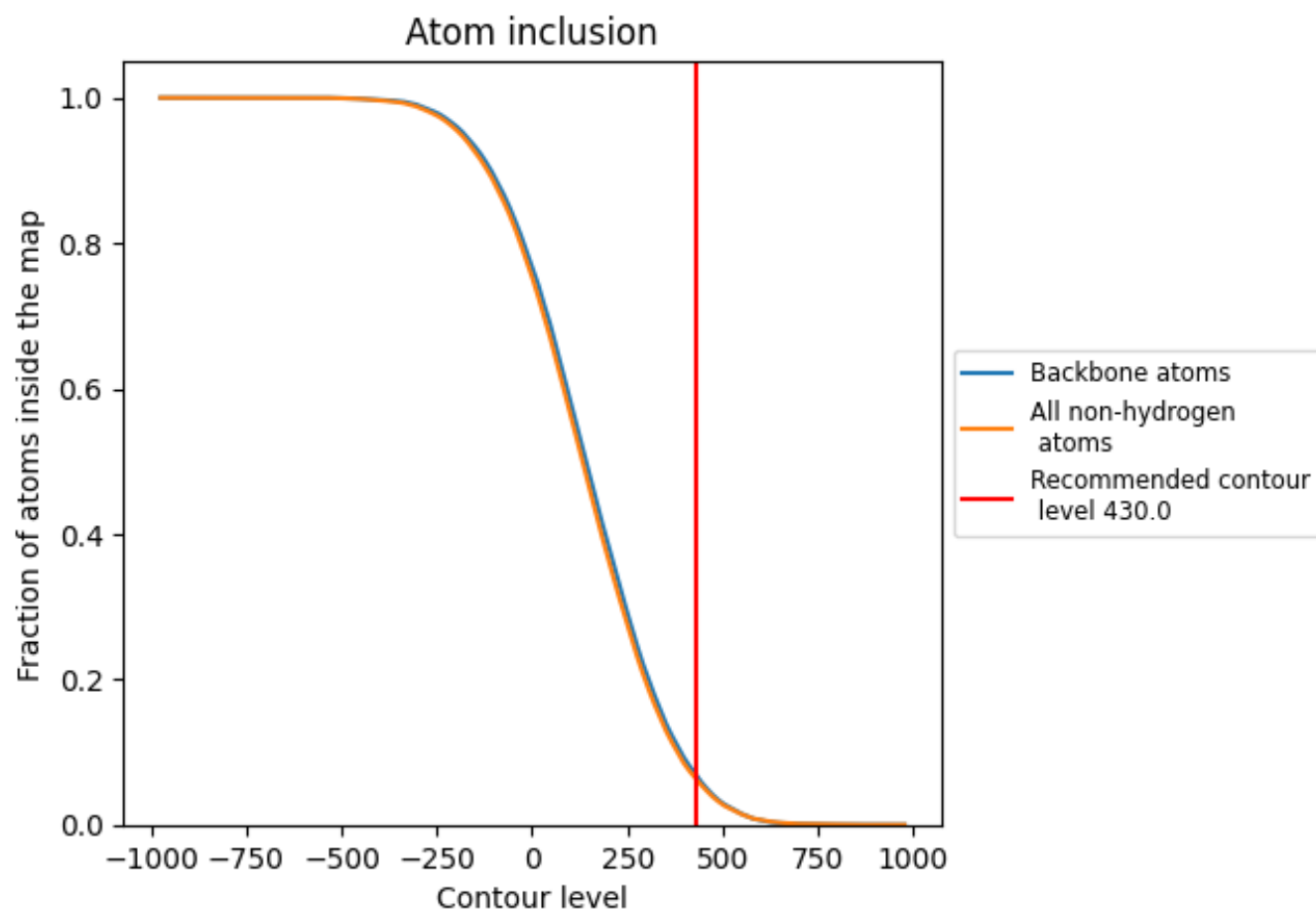
## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (430.0).

































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 7% of all backbone atoms, 6% 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 (430.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.0633	 0.0210
A	 0.0667	 0.0210
B	 0.0967	 0.0030
C	 0.1087	 0.0310
D	 0.0811	 0.0140
E	 0.0781	 0.0340
F	 0.0812	 0.0260
G	 0.0642	 0.0240
H	 0.0344	 0.0130
I	 0.0133	 0.0240
J	 0.0301	 0.0110
K	 0.0326	 0.0240
L	 0.0564	 0.0330
M	 0.0740	 0.0240
N	 0.0699	 0.0110

