



## Full wwPDB EM Validation Report ⓘ

May 11, 2026 – 06:33 PM JST

PDB ID : 24MC / pdb\_000024mc  
EMDB ID : EMD-69647  
Title : Structure of oocyte cytoplasmic lattices  
Authors : Liu, Q.; Gui, M.  
Deposited on : 2026-03-10  
Resolution : 3.40 Å(reported)

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:

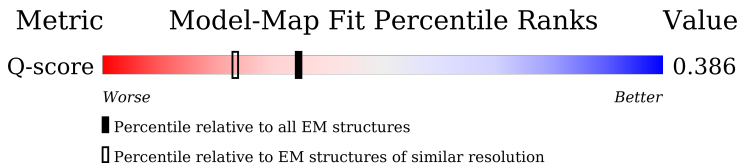
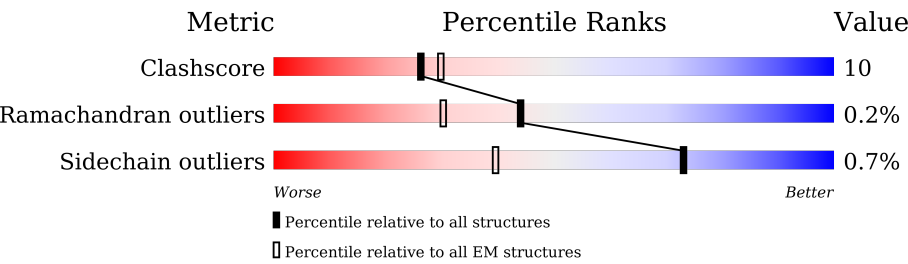
EMDB validation analysis : 0.0.1.dev132  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (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 i

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

The reported resolution of this entry is 3.40 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.



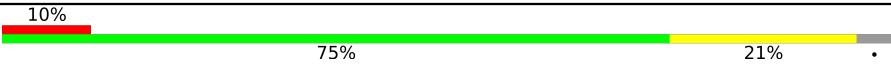

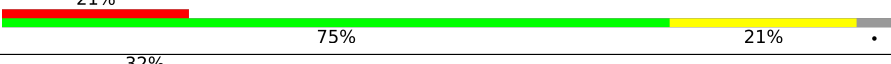
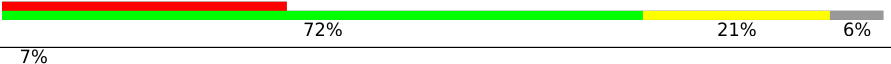
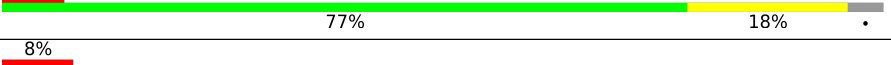
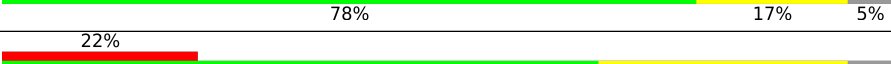
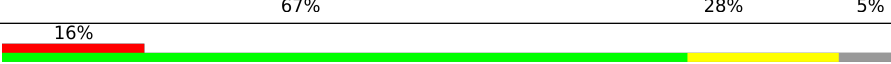
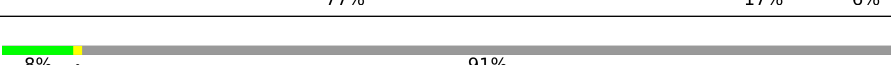
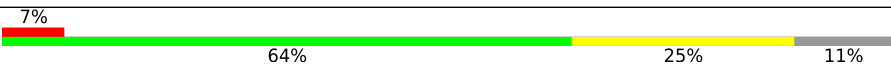






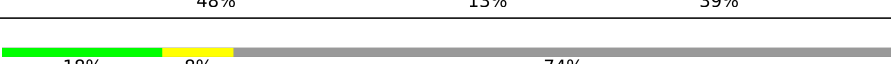
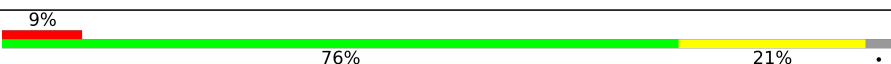
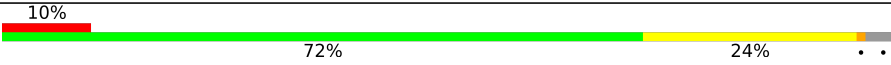


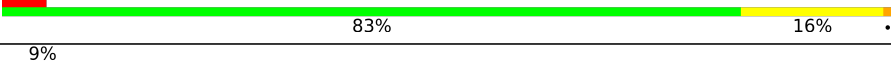

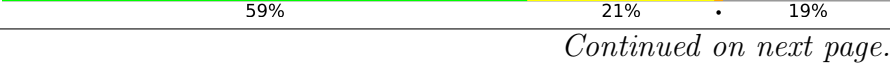


Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14717 ( 2.90 - 3.90 )

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	m	466	<div><div>16%</div><div>61%</div><div>36%</div><div>..</div></div>
2	p	468	<div><div>11%</div><div>60%</div><div>36%</div><div>...</div></div>
3	A	682	<div><div>20%</div><div>74%</div><div>21%</div><div>5%</div></div>
3	B	682	<div><div>10%</div><div>73%</div><div>23%</div><div>.</div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	C	682	
3	D	682	
3	E	682	
3	F	682	
3	G	682	
3	H	682	
3	I	682	
3	K	682	
4	M	937	
4	R	937	
5	N	164	
5	U	164	
6	O	346	
7	P	1163	
7	S	1163	
8	Q	581	
8	T	581	
9	V	228	
10	W	445	
10	Z	445	
11	X	449	
11	Y	449	
12	a	147	
12	c	147	
13	b	782	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
13	d	782	<div><div></div><div>31%56%22%21%</div></div>
14	e	993	<div><div></div><div>42%69%28%. .</div></div>
14	f	993	<div><div></div><div>41%61%35%. .</div></div>
15	h	163	<div><div></div><div>16%57%30%13%</div></div>
15	j	163	<div><div></div><div>26%54%34%12%</div></div>
15	l	163	<div><div></div><div>46%56%25%. 18%</div></div>
16	n	469	<div><div></div><div>. 81%18%</div></div>

## 2 Entry composition [i](#)

There are 20 unique types of molecules in this entry. The entry contains 138959 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 F-box and WD-40 domain protein 19.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	m	461	Total	C	N	O	S	0	0
			3723	2394	638	662	29		

- Molecule 2 is a protein called F-box and WD-40 domain protein 21.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	p	464	Total	C	N	O	S	0	0
			3804	2465	636	678	25		

- Molecule 3 is a protein called Inactive protein-arginine deiminase type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	651	Total	C	N	O	S	0	0
			5161	3309	846	967	39		
3	B	655	Total	C	N	O	S	0	0
			5188	3323	853	973	39		
3	C	655	Total	C	N	O	S	0	0
			5188	3323	853	973	39		
3	D	650	Total	C	N	O	S	0	0
			5154	3304	845	966	39		
3	E	655	Total	C	N	O	S	0	0
			5188	3323	853	973	39		
3	F	639	Total	C	N	O	S	0	0
			5059	3247	825	948	39		
3	G	655	Total	C	N	O	S	0	0
			5188	3323	853	973	39		
3	H	650	Total	C	N	O	S	0	0
			5148	3299	847	963	39		
3	I	651	Total	C	N	O	S	0	0
			5161	3309	846	967	39		
3	K	643	Total	C	N	O	S	0	0
			5102	3273	837	953	39		

- Molecule 4 is a protein called NLR family, pyrin domain containing 4F.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	M	88	Total	C	N	O	S	0	0
			728	470	125	130	3		
4	R	838	Total	C	N	O	S	0	0
			6735	4297	1118	1253	67		

- Molecule 5 is a protein called Oocyte-expressed protein homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	N	120	Total	C	N	O	S	0	0
			967	619	167	176	5		
5	U	87	Total	C	N	O	S	0	0
			701	449	120	127	5		

- Molecule 6 is a protein called Isoform 2 of KH domain-containing protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	O	128	Total	C	N	O	S	0	0
			1066	688	191	179	8		

- Molecule 7 is a protein called NACHT, LRR and PYD domains-containing protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	P	940	Total	C	N	O	S	0	0
			7419	4722	1255	1377	65		
7	S	949	Total	C	N	O	S	0	0
			7476	4757	1266	1388	65		

- Molecule 8 is a protein called Transducin-like enhancer protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Q	365	Total	C	N	O	S	0	0
			2884	1830	505	529	20		
8	T	355	Total	C	N	O	S	0	0
			2803	1778	493	512	20		

- Molecule 9 is a protein called Zinc finger BED domain-containing protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	V	59	Total	C	N	O	S	0	0
			476	303	87	80	6		

- Molecule 10 is a protein called Tubulin beta-2A chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	W	431	Total	C	N	O	S	0	0
			3387	2125	580	656	26		
10	Z	428	Total	C	N	O	S	0	0
			3368	2115	576	651	26		

- Molecule 11 is a protein called Tubulin alpha-1C chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	X	418	Total	C	N	O	S	0	0
			3287	2083	558	624	22		
11	Y	423	Total	C	N	O	S	0	0
			3303	2091	562	628	22		

- Molecule 12 is a protein called Ubiquitin-conjugating enzyme E2 D3.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	a	147	Total	C	N	O	S	0	0
			1173	751	200	214	8		
12	c	147	Total	C	N	O	S	0	0
			1173	751	200	214	8		

- Molecule 13 is a protein called E3 ubiquitin-protein ligase UHRF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	b	630	Total	C	N	O	S	0	0
			5084	3180	930	941	33		
13	d	616	Total	C	N	O	S	0	0
			4985	3121	914	917	33		

- Molecule 14 is a protein called NACHT, LRR and PYD domains-containing protein 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	e	967	Total	C	N	O	S	0	0
			7723	4911	1322	1426	64		
14	f	963	Total	C	N	O	S	0	0
			7695	4897	1318	1416	64		

- Molecule 15 is a protein called S-phase kinase-associated protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	h	142	Total	C	N	O	S	0	0
			1151	732	189	225	5		

*Continued on next page...*

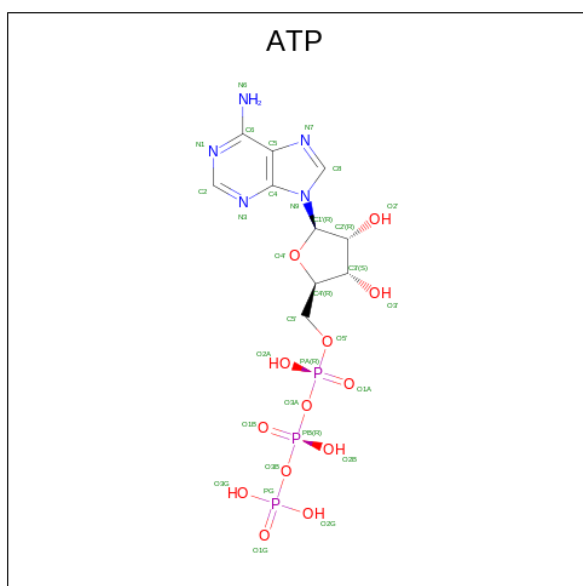
Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
15	j	144	Total	C	N	O	S	0	0
			1160	733	191	231	5		
15	l	133	Total	C	N	O	S	0	0
			1071	683	174	209	5		

- Molecule 16 is a protein called Expressed sequence C85627.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	n	467	Total	C	N	O	S	0	0
			3787	2443	629	685	30		

- Molecule 17 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ) (labeled as "Ligand of Interest" by depositor).

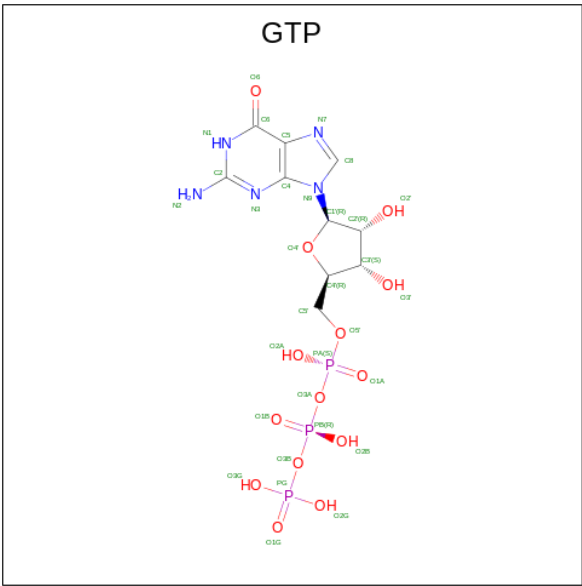


Mol	Chain	Residues	Atoms					AltConf
17	P	1	Total	C	N	O	P	0
			31	10	5	13	3	
17	R	1	Total	C	N	O	P	0
			31	10	5	13	3	
17	S	1	Total	C	N	O	P	0
			31	10	5	13	3	
17	e	1	Total	C	N	O	P	0
			31	10	5	13	3	
17	f	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 18 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula:  $C_{10}H_{16}N_5O_{14}P_3$ )



(labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
18	W	1	Total	C	N	O	P	0
			32	10	5	14	3	
18	X	1	Total	C	N	O	P	0
			32	10	5	14	3	
18	Y	1	Total	C	N	O	P	0
			32	10	5	14	3	
18	Z	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 19 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
19	W	1	Total	Mg	0
			1	1	
19	X	1	Total	Mg	0
			1	1	
19	Y	1	Total	Mg	0
			1	1	
19	Z	1	Total	Mg	0
			1	1	

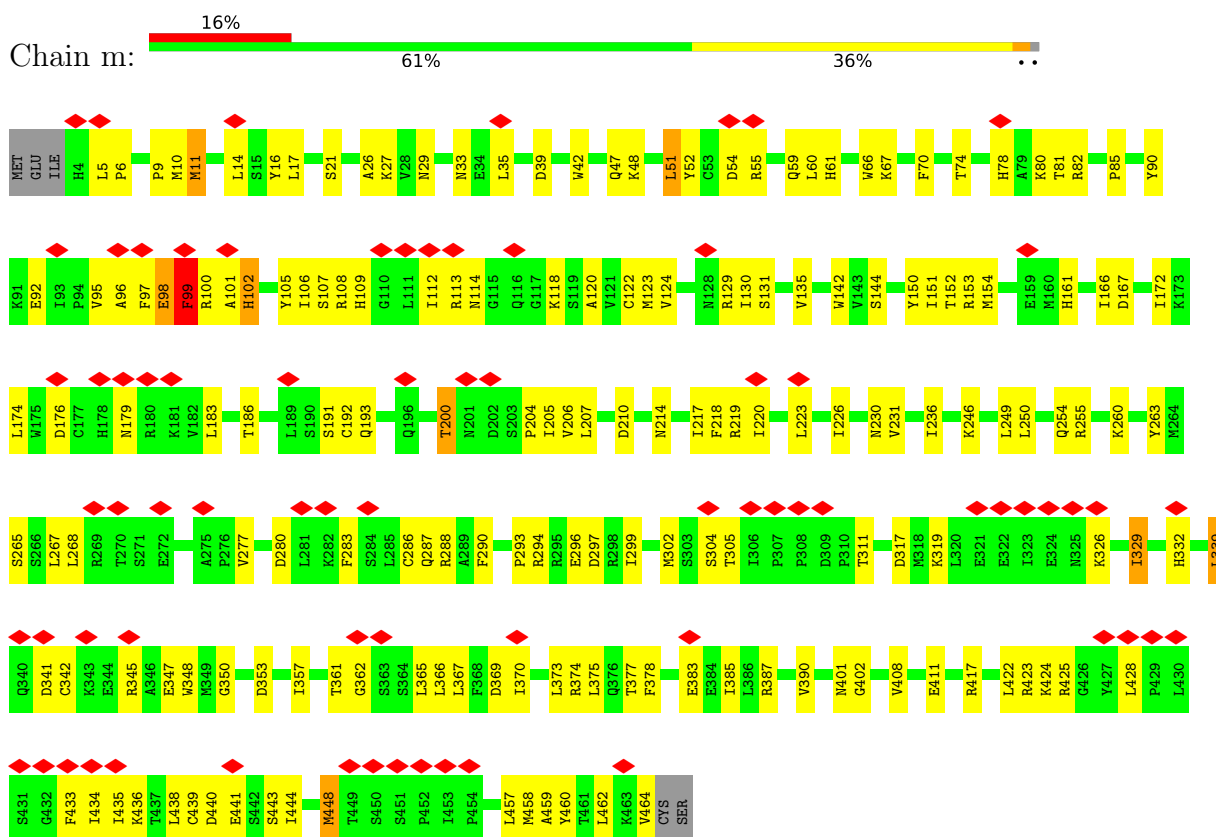
- Molecule 20 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
20	b	3	Total 3	Zn 3	0
20	d	3	Total 3	Zn 3	0

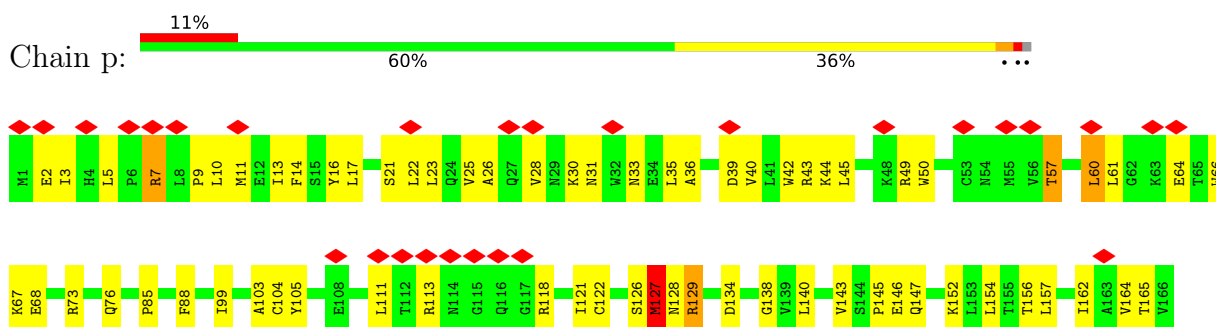
### 3 Residue-property plots

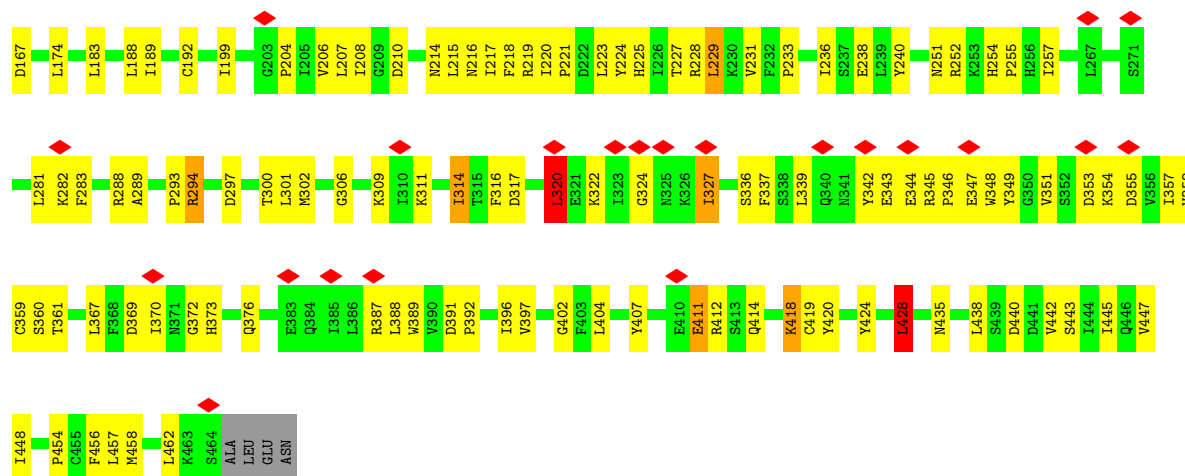
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: F-box and WD-40 domain protein 19

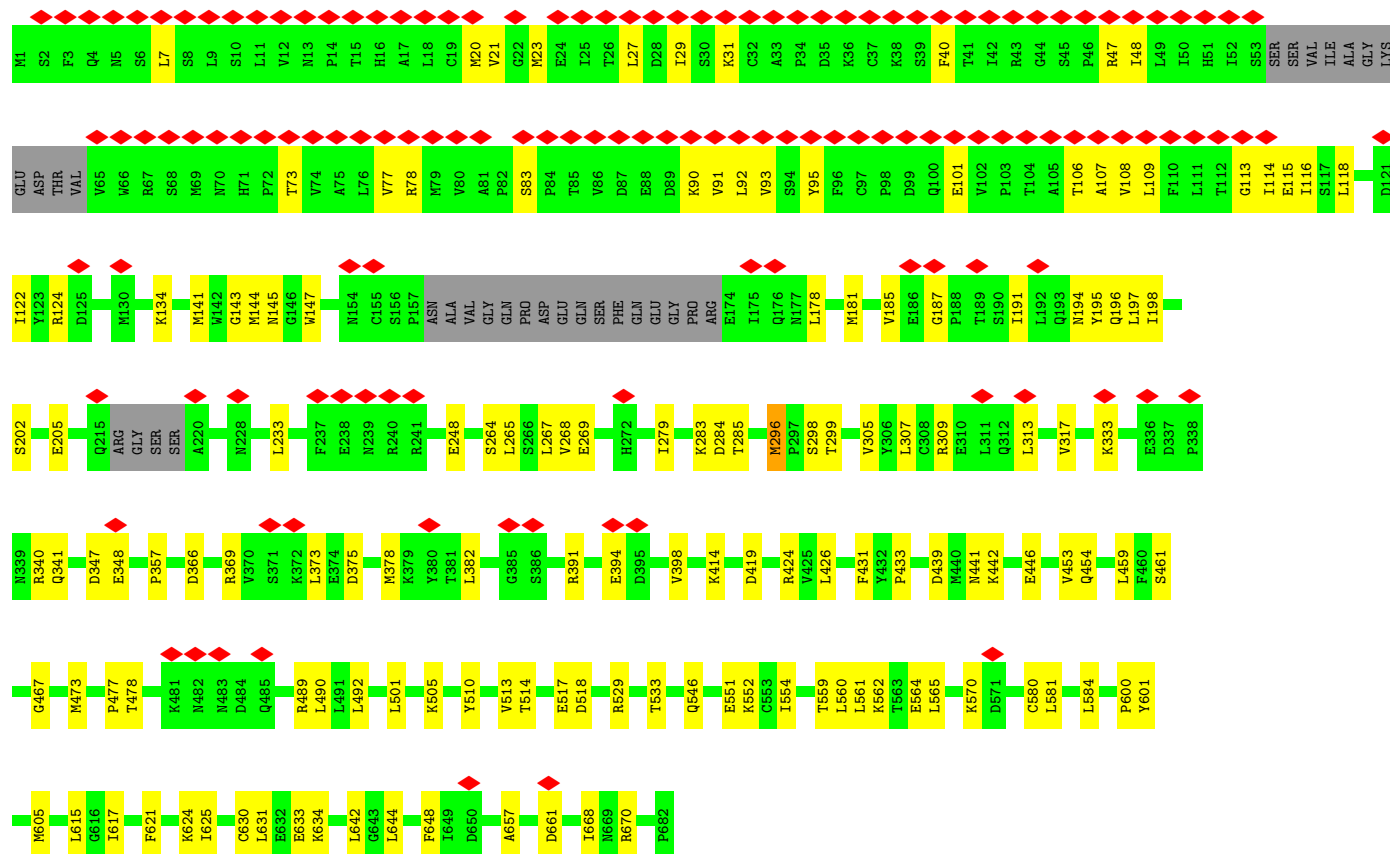
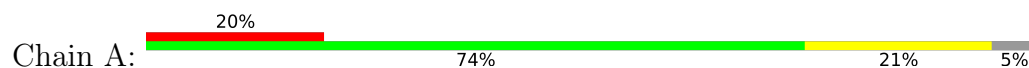


- Molecule 2: F-box and WD-40 domain protein 21

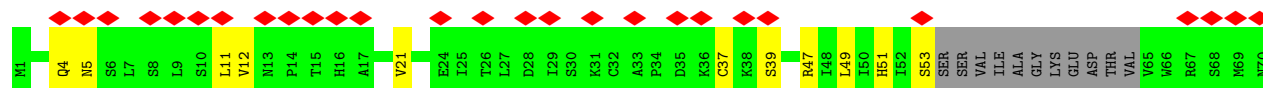


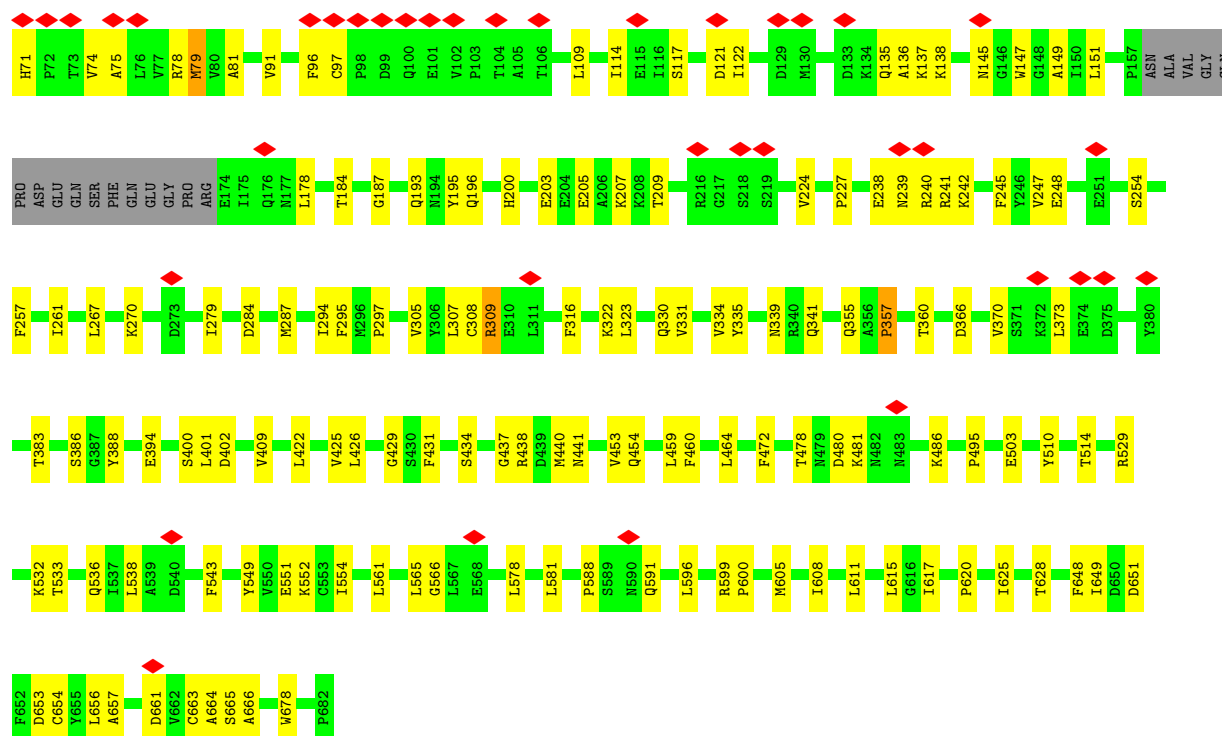


• Molecule 3: Inactive protein-arginine deiminase type-6

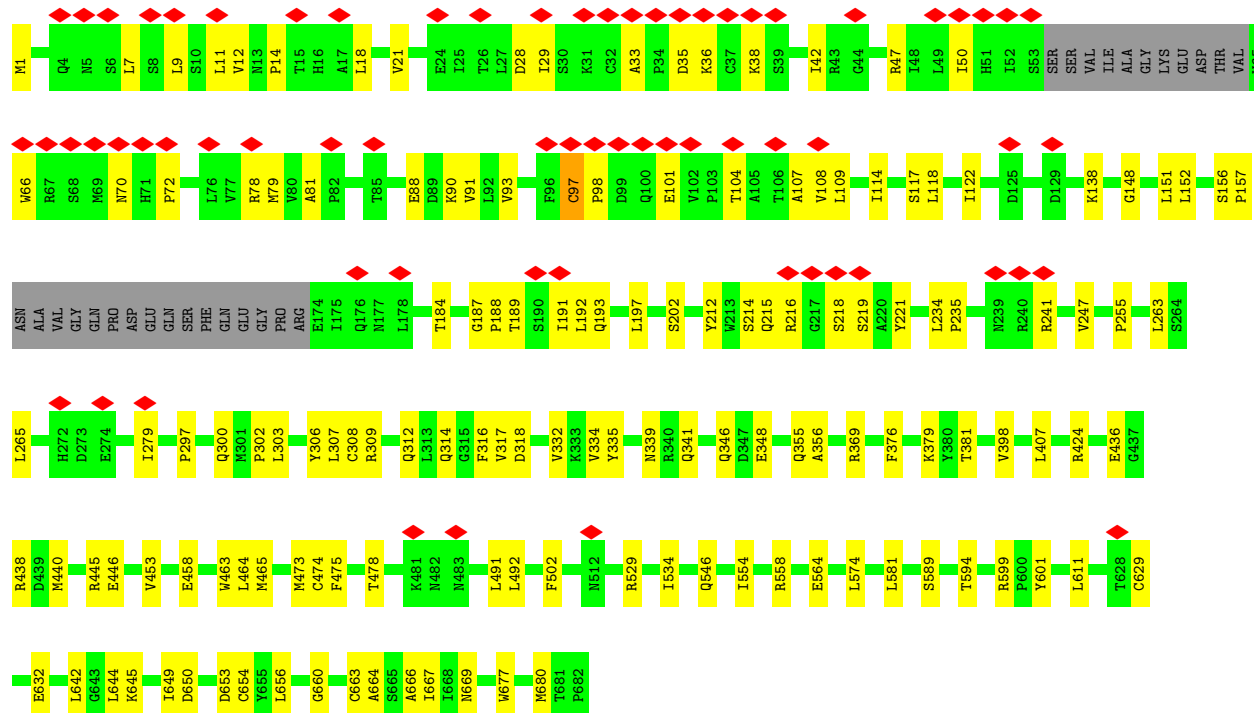
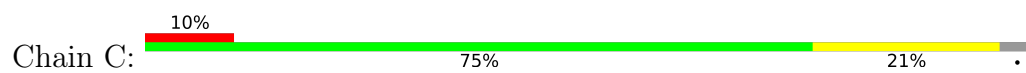


• Molecule 3: Inactive protein-arginine deiminase type-6

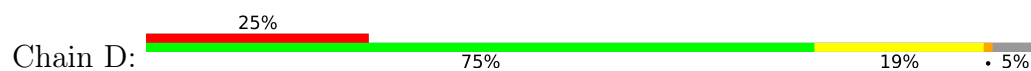


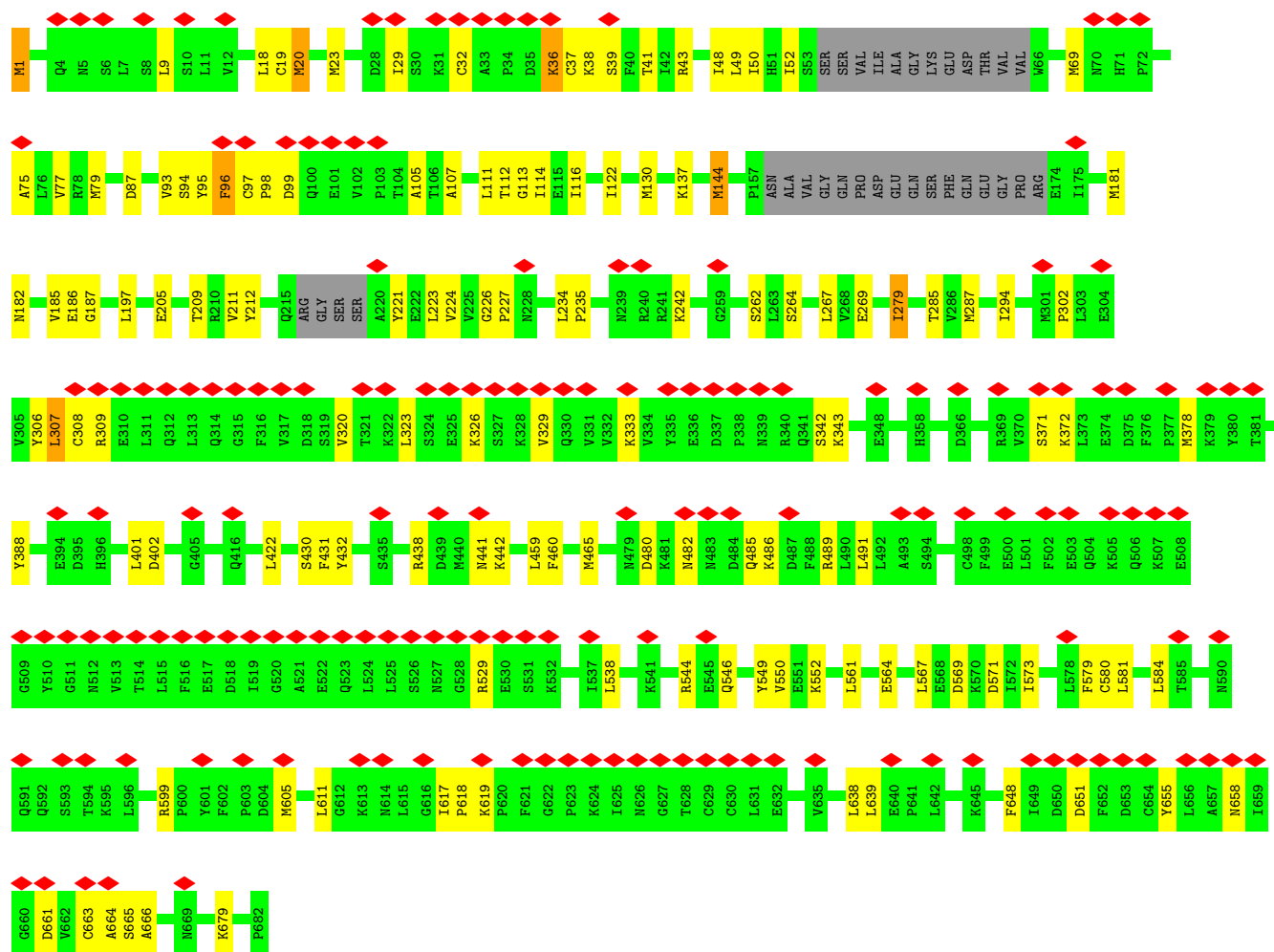


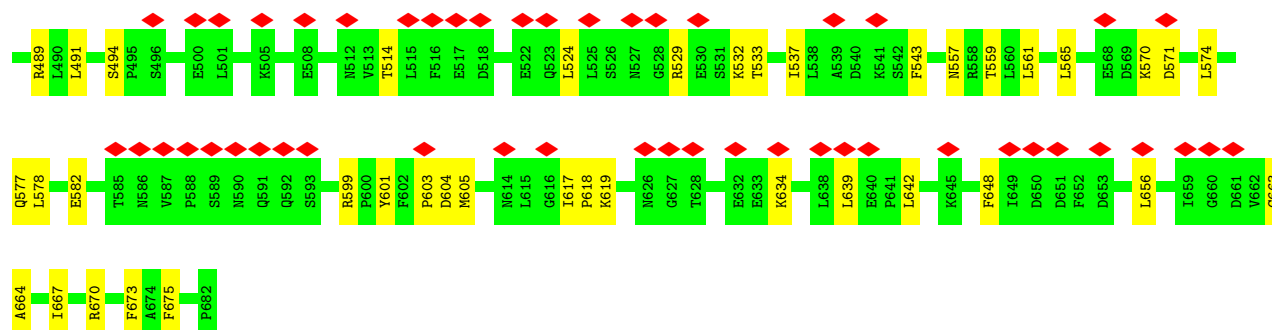
• Molecule 3: Inactive protein-arginine deiminase type-6



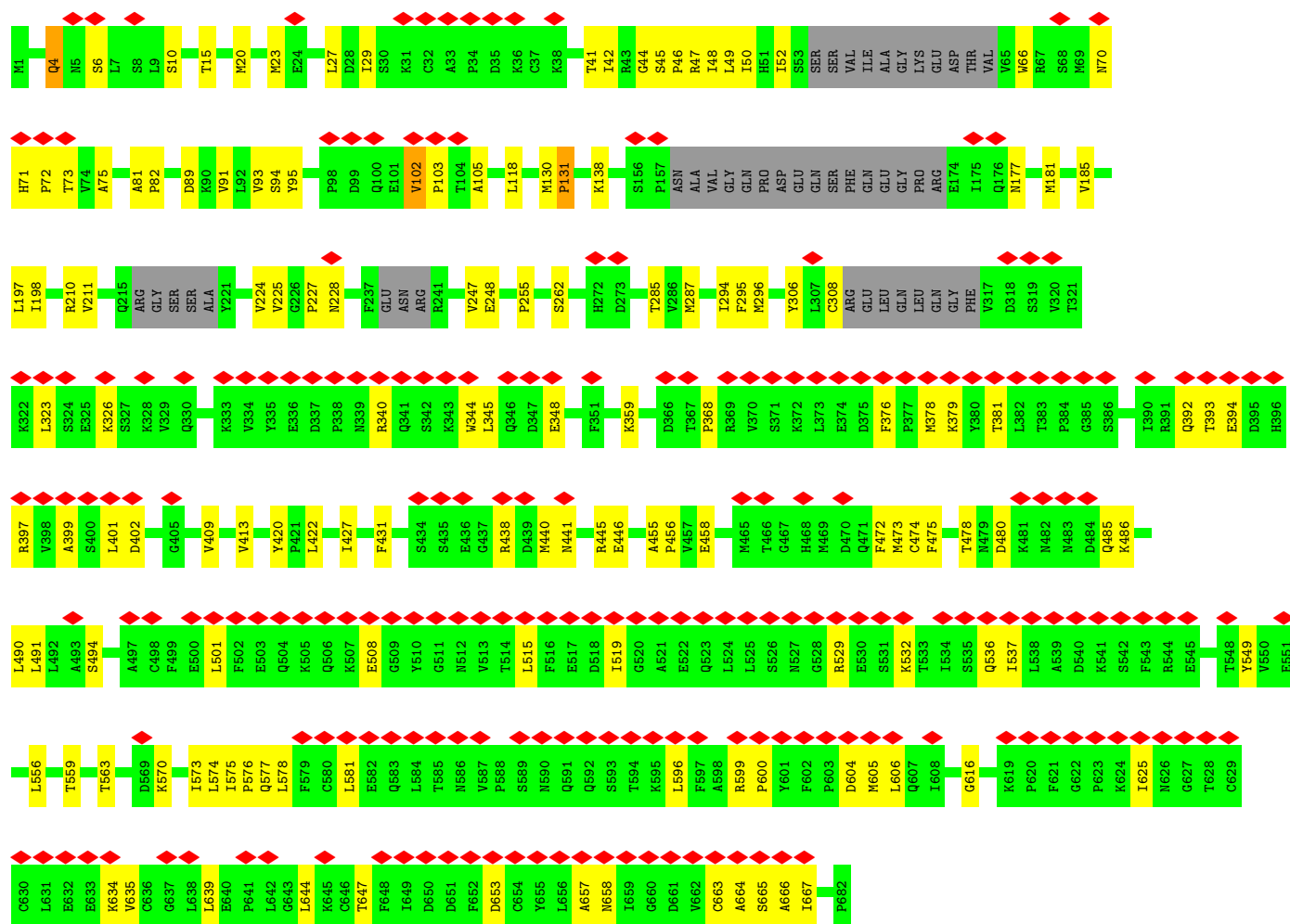
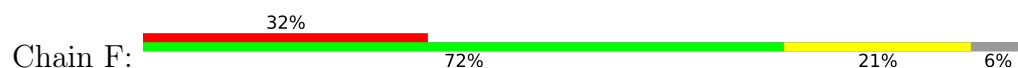
• Molecule 3: Inactive protein-arginine deiminase type-6



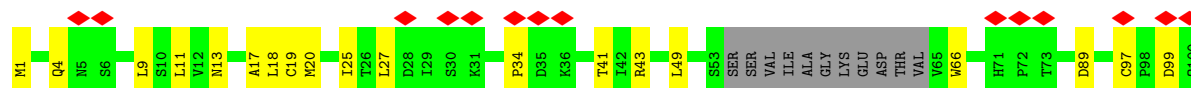
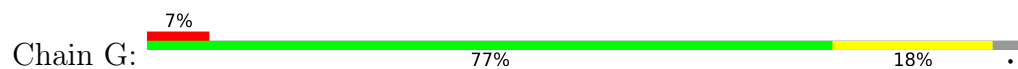


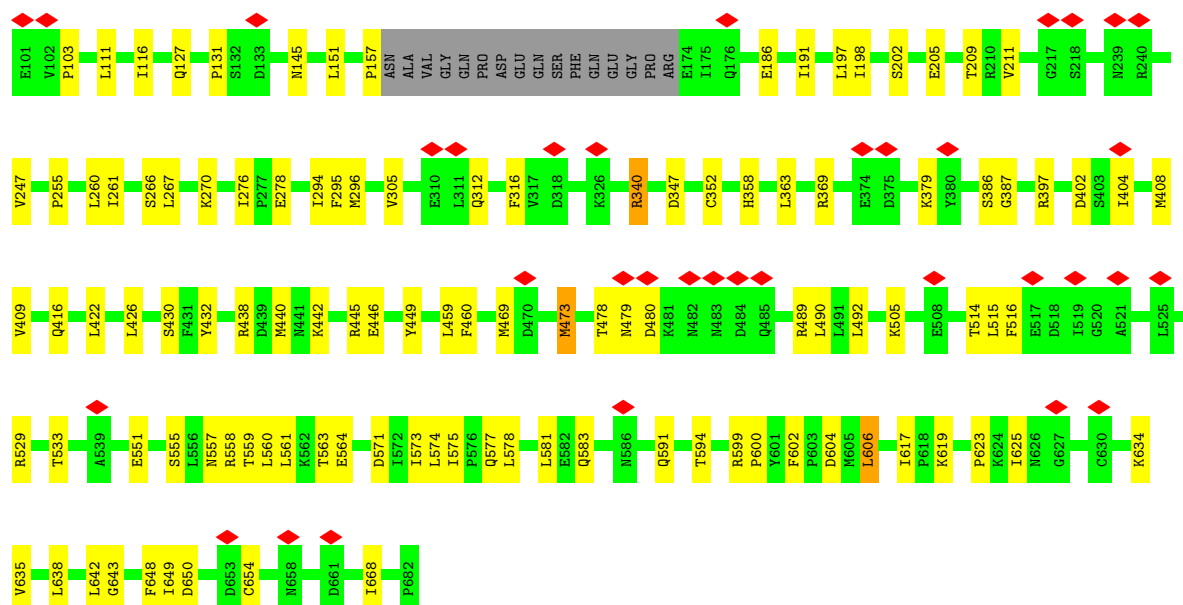


• Molecule 3: Inactive protein-arginine deiminase type-6

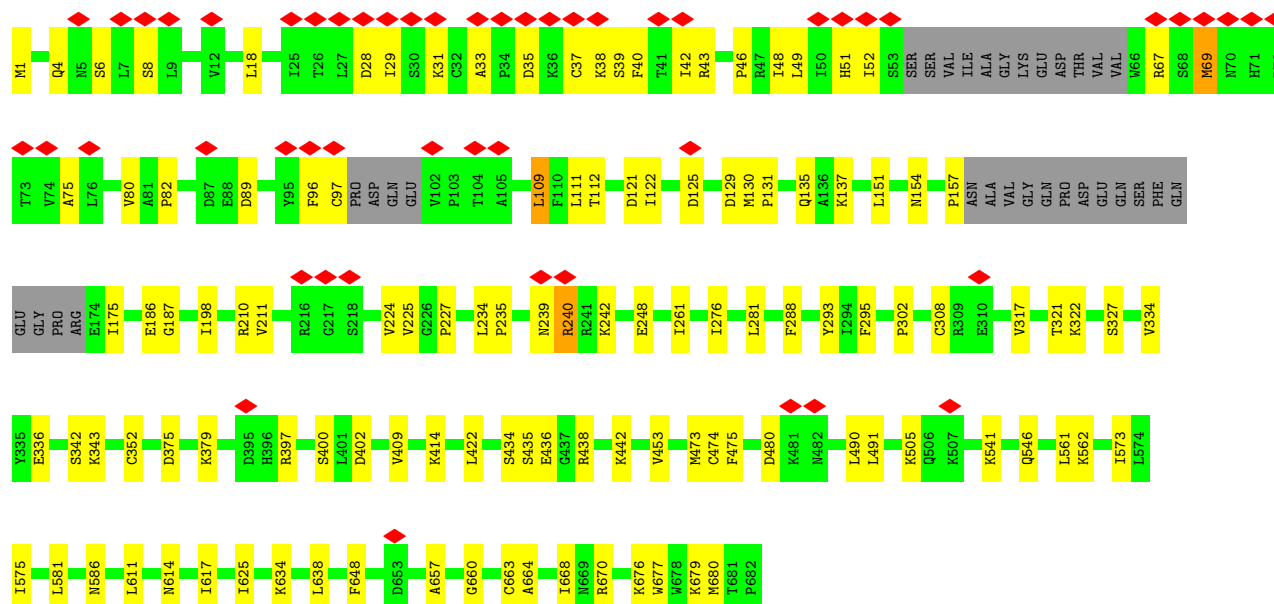
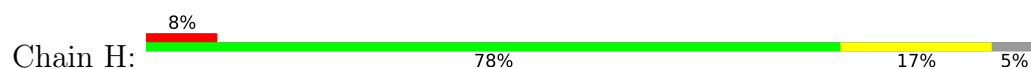


• Molecule 3: Inactive protein-arginine deiminase type-6

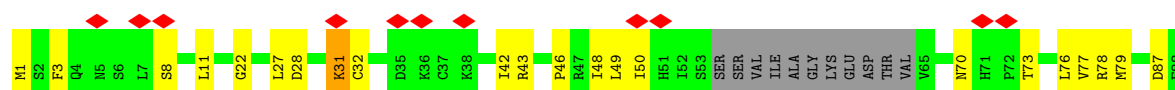




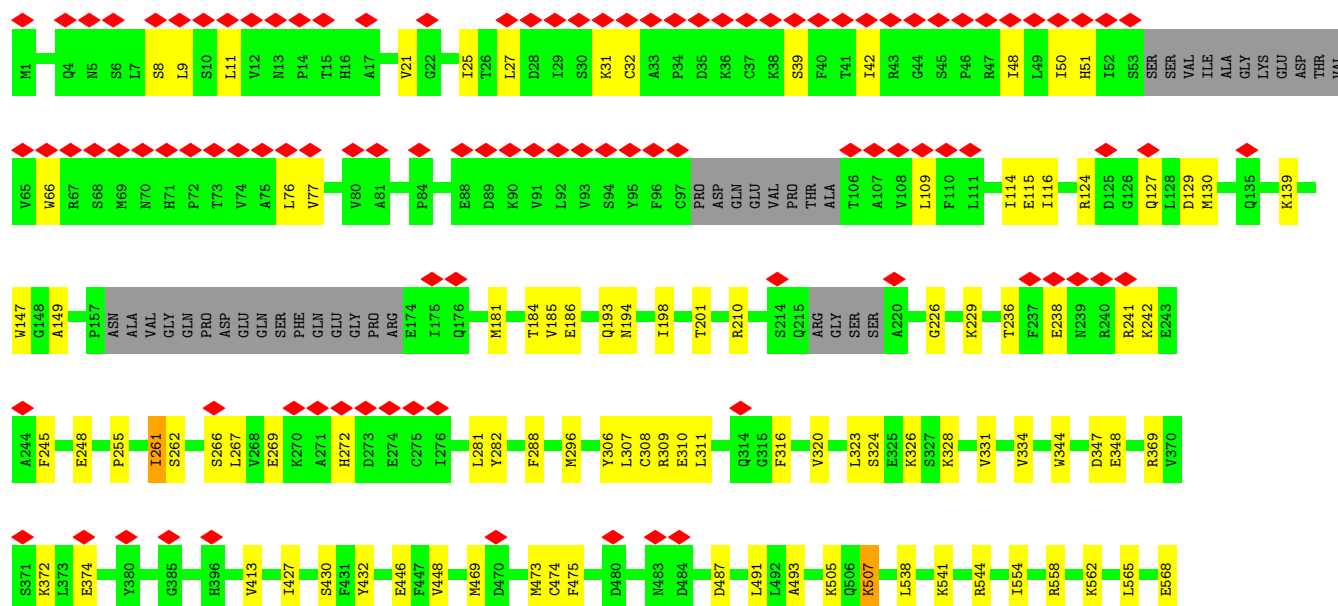
• Molecule 3: Inactive protein-arginine deiminase type-6

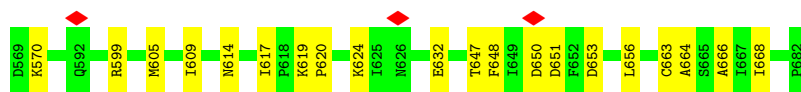


• Molecule 3: Inactive protein-arginine deiminase type-6



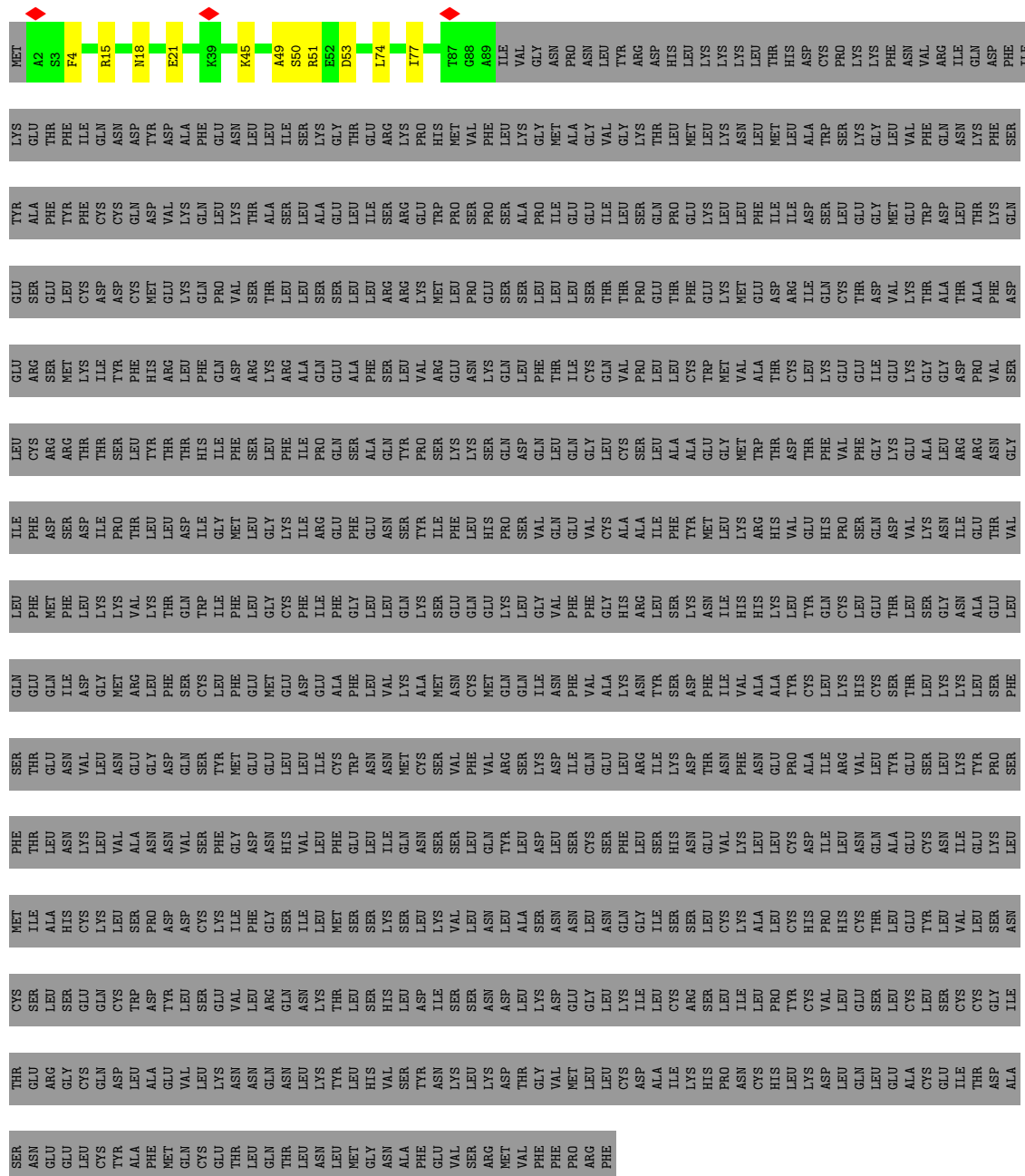






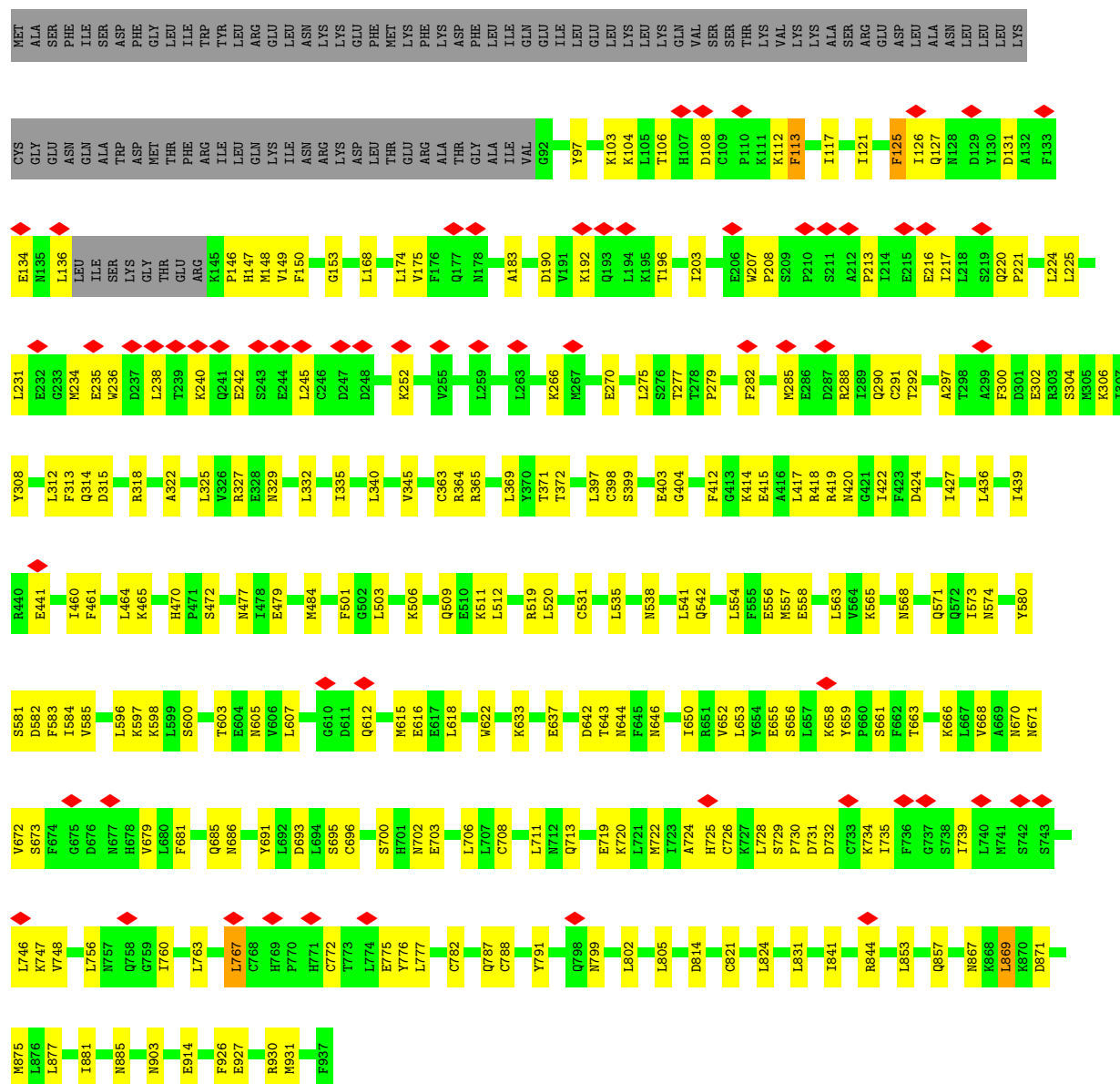
- Molecule 4: NLR family, pyrin domain containing 4F

Chain M:  8% . 91%

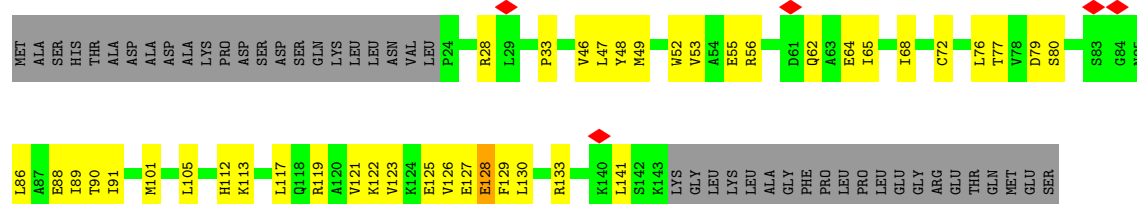


- Molecule 4: NLR family, pyrin domain containing 4F

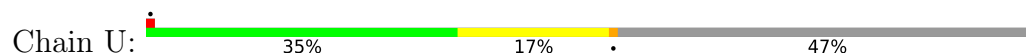
Chain R:  7% 64% 25% 11%



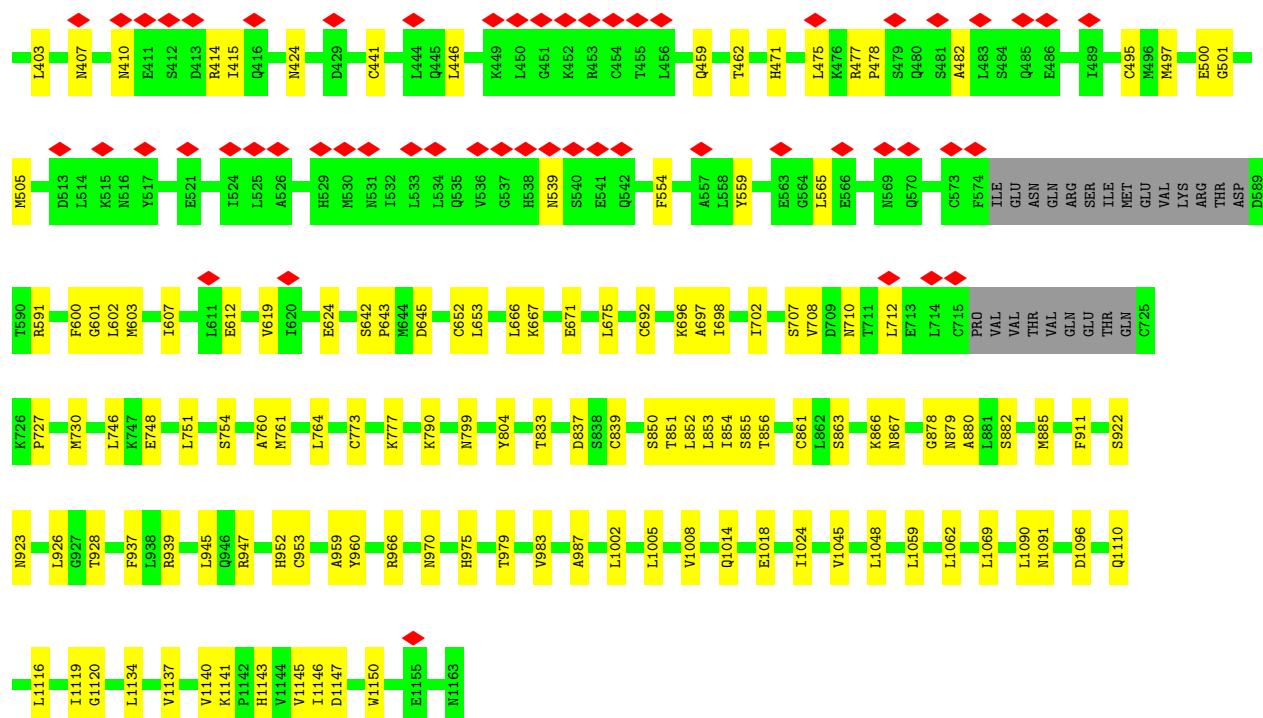
• Molecule 5: Oocyte-expressed protein homolog



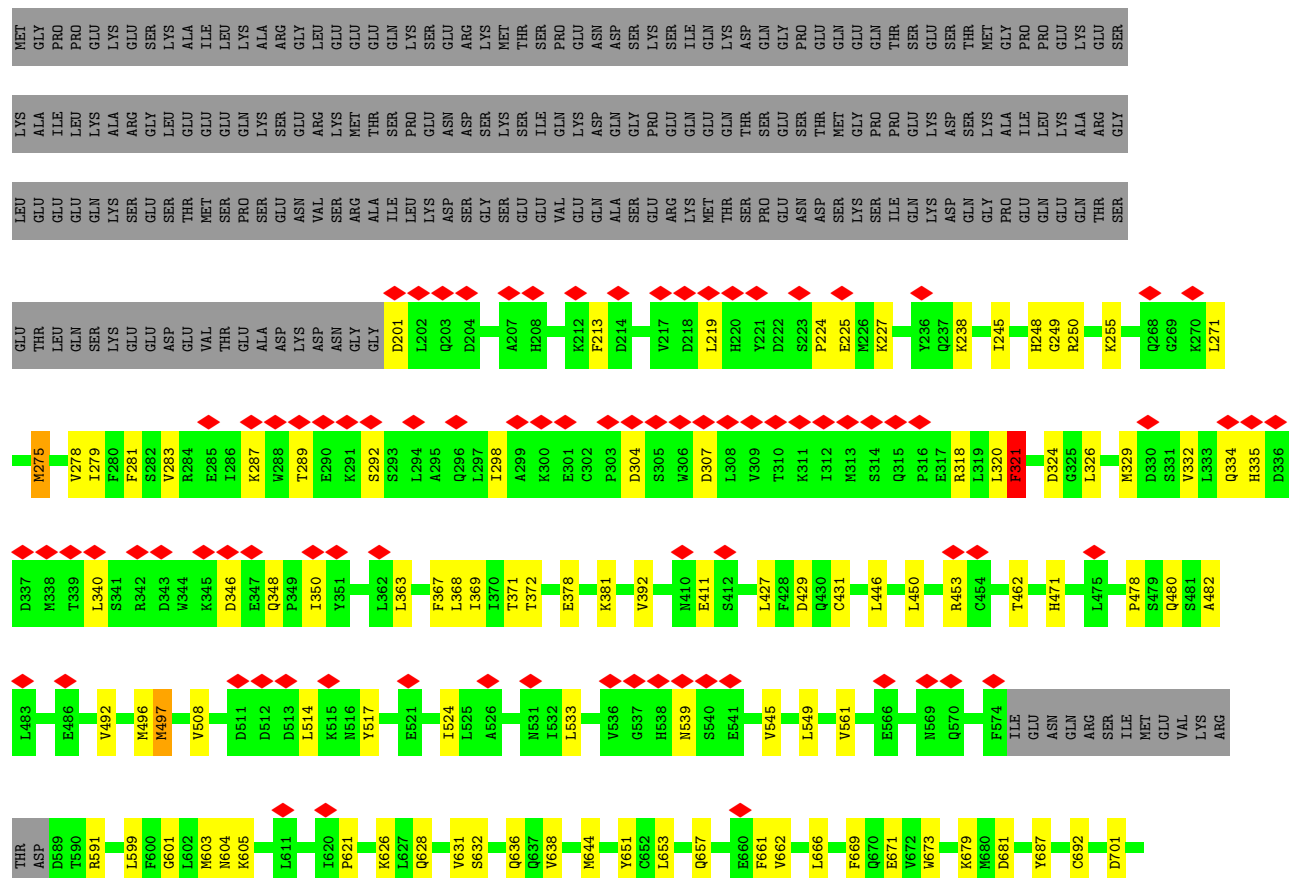
• Molecule 5: Oocyte-expressed protein homolog



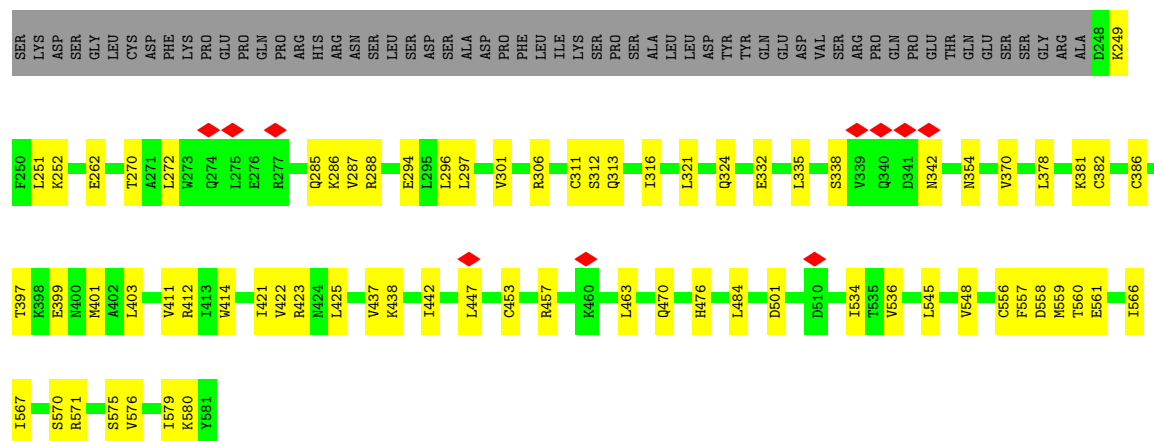




• Molecule 7: NACHT, LRR and PYD domains-containing protein 5

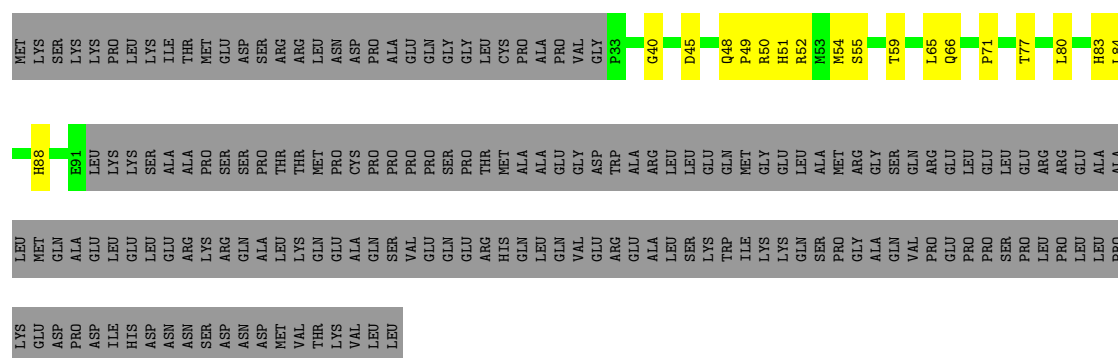






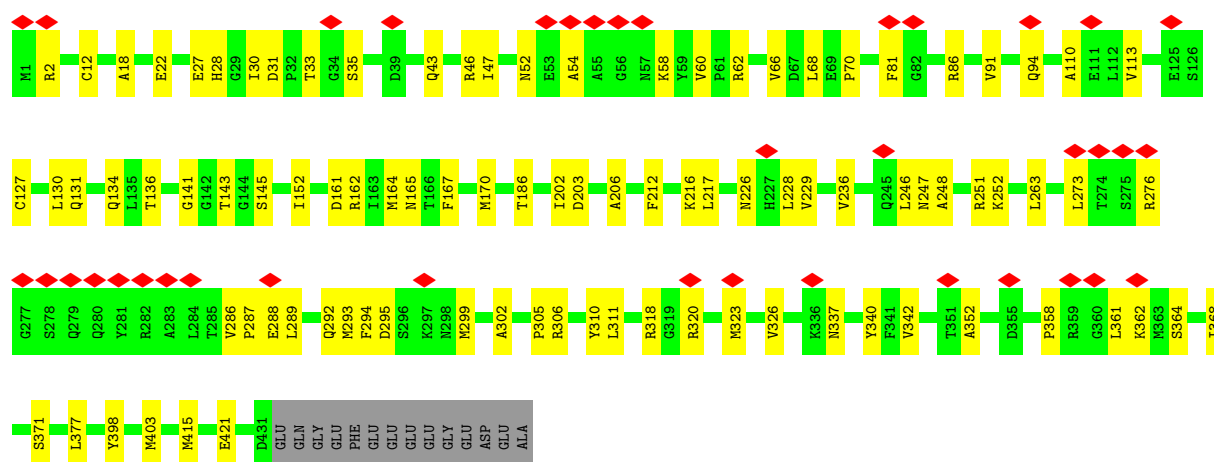
• Molecule 9: Zinc finger BED domain-containing protein 3

Chain V: 18% 8% 74%



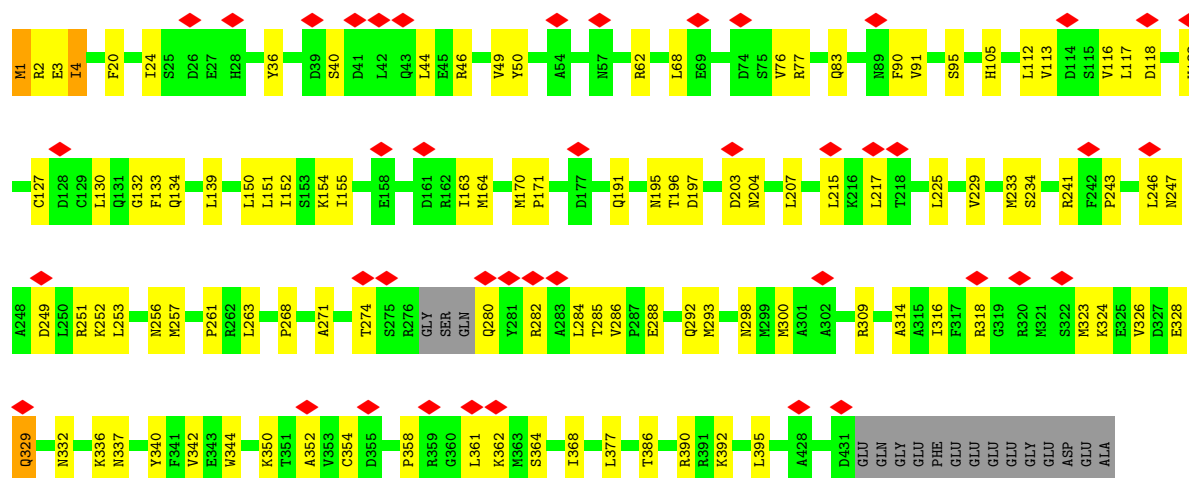
• Molecule 10: Tubulin beta-2A chain

Chain W: 9% 76% 21%

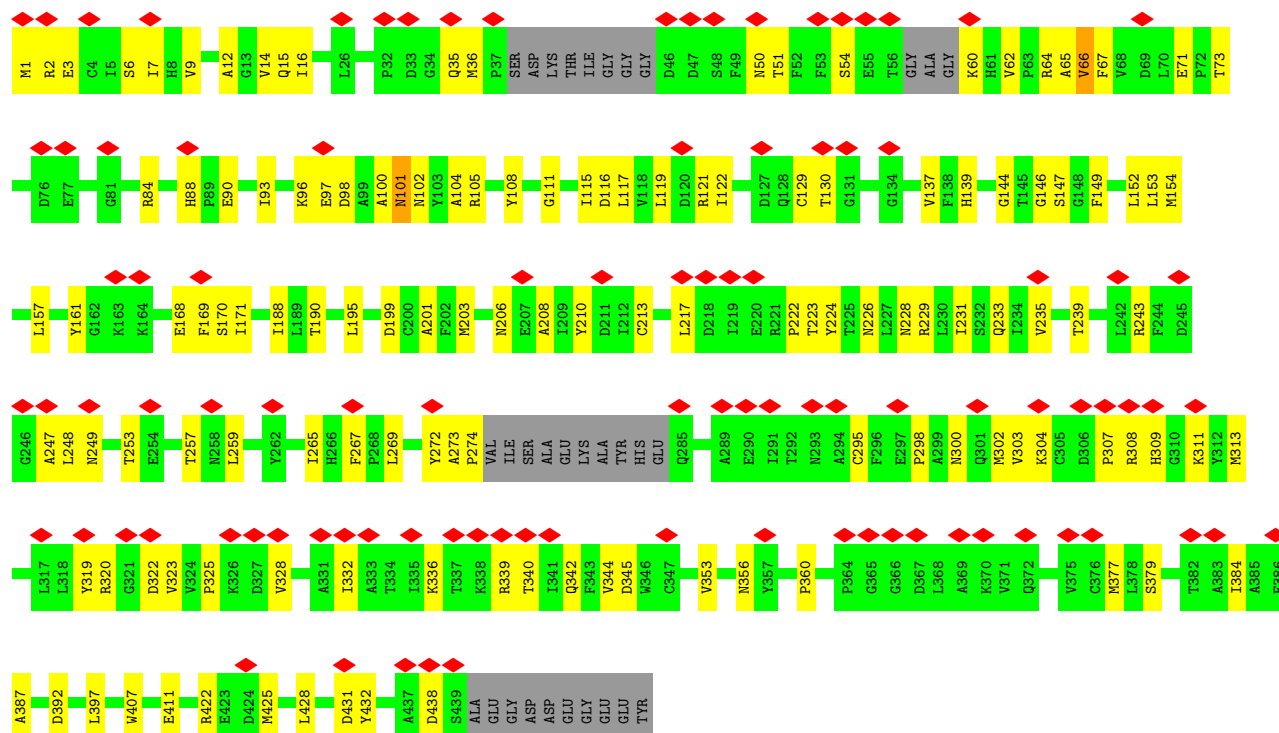


• Molecule 10: Tubulin beta-2A chain

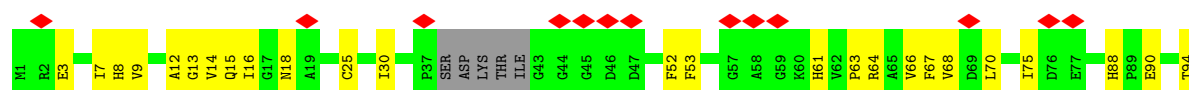
Chain Z: 10% 72% 24%



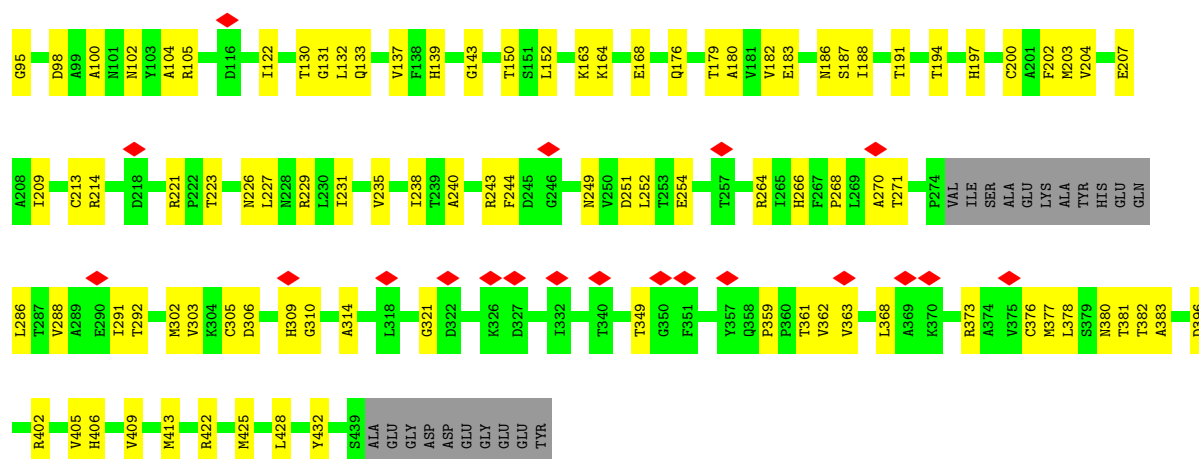
• Molecule 11: Tubulin alpha-1C chain



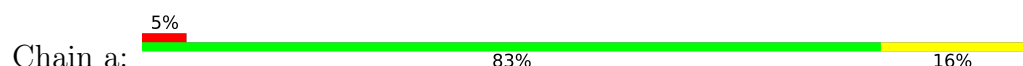
• Molecule 11: Tubulin alpha-1C chain



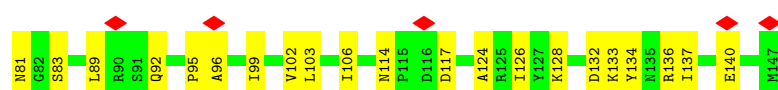
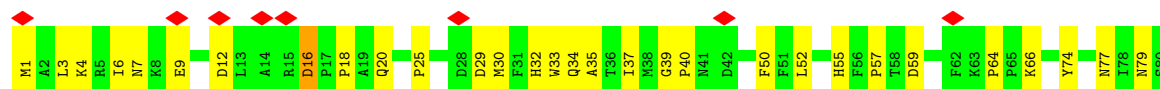




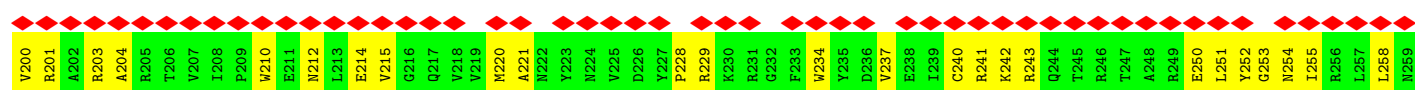
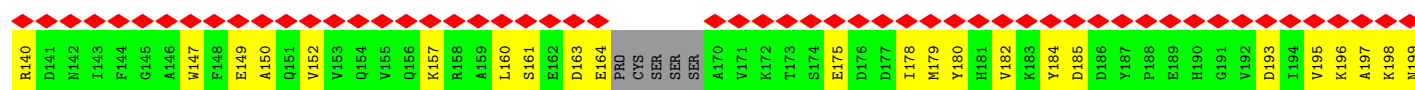
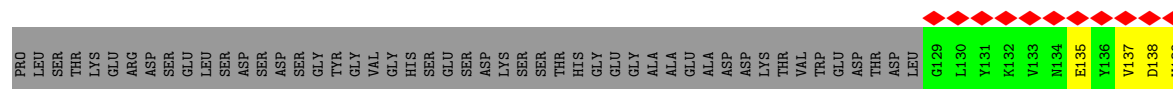
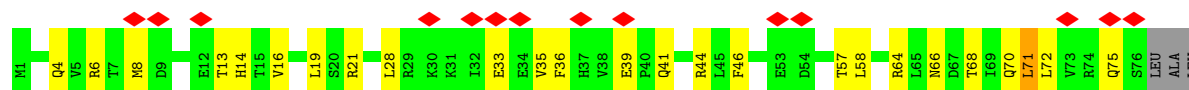
• Molecule 12: Ubiquitin-conjugating enzyme E2 D3

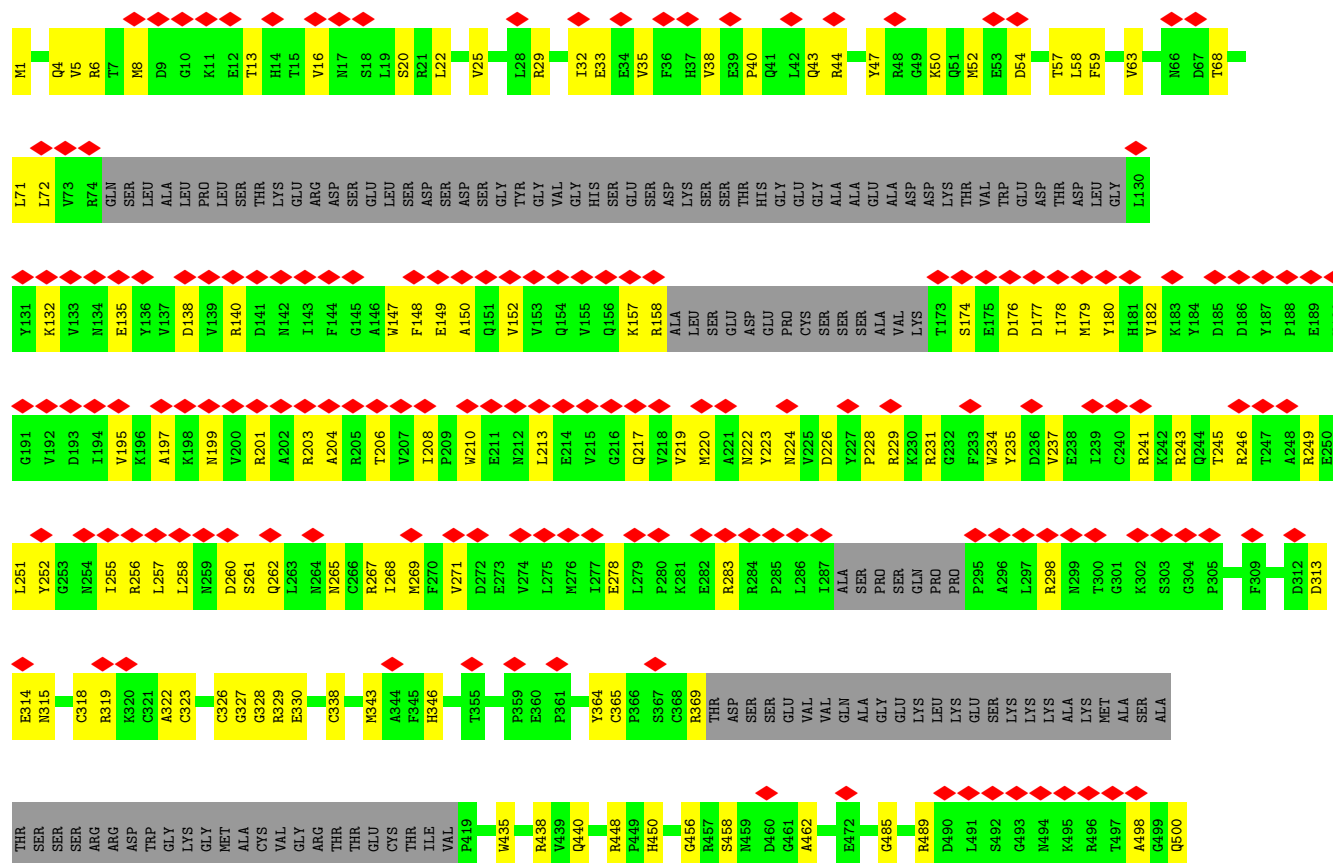


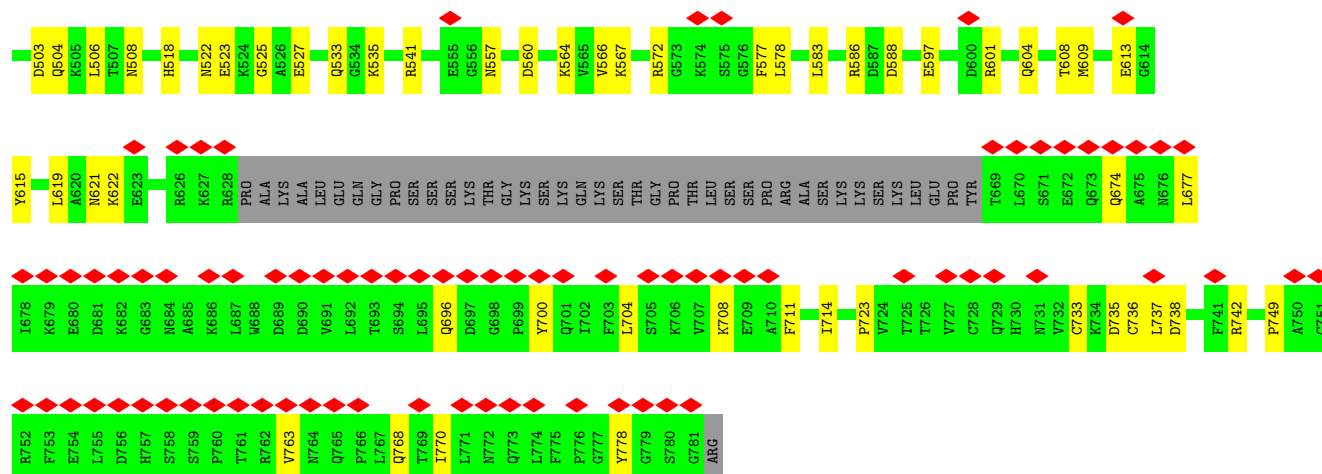
• Molecule 12: Ubiquitin-conjugating enzyme E2 D3



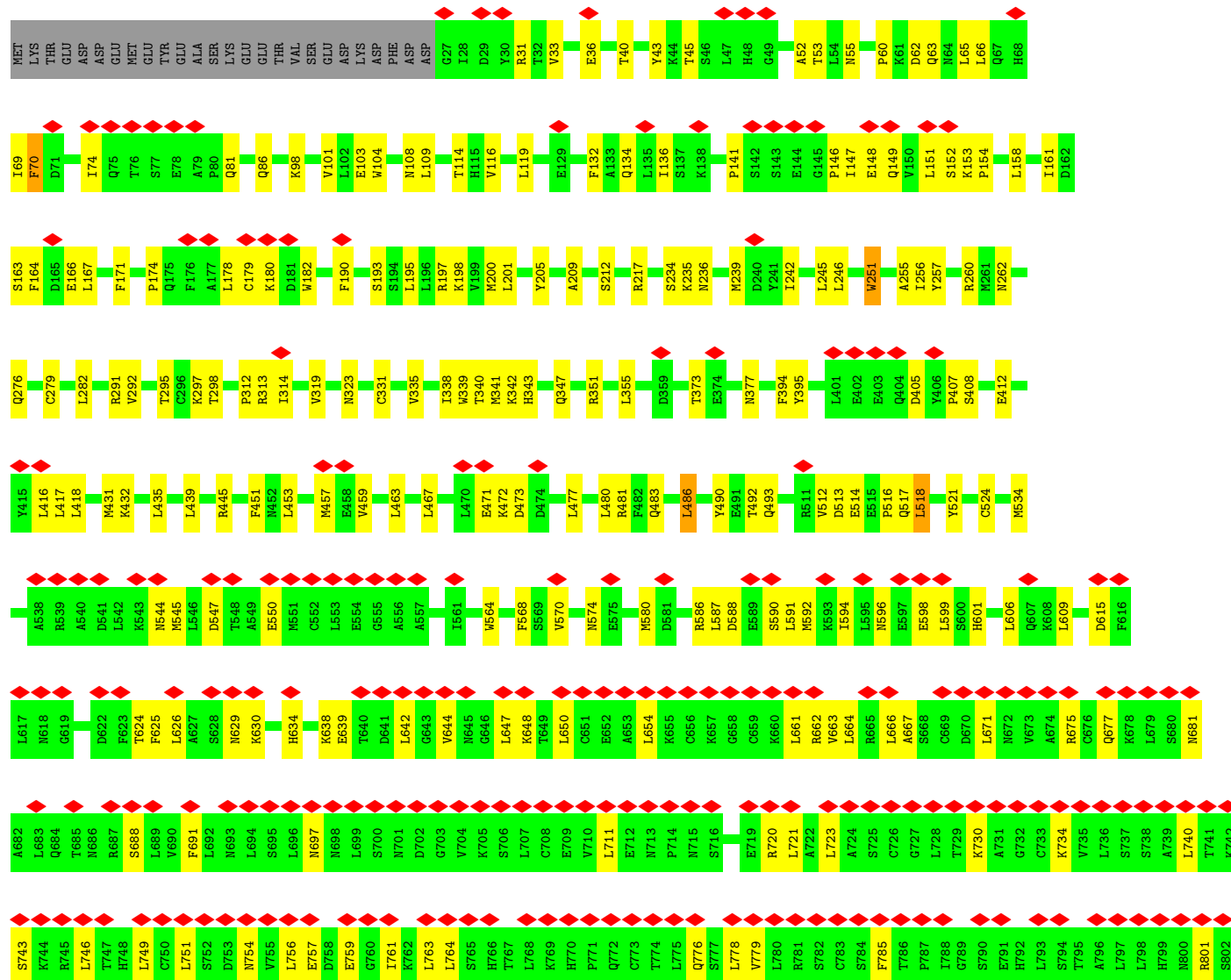
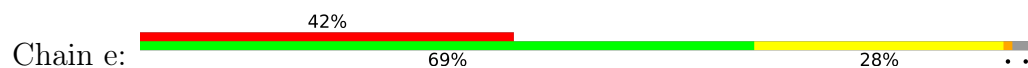
• Molecule 13: E3 ubiquitin-protein ligase UHRF1





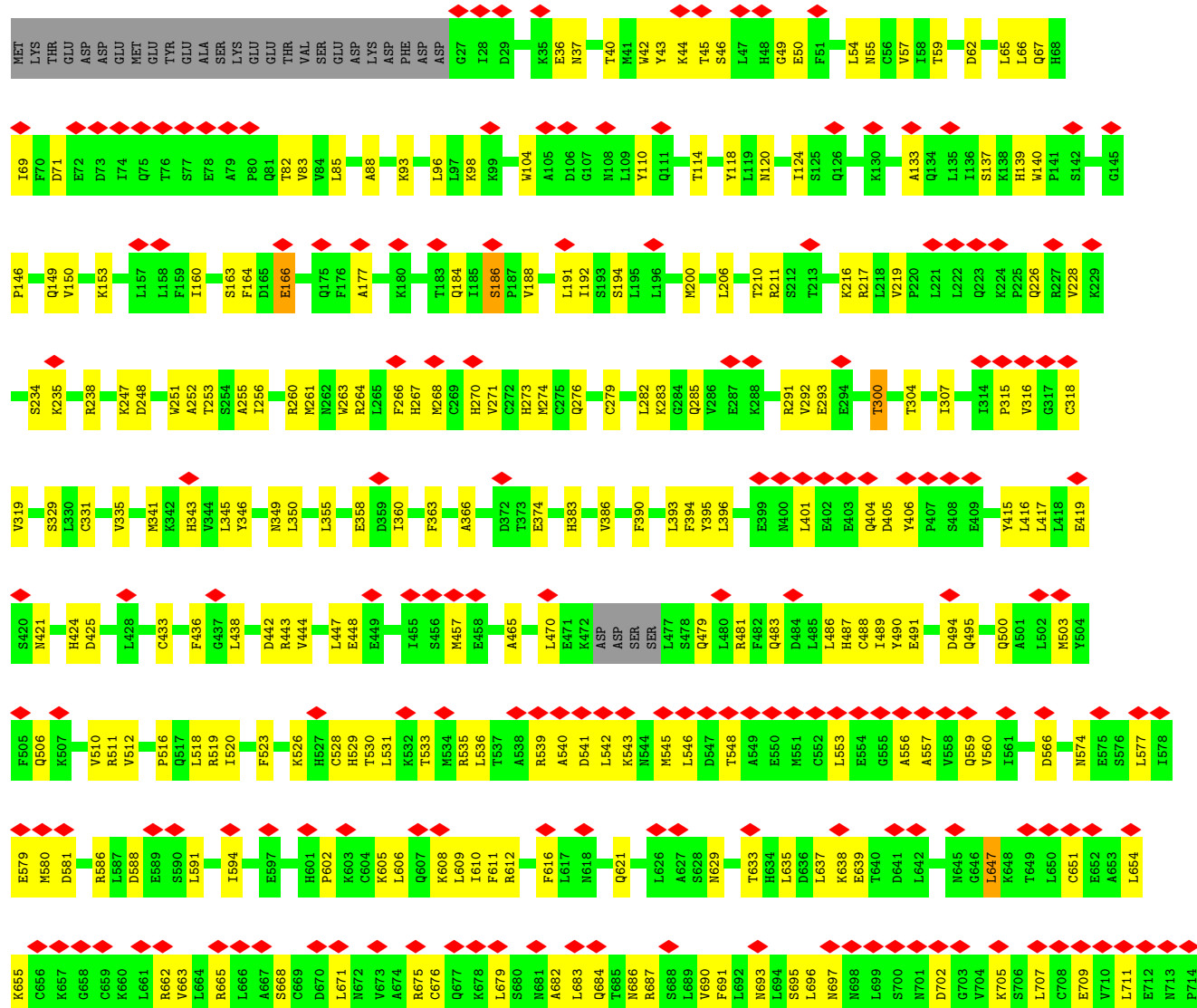
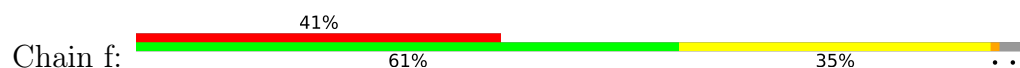


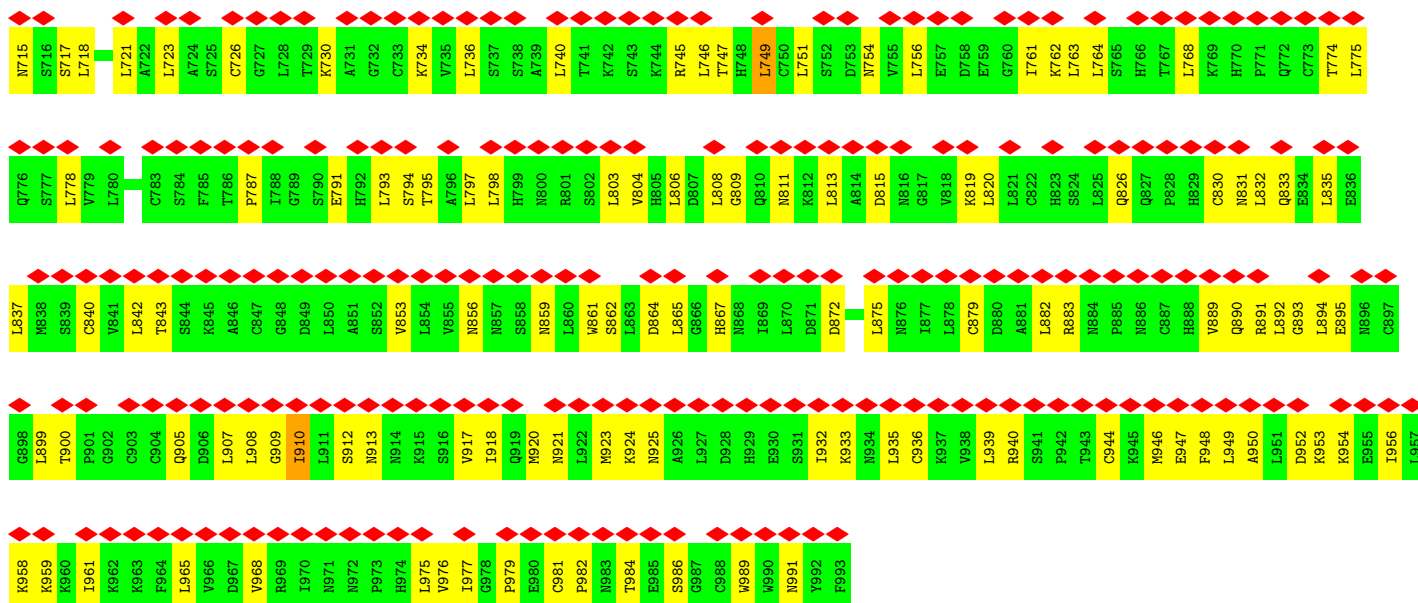
• Molecule 14: NACHT, LRR and PYD domains-containing protein 14



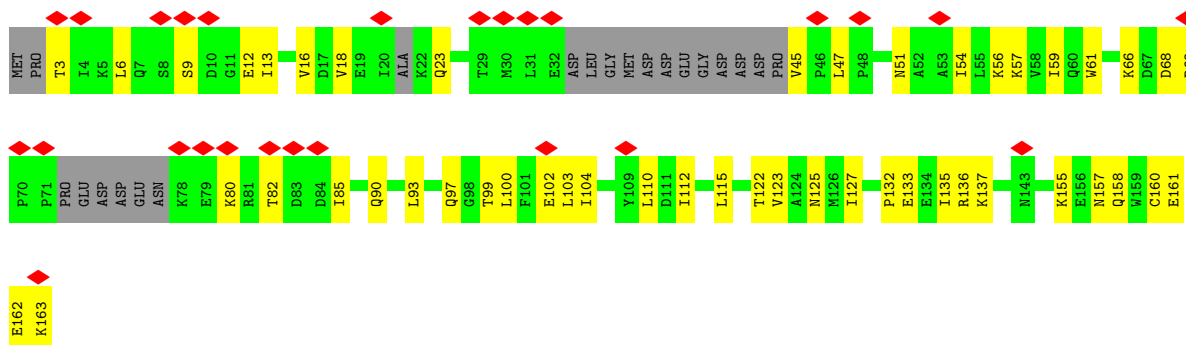


• Molecule 14: NACHT, LRR and PYD domains-containing protein 14

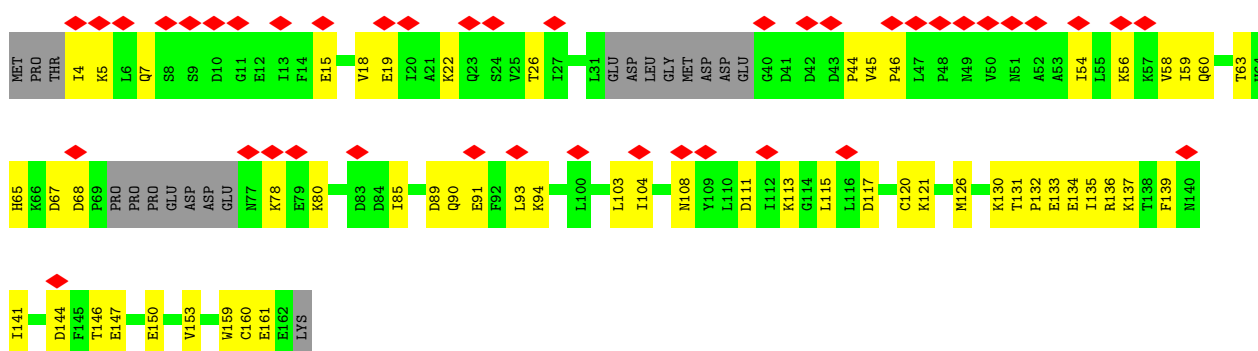




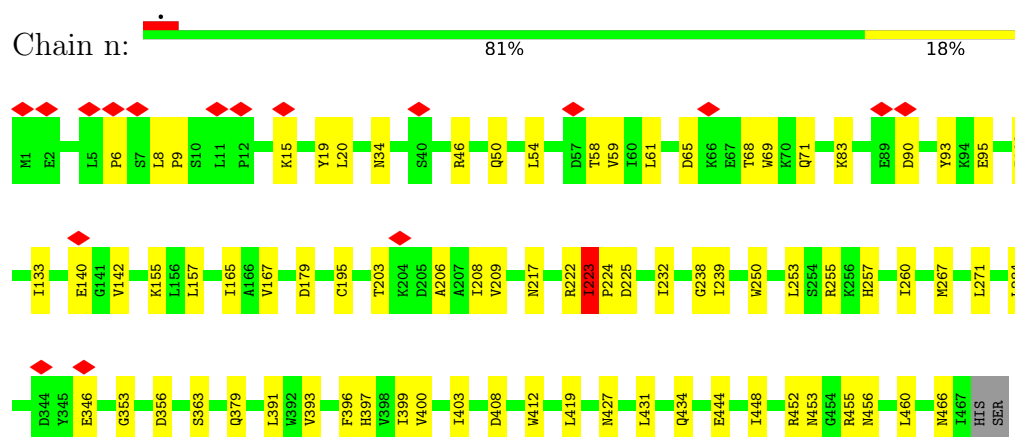
• Molecule 15: S-phase kinase-associated protein 1



• Molecule 15: S-phase kinase-associated protein 1



• Molecule 15: S-phase kinase-associated protein 1



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	288673	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	0.041	Depositor
Minimum map value	0.000	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.004	Depositor
Map size (Å)	372.0, 372.0, 372.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.93, 0.93, 0.93	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, GTP, ZN, MG

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	m	0.36	0/3815	0.78	6/5180 (0.1%)
2	p	0.38	1/3906 (0.0%)	0.83	7/5299 (0.1%)
3	A	0.24	0/5278	0.58	1/7156 (0.0%)
3	B	0.25	0/5306	0.58	1/7194 (0.0%)
3	C	0.22	0/5306	0.56	2/7194 (0.0%)
3	D	0.26	0/5271	0.57	9/7146 (0.1%)
3	E	0.27	0/5306	0.64	3/7194 (0.0%)
3	F	0.25	0/5173	0.57	2/7014 (0.0%)
3	G	0.23	0/5306	0.56	1/7195 (0.0%)
3	H	0.22	0/5264	0.49	2/7134 (0.0%)
3	I	0.27	0/5278	0.61	3/7156 (0.0%)
3	K	0.21	0/5216	0.51	2/7067 (0.0%)
4	M	0.27	0/738	0.54	0/984
4	R	0.27	0/6865	0.63	6/9252 (0.1%)
5	N	0.38	0/986	0.80	2/1336 (0.1%)
5	U	0.32	0/718	0.70	1/980 (0.1%)
6	O	0.33	0/1096	0.70	2/1480 (0.1%)
7	P	0.22	0/7549	0.51	1/10205 (0.0%)
7	S	0.25	0/7608	0.57	3/10289 (0.0%)
8	Q	0.21	0/2950	0.54	1/4005 (0.0%)
8	T	0.22	0/2864	0.52	0/3883
9	V	0.25	0/494	0.55	0/672
10	W	0.27	0/3462	0.60	0/4689
10	Z	0.32	1/3442 (0.0%)	0.70	8/4661 (0.2%)
11	X	0.26	0/3360	0.58	0/4560
11	Y	0.26	0/3377	0.60	0/4583
12	a	0.25	0/1208	0.61	0/1647
12	c	0.35	0/1208	0.78	2/1647 (0.1%)
13	b	0.25	0/5196	0.56	1/7016 (0.0%)
13	d	0.29	1/5096 (0.0%)	0.62	1/6880 (0.0%)
14	e	0.26	0/7868	0.62	1/10637 (0.0%)
14	f	0.32	0/7839	0.76	6/10596 (0.1%)



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
15	h	0.29	0/1168	0.65	0/1575
15	j	0.29	0/1177	0.69	0/1589
15	l	0.34	0/1086	0.72	1/1461 (0.1%)
16	n	0.26	1/3881 (0.0%)	0.56	2/5275 (0.0%)
All	All	0.27	4/141661 (0.0%)	0.61	77/191831 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	D	0	1
3	F	0	1
3	G	0	1
12	a	0	2
All	All	0	5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	d	283	ARG	C-N	6.39	1.43	1.32
2	p	428	LEU	C-O	5.58	1.26	1.23
16	n	223	ILE	C-N	5.50	1.41	1.34
10	Z	243	PRO	CG-CD	-5.12	1.33	1.50

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	Z	243	PRO	CA-N-CD	-13.67	92.87	112.00
3	E	131	PRO	CA-N-CD	-11.51	95.89	112.00
7	P	478	PRO	CA-N-CD	-9.75	98.35	112.00
2	p	392	PRO	CA-N-CD	-9.62	98.53	112.00
3	F	131	PRO	CA-N-CD	-9.43	98.80	112.00
10	Z	243	PRO	N-CD-CG	-8.69	90.17	103.20
4	R	221	PRO	CA-N-CD	-8.41	100.23	112.00
10	Z	1	MET	CA-CB-CG	7.89	129.89	114.10
5	N	127	GLU	CA-CB-CG	7.62	129.33	114.10
6	O	101	MET	CA-CB-CG	7.59	129.28	114.10
16	n	58	THR	CA-C-N	7.59	135.63	121.97
16	n	58	THR	C-N-CA	7.59	135.63	121.97
1	m	99	PHE	N-CA-C	-7.30	102.50	111.33

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	357	PRO	CA-N-CD	-7.09	102.08	112.00
3	C	339	ASN	N-CA-C	7.04	120.38	109.60
1	m	11	MET	CB-CG-SD	6.90	133.41	112.70
10	Z	1	MET	CB-CA-C	6.89	123.18	110.10
2	p	428	LEU	CA-CB-CG	6.46	138.90	116.30
2	p	418	LYS	CA-CB-CG	6.45	127.00	114.10
4	R	125	PHE	CA-C-N	6.34	133.39	121.97
4	R	125	PHE	C-N-CA	6.34	133.39	121.97
13	d	564	LYS	CB-CG-CD	6.27	125.73	111.30
6	O	128	MET	CB-CG-SD	6.21	131.34	112.70
7	S	321	PHE	N-CA-C	6.14	119.82	111.17
2	p	314	ILE	CB-CG1-CD1	6.04	126.47	113.80
1	m	60	LEU	CA-CB-CG	6.03	137.40	116.30
7	S	275	MET	CB-CG-SD	6.00	130.71	112.70
14	f	494	ASP	CA-C-N	5.99	132.97	121.54
14	f	494	ASP	C-N-CA	5.99	132.97	121.54
3	I	342	SER	CB-CA-C	-5.91	109.75	116.54
3	F	4	GLN	N-CA-C	-5.88	107.35	114.75
2	p	320	LEU	N-CA-C	-5.83	101.49	109.71
2	p	428	LEU	CB-CG-CD2	-5.81	93.28	110.70
2	p	391	ASP	N-CA-C	-5.80	102.74	109.93
3	C	654	CYS	CA-CB-SG	5.77	127.68	114.40
3	D	99	ASP	CA-C-N	-5.75	115.60	122.44
3	D	99	ASP	C-N-CA	-5.75	115.60	122.44
14	f	285	GLN	CB-CG-CD	5.67	122.24	112.60
1	m	54	ASP	CA-C-N	5.64	132.32	121.54
1	m	54	ASP	C-N-CA	5.64	132.32	121.54
10	Z	1	MET	CB-CG-SD	5.63	129.59	112.70
3	K	372	LYS	CB-CG-CD	5.56	124.09	111.30
10	Z	91	VAL	CB-CA-C	5.51	120.33	111.29
3	D	96	PHE	CA-C-N	-5.46	112.81	122.48
3	D	96	PHE	C-N-CA	-5.46	112.81	122.48
12	c	117	ASP	CB-CA-C	5.46	115.91	109.47
3	I	31	LYS	CA-CB-CG	5.42	124.94	114.10
3	D	36	LYS	CA-C-N	-5.40	114.33	122.81
3	D	36	LYS	C-N-CA	-5.40	114.33	122.81
3	G	186	GLU	CA-CB-CG	5.40	124.90	114.10
3	K	507	LYS	CB-CG-CD	5.35	123.60	111.30
3	H	69	MET	CB-CG-SD	5.32	128.66	112.70
7	S	942	GLU	CA-CB-CG	5.31	124.72	114.10
5	N	128	GLU	CA-CB-CG	5.30	124.71	114.10
3	D	20	MET	CB-CG-SD	-5.30	96.81	112.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	465	MET	CB-CG-SD	5.28	128.53	112.70
5	U	56	ARG	CD-NE-CZ	5.25	131.75	124.40
15	l	94	LYS	CB-CG-CD	5.23	123.33	111.30
13	b	336	LEU	CB-CG-CD2	5.19	126.27	110.70
3	E	130	MET	C-N-CD	-5.18	103.76	125.00
10	Z	91	VAL	CA-CB-CG1	5.17	119.19	110.40
8	Q	154	GLU	CB-CA-C	5.16	115.60	110.33
3	E	5	ASN	CA-CB-CG	5.15	117.75	112.60
3	D	97	CYS	CA-CB-SG	-5.15	102.55	114.40
1	m	448	MET	CA-CB-CG	5.13	124.36	114.10
3	A	296	MET	CB-CG-SD	5.12	128.06	112.70
14	f	448	GLU	CA-C-N	-5.11	112.56	122.06
14	f	448	GLU	C-N-CA	-5.11	112.56	122.06
14	e	723	LEU	CA-CB-CG	5.06	134.00	116.30
14	f	292	VAL	CG1-CB-CG2	-5.06	99.67	110.80
3	H	240	ARG	CA-CB-CG	5.05	124.20	114.10
3	D	114	ILE	CA-CB-CG1	5.04	118.97	110.40
4	R	103	LYS	CA-CB-CG	5.03	124.15	114.10
10	Z	4	ILE	CA-CB-CG2	5.03	119.04	110.50
12	c	117	ASP	CA-CB-CG	5.02	117.62	112.60
4	R	240	LYS	CA-CB-CG	5.01	124.13	114.10
4	R	113	PHE	N-CA-C	5.01	114.85	108.24

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	36	LYS	Peptide
3	F	445	ARG	Sidechain
3	G	340	ARG	Sidechain
12	a	136	ARG	Sidechain
12	a	72	ARG	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	m	3723	0	3777	130	0
2	p	3804	0	3819	128	0
3	A	5161	0	5172	96	0
3	B	5188	0	5201	99	0
3	C	5188	0	5201	84	0
3	D	5154	0	5163	85	0
3	E	5188	0	5201	89	0
3	F	5059	0	5073	91	0
3	G	5188	0	5203	81	0
3	H	5148	0	5166	75	0
3	I	5161	0	5176	131	0
3	K	5102	0	5120	69	0
4	M	728	0	763	7	0
4	R	6735	0	6754	154	0
5	N	967	0	991	29	0
5	U	701	0	694	27	0
6	O	1066	0	1077	22	0
7	P	7419	0	7514	124	0
7	S	7476	0	7557	123	0
8	Q	2884	0	2862	51	0
8	T	2803	0	2795	51	0
9	V	476	0	447	16	0
10	W	3387	0	3264	62	0
10	Z	3368	0	3247	83	0
11	X	3287	0	3201	90	0
11	Y	3303	0	3214	79	0
12	a	1173	0	1159	19	0
12	c	1173	0	1159	36	0
13	b	5084	0	4971	118	0
13	d	4985	0	4876	119	0
14	e	7723	0	7829	193	0
14	f	7695	0	7808	241	0
15	h	1151	0	1160	33	0
15	j	1160	0	1154	39	0
15	l	1071	0	1078	35	0
16	n	3787	0	3806	52	0
17	P	31	0	12	1	0
17	R	31	0	12	2	0
17	S	31	0	12	1	0
17	e	31	0	12	0	0
17	f	31	0	12	1	0
18	W	32	0	12	2	0
18	X	32	0	12	4	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	Y	32	0	12	1	0
18	Z	32	0	12	0	0
19	W	1	0	0	0	0
19	X	1	0	0	0	0
19	Y	1	0	0	0	0
19	Z	1	0	0	0	0
20	b	3	0	0	0	0
20	d	3	0	0	0	0
All	All	138959	0	138760	2817	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 10.

All (2817) 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)
13:d:733:CYS:HB2	13:d:736:CYS:SG	1.90	1.10
3:F:130:MET:HE1	3:G:43:ARG:HE	1.37	0.87
10:Z:191:GLN:O	10:Z:195:ASN:HB2	1.74	0.86
3:F:639:LEU:HB3	3:F:644:LEU:HD11	1.57	0.86
12:a:103:LEU:O	12:a:107:CYS:HB2	1.76	0.85
2:p:30:LYS:HE2	15:l:144:ASP:HB2	1.61	0.82
14:f:954:LYS:O	14:f:958:LYS:HB2	1.79	0.82
3:I:344:TRP:O	3:I:348:GLU:HB2	1.79	0.81
10:Z:207:LEU:HD13	10:Z:225:LEU:HB3	1.66	0.77
3:D:116:ILE:HG22	3:D:185:VAL:HG12	1.66	0.76
1:m:47:GLN:HB3	1:m:51:LEU:HD12	1.67	0.76
7:S:392:VAL:HG22	5:U:28:ARG:HH12	1.51	0.76
14:e:116:VAL:HG23	14:e:158:LEU:HB3	1.67	0.75
1:m:433:PHE:O	1:m:448:MET:HA	1.88	0.74
3:B:394:GLU:HG2	3:B:441:ASN:HD22	1.52	0.74
4:R:821:CYS:HA	4:R:824:LEU:HB2	1.68	0.74
1:m:55:ARG:HH12	1:m:108:ARG:HD3	1.53	0.73
14:e:948:PHE:HA	14:e:976:VAL:O	1.88	0.73
12:c:1:MET:HE3	12:c:3:LEU:H	1.52	0.73
15:h:90:GLN:HA	15:h:93:LEU:HG	1.68	0.73
16:n:50:GLN:O	16:n:54:LEU:HB2	1.89	0.73
2:p:233:PRO:HD2	2:p:257:ILE:HD11	1.71	0.72
7:P:675:LEU:HD11	8:Q:261:LEU:HD22	1.70	0.72
7:S:1120:GLY:HA2	7:S:1147:ASP:O	1.90	0.72
7:S:462:THR:HG21	7:S:601:GLY:HA3	1.71	0.72

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:p:39:ASP:HB3	2:p:66:TRP:HD1	1.54	0.72
4:R:574:ASN:HA	4:R:600:SER:O	1.88	0.72
5:U:52:TRP:HD1	5:U:56:ARG:HH22	1.36	0.72
4:R:582:ASP:HA	4:R:585:VAL:HG12	1.71	0.71
3:G:294:ILE:HG21	3:G:422:LEU:HD12	1.70	0.71
3:E:116:ILE:HA	3:E:184:THR:O	1.90	0.71
3:I:89:ASP:HB2	3:I:111:LEU:O	1.90	0.71
3:E:114:ILE:HG22	3:E:187:GLY:HA3	1.72	0.71
2:p:214:ASN:HB3	2:p:228:ARG:HD3	1.73	0.71
10:W:62:ARG:NH1	10:W:127:CYS:SG	2.64	0.71
3:D:18:LEU:HA	3:D:112:THR:O	1.90	0.70
7:S:874:MET:HE2	7:S:906:LEU:HB2	1.73	0.70
14:e:136:ILE:HD11	14:e:151:LEU:HD21	1.71	0.70
14:e:534:MET:HE3	14:e:570:VAL:HG11	1.72	0.70
14:e:954:LYS:O	14:e:958:LYS:HB2	1.90	0.70
13:d:8:MET:N	13:d:8:MET:SD	2.63	0.70
3:D:480:ASP:HB3	3:D:485:GLN:HE21	1.55	0.70
14:f:318:CYS:SG	14:f:319:VAL:N	2.64	0.70
3:C:663:CYS:SG	3:C:664:ALA:N	2.64	0.70
14:f:163:SER:HB3	14:f:166:GLU:HG2	1.73	0.70
3:H:37:CYS:HA	3:H:97:CYS:HA	1.72	0.70
4:R:213:PRO:HB2	4:R:216:GLU:HB3	1.73	0.69
2:p:448:ILE:HD11	2:p:458:MET:HG2	1.74	0.69
7:P:407:ASN:ND2	7:P:441:CYS:SG	2.65	0.69
8:Q:311:CYS:HB2	8:Q:316:ILE:HG12	1.73	0.69
1:m:107:SER:HB3	1:m:120:ALA:HB3	1.75	0.69
3:A:29:ILE:HG12	3:A:93:VAL:HG11	1.73	0.69
3:I:411:PRO:HD2	3:I:475:PHE:HD2	1.58	0.69
4:R:615:MET:HA	4:R:618:LEU:HB2	1.72	0.69
13:d:489:ARG:HB2	13:d:500:GLN:HA	1.75	0.69
14:e:861:TRP:HA	14:e:889:VAL:HA	1.75	0.69
3:B:294:ILE:HG21	3:B:422:LEU:HD12	1.74	0.69
10:W:186:THR:HA	10:W:415:MET:HE1	1.75	0.69
11:Y:270:ALA:HA	11:Y:377:MET:O	1.92	0.68
3:A:115:GLU:O	3:A:185:VAL:HA	1.92	0.68
10:Z:77:ARG:HH12	10:Z:83:GLN:HA	1.58	0.68
10:Z:132:GLY:HA2	10:Z:163:ILE:O	1.94	0.68
4:R:112:LYS:HD2	17:R:1001:ATP:H3'	1.76	0.68
7:S:827:PRO:O	16:n:455:ARG:NH1	2.27	0.68
14:f:965:LEU:HD13	14:f:977:ILE:HG21	1.76	0.68
3:H:586:ASN:HD21	13:b:508:ASN:H	1.42	0.68

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:562:LYS:HE3	3:B:5:ASN:HB3	1.76	0.68
8:Q:403:LEU:HD22	8:Q:413:ILE:HG12	1.76	0.68
8:T:399:GLU:HB3	8:T:401:MET:HE2	1.76	0.68
3:E:559:THR:HA	3:F:4:GLN:HE22	1.59	0.68
14:f:104:TRP:HD1	14:f:110:TYR:HB2	1.58	0.68
13:b:720:VAL:HB	13:b:723:PRO:HB3	1.76	0.67
15:l:136:ARG:HA	15:l:141:ILE:HB	1.76	0.67
5:U:78:VAL:HG22	5:U:89:ILE:HG12	1.75	0.67
11:Y:271:THR:O	11:Y:376:CYS:HA	1.94	0.67
11:Y:98:ASP:OD1	10:Z:2:ARG:NH2	2.28	0.67
14:f:118:TYR:HA	14:f:160:ILE:HB	1.76	0.67
16:n:250:TRP:NE1	16:n:300:ASP:OD1	2.23	0.67
4:R:756:LEU:HD23	4:R:782:CYS:HB3	1.77	0.67
3:G:97:CYS:HB2	3:G:103:PRO:HA	1.76	0.67
3:B:605:MET:HE1	3:B:620:PRO:HG3	1.75	0.67
3:C:29:ILE:O	3:C:33:ALA:HB2	1.94	0.67
3:G:445:ARG:HE	3:G:449:TYR:HE1	1.43	0.67
1:m:174:LEU:HD22	1:m:223:LEU:HD13	1.76	0.67
11:Y:240:ALA:O	11:Y:244:PHE:HB2	1.95	0.67
3:D:93:VAL:HB	3:D:107:ALA:HB3	1.76	0.66
10:Z:4:ILE:HD12	10:Z:134:GLN:HE21	1.60	0.66
14:f:936:CYS:HB3	14:f:940:ARG:HH12	1.59	0.66
10:W:46:ARG:HH22	10:W:248:ALA:HB1	1.60	0.66
13:b:140:ARG:H	13:b:199:ASN:HB3	1.61	0.66
13:d:243:ARG:HG2	13:d:245:THR:HG22	1.77	0.66
3:H:657:ALA:HA	13:b:457:ARG:HH22	1.59	0.66
3:H:157:PRO:HB3	3:H:379:LYS:HE2	1.76	0.66
7:S:1061:ARG:HG3	7:S:1089:SER:HB2	1.77	0.66
14:f:932:ILE:HG21	14:f:961:ILE:HG23	1.76	0.66
1:m:214:ASN:OD1	1:m:230:ASN:ND2	2.29	0.66
11:X:239:THR:OG1	11:X:243:ARG:NH1	2.29	0.66
14:f:948:PHE:HB3	14:f:982:PRO:HG3	1.78	0.66
3:K:473:MET:HA	3:K:491:LEU:O	1.96	0.66
10:Z:3:GLU:HB2	10:Z:130:LEU:HD12	1.76	0.66
3:C:42:ILE:HD12	3:C:50:ILE:HG21	1.77	0.65
11:X:137:VAL:HG21	11:X:154:MET:HE1	1.77	0.65
3:F:663:CYS:SG	3:F:664:ALA:N	2.68	0.65
1:m:97:PHE:O	1:m:98:GLU:HB2	1.94	0.65
8:T:311:CYS:HB3	8:T:316:ILE:HG12	1.78	0.65
14:e:598:GLU:HA	14:e:601:HIS:CE1	2.31	0.65
10:W:263:LEU:HD21	10:W:421:GLU:HG2	1.79	0.65

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:S:320:LEU:HA	7:S:367:PHE:HB2	1.78	0.65
10:W:252:LYS:NZ	11:X:101:ASN:OD1	2.23	0.65
13:b:728:CYS:HB3	13:b:753:PHE:HD2	1.62	0.65
7:P:410:ASN:HA	7:P:414:ARG:HB2	1.78	0.64
12:c:55:HIS:HB2	12:c:66:LYS:HB2	1.78	0.64
16:n:379:GLN:HE22	16:n:419:LEU:H	1.44	0.64
15:l:4:ILE:HG21	15:l:21:ALA:HB2	1.78	0.64
3:A:114:ILE:HG22	3:A:187:GLY:HA3	1.78	0.64
3:F:42:ILE:HG12	3:F:50:ILE:HG12	1.78	0.64
3:F:399:ALA:O	3:F:438:ARG:NH1	2.31	0.64
3:I:465:MET:HG2	3:I:599:ARG:HG3	1.79	0.64
4:R:777:LEU:HD22	4:R:802:LEU:HD11	1.78	0.64
10:Z:392:LYS:HD3	10:Z:395:LEU:HB3	1.79	0.64
14:f:264:ARG:NH1	14:f:433:CYS:SG	2.69	0.64
2:p:238:GLU:OE2	2:p:251:ASN:ND2	2.29	0.64
3:C:473:MET:HA	3:C:491:LEU:O	1.97	0.64
4:R:125:PHE:HD1	4:R:126:ILE:H	1.42	0.64
13:d:241:ARG:HB2	13:d:252:TYR:HB2	1.80	0.64
2:p:342:TYR:O	2:p:345:ARG:NH2	2.31	0.64
11:X:3:GLU:HA	11:X:51:THR:HG23	1.80	0.64
11:X:269:LEU:HD13	11:X:303:VAL:HG12	1.78	0.64
11:Y:188:ILE:HD12	11:Y:425:MET:HG3	1.80	0.64
7:S:275:MET:HE3	7:S:318:ARG:HG3	1.79	0.64
13:b:152:VAL:HA	13:b:182:VAL:HG12	1.80	0.64
3:I:514:THR:HA	3:I:533:THR:HA	1.79	0.64
13:d:38:VAL:HG21	13:d:71:LEU:HD21	1.80	0.64
2:p:76:GLN:HG2	2:p:111:LEU:HD12	1.80	0.64
13:d:257:LEU:H	13:d:261:SER:HB2	1.62	0.64
14:e:932:ILE:HD13	14:e:935:LEU:HD13	1.80	0.64
1:m:192:CYS:HA	1:m:210:ASP:HA	1.80	0.63
3:C:47:ARG:HG3	3:C:81:ALA:HB3	1.80	0.63
10:Z:1:MET:HE3	10:Z:2:ARG:H	1.63	0.63
3:A:40:PHE:HA	3:A:95:TYR:HA	1.80	0.63
3:A:118:LEU:HD21	3:A:265:LEU:HB3	1.79	0.63
14:f:936:CYS:HA	14:f:939:LEU:HB2	1.81	0.63
1:m:347:GLU:HG3	1:m:348:TRP:CD1	2.33	0.63
5:U:52:TRP:CD1	5:U:56:ARG:HH22	2.15	0.63
1:m:305:THR:HG21	1:m:311:THR:HA	1.80	0.63
5:U:112:HIS:HE2	9:V:71:PRO:HB2	1.63	0.63
1:m:78:HIS:HB2	15:h:160:CYS:HB2	1.80	0.63
2:p:320:LEU:HD22	2:p:327:ILE:HG22	1.80	0.63

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:P:671:GLU:HG3	7:P:697:ALA:HB3	1.79	0.63
15:j:56:LYS:O	15:j:56:LYS:NZ	2.32	0.63
2:p:240:TYR:OH	2:p:288:ARG:NH1	2.32	0.63
11:X:50:ASN:O	11:X:64:ARG:NH2	2.32	0.63
11:Y:53:PHE:HA	11:Y:63:PRO:HA	1.81	0.63
13:d:44:ARG:HB2	13:d:72:LEU:HB3	1.80	0.63
14:f:556:ALA:O	14:f:560:VAL:N	2.30	0.63
3:K:238:GLU:HB2	3:K:241:ARG:HD2	1.81	0.63
10:W:66:VAL:HG12	10:W:91:VAL:HB	1.81	0.63
14:f:840:CYS:HB3	14:f:842:LEU:HD22	1.81	0.63
10:Z:314:ALA:HB3	10:Z:368:ILE:HG13	1.81	0.62
13:b:215:VAL:HG12	13:b:240:CYS:HA	1.79	0.62
14:f:606:LEU:HD21	14:f:629:ASN:HD21	1.64	0.62
15:l:104:ILE:HG22	15:l:119:THR:HB	1.81	0.62
3:F:295:PHE:HB2	3:F:409:VAL:HG11	1.81	0.62
14:f:893:GLY:HA2	14:f:921:ASN:HB3	1.81	0.62
3:C:188:PRO:HG2	3:C:191:ILE:HD11	1.81	0.62
3:H:39:SER:HB3	3:H:96:PHE:HB3	1.80	0.62
3:E:619:LYS:HG2	3:E:648:PHE:HB3	1.81	0.62
4:R:655:GLU:HA	4:R:658:LYS:HB2	1.81	0.62
11:X:308:ARG:HD2	11:X:340:THR:HB	1.82	0.62
14:f:574:ASN:HD22	14:f:577:LEU:HB2	1.64	0.62
1:m:59:GLN:HE21	1:m:61:HIS:HB3	1.63	0.62
3:B:510:TYR:HB3	3:B:625:ILE:HD12	1.80	0.62
3:F:402:ASP:HA	3:F:440:MET:HG3	1.81	0.62
9:V:77:THR:HA	9:V:80:LEU:HD12	1.82	0.62
14:e:734:LYS:HD3	14:e:763:LEU:HB3	1.81	0.62
1:m:101:ALA:HA	1:m:124:VAL:HG22	1.82	0.62
1:m:107:SER:HB2	1:m:161:HIS:HE1	1.65	0.62
2:p:128:ASN:O	2:p:146:GLU:HA	1.99	0.62
3:E:176:GLN:HE21	3:E:359:LYS:HE3	1.63	0.62
7:S:638:VAL:HG13	8:T:249:LYS:HZ3	1.64	0.62
8:T:567:ILE:HG13	8:T:576:VAL:HG12	1.81	0.62
15:l:57:LYS:HB2	15:l:103:LEU:HD21	1.82	0.62
2:p:157:LEU:HB2	2:p:162:ILE:HG12	1.81	0.62
4:R:231:LEU:HD23	4:R:234:MET:HE2	1.82	0.62
1:m:205:ILE:HD12	1:m:207:LEU:HD21	1.81	0.62
3:B:316:PHE:HD1	3:B:649:ILE:HG21	1.65	0.62
3:F:308:CYS:HB2	3:F:665:SER:H	1.63	0.62
3:G:459:LEU:HD12	3:G:469:MET:HE1	1.81	0.62
7:S:225:GLU:HB2	5:U:28:ARG:HG2	1.80	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:b:323:CYS:SG	13:b:327:GLY:N	2.73	0.62
7:S:926:LEU:HB2	7:S:953:CYS:HB3	1.82	0.61
14:e:171:PHE:HE1	14:e:193:SER:HA	1.64	0.61
3:A:134:LYS:NZ	3:A:283:LYS:O	2.34	0.61
7:P:505:MET:HG2	7:P:591:ARG:HD2	1.81	0.61
4:R:149:VAL:O	4:R:275:LEU:HB2	2.00	0.61
13:d:319:ARG:NH2	13:d:343:MET:SD	2.73	0.61
3:A:279:ILE:HD12	3:B:552:LYS:HD2	1.83	0.61
3:I:295:PHE:O	3:I:454:GLN:NE2	2.32	0.61
10:W:293:MET:HB3	10:W:294:PHE:HD2	1.66	0.61
10:Z:170:MET:HB3	10:Z:203:ASP:HA	1.81	0.61
2:p:128:ASN:O	2:p:129:ARG:HB3	2.00	0.61
3:D:130:MET:HE1	3:E:43:ARG:HD3	1.82	0.61
4:R:658:LYS:HE2	4:R:686:ASN:HD21	1.65	0.61
3:B:426:LEU:HD11	3:B:565:LEU:HD21	1.81	0.61
3:G:296:MET:N	3:G:296:MET:SD	2.74	0.61
7:S:747:LYS:HD2	7:S:776:GLN:HG3	1.82	0.61
10:W:141:GLY:O	10:W:145:SER:HB3	2.01	0.61
13:b:308:ARG:HH21	14:e:407:PRO:HD2	1.66	0.61
1:m:287:GLN:HB3	1:m:304:SER:HB2	1.83	0.61
2:p:5:LEU:HB3	2:p:10:LEU:HG	1.83	0.61
4:R:571:GLN:HE21	4:R:597:LYS:HB2	1.66	0.61
10:W:295:ASP:HA	10:W:306:ARG:HH22	1.66	0.61
2:p:214:ASN:HA	2:p:229:LEU:O	2.01	0.61
3:E:135:GLN:NE2	3:F:563:THR:OG1	2.33	0.61
4:R:329:ASN:ND2	4:R:363:CYS:O	2.34	0.61
15:h:85:ILE:HG21	15:h:93:LEU:HD11	1.82	0.61
3:A:23:MET:O	3:A:78:ARG:NH1	2.33	0.61
3:I:309:ARG:HE	3:I:317:VAL:HG11	1.66	0.61
11:Y:100:ALA:HA	10:Z:252:LYS:HE2	1.82	0.61
13:b:326:CYS:SG	13:b:346:HIS:ND1	2.68	0.61
3:F:653:ASP:O	3:F:657:ALA:HB2	2.01	0.60
8:T:453:CYS:HB3	8:T:463:LEU:HB3	1.83	0.60
14:e:626:LEU:HD11	14:e:661:LEU:HD22	1.82	0.60
1:m:443:SER:HA	1:m:460:TYR:O	2.01	0.60
3:D:342:SER:OG	3:D:343:LYS:N	2.31	0.60
11:Y:249:ASN:H	14:f:49:GLY:HA2	1.65	0.60
14:e:599:LEU:O	14:e:629:ASN:ND2	2.33	0.60
14:f:895:GLU:HG2	14:f:923:MET:HB3	1.83	0.60
3:A:347:ASP:OD2	3:A:369:ARG:NH2	2.34	0.60
3:D:430:SER:OG	3:D:432:TYR:O	2.19	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:261:ILE:HG23	3:E:288:PHE:HB2	1.83	0.60
14:e:163:SER:H	14:e:209:ALA:HB3	1.66	0.60
14:f:346:TYR:O	14:f:350:LEU:HB2	2.01	0.60
14:f:832:LEU:HB3	14:f:835:LEU:HD23	1.82	0.60
8:T:297:LEU:HB2	8:T:312:SER:HB2	1.84	0.60
14:e:33:VAL:HG21	14:e:141:PRO:HG3	1.83	0.60
14:f:416:LEU:HA	14:f:419:GLU:HG2	1.84	0.60
3:F:296:MET:N	3:F:296:MET:SD	2.74	0.60
8:Q:453:CYS:SG	8:Q:500:ARG:NH2	2.75	0.60
4:R:234:MET:HE1	4:R:236:TRP:HB3	1.82	0.60
7:S:250:ARG:HH12	7:S:429:ASP:HB3	1.67	0.60
3:E:178:LEU:HD23	3:E:246:TYR:HB3	1.83	0.60
8:T:381:LYS:NZ	8:T:382:CYS:SG	2.74	0.60
8:T:423:ARG:HH12	8:T:457:ARG:HA	1.66	0.60
14:f:671:LEU:HG	14:f:675:ARG:HD2	1.84	0.60
3:I:178:LEU:HD13	3:I:248:GLU:HB2	1.84	0.60
4:R:691:TYR:CE2	4:R:693:ASP:HB2	2.37	0.60
3:C:332:VAL:HA	12:c:81:ASN:HD21	1.66	0.60
3:E:87:ASP:HB3	3:E:110:PHE:HB3	1.82	0.60
2:p:322:LYS:HG3	2:p:327:ILE:HG12	1.83	0.60
3:K:255:PRO:HG3	3:K:446:GLU:HB3	1.84	0.60
4:R:696:CYS:HA	4:R:725:HIS:HB2	1.83	0.60
12:c:74:TYR:HE2	12:c:134:TYR:HA	1.66	0.60
14:e:217:ARG:HG3	14:e:341:MET:HE2	1.82	0.60
14:e:897:CYS:HB2	14:e:899:LEU:HD23	1.84	0.60
14:f:933:LYS:HA	14:f:936:CYS:HB2	1.84	0.60
14:f:949:LEU:HB3	14:f:977:ILE:HG13	1.84	0.60
8:Q:492:HIS:HB2	8:Q:507:ASP:HB3	1.83	0.60
14:e:654:LEU:HD21	14:e:661:LEU:HD23	1.84	0.60
14:e:946:MET:HE2	14:e:975:LEU:HD13	1.84	0.60
14:e:952:ASP:HB3	14:e:955:GLU:HG2	1.84	0.60
15:j:126:MET:O	15:j:130:LYS:NZ	2.35	0.60
1:m:374:ARG:NH1	1:m:377:THR:OG1	2.35	0.59
2:p:14:PHE:HE1	2:p:35:LEU:HB2	1.67	0.59
3:A:514:THR:HA	3:A:533:THR:HA	1.83	0.59
3:I:515:LEU:HG	3:I:623:PRO:HD3	1.84	0.59
4:R:685:GLN:HE22	4:R:713:GLN:HE22	1.50	0.59
4:R:708:CYS:HA	4:R:739:ILE:HD13	1.84	0.59
13:b:503:ASP:HB3	13:b:577:PHE:HB2	1.84	0.59
15:h:158:GLN:HE22	15:h:162:GLU:HB2	1.66	0.59
1:m:424:LYS:HD3	1:m:428:LEU:HB2	1.84	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:297:PRO:HD2	3:C:300:GLN:HE22	1.67	0.59
3:C:407:LEU:HD21	3:C:440:MET:HE1	1.83	0.59
3:D:307:LEU:HD11	3:D:320:VAL:HG11	1.83	0.59
3:B:663:CYS:SG	3:B:664:ALA:N	2.74	0.59
11:Y:264:ARG:HD2	14:f:248:ASP:HB3	1.83	0.59
13:b:212:ASN:ND2	14:e:970:ILE:O	2.36	0.59
1:m:174:LEU:HD21	1:m:220:ILE:HG23	1.83	0.59
4:R:501:PHE:HD2	4:R:557:MET:HB2	1.68	0.59
9:V:51:HIS:ND1	9:V:52:ARG:O	2.35	0.59
13:b:243:ARG:HB3	13:b:250:GLU:HB2	1.83	0.59
11:Y:321:GLY:HA2	11:Y:359:PRO:HA	1.83	0.59
1:m:297:ASP:O	1:m:317:ASP:HA	2.03	0.59
3:B:533:THR:H	3:B:536:GLN:HE21	1.50	0.59
3:E:491:LEU:HD11	3:E:639:LEU:HD21	1.83	0.59
8:Q:431:SER:OG	8:Q:452:ARG:NH1	2.35	0.59
7:S:883:SER:HB2	16:n:155:LYS:HE3	1.83	0.59
1:m:255:ARG:HH21	1:m:287:GLN:HA	1.68	0.59
1:m:326:LYS:HE3	7:S:1079:LEU:HD13	1.85	0.59
3:B:330:GLN:NE2	3:B:331:VAL:O	2.36	0.59
3:D:1:MET:SD	3:D:1:MET:N	2.65	0.59
3:F:102:VAL:HG22	3:F:103:PRO:HD2	1.84	0.59
4:R:372:THR:OG1	4:R:511:LYS:NZ	2.36	0.59
4:R:460:ILE:HD12	4:R:512:LEU:HD11	1.84	0.59
14:f:695:SER:HA	14:f:723:LEU:HA	1.83	0.59
15:l:112:ILE:HG12	15:l:115:LEU:H	1.68	0.59
3:I:100:GLN:HG3	3:I:103:PRO:HD3	1.85	0.59
4:R:691:TYR:HD1	4:R:720:LYS:HE3	1.68	0.59
4:R:719:GLU:HG3	4:R:747:LYS:HE2	1.84	0.59
11:Y:25:CYS:HA	11:Y:30:ILE:HD12	1.85	0.59
13:d:152:VAL:HA	13:d:182:VAL:HG12	1.84	0.59
14:f:921:ASN:HA	14:f:950:ALA:HB3	1.84	0.59
2:p:311:LYS:NZ	2:p:346:PRO:O	2.36	0.59
3:E:48:ILE:HD11	3:E:111:LEU:HD11	1.85	0.59
3:H:660:GLY:O	13:b:508:ASN:ND2	2.35	0.59
3:I:431:PHE:HZ	3:I:560:LEU:HD22	1.67	0.59
7:P:612:GLU:HG2	7:P:619:VAL:H	1.66	0.59
10:Z:249:ASP:HB3	10:Z:252:LYS:HG3	1.84	0.59
14:f:483:GLN:OE1	14:f:511:ARG:NH1	2.36	0.59
14:f:542:LEU:O	14:f:546:LEU:HB2	2.03	0.59
13:b:44:ARG:HD3	13:b:72:LEU:HD22	1.85	0.59
14:e:251:TRP:HZ2	14:e:282:LEU:HB3	1.68	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:302:GLU:OE2	4:R:327:ARG:NH2	2.36	0.58
13:d:38:VAL:O	13:d:43:GLN:NE2	2.36	0.58
13:d:674:GLN:NE2	13:d:700:TYR:OH	2.36	0.58
16:n:453:ASN:HB3	16:n:456:ASN:HB2	1.85	0.58
1:m:411:GLU:OE1	1:m:417:ARG:NH2	2.36	0.58
3:D:323:LEU:HG	3:D:611:LEU:HD23	1.85	0.58
3:G:116:ILE:HD12	3:G:267:LEU:HD22	1.85	0.58
3:I:235:PRO:HG2	3:I:237:PHE:CE1	2.38	0.58
7:S:250:ARG:O	7:S:255:LYS:NZ	2.36	0.58
11:X:105:ARG:HG3	11:X:411:GLU:HG3	1.85	0.58
14:e:801:ARG:HD3	14:e:829:HIS:HB2	1.84	0.58
2:p:99:ILE:HA	2:p:454:PRO:HG3	1.83	0.58
3:A:23:MET:SD	3:A:23:MET:N	2.77	0.58
3:C:138:LYS:NZ	3:D:564:GLU:OE2	2.36	0.58
3:I:468:HIS:HB2	3:I:471:GLN:HG3	1.85	0.58
4:R:242:GLU:HA	4:R:245:LEU:HB2	1.85	0.58
11:X:377:MET:SD	11:X:379:SER:OG	2.58	0.58
11:Y:238:ILE:HG21	11:Y:378:LEU:HD21	1.85	0.58
15:j:5:LYS:HD2	15:j:15:GLU:HG3	1.84	0.58
3:D:529:ARG:NH1	3:D:580:CYS:SG	2.76	0.58
3:G:295:PHE:HB3	3:G:409:VAL:HG21	1.85	0.58
13:d:237:VAL:HG12	13:d:255:ILE:HA	1.86	0.58
3:D:144:MET:SD	3:D:144:MET:N	2.72	0.58
14:f:633:THR:HB	14:f:662:ARG:HG2	1.85	0.58
4:R:312:LEU:O	4:R:314:GLN:NE2	2.36	0.58
3:E:3:PHE:HZ	3:E:7:LEU:HA	1.69	0.58
3:E:412:PRO:HG3	3:E:673:PHE:HZ	1.69	0.58
3:I:87:ASP:H	3:I:112:THR:HG22	1.69	0.58
10:Z:234:SER:O	10:Z:241:ARG:NH2	2.34	0.58
13:d:224:ASN:ND2	13:d:226:ASP:OD1	2.37	0.58
13:d:246:ARG:HD3	14:f:465:ALA:HB1	1.85	0.58
14:f:539:ARG:HB3	14:f:541:ASP:H	1.69	0.58
7:P:328:ASP:N	7:P:328:ASP:OD1	2.37	0.58
10:W:323:MET:HA	10:W:326:VAL:HG22	1.86	0.58
14:e:340:THR:HB	14:e:342:LYS:HE3	1.86	0.58
7:P:237:GLN:HG2	7:P:239:THR:H	1.67	0.58
4:R:279:PRO:HA	4:R:282:PHE:HB3	1.84	0.58
4:R:772:CYS:SG	4:R:799:ASN:ND2	2.76	0.58
13:b:228:PRO:HB2	13:b:229:ARG:HH21	1.69	0.58
14:e:776:GLN:HA	14:e:803:LEU:HA	1.86	0.58
14:e:896:ASN:HB3	14:e:924:LYS:HB2	1.86	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:f:665:ARG:NH1	14:f:991:ASN:O	2.37	0.58
14:f:861:TRP:HA	14:f:889:VAL:HA	1.84	0.58
1:m:231:VAL:HG11	1:m:250:LEU:HD12	1.84	0.58
2:p:105:TYR:O	2:p:156:THR:OG1	2.21	0.58
3:B:532:LYS:HG2	3:B:536:GLN:HG3	1.85	0.58
3:C:346:GLN:HA	3:C:667:ILE:HD11	1.85	0.58
3:F:494:SER:HB2	3:F:574:LEU:HD22	1.85	0.58
3:F:515:LEU:HD11	3:F:537:ILE:HD11	1.85	0.58
3:G:116:ILE:HD13	3:G:197:LEU:HD21	1.85	0.58
13:b:542:ASN:ND2	13:b:557:ASN:OD1	2.37	0.58
14:e:751:LEU:HD12	14:e:754:ASN:HB2	1.85	0.58
1:m:365:LEU:HB3	1:m:378:PHE:HB2	1.86	0.57
3:F:491:LEU:HB2	3:F:606:LEU:HD21	1.86	0.57
3:I:501:LEU:HD11	3:I:634:LYS:HG2	1.86	0.57
5:N:126:VAL:HG21	6:O:69:LEU:HD21	1.86	0.57
11:Y:98:ASP:O	11:Y:105:ARG:NH2	2.37	0.57
10:Z:207:LEU:HB3	10:Z:225:LEU:HD23	1.86	0.57
1:m:108:ARG:NH2	1:m:439:CYS:O	2.36	0.57
2:p:42:TRP:CE2	2:p:67:LYS:HG3	2.39	0.57
3:A:489:ARG:NH2	3:A:570:LYS:O	2.36	0.57
3:B:438:ARG:NH2	3:B:464:LEU:O	2.37	0.57
3:H:546:GLN:HG2	3:H:581:LEU:HD12	1.85	0.57
6:O:92:PRO:HA	6:O:95:ARG:HE	1.68	0.57
11:X:311:LYS:HB2	11:X:344:VAL:HG12	1.86	0.57
12:c:37:ILE:HG23	12:c:50:PHE:HB2	1.86	0.57
14:f:234:SER:O	14:f:238:ARG:HB2	2.04	0.57
14:f:457:MET:N	14:f:457:MET:SD	2.77	0.57
16:n:208:ILE:HD13	16:n:271:LEU:HD21	1.85	0.57
16:n:225:ASP:N	16:n:225:ASP:OD1	2.36	0.57
3:A:478:THR:HG22	3:A:642:LEU:HB3	1.86	0.57
3:I:543:PHE:HZ	3:I:578:LEU:HB3	1.69	0.57
10:W:130:LEU:O	10:W:162:ARG:NE	2.37	0.57
11:X:35:GLN:OE1	11:X:60:LYS:N	2.37	0.57
15:j:67:ASP:OD1	15:j:67:ASP:N	2.37	0.57
3:H:125:ASP:OD2	3:I:43:ARG:NH2	2.37	0.57
4:R:332:LEU:HD13	4:R:335:ILE:HD11	1.87	0.57
11:Y:310:GLY:HA3	11:Y:383:ALA:HB2	1.86	0.57
14:e:834:GLU:OE2	14:e:861:TRP:NE1	2.37	0.57
14:f:908:LEU:HB3	14:f:935:LEU:HA	1.84	0.57
1:m:260:LYS:HG2	1:m:280:ASP:OD2	2.05	0.57
3:A:91:VAL:O	3:A:108:VAL:HA	2.04	0.57

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:453:VAL:HG12	3:A:454:GLN:HG3	1.86	0.57
3:A:529:ARG:NH2	3:A:580:CYS:SG	2.77	0.57
3:B:308:CYS:HA	3:B:334:VAL:HG22	1.85	0.57
3:G:209:THR:HB	3:G:261:ILE:HD13	1.86	0.57
3:G:397:ARG:HG2	3:G:591:GLN:HG2	1.85	0.57
4:R:131:ASP:HB3	4:R:175:VAL:HB	1.86	0.57
14:e:257:TYR:HD1	14:e:550:GLU:HB3	1.70	0.57
3:G:478:THR:OG1	3:G:480:ASP:OD1	2.23	0.57
3:K:8:SER:HB3	3:K:31:LYS:HG2	1.86	0.57
4:M:49:ALA:HB1	4:M:53:ASP:HB3	1.86	0.57
14:e:451:PHE:HB3	14:e:453:LEU:HD13	1.85	0.57
3:B:11:LEU:HD23	3:B:12:VAL:HG23	1.86	0.57
3:C:47:ARG:NH1	3:C:88:GLU:OE1	2.36	0.57
3:G:408:MET:HE1	3:G:473:MET:HG2	1.86	0.57
7:P:702:ILE:H	7:P:754:SER:HB3	1.68	0.57
7:P:773:CYS:SG	7:P:799:ASN:ND2	2.77	0.57
4:R:127:GLN:HE22	4:R:174:LEU:HD12	1.70	0.57
7:S:628:GLN:HE21	7:S:661:PHE:HD1	1.51	0.57
8:T:556:CYS:SG	8:T:557:PHE:N	2.77	0.57
11:X:309:HIS:O	11:X:311:LYS:NZ	2.36	0.57
14:f:404:GLN:NE2	14:f:405:ASP:O	2.37	0.57
3:A:93:VAL:O	3:A:106:THR:HA	2.04	0.57
3:C:306:TYR:O	3:C:666:ALA:HA	2.05	0.57
7:P:866:LYS:HD3	8:Q:273:TRP:HD1	1.70	0.57
7:P:1120:GLY:HA2	7:P:1147:ASP:O	2.05	0.57
8:Q:302:SER:HB2	8:Q:351:LEU:HD21	1.87	0.57
13:b:440:GLN:NE2	13:b:610:GLN:O	2.37	0.57
13:b:741:PHE:O	13:b:744:GLN:NE2	2.37	0.57
14:e:239:MET:SD	14:e:260:ARG:NE	2.76	0.57
1:m:80:LYS:NZ	1:m:439:CYS:SG	2.72	0.57
2:p:219:ARG:HB2	2:p:224:TYR:H	1.70	0.57
3:F:177:ASN:HA	3:F:359:LYS:HD2	1.86	0.57
7:P:266:TRP:NE1	7:P:276:SER:O	2.36	0.57
7:P:1045:VAL:HG21	7:P:1069:LEU:HD11	1.86	0.57
4:R:364:ARG:NH2	4:R:558:GLU:OE1	2.37	0.57
11:Y:200:CYS:H	11:Y:266:HIS:HB2	1.70	0.57
13:b:135:GLU:HG2	13:b:137:VAL:HG13	1.87	0.57
13:d:138:ASP:OD2	13:d:298:ARG:NH2	2.33	0.57
1:m:96:ALA:HB1	1:m:99:PHE:HD2	1.70	0.57
1:m:70:PHE:O	1:m:74:THR:OG1	2.19	0.56
2:p:40:VAL:HG13	2:p:43:ARG:HH21	1.70	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:93:VAL:HG12	3:A:107:ALA:HB3	1.87	0.56
3:A:269:GLU:HB3	3:A:279:ILE:HB	1.86	0.56
3:C:312:GLN:OE1	13:d:448:ARG:NH2	2.38	0.56
3:E:135:GLN:HA	3:E:138:LYS:HE2	1.86	0.56
5:N:91:ILE:HD12	5:N:101:MET:HG2	1.85	0.56
13:d:228:PRO:HG2	14:f:406:TYR:HD2	1.70	0.56
13:d:586:ARG:NH2	13:d:588:ASP:OD2	2.38	0.56
1:m:402:GLY:HA2	1:m:434:ILE:HD11	1.86	0.56
3:F:480:ASP:OD1	3:F:480:ASP:N	2.37	0.56
13:b:552:ALA:O	14:e:323:ASN:ND2	2.38	0.56
14:e:779:VAL:HG11	14:e:989:TRP:HE1	1.70	0.56
1:m:193:GLN:NE2	1:m:236:ILE:O	2.38	0.56
3:F:485:GLN:HG3	3:F:570:LYS:HD3	1.88	0.56
3:H:154:ASN:HB2	3:H:248:GLU:OE1	2.05	0.56
3:H:663:CYS:SG	3:H:664:ALA:N	2.78	0.56
3:I:676:LYS:HB2	3:I:679:LYS:HB2	1.88	0.56
3:K:261:ILE:HG22	3:K:288:PHE:HB2	1.87	0.56
8:Q:493:CYS:HB3	8:Q:505:THR:HG22	1.88	0.56
4:R:729:SER:OG	4:R:732:ASP:OD1	2.24	0.56
11:X:210:TYR:HE1	11:X:222:PRO:HD2	1.70	0.56
13:b:241:ARG:HB3	13:b:252:TYR:HB2	1.87	0.56
13:b:462:ALA:N	13:b:516:ASN:OD1	2.35	0.56
13:d:138:ASP:HA	13:d:149:GLU:HA	1.86	0.56
14:f:44:LYS:HZ1	14:f:374:GLU:HA	1.71	0.56
14:f:809:GLY:O	14:f:811:ASN:ND2	2.38	0.56
14:f:826:GLN:HG3	14:f:853:VAL:HG12	1.88	0.56
3:A:492:LEU:HD22	3:A:554:ILE:HD11	1.87	0.56
2:p:283:PHE:HE2	2:p:314:ILE:HG12	1.71	0.56
3:D:43:ARG:NH2	3:E:131:PRO:O	2.38	0.56
3:E:514:THR:HA	3:E:533:THR:HA	1.87	0.56
3:I:463:TRP:CD1	3:I:553:CYS:HG	2.24	0.56
7:P:285:GLU:OE1	7:P:539:ASN:ND2	2.38	0.56
7:P:708:VAL:HG22	7:P:710:ASN:H	1.71	0.56
7:P:837:ASP:OD1	7:P:863:SER:OG	2.22	0.56
7:S:320:LEU:C	7:S:367:PHE:O	2.48	0.56
10:W:110:ALA:HA	10:W:113:VAL:HG12	1.85	0.56
11:Y:14:VAL:HG22	11:Y:67:PHE:HB3	1.87	0.56
14:f:883:ARG:NH1	14:f:913:ASN:OD1	2.39	0.56
2:p:25:VAL:HA	2:p:28:VAL:HG23	1.86	0.56
2:p:428:LEU:H	2:p:456:PHE:HZ	1.52	0.56
3:H:48:ILE:HD11	3:H:89:ASP:HB3	1.87	0.56

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:P:362:LEU:HD23	7:P:363:LEU:HD23	1.86	0.56
4:R:414:LYS:HA	4:R:417:LEU:HD12	1.87	0.56
11:X:319:TYR:HB3	11:X:323:VAL:HG21	1.88	0.56
13:b:57:THR:OG1	13:b:58:LEU:N	2.38	0.56
14:e:948:PHE:HD1	14:e:976:VAL:HG23	1.69	0.56
14:f:83:VAL:HG13	14:f:226:GLN:HG3	1.86	0.56
14:f:531:LEU:H	14:f:574:ASN:HD21	1.54	0.56
14:f:717:SER:HA	14:f:745:ARG:HG3	1.86	0.56
16:n:102:ILE:HD13	16:n:130:MET:HE3	1.86	0.56
15:j:89:ASP:O	15:j:93:LEU:HB2	2.06	0.56
3:C:558:ARG:HH12	3:C:574:LEU:HD21	1.70	0.56
3:I:227:PRO:O	3:I:228:ASN:ND2	2.39	0.56
7:P:338:MET:HE1	7:P:340:LEU:HB2	1.87	0.56
11:Y:53:PHE:HD1	11:Y:61:HIS:HB2	1.71	0.56
11:Y:306:ASP:HB3	11:Y:309:HIS:HB2	1.87	0.56
13:b:278:GLU:HB3	13:b:283:ARG:HG3	1.88	0.56
13:d:47:TYR:HB3	13:d:52:MET:HE1	1.88	0.56
2:p:217:ILE:HD12	2:p:227:THR:HB	1.88	0.56
3:C:216:ARG:HD2	3:C:241:ARG:HH11	1.69	0.56
3:C:445:ARG:NH1	3:C:458:GLU:OE2	2.39	0.56
3:D:1:MET:HE2	3:D:267:LEU:HD12	1.87	0.56
7:P:319:LEU:HD22	7:P:367:PHE:H	1.70	0.56
7:S:411:GLU:N	7:S:411:GLU:OE1	2.38	0.56
7:S:898:LEU:HB2	7:S:924:ASN:HB3	1.87	0.56
13:b:336:LEU:HD22	13:b:363:TRP:HE3	1.71	0.56
14:f:924:LYS:H	14:f:952:ASP:HB3	1.70	0.56
6:O:46:VAL:O	6:O:84:ALA:HB3	2.06	0.56
8:Q:254:LEU:HD23	8:Q:288:ARG:HH12	1.71	0.56
7:S:378:GLU:HA	7:S:381:LYS:HE2	1.88	0.56
5:U:100:ARG:NH1	9:V:45:ASP:O	2.38	0.56
11:X:223:THR:H	11:X:226:ASN:HD22	1.52	0.56
13:d:33:GLU:HG3	13:d:40:PRO:HD3	1.88	0.56
13:d:228:PRO:HG2	14:f:406:TYR:CD2	2.41	0.56
13:d:249:ARG:HE	13:d:271:VAL:HG21	1.71	0.56
3:B:254:SER:H	3:B:257:PHE:HB3	1.71	0.56
3:D:87:ASP:H	3:D:112:THR:HB	1.71	0.56
3:E:309:ARG:HG3	3:E:317:VAL:HG11	1.88	0.56
3:F:529:ARG:NH2	3:F:600:PRO:O	2.38	0.56
7:P:1110:GLN:HB3	7:P:1137:VAL:HG22	1.88	0.56
12:c:64:PRO:O	12:c:66:LYS:NZ	2.39	0.56
2:p:367:LEU:HD13	2:p:376:GLN:HB3	1.87	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:234:LEU:HD12	3:E:235:PRO:HD2	1.88	0.55
4:R:927:GLU:HA	4:R:930:ARG:HG2	1.87	0.55
5:U:30:ARG:HD3	5:U:75:LEU:HB3	1.87	0.55
13:b:541:ARG:NH1	13:b:560:ASP:OD2	2.38	0.55
14:e:66:LEU:HA	14:e:69:ILE:HD12	1.88	0.55
3:A:95:TYR:OH	3:A:101:GLU:O	2.23	0.55
3:B:37:CYS:HA	3:B:97:CYS:HA	1.88	0.55
3:D:294:ILE:HG12	3:D:422:LEU:HD13	1.86	0.55
11:X:2:ARG:HH22	11:X:249:ASN:HB2	1.72	0.55
11:Y:221:ARG:HE	10:Z:324:LYS:HB2	1.71	0.55
14:f:663:VAL:HG22	14:f:691:PHE:HB2	1.89	0.55
7:P:653:LEU:HD12	7:P:666:LEU:HD23	1.88	0.55
7:S:859:LEU:HD21	7:S:862:LEU:HD13	1.88	0.55
7:S:872:LYS:HA	7:S:875:ILE:HD12	1.88	0.55
11:X:213:CYS:HA	11:X:217:LEU:HB2	1.88	0.55
13:d:323:CYS:SG	13:d:327:GLY:N	2.80	0.55
3:K:605:MET:HE2	3:K:620:PRO:HB3	1.88	0.55
7:P:250:ARG:O	7:P:255:LYS:NZ	2.39	0.55
4:R:190:ASP:N	4:R:190:ASP:OD1	2.38	0.55
7:S:922:SER:OG	7:S:923:ASN:ND2	2.40	0.55
7:S:1102:MET:HG3	7:S:1130:VAL:HG21	1.89	0.55
13:b:466:VAL:HG22	13:b:540:VAL:HB	1.89	0.55
12:c:1:MET:HB3	12:c:4:LYS:HE2	1.87	0.55
3:H:121:ASP:OD1	3:H:121:ASP:N	2.39	0.55
8:Q:288:ARG:HH21	8:Q:324:GLN:HA	1.71	0.55
8:T:566:ILE:HG13	8:T:579:ILE:HD11	1.89	0.55
10:Z:164:MET:O	10:Z:196:THR:OG1	2.24	0.55
14:f:862:SER:HA	14:f:891:ARG:HB2	1.89	0.55
16:n:257:HIS:HB3	16:n:260:ILE:HB	1.88	0.55
3:G:402:ASP:HA	3:G:440:MET:HG3	1.89	0.55
3:H:43:ARG:HH21	3:I:123:TYR:HB2	1.72	0.55
4:R:150:PHE:HE1	4:R:277:THR:HB	1.71	0.55
12:c:6:ILE:HB	12:c:30:MET:HE1	1.87	0.55
13:d:8:MET:HG2	14:f:177:ALA:HB1	1.88	0.55
14:e:514:GLU:HG3	14:e:516:PRO:HD2	1.88	0.55
3:G:416:GLN:NE2	3:H:135:GLN:OE1	2.40	0.55
3:H:42:ILE:HD13	3:H:52:ILE:HD11	1.89	0.55
3:I:490:LEU:HD23	3:I:572:ILE:HG12	1.89	0.55
11:Y:288:VAL:O	11:Y:292:THR:HG23	2.07	0.55
3:B:294:ILE:HG12	3:B:453:VAL:HG11	1.88	0.55
3:K:617:ILE:O	3:K:648:PHE:HA	2.07	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:N:77:THR:OG1	5:N:90:THR:OG1	2.20	0.55
7:P:1090:LEU:O	7:P:1119:ILE:HA	2.07	0.55
7:S:329:MET:HA	7:S:332:VAL:HG12	1.88	0.55
13:b:551:TYR:O	13:b:558:ARG:NH2	2.40	0.55
13:d:518:HIS:CE1	13:d:533:GLN:HG3	2.42	0.55
14:f:683:LEU:HA	14:f:686:ASN:HB2	1.87	0.55
16:n:434:GLN:NE2	16:n:452:ARG:O	2.39	0.55
3:C:218:SER:OG	3:C:219:SER:N	2.37	0.55
3:C:589:SER:HB3	13:d:523:GLU:HG2	1.87	0.55
3:F:401:LEU:HG	3:F:438:ARG:HG2	1.88	0.55
5:N:46:VAL:HG22	5:N:90:THR:HG22	1.89	0.55
14:f:808:LEU:HD11	14:f:813:LEU:HD22	1.88	0.55
14:f:892:LEU:HD11	14:f:920:MET:HB3	1.87	0.55
1:m:151:ILE:HA	1:m:167:ASP:HA	1.88	0.55
2:p:76:GLN:NE2	2:p:111:LEU:O	2.39	0.55
3:B:145:ASN:O	3:C:66:TRP:NE1	2.40	0.55
3:G:583:GLN:HE21	3:G:594:THR:HA	1.72	0.55
3:I:629:CYS:HB3	3:I:632:GLU:HB2	1.88	0.55
10:Z:113:VAL:HA	10:Z:116:VAL:HG22	1.88	0.55
13:b:21:ARG:NH1	13:b:320:LYS:O	2.40	0.55
14:e:490:TYR:O	14:e:493:GLN:NE2	2.39	0.55
14:f:238:ARG:NH1	14:f:266:PHE:O	2.38	0.55
2:p:164:VAL:HG22	2:p:174:LEU:HG	1.88	0.54
2:p:402:GLY:HA2	2:p:424:TYR:CE2	2.42	0.54
3:D:50:ILE:HG12	3:D:77:VAL:HG12	1.88	0.54
4:R:719:GLU:HB2	4:R:747:LYS:HG3	1.89	0.54
14:f:892:LEU:HD23	14:f:917:VAL:HG11	1.89	0.54
3:A:198:ILE:HG22	3:A:233:LEU:HA	1.88	0.54
3:C:91:VAL:HB	3:C:109:LEU:HB3	1.88	0.54
3:E:41:THR:OG1	3:E:94:SER:OG	2.24	0.54
3:H:122:ILE:HD13	3:H:137:LYS:HG2	1.89	0.54
3:K:568:GLU:OE2	3:K:570:LYS:NZ	2.40	0.54
7:P:359:ARG:HH21	7:P:384:VAL:HA	1.71	0.54
13:b:198:LYS:NZ	13:b:199:ASN:OD1	2.40	0.54
15:j:113:LYS:NZ	15:j:117:ASP:OD2	2.41	0.54
3:C:212:TYR:HB3	3:C:221:TYR:HB3	1.89	0.54
3:D:95:TYR:HB2	3:D:105:ALA:HB3	1.89	0.54
3:G:442:LYS:HA	3:G:445:ARG:HG2	1.88	0.54
3:G:557:ASN:HA	3:G:560:LEU:HD12	1.89	0.54
7:P:287:LYS:HB3	7:P:290:GLU:HG2	1.89	0.54
7:P:698:ILE:HG22	7:P:746:LEU:HD11	1.89	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Q:351:LEU:HD13	8:Q:358:LEU:HD12	1.89	0.54
11:Y:9:VAL:HG12	11:Y:68:VAL:HG22	1.89	0.54
10:Z:68:LEU:HD22	10:Z:95:SER:HB2	1.89	0.54
10:Z:282:ARG:HH21	10:Z:285:THR:HG21	1.71	0.54
12:c:96:ALA:HB2	13:d:714:ILE:HD11	1.89	0.54
13:d:256:ARG:HA	13:d:261:SER:O	2.08	0.54
14:e:512:VAL:HG22	14:e:521:TYR:HD2	1.73	0.54
14:e:513:ASP:OD2	14:e:544:ASN:ND2	2.41	0.54
16:n:222:ARG:HG2	16:n:224:PRO:HD2	1.88	0.54
2:p:3:ILE:HB	15:l:101:PHE:HE1	1.73	0.54
3:D:538:LEU:HD13	3:D:544:ARG:HH12	1.72	0.54
3:E:41:THR:HG22	3:E:66:TRP:HB3	1.90	0.54
3:E:529:ARG:HE	3:E:656:LEU:HD13	1.73	0.54
3:E:663:CYS:SG	3:E:664:ALA:N	2.80	0.54
3:H:400:SER:OG	3:H:402:ASP:OD2	2.24	0.54
3:I:205:GLU:HB3	3:I:261:ILE:HG23	1.89	0.54
4:R:136:LEU:HD22	4:R:147:HIS:HE1	1.72	0.54
7:S:224:PRO:HA	7:S:227:LYS:HD2	1.88	0.54
9:V:50:ARG:O	9:V:52:ARG:NH1	2.40	0.54
12:a:46:GLN:HE22	14:e:445:ARG:HH22	1.55	0.54
14:f:67:GLN:O	14:f:71:ASP:HB3	2.06	0.54
14:f:271:VAL:HB	14:f:274:MET:HG2	1.89	0.54
3:B:459:LEU:HD11	3:B:561:LEU:HD13	1.90	0.54
3:D:489:ARG:NH1	3:D:571:ASP:OD1	2.41	0.54
3:E:474:CYS:SG	3:E:475:PHE:N	2.81	0.54
3:I:311:LEU:HD12	7:S:794:LYS:HB2	1.88	0.54
8:Q:469:SER:HB2	8:Q:487:LEU:HB3	1.88	0.54
4:R:732:ASP:HA	4:R:735:ILE:HD12	1.89	0.54
8:T:370:VAL:HB	8:T:382:CYS:HB2	1.90	0.54
12:a:21:CYS:HA	12:a:37:ILE:HG13	1.90	0.54
13:d:234:TRP:HB2	13:d:298:ARG:HH11	1.72	0.54
13:d:235:TYR:HB2	13:d:237:VAL:HG13	1.90	0.54
14:e:921:ASN:HA	14:e:950:ALA:HB3	1.89	0.54
15:j:4:ILE:HD11	15:j:18:VAL:HG23	1.90	0.54
2:p:435:ASN:HD22	2:p:447:VAL:HG12	1.73	0.54
3:B:49:LEU:HB3	3:B:78:ARG:H	1.73	0.54
3:B:135:GLN:HE22	3:B:138:LYS:HE3	1.73	0.54
3:C:21:VAL:HA	3:C:79:MET:HB2	1.88	0.54
3:C:629:CYS:HB3	3:C:632:GLU:HB2	1.87	0.54
3:D:223:LEU:HD21	3:D:227:PRO:HD2	1.90	0.54
3:I:121:ASP:OD1	3:I:121:ASP:N	2.40	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:663:CYS:SG	3:K:664:ALA:N	2.80	0.54
4:R:668:VAL:HA	4:R:693:ASP:HB3	1.88	0.54
12:c:16:ASP:OD1	12:c:16:ASP:N	2.40	0.54
14:f:273:HIS:HA	14:f:276:GLN:HG2	1.90	0.54
2:p:216:ASN:OD1	2:p:225:HIS:NE2	2.37	0.54
3:G:650:ASP:OD1	3:G:650:ASP:N	2.41	0.54
3:I:489:ARG:NH2	3:I:571:ASP:OD1	2.40	0.54
5:N:28:ARG:HH22	7:P:226:MET:HG2	1.73	0.54
7:P:333:LEU:HD13	7:P:335:HIS:HB3	1.90	0.54
4:R:695:SER:HB2	4:R:724:ALA:HB3	1.90	0.54
4:R:719:GLU:HA	4:R:746:LEU:HA	1.89	0.54
14:f:526:LYS:HG3	14:f:566:ASP:HB3	1.88	0.54
14:f:986:SER:HA	14:f:989:TRP:HB3	1.89	0.54
3:H:6:SER:HB3	3:H:8:SER:H	1.72	0.54
7:P:281:PHE:HB2	7:P:323:ILE:HG23	1.90	0.54
7:P:495:CYS:HB3	7:P:559:TYR:HB2	1.89	0.54
16:n:65:ASP:N	16:n:65:ASP:OD1	2.39	0.54
1:m:11:MET:HE2	1:m:35:LEU:HD23	1.90	0.54
3:F:639:LEU:HD22	3:F:644:LEU:HD21	1.90	0.54
4:R:345:VAL:HA	4:R:369:LEU:HD21	1.90	0.54
12:c:103:LEU:HA	12:c:106:ILE:HD12	1.88	0.54
14:e:198:LYS:NZ	14:e:201:LEU:O	2.41	0.54
16:n:68:THR:OG1	16:n:71:GLN:OE1	2.25	0.54
2:p:40:VAL:HG12	2:p:44:LYS:HE3	1.90	0.54
2:p:210:ASP:OD1	2:p:214:ASN:N	2.41	0.54
7:P:501:GLY:O	7:P:505:MET:HA	2.07	0.54
7:S:839:CYS:O	7:S:867:ASN:ND2	2.40	0.54
5:U:46:VAL:HG22	5:U:90:THR:HG22	1.90	0.54
13:d:204:ALA:HA	13:d:278:GLU:HG3	1.89	0.54
14:f:279:CYS:O	14:f:283:LYS:NZ	2.41	0.54
14:f:804:VAL:HA	14:f:832:LEU:HG	1.88	0.54
15:j:159:TRP:O	15:j:161:GLU:N	2.41	0.54
2:p:39:ASP:HB3	2:p:66:TRP:CD1	2.40	0.53
3:E:605:MET:HA	3:E:618:PRO:HB2	1.90	0.53
7:P:446:LEU:HD11	7:P:471:HIS:CG	2.43	0.53
11:X:101:ASN:HA	11:X:144:GLY:H	1.73	0.53
14:f:483:GLN:HB2	14:f:511:ARG:HH22	1.73	0.53
14:f:690:VAL:O	14:f:718:LEU:HA	2.08	0.53
2:p:26:ALA:HA	2:p:33:ASN:HA	1.89	0.53
3:B:51:HIS:O	3:B:75:ALA:HA	2.08	0.53
3:B:316:PHE:N	3:B:651:ASP:OD1	2.41	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:660:GLY:O	13:d:508:ASN:ND2	2.41	0.53
5:U:93:GLY:O	5:U:98:GLN:NE2	2.42	0.53
12:c:18:PRO:O	13:d:621:ASN:ND2	2.41	0.53
14:e:439:LEU:HA	14:e:457:MET:HE1	1.90	0.53
14:f:842:LEU:HG	14:f:843:THR:HG22	1.88	0.53
3:E:323:LEU:HA	3:E:326:LYS:HD3	1.91	0.53
3:E:460:PHE:HB3	3:E:557:ASN:HD21	1.73	0.53
8:Q:363:TYR:HA	8:Q:390:SER:HB2	1.88	0.53
11:X:9:VAL:HG12	11:X:146:GLY:HA2	1.90	0.53
13:b:747:SER:HA	13:b:754:GLU:HA	1.90	0.53
3:A:307:LEU:HD13	3:A:317:VAL:HG23	1.90	0.53
3:G:581:LEU:HD21	3:H:276:ILE:HG22	1.89	0.53
7:P:947:ARG:HG2	7:P:975:HIS:HB2	1.91	0.53
4:R:479:GLU:HG3	4:R:531:CYS:HB2	1.89	0.53
8:T:335:LEU:HD21	8:T:378:LEU:HD23	1.91	0.53
10:Z:337:ASN:HB3	10:Z:340:TYR:HB2	1.90	0.53
13:b:203:ARG:NH1	13:b:295:PRO:O	2.42	0.53
13:b:221:ALA:HB1	13:b:268:ILE:HG21	1.91	0.53
14:f:43:TYR:HE1	14:f:54:LEU:HD21	1.73	0.53
15:j:150:GLU:HA	15:j:153:VAL:HG12	1.90	0.53
15:l:7:GLN:NE2	15:l:8:SER:O	2.40	0.53
3:A:47:ARG:HH21	3:A:83:SER:HA	1.72	0.53
3:D:182:ASN:HD22	3:D:242:LYS:HE2	1.73	0.53
3:E:319:SER:HA	3:E:322:LYS:HG3	1.90	0.53
3:I:425:VAL:O	3:I:456:PRO:HA	2.09	0.53
5:N:117:LEU:O	5:N:121:VAL:HG22	2.08	0.53
4:R:397:LEU:HD21	4:R:436:LEU:HD21	1.90	0.53
7:S:514:LEU:HD21	7:S:533:LEU:HD11	1.89	0.53
13:d:541:ARG:O	13:d:557:ASN:HA	2.09	0.53
14:f:654:LEU:HB3	14:f:682:ALA:HB1	1.90	0.53
14:f:965:LEU:HB3	14:f:977:ILE:HD13	1.90	0.53
3:B:238:GLU:OE1	3:B:241:ARG:NH1	2.41	0.53
3:D:371:SER:OG	3:D:372:LYS:NZ	2.42	0.53
3:F:581:LEU:HD21	3:F:596:LEU:HD13	1.90	0.53
3:G:558:ARG:HH12	3:G:574:LEU:HD21	1.73	0.53
3:I:70:ASN:O	3:I:73:THR:OG1	2.26	0.53
4:M:50:SER:OG	4:M:51:ARG:N	2.37	0.53
5:U:112:HIS:NE2	9:V:71:PRO:HB2	2.23	0.53
11:Y:396:ASP:OD2	11:Y:422:ARG:NH2	2.41	0.53
14:f:419:GLU:HA	14:f:481:ARG:HE	1.74	0.53
14:f:711:LEU:HD21	14:f:718:LEU:HG	1.91	0.53

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:l:158:GLN:NE2	15:l:159:TRP:O	2.42	0.53
2:p:311:LYS:HE3	2:p:346:PRO:HG2	1.89	0.53
3:I:295:PHE:HB3	3:I:409:VAL:HG21	1.90	0.53
11:Y:8:HIS:ND1	11:Y:13:GLY:O	2.42	0.53
10:Z:46:ARG:HH11	10:Z:49:VAL:HG21	1.73	0.53
13:b:487:GLY:O	13:b:504:GLN:NE2	2.41	0.53
14:f:164:PHE:HB3	14:f:210:THR:HB	1.91	0.53
14:f:609:LEU:O	14:f:635:LEU:HA	2.07	0.53
1:m:186:THR:HG23	1:m:223:LEU:HD23	1.91	0.53
2:p:7:ARG:NH2	2:p:11:MET:SD	2.81	0.53
3:B:114:ILE:HD13	3:B:187:GLY:HA3	1.90	0.53
3:I:327:SER:HB3	3:I:614:ASN:HD21	1.73	0.53
5:U:103:ASN:HD22	9:V:48:GLN:HE22	1.57	0.53
11:X:90:GLU:O	11:X:121:ARG:NH1	2.41	0.53
11:Y:179:THR:HA	10:Z:246:LEU:HD12	1.90	0.53
13:b:150:ALA:HA	13:b:185:ASP:H	1.74	0.53
13:b:179:MET:HA	13:b:195:VAL:O	2.08	0.53
14:e:163:SER:HB2	14:e:166:GLU:HG3	1.89	0.53
14:f:383:HIS:HB2	14:f:386:VAL:HG22	1.90	0.53
16:n:396:PHE:HA	16:n:412:TRP:HB2	1.90	0.53
1:m:341:ASP:OD1	1:m:341:ASP:N	2.38	0.53
3:A:529:ARG:HH21	3:A:601:TYR:HA	1.74	0.53
3:F:44:GLY:HA2	3:F:91:VAL:HG22	1.90	0.53
3:K:48:ILE:HD11	3:K:77:VAL:HB	1.91	0.53
7:S:863:SER:HB2	7:S:892:ILE:HD12	1.91	0.53
11:Y:3:GLU:O	11:Y:133:GLN:N	2.41	0.53
11:Y:132:LEU:HB3	11:Y:164:LYS:NZ	2.24	0.53
3:A:197:LEU:HD12	3:A:265:LEU:HD11	1.91	0.53
3:E:582:GLU:OE2	3:E:599:ARG:NH2	2.41	0.53
7:P:979:THR:HG23	7:P:1008:VAL:HB	1.89	0.53
4:R:403:GLU:HB2	4:R:470:HIS:CE1	2.44	0.53
10:Z:358:PRO:HG3	10:Z:364:SER:HB3	1.91	0.53
14:f:69:ILE:HD11	14:f:228:VAL:HG11	1.91	0.53
14:f:150:VAL:HA	14:f:153:LYS:HE3	1.91	0.53
16:n:217:ASN:ND2	16:n:232:ILE:O	2.41	0.53
15:j:85:ILE:HG23	15:j:89:ASP:HB2	1.91	0.53
15:l:54:ILE:HD12	15:l:106:ALA:HB2	1.91	0.53
3:B:240:ARG:HH12	3:B:242:LYS:HZ2	1.56	0.52
3:B:339:ASN:N	3:B:339:ASN:OD1	2.42	0.52
3:G:127:GLN:OE1	3:G:127:GLN:N	2.42	0.52
3:I:305:VAL:HG22	3:I:668:ILE:HG23	1.92	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:P:923:ASN:HA	7:P:952:HIS:HB3	1.90	0.52
5:U:103:ASN:ND2	9:V:55:SER:HB2	2.24	0.52
13:d:5:VAL:HG21	13:d:32:ILE:HD11	1.91	0.52
14:e:312:PRO:HD2	14:e:319:VAL:HG21	1.91	0.52
14:f:612:ARG:HG2	14:f:638:LYS:HB3	1.90	0.52
14:f:826:GLN:HG2	14:f:856:ASN:HD22	1.72	0.52
1:m:176:ASP:OD2	1:m:179:ASN:ND2	2.39	0.52
2:p:355:ASP:HB3	2:p:370:ILE:HB	1.90	0.52
3:A:546:GLN:HG2	3:A:581:LEU:HD12	1.91	0.52
3:D:459:LEU:HD11	3:D:561:LEU:HD13	1.90	0.52
3:K:127:GLN:NE2	3:K:130:MET:SD	2.82	0.52
4:R:659:TYR:HE1	4:R:661:SER:HB3	1.74	0.52
8:T:560:THR:OG1	8:T:561:GLU:N	2.42	0.52
13:d:735:ASP:N	13:d:735:ASP:OD1	2.40	0.52
14:f:682:ALA:O	14:f:686:ASN:HB2	2.09	0.52
14:f:907:LEU:HB3	14:f:935:LEU:HD21	1.91	0.52
4:R:643:THR:O	4:R:672:VAL:HA	2.10	0.52
7:S:278:VAL:HG22	7:S:320:LEU:HB3	1.90	0.52
7:S:631:VAL:HG21	7:S:653:LEU:HD21	1.91	0.52
13:b:503:ASP:OD1	13:b:503:ASP:N	2.42	0.52
14:e:911:LEU:HD12	14:e:935:LEU:HB3	1.91	0.52
14:f:808:LEU:HB3	14:f:837:LEU:HA	1.90	0.52
1:m:287:GLN:HG3	1:m:288:ARG:HD2	1.92	0.52
3:A:473:MET:HG3	3:A:490:LEU:HD11	1.90	0.52
3:A:630:CYS:HA	3:A:633:GLU:HG3	1.91	0.52
3:B:117:SER:OG	3:B:184:THR:OG1	2.22	0.52
3:D:485:GLN:OE1	3:D:485:GLN:N	2.43	0.52
3:E:1:MET:SD	3:E:1:MET:N	2.74	0.52
4:M:45:LYS:O	4:M:49:ALA:HB2	2.08	0.52
11:Y:251:ASP:HB2	11:Y:254:GLU:HB2	1.92	0.52
11:Y:422:ARG:O	11:Y:422:ARG:NH1	2.39	0.52
14:f:608:LYS:HZ3	14:f:610:ILE:HD11	1.74	0.52
2:p:252:ARG:HB3	2:p:257:ILE:HG21	1.91	0.52
3:B:581:LEU:HG	3:B:596:LEU:HB3	1.90	0.52
3:C:189:THR:HG23	3:C:193:GLN:HE21	1.75	0.52
3:D:619:LYS:HG2	3:D:648:PHE:HB3	1.91	0.52
3:E:603:PRO:HD3	3:E:656:LEU:HD11	1.90	0.52
6:O:88:ILE:HD13	6:O:98:VAL:HG23	1.91	0.52
7:P:395:LEU:O	7:P:400:ARG:NH1	2.43	0.52
10:Z:62:ARG:NH1	10:Z:127:CYS:SG	2.83	0.52
10:Z:323:MET:HA	10:Z:326:VAL:HB	1.91	0.52

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:e:103:GLU:HB3	14:e:109:LEU:HD23	1.92	0.52
14:e:331:CYS:HB3	14:e:394:PHE:HB2	1.91	0.52
14:e:471:GLU:O	14:e:473:ASP:N	2.41	0.52
16:n:208:ILE:HD11	16:n:267:MET:HE1	1.91	0.52
1:m:347:GLU:HG3	1:m:348:TRP:HD1	1.71	0.52
2:p:254:HIS:HB3	2:p:257:ILE:HB	1.92	0.52
3:A:617:ILE:O	3:A:648:PHE:HA	2.09	0.52
3:B:529:ARG:NH2	3:B:600:PRO:O	2.40	0.52
3:E:470:ASP:N	3:E:470:ASP:OD1	2.43	0.52
3:K:226:GLY:H	3:K:229:LYS:HB3	1.75	0.52
4:M:4:PHE:HB3	5:N:64:GLU:HG2	1.90	0.52
4:R:775:GLU:N	4:R:775:GLU:OE2	2.43	0.52
10:W:30:ILE:HD11	10:W:47:ILE:HD11	1.90	0.52
10:W:134:GLN:HA	10:W:165:ASN:O	2.10	0.52
13:d:527:GLU:HG2	13:d:567:LYS:HB3	1.92	0.52
14:e:606:LEU:HD21	14:e:609:LEU:HB2	1.92	0.52
1:m:90:TYR:HB2	1:m:425:ARG:HH11	1.73	0.52
2:p:188:LEU:HD12	2:p:189:ILE:H	1.75	0.52
3:C:117:SER:OG	3:C:184:THR:OG1	2.25	0.52
3:D:491:LEU:HD21	3:D:639:LEU:HD21	1.91	0.52
3:E:188:PRO:O	3:E:192:LEU:HB2	2.09	0.52
11:X:392:ASP:HB2	11:X:425:MET:HE2	1.92	0.52
13:d:456:GLY:HA3	13:d:462:ALA:HA	1.90	0.52
14:f:872:ASP:OD2	14:f:900:THR:OG1	2.28	0.52
1:m:124:VAL:HA	1:m:129:ARG:O	2.09	0.52
3:B:308:CYS:SG	3:B:665:SER:N	2.81	0.52
3:F:211:VAL:HG12	3:F:247:VAL:HG13	1.90	0.52
3:H:211:VAL:N	3:H:225:VAL:O	2.41	0.52
7:P:1141:LYS:HB3	7:P:1143:HIS:CE1	2.44	0.52
10:Z:328:GLU:OE2	10:Z:332:ASN:ND2	2.43	0.52
13:b:175:GLU:O	13:b:198:LYS:N	2.43	0.52
13:d:364:TYR:HB2	13:d:369:ARG:HD3	1.92	0.52
15:h:3:THR:HA	15:h:16:VAL:O	2.10	0.52
16:n:6:PRO:HB3	16:n:34:ASN:HD21	1.74	0.52
3:B:431:PHE:H	3:B:460:PHE:HD2	1.58	0.52
3:C:38:LYS:HB2	3:C:98:PRO:HD3	1.90	0.52
3:D:39:SER:HB2	3:D:96:PHE:HB2	1.90	0.52
3:F:10:SER:HG	3:F:15:THR:HG1	1.58	0.52
3:H:18:LEU:HA	3:H:112:THR:O	2.09	0.52
7:P:315:GLN:HB3	7:P:319:LEU:HD12	1.92	0.52
4:R:470:HIS:CD2	4:R:472:SER:H	2.28	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:X:188:ILE:HD12	11:X:425:MET:HG3	1.92	0.52
10:Z:151:LEU:HD12	10:Z:155:ILE:HD11	1.91	0.52
14:e:568:PHE:HB3	14:e:598:GLU:HG3	1.92	0.52
14:e:734:LYS:HB2	14:e:763:LEU:HD13	1.91	0.52
16:n:448:ILE:HB	16:n:460:LEU:HD11	1.92	0.52
2:p:238:GLU:HB2	2:p:251:ASN:HB3	1.91	0.52
3:A:305:VAL:HG22	3:A:668:ILE:HG12	1.92	0.52
3:B:402:ASP:OD1	3:B:402:ASP:N	2.42	0.52
3:C:93:VAL:HB	3:C:107:ALA:HB3	1.92	0.52
3:C:234:LEU:HD12	3:C:235:PRO:HD2	1.92	0.52
3:D:52:ILE:HA	3:D:75:ALA:HA	1.91	0.52
7:P:477:ARG:NH2	7:P:482:ALA:O	2.43	0.52
8:T:447:LEU:HA	8:T:470:GLN:HB3	1.91	0.52
13:d:326:CYS:SG	13:d:346:HIS:ND1	2.72	0.52
14:e:720:ARG:HH11	14:e:989:TRP:HE3	1.58	0.52
1:m:55:ARG:NH1	1:m:108:ARG:HD3	2.22	0.51
3:A:309:ARG:HH12	3:A:333:LYS:HB3	1.75	0.51
3:F:138:LYS:HG2	3:F:285:THR:HB	1.92	0.51
3:I:439:ASP:OD1	3:I:440:MET:N	2.43	0.51
13:d:237:VAL:HG11	13:d:255:ILE:HD13	1.92	0.51
14:f:936:CYS:HB3	14:f:940:ARG:NH1	2.23	0.51
1:m:383:GLU:OE2	1:m:401:ASN:ND2	2.41	0.51
3:B:195:TYR:HB3	3:B:267:LEU:HD11	1.92	0.51
3:E:489:ARG:HE	3:E:571:ASP:HA	1.74	0.51
5:N:52:TRP:HA	5:N:55:GLU:HG3	1.91	0.51
8:Q:536:VAL:HG23	8:Q:545:LEU:HB2	1.91	0.51
8:T:501:ASP:OD1	8:T:501:ASP:N	2.44	0.51
5:U:103:ASN:ND2	9:V:48:GLN:OE1	2.42	0.51
11:X:303:VAL:HG11	11:X:384:ILE:HD13	1.92	0.51
10:Z:292:GLN:O	10:Z:298:ASN:ND2	2.43	0.51
14:f:608:LYS:NZ	14:f:610:ILE:HD11	2.24	0.51
14:f:861:TRP:HB2	14:f:890:GLN:HB2	1.92	0.51
1:m:200:THR:HG21	1:m:268:LEU:HD11	1.93	0.51
3:C:302:PRO:HG3	3:C:611:LEU:HA	1.93	0.51
3:I:599:ARG:HH22	3:I:656:LEU:HA	1.75	0.51
7:P:275:MET:HB3	7:P:320:LEU:HB2	1.92	0.51
4:R:113:PHE:CG	4:R:117:ILE:HD11	2.46	0.51
4:R:203:ILE:HD13	4:R:217:ILE:HG21	1.91	0.51
4:R:653:LEU:O	4:R:656:SER:OG	2.26	0.51
7:S:334:GLN:O	7:S:335:HIS:ND1	2.43	0.51
7:S:450:LEU:HD13	7:S:453:ARG:HB2	1.93	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:X:15:GLN:HB3	11:X:228:ASN:HD21	1.75	0.51
11:X:298:PRO:HB3	11:X:307:PRO:HD2	1.92	0.51
14:f:947:GLU:HG2	14:f:948:PHE:HB2	1.91	0.51
3:G:255:PRO:HG3	3:G:446:GLU:HB3	1.92	0.51
6:O:55:PHE:CG	6:O:62:ILE:HD11	2.46	0.51
7:S:666:LEU:HB3	7:S:692:CYS:HB3	1.92	0.51
10:W:2:ARG:NH1	11:X:98:ASP:OD2	2.43	0.51
10:Z:215:LEU:HG	10:Z:217:LEU:HG	1.92	0.51
10:Z:247:ASN:HD21	10:Z:256:ASN:HD22	1.57	0.51
13:b:204:ALA:HA	13:b:278:GLU:HG2	1.92	0.51
12:c:34:GLN:HE21	13:d:613:GLU:HG3	1.75	0.51
13:d:1:MET:HE1	13:d:20:SER:HA	1.93	0.51
14:f:118:TYR:OH	14:f:120:ASN:ND2	2.44	0.51
3:F:255:PRO:HG3	3:F:446:GLU:HB3	1.92	0.51
3:I:200:HIS:NE2	3:I:266:SER:OG	2.44	0.51
14:e:761:ILE:HG13	14:e:785:PHE:HB3	1.90	0.51
16:n:363:SER:HB3	16:n:391:LEU:HD11	1.92	0.51
15:j:103:LEU:HD22	15:j:115:LEU:HD11	1.93	0.51
1:m:109:HIS:HE2	1:m:441:GLU:HB3	1.75	0.51
1:m:277:VAL:HG22	1:m:329:ILE:HG22	1.91	0.51
2:p:354:LYS:HD2	2:p:414:GLN:HB3	1.92	0.51
3:A:141:MET:HG2	3:A:143:GLY:H	1.76	0.51
3:B:533:THR:HG23	3:B:536:GLN:HE21	1.75	0.51
3:D:599:ARG:HH12	3:D:658:ASN:HD22	1.57	0.51
3:E:194:ASN:HD21	3:E:272:HIS:HE1	1.59	0.51
3:I:254:SER:HB3	3:I:257:PHE:HB3	1.93	0.51
3:I:401:LEU:HD13	3:I:429:GLY:HA2	1.93	0.51
3:I:494:SER:HB3	3:I:574:LEU:HD12	1.92	0.51
5:N:113:LYS:HD2	7:P:712:LEU:HD11	1.91	0.51
4:R:857:GLN:NE2	4:R:885:ASN:O	2.40	0.51
7:S:895:ASN:HD21	8:T:272:LEU:HA	1.76	0.51
11:X:102:ASN:HD21	11:X:407:TRP:HB3	1.75	0.51
11:Y:286:LEU:HA	11:Y:373:ARG:HH21	1.75	0.51
13:d:315:ASN:HB3	13:d:567:LYS:HZ3	1.76	0.51
13:d:738:ASP:OD1	13:d:742:ARG:NH2	2.44	0.51
14:e:260:ARG:NH1	14:e:547:ASP:O	2.44	0.51
14:f:188:VAL:HA	14:f:191:LEU:HD23	1.92	0.51
14:f:490:TYR:HB2	14:f:520:ILE:HG23	1.93	0.51
14:f:795:THR:HA	14:f:798:LEU:HD12	1.92	0.51
3:E:116:ILE:HD13	3:E:197:LEU:HD21	1.91	0.51
3:E:577:GLN:HE21	3:E:604:ASP:HA	1.76	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:508:GLU:HG2	3:F:625:ILE:HG21	1.93	0.51
3:I:307:LEU:HB2	3:I:333:LYS:HG2	1.93	0.51
4:R:134:GLU:HG2	4:R:149:VAL:HG21	1.93	0.51
4:R:146:PRO:HG3	4:R:270:GLU:HA	1.93	0.51
12:c:20:GLN:HE22	13:d:622:LYS:HD3	1.74	0.51
14:f:791:GLU:HG3	14:f:820:LEU:HD13	1.92	0.51
1:m:105:TYR:CZ	1:m:440:ASP:HB2	2.46	0.51
3:E:559:THR:HA	3:F:4:GLN:NE2	2.26	0.51
3:G:529:ARG:HH22	3:G:599:ARG:HG2	1.76	0.51
7:S:1154:ASP:N	7:S:1154:ASP:OD1	2.43	0.51
10:W:27:GLU:OE1	10:W:318:ARG:NH2	2.39	0.51
10:W:361:LEU:HD12	10:W:362:LYS:H	1.75	0.51
10:W:398:TYR:HB3	10:W:403:MET:HG3	1.92	0.51
13:d:178:ILE:HB	13:d:197:ALA:HB2	1.91	0.51
14:e:338:ILE:HD13	14:e:343:HIS:HD2	1.76	0.51
14:f:114:THR:OG1	14:f:153:LYS:NZ	2.42	0.51
14:f:253:THR:HB	14:f:553:LEU:HD21	1.93	0.51
14:f:329:SER:HB2	14:f:355:LEU:HD21	1.92	0.51
2:p:14:PHE:O	2:p:22:LEU:HD21	2.11	0.51
3:D:116:ILE:HD13	3:D:267:LEU:HG	1.92	0.51
3:D:264:SER:HG	3:D:285:THR:HG1	1.58	0.51
3:D:401:LEU:HG	3:D:438:ARG:HG3	1.93	0.51
3:D:482:ASN:HB3	3:D:485:GLN:HE22	1.75	0.51
3:D:546:GLN:HG2	3:D:581:LEU:HG	1.93	0.51
3:F:376:PHE:HB2	3:F:379:LYS:HD3	1.93	0.51
3:G:573:ILE:HG23	3:G:638:LEU:HD22	1.93	0.51
3:H:210:ARG:HG2	3:H:227:PRO:HD3	1.93	0.51
7:P:462:THR:HG21	7:P:601:GLY:HA3	1.93	0.51
4:R:767:LEU:O	4:R:799:ASN:ND2	2.43	0.51
7:S:651:TYR:OH	7:S:681:ASP:OD1	2.27	0.51
11:Y:70:LEU:HA	11:Y:95:GLY:HA3	1.92	0.51
10:Z:318:ARG:HG2	10:Z:354:CYS:HB3	1.92	0.51
14:f:253:THR:HA	14:f:256:ILE:HD12	1.92	0.51
15:h:6:LEU:HA	15:h:45:VAL:HG22	1.92	0.51
1:m:14:LEU:HA	1:m:17:LEU:HG	1.92	0.51
3:C:307:LEU:HD21	3:C:317:VAL:HG13	1.93	0.51
5:N:130:LEU:HD11	6:O:65:LEU:HD12	1.91	0.51
7:S:392:VAL:HG22	5:U:28:ARG:NH1	2.23	0.51
7:S:496:MET:HG2	7:S:517:TYR:CE1	2.46	0.51
7:S:769:ARG:HG3	7:S:798:SER:HB3	1.93	0.51
7:S:923:ASN:HA	7:S:952:HIS:HB3	1.93	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:W:246:LEU:HD23	10:W:352:ALA:HB2	1.93	0.51
14:e:339:TRP:HH2	14:e:416:LEU:HB2	1.76	0.51
14:e:570:VAL:O	14:e:574:ASN:HB2	2.11	0.51
14:f:910:ILE:O	14:f:913:ASN:C	2.54	0.51
16:n:113:GLY:HA3	16:n:444:GLU:OE1	2.11	0.51
2:p:17:LEU:HD13	2:p:21:SER:HB2	1.92	0.50
3:B:599:ARG:NH2	3:B:656:LEU:O	2.42	0.50
3:C:1:MET:SD	3:C:18:LEU:HB2	2.50	0.50
3:C:492:LEU:HD22	3:C:554:ILE:HG23	1.93	0.50
3:G:617:ILE:O	3:G:648:PHE:HA	2.12	0.50
3:K:487:ASP:OD1	3:K:487:ASP:N	2.44	0.50
14:e:957:LEU:HA	14:e:962:LYS:HB2	1.92	0.50
14:f:140:TRP:HZ2	14:f:150:VAL:HG21	1.76	0.50
14:f:216:LYS:HA	14:f:219:VAL:HG22	1.93	0.50
14:f:421:ASN:HB2	14:f:424:HIS:HB3	1.93	0.50
14:f:425:ASP:OD1	14:f:425:ASP:N	2.44	0.50
15:l:130:LYS:NZ	15:l:138:THR:OG1	2.43	0.50
3:A:196:GLN:N	3:A:268:VAL:O	2.45	0.50
3:B:400:SER:OG	3:B:402:ASP:OD1	2.28	0.50
4:R:236:TRP:CD1	4:R:236:TRP:H	2.30	0.50
7:S:1006:GLU:OE2	7:S:1061:ARG:NH2	2.44	0.50
11:X:208:ALA:HB2	11:X:304:LYS:HG2	1.94	0.50
11:Y:268:PRO:HB3	11:Y:380:ASN:HB2	1.94	0.50
1:m:462:LEU:HB3	1:m:464:VAL:HG13	1.93	0.50
2:p:206:VAL:HG23	2:p:220:ILE:HD11	1.93	0.50
2:p:360:SER:HB2	2:p:388:LEU:HD22	1.93	0.50
2:p:407:TYR:HD2	2:p:418:LYS:HA	1.75	0.50
3:B:205:GLU:OE2	3:B:205:GLU:N	2.45	0.50
3:D:212:TYR:HB3	3:D:221:TYR:HB3	1.92	0.50
3:K:25:ILE:HB	3:K:77:VAL:HG23	1.93	0.50
13:d:140:ARG:HA	13:d:147:TRP:HA	1.92	0.50
2:p:314:ILE:HD12	2:p:336:SER:HB2	1.93	0.50
3:G:202:SER:OG	3:G:205:GLU:OE1	2.29	0.50
3:H:342:SER:OG	3:H:343:LYS:N	2.42	0.50
3:K:42:ILE:HG12	3:K:50:ILE:HG12	1.92	0.50
10:W:226:ASN:OD1	18:W:501:GTP:N1	2.45	0.50
11:X:168:GLU:HB2	11:X:201:ALA:HA	1.93	0.50
11:Y:132:LEU:HB3	11:Y:164:LYS:HZ2	1.76	0.50
13:d:29:ARG:HB3	13:d:40:PRO:HB3	1.94	0.50
14:e:721:LEU:HD23	14:e:749:LEU:HD13	1.94	0.50
14:f:42:TRP:O	14:f:45:THR:OG1	2.26	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:j:7:GLN:HB2	15:j:44:PRO:HB2	1.94	0.50
15:j:136:ARG:O	15:j:141:ILE:N	2.41	0.50
2:p:208:ILE:O	2:p:215:LEU:HA	2.12	0.50
2:p:293:PRO:HD3	2:p:351:VAL:HG23	1.94	0.50
3:A:561:LEU:O	3:A:565:LEU:HB2	2.12	0.50
3:C:314:GLN:HA	3:C:318:ASP:HB2	1.92	0.50
3:I:294:ILE:HD12	3:I:453:VAL:HG11	1.92	0.50
7:S:892:ILE:HD13	7:S:1161:TRP:HA	1.94	0.50
5:U:42:SER:OG	5:U:43:ASN:ND2	2.44	0.50
11:Y:204:VAL:HA	11:Y:302:MET:HE2	1.94	0.50
13:b:517:CYS:SG	13:b:518:HIS:N	2.84	0.50
12:c:77:ASN:HD21	12:c:114:ASN:H	1.59	0.50
12:c:133:LYS:O	12:c:137:ILE:HD12	2.11	0.50
13:d:243:ARG:HH22	13:d:246:ARG:HH12	1.58	0.50
15:j:7:GLN:HB3	15:j:46:PRO:HA	1.92	0.50
3:B:91:VAL:HB	3:B:109:LEU:HB3	1.93	0.50
3:F:306:TYR:O	3:F:666:ALA:HA	2.11	0.50
7:S:287:LYS:HG2	7:S:289:THR:H	1.77	0.50
7:S:1070:THR:OG1	7:S:1072:ASN:OD1	2.28	0.50
8:T:397:THR:HG23	8:T:399:GLU:H	1.77	0.50
8:T:423:ARG:NH2	8:T:457:ARG:O	2.44	0.50
11:X:336:LYS:O	11:X:339:ARG:NH2	2.44	0.50
13:b:4:GLN:NE2	13:b:66:ASN:OD1	2.44	0.50
13:b:184:TYR:HE1	13:b:193:ASP:HB2	1.76	0.50
13:b:240:CYS:HB2	13:b:253:GLY:HA2	1.93	0.50
13:b:254:ASN:ND2	13:b:262:GLN:OE1	2.45	0.50
14:f:261:MET:SD	14:f:519:ARG:NE	2.77	0.50
14:f:518:LEU:HB2	14:f:542:LEU:HD23	1.92	0.50
14:f:668:SER:H	14:f:696:LEU:HB3	1.77	0.50
1:m:90:TYR:HB2	1:m:425:ARG:NH1	2.26	0.50
3:B:588:PRO:HG2	3:B:591:GLN:HE22	1.77	0.50
3:D:234:LEU:HD12	3:D:235:PRO:HD2	1.92	0.50
3:E:250:THR:HG23	3:E:251:GLU:HG2	1.93	0.50
3:F:47:ARG:NH1	3:F:89:ASP:OD1	2.44	0.50
3:F:576:PRO:HG3	3:F:634:LYS:HD3	1.93	0.50
3:G:563:THR:OG1	3:H:135:GLN:NE2	2.44	0.50
3:K:21:VAL:N	3:K:114:ILE:O	2.36	0.50
8:Q:254:LEU:HA	8:Q:260:VAL:HG12	1.94	0.50
4:R:841:ILE:H	4:R:867:ASN:HD22	1.59	0.50
13:d:260:ASP:OD1	13:d:262:GLN:NE2	2.45	0.50
14:e:146:PRO:HG2	14:e:149:GLN:HB2	1.93	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:e:164:PHE:HA	14:e:167:LEU:HD12	1.93	0.50
14:e:477:LEU:HB3	14:e:481:ARG:HH11	1.77	0.50
14:e:740:LEU:O	14:e:743:SER:C	2.54	0.50
14:f:531:LEU:HD12	14:f:577:LEU:HD22	1.93	0.50
1:m:311:THR:HB	1:m:339:LEU:HD22	1.93	0.50
2:p:28:VAL:HG22	15:l:135:ILE:HG21	1.94	0.50
3:E:438:ARG:NH2	3:E:464:LEU:O	2.44	0.50
3:E:524:LEU:HD22	3:E:529:ARG:HB2	1.94	0.50
3:G:489:ARG:NH1	3:G:571:ASP:OD1	2.43	0.50
3:I:382:LEU:HD13	3:I:386:SER:HB3	1.94	0.50
4:R:877:LEU:O	4:R:881:ILE:HG13	2.12	0.50
11:X:269:LEU:HD11	11:X:302:MET:H	1.76	0.50
13:d:541:ARG:NH1	13:d:560:ASP:OD2	2.35	0.50
13:d:723:PRO:HD2	13:d:763:VAL:HG13	1.94	0.50
14:e:534:MET:HG2	14:e:580:MET:HE2	1.93	0.50
14:f:556:ALA:HA	14:f:559:GLN:HB2	1.93	0.50
15:l:8:SER:OG	15:l:9:SER:N	2.42	0.50
3:E:401:LEU:HD21	3:E:467:GLY:HA3	1.92	0.50
3:G:312:GLN:NE2	3:G:654:CYS:SG	2.85	0.50
7:P:939:ARG:HH22	7:S:997:GLU:HA	1.75	0.50
15:h:161:GLU:OE1	15:h:161:GLU:N	2.45	0.50
2:p:297:ASP:O	2:p:317:ASP:HA	2.12	0.49
2:p:300:THR:O	2:p:349:TYR:OH	2.30	0.49
3:F:323:LEU:HD11	3:F:616:GLY:HA3	1.94	0.49
3:H:295:PHE:HB2	3:H:409:VAL:HG21	1.93	0.49
4:R:364:ARG:O	4:R:365:ARG:NH1	2.44	0.49
14:e:171:PHE:CE1	14:e:193:SER:HA	2.44	0.49
14:f:734:LYS:HG2	14:f:763:LEU:HD22	1.94	0.49
15:l:146:THR:OG1	15:l:149:GLU:OE1	2.30	0.49
2:p:85:PRO:HG3	2:p:420:TYR:HB2	1.94	0.49
3:A:439:ASP:OD2	3:A:439:ASP:N	2.45	0.49
10:W:247:ASN:N	10:W:247:ASN:OD1	2.45	0.49
10:Z:318:ARG:HA	10:Z:354:CYS:O	2.11	0.49
13:d:223:TYR:CE2	13:d:228:PRO:HB3	2.46	0.49
14:e:291:ARG:O	14:e:295:THR:OG1	2.26	0.49
14:f:909:GLY:O	14:f:912:SER:OG	2.26	0.49
15:j:78:LYS:HB2	15:j:80:LYS:HG3	1.94	0.49
15:l:136:ARG:O	15:l:141:ILE:N	2.38	0.49
3:E:543:PHE:HE2	3:E:578:LEU:HD13	1.77	0.49
3:F:262:SER:OG	3:F:287:MET:SD	2.68	0.49
3:G:11:LEU:HD21	3:G:34:PRO:HD3	1.94	0.49

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:551:GLU:OE2	3:G:555:SER:OG	2.30	0.49
3:I:8:SER:HA	3:I:31:LYS:HG3	1.94	0.49
4:R:581:SER:HA	4:R:584:ILE:HD12	1.94	0.49
4:R:777:LEU:HD21	4:R:805:LEU:HD13	1.95	0.49
11:X:97:GLU:OE2	11:X:105:ARG:NH2	2.34	0.49
10:Z:76:VAL:HG23	10:Z:90:PHE:HE2	1.77	0.49
12:c:137:ILE:HA	12:c:140:GLU:HG3	1.92	0.49
1:m:26:ALA:HA	1:m:33:ASN:HA	1.95	0.49
1:m:283:PHE:HD2	1:m:286:CYS:HB2	1.78	0.49
3:B:209:THR:HB	3:B:261:ILE:HD13	1.95	0.49
3:F:45:SER:HB2	3:F:48:ILE:HG12	1.93	0.49
3:F:326:LYS:NZ	3:F:647:THR:OG1	2.44	0.49
3:G:432:TYR:HB2	3:H:198:ILE:HD11	1.93	0.49
3:I:365:LEU:HD13	3:I:389:LEU:HB3	1.94	0.49
3:I:407:LEU:HB3	3:I:427:ILE:HG22	1.94	0.49
3:I:557:ASN:O	3:I:561:LEU:HD13	2.12	0.49
7:P:237:GLN:HE21	7:P:239:THR:HB	1.78	0.49
7:P:642:SER:OG	7:P:645:ASP:OD2	2.23	0.49
4:R:97:TYR:OH	4:R:183:ALA:O	2.27	0.49
13:d:174:SER:OG	13:d:176:ASP:OD1	2.30	0.49
13:d:313:ASP:O	13:d:329:ARG:NE	2.45	0.49
14:f:864:ASP:HB2	14:f:891:ARG:HD2	1.95	0.49
1:m:9:PRO:HB2	1:m:10:MET:HE2	1.93	0.49
3:A:378:MET:O	3:A:382:LEU:HB2	2.12	0.49
3:H:586:ASN:ND2	13:b:508:ASN:H	2.08	0.49
3:K:116:ILE:HG23	3:K:185:VAL:HG22	1.94	0.49
4:R:607:LEU:O	4:R:646:ASN:ND2	2.46	0.49
7:S:979:THR:HG23	7:S:1008:VAL:HB	1.95	0.49
11:Y:213:CYS:SG	11:Y:226:ASN:ND2	2.75	0.49
14:f:44:LYS:HZ1	14:f:374:GLU:HG2	1.78	0.49
14:f:540:ALA:H	14:f:586:ARG:HB2	1.78	0.49
3:A:513:VAL:HG11	3:A:625:ILE:HD11	1.95	0.49
3:D:262:SER:OG	3:D:287:MET:SD	2.68	0.49
3:F:94:SER:HA	3:F:105:ALA:HB3	1.94	0.49
3:I:264:SER:HB3	3:I:285:THR:HB	1.94	0.49
3:I:504:GLN:HA	3:I:507:LYS:HD2	1.95	0.49
3:I:581:LEU:HA	3:I:598:ALA:HA	1.94	0.49
7:P:219:LEU:O	7:P:261:SER:OG	2.29	0.49
10:W:54:ALA:HB3	10:W:58:LYS:HB2	1.95	0.49
11:X:247:ALA:HB2	11:X:356:ASN:HB2	1.95	0.49
11:X:320:ARG:HE	11:X:360:PRO:HB3	1.77	0.49

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:f:188:VAL:O	14:f:192:ILE:HD12	2.13	0.49
14:f:764:LEU:O	14:f:768:LEU:HG	2.13	0.49
15:h:97:GLN:HA	15:h:100:LEU:HG	1.94	0.49
1:m:294:ARG:O	1:m:296:GLU:N	2.46	0.49
2:p:288:ARG:NH2	2:p:289:ALA:O	2.45	0.49
3:A:264:SER:HB2	3:A:285:THR:HG22	1.94	0.49
3:A:605:MET:HE1	3:A:631:LEU:HB3	1.95	0.49
3:B:47:ARG:HD3	3:B:81:ALA:HB3	1.95	0.49
3:C:650:ASP:OD1	3:C:650:ASP:N	2.44	0.49
3:F:394:GLU:OE2	3:F:441:ASN:ND2	2.42	0.49
3:G:559:THR:HG23	3:H:4:GLN:HG3	1.93	0.49
11:X:147:SER:HB2	11:X:190:THR:HB	1.93	0.49
11:X:199:ASP:OD1	11:X:199:ASP:N	2.46	0.49
14:e:60:PRO:HA	14:e:63:GLN:HB2	1.94	0.49
14:e:740:LEU:O	14:e:743:SER:O	2.31	0.49
14:f:647:LEU:HD13	14:f:675:ARG:HD3	1.95	0.49
1:m:106:ILE:HB	1:m:122:CYS:HB2	1.94	0.49
2:p:152:LYS:H	2:p:167:ASP:HA	1.78	0.49
3:D:617:ILE:O	3:D:648:PHE:HA	2.13	0.49
3:E:532:LYS:HG3	3:E:537:ILE:HG13	1.93	0.49
8:Q:431:SER:HA	8:Q:446:GLY:HA3	1.94	0.49
8:Q:441:ASN:HD22	8:Q:500:ARG:HH22	1.61	0.49
10:W:68:LEU:HD23	10:W:143:THR:HG23	1.93	0.49
11:X:384:ILE:HD12	11:X:387:ALA:HB3	1.95	0.49
14:e:179:CYS:SG	14:e:180:LYS:N	2.86	0.49
14:e:711:LEU:HD13	14:e:746:LEU:HD21	1.95	0.49
3:A:461:SER:OG	3:A:467:GLY:O	2.31	0.49
3:B:137:LYS:NZ	3:B:284:ASP:OD1	2.40	0.49
3:B:196:GLN:HB2	3:B:270:LYS:HE3	1.95	0.49
3:C:312:GLN:HA	13:d:448:ARG:HH22	1.78	0.49
3:I:516:PHE:HD2	3:I:531:SER:HA	1.78	0.49
7:S:346:ASP:HB3	7:S:348:GLN:HE22	1.77	0.49
8:T:421:ILE:H	8:T:421:ILE:HD12	1.78	0.49
11:Y:88:HIS:CE1	11:Y:90:GLU:HB3	2.48	0.49
12:a:46:GLN:NE2	14:e:445:ARG:HH22	2.11	0.49
13:b:480:TYR:CZ	13:b:585:ARG:HD2	2.48	0.49
14:e:53:THR:OG1	14:e:55:ASN:OD1	2.31	0.49
14:e:677:GLN:O	14:e:681:ASN:ND2	2.46	0.49
3:H:327:SER:HB3	3:H:614:ASN:HD21	1.78	0.49
4:M:18:ASN:ND2	4:M:21:GLU:OE2	2.46	0.49
7:P:284:ARG:NH1	17:P:1201:ATP:O3G	2.43	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:P:286:ILE:HD12	7:P:350:ILE:HD11	1.95	0.49
4:R:554:LEU:HB3	4:R:563:LEU:HD12	1.94	0.49
10:Z:4:ILE:HD11	10:Z:50:TYR:CE1	2.48	0.49
13:b:691:VAL:HG22	13:b:706:LYS:HE2	1.94	0.49
3:D:302:PRO:HG3	3:D:611:LEU:HD12	1.95	0.48
3:F:227:PRO:O	3:F:228:ASN:ND2	2.46	0.48
3:I:211:VAL:HG22	3:I:247:VAL:HG12	1.95	0.48
3:I:340:ARG:NH1	3:I:348:GLU:OE1	2.46	0.48
3:K:430:SER:OG	3:K:432:TYR:O	2.30	0.48
5:N:68:ILE:O	5:N:72:CYS:HB2	2.12	0.48
7:S:835:ARG:HA	7:S:863:SER:HB3	1.95	0.48
8:T:249:LYS:HA	8:T:249:LYS:HD2	1.65	0.48
8:T:422:VAL:HG12	8:T:423:ARG:HG2	1.95	0.48
10:W:52:ASN:HA	10:W:62:ARG:HH21	1.78	0.48
10:Z:323:MET:N	10:Z:323:MET:SD	2.85	0.48
12:c:92:GLN:OE1	12:c:92:GLN:N	2.45	0.48
14:e:235:LYS:NZ	14:e:545:MET:SD	2.74	0.48
14:f:36:GLU:O	14:f:40:THR:OG1	2.23	0.48
15:j:56:LYS:NZ	15:j:60:GLN:HB3	2.28	0.48
2:p:447:VAL:HA	2:p:457:LEU:HD22	1.95	0.48
3:A:501:LEU:HD22	3:A:634:LYS:HD2	1.95	0.48
3:B:402:ASP:HB3	3:B:440:MET:HA	1.95	0.48
3:C:151:LEU:HD21	3:C:247:VAL:HG12	1.95	0.48
3:G:41:THR:HG22	3:G:66:TRP:HA	1.95	0.48
3:H:234:LEU:HD12	3:H:235:PRO:HD2	1.94	0.48
3:I:438:ARG:NH1	3:I:462:ASP:O	2.41	0.48
3:K:210:ARG:HB2	3:K:248:GLU:HG2	1.94	0.48
7:P:554:PHE:HE1	7:P:602:LEU:HD21	1.79	0.48
14:f:875:LEU:HD11	14:f:894:LEU:HD13	1.93	0.48
15:h:93:LEU:HD13	15:h:122:THR:OG1	2.13	0.48
1:m:135:VAL:HG13	1:m:459:ALA:HB1	1.95	0.48
3:C:502:PHE:HA	3:C:534:ILE:HD11	1.95	0.48
3:K:308:CYS:HA	3:K:334:VAL:HG12	1.96	0.48
5:N:125:GLU:HA	5:N:128:GLU:OE2	2.13	0.48
7:P:359:ARG:NE	7:P:383:MET:O	2.46	0.48
7:P:1018:GLU:OE2	7:P:1018:GLU:N	2.43	0.48
7:S:255:LYS:HG2	7:S:392:VAL:HG21	1.95	0.48
11:X:3:GLU:OE1	11:X:64:ARG:NH1	2.46	0.48
11:Y:133:GLN:HG2	11:Y:252:LEU:HB2	1.94	0.48
10:Z:285:THR:HG23	10:Z:288:GLU:HG2	1.95	0.48
13:d:4:GLN:O	13:d:68:THR:HA	2.13	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:e:964:PHE:HA	14:e:967:ASP:HB2	1.96	0.48
14:f:315:PRO:HG2	14:f:318:CYS:HB2	1.95	0.48
14:f:506:GLN:NE2	14:f:530:THR:OG1	2.39	0.48
1:m:361:THR:HG22	1:m:362:GLY:H	1.79	0.48
3:H:82:PRO:HG2	3:H:186:GLU:HG2	1.94	0.48
3:K:558:ARG:HE	3:K:562:LYS:HZ2	1.60	0.48
4:R:282:PHE:HA	4:R:285:MET:HG2	1.96	0.48
4:R:535:LEU:HA	4:R:541:LEU:HD23	1.96	0.48
11:X:319:TYR:CE2	11:X:328:VAL:HG22	2.49	0.48
14:f:751:LEU:HA	14:f:754:ASN:HB2	1.95	0.48
2:p:199:ILE:HA	2:p:204:PRO:HA	1.95	0.48
3:D:197:LEU:HD11	3:D:234:LEU:HD23	1.94	0.48
3:I:90:LYS:HZ3	3:I:108:VAL:HG23	1.77	0.48
4:R:365:ARG:NH2	4:R:556:GLU:OE2	2.46	0.48
4:R:841:ILE:HB	4:R:867:ASN:HD22	1.79	0.48
13:b:138:ASP:HA	13:b:149:GLU:HA	1.94	0.48
14:f:124:ILE:HD12	14:f:192:ILE:HG12	1.96	0.48
3:A:202:SER:OG	3:A:205:GLU:OE1	2.31	0.48
3:A:394:GLU:HB2	3:A:441:ASN:HD22	1.78	0.48
3:B:122:ILE:HG22	3:B:149:ALA:HB2	1.94	0.48
3:B:608:ILE:HG21	3:B:615:LEU:HD13	1.95	0.48
3:D:569:ASP:N	3:D:569:ASP:OD1	2.46	0.48
3:G:347:ASP:OD2	3:G:369:ARG:NH2	2.46	0.48
3:I:50:ILE:HG12	3:I:77:VAL:HG22	1.95	0.48
3:I:486:LYS:H	3:I:489:ARG:HH22	1.60	0.48
6:O:98:VAL:O	6:O:101:MET:HB3	2.13	0.48
8:Q:570:SER:OG	8:Q:571:ARG:N	2.46	0.48
11:Y:349:THR:HG22	14:f:57:VAL:HB	1.95	0.48
13:b:515:LEU:HD13	13:b:521:ILE:HD11	1.94	0.48
14:e:891:ARG:NH1	14:e:983:ASN:O	2.46	0.48
14:f:734:LYS:HB2	14:f:763:LEU:HD13	1.94	0.48
16:n:203:THR:OG1	16:n:206:ALA:O	2.31	0.48
16:n:356:ASP:OD1	16:n:356:ASP:N	2.47	0.48
1:m:61:HIS:CE1	1:m:113:ARG:HG3	2.49	0.48
1:m:97:PHE:O	7:P:856:THR:OG1	2.29	0.48
2:p:128:ASN:HB2	2:p:146:GLU:OE2	2.14	0.48
3:E:8:SER:HB2	3:E:31:LYS:HG2	1.95	0.48
3:G:460:PHE:O	3:G:557:ASN:ND2	2.41	0.48
3:I:48:ILE:HD11	3:I:89:ASP:HB3	1.94	0.48
3:I:402:ASP:HB2	3:I:440:MET:HA	1.95	0.48
6:O:23:ILE:HD11	6:O:33:PHE:HE2	1.78	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:W:236:VAL:HG22	10:W:368:ILE:HG12	1.95	0.48
11:X:7:ILE:HD13	11:X:153:LEU:HD21	1.95	0.48
11:X:319:TYR:CZ	11:X:328:VAL:HG22	2.48	0.48
13:b:6:ARG:HB3	13:b:13:THR:HG23	1.96	0.48
13:b:229:ARG:NE	14:e:405:ASP:OD2	2.46	0.48
14:e:785:PHE:HZ	14:e:808:LEU:HB2	1.79	0.48
14:f:535:ARG:HA	14:f:581:ASP:O	2.14	0.48
15:j:59:ILE:O	15:j:63:THR:HG23	2.14	0.48
2:p:238:GLU:HB3	2:p:240:TYR:CE2	2.49	0.48
2:p:339:LEU:HD13	2:p:346:PRO:HG3	1.96	0.48
3:C:645:LYS:HE3	3:K:624:LYS:HE2	1.96	0.48
3:D:48:ILE:HA	3:D:79:MET:HA	1.96	0.48
3:G:18:LEU:HD21	3:G:191:ILE:HD13	1.94	0.48
3:G:563:THR:HG23	3:G:564:GLU:HG2	1.96	0.48
3:H:308:CYS:HA	3:H:334:VAL:HB	1.96	0.48
3:H:668:ILE:HD13	3:H:670:ARG:HH21	1.79	0.48
3:I:321:THR:HG22	3:I:331:VAL:HG11	1.95	0.48
3:I:347:ASP:O	3:I:403:SER:OG	2.32	0.48
8:Q:534:ILE:HD13	8:Q:568:THR:HG21	1.95	0.48
4:R:670:ASN:OD1	4:R:695:SER:OG	2.31	0.48
4:R:729:SER:OG	4:R:731:ASP:OD1	2.25	0.48
10:W:206:ALA:HB2	10:W:302:ALA:HA	1.96	0.48
14:f:528:CYS:SG	14:f:529:HIS:N	2.87	0.48
15:h:12:GLU:OE1	15:h:13:ILE:N	2.47	0.48
16:n:90:ASP:OD1	16:n:466:ASN:ND2	2.47	0.48
15:j:85:ILE:O	15:j:90:GLN:NE2	2.46	0.48
2:p:183:LEU:HD21	2:p:221:PRO:HB2	1.95	0.48
3:B:366:ASP:OD2	3:B:388:TYR:OH	2.23	0.48
3:C:546:GLN:HB3	3:C:581:LEU:HD23	1.96	0.48
3:F:345:LEU:HD13	3:F:667:ILE:HG22	1.95	0.48
3:I:235:PRO:HG2	3:I:237:PHE:HE1	1.78	0.48
3:I:348:GLU:OE2	3:I:369:ARG:N	2.47	0.48
3:K:316:PHE:N	3:K:651:ASP:OD2	2.46	0.48
3:K:326:LYS:HG2	3:K:614:ASN:HD22	1.79	0.48
6:O:60:GLU:OE2	6:O:60:GLU:N	2.38	0.48
4:R:583:PHE:HZ	4:R:603:THR:HB	1.78	0.48
9:V:65:LEU:HD13	9:V:83:HIS:CE1	2.48	0.48
13:b:472:GLU:OE1	13:b:472:GLU:N	2.47	0.48
1:m:82:ARG:NE	15:h:161:GLU:O	2.47	0.48
1:m:102:HIS:HB2	1:m:154:MET:HE3	1.95	0.48
3:F:294:ILE:HG21	3:F:422:LEU:HD13	1.95	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:90:LYS:NZ	3:I:92:LEU:HD13	2.29	0.48
3:I:306:TYR:HB2	3:I:667:ILE:HG23	1.94	0.48
3:K:599:ARG:NH2	3:K:656:LEU:O	2.45	0.48
5:N:79:ASP:HB2	5:N:88:GLU:HG2	1.96	0.48
7:S:940:ASN:HD22	16:n:257:HIS:CD2	2.32	0.48
5:U:100:ARG:NE	9:V:55:SER:OG	2.44	0.48
10:W:33:THR:C	10:W:58:LYS:HZ1	2.21	0.48
10:W:152:ILE:HG12	10:W:164:MET:HE2	1.96	0.48
13:b:220:MET:SD	13:b:234:TRP:HB3	2.54	0.48
13:b:713:CYS:O	13:b:717:GLN:N	2.47	0.48
14:e:119:LEU:HD12	14:e:161:ILE:HG22	1.95	0.48
14:e:642:LEU:HD11	14:e:666:LEU:HD13	1.96	0.48
14:f:263:TRP:O	14:f:267:HIS:ND1	2.42	0.48
14:f:487:HIS:HD2	14:f:520:ILE:HG21	1.79	0.48
3:A:27:LEU:HD22	3:A:91:VAL:HG11	1.96	0.47
3:A:195:TYR:HB3	3:A:267:LEU:HD11	1.95	0.47
3:C:279:ILE:HG13	3:D:552:LYS:HD3	1.95	0.47
3:F:73:THR:OG1	3:F:73:THR:O	2.29	0.47
3:H:397:ARG:HH22	3:H:438:ARG:HG2	1.79	0.47
3:K:193:GLN:HE22	3:K:236:THR:HG21	1.78	0.47
7:S:561:VAL:HG13	7:S:621:PRO:HG3	1.96	0.47
10:W:70:PRO:HG3	10:W:94:GLN:HA	1.96	0.47
11:X:206:ASN:OD1	18:X:501:GTP:N2	2.47	0.47
12:a:37:ILE:HD11	12:a:103:LEU:HD22	1.96	0.47
3:A:29:ILE:HB	3:A:73:THR:OG1	2.14	0.47
3:A:178:LEU:HD23	3:A:248:GLU:HB3	1.96	0.47
3:B:309:ARG:HH21	3:B:335:TYR:HA	1.80	0.47
3:C:308:CYS:HA	3:C:334:VAL:HG12	1.96	0.47
3:H:505:LYS:HE2	3:H:625:ILE:HG13	1.96	0.47
7:S:427:LEU:O	7:S:431:CYS:HB2	2.14	0.47
10:W:286:VAL:HG23	10:W:287:PRO:HD3	1.94	0.47
13:b:8:MET:HG3	13:b:72:LEU:HD12	1.95	0.47
13:b:16:VAL:HG22	13:b:35:VAL:HG21	1.95	0.47
13:d:315:ASN:HB3	13:d:567:LYS:NZ	2.29	0.47
14:e:662:ARG:HH22	14:e:688:SER:HB3	1.79	0.47
14:e:666:LEU:O	14:e:697:ASN:ND2	2.35	0.47
14:f:291:ARG:HH12	14:f:293:GLU:HB2	1.79	0.47
14:f:665:ARG:HA	14:f:693:ASN:HB3	1.96	0.47
2:p:281:LEU:HD13	2:p:301:LEU:HD11	1.95	0.47
2:p:354:LYS:NZ	2:p:412:ARG:O	2.47	0.47
3:E:47:ARG:HD2	3:E:81:ALA:HB3	1.96	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:544:ARG:O	3:I:548:THR:HG23	2.13	0.47
3:K:538:LEU:O	3:K:544:ARG:NH2	2.39	0.47
7:P:1002:LEU:HD21	7:P:1005:LEU:HD13	1.96	0.47
4:R:216:GLU:O	4:R:220:GLN:NE2	2.40	0.47
7:S:304:ASP:N	7:S:304:ASP:OD1	2.45	0.47
13:b:161:SER:OG	13:b:163:ASP:OD1	2.31	0.47
14:e:132:PHE:HD2	14:e:182:TRP:HB2	1.79	0.47
14:e:596:ASN:ND2	14:e:624:THR:OG1	2.46	0.47
15:l:26:THR:HG22	15:l:110:LEU:HD13	1.95	0.47
2:p:306:GLY:O	2:p:309:LYS:NZ	2.47	0.47
3:C:7:LEU:HB2	3:C:9:LEU:HD13	1.95	0.47
3:C:279:ILE:HD11	3:D:549:TYR:CD2	2.49	0.47
3:C:316:PHE:HA	3:C:649:ILE:HD11	1.97	0.47
3:F:501:LEU:HD13	3:F:634:LYS:HD2	1.95	0.47
3:H:130:MET:HE2	3:H:130:MET:HB3	1.82	0.47
3:I:48:ILE:HG23	3:I:77:VAL:HG13	1.96	0.47
7:P:277:PHE:HB3	7:P:315:GLN:HE22	1.80	0.47
5:U:74:ALA:HB2	5:U:97:ALA:HB1	1.97	0.47
11:X:325:PRO:HA	11:X:328:VAL:HB	1.96	0.47
11:Y:70:LEU:HB2	11:Y:98:ASP:HA	1.96	0.47
15:j:146:THR:OG1	15:j:147:GLU:N	2.47	0.47
2:p:104:CYS:HB3	2:p:156:THR:HG23	1.95	0.47
2:p:288:ARG:HB2	2:p:302:MET:HE2	1.96	0.47
3:B:486:LYS:NZ	3:B:566:GLY:O	2.47	0.47
3:F:224:VAL:HG23	3:F:225:VAL:HG23	1.96	0.47
3:H:29:ILE:HG21	3:H:69:MET:HE1	1.97	0.47
5:N:123:VAL:HG12	6:O:69:LEU:HD11	1.96	0.47
7:P:603:MET:HE3	7:P:624:GLU:HB3	1.96	0.47
13:b:178:ILE:HB	13:b:197:ALA:HB2	1.96	0.47
13:d:179:MET:HA	13:d:195:VAL:O	2.15	0.47
14:f:216:LYS:NZ	14:f:341:MET:SD	2.88	0.47
14:f:793:LEU:HB3	14:f:806:LEU:HD11	1.97	0.47
15:h:82:THR:OG1	15:h:82:THR:O	2.28	0.47
1:m:6:PRO:HB2	1:m:9:PRO:HD2	1.95	0.47
3:E:371:SER:H	3:E:396:HIS:HE1	1.61	0.47
3:I:122:ILE:O	3:I:148:GLY:N	2.48	0.47
10:W:161:ASP:O	10:W:251:ARG:NH2	2.46	0.47
10:W:286:VAL:HA	10:W:289:LEU:HB2	1.95	0.47
11:X:273:ALA:HB2	11:X:295:CYS:HB3	1.96	0.47
10:Z:4:ILE:HD11	10:Z:50:TYR:CD1	2.50	0.47
13:d:158:ARG:HB2	13:d:177:ASP:O	2.14	0.47

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:e:861:TRP:HE3	14:e:890:GLN:HB2	1.80	0.47
14:e:867:HIS:HD2	14:e:895:GLU:HB2	1.80	0.47
15:l:94:LYS:HA	15:l:94:LYS:HE3	1.97	0.47
1:m:81:THR:HG23	1:m:408:VAL:HG11	1.96	0.47
1:m:99:PHE:HA	1:m:150:TYR:OH	2.15	0.47
2:p:57:THR:HG22	2:p:66:TRP:CZ3	2.49	0.47
3:A:657:ALA:HB1	3:A:661:ASP:HB2	1.97	0.47
3:E:122:ILE:HG23	3:E:123:TYR:HD1	1.79	0.47
3:F:210:ARG:HB2	3:F:248:GLU:HG2	1.95	0.47
3:K:39:SER:HB3	3:K:66:TRP:HB3	1.97	0.47
5:N:76:LEU:HD11	5:N:105:LEU:HD11	1.96	0.47
7:P:201:ASP:N	7:P:204:ASP:OD2	2.48	0.47
7:P:854:ILE:HD11	7:P:880:ALA:HA	1.95	0.47
8:Q:289:VAL:HG13	8:Q:573:CYS:HB2	1.97	0.47
4:R:329:ASN:HD22	4:R:332:LEU:HD23	1.80	0.47
7:S:626:LYS:HE2	8:T:165:GLY:HA3	1.96	0.47
8:T:285:GLN:HE21	8:T:580:LYS:HD2	1.80	0.47
11:X:93:ILE:HD11	11:X:121:ARG:HG3	1.97	0.47
11:X:332:ILE:HD11	11:X:353:VAL:HG21	1.96	0.47
13:b:28:LEU:HD22	13:b:58:LEU:HD21	1.95	0.47
13:b:157:LYS:HA	13:b:178:ILE:HA	1.95	0.47
13:b:210:TRP:CE2	13:b:242:LYS:HE2	2.49	0.47
14:e:590:SER:O	14:e:594:ILE:HG12	2.14	0.47
14:e:647:LEU:HD12	14:e:650:LEU:HD23	1.95	0.47
14:e:661:LEU:HD21	14:e:664:LEU:HD22	1.97	0.47
14:f:37:ASN:HD21	14:f:139:HIS:CD2	2.32	0.47
14:f:393:LEU:HD22	14:f:438:LEU:HD11	1.96	0.47
14:f:516:PRO:HD3	14:f:545:MET:HB2	1.96	0.47
14:f:611:PHE:HB2	14:f:637:LEU:HD23	1.96	0.47
14:f:797:LEU:HB3	14:f:830:CYS:HB2	1.96	0.47
14:f:925:ASN:N	14:f:952:ASP:OD2	2.47	0.47
2:p:23:LEU:HD11	15:l:157:ASN:HB2	1.95	0.47
2:p:25:VAL:HG23	2:p:36:ALA:HB2	1.97	0.47
3:G:211:VAL:HG12	3:G:247:VAL:HG13	1.95	0.47
8:Q:301:VAL:HG11	8:Q:560:THR:HG22	1.96	0.47
4:R:308:TYR:O	4:R:312:LEU:HD12	2.15	0.47
10:W:310:TYR:CD1	10:W:371:SER:HB2	2.49	0.47
11:X:224:TYR:HE2	18:X:501:GTP:C5	2.33	0.47
11:Y:7:ILE:HB	11:Y:137:VAL:HG12	1.97	0.47
13:b:64:ARG:HE	13:b:337:LEU:HD22	1.78	0.47
14:f:442:ASP:OD2	14:f:443:ARG:NH1	2.48	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:f:588:ASP:HB2	14:f:591:LEU:HD13	1.96	0.47
15:j:131:THR:O	15:j:134:GLU:HG2	2.15	0.47
15:l:113:LYS:HA	15:l:116:LEU:HB2	1.96	0.47
1:m:16:TYR:HD1	15:h:80:LYS:HZ3	1.63	0.47
1:m:411:GLU:H	1:m:411:GLU:CD	2.23	0.47
3:B:355:GLN:NE2	3:B:360:THR:OG1	2.48	0.47
3:H:51:HIS:O	3:H:75:ALA:HA	2.14	0.47
7:P:565:LEU:HD21	7:P:619:VAL:HG13	1.96	0.47
4:R:266:LYS:HB2	4:R:266:LYS:HE3	1.75	0.47
11:Y:102:ASN:HB3	11:Y:105:ARG:HB2	1.97	0.47
11:Y:130:THR:OG1	11:Y:131:GLY:N	2.47	0.47
11:Y:303:VAL:HG13	11:Y:305:CYS:H	1.80	0.47
13:d:438:ARG:NH2	13:d:450:HIS:O	2.43	0.47
14:e:347:GLN:HG3	14:e:351:ARG:HH12	1.80	0.47
14:f:341:MET:HE2	14:f:341:MET:HB3	1.61	0.47
16:n:46:ARG:HD2	16:n:69:TRP:CD1	2.50	0.47
16:n:165:ILE:HD13	16:n:179:ASP:HA	1.97	0.47
1:m:85:PRO:O	1:m:425:ARG:NH2	2.48	0.47
3:B:401:LEU:HD21	3:B:429:GLY:HA2	1.97	0.47
3:F:397:ARG:HD2	3:F:438:ARG:HH12	1.80	0.47
3:H:293:TYR:HB2	3:H:352:CYS:HB3	1.97	0.47
3:H:434:SER:OG	3:H:435:SER:N	2.48	0.47
3:H:453:VAL:HG12	3:H:680:MET:HE1	1.97	0.47
3:H:617:ILE:O	3:H:648:PHE:HA	2.15	0.47
3:I:397:ARG:H	3:I:397:ARG:HG2	1.54	0.47
7:P:730:MET:HE1	7:P:760:ALA:HA	1.96	0.47
8:Q:348:THR:HG23	8:Q:394:LEU:HD12	1.97	0.47
8:T:438:LYS:HA	8:T:438:LYS:HD3	1.80	0.47
11:X:16:ILE:HG13	11:X:231:ILE:HD12	1.96	0.47
11:Y:66:VAL:HG11	11:Y:122:ILE:HD11	1.97	0.47
12:a:72:ARG:HH11	12:a:145:TYR:HE1	1.63	0.47
14:f:671:LEU:HB2	14:f:697:ASN:HB3	1.97	0.47
1:m:27:LYS:NZ	15:h:157:ASN:HB2	2.30	0.46
1:m:191:SER:OG	7:P:879:ASN:OD1	2.23	0.46
1:m:423:ARG:O	1:m:425:ARG:HD2	2.15	0.46
3:A:21:VAL:HA	3:A:78:ARG:HH22	1.80	0.46
3:A:90:LYS:HA	3:A:109:LEU:O	2.15	0.46
3:B:657:ALA:HB1	3:B:661:ASP:HB2	1.96	0.46
3:C:114:ILE:HG13	3:C:187:GLY:HA3	1.96	0.46
3:H:151:LEU:HG	3:H:288:PHE:HB3	1.97	0.46
3:I:466:THR:HA	3:I:659:ILE:HD12	1.97	0.46

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:296:MET:N	3:K:296:MET:SD	2.89	0.46
8:T:316:ILE:HB	8:T:335:LEU:HB2	1.95	0.46
10:W:202:ILE:HG21	10:W:229:VAL:HG22	1.97	0.46
11:X:71:GLU:HG3	11:X:73:THR:HG23	1.97	0.46
11:Y:179:THR:O	10:Z:256:ASN:ND2	2.48	0.46
12:a:139:ARG:O	12:a:143:GLN:HG3	2.14	0.46
13:b:214:GLU:HG2	13:b:215:VAL:O	2.15	0.46
13:d:435:TRP:HB3	13:d:440:GLN:HB2	1.97	0.46
13:d:704:LEU:O	13:d:708:LYS:HG2	2.15	0.46
14:e:932:ILE:HB	14:e:961:ILE:HD12	1.96	0.46
2:p:154:LEU:HD13	2:p:165:THR:HG22	1.97	0.46
3:C:341:GLN:HE22	3:C:398:VAL:HA	1.79	0.46
3:D:550:VAL:HG21	3:D:579:PHE:HB2	1.96	0.46
3:H:49:LEU:HD22	3:H:80:VAL:HG13	1.97	0.46
3:K:127:GLN:HE21	3:K:129:ASP:H	1.63	0.46
3:K:413:VAL:HG21	3:K:565:LEU:HD22	1.96	0.46
8:T:157:PHE:HE1	8:T:251:LEU:HB2	1.80	0.46
11:X:12:ALA:HB2	18:X:501:GTP:C8	2.50	0.46
11:Y:362:VAL:HG23	11:Y:368:LEU:HD22	1.97	0.46
12:a:60:TYR:O	13:b:739:ARG:NH2	2.48	0.46
12:c:89:LEU:HD21	12:c:102:VAL:HB	1.98	0.46
13:d:180:TYR:HB3	13:d:182:VAL:HG13	1.98	0.46
1:m:17:LEU:HB3	1:m:21:SER:HB2	1.97	0.46
1:m:105:TYR:HH	1:m:443:SER:HG	1.58	0.46
1:m:319:LYS:HD2	1:m:332:HIS:CE1	2.51	0.46
4:R:622:TRP:HD1	4:R:652:VAL:HB	1.80	0.46
11:Y:187:SER:O	11:Y:191:THR:HG23	2.15	0.46
10:Z:1:MET:CE	10:Z:2:ARG:H	2.27	0.46
12:c:126:ILE:HD12	12:c:133:LYS:NZ	2.30	0.46
13:d:489:ARG:HD3	13:d:498:ALA:H	1.79	0.46
14:f:751:LEU:HD12	14:f:756:LEU:HD11	1.96	0.46
15:h:155:LYS:HA	15:h:155:LYS:HD2	1.59	0.46
16:n:103:TRP:CZ3	16:n:452:ARG:HD2	2.50	0.46
2:p:49:ARG:HG3	2:p:294:ARG:HE	1.80	0.46
2:p:152:LYS:NZ	2:p:192:CYS:O	2.48	0.46
3:C:197:LEU:HD22	3:C:265:LEU:HD11	1.98	0.46
3:D:211:VAL:HG13	3:D:224:VAL:HG23	1.98	0.46
3:H:187:GLY:H	3:H:239:ASN:HD21	1.62	0.46
4:R:691:TYR:HE2	4:R:693:ASP:HB2	1.80	0.46
8:T:294:GLU:HG2	8:T:313:GLN:HG2	1.97	0.46
8:T:534:ILE:HG23	8:T:548:VAL:HB	1.97	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:b:438:ARG:HH12	13:b:466:VAL:HG11	1.79	0.46
14:e:70:PHE:HZ	14:e:205:TYR:HB3	1.81	0.46
14:e:940:ARG:HG3	14:e:968:VAL:HG22	1.97	0.46
14:f:360:ILE:HA	14:f:363:PHE:HD1	1.80	0.46
14:f:396:LEU:HD21	14:f:444:VAL:HG23	1.97	0.46
1:m:217:ILE:HD11	1:m:267:LEU:HD13	1.97	0.46
2:p:42:TRP:CD2	2:p:67:LYS:HG3	2.51	0.46
3:A:461:SER:OG	3:A:461:SER:O	2.34	0.46
3:B:187:GLY:H	3:B:239:ASN:HD22	1.64	0.46
3:C:348:GLU:OE2	3:C:369:ARG:NE	2.44	0.46
3:E:529:ARG:NE	3:E:601:TYR:O	2.48	0.46
3:G:479:ASN:HD21	3:G:643:GLY:HA3	1.80	0.46
5:N:119:ARG:HA	5:N:119:ARG:HD2	1.63	0.46
7:P:602:LEU:HD22	7:P:607:ILE:HG21	1.98	0.46
7:P:748:GLU:HG3	7:P:777:LYS:HB2	1.97	0.46
4:R:484:MET:HE2	4:R:484:MET:HB2	1.81	0.46
10:W:66:VAL:HA	10:W:91:VAL:O	2.14	0.46
11:Y:214:ARG:HH21	10:Z:324:LYS:NZ	2.13	0.46
13:b:195:VAL:HB	13:b:199:ASN:HD22	1.80	0.46
13:d:149:GLU:HG2	13:d:298:ARG:HE	1.80	0.46
14:f:184:GLN:HE22	14:f:186:SER:HB3	1.81	0.46
14:f:260:ARG:HG3	14:f:548:THR:HG21	1.98	0.46
14:f:331:CYS:HB3	14:f:390:PHE:O	2.16	0.46
16:n:83:LYS:HB3	16:n:397:HIS:CE1	2.51	0.46
1:m:98:GLU:O	1:m:99:PHE:C	2.59	0.46
2:p:218:PHE:HB3	2:p:223:LEU:HD23	1.98	0.46
3:A:116:ILE:HA	3:A:185:VAL:HG12	1.97	0.46
3:D:308:CYS:HB3	3:D:665:SER:H	1.80	0.46
3:I:22:GLY:N	3:I:79:MET:O	2.45	0.46
12:a:31:PHE:HE2	12:a:58:THR:HA	1.80	0.46
13:b:210:TRP:CZ2	13:b:242:LYS:HG2	2.51	0.46
12:c:79:ASN:ND2	12:c:81:ASN:OD1	2.49	0.46
14:e:642:LEU:HD13	14:e:647:LEU:HD13	1.97	0.46
14:e:663:VAL:HG13	14:e:691:PHE:CD2	2.51	0.46
16:n:9:PRO:HG2	15:j:108:ASN:HD21	1.81	0.46
15:j:133:GLU:HA	15:j:136:ARG:HG2	1.98	0.46
3:C:35:ASP:OD1	3:C:36:LYS:NZ	2.48	0.46
3:D:19:CYS:O	3:D:113:GLY:CA	2.64	0.46
3:E:413:VAL:HG11	3:E:565:LEU:HD22	1.98	0.46
3:F:49:LEU:HD22	3:G:49:LEU:HD11	1.96	0.46
3:I:475:PHE:HE1	3:I:490:LEU:HD13	1.79	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:9:LEU:HG	3:K:27:LEU:HD12	1.96	0.46
5:N:49:MET:HE3	5:N:53:VAL:HG12	1.98	0.46
7:P:263:VAL:HG21	7:P:280:PHE:HD2	1.79	0.46
7:P:265:GLY:HA3	7:P:271:LEU:HD22	1.97	0.46
8:Q:557:PHE:HB2	8:Q:568:THR:HG22	1.96	0.46
4:R:681:PHE:HD2	4:R:706:LEU:HD12	1.81	0.46
4:R:787:GLN:HE21	4:R:791:TYR:HE1	1.62	0.46
5:U:76:LEU:HD12	5:U:101:MET:SD	2.56	0.46
10:W:12:CYS:HB2	18:W:501:GTP:C8	2.50	0.46
10:W:52:ASN:N	10:W:60:VAL:O	2.47	0.46
13:d:147:TRP:HB3	13:d:201:ARG:NH1	2.31	0.46
14:e:31:ARG:NH2	14:e:104:TRP:O	2.48	0.46
14:e:101:VAL:HG23	14:e:116:VAL:HG11	1.98	0.46
14:e:833:GLN:NE2	14:e:859:ASN:O	2.41	0.46
14:f:300:THR:O	14:f:304:THR:HG23	2.16	0.46
14:f:479:GLN:O	14:f:511:ARG:NH2	2.48	0.46
16:n:155:LYS:NZ	16:n:195:CYS:O	2.41	0.46
16:n:239:ILE:HD13	16:n:253:LEU:HD22	1.98	0.46
3:A:431:PHE:HZ	3:A:560:LEU:HG	1.81	0.46
3:A:442:LYS:O	3:A:446:GLU:HG2	2.15	0.46
3:F:118:LEU:HD22	3:F:181:MET:HE2	1.98	0.46
3:F:556:LEU:O	3:F:559:THR:OG1	2.32	0.46
3:G:386:SER:OG	3:G:387:GLY:N	2.47	0.46
7:P:341:SER:O	7:P:356:SER:OG	2.34	0.46
4:R:148:MET:O	4:R:292:THR:OG1	2.31	0.46
10:W:217:LEU:HD12	10:W:276:ARG:HB2	1.98	0.46
10:Z:152:ILE:HG23	10:Z:164:MET:HE3	1.97	0.46
12:a:45:TYR:OH	12:a:74:TYR:O	2.32	0.46
14:e:377:ASN:OD1	14:e:377:ASN:N	2.49	0.46
14:e:757:GLU:O	14:e:761:ILE:HG12	2.16	0.46
14:e:860:LEU:HD12	14:e:862:SER:H	1.79	0.46
14:f:65:LEU:HD11	14:f:96:LEU:HD12	1.97	0.46
14:f:273:HIS:CE1	17:f:1001:ATP:H1'	2.50	0.46
14:f:557:ALA:HA	14:f:560:VAL:HG22	1.98	0.46
14:f:616:PHE:HB3	14:f:621:GLN:HG2	1.98	0.46
15:l:53:ALA:O	15:l:57:LYS:NZ	2.44	0.46
3:B:307:LEU:HD13	3:B:666:ALA:HB2	1.98	0.46
3:B:543:PHE:HE1	3:B:578:LEU:HD13	1.81	0.46
3:B:617:ILE:O	3:B:648:PHE:HA	2.16	0.46
3:C:152:LEU:HD23	3:C:152:LEU:HA	1.81	0.46
3:D:465:MET:HE1	3:D:584:LEU:HA	1.97	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:663:CYS:SG	3:D:664:ALA:N	2.88	0.46
3:E:255:PRO:HG3	3:E:446:GLU:HB3	1.96	0.46
3:F:427:ILE:HG23	3:F:458:GLU:HA	1.97	0.46
3:I:42:ILE:HG23	3:I:93:VAL:HG12	1.97	0.46
3:I:137:LYS:NZ	3:I:284:ASP:OD2	2.49	0.46
8:Q:286:LYS:HD3	8:Q:575:SER:HB3	1.98	0.46
8:Q:492:HIS:HE1	8:Q:513:ILE:HG13	1.81	0.46
7:S:1110:GLN:HG2	7:S:1137:VAL:HG22	1.98	0.46
8:T:288:ARG:HH21	8:T:324:GLN:HA	1.81	0.46
11:X:116:ASP:OD1	11:X:117:LEU:N	2.49	0.46
10:Z:1:MET:HE3	10:Z:2:ARG:N	2.31	0.46
10:Z:274:THR:HG21	10:Z:280:GLN:HA	1.98	0.46
13:b:147:TRP:HB2	13:b:201:ARG:HH21	1.80	0.46
13:d:572:ARG:HD3	13:d:577:PHE:HA	1.98	0.46
14:e:62:ASP:HA	14:e:65:LEU:HB2	1.98	0.46
14:e:262:ASN:ND2	14:e:297:LYS:O	2.49	0.46
14:e:895:GLU:HG2	14:e:923:MET:HG2	1.97	0.46
14:f:82:THR:HA	14:f:206:LEU:HD12	1.97	0.46
15:l:100:LEU:HA	15:l:103:LEU:HB2	1.98	0.46
3:B:654:CYS:HA	3:B:657:ALA:HB2	1.98	0.46
3:D:9:LEU:HD13	3:D:32:CYS:HB2	1.98	0.46
3:G:642:LEU:HD23	3:G:642:LEU:HA	1.85	0.46
3:K:344:TRP:O	3:K:348:GLU:HB2	2.16	0.46
7:P:497:MET:HA	7:P:500:GLU:HG2	1.97	0.46
7:P:565:LEU:HD11	7:P:619:VAL:HA	1.97	0.46
7:P:983:VAL:HG23	7:P:987:ALA:HB3	1.97	0.46
4:R:148:MET:HB2	4:R:292:THR:HG23	1.97	0.46
4:R:415:GLU:HA	4:R:418:ARG:HE	1.81	0.46
11:Y:406:HIS:HA	11:Y:409:VAL:HG22	1.99	0.46
10:Z:358:PRO:HG2	10:Z:361:LEU:HB3	1.97	0.46
14:f:386:VAL:O	14:f:390:PHE:HD2	1.99	0.46
14:f:500:GLN:HA	14:f:503:MET:HG3	1.98	0.46
15:j:136:ARG:HB2	15:j:141:ILE:HB	1.97	0.46
1:m:55:ARG:NH1	1:m:108:ARG:HH11	2.14	0.45
1:m:150:TYR:HD2	7:P:851:THR:HG23	1.80	0.45
1:m:153:ARG:NH2	1:m:193:GLN:O	2.49	0.45
2:p:22:LEU:HA	2:p:25:VAL:HG22	1.98	0.45
3:C:303:LEU:N	3:C:669:ASN:O	2.44	0.45
3:E:20:MET:HE2	3:E:282:TYR:HD2	1.81	0.45
3:F:478:THR:OG1	3:F:480:ASP:OD1	2.26	0.45
3:G:505:LYS:HA	3:G:505:LYS:HD3	1.73	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:9:LEU:HD23	3:K:109:LEU:HD13	1.98	0.45
3:K:51:HIS:HB2	3:K:76:LEU:HB2	1.98	0.45
3:K:124:ARG:HH12	3:K:147:TRP:HA	1.81	0.45
3:K:650:ASP:OD1	3:K:650:ASP:N	2.43	0.45
6:O:51:LEU:O	6:O:55:PHE:HB2	2.16	0.45
4:R:302:GLU:O	4:R:306:LYS:HG3	2.16	0.45
12:a:29:ASP:OD1	12:a:31:PHE:N	2.42	0.45
13:b:251:LEU:HD12	13:b:268:ILE:HB	1.98	0.45
13:b:302:LYS:HB3	13:b:303:SER:H	1.58	0.45
13:b:609:MET:HE2	13:b:609:MET:HB2	1.82	0.45
14:f:734:LYS:HD3	14:f:763:LEU:HB3	1.97	0.45
14:f:833:GLN:HG3	14:f:861:TRP:CZ2	2.51	0.45
15:l:133:GLU:HA	15:l:136:ARG:HG2	1.98	0.45
2:p:369:ASP:OD1	2:p:372:GLY:N	2.50	0.45
3:B:178:LEU:HD22	3:B:248:GLU:HB3	1.97	0.45
3:H:676:LYS:HB2	3:H:679:LYS:HG3	1.97	0.45
3:I:141:MET:HE1	3:I:147:TRP:CE2	2.52	0.45
3:K:469:MET:HB2	3:K:469:MET:HE2	1.72	0.45
8:T:412:ARG:HE	8:T:421:ILE:HG21	1.81	0.45
14:e:251:TRP:CD1	14:e:292:VAL:HG21	2.51	0.45
14:f:946:MET:HG3	14:f:975:LEU:HD13	1.97	0.45
14:f:981:CYS:O	14:f:984:THR:OG1	2.32	0.45
1:m:369:ASP:OD1	1:m:373:LEU:N	2.49	0.45
2:p:23:LEU:HD12	2:p:23:LEU:HA	1.68	0.45
2:p:442:VAL:HA	2:p:462:LEU:HD13	1.99	0.45
3:A:373:LEU:HD23	3:A:373:LEU:HA	1.87	0.45
3:B:357:PRO:HD3	3:B:678:TRP:CH2	2.51	0.45
3:C:599:ARG:NH1	3:C:656:LEU:O	2.43	0.45
3:D:378:MET:HE2	3:D:388:TYR:HE1	1.82	0.45
3:E:378:MET:HE3	3:E:381:THR:HB	1.98	0.45
3:E:446:GLU:HA	3:E:449:TYR:HB2	1.97	0.45
3:G:198:ILE:HG13	3:G:266:SER:HB2	1.98	0.45
7:P:839:CYS:O	7:P:867:ASN:ND2	2.50	0.45
10:W:170:MET:HB2	10:W:203:ASP:HA	1.97	0.45
11:Y:176:GLN:NE2	11:Y:207:GLU:OE2	2.49	0.45
11:Y:402:ARG:HD2	11:Y:405:VAL:HG11	1.98	0.45
13:b:150:ALA:HB1	13:b:182:VAL:HB	1.98	0.45
14:e:234:SER:OG	14:e:236:ASN:OD1	2.33	0.45
14:e:246:LEU:HD21	14:e:279:CYS:HB2	1.99	0.45
14:e:599:LEU:HD13	14:e:625:PHE:CD2	2.51	0.45
14:f:433:CYS:HB3	14:f:491:GLU:HG2	1.97	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:p:2:GLU:HG2	15:l:141:ILE:HG23	1.98	0.45
3:A:20:MET:HA	3:A:113:GLY:HA3	1.98	0.45
3:E:306:TYR:HB2	3:E:667:ILE:HG23	1.99	0.45
3:G:1:MET:HE3	3:G:1:MET:HB3	1.78	0.45
3:H:422:LEU:HD11	3:H:677:TRP:HB3	1.99	0.45
3:I:508:GLU:HB3	3:I:510:TYR:HE1	1.81	0.45
3:I:527:ASN:HD21	3:I:656:LEU:HD12	1.82	0.45
3:I:575:ILE:HA	3:I:576:PRO:HD2	1.81	0.45
4:R:612:GLN:O	4:R:616:GLU:HG2	2.17	0.45
7:S:632:SER:O	7:S:636:GLN:HG2	2.16	0.45
10:W:293:MET:HB3	10:W:294:PHE:CD2	2.50	0.45
13:b:589:THR:OG1	13:b:590:GLU:OE1	2.34	0.45
14:e:518:LEU:HD11	14:e:564:TRP:CE2	2.52	0.45
14:e:730:LYS:HG2	14:e:759:GLU:HB2	1.98	0.45
3:B:39:SER:HB2	3:B:96:PHE:CE2	2.52	0.45
3:B:653:ASP:OD1	3:B:653:ASP:N	2.50	0.45
3:G:514:THR:HB	3:G:533:THR:HG22	1.98	0.45
3:G:634:LYS:O	3:G:638:LEU:HD12	2.16	0.45
3:I:1:MET:HG3	3:I:3:PHE:HE1	1.81	0.45
3:I:50:ILE:HA	3:I:76:LEU:O	2.15	0.45
5:N:56:ARG:HG2	5:N:112:HIS:CE1	2.51	0.45
7:P:667:LYS:HD3	7:P:667:LYS:HA	1.83	0.45
4:R:106:THR:HG23	4:R:168:LEU:HD11	1.98	0.45
4:R:693:ASP:HA	4:R:722:MET:HB2	1.99	0.45
7:S:245:ILE:O	7:S:369:ILE:HA	2.17	0.45
7:S:381:LYS:HD2	8:T:332:GLU:HA	1.98	0.45
12:a:85:CYS:HB2	12:a:119:LEU:HD23	1.98	0.45
13:b:139:VAL:HG12	13:b:200:VAL:HA	1.99	0.45
16:n:20:LEU:HD23	16:n:20:LEU:HA	1.80	0.45
15:l:54:ILE:HG22	15:l:103:LEU:HG	1.98	0.45
15:l:121:LYS:O	15:l:125:ASN:ND2	2.50	0.45
15:l:122:THR:O	15:l:126:MET:HG3	2.16	0.45
1:m:131:SER:HA	1:m:142:TRP:O	2.16	0.45
2:p:113:ARG:H	2:p:113:ARG:HD2	1.81	0.45
3:A:21:VAL:HA	3:A:78:ARG:NH2	2.31	0.45
3:A:299:THR:HG23	3:A:477:PRO:HB3	1.99	0.45
3:A:584:LEU:HD23	3:A:584:LEU:HA	1.82	0.45
3:B:238:GLU:HB3	3:B:241:ARG:HD2	1.99	0.45
3:C:122:ILE:O	3:C:148:GLY:N	2.46	0.45
3:C:376:PHE:HB2	3:C:379:LYS:HG3	1.98	0.45
3:D:573:ILE:HG23	3:D:638:LEU:HD12	1.99	0.45

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:40:PHE:CE1	3:H:67:ARG:HB2	2.51	0.45
7:S:996:LYS:HG3	7:S:1023:MET:HA	1.98	0.45
10:W:305:PRO:HG2	10:W:306:ARG:HH11	1.82	0.45
13:b:338:CYS:HB2	13:b:365:CYS:HB3	1.82	0.45
13:d:314:GLU:OE2	13:d:567:LYS:NZ	2.49	0.45
13:d:566:VAL:HB	13:d:583:LEU:HD23	1.98	0.45
14:e:148:GLU:O	14:e:152:SER:HB3	2.17	0.45
14:f:639:GLU:HA	14:f:668:SER:HB3	1.99	0.45
16:n:167:VAL:HG21	16:n:209:VAL:HG11	1.97	0.45
1:m:367:LEU:O	1:m:375:LEU:N	2.50	0.45
3:H:414:LYS:HB3	3:H:414:LYS:HE2	1.76	0.45
7:P:960:TYR:CZ	7:P:983:VAL:HB	2.52	0.45
4:R:322:ALA:HA	4:R:325:LEU:HD12	1.97	0.45
4:R:580:TYR:CZ	4:R:584:ILE:HD11	2.52	0.45
4:R:644:ASN:OD1	4:R:673:SER:OG	2.34	0.45
7:S:669:PHE:O	7:S:671:GLU:N	2.50	0.45
11:X:6:SER:O	11:X:65:ALA:HA	2.17	0.45
14:e:245:LEU:HD12	14:e:245:LEU:HA	1.85	0.45
16:n:399:ILE:HA	16:n:408:ASP:O	2.17	0.45
2:p:322:LYS:HG3	2:p:327:ILE:HG23	1.99	0.45
2:p:346:PRO:HB3	2:p:359:CYS:SG	2.57	0.45
3:B:370:VAL:HG13	3:B:373:LEU:HD21	1.99	0.45
3:C:529:ARG:HH12	3:C:601:TYR:HA	1.82	0.45
3:D:29:ILE:HD12	3:D:93:VAL:HG11	1.97	0.45
3:E:119:GLU:OE2	3:E:184:THR:OG1	2.22	0.45
3:E:283:LYS:HG2	3:F:431:PHE:CZ	2.51	0.45
3:E:337:ASP:HB2	3:E:340:ARG:HG3	1.98	0.45
3:K:184:THR:OG1	3:K:242:LYS:NZ	2.44	0.45
7:P:278:VAL:HA	7:P:320:LEU:O	2.16	0.45
7:P:307:ASP:O	7:P:311:LYS:HB2	2.16	0.45
4:R:192:LYS:HD3	4:R:235:GLU:H	1.80	0.45
4:R:926:PHE:O	4:R:927:GLU:HG2	2.17	0.45
7:S:824:LEU:HD12	7:S:852:LEU:HD11	1.98	0.45
8:T:158:CYS:SG	8:T:159:GLN:N	2.90	0.45
11:X:259:LEU:HD23	11:X:259:LEU:HA	1.86	0.45
11:Y:180:ALA:HB3	11:Y:183:GLU:HG3	1.99	0.45
13:b:717:GLN:HE21	13:b:717:GLN:HB3	1.54	0.45
13:b:762:ARG:HH21	13:b:765:GLN:HG2	1.81	0.45
13:d:210:TRP:HA	13:d:213:LEU:HG	1.99	0.45
13:d:330:GLU:O	13:d:346:HIS:NE2	2.50	0.45
14:f:401:LEU:HB2	14:f:404:GLN:HB3	1.98	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:j:65:HIS:ND1	15:j:68:ASP:OD2	2.44	0.45
1:m:51:LEU:HD23	1:m:52:TYR:H	1.82	0.45
1:m:174:LEU:O	1:m:183:LEU:N	2.48	0.45
3:B:184:THR:HG22	3:B:242:LYS:HG2	1.99	0.45
3:D:431:PHE:HB2	3:D:460:PHE:HB2	1.99	0.45
3:F:185:VAL:HG21	3:F:197:LEU:HD21	1.99	0.45
4:R:439:ILE:HG22	4:R:441:GLU:H	1.82	0.45
4:R:565:LYS:HB2	4:R:565:LYS:HE2	1.75	0.45
4:R:730:PRO:O	4:R:734:LYS:HG2	2.16	0.45
4:R:824:LEU:HD21	4:R:831:LEU:HD11	1.99	0.45
7:S:283:VAL:HG21	7:S:326:LEU:H	1.81	0.45
10:W:252:LYS:HZ1	11:X:100:ALA:HA	1.81	0.45
11:Y:139:HIS:NE2	11:Y:168:GLU:OE1	2.34	0.45
12:a:5:ARG:O	12:a:9:GLU:HB3	2.16	0.45
13:b:46:PHE:CE1	14:e:174:PRO:HD3	2.52	0.45
12:c:1:MET:HE2	12:c:3:LEU:HD23	1.99	0.45
13:d:132:LYS:N	13:d:135:GLU:OE1	2.50	0.45
14:e:907:LEU:HD13	14:e:935:LEU:HD21	1.98	0.45
15:j:26:THR:OG1	15:j:111:ASP:OD2	2.24	0.45
1:m:288:ARG:HD3	1:m:302:MET:HE1	1.99	0.45
2:p:103:ALA:HB1	2:p:121:ILE:HD11	1.98	0.45
2:p:215:LEU:O	2:p:228:ARG:HA	2.17	0.45
3:B:21:VAL:HA	3:B:79:MET:HB3	1.99	0.45
3:C:214:SER:HB3	3:C:221:TYR:CD1	2.52	0.45
3:F:344:TRP:CD1	3:F:344:TRP:H	2.34	0.45
7:P:324:ASP:HA	7:P:371:THR:HB	1.98	0.45
8:Q:291:LYS:HD2	8:Q:329:ARG:HH12	1.82	0.45
4:R:506:LYS:HA	4:R:509:GLN:HB2	1.98	0.45
7:S:843:ILE:O	7:S:847:GLU:HG2	2.17	0.45
7:S:1059:LEU:HD21	7:S:1062:LEU:HD13	1.99	0.45
5:U:39:GLN:HE21	5:U:39:GLN:HB2	1.60	0.45
10:W:286:VAL:HG11	10:W:326:VAL:HG12	1.99	0.45
11:X:88:HIS:CD2	11:X:90:GLU:H	2.34	0.45
11:X:311:LYS:HD2	11:X:342:GLN:HB2	1.99	0.45
11:Y:288:VAL:HA	11:Y:291:ILE:HD12	1.99	0.45
11:Y:314:ALA:HB3	11:Y:380:ASN:HB3	1.98	0.45
14:e:417:LEU:HD13	14:e:431:MET:HE3	1.97	0.45
14:e:638:LYS:HA	14:e:667:ALA:HB3	1.99	0.45
14:f:815:ASP:O	14:f:819:LYS:HD3	2.17	0.45
14:f:953:LYS:H	14:f:953:LYS:HG2	1.50	0.45
1:m:280:ASP:HB2	7:S:1054:GLN:OE1	2.16	0.44

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:348:GLU:OE1	3:A:369:ARG:N	2.45	0.44
3:A:424:ARG:NH1	3:A:564:GLU:OE1	2.43	0.44
3:C:436:GLU:OE2	3:C:594:THR:OG1	2.30	0.44
3:G:515:LEU:HG	3:G:623:PRO:HD3	2.00	0.44
7:P:424:ASN:HB2	7:P:459:GLN:HE22	1.82	0.44
8:Q:480:GLU:HB3	8:Q:482:TRP:HD1	1.82	0.44
7:S:292:SER:HB3	7:S:350:ILE:HD11	1.98	0.44
8:T:558:ASP:OD1	8:T:559:MET:N	2.50	0.44
10:Z:20:PHE:O	10:Z:24:ILE:HG12	2.17	0.44
10:Z:118:ASP:O	10:Z:122:LYS:NZ	2.50	0.44
13:d:246:ARG:NE	14:f:465:ALA:O	2.49	0.44
14:e:45:THR:HG23	14:e:373:THR:HB	1.98	0.44
14:e:862:SER:HA	14:e:891:ARG:HB3	1.98	0.44
14:f:486:LEU:HA	14:f:489:ILE:HG12	1.98	0.44
15:h:57:LYS:HE2	15:h:57:LYS:HB2	1.67	0.44
16:n:353:GLY:HA3	16:n:393:VAL:HB	1.98	0.44
1:m:152:THR:N	1:m:166:ILE:O	2.48	0.44
1:m:204:PRO:HB2	1:m:220:ILE:HD12	1.99	0.44
3:B:53:SER:HB2	3:B:74:VAL:HG13	1.99	0.44
3:C:114:ILE:HD11	3:C:192:LEU:HD13	1.98	0.44
5:N:80:SER:O	5:N:80:SER:OG	2.35	0.44
7:P:237:GLN:HE22	7:P:240:PHE:HB3	1.82	0.44
7:P:323:ILE:HG22	7:P:326:LEU:HD11	2.00	0.44
8:Q:426:LYS:HA	8:Q:426:LYS:HD2	1.84	0.44
8:Q:484:LEU:HD11	8:Q:492:HIS:HB3	1.99	0.44
4:R:871:ASP:O	4:R:875:MET:HG2	2.18	0.44
7:S:812:MET:HE1	7:S:836:LEU:HD22	1.99	0.44
8:T:403:LEU:HD21	8:T:437:VAL:HG21	1.99	0.44
10:Z:77:ARG:NH1	10:Z:77:ARG:O	2.50	0.44
13:b:251:LEU:HB2	13:b:268:ILE:HD12	1.98	0.44
14:e:751:LEU:HD21	14:e:756:LEU:HD22	1.97	0.44
14:f:146:PRO:HG2	14:f:149:GLN:HB3	1.99	0.44
14:f:899:LEU:HD21	14:f:925:ASN:HA	1.99	0.44
15:j:134:GLU:HA	15:j:137:LYS:HG2	2.00	0.44
3:A:92:LEU:HD12	3:A:108:VAL:HG12	1.99	0.44
3:D:323:LEU:HA	3:D:326:LYS:HD3	1.99	0.44
3:F:20:MET:HE2	3:F:20:MET:HB2	1.55	0.44
3:K:11:LEU:HB2	3:K:32:CYS:HB2	1.99	0.44
3:K:269:GLU:HB2	3:K:281:LEU:HD11	2.00	0.44
3:K:507:LYS:HA	3:K:507:LYS:HE3	1.98	0.44
5:N:52:TRP:CZ3	5:N:53:VAL:HG23	2.53	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:N:62:GLN:HA	5:N:65:ILE:HG12	1.99	0.44
4:R:650:ILE:HD12	4:R:679:VAL:HB	1.99	0.44
4:R:695:SER:HA	4:R:724:ALA:H	1.81	0.44
4:R:726:CYS:HB3	4:R:728:LEU:HD12	2.00	0.44
5:U:76:LEU:HD11	5:U:105:LEU:HD11	1.99	0.44
11:Y:209:ILE:HG22	11:Y:227:LEU:HD22	1.99	0.44
11:Y:229:ARG:NE	11:Y:363:VAL:HG11	2.33	0.44
10:Z:336:LYS:HA	10:Z:336:LYS:HD3	1.77	0.44
13:d:16:VAL:HG22	13:d:35:VAL:HG11	1.98	0.44
13:d:255:ILE:HG22	13:d:257:LEU:HG	2.00	0.44
14:e:989:TRP:CD1	14:e:989:TRP:H	2.34	0.44
14:f:46:SER:O	14:f:46:SER:OG	2.31	0.44
14:f:217:ARG:HH12	14:f:341:MET:HG3	1.81	0.44
14:f:395:TYR:HE2	14:f:417:LEU:HD22	1.83	0.44
16:n:400:VAL:HB	16:n:408:ASP:HB2	1.99	0.44
15:j:117:ASP:O	15:j:121:LYS:HG2	2.17	0.44
3:B:121:ASP:OD1	3:B:121:ASP:N	2.46	0.44
3:B:478:THR:HG22	3:B:480:ASP:H	1.81	0.44
3:C:653:ASP:N	3:C:653:ASP:OD1	2.46	0.44
3:G:11:LEU:O	3:G:13:ASN:N	2.50	0.44
3:K:267:LEU:HB3	3:K:282:TYR:HB3	1.99	0.44
7:P:372:THR:OG1	7:P:373:ARG:N	2.51	0.44
7:P:696:LYS:HB3	7:P:696:LYS:HE2	1.77	0.44
8:Q:397:THR:HG22	8:Q:437:VAL:HG11	1.98	0.44
11:Y:223:THR:H	11:Y:226:ASN:HB3	1.82	0.44
10:Z:117:LEU:HD11	10:Z:154:LYS:HB3	1.99	0.44
10:Z:309:ARG:HD2	10:Z:342:VAL:HG12	2.00	0.44
10:Z:314:ALA:HA	10:Z:350:LYS:HG2	1.99	0.44
13:b:6:ARG:O	13:b:70:GLN:HA	2.17	0.44
13:b:421:ASN:HB3	13:b:463:TYR:CZ	2.52	0.44
12:c:124:ALA:O	12:c:128:LYS:HG2	2.18	0.44
1:m:118:LYS:HA	1:m:118:LYS:HD3	1.82	0.44
2:p:31:ASN:O	2:p:35:LEU:HG	2.17	0.44
2:p:145:PRO:O	2:p:147:GLN:NE2	2.50	0.44
3:A:118:LEU:HD23	3:A:284:ASP:HB3	1.98	0.44
3:A:391:ARG:HA	3:A:391:ARG:HD2	1.83	0.44
3:E:68:SER:OG	3:E:70:ASN:OD1	2.35	0.44
3:F:577:GLN:NE2	3:F:578:LEU:O	2.50	0.44
3:G:4:GLN:HA	3:G:25:ILE:HG12	1.99	0.44
3:I:97:CYS:HB2	3:I:103:PRO:HA	2.00	0.44
7:P:852:LEU:O	7:P:855:SER:OG	2.33	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:642:ASP:OD1	4:R:671:ASN:ND2	2.49	0.44
8:T:287:VAL:HG23	8:T:576:VAL:HG23	1.99	0.44
8:T:437:VAL:HG22	8:T:442:ILE:HG13	2.00	0.44
10:Z:392:LYS:HE2	10:Z:395:LEU:HD23	1.98	0.44
13:b:521:ILE:H	13:b:521:ILE:HD12	1.83	0.44
12:c:3:LEU:O	12:c:7:ASN:ND2	2.50	0.44
12:c:29:ASP:OD2	12:c:32:HIS:ND1	2.50	0.44
12:c:95:PRO:HG2	13:d:749:PRO:HB3	1.99	0.44
13:d:20:SER:OG	13:d:22:LEU:O	2.35	0.44
13:d:615:TYR:CE1	13:d:619:LEU:HD21	2.53	0.44
14:e:908:LEU:HD21	14:e:934:ASN:HB2	1.98	0.44
1:m:411:GLU:OE1	15:h:161:GLU:HG2	2.17	0.44
2:p:344:GLU:HB3	2:p:361:THR:HB	2.00	0.44
3:A:414:LYS:HG3	3:A:419:ASP:HB3	2.00	0.44
3:A:615:LEU:HD11	3:A:644:LEU:HD13	1.98	0.44
3:H:541:LYS:HA	3:H:541:LYS:HD2	1.76	0.44
3:I:328:LYS:HA	3:I:328:LYS:HD2	1.81	0.44
6:O:73:ILE:HG22	6:O:88:ILE:HG12	1.99	0.44
8:Q:514:LEU:HD11	8:Q:530:MET:HG2	1.99	0.44
4:R:464:LEU:HD12	4:R:465:LYS:H	1.82	0.44
7:S:653:LEU:HD12	7:S:662:VAL:HG22	2.00	0.44
11:Y:361:THR:OG1	11:Y:362:VAL:N	2.51	0.44
10:Z:3:GLU:HG3	10:Z:127:CYS:HB3	1.98	0.44
12:c:25:PRO:HA	12:c:33:TRP:HD1	1.82	0.44
13:d:251:LEU:HD12	13:d:268:ILE:HB	1.98	0.44
14:e:662:ARG:NH1	14:e:688:SER:O	2.50	0.44
14:f:707:LEU:HD13	14:f:721:LEU:HD22	2.00	0.44
15:l:132:PRO:HA	15:l:135:ILE:HG22	2.00	0.44
1:m:219:ARG:HB2	1:m:226:ILE:HD11	2.00	0.44
1:m:290:PHE:HE2	1:m:293:PRO:HD3	1.82	0.44
3:A:144:MET:SD	3:A:145:ASN:ND2	2.91	0.44
3:A:442:LYS:HE3	3:A:442:LYS:HB3	1.71	0.44
3:B:503:GLU:HG3	3:B:538:LEU:HD22	1.99	0.44
3:D:41:THR:HG22	3:D:94:SER:OG	2.17	0.44
3:D:205:GLU:O	3:D:209:THR:HG22	2.18	0.44
3:D:605:MET:HA	3:D:618:PRO:HD2	2.00	0.44
3:E:297:PRO:HG2	3:E:300:GLN:HG2	1.99	0.44
3:E:489:ARG:NH2	3:E:570:LYS:O	2.43	0.44
3:I:543:PHE:CZ	3:I:578:LEU:HB3	2.51	0.44
4:M:15:ARG:NH2	7:P:707:SER:OG	2.48	0.44
7:P:928:THR:HG23	7:P:959:ALA:HB2	1.99	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Q:451:LEU:HD22	8:Q:485:LEU:HD21	2.00	0.44
4:R:598:LYS:HG3	4:R:637:GLU:HB2	1.99	0.44
8:T:438:LYS:HG2	8:T:476:HIS:CE1	2.53	0.44
11:X:223:THR:HG22	11:X:224:TYR:H	1.83	0.44
11:X:345:ASP:H	11:X:438:ASP:HA	1.81	0.44
10:Z:196:THR:OG1	10:Z:197:ASP:N	2.50	0.44
10:Z:316:ILE:HG12	10:Z:352:ALA:HB3	1.99	0.44
12:a:5:ARG:HA	12:a:8:LYS:HG2	2.00	0.44
13:b:596:ARG:HD2	13:b:596:ARG:HA	1.84	0.44
15:l:4:ILE:HD12	15:l:4:ILE:HA	1.86	0.44
1:m:82:ARG:HG3	15:h:163:LYS:HE2	1.98	0.44
1:m:357:ILE:HD11	1:m:370:ILE:HG22	1.99	0.44
2:p:396:ILE:HG23	2:p:404:LEU:HD11	1.99	0.44
3:A:181:MET:HE2	3:A:181:MET:HB3	1.86	0.44
3:B:224:VAL:HG21	3:B:245:PHE:HE2	1.83	0.44
3:G:430:SER:OG	3:G:438:ARG:O	2.35	0.44
3:K:474:CYS:SG	3:K:475:PHE:N	2.91	0.44
7:P:360:LYS:NZ	7:P:366:SER:O	2.50	0.44
4:R:700:SER:OG	4:R:702:ASN:OD1	2.34	0.44
10:W:141:GLY:O	10:W:145:SER:CB	2.66	0.44
11:X:7:ILE:HG13	11:X:66:VAL:HG13	1.99	0.44
11:X:229:ARG:O	11:X:233:GLN:HG2	2.18	0.44
11:X:253:THR:O	11:X:257:THR:HG23	2.18	0.44
11:Y:64:ARG:HA	11:Y:64:ARG:HD3	1.76	0.44
10:Z:3:GLU:HB2	10:Z:130:LEU:HA	1.99	0.44
10:Z:77:ARG:NH2	10:Z:83:GLN:OE1	2.51	0.44
10:Z:253:LEU:O	10:Z:257:MET:HB2	2.17	0.44
13:b:682:LYS:H	13:b:682:LYS:HG2	1.56	0.44
13:d:203:ARG:HE	13:d:203:ARG:HB2	1.47	0.44
14:e:671:LEU:HA	14:e:675:ARG:HH12	1.83	0.44
14:e:764:LEU:HD22	14:e:778:LEU:HD11	2.00	0.44
3:C:14:PRO:HG3	3:C:108:VAL:HG23	2.00	0.44
3:D:306:TYR:O	3:D:666:ALA:HA	2.18	0.44
3:E:279:ILE:HD11	3:F:549:TYR:CD1	2.53	0.44
3:E:379:LYS:HA	3:E:382:LEU:HD23	2.00	0.44
3:F:6:SER:HA	3:F:27:LEU:HA	2.00	0.44
3:F:66:TRP:HD1	3:G:145:ASN:HA	1.82	0.44
3:F:475:PHE:CE1	3:F:490:LEU:HD12	2.53	0.44
3:I:49:LEU:HG	3:I:78:ARG:HG2	2.00	0.44
3:K:181:MET:SD	3:K:245:PHE:HB2	2.58	0.44
4:R:104:LYS:HD3	4:R:108:ASP:HB2	2.00	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:371:THR:HG21	4:R:503:LEU:HD21	2.00	0.44
4:R:711:LEU:HD23	4:R:711:LEU:HA	1.85	0.44
4:R:760:ILE:HG12	4:R:788:CYS:HB3	1.99	0.44
7:S:524:ILE:HG21	7:S:533:LEU:HD22	2.00	0.44
7:S:662:VAL:O	7:S:666:LEU:HB2	2.17	0.44
7:S:1020:LEU:HB3	7:S:1048:LEU:HD21	1.99	0.44
11:X:35:GLN:NE2	11:X:36:MET:O	2.50	0.44
10:Z:112:LEU:HD12	10:Z:112:LEU:HA	1.83	0.44
10:Z:139:LEU:HB2	10:Z:171:PRO:HD3	2.00	0.44
12:a:20:GLN:HA	13:b:622:LYS:HZ1	1.83	0.44
12:c:132:ASP:OD1	12:c:133:LYS:N	2.50	0.44
14:e:98:LYS:HA	14:e:101:VAL:HG12	2.00	0.44
14:e:314:ILE:H	14:e:314:ILE:HG13	1.63	0.44
14:e:882:LEU:HD22	14:e:917:VAL:HG13	1.98	0.44
14:f:543:LYS:HA	14:f:546:LEU:HB3	1.99	0.44
2:p:369:ASP:OD1	2:p:373:HIS:N	2.50	0.43
3:A:625:ILE:HD13	3:A:625:ILE:HA	1.79	0.43
3:B:203:GLU:O	3:B:207:LYS:HG3	2.17	0.43
3:D:48:ILE:HD11	3:D:77:VAL:HB	1.99	0.43
3:F:46:PRO:HG3	3:G:131:PRO:HD3	2.00	0.43
3:I:11:LEU:HG	3:I:32:CYS:HB2	2.00	0.43
3:I:391:ARG:HA	3:I:391:ARG:HD2	1.81	0.43
4:M:74:LEU:HA	4:M:77:ILE:HB	1.99	0.43
7:P:761:MET:HE3	7:P:764:LEU:HD23	2.00	0.43
8:Q:426:LYS:NZ	8:Q:427:GLY:O	2.49	0.43
8:Q:441:ASN:HA	8:Q:454:TRP:O	2.18	0.43
4:R:763:LEU:HD23	4:R:763:LEU:HA	1.89	0.43
4:R:814:ASP:HB2	4:R:844:ARG:HG3	1.99	0.43
10:Z:36:TYR:OH	10:Z:40:SER:O	2.32	0.43
10:Z:344:TRP:CD1	10:Z:344:TRP:H	2.36	0.43
13:b:70:GLN:HE22	14:e:190:PHE:HB2	1.83	0.43
14:e:931:SER:OG	14:e:932:ILE:N	2.51	0.43
14:f:346:TYR:HB2	14:f:349:ASN:ND2	2.33	0.43
14:f:918:ILE:HG22	14:f:946:MET:HA	2.00	0.43
1:m:350:GLY:HA3	1:m:390:VAL:HG21	2.00	0.43
2:p:10:LEU:HD23	2:p:13:ILE:HD12	1.99	0.43
2:p:88:PHE:CE2	2:p:462:LEU:HG	2.53	0.43
3:B:193:GLN:O	3:B:270:LYS:NZ	2.51	0.43
3:B:514:THR:HA	3:B:533:THR:HA	1.99	0.43
3:C:78:ARG:C	3:C:79:MET:HE2	2.43	0.43
3:F:486:LYS:HB3	3:F:486:LYS:HE2	1.89	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:300:PHE:O	4:R:304:SER:OG	2.34	0.43
4:R:364:ARG:HG3	4:R:365:ARG:HG2	1.99	0.43
4:R:538:ASN:O	4:R:542:GLN:NE2	2.51	0.43
7:S:657:GLN:O	7:S:687:TYR:OH	2.36	0.43
8:T:411:VAL:O	8:T:425:LEU:HB2	2.17	0.43
10:W:228:LEU:HD13	10:W:273:LEU:HD22	2.00	0.43
13:d:157:LYS:HA	13:d:178:ILE:HA	2.00	0.43
13:d:506:LEU:HD12	13:d:506:LEU:HA	1.86	0.43
14:f:59:THR:HB	14:f:62:ASP:HB3	1.98	0.43
15:j:54:ILE:O	15:j:58:VAL:HG12	2.18	0.43
1:m:436:LYS:HD2	1:m:438:LEU:HD21	2.00	0.43
2:p:438:LEU:HD12	2:p:445:ILE:HD11	1.99	0.43
3:D:37:CYS:HA	3:D:98:PRO:HD2	2.00	0.43
3:F:131:PRO:O	3:F:131:PRO:HD2	2.18	0.43
3:F:368:PRO:O	3:F:393:THR:OG1	2.33	0.43
3:H:35:ASP:OD1	3:H:35:ASP:N	2.50	0.43
3:H:175:ILE:HD13	3:H:175:ILE:HA	1.84	0.43
3:K:307:LEU:HD23	3:K:331:VAL:HG13	1.99	0.43
7:P:643:PRO:HB2	7:P:675:LEU:HD12	2.00	0.43
7:S:508:VAL:HG12	7:S:545:VAL:HB	2.00	0.43
7:S:599:LEU:O	7:S:603:MET:HG2	2.18	0.43
7:S:937:PHE:HE2	7:S:945:LEU:HD22	1.83	0.43
10:W:358:PRO:CG	10:W:364:SER:HB3	2.47	0.43
11:X:157:LEU:HD22	11:X:161:TYR:HE2	1.84	0.43
10:Z:284:LEU:HB2	10:Z:362:LYS:HZ3	1.82	0.43
13:b:180:TYR:HB3	13:b:182:VAL:HG13	2.00	0.43
13:b:479:ASN:O	13:b:585:ARG:HA	2.17	0.43
13:d:57:THR:HG23	13:d:59:PHE:H	1.82	0.43
13:d:217:GLN:HG3	13:d:219:VAL:HG13	2.01	0.43
14:e:629:ASN:OD1	14:e:630:LYS:N	2.48	0.43
14:f:447:LEU:HD23	14:f:447:LEU:HA	1.75	0.43
14:f:787:PRO:HG3	14:f:813:LEU:HA	2.01	0.43
2:p:126:SER:O	2:p:127:MET:C	2.60	0.43
2:p:281:LEU:HD23	2:p:281:LEU:HA	1.77	0.43
3:C:152:LEU:HG	3:C:356:ALA:HB2	2.01	0.43
3:D:144:MET:HA	3:D:679:LYS:HD2	2.00	0.43
3:D:329:VAL:HG21	3:D:611:LEU:HD11	2.00	0.43
3:E:36:LYS:H	3:E:36:LYS:HG2	1.61	0.43
3:F:138:LYS:HB2	3:F:138:LYS:HE3	1.80	0.43
3:F:599:ARG:HH12	3:F:658:ASN:HA	1.83	0.43
3:I:652:PHE:O	3:I:656:LEU:HB2	2.18	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:P:591:ARG:HE	7:P:591:ARG:HB2	1.62	0.43
11:Y:104:ALA:HB2	11:Y:413:MET:HE2	2.01	0.43
11:Y:139:HIS:CD2	11:Y:150:THR:HG21	2.53	0.43
11:Y:381:THR:OG1	11:Y:382:THR:N	2.52	0.43
12:a:60:TYR:CD2	12:a:61:PRO:HA	2.53	0.43
14:f:85:LEU:HD23	14:f:228:VAL:HB	2.01	0.43
14:f:778:LEU:HD23	14:f:803:LEU:HD21	2.00	0.43
14:f:865:LEU:HD23	14:f:893:GLY:H	1.83	0.43
1:m:366:LEU:HD23	1:m:374:ARG:HD2	2.00	0.43
3:A:551:GLU:HA	3:A:554:ILE:HG22	2.00	0.43
3:C:215:GLN:H	3:C:215:GLN:HG2	1.67	0.43
3:E:155:CYS:SG	3:E:387:GLY:HA3	2.58	0.43
7:P:1014:GLN:H	7:P:1014:GLN:HG3	1.61	0.43
8:Q:347:ARG:H	8:Q:362:GLY:HA2	1.83	0.43
4:R:150:PHE:HB2	4:R:291:CYS:SG	2.58	0.43
4:R:477:ASN:ND2	4:R:479:GLU:OE1	2.52	0.43
7:S:238:LYS:HA	7:S:238:LYS:HD3	1.78	0.43
7:S:1091:ASN:HB2	7:S:1150:TRP:CD2	2.53	0.43
13:d:768:GLN:NE2	13:d:778:TYR:OH	2.52	0.43
14:e:81:GLN:HA	14:e:205:TYR:HD1	1.84	0.43
14:e:486:LEU:HD23	14:e:486:LEU:HA	1.93	0.43
14:e:517:GLN:NE2	14:e:521:TYR:OH	2.52	0.43
14:e:630:LYS:HA	14:e:630:LYS:HD2	1.85	0.43
14:e:852:SER:HA	14:e:855:VAL:HG12	2.01	0.43
15:j:56:LYS:HZ1	15:j:60:GLN:HB3	1.82	0.43
15:l:20:ILE:HD13	15:l:20:ILE:HA	1.93	0.43
1:m:42:TRP:CD2	1:m:67:LYS:HG3	2.54	0.43
1:m:365:LEU:HD12	1:m:365:LEU:HA	1.86	0.43
1:m:422:LEU:HD23	1:m:422:LEU:HA	1.90	0.43
2:p:337:PHE:HZ	2:p:357:ILE:HD12	1.84	0.43
3:A:561:LEU:HD12	3:A:561:LEU:HA	1.83	0.43
3:F:532:LYS:HE3	3:F:536:GLN:HG3	2.01	0.43
3:H:29:ILE:O	3:H:33:ALA:HB2	2.18	0.43
3:H:240:ARG:HH12	3:H:242:LYS:HE2	1.83	0.43
3:I:419:ASP:OD1	3:I:420:TYR:N	2.52	0.43
3:K:201:THR:OG1	3:K:262:SER:O	2.31	0.43
6:O:14:ASP:O	6:O:16:LYS:NZ	2.52	0.43
4:R:465:LYS:NZ	4:R:520:LEU:O	2.51	0.43
8:T:338:SER:O	8:T:342:ASN:HA	2.18	0.43
8:T:386:CYS:HB3	8:T:414:TRP:HZ2	1.84	0.43
10:W:52:ASN:HD22	10:W:86:ARG:HH22	1.64	0.43

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:X:111:GLY:O	11:X:115:ILE:HB	2.18	0.43
11:X:171:ILE:HG21	18:X:501:GTP:N3	2.34	0.43
11:X:195:LEU:HD11	11:X:428:LEU:HD12	2.01	0.43
11:X:203:MET:HE3	11:X:267:PHE:HB3	1.99	0.43
13:b:258:LEU:H	13:b:261:SER:HB3	1.84	0.43
13:b:619:LEU:HD21	14:e:313:ARG:HG3	1.99	0.43
13:d:220:MET:N	13:d:220:MET:SD	2.91	0.43
14:e:486:LEU:HD22	14:e:524:CYS:SG	2.59	0.43
14:e:639:GLU:H	14:e:667:ALA:HB3	1.84	0.43
14:e:785:PHE:H	14:e:811:ASN:HD21	1.65	0.43
14:e:949:LEU:HB3	14:e:977:ILE:HG23	2.00	0.43
14:f:69:ILE:HG12	14:f:228:VAL:HG21	2.00	0.43
14:f:794:SER:HA	14:f:797:LEU:HG	2.00	0.43
14:f:867:HIS:HA	14:f:895:GLU:HB2	1.99	0.43
2:p:122:CYS:HB3	2:p:156:THR:HG21	2.01	0.43
2:p:207:LEU:HD22	2:p:215:LEU:HD21	2.00	0.43
3:A:505:LYS:HG3	3:A:510:TYR:CE1	2.54	0.43
3:A:529:ARG:NH2	3:A:600:PRO:O	2.52	0.43
3:G:305:VAL:HG22	3:G:668:ILE:HG23	2.01	0.43
3:I:340:ARG:HB3	3:I:344:TRP:CD1	2.54	0.43
3:K:115:GLU:N	3:K:186:GLU:OE2	2.52	0.43
7:P:1024:ILE:HD12	7:P:1048:LEU:HD11	2.01	0.43
8:Q:299:VAL:HG12	8:Q:310:THR:HG22	1.99	0.43
7:S:321:PHE:HB2	7:S:367:PHE:O	2.19	0.43
9:V:54:MET:HB3	9:V:54:MET:HE2	1.69	0.43
11:Y:8:HIS:HE1	11:Y:16:ILE:HG22	1.83	0.43
11:Y:122:ILE:HD13	11:Y:122:ILE:HA	1.89	0.43
10:Z:122:LYS:HA	10:Z:122:LYS:HD3	1.81	0.43
13:b:564:LYS:HG2	13:b:587:ASP:HB3	2.01	0.43
13:d:222:ASN:ND2	13:d:231:ARG:HB2	2.33	0.43
13:d:252:TYR:HB3	13:d:265:ASN:HA	2.01	0.43
15:h:47:LEU:HD21	15:h:110:LEU:HD21	1.99	0.43
15:j:132:PRO:HA	15:j:135:ILE:HG12	1.99	0.43
15:l:54:ILE:O	15:l:58:VAL:HG23	2.18	0.43
3:B:305:VAL:HB	3:B:331:VAL:HG12	2.00	0.43
3:C:478:THR:HG22	3:C:642:LEU:HB3	1.99	0.43
3:E:200:HIS:CE1	3:E:264:SER:HB2	2.54	0.43
3:E:212:TYR:O	3:E:246:TYR:N	2.46	0.43
3:I:321:THR:O	3:I:325:GLU:HG2	2.19	0.43
3:I:370:VAL:HB	3:I:373:LEU:HG	2.00	0.43
6:O:8:GLN:HE21	6:O:60:GLU:HA	1.83	0.43

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:U:75:LEU:O	5:U:91:ILE:HA	2.19	0.43
9:V:48:GLN:HA	9:V:49:PRO:HD3	1.86	0.43
10:W:28:HIS:HA	10:W:43:GLN:HB3	2.01	0.43
11:X:313:MET:HG3	11:X:344:VAL:HG11	2.00	0.43
11:Y:98:ASP:OD2	10:Z:2:ARG:NH1	2.51	0.43
10:Z:133:PHE:HB2	10:Z:164:MET:HG3	2.01	0.43
10:Z:386:THR:O	10:Z:390:ARG:HB2	2.19	0.43
13:b:160:LEU:HD22	13:b:164:GLU:HG3	2.00	0.43
13:d:522:ASN:ND2	13:d:525:GLY:O	2.47	0.43
14:e:764:LEU:HD13	14:e:778:LEU:HD21	2.00	0.43
14:f:88:ALA:O	14:f:93:LYS:NZ	2.52	0.43
14:f:234:SER:OG	14:f:235:LYS:N	2.52	0.43
14:f:651:CYS:O	14:f:655:LYS:HG2	2.19	0.43
14:f:684:GLN:NE2	14:f:709:GLU:O	2.49	0.43
14:f:905:GLN:HE21	14:f:905:GLN:HB2	1.66	0.43
1:m:444:ILE:O	1:m:460:TYR:HB2	2.19	0.43
3:A:518:ASP:HB2	3:A:624:LYS:HE2	2.01	0.43
3:E:263:LEU:HD23	3:E:263:LEU:HA	1.91	0.43
3:F:392:GLN:NE2	3:F:393:THR:O	2.51	0.43
3:G:260:LEU:HD23	3:G:260:LEU:HA	1.92	0.43
3:H:634:LYS:O	3:H:638:LEU:HG	2.18	0.43
3:I:459:LEU:HD23	3:I:459:LEU:HA	1.76	0.43
5:N:141:LEU:HD11	6:O:49:ARG:HH22	1.84	0.43
7:P:966:ARG:O	7:P:970:ASN:HB2	2.19	0.43
4:R:633:LYS:HB3	4:R:663:THR:HG21	2.00	0.43
7:S:872:LYS:HE2	7:S:872:LYS:HB3	1.53	0.43
11:Y:406:HIS:CG	10:Z:261:PRO:HG3	2.54	0.43
10:Z:170:MET:SD	10:Z:377:LEU:HD11	2.58	0.43
13:d:503:ASP:HB2	13:d:578:LEU:HB2	2.01	0.43
14:f:268:MET:HE3	14:f:274:MET:HB3	2.01	0.43
14:f:510:VAL:HG12	14:f:512:VAL:HG23	2.01	0.43
14:f:602:PRO:O	14:f:605:LYS:NZ	2.50	0.43
15:h:112:ILE:HG13	15:h:115:LEU:HB2	2.00	0.43
1:m:5:LEU:HA	1:m:6:PRO:HD3	1.86	0.43
1:m:100:ARG:HH12	1:m:435:ILE:HB	1.84	0.43
2:p:16:TYR:CE2	15:l:121:LYS:HG2	2.53	0.43
3:B:549:TYR:HA	3:B:552:LYS:HE3	2.01	0.43
3:F:378:MET:HA	3:F:381:THR:HG22	1.99	0.43
3:F:575:ILE:HD12	3:F:635:VAL:HG22	2.01	0.43
3:K:139:LYS:HG3	3:K:147:TRP:HE1	1.83	0.43
3:K:194:ASN:HD21	3:K:272:HIS:HE1	1.67	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:N:48:TYR:HD2	5:N:86:LEU:HD11	1.84	0.43
5:N:129:PHE:O	5:N:133:ARG:HG2	2.18	0.43
7:P:1059:LEU:HD21	7:P:1062:LEU:HD13	2.00	0.43
4:R:238:LEU:HB3	4:R:288:ARG:HG2	2.00	0.43
4:R:681:PHE:CE2	4:R:703:GLU:HG3	2.54	0.43
10:W:299:MET:HA	10:W:299:MET:HE2	2.01	0.43
10:W:398:TYR:HB3	10:W:403:MET:CG	2.49	0.43
11:X:14:VAL:HG23	11:X:67:PHE:CD2	2.54	0.43
11:X:152:LEU:HD12	11:X:152:LEU:HA	1.87	0.43
11:X:397:LEU:HD23	11:X:397:LEU:HA	1.91	0.43
11:Y:231:ILE:O	11:Y:235:VAL:HG12	2.19	0.43
14:e:459:VAL:O	14:e:463:LEU:HG	2.19	0.43
14:f:104:TRP:HB2	14:f:110:TYR:HD2	1.84	0.43
14:f:436:PHE:CG	14:f:488:CYS:HB3	2.54	0.43
14:f:580:MET:HE1	14:f:606:LEU:HB2	2.01	0.43
14:f:736:LEU:HD11	14:f:749:LEU:HD21	2.01	0.43
3:A:122:ILE:HG22	3:A:147:TRP:HB2	2.01	0.42
3:A:426:LEU:HB3	3:A:459:LEU:HD12	2.01	0.42
3:E:1:MET:HG2	3:E:281:LEU:HD13	2.01	0.42
3:F:71:HIS:CD2	3:F:72:PRO:HD3	2.53	0.42
3:I:186:GLU:HG2	3:I:240:ARG:H	1.83	0.42
3:K:505:LYS:HD3	3:K:505:LYS:HA	1.82	0.42
3:K:619:LYS:NZ	3:K:632:GLU:OE2	2.37	0.42
4:R:748:VAL:HG13	4:R:776:TYR:HB2	2.01	0.42
7:S:679:LYS:HE2	7:S:679:LYS:HB2	1.87	0.42
11:X:3:GLU:HB2	11:X:129:CYS:SG	2.59	0.42
11:Y:202:PHE:HE2	11:Y:378:LEU:HD22	1.83	0.42
10:Z:204:ASN:HA	10:Z:207:LEU:HB2	2.00	0.42
10:Z:268:PRO:HG2	10:Z:300:MET:HB2	2.01	0.42
13:b:234:TRP:HB2	13:b:298:ARG:NH2	2.34	0.42
12:c:133:LYS:O	12:c:136:ARG:HG2	2.19	0.42
13:d:140:ARG:HH21	13:d:258:LEU:HA	1.84	0.42
14:e:114:THR:OG1	14:e:153:LYS:NZ	2.51	0.42
14:f:831:ASN:HB2	14:f:859:ASN:HB2	2.01	0.42
16:n:238:GLY:O	16:n:255:ARG:NH1	2.51	0.42
1:m:362:GLY:O	1:m:385:ILE:N	2.45	0.42
3:C:263:LEU:HD12	3:C:263:LEU:HA	1.93	0.42
3:D:52:ILE:HG13	3:D:75:ALA:HB2	2.02	0.42
3:E:18:LEU:HG	3:E:112:THR:HB	2.01	0.42
3:E:297:PRO:HA	3:E:409:VAL:HG13	2.01	0.42
3:E:617:ILE:O	3:E:648:PHE:HA	2.20	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:17:ALA:O	3:G:111:LEU:HA	2.20	0.42
3:H:473:MET:HA	3:H:491:LEU:O	2.19	0.42
3:I:378:MET:O	3:I:382:LEU:HB2	2.19	0.42
3:I:459:LEU:HD12	3:I:469:MET:HE1	2.00	0.42
6:O:98:VAL:HA	6:O:101:MET:HB2	2.01	0.42
7:P:1140:VAL:HG12	7:P:1141:LYS:HG3	2.01	0.42
8:Q:249:LYS:HA	8:Q:249:LYS:HD2	1.85	0.42
8:T:252:LYS:HD3	8:T:262:GLU:HB3	2.00	0.42
10:Z:286:VAL:HG11	10:Z:326:VAL:HG22	2.01	0.42
13:b:139:VAL:HG12	13:b:200:VAL:HG22	2.02	0.42
13:d:267:ARG:HH21	13:d:269:MET:HB3	1.84	0.42
13:d:323:CYS:SG	13:d:328:GLY:N	2.92	0.42
14:e:200:MET:HE2	14:e:200:MET:HB2	1.94	0.42
14:e:927:LEU:HG	14:e:932:ILE:HD11	1.99	0.42
1:m:105:TYR:OH	1:m:443:SER:OG	2.28	0.42
3:A:296:MET:HE3	3:A:296:MET:HA	2.02	0.42
3:G:606:LEU:HD13	3:G:606:LEU:HA	1.90	0.42
3:I:340:ARG:HD3	3:I:340:ARG:HA	1.75	0.42
3:I:431:PHE:CD1	3:I:460:PHE:HB2	2.54	0.42
3:I:613:LYS:HD2	3:I:613:LYS:HA	1.82	0.42
6:O:88:ILE:HG22	6:O:95:ARG:HG2	2.02	0.42
7:P:790:LYS:HE3	7:P:790:LYS:HB2	1.93	0.42
7:P:926:LEU:HB2	7:P:953:CYS:HB3	2.01	0.42
7:S:856:THR:O	7:S:856:THR:OG1	2.31	0.42
7:S:1161:TRP:CD1	7:S:1161:TRP:H	2.37	0.42
8:T:286:LYS:HD3	8:T:575:SER:HB3	2.01	0.42
9:V:59:THR:HA	9:V:66:GLN:HB2	2.00	0.42
11:X:210:TYR:CE1	11:X:222:PRO:HD2	2.54	0.42
10:Z:1:MET:O	10:Z:3:GLU:HG2	2.19	0.42
13:b:309:PHE:HD1	13:b:320:LYS:HD3	1.83	0.42
14:e:154:PRO:HB3	14:e:201:LEU:HD22	2.01	0.42
14:e:432:LYS:HB3	14:e:432:LYS:HE2	1.89	0.42
14:f:574:ASN:HD22	14:f:577:LEU:CB	2.30	0.42
14:f:723:LEU:HD13	14:f:726:CYS:HB2	2.02	0.42
14:f:740:LEU:HD11	14:f:774:THR:OG1	2.19	0.42
15:h:61:TRP:CZ2	15:h:93:LEU:HD23	2.54	0.42
15:h:137:LYS:HE3	15:h:137:LYS:HB3	1.71	0.42
16:n:114:LEU:HD23	16:n:114:LEU:HA	1.81	0.42
3:B:207:LYS:HA	3:B:227:PRO:HA	2.01	0.42
3:C:255:PRO:HB3	3:C:446:GLU:HB3	2.01	0.42
3:C:465:MET:HE2	3:C:599:ARG:HB2	2.01	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:269:GLU:HG3	3:D:279:ILE:O	2.20	0.42
3:E:407:LEU:HB3	3:E:427:ILE:HD13	2.02	0.42
3:G:20:MET:HE3	3:G:20:MET:HB2	1.91	0.42
3:I:253:PRO:O	3:I:451:GLN:NE2	2.52	0.42
3:I:295:PHE:HB3	3:I:409:VAL:CG2	2.50	0.42
3:K:198:ILE:HG13	3:K:266:SER:HB2	2.01	0.42
3:K:320:VAL:O	3:K:324:SER:OG	2.30	0.42
3:K:609:ILE:HG23	3:K:668:ILE:HD11	2.00	0.42
3:K:653:ASP:N	3:K:653:ASP:OD1	2.50	0.42
7:P:777:LYS:HB3	7:P:804:TYR:HD2	1.84	0.42
4:R:607:LEU:HD22	4:R:646:ASN:HD21	1.83	0.42
10:W:18:ALA:HB1	10:W:81:PHE:CG	2.55	0.42
10:W:358:PRO:HG3	10:W:364:SER:HB3	2.00	0.42
11:X:273:ALA:HA	11:X:300:ASN:HD21	1.84	0.42
11:Y:3:GLU:HG3	11:Y:64:ARG:HG3	2.02	0.42
13:d:252:TYR:HH	14:f:415:TYR:HH	1.67	0.42
14:e:74:ILE:HD12	14:e:74:ILE:HA	1.89	0.42
14:f:510:VAL:HB	14:f:536:LEU:HA	2.01	0.42
14:f:879:CYS:HA	14:f:882:LEU:HD12	2.02	0.42
15:j:19:GLU:HA	15:j:22:LYS:HG3	2.00	0.42
1:m:48:LYS:HD2	1:m:48:LYS:HA	1.86	0.42
3:B:323:LEU:HB3	3:B:611:LEU:HD13	2.01	0.42
3:C:18:LEU:HD11	3:C:191:ILE:HD12	2.00	0.42
3:E:570:LYS:HB2	3:E:570:LYS:HE3	1.86	0.42
3:G:4:GLN:HE22	3:H:562:LYS:HD3	1.84	0.42
3:G:516:PHE:HZ	3:G:602:PHE:HA	1.84	0.42
3:I:215:GLN:H	3:I:215:GLN:HG3	1.72	0.42
3:I:424:ARG:HE	3:I:424:ARG:HB3	1.75	0.42
3:K:306:TYR:O	3:K:666:ALA:HA	2.19	0.42
3:K:328:LYS:HB3	3:K:328:LYS:HE3	1.88	0.42
4:R:313:PHE:HD2	4:R:318:ARG:HB3	1.85	0.42
4:R:315:ASP:OD2	4:R:318:ARG:N	2.48	0.42
4:R:404:GLY:HA3	4:R:412:PHE:HE1	1.84	0.42
7:S:1051:GLY:HA2	7:S:1054:GLN:HG2	2.01	0.42
10:W:31:ASP:OD1	10:W:35:SER:N	2.52	0.42
10:W:288:GLU:OE1	10:W:292:GLN:NE2	2.53	0.42
10:Z:329:GLN:HA	10:Z:332:ASN:ND2	2.35	0.42
14:e:923:MET:N	14:e:923:MET:SD	2.93	0.42
3:A:48:ILE:HG23	3:A:77:VAL:HG13	2.01	0.42
3:D:459:LEU:HD23	3:D:459:LEU:HA	1.89	0.42
3:D:651:ASP:O	3:D:655:TYR:HB2	2.20	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:479:ASN:ND2	3:E:642:LEU:O	2.51	0.42
3:G:157:PRO:HB3	3:G:379:LYS:HE2	2.01	0.42
7:P:358:LEU:HB3	7:P:359:ARG:NH2	2.35	0.42
7:P:850:SER:HB3	7:P:880:ALA:HB2	2.01	0.42
7:P:1091:ASN:HB3	7:P:1150:TRP:CG	2.54	0.42
7:S:1051:GLY:O	7:S:1054:GLN:HB2	2.20	0.42
11:Y:52:PHE:HE1	11:Y:243:ARG:HE	1.66	0.42
10:Z:271:ALA:HB2	10:Z:293:MET:HG2	2.02	0.42
14:f:730:LYS:H	14:f:730:LYS:HG3	1.70	0.42
14:f:762:LYS:HD2	14:f:762:LYS:HA	1.83	0.42
16:n:112:ARG:HH21	16:n:119:GLN:HA	1.84	0.42
3:A:116:ILE:HG12	3:A:185:VAL:HG12	2.02	0.42
3:D:550:VAL:HG11	3:D:579:PHE:CD1	2.55	0.42
3:E:69:MET:SD	3:E:95:TYR:OH	2.70	0.42
3:G:316:PHE:HD1	3:G:649:ILE:HG21	1.83	0.42
3:H:28:ASP:HB3	3:H:31:LYS:HG2	2.00	0.42
3:H:46:PRO:HG3	3:I:131:PRO:HD3	2.01	0.42
3:I:212:TYR:HB3	3:I:221:TYR:HB3	2.01	0.42
3:K:310:GLU:HB3	3:K:311:LEU:H	1.68	0.42
3:K:347:ASP:OD1	3:K:369:ARG:NH1	2.53	0.42
3:K:427:ILE:HD11	3:K:448:VAL:HG11	2.00	0.42
5:N:47:LEU:HG	5:N:89:ILE:HB	2.00	0.42
6:O:50:LEU:HD23	6:O:53:ILE:HD13	2.02	0.42
7:P:288:TRP:CD1	7:P:332:VAL:HG11	2.55	0.42
7:P:833:THR:HG23	7:P:861:CYS:HB3	2.02	0.42
8:Q:413:ILE:HB	8:Q:423:ARG:HB3	2.01	0.42
4:R:668:VAL:HG22	4:R:691:TYR:HE2	1.84	0.42
7:S:673:TRP:NE1	7:S:701:ASP:OD2	2.48	0.42
5:U:77:THR:OG1	5:U:90:THR:OG1	2.22	0.42
13:b:237:VAL:HG11	13:b:268:ILE:HD11	2.00	0.42
13:d:229:ARG:HD3	14:f:406:TYR:HB2	2.02	0.42
13:d:733:CYS:O	13:d:737:LEU:HD12	2.19	0.42
14:e:86:GLN:HG2	14:e:212:SER:HA	2.02	0.42
14:e:251:TRP:NE1	14:e:255:ALA:HB2	2.35	0.42
14:f:66:LEU:HD13	14:f:110:TYR:OH	2.19	0.42
14:f:747:THR:HA	14:f:775:LEU:HA	2.01	0.42
15:j:144:ASP:OD1	15:j:144:ASP:N	2.46	0.42
1:m:98:GLU:HB3	7:P:855:SER:HA	2.02	0.42
2:p:347:GLU:HB2	2:p:348:TRP:HD1	1.83	0.42
2:p:353:ASP:OD1	2:p:353:ASP:N	2.52	0.42
3:B:295:PHE:HB3	3:B:409:VAL:HG21	2.02	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:561:LEU:HD23	3:E:561:LEU:HA	1.82	0.42
3:G:404:ILE:HD12	3:G:404:ILE:HA	1.96	0.42
3:G:505:LYS:HD2	3:G:625:ILE:HG13	2.02	0.42
8:Q:441:ASN:ND2	8:Q:500:ARG:HH22	2.18	0.42
7:S:777:LYS:HA	7:S:804:TYR:HB3	2.01	0.42
11:X:149:PHE:O	11:X:153:LEU:HB2	2.20	0.42
11:Y:12:ALA:HB2	18:Y:501:GTP:C8	2.54	0.42
14:e:418:LEU:HD21	14:e:467:LEU:HD23	2.01	0.42
14:f:594:ILE:HD12	14:f:594:ILE:HA	1.82	0.42
15:l:7:GLN:HG2	15:l:11:GLY:HA2	2.02	0.42
2:p:36:ALA:O	2:p:42:TRP:NE1	2.53	0.42
3:D:486:LYS:HE3	3:D:567:LEU:HD23	2.02	0.42
3:G:151:LEU:HD21	3:G:247:VAL:HG12	2.01	0.42
3:I:401:LEU:HD23	3:I:401:LEU:HA	1.90	0.42
7:P:403:LEU:HD21	7:P:441:CYS:HB2	2.01	0.42
7:P:600:PHE:CG	7:P:652:CYS:HB3	2.54	0.42
7:P:727:PRO:HG2	7:P:730:MET:HB2	2.02	0.42
8:Q:284:LEU:HD23	8:Q:579:ILE:HA	2.02	0.42
8:Q:505:THR:O	8:Q:505:THR:OG1	2.30	0.42
4:R:196:THR:HB	4:R:252:LYS:HG3	2.02	0.42
7:S:271:LEU:HD23	7:S:271:LEU:HA	1.86	0.42
7:S:279:ILE:HD13	7:S:298:ILE:HG23	2.02	0.42
7:S:480:GLN:HE22	7:S:482:ALA:HB3	1.85	0.42
7:S:497:MET:HE1	7:S:514:LEU:HD23	2.02	0.42
7:S:849:ILE:HD13	7:S:864:LEU:HD21	2.02	0.42
8:T:306:ARG:HE	8:T:306:ARG:HB2	1.69	0.42
9:V:84:LEU:HD23	9:V:88:HIS:HD2	1.84	0.42
11:X:54:SER:OG	11:X:62:VAL:O	2.35	0.42
10:Z:207:LEU:HD11	10:Z:229:VAL:HG13	2.01	0.42
12:a:136:ARG:HH12	13:b:494:ASN:HA	1.85	0.42
14:e:195:LEU:HD23	14:e:195:LEU:HA	1.84	0.42
14:e:480:LEU:HA	14:e:483:GLN:HG2	2.02	0.42
14:e:634:HIS:HA	14:e:663:VAL:HB	2.02	0.42
14:e:933:LYS:HE2	14:e:933:LYS:HB3	1.77	0.42
14:f:211:ARG:HD2	14:f:343:HIS:HD2	1.84	0.42
14:f:291:ARG:NH1	14:f:293:GLU:HB2	2.35	0.42
14:f:345:LEU:HD23	14:f:345:LEU:HA	1.90	0.42
15:h:123:VAL:O	15:h:127:ILE:HG22	2.20	0.42
16:n:19:TYR:CE1	15:j:80:LYS:HB3	2.55	0.42
1:m:29:ASN:O	1:m:33:ASN:N	2.50	0.42
1:m:109:HIS:NE2	1:m:441:GLU:HB3	2.34	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:m:254:GLN:HG2	7:P:911:PHE:CZ	2.55	0.42
3:C:438:ARG:NH2	3:C:464:LEU:O	2.53	0.42
3:C:474:CYS:SG	3:C:475:PHE:N	2.93	0.42
3:D:269:GLU:OE2	3:D:279:ILE:HD12	2.20	0.42
3:E:191:ILE:HD12	3:E:191:ILE:HA	1.93	0.42
3:F:340:ARG:NH1	3:F:348:GLU:OE2	2.53	0.42
3:G:426:LEU:HD13	3:G:459:LEU:HD11	2.02	0.42
3:G:600:PRO:HG3	3:G:604:ASP:HB2	2.02	0.42
3:H:322:LYS:HA	3:H:322:LYS:HD3	1.74	0.42
3:H:336:GLU:H	3:H:336:GLU:HG3	1.73	0.42
3:I:28:ASP:HB3	3:I:31:LYS:HE2	2.02	0.42
3:I:453:VAL:HG12	3:I:454:GLN:HG3	2.01	0.42
7:P:235:PRO:HD3	7:P:241:GLN:HG3	2.02	0.42
7:P:937:PHE:HE2	7:P:945:LEU:HD22	1.83	0.42
8:Q:248:ASP:OD1	8:Q:248:ASP:N	2.53	0.42
4:R:903:ASN:HA	4:R:931:MET:HE1	2.02	0.42
7:S:644:MET:HA	7:S:644:MET:HE3	2.02	0.42
7:S:1162:LYS:HG2	8:T:270:THR:HG22	2.00	0.42
10:W:2:ARG:HB3	10:W:131:GLN:HB2	2.02	0.42
10:W:293:MET:HE2	10:W:293:MET:HB2	1.73	0.42
11:Y:9:VAL:HG23	11:Y:139:HIS:HB3	2.02	0.42
10:Z:112:LEU:O	10:Z:116:VAL:HG13	2.20	0.42
13:b:554:ALA:HA	14:e:323:ASN:HB3	2.02	0.42
14:e:236:ASN:OD1	14:e:236:ASN:N	2.51	0.42
14:f:358:GLU:N	14:f:358:GLU:OE1	2.51	0.42
14:f:523:PHE:HA	14:f:526:LYS:HE3	2.02	0.42
15:h:54:ILE:HD13	15:h:102:GLU:HB2	2.00	0.42
16:n:284:LEU:HD23	16:n:304:LEU:HD11	2.00	0.42
3:A:433:PRO:HD3	3:B:200:HIS:CE1	2.55	0.41
3:B:39:SER:HB2	3:B:96:PHE:HE2	1.85	0.41
3:B:625:ILE:N	3:B:628:THR:O	2.50	0.41
3:E:484:ASP:N	3:E:484:ASP:OD1	2.48	0.41
3:F:472:PHE:CD2	3:F:473:MET:HG2	2.55	0.41
3:G:352:CYS:HB2	3:G:363:LEU:HB3	2.02	0.41
3:H:1:MET:HB3	3:H:281:LEU:HD22	2.02	0.41
3:I:283:LYS:HB2	3:I:283:LYS:HE3	1.85	0.41
6:O:15:HIS:CE1	6:O:76:ASN:HD22	2.38	0.41
7:P:853:LEU:HD23	7:P:853:LEU:HA	1.89	0.41
7:S:320:LEU:O	7:S:368:LEU:HA	2.20	0.41
7:S:340:LEU:HD23	7:S:340:LEU:HA	1.86	0.41
7:S:837:ASP:HB3	7:S:865:ALA:HB3	2.02	0.41

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:X:122:ILE:HD12	11:X:122:ILE:HA	1.85	0.41
11:X:422:ARG:O	11:X:422:ARG:NH1	2.54	0.41
13:b:693:THR:O	13:b:696:GLN:NE2	2.53	0.41
13:d:6:ARG:HD2	13:d:13:THR:HG22	2.02	0.41
14:f:924:LYS:N	14:f:952:ASP:HB3	2.33	0.41
1:m:95:VAL:HG22	1:m:123:MET:SD	2.60	0.41
1:m:113:ARG:NH2	1:m:114:ASN:O	2.53	0.41
2:p:5:LEU:HD21	2:p:9:PRO:HB2	2.02	0.41
3:A:340:ARG:NH2	3:A:366:ASP:OD1	2.53	0.41
3:B:341:GLN:H	3:B:341:GLN:HG3	1.73	0.41
3:C:424:ARG:NH1	3:C:564:GLU:O	2.52	0.41
3:D:181:MET:HE2	3:D:181:MET:HB3	1.82	0.41
3:D:223:LEU:HD11	3:D:226:GLY:HA3	2.02	0.41
3:E:283:LYS:HB3	3:E:283:LYS:HE3	1.97	0.41
3:E:673:PHE:HD2	3:E:675:PHE:H	1.67	0.41
3:F:20:MET:HB3	3:F:23:MET:HB3	2.01	0.41
3:F:29:ILE:HB	3:F:95:TYR:HE1	1.85	0.41
3:H:302:PRO:HG3	3:H:611:LEU:HA	2.02	0.41
3:I:141:MET:HE1	3:I:147:TRP:CD2	2.56	0.41
7:P:315:GLN:O	7:P:319:LEU:HB2	2.21	0.41
7:P:340:LEU:O	7:P:342:ARG:NH1	2.53	0.41
4:R:117:ILE:O	4:R:121:ILE:HG13	2.20	0.41
7:S:604:ASN:OD1	7:S:605:LYS:N	2.52	0.41
10:Z:163:ILE:HG12	10:Z:251:ARG:HE	1.85	0.41
13:b:33:GLU:HG2	13:b:39:GLU:HA	2.01	0.41
12:c:66:LYS:HD3	12:c:66:LYS:HA	1.75	0.41
13:d:206:THR:OG1	13:d:278:GLU:OE2	2.38	0.41
13:d:222:ASN:HD22	13:d:231:ARG:HB2	1.85	0.41
13:d:338:CYS:HB2	13:d:365:CYS:HB3	1.92	0.41
13:d:677:LEU:HB2	13:d:770:ILE:HD12	2.01	0.41
14:e:108:ASN:HB2	14:e:109:LEU:HD22	2.02	0.41
14:e:178:LEU:HD11	14:e:197:ARG:HD2	2.01	0.41
14:e:588:ASP:O	14:e:592:MET:HG2	2.21	0.41
14:e:839:SER:N	14:e:866:GLY:O	2.52	0.41
14:e:940:ARG:HG2	14:e:971:ASN:HD21	1.84	0.41
14:f:335:VAL:HG11	14:f:394:PHE:CD2	2.55	0.41
14:f:756:LEU:HD22	14:f:764:LEU:HD21	2.02	0.41
15:h:23:GLN:HG3	15:h:66:LYS:HA	2.01	0.41
16:n:133:ILE:HG21	16:n:157:LEU:HD13	2.02	0.41
1:m:39:ASP:HB2	1:m:66:TRP:HD1	1.85	0.41
1:m:90:TYR:HE1	1:m:458:MET:HG2	1.85	0.41

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:p:10:LEU:HD23	2:p:10:LEU:HA	1.91	0.41
2:p:60:LEU:HD22	2:p:113:ARG:NH2	2.35	0.41
3:A:7:LEU:HB3	3:A:31:LYS:HE2	2.02	0.41
3:B:297:PRO:HB3	3:B:409:VAL:HG12	2.02	0.41
3:C:453:VAL:HA	3:C:680:MET:HE1	2.01	0.41
3:E:18:LEU:HD21	3:E:191:ILE:HG12	2.02	0.41
3:E:210:ARG:HG3	3:E:227:PRO:HD3	2.03	0.41
3:F:52:ILE:HD12	3:F:75:ALA:HB2	2.02	0.41
3:H:109:LEU:HG	3:H:111:LEU:HG	2.02	0.41
3:H:131:PRO:HG2	3:I:46:PRO:HB3	2.02	0.41
3:H:573:ILE:HD13	3:H:573:ILE:HA	1.93	0.41
3:I:541:LYS:HA	3:I:541:LYS:HD2	1.89	0.41
7:S:922:SER:HB2	7:S:951:ASN:HB2	2.02	0.41
7:S:1020:LEU:O	7:S:1024:ILE:HG13	2.21	0.41
10:W:22:GLU:HG2	10:W:81:PHE:HB3	2.03	0.41
10:W:136:THR:HG22	10:W:167:PHE:HB2	2.03	0.41
11:Y:143:GLY:O	11:Y:186:ASN:ND2	2.43	0.41
14:f:363:PHE:HA	14:f:366:ALA:HB3	2.02	0.41
14:f:702:ASP:HA	14:f:705:LYS:HD2	2.02	0.41
15:h:132:PRO:HA	15:h:135:ILE:HD12	2.02	0.41
15:j:126:MET:HE3	15:j:126:MET:HB3	1.81	0.41
2:p:254:HIS:CD2	2:p:255:PRO:HD2	2.56	0.41
2:p:387:ARG:O	2:p:397:VAL:HA	2.21	0.41
3:A:21:VAL:HB	3:A:115:GLU:HB2	2.02	0.41
3:A:459:LEU:HD11	3:A:561:LEU:HD13	2.02	0.41
3:B:425:VAL:H	3:B:454:GLN:HB3	1.85	0.41
3:B:472:PHE:HB2	3:B:554:ILE:HD11	2.01	0.41
3:F:95:TYR:H	3:F:105:ALA:HB3	1.85	0.41
3:F:491:LEU:HD22	3:F:573:ILE:HB	2.01	0.41
3:I:138:LYS:HG2	3:I:285:THR:HG23	2.01	0.41
3:I:560:LEU:HD12	3:I:560:LEU:HA	1.82	0.41
7:P:360:LYS:HE3	7:P:368:LEU:HD23	2.03	0.41
4:R:605:ASN:OD1	4:R:644:ASN:ND2	2.53	0.41
7:S:320:LEU:O	7:S:367:PHE:O	2.38	0.41
7:S:1013:THR:HG22	7:S:1014:GLN:H	1.86	0.41
13:d:597:GLU:O	13:d:601:ARG:HG2	2.20	0.41
14:e:242:ILE:HG21	14:e:256:ILE:HD13	2.02	0.41
14:e:671:LEU:HA	14:e:675:ARG:NH1	2.35	0.41
14:e:931:SER:O	14:e:935:LEU:HD12	2.20	0.41
15:h:99:THR:O	15:h:103:LEU:HD12	2.20	0.41
1:m:172:ILE:HG22	1:m:223:LEU:HD21	2.01	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:p:282:LYS:HE3	2:p:316:PHE:HE2	1.85	0.41
2:p:343:GLU:O	2:p:345:ARG:NH1	2.40	0.41
2:p:389:TRP:HB3	2:p:396:ILE:HB	2.02	0.41
3:A:298:SER:O	3:A:670:ARG:NH2	2.53	0.41
3:B:495:PRO:HD2	3:B:551:GLU:HB2	2.01	0.41
3:C:355:GLN:HB3	3:C:677:TRP:HD1	1.85	0.41
3:D:20:MET:HB2	3:D:23:MET:HE3	2.02	0.41
3:D:442:LYS:HD2	3:D:442:LYS:HA	1.82	0.41
3:F:41:THR:O	3:F:93:VAL:HA	2.20	0.41
3:G:270:LYS:HA	3:G:278:GLU:HG2	2.03	0.41
3:G:575:ILE:HD12	3:G:635:VAL:HG23	2.01	0.41
3:G:619:LYS:HA	3:G:648:PHE:HD2	1.85	0.41
3:H:561:LEU:HD12	3:H:561:LEU:HA	1.92	0.41
3:I:295:PHE:HZ	3:I:404:ILE:HD11	1.86	0.41
3:I:300:GLN:HB2	3:I:670:ARG:HB3	2.02	0.41
5:N:53:VAL:HG21	5:N:113:LYS:HE3	2.03	0.41
4:R:869:LEU:HD12	4:R:869:LEU:HA	1.81	0.41
7:S:249:GLY:HA3	7:S:392:VAL:HB	2.03	0.41
7:S:363:LEU:HD12	7:S:363:LEU:HA	1.93	0.41
8:T:301:VAL:HG22	8:T:567:ILE:HD13	2.02	0.41
8:T:484:LEU:HD23	8:T:484:LEU:HA	1.80	0.41
11:X:272:TYR:CD1	11:X:274:PRO:HD2	2.56	0.41
10:Z:36:TYR:CZ	10:Z:44:LEU:HG	2.55	0.41
12:a:62:PHE:HB3	13:b:745:VAL:HG21	2.02	0.41
13:b:685:ALA:HA	13:b:688:TRP:CE3	2.55	0.41
13:d:140:ARG:H	13:d:199:ASN:HB3	1.85	0.41
14:e:955:GLU:OE1	14:e:958:LYS:NZ	2.43	0.41
15:j:139:PHE:HB2	15:j:141:ILE:HG13	2.02	0.41
1:m:130:ILE:HB	1:m:144:SER:HB3	2.02	0.41
1:m:246:LYS:HB3	1:m:296:GLU:OE1	2.21	0.41
2:p:61:LEU:HD13	2:p:66:TRP:CD2	2.56	0.41
3:B:383:THR:O	3:B:386:SER:OG	2.30	0.41
3:D:661:ASP:OD1	3:D:661:ASP:N	2.53	0.41
3:I:205:GLU:HA	3:I:208:LYS:HB2	2.02	0.41
7:P:1116:LEU:HD22	7:P:1119:ILE:HG22	2.02	0.41
4:R:399:SER:OG	4:R:420:ASN:OD1	2.34	0.41
7:S:248:HIS:HA	7:S:372:THR:O	2.21	0.41
11:X:139:HIS:O	11:X:170:SER:HA	2.20	0.41
11:Y:15:GLN:HA	11:Y:18:ASN:HD21	1.85	0.41
11:Y:152:LEU:HD23	11:Y:152:LEU:HA	1.92	0.41
13:d:50:LYS:HB3	13:d:50:LYS:HE2	1.67	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:d:318:CYS:H	13:d:322:ALA:HB2	1.86	0.41
14:e:355:LEU:HD12	14:e:355:LEU:HA	1.95	0.41
14:e:518:LEU:HD23	14:e:518:LEU:HA	1.93	0.41
14:f:270:HIS:CD2	14:f:271:VAL:HG23	2.55	0.41
16:n:140:GLU:HB2	16:n:142:VAL:HG12	2.03	0.41
16:n:427:ASN:HD21	16:n:431:LEU:HD12	1.85	0.41
1:m:206:VAL:HB	1:m:218:PHE:HB2	2.02	0.41
1:m:302:MET:HB3	1:m:302:MET:HE2	1.78	0.41
2:p:64:GLU:HG3	2:p:68:GLU:HG2	2.02	0.41
2:p:140:LEU:HD21	2:p:143:VAL:HB	2.02	0.41
3:C:202:SER:OG	3:D:442:LYS:NZ	2.38	0.41
3:D:19:CYS:HB2	3:D:111:LEU:HD22	2.02	0.41
3:D:309:ARG:HH12	3:D:333:LYS:HD2	1.85	0.41
3:E:213:TRP:HE3	3:E:224:VAL:HG11	1.86	0.41
3:F:70:ASN:OD1	3:F:72:PRO:HD2	2.20	0.41
3:F:81:ALA:HA	3:F:82:PRO:HD3	1.88	0.41
3:F:130:MET:HB3	3:F:130:MET:HE2	1.42	0.41
3:F:474:CYS:SG	3:F:475:PHE:N	2.93	0.41
3:H:375:ASP:OD1	3:H:375:ASP:N	2.53	0.41
3:I:492:LEU:HD13	3:I:558:ARG:HH11	1.84	0.41
7:P:381:LYS:HE2	8:Q:332:GLU:HA	2.02	0.41
4:R:666:LYS:HE3	4:R:666:LYS:HB2	1.89	0.41
4:R:853:LEU:HD23	4:R:853:LEU:HA	1.84	0.41
7:S:324:ASP:HA	7:S:371:THR:HB	2.02	0.41
7:S:446:LEU:HD11	7:S:471:HIS:CD2	2.55	0.41
8:T:354:ASN:ND2	9:V:40:GLY:O	2.43	0.41
10:W:311:LEU:HD23	10:W:342:VAL:HG11	2.02	0.41
11:X:1:MET:O	11:X:130:THR:OG1	2.37	0.41
12:c:39:GLY:HA2	12:c:40:PRO:HD3	1.93	0.41
14:e:43:TYR:HA	14:e:52:ALA:HB1	2.03	0.41
14:f:98:LYS:HE3	14:f:98:LYS:HB2	1.86	0.41
14:f:647:LEU:O	14:f:651:CYS:HB2	2.20	0.41
14:f:833:GLN:HG3	14:f:861:TRP:CH2	2.56	0.41
14:f:953:LYS:HA	14:f:956:ILE:HD12	2.02	0.41
15:h:68:ASP:HA	15:h:69:PRO:HD2	1.95	0.41
1:m:82:ARG:HD3	1:m:82:ARG:HA	1.87	0.41
2:p:231:VAL:HB	2:p:236:ILE:HD11	2.03	0.41
2:p:418:LYS:HD2	2:p:419:CYS:N	2.35	0.41
3:B:136:ALA:O	3:B:147:TRP:NE1	2.50	0.41
3:B:402:ASP:HB3	3:B:441:ASN:H	1.85	0.41
3:C:70:ASN:HB3	3:C:72:PRO:HD2	2.02	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:177:ASN:HB2	3:F:359:LYS:HZ2	1.85	0.41
3:H:474:CYS:SG	3:H:475:PHE:N	2.94	0.41
3:I:116:ILE:HD13	3:I:267:LEU:HD13	2.03	0.41
3:I:339:ASN:HB3	3:I:373:LEU:HD13	2.02	0.41
3:K:238:GLU:HB2	3:K:241:ARG:HH11	1.85	0.41
4:R:403:GLU:OE2	4:R:419:ARG:NH2	2.54	0.41
8:T:285:GLN:NE2	8:T:580:LYS:HD2	2.36	0.41
10:W:247:ASN:HB3	10:W:252:LYS:HG3	2.02	0.41
11:X:14:VAL:HG23	11:X:67:PHE:HD2	1.85	0.41
11:X:322:ASP:OD1	11:X:322:ASP:N	2.36	0.41
12:c:99:ILE:HA	12:c:102:VAL:HG22	2.03	0.41
13:d:535:LYS:HE3	13:d:535:LYS:HB2	1.81	0.41
14:e:147:ILE:HG13	14:e:151:LEU:HD23	2.03	0.41
14:f:46:SER:OG	14:f:50:GLU:O	2.35	0.41
14:f:251:TRP:HD1	14:f:255:ALA:HB2	1.86	0.41
14:f:687:ARG:NE	14:f:715:ASN:O	2.50	0.41
1:m:174:LEU:HB3	1:m:183:LEU:HB3	2.03	0.41
1:m:387:ARG:NH1	1:m:434:ILE:O	2.54	0.41
2:p:204:PRO:HB2	2:p:220:ILE:HB	2.02	0.41
2:p:349:TYR:HA	2:p:358:VAL:O	2.21	0.41
3:A:552:LYS:HD2	3:B:279:ILE:HD12	2.02	0.41
3:B:151:LEU:HD21	3:B:247:VAL:HG22	2.03	0.41
3:B:434:SER:OG	3:B:437:GLY:O	2.31	0.41
3:B:532:LYS:CG	3:B:536:GLN:HG3	2.51	0.41
3:E:559:THR:CA	3:F:4:GLN:HE22	2.30	0.41
3:E:634:LYS:HA	3:E:634:LYS:HD3	1.78	0.41
3:F:600:PRO:HB3	3:F:604:ASP:HB2	2.03	0.41
3:G:1:MET:SD	3:G:1:MET:N	2.83	0.41
3:G:490:LEU:HD21	3:G:561:LEU:HD13	2.02	0.41
3:I:340:ARG:HB3	3:I:344:TRP:CG	2.56	0.41
3:I:523:GLN:H	3:I:523:GLN:HG2	1.68	0.41
3:K:149:ALA:HB3	3:K:288:PHE:HD1	1.86	0.41
3:K:374:GLU:OE1	3:K:374:GLU:N	2.54	0.41
3:K:541:LYS:HA	3:K:541:LYS:HD2	1.81	0.41
7:P:854:ILE:HG23	7:P:885:MET:HB2	2.01	0.41
7:P:1134:LEU:HD22	7:P:1146:ILE:HD13	2.03	0.41
8:Q:528:VAL:HG12	8:Q:534:ILE:HG12	2.02	0.41
4:R:290:GLN:H	4:R:290:GLN:HG3	1.66	0.41
4:R:340:LEU:HD11	17:R:1001:ATP:H1'	2.03	0.41
4:R:398:CYS:HB3	4:R:461:PHE:HB2	2.02	0.41
4:R:414:LYS:HE2	4:R:418:ARG:HD3	2.03	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:S:549:LEU:HD22	7:S:591:ARG:HH22	1.85	0.41
7:S:821:CYS:SG	7:S:848:MET:HB3	2.61	0.41
7:S:960:TYR:CE1	7:S:983:VAL:HG22	2.56	0.41
8:T:570:SER:OG	8:T:571:ARG:N	2.54	0.41
5:U:31:THR:O	5:U:31:THR:OG1	2.38	0.41
5:U:42:SER:OG	5:U:43:ASN:N	2.54	0.41
5:U:104:ILE:O	5:U:108:MET:HG2	2.20	0.41
11:X:298:PRO:HG3	11:X:308:ARG:HG2	2.02	0.41
11:Y:75:ILE:HG21	11:Y:94:THR:HB	2.02	0.41
10:Z:229:VAL:O	10:Z:233:MET:HG2	2.20	0.41
10:Z:229:VAL:HB	10:Z:233:MET:HE3	2.03	0.41
13:b:212:ASN:HB3	14:e:970:ILE:HG23	2.03	0.41
13:b:237:VAL:HG22	13:b:255:ILE:HG23	2.02	0.41
13:b:725:THR:HA	13:b:731:ASN:HA	2.02	0.41
12:c:79:ASN:OD1	12:c:83:SER:N	2.45	0.41
13:d:25:VAL:HG11	13:d:54:ASP:HA	2.03	0.41
13:d:150:ALA:HB1	13:d:182:VAL:HB	2.02	0.41
13:d:485:GLY:O	13:d:504:GLN:NE2	2.39	0.41
13:d:696:GLN:H	13:d:696:GLN:HG3	1.61	0.41
14:e:395:TYR:HD2	14:e:435:LEU:HD22	1.86	0.41
14:e:439:LEU:HB2	14:e:492:THR:HG23	2.03	0.41
14:e:847:CYS:HA	14:e:850:LEU:HD12	2.01	0.41
15:h:82:THR:OG1	15:h:125:ASN:OD1	2.34	0.41
16:n:15:LYS:HG3	15:j:120:CYS:SG	2.61	0.41
1:m:92:GLU:HA	1:m:457:LEU:O	2.20	0.41
1:m:462:LEU:HD12	1:m:462:LEU:HA	1.88	0.41
2:p:126:SER:O	2:p:126:SER:OG	2.32	0.41
3:B:481:LYS:HZ2	3:B:481:LYS:HG3	1.72	0.41
3:C:156:SER:HA	3:C:157:PRO:HD3	1.90	0.41
3:C:335:TYR:H	3:C:381:THR:HG21	1.85	0.41
3:C:463:TRP:CD1	3:C:463:TRP:H	2.39	0.41
3:D:402:ASP:OD2	3:D:441:ASN:ND2	2.54	0.41
3:E:296:MET:HB2	3:E:670:ARG:HB2	2.02	0.41
3:E:494:SER:HB2	3:E:574:LEU:HB3	2.03	0.41
3:G:19:CYS:SG	3:G:20:MET:N	2.94	0.41
3:G:340:ARG:H	3:G:340:ARG:HG2	1.55	0.41
3:I:389:LEU:HD23	3:I:389:LEU:HA	1.89	0.41
3:K:605:MET:HB2	3:K:605:MET:HE3	1.88	0.41
6:O:4:LEU:HG	6:O:5:LYS:HG3	2.03	0.41
7:P:415:ILE:HD13	7:P:415:ILE:HA	1.96	0.41
7:S:279:ILE:HD12	7:S:281:PHE:CE1	2.56	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:S:726:LYS:HE3	7:S:726:LYS:HB2	1.71	0.41
8:T:536:VAL:HG23	8:T:545:LEU:HB2	2.02	0.41
10:Z:105:HIS:NE2	10:Z:150:LEU:HD13	2.36	0.41
13:b:210:TRP:NE1	13:b:242:LYS:HE2	2.36	0.41
13:d:608:THR:OG1	13:d:609:MET:N	2.54	0.41
14:e:851:ALA:HB1	14:e:881:ALA:HB2	2.03	0.41
14:e:961:ILE:HD13	14:e:961:ILE:HA	1.84	0.41
14:f:133:ALA:O	14:f:137:SER:HB3	2.21	0.41
14:f:687:ARG:H	14:f:687:ARG:HG2	1.75	0.41
14:f:761:ILE:HD13	14:f:764:LEU:HD23	2.02	0.41
15:l:58:VAL:HG11	15:l:110:LEU:HG	2.03	0.41
1:m:263:TYR:CE2	1:m:265:SER:HB2	2.57	0.40
2:p:411:GLU:OE2	15:l:161:GLU:HG3	2.21	0.40
3:A:313:LEU:HD23	3:A:313:LEU:HA	1.90	0.40
3:B:322:LYS:O	3:B:322:LYS:NZ	2.51	0.40
3:C:118:LEU:HD23	3:C:118:LEU:HA	1.90	0.40
3:G:89:ASP:N	3:G:89:ASP:OD1	2.54	0.40
3:H:317:VAL:O	3:H:321:THR:OG1	2.33	0.40
3:H:436:GLU:H	3:H:436:GLU:HG2	1.71	0.40
3:I:310:GLU:HG2	3:I:311:LEU:HD23	2.02	0.40
3:I:508:GLU:HB3	3:I:510:TYR:CE1	2.56	0.40
3:K:323:LEU:HD21	3:K:647:THR:HB	2.03	0.40
7:P:666:LEU:HD13	7:P:692:CYS:HB3	2.03	0.40
7:P:751:LEU:HA	7:P:751:LEU:HD23	1.81	0.40
8:Q:412:ARG:HD3	8:Q:414:TRP:HE1	1.86	0.40
4:R:573:ILE:HG22	4:R:596:LEU:HD21	2.04	0.40
4:R:881:ILE:HG13	4:R:881:ILE:H	1.67	0.40
7:S:219:LEU:HD11	17:S:1201:ATP:HN61	1.87	0.40
7:S:761:MET:HB2	7:S:761:MET:HE2	1.78	0.40
7:S:796:LEU:HD21	7:S:805:LEU:HD22	2.03	0.40
7:S:976:LEU:HB3	7:S:1002:LEU:HD11	2.04	0.40
7:S:1101:GLY:HA2	7:S:1104:LYS:HE2	2.03	0.40
5:U:94:GLN:HG2	5:U:95:PRO:HD2	2.04	0.40
13:b:13:THR:O	13:b:14:HIS:ND1	2.54	0.40
13:b:39:GLU:OE1	13:b:41:GLN:NE2	2.47	0.40
14:e:875:LEU:HD12	14:e:878:LEU:HD21	2.03	0.40
14:f:654:LEU:O	14:f:686:ASN:ND2	2.54	0.40
15:h:100:LEU:O	15:h:104:ILE:HG23	2.21	0.40
16:n:46:ARG:HH21	16:n:50:GLN:HE21	1.69	0.40
16:n:61:LEU:HD23	16:n:61:LEU:H	1.85	0.40
16:n:93:TYR:OH	16:n:95:GLU:OE2	2.27	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:m:342:CYS:O	1:m:345:ARG:NH1	2.55	0.40
2:p:67:LYS:NZ	15:l:157:ASN:HB3	2.37	0.40
2:p:118:ARG:H	2:p:118:ARG:HD3	1.86	0.40
3:C:97:CYS:HB2	3:C:101:GLU:HB3	2.02	0.40
3:G:9:LEU:HD21	3:G:27:LEU:HD13	2.03	0.40
3:H:49:LEU:HD13	3:I:49:LEU:HD22	2.03	0.40
3:I:267:LEU:HD23	3:I:281:LEU:HB2	2.03	0.40
3:I:322:LYS:O	3:I:326:LYS:HG2	2.22	0.40
3:K:493:ALA:HB3	3:K:554:ILE:HD13	2.03	0.40
5:N:77:THR:HG1	5:N:90:THR:HG1	1.52	0.40
5:N:123:VAL:HB	6:O:101:MET:HE3	2.03	0.40
7:P:471:HIS:CE1	7:P:475:LEU:HD12	2.56	0.40
7:P:878:GLY:O	7:P:882:SER:HB3	2.21	0.40
7:P:1145:VAL:HG12	7:P:1147:ASP:HB2	2.04	0.40
8:Q:417:ARG:H	8:Q:417:ARG:HG3	1.67	0.40
4:R:417:LEU:HB3	4:R:422:ILE:HB	2.04	0.40
4:R:802:LEU:HD12	4:R:802:LEU:HA	1.93	0.40
7:S:762:LYS:HB2	7:S:791:HIS:CE1	2.56	0.40
7:S:1017:CYS:SG	7:S:1047:THR:HB	2.61	0.40
11:X:104:ALA:O	11:X:108:TYR:HB2	2.21	0.40
11:Y:194:THR:HA	11:Y:197:HIS:HB2	2.03	0.40
11:Y:252:LEU:HD23	11:Y:252:LEU:HA	1.85	0.40
11:Y:428:LEU:HG	11:Y:432:TYR:HE1	1.87	0.40
12:a:99:ILE:HD13	12:a:99:ILE:HA	1.89	0.40
13:b:6:ARG:HH11	13:b:68:THR:HG21	1.86	0.40
13:b:334:LYS:HA	13:b:334:LYS:HD2	1.75	0.40
13:d:140:ARG:HG3	13:d:147:TRP:CD1	2.56	0.40
14:e:36:GLU:O	14:e:40:THR:HG22	2.21	0.40
14:e:134:GLN:H	14:e:134:GLN:HG2	1.63	0.40
14:e:408:SER:HB2	14:e:412:GLU:HB2	2.03	0.40
14:e:967:ASP:HA	14:e:970:ILE:HG12	2.03	0.40
14:f:194:SER:HB2	14:f:200:MET:HG2	2.03	0.40
14:f:470:LEU:HA	14:f:470:LEU:HD12	1.86	0.40
14:f:965:LEU:O	14:f:968:VAL:HG22	2.20	0.40
15:h:9:SER:HB3	15:h:51:ASN:HA	2.03	0.40
1:m:205:ILE:HD13	1:m:268:LEU:HD21	2.03	0.40
3:A:369:ARG:NH1	3:A:398:VAL:O	2.55	0.40
3:B:552:LYS:HB3	3:B:552:LYS:HE2	1.84	0.40
3:C:478:THR:HA	3:C:644:LEU:HD11	2.03	0.40
3:D:186:GLU:OE2	3:D:187:GLY:N	2.54	0.40
3:E:149:ALA:HB3	3:E:287:MET:O	2.22	0.40

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:455:ALA:HA	3:F:456:PRO:HD3	1.83	0.40
3:G:473:MET:HB2	3:G:492:LEU:HD23	2.04	0.40
3:H:129:ASP:OD1	3:H:129:ASP:N	2.50	0.40
3:I:209:THR:HB	3:I:261:ILE:HD13	2.03	0.40
6:O:53:ILE:HD12	6:O:53:ILE:H	1.86	0.40
4:R:153:GLY:HA3	4:R:297:ALA:HB2	2.02	0.40
4:R:183:ALA:HA	4:R:225:LEU:O	2.21	0.40
4:R:207:TRP:CD2	4:R:208:PRO:HD2	2.56	0.40
10:W:212:PHE:O	10:W:216:LYS:HD3	2.21	0.40
10:W:337:ASN:HB3	10:W:340:TYR:HB2	2.03	0.40
11:X:84:ARG:H	11:X:84:ARG:HG3	1.71	0.40
11:X:96:LYS:HA	11:X:96:LYS:HD2	1.82	0.40
11:X:119:LEU:HD12	11:X:119:LEU:HA	1.89	0.40
13:b:196:LYS:O	13:b:200:VAL:HG23	2.22	0.40
13:b:203:ARG:HE	13:b:203:ARG:HB2	1.69	0.40
12:c:9:GLU:HA	12:c:12:ASP:OD2	2.21	0.40
13:d:58:LEU:HB3	13:d:63:VAL:HG22	2.03	0.40
14:e:477:LEU:HD12	14:e:477:LEU:HA	1.91	0.40
14:e:586:ARG:NH1	14:e:615:ASP:OD2	2.54	0.40
14:e:644:VAL:HG12	14:e:675:ARG:HD2	2.03	0.40
14:e:884:ASN:HA	14:e:885:PRO:HD3	1.91	0.40
14:f:137:SER:O	14:f:137:SER:OG	2.30	0.40
14:f:307:ILE:HD13	14:f:307:ILE:HA	1.90	0.40
14:f:533:THR:HA	14:f:579:GLU:HB3	2.03	0.40
14:f:918:ILE:HA	14:f:946:MET:HB2	2.01	0.40
15:h:133:GLU:HG3	15:h:136:ARG:HH21	1.86	0.40
15:j:5:LYS:O	15:j:45:VAL:HG12	2.22	0.40
15:j:91:GLU:HA	15:j:94:LYS:HG2	2.03	0.40
1:m:249:LEU:HD13	1:m:299:ILE:HD13	2.04	0.40
1:m:353:ASP:OD1	1:m:353:ASP:N	2.53	0.40
2:p:50:TRP:NE1	2:p:73:ARG:HB3	2.36	0.40
2:p:134:ASP:O	2:p:138:GLY:N	2.53	0.40
3:A:124:ARG:HG2	3:A:357:PRO:HG3	2.04	0.40
3:A:621:PHE:HD1	3:A:621:PHE:HA	1.77	0.40
3:C:90:LYS:HA	3:C:109:LEU:O	2.22	0.40
3:D:38:LYS:O	3:D:69:MET:HB2	2.21	0.40
3:D:122:ILE:HD13	3:D:137:LYS:HG2	2.02	0.40
3:F:413:VAL:HG23	3:F:420:TYR:HB2	2.02	0.40
3:G:577:GLN:OE1	3:G:578:LEU:N	2.49	0.40
3:H:261:ILE:HG12	3:H:288:PHE:HB2	2.03	0.40
3:I:157:PRO:HG2	3:I:379:LYS:HD2	2.03	0.40

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:414:LYS:HE3	3:I:414:LYS:HB3	1.78	0.40
5:N:33:PRO:HB3	8:Q:376:PRO:HA	2.03	0.40
8:Q:297:LEU:HD23	8:Q:297:LEU:HA	1.85	0.40
4:R:424:ASP:HA	4:R:427:ILE:HD12	2.03	0.40
4:R:465:LYS:HE2	4:R:519:ARG:HA	2.02	0.40
4:R:841:ILE:HD13	4:R:841:ILE:HA	1.86	0.40
7:S:201:ASP:HB3	7:S:307:ASP:HB2	2.04	0.40
11:X:169:PHE:CD1	11:X:235:VAL:HG22	2.56	0.40
11:X:265:ILE:HG23	11:X:432:TYR:CE2	2.57	0.40
13:b:220:MET:HA	13:b:220:MET:HE2	2.03	0.40
13:b:623:GLU:HG3	14:e:314:ILE:HG12	2.04	0.40
13:d:148:PHE:HA	13:d:298:ARG:HD2	2.02	0.40
13:d:601:ARG:HA	13:d:604:GLN:HB2	2.03	0.40
14:e:335:VAL:HG11	14:e:394:PHE:CD2	2.57	0.40
14:e:648:LYS:HB2	14:e:648:LYS:HE2	1.90	0.40
14:e:779:VAL:HG12	14:e:807:ASP:H	1.85	0.40
14:f:736:LEU:HG	14:f:746:LEU:HD21	2.03	0.40
15:h:56:LYS:O	15:h:59:ILE:HG22	2.21	0.40
16:n:8:LEU:HD11	15:j:104:ILE:HG21	2.04	0.40
16:n:223:ILE:HD12	16:n:223:ILE:HA	1.86	0.40
16:n:403:ILE:HD12	16:n:403:ILE:HA	1.84	0.40
2:p:440:ASP:OD1	2:p:443:SER:OG	2.33	0.40
3:A:191:ILE:HA	3:A:194:ASN:HD22	1.87	0.40
3:A:375:ASP:OD1	3:A:375:ASP:N	2.53	0.40
3:A:559:THR:HG23	3:B:4:GLN:HB2	2.03	0.40
3:F:130:MET:H	3:F:130:MET:HG2	1.45	0.40
3:H:480:ASP:OD1	3:H:480:ASP:N	2.53	0.40
3:I:94:SER:HA	3:I:105:ALA:O	2.21	0.40
3:I:252:PHE:HZ	3:I:354:THR:HG21	1.86	0.40
3:I:475:PHE:CE1	3:I:490:LEU:HD13	2.56	0.40
3:K:116:ILE:HG12	3:K:185:VAL:HG13	2.03	0.40
7:P:922:SER:OG	7:P:923:ASN:OD1	2.36	0.40
7:P:1096:ASP:OD1	7:P:1096:ASP:N	2.45	0.40
8:Q:453:CYS:HB3	8:Q:463:LEU:HB2	2.03	0.40
8:Q:566:ILE:HG13	8:Q:579:ILE:HD11	2.04	0.40
7:S:478:PRO:HB2	7:S:480:GLN:HG3	2.03	0.40
8:T:321:LEU:HD23	8:T:321:LEU:HA	1.92	0.40
13:b:36:PHE:HD2	13:b:71:LEU:HD13	1.87	0.40
13:b:350:LEU:HD23	13:b:350:LEU:HA	1.89	0.40
13:b:506:LEU:HD12	13:b:506:LEU:HA	1.94	0.40
12:c:35:ALA:HB3	12:c:52:LEU:HB2	2.04	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:c:74:TYR:OH	12:c:137:ILE:HD13	2.21	0.40
14:e:245:LEU:HD21	14:e:276:GLN:HG2	2.04	0.40
14:e:587:LEU:HA	14:e:591:LEU:HD11	2.04	0.40
14:f:676:CYS:HA	14:f:679:LEU:HB3	2.03	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	m	459/466 (98%)	425 (93%)	32 (7%)	2 (0%)	30	59
2	p	462/468 (99%)	424 (92%)	34 (7%)	4 (1%)	14	42
3	A	643/682 (94%)	609 (95%)	33 (5%)	1 (0%)	43	71
3	B	649/682 (95%)	615 (95%)	32 (5%)	2 (0%)	36	65
3	C	649/682 (95%)	626 (96%)	20 (3%)	3 (0%)	24	54
3	D	642/682 (94%)	619 (96%)	23 (4%)	0	100	100
3	E	649/682 (95%)	618 (95%)	29 (4%)	2 (0%)	36	65
3	F	627/682 (92%)	594 (95%)	31 (5%)	2 (0%)	36	65
3	G	649/682 (95%)	620 (96%)	28 (4%)	1 (0%)	43	71
3	H	642/682 (94%)	621 (97%)	21 (3%)	0	100	100
3	I	643/682 (94%)	621 (97%)	20 (3%)	2 (0%)	36	65
3	K	633/682 (93%)	606 (96%)	26 (4%)	1 (0%)	43	71
4	M	86/937 (9%)	81 (94%)	5 (6%)	0	100	100
4	R	834/937 (89%)	803 (96%)	31 (4%)	0	100	100
5	N	118/164 (72%)	115 (98%)	3 (2%)	0	100	100
5	U	85/164 (52%)	77 (91%)	8 (9%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	O	126/346 (36%)	122 (97%)	4 (3%)	0	100	100
7	P	934/1163 (80%)	898 (96%)	36 (4%)	0	100	100
7	S	945/1163 (81%)	907 (96%)	37 (4%)	1 (0%)	48	78
8	Q	361/581 (62%)	334 (92%)	25 (7%)	2 (1%)	21	50
8	T	351/581 (60%)	335 (95%)	16 (5%)	0	100	100
9	V	57/228 (25%)	53 (93%)	4 (7%)	0	100	100
10	W	429/445 (96%)	414 (96%)	15 (4%)	0	100	100
10	Z	424/445 (95%)	398 (94%)	26 (6%)	0	100	100
11	X	410/449 (91%)	397 (97%)	12 (3%)	1 (0%)	43	71
11	Y	417/449 (93%)	383 (92%)	34 (8%)	0	100	100
12	a	145/147 (99%)	138 (95%)	7 (5%)	0	100	100
12	c	145/147 (99%)	132 (91%)	12 (8%)	1 (1%)	18	47
13	b	618/782 (79%)	572 (93%)	46 (7%)	0	100	100
13	d	604/782 (77%)	565 (94%)	39 (6%)	0	100	100
14	e	965/993 (97%)	881 (91%)	83 (9%)	1 (0%)	48	78
14	f	959/993 (97%)	869 (91%)	85 (9%)	5 (0%)	24	54
15	h	134/163 (82%)	127 (95%)	7 (5%)	0	100	100
15	j	138/163 (85%)	132 (96%)	5 (4%)	1 (1%)	18	47
15	l	125/163 (77%)	117 (94%)	8 (6%)	0	100	100
16	n	465/469 (99%)	440 (95%)	23 (5%)	2 (0%)	30	59
All	All	17222/20608 (84%)	16288 (95%)	900 (5%)	34 (0%)	44	71

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	p	129	ARG
3	G	99	ASP
7	S	942	GLU
14	f	495	GLN
14	f	959	LYS
16	n	59	VAL
15	j	160	CYS
3	B	71	HIS
11	X	101	ASN
1	m	51	LEU

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type
2	p	127	MET
2	p	294	ARG
3	A	341	GLN
3	C	12	VAL
3	C	104	THR
3	C	309	ARG
3	E	104	THR
3	F	102	VAL
3	B	309	ARG
3	E	5	ASN
3	I	99	ASP
3	I	104	THR
12	c	57	PRO
14	e	472	LYS
3	K	309	ARG
8	Q	313	GLN
14	f	247	LYS
14	f	252	ALA
8	Q	279	THR
14	f	979	PRO
16	n	346	GLU
2	p	324	GLY
3	F	519	ILE
1	m	112	ILE

### 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	m	425/430 (99%)	419 (99%)	6 (1%)	59	70
2	p	428/431 (99%)	418 (98%)	10 (2%)	44	63
3	A	588/613 (96%)	587 (100%)	1 (0%)	87	85
3	B	591/613 (96%)	589 (100%)	2 (0%)	86	84
3	C	591/613 (96%)	588 (100%)	3 (0%)	81	81

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	D	587/613 (96%)	582 (99%)	5 (1%)	70	76
3	E	591/613 (96%)	587 (99%)	4 (1%)	76	78
3	F	578/613 (94%)	576 (100%)	2 (0%)	86	84
3	G	591/613 (96%)	587 (99%)	4 (1%)	76	78
3	H	586/613 (96%)	580 (99%)	6 (1%)	68	75
3	I	588/613 (96%)	585 (100%)	3 (0%)	81	81
3	K	581/613 (95%)	580 (100%)	1 (0%)	87	85
4	M	79/862 (9%)	79 (100%)	0	100	100
4	R	773/862 (90%)	768 (99%)	5 (1%)	78	80
5	N	107/143 (75%)	106 (99%)	1 (1%)	70	76
5	U	76/143 (53%)	76 (100%)	0	100	100
6	O	115/278 (41%)	114 (99%)	1 (1%)	70	76
7	P	843/1054 (80%)	842 (100%)	1 (0%)	88	89
7	S	847/1054 (80%)	839 (99%)	8 (1%)	70	76
8	Q	322/516 (62%)	322 (100%)	0	100	100
8	T	313/516 (61%)	311 (99%)	2 (1%)	78	80
9	V	50/197 (25%)	50 (100%)	0	100	100
10	W	371/382 (97%)	369 (100%)	2 (0%)	81	81
10	Z	369/382 (97%)	367 (100%)	2 (0%)	81	81
11	X	356/376 (95%)	353 (99%)	3 (1%)	73	77
11	Y	355/376 (94%)	352 (99%)	3 (1%)	73	77
12	a	132/132 (100%)	132 (100%)	0	100	100
12	c	132/132 (100%)	130 (98%)	2 (2%)	57	69
13	b	555/682 (81%)	547 (99%)	8 (1%)	59	70
13	d	544/682 (80%)	541 (99%)	3 (1%)	78	80
14	e	884/909 (97%)	876 (99%)	8 (1%)	70	76
14	f	880/909 (97%)	869 (99%)	11 (1%)	61	71
15	h	132/150 (88%)	131 (99%)	1 (1%)	73	77
15	j	132/150 (88%)	132 (100%)	0	100	100
15	l	121/150 (81%)	120 (99%)	1 (1%)	73	77
16	n	433/435 (100%)	432 (100%)	1 (0%)	87	85

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	15646/18463 (85%)	15536 (99%)	110 (1%)	73	78

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	m	98	GLU
1	m	99	PHE
1	m	102	HIS
1	m	200	THR
1	m	329	ILE
1	m	339	LEU
2	p	7	ARG
2	p	45	LEU
2	p	57	THR
2	p	60	LEU
2	p	127	MET
2	p	229	LEU
2	p	320	LEU
2	p	327	ILE
2	p	411	GLU
2	p	428	LEU
3	A	517	GLU
3	B	79	MET
3	B	287	MET
3	C	11	LEU
3	C	28	ASP
3	C	97	CYS
3	D	1	MET
3	D	49	LEU
3	D	144	MET
3	D	279	ILE
3	D	307	LEU
3	E	65	VAL
3	E	80	VAL
3	E	261	ILE
3	E	389	LEU
3	F	198	ILE
3	F	605	MET
3	G	276	ILE
3	G	358	HIS
3	G	473	MET
3	G	606	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
3	H	38	LYS
3	H	109	LEU
3	H	224	VAL
3	H	442	LYS
3	H	490	LEU
3	H	575	ILE
3	I	27	LEU
3	I	92	LEU
3	I	236	THR
3	K	261	ILE
5	N	122	LYS
6	O	128	MET
7	P	320	LEU
4	R	224	LEU
4	R	568	ASN
4	R	767	LEU
4	R	869	LEU
4	R	914	GLU
7	S	213	PHE
7	S	321	PHE
7	S	492	VAL
7	S	497	MET
7	S	539	ASN
7	S	841	LEU
7	S	932	GLN
7	S	1155	GLU
8	T	171	MET
8	T	296	LEU
10	W	320	ARG
10	W	377	LEU
11	X	66	VAL
11	X	248	LEU
11	X	431	ASP
11	Y	163	LYS
11	Y	182	VAL
11	Y	203	MET
10	Z	263	LEU
10	Z	329	GLN
13	b	19	LEU
13	b	71	LEU
13	b	75	GLN
13	b	507	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
13	b	684	ASN
13	b	688	TRP
13	b	745	VAL
13	b	775	PHE
12	c	16	ASP
12	c	59	ASP
13	d	208	ILE
13	d	458	SER
13	d	711	PHE
14	e	70	PHE
14	e	251	TRP
14	e	298	THR
14	e	486	LEU
14	e	518	LEU
14	e	803	LEU
14	e	886	ASN
14	e	938	VAL
14	f	55	ASN
14	f	166	GLU
14	f	186	SER
14	f	282	LEU
14	f	300	THR
14	f	316	VAL
14	f	647	LEU
14	f	749	LEU
14	f	910	ILE
14	f	944	CYS
14	f	976	VAL
15	h	18	VAL
16	n	223	ILE
15	l	159	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (316) such sidechains are listed below:

Mol	Chain	Res	Type
1	m	136	HIS
1	m	161	HIS
1	m	230	ASN
1	m	240	HIS
2	p	4	HIS
2	p	109	HIS
2	p	128	ASN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
2	p	136	HIS
2	p	179	ASN
2	p	341	ASN
2	p	427	HIS
3	A	127	GLN
3	A	145	ASN
3	A	177	ASN
3	A	200	HIS
3	A	330	GLN
3	A	392	GLN
3	A	416	GLN
3	A	441	ASN
3	A	479	ASN
3	A	504	GLN
3	A	583	GLN
3	A	592	GLN
3	B	127	GLN
3	B	135	GLN
3	B	228	ASN
3	B	239	ASN
3	B	330	GLN
3	B	355	GLN
3	B	392	GLN
3	B	406	ASN
3	B	416	GLN
3	B	441	ASN
3	B	468	HIS
3	B	536	GLN
3	B	592	GLN
3	B	669	ASN
3	C	13	ASN
3	C	154	ASN
3	C	193	GLN
3	C	468	HIS
3	C	504	GLN
3	C	614	ASN
3	D	4	GLN
3	D	182	ASN
3	D	215	GLN
3	D	358	HIS
3	D	577	GLN
3	D	626	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
3	D	658	ASN
3	E	13	ASN
3	E	51	HIS
3	E	182	ASN
3	E	272	HIS
3	E	300	GLN
3	E	355	GLN
3	E	557	ASN
3	E	592	GLN
3	E	607	GLN
3	E	658	ASN
3	F	4	GLN
3	F	5	ASN
3	F	177	ASN
3	F	182	ASN
3	F	228	ASN
3	F	346	GLN
3	F	392	GLN
3	F	406	ASN
3	F	471	GLN
3	F	536	GLN
3	F	586	ASN
3	F	607	GLN
3	G	4	GLN
3	G	177	ASN
3	G	196	GLN
3	G	396	HIS
3	G	416	GLN
3	G	451	GLN
3	G	527	ASN
3	G	583	GLN
3	H	51	HIS
3	H	70	ASN
3	H	135	GLN
3	H	239	ASN
3	H	346	GLN
3	H	392	GLN
3	H	406	ASN
3	H	452	GLN
3	H	485	GLN
3	H	586	ASN
3	H	614	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
3	I	51	HIS
3	I	177	ASN
3	I	194	ASN
3	I	239	ASN
3	I	346	GLN
3	I	392	GLN
3	I	451	GLN
3	I	626	ASN
3	I	658	ASN
3	K	51	HIS
3	K	70	ASN
3	K	127	GLN
3	K	177	ASN
3	K	193	GLN
3	K	239	ASN
3	K	272	HIS
3	K	416	GLN
3	K	471	GLN
3	K	506	GLN
3	K	557	ASN
3	K	607	GLN
4	M	31	GLN
4	M	40	GLN
4	M	56	ASN
4	M	65	GLN
4	M	75	GLN
5	N	73	GLN
5	N	115	ASN
6	O	8	GLN
6	O	15	HIS
6	O	64	HIS
6	O	70	HIS
7	P	268	GLN
7	P	273	GLN
7	P	315	GLN
7	P	334	GLN
7	P	402	GLN
7	P	407	ASN
7	P	459	GLN
7	P	471	HIS
7	P	516	ASN
7	P	539	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
7	P	571	HIS
7	P	604	ASN
7	P	637	GLN
7	P	770	ASN
7	P	799	ASN
7	P	867	ASN
7	P	895	ASN
7	P	915	ASN
7	P	1088	ASN
7	P	1159	ASN
8	Q	175	GLN
8	Q	285	GLN
8	Q	313	GLN
8	Q	342	ASN
8	Q	354	ASN
8	Q	396	ASN
8	Q	492	HIS
4	R	93	ASN
4	R	127	GLN
4	R	147	HIS
4	R	329	ASN
4	R	331	GLN
4	R	337	GLN
4	R	470	HIS
4	R	477	ASN
4	R	492	GLN
4	R	571	GLN
4	R	623	ASN
4	R	685	GLN
4	R	686	ASN
4	R	787	GLN
4	R	798	GLN
4	R	903	ASN
7	S	296	GLN
7	S	334	GLN
7	S	374	ASN
7	S	419	HIS
7	S	425	HIS
7	S	459	GLN
7	S	471	HIS
7	S	480	GLN
7	S	539	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
7	S	628	GLN
7	S	636	GLN
7	S	639	ASN
7	S	670	GLN
7	S	693	GLN
7	S	791	HIS
7	S	799	ASN
7	S	867	ASN
7	S	889	GLN
7	S	895	ASN
7	S	904	HIS
7	S	913	ASN
7	S	923	ASN
7	S	940	ASN
7	S	946	GLN
7	S	1143	HIS
7	S	1159	ASN
8	T	274	GLN
8	T	285	GLN
8	T	292	HIS
8	T	383	GLN
8	T	392	GLN
8	T	396	ASN
8	T	502	GLN
8	T	547	GLN
5	U	39	GLN
5	U	43	ASN
5	U	103	ASN
9	V	48	GLN
9	V	83	HIS
9	V	88	HIS
10	W	43	GLN
10	W	131	GLN
10	W	165	ASN
10	W	329	GLN
10	W	332	ASN
10	W	375	GLN
11	X	28	HIS
11	X	50	ASN
11	X	102	ASN
11	X	139	HIS
11	X	197	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
11	X	226	ASN
11	Y	28	HIS
11	Y	50	ASN
11	Y	88	HIS
11	Y	176	GLN
10	Z	8	GLN
10	Z	43	GLN
10	Z	131	GLN
10	Z	134	GLN
10	Z	245	GLN
10	Z	247	ASN
10	Z	337	ASN
10	Z	375	GLN
12	a	20	GLN
12	a	46	GLN
12	a	114	ASN
13	b	4	GLN
13	b	43	GLN
13	b	66	ASN
13	b	70	GLN
13	b	217	GLN
13	b	224	ASN
13	b	264	ASN
13	b	717	GLN
13	b	768	GLN
13	b	773	GLN
12	c	20	GLN
12	c	55	HIS
12	c	77	ASN
12	c	135	ASN
13	d	43	GLN
13	d	190	HIS
13	d	217	GLN
13	d	335	GLN
13	d	477	ASN
13	d	518	HIS
13	d	548	HIS
13	d	621	ASN
13	d	674	GLN
13	d	731	ASN
13	d	744	GLN
13	d	765	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
13	d	768	GLN
13	d	773	GLN
14	e	75	GLN
14	e	120	ASN
14	e	139	HIS
14	e	175	GLN
14	e	262	ASN
14	e	273	HIS
14	e	347	GLN
14	e	353	HIS
14	e	452	ASN
14	e	495	GLN
14	e	517	GLN
14	e	596	ASN
14	e	601	HIS
14	e	677	GLN
14	e	713	ASN
14	e	766	HIS
14	e	811	ASN
14	e	867	HIS
14	e	884	ASN
14	f	111	GLN
14	f	120	ASN
14	f	139	HIS
14	f	149	GLN
14	f	184	GLN
14	f	270	HIS
14	f	273	HIS
14	f	349	ASN
14	f	383	HIS
14	f	479	GLN
14	f	487	HIS
14	f	574	ASN
14	f	629	ASN
14	f	634	HIS
14	f	645	ASN
14	f	686	ASN
14	f	697	ASN
14	f	713	ASN
14	f	754	ASN
14	f	827	GLN
14	f	856	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
14	f	905	GLN
14	f	971	ASN
15	h	7	GLN
15	h	23	GLN
15	h	158	GLN
16	n	196	GLN
16	n	427	ASN
15	j	23	GLN
15	j	90	GLN
15	j	108	ASN
15	j	125	ASN
15	l	108	ASN
15	l	125	ASN
15	l	140	ASN
15	l	158	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 10 are monoatomic - leaving 9 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
17	ATP	e	1001	-	29,33,33	0.28	0	44,52,52	0.46	1 (2%)
18	GTP	X	501	19	30,34,34	0.84	1 (3%)	46,54,54	1.85	11 (23%)
18	GTP	Y	501	19	30,34,34	0.83	1 (3%)	46,54,54	1.78	11 (23%)
18	GTP	Z	501	19	30,34,34	0.86	1 (3%)	46,54,54	1.73	12 (26%)
17	ATP	S	1201	-	29,33,33	0.29	0	44,52,52	0.46	0
17	ATP	f	1001	-	29,33,33	0.29	0	44,52,52	0.61	1 (2%)
18	GTP	W	501	19	30,34,34	0.85	1 (3%)	46,54,54	1.78	11 (23%)
17	ATP	R	1001	-	29,33,33	0.28	0	44,52,52	0.51	1 (2%)
17	ATP	P	1201	-	29,33,33	0.28	0	44,52,52	0.45	1 (2%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	ATP	e	1001	-	-	9/22/38/38	0/3/3/3
18	GTP	X	501	19	-	3/22/38/38	0/3/3/3
18	GTP	Y	501	19	-	6/22/38/38	0/3/3/3
18	GTP	Z	501	19	-	7/22/38/38	0/3/3/3
17	ATP	S	1201	-	-	5/22/38/38	0/3/3/3
17	ATP	f	1001	-	-	8/22/38/38	0/3/3/3
18	GTP	W	501	19	-	3/22/38/38	0/3/3/3
17	ATP	R	1001	-	-	7/22/38/38	0/3/3/3
17	ATP	P	1201	-	-	5/22/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	Z	501	GTP	C2-N3	2.22	1.38	1.33
18	Y	501	GTP	C2-N3	2.19	1.38	1.33
18	W	501	GTP	C2-N3	2.17	1.38	1.33
18	X	501	GTP	C2-N3	2.15	1.38	1.33

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	X	501	GTP	C5-C4-N3	-5.23	119.97	128.46

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	Y	501	GTP	C5-C4-N3	-5.03	120.31	128.46
18	W	501	GTP	C5-C4-N3	-4.97	120.39	128.46
18	X	501	GTP	C2-N3-C4	4.87	120.97	112.30
18	Z	501	GTP	C5-C4-N3	-4.78	120.70	128.46
18	Y	501	GTP	C2-N3-C4	4.58	120.45	112.30
18	W	501	GTP	C2-N3-C4	4.45	120.23	112.30
18	Z	501	GTP	C2-N3-C4	4.40	120.13	112.30
18	X	501	GTP	PB-O3B-PG	-4.11	118.72	132.83
18	Y	501	GTP	PB-O3B-PG	-3.63	120.38	132.83
18	W	501	GTP	PB-O3B-PG	-3.58	120.55	132.83
18	X	501	GTP	N9-C4-N3	3.36	132.68	125.94
18	W	501	GTP	N9-C4-N3	3.34	132.65	125.94
18	W	501	GTP	PA-O3A-PB	-3.31	121.48	132.83
18	Y	501	GTP	PA-O3A-PB	-3.27	121.62	132.83
18	Y	501	GTP	N9-C4-N3	3.21	132.39	125.94
18	Z	501	GTP	N9-C4-N3	3.15	132.26	125.94
18	Z	501	GTP	PB-O3B-PG	-3.13	122.10	132.83
18	X	501	GTP	PA-O3A-PB	-3.02	122.46	132.83
18	Y	501	GTP	C2-N1-C6	-2.93	119.75	125.10
18	X	501	GTP	C2-N1-C6	-2.93	119.76	125.10
18	W	501	GTP	C2-N1-C6	-2.90	119.81	125.10
18	Z	501	GTP	C2-N1-C6	-2.88	119.85	125.10
18	Z	501	GTP	PA-O3A-PB	-2.88	122.95	132.83
18	Y	501	GTP	N9-C8-N7	-2.72	108.26	113.39
18	X	501	GTP	N9-C8-N7	-2.65	108.41	113.39
18	Z	501	GTP	N9-C8-N7	-2.63	108.44	113.39
18	Z	501	GTP	C5-C6-N1	2.61	119.82	113.19
18	Y	501	GTP	C8-N7-C5	2.59	108.93	104.24
18	X	501	GTP	C5-C6-N1	2.59	119.76	113.19
18	W	501	GTP	N9-C8-N7	-2.57	108.56	113.39
18	W	501	GTP	C5-C6-N1	2.57	119.70	113.19
18	Y	501	GTP	C5-C6-N1	2.54	119.65	113.19
18	X	501	GTP	C8-N7-C5	2.52	108.81	104.24
18	Z	501	GTP	O6-C6-C5	-2.50	119.96	126.60
18	X	501	GTP	O6-C6-C5	-2.50	119.96	126.60
18	W	501	GTP	O6-C6-C5	-2.43	120.15	126.60
18	Y	501	GTP	O6-C6-C5	-2.42	120.19	126.60
18	Z	501	GTP	C8-N7-C5	2.41	108.60	104.24
18	W	501	GTP	C8-N7-C5	2.37	108.52	104.24
18	W	501	GTP	C3'-C2'-C1'	2.21	105.62	101.43
18	Y	501	GTP	C3'-C2'-C1'	2.15	105.51	101.43
18	X	501	GTP	C3'-C2'-C1'	2.11	105.43	101.43

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	R	1001	ATP	PB-O3B-PG	2.04	139.84	132.83
17	f	1001	ATP	PB-O3B-PG	2.04	139.82	132.83
18	Z	501	GTP	C2'-C3'-C4'	2.03	106.58	102.64
18	Z	501	GTP	C3'-C2'-C1'	2.02	105.27	101.43
17	P	1201	ATP	PB-O3B-PG	2.01	139.72	132.83
17	e	1001	ATP	PB-O3B-PG	2.00	139.70	132.83

There are no chirality outliers.

All (53) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	P	1201	ATP	PB-O3B-PG-O3G
17	R	1001	ATP	C5'-O5'-PA-O1A
17	R	1001	ATP	C5'-O5'-PA-O2A
17	R	1001	ATP	C3'-C4'-C5'-O5'
17	e	1001	ATP	PB-O3B-PG-O3G
17	e	1001	ATP	C5'-O5'-PA-O1A
17	e	1001	ATP	C5'-O5'-PA-O2A
17	e	1001	ATP	C3'-C4'-C5'-O5'
17	f	1001	ATP	C5'-O5'-PA-O1A
17	f	1001	ATP	C5'-O5'-PA-O3A
18	W	501	GTP	C3'-C4'-C5'-O5'
18	X	501	GTP	C5'-O5'-PA-O3A
18	X	501	GTP	C5'-O5'-PA-O2A
18	Y	501	GTP	C5'-O5'-PA-O1A
18	Z	501	GTP	C5'-O5'-PA-O1A
18	Z	501	GTP	C5'-O5'-PA-O2A
18	Z	501	GTP	C3'-C4'-C5'-O5'
17	P	1201	ATP	O4'-C4'-C5'-O5'
18	Y	501	GTP	C3'-C4'-C5'-O5'
17	P	1201	ATP	C3'-C4'-C5'-O5'
17	e	1001	ATP	O4'-C4'-C5'-O5'
18	Y	501	GTP	O4'-C4'-C5'-O5'
18	Z	501	GTP	O4'-C4'-C5'-O5'
17	R	1001	ATP	O4'-C4'-C5'-O5'
18	W	501	GTP	O4'-C4'-C5'-O5'
18	W	501	GTP	C4'-C5'-O5'-PA
17	S	1201	ATP	PA-O3A-PB-O1B
17	f	1001	ATP	PG-O3B-PB-O1B
17	S	1201	ATP	C3'-C4'-C5'-O5'
18	X	501	GTP	C4'-C5'-O5'-PA
18	Z	501	GTP	C4'-C5'-O5'-PA

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
17	e	1001	ATP	C4'-C5'-O5'-PA
18	Z	501	GTP	PB-O3A-PA-O5'
17	P	1201	ATP	C4'-C5'-O5'-PA
17	f	1001	ATP	C4'-C5'-O5'-PA
17	R	1001	ATP	C5'-O5'-PA-O3A
18	Y	501	GTP	C5'-O5'-PA-O3A
18	Y	501	GTP	C5'-O5'-PA-O2A
17	P	1201	ATP	PG-O3B-PB-O2B
18	Y	501	GTP	PB-O3A-PA-O2A
17	R	1001	ATP	PA-O3A-PB-O3B
17	f	1001	ATP	O4'-C1'-N9-C8
17	f	1001	ATP	PG-O3B-PB-O2B
17	f	1001	ATP	C2'-C1'-N9-C8
17	f	1001	ATP	C2'-C1'-N9-C4
17	e	1001	ATP	PB-O3B-PG-O2G
17	S	1201	ATP	C5'-O5'-PA-O3A
17	e	1001	ATP	C5'-O5'-PA-O3A
18	Z	501	GTP	C5'-O5'-PA-O3A
17	R	1001	ATP	PA-O3A-PB-O1B
17	S	1201	ATP	PG-O3B-PB-O2B
17	S	1201	ATP	C5'-O5'-PA-O2A
17	e	1001	ATP	PB-O3B-PG-O1G

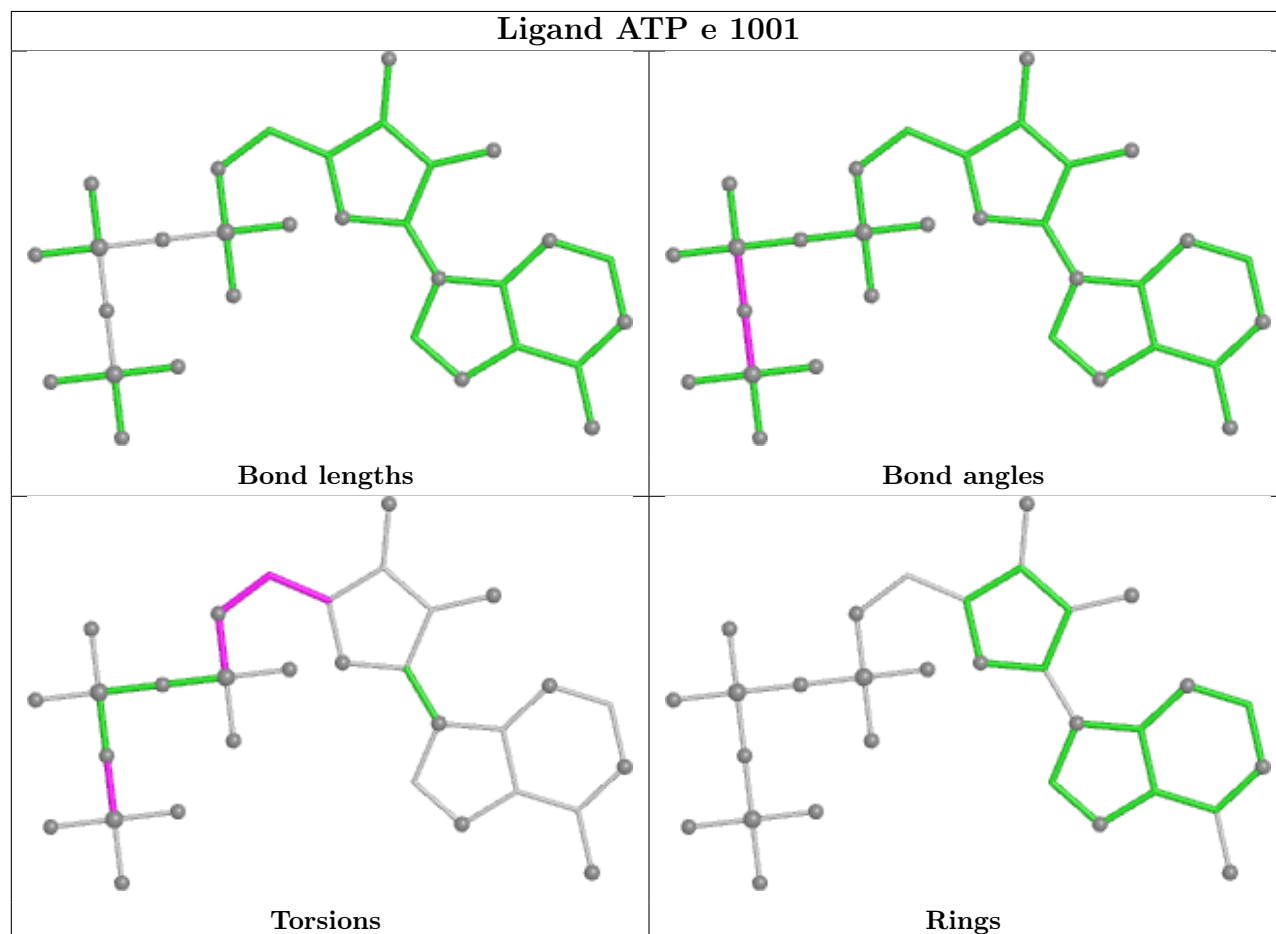
There are no ring outliers.

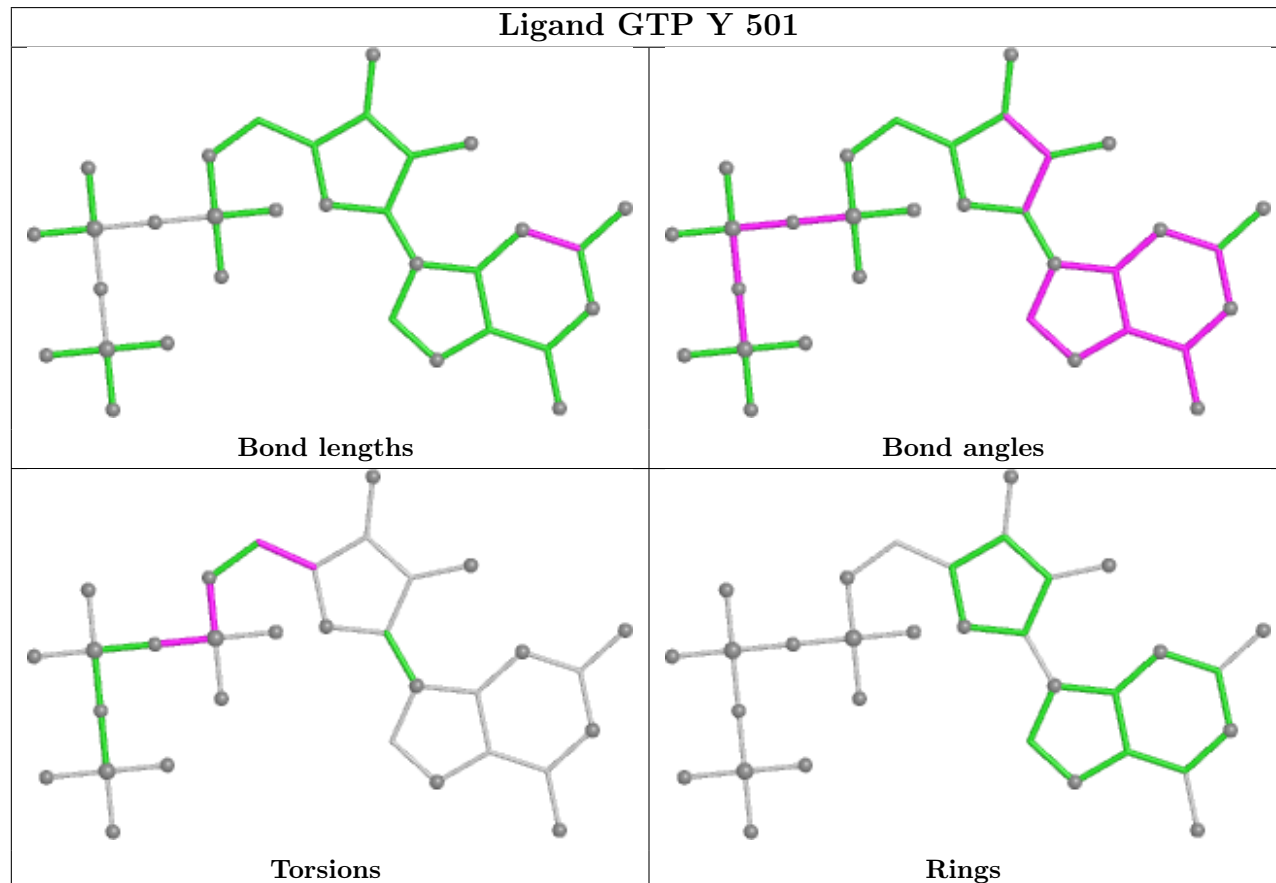
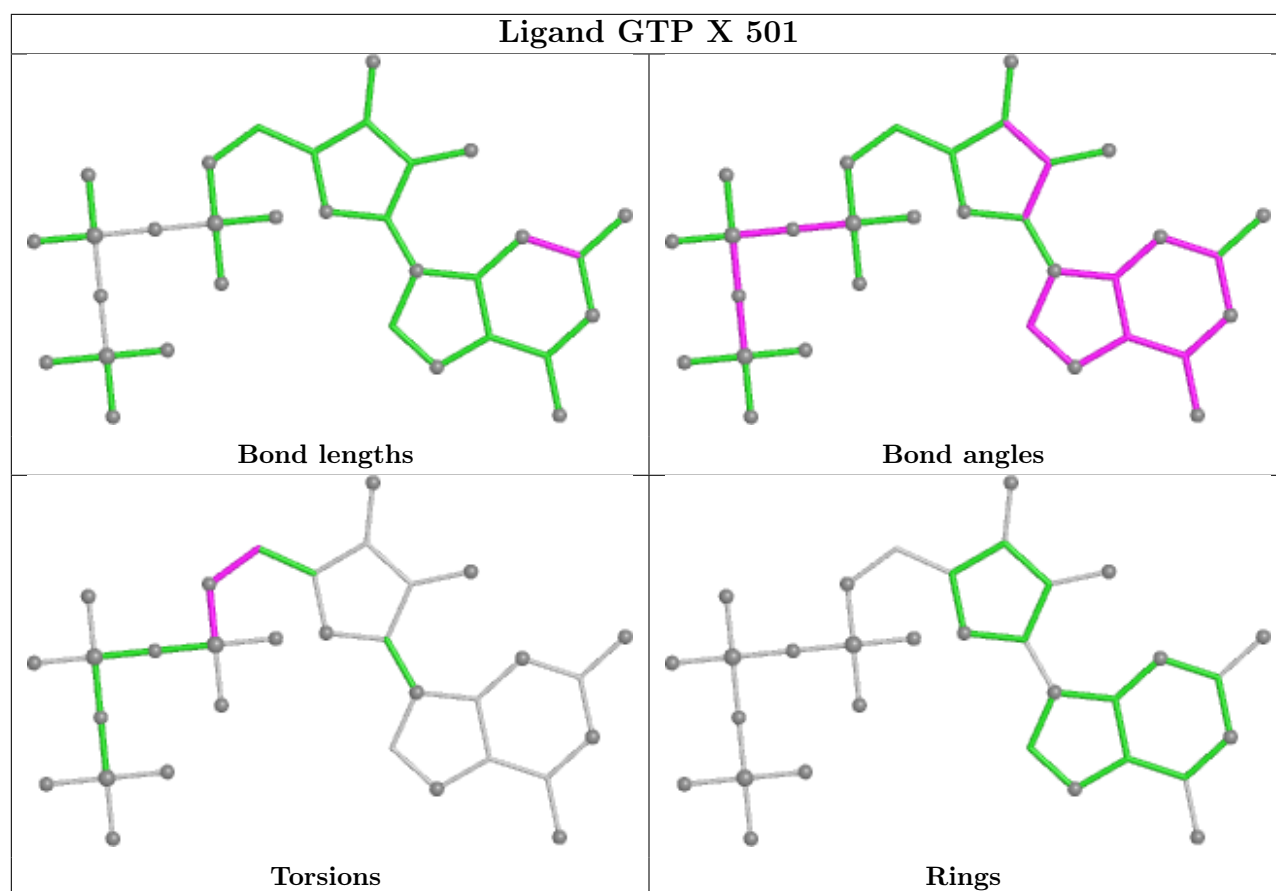
7 monomers are involved in 12 short contacts:

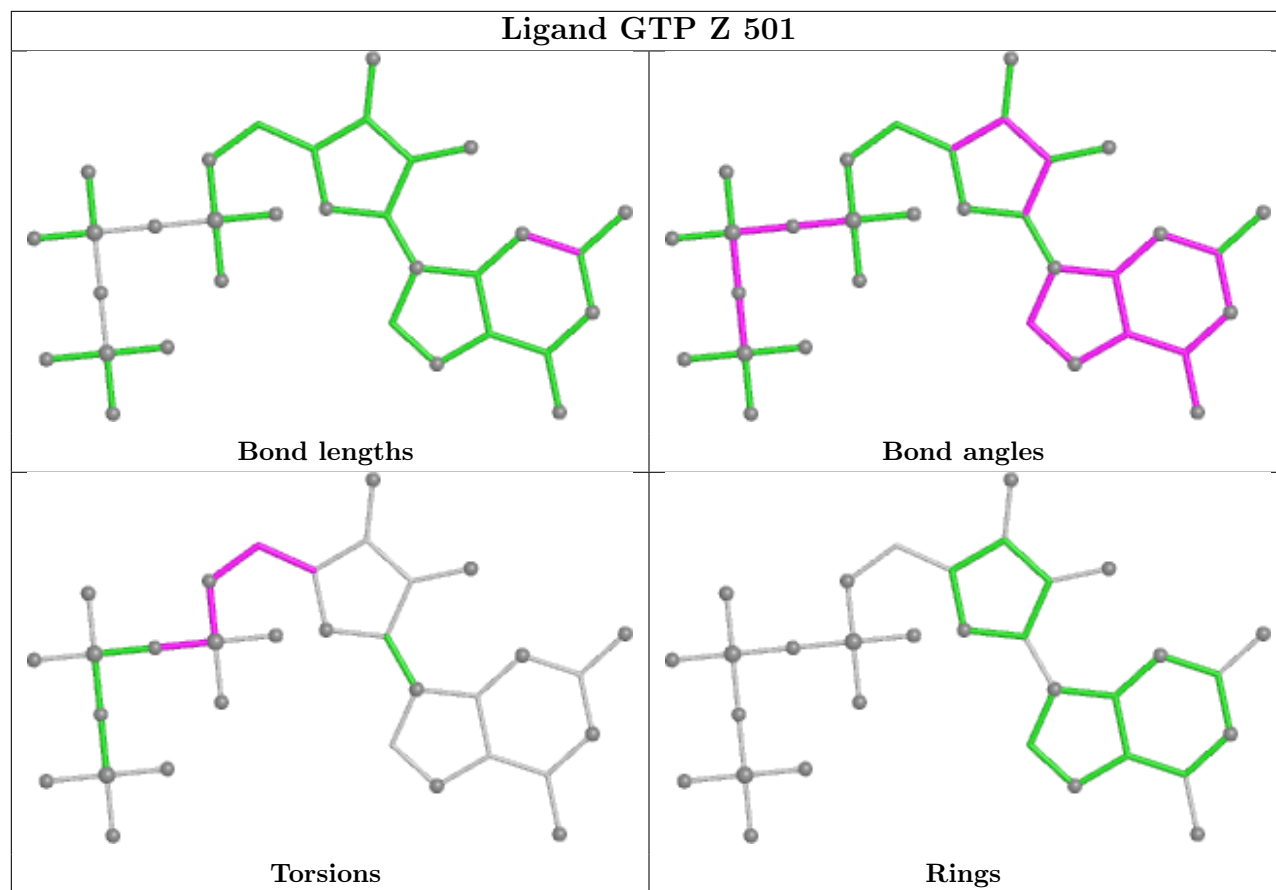
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	X	501	GTP	4	0
18	Y	501	GTP	1	0
17	S	1201	ATP	1	0
17	f	1001	ATP	1	0
18	W	501	GTP	2	0
17	R	1001	ATP	2	0
17	P	1201	ATP	1	0

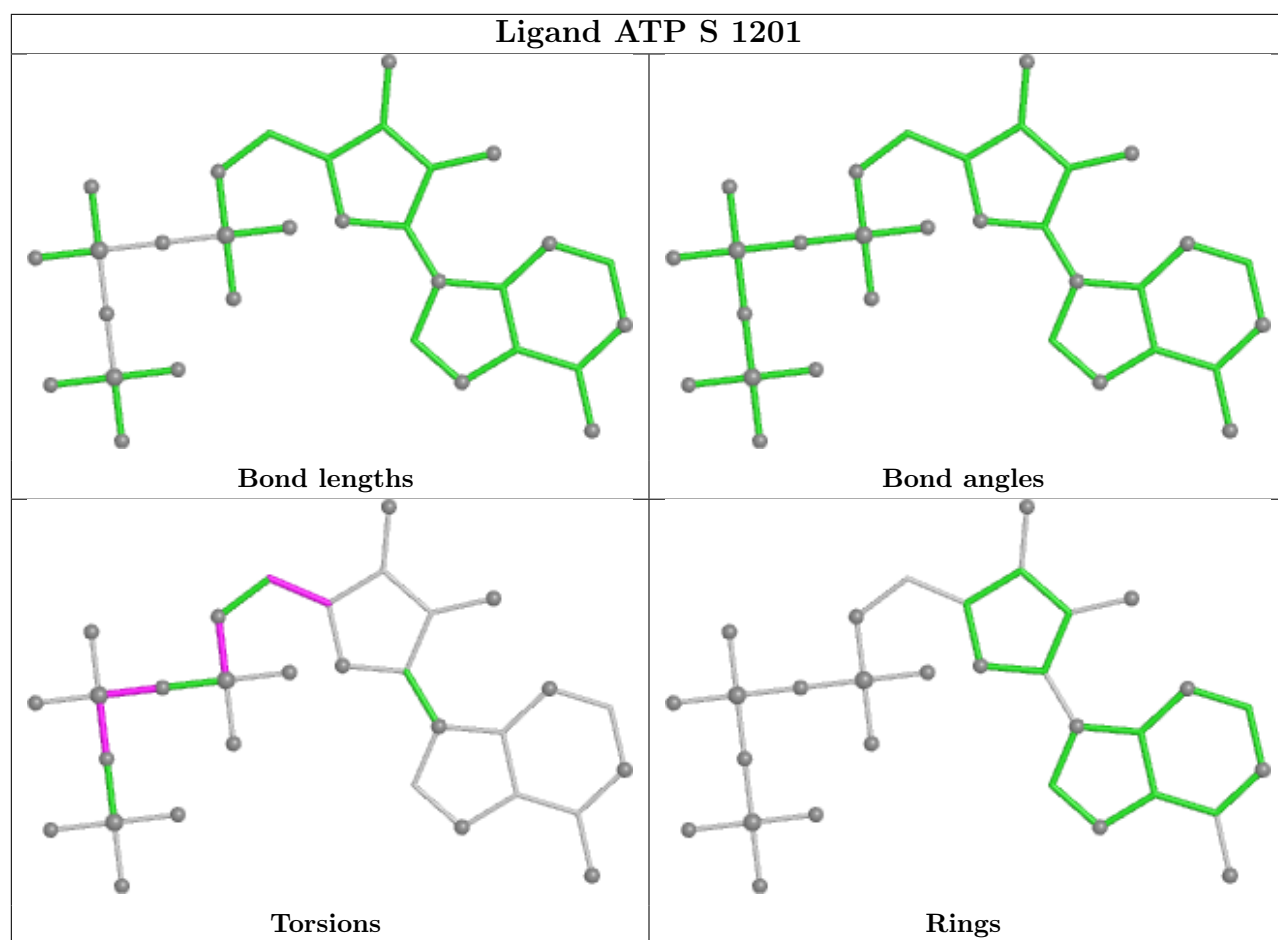
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

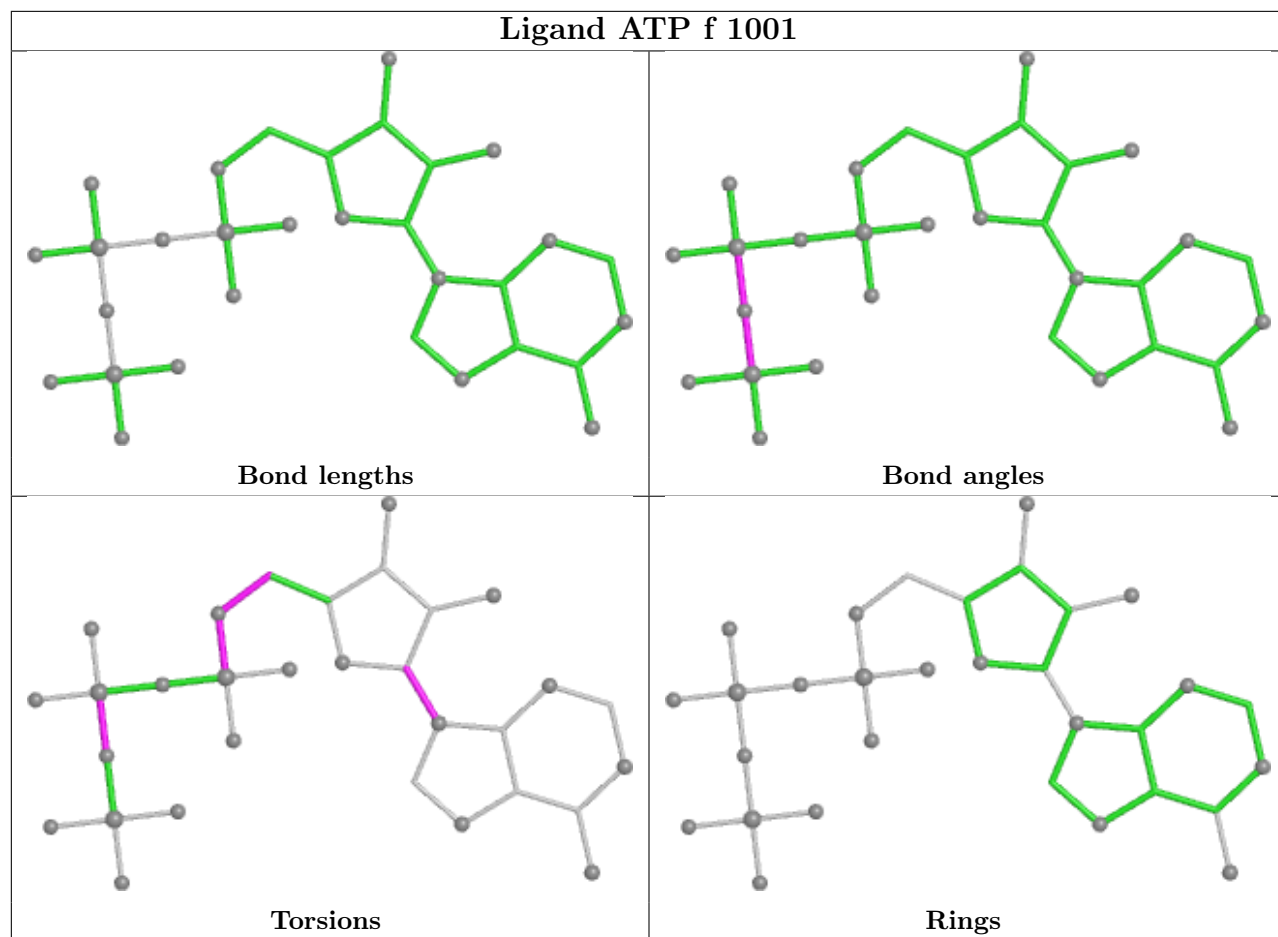


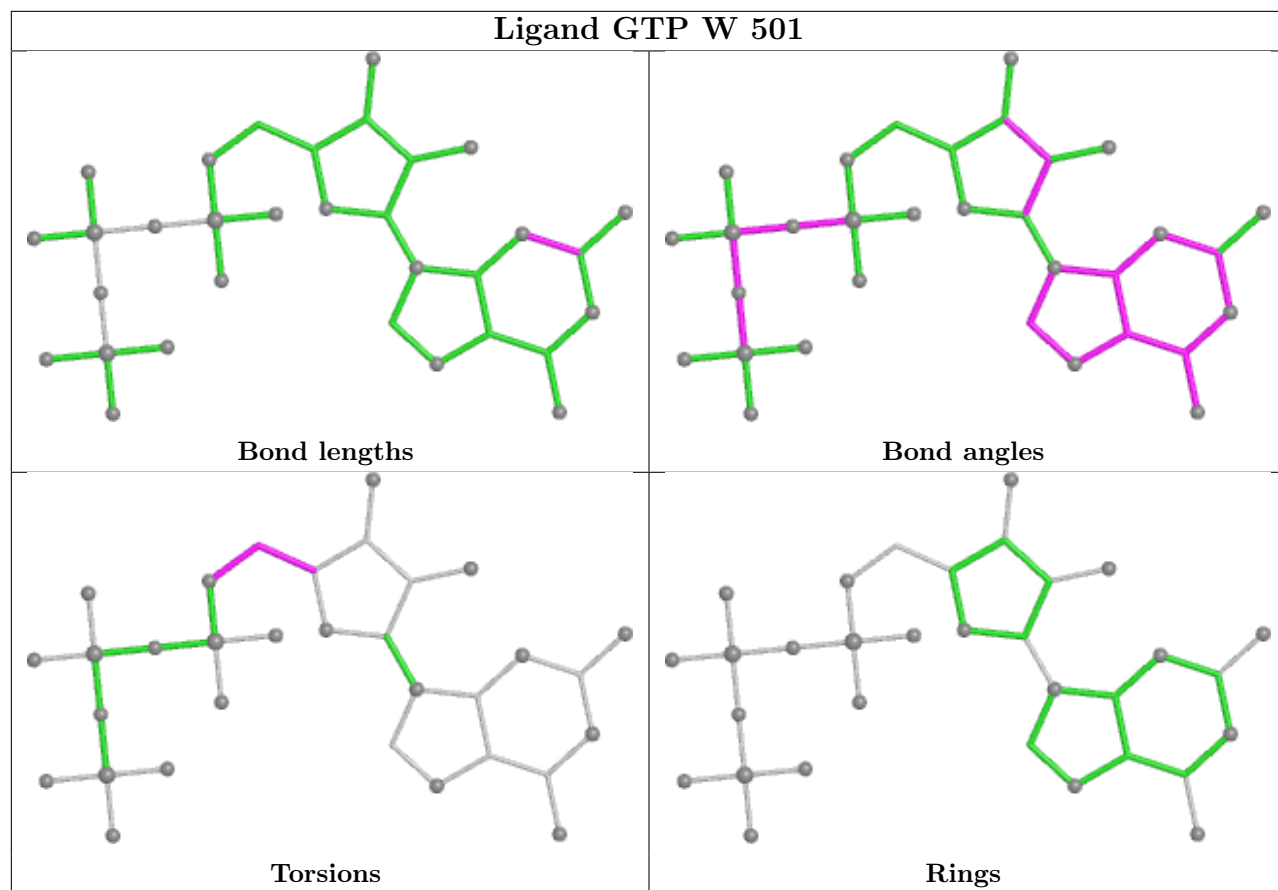


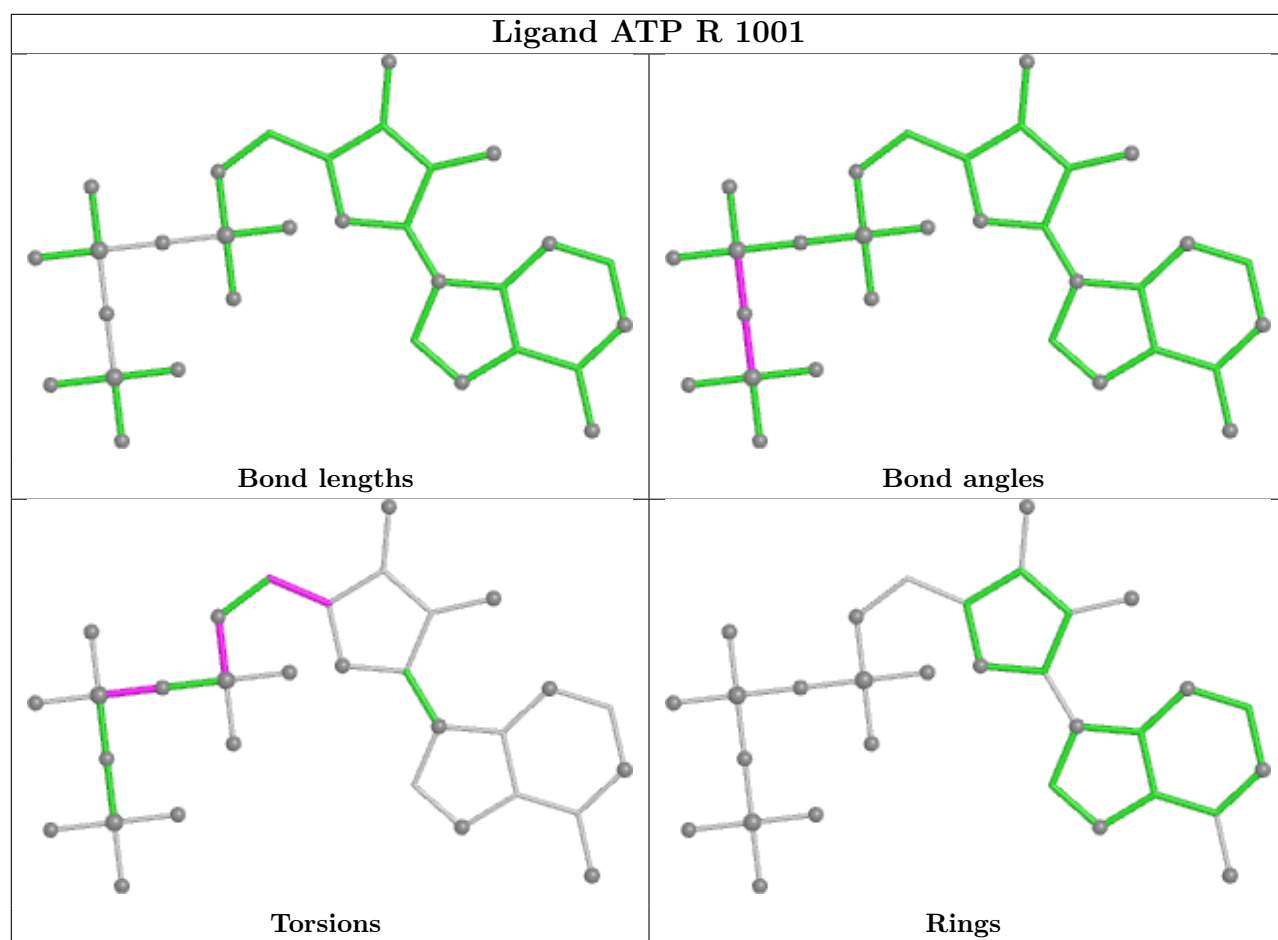


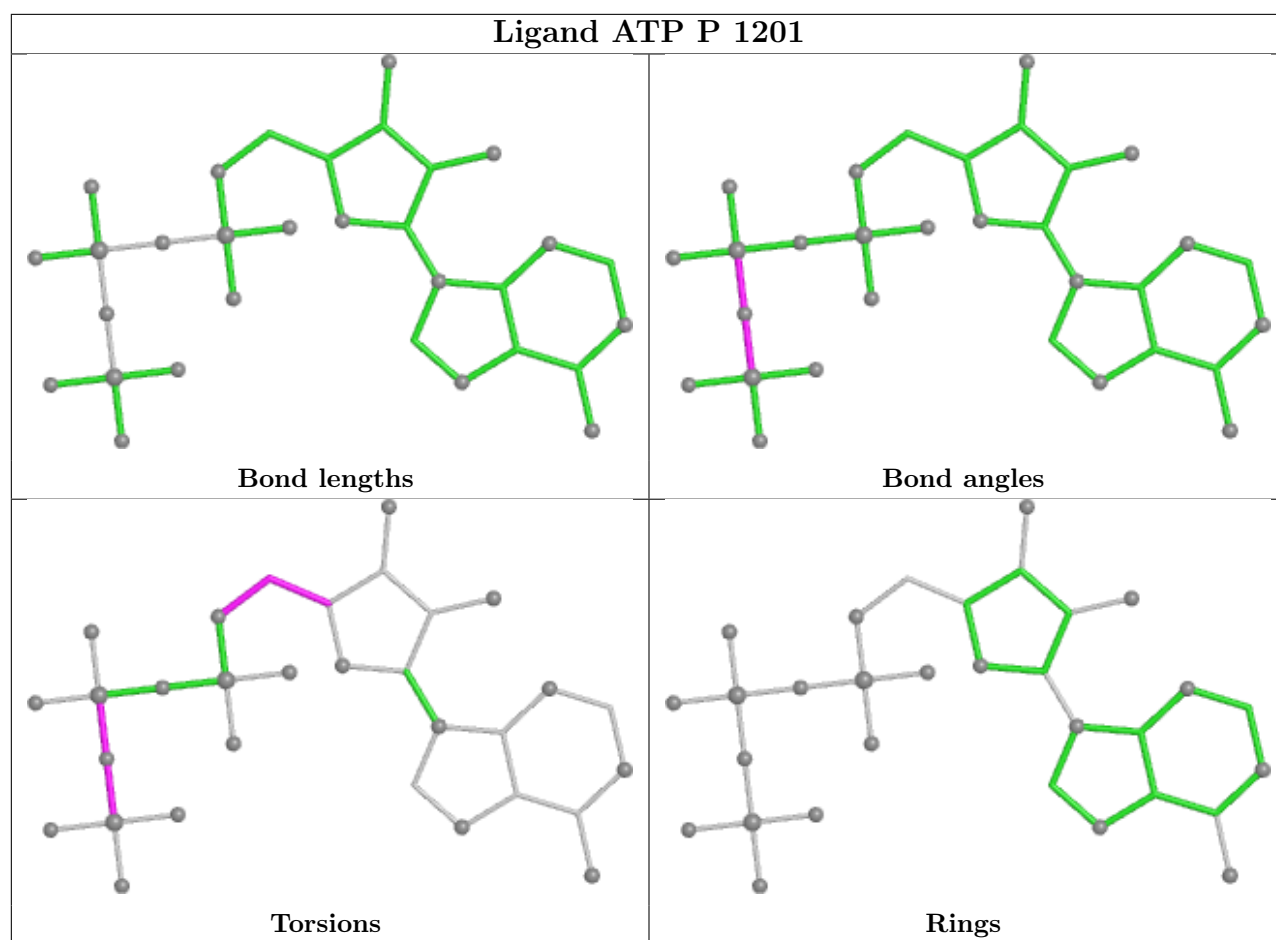












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

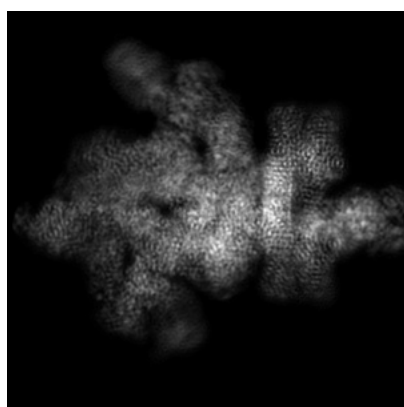
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-69647. These allow visual inspection of the internal detail of the map and identification of artifacts.

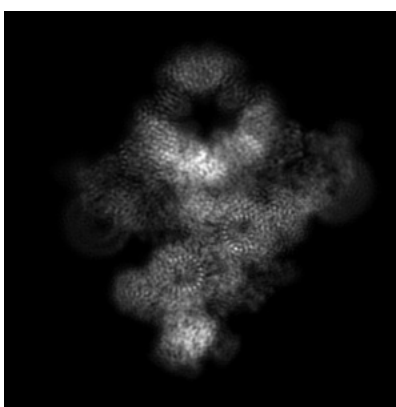
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

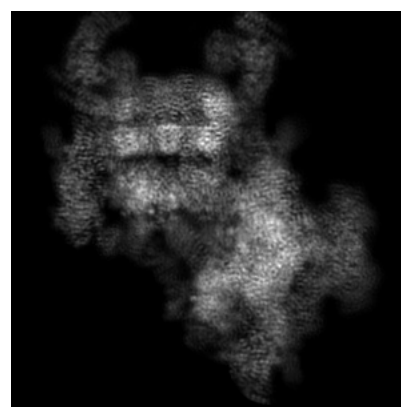
#### 6.1.1 Primary map



X



Y

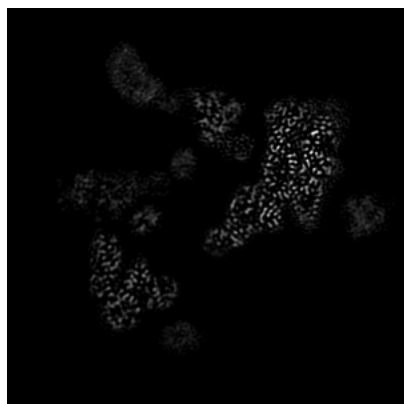


Z

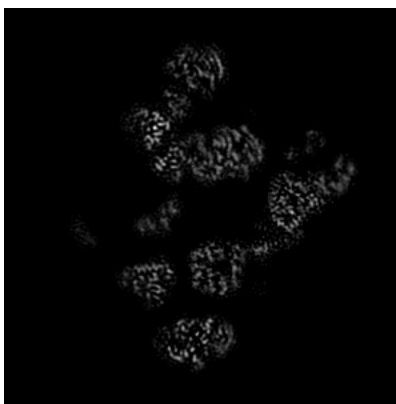
The images above show the map projected in three orthogonal directions.

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

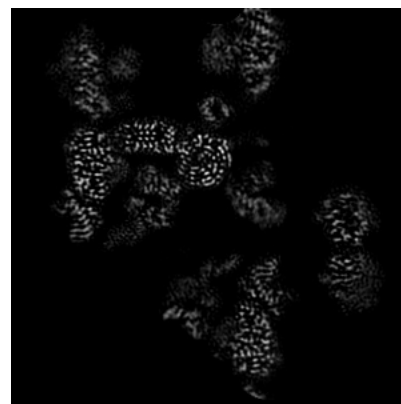
#### 6.2.1 Primary map



X Index: 200



Y Index: 200

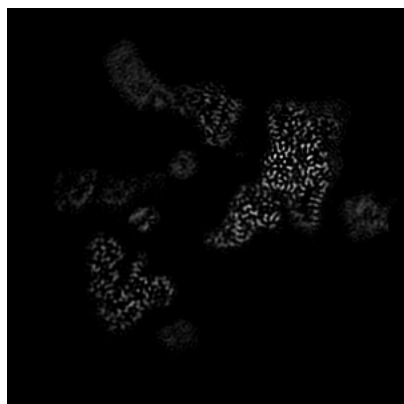


Z Index: 200

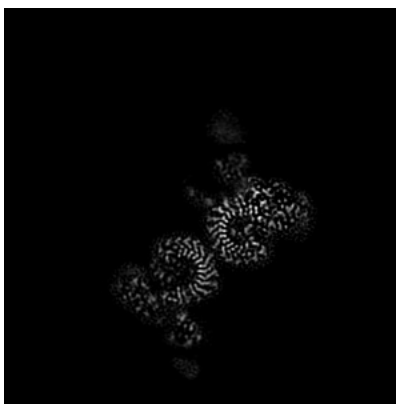
The images above show central slices of the map in three orthogonal directions.

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

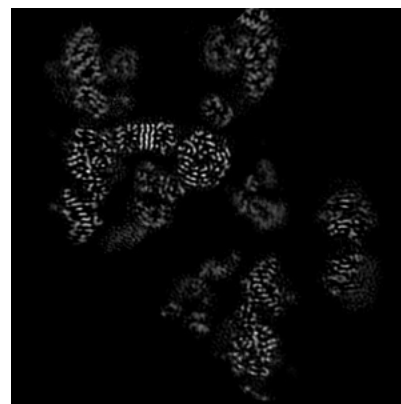
### 6.3.1 Primary map



X Index: 204



Y Index: 282

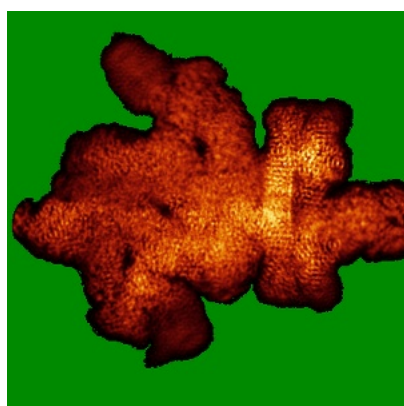


Z Index: 197

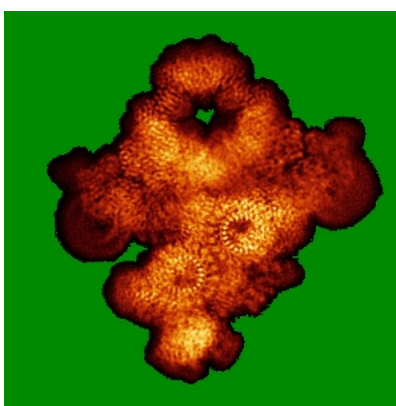
The images above show the largest variance slices of the map in three orthogonal directions.

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

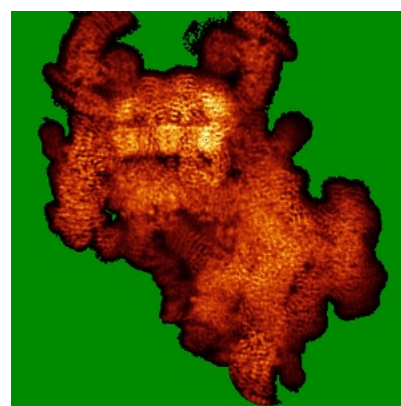
### 6.4.1 Primary map



X



Y

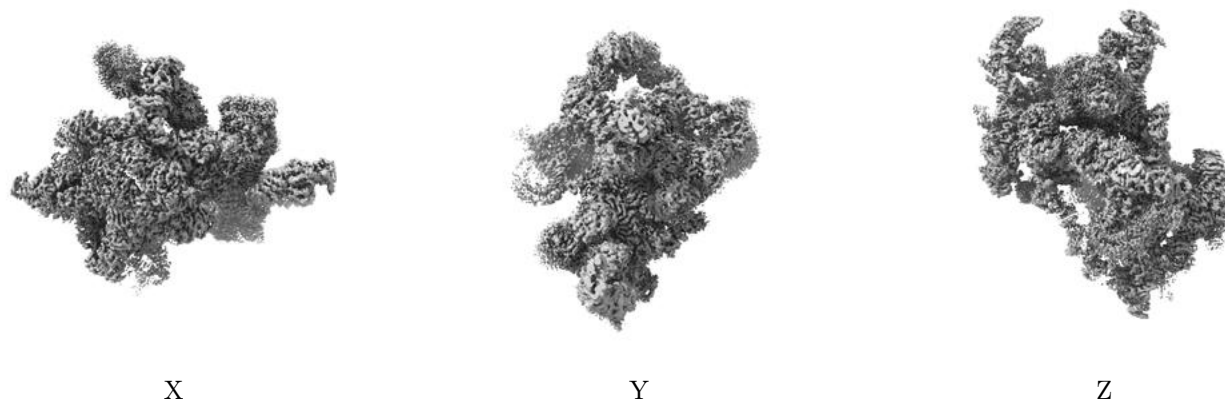


Z

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

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

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.004. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

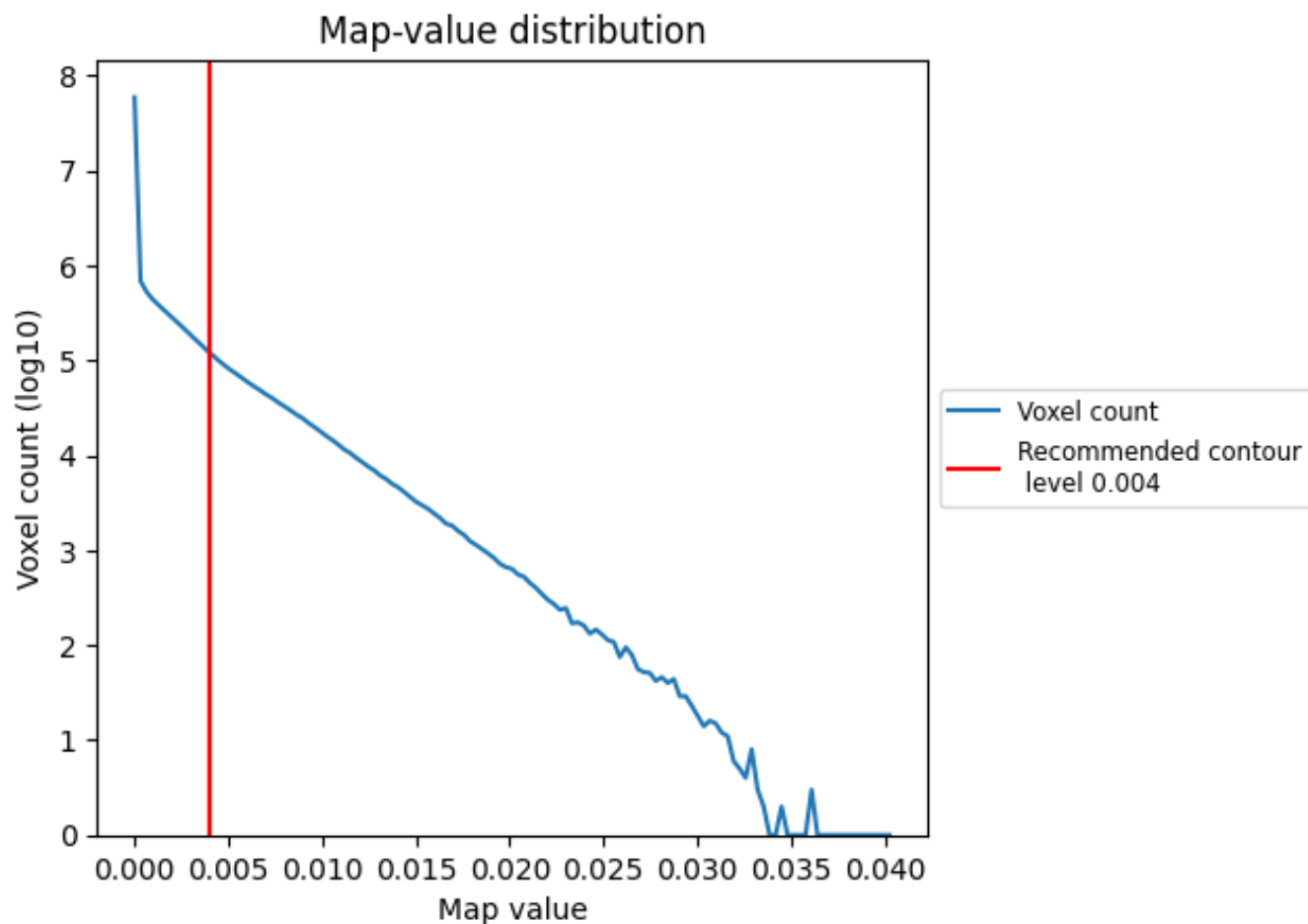
## 6.6 Mask visualisation [i](#)

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.

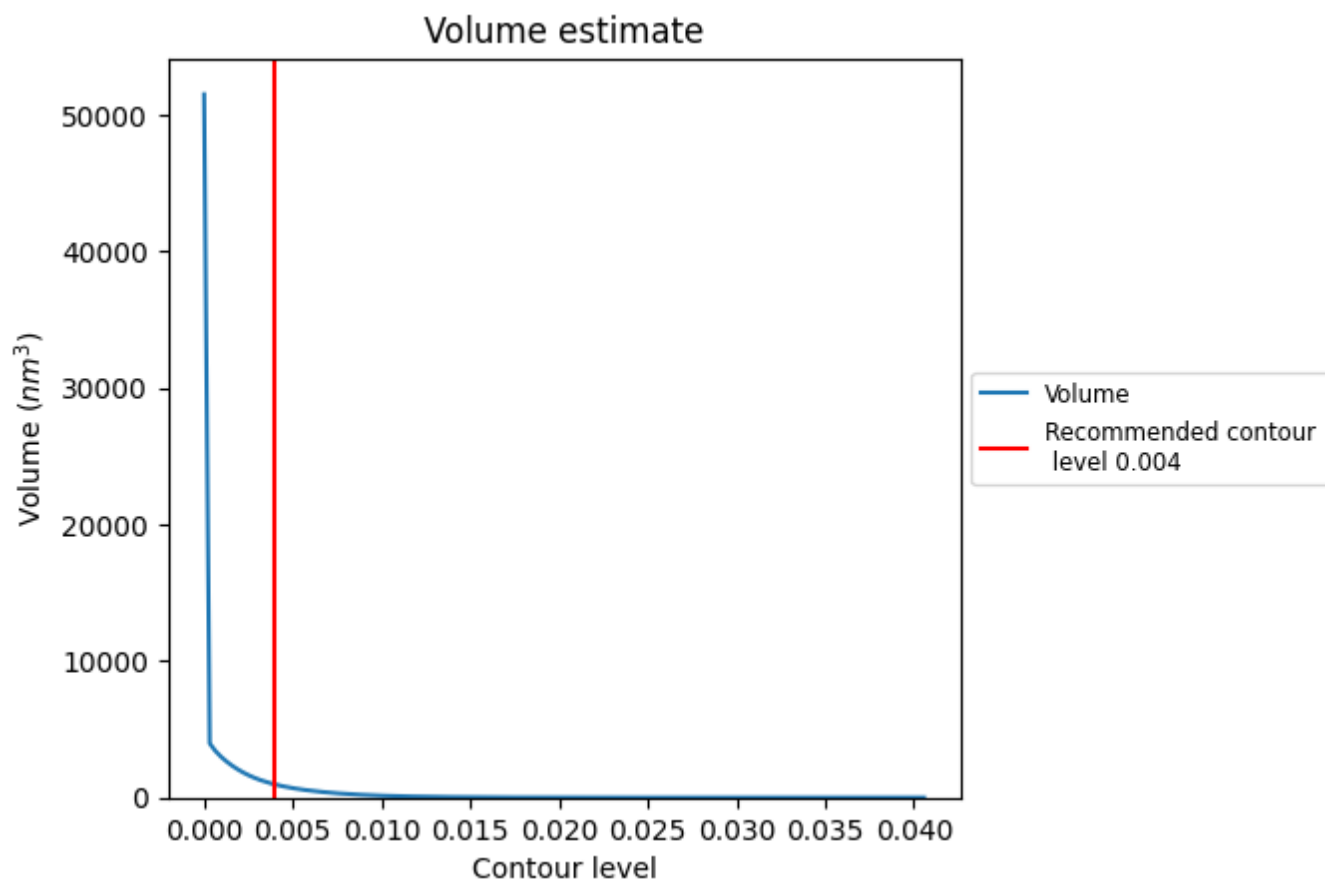
### 7.1 Map-value distribution [i](#)



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.



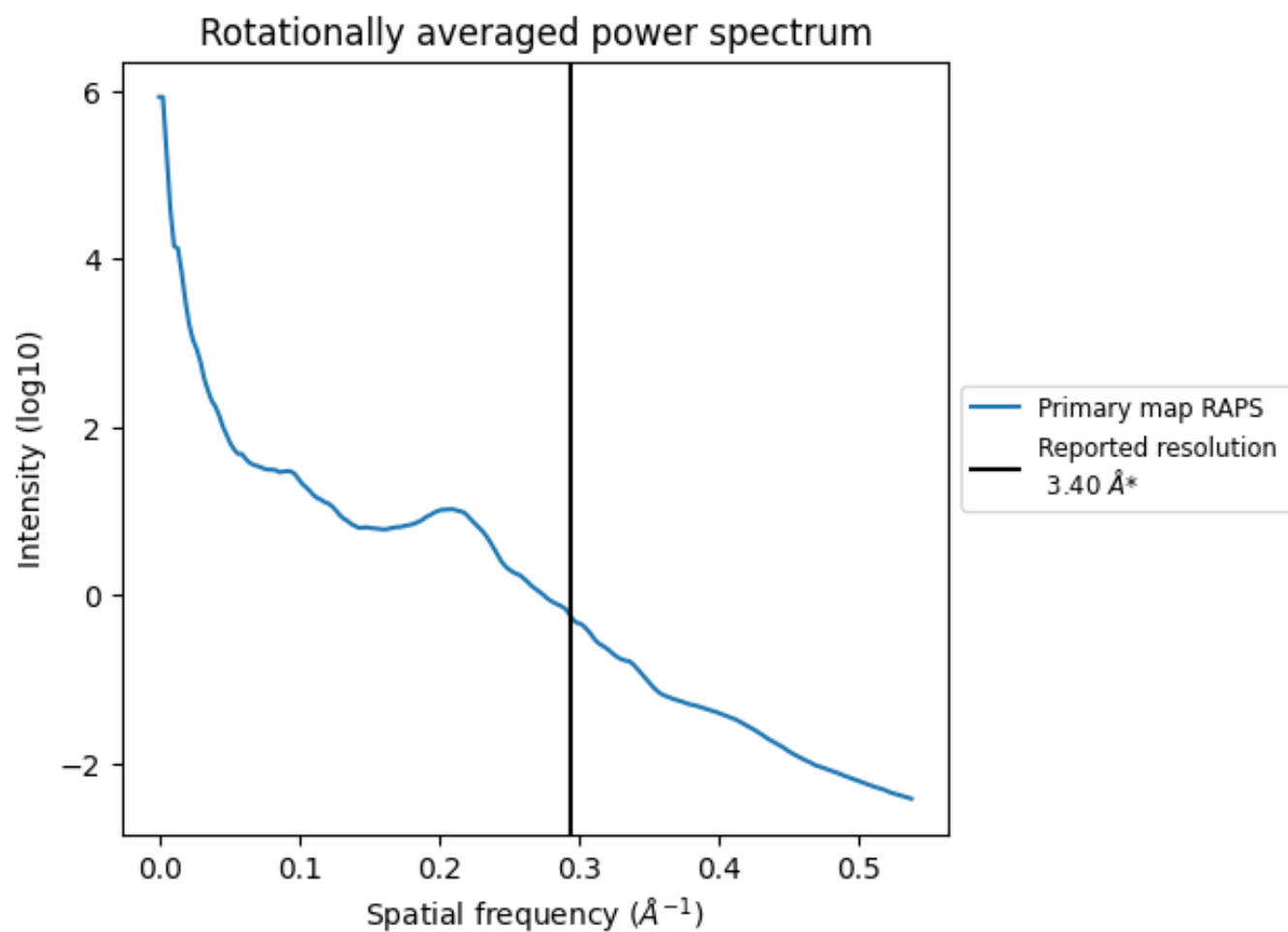
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 960  $\text{nm}^3$ ; this corresponds to an approximate mass of 867 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 0.294 Å<sup>-1</sup>

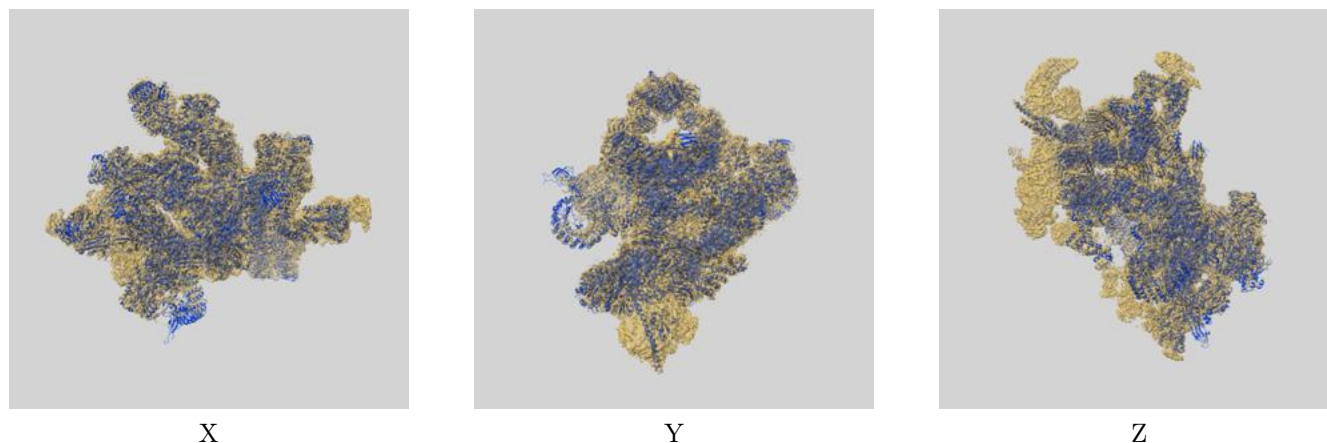
## 8 Fourier-Shell correlation

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

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

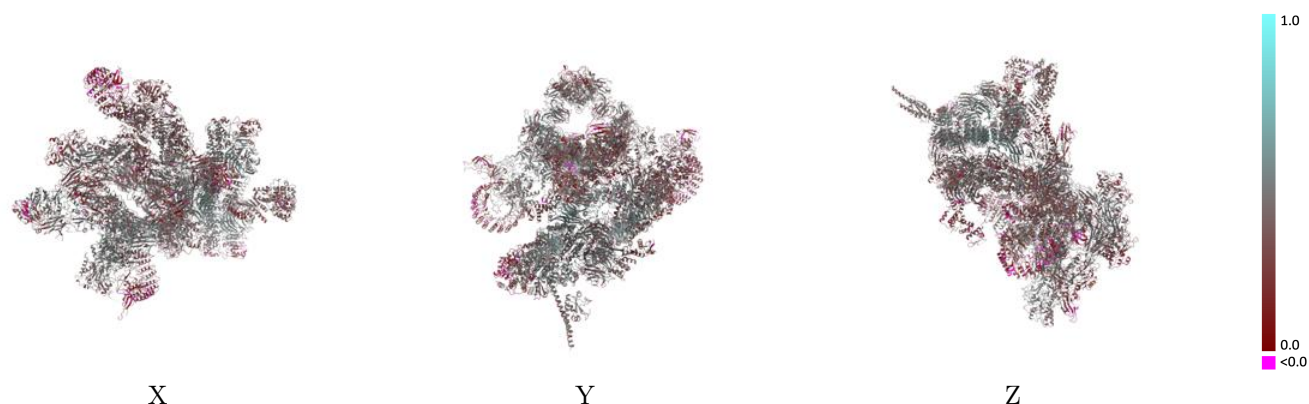
This section contains information regarding the fit between EMDB map EMD-69647 and PDB model 24MC. Per-residue inclusion information can be found in section 3 on page 11.

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



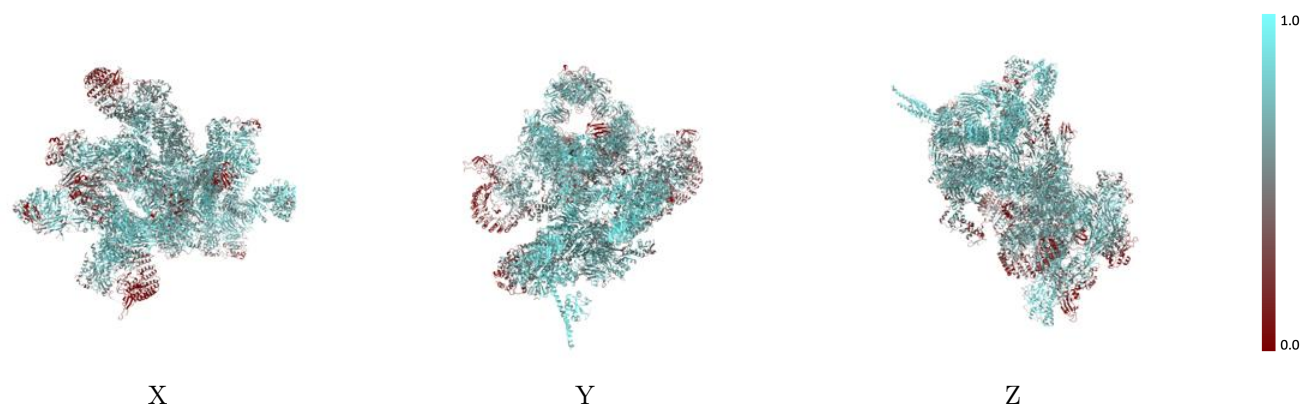
The images above show the 3D surface view of the map at the recommended contour level 0.004 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



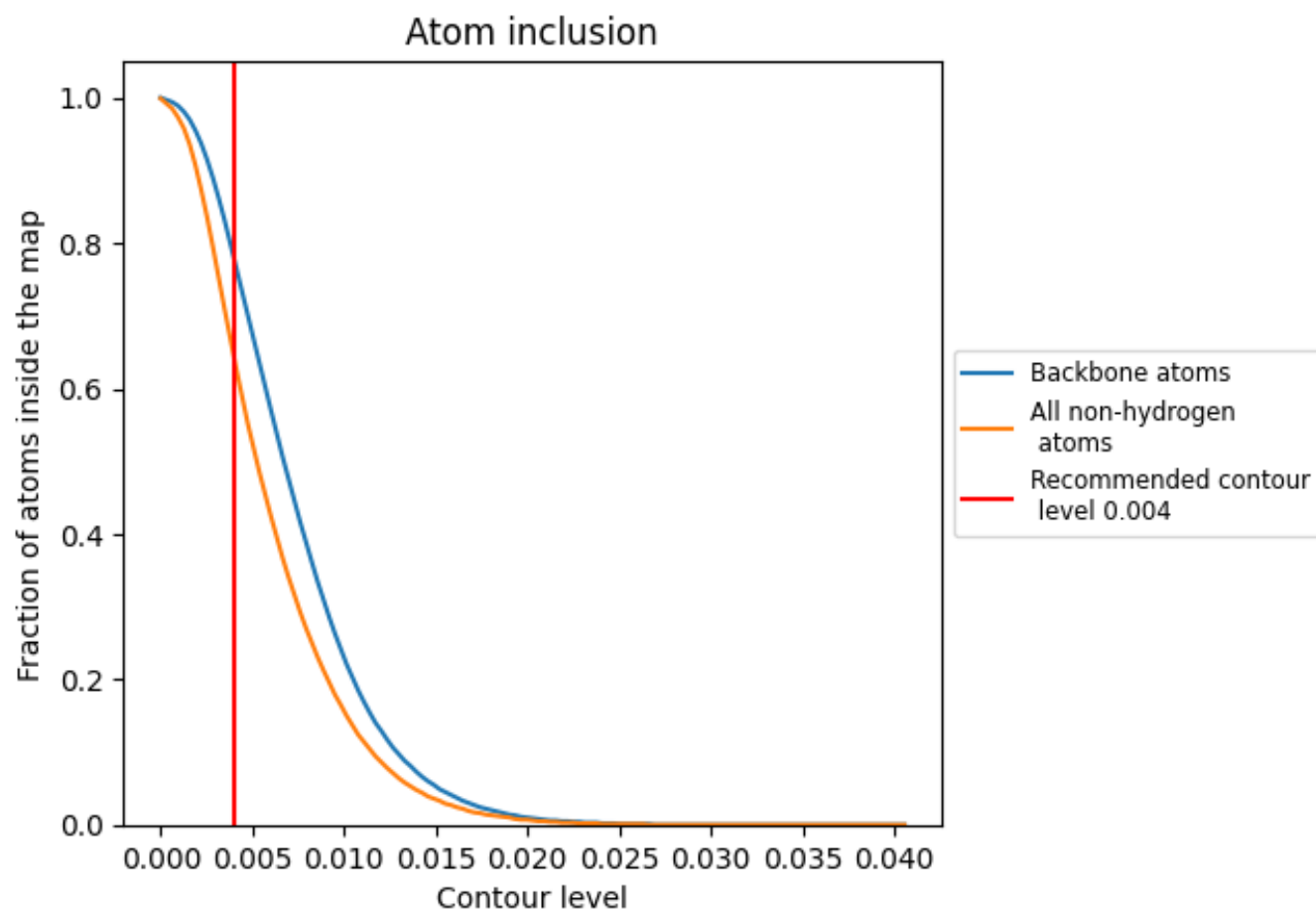
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.004).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 64% 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 (0.004) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6430	 0.3860
A	 0.6070	 0.3960
B	 0.7210	 0.4290
C	 0.7040	 0.4020
D	 0.5740	 0.3740
E	 0.6140	 0.3770
F	 0.5260	 0.3670
G	 0.7220	 0.4340
H	 0.7530	 0.4700
I	 0.5920	 0.3570
K	 0.6390	 0.3440
M	 0.7730	 0.4590
N	 0.8140	 0.4400
O	 0.8050	 0.4140
P	 0.7080	 0.4240
Q	 0.7940	 0.4770
R	 0.6930	 0.3650
S	 0.7750	 0.4600
T	 0.8340	 0.4820
U	 0.8420	 0.4610
V	 0.9070	 0.4870
W	 0.6950	 0.4190
X	 0.5720	 0.3580
Y	 0.6860	 0.3830
Z	 0.6760	 0.3830
a	 0.7800	 0.4720
b	 0.5300	 0.3730
c	 0.6610	 0.3280
d	 0.4870	 0.2720
e	 0.4480	 0.3340
f	 0.4570	 0.2700
h	 0.6090	 0.3250
j	 0.5100	 0.3120
l	 0.3600	 0.2400
m	 0.6430	 0.3930



*Continued on next page...*

*Continued from previous page...*

Chain	Atom inclusion	Q-score
n	 0.8230	 0.4820
p	 0.6730	 0.3690