



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 08:03 AM UTC

PDB ID : 7SP4 / pdb_00007sp4
EMDB ID : EMD-25365
Title : In situ cryo-EM structure of bacteriophage Sf6 gp3:gp7:gp5 complex in con-
formation 2 at 3.71Å resolution
Authors : Li, F.; Cingolani, G.; Hou, C.; Yang, R.
Deposited on : 2021-11-02
Resolution : 3.71 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

A user guide is available at

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

The types of validation reports are described at

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

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

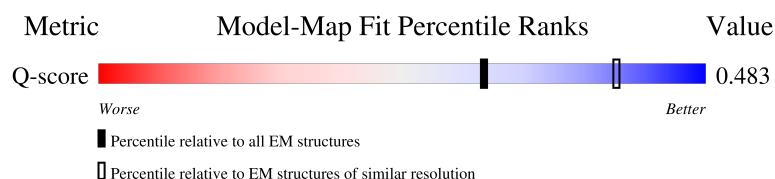
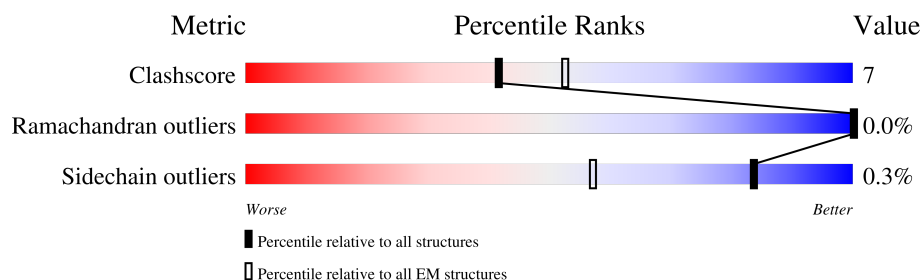
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.71 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	10534 (3.21 - 4.21)

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

Mol	Chain	Length	Quality of chain
1	0	160	9% 73% 20% 7%
1	1	160	9% 71% 22% 7%
1	c	160	8% 71% 21% 8%
1	h	160	14% 70% 27% .

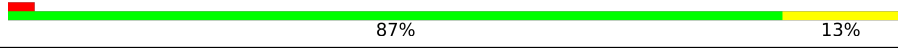
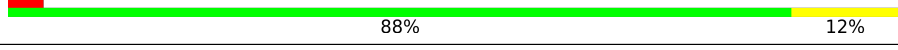
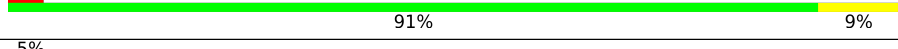
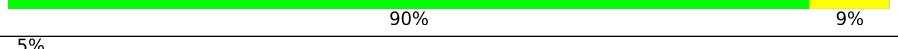
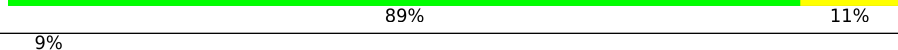
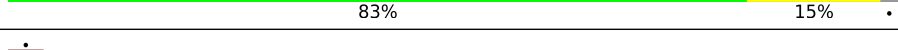
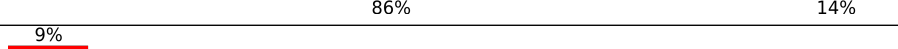
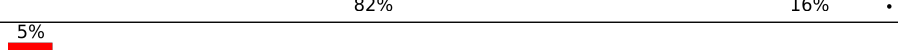
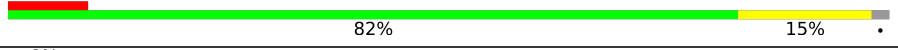
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	m	160	
1	r	160	
1	s	160	
1	u	160	
1	v	160	
1	w	160	
1	x	160	
1	z	160	
2	A	708	
2	B	708	
2	C	708	
2	D	708	
2	E	708	
2	F	708	
2	G	708	
2	H	708	
2	I	708	
2	J	708	
2	K	708	
2	L	708	
3	M	423	
3	N	423	
3	O	423	
3	P	423	
3	Q	423	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	R	423	
3	S	423	
3	T	423	
3	U	423	
3	V	423	
3	W	423	
3	X	423	
3	Y	423	
3	Z	423	
3	a	423	
3	b	423	
3	d	423	
3	e	423	
3	f	423	
3	g	423	
3	i	423	
3	j	423	
3	k	423	
3	l	423	
3	n	423	
3	o	423	
3	p	423	
3	q	423	
3	t	423	
3	y	423	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 169849 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 Gene 7 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	149	Total	C	N	O	S	0	0
			1166	735	192	233	6		
1	1	149	Total	C	N	O	S	0	0
			1168	737	192	233	6		
1	c	148	Total	C	N	O	S	0	0
			1161	732	191	232	6		
1	h	155	Total	C	N	O	S	0	0
			1212	765	198	243	6		
1	m	148	Total	C	N	O	S	0	0
			1161	732	191	232	6		
1	r	156	Total	C	N	O	S	0	0
			1219	770	199	244	6		
1	s	148	Total	C	N	O	S	0	0
			1161	732	191	232	6		
1	u	158	Total	C	N	O	S	0	0
			1229	774	202	247	6		
1	v	155	Total	C	N	O	S	0	0
			1212	765	198	243	6		
1	w	157	Total	C	N	O	S	0	0
			1227	774	201	246	6		
1	x	148	Total	C	N	O	S	0	0
			1161	732	191	232	6		
1	z	148	Total	C	N	O	S	0	0
			1161	732	191	232	6		

- Molecule 2 is a protein called Gene 3 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	628	Total	C	N	O	S	0	0
			4973	3112	879	959	23		
2	B	628	Total	C	N	O	S	0	0
			4973	3112	879	959	23		
2	C	628	Total	C	N	O	S	0	0
			4973	3112	879	959	23		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	628	Total	C	N	O	S	0	0
			4973	3112	879	959	23		
2	E	628	Total	C	N	O	S	0	0
			4973	3112	879	959	23		
2	F	628	Total	C	N	O	S	0	0
			4973	3112	879	959	23		
2	G	628	Total	C	N	O	S	0	0
			4973	3112	879	959	23		
2	H	628	Total	C	N	O	S	0	0
			4973	3112	879	959	23		
2	I	628	Total	C	N	O	S	0	0
			4973	3112	879	959	23		
2	J	628	Total	C	N	O	S	0	0
			4973	3112	879	959	23		
2	K	628	Total	C	N	O	S	0	0
			4973	3112	879	959	23		
2	L	628	Total	C	N	O	S	0	0
			4973	3112	879	959	23		

- Molecule 3 is a protein called Gene 5 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	M	422	Total	C	N	O	S	0	0
			3209	2018	550	631	10		
3	N	422	Total	C	N	O	S	0	0
			3209	2018	550	631	10		
3	O	422	Total	C	N	O	S	0	0
			3209	2018	550	631	10		
3	P	422	Total	C	N	O	S	0	0
			3209	2018	550	631	10		
3	Q	422	Total	C	N	O	S	0	0
			3209	2018	550	631	10		
3	R	422	Total	C	N	O	S	0	0
			3209	2018	550	631	10		
3	S	422	Total	C	N	O	S	0	0
			3209	2018	550	631	10		
3	T	422	Total	C	N	O	S	0	0
			3209	2018	550	631	10		
3	U	422	Total	C	N	O	S	0	0
			3209	2018	550	631	10		
3	V	422	Total	C	N	O	S	0	0
			3209	2018	550	631	10		

Continued on next page...

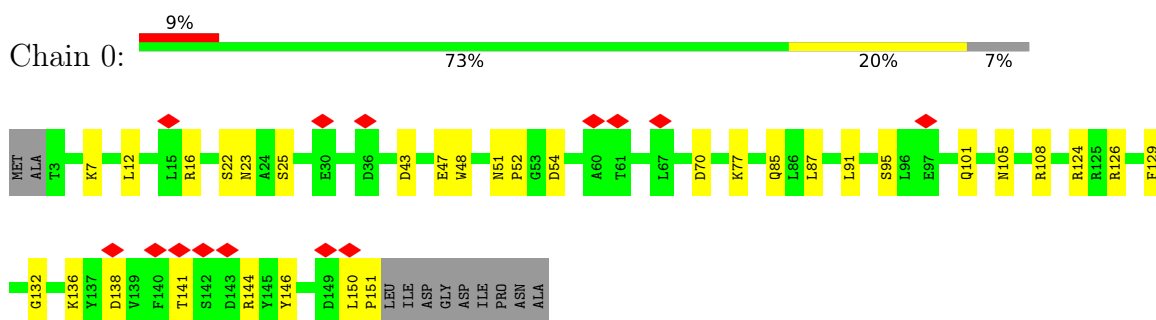
Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
3	W	422	Total	C	N	O	S	0	0
			3209	2018	550	631	10		
3	X	422	Total	C	N	O	S	0	0
			3209	2018	550	631	10		
3	Y	414	Total	C	N	O	S	0	0
			3149	1983	539	617	10		
3	Z	421	Total	C	N	O	S	0	0
			3202	2013	549	630	10		
3	a	414	Total	C	N	O	S	0	0
			3149	1983	539	617	10		
3	b	422	Total	C	N	O	S	0	0
			3209	2018	550	631	10		
3	d	422	Total	C	N	O	S	0	0
			3209	2018	550	631	10		
3	e	414	Total	C	N	O	S	0	0
			3149	1983	539	617	10		
3	f	422	Total	C	N	O	S	0	0
			3209	2018	550	631	10		
3	g	422	Total	C	N	O	S	0	0
			3209	2018	550	631	10		
3	i	421	Total	C	N	O	S	0	0
			3202	2013	549	630	10		
3	j	422	Total	C	N	O	S	0	0
			3209	2018	550	631	10		
3	k	421	Total	C	N	O	S	0	0
			3202	2013	549	630	10		
3	l	421	Total	C	N	O	S	0	0
			3202	2013	549	630	10		
3	n	421	Total	C	N	O	S	0	0
			3202	2013	549	630	10		
3	o	422	Total	C	N	O	S	0	0
			3209	2018	550	631	10		
3	p	414	Total	C	N	O	S	0	0
			3149	1983	539	617	10		
3	q	414	Total	C	N	O	S	0	0
			3149	1983	539	617	10		
3	t	422	Total	C	N	O	S	0	0
			3209	2018	550	631	10		
3	y	422	Total	C	N	O	S	0	0
			3209	2018	550	631	10		

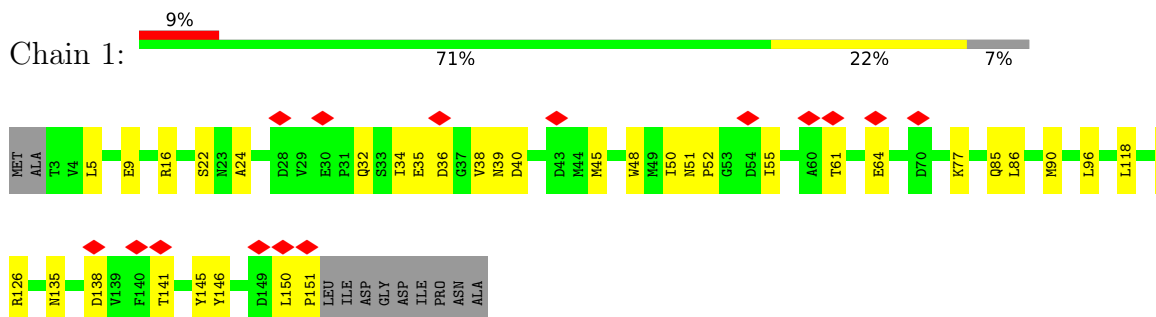
3 Residue-property plots [i](#)

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.

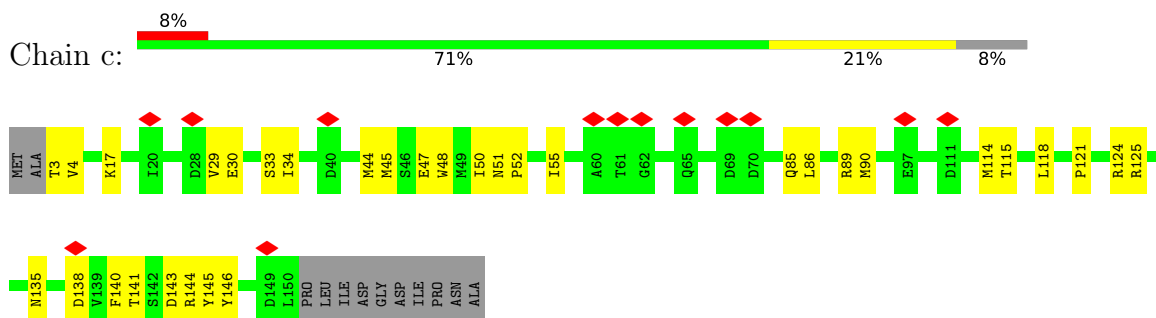
- Molecule 1: Gene 7 protein



- Molecule 1: Gene 7 protein

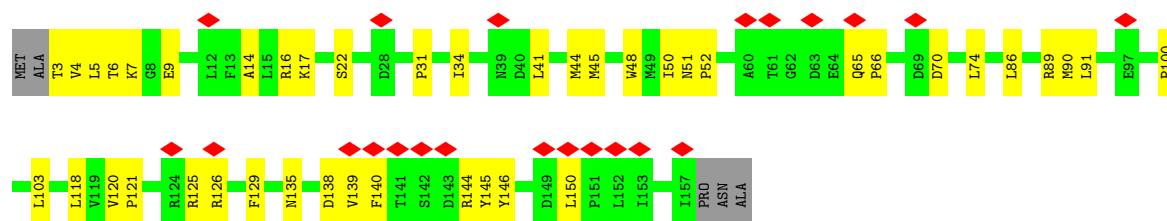


- Molecule 1: Gene 7 protein

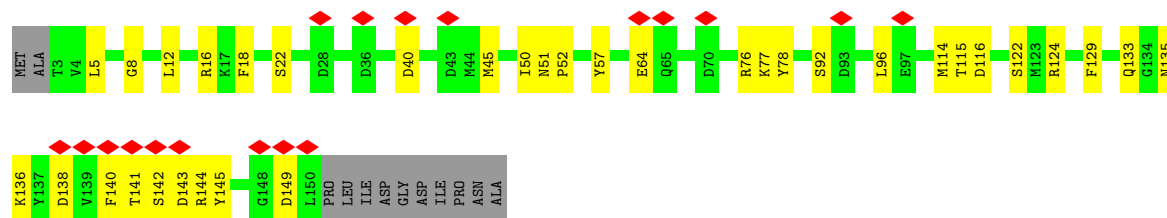


- Molecule 1: Gene 7 protein

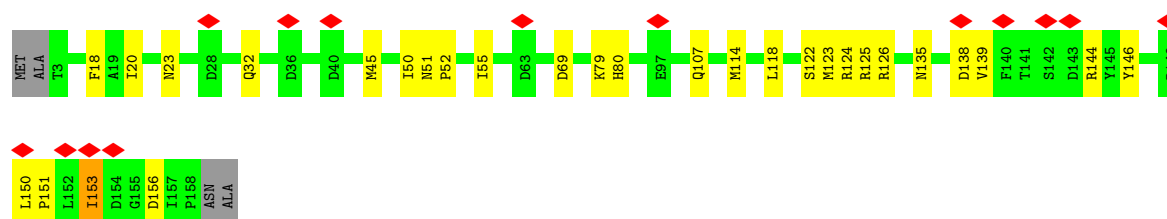
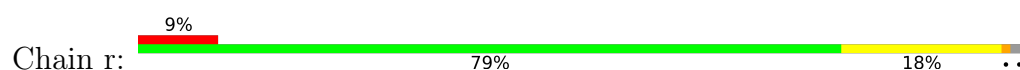




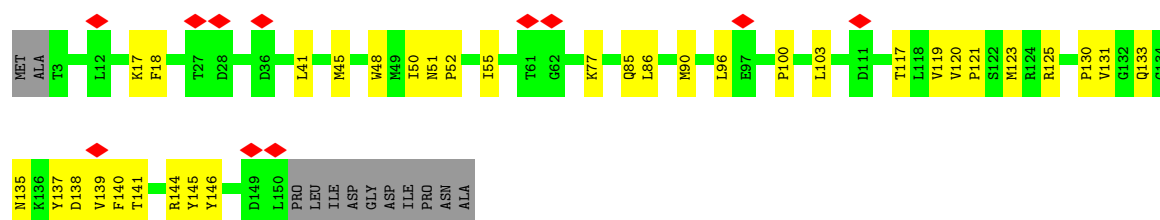
• Molecule 1: Gene 7 protein



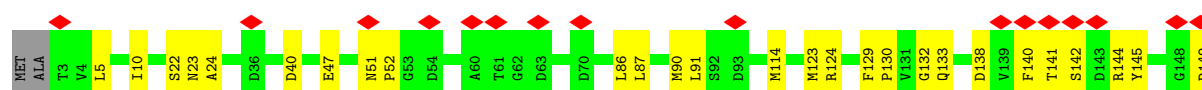
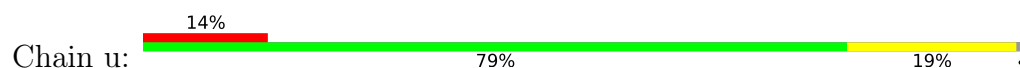
• Molecule 1: Gene 7 protein



• Molecule 1: Gene 7 protein

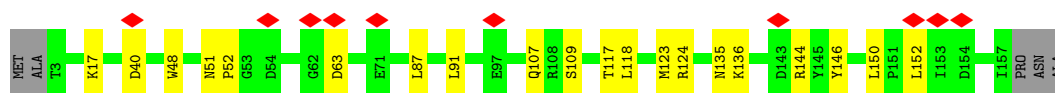
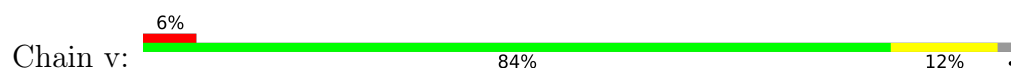


• Molecule 1: Gene 7 protein

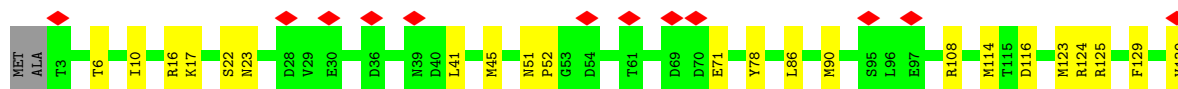
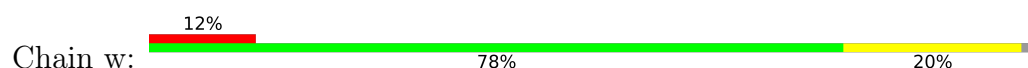




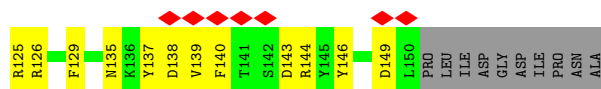
- Molecule 1: Gene 7 protein



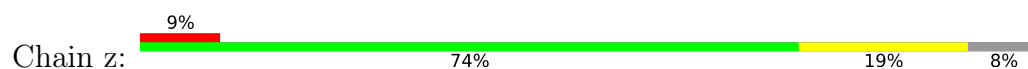
- Molecule 1: Gene 7 protein



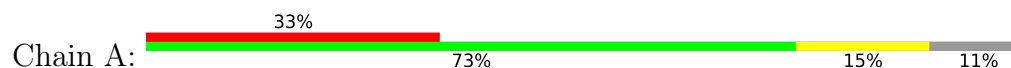
- Molecule 1: Gene 7 protein

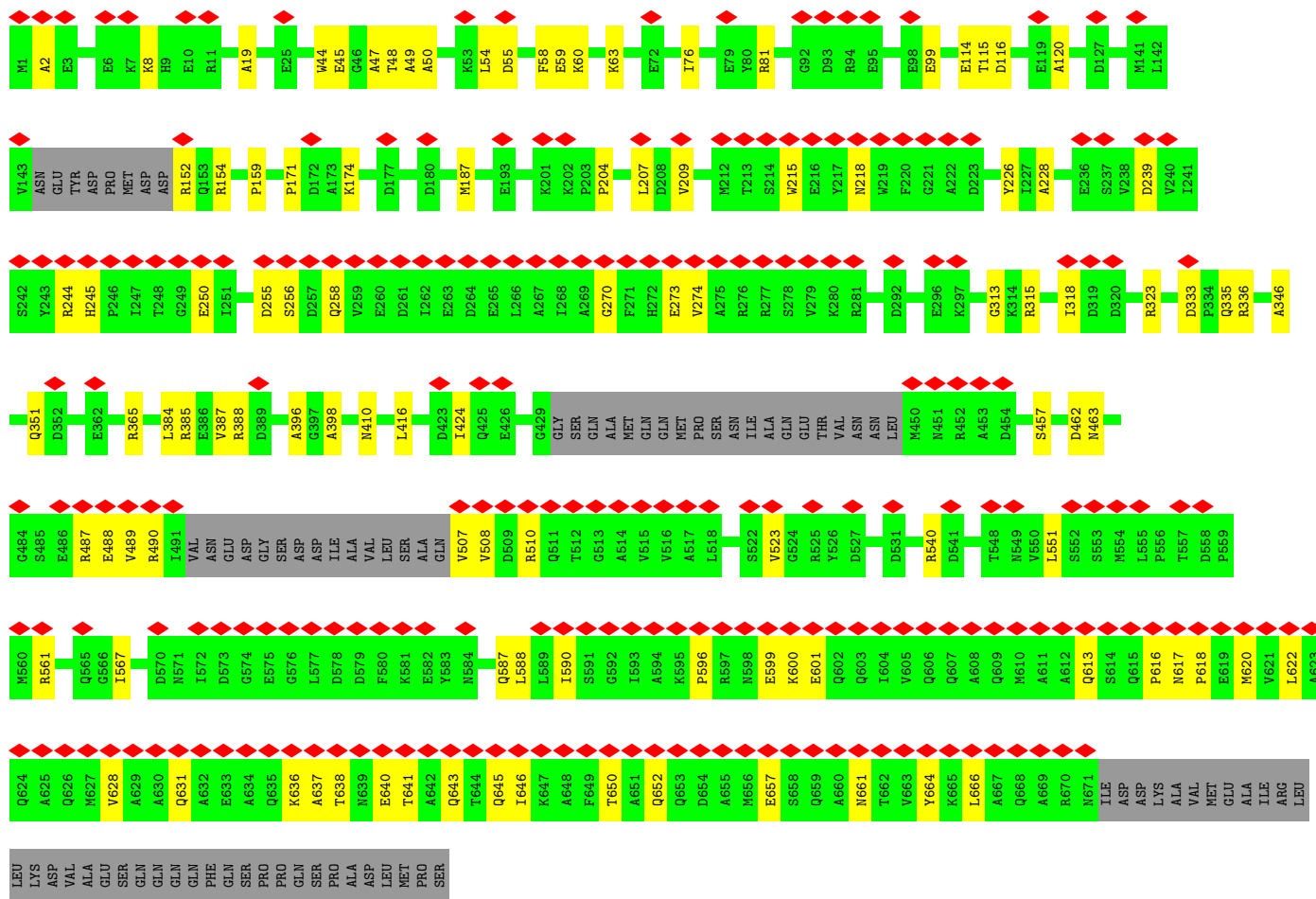


- Molecule 1: Gene 7 protein

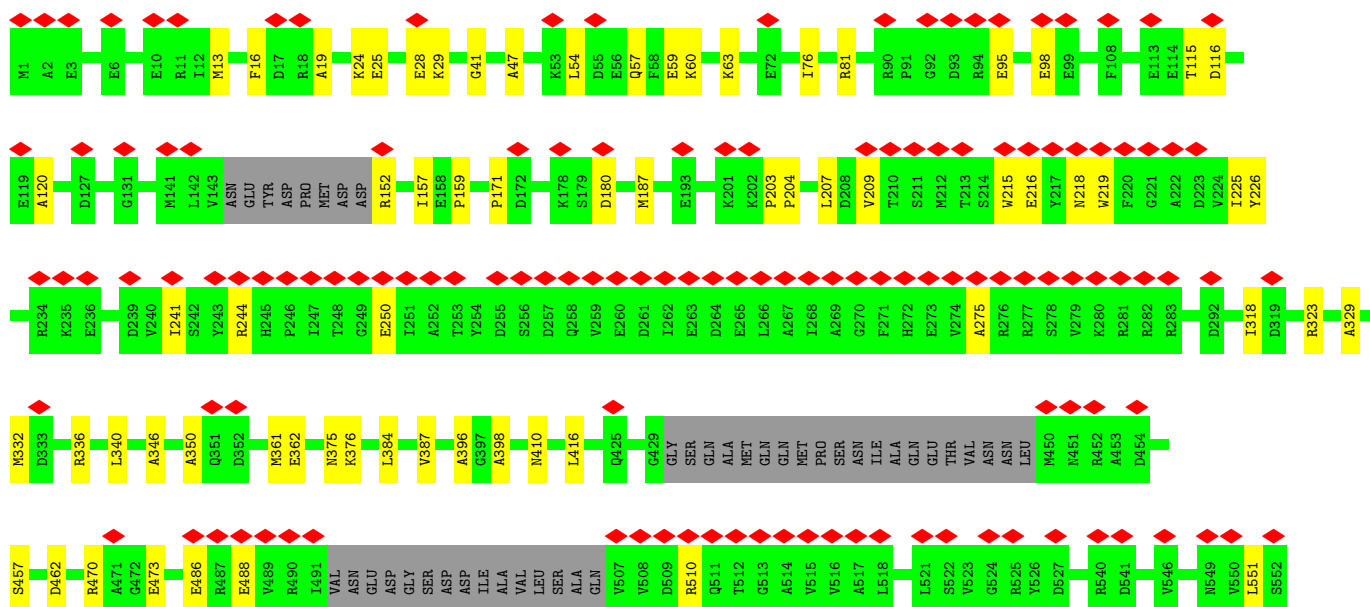
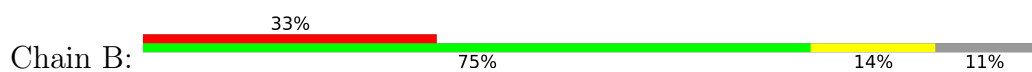


- Molecule 2: Gene 3 protein

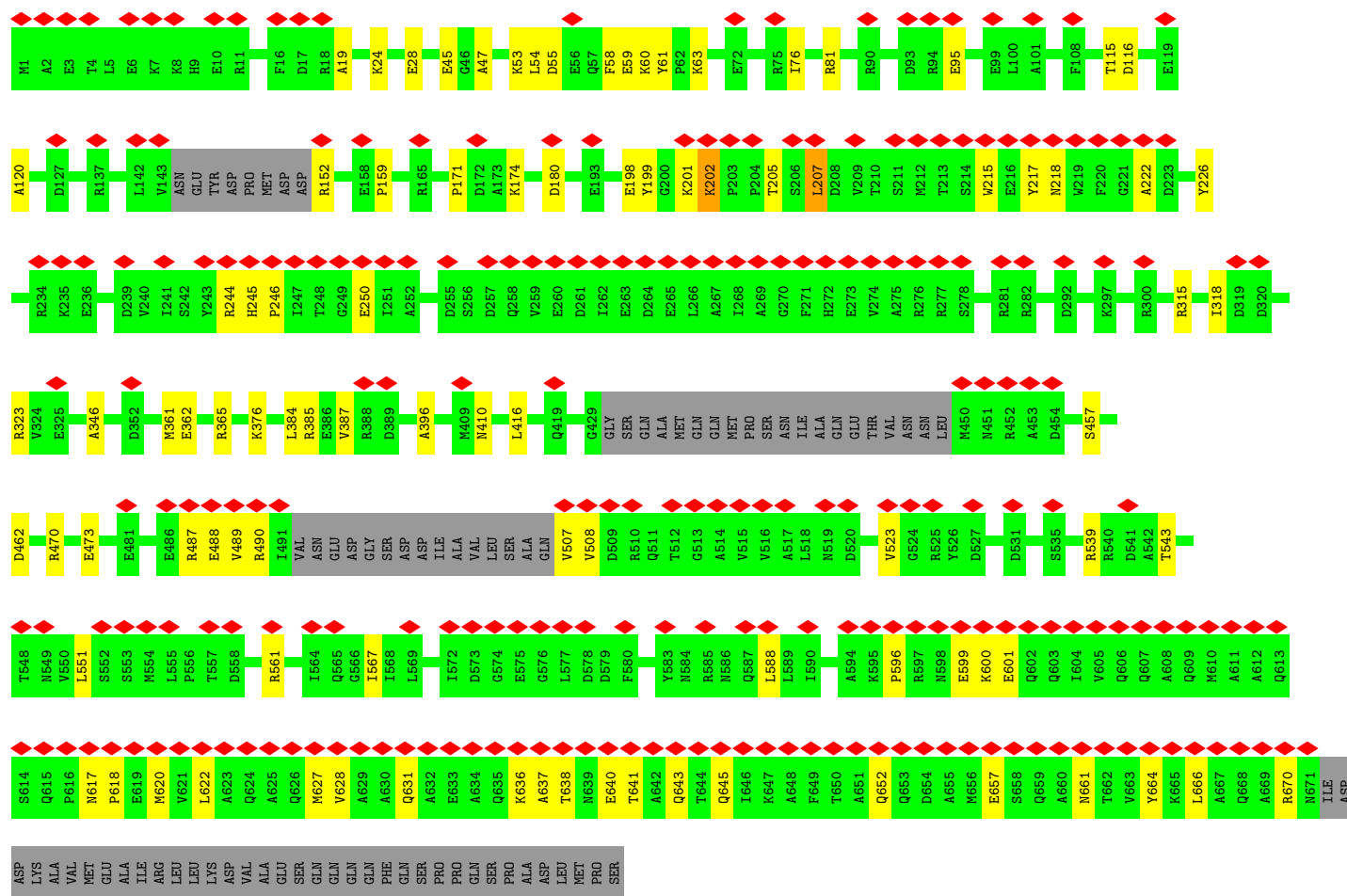
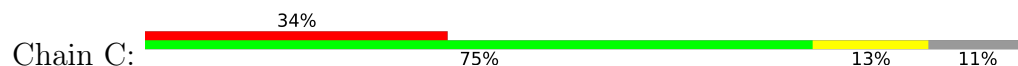




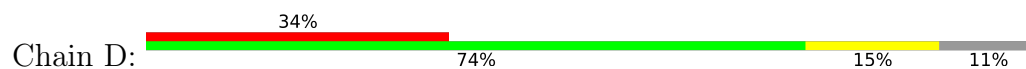
• Molecule 2: Gene 3 protein

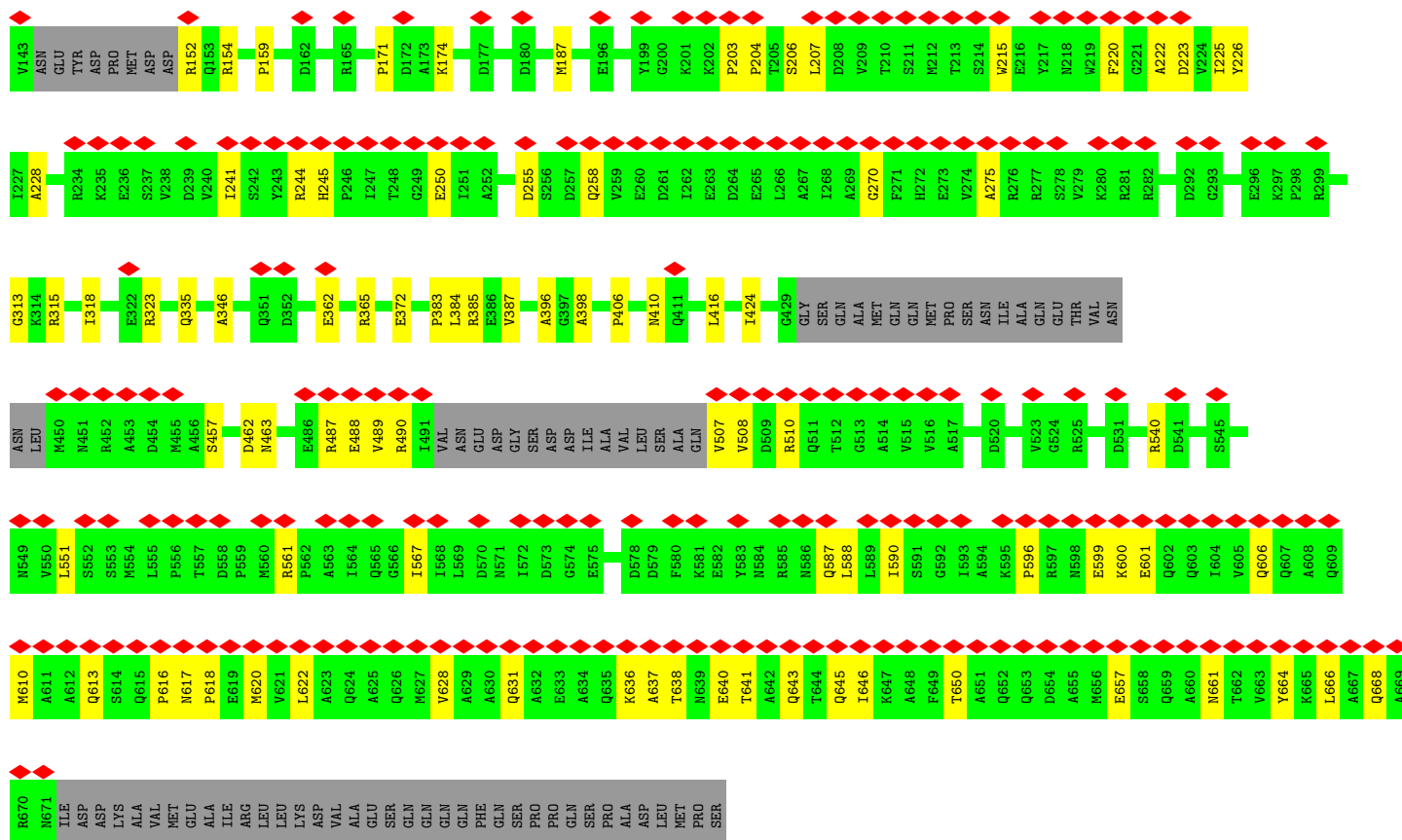


- Molecule 2: Gene 3 protein

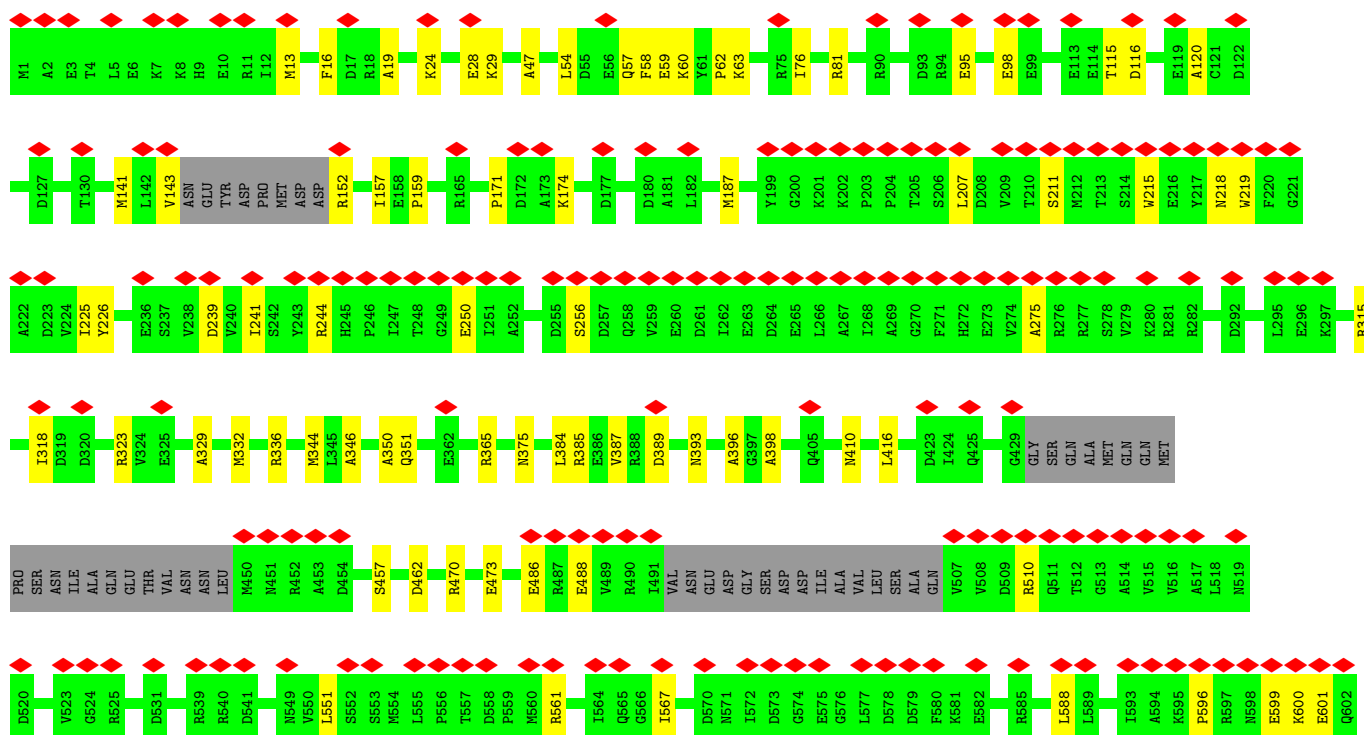
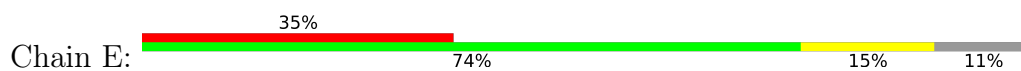


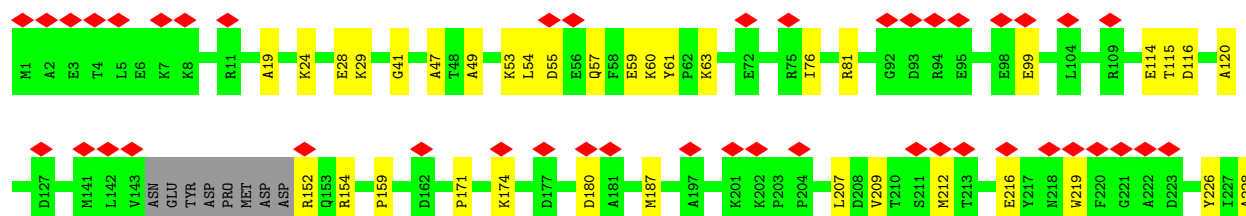
- Molecule 2: Gene 3 protein

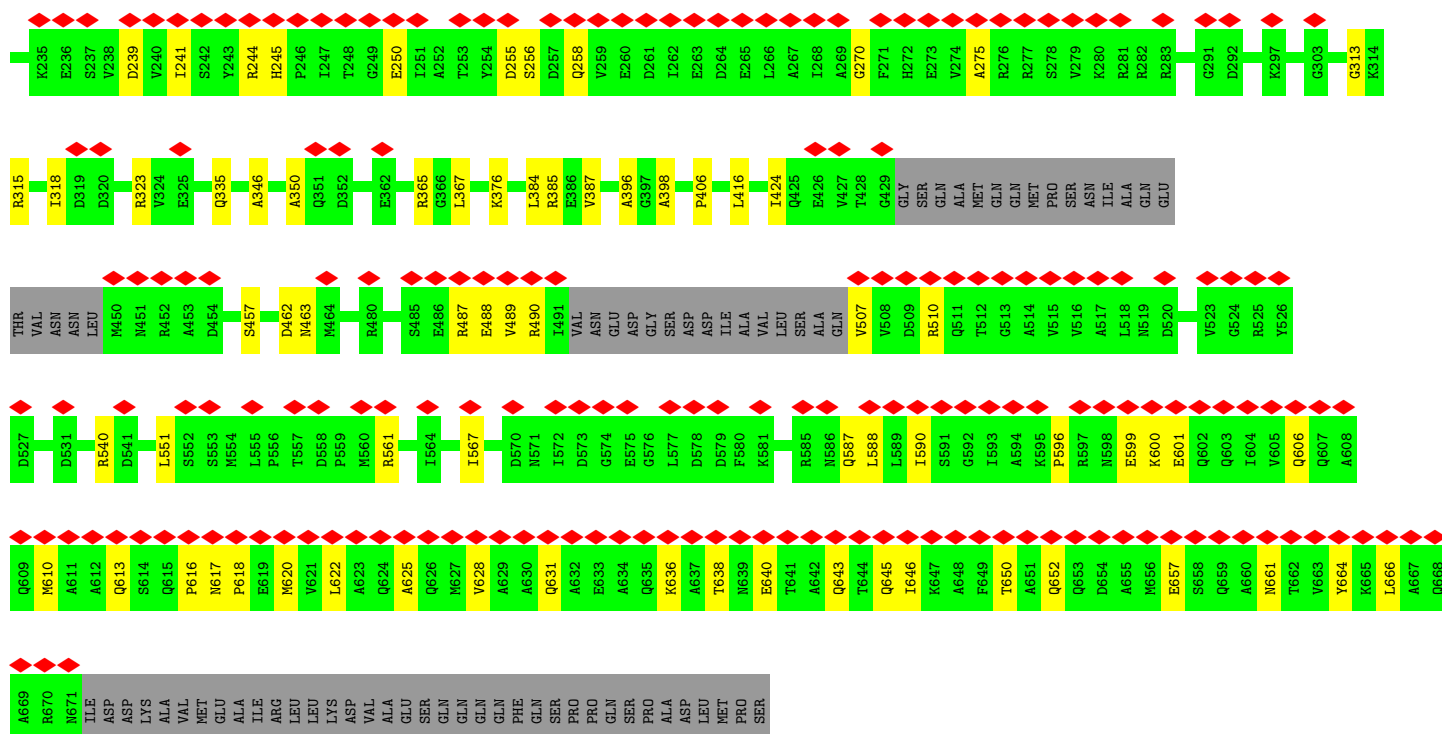




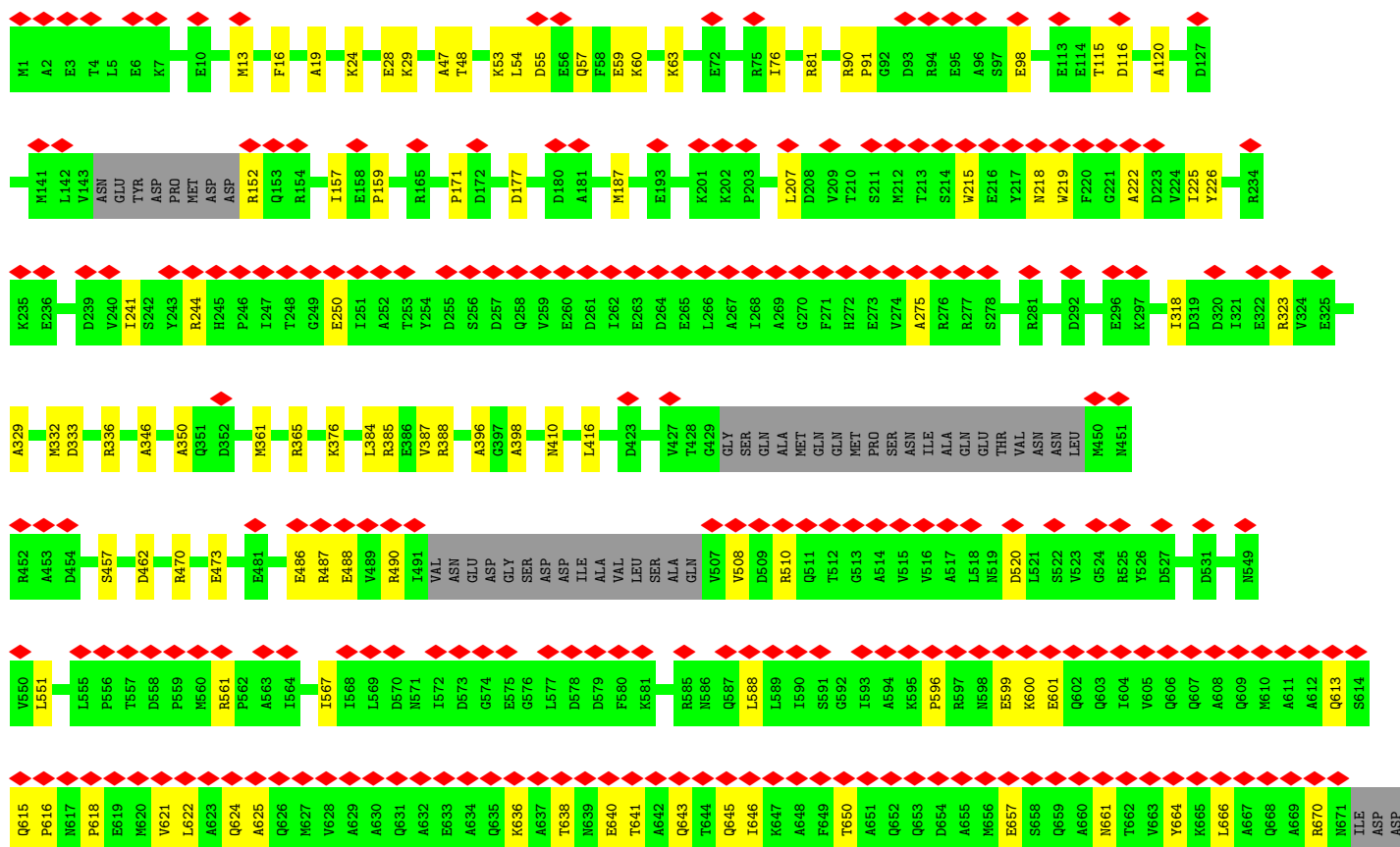
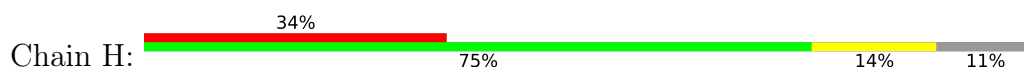
• Molecule 2: Gene 3 protein







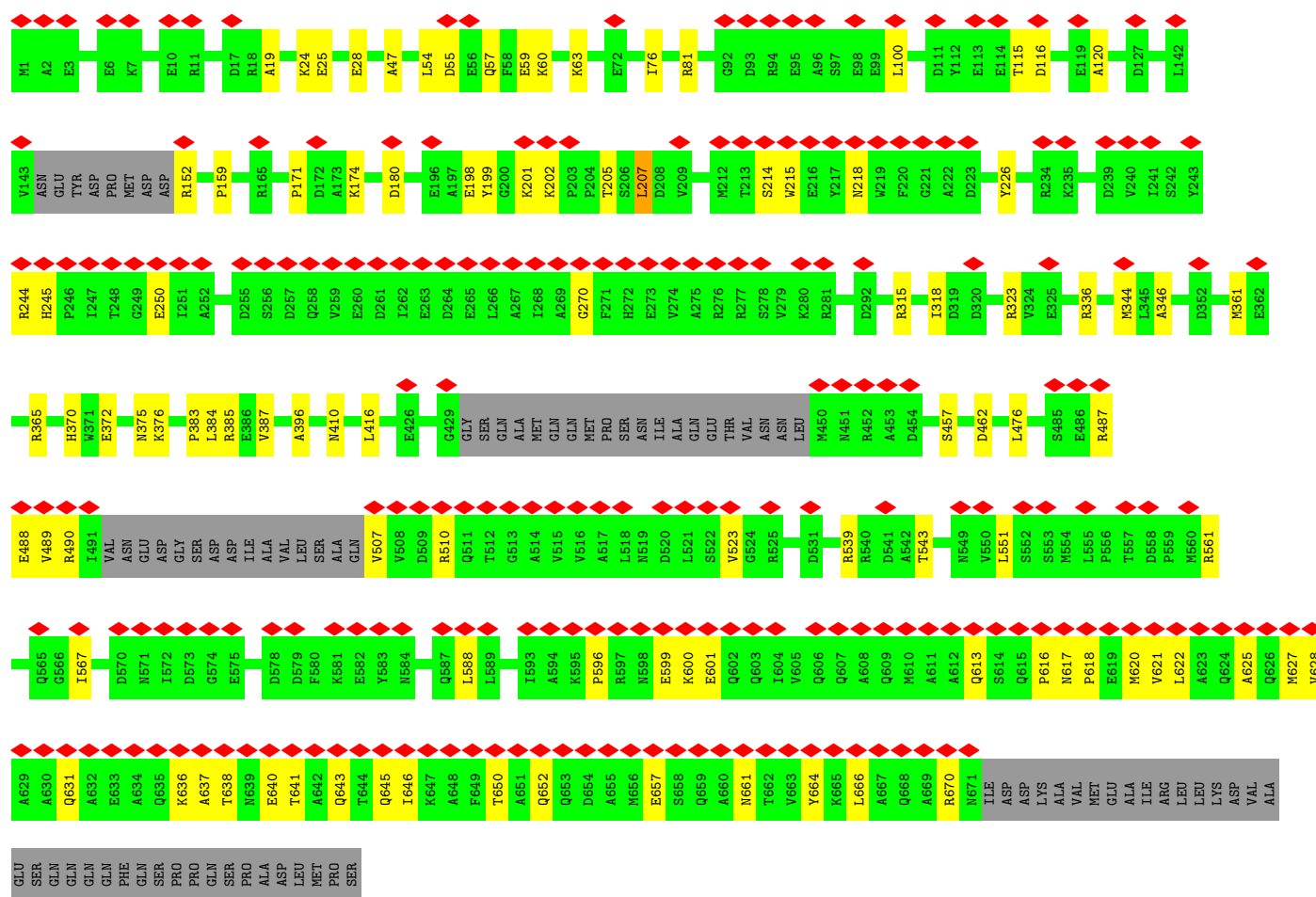
• Molecule 2: Gene 3 protein



LYS
ALA
VAL
MET
GLU
GLU
ALA
TLE
ARG
LEU
LYS
LYS
ASP
VAL
ALA
SER
GLN
GLN
GLN
PHE
GLN
SER
PRO
PRO
GLN
SER
PRO
PRO
ALA
ASP
LEU
MET
PRO
SER

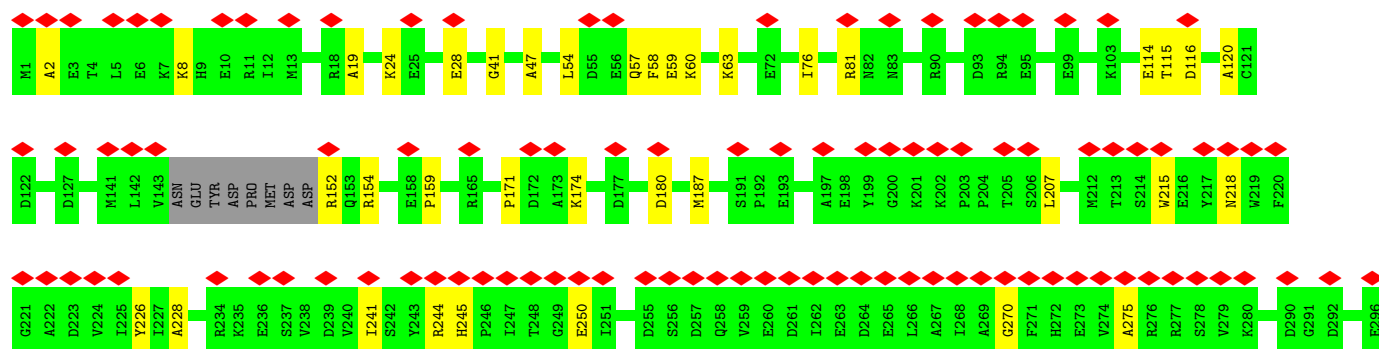
• Molecule 2: Gene 3 protein

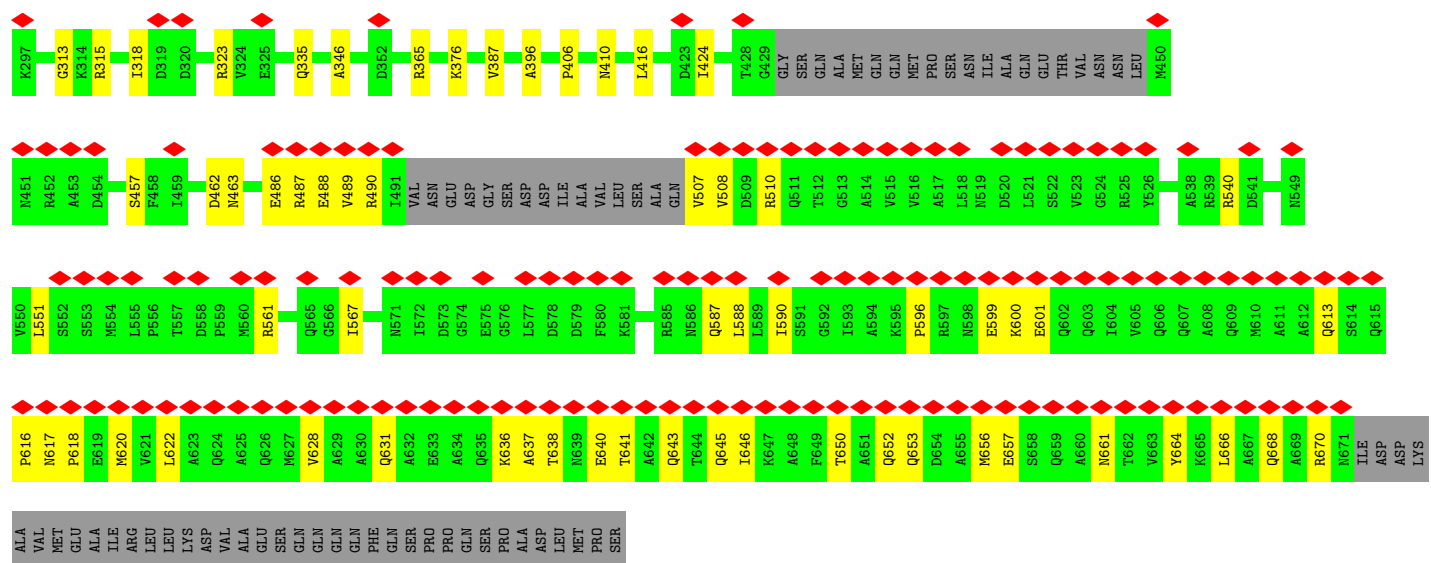
Chain I: 32% 74% 14% 11%



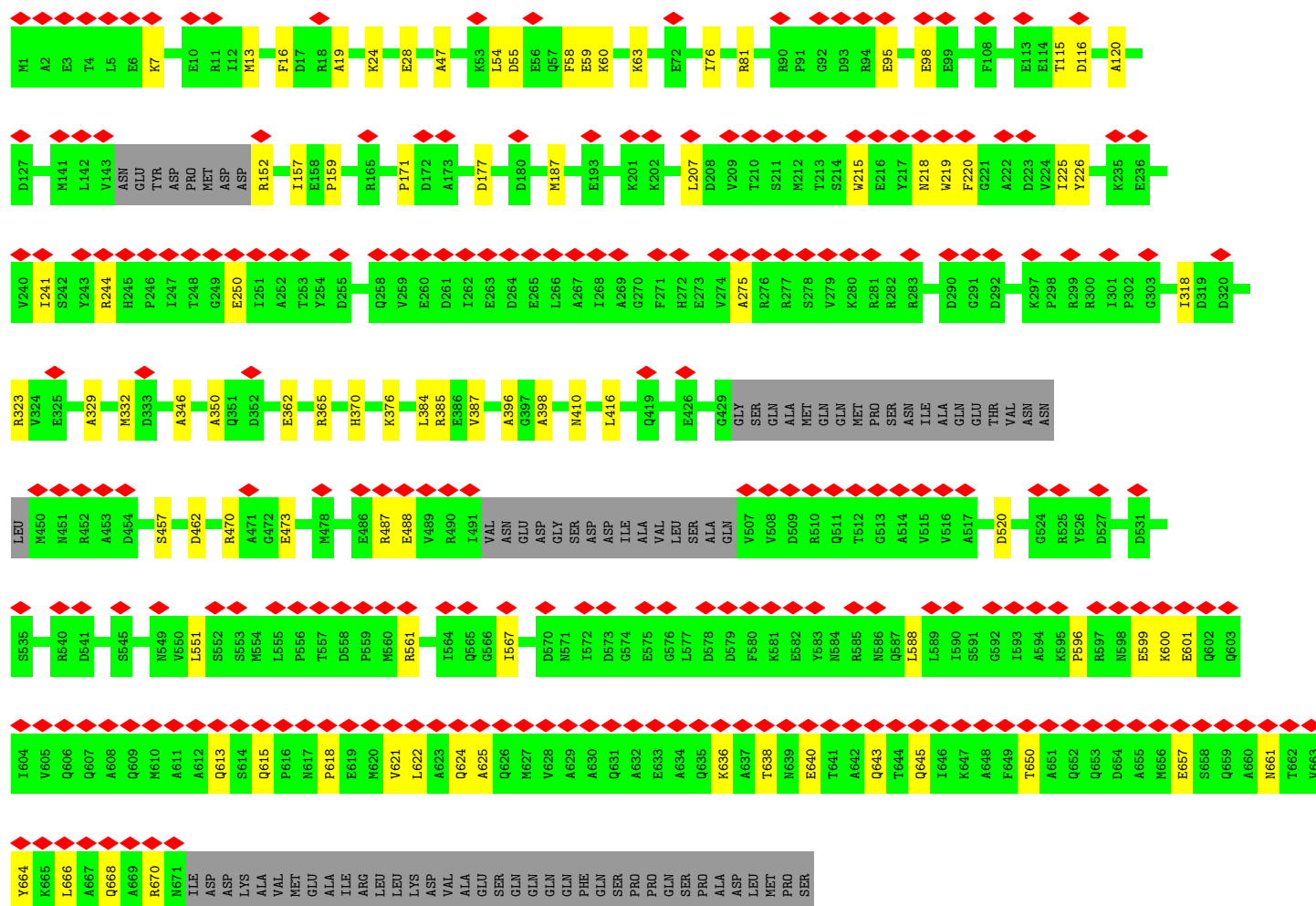
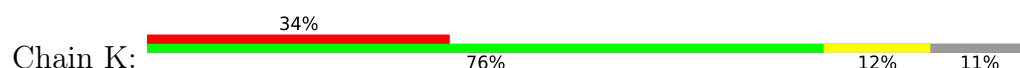
• Molecule 2: Gene 3 protein

Chain J: 35% 75% 14% 11%

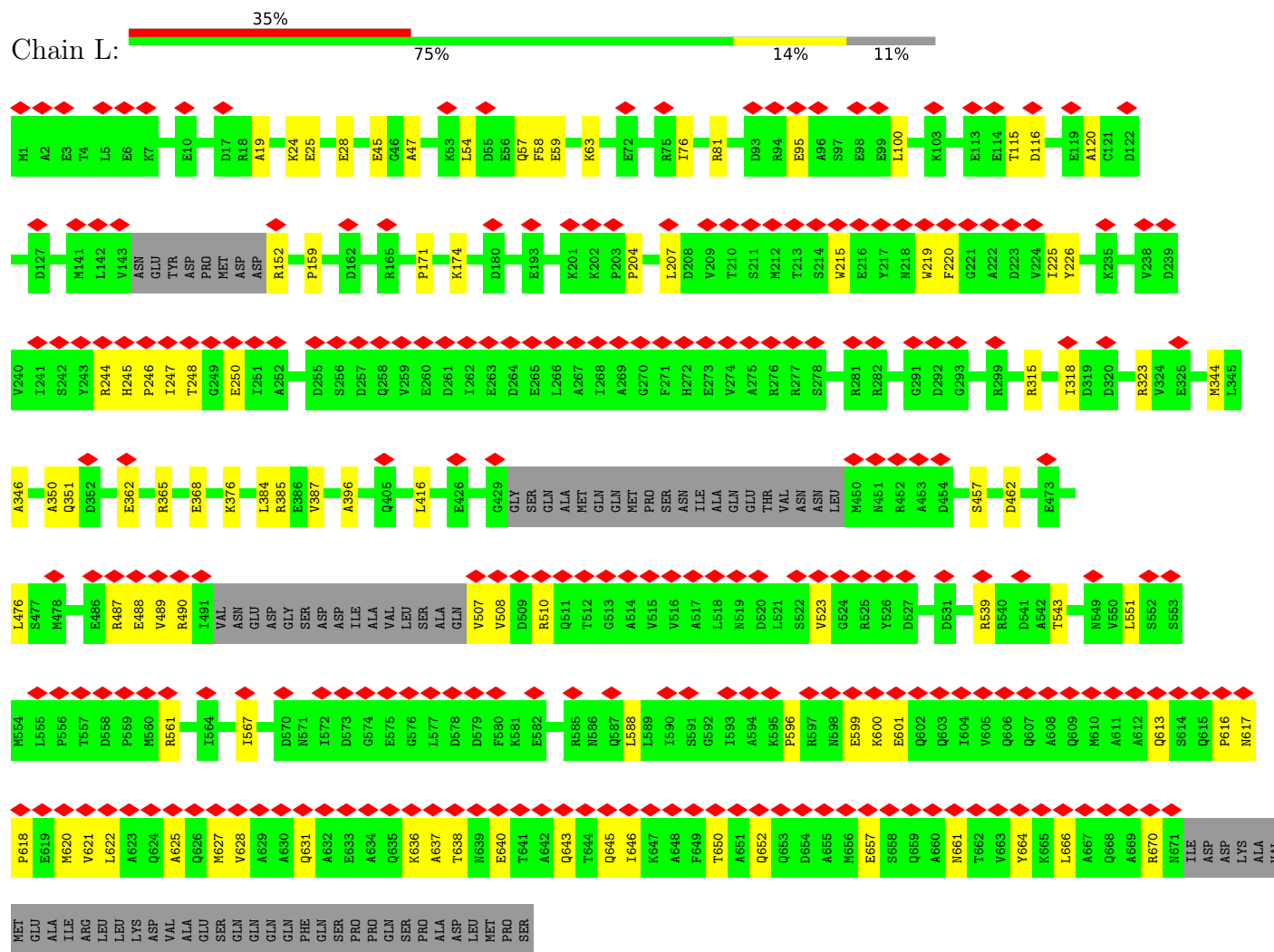




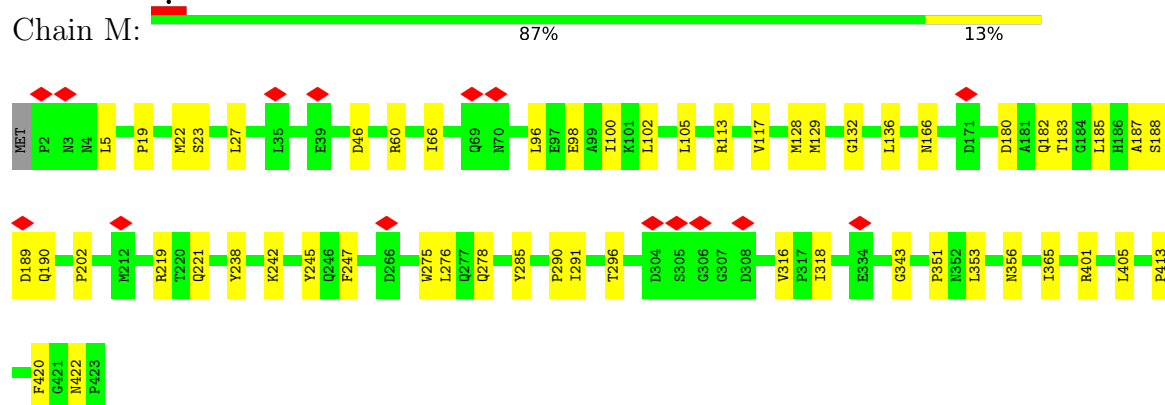
• Molecule 2: Gene 3 protein



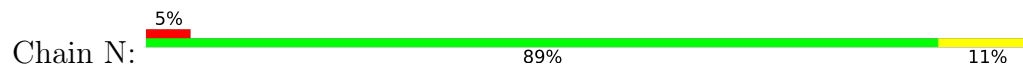
Chain L:

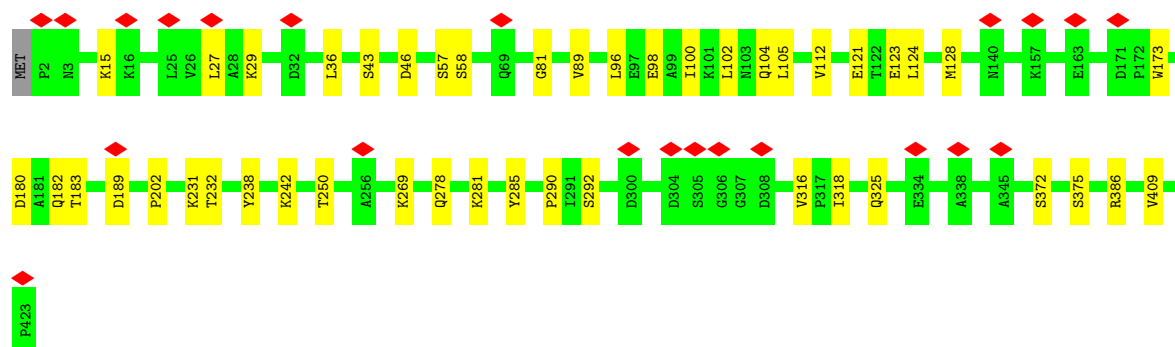


Chain M:

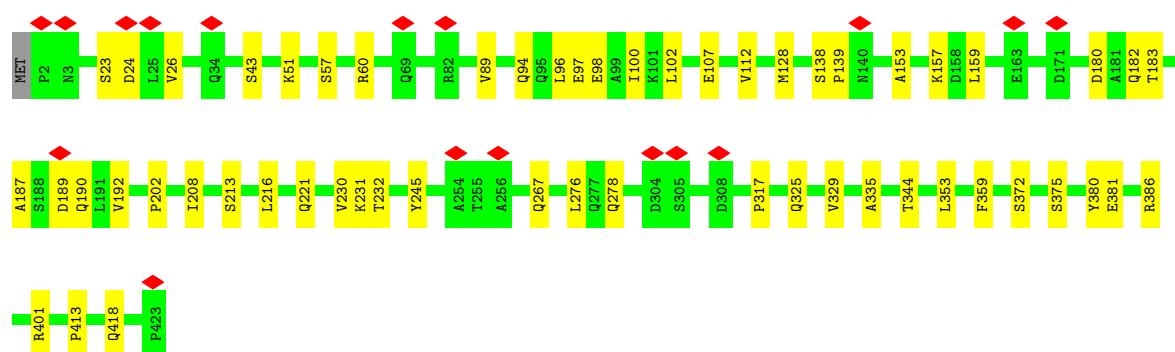
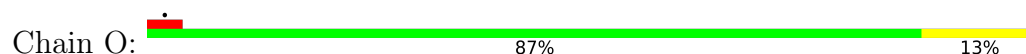


Chain N:

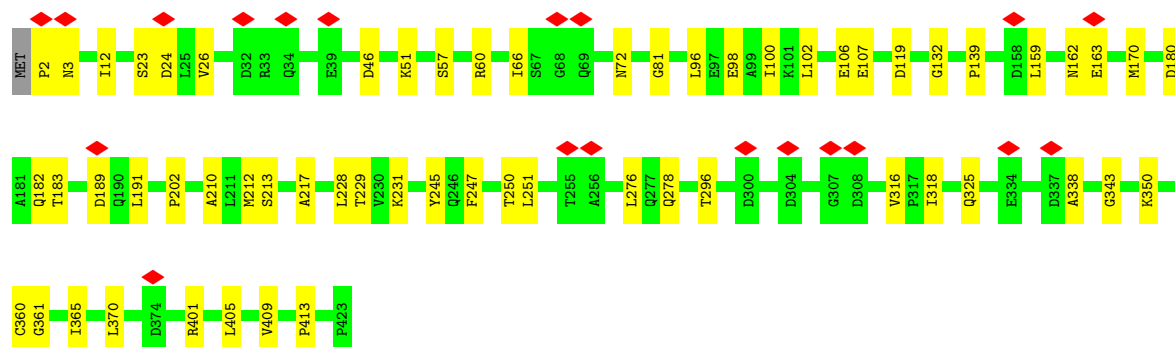
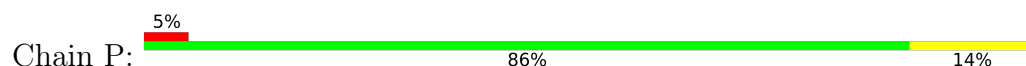




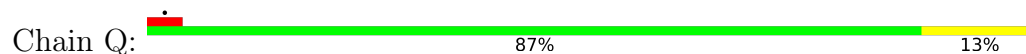
• Molecule 3: Gene 5 protein

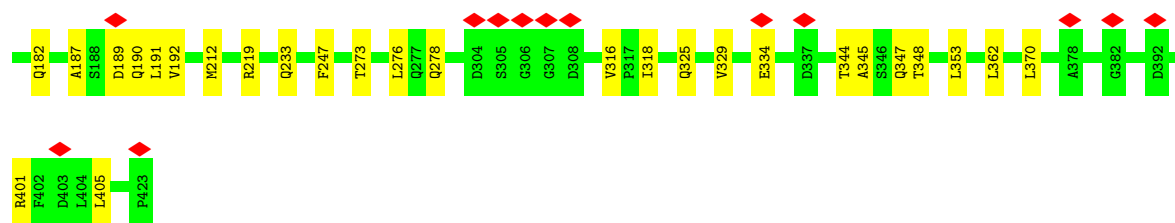


• Molecule 3: Gene 5 protein

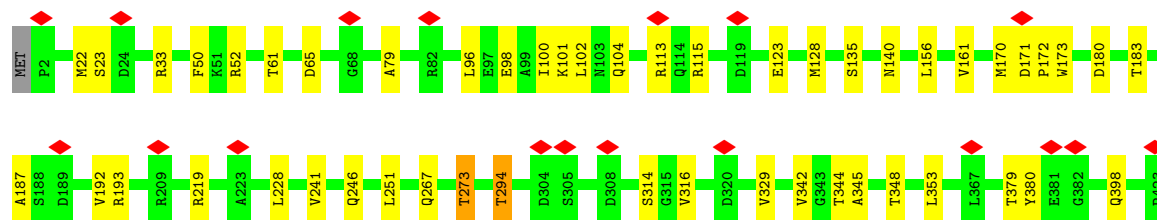
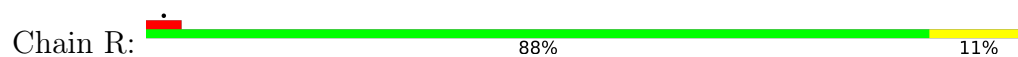


• Molecule 3: Gene 5 protein

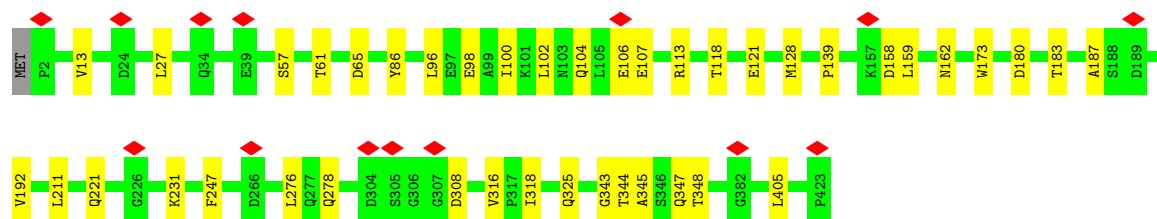
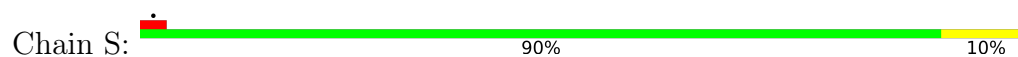




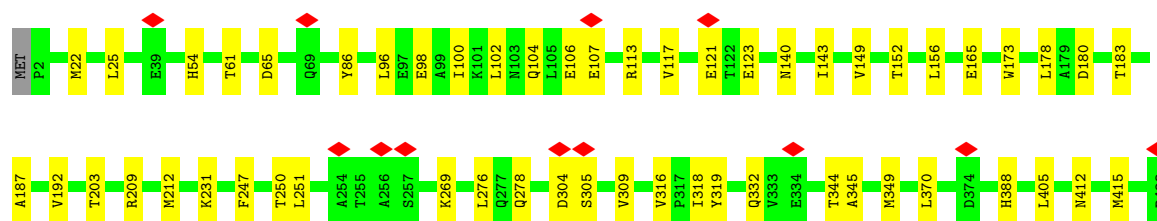
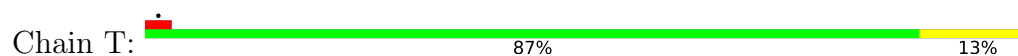
• Molecule 3: Gene 5 protein



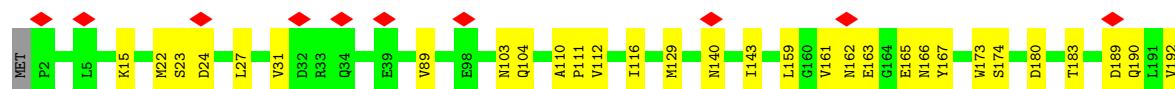
• Molecule 3: Gene 5 protein

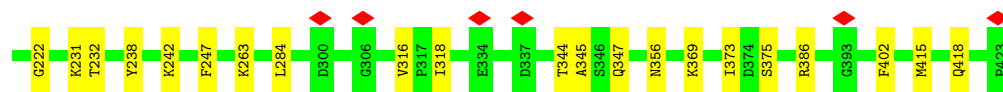


• Molecule 3: Gene 5 protein

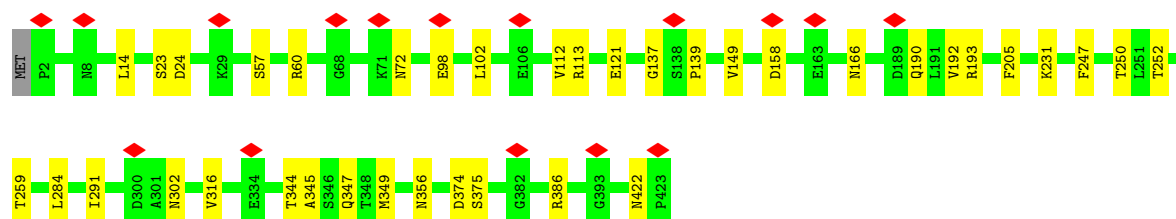


• Molecule 3: Gene 5 protein

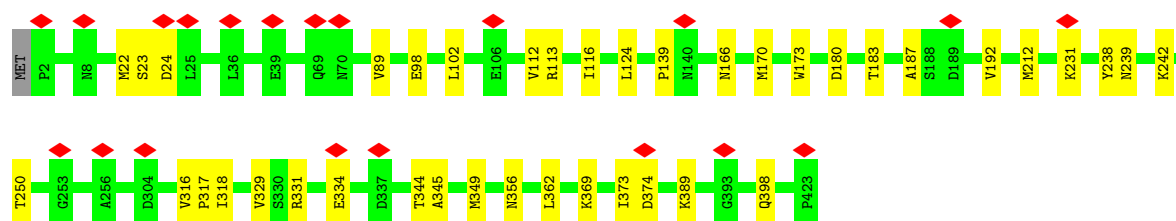




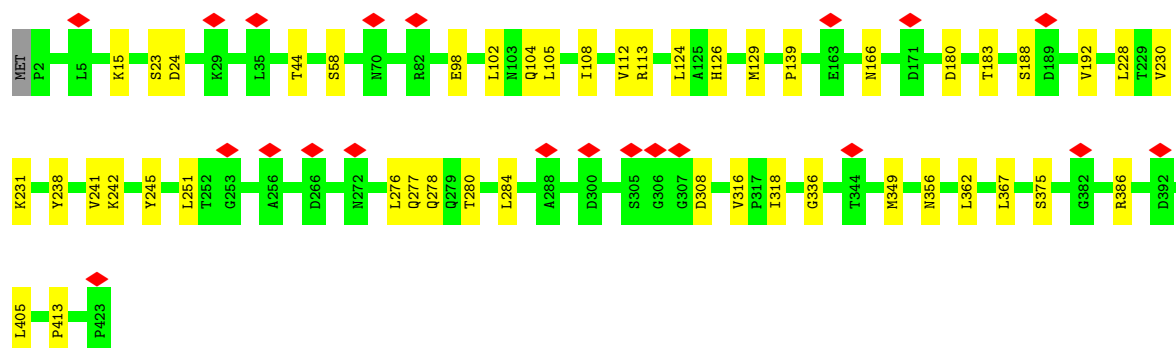
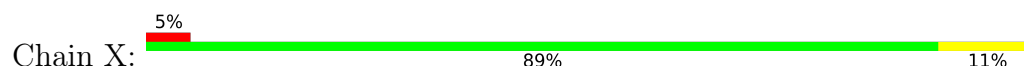
• Molecule 3: Gene 5 protein



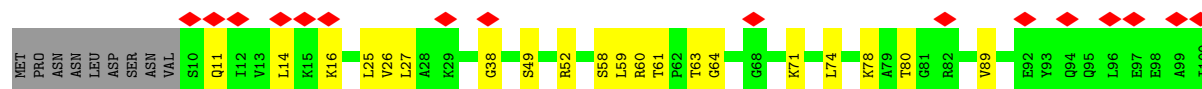
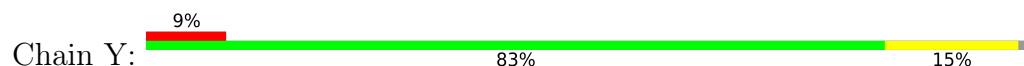
• Molecule 3: Gene 5 protein

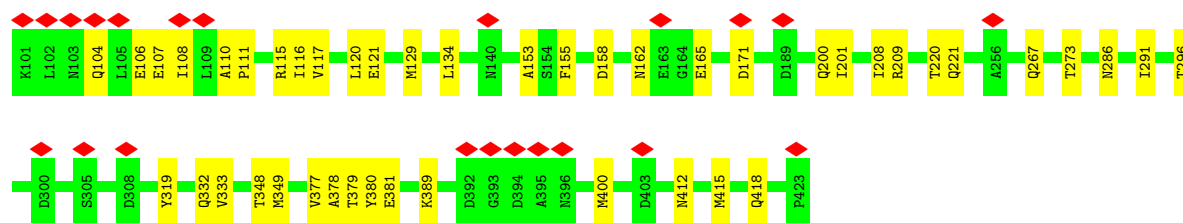


• Molecule 3: Gene 5 protein

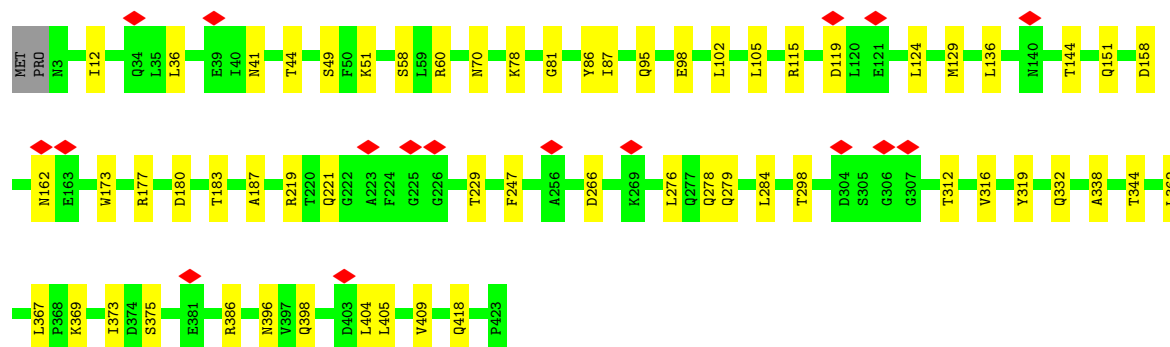
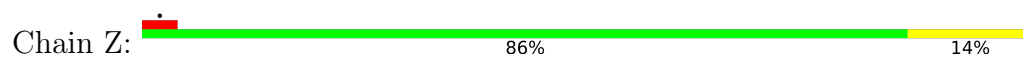


• Molecule 3: Gene 5 protein

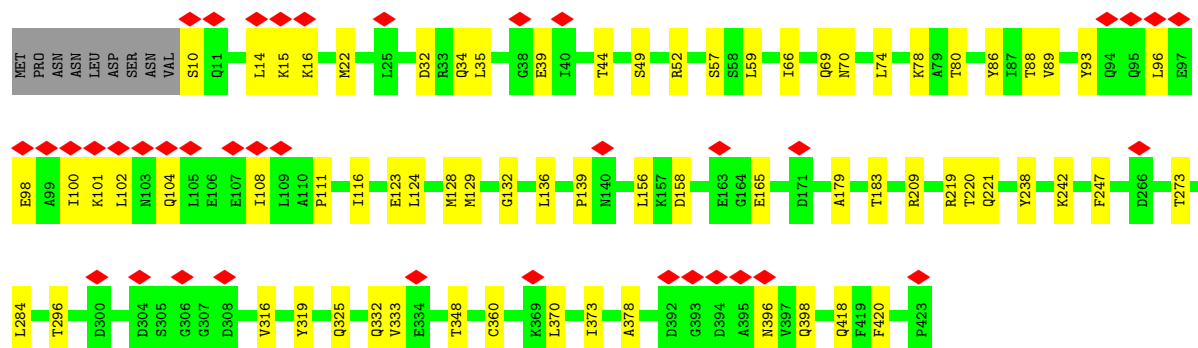
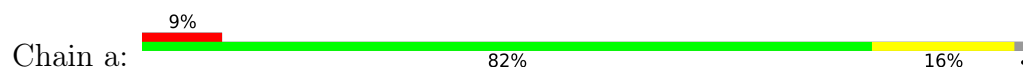




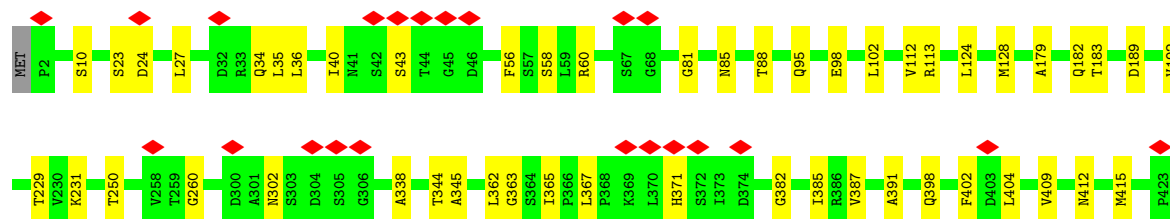
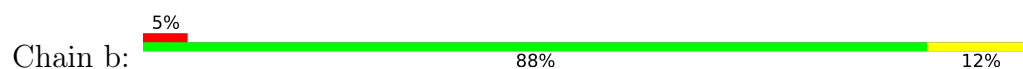
• Molecule 3: Gene 5 protein



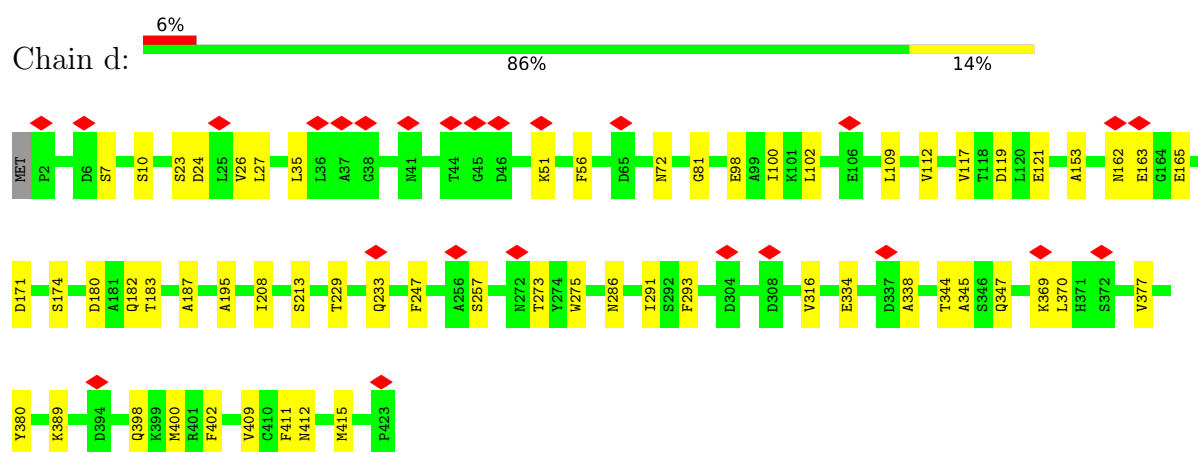
• Molecule 3: Gene 5 protein



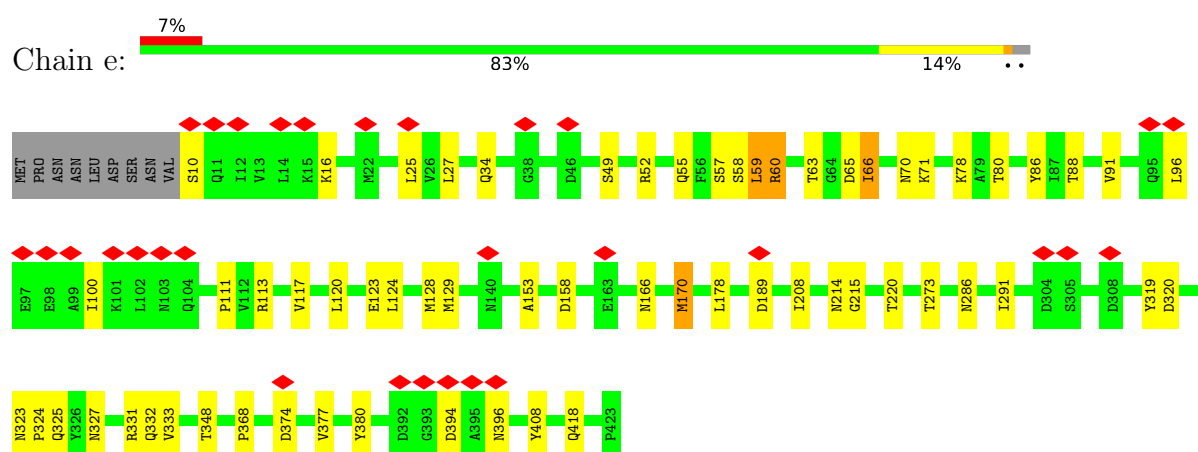
• Molecule 3: Gene 5 protein



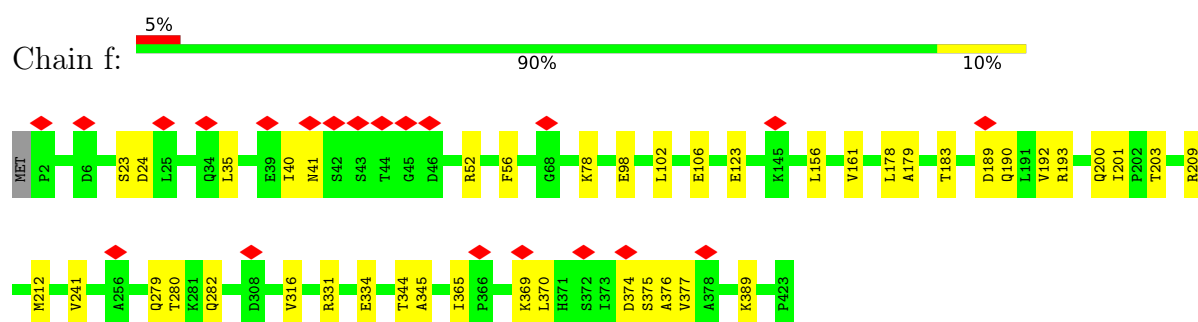
• Molecule 3: Gene 5 protein



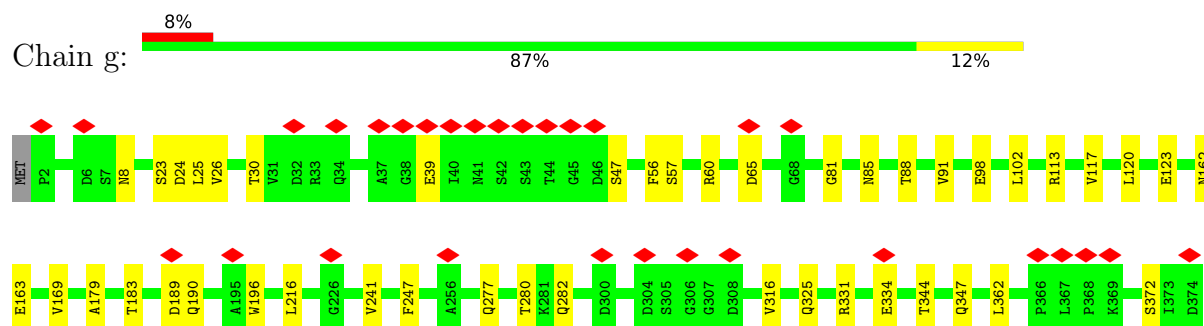
• Molecule 3: Gene 5 protein

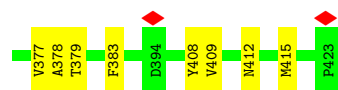


• Molecule 3: Gene 5 protein

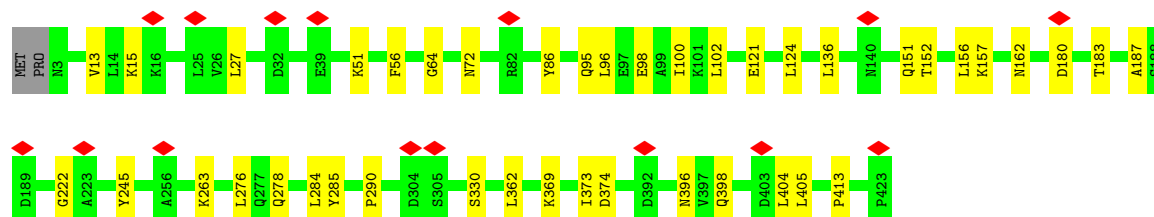
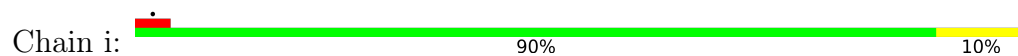


• Molecule 3: Gene 5 protein

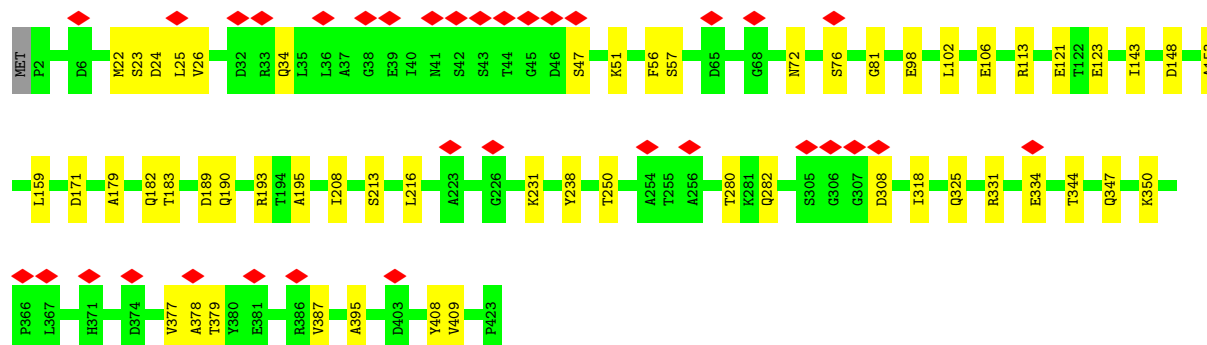
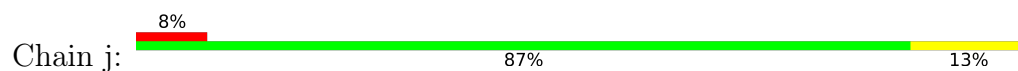




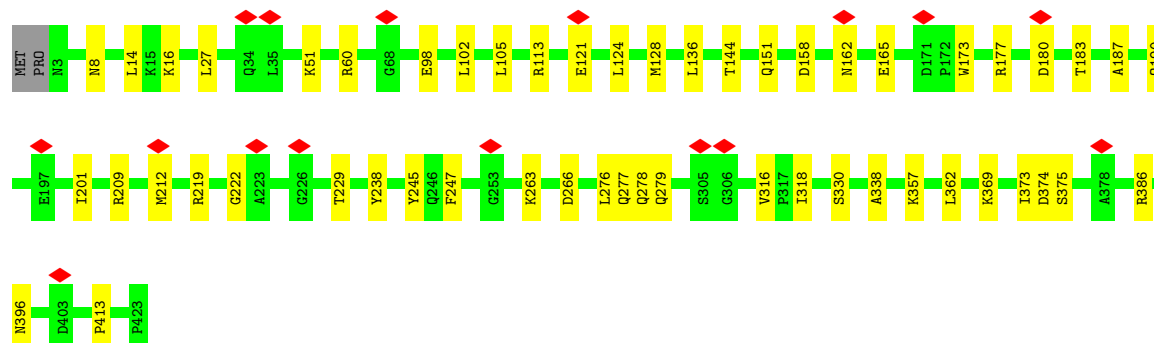
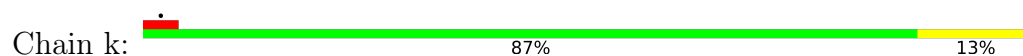
- Molecule 3: Gene 5 protein



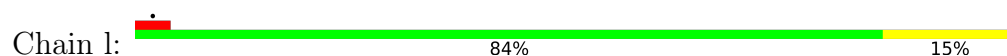
- Molecule 3: Gene 5 protein

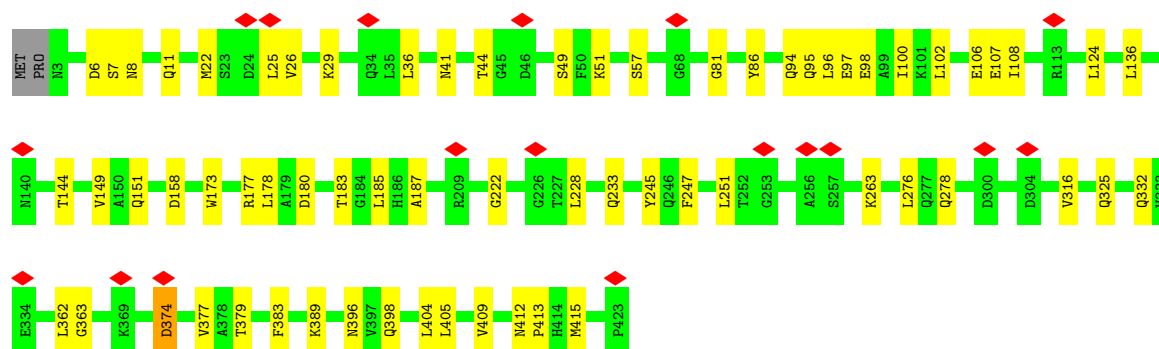


- Molecule 3: Gene 5 protein

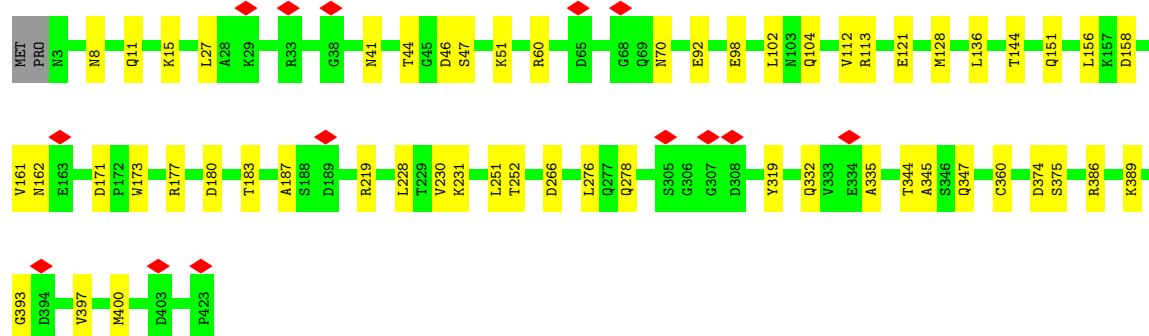
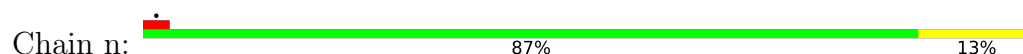


- Molecule 3: Gene 5 protein

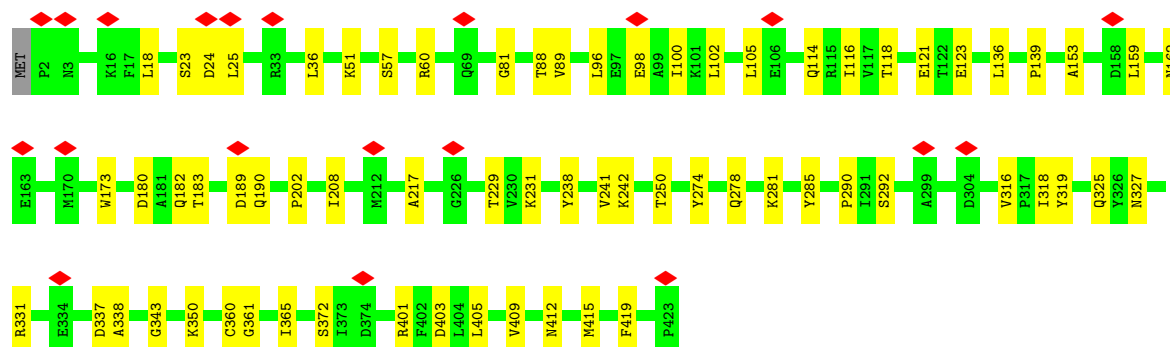
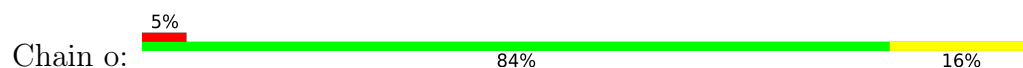




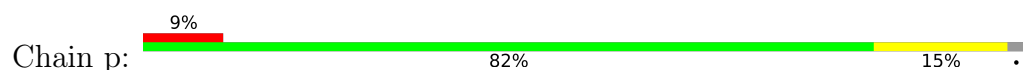
• Molecule 3: Gene 5 protein

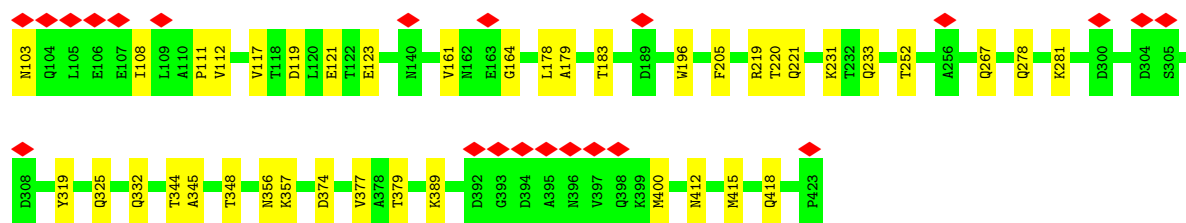


• Molecule 3: Gene 5 protein

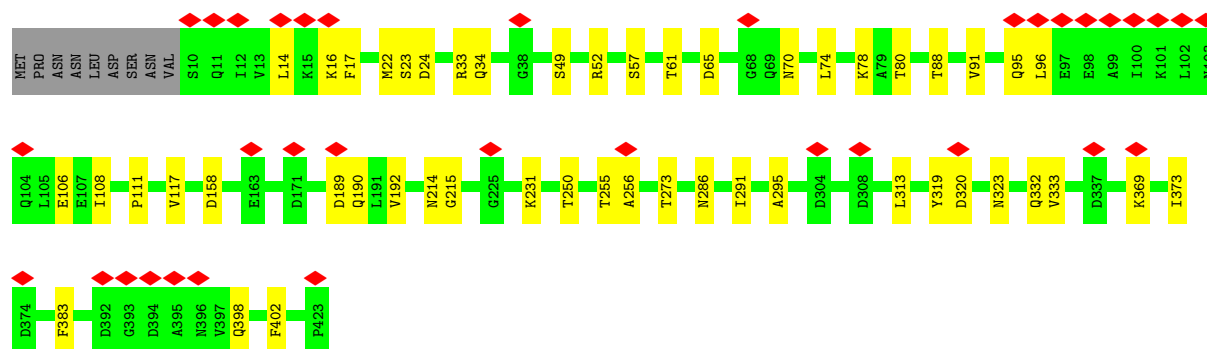
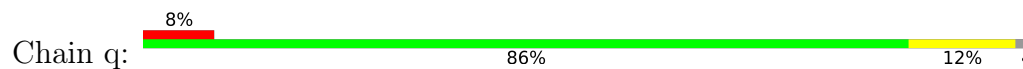


• Molecule 3: Gene 5 protein

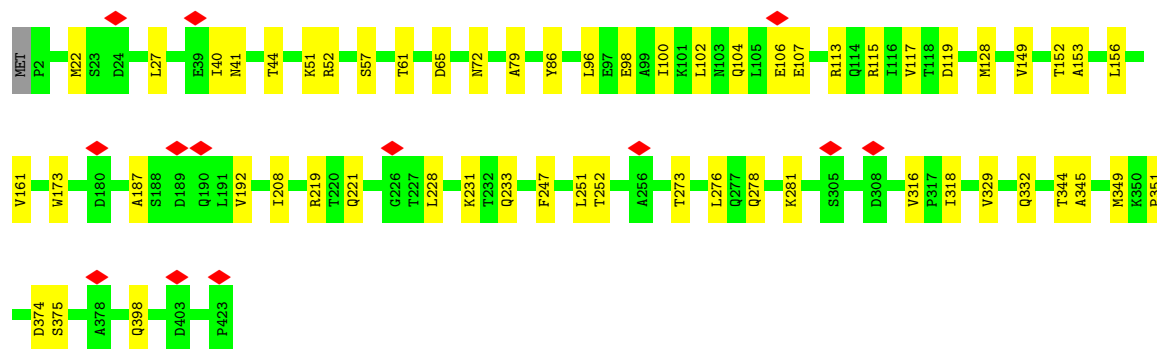
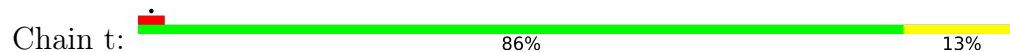




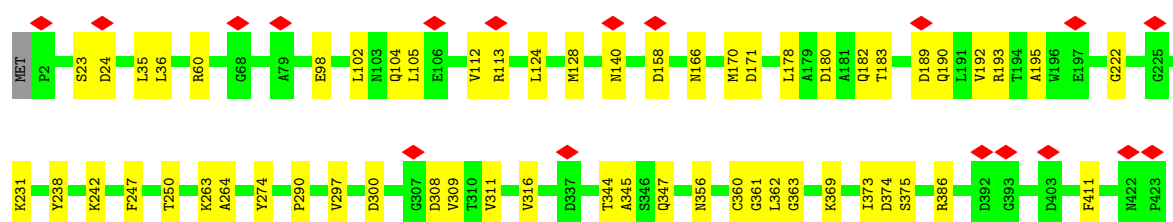
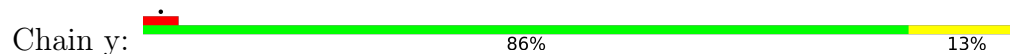
• Molecule 3: Gene 5 protein



• Molecule 3: Gene 5 protein



• Molecule 3: Gene 5 protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	39000	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)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	13.410	Depositor
Minimum map value	-6.586	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	3.6	Depositor
Map size ($\text{\AA}$)	574.464, 574.464, 574.464	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.122, 1.122, 1.122	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0	0.14	0/1191	0.34	1/1618 (0.1%)
1	1	0.12	0/1194	0.31	0/1623
1	c	0.13	0/1186	0.32	0/1611
1	h	0.13	0/1238	0.34	0/1683
1	m	0.12	0/1186	0.30	0/1611
1	r	0.28	0/1246	0.47	1/1695 (0.1%)
1	s	0.14	0/1186	0.37	0/1611
1	u	0.13	0/1256	0.29	0/1709
1	v	0.12	0/1238	0.27	0/1683
1	w	0.14	0/1254	0.32	0/1706
1	x	0.12	0/1186	0.32	0/1611
1	z	0.13	0/1186	0.28	0/1611
2	A	0.11	0/5064	0.31	0/6846
2	B	0.11	0/5064	0.32	0/6846
2	C	0.16	0/5064	0.34	0/6846
2	D	0.11	0/5064	0.31	0/6846
2	E	0.11	0/5064	0.32	0/6846
2	F	0.11	0/5064	0.30	0/6846
2	G	0.11	0/5064	0.31	0/6846
2	H	0.11	0/5064	0.32	0/6846
2	I	0.17	0/5064	0.35	0/6846
2	J	0.11	0/5064	0.31	0/6846
2	K	0.11	0/5064	0.32	0/6846
2	L	0.11	0/5064	0.30	0/6846
3	M	0.14	0/3274	0.33	0/4455
3	N	0.13	0/3274	0.32	0/4455
3	O	0.13	0/3274	0.30	0/4455
3	P	0.21	0/3274	0.36	0/4455
3	Q	0.30	0/3274	0.48	2/4455 (0.0%)
3	R	0.30	0/3274	0.50	2/4455 (0.0%)
3	S	0.28	0/3274	0.46	2/4455 (0.0%)
3	T	0.13	0/3274	0.30	0/4455
3	U	0.25	0/3274	0.45	0/4455
3	V	0.13	0/3274	0.32	0/4455

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	W	0.13	0/3274	0.32	0/4455
3	X	0.12	0/3274	0.31	0/4455
3	Y	0.37	0/3213	0.59	1/4371 (0.0%)
3	Z	0.12	0/3266	0.28	0/4444
3	a	0.28	0/3213	0.47	0/4371
3	b	0.14	0/3274	0.32	0/4455
3	d	0.14	0/3274	0.32	0/4455
3	e	0.30	0/3213	0.48	1/4371 (0.0%)
3	f	0.14	0/3274	0.31	0/4455
3	g	0.14	0/3274	0.32	0/4455
3	i	0.23	0/3266	0.39	0/4444
3	j	0.18	0/3274	0.33	0/4455
3	k	0.21	0/3266	0.38	0/4444
3	l	0.24	0/3266	0.39	1/4444 (0.0%)
3	n	0.22	0/3266	0.39	0/4444
3	o	0.12	0/3274	0.29	0/4455
3	p	0.30	0/3213	0.52	3/4371 (0.1%)
3	q	0.31	0/3213	0.48	0/4371
3	t	0.12	0/3274	0.27	0/4455
3	y	0.11	0/3274	0.29	0/4455
All	All	0.18	0/173190	0.36	14/235099 (0.0%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	R	170	MET	CA-C-N	8.23	132.18	120.49
3	R	170	MET	C-N-CA	8.23	132.18	120.49
3	p	66	ILE	N-CA-C	-7.11	104.37	111.77
1	0	151	PRO	N-CA-CB	6.73	110.41	103.00
3	p	164	GLY	CA-C-O	-6.68	117.50	122.37
3	e	66	ILE	N-CA-C	-6.53	106.16	112.29
1	r	156	ASP	N-CA-C	-6.21	105.83	113.41
3	S	343	GLY	CA-C-O	-6.07	117.94	122.37
3	p	63	THR	N-CA-C	-5.79	100.45	109.72
3	Y	63	THR	CB-CA-C	-5.67	102.72	111.74
3	Q	130	ASN	CA-C-N	-5.57	113.86	122.49
3	Q	130	ASN	C-N-CA	-5.57	113.86	122.49
3	S	345	ALA	N-CA-C	5.30	116.75	111.07
3	l	374	ASP	CB-CA-C	5.16	118.47	109.65

There are no chirality outliers.

There are no planarity outliers.

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	0	1166	0	1116	36	0
1	1	1168	0	1129	47	0
1	c	1161	0	1122	56	0
1	h	1212	0	1171	49	0
1	m	1161	0	1122	53	0
1	r	1219	0	1172	49	0
1	s	1161	0	1122	46	0
1	u	1229	0	1178	54	0
1	v	1212	0	1173	30	0
1	w	1227	0	1182	46	0
1	x	1161	0	1121	44	0
1	z	1161	0	1121	51	0
2	A	4973	0	4892	121	0
2	B	4973	0	4894	116	0
2	C	4973	0	4895	108	0
2	D	4973	0	4895	108	0
2	E	4973	0	4894	129	0
2	F	4973	0	4893	103	0
2	G	4973	0	4893	129	0
2	H	4973	0	4895	115	0
2	I	4973	0	4895	112	0
2	J	4973	0	4894	104	0
2	K	4973	0	4895	99	0
2	L	4973	0	4895	105	0
3	M	3209	0	3149	38	0
3	N	3209	0	3149	29	0
3	O	3209	0	3149	34	0
3	P	3209	0	3149	39	0
3	Q	3209	0	3149	38	0
3	R	3209	0	3149	35	0
3	S	3209	0	3149	27	0
3	T	3209	0	3149	35	0
3	U	3209	0	3149	38	0
3	V	3209	0	3149	25	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	W	3209	0	3149	25	0
3	X	3209	0	3149	27	0
3	Y	3149	0	3094	63	0
3	Z	3202	0	3141	39	0
3	a	3149	0	3093	58	0
3	b	3209	0	3149	61	0
3	d	3209	0	3148	39	0
3	e	3149	0	3094	56	0
3	f	3209	0	3149	46	0
3	g	3209	0	3149	48	0
3	i	3202	0	3141	33	0
3	j	3209	0	3149	56	0
3	k	3202	0	3141	37	0
3	l	3202	0	3141	43	0
3	n	3202	0	3141	40	0
3	o	3209	0	3149	42	0
3	p	3149	0	3090	67	0
3	q	3149	0	3092	43	0
3	t	3209	0	3149	35	0
3	y	3209	0	3149	36	0
All	All	169849	0	166606	2299	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (2299) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:209:VAL:HG21	3:g:378:ALA:CA	1.28	1.57
2:B:209:VAL:CG2	3:g:378:ALA:HA	1.30	1.57
2:H:222:ALA:CB	3:p:377:VAL:HG11	1.23	1.57
2:I:57:GLN:CG	1:c:124:ARG:NH2	1.74	1.51
2:G:61:TYR:CD2	1:z:128:ASP:OD2	1.68	1.47
2:J:215:TRP:CH2	1:c:138:ASP:OD2	1.68	1.44
2:E:57:GLN:CA	3:e:96:LEU:HG	1.37	1.41
2:H:222:ALA:HB2	3:p:377:VAL:CB	1.49	1.41
2:I:57:GLN:CG	1:c:124:ARG:HH21	1.31	1.39
2:H:222:ALA:CB	3:p:377:VAL:CG1	1.98	1.38
2:D:222:ALA:CB	3:j:378:ALA:HA	1.48	1.38
2:H:215:TRP:CH2	1:m:144:ARG:NH2	1.94	1.33
2:J:215:TRP:CZ2	1:c:138:ASP:OD1	1.81	1.31

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:49:ALA:HB2	3:b:371:HIS:CG	1.63	1.31
2:I:25:GLU:HG2	1:h:139:VAL:CG1	1.58	1.30
2:G:41:GLY:O	1:m:136:LYS:NZ	1.63	1.29
2:H:222:ALA:HB2	3:p:377:VAL:CG1	1.61	1.28
2:E:57:GLN:HA	3:e:96:LEU:CG	1.51	1.27
2:L:220:PHE:HA	3:Y:16:LYS:NZ	1.50	1.26
3:p:59:LEU:CD1	3:p:66:ILE:HD11	1.65	1.26
2:F:49:ALA:HB2	3:b:371:HIS:ND1	1.46	1.26
2:E:57:GLN:NE2	3:e:396:ASN:HD22	1.33	1.26
2:D:222:ALA:CB	3:j:378:ALA:CA	2.15	1.24
2:E:57:GLN:HB3	3:e:96:LEU:CD1	1.59	1.23
2:C:217:TYR:O	3:a:104:GLN:HG2	1.36	1.23
2:K:219:TRP:O	3:f:375:SER:O	1.58	1.20
2:C:217:TYR:O	3:a:104:GLN:CG	1.89	1.19
2:H:222:ALA:HB1	3:p:377:VAL:CG1	1.69	1.17
1:0:144:ARG:HD2	2:C:45:GLU:O	1.42	1.16
2:J:215:TRP:HZ2	1:c:138:ASP:OD1	1.15	1.16
2:C:217:TYR:O	3:a:104:GLN:CD	1.88	1.15
2:C:63:LYS:NZ	1:r:135:ASN:HD21	1.40	1.15
2:I:55:ASP:OD2	1:c:121:PRO:O	1.61	1.15
2:K:220:PHE:O	3:f:376:ALA:HB1	1.46	1.15
2:I:218:ASN:HB2	1:c:140:PHE:CZ	1.81	1.14
2:B:376:LYS:HG2	1:r:126:ARG:HD3	1.28	1.14
2:G:216:GLU:OE1	1:z:139:VAL:O	1.62	1.14
2:I:57:GLN:HG3	1:c:124:ARG:NH2	0.79	1.12
2:F:215:TRP:CH2	1:w:144:ARG:NH2	2.17	1.11
2:D:222:ALA:HB2	3:j:378:ALA:CA	1.76	1.11
2:A:55:ASP:OD2	1:s:121:PRO:O	1.68	1.11
2:D:222:ALA:HB1	3:j:378:ALA:HA	1.12	1.11
2:E:57:GLN:NE2	3:e:396:ASN:ND2	1.98	1.11
2:H:222:ALA:HB2	3:p:377:VAL:HB	1.25	1.11
2:I:215:TRP:CH2	1:h:144:ARG:NH2	2.18	1.11
2:E:365:ARG:NH1	1:z:117:THR:OG1	1.84	1.10
2:I:25:GLU:CG	1:h:139:VAL:HG12	1.81	1.10
3:R:22:MET:SD	3:k:162:ASN:ND2	2.25	1.10
1:0:138:ASP:OD2	2:C:215:TRP:CH2	2.03	1.09
2:E:57:GLN:CB	3:e:96:LEU:HD11	1.76	1.09
2:H:55:ASP:OD2	1:h:121:PRO:O	1.68	1.09
2:K:220:PHE:HA	3:f:376:ALA:CA	1.83	1.08
3:p:59:LEU:HD13	3:p:66:ILE:HD11	1.22	1.07
2:K:220:PHE:CA	3:f:376:ALA:HA	1.83	1.07

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:215:TRP:CZ3	1:m:144:ARG:NH2	2.24	1.06
2:C:222:ALA:HB3	3:a:378:ALA:HA	1.38	1.06
2:L:57:GLN:HG3	1:u:124:ARG:NH2	1.71	1.06
2:L:215:TRP:CZ2	1:x:138:ASP:OD1	1.92	1.06
3:p:59:LEU:HD13	3:p:66:ILE:CD1	1.85	1.05
2:F:49:ALA:CB	3:b:371:HIS:CG	2.38	1.05
2:J:215:TRP:CZ2	1:c:138:ASP:CG	2.35	1.04
2:B:375:ASN:ND2	1:r:126:ARG:HE	1.56	1.03
2:J:63:LYS:HD2	1:v:135:ASN:OD1	1.59	1.03
2:B:25:GLU:HG2	1:s:139:VAL:HG11	1.40	1.03
2:K:55:ASP:OD2	1:x:121:PRO:O	1.76	1.03
2:G:61:TYR:CD2	1:z:128:ASP:CG	2.36	1.02
2:A:50:ALA:HA	1:u:149:ASP:HB2	1.41	1.02
2:C:217:TYR:C	3:a:104:GLN:CD	2.26	1.01
2:L:58:PHE:CE1	3:Y:11:GLN:NE2	2.28	1.01
2:G:219:TRP:HB3	3:b:34:GLN:NE2	1.74	1.00
2:G:219:TRP:HB3	3:b:34:GLN:HE22	1.25	1.00
2:F:365:ARG:NH1	1:m:114:MET:SD	2.21	1.00
2:G:212:MET:O	1:z:140:PHE:CE2	2.14	1.00
2:L:220:PHE:HA	3:Y:16:LYS:HZ1	0.83	1.00
2:C:58:PHE:CE1	3:a:96:LEU:HD13	1.97	0.99
2:G:209:VAL:HG21	3:b:382:GLY:H	1.25	0.98
2:I:25:GLU:HG2	1:h:139:VAL:HG12	1.01	0.98
2:F:63:LYS:HD2	1:z:135:ASN:ND2	1.79	0.97
2:H:29:LYS:HD3	1:m:138:ASP:OD1	1.61	0.97
2:A:204:PRO:CD	3:Y:38:GLY:HA3	1.93	0.97
2:G:209:VAL:HG21	3:b:382:GLY:N	1.78	0.97
2:F:215:TRP:CZ2	1:w:144:ARG:NH2	2.32	0.97
2:E:57:GLN:HE22	3:e:396:ASN:HD22	1.06	0.97
2:J:215:TRP:CH2	1:c:138:ASP:CG	2.40	0.97
1:1:141:THR:HG23	2:E:215:TRP:HD1	1.29	0.97
2:E:57:GLN:CB	3:e:96:LEU:HG	1.86	0.96
2:L:219:TRP:O	3:Y:16:LYS:NZ	1.97	0.96
2:L:220:PHE:CA	3:Y:16:LYS:HZ1	1.77	0.96
2:G:41:GLY:C	1:m:136:LYS:NZ	2.24	0.95
2:I:218:ASN:HB2	1:c:140:PHE:HZ	1.17	0.95
2:I:218:ASN:ND2	1:c:140:PHE:HE1	1.62	0.95
2:G:53:LYS:NZ	3:p:11:GLN:HG3	1.82	0.95
1:O:144:ARG:CD	2:C:45:GLU:O	2.15	0.94
2:D:222:ALA:HB3	3:j:379:THR:N	1.81	0.94
2:I:60:LYS:O	1:c:146:TYR:OH	1.84	0.94

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:361:MET:SD	1:v:118:LEU:HD21	2.07	0.94
2:I:215:TRP:CZ2	1:h:144:ARG:NH2	2.32	0.93
2:B:375:ASN:ND2	1:r:126:ARG:NE	2.15	0.93
2:B:209:VAL:HG22	3:g:377:VAL:O	1.68	0.93
2:B:215:TRP:CZ2	1:s:144:ARG:NH2	2.37	0.92
2:I:57:GLN:CB	1:c:124:ARG:HH21	1.82	0.92
2:A:45:GLU:O	1:u:144:ARG:HD2	1.69	0.92
2:J:58:PHE:HB2	3:q:96:LEU:HA	1.49	0.92
2:D:206:SER:HB2	3:j:106:GLU:OE2	1.68	0.92
2:J:215:TRP:HH2	1:c:138:ASP:OD2	1.29	0.91
2:C:63:LYS:HZ2	1:r:135:ASN:HD21	1.07	0.91
2:J:41:GLY:HA3	1:v:136:LYS:HZ3	1.34	0.91
2:A:58:PHE:CE1	1:u:150:LEU:O	2.23	0.91
2:A:58:PHE:CZ	1:u:150:LEU:O	2.24	0.90
2:H:215:TRP:CZ2	1:m:144:ARG:NH2	2.25	0.90
2:C:58:PHE:HE1	3:a:96:LEU:HD13	1.36	0.90
2:E:57:GLN:CB	3:e:96:LEU:CG	2.34	0.90
1:I:146:TYR:OH	2:D:60:LYS:O	1.89	0.89
2:G:41:GLY:C	1:m:136:LYS:HZ1	1.79	0.89
2:A:204:PRO:HG3	3:Y:38:GLY:CA	2.02	0.89
2:G:61:TYR:HD2	1:z:128:ASP:OD2	1.53	0.89
2:C:217:TYR:C	3:a:104:GLN:OE1	2.15	0.89
2:G:212:MET:O	1:z:140:PHE:CZ	2.25	0.89
2:J:58:PHE:CB	3:q:96:LEU:HA	2.03	0.89
2:D:222:ALA:CB	3:j:378:ALA:C	2.46	0.88
2:G:209:VAL:CG2	3:b:382:GLY:HA2	2.02	0.88
2:E:57:GLN:CA	3:e:96:LEU:CG	2.05	0.87
2:I:365:ARG:NH1	1:v:117:THR:OG1	2.07	0.86
2:F:60:LYS:O	1:z:146:TYR:OH	1.93	0.86
2:D:222:ALA:HB2	3:j:378:ALA:N	1.90	0.86
2:I:25:GLU:HG2	1:h:139:VAL:HG11	1.57	0.86
2:A:204:PRO:HG3	3:Y:38:GLY:HA2	1.56	0.86
2:E:375:ASN:O	1:z:126:ARG:NH1	2.09	0.86
2:H:618:PRO:O	2:H:622:LEU:HB2	1.75	0.85
2:J:57:GLN:O	3:q:96:LEU:HG	1.48	0.85
2:F:49:ALA:CB	3:b:371:HIS:ND1	2.35	0.85
2:G:53:LYS:HZ3	3:p:11:GLN:HG3	1.37	0.85
2:H:388:ARG:CZ	1:v:107:GLN:NE2	2.39	0.85
2:C:63:LYS:NZ	1:r:135:ASN:ND2	2.24	0.85
1:I:141:THR:O	2:E:215:TRP:NE1	2.09	0.85
2:G:63:LYS:HZ2	1:m:135:ASN:HD21	1.21	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:209:VAL:HG21	3:b:382:GLY:CA	2.07	0.85
2:E:57:GLN:HB3	3:e:96:LEU:HD11	0.87	0.84
2:C:55:ASP:HB2	1:r:124:ARG:NH2	1.91	0.84
2:E:618:PRO:O	2:E:622:LEU:HB2	1.77	0.84
2:H:222:ALA:CB	3:p:377:VAL:CB	2.38	0.84
2:I:57:GLN:HG3	1:c:124:ARG:HH22	1.03	0.84
2:L:376:LYS:HE3	1:s:125:ARG:O	1.77	0.84
3:p:59:LEU:CD1	3:p:66:ILE:CD1	2.50	0.84
2:A:388:ARG:NH2	1:r:107:GLN:NE2	2.25	0.83
2:G:41:GLY:CA	1:m:136:LYS:HZ2	1.91	0.83
2:J:365:ARG:CZ	1:x:114:MET:HE1	2.08	0.83
2:K:618:PRO:O	2:K:622:LEU:HB2	1.76	0.83
1:c:86:LEU:HG	1:c:90:MET:HE2	1.60	0.83
1:1:118:LEU:CD1	2:C:361:MET:HG2	2.09	0.83
3:p:59:LEU:HD12	3:p:66:ILE:HD11	1.57	0.83
1:0:146:TYR:OH	2:B:60:LYS:O	1.96	0.83
2:A:45:GLU:O	1:u:144:ARG:CD	2.25	0.83
1:1:141:THR:HG23	2:E:215:TRP:CD1	2.14	0.83
2:D:222:ALA:HB3	3:j:378:ALA:C	2.04	0.82
2:A:204:PRO:CG	3:Y:38:GLY:CA	2.57	0.82
2:D:362:GLU:HG3	1:w:114:MET:HE1	1.59	0.82
2:J:365:ARG:CZ	1:x:114:MET:CE	2.56	0.82
2:J:215:TRP:CH2	1:c:144:ARG:NH2	2.46	0.82
2:J:376:LYS:HE3	1:x:125:ARG:O	1.80	0.82
2:A:209:VAL:HG21	3:Y:378:ALA:HA	1.62	0.82
2:A:209:VAL:HG12	3:Y:379:THR:HB	1.61	0.81
2:G:376:LYS:HE3	1:h:125:ARG:O	1.80	0.81
2:H:222:ALA:HB1	3:p:377:VAL:HG11	0.82	0.81
3:a:10:SER:N	3:g:47:SER:HG	1.77	0.81
2:B:29:LYS:NZ	1:s:133:GLN:HE21	1.79	0.81
2:K:59:GLU:OE1	1:x:125:ARG:HG3	1.81	0.81
1:0:138:ASP:OD2	2:C:215:TRP:HH2	1.22	0.81
2:A:204:PRO:HD3	3:Y:38:GLY:HA3	1.62	0.80
3:g:81:GLY:HA3	3:g:409:VAL:HG12	1.63	0.80
1:1:118:LEU:HD11	2:C:361:MET:HG2	1.63	0.80
2:G:63:LYS:NZ	1:m:135:ASN:HD21	1.79	0.80
2:J:57:GLN:O	3:q:96:LEU:CG	2.08	0.80
2:G:61:TYR:HD2	1:z:128:ASP:CG	1.83	0.80
3:e:27:LEU:HD12	3:e:128:MET:HE1	1.62	0.80
2:D:362:GLU:CG	1:w:114:MET:HE1	2.12	0.79
2:D:222:ALA:HB2	3:j:377:VAL:C	2.07	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:344:MET:HE3	1:x:126:ARG:HH12	1.46	0.79
2:B:209:VAL:HG21	3:g:378:ALA:C	2.07	0.79
2:B:375:ASN:HD22	1:r:126:ARG:HE	1.27	0.79
2:C:63:LYS:HZ3	1:r:135:ASN:HD21	1.28	0.79
2:B:25:GLU:HG2	1:s:139:VAL:CG1	2.11	0.79
2:B:618:PRO:O	2:B:622:LEU:HB2	1.82	0.79
1:1:126:ARG:HH12	2:E:344:MET:HG2	1.47	0.79
2:I:344:MET:HE3	1:h:126:ARG:NH1	1.98	0.79
2:E:636:LYS:HD2	2:F:638:THR:HA	1.65	0.78
2:G:41:GLY:HA3	1:m:136:LYS:HZ2	1.48	0.78
2:H:207:LEU:HD21	3:p:379:THR:HG21	1.65	0.78
2:L:58:PHE:HE1	3:Y:11:GLN:NE2	1.81	0.78
2:L:115:THR:HG22	2:L:116:ASP:H	1.48	0.78
2:A:636:LYS:HD2	2:B:638:THR:HA	1.65	0.78
2:C:115:THR:HG22	2:C:116:ASP:H	1.48	0.78
2:E:54:LEU:CD2	1:w:124:ARG:CD	2.60	0.78
2:H:57:GLN:HE22	1:h:150:LEU:HD13	1.48	0.78
2:H:636:LYS:HD2	2:I:638:THR:HA	1.65	0.78
2:J:636:LYS:HD2	2:K:638:THR:HA	1.66	0.78
2:J:215:TRP:CZ3	1:c:144:ARG:NH2	2.51	0.78
2:B:209:VAL:CG2	3:g:378:ALA:CA	2.15	0.78
2:D:215:TRP:CH2	1:r:138:ASP:OD1	2.36	0.77
2:F:49:ALA:HB2	3:b:371:HIS:CB	2.13	0.77
2:F:115:THR:HG22	2:F:116:ASP:H	1.48	0.77
2:B:636:LYS:HD2	2:C:638:THR:HA	1.65	0.77
2:I:115:THR:HG22	2:I:116:ASP:H	1.48	0.77
2:G:350:ALA:CB	1:m:129:PHE:HE2	1.97	0.77
3:i:98:GLU:HA	3:i:102:LEU:HB2	1.65	0.77
2:H:222:ALA:HB2	3:p:377:VAL:CG2	2.14	0.77
2:K:636:LYS:HD2	2:L:638:THR:HA	1.65	0.77
2:D:206:SER:CB	3:j:106:GLU:OE2	2.31	0.77
2:B:115:THR:HG22	2:B:116:ASP:H	1.49	0.77
3:l:98:GLU:HA	3:l:102:LEU:HB2	1.65	0.77
2:E:596:PRO:HB3	2:E:601:GLU:HG3	1.67	0.77
2:H:57:GLN:NE2	1:h:150:LEU:HD13	2.00	0.77
2:H:57:GLN:HE22	1:h:150:LEU:CD1	1.97	0.77
2:K:115:THR:HG22	2:K:116:ASP:H	1.49	0.76
2:G:61:TYR:CG	1:z:128:ASP:OD2	2.37	0.76
2:J:63:LYS:CD	1:v:135:ASN:OD1	2.33	0.76
3:M:221:GLN:HE22	3:M:343:GLY:HA3	1.47	0.76
2:J:218:ASN:OD1	3:q:106:GLU:OE1	2.02	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:209:VAL:HG21	3:b:382:GLY:HA2	1.64	0.76
2:A:596:PRO:HB3	2:A:601:GLU:HG3	1.67	0.76
2:E:115:THR:HG22	2:E:116:ASP:H	1.49	0.76
2:I:596:PRO:HB3	2:I:601:GLU:HG3	1.67	0.76
2:J:63:LYS:NZ	1:v:135:ASN:OD1	2.17	0.76
2:C:636:LYS:HD2	2:D:638:THR:HA	1.67	0.76
2:D:115:THR:HG22	2:D:116:ASP:H	1.49	0.76
2:D:636:LYS:HD2	2:E:638:THR:HA	1.66	0.76
2:J:596:PRO:HB3	2:J:601:GLU:HG3	1.67	0.76
2:D:223:ASP:OD1	3:j:379:THR:CG2	2.34	0.76
2:G:636:LYS:HD2	2:H:638:THR:HA	1.66	0.75
2:I:218:ASN:HB2	1:c:140:PHE:CE1	2.20	0.75
2:L:344:MET:HE3	1:x:126:ARG:NH1	2.01	0.75
3:Z:98:GLU:HA	3:Z:102:LEU:HB2	1.68	0.75
2:I:218:ASN:CB	1:c:140:PHE:CZ	2.68	0.75
2:A:115:THR:HG22	2:A:116:ASP:H	1.49	0.75
2:G:115:THR:HG22	2:G:116:ASP:H	1.50	0.75
2:H:115:THR:HG22	2:H:116:ASP:H	1.49	0.75
2:L:596:PRO:HB3	2:L:601:GLU:HG3	1.67	0.75
2:A:638:THR:HA	2:L:636:LYS:HD2	1.68	0.75
2:H:596:PRO:HB3	2:H:601:GLU:HG3	1.67	0.75
2:J:115:THR:HG22	2:J:116:ASP:H	1.49	0.75
2:B:596:PRO:HB3	2:B:601:GLU:HG3	1.67	0.75
2:K:218:ASN:HD22	1:x:140:PHE:HE1	1.33	0.75
2:K:596:PRO:HB3	2:K:601:GLU:HG3	1.67	0.75
2:A:44:TRP:C	1:u:144:ARG:HH12	1.94	0.75
2:F:596:PRO:HB3	2:F:601:GLU:HG3	1.67	0.74
2:B:375:ASN:CG	1:r:126:ARG:NE	2.45	0.74
2:C:596:PRO:HB3	2:C:601:GLU:HG3	1.67	0.74
2:D:223:ASP:CG	3:j:379:THR:HG21	2.13	0.74
2:G:53:LYS:NZ	3:p:11:GLN:CG	2.49	0.74
2:A:388:ARG:CZ	1:r:107:GLN:NE2	2.51	0.74
2:D:596:PRO:HB3	2:D:601:GLU:HG3	1.67	0.74
2:G:596:PRO:HB3	2:G:601:GLU:HG3	1.67	0.74
2:I:383:PRO:HG3	1:x:118:LEU:HD21	1.69	0.74
3:b:81:GLY:HA3	3:b:409:VAL:HG12	1.70	0.74
2:I:636:LYS:HD2	2:J:638:THR:HA	1.68	0.74
2:J:365:ARG:NH2	1:x:114:MET:HE3	2.03	0.74
2:E:57:GLN:HA	3:e:96:LEU:CB	2.18	0.73
2:G:29:LYS:NZ	1:z:133:GLN:HE21	1.86	0.73
2:K:7:LYS:CE	3:q:34:GLN:HE22	2.00	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:60:LYS:O	1:x:146:TYR:OH	2.04	0.73
2:F:636:LYS:HD2	2:G:638:THR:HA	1.68	0.73
2:E:351:GLN:HE21	1:w:123:MET:CE	2.02	0.73
2:I:218:ASN:ND2	1:c:140:PHE:CE1	2.53	0.73
3:Q:57:SER:HB3	3:Q:325:GLN:HB3	1.70	0.73
2:K:220:PHE:O	3:f:376:ALA:CB	2.34	0.73
1:1:118:LEU:CD1	2:C:361:MET:SD	2.77	0.73
2:H:207:LEU:CD2	3:p:379:THR:HG21	2.18	0.73
3:b:60:ARG:NH1	3:p:123:GLU:OE1	2.22	0.73
3:R:115:ARG:NH2	3:k:279:GLN:OE1	2.22	0.72
3:n:344:THR:HG22	3:n:345:ALA:H	1.54	0.72
2:K:370:HIS:CE1	1:s:120:VAL:HG21	2.25	0.72
2:L:351:GLN:HE21	1:u:123:MET:HE2	1.55	0.72
3:k:98:GLU:HA	3:k:102:LEU:HB2	1.70	0.72
2:B:207:LEU:HD21	3:g:379:THR:HG22	1.69	0.72
2:D:215:TRP:HH2	1:r:138:ASP:OD1	1.72	0.72
2:F:49:ALA:CB	3:b:371:HIS:CB	2.68	0.72
2:E:62:PRO:HD3	1:w:125:ARG:NH2	2.04	0.72
2:I:59:GLU:OE1	1:c:125:ARG:HG2	1.89	0.72
1:x:44:MET:HE1	1:x:85:GLN:HB3	1.71	0.72
2:A:209:VAL:CG1	3:Y:379:THR:HB	2.20	0.71
2:F:49:ALA:CB	3:b:371:HIS:HB3	2.19	0.71
2:H:207:LEU:HD21	3:p:379:THR:CG2	2.20	0.71
1:0:51:ASN:HB3	1:0:52:PRO:HD3	1.70	0.71
2:I:25:GLU:CG	1:h:139:VAL:CG1	2.51	0.71
2:H:376:LYS:HE3	1:c:125:ARG:O	1.90	0.71
2:K:59:GLU:OE1	1:x:125:ARG:CG	2.38	0.71
2:G:61:TYR:CE2	1:z:128:ASP:OD2	2.41	0.71
1:1:126:ARG:NH1	2:E:344:MET:SD	2.64	0.71
2:E:351:GLN:HE21	1:w:123:MET:HE2	1.55	0.71
2:G:41:GLY:HA3	1:m:136:LYS:NZ	2.06	0.71
2:L:25:GLU:HG2	1:x:139:VAL:HG23	1.72	0.71
2:B:376:LYS:HG2	1:r:126:ARG:CD	2.16	0.70
2:A:388:ARG:NH2	1:r:107:GLN:HE22	1.88	0.70
2:K:220:PHE:HA	3:f:376:ALA:HA	0.89	0.70
2:G:209:VAL:HG23	3:b:382:GLY:HA2	1.73	0.70
2:I:218:ASN:CG	1:c:140:PHE:HE1	1.98	0.70
2:A:215:TRP:HE1	1:u:141:THR:N	1.89	0.70
3:g:189:ASP:OD2	3:g:190:GLN:N	2.24	0.70
3:g:241:VAL:HG21	3:g:316:VAL:HG11	1.72	0.70
3:o:412:ASN:HB3	3:o:415:MET:HE2	1.74	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:77:LYS:HD2	1:s:50:ILE:HD11	1.73	0.70
2:G:29:LYS:NZ	1:z:133:GLN:NE2	2.40	0.69
3:R:98:GLU:HA	3:R:102:LEU:HB2	1.73	0.69
2:B:215:TRP:CE2	1:s:144:ARG:NH2	2.60	0.69
2:J:60:LYS:O	1:v:146:TYR:OH	2.10	0.69
2:I:218:ASN:CB	1:c:140:PHE:CE1	2.75	0.69
2:J:653:GLN:HA	2:J:656:MET:HE3	1.74	0.69
3:S:98:GLU:HA	3:S:102:LEU:HB2	1.74	0.69
3:T:344:THR:HG22	3:T:345:ALA:H	1.58	0.69
2:A:215:TRP:CD1	1:u:140:PHE:C	2.66	0.69
2:B:209:VAL:CG2	3:g:378:ALA:C	2.64	0.69
2:G:29:LYS:HZ3	1:z:133:GLN:HE21	1.39	0.69
2:G:41:GLY:HA3	1:m:136:LYS:CE	2.22	0.69
3:e:52:ARG:NH1	3:e:78:LYS:O	2.26	0.69
2:F:49:ALA:HB2	3:b:371:HIS:HD1	1.54	0.69
2:D:25:GLU:HG2	1:r:139:VAL:CG1	2.23	0.69
1:s:51:ASN:HB3	1:s:52:PRO:HD3	1.73	0.69
2:F:59:GLU:OE1	1:z:125:ARG:HG2	1.91	0.68
2:B:29:LYS:HZ3	1:s:133:GLN:HE21	1.38	0.68
3:j:98:GLU:HA	3:j:102:LEU:HB2	1.75	0.68
2:J:215:TRP:CZ2	1:c:138:ASP:OD2	2.33	0.68
3:d:98:GLU:OE2	3:d:398:GLN:NE2	2.24	0.68
3:O:267:GLN:NE2	3:O:418:GLN:OE1	2.26	0.68
2:H:388:ARG:NH2	1:v:107:GLN:HE21	1.92	0.68
2:K:7:LYS:HD3	3:q:34:GLN:HE22	1.59	0.68
1:1:118:LEU:HD12	2:C:361:MET:SD	2.32	0.68
2:E:54:LEU:HD21	1:w:124:ARG:CD	2.22	0.68
2:A:209:VAL:CG2	3:Y:378:ALA:HA	2.23	0.68
3:d:98:GLU:HA	3:d:102:LEU:HB2	1.74	0.68
3:i:86:TYR:HB3	3:i:405:LEU:HD23	1.76	0.68
2:A:49:ALA:HB1	1:u:151:PRO:HB2	1.74	0.67
2:F:63:LYS:HD2	1:z:135:ASN:HD22	1.59	0.67
2:H:59:GLU:OE1	1:h:125:ARG:CG	2.43	0.67
2:I:218:ASN:HD22	1:c:140:PHE:HE1	1.41	0.67
3:g:277:GLN:OE1	3:g:280:THR:HG22	1.93	0.67
2:D:223:ASP:OD1	3:j:379:THR:HG21	1.95	0.67
2:F:63:LYS:NZ	1:z:135:ASN:HD21	1.92	0.67
2:G:41:GLY:CA	1:m:136:LYS:NZ	2.53	0.67
2:J:63:LYS:HZ3	1:v:135:ASN:CG	2.02	0.67
2:D:25:GLU:HG2	1:r:139:VAL:HG11	1.76	0.67
1:m:141:THR:HG22	1:m:143:ASP:H	1.60	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:s:17:LYS:NZ	1:u:40:ASP:OD2	2.23	0.67
3:Q:344:THR:HG22	3:Q:345:ALA:H	1.59	0.67
3:l:86:TYR:HB3	3:l:405:LEU:HD23	1.76	0.67
2:A:49:ALA:HB1	1:u:151:PRO:CB	2.24	0.67
2:K:362:GLU:HA	1:u:114:MET:HE1	1.77	0.67
2:G:53:LYS:HZ3	3:p:11:GLN:CG	2.05	0.67
3:l:94:GLN:HB2	3:l:97:GLU:HG3	1.77	0.67
3:Q:98:GLU:HA	3:Q:102:LEU:HB2	1.76	0.67
3:f:98:GLU:HA	3:f:102:LEU:HB2	1.77	0.67
2:G:61:TYR:CD2	1:z:128:ASP:OD1	2.47	0.67
2:H:59:GLU:OE1	1:h:125:ARG:HG2	1.93	0.67
3:t:344:THR:HG22	3:t:345:ALA:H	1.60	0.67
3:p:52:ARG:NH1	3:p:78:LYS:O	2.28	0.66
2:A:209:VAL:HG11	3:Y:379:THR:H	1.60	0.66
2:L:45:GLU:CB	1:x:144:ARG:HH22	2.08	0.66
1:c:141:THR:HG22	1:c:143:ASP:H	1.60	0.66
3:P:276:LEU:O	3:P:278:GLN:NE2	2.29	0.66
2:K:215:TRP:CH2	1:v:144:ARG:NH2	2.63	0.66
3:q:52:ARG:NH1	3:q:78:LYS:O	2.28	0.66
2:C:222:ALA:CB	3:a:378:ALA:HA	2.23	0.66
2:F:215:TRP:CZ3	1:w:144:ARG:NH2	2.63	0.66
3:p:356:ASN:OD1	3:p:357:LYS:N	2.28	0.66
2:A:47:ALA:N	1:u:144:ARG:NH2	2.31	0.66
2:E:54:LEU:CD2	1:w:124:ARG:HD2	2.25	0.66
3:R:344:THR:HG22	3:R:345:ALA:H	1.61	0.66
2:F:63:LYS:HD2	1:z:135:ASN:HD21	1.60	0.66
2:F:370:HIS:CE1	1:h:120:VAL:HG21	2.31	0.66
1:l:35:GLU:O	1:l:39:ASN:ND2	2.29	0.66
3:t:57:SER:H	3:t:72:ASN:HD21	1.44	0.66
2:H:63:LYS:HD2	1:h:135:ASN:ND2	2.12	0.65
2:L:57:GLN:HG3	1:u:124:ARG:HH21	1.56	0.65
2:A:204:PRO:CG	3:Y:38:GLY:HA3	2.21	0.65
1:l:141:THR:C	2:E:215:TRP:HE1	2.03	0.65
2:E:57:GLN:HA	3:e:96:LEU:HG	0.70	0.65
3:j:344:THR:HB	3:j:347:GLN:HB2	1.79	0.65
2:E:58:PHE:CE2	3:e:100:ILE:HA	2.32	0.65
3:V:247:PHE:HD1	3:V:316:VAL:HG12	1.61	0.65
3:d:72:ASN:HB2	3:q:91:VAL:HG12	1.79	0.65
2:F:63:LYS:CD	1:z:135:ASN:ND2	2.58	0.65
1:v:51:ASN:HB3	1:v:52:PRO:HD3	1.79	0.65
2:G:29:LYS:HZ1	1:z:133:GLN:NE2	1.95	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:d:81:GLY:HA3	3:d:409:VAL:HG22	1.78	0.65
3:n:98:GLU:HA	3:n:102:LEU:HB2	1.79	0.64
1:x:42:GLU:HG3	1:x:66:PRO:HG3	1.78	0.64
3:Q:276:LEU:O	3:Q:278:GLN:NE2	2.30	0.64
3:S:173:TRP:NE1	3:l:158:ASP:OD2	2.29	0.64
3:a:129:MET:HB2	3:a:418:GLN:HE21	1.62	0.64
1:0:124:ARG:HH12	1:0:150:LEU:HD23	1.61	0.64
2:F:63:LYS:CD	1:z:135:ASN:HD21	2.10	0.64
3:T:143:ILE:HG22	3:T:178:LEU:HD21	1.79	0.64
1:0:22:SER:H	1:0:25:SER:HB3	1.61	0.64
2:G:219:TRP:CB	3:b:34:GLN:HE22	2.07	0.64
2:J:365:ARG:CZ	1:x:114:MET:HE3	2.26	0.64
3:S:192:VAL:HG11	3:l:187:ALA:HB3	1.79	0.64
2:B:215:TRP:HH2	1:s:138:ASP:OD1	1.80	0.64
2:I:24:LYS:NZ	2:I:28:GLU:OE2	2.28	0.64
1:c:51:ASN:HB3	1:c:52:PRO:HD3	1.79	0.64
1:1:118:LEU:CD1	2:C:361:MET:CG	2.76	0.64
2:C:63:LYS:HZ3	1:r:135:ASN:ND2	1.90	0.64
3:P:81:GLY:HA3	3:P:409:VAL:HG22	1.79	0.64
3:t:219:ARG:HD3	3:t:351:PRO:HG3	1.80	0.64
2:B:209:VAL:CG2	3:g:377:VAL:O	2.42	0.64
2:C:53:LYS:NZ	3:a:396:ASN:HD22	1.96	0.64
3:k:229:THR:HG22	3:k:338:ALA:HA	1.80	0.64
2:J:41:GLY:HA3	1:v:136:LYS:NZ	2.09	0.64
3:V:375:SER:OG	3:V:386:ARG:NH1	2.31	0.64
3:a:52:ARG:NH1	3:a:78:LYS:O	2.31	0.63
3:y:247:PHE:HD1	3:y:316:VAL:HG12	1.63	0.63
2:A:255:ASP:OD1	2:A:258:GLN:NE2	2.32	0.63
2:E:488:GLU:OE1	2:E:510:ARG:NH1	2.29	0.63
3:Y:52:ARG:NH1	3:Y:78:LYS:O	2.31	0.63
2:A:58:PHE:CE2	1:u:151:PRO:HA	2.34	0.63
2:K:7:LYS:CD	3:q:34:GLN:HE22	2.12	0.63
3:o:81:GLY:HA3	3:o:409:VAL:HG22	1.80	0.63
1:0:101:GLN:NE2	1:0:105:ASN:OD1	2.31	0.63
2:B:207:LEU:HD21	3:g:379:THR:CG2	2.29	0.63
3:U:89:VAL:HG12	3:U:116:ILE:HD11	1.81	0.63
3:q:33:ARG:HH12	3:q:383:PHE:HE2	1.45	0.63
2:B:375:ASN:OD1	1:r:123:MET:HE3	1.99	0.62
2:B:376:LYS:CG	1:r:126:ARG:HD3	2.18	0.62
2:D:255:ASP:OD1	2:D:258:GLN:NE2	2.32	0.62
3:O:231:LYS:HG2	3:O:232:THR:HG23	1.81	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:123:GLU:HG3	3:k:60:ARG:HH12	1.62	0.62
3:X:375:SER:OG	3:X:386:ARG:NH1	2.32	0.62
1:s:45:MET:HE1	1:s:55:ILE:HD11	1.81	0.62
2:G:255:ASP:OD1	2:G:258:GLN:NE2	2.32	0.62
2:H:361:MET:HE1	1:c:115:THR:OG1	2.00	0.62
2:L:57:GLN:CG	1:u:124:ARG:NH2	2.55	0.62
3:b:112:VAL:HG21	3:b:402:PHE:HE2	1.64	0.62
3:Z:276:LEU:O	3:Z:278:GLN:NE2	2.31	0.62
3:y:140:ASN:OD1	3:y:347:GLN:NE2	2.28	0.62
2:G:57:GLN:O	3:p:11:GLN:NE2	2.32	0.62
2:J:24:LYS:NZ	2:J:28:GLU:OE2	2.29	0.62
3:P:57:SER:HB3	3:P:325:GLN:HG3	1.82	0.62
3:b:98:GLU:HA	3:b:102:LEU:HB2	1.81	0.62
1:s:86:LEU:HD23	1:s:90:MET:HE2	1.80	0.62
2:C:362:GLU:OE2	1:w:108:ARG:NH2	2.32	0.62
2:G:618:PRO:O	2:G:622:LEU:HB2	1.99	0.62
3:b:27:LEU:HD13	3:b:128:MET:HE2	1.81	0.62
1:x:45:MET:HE1	1:x:55:ILE:HD11	1.80	0.62
2:E:60:LYS:O	1:w:146:TYR:OH	2.10	0.62
2:F:63:LYS:HZ2	1:z:135:ASN:HD21	1.47	0.62
2:F:336:ARG:NH1	1:w:145:TYR:OH	2.33	0.62
2:L:220:PHE:CA	3:Y:16:LYS:NZ	2.45	0.62
2:B:488:GLU:OE1	2:B:510:ARG:NH1	2.30	0.62
2:K:219:TRP:O	3:f:375:SER:C	2.41	0.62
3:Y:26:VAL:HG23	3:Y:27:LEU:HD12	1.82	0.62
2:A:48:THR:HG23	1:s:135:ASN:HA	1.81	0.62
3:y:166:ASN:OD1	3:y:356:ASN:ND2	2.33	0.62
2:C:618:PRO:O	2:C:622:LEU:HB2	2.00	0.61
2:K:346:ALA:HA	2:L:416:LEU:HD11	1.82	0.61
3:M:187:ALA:HB3	3:b:192:VAL:HG11	1.81	0.61
1:r:18:PHE:HD2	1:r:20:ILE:HG13	1.65	0.61
1:0:126:ARG:HD3	2:C:61:TYR:OH	2.01	0.61
2:H:346:ALA:HA	2:I:416:LEU:HD11	1.82	0.61
2:L:58:PHE:HE1	3:Y:11:GLN:HE22	1.46	0.61
2:E:346:ALA:HA	2:F:416:LEU:HD11	1.83	0.61
3:e:124:LEU:HG	3:e:128:MET:HE2	1.83	0.61
3:g:162:ASN:OD1	3:g:163:GLU:N	2.32	0.61
3:S:276:LEU:O	3:S:278:GLN:NE2	2.33	0.61
3:W:98:GLU:HA	3:W:102:LEU:HB2	1.81	0.61
3:g:247:PHE:HD1	3:g:316:VAL:HG12	1.64	0.61
3:Z:115:ARG:NH2	3:Z:119:ASP:OD1	2.33	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:u:51:ASN:HB3	1:u:52:PRO:HD3	1.82	0.61
1:0:141:THR:OG1	3:a:15:LYS:NZ	2.33	0.61
2:B:346:ALA:HA	2:C:416:LEU:HD11	1.83	0.61
3:i:276:LEU:O	3:i:278:GLN:NE2	2.34	0.61
3:p:49:SER:HB3	3:p:80:THR:HG22	1.83	0.61
2:A:388:ARG:CZ	1:r:107:GLN:HE22	2.11	0.61
2:I:57:GLN:CG	1:c:124:ARG:HH22	1.77	0.61
3:Z:51:LYS:NZ	3:t:104:GLN:OE1	2.33	0.61
3:q:369:LYS:NZ	3:q:373:ILE:O	2.34	0.61
1:0:129:PHE:HE2	2:B:350:ALA:CB	2.14	0.61
2:F:346:ALA:HA	2:G:416:LEU:HD11	1.83	0.61
2:H:222:ALA:CB	3:p:377:VAL:HG21	2.30	0.61
3:U:162:ASN:OD1	3:U:163:GLU:N	2.33	0.61
3:Z:86:TYR:HB3	3:Z:405:LEU:HD23	1.82	0.61
2:C:346:ALA:HA	2:D:416:LEU:HD11	1.82	0.60
3:N:81:GLY:HA3	3:N:409:VAL:HG22	1.83	0.60
2:C:63:LYS:HZ2	1:r:135:ASN:ND2	1.90	0.60
2:L:219:TRP:C	3:Y:16:LYS:HZ2	1.99	0.60
2:F:361:MET:HE1	1:m:115:THR:OG1	2.02	0.60
2:J:618:PRO:O	2:J:622:LEU:HB2	2.02	0.60
3:R:135:SER:HB3	3:R:294:THR:HG21	1.83	0.60
3:b:36:LEU:HD22	3:b:363:GLY:HA3	1.83	0.60
2:F:215:TRP:CZ2	1:w:139:VAL:N	2.69	0.60
3:o:173:TRP:NE1	3:y:158:ASP:OD2	2.34	0.60
1:z:51:ASN:HB3	1:z:52:PRO:HD3	1.82	0.60
2:A:416:LEU:HD11	2:L:346:ALA:HA	1.82	0.60
2:A:618:PRO:O	2:A:622:LEU:HB2	2.01	0.60
2:B:216:GLU:OE1	1:s:144:ARG:NH2	2.35	0.60
2:H:388:ARG:NH2	1:v:107:GLN:NE2	2.49	0.60
2:I:346:ALA:HA	2:J:416:LEU:HD11	1.82	0.60
3:Q:170:MET:HE1	3:Q:178:LEU:HD12	1.82	0.60
2:L:25:GLU:HG2	1:x:139:VAL:CG2	2.31	0.60
3:N:173:TRP:NE1	3:V:158:ASP:OD2	2.35	0.60
3:b:387:VAL:HG13	3:b:402:PHE:HE1	1.67	0.60
2:E:81:ARG:NH2	2:F:462:ASP:OD2	2.35	0.60
2:G:219:TRP:CB	3:b:34:GLN:NE2	2.57	0.60
3:T:61:THR:HG21	3:T:65:ASP:H	1.67	0.60
3:f:374:ASP:HB3	3:f:389:LYS:HE3	1.83	0.60
3:i:95:GLN:OE1	3:i:396:ASN:ND2	2.35	0.60
2:C:54:LEU:HG	1:r:124:ARG:CD	2.23	0.60
3:M:182:GLN:HE22	3:M:202:PRO:HD3	1.67	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:k:209:ARG:NH1	3:k:209:ARG:HB3	2.17	0.60
3:p:344:THR:HG22	3:p:345:ALA:H	1.66	0.60
2:E:58:PHE:HB2	3:e:96:LEU:O	2.01	0.59
2:I:63:LYS:HD2	1:c:135:ASN:OD1	2.01	0.59
2:J:376:LYS:CE	1:x:125:ARG:O	2.50	0.59
3:O:98:GLU:HA	3:O:102:LEU:HB2	1.83	0.59
3:V:112:VAL:HG23	3:V:113:ARG:HD3	1.84	0.59
3:d:51:LYS:HE2	3:q:17:PHE:HE1	1.67	0.59
3:g:98:GLU:HA	3:g:102:LEU:HB2	1.84	0.59
3:j:231:LYS:NZ	3:j:308:ASP:OD2	2.32	0.59
3:l:276:LEU:O	3:l:278:GLN:NE2	2.34	0.59
2:K:618:PRO:O	2:K:622:LEU:CB	2.50	0.59
1:s:100:PRO:HA	1:s:103:LEU:HD12	1.83	0.59
1:w:6:THR:HA	1:w:71:GLU:HA	1.83	0.59
2:B:81:ARG:NH2	2:C:462:ASP:OD2	2.35	0.59
2:C:59:GLU:OE1	1:r:125:ARG:HD3	2.03	0.59
2:F:24:LYS:NZ	2:F:28:GLU:OE2	2.28	0.59
3:o:25:LEU:HD22	3:o:121:GLU:HG2	1.84	0.59
3:e:111:PRO:HG2	3:j:56:PHE:HE2	1.67	0.59
3:U:143:ILE:HD11	3:U:174:SER:HB3	1.85	0.59
3:l:6:ASP:OD1	3:l:7:SER:N	2.35	0.59
2:G:49:ALA:HB2	1:m:140:PHE:CZ	2.37	0.59
3:o:365:ILE:HD11	3:o:405:LEU:HD23	1.85	0.59
1:w:157:ILE:HG23	1:w:158:PRO:HD3	1.83	0.59
2:B:215:TRP:CH2	1:s:138:ASP:OD1	2.55	0.59
3:e:57:SER:HB3	3:e:325:GLN:HB3	1.84	0.59
3:k:219:ARG:NH1	3:k:266:ASP:OD1	2.34	0.59
3:Z:81:GLY:HA3	3:Z:409:VAL:HG22	1.83	0.59
3:d:112:VAL:HG21	3:d:402:PHE:HE2	1.67	0.59
3:j:81:GLY:HA3	3:j:409:VAL:HG12	1.84	0.59
2:D:24:LYS:NZ	2:D:28:GLU:OE2	2.28	0.59
2:G:61:TYR:CE2	1:z:128:ASP:CG	2.80	0.59
2:L:24:LYS:NZ	2:L:28:GLU:OE2	2.28	0.59
3:f:241:VAL:HG21	3:f:316:VAL:HG21	1.85	0.59
2:C:24:LYS:NZ	2:C:28:GLU:OE2	2.28	0.59
2:K:7:LYS:HE2	3:q:34:GLN:NE2	2.18	0.59
2:K:81:ARG:NH2	2:L:462:ASP:OD2	2.35	0.59
2:K:370:HIS:HE1	1:s:120:VAL:HG21	1.67	0.59
3:O:187:ALA:HB3	3:f:192:VAL:HG11	1.85	0.59
3:W:369:LYS:NZ	3:W:373:ILE:O	2.36	0.59
3:a:49:SER:HB3	3:a:80:THR:HG22	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:k:276:LEU:O	3:k:278:GLN:NE2	2.36	0.59
3:T:412:ASN:HB3	3:T:415:MET:HE3	1.85	0.58
3:a:165:GLU:OE2	3:a:209:ARG:NH1	2.35	0.58
2:H:222:ALA:CB	3:p:377:VAL:CG2	2.79	0.58
2:L:618:PRO:O	2:L:622:LEU:HB2	2.03	0.58
2:E:62:PRO:HD3	1:w:125:ARG:HH21	1.65	0.58
3:Z:173:TRP:NE1	3:e:158:ASP:OD2	2.35	0.58
3:i:98:GLU:OE2	3:i:398:GLN:NE2	2.35	0.58
3:n:112:VAL:HG23	3:n:113:ARG:HD3	1.85	0.58
2:D:346:ALA:HA	2:E:416:LEU:HD11	1.85	0.58
2:K:220:PHE:C	3:f:376:ALA:HB1	2.27	0.58
3:Y:49:SER:HB3	3:Y:80:THR:HG22	1.85	0.58
2:F:618:PRO:O	2:F:622:LEU:HB2	2.03	0.58
2:G:346:ALA:HA	2:H:416:LEU:HD11	1.85	0.58
3:d:112:VAL:HG21	3:d:402:PHE:CE2	2.39	0.58
3:o:88:THR:OG1	3:o:403:ASP:OD1	2.20	0.58
2:H:81:ARG:NH2	2:I:462:ASP:OD2	2.35	0.58
2:K:636:LYS:NZ	2:L:637:ALA:O	2.31	0.58
3:U:166:ASN:OD1	3:U:356:ASN:ND2	2.37	0.58
1:c:50:ILE:HG13	1:c:51:ASN:N	2.19	0.58
2:D:362:GLU:HG2	1:w:114:MET:SD	2.43	0.58
3:Q:140:ASN:OD1	3:Q:344:THR:OG1	2.21	0.58
3:V:139:PRO:HB3	3:V:349:MET:HE1	1.86	0.58
1:r:51:ASN:HB3	1:r:52:PRO:HD3	1.86	0.58
3:y:369:LYS:NZ	3:y:373:ILE:O	2.37	0.58
2:A:336:ARG:HD2	1:u:130:PRO:HB3	1.85	0.58
2:L:58:PHE:CZ	3:Y:11:GLN:NE2	2.71	0.58
3:U:15:LYS:HE2	3:U:103:ASN:HD22	1.68	0.58
3:W:166:ASN:OD1	3:W:356:ASN:ND2	2.36	0.58
3:a:98:GLU:HG2	3:a:102:LEU:HD12	1.86	0.58
2:A:49:ALA:CB	1:u:151:PRO:HB2	2.33	0.58
2:G:81:ARG:NH2	2:H:462:ASP:OD2	2.37	0.58
2:J:346:ALA:HA	2:K:416:LEU:HD11	1.85	0.58
3:y:190:GLN:OE1	3:y:193:ARG:NH2	2.36	0.58
1:1:141:THR:HA	2:E:215:TRP:HE1	1.69	0.58
3:b:43:SER:HB3	1:z:147:PRO:HB3	1.86	0.58
3:e:59:LEU:CD1	3:e:66:ILE:HG22	2.34	0.58
3:j:189:ASP:OD1	3:j:190:GLN:N	2.37	0.58
3:y:98:GLU:HA	3:y:102:LEU:HB2	1.85	0.58
3:y:102:LEU:HD12	3:y:105:LEU:HD13	1.86	0.58
2:B:215:TRP:CH2	1:s:144:ARG:NH2	2.71	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:173:TRP:NE1	3:n:158:ASP:OD2	2.37	0.57
3:n:375:SER:OG	3:n:386:ARG:NH1	2.37	0.57
2:J:58:PHE:CG	3:q:96:LEU:HA	2.38	0.57
2:K:7:LYS:CE	3:q:34:GLN:NE2	2.66	0.57
3:e:25:LEU:HD21	3:e:117:VAL:HG11	1.85	0.57
3:j:193:ARG:NH2	3:o:190:GLN:OE1	2.37	0.57
1:l:51:ASN:HB3	1:l:52:PRO:HD3	1.86	0.57
3:T:187:ALA:HB3	3:X:192:VAL:HG21	1.85	0.57
2:A:346:ALA:HA	2:B:416:LEU:HD11	1.86	0.57
2:J:57:GLN:C	3:q:96:LEU:HD21	2.23	0.57
3:M:188:SER:HA	3:b:189:ASP:OD1	2.04	0.57
3:S:104:GLN:OE1	3:l:51:LYS:NZ	2.30	0.57
3:U:344:THR:HG22	3:U:345:ALA:H	1.68	0.57
3:t:51:LYS:NZ	3:y:104:GLN:OE1	2.33	0.57
3:O:189:ASP:OD1	3:O:190:GLN:N	2.37	0.57
1:m:51:ASN:HB3	1:m:52:PRO:HD3	1.86	0.57
1:l:126:ARG:NH1	2:E:344:MET:HG2	2.17	0.57
2:B:621:VAL:HA	2:B:624:GLN:HE21	1.70	0.57
2:D:99:GLU:HB3	2:D:510:ARG:HD2	1.87	0.57
2:G:53:LYS:HZ2	3:p:11:GLN:CG	2.17	0.57
2:G:99:GLU:HB3	2:G:510:ARG:HD2	1.87	0.57
3:Z:124:LEU:HD12	3:Z:362:LEU:HD13	1.87	0.57
2:G:628:VAL:HA	2:G:631:GLN:HG2	1.86	0.57
3:M:276:LEU:O	3:M:278:GLN:NE2	2.38	0.57
3:Q:233:GLN:HG3	3:Q:334:GLU:HA	1.85	0.57
3:S:162:ASN:ND2	3:W:22:MET:SD	2.74	0.57
3:k:144:THR:HG22	3:k:177:ARG:HD2	1.87	0.57
3:n:136:LEU:HD13	3:n:151:GLN:HG3	1.86	0.57
1:l:135:ASN:HD21	2:D:63:LYS:NZ	2.03	0.57
2:A:81:ARG:NH2	2:B:462:ASP:OD2	2.37	0.57
2:C:81:ARG:NH2	2:D:462:ASP:OD2	2.38	0.57
2:H:636:LYS:NZ	2:I:637:ALA:O	2.32	0.57
2:J:652:GLN:HG3	2:J:656:MET:HE2	1.86	0.57
3:y:360:CYS:SG	3:y:361:GLY:N	2.78	0.57
2:B:625:ALA:HB3	2:C:627:MET:HE2	1.86	0.57
2:K:215:TRP:CZ2	1:v:144:ARG:NH2	2.71	0.57
1:w:51:ASN:HB3	1:w:52:PRO:HD3	1.87	0.57
2:D:618:PRO:O	2:D:622:LEU:HB2	2.05	0.56
2:J:81:ARG:NH2	2:K:462:ASP:OD2	2.37	0.56
3:W:170:MET:HE3	3:W:212:MET:HE1	1.87	0.56
3:k:173:TRP:NE1	3:q:158:ASP:OD2	2.34	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:99:GLU:HB3	2:A:510:ARG:HD2	1.87	0.56
2:C:198:GLU:O	2:C:199:TYR:C	2.48	0.56
2:D:81:ARG:NH2	2:E:462:ASP:OD2	2.37	0.56
2:D:220:PHE:C	3:j:377:VAL:HG21	2.30	0.56
2:H:222:ALA:HB3	3:p:377:VAL:HG21	1.87	0.56
3:T:203:THR:HG22	3:T:209:ARG:HH12	1.71	0.56
3:Z:219:ARG:NH1	3:Z:266:ASP:OD1	2.38	0.56
1:z:32:GLN:NE2	1:z:35:GLU:OE2	2.38	0.56
2:I:57:GLN:CB	1:c:124:ARG:NH2	2.52	0.56
3:Z:95:GLN:OE1	3:Z:396:ASN:ND2	2.39	0.56
3:n:144:THR:HG22	3:n:177:ARG:HD2	1.88	0.56
1:1:36:ASP:HA	1:1:39:ASN:HD22	1.70	0.56
2:A:58:PHE:CZ	1:u:150:LEU:C	2.83	0.56
2:I:618:PRO:O	2:I:622:LEU:HB2	2.05	0.56
3:R:61:THR:HG21	3:R:65:ASP:H	1.68	0.56
3:Z:369:LYS:NZ	3:Z:373:ILE:O	2.31	0.56
3:o:182:GLN:HE22	3:o:202:PRO:HD3	1.71	0.56
2:I:344:MET:HE3	1:h:126:ARG:HH11	1.71	0.56
3:N:124:LEU:HD23	3:N:128:MET:HE2	1.86	0.56
3:O:96:LEU:O	3:O:100:ILE:HG12	2.06	0.56
3:Q:111:PRO:HG2	3:i:56:PHE:HE2	1.71	0.56
3:y:189:ASP:OD1	3:y:190:GLN:N	2.39	0.56
2:F:350:ALA:CB	1:z:129:PHE:HE2	2.18	0.56
2:G:63:LYS:NZ	1:m:135:ASN:ND2	2.50	0.56
2:H:215:TRP:CE2	1:m:144:ARG:NH2	2.73	0.56
3:R:140:ASN:OD1	3:R:344:THR:OG1	2.23	0.56
3:Z:229:THR:HG22	3:Z:338:ALA:HA	1.86	0.56
2:I:81:ARG:NH2	2:J:462:ASP:OD2	2.38	0.56
3:l:95:GLN:OE1	3:l:396:ASN:ND2	2.39	0.56
2:F:81:ARG:NH2	2:G:462:ASP:OD2	2.38	0.56
2:G:209:VAL:CG2	3:b:382:GLY:CA	2.72	0.56
3:Z:187:ALA:HB3	3:t:192:VAL:HG21	1.87	0.56
3:b:58:SER:OG	3:p:119:ASP:OD2	2.21	0.56
3:Q:187:ALA:HB3	3:U:192:VAL:HG21	1.86	0.56
2:H:361:MET:HE1	1:c:115:THR:HG1	1.71	0.55
3:Z:158:ASP:OD2	3:t:173:TRP:NE1	2.39	0.55
3:n:276:LEU:O	3:n:278:GLN:NE2	2.38	0.55
3:g:372:SER:OG	1:u:154:ASP:OD2	2.24	0.55
3:o:180:ASP:O	3:o:183:THR:OG1	2.24	0.55
3:M:129:MET:HE3	3:M:351:PRO:HG2	1.86	0.55
3:M:180:ASP:O	3:M:183:THR:OG1	2.25	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:273:THR:HG22	3:Q:329:VAL:HG22	1.88	0.55
3:R:173:TRP:NE1	3:k:158:ASP:OD2	2.39	0.55
3:e:153:ALA:HB2	3:e:208:ILE:HB	1.88	0.55
2:A:462:ASP:OD2	2:L:81:ARG:NH2	2.38	0.55
3:U:375:SER:OG	3:U:386:ARG:NH1	2.40	0.55
3:o:360:CYS:SG	3:o:361:GLY:N	2.80	0.55
2:A:47:ALA:H	1:u:144:ARG:NH2	2.04	0.55
2:B:599:GLU:HG2	2:B:600:LYS:N	2.22	0.55
3:P:96:LEU:O	3:P:100:ILE:HG12	2.07	0.55
3:Y:273:THR:HG21	3:Y:333:VAL:HG22	1.87	0.55
3:e:49:SER:HB3	3:e:80:THR:HG22	1.88	0.55
2:E:58:PHE:CB	3:e:96:LEU:O	2.55	0.55
2:K:599:GLU:HG2	2:K:600:LYS:N	2.22	0.55
3:i:369:LYS:NZ	3:i:373:ILE:O	2.36	0.55
2:E:365:ARG:CZ	1:z:117:THR:OG1	2.54	0.55
2:F:63:LYS:C	1:z:132:GLY:HA3	2.32	0.55
2:I:599:GLU:HG2	2:I:600:LYS:N	2.22	0.55
3:R:187:ALA:HB3	3:V:192:VAL:HG21	1.89	0.55
3:R:193:ARG:NH2	3:k:190:GLN:OE1	2.38	0.55
3:S:61:THR:HG21	3:S:65:ASP:H	1.72	0.55
3:g:123:GLU:OE2	3:g:408:TYR:OH	2.21	0.55
1:O:144:ARG:HH12	2:C:45:GLU:HA	1.69	0.55
1:l:77:LYS:HD3	1:r:50:ILE:HD11	1.87	0.55
2:E:57:GLN:CD	3:e:396:ASN:ND2	2.63	0.55
2:L:599:GLU:HG2	2:L:600:LYS:N	2.22	0.55
3:Q:128:MET:HE3	3:Q:353:LEU:HD22	1.88	0.55
3:t:27:LEU:HD22	3:t:128:MET:HE1	1.88	0.55
2:B:29:LYS:HZ1	1:s:133:GLN:HE21	1.55	0.55
2:K:63:LYS:HD2	1:x:135:ASN:OD1	2.07	0.55
2:L:45:GLU:HB3	1:x:144:ARG:HH22	1.72	0.55
2:L:351:GLN:HE21	1:u:123:MET:CE	2.20	0.55
3:T:104:GLN:OE1	3:n:51:LYS:NZ	2.33	0.55
3:k:209:ARG:HB3	3:k:209:ARG:HH11	1.72	0.55
1:l:118:LEU:HD12	2:C:361:MET:CG	2.37	0.54
2:I:218:ASN:CG	1:c:140:PHE:CE1	2.83	0.54
2:J:58:PHE:HB2	3:q:96:LEU:CA	1.99	0.54
2:L:57:GLN:CG	1:u:124:ARG:HH21	2.16	0.54
1:h:51:ASN:HB3	1:h:52:PRO:HD3	1.87	0.54
3:o:96:LEU:O	3:o:100:ILE:HG12	2.07	0.54
2:F:48:THR:HG22	3:b:371:HIS:HE1	1.72	0.54
3:M:27:LEU:HD22	3:M:128:MET:HE1	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:276:LEU:O	3:O:278:GLN:NE2	2.40	0.54
3:Y:162:ASN:ND2	3:l:22:MET:SD	2.66	0.54
3:j:25:LEU:HD13	3:j:121:GLU:OE1	2.07	0.54
1:l:141:THR:HA	2:E:215:TRP:NE1	2.22	0.54
2:B:207:LEU:HD11	3:g:379:THR:HG21	1.88	0.54
2:D:599:GLU:HG2	2:D:600:LYS:N	2.22	0.54
2:J:57:GLN:C	3:q:96:LEU:CD2	2.53	0.54
2:L:376:LYS:CE	1:s:125:ARG:O	2.53	0.54
3:Y:104:GLN:NE2	1:u:140:PHE:HB3	2.22	0.54
3:a:219:ARG:NH1	3:a:221:GLN:OE1	2.41	0.54
2:E:599:GLU:HG2	2:E:600:LYS:N	2.22	0.54
2:G:24:LYS:NZ	2:G:28:GLU:OE2	2.28	0.54
2:G:599:GLU:HG2	2:G:600:LYS:N	2.22	0.54
3:N:96:LEU:O	3:N:100:ILE:HG12	2.07	0.54
3:P:98:GLU:HA	3:P:102:LEU:HB2	1.89	0.54
3:t:233:GLN:OE1	3:t:332:GLN:NE2	2.41	0.54
2:G:350:ALA:HB2	1:m:129:PHE:HE2	1.73	0.54
3:Q:344:THR:HB	3:Q:347:GLN:HG2	1.87	0.54
3:Y:104:GLN:OE1	1:u:141:THR:OG1	2.25	0.54
3:p:59:LEU:HD13	3:p:66:ILE:HD12	1.82	0.54
3:y:231:LYS:HB3	3:y:250:THR:HG23	1.89	0.54
2:A:599:GLU:HG2	2:A:600:LYS:N	2.22	0.54
2:I:57:GLN:HG3	1:c:124:ARG:HH21	0.74	0.54
3:Z:60:ARG:NE	3:t:86:TYR:O	2.34	0.54
3:f:189:ASP:OD1	3:f:190:GLN:N	2.40	0.54
3:j:250:THR:OG1	3:j:308:ASP:OD1	2.25	0.54
2:C:63:LYS:HD2	1:r:135:ASN:ND2	2.23	0.54
2:K:58:PHE:CE1	1:v:150:LEU:HD13	2.43	0.54
2:L:368:GLU:CD	1:s:119:VAL:HG21	2.33	0.54
3:Z:136:LEU:HD13	3:Z:151:GLN:HG3	1.89	0.54
3:d:344:THR:HB	3:d:347:GLN:HB2	1.90	0.54
1:m:142:SER:HB3	3:p:103:ASN:HB2	1.90	0.54
3:n:393:GLY:O	3:o:401:ARG:NH1	2.41	0.54
2:A:49:ALA:CB	1:u:151:PRO:CB	2.86	0.54
2:B:95:GLU:H	2:B:95:GLU:CD	2.15	0.54
2:H:365:ARG:HG2	1:c:114:MET:HE1	1.89	0.54
2:L:204:PRO:HB3	3:f:209:ARG:NH2	2.22	0.54
3:Y:14:LEU:HG	3:Y:16:LYS:H	1.72	0.54
3:p:95:GLN:HG2	3:p:96:LEU:HD22	1.89	0.54
2:D:383:PRO:HG3	1:z:118:LEU:HD21	1.89	0.54
2:F:599:GLU:HG2	2:F:600:LYS:N	2.22	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:104:GLN:OE1	3:k:51:LYS:NZ	2.37	0.54
1:w:151:PRO:HB2	1:w:153:ILE:HG12	1.89	0.54
1:O:124:ARG:HH21	2:B:59:GLU:HG3	1.72	0.54
2:A:50:ALA:HA	1:u:149:ASP:CB	2.28	0.54
2:F:63:LYS:NZ	1:z:135:ASN:ND2	2.56	0.54
2:H:599:GLU:HG2	2:H:600:LYS:N	2.22	0.54
2:H:618:PRO:O	2:H:622:LEU:CB	2.50	0.54
3:M:189:ASP:OD1	3:M:190:GLN:N	2.41	0.54
3:Y:89:VAL:HG12	3:Y:116:ILE:HD11	1.89	0.54
3:a:34:GLN:HG3	3:a:35:LEU:HD12	1.89	0.54
2:A:351:GLN:HE21	1:s:123:MET:CE	2.21	0.53
3:P:247:PHE:HD1	3:P:316:VAL:HG12	1.72	0.53
3:f:41:ASN:ND2	1:x:143:ASP:OD1	2.41	0.53
3:p:86:TYR:HB3	3:p:88:THR:HG23	1.90	0.53
2:C:55:ASP:CB	1:r:124:ARG:NH2	2.47	0.53
2:C:599:GLU:HG2	2:C:600:LYS:N	2.22	0.53
2:H:57:GLN:NE2	1:h:150:LEU:CD1	2.67	0.53
3:M:98:GLU:HA	3:M:102:LEU:HB2	1.90	0.53
3:N:27:LEU:HD13	3:N:128:MET:HE1	1.89	0.53
3:o:189:ASP:N	3:o:189:ASP:OD1	2.42	0.53
1:x:51:ASN:HB3	1:x:52:PRO:HD3	1.88	0.53
2:J:599:GLU:HG2	2:J:600:LYS:N	2.22	0.53
3:o:57:SER:HB3	3:o:325:GLN:HG3	1.90	0.53
3:o:102:LEU:HD13	3:o:105:LEU:HD13	1.90	0.53
3:R:192:VAL:HG21	3:k:187:ALA:HB3	1.90	0.53
3:b:112:VAL:HG21	3:b:402:PHE:CE2	2.42	0.53
3:o:123:GLU:OE1	3:y:60:ARG:NH1	2.39	0.53
2:E:54:LEU:HD21	1:w:124:ARG:HD2	1.89	0.53
1:l:24:ALA:HB2	1:r:32:GLN:HG2	1.91	0.53
2:D:222:ALA:CB	3:j:379:THR:N	2.60	0.53
2:E:95:GLU:H	2:E:95:GLU:CD	2.15	0.53
3:N:27:LEU:HB2	3:N:121:GLU:OE2	2.09	0.53
3:P:60:ARG:HH11	3:g:85:ASN:HB2	1.74	0.53
3:U:231:LYS:HG2	3:U:232:THR:HG23	1.90	0.53
3:W:344:THR:HG22	3:W:345:ALA:H	1.72	0.53
3:l:98:GLU:OE2	3:l:398:GLN:NE2	2.35	0.53
2:A:120:ALA:HA	2:A:159:PRO:HB3	1.91	0.53
2:D:222:ALA:CB	3:j:377:VAL:O	2.57	0.53
2:D:222:ALA:HB2	3:j:378:ALA:C	2.23	0.53
2:G:61:TYR:HD2	1:z:128:ASP:OD1	1.86	0.53
3:O:26:VAL:HG21	3:O:213:SER:HB2	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:231:LYS:HB3	3:P:250:THR:HG23	1.90	0.53
3:X:102:LEU:HD12	3:X:105:LEU:HD13	1.89	0.53
3:p:161:VAL:HG11	3:p:415:MET:HG2	1.89	0.53
3:y:375:SER:OG	3:y:386:ARG:NH1	2.42	0.53
1:0:7:LYS:HD2	1:0:70:ASP:HB2	1.91	0.53
2:B:636:LYS:NZ	2:C:637:ALA:O	2.33	0.53
2:G:350:ALA:CB	1:m:129:PHE:CE2	2.86	0.53
3:X:98:GLU:HA	3:X:102:LEU:HB2	1.91	0.53
3:Y:412:ASN:HB3	3:Y:415:MET:HE2	1.90	0.53
3:a:111:PRO:HG2	3:g:56:PHE:HE2	1.74	0.53
3:l:245:TYR:HD2	3:l:413:PRO:HD2	1.74	0.53
2:G:53:LYS:HZ2	3:p:11:GLN:HG3	1.68	0.53
3:o:331:ARG:NH1	3:o:337:ASP:OD2	2.33	0.53
2:E:486:GLU:HB3	2:E:510:ARG:HD2	1.91	0.53
2:E:636:LYS:NZ	2:F:637:ALA:O	2.32	0.53
2:G:63:LYS:HZ2	1:m:135:ASN:ND2	2.00	0.53
3:P:365:ILE:HD11	3:P:405:LEU:HD23	1.91	0.53
3:Y:158:ASP:OD2	3:l:173:TRP:NE1	2.42	0.53
2:I:376:LYS:NZ	1:v:124:ARG:O	2.41	0.52
3:P:401:ARG:NH2	3:l:396:ASN:OD1	2.41	0.52
3:n:180:ASP:O	3:n:183:THR:OG1	2.27	0.52
1:r:45:MET:HE1	1:r:55:ILE:HD11	1.90	0.52
1:l:141:THR:CA	2:E:215:TRP:HE1	2.22	0.52
2:F:49:ALA:HB1	3:b:371:HIS:CG	2.41	0.52
2:G:41:GLY:C	1:m:136:LYS:HZ2	2.02	0.52
2:H:54:LEU:HD23	2:H:59:GLU:HB2	1.92	0.52
2:I:54:LEU:HD23	2:I:59:GLU:HB2	1.92	0.52
3:O:372:SER:OG	3:k:374:ASP:OD1	2.23	0.52
3:l:36:LEU:HD22	3:l:363:GLY:HA3	1.90	0.52
3:y:112:VAL:HG23	3:y:113:ARG:HD3	1.91	0.52
1:0:108:ARG:NH2	2:L:362:GLU:OE2	2.40	0.52
2:F:209:VAL:HG21	3:e:377:VAL:HG21	1.91	0.52
2:H:76:ILE:HG12	2:H:457:SER:HB3	1.91	0.52
2:J:365:ARG:NH1	1:x:114:MET:HE1	2.23	0.52
3:S:231:LYS:NZ	3:S:308:ASP:OD2	2.29	0.52
3:V:166:ASN:OD1	3:V:356:ASN:ND2	2.42	0.52
3:Z:98:GLU:OE2	3:Z:398:GLN:NE2	2.41	0.52
1:h:138:ASP:OD1	1:h:139:VAL:N	2.43	0.52
3:y:23:SER:OG	3:y:24:ASP:N	2.41	0.52
2:A:58:PHE:CZ	1:u:149:ASP:O	2.63	0.52
2:H:19:ALA:HA	2:H:171:PRO:HG3	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:318:ILE:HB	2:J:323:ARG:HE	1.75	0.52
2:L:628:VAL:HA	2:L:631:GLN:HG2	1.92	0.52
3:M:128:MET:HE3	3:M:353:LEU:HD13	1.91	0.52
1:h:31:PRO:HA	1:h:34:ILE:HD12	1.90	0.52
2:A:60:LYS:O	1:s:146:TYR:OH	2.21	0.52
2:E:24:LYS:NZ	2:E:28:GLU:OE2	2.31	0.52
2:K:95:GLU:CD	2:K:95:GLU:H	2.16	0.52
3:Y:25:LEU:HD11	3:Y:117:VAL:HG11	1.92	0.52
1:u:22:SER:OG	1:u:23:ASN:N	2.42	0.52
2:B:318:ILE:HB	2:B:323:ARG:HE	1.75	0.52
2:F:49:ALA:HB2	3:b:371:HIS:HB3	1.83	0.52
2:H:486:GLU:HB3	2:H:510:ARG:HD2	1.91	0.52
2:K:551:LEU:HD11	2:K:561:ARG:HG3	1.92	0.52
2:F:318:ILE:HB	2:F:323:ARG:HE	1.75	0.52
2:J:54:LEU:HD23	2:J:59:GLU:HB2	1.92	0.52
2:K:54:LEU:HD23	2:K:59:GLU:HB2	1.92	0.52
3:U:15:LYS:HE2	3:U:103:ASN:ND2	2.25	0.52
3:W:331:ARG:NH2	3:W:334:GLU:OE1	2.43	0.52
3:Y:115:ARG:NH2	3:f:279:GLN:O	2.40	0.52
2:D:120:ALA:HA	2:D:159:PRO:HB3	1.91	0.52
2:F:54:LEU:HD23	2:F:59:GLU:HB2	1.92	0.52
2:G:54:LEU:HD23	2:G:59:GLU:HB2	1.92	0.52
2:G:120:ALA:HA	2:G:159:PRO:HB3	1.91	0.52
2:A:318:ILE:HB	2:A:323:ARG:HE	1.74	0.52
2:H:318:ILE:HB	2:H:323:ARG:HE	1.75	0.52
3:O:375:SER:OG	3:O:386:ARG:NH1	2.43	0.52
3:W:124:LEU:HD12	3:W:362:LEU:HD13	1.92	0.52
3:Y:25:LEU:HD11	3:Y:117:VAL:CG1	2.40	0.52
3:Y:129:MET:HB2	3:Y:418:GLN:HE21	1.74	0.52
1:m:78:TYR:OH	1:m:116:ASP:OD2	2.23	0.52
2:E:54:LEU:HD23	2:E:59:GLU:HB2	1.92	0.52
2:E:58:PHE:CD2	3:e:100:ILE:HA	2.45	0.52
2:E:76:ILE:HG12	2:E:457:SER:HB3	1.92	0.52
2:I:318:ILE:HB	2:I:323:ARG:HE	1.75	0.52
2:J:120:ALA:HA	2:J:159:PRO:HB3	1.91	0.52
2:L:318:ILE:HB	2:L:323:ARG:HE	1.75	0.52
3:V:344:THR:HG22	3:V:345:ALA:H	1.75	0.52
1:z:48:TRP:HZ2	1:z:85:GLN:HG3	1.75	0.52
1:1:34:ILE:O	1:1:38:VAL:HG23	2.10	0.51
2:D:318:ILE:HB	2:D:323:ARG:HE	1.75	0.51
2:E:318:ILE:HB	2:E:323:ARG:HE	1.75	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:61:TYR:CE2	1:z:128:ASP:OD1	2.64	0.51
3:T:304:ASP:OD1	3:T:305:SER:N	2.43	0.51
3:U:140:ASN:OD1	3:U:347:GLN:NE2	2.42	0.51
3:X:166:ASN:OD1	3:X:356:ASN:ND2	2.42	0.51
3:d:344:THR:HG22	3:d:345:ALA:H	1.75	0.51
1:1:118:LEU:HD13	2:C:361:MET:SD	2.49	0.51
1:1:135:ASN:HD21	2:D:63:LYS:HZ3	1.58	0.51
2:F:628:VAL:HA	2:F:631:GLN:HG2	1.92	0.51
2:G:41:GLY:HA3	1:m:136:LYS:HE3	1.92	0.51
2:G:318:ILE:HB	2:G:323:ARG:HE	1.75	0.51
2:H:551:LEU:HD11	2:H:561:ARG:HG3	1.92	0.51
3:O:401:ARG:NH1	3:k:396:ASN:OD1	2.42	0.51
3:Y:200:GLN:NE2	3:Y:201:ILE:O	2.42	0.51
1:h:41:LEU:HD12	1:h:86:LEU:HD22	1.91	0.51
3:n:219:ARG:NH1	3:n:266:ASP:OD1	2.43	0.51
2:C:76:ILE:HG12	2:C:457:SER:HB3	1.90	0.51
2:F:347:ASP:HB2	1:z:125:ARG:HH12	1.75	0.51
2:H:215:TRP:CE3	1:m:144:ARG:NH2	2.76	0.51
2:L:54:LEU:HD23	2:L:59:GLU:HB2	1.92	0.51
3:i:86:TYR:OH	3:p:64:GLY:N	2.44	0.51
3:p:267:GLN:NE2	3:p:418:GLN:OE1	2.42	0.51
3:q:189:ASP:OD1	3:q:190:GLN:N	2.43	0.51
3:t:52:ARG:HH21	3:t:79:ALA:HB2	1.75	0.51
3:t:61:THR:HG21	3:t:65:ASP:H	1.76	0.51
3:t:98:GLU:OE1	3:t:398:GLN:NE2	2.43	0.51
2:A:48:THR:HG21	1:s:140:PHE:CD2	2.46	0.51
2:E:19:ALA:HA	2:E:171:PRO:HG3	1.92	0.51
2:I:372:GLU:O	1:v:123:MET:HG2	2.10	0.51
3:S:187:ALA:HB3	3:W:192:VAL:HG21	1.91	0.51
2:B:551:LEU:HD11	2:B:561:ARG:HG3	1.92	0.51
2:D:54:LEU:HD23	2:D:59:GLU:HB2	1.92	0.51
2:G:219:TRP:C	3:b:34:GLN:HE21	2.18	0.51
2:H:336:ARG:NH1	1:m:145:TYR:OH	2.43	0.51
3:S:158:ASP:OD2	3:W:173:TRP:NE1	2.44	0.51
3:o:23:SER:OG	3:o:24:ASP:N	2.44	0.51
2:C:636:LYS:NZ	2:D:637:ALA:O	2.34	0.51
3:k:102:LEU:HD22	3:k:105:LEU:HD13	1.93	0.51
3:p:219:ARG:NH1	3:p:221:GLN:OE1	2.42	0.51
2:A:58:PHE:CZ	1:u:151:PRO:HA	2.46	0.51
2:B:486:GLU:HB3	2:B:510:ARG:HD2	1.91	0.51
2:C:640:GLU:HA	2:D:645:GLN:HE21	1.76	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:362:GLU:HG3	1:w:114:MET:CE	2.38	0.51
2:F:640:GLU:HA	2:G:645:GLN:HE21	1.76	0.51
2:I:344:MET:HE3	1:h:126:ARG:HH12	1.73	0.51
2:K:618:PRO:HA	2:K:621:VAL:HG12	1.93	0.51
3:V:231:LYS:HB3	3:V:250:THR:HG23	1.92	0.51
3:X:367:LEU:HD21	3:X:405:LEU:HD12	1.92	0.51
3:b:391:ALA:HB2	3:b:398:GLN:HG3	1.92	0.51
3:d:286:ASN:HB2	3:d:291:ILE:HD11	1.93	0.51
1:s:48:TRP:HZ2	1:s:85:GLN:HG3	1.75	0.51
2:A:54:LEU:HD23	2:A:59:GLU:HB2	1.92	0.51
2:C:246:PRO:HA	2:C:250:GLU:HB3	1.92	0.51
2:H:60:LYS:O	1:h:146:TYR:OH	2.21	0.51
2:I:628:VAL:HA	2:I:631:GLN:HG2	1.92	0.51
3:P:360:CYS:SG	3:P:361:GLY:N	2.83	0.51
3:X:241:VAL:HG11	3:X:316:VAL:HG21	1.92	0.51
1:l:126:ARG:HH12	2:E:344:MET:CG	2.20	0.51
2:B:470:ARG:NH1	2:B:473:GLU:OE1	2.43	0.51
2:B:618:PRO:HA	2:B:621:VAL:HG12	1.93	0.51
2:C:54:LEU:HD23	2:C:59:GLU:HB2	1.92	0.51
2:C:318:ILE:HB	2:C:323:ARG:HE	1.75	0.51
2:L:657:GLU:HG2	2:L:661:ASN:HD21	1.76	0.51
3:T:96:LEU:O	3:T:100:ILE:HG12	2.10	0.51
2:B:76:ILE:HG12	2:B:457:SER:HB3	1.92	0.51
2:B:336:ARG:NH1	1:s:145:TYR:OH	2.44	0.51
2:L:246:PRO:HA	2:L:250:GLU:HB3	1.92	0.51
3:o:316:VAL:HG13	3:o:318:ILE:HG13	1.93	0.51
3:q:49:SER:HB3	3:q:80:THR:HG22	1.92	0.51
2:B:54:LEU:HD23	2:B:59:GLU:HB2	1.92	0.50
2:D:76:ILE:HG12	2:D:457:SER:HB3	1.92	0.50
2:D:222:ALA:HB2	3:j:377:VAL:O	2.10	0.50
2:J:47:ALA:HB2	1:c:145:TYR:CD2	2.45	0.50
2:K:318:ILE:HB	2:K:323:ARG:HE	1.75	0.50
2:L:152:ARG:HH11	2:L:152:ARG:HG3	1.77	0.50
3:U:129:MET:HB2	3:U:418:GLN:HE21	1.77	0.50
3:k:201:ILE:HG12	3:k:212:MET:HE2	1.93	0.50
1:l:86:LEU:O	1:l:90:MET:HG3	2.10	0.50
2:A:636:LYS:NZ	2:B:637:ALA:O	2.37	0.50
2:E:47:ALA:O	2:E:63:LYS:HE2	2.12	0.50
2:G:376:LYS:CE	1:h:125:ARG:O	2.55	0.50
3:O:60:ARG:NH2	3:f:123:GLU:OE1	2.41	0.50
3:P:162:ASN:OD1	3:P:163:GLU:N	2.44	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:V:190:GLN:OE1	3:V:193:ARG:NH1	2.45	0.50
3:b:385:ILE:HG12	3:b:404:LEU:HD12	1.93	0.50
3:d:412:ASN:HD22	3:d:415:MET:HE3	1.77	0.50
3:i:27:LEU:HB2	3:i:121:GLU:OE2	2.11	0.50
3:l:144:THR:HG22	3:l:177:ARG:HD2	1.93	0.50
3:y:344:THR:HG22	3:y:345:ALA:H	1.76	0.50
2:A:333:ASP:OD2	1:u:133:GLN:HG3	2.12	0.50
2:B:120:ALA:HA	2:B:159:PRO:HB3	1.93	0.50
2:B:209:VAL:CG2	3:g:379:THR:N	2.73	0.50
2:E:470:ARG:NH1	2:E:473:GLU:OE1	2.43	0.50
2:K:668:GLN:OE1	2:L:670:ARG:NH1	2.42	0.50
3:Q:192:VAL:HG21	3:i:187:ALA:HB3	1.93	0.50
3:a:158:ASP:OD2	3:n:173:TRP:NE1	2.42	0.50
3:e:10:SER:N	3:j:47:SER:HG	2.09	0.50
3:i:136:LEU:HD13	3:i:151:GLN:HG3	1.93	0.50
1:u:24:ALA:HB2	1:x:32:GLN:HG2	1.94	0.50
2:B:47:ALA:O	2:B:63:LYS:HE2	2.12	0.50
2:E:120:ALA:HA	2:E:159:PRO:HB3	1.93	0.50
2:H:120:ALA:HA	2:H:159:PRO:HB3	1.93	0.50
2:A:152:ARG:HH11	2:A:152:ARG:HG3	1.76	0.50
2:C:95:GLU:CD	2:C:95:GLU:H	2.19	0.50
2:C:628:VAL:HA	2:C:631:GLN:HG2	1.93	0.50
2:D:152:ARG:HH11	2:D:152:ARG:HG3	1.77	0.50
2:E:152:ARG:HH11	2:E:152:ARG:HG3	1.76	0.50
3:P:51:LYS:NZ	3:l:8:ASN:OD1	2.33	0.50
3:b:182:GLN:OE1	3:p:196:TRP:NE1	2.40	0.50
3:n:8:ASN:OD1	3:o:51:LYS:NZ	2.33	0.50
2:B:25:GLU:CG	1:s:139:VAL:CG1	2.87	0.50
2:C:152:ARG:HG3	2:C:152:ARG:HH11	1.77	0.50
2:F:76:ILE:HG12	2:F:457:SER:HB3	1.93	0.50
2:H:618:PRO:HA	2:H:621:VAL:HG12	1.92	0.50
3:N:372:SER:OG	3:i:374:ASP:OD1	2.29	0.50
3:j:216:LEU:O	3:j:350:LYS:NZ	2.43	0.50
3:k:136:LEU:HD13	3:k:151:GLN:HG3	1.94	0.50
3:l:180:ASP:O	3:l:183:THR:OG1	2.30	0.50
3:l:247:PHE:HD1	3:l:316:VAL:HG12	1.77	0.50
3:y:374:ASP:N	3:y:374:ASP:OD1	2.42	0.50
2:A:49:ALA:HB1	1:u:151:PRO:HB3	1.94	0.50
2:A:76:ILE:HG12	2:A:457:SER:HB3	1.94	0.50
2:B:19:ALA:HA	2:B:171:PRO:HG3	1.93	0.50
2:C:657:GLU:HG2	2:C:661:ASN:HD21	1.76	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:57:GLN:HE22	3:e:396:ASN:ND2	1.84	0.50
2:E:211:SER:OG	3:j:34:GLN:HB2	2.11	0.50
2:I:57:GLN:CD	1:c:124:ARG:HH22	2.19	0.50
2:K:19:ALA:HA	2:K:171:PRO:HG3	1.93	0.50
2:K:657:GLU:HG2	2:K:661:ASN:HD21	1.77	0.50
3:S:27:LEU:HD22	3:S:128:MET:HE1	1.94	0.50
3:Z:279:GLN:O	3:t:115:ARG:NH1	2.45	0.50
3:t:98:GLU:HA	3:t:102:LEU:HB2	1.93	0.50
2:I:640:GLU:HA	2:J:645:GLN:HE21	1.75	0.50
2:J:152:ARG:HH11	2:J:152:ARG:HG3	1.77	0.50
2:L:76:ILE:HG12	2:L:457:SER:HB3	1.93	0.50
1:c:47:GLU:O	1:c:50:ILE:HG12	2.12	0.50
2:A:204:PRO:CD	3:Y:38:GLY:CA	2.75	0.50
2:H:59:GLU:OE1	1:h:125:ARG:HG3	2.10	0.50
2:H:388:ARG:CZ	1:v:107:GLN:HE21	2.18	0.50
3:W:374:ASP:OD1	3:W:374:ASP:N	2.45	0.50
3:t:187:ALA:HB3	3:y:192:VAL:HG21	1.93	0.50
2:A:645:GLN:HE21	2:L:640:GLU:HA	1.76	0.49
2:G:350:ALA:HB3	1:m:129:PHE:HE2	1.75	0.49
2:H:488:GLU:HB3	2:H:510:ARG:HH21	1.77	0.49
2:K:120:ALA:HA	2:K:159:PRO:HB3	1.93	0.49
3:U:165:GLU:OE2	3:U:167:TYR:OH	2.24	0.49
3:g:344:THR:HB	3:g:347:GLN:HB2	1.94	0.49
3:p:389:LYS:HG2	3:p:400:MET:HE3	1.93	0.49
3:q:320:ASP:OD2	3:q:323:ASN:ND2	2.45	0.49
3:t:96:LEU:O	3:t:100:ILE:HG12	2.12	0.49
2:B:152:ARG:HH11	2:B:152:ARG:HG3	1.77	0.49
2:B:618:PRO:O	2:B:622:LEU:CB	2.57	0.49
2:D:206:SER:OG	3:j:106:GLU:OE2	2.29	0.49
2:E:551:LEU:HD11	2:E:561:ARG:HG3	1.94	0.49
2:G:54:LEU:HD12	1:m:122:SER:OG	2.11	0.49
2:G:152:ARG:HH11	2:G:152:ARG:HG3	1.76	0.49
2:I:370:HIS:CE1	1:x:120:VAL:HG21	2.47	0.49
3:P:139:PRO:HG2	3:P:343:GLY:HA2	1.94	0.49
2:A:628:VAL:HA	2:A:631:GLN:HG2	1.94	0.49
2:F:246:PRO:HA	2:F:250:GLU:HB3	1.93	0.49
2:F:657:GLU:HG2	2:F:661:ASN:HD21	1.76	0.49
2:K:47:ALA:O	2:K:63:LYS:HE2	2.12	0.49
3:M:96:LEU:O	3:M:100:ILE:HG12	2.11	0.49
3:N:231:LYS:HG2	3:N:232:THR:HG23	1.93	0.49
3:O:192:VAL:HG21	3:W:187:ALA:HB3	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:96:LEU:O	3:S:100:ILE:HG12	2.12	0.49
2:E:57:GLN:C	3:e:96:LEU:HB3	2.37	0.49
2:F:152:ARG:HG3	2:F:152:ARG:HH11	1.77	0.49
2:H:152:ARG:HH11	2:H:152:ARG:HG3	1.76	0.49
3:O:23:SER:OG	3:O:24:ASP:N	2.44	0.49
3:O:216:LEU:HD11	3:O:353:LEU:HD12	1.93	0.49
3:a:123:GLU:CD	3:g:60:ARG:HH22	2.19	0.49
1:h:17:LYS:O	1:m:92:SER:OG	2.24	0.49
3:y:182:GLN:HE21	3:y:195:ALA:HB2	1.78	0.49
1:1:126:ARG:NH1	2:E:344:MET:CG	2.76	0.49
2:H:599:GLU:HG2	2:H:600:LYS:H	1.78	0.49
2:J:76:ILE:HG12	2:J:457:SER:HB3	1.94	0.49
2:K:76:ILE:HG12	2:K:457:SER:HB3	1.92	0.49
3:P:245:TYR:HD2	3:P:413:PRO:HD2	1.78	0.49
3:Z:86:TYR:HB2	3:Z:404:LEU:O	2.11	0.49
3:a:319:TYR:CD2	3:a:332:GLN:HB2	2.48	0.49
3:e:91:VAL:HG12	3:j:72:ASN:HB2	1.94	0.49
1:u:138:ASP:OD1	1:u:138:ASP:N	2.45	0.49
3:y:124:LEU:HD12	3:y:362:LEU:HD13	1.94	0.49
2:A:640:GLU:HA	2:B:645:GLN:HE21	1.78	0.49
2:E:54:LEU:HD21	1:w:124:ARG:HD3	1.93	0.49
2:F:47:ALA:O	2:F:63:LYS:HE2	2.13	0.49
2:G:599:GLU:HG2	2:G:600:LYS:H	1.78	0.49
2:K:152:ARG:HG3	2:K:152:ARG:HH11	1.77	0.49
3:Y:111:PRO:HG2	3:f:56:PHE:HE2	1.77	0.49
3:d:182:GLN:NE2	3:d:195:ALA:HB2	2.28	0.49
3:k:180:ASP:O	3:k:183:THR:OG1	2.29	0.49
3:l:222:GLY:HA3	3:l:263:LYS:HG3	1.94	0.49
3:q:22:MET:HA	3:q:22:MET:HE2	1.95	0.49
1:1:32:GLN:HB3	1:w:23:ASN:HD22	1.76	0.49
2:C:47:ALA:O	2:C:63:LYS:HE2	2.13	0.49
2:E:599:GLU:HG2	2:E:600:LYS:H	1.78	0.49
2:G:180:ASP:OD1	2:G:180:ASP:N	2.45	0.49
3:O:94:GLN:HB2	3:O:97:GLU:OE1	2.12	0.49
3:Q:86:TYR:CE1	3:Q:405:LEU:HD21	2.48	0.49
2:E:13:MET:HE2	2:E:13:MET:HA	1.95	0.49
2:K:219:TRP:C	3:f:375:SER:O	2.50	0.49
2:L:95:GLU:CD	2:L:95:GLU:H	2.20	0.49
3:O:182:GLN:HE22	3:O:202:PRO:HD3	1.78	0.49
3:e:129:MET:HB2	3:e:418:GLN:HE21	1.77	0.49
1:h:50:ILE:HG13	1:h:51:ASN:N	2.28	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:o:278:GLN:O	3:o:281:LYS:NZ	2.37	0.49
3:q:23:SER:OG	3:q:24:ASP:N	2.45	0.49
1:v:152:LEU:HD23	1:v:152:LEU:H	1.78	0.49
2:A:209:VAL:CG1	3:Y:379:THR:H	2.23	0.49
2:E:59:GLU:OE1	1:w:125:ARG:HG2	2.12	0.49
2:I:76:ILE:HG12	2:I:457:SER:HB3	1.93	0.49
2:I:152:ARG:HH11	2:I:152:ARG:HG3	1.77	0.49
2:L:368:GLU:HG2	1:s:119:VAL:HG21	1.95	0.49
3:R:246:GLN:HG2	3:R:314:SER:HA	1.94	0.49
3:a:10:SER:N	3:g:47:SER:OG	2.42	0.49
3:d:7:SER:HB3	3:p:78:LYS:HG3	1.94	0.49
2:D:628:VAL:HA	2:D:631:GLN:HG2	1.94	0.49
2:H:47:ALA:O	2:H:63:LYS:HE2	2.12	0.49
2:J:640:GLU:HA	2:K:645:GLN:HE21	1.78	0.49
2:K:621:VAL:HA	2:K:624:GLN:HE21	1.77	0.49
3:X:231:LYS:NZ	3:X:308:ASP:OD1	2.41	0.49
3:Y:267:GLN:NE2	3:Y:296:THR:OG1	2.42	0.49
3:a:32:ASP:OD1	3:a:34:GLN:HG2	2.13	0.49
1:c:44:MET:HG3	1:c:89:ARG:HH11	1.76	0.49
3:p:25:LEU:HG	3:p:121:GLU:OE1	2.13	0.49
2:A:49:ALA:O	1:u:149:ASP:OD2	2.30	0.48
2:D:599:GLU:HG2	2:D:600:LYS:H	1.78	0.48
2:I:100:LEU:HD13	2:I:510:ARG:NH1	2.28	0.48
2:J:628:VAL:HA	2:J:631:GLN:HG2	1.94	0.48
3:R:171:ASP:OD1	3:R:172:PRO:HD2	2.13	0.48
3:R:219:ARG:O	3:R:348:THR:OG1	2.19	0.48
3:S:86:TYR:CE1	3:S:405:LEU:HD21	2.48	0.48
3:d:27:LEU:HB2	3:d:121:GLU:OE1	2.13	0.48
3:e:320:ASP:OD2	3:e:323:ASN:ND2	2.46	0.48
2:B:657:GLU:HG2	2:B:661:ASN:HD21	1.77	0.48
2:H:657:GLU:HG2	2:H:661:ASN:HD21	1.77	0.48
2:J:599:GLU:HG2	2:J:600:LYS:H	1.77	0.48
3:p:26:VAL:HG23	3:p:27:LEU:HD22	1.94	0.48
2:A:351:GLN:HE21	1:s:123:MET:HE3	1.78	0.48
2:D:640:GLU:HA	2:E:645:GLN:HE21	1.78	0.48
2:F:487:ARG:HH21	2:F:523:VAL:HG22	1.78	0.48
2:H:13:MET:HE2	2:H:13:MET:HA	1.95	0.48
2:H:350:ALA:CB	1:h:129:PHE:HE1	2.26	0.48
3:R:52:ARG:HH21	3:R:79:ALA:HB2	1.77	0.48
3:V:23:SER:OG	3:V:24:ASP:N	2.45	0.48
3:Z:87:ILE:HG23	3:e:58:SER:HB2	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:l:124:LEU:HD12	3:l:362:LEU:HD13	1.95	0.48
1:r:69:ASP:N	1:r:69:ASP:OD1	2.47	0.48
2:E:350:ALA:CB	1:w:129:PHE:HE2	2.26	0.48
2:E:657:GLU:HG2	2:E:661:ASN:HD21	1.77	0.48
2:G:76:ILE:HG12	2:G:457:SER:HB3	1.93	0.48
3:M:66:ILE:HD13	3:b:88:THR:HG21	1.95	0.48
3:g:57:SER:HB3	3:g:325:GLN:HG3	1.95	0.48
1:h:3:THR:OG1	1:h:4:VAL:N	2.47	0.48
1:m:50:ILE:HG13	1:m:51:ASN:N	2.28	0.48
2:K:218:ASN:ND2	1:x:140:PHE:HE1	2.08	0.48
2:K:599:GLU:HG2	2:K:600:LYS:H	1.78	0.48
3:M:60:ARG:HH11	3:b:85:ASN:HB2	1.77	0.48
3:Q:56:PHE:HE2	3:U:111:PRO:HG2	1.78	0.48
3:Q:96:LEU:O	3:Q:100:ILE:HG12	2.14	0.48
3:d:162:ASN:OD1	3:d:163:GLU:N	2.47	0.48
2:K:13:MET:HE2	2:K:13:MET:HA	1.95	0.48
3:N:189:ASP:OD1	3:N:189:ASP:N	2.46	0.48
3:T:98:GLU:HA	3:T:102:LEU:HB2	1.96	0.48
3:U:344:THR:HB	3:U:347:GLN:HG2	1.95	0.48
3:X:139:PRO:HB3	3:X:349:MET:SD	2.54	0.48
3:Y:107:GLU:HG3	3:Y:108:ILE:HD12	1.95	0.48
3:d:229:THR:HG22	3:d:338:ALA:HA	1.95	0.48
3:g:247:PHE:CD1	3:g:316:VAL:HG12	2.48	0.48
3:j:123:GLU:OE2	3:o:60:ARG:NH1	2.47	0.48
1:w:16:ARG:HA	1:w:22:SER:HB3	1.96	0.48
2:I:664:TYR:CD2	2:J:666:LEU:HD22	2.48	0.48
2:L:204:PRO:HD2	3:f:203:THR:HG21	1.96	0.48
1:u:5:LEU:HD21	1:u:10:ILE:HD11	1.95	0.48
1:0:48:TRP:HZ2	1:0:85:GLN:HG3	1.79	0.48
1:0:129:PHE:HE2	2:B:350:ALA:HB3	1.79	0.48
1:1:61:THR:HB	1:1:64:GLU:HB2	1.96	0.48
2:A:599:GLU:HG2	2:A:600:LYS:H	1.77	0.48
2:B:13:MET:HE2	2:B:13:MET:HA	1.95	0.48
2:B:362:GLU:HA	1:r:114:MET:CE	2.44	0.48
2:I:47:ALA:O	2:I:63:LYS:HE2	2.12	0.48
2:I:375:ASN:OD1	1:v:123:MET:CE	2.61	0.48
2:L:220:PHE:HA	3:Y:16:LYS:CE	2.38	0.48
3:M:401:ARG:NH2	3:Z:396:ASN:OD1	2.47	0.48
3:Z:180:ASP:O	3:Z:183:THR:OG1	2.30	0.48
3:y:308:ASP:OD1	3:y:309:VAL:N	2.47	0.48
2:B:650:THR:HG22	2:C:652:GLN:HE21	1.79	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:53:LYS:HZ3	3:a:396:ASN:HD22	1.62	0.48
2:G:640:GLU:HA	2:H:645:GLN:HE21	1.77	0.48
2:I:207:LEU:HD12	2:I:226:TYR:HD2	1.79	0.48
2:K:664:TYR:CD2	2:L:666:LEU:HD22	2.49	0.48
2:L:47:ALA:O	2:L:63:LYS:HE2	2.12	0.48
2:L:487:ARG:HH21	2:L:523:VAL:HG22	1.78	0.48
2:L:599:GLU:HG2	2:L:600:LYS:H	1.78	0.48
3:S:139:PRO:HB2	3:S:347:GLN:HE22	1.78	0.48
3:V:231:LYS:HB2	3:V:252:THR:HG23	1.94	0.48
3:X:316:VAL:HG13	3:X:318:ILE:HG13	1.96	0.48
3:b:124:LEU:HD22	3:b:362:LEU:HD22	1.96	0.48
3:n:92:GLU:HG3	3:n:397:VAL:CG1	2.44	0.48
2:A:657:GLU:HG2	2:A:661:ASN:HD21	1.79	0.48
2:C:487:ARG:HH21	2:C:523:VAL:HG22	1.79	0.48
3:O:190:GLN:OE1	3:f:193:ARG:NH2	2.47	0.48
3:T:231:LYS:HB3	3:T:250:THR:HG23	1.96	0.48
3:n:389:LYS:HG2	3:n:400:MET:HE3	1.96	0.48
2:C:54:LEU:HG	1:r:124:ARG:HD3	1.94	0.47
2:D:636:LYS:NZ	2:E:637:ALA:O	2.37	0.47
3:R:96:LEU:O	3:R:100:ILE:HG12	2.13	0.47
3:R:273:THR:HG22	3:R:329:VAL:HG22	1.96	0.47
3:W:139:PRO:HB3	3:W:349:MET:SD	2.54	0.47
1:h:3:THR:N	1:m:64:GLU:OE1	2.47	0.47
2:B:622:LEU:HG	2:C:627:MET:HE1	1.96	0.47
2:C:58:PHE:HE1	3:a:96:LEU:CD1	2.16	0.47
2:E:62:PRO:CD	1:w:125:ARG:HH21	2.27	0.47
2:E:650:THR:HG22	2:F:652:GLN:HE21	1.79	0.47
2:J:668:GLN:OE1	2:K:670:ARG:NH1	2.45	0.47
1:c:29:VAL:HG21	1:c:34:ILE:HD11	1.95	0.47
2:B:599:GLU:HG2	2:B:600:LYS:H	1.78	0.47
2:C:218:ASN:N	3:a:104:GLN:OE1	2.44	0.47
2:E:664:TYR:CD2	2:F:666:LEU:HD22	2.49	0.47
2:G:187:MET:HG2	2:G:228:ALA:HB2	1.95	0.47
2:K:470:ARG:NH1	2:K:473:GLU:OE1	2.43	0.47
3:Q:28:ALA:O	3:Q:33:ARG:NH2	2.44	0.47
3:Q:56:PHE:CE2	3:U:111:PRO:HG2	2.50	0.47
3:T:165:GLU:N	3:T:165:GLU:OE2	2.47	0.47
3:Y:319:TYR:CD2	3:Y:332:GLN:HB2	2.49	0.47
3:Y:389:LYS:HD2	3:Y:400:MET:HE3	1.95	0.47
3:a:86:TYR:HB3	3:a:88:THR:HG23	1.97	0.47
3:a:100:ILE:HG22	3:a:101:LYS:HG3	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:b:23:SER:OG	3:b:24:ASP:N	2.47	0.47
3:j:123:GLU:OE1	3:j:408:TYR:OH	2.26	0.47
3:o:139:PRO:HG2	3:o:343:GLY:HA2	1.96	0.47
1:l:5:LEU:HD12	1:l:9:GLU:OE2	2.14	0.47
2:A:664:TYR:CD2	2:B:666:LEU:HD22	2.50	0.47
2:B:640:GLU:HA	2:C:645:GLN:HE21	1.79	0.47
2:B:664:TYR:CD2	2:C:666:LEU:HD22	2.49	0.47
2:C:664:TYR:CD2	2:D:666:LEU:HD22	2.49	0.47
2:D:657:GLU:HG2	2:D:661:ASN:HD21	1.79	0.47
2:F:120:ALA:HA	2:F:159:PRO:HB3	1.96	0.47
2:F:599:GLU:HG2	2:F:600:LYS:H	1.78	0.47
2:I:120:ALA:HA	2:I:159:PRO:HB3	1.96	0.47
2:I:599:GLU:HG2	2:I:600:LYS:H	1.78	0.47
2:J:47:ALA:O	2:J:63:LYS:HE2	2.14	0.47
2:K:59:GLU:OE1	1:x:125:ARG:HG2	2.15	0.47
3:M:22:MET:HG2	3:M:23:SER:N	2.28	0.47
3:T:276:LEU:O	3:T:278:GLN:NE2	2.47	0.47
3:Z:221:GLN:HG2	3:Z:344:THR:O	2.15	0.47
3:i:245:TYR:HD2	3:i:413:PRO:HD2	1.79	0.47
3:o:18:LEU:HD13	3:y:411:PHE:HB3	1.97	0.47
3:o:114:GLN:NE2	3:o:118:THR:OG1	2.47	0.47
3:p:344:THR:HG22	3:p:345:ALA:N	2.28	0.47
3:q:286:ASN:HB2	3:q:291:ILE:HG12	1.95	0.47
2:A:48:THR:HG21	1:s:140:PHE:HD2	1.78	0.47
2:A:587:GLN:HA	2:A:590:ILE:HG12	1.97	0.47
2:A:666:LEU:HD22	2:L:664:TYR:CD2	2.49	0.47
2:D:187:MET:HG2	2:D:228:ALA:HB2	1.96	0.47
2:I:180:ASP:OD1	2:I:180:ASP:N	2.47	0.47
2:J:41:GLY:CA	1:v:136:LYS:NZ	2.77	0.47
3:Q:120:LEU:HD21	3:Q:362:LEU:HD11	1.96	0.47
3:Y:134:LEU:HD13	3:Y:155:PHE:HE2	1.80	0.47
3:Y:286:ASN:HB2	3:Y:291:ILE:HG12	1.95	0.47
1:c:48:TRP:O	1:c:52:PRO:HD2	2.14	0.47
3:d:180:ASP:O	3:d:183:THR:OG1	2.32	0.47
1:m:5:LEU:HD12	1:m:76:ARG:HD2	1.95	0.47
3:y:238:TYR:O	3:y:242:LYS:HB3	2.14	0.47
2:A:187:MET:HG2	2:A:228:ALA:HB2	1.96	0.47
2:C:120:ALA:HA	2:C:159:PRO:HB3	1.96	0.47
2:C:599:GLU:HG2	2:C:600:LYS:H	1.78	0.47
2:D:567:ILE:HD13	2:D:588:LEU:HD21	1.97	0.47
2:E:62:PRO:CD	1:w:125:ARG:NH2	2.77	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:587:GLN:HA	2:J:590:ILE:HG12	1.97	0.47
2:J:664:TYR:CD2	2:K:666:LEU:HD22	2.49	0.47
2:L:120:ALA:HA	2:L:159:PRO:HB3	1.96	0.47
3:M:245:TYR:HD2	3:M:413:PRO:HD2	1.79	0.47
3:Q:182:GLN:NE2	3:Q:191:LEU:O	2.44	0.47
3:e:123:GLU:OE2	3:e:408:TYR:OH	2.25	0.47
3:f:331:ARG:NH2	3:f:334:GLU:OE1	2.46	0.47
3:f:344:THR:HG22	3:f:345:ALA:H	1.79	0.47
1:u:86:LEU:O	1:u:90:MET:HG2	2.14	0.47
2:A:388:ARG:NH2	1:r:107:GLN:HE21	2.11	0.47
2:C:19:ALA:HA	2:C:171:PRO:HG3	1.96	0.47
2:D:220:PHE:CA	3:j:377:VAL:HG21	2.44	0.47
2:D:406:PRO:HB2	2:E:410:ASN:HB3	1.96	0.47
2:F:628:VAL:HG22	2:F:631:GLN:NE2	2.30	0.47
2:G:567:ILE:HD13	2:G:588:LEU:HD21	1.97	0.47
2:G:664:TYR:CD2	2:H:666:LEU:HD22	2.49	0.47
2:H:664:TYR:CD2	2:I:666:LEU:HD22	2.49	0.47
2:J:187:MET:HG2	2:J:228:ALA:HB2	1.96	0.47
2:J:313:GLY:O	2:J:463:ASN:ND2	2.47	0.47
2:J:406:PRO:HB2	2:K:410:ASN:HB3	1.96	0.47
2:J:486:GLU:HB3	2:J:510:ARG:HD2	1.96	0.47
2:K:220:PHE:HB2	3:f:377:VAL:H	1.79	0.47
2:K:622:LEU:HA	2:K:625:ALA:HB2	1.96	0.47
2:K:650:THR:HG22	2:L:652:GLN:HE21	1.80	0.47
2:L:628:VAL:HG22	2:L:631:GLN:NE2	2.30	0.47
3:O:107:GLU:OE2	3:O:107:GLU:N	2.46	0.47
3:Q:316:VAL:HG23	3:Q:318:ILE:HG13	1.96	0.47
3:R:100:ILE:HG13	3:R:101:LYS:HG3	1.95	0.47
3:V:284:LEU:HB3	3:V:291:ILE:HD12	1.97	0.47
3:b:412:ASN:HD22	3:b:415:MET:HE3	1.79	0.47
3:n:46:ASP:OD1	3:n:47:SER:N	2.48	0.47
3:t:149:VAL:O	3:t:152:THR:OG1	2.32	0.47
3:t:276:LEU:O	3:t:278:GLN:NE2	2.48	0.47
1:l:118:LEU:HD12	2:C:361:MET:HG2	1.91	0.47
2:E:141:MET:HE3	2:E:143:VAL:HG21	1.97	0.47
2:F:180:ASP:OD1	2:F:180:ASP:N	2.47	0.47
2:H:488:GLU:HB3	2:H:510:ARG:NH2	2.30	0.47
2:H:622:LEU:HA	2:H:625:ALA:HB2	1.96	0.47
2:I:617:ASN:HA	2:I:620:MET:HG2	1.97	0.47
2:L:204:PRO:HB3	3:f:209:ARG:CZ	2.44	0.47
3:M:365:ILE:HD11	3:M:405:LEU:HD23	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:V:98:GLU:HA	3:V:102:LEU:HB2	1.97	0.47
3:X:228:LEU:HB3	3:X:251:LEU:HD23	1.95	0.47
3:Z:162:ASN:ND2	3:t:22:MET:HE3	2.30	0.47
3:g:25:LEU:HD11	3:g:117:VAL:HG11	1.95	0.47
3:k:27:LEU:HB2	3:k:121:GLU:OE2	2.15	0.47
2:A:58:PHE:CE1	1:u:149:ASP:O	2.68	0.47
2:D:664:TYR:CD2	2:E:666:LEU:HD22	2.50	0.47
2:E:617:ASN:HA	2:E:620:MET:HG2	1.96	0.47
2:G:587:GLN:HA	2:G:590:ILE:HG12	1.97	0.47
2:G:657:GLU:HG2	2:G:661:ASN:HD21	1.79	0.47
2:H:470:ARG:NH1	2:H:473:GLU:OE1	2.43	0.47
3:O:157:LYS:HE2	3:f:212:MET:HE1	1.95	0.47
3:U:23:SER:OG	3:U:24:ASP:N	2.48	0.47
3:W:112:VAL:HG23	3:W:113:ARG:HD3	1.97	0.47
3:f:23:SER:OG	3:f:24:ASP:N	2.47	0.47
1:h:100:PRO:HA	1:h:103:LEU:HD12	1.96	0.47
3:t:41:ASN:H	3:t:44:THR:HG22	1.80	0.47
1:O:124:ARG:NH2	2:B:57:GLN:HG3	2.30	0.47
2:F:19:ALA:HA	2:F:171:PRO:HG3	1.96	0.47
2:F:664:TYR:CD2	2:G:666:LEU:HD22	2.49	0.47
2:J:245:HIS:HB2	2:J:270:GLY:HA2	1.97	0.47
3:T:316:VAL:HG23	3:T:318:ILE:HG13	1.96	0.47
1:h:44:MET:HG3	1:h:89:ARG:HE	1.80	0.47
3:l:374:ASP:OD2	3:l:389:LYS:HB2	2.15	0.47
2:A:245:HIS:HB2	2:A:270:GLY:HA2	1.96	0.46
2:F:551:LEU:HD11	2:F:561:ARG:HG3	1.97	0.46
2:F:617:ASN:HA	2:F:620:MET:HG2	1.97	0.46
2:H:640:GLU:HA	2:I:645:GLN:HE21	1.80	0.46
2:I:19:ALA:HA	2:I:171:PRO:HG3	1.96	0.46
3:P:182:GLN:NE2	3:P:191:LEU:HD11	2.30	0.46
3:b:229:THR:HG22	3:b:338:ALA:HA	1.96	0.46
3:d:10:SER:HB3	3:i:13:VAL:H	1.79	0.46
3:n:228:LEU:HD13	3:n:251:LEU:HD23	1.97	0.46
1:O:141:THR:HG23	3:a:15:LYS:CD	2.46	0.46
1:1:16:ARG:HG3	1:1:22:SER:HA	1.96	0.46
2:B:209:VAL:HG23	3:g:378:ALA:C	2.39	0.46
2:C:202:LYS:HB2	2:C:202:LYS:HE2	1.76	0.46
2:C:551:LEU:HD11	2:C:561:ARG:HG3	1.97	0.46
2:E:618:PRO:O	2:E:622:LEU:CB	2.55	0.46
2:G:617:ASN:HA	2:G:620:MET:HG2	1.97	0.46
3:N:180:ASP:O	3:N:183:THR:OG1	2.33	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:12:ILE:HD13	3:X:44:THR:HG23	1.96	0.46
1:v:48:TRP:O	1:v:52:PRO:HD2	2.15	0.46
2:A:313:GLY:O	2:A:463:ASN:ND2	2.48	0.46
2:D:29:LYS:HD3	1:r:138:ASP:OD2	2.14	0.46
2:D:47:ALA:O	2:D:63:LYS:HE2	2.15	0.46
2:I:657:GLU:HG2	2:I:661:ASN:HD21	1.79	0.46
2:J:490:ARG:HB3	2:J:507:VAL:N	2.31	0.46
3:O:43:SER:O	3:O:43:SER:OG	2.32	0.46
3:O:51:LYS:NZ	3:k:8:ASN:OD1	2.31	0.46
1:c:89:ARG:NH2	1:v:109:SER:OG	2.49	0.46
3:j:26:VAL:HG21	3:j:213:SER:HB2	1.96	0.46
3:j:51:LYS:HE3	3:j:76:SER:HB3	1.97	0.46
3:o:229:THR:HG22	3:o:338:ALA:HA	1.97	0.46
3:t:40:ILE:HA	3:t:44:THR:HG21	1.98	0.46
1:x:119:VAL:HG23	1:x:120:VAL:H	1.80	0.46
2:G:313:GLY:O	2:G:463:ASN:ND2	2.48	0.46
2:I:487:ARG:HH21	2:I:523:VAL:HG22	1.80	0.46
2:J:57:GLN:CA	3:q:96:LEU:HD21	2.46	0.46
2:K:350:ALA:CB	1:x:129:PHE:HE1	2.29	0.46
3:Q:162:ASN:HD22	3:U:22:MET:HG2	1.81	0.46
3:i:152:THR:O	3:i:156:LEU:HD23	2.16	0.46
2:A:47:ALA:O	2:A:63:LYS:HE2	2.15	0.46
2:A:567:ILE:HD13	2:A:588:LEU:HD21	1.97	0.46
2:D:587:GLN:HA	2:D:590:ILE:HG12	1.97	0.46
2:I:198:GLU:O	2:I:199:TYR:C	2.59	0.46
2:I:628:VAL:HG22	2:I:631:GLN:NE2	2.30	0.46
3:N:57:SER:HB3	3:N:325:GLN:HG3	1.96	0.46
3:Q:22:MET:HE3	3:i:162:ASN:HB3	1.98	0.46
3:a:128:MET:HE3	3:a:360:CYS:HB2	1.96	0.46
1:c:50:ILE:HG13	1:c:51:ASN:H	1.79	0.46
3:f:52:ARG:NH1	3:f:78:LYS:O	2.48	0.46
1:h:6:THR:N	1:h:9:GLU:OE2	2.39	0.46
3:o:217:ALA:O	3:o:350:LYS:NZ	2.48	0.46
3:p:220:THR:HG23	3:p:348:THR:HG22	1.96	0.46
3:q:14:LEU:HG	3:q:16:LYS:H	1.80	0.46
3:t:231:LYS:HE3	3:t:252:THR:HB	1.98	0.46
1:u:87:LEU:O	1:u:91:LEU:HG	2.14	0.46
1:x:137:TYR:CD2	1:x:144:ARG:HG2	2.51	0.46
2:A:207:LEU:HD21	3:Y:377:VAL:HG11	1.98	0.46
2:G:406:PRO:HB2	2:H:410:ASN:HB3	1.97	0.46
2:K:567:ILE:HD13	2:K:588:LEU:HD21	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:617:ASN:HA	2:L:620:MET:HG2	1.97	0.46
3:U:247:PHE:CD1	3:U:316:VAL:HG12	2.50	0.46
3:W:23:SER:OG	3:W:24:ASP:N	2.49	0.46
3:W:238:TYR:O	3:W:242:LYS:HB3	2.15	0.46
3:q:319:TYR:CD2	3:q:332:GLN:HB2	2.50	0.46
2:A:204:PRO:CG	3:Y:38:GLY:N	2.79	0.46
2:F:207:LEU:H	2:F:207:LEU:HD23	1.80	0.46
2:F:350:ALA:HB2	1:z:129:PHE:HE2	1.80	0.46
2:G:47:ALA:O	2:G:63:LYS:HE2	2.15	0.46
2:J:567:ILE:HD13	2:J:588:LEU:HD21	1.97	0.46
2:L:551:LEU:HD11	2:L:561:ARG:HG3	1.98	0.46
3:M:285:TYR:CE1	3:M:290:PRO:HB3	2.51	0.46
3:P:182:GLN:HE22	3:P:202:PRO:HD3	1.81	0.46
3:p:278:GLN:O	3:p:281:LYS:NZ	2.41	0.46
1:x:78:TYR:OH	1:x:116:ASP:OD2	2.28	0.46
2:A:174:LYS:O	2:A:315:ARG:NH2	2.48	0.46
2:A:387:VAL:HB	2:A:396:ALA:HB3	1.98	0.46
2:E:115:THR:HG21	2:E:157:ILE:H	1.81	0.46
2:F:350:ALA:CB	1:z:129:PHE:CE2	2.99	0.46
2:G:174:LYS:O	2:G:315:ARG:NH2	2.48	0.46
2:I:551:LEU:HD11	2:I:561:ARG:HG3	1.97	0.46
2:J:174:LYS:O	2:J:315:ARG:NH2	2.48	0.46
2:J:617:ASN:HA	2:J:620:MET:HG2	1.97	0.46
3:a:93:TYR:CZ	3:a:398:GLN:HB2	2.51	0.46
2:H:650:THR:HG22	2:I:652:GLN:HE21	1.81	0.46
3:M:5:LEU:HD23	3:M:5:LEU:HA	1.83	0.46
3:P:316:VAL:HG23	3:P:318:ILE:HG13	1.98	0.46
3:Q:91:VAL:HG12	3:i:72:ASN:HB2	1.96	0.46
3:T:22:MET:HE2	3:n:162:ASN:HB2	1.97	0.46
3:b:56:PHE:HE2	3:p:111:PRO:HG2	1.81	0.46
3:d:165:GLU:OE1	3:d:165:GLU:N	2.49	0.46
3:j:153:ALA:HB2	3:j:208:ILE:HB	1.97	0.46
3:j:171:ASP:OD1	3:j:171:ASP:N	2.49	0.46
3:l:247:PHE:CD1	3:l:316:VAL:HG12	2.51	0.46
3:n:128:MET:HE3	3:n:360:CYS:SG	2.56	0.46
3:q:231:LYS:HG2	3:q:250:THR:HG23	1.98	0.46
3:y:222:GLY:HA3	3:y:263:LYS:HG3	1.98	0.46
1:l:50:ILE:HD13	1:w:116:ASP:HB2	1.98	0.46
2:A:661:ASN:HA	2:B:666:LEU:HD11	1.98	0.46
2:B:567:ILE:HD13	2:B:588:LEU:HD21	1.97	0.46
2:D:19:ALA:HA	2:D:171:PRO:HG3	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:567:ILE:HD13	2:H:588:LEU:HD21	1.98	0.46
2:L:19:ALA:HA	2:L:171:PRO:HG3	1.96	0.46
2:L:207:LEU:HD23	2:L:207:LEU:H	1.81	0.46
3:f:369:LYS:HD3	3:f:370:LEU:O	2.16	0.46
2:D:661:ASN:HA	2:E:666:LEU:HD11	1.98	0.45
2:G:19:ALA:HA	2:G:171:PRO:HG3	1.98	0.45
2:G:60:LYS:NZ	1:m:140:PHE:CE2	2.84	0.45
3:N:98:GLU:HA	3:N:102:LEU:HB2	1.98	0.45
3:P:180:ASP:O	3:P:183:THR:OG1	2.33	0.45
1:m:16:ARG:HG3	1:m:22:SER:HB2	1.98	0.45
3:p:25:LEU:HD21	3:p:117:VAL:HG11	1.98	0.45
1:l:145:TYR:OH	2:E:336:ARG:NH1	2.49	0.45
2:C:58:PHE:CZ	3:a:96:LEU:HD13	2.49	0.45
2:H:115:THR:HG21	2:H:157:ILE:H	1.81	0.45
2:K:177:ASP:OD1	2:K:177:ASP:N	2.45	0.45
2:K:350:ALA:HB2	1:x:129:PHE:HE1	1.80	0.45
3:Q:100:ILE:HG13	3:Q:101:LYS:HG3	1.98	0.45
3:Q:104:GLN:OE1	3:i:51:LYS:NZ	2.38	0.45
3:T:25:LEU:HD23	3:T:121:GLU:HB2	1.99	0.45
3:T:247:PHE:CD1	3:T:316:VAL:HG12	2.52	0.45
3:Y:104:GLN:CD	1:u:140:PHE:HB3	2.40	0.45
3:b:95:GLN:NE2	3:e:368:PRO:O	2.47	0.45
3:d:275:TRP:HD1	3:d:291:ILE:HG22	1.81	0.45
3:k:27:LEU:HD22	3:k:128:MET:HE1	1.98	0.45
1:w:149:ASP:OD1	1:w:149:ASP:N	2.48	0.45
1:z:32:GLN:O	1:z:35:GLU:HG3	2.17	0.45
2:D:313:GLY:O	2:D:463:ASN:ND2	2.48	0.45
2:G:207:LEU:HD23	2:G:207:LEU:H	1.82	0.45
2:J:114:GLU:HB2	2:J:154:ARG:NH2	2.31	0.45
2:L:204:PRO:CB	3:f:209:ARG:CZ	2.95	0.45
3:M:129:MET:HE1	3:M:219:ARG:HD3	1.98	0.45
3:V:374:ASP:N	3:V:374:ASP:OD1	2.44	0.45
3:a:179:ALA:O	3:a:183:THR:HG23	2.17	0.45
3:j:280:THR:HG22	3:j:282:GLN:HG2	1.97	0.45
3:n:156:LEU:HD12	3:n:161:VAL:HG21	1.98	0.45
3:p:374:ASP:OD1	3:p:374:ASP:N	2.46	0.45
2:A:617:ASN:HA	2:A:620:MET:HG2	1.97	0.45
2:B:207:LEU:HD23	2:B:207:LEU:H	1.82	0.45
2:D:207:LEU:HB2	2:D:226:TYR:H	1.81	0.45
2:E:207:LEU:HD23	2:E:207:LEU:H	1.82	0.45
2:E:211:SER:OG	3:j:34:GLN:CB	2.64	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:640:GLU:HA	2:F:645:GLN:HE21	1.80	0.45
3:M:129:MET:CE	3:M:219:ARG:HD3	2.47	0.45
3:Q:32:ASP:OD1	3:Q:33:ARG:N	2.49	0.45
3:S:183:THR:HA	3:S:192:VAL:HG23	1.98	0.45
3:U:369:LYS:NZ	3:U:373:ILE:O	2.46	0.45
3:W:389:LYS:NZ	3:W:398:GLN:OE1	2.47	0.45
3:X:230:VAL:HG23	3:X:336:GLY:H	1.81	0.45
3:i:222:GLY:HA3	3:i:263:LYS:HG3	1.98	0.45
3:l:228:LEU:HD13	3:l:251:LEU:HD23	1.97	0.45
3:o:153:ALA:HB2	3:o:208:ILE:HB	1.97	0.45
2:C:617:ASN:HA	2:C:620:MET:HG2	1.97	0.45
2:F:488:GLU:HB3	2:F:510:ARG:HE	1.82	0.45
2:G:207:LEU:HB2	2:G:226:TYR:H	1.81	0.45
3:M:166:ASN:OD1	3:M:356:ASN:ND2	2.49	0.45
3:R:98:GLU:OE2	3:R:398:GLN:NE2	2.50	0.45
3:T:192:VAL:HG21	3:n:187:ALA:HB3	1.98	0.45
3:e:273:THR:HG22	3:e:331:ARG:HG3	1.98	0.45
3:g:331:ARG:NH2	3:g:334:GLU:OE1	2.49	0.45
3:i:276:LEU:HD11	3:i:330:SER:HB3	1.99	0.45
3:k:247:PHE:CD1	3:k:316:VAL:HG12	2.51	0.45
3:y:264:ALA:N	3:y:300:ASP:OD1	2.49	0.45
1:l:125:ARG:O	2:C:376:LYS:HE3	2.16	0.45
2:B:362:GLU:HA	1:r:114:MET:HE1	1.98	0.45
2:B:387:VAL:HB	2:B:396:ALA:HB3	1.99	0.45
2:I:636:LYS:NZ	2:J:637:ALA:O	2.35	0.45
2:J:207:LEU:HB2	2:J:226:TYR:H	1.81	0.45
2:J:241:ILE:HG23	2:J:275:ALA:HB2	1.98	0.45
2:K:24:LYS:NZ	2:K:28:GLU:OE2	2.31	0.45
2:L:365:ARG:O	2:L:385:ARG:NH1	2.42	0.45
3:S:107:GLU:CD	3:S:107:GLU:H	2.25	0.45
3:b:40:ILE:HG23	3:b:365:ILE:HD11	1.98	0.45
1:0:132:GLY:HA3	2:B:63:LYS:C	2.42	0.45
2:A:209:VAL:CB	3:Y:379:THR:H	2.29	0.45
2:A:637:ALA:O	2:L:636:LYS:NZ	2.35	0.45
2:B:115:THR:HG21	2:B:157:ILE:H	1.81	0.45
2:B:488:GLU:OE1	2:B:488:GLU:N	2.50	0.45
2:D:617:ASN:HA	2:D:620:MET:HG2	1.97	0.45
2:L:204:PRO:CD	3:f:203:THR:HG21	2.47	0.45
3:d:187:ALA:HB3	3:q:192:VAL:HG11	1.98	0.45
3:i:124:LEU:HD12	3:i:362:LEU:HD13	1.98	0.45
3:p:179:ALA:O	3:p:183:THR:HG23	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:y:274:TYR:CE1	3:y:290:PRO:HG2	2.52	0.45
2:K:115:THR:HG21	2:K:157:ILE:H	1.80	0.45
3:N:46:ASP:OD1	3:N:46:ASP:N	2.50	0.45
3:S:316:VAL:HG23	3:S:318:ILE:HG13	1.99	0.45
3:Z:375:SER:OG	3:Z:386:ARG:NH1	2.50	0.45
3:l:233:GLN:HE22	3:l:332:GLN:HB3	1.81	0.45
3:n:92:GLU:HG3	3:n:397:VAL:HG13	1.99	0.45
3:n:344:THR:H	3:n:347:GLN:HE22	1.65	0.45
2:E:488:GLU:OE1	2:E:488:GLU:N	2.50	0.45
2:G:114:GLU:HB2	2:G:154:ARG:NH2	2.31	0.45
2:H:207:LEU:HD23	2:H:207:LEU:H	1.82	0.45
2:K:207:LEU:HD23	2:K:207:LEU:H	1.82	0.45
2:L:365:ARG:NH2	1:s:117:THR:O	2.50	0.45
2:L:488:GLU:HB3	2:L:510:ARG:HE	1.81	0.45
3:R:33:ARG:HE	3:R:33:ARG:HB3	1.64	0.45
3:U:238:TYR:O	3:U:242:LYS:HB3	2.17	0.45
3:d:26:VAL:HG21	3:d:213:SER:HB2	1.99	0.45
3:e:16:LYS:HB3	3:e:16:LYS:HE2	1.82	0.45
3:j:57:SER:HB3	3:j:325:GLN:HG3	1.98	0.45
1:s:41:LEU:HB2	1:s:86:LEU:HD11	1.97	0.45
2:C:245:HIS:HD2	2:C:246:PRO:HD2	1.82	0.45
2:D:114:GLU:HB2	2:D:154:ARG:NH2	2.31	0.45
2:E:622:LEU:HA	2:E:625:ALA:HB2	1.99	0.45
2:H:376:LYS:CE	1:c:125:ARG:O	2.61	0.45
2:J:207:LEU:HD23	2:J:207:LEU:H	1.82	0.45
2:K:362:GLU:CA	1:u:114:MET:HE1	2.43	0.45
3:O:245:TYR:HD2	3:O:413:PRO:HD2	1.82	0.45
3:U:110:ALA:N	3:U:111:PRO:HD2	2.31	0.45
3:Z:49:SER:OG	3:Z:78:LYS:NZ	2.49	0.45
1:v:87:LEU:O	1:v:91:LEU:HG	2.17	0.45
1:w:41:LEU:O	1:w:45:MET:HG2	2.17	0.45
1:w:78:TYR:OH	1:w:116:ASP:OD2	2.23	0.45
2:D:174:LYS:O	2:D:315:ARG:NH2	2.48	0.44
2:D:207:LEU:HD23	2:D:207:LEU:H	1.82	0.44
2:E:211:SER:OG	3:j:34:GLN:OE1	2.34	0.44
2:E:567:ILE:HD13	2:E:588:LEU:HD21	1.98	0.44
2:G:487:ARG:HG3	2:G:489:VAL:HG23	2.00	0.44
2:H:207:LEU:HB2	2:H:226:TYR:H	1.83	0.44
2:H:241:ILE:HG23	2:H:275:ALA:HB2	1.99	0.44
2:I:55:ASP:CG	1:c:121:PRO:O	2.53	0.44
2:K:640:GLU:HA	2:L:645:GLN:HE21	1.80	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:23:SER:HB3	3:k:277:GLN:NE2	2.31	0.44
3:R:113:ARG:NH2	3:R:379:THR:O	2.50	0.44
3:Z:298:THR:HB	3:Z:312:THR:HG23	1.99	0.44
3:Z:367:LEU:HD21	3:Z:405:LEU:HD12	1.98	0.44
1:c:45:MET:HE1	1:c:55:ILE:HD11	1.99	0.44
3:l:379:THR:HA	3:l:383:PHE:O	2.17	0.44
3:o:136:LEU:HB2	3:o:419:PHE:HB2	1.98	0.44
1:u:141:THR:HG22	1:u:142:SER:N	2.32	0.44
1:1:138:ASP:OD2	2:E:29:LYS:HD3	2.17	0.44
2:A:19:ALA:HA	2:A:171:PRO:HG3	1.98	0.44
2:B:661:ASN:HA	2:C:666:LEU:HD11	2.00	0.44
2:E:241:ILE:HG23	2:E:275:ALA:HB2	1.99	0.44
2:J:19:ALA:HA	2:J:171:PRO:HG3	1.98	0.44
2:K:220:PHE:C	3:f:376:ALA:CB	2.89	0.44
3:N:182:GLN:HE22	3:N:202:PRO:HD3	1.80	0.44
3:N:316:VAL:HG23	3:N:318:ILE:HG13	1.99	0.44
3:P:2:PRO:HB2	3:P:3:ASN:H	1.56	0.44
3:e:214:ASN:OD1	3:e:215:GLY:N	2.50	0.44
3:i:285:TYR:HE1	3:i:290:PRO:HB3	1.81	0.44
1:x:16:ARG:HG3	1:x:22:SER:HB3	1.99	0.44
1:O:126:ARG:CD	2:C:61:TYR:OH	2.57	0.44
2:A:207:LEU:HD23	2:A:207:LEU:H	1.82	0.44
2:A:207:LEU:HB2	2:A:226:TYR:H	1.81	0.44
2:G:661:ASN:HA	2:H:666:LEU:HD11	1.99	0.44
2:H:643:GLN:HB3	2:I:645:GLN:NE2	2.33	0.44
2:K:207:LEU:HB2	2:K:226:TYR:H	1.82	0.44
3:N:89:VAL:HG11	3:N:112:VAL:HG13	2.00	0.44
3:O:380:TYR:CE1	3:O:381:GLU:HG2	2.53	0.44
3:P:106:GLU:HG2	3:P:107:GLU:N	2.32	0.44
3:Q:189:ASP:OD1	3:Q:190:GLN:N	2.50	0.44
3:S:180:ASP:O	3:S:183:THR:OG1	2.35	0.44
3:T:123:GLU:OE1	3:n:60:ARG:NH2	2.47	0.44
3:d:35:LEU:HD23	3:d:411:PHE:CZ	2.51	0.44
3:d:56:PHE:HE2	3:q:111:PRO:HG2	1.82	0.44
1:m:45:MET:HG2	1:m:57:TYR:CG	2.52	0.44
3:p:178:LEU:HD12	3:p:205:PHE:CZ	2.52	0.44
3:p:231:LYS:HB2	3:p:252:THR:HG23	1.99	0.44
2:B:241:ILE:HG23	2:B:275:ALA:HB2	2.00	0.44
2:D:241:ILE:HG23	2:D:275:ALA:HB2	2.00	0.44
2:D:387:VAL:HB	2:D:396:ALA:HB3	1.99	0.44
2:H:384:LEU:HD23	2:H:398:ALA:O	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:387:VAL:HB	2:K:396:ALA:HB3	1.99	0.44
3:M:22:MET:HB3	3:U:162:ASN:HD22	1.82	0.44
3:W:317:PRO:HB2	3:W:329:VAL:HG11	2.00	0.44
1:0:12:LEU:O	1:0:16:ARG:HG3	2.16	0.44
2:B:643:GLN:HB3	2:C:645:GLN:NE2	2.33	0.44
2:D:540:ARG:NH2	2:E:98:GLU:OE1	2.51	0.44
2:G:387:VAL:HB	2:G:396:ALA:HB3	1.99	0.44
2:H:488:GLU:OE1	2:H:488:GLU:N	2.51	0.44
2:K:643:GLN:HB3	2:L:645:GLN:NE2	2.33	0.44
2:K:661:ASN:HA	2:L:666:LEU:HD11	2.00	0.44
3:M:247:PHE:HD1	3:M:316:VAL:HG12	1.82	0.44
3:P:66:ILE:HD13	3:g:88:THR:HG21	1.98	0.44
3:V:137:GLY:HA2	3:V:422:ASN:HB3	1.98	0.44
3:b:113:ARG:HE	3:b:113:ARG:HB2	1.70	0.44
3:j:179:ALA:O	3:j:183:THR:HG23	2.18	0.44
1:z:112:ALA:O	1:z:115:THR:HG22	2.17	0.44
2:A:114:GLU:HB2	2:A:154:ARG:NH2	2.32	0.44
2:A:488:GLU:OE1	2:A:488:GLU:N	2.51	0.44
2:D:245:HIS:HB2	2:D:270:GLY:HA2	2.00	0.44
2:L:207:LEU:HB2	2:L:226:TYR:H	1.82	0.44
3:M:46:ASP:OD1	3:M:46:ASP:N	2.45	0.44
3:M:102:LEU:HD13	3:M:105:LEU:HD13	1.99	0.44
3:N:58:SER:OG	3:d:119:ASP:OD2	2.28	0.44
3:P:170:MET:HE1	3:P:210:ALA:HB1	1.99	0.44
3:Q:111:PRO:HG2	3:i:56:PHE:CE2	2.52	0.44
3:S:57:SER:HB3	3:S:325:GLN:HB3	2.00	0.44
3:T:140:ASN:OD1	3:T:344:THR:OG1	2.35	0.44
3:W:231:LYS:HB3	3:W:250:THR:HG23	1.99	0.44
3:Z:12:ILE:HA	3:b:10:SER:HB2	1.99	0.44
3:d:117:VAL:HG21	3:d:380:TYR:HD2	1.82	0.44
3:d:247:PHE:HD1	3:d:316:VAL:HG12	1.83	0.44
3:g:8:ASN:HD21	3:l:108:ILE:HD11	1.83	0.44
3:k:165:GLU:H	3:k:357:LYS:HB2	1.83	0.44
3:o:98:GLU:HA	3:o:102:LEU:HB2	1.99	0.44
1:r:153:ILE:H	1:r:153:ILE:HG13	1.47	0.44
3:t:316:VAL:HG23	3:t:318:ILE:HG13	2.00	0.44
1:0:48:TRP:O	1:0:52:PRO:HD2	2.18	0.44
2:A:645:GLN:NE2	2:L:643:GLN:HB3	2.33	0.44
2:C:365:ARG:O	2:C:385:ARG:NH1	2.42	0.44
2:E:668:GLN:OE1	2:F:670:ARG:NH1	2.44	0.44
2:G:540:ARG:NH2	2:H:98:GLU:OE1	2.51	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:365:ARG:O	2:H:385:ARG:NH1	2.48	0.44
2:J:657:GLU:HG2	2:J:661:ASN:HD21	1.82	0.44
2:K:241:ILE:HG23	2:K:275:ALA:HB2	2.00	0.44
3:O:128:MET:HG3	3:O:359:PHE:HE2	1.82	0.44
3:e:286:ASN:HB2	3:e:291:ILE:HG12	1.99	0.44
3:g:120:LEU:HD12	3:g:123:GLU:OE2	2.18	0.44
1:h:65:GLN:HG2	1:h:66:PRO:HD2	2.00	0.44
3:k:369:LYS:NZ	3:k:373:ILE:O	2.43	0.44
3:l:81:GLY:HA3	3:l:409:VAL:HG22	2.00	0.44
3:l:86:TYR:HB2	3:l:404:LEU:O	2.18	0.44
3:n:41:ASN:HB2	3:n:44:THR:HG23	1.99	0.44
3:n:344:THR:HB	3:n:347:GLN:OE1	2.17	0.44
3:o:136:LEU:HD23	3:o:136:LEU:HA	1.86	0.44
3:p:60:ARG:HE	3:p:60:ARG:HB3	1.27	0.44
1:w:10:ILE:HG22	1:w:86:LEU:HD21	1.99	0.44
1:l:45:MET:HE1	1:l:55:ILE:HD11	1.98	0.44
2:A:613:GLN:O	2:A:613:GLN:NE2	2.50	0.44
2:G:239:ASP:O	2:G:256:SER:OG	2.22	0.44
2:G:245:HIS:HB2	2:G:270:GLY:HA2	1.99	0.44
2:I:215:TRP:CE2	1:h:144:ARG:NH2	2.85	0.44
2:J:540:ARG:NH2	2:K:98:GLU:OE1	2.50	0.44
3:N:231:LYS:HB3	3:N:250:THR:HG23	1.99	0.44
3:P:23:SER:OG	3:P:24:ASP:N	2.51	0.44
3:R:128:MET:HE2	3:R:353:LEU:HD13	2.00	0.44
3:S:139:PRO:HB2	3:S:347:GLN:NE2	2.33	0.44
3:d:233:GLN:HE22	3:d:334:GLU:HA	1.83	0.44
3:l:106:GLU:HG2	3:l:107:GLU:N	2.33	0.44
3:n:70:ASN:OD1	3:n:70:ASN:N	2.51	0.44
1:z:49:MET:HE1	1:z:54:ASP:OD1	2.17	0.44
2:C:207:LEU:HD12	2:C:226:TYR:HD2	1.83	0.44
2:E:207:LEU:HB2	2:E:226:TYR:H	1.83	0.44
3:P:217:ALA:O	3:P:350:LYS:NZ	2.51	0.44
3:f:280:THR:HG22	3:f:282:GLN:HG2	2.00	0.44
1:l:48:TRP:HZ2	1:l:85:GLN:HG3	1.82	0.43
2:E:661:ASN:HA	2:F:666:LEU:HD11	2.00	0.43
2:F:95:GLU:CD	2:F:95:GLU:H	2.26	0.43
2:F:207:LEU:HB2	2:F:226:TYR:H	1.83	0.43
2:G:59:GLU:OE2	1:m:124:ARG:HG2	2.18	0.43
2:G:241:ILE:HG23	2:G:275:ALA:HB2	2.00	0.43
2:G:488:GLU:OE1	2:G:488:GLU:N	2.51	0.43
3:V:139:PRO:CB	3:V:349:MET:HE1	2.46	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:a:132:GLY:O	3:a:296:THR:OG1	2.32	0.43
3:d:344:THR:HG22	3:d:345:ALA:N	2.33	0.43
1:m:18:PHE:CE2	1:m:96:LEU:HD13	2.53	0.43
1:v:40:ASP:OD1	1:x:16:ARG:NH2	2.51	0.43
1:l:150:LEU:HG	1:l:151:PRO:HD2	2.00	0.43
2:A:273:GLU:OE1	2:A:274:VAL:HG12	2.18	0.43
2:C:53:LYS:HZ2	3:a:396:ASN:HD22	1.66	0.43
2:F:244:ARG:HA	2:F:250:GLU:O	2.18	0.43
2:I:385:ARG:NH2	1:v:51:ASN:HD21	2.16	0.43
3:N:269:LYS:NZ	3:N:292:SER:HB2	2.33	0.43
3:Q:110:ALA:N	3:Q:111:PRO:HD2	2.33	0.43
3:R:156:LEU:HD22	3:R:161:VAL:HG21	2.00	0.43
3:U:162:ASN:OD1	3:U:163:GLU:HG3	2.18	0.43
3:X:180:ASP:O	3:X:183:THR:HG22	2.18	0.43
3:d:153:ALA:HB2	3:d:208:ILE:HB	1.99	0.43
1:h:7:LYS:HE2	1:h:70:ASP:HB2	2.00	0.43
3:k:14:LEU:HD23	3:k:16:LYS:HD3	2.01	0.43
3:k:113:ARG:HE	3:k:113:ARG:HB2	1.63	0.43
3:l:96:LEU:O	3:l:100:ILE:HG12	2.18	0.43
1:u:144:ARG:HG3	1:u:145:TYR:HD1	1.83	0.43
2:D:384:LEU:HD23	2:D:398:ALA:O	2.18	0.43
2:D:487:ARG:HG3	2:D:489:VAL:HG23	2.00	0.43
2:F:6:GLU:HB2	3:e:34:GLN:HE22	1.82	0.43
2:I:490:ARG:HB3	2:I:507:VAL:N	2.33	0.43
2:L:245:HIS:HD2	2:L:246:PRO:HD2	1.82	0.43
3:M:316:VAL:HG23	3:M:318:ILE:HG13	2.00	0.43
3:Y:108:ILE:HG23	3:f:56:PHE:CZ	2.53	0.43
3:a:16:LYS:HB3	3:a:16:LYS:HE2	1.79	0.43
3:a:89:VAL:HG12	3:a:116:ILE:HD11	2.01	0.43
3:a:220:THR:HG23	3:a:348:THR:HG22	2.01	0.43
3:e:220:THR:HG23	3:e:348:THR:HG22	1.99	0.43
1:h:118:LEU:HD23	1:h:118:LEU:HA	1.87	0.43
3:p:319:TYR:CD2	3:p:332:GLN:HB2	2.53	0.43
1:s:18:PHE:CE2	1:s:96:LEU:HD13	2.52	0.43
1:s:137:TYR:HA	1:s:141:THR:HG22	1.99	0.43
1:0:47:GLU:OE1	1:r:80:HIS:HB2	2.18	0.43
2:A:540:ARG:NH2	2:B:98:GLU:OE1	2.51	0.43
2:C:636:LYS:HZ3	2:D:641:THR:N	2.17	0.43
2:D:490:ARG:HB3	2:D:507:VAL:N	2.33	0.43
2:I:643:GLN:HB3	2:J:645:GLN:NE2	2.33	0.43
2:L:368:GLU:CG	1:s:119:VAL:HG21	2.48	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:212:MET:HE3	3:Q:212:MET:HB3	1.83	0.43
3:U:180:ASP:O	3:U:183:THR:HG22	2.18	0.43
1:h:17:LYS:NZ	1:m:40:ASP:OD2	2.50	0.43
3:p:89:VAL:HG11	3:p:112:VAL:HG13	1.99	0.43
3:q:95:GLN:HB3	3:q:398:GLN:OE1	2.18	0.43
1:w:124:ARG:HD3	1:w:124:ARG:HA	1.79	0.43
1:1:141:THR:CG2	2:E:215:TRP:CD1	2.96	0.43
2:A:643:GLN:HB3	2:B:645:GLN:NE2	2.33	0.43
2:B:218:ASN:OD1	2:B:219:TRP:N	2.51	0.43
2:C:244:ARG:HA	2:C:250:GLU:O	2.18	0.43
2:G:207:LEU:HD12	2:G:226:TYR:HD2	1.83	0.43
2:L:539:ARG:NH1	2:L:543:THR:OG1	2.52	0.43
3:Q:247:PHE:CD1	3:Q:316:VAL:HG12	2.52	0.43
3:k:222:GLY:HA3	3:k:263:LYS:HG3	1.99	0.43
3:l:41:ASN:HB3	3:l:44:THR:HG23	2.00	0.43
3:t:156:LEU:HD22	3:t:161:VAL:HG21	2.00	0.43
2:B:668:GLN:OE1	2:C:670:ARG:NH1	2.44	0.43
2:C:487:ARG:HG3	2:C:489:VAL:HG23	2.00	0.43
2:C:643:GLN:HB3	2:D:645:GLN:NE2	2.34	0.43
2:D:488:GLU:OE1	2:D:488:GLU:N	2.51	0.43
2:D:643:GLN:HB3	2:E:645:GLN:NE2	2.34	0.43
2:E:365:ARG:O	2:E:385:ARG:NH1	2.48	0.43
2:E:643:GLN:HB3	2:F:645:GLN:NE2	2.33	0.43
2:I:244:ARG:HA	2:I:250:GLU:O	2.18	0.43
2:I:336:ARG:NH1	1:h:145:TYR:OH	2.48	0.43
2:J:180:ASP:OD1	2:J:180:ASP:N	2.45	0.43
2:L:244:ARG:HA	2:L:250:GLU:O	2.18	0.43
3:R:22:MET:SD	3:R:22:MET:N	2.92	0.43
3:Y:381:GLU:N	3:Y:381:GLU:OE2	2.51	0.43
3:g:179:ALA:O	3:g:183:THR:HG23	2.19	0.43
3:i:284:LEU:HD23	3:i:284:LEU:HA	1.91	0.43
2:G:490:ARG:HB3	2:G:507:VAL:N	2.33	0.43
2:G:643:GLN:HB3	2:H:645:GLN:NE2	2.34	0.43
2:J:207:LEU:HD12	2:J:226:TYR:HD2	1.84	0.43
2:J:387:VAL:HB	2:J:396:ALA:HB3	2.00	0.43
2:K:59:GLU:HG3	1:x:124:ARG:NH2	2.33	0.43
2:K:622:LEU:HD23	2:L:627:MET:HE1	2.01	0.43
3:P:132:GLY:O	3:P:296:THR:OG1	2.28	0.43
3:W:316:VAL:HG13	3:W:318:ILE:HG13	1.99	0.43
3:Y:110:ALA:HB3	3:Y:111:PRO:HD3	2.01	0.43
3:l:26:VAL:HA	3:l:29:LYS:NZ	2.34	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:174:LYS:O	2:F:315:ARG:NH2	2.51	0.43
2:G:384:LEU:HD23	2:G:398:ALA:O	2.19	0.43
3:M:182:GLN:O	3:M:185:LEU:HD23	2.19	0.43
3:R:113:ARG:NH2	3:R:380:TYR:HB2	2.34	0.43
3:S:13:VAL:HG22	3:l:49:SER:HB2	2.00	0.43
3:T:269:LYS:HZ3	3:T:269:LYS:HG3	1.67	0.43
3:Z:41:ASN:HB2	3:Z:44:THR:HG23	2.01	0.43
3:a:139:PRO:HA	3:a:420:PHE:CG	2.53	0.43
3:b:179:ALA:O	3:b:183:THR:HG23	2.18	0.43
3:b:231:LYS:HB3	3:b:250:THR:HG23	2.00	0.43
1:c:17:LYS:HD3	1:c:17:LYS:HA	1.85	0.43
3:e:86:TYR:HB3	3:e:88:THR:HG23	2.01	0.43
3:e:394:ASP:HB2	1:w:152:LEU:HD22	2.01	0.43
3:g:113:ARG:HE	3:g:113:ARG:HB2	1.73	0.43
1:h:41:LEU:O	1:h:45:MET:HG2	2.18	0.43
3:k:276:LEU:HD11	3:k:330:SER:HB3	2.01	0.43
3:l:374:ASP:OD2	3:l:389:LYS:HE2	2.19	0.43
3:o:319:TYR:HA	3:o:327:ASN:OD1	2.19	0.43
2:A:490:ARG:HB3	2:A:507:VAL:N	2.33	0.43
2:A:636:LYS:HZ3	2:B:641:THR:N	2.17	0.43
2:D:244:ARG:HA	2:D:250:GLU:O	2.19	0.43
2:E:387:VAL:HB	2:E:396:ALA:HB3	1.99	0.43
2:F:245:HIS:HD2	2:F:246:PRO:HD2	1.82	0.43
2:F:643:GLN:HB3	2:G:645:GLN:NE2	2.33	0.43
2:I:365:ARG:O	2:I:385:ARG:NH1	2.41	0.43
2:L:57:GLN:HG3	1:u:124:ARG:HH22	1.69	0.43
3:P:228:LEU:HD12	3:P:251:LEU:HB3	2.01	0.43
3:U:27:LEU:O	3:U:31:VAL:HG13	2.18	0.43
3:U:316:VAL:HG23	3:U:318:ILE:HG13	2.00	0.43
3:a:124:LEU:O	3:a:128:MET:HG3	2.19	0.43
3:p:16:LYS:HB3	3:p:16:LYS:HE2	1.78	0.43
2:B:244:ARG:HA	2:B:250:GLU:O	2.19	0.43
2:G:335:GLN:HA	2:G:424:ILE:HD11	2.01	0.43
2:I:650:THR:HG22	2:J:652:GLN:HE21	1.84	0.43
2:J:487:ARG:HG3	2:J:489:VAL:HG23	2.01	0.43
2:K:613:GLN:O	2:K:613:GLN:NE2	2.52	0.43
3:N:375:SER:OG	3:N:386:ARG:NH1	2.52	0.43
3:Q:212:MET:HE1	3:i:157:LYS:HE2	2.00	0.43
3:Y:117:VAL:HG21	3:Y:380:TYR:HD2	1.84	0.43
1:c:3:THR:OG1	1:c:4:VAL:N	2.48	0.43
3:g:280:THR:HG23	3:g:282:GLN:HG2	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:n:344:THR:HB	3:n:347:GLN:CD	2.44	0.43
3:o:238:TYR:O	3:o:242:LYS:HB3	2.19	0.43
1:u:153:ILE:O	1:u:153:ILE:HG22	2.19	0.43
3:y:180:ASP:O	3:y:183:THR:HG22	2.19	0.43
1:0:87:LEU:O	1:0:91:LEU:HG	2.18	0.42
1:0:136:LYS:HE2	2:B:41:GLY:HA3	2.01	0.42
1:0:141:THR:N	3:a:15:LYS:HD2	2.33	0.42
2:B:329:ALA:HA	2:B:332:MET:HE3	2.01	0.42
2:D:207:LEU:HD12	2:D:226:TYR:HD2	1.83	0.42
2:D:636:LYS:HZ3	2:E:641:THR:N	2.17	0.42
2:E:16:PHE:HZ	2:E:187:MET:HE3	1.84	0.42
2:F:539:ARG:NH1	2:F:543:THR:OG1	2.52	0.42
2:H:387:VAL:HB	2:H:396:ALA:HB3	2.01	0.42
2:H:621:VAL:HA	2:H:624:GLN:HE21	1.83	0.42
2:H:661:ASN:HA	2:I:666:LEU:HD11	2.01	0.42
2:I:621:VAL:O	2:I:625:ALA:HB2	2.19	0.42
2:J:410:ASN:OD1	2:J:410:ASN:N	2.52	0.42
2:K:218:ASN:OD1	2:K:219:TRP:N	2.51	0.42
3:N:36:LEU:HD22	3:N:409:VAL:HG23	2.00	0.42
3:T:180:ASP:O	3:T:183:THR:OG1	2.36	0.42
3:U:112:VAL:HG11	3:U:402:PHE:CE1	2.54	0.42
3:U:161:VAL:HG13	3:U:415:MET:HE3	2.01	0.42
3:W:180:ASP:O	3:W:183:THR:HG22	2.20	0.42
3:Y:64:GLY:N	3:l:86:TYR:OH	2.52	0.42
3:Z:144:THR:HG22	3:Z:177:ARG:HD2	2.00	0.42
3:e:319:TYR:CD2	3:e:332:GLN:HB2	2.54	0.42
3:n:374:ASP:OD1	3:o:372:SER:OG	2.34	0.42
3:o:241:VAL:HG21	3:o:316:VAL:HG21	2.00	0.42
1:z:125:ARG:HG3	1:z:146:TYR:CD2	2.54	0.42
2:B:207:LEU:HB2	2:B:226:TYR:H	1.82	0.42
2:G:365:ARG:O	2:G:385:ARG:NH1	2.49	0.42
2:K:376:LYS:NZ	1:u:124:ARG:O	2.49	0.42
3:Q:401:ARG:NH2	3:i:64:GLY:O	2.52	0.42
3:a:57:SER:HB3	3:a:325:GLN:HB3	2.00	0.42
3:f:200:GLN:HG3	3:f:201:ILE:H	1.84	0.42
3:k:362:LEU:HD12	3:k:362:LEU:HA	1.91	0.42
3:o:36:LEU:HD21	3:o:409:VAL:HG21	2.02	0.42
3:o:285:TYR:CE1	3:o:290:PRO:HB3	2.53	0.42
1:v:63:ASP:HA	1:x:3:THR:HG23	2.00	0.42
1:l:40:ASP:OD2	1:w:17:LYS:NZ	2.52	0.42
2:A:218:ASN:HB2	1:s:140:PHE:CE1	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:57:GLN:CB	3:e:96:LEU:CD1	2.23	0.42
2:F:476:LEU:HD12	2:F:476:LEU:HA	1.94	0.42
2:I:539:ARG:NH1	2:I:543:THR:OG1	2.52	0.42
2:J:335:GLN:HA	2:J:424:ILE:HD11	2.01	0.42
3:Q:149:VAL:O	3:Q:152:THR:OG1	2.37	0.42
3:R:113:ARG:HH21	3:R:380:TYR:HB2	1.83	0.42
3:a:22:MET:HB3	3:g:162:ASN:HD22	1.84	0.42
3:a:108:ILE:O	3:a:111:PRO:HD2	2.19	0.42
3:b:387:VAL:HG22	3:b:402:PHE:CE1	2.54	0.42
3:e:189:ASP:OD1	3:e:189:ASP:N	2.52	0.42
3:g:412:ASN:HB3	3:g:415:MET:HG3	2.01	0.42
3:n:319:TYR:CD1	3:n:332:GLN:HG3	2.55	0.42
3:n:344:THR:HG22	3:n:345:ALA:N	2.29	0.42
3:o:159:LEU:HD23	3:o:159:LEU:HA	1.91	0.42
3:t:273:THR:HG22	3:t:329:VAL:HG22	2.01	0.42
2:A:218:ASN:HB2	1:s:140:PHE:CZ	2.55	0.42
2:C:539:ARG:NH1	2:C:543:THR:OG1	2.52	0.42
2:D:664:TYR:OH	2:E:670:ARG:HG2	2.19	0.42
2:F:49:ALA:CA	3:b:371:HIS:CE1	3.03	0.42
2:J:63:LYS:CE	1:v:135:ASN:OD1	2.67	0.42
2:L:567:ILE:HD13	2:L:588:LEU:HD21	2.01	0.42
3:O:180:ASP:O	3:O:183:THR:OG1	2.38	0.42
3:R:50:PHE:CE1	3:V:14:LEU:HD12	2.54	0.42
3:T:149:VAL:O	3:T:152:THR:OG1	2.34	0.42
3:X:23:SER:OG	3:X:24:ASP:N	2.52	0.42
3:Y:153:ALA:HB2	3:Y:208:ILE:HB	2.01	0.42
3:e:60:ARG:HE	3:e:60:ARG:HB3	1.36	0.42
3:g:169:VAL:HG12	3:g:216:LEU:HD11	2.02	0.42
3:j:238:TYR:HD1	3:j:318:ILE:HD13	1.84	0.42
3:k:375:SER:OG	3:k:386:ARG:NH1	2.52	0.42
3:l:25:LEU:O	3:l:29:LYS:NZ	2.52	0.42
3:n:230:VAL:HG23	3:n:335:ALA:HA	2.01	0.42
1:v:17:LYS:HA	1:v:17:LYS:HD3	1.77	0.42
3:y:297:VAL:HG22	3:y:311:VAL:HG21	2.01	0.42
2:F:49:ALA:HA	3:b:371:HIS:CE1	2.54	0.42
2:F:215:TRP:CE2	1:w:144:ARG:NH2	2.85	0.42
2:G:55:ASP:HB2	1:m:124:ARG:NH2	2.34	0.42
2:H:16:PHE:HZ	2:H:187:MET:HE3	1.85	0.42
2:I:476:LEU:HD12	2:I:476:LEU:HA	1.93	0.42
2:L:621:VAL:O	2:L:625:ALA:HB2	2.19	0.42
3:P:26:VAL:HG21	3:P:213:SER:HB2	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:106:GLU:H	3:S:106:GLU:CD	2.27	0.42
3:T:113:ARG:O	3:T:117:VAL:HG23	2.20	0.42
3:T:319:TYR:CD1	3:T:332:GLN:HB2	2.55	0.42
3:W:239:ASN:HA	3:W:242:LYS:HD3	2.02	0.42
3:f:156:LEU:O	3:f:161:VAL:HG22	2.20	0.42
3:l:57:SER:HB3	3:l:325:GLN:HG3	2.02	0.42
1:s:117:THR:O	1:s:117:THR:HG22	2.19	0.42
1:0:54:ASP:N	1:0:54:ASP:OD1	2.49	0.42
2:B:16:PHE:HZ	2:B:187:MET:HE3	1.85	0.42
2:B:24:LYS:NZ	2:B:28:GLU:OE2	2.31	0.42
2:B:47:ALA:HB2	1:s:145:TYR:CG	2.54	0.42
2:D:668:GLN:OE1	2:E:670:ARG:NH1	2.44	0.42
2:F:487:ARG:HG3	2:F:489:VAL:HG23	2.01	0.42
2:H:329:ALA:HA	2:H:332:MET:HE3	2.01	0.42
2:I:245:HIS:HB2	2:I:270:GLY:HA2	2.02	0.42
2:I:567:ILE:HD13	2:I:588:LEU:HD21	2.01	0.42
3:N:29:LYS:H	3:N:29:LYS:HG2	1.67	0.42
3:N:102:LEU:HD13	3:N:105:LEU:HD13	2.01	0.42
3:O:57:SER:HB3	3:O:325:GLN:HG3	2.00	0.42
3:P:229:THR:HG22	3:P:338:ALA:HA	2.01	0.42
3:T:349:MET:N	3:T:349:MET:SD	2.93	0.42
3:U:222:GLY:HA3	3:U:263:LYS:HG3	2.01	0.42
3:W:344:THR:HG22	3:W:345:ALA:N	2.35	0.42
3:X:245:TYR:HD2	3:X:413:PRO:HD2	1.84	0.42
3:Z:319:TYR:CD1	3:Z:332:GLN:HG3	2.55	0.42
3:d:389:LYS:HG2	3:d:400:MET:HE2	2.01	0.42
1:h:91:LEU:HD23	1:h:91:LEU:HA	1.87	0.42
3:q:117:VAL:HG22	3:q:383:PHE:HD1	1.84	0.42
2:A:410:ASN:OD1	2:A:410:ASN:N	2.52	0.42
2:A:664:TYR:OH	2:B:670:ARG:HG2	2.19	0.42
2:B:628:VAL:HA	2:B:631:GLN:HG2	2.02	0.42
2:C:490:ARG:HD2	2:C:508:VAL:HG22	2.02	0.42
2:D:203:PRO:HA	2:D:204:PRO:HD2	1.95	0.42
2:D:335:GLN:HA	2:D:424:ILE:HD11	2.01	0.42
2:E:218:ASN:OD1	2:E:219:TRP:N	2.53	0.42
2:F:384:LEU:HD12	2:F:384:LEU:HA	1.91	0.42
2:G:244:ARG:HA	2:G:250:GLU:O	2.18	0.42
2:H:48:THR:HG21	1:h:140:PHE:CE2	2.54	0.42
2:H:622:LEU:HD23	2:I:627:MET:HE1	2.00	0.42
2:I:487:ARG:HG3	2:I:489:VAL:HG23	2.01	0.42
2:L:384:LEU:HD12	2:L:384:LEU:HA	1.91	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:488:GLU:HB3	2:L:510:ARG:NE	2.35	0.42
3:V:344:THR:HB	3:V:347:GLN:HG2	2.01	0.42
3:W:89:VAL:HG12	3:W:116:ILE:HD11	2.02	0.42
3:X:284:LEU:HD23	3:X:284:LEU:HA	1.89	0.42
3:Z:58:SER:OG	3:t:119:ASP:OD2	2.23	0.42
3:a:136:LEU:HD23	3:a:136:LEU:HA	1.92	0.42
3:a:238:TYR:O	3:a:242:LYS:HB3	2.20	0.42
3:b:344:THR:HG22	3:b:345:ALA:H	1.85	0.42
3:e:113:ARG:HD2	3:e:380:TYR:CG	2.55	0.42
3:j:331:ARG:NH2	3:j:334:GLU:OE1	2.53	0.42
3:l:412:ASN:HB3	3:l:415:MET:HG3	2.01	0.42
1:z:13:PHE:O	1:z:17:LYS:HG2	2.20	0.42
2:A:2:ALA:O	2:A:8:LYS:NZ	2.39	0.42
2:B:361:MET:SD	1:r:118:LEU:HD22	2.60	0.42
2:E:207:LEU:HB3	2:E:225:ILE:HG23	2.02	0.42
2:E:329:ALA:HA	2:E:332:MET:HE3	2.01	0.42
2:F:488:GLU:OE1	2:F:488:GLU:N	2.53	0.42
2:G:41:GLY:CA	1:m:136:LYS:CE	2.97	0.42
2:H:244:ARG:HA	2:H:250:GLU:O	2.19	0.42
2:L:490:ARG:HB3	2:L:507:VAL:N	2.35	0.42
3:P:170:MET:HE3	3:P:170:MET:HB2	1.86	0.42
3:Q:219:ARG:O	3:Q:348:THR:OG1	2.27	0.42
3:Q:370:LEU:HD23	3:Q:370:LEU:HA	1.88	0.42
3:S:159:LEU:HD23	3:S:159:LEU:HA	1.95	0.42
3:T:370:LEU:HD23	3:T:370:LEU:HA	1.87	0.42
3:U:284:LEU:HD23	3:U:284:LEU:HA	1.90	0.42
3:X:276:LEU:O	3:X:278:GLN:NE2	2.53	0.42
3:X:277:GLN:HG2	3:X:280:THR:H	1.85	0.42
3:Z:129:MET:HG3	3:Z:418:GLN:NE2	2.35	0.42
3:d:109:LEU:O	3:d:112:VAL:HG22	2.20	0.42
3:j:25:LEU:HA	3:j:121:GLU:OE1	2.19	0.42
3:n:15:LYS:HB3	3:n:104:GLN:NE2	2.35	0.42
3:q:88:THR:HA	3:q:402:PHE:O	2.20	0.42
3:t:247:PHE:HD1	3:t:316:VAL:HG12	1.84	0.42
3:y:170:MET:HE1	3:y:178:LEU:HD12	2.01	0.42
2:A:384:LEU:HD23	2:A:398:ALA:O	2.19	0.42
2:A:487:ARG:HH21	2:A:523:VAL:HG22	1.85	0.42
2:A:641:THR:N	2:L:636:LYS:HZ3	2.18	0.42
2:B:384:LEU:HD23	2:B:398:ALA:O	2.20	0.42
2:E:174:LYS:O	2:E:315:ARG:NH2	2.53	0.42
2:E:207:LEU:HD12	2:E:226:TYR:HD2	1.85	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:244:ARG:HA	2:E:250:GLU:O	2.19	0.42
2:F:490:ARG:HB3	2:F:507:VAL:N	2.34	0.42
2:G:367:LEU:CD2	1:c:118:LEU:CD1	2.97	0.42
2:H:24:LYS:NZ	2:H:28:GLU:OE2	2.31	0.42
2:K:152:ARG:HG3	2:K:152:ARG:NH1	2.35	0.42
2:K:207:LEU:HB3	2:K:225:ILE:HG23	2.02	0.42
2:L:488:GLU:OE1	2:L:488:GLU:N	2.53	0.42
3:N:123:GLU:OE1	3:V:60:ARG:NH1	2.49	0.42
3:S:247:PHE:CD1	3:S:316:VAL:HG12	2.55	0.42
3:Z:247:PHE:CD1	3:Z:316:VAL:HG12	2.55	0.42
3:f:178:LEU:HD23	3:f:178:LEU:HA	1.91	0.42
3:g:23:SER:OG	3:g:24:ASP:N	2.51	0.42
3:l:11:GLN:N	3:l:11:GLN:OE1	2.52	0.42
3:o:231:LYS:HB3	3:o:250:THR:HG23	2.01	0.42
3:q:332:GLN:NE2	3:q:333:VAL:O	2.53	0.42
1:s:131:VAL:HG22	1:s:135:ASN:HD21	1.84	0.42
3:t:221:GLN:HE21	3:t:349:MET:HE1	1.85	0.42
3:y:36:LEU:HD22	3:y:363:GLY:HA3	2.01	0.42
2:A:207:LEU:HD12	2:A:226:TYR:HD2	1.84	0.42
2:A:487:ARG:HG3	2:A:489:VAL:HG23	2.01	0.42
2:B:152:ARG:HG3	2:B:152:ARG:NH1	2.35	0.42
2:C:54:LEU:HD12	1:r:122:SER:HB3	2.01	0.42
2:C:488:GLU:OE1	2:C:488:GLU:N	2.53	0.42
2:D:222:ALA:HB3	3:j:379:THR:H	1.76	0.42
2:G:664:TYR:OH	2:H:670:ARG:HG2	2.19	0.42
2:J:488:GLU:N	2:J:488:GLU:OE1	2.53	0.42
2:K:244:ARG:HA	2:K:250:GLU:O	2.19	0.42
3:N:278:GLN:O	3:N:281:LYS:NZ	2.42	0.42
3:O:89:VAL:HG11	3:O:112:VAL:HG13	2.02	0.42
3:O:159:LEU:HD23	3:O:159:LEU:HA	1.94	0.42
3:T:370:LEU:H	3:T:388:HIS:CE1	2.38	0.42
3:e:170:MET:HE2	3:e:170:MET:HB3	1.63	0.42
3:j:143:ILE:HG23	3:j:148:ASP:HB2	2.01	0.42
3:n:344:THR:N	3:n:347:GLN:HE22	2.18	0.42
2:A:209:VAL:HG11	3:Y:379:THR:N	2.31	0.41
2:A:244:ARG:HA	2:A:250:GLU:O	2.20	0.41
2:C:180:ASP:OD1	2:C:180:ASP:N	2.47	0.41
2:C:387:VAL:HB	2:C:396:ALA:HB3	2.02	0.41
2:D:365:ARG:O	2:D:385:ARG:NH1	2.51	0.41
2:F:58:PHE:CE1	1:w:151:PRO:HB3	2.55	0.41
2:H:177:ASP:OD1	2:H:177:ASP:N	2.45	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:490:ARG:HD2	2:H:508:VAL:HG22	2.02	0.41
2:I:63:LYS:C	1:c:132:GLY:HA3	2.45	0.41
2:J:613:GLN:O	2:J:616:PRO:HD2	2.20	0.41
2:J:646:ILE:O	2:J:650:THR:HG23	2.20	0.41
3:M:351:PRO:HB3	3:M:420:PHE:CZ	2.55	0.41
3:N:43:SER:HB2	3:i:15:LYS:HZ1	1.85	0.41
3:P:159:LEU:HD23	3:P:159:LEU:HA	1.91	0.41
3:a:59:LEU:HD13	3:a:66:ILE:HD11	2.01	0.41
3:b:35:LEU:HD23	3:b:35:LEU:HA	1.93	0.41
3:f:200:GLN:HG3	3:f:201:ILE:N	2.35	0.41
3:j:159:LEU:HD23	3:j:159:LEU:HA	1.95	0.41
3:k:124:LEU:O	3:k:128:MET:HG3	2.20	0.41
3:p:57:SER:HB3	3:p:325:GLN:HB3	2.01	0.41
3:q:108:ILE:O	3:q:111:PRO:HD2	2.20	0.41
3:q:214:ASN:OD1	3:q:215:GLY:N	2.53	0.41
1:r:23:ASN:C	1:r:23:ASN:HD22	2.27	0.41
3:t:113:ARG:O	3:t:117:VAL:HG23	2.20	0.41
1:z:48:TRP:O	1:z:52:PRO:HD2	2.19	0.41
1:0:43:ASP:CG	1:r:79:LYS:HD3	2.45	0.41
1:0:141:THR:H	3:a:15:LYS:HZ2	1.68	0.41
2:E:384:LEU:HD23	2:E:398:ALA:O	2.20	0.41
2:F:567:ILE:HD13	2:F:588:LEU:HD21	2.01	0.41
2:H:333:ASP:OD2	1:m:133:GLN:HG3	2.20	0.41
2:H:615:GLN:O	2:H:618:PRO:HD2	2.21	0.41
2:J:244:ARG:HA	2:J:250:GLU:O	2.20	0.41
2:K:329:ALA:HA	2:K:332:MET:HE3	2.02	0.41
3:P:46:ASP:OD1	3:P:46:ASP:N	2.53	0.41
3:R:180:ASP:O	3:R:183:THR:OG1	2.33	0.41
3:a:284:LEU:HD23	3:a:284:LEU:HA	1.93	0.41
3:b:60:ARG:HH21	3:p:85:ASN:HB2	1.84	0.41
3:d:23:SER:OG	3:d:24:ASP:N	2.53	0.41
3:d:369:LYS:HG2	3:d:370:LEU:N	2.35	0.41
3:i:86:TYR:HB2	3:i:404:LEU:O	2.20	0.41
3:j:182:GLN:NE2	3:j:195:ALA:HB2	2.34	0.41
1:m:149:ASP:HB2	3:p:96:LEU:HD12	2.01	0.41
3:p:412:ASN:HB3	3:p:415:MET:CE	2.49	0.41
1:s:77:LYS:O	1:u:47:GLU:HG2	2.20	0.41
3:y:182:GLN:NE2	3:y:195:ALA:HB2	2.35	0.41
2:A:365:ARG:O	2:A:385:ARG:NH1	2.50	0.41
2:E:613:GLN:O	2:E:616:PRO:HD2	2.20	0.41
2:G:510:ARG:HD3	2:G:510:ARG:H	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:613:GLN:O	2:G:613:GLN:NE2	2.51	0.41
2:G:646:ILE:O	2:G:650:THR:HG23	2.20	0.41
2:H:207:LEU:HB3	2:H:225:ILE:HG23	2.02	0.41
2:I:410:ASN:OD1	2:I:410:ASN:N	2.53	0.41
2:I:488:GLU:OE1	2:I:488:GLU:N	2.54	0.41
2:J:2:ALA:O	2:J:8:LYS:NZ	2.38	0.41
2:J:57:GLN:CA	3:q:96:LEU:CD2	2.97	0.41
2:J:57:GLN:HA	3:q:96:LEU:CD2	2.50	0.41
2:J:643:GLN:HB3	2:K:645:GLN:NE2	2.34	0.41
2:L:100:LEU:HD13	2:L:510:ARG:HH11	1.85	0.41
3:M:19:PRO:HB3	3:U:163:GLU:OE1	2.21	0.41
3:N:15:LYS:HB3	3:N:104:GLN:OE1	2.21	0.41
3:P:119:ASP:OD2	3:X:58:SER:OG	2.23	0.41
3:R:267:GLN:O	3:R:342:VAL:HG12	2.19	0.41
3:S:118:THR:O	3:S:121:GLU:HG3	2.19	0.41
3:Y:221:GLN:HG2	3:Y:349:MET:HE1	2.01	0.41
3:a:370:LEU:HD23	3:a:373:ILE:HD12	2.02	0.41
3:d:273:THR:HG23	3:d:293:PHE:HB3	2.02	0.41
3:f:179:ALA:O	3:f:183:THR:HG23	2.20	0.41
3:k:245:TYR:HD2	3:k:413:PRO:HD2	1.85	0.41
3:l:149:VAL:HG21	3:l:178:LEU:HD11	2.01	0.41
3:o:274:TYR:HA	3:o:292:SER:HA	2.01	0.41
1:1:125:ARG:HD3	2:D:59:GLU:OE1	2.20	0.41
2:B:207:LEU:HB3	2:B:225:ILE:HG23	2.02	0.41
2:D:510:ARG:HD3	2:D:510:ARG:H	1.86	0.41
2:D:613:GLN:O	2:D:613:GLN:NE2	2.51	0.41
2:E:239:ASP:O	2:E:256:SER:OG	2.25	0.41
2:E:615:GLN:O	2:E:618:PRO:HD2	2.20	0.41
2:F:351:GLN:HE21	1:z:123:MET:HE2	1.85	0.41
2:F:387:VAL:HB	2:F:396:ALA:HB3	2.02	0.41
2:H:207:LEU:HD12	2:H:226:TYR:HD2	1.85	0.41
2:J:490:ARG:HD2	2:J:508:VAL:HG22	2.01	0.41
2:K:16:PHE:HZ	2:K:187:MET:HE3	1.85	0.41
2:L:207:LEU:HB3	2:L:225:ILE:HG23	2.02	0.41
3:U:344:THR:HG22	3:U:345:ALA:N	2.34	0.41
3:Y:165:GLU:OE2	3:Y:209:ARG:NE	2.54	0.41
3:a:156:LEU:HD23	3:a:156:LEU:HA	1.89	0.41
1:c:48:TRP:HZ2	1:c:85:GLN:HG3	1.86	0.41
3:d:171:ASP:OD1	3:d:174:SER:OG	2.26	0.41
3:j:22:MET:HG2	3:o:162:ASN:HD22	1.85	0.41
1:w:139:VAL:O	1:w:140:PHE:HB3	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:510:ARG:HD3	2:A:510:ARG:H	1.86	0.41
2:E:54:LEU:HD23	1:w:124:ARG:HD2	2.01	0.41
2:E:664:TYR:OH	2:F:670:ARG:HG2	2.20	0.41
2:L:387:VAL:HB	2:L:396:ALA:HB3	2.02	0.41
2:L:613:GLN:O	2:L:616:PRO:HD2	2.21	0.41
3:M:136:LEU:HD23	3:M:136:LEU:HA	1.89	0.41
3:M:238:TYR:O	3:M:242:LYS:HB3	2.20	0.41
3:O:153:ALA:HB2	3:O:208:ILE:HB	2.03	0.41
3:R:241:VAL:HG11	3:R:316:VAL:HG21	2.03	0.41
3:U:165:GLU:CD	3:U:167:TYR:HH	2.22	0.41
3:U:189:ASP:OD2	3:U:190:GLN:N	2.53	0.41
3:V:57:SER:H	3:V:72:ASN:ND2	2.19	0.41
3:a:273:THR:HG21	3:a:333:VAL:HG22	2.03	0.41
3:b:260:GLY:N	3:b:302:ASN:OD1	2.33	0.41
3:g:102:LEU:HD23	3:g:102:LEU:HA	1.94	0.41
3:g:362:LEU:HD21	3:g:383:PHE:HZ	1.85	0.41
1:h:14:ALA:C	1:h:16:ARG:H	2.28	0.41
3:i:285:TYR:CE1	3:i:290:PRO:HB3	2.55	0.41
3:n:231:LYS:HB2	3:n:252:THR:HG23	2.02	0.41
1:x:100:PRO:HA	1:x:103:LEU:HD12	2.03	0.41
1:z:100:PRO:HA	1:z:103:LEU:HD12	2.02	0.41
1:0:43:ASP:HB2	1:r:80:HIS:NE2	2.35	0.41
2:B:207:LEU:HD12	2:B:226:TYR:HD2	1.85	0.41
2:B:410:ASN:OD1	2:B:410:ASN:N	2.53	0.41
2:C:53:LYS:NZ	3:a:396:ASN:ND2	2.67	0.41
2:C:470:ARG:NH1	2:C:473:GLU:OE1	2.53	0.41
2:D:613:GLN:O	2:D:616:PRO:HD2	2.21	0.41
2:F:621:VAL:O	2:F:625:ALA:HB2	2.21	0.41
2:I:174:LYS:O	2:I:315:ARG:NH2	2.51	0.41
2:I:214:SER:OG	3:d:377:VAL:HG21	2.21	0.41
2:K:488:GLU:OE1	2:K:488:GLU:N	2.53	0.41
2:L:174:LYS:O	2:L:315:ARG:NH2	2.51	0.41
3:P:182:GLN:HE21	3:g:196:TRP:NE1	2.18	0.41
3:P:247:PHE:CD1	3:P:316:VAL:HG12	2.55	0.41
3:T:106:GLU:HG2	3:T:107:GLU:N	2.36	0.41
3:T:251:LEU:HB2	3:T:309:VAL:HG23	2.01	0.41
3:f:35:LEU:HD23	3:f:35:LEU:HA	1.92	0.41
3:p:233:GLN:OE1	3:p:332:GLN:NE2	2.54	0.41
3:q:273:THR:HG21	3:q:333:VAL:HG22	2.01	0.41
1:r:150:LEU:HA	1:r:151:PRO:HD3	1.96	0.41
3:t:374:ASP:OD1	3:t:375:SER:N	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:y:344:THR:HG22	3:y:345:ALA:N	2.35	0.41
1:z:150:LEU:HD12	1:z:150:LEU:HA	1.94	0.41
1:1:141:THR:CG2	2:E:215:TRP:HD1	2.15	0.41
2:A:335:GLN:HA	2:A:424:ILE:HD11	2.02	0.41
2:A:490:ARG:HD2	2:A:508:VAL:HG22	2.02	0.41
2:C:384:LEU:HD12	2:C:384:LEU:HA	1.91	0.41
2:D:646:ILE:O	2:D:650:THR:HG23	2.20	0.41
2:F:90:ARG:HA	2:F:91:PRO:HD3	1.94	0.41
2:H:664:TYR:OH	2:I:670:ARG:HG2	2.21	0.41
2:I:387:VAL:HB	2:I:396:ALA:HB3	2.02	0.41
2:K:207:LEU:HD12	2:K:226:TYR:HD2	1.85	0.41
2:K:384:LEU:HD23	2:K:398:ALA:O	2.20	0.41
3:S:221:GLN:HG3	3:S:347:GLN:HG2	2.02	0.41
3:V:149:VAL:HG11	3:V:205:PHE:HD2	1.85	0.41
3:X:15:LYS:HB3	3:X:104:GLN:NE2	2.35	0.41
3:X:112:VAL:HG23	3:X:113:ARG:HD3	2.02	0.41
3:Y:220:THR:HG23	3:Y:348:THR:HG22	2.03	0.41
3:d:100:ILE:HD12	3:p:46:ASP:HB3	2.01	0.41
3:f:102:LEU:HD23	3:f:102:LEU:HA	1.94	0.41
1:m:77:LYS:H	1:m:77:LYS:HG2	1.62	0.41
3:y:35:LEU:HD23	3:y:35:LEU:HA	1.92	0.41
2:B:340:LEU:HD22	1:s:130:PRO:HD3	2.02	0.41
2:I:510:ARG:HD3	2:I:510:ARG:HA	1.82	0.41
2:I:636:LYS:HZ3	2:J:641:THR:N	2.18	0.41
2:L:646:ILE:O	2:L:650:THR:HG23	2.21	0.41
3:O:317:PRO:HB2	3:O:329:VAL:HG11	2.03	0.41
3:P:72:ASN:HB2	3:g:91:VAL:HG12	2.02	0.41
3:W:170:MET:HE3	3:W:212:MET:CE	2.49	0.41
3:Z:284:LEU:HD23	3:Z:284:LEU:HA	1.90	0.41
3:a:247:PHE:CD1	3:a:316:VAL:HG12	2.56	0.41
3:i:96:LEU:O	3:i:100:ILE:HG12	2.20	0.41
3:n:11:GLN:OE1	3:n:11:GLN:N	2.54	0.41
1:0:22:SER:OG	1:0:23:ASN:N	2.54	0.41
1:0:95:SER:O	1:0:95:SER:OG	2.37	0.41
2:A:551:LEU:HD11	2:A:561:ARG:HG3	2.03	0.41
2:B:203:PRO:HA	2:B:204:PRO:HD2	2.01	0.41
2:C:567:ILE:HD13	2:C:588:LEU:HD21	2.02	0.41
2:D:29:LYS:CD	1:r:138:ASP:OD2	2.68	0.41
2:D:410:ASN:OD1	2:D:410:ASN:N	2.52	0.41
2:D:551:LEU:HD11	2:D:561:ARG:HG3	2.03	0.41
2:E:636:LYS:HZ3	2:F:641:THR:N	2.19	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:63:LYS:O	1:z:132:GLY:HA3	2.20	0.41
2:H:487:ARG:NH2	2:H:520:ASP:OD2	2.54	0.41
2:I:244:ARG:NH1	2:I:250:GLU:OE1	2.54	0.41
2:I:613:GLN:O	2:I:616:PRO:HD2	2.21	0.41
2:J:365:ARG:NH2	1:x:114:MET:CE	2.75	0.41
2:K:365:ARG:O	2:K:385:ARG:NH1	2.49	0.41
2:K:664:TYR:OH	2:L:670:ARG:HG2	2.21	0.41
3:M:113:ARG:O	3:M:117:VAL:HG23	2.21	0.41
3:O:138:SER:HA	3:O:139:PRO:HD3	1.98	0.41
3:Q:158:ASP:OD2	3:U:173:TRP:NE1	2.54	0.41
3:R:156:LEU:HD23	3:R:156:LEU:HA	1.90	0.41
3:T:212:MET:HE3	3:T:212:MET:HB3	1.77	0.41
3:U:159:LEU:HD23	3:U:159:LEU:HA	1.92	0.41
3:e:273:THR:HG21	3:e:333:VAL:HG22	2.03	0.41
3:e:324:PRO:O	3:e:327:ASN:ND2	2.54	0.41
3:f:106:GLU:H	3:f:106:GLU:CD	2.28	0.41
1:h:5:LEU:HD23	1:h:74:LEU:HB2	2.02	0.41
1:h:16:ARG:HG3	1:h:22:SER:HB3	2.03	0.41
1:h:86:LEU:HG	1:h:90:MET:SD	2.60	0.41
3:i:374:ASP:OD1	3:i:374:ASP:N	2.52	0.41
3:k:238:TYR:HD1	3:k:318:ILE:HD13	1.86	0.41
1:m:124:ARG:NH1	1:m:124:ARG:HB2	2.36	0.41
3:n:27:LEU:HB2	3:n:121:GLU:OE2	2.20	0.41
3:q:295:ALA:HB1	3:q:313:LEU:HB3	2.01	0.41
1:u:149:ASP:OD1	1:u:151:PRO:HD3	2.20	0.41
1:x:149:ASP:OD1	1:x:149:ASP:N	2.54	0.41
3:y:124:LEU:HD21	3:y:128:MET:HE2	2.03	0.41
3:y:171:ASP:OD1	3:y:171:ASP:N	2.53	0.41
1:1:96:LEU:HD23	1:1:96:LEU:HA	1.95	0.41
2:C:115:THR:HG22	2:C:116:ASP:N	2.26	0.41
2:C:174:LYS:O	2:C:315:ARG:NH2	2.51	0.41
2:C:410:ASN:N	2:C:410:ASN:OD1	2.54	0.41
2:D:215:TRP:CH2	1:r:144:ARG:NH1	2.89	0.41
2:F:207:LEU:HB3	2:F:225:ILE:HG23	2.03	0.41
2:H:613:GLN:O	2:H:616:PRO:HD2	2.21	0.41
2:I:385:ARG:NH2	1:x:115:THR:HG21	2.36	0.41
2:I:646:ILE:O	2:I:650:THR:HG23	2.21	0.41
2:K:487:ARG:NH2	2:K:520:ASP:OD2	2.54	0.41
2:L:350:ALA:CB	1:u:129:PHE:HE1	2.33	0.41
2:L:487:ARG:HG3	2:L:489:VAL:HG23	2.02	0.41
2:L:490:ARG:HD2	2:L:508:VAL:HG22	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:212:MET:HE3	3:P:212:MET:HB3	1.86	0.41
3:V:121:GLU:OE2	3:V:121:GLU:HA	2.21	0.41
3:V:259:THR:HA	3:V:302:ASN:HB3	2.02	0.41
3:Z:70:ASN:OD1	3:Z:70:ASN:N	2.53	0.41
3:f:344:THR:HG22	3:f:345:ALA:N	2.35	0.41
3:o:89:VAL:HG12	3:o:116:ILE:HD11	2.03	0.41
3:p:108:ILE:O	3:p:111:PRO:HD2	2.21	0.41
2:A:239:ASP:O	2:A:256:SER:OG	2.23	0.40
2:B:646:ILE:O	2:B:650:THR:HG23	2.21	0.40
2:C:490:ARG:HB3	2:C:507:VAL:N	2.35	0.40
2:E:610:MET:HE2	2:E:610:MET:HA	2.02	0.40
2:H:218:ASN:OD1	2:H:219:TRP:N	2.54	0.40
2:H:636:LYS:HZ3	2:I:641:THR:N	2.19	0.40
3:M:422:ASN:OD1	3:M:422:ASN:N	2.53	0.40
3:N:238:TYR:O	3:N:242:LYS:HB3	2.21	0.40
3:V:344:THR:HG22	3:V:345:ALA:N	2.35	0.40
3:Y:111:PRO:HG2	3:f:56:PHE:CE2	2.56	0.40
1:c:30:GLU:O	1:c:33:SER:OG	2.31	0.40
3:i:95:GLN:HB2	3:i:396:ASN:HB3	2.03	0.40
3:t:106:GLU:HG2	3:t:107:GLU:N	2.36	0.40
1:w:45:MET:HE3	1:w:45:MET:HA	2.02	0.40
2:B:29:LYS:HD3	1:s:138:ASP:OD2	2.20	0.40
2:E:621:VAL:HA	2:E:624:GLN:HE21	1.86	0.40
2:F:247:ILE:HG22	2:F:248:THR:HG23	2.03	0.40
2:G:60:LYS:NZ	1:m:140:PHE:HE2	2.18	0.40
2:G:606:GLN:O	2:G:610:MET:HG2	2.21	0.40
2:G:613:GLN:O	2:G:616:PRO:HD2	2.21	0.40
2:H:90:ARG:HA	2:H:91:PRO:HD3	1.92	0.40
2:J:551:LEU:HD11	2:J:561:ARG:HG3	2.03	0.40
2:L:476:LEU:HD12	2:L:476:LEU:HA	1.94	0.40
3:Z:36:LEU:HD22	3:Z:409:VAL:HG23	2.03	0.40
3:Z:102:LEU:HD22	3:Z:105:LEU:HD13	2.02	0.40
3:b:36:LEU:O	3:b:36:LEU:HD23	2.21	0.40
3:d:257:SER:O	3:d:257:SER:OG	2.38	0.40
1:m:116:ASP:HB2	1:z:50:ILE:HD13	2.03	0.40
3:t:153:ALA:HB2	3:t:208:ILE:HB	2.03	0.40
3:t:228:LEU:HB3	3:t:251:LEU:HD23	2.03	0.40
1:x:7:LYS:NZ	1:x:57:TYR:OH	2.52	0.40
1:l:5:LEU:HA	1:l:9:GLU:OE2	2.21	0.40
2:A:646:ILE:O	2:A:650:THR:HG23	2.21	0.40
2:B:664:TYR:OH	2:C:670:ARG:HG2	2.20	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:60:LYS:O	1:r:146:TYR:OH	2.29	0.40
2:D:362:GLU:CG	1:w:114:MET:CE	2.91	0.40
2:D:490:ARG:HD2	2:D:508:VAL:HG22	2.03	0.40
2:I:661:ASN:HA	2:J:666:LEU:HD11	2.02	0.40
2:I:664:TYR:OH	2:J:670:ARG:HG2	2.22	0.40
2:J:613:GLN:O	2:J:613:GLN:NE2	2.51	0.40
2:K:615:GLN:O	2:K:618:PRO:HD2	2.20	0.40
2:L:63:LYS:C	1:u:132:GLY:HA3	2.46	0.40
2:L:204:PRO:HG2	3:f:209:ARG:NE	2.36	0.40
2:L:247:ILE:HG22	2:L:248:THR:HG23	2.03	0.40
3:M:132:GLY:O	3:M:296:THR:OG1	2.30	0.40
3:N:285:TYR:CE1	3:N:290:PRO:HB3	2.56	0.40
3:P:189:ASP:OD1	3:X:188:SER:HA	2.21	0.40
3:R:228:LEU:HB3	3:R:251:LEU:HD23	2.02	0.40
3:T:54:HIS:CE1	3:X:108:ILE:HG12	2.57	0.40
3:T:156:LEU:HD23	3:T:156:LEU:HA	1.93	0.40
3:X:124:LEU:HD12	3:X:362:LEU:HD13	2.03	0.40
3:Y:104:GLN:NE2	3:Y:106:GLU:HB2	2.37	0.40
1:h:48:TRP:O	1:h:52:PRO:HD2	2.21	0.40
3:j:113:ARG:HE	3:j:113:ARG:HB2	1.63	0.40
3:l:136:LEU:HD13	3:l:151:GLN:HG3	2.03	0.40
3:n:400:MET:HE2	3:n:400:MET:HB3	1.90	0.40
3:q:255:THR:HG22	3:q:256:ALA:N	2.36	0.40
2:B:180:ASP:OD1	2:B:180:ASP:N	2.48	0.40
2:B:636:LYS:HZ3	2:C:641:THR:N	2.19	0.40
2:D:207:LEU:HB3	2:D:225:ILE:HG23	2.04	0.40
2:D:372:GLU:O	1:w:123:MET:HG2	2.21	0.40
2:F:365:ARG:O	2:F:385:ARG:NH1	2.43	0.40
2:F:650:THR:HG22	2:G:652:GLN:HE21	1.86	0.40
2:G:219:TRP:O	3:b:34:GLN:HB3	2.21	0.40
2:G:551:LEU:HD11	2:G:561:ARG:HG3	2.03	0.40
2:G:622:LEU:HA	2:G:625:ALA:HB3	2.04	0.40
2:G:636:LYS:HZ3	2:H:641:THR:N	2.19	0.40
2:H:53:LYS:HD3	2:H:57:GLN:O	2.22	0.40
2:I:637:ALA:HA	2:I:640:GLU:HB2	2.03	0.40
3:M:247:PHE:CD1	3:M:316:VAL:HG12	2.57	0.40
3:O:221:GLN:HG2	3:O:344:THR:O	2.21	0.40
3:O:230:VAL:HG23	3:O:335:ALA:HA	2.03	0.40
3:S:113:ARG:HD3	3:S:113:ARG:H	1.87	0.40
3:T:86:TYR:CE1	3:T:405:LEU:HD21	2.56	0.40
3:U:15:LYS:HB3	3:U:104:GLN:HE22	1.86	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:126:HIS:HA	3:X:129:MET:HG2	2.03	0.40
3:X:238:TYR:O	3:X:242:LYS:HB3	2.21	0.40
3:a:14:LEU:HD11	3:g:39:GLU:CD	2.47	0.40
3:a:39:GLU:O	3:a:44:THR:HG21	2.21	0.40
3:g:26:VAL:O	3:g:30:THR:HG23	2.22	0.40
1:u:141:THR:HG22	1:u:142:SER:H	1.87	0.40
1:w:86:LEU:O	1:w:90:MET:HG2	2.22	0.40
1:0:132:GLY:HA3	2:B:63:LYS:O	2.22	0.40
2:A:613:GLN:O	2:A:616:PRO:HD2	2.21	0.40
2:A:652:GLN:HE21	2:L:650:THR:HG22	1.85	0.40
2:B:569:LEU:HD22	2:B:580:PHE:HZ	1.87	0.40
2:D:606:GLN:O	2:D:610:MET:HG2	2.21	0.40
2:E:389:ASP:OD1	2:E:393:ASN:N	2.54	0.40
2:F:100:LEU:HD13	2:F:510:ARG:HH11	1.85	0.40
2:H:215:TRP:CZ2	1:m:144:ARG:CZ	2.98	0.40
2:H:646:ILE:O	2:H:650:THR:HG23	2.22	0.40
2:I:384:LEU:HD12	2:I:384:LEU:HA	1.91	0.40
2:J:664:TYR:OH	2:K:670:ARG:HG2	2.21	0.40
3:M:275:TRP:HD1	3:M:291:ILE:HG22	1.86	0.40
3:b:367:LEU:HD23	3:b:367:LEU:HA	1.91	0.40
3:e:120:LEU:O	3:e:123:GLU:HG3	2.22	0.40
3:e:374:ASP:N	3:e:374:ASP:OD1	2.52	0.40
3:f:40:ILE:HG23	3:f:365:ILE:HG12	2.02	0.40
3:g:65:ASP:OD2	3:j:395:ALA:HA	2.22	0.40
3:i:180:ASP:O	3:i:183:THR:OG1	2.39	0.40
3:j:23:SER:OG	3:j:24:ASP:N	2.55	0.40
3:l:185:LEU:HD23	3:l:185:LEU:HA	1.94	0.40
1:m:8:GLY:O	1:m:12:LEU:HD23	2.21	0.40
3:n:171:ASP:OD1	3:n:171:ASP:N	2.53	0.40
3:p:23:SER:OG	3:p:24:ASP:N	2.54	0.40
3:t:281:LYS:HA	3:t:281:LYS:HD3	1.98	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	147/160 (92%)	141 (96%)	6 (4%)	0	100	100
1	1	147/160 (92%)	136 (92%)	11 (8%)	0	100	100
1	c	146/160 (91%)	135 (92%)	11 (8%)	0	100	100
1	h	153/160 (96%)	141 (92%)	12 (8%)	0	100	100
1	m	146/160 (91%)	135 (92%)	11 (8%)	0	100	100
1	r	154/160 (96%)	147 (96%)	7 (4%)	0	100	100
1	s	146/160 (91%)	131 (90%)	15 (10%)	0	100	100
1	u	156/160 (98%)	143 (92%)	13 (8%)	0	100	100
1	v	153/160 (96%)	144 (94%)	9 (6%)	0	100	100
1	w	155/160 (97%)	149 (96%)	6 (4%)	0	100	100
1	x	146/160 (91%)	135 (92%)	11 (8%)	0	100	100
1	z	146/160 (91%)	139 (95%)	7 (5%)	0	100	100
2	A	620/708 (88%)	590 (95%)	30 (5%)	0	100	100
2	B	620/708 (88%)	591 (95%)	29 (5%)	0	100	100
2	C	620/708 (88%)	591 (95%)	29 (5%)	0	100	100
2	D	620/708 (88%)	591 (95%)	29 (5%)	0	100	100
2	E	620/708 (88%)	594 (96%)	26 (4%)	0	100	100
2	F	620/708 (88%)	592 (96%)	28 (4%)	0	100	100
2	G	620/708 (88%)	591 (95%)	29 (5%)	0	100	100
2	H	620/708 (88%)	593 (96%)	27 (4%)	0	100	100
2	I	620/708 (88%)	592 (96%)	28 (4%)	0	100	100
2	J	620/708 (88%)	592 (96%)	28 (4%)	0	100	100
2	K	620/708 (88%)	592 (96%)	28 (4%)	0	100	100
2	L	620/708 (88%)	593 (96%)	27 (4%)	0	100	100
3	M	420/423 (99%)	406 (97%)	14 (3%)	0	100	100
3	N	420/423 (99%)	408 (97%)	12 (3%)	0	100	100
3	O	420/423 (99%)	405 (96%)	15 (4%)	0	100	100
3	P	420/423 (99%)	412 (98%)	8 (2%)	0	100	100
3	Q	420/423 (99%)	410 (98%)	10 (2%)	0	100	100
3	R	420/423 (99%)	409 (97%)	11 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	S	420/423 (99%)	412 (98%)	8 (2%)	0	100	100
3	T	420/423 (99%)	405 (96%)	15 (4%)	0	100	100
3	U	420/423 (99%)	408 (97%)	12 (3%)	0	100	100
3	V	420/423 (99%)	401 (96%)	19 (4%)	0	100	100
3	W	420/423 (99%)	405 (96%)	15 (4%)	0	100	100
3	X	420/423 (99%)	400 (95%)	20 (5%)	0	100	100
3	Y	412/423 (97%)	391 (95%)	21 (5%)	0	100	100
3	Z	419/423 (99%)	404 (96%)	15 (4%)	0	100	100
3	a	412/423 (97%)	394 (96%)	18 (4%)	0	100	100
3	b	420/423 (99%)	408 (97%)	12 (3%)	0	100	100
3	d	420/423 (99%)	414 (99%)	6 (1%)	0	100	100
3	e	412/423 (97%)	393 (95%)	18 (4%)	1 (0%)	43	71
3	f	420/423 (99%)	408 (97%)	12 (3%)	0	100	100
3	g	420/423 (99%)	410 (98%)	10 (2%)	0	100	100
3	i	419/423 (99%)	396 (94%)	23 (6%)	0	100	100
3	j	420/423 (99%)	411 (98%)	9 (2%)	0	100	100
3	k	419/423 (99%)	399 (95%)	20 (5%)	0	100	100
3	l	419/423 (99%)	404 (96%)	15 (4%)	0	100	100
3	n	419/423 (99%)	399 (95%)	20 (5%)	0	100	100
3	o	420/423 (99%)	407 (97%)	13 (3%)	0	100	100
3	p	412/423 (97%)	397 (96%)	15 (4%)	0	100	100
3	q	412/423 (97%)	395 (96%)	17 (4%)	0	100	100
3	t	420/423 (99%)	408 (97%)	12 (3%)	0	100	100
3	y	420/423 (99%)	398 (95%)	22 (5%)	0	100	100
All	All	21790/23106 (94%)	20895 (96%)	894 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	e	70	ASN

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	0	128/137 (93%)	128 (100%)	0	100	100
1	1	129/137 (94%)	129 (100%)	0	100	100
1	c	128/137 (93%)	128 (100%)	0	100	100
1	h	134/137 (98%)	134 (100%)	0	100	100
1	m	128/137 (93%)	128 (100%)	0	100	100
1	r	135/137 (98%)	134 (99%)	1 (1%)	76	77
1	s	128/137 (93%)	128 (100%)	0	100	100
1	u	135/137 (98%)	135 (100%)	0	100	100
1	v	134/137 (98%)	134 (100%)	0	100	100
1	w	136/137 (99%)	136 (100%)	0	100	100
1	x	128/137 (93%)	128 (100%)	0	100	100
1	z	128/137 (93%)	128 (100%)	0	100	100
2	A	522/592 (88%)	522 (100%)	0	100	100
2	B	522/592 (88%)	522 (100%)	0	100	100
2	C	522/592 (88%)	518 (99%)	4 (1%)	73	76
2	D	522/592 (88%)	522 (100%)	0	100	100
2	E	522/592 (88%)	522 (100%)	0	100	100
2	F	522/592 (88%)	522 (100%)	0	100	100
2	G	522/592 (88%)	522 (100%)	0	100	100
2	H	522/592 (88%)	522 (100%)	0	100	100
2	I	522/592 (88%)	518 (99%)	4 (1%)	73	76
2	J	522/592 (88%)	522 (100%)	0	100	100
2	K	522/592 (88%)	522 (100%)	0	100	100
2	L	522/592 (88%)	522 (100%)	0	100	100
3	M	350/351 (100%)	350 (100%)	0	100	100
3	N	350/351 (100%)	350 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	O	350/351 (100%)	350 (100%)	0	100	100
3	P	350/351 (100%)	349 (100%)	1 (0%)	86	83
3	Q	350/351 (100%)	348 (99%)	2 (1%)	78	79
3	R	350/351 (100%)	348 (99%)	2 (1%)	78	79
3	S	350/351 (100%)	347 (99%)	3 (1%)	70	75
3	T	350/351 (100%)	350 (100%)	0	100	100
3	U	350/351 (100%)	350 (100%)	0	100	100
3	V	350/351 (100%)	350 (100%)	0	100	100
3	W	350/351 (100%)	350 (100%)	0	100	100
3	X	350/351 (100%)	350 (100%)	0	100	100
3	Y	342/351 (97%)	333 (97%)	9 (3%)	40	60
3	Z	349/351 (99%)	349 (100%)	0	100	100
3	a	342/351 (97%)	339 (99%)	3 (1%)	70	75
3	b	350/351 (100%)	350 (100%)	0	100	100
3	d	350/351 (100%)	350 (100%)	0	100	100
3	e	342/351 (97%)	333 (97%)	9 (3%)	40	60
3	f	350/351 (100%)	350 (100%)	0	100	100
3	g	350/351 (100%)	350 (100%)	0	100	100
3	i	349/351 (99%)	349 (100%)	0	100	100
3	j	350/351 (100%)	349 (100%)	1 (0%)	86	83
3	k	349/351 (99%)	349 (100%)	0	100	100
3	l	349/351 (99%)	348 (100%)	1 (0%)	86	83
3	n	349/351 (99%)	349 (100%)	0	100	100
3	o	350/351 (100%)	350 (100%)	0	100	100
3	p	342/351 (97%)	337 (98%)	5 (2%)	57	68
3	q	342/351 (97%)	337 (98%)	5 (2%)	57	68
3	t	350/351 (100%)	350 (100%)	0	100	100
3	y	350/351 (100%)	350 (100%)	0	100	100
All	All	18290/19278 (95%)	18240 (100%)	50 (0%)	84	83

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	201	LYS
2	C	202	LYS
2	C	205	THR
2	C	207	LEU
2	I	201	LYS
2	I	202	LYS
2	I	205	THR
2	I	207	LEU
3	P	370	LEU
3	Q	58	SER
3	Q	119	ASP
3	R	273	THR
3	R	294	THR
3	S	211	LEU
3	S	344	THR
3	S	348	THR
3	Y	58	SER
3	Y	59	LEU
3	Y	60	ARG
3	Y	61	THR
3	Y	71	LYS
3	Y	74	LEU
3	Y	120	LEU
3	Y	121	GLU
3	Y	171	ASP
3	a	69	GLN
3	a	70	ASN
3	a	74	LEU
3	e	55	GLN
3	e	59	LEU
3	e	60	ARG
3	e	63	THR
3	e	65	ASP
3	e	71	LYS
3	e	166	ASN
3	e	170	MET
3	e	178	LEU
3	j	387	VAL
3	l	377	VAL
3	p	60	ARG
3	p	65	ASP
3	p	66	ILE
3	p	67	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	p	69	GLN
3	q	57	SER
3	q	61	THR
3	q	65	ASP
3	q	70	ASN
3	q	74	LEU
1	r	153	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (185) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	32	GLN
1	1	39	ASN
1	1	107	GLN
1	1	135	ASN
2	A	153	GLN
2	A	258	GLN
2	A	351	GLN
2	A	393	ASN
2	A	598	ASN
2	A	645	GLN
2	A	652	GLN
2	B	375	ASN
2	B	652	GLN
2	C	519	ASN
2	C	598	ASN
2	C	631	GLN
2	C	645	GLN
2	D	153	GLN
2	D	258	GLN
2	D	393	ASN
2	D	598	ASN
2	D	645	GLN
2	D	652	GLN
2	E	57	GLN
2	E	351	GLN
2	E	598	ASN
2	E	624	GLN
2	E	652	GLN
2	F	519	ASN
2	F	645	GLN
2	G	153	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	G	258	GLN
2	G	393	ASN
2	G	598	ASN
2	G	645	GLN
2	G	652	GLN
2	H	57	GLN
2	H	370	HIS
2	H	624	GLN
2	H	645	GLN
2	I	519	ASN
2	I	598	ASN
2	J	153	GLN
2	J	393	ASN
2	J	598	ASN
2	J	645	GLN
2	K	370	HIS
2	K	645	GLN
2	K	652	GLN
2	L	351	GLN
2	L	598	ASN
2	L	645	GLN
3	M	69	GLN
3	M	221	GLN
3	M	239	ASN
3	M	272	ASN
3	M	332	GLN
3	M	388	HIS
3	N	55	GLN
3	N	104	GLN
3	N	239	ASN
3	N	388	HIS
3	O	85	ASN
3	O	267	GLN
3	O	332	GLN
3	O	418	GLN
3	P	126	HIS
3	P	182	GLN
3	P	332	GLN
3	R	233	GLN
3	S	233	GLN
3	S	332	GLN
3	T	69	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	T	166	ASN
3	T	198	ASN
3	T	388	HIS
3	U	34	GLN
3	U	55	GLN
3	U	104	GLN
3	U	176	GLN
3	U	186	HIS
3	U	418	GLN
3	V	176	GLN
3	V	182	GLN
3	V	279	GLN
3	V	356	ASN
3	W	186	HIS
3	X	34	GLN
3	X	186	HIS
3	X	356	ASN
3	Y	85	ASN
3	Y	198	ASN
3	Y	352	ASN
3	Y	356	ASN
3	Z	3	ASN
3	Z	176	GLN
3	Z	204	ASN
3	Z	278	GLN
3	Z	286	ASN
3	Z	418	GLN
3	a	396	ASN
3	b	34	GLN
3	b	104	GLN
3	b	388	HIS
3	d	55	GLN
3	d	72	ASN
3	d	190	GLN
3	d	347	GLN
3	e	34	GLN
3	e	55	GLN
3	e	332	GLN
3	e	356	ASN
3	f	54	HIS
3	f	186	HIS
3	f	214	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	f	282	GLN
3	f	323	ASN
3	g	103	ASN
3	g	182	GLN
3	g	186	HIS
3	g	347	GLN
3	g	396	ASN
1	h	51	ASN
1	h	85	GLN
1	h	135	ASN
3	i	72	ASN
3	i	204	ASN
3	i	221	GLN
3	i	278	GLN
3	i	279	GLN
3	i	286	ASN
3	j	166	ASN
3	j	186	HIS
3	k	3	ASN
3	k	166	ASN
3	k	204	ASN
3	k	277	GLN
3	k	278	GLN
3	k	286	ASN
3	k	347	GLN
3	l	131	ASN
3	l	140	ASN
3	l	166	ASN
3	l	186	HIS
3	l	286	ASN
1	m	101	GLN
1	m	133	GLN
1	m	135	ASN
3	n	72	ASN
3	n	73	ASN
3	n	131	ASN
3	n	182	GLN
3	n	190	GLN
3	n	204	ASN
3	o	272	ASN
3	o	332	GLN
3	p	55	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	p	166	ASN
3	p	176	GLN
3	p	332	GLN
3	p	371	HIS
3	q	34	GLN
3	q	114	GLN
3	q	176	GLN
3	q	332	GLN
3	q	356	ASN
1	r	105	ASN
1	r	107	GLN
1	r	135	ASN
1	s	23	ASN
1	s	133	GLN
3	t	69	GLN
3	t	198	ASN
3	t	233	GLN
3	t	332	GLN
1	v	51	ASN
1	v	107	GLN
1	x	133	GLN
3	y	72	ASN
3	y	182	GLN
3	y	186	HIS
3	y	418	GLN
1	z	105	ASN
1	z	133	GLN
1	z	135	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

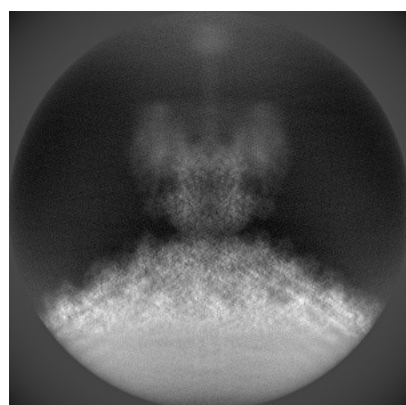
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25365. These allow visual inspection of the internal detail of the map and identification of artifacts.

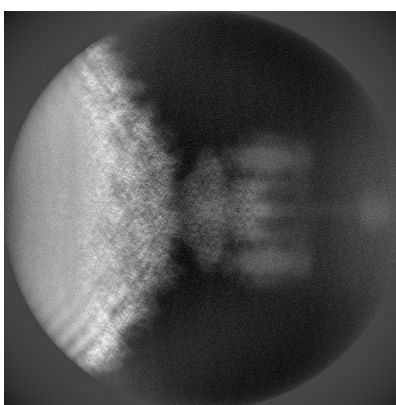
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

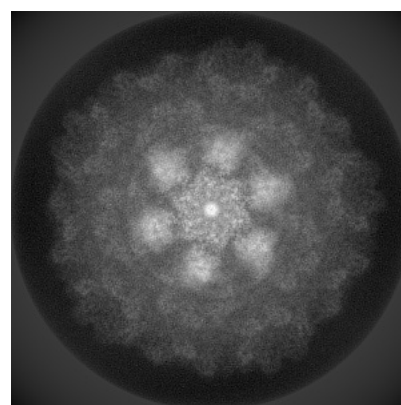
6.1.1 Primary map



X



Y

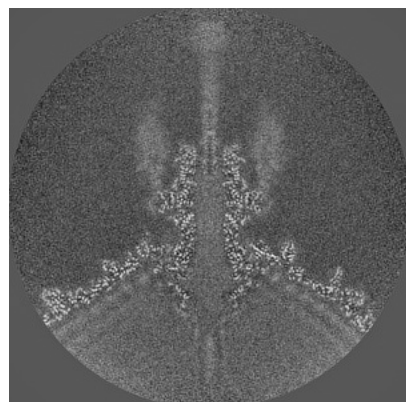


Z

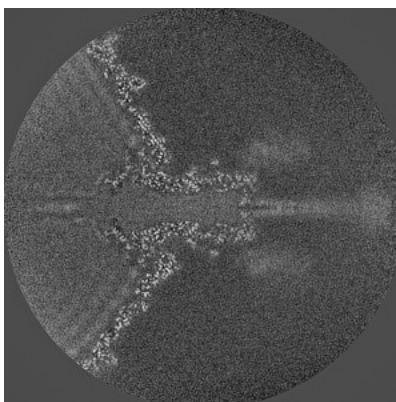
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

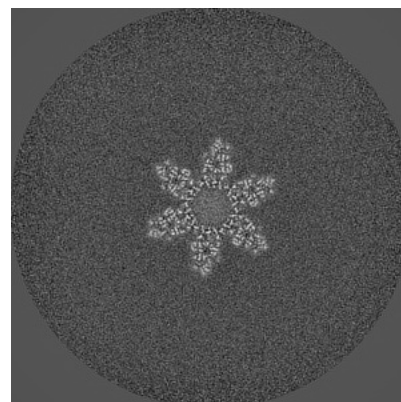
6.2.1 Primary map



X Index: 256



Y Index: 256

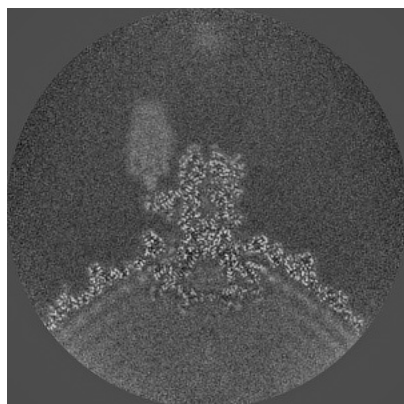


Z Index: 256

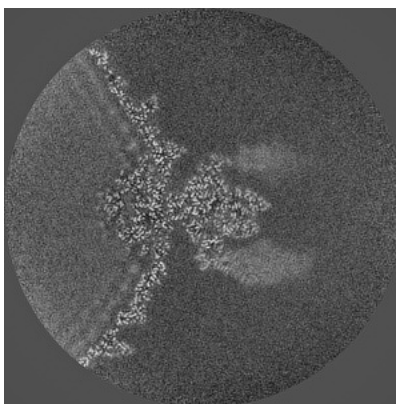
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

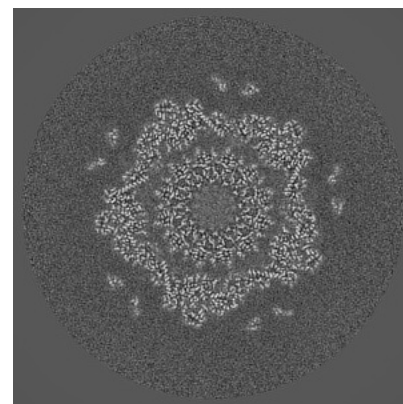
6.3.1 Primary map



X Index: 236



Y Index: 224

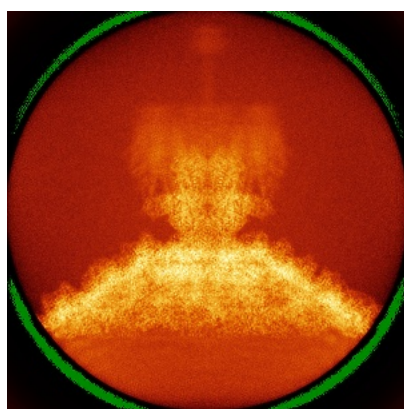


Z Index: 177

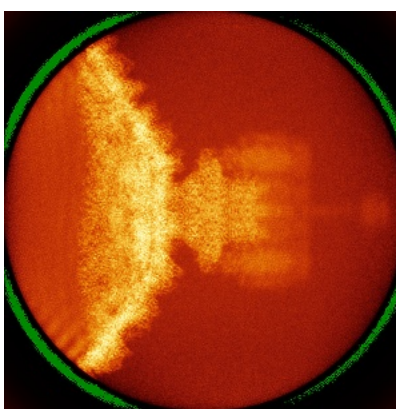
The images above show the largest variance slices of the map in three orthogonal directions.

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

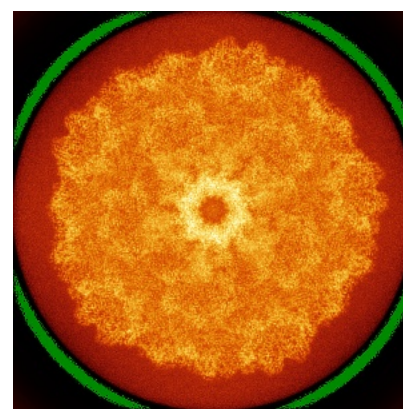
6.4.1 Primary map



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

This section was not generated.

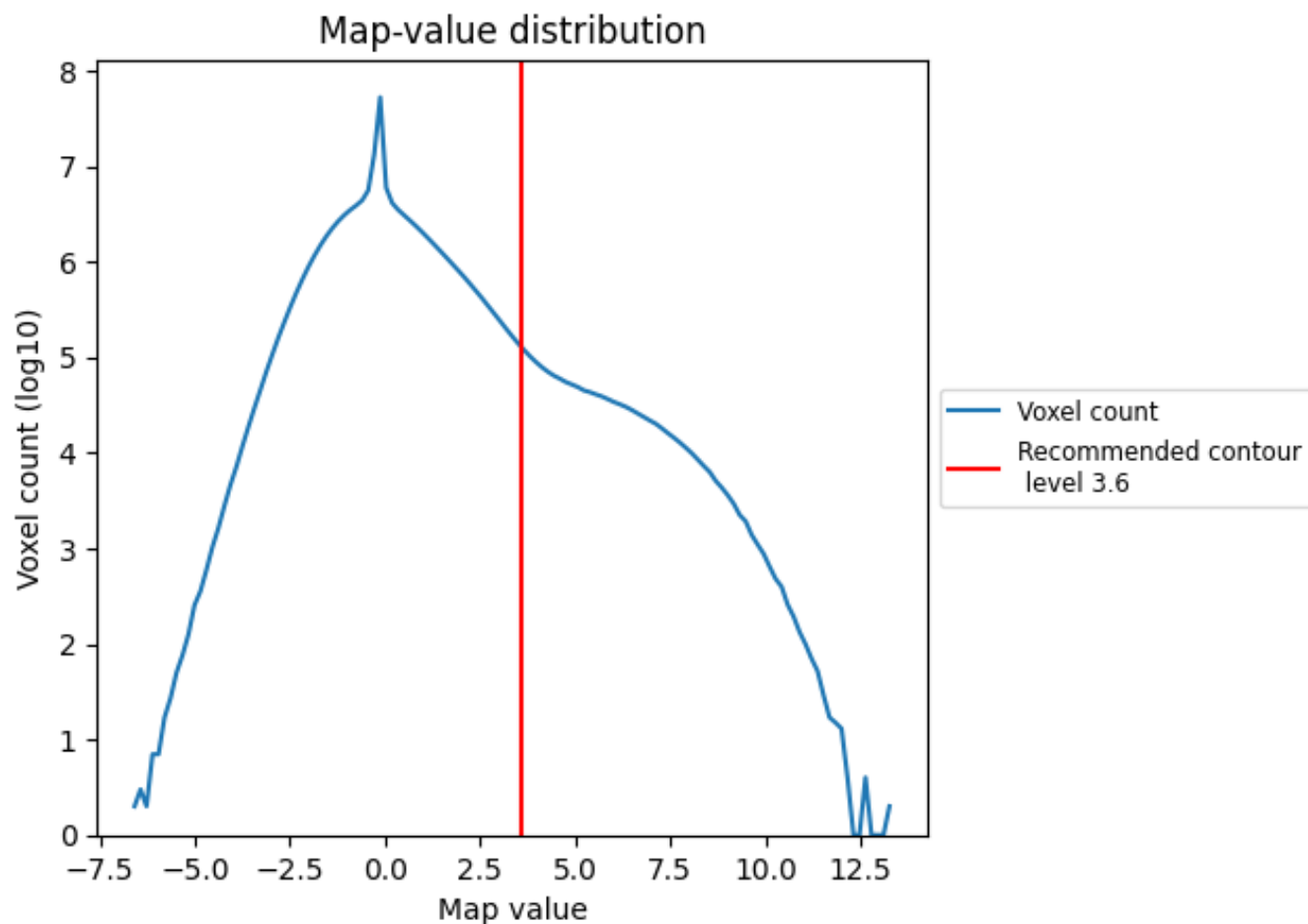
6.6 Mask visualisation

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

7 Map analysis [i](#)

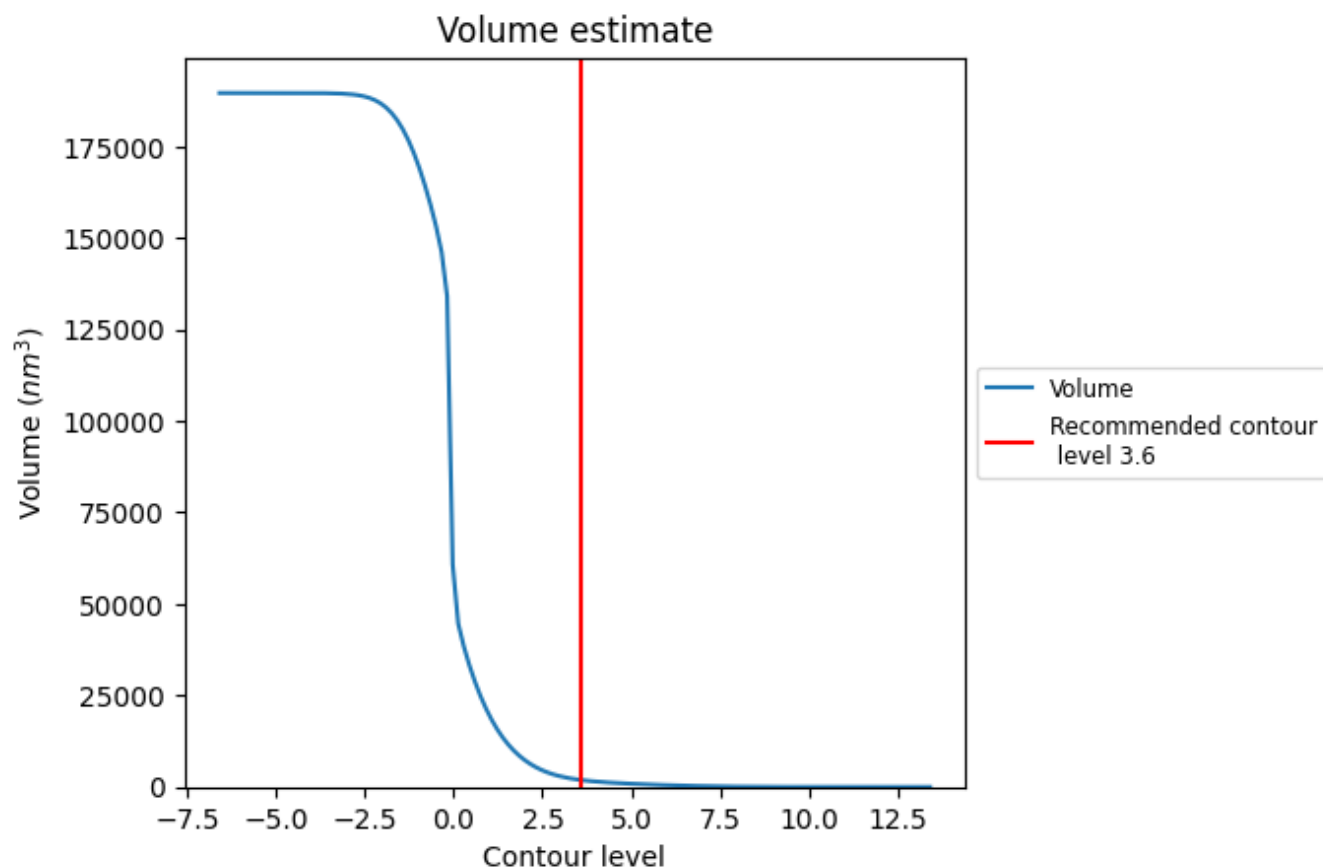
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

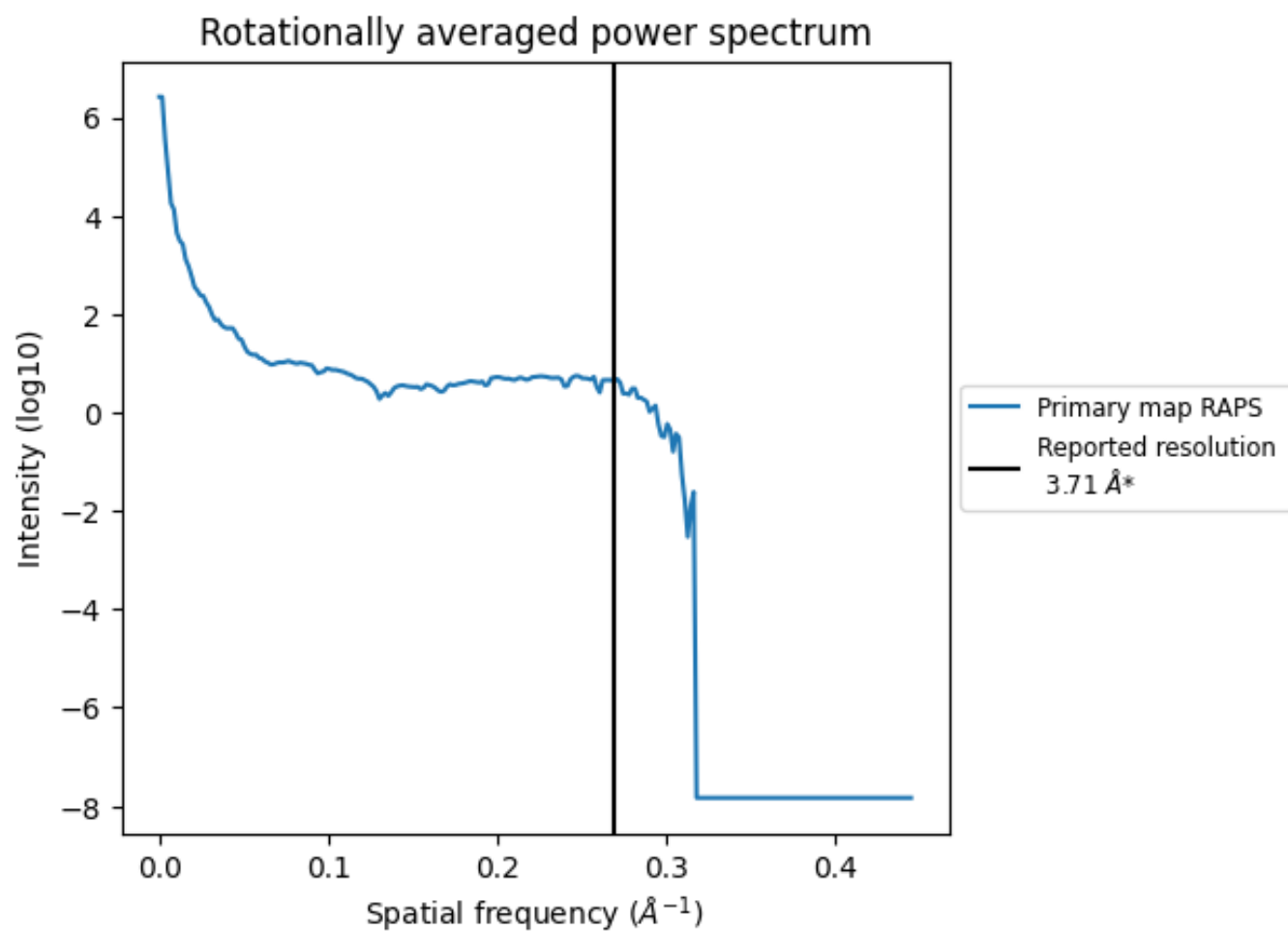
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1878 nm³; this corresponds to an approximate mass of 1696 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 ⓘ

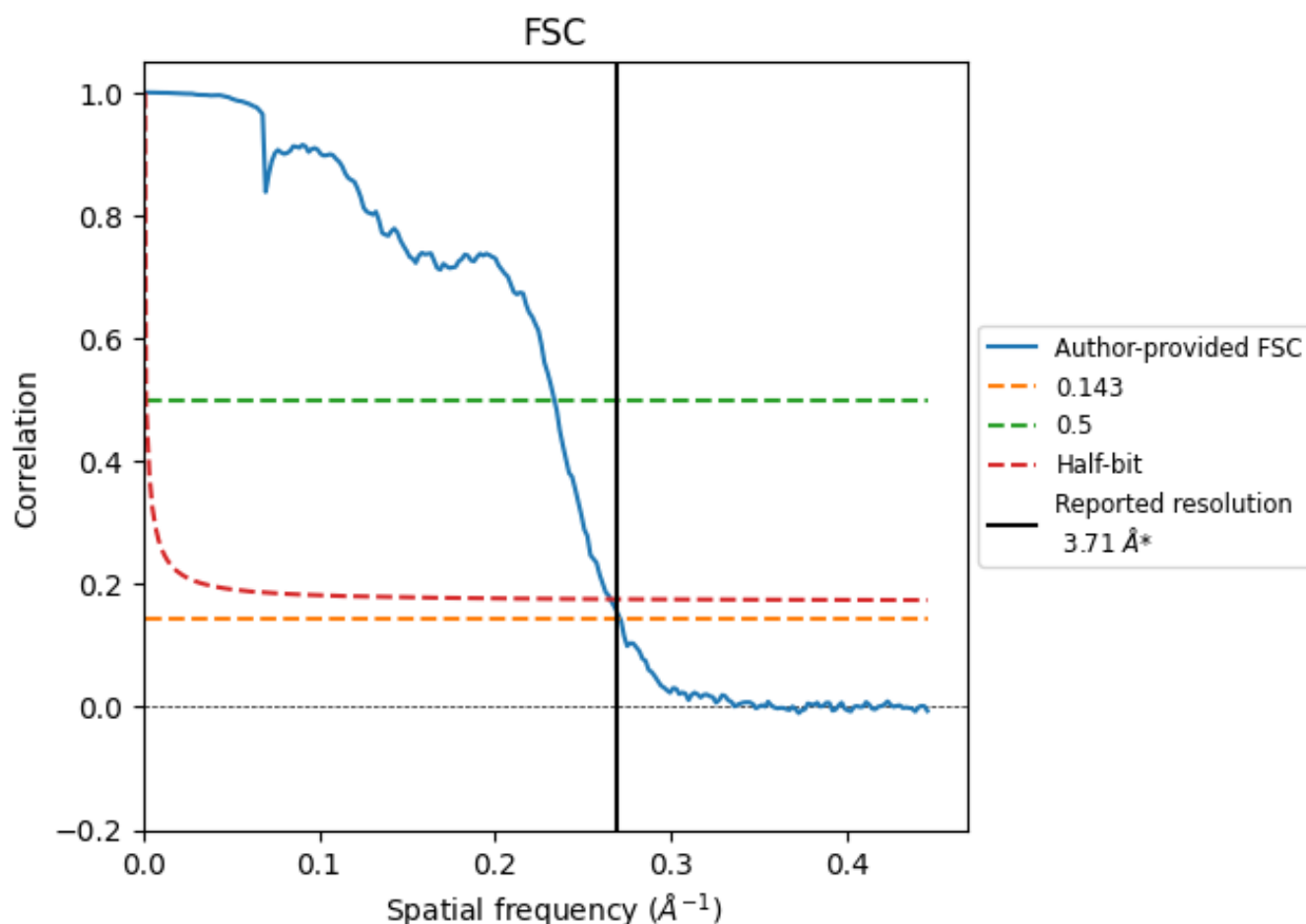


*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

8.2 Resolution estimates [i](#)

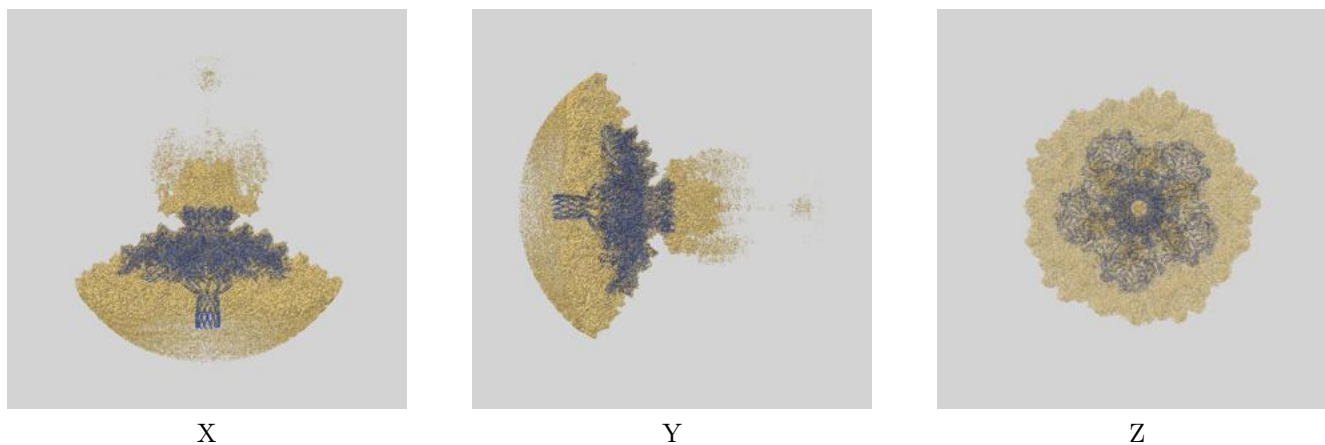
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.71	-	-
Author-provided FSC curve	3.69	4.28	3.77
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

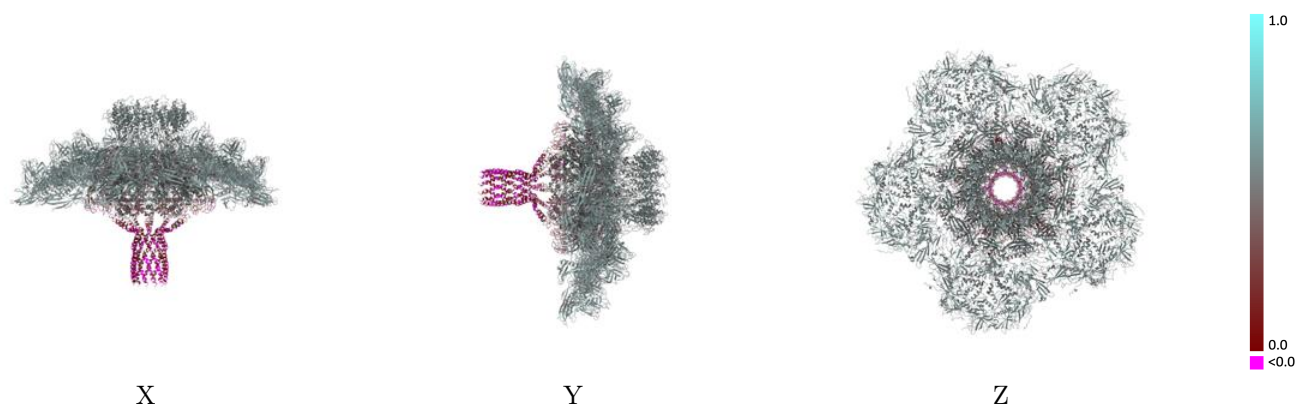
This section contains information regarding the fit between EMDB map EMD-25365 and PDB model 7SP4. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



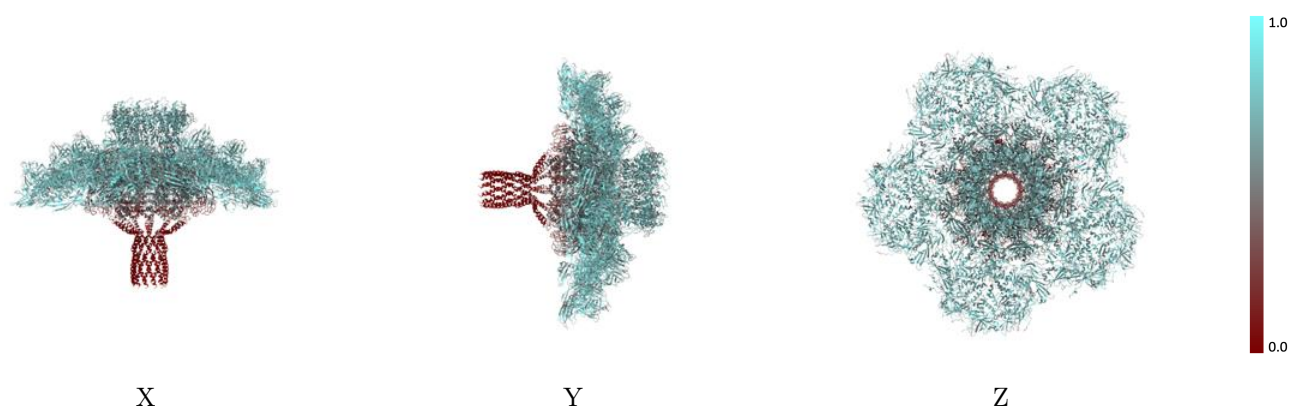
The images above show the 3D surface view of the map at the recommended contour level 3.6 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



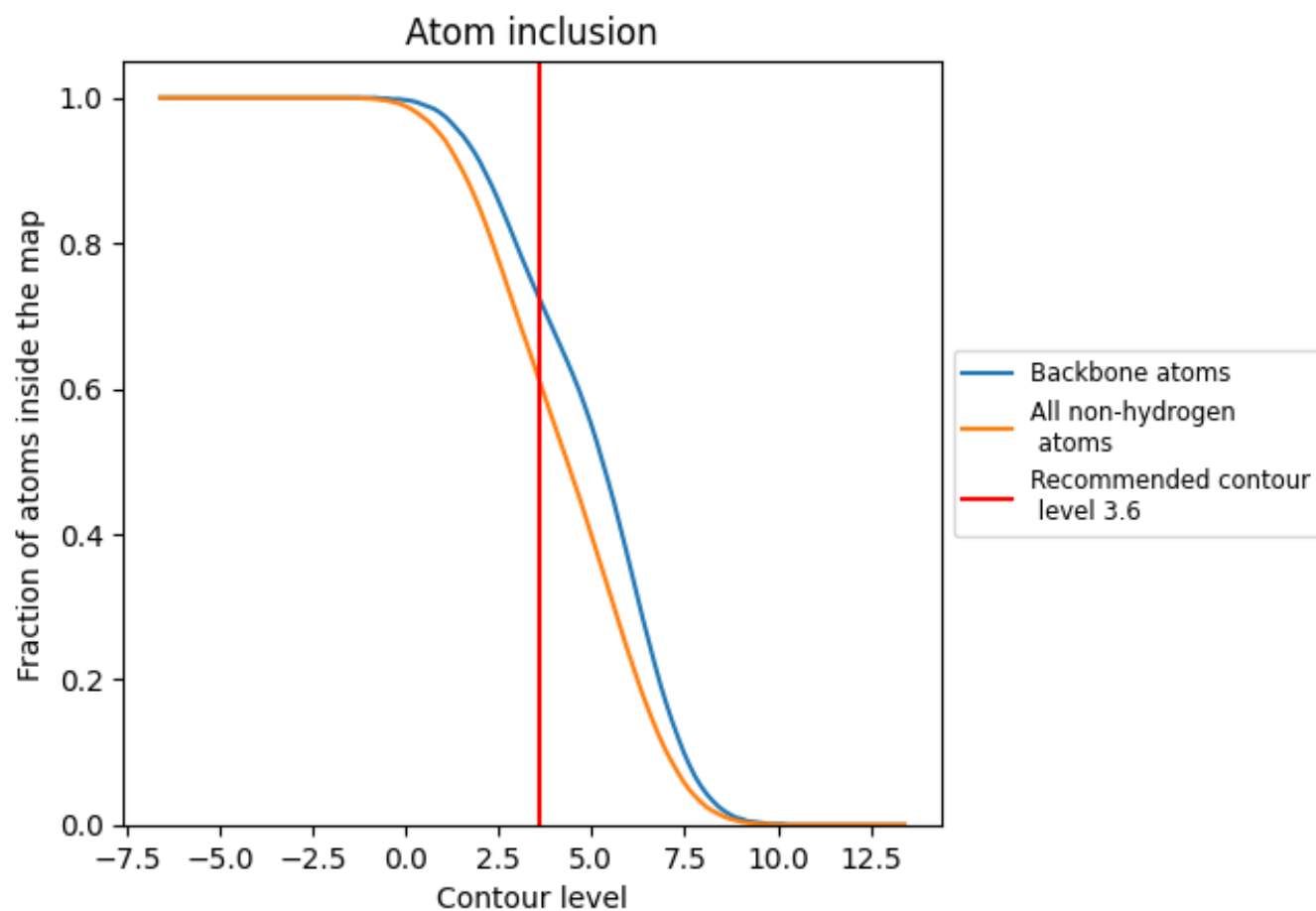
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3.6).

9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 61% 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 (3.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6100	 0.4830
0	 0.6640	 0.5110
1	 0.6770	 0.5160
A	 0.4610	 0.4040
B	 0.4560	 0.4070
C	 0.4500	 0.4060
D	 0.4470	 0.4040
E	 0.4490	 0.4020
F	 0.4490	 0.4070
G	 0.4600	 0.4020
H	 0.4510	 0.4010
I	 0.4600	 0.4070
J	 0.4500	 0.3990
K	 0.4500	 0.3980
L	 0.4490	 0.3960
M	 0.7020	 0.5310
N	 0.7040	 0.5300
O	 0.7050	 0.5280
P	 0.7000	 0.5290
Q	 0.6990	 0.5290
R	 0.7040	 0.5320
S	 0.7090	 0.5300
T	 0.7130	 0.5320
U	 0.7040	 0.5290
V	 0.7050	 0.5280
W	 0.6920	 0.5270
X	 0.6860	 0.5260
Y	 0.6810	 0.5110
Z	 0.7120	 0.5360
a	 0.6710	 0.5150
b	 0.6960	 0.5270
c	 0.6800	 0.5190
d	 0.6940	 0.5330
e	 0.6910	 0.5290
f	 0.7020	 0.5290



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
g	 0.6850	 0.5250
h	 0.6390	 0.5140
i	 0.7030	 0.5320
j	 0.6830	 0.5350
k	 0.6970	 0.5310
l	 0.6980	 0.5290
m	 0.6400	 0.5040
n	 0.7060	 0.5310
o	 0.7020	 0.5370
p	 0.6820	 0.5120
q	 0.6830	 0.5180
r	 0.6880	 0.5190
s	 0.6760	 0.5150
t	 0.7170	 0.5380
u	 0.6460	 0.4980
v	 0.6700	 0.5220
w	 0.6560	 0.5080
x	 0.6640	 0.5140
y	 0.7070	 0.5310
z	 0.6810	 0.5230