



Full wwPDB EM Validation Report ⓘ

Mar 26, 2026 – 07:33 AM UTC

PDB ID : 8KEA / pdb_00008kea
EMDB ID : EMD-37151
Title : Cyanophage A-1(L) baseplate-initiators
Authors : Yu, R.C.; Li, Q.; Zhou, C.Z.
Deposited on : 2023-08-11
Resolution : 3.44 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:

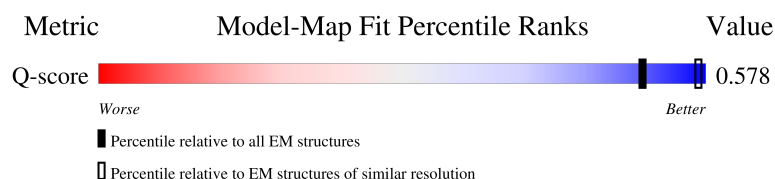
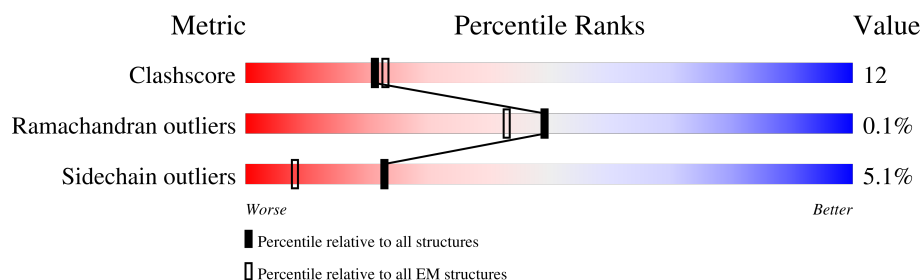
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.44 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	13877 (2.94 - 3.94)

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	A	899	 12% 73% 24% ..
1	B	899	 13% 71% 25% ..
1	C	899	 12% 70% 25% ..
2	D	270	 17% 59% 28% 9%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	E	270	
2	F	270	
3	G	689	
3	H	689	
3	I	689	
4	J	155	
4	K	155	
4	L	155	
4	M	155	
4	N	155	
4	O	155	
5	P	282	
5	Q	282	
5	R	282	
5	S	282	
5	T	282	
5	U	282	
6	V	114	
6	W	114	
6	X	114	
6	Y	114	
6	Z	114	
6	a	114	
7	b	390	
7	d	390	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
7	e	390	
7	g	390	
7	h	390	
7	j	390	
7	k	390	
7	m	390	
7	n	390	
7	p	390	
7	q	390	
7	s	390	
8	c	191	
8	f	191	
8	i	191	
8	l	191	
8	o	191	
8	r	191	

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 97165 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 hub.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	878	Total	C	N	O	S	0	0
			6783	4258	1169	1345	11		
1	B	878	Total	C	N	O	S	0	0
			6783	4258	1169	1345	11		
1	C	878	Total	C	N	O	S	0	0
			6783	4258	1169	1345	11		

- Molecule 2 is a protein called central spike.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	245	Total	C	N	O	S	0	0
			1899	1178	335	380	6		
2	E	245	Total	C	N	O	S	0	0
			1899	1178	335	380	6		
2	F	245	Total	C	N	O	S	0	0
			1899	1178	335	380	6		

- Molecule 3 is a protein called tmp.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	G	24	Total	C	N	O	0	0
			187	118	31	38		
3	H	24	Total	C	N	O	0	0
			187	118	31	38		
3	I	24	Total	C	N	O	0	0
			187	118	31	38		

- Molecule 4 is a protein called baseplate gp16.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	J	151	Total	C	N	O	S	0	0
			1173	742	191	239	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
4	K	154	Total	C	N	O	S	0	0
			1198	755	196	246	1		
4	L	151	Total	C	N	O	S	0	0
			1173	742	191	239	1		
4	M	153	Total	C	N	O	S	0	0
			1188	750	194	243	1		
4	N	151	Total	C	N	O	S	0	0
			1173	742	191	239	1		
4	O	153	Total	C	N	O	S	0	0
			1188	750	194	243	1		

- Molecule 5 is a protein called tube initiator.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	P	279	Total	C	N	O	S	0	0
			2217	1413	379	417	8		
5	Q	279	Total	C	N	O	S	0	0
			2217	1413	379	417	8		
5	R	281	Total	C	N	O	S	0	0
			2238	1424	385	421	8		
5	S	279	Total	C	N	O	S	0	0
			2217	1413	379	417	8		
5	T	279	Total	C	N	O	S	0	0
			2217	1413	379	417	8		
5	U	279	Total	C	N	O	S	0	0
			2217	1413	379	417	8		

- Molecule 6 is a protein called sheath initiator.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	V	113	Total	C	N	O	S	0	0
			907	586	142	178	1		
6	W	113	Total	C	N	O	S	0	0
			907	586	142	178	1		
6	X	113	Total	C	N	O	S	0	0
			907	586	142	178	1		
6	Y	113	Total	C	N	O	S	0	0
			907	586	142	178	1		
6	Z	113	Total	C	N	O	S	0	0
			907	586	142	178	1		
6	a	113	Total	C	N	O	S	0	0
			907	586	142	178	1		

- Molecule 7 is a protein called wedge protein gp31.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	b	386	Total	C	N	O	S	0	0
			2952	1882	479	582	9		
7	d	382	Total	C	N	O	S	0	0
			2918	1863	474	572	9		
7	e	386	Total	C	N	O	S	0	0
			2952	1882	479	582	9		
7	g	382	Total	C	N	O	S	0	0
			2918	1863	474	572	9		
7	h	386	Total	C	N	O	S	0	0
			2952	1882	479	582	9		
7	j	382	Total	C	N	O	S	0	0
			2918	1863	474	572	9		
7	k	386	Total	C	N	O	S	0	0
			2952	1882	479	582	9		
7	m	382	Total	C	N	O	S	0	0
			2918	1863	474	572	9		
7	n	386	Total	C	N	O	S	0	0
			2952	1882	479	582	9		
7	p	382	Total	C	N	O	S	0	0
			2918	1863	474	572	9		
7	q	386	Total	C	N	O	S	0	0
			2952	1882	479	582	9		
7	s	382	Total	C	N	O	S	0	0
			2918	1863	474	572	9		

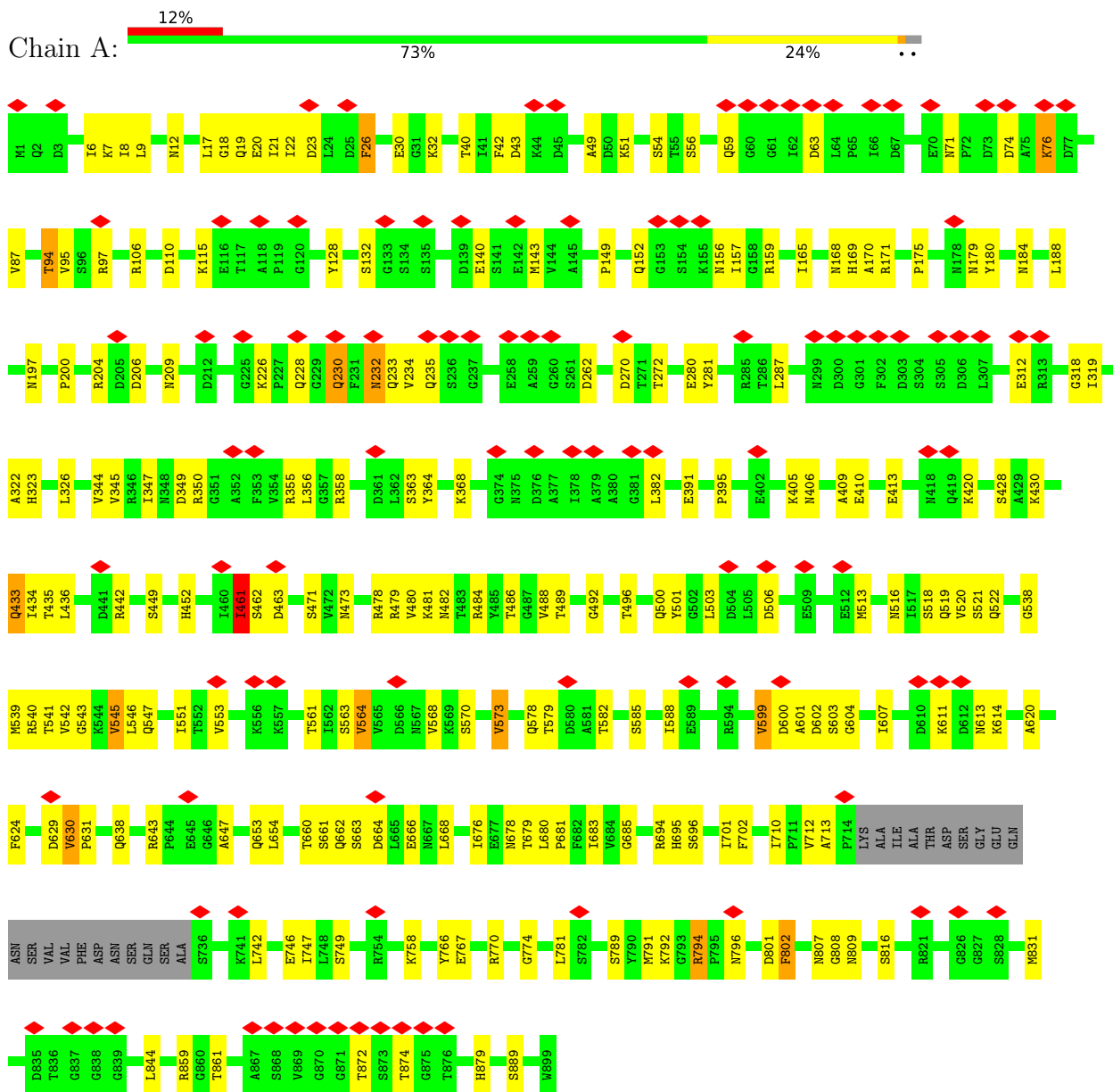
- Molecule 8 is a protein called wedge protein gp32.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	c	190	Total	C	N	O	S	0	0
			1580	1032	254	289	5		
8	f	190	Total	C	N	O	S	0	0
			1580	1032	254	289	5		
8	i	190	Total	C	N	O	S	0	0
			1580	1032	254	289	5		
8	l	190	Total	C	N	O	S	0	0
			1580	1032	254	289	5		
8	o	190	Total	C	N	O	S	0	0
			1580	1032	254	289	5		
8	r	190	Total	C	N	O	S	0	0
			1580	1032	254	289	5		

3 Residue-property plots

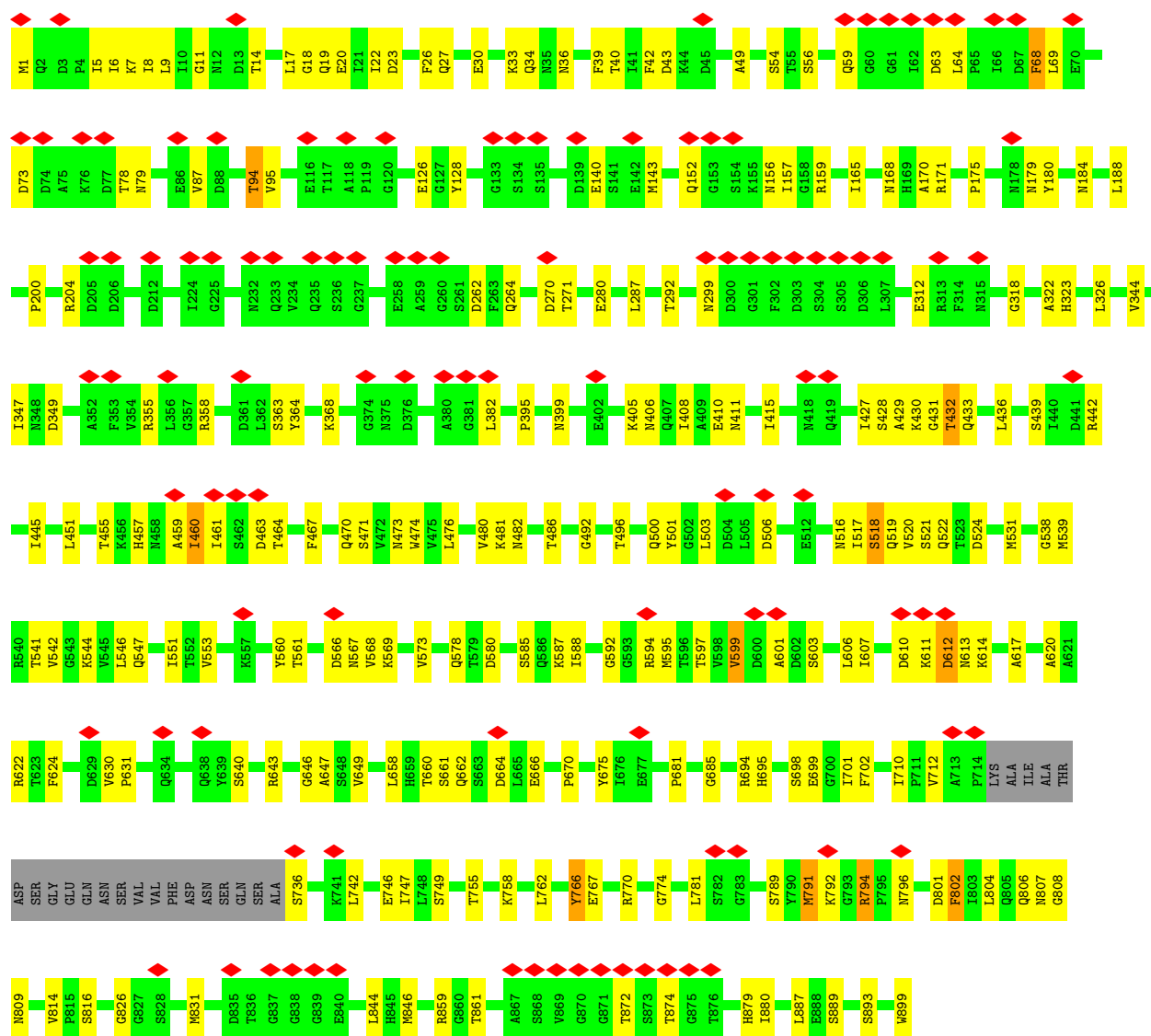
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: hub



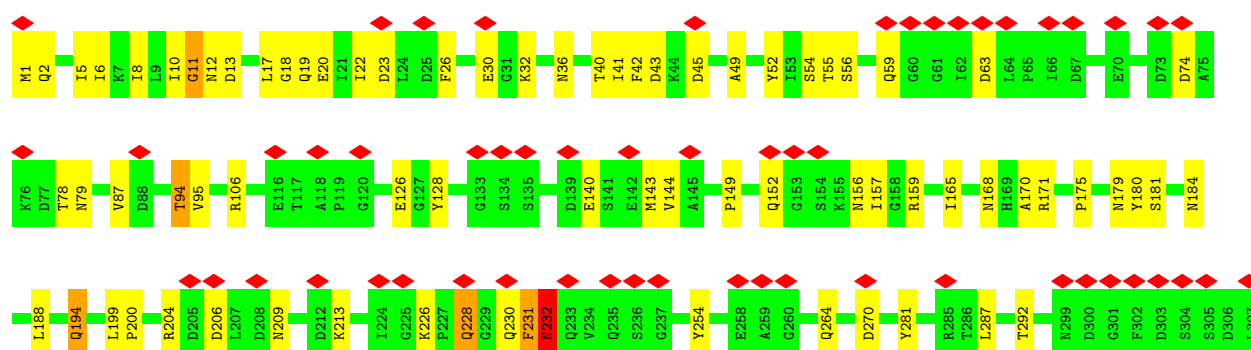
- Molecule 1: hub

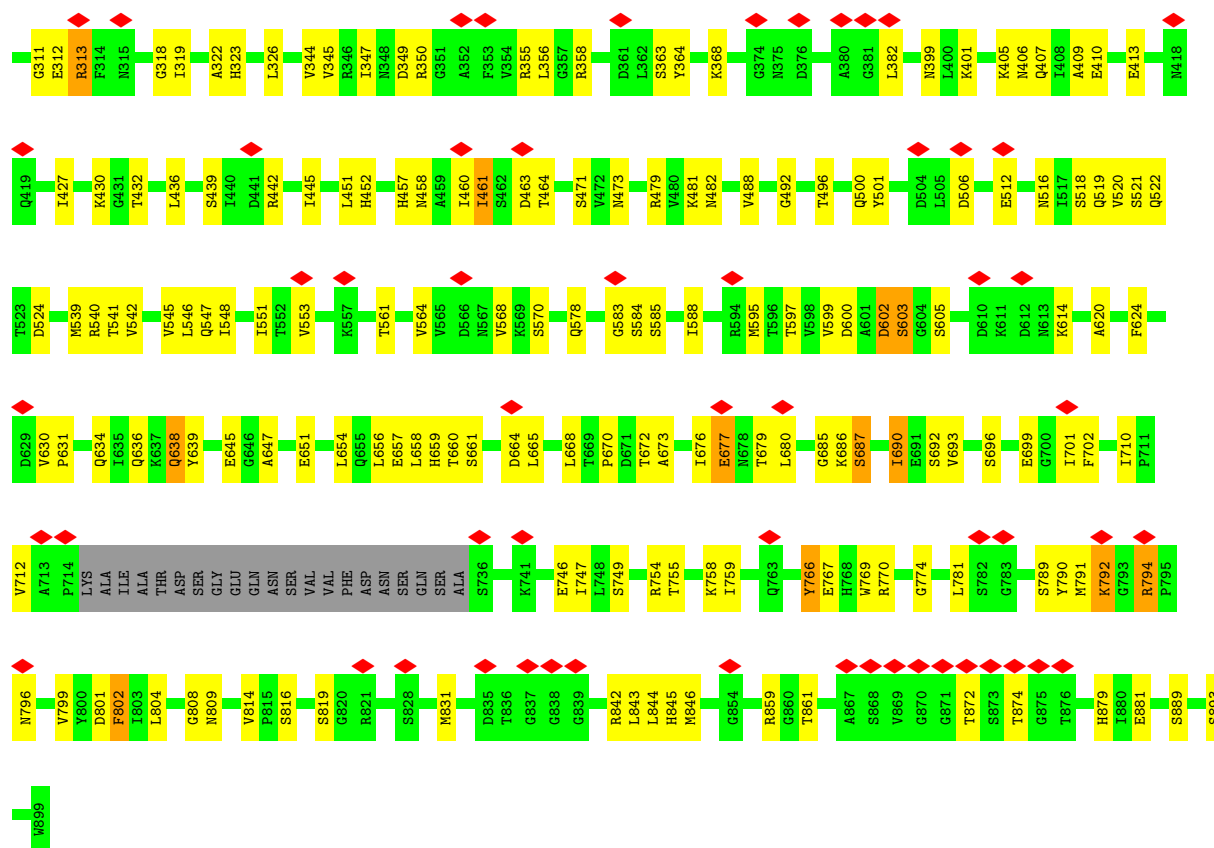
Chain B: 13% 71% 25% ..



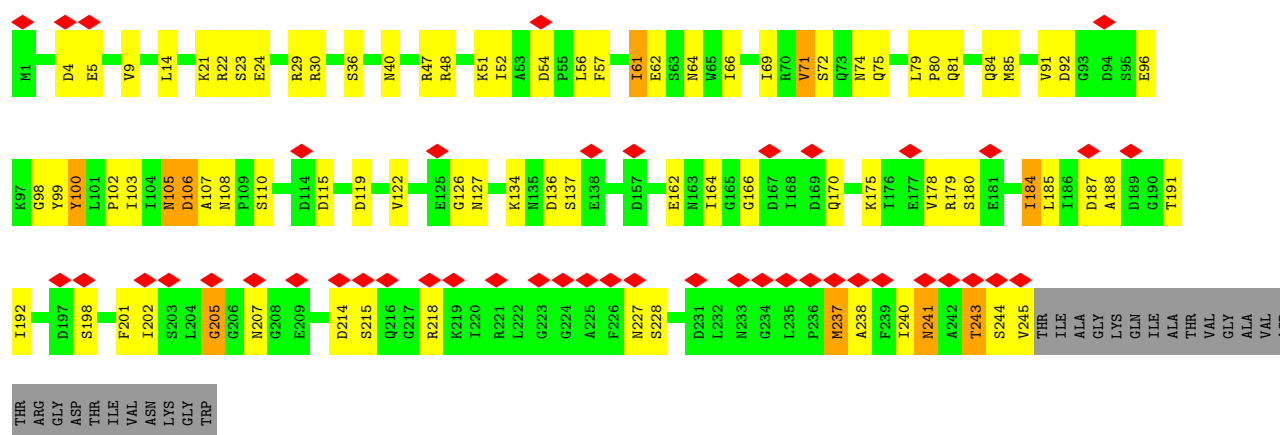
• Molecule 1: hub

Chain C: 12% 70% 25% ..

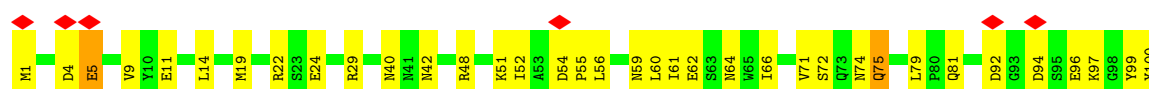




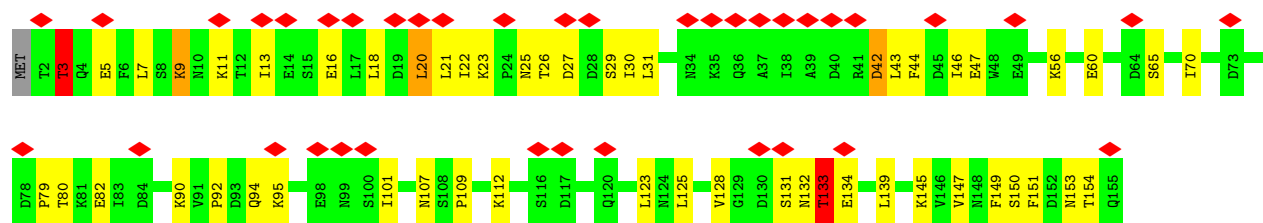
• Molecule 2: central spike



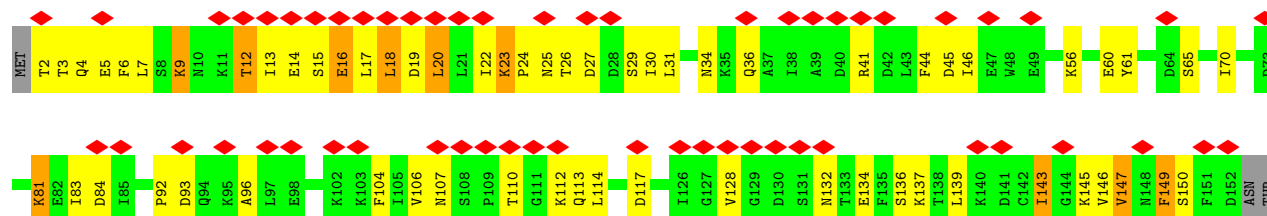
• Molecule 2: central spike





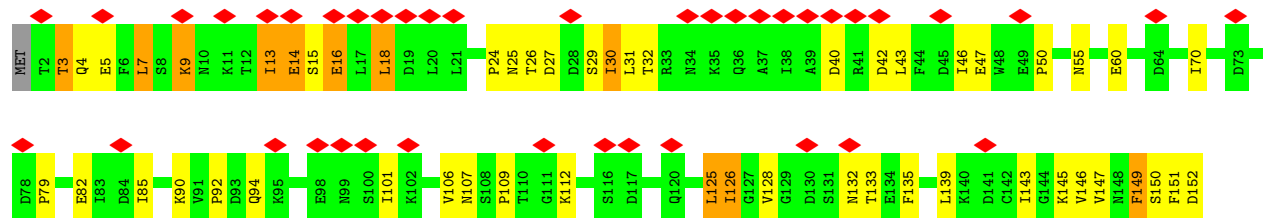


• Molecule 4: baseplate gp16



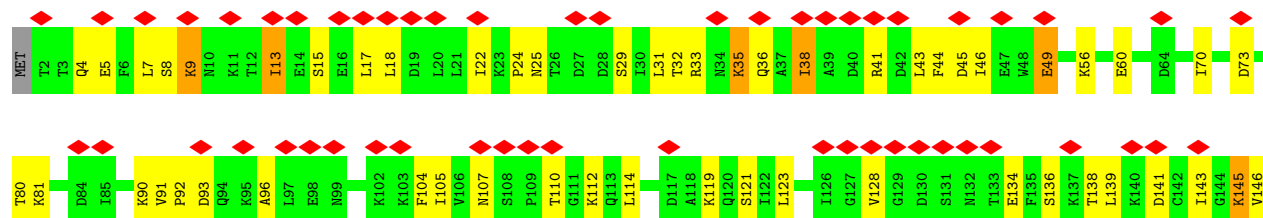
GLN

• Molecule 4: baseplate gp16



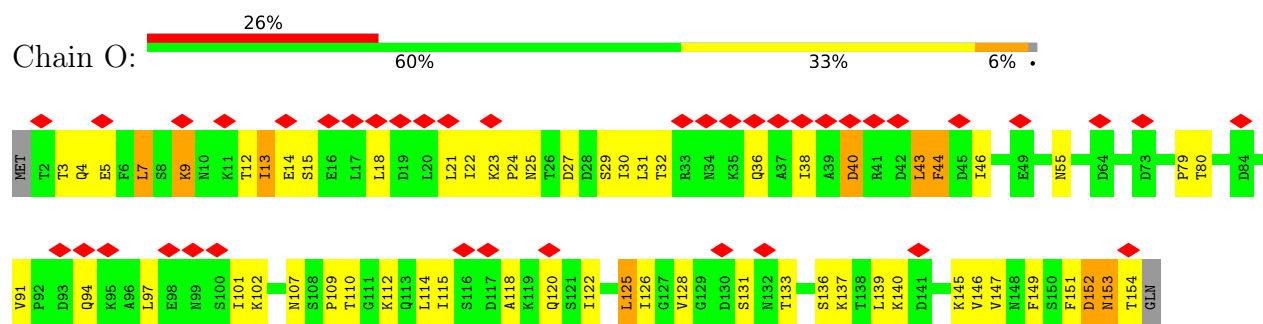
N153
T154
GLN

• Molecule 4: baseplate gp16

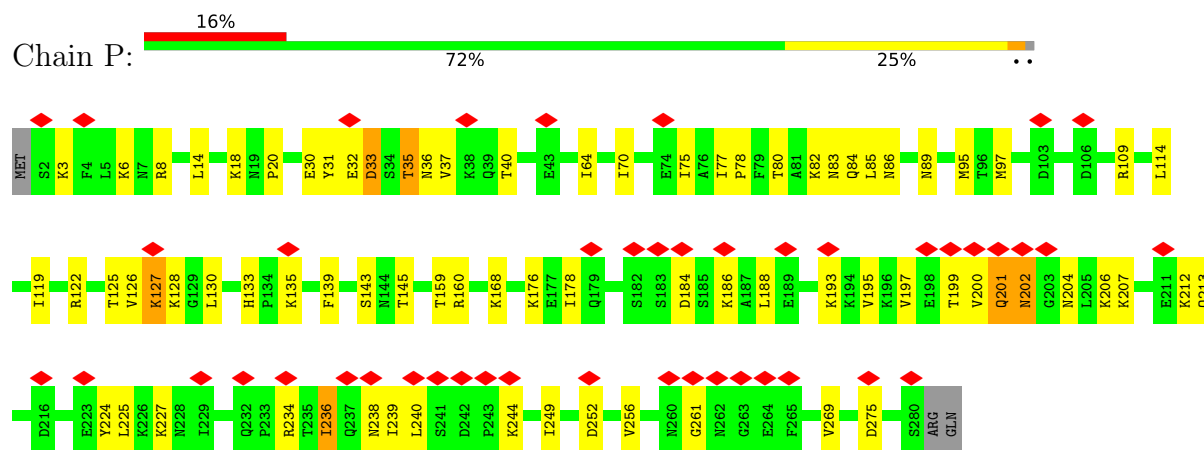


V147
N148
F151
D152
ASN
THR
GLN

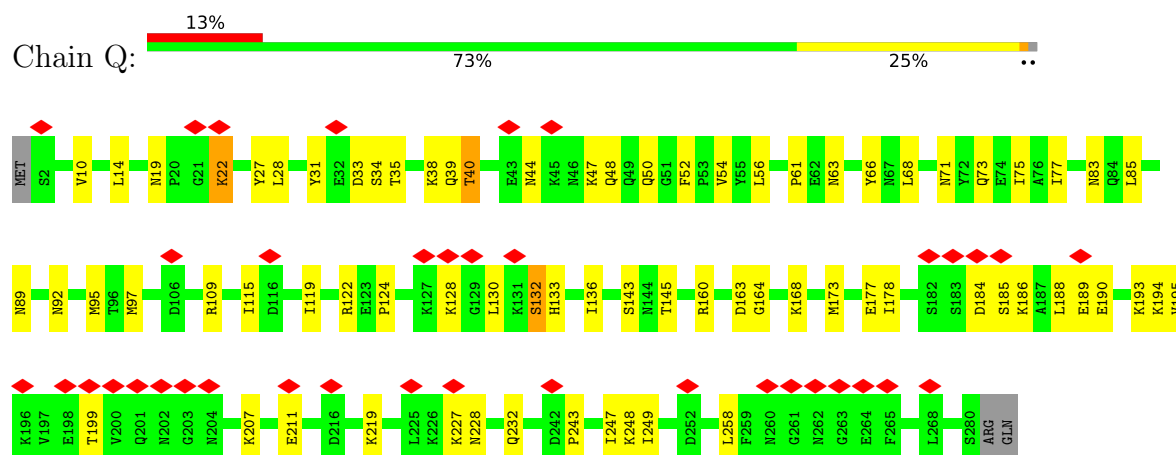
- Molecule 4: baseplate gp16



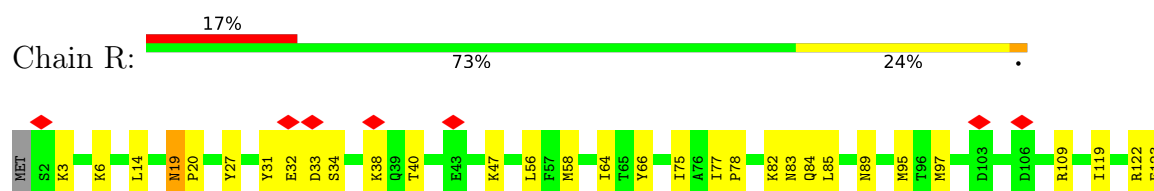
- Molecule 5: tube initiator

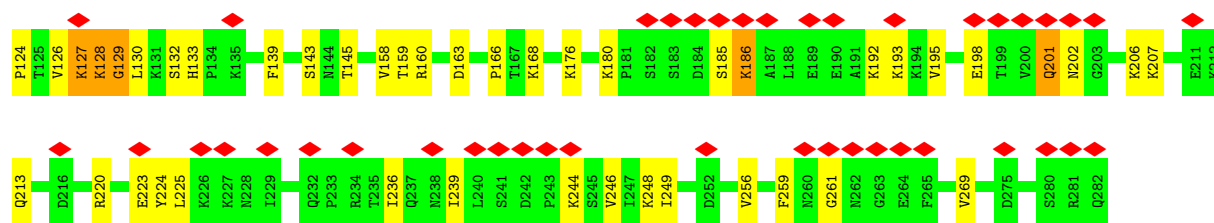


- Molecule 5: tube initiator

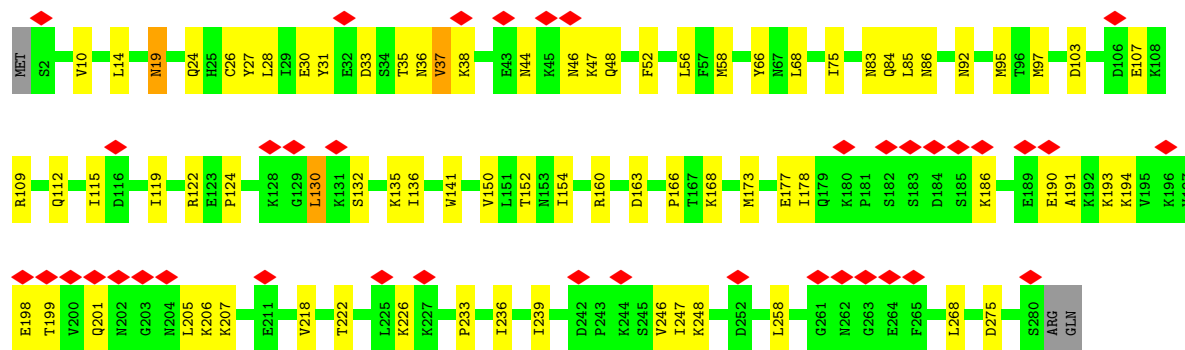


- Molecule 5: tube initiator

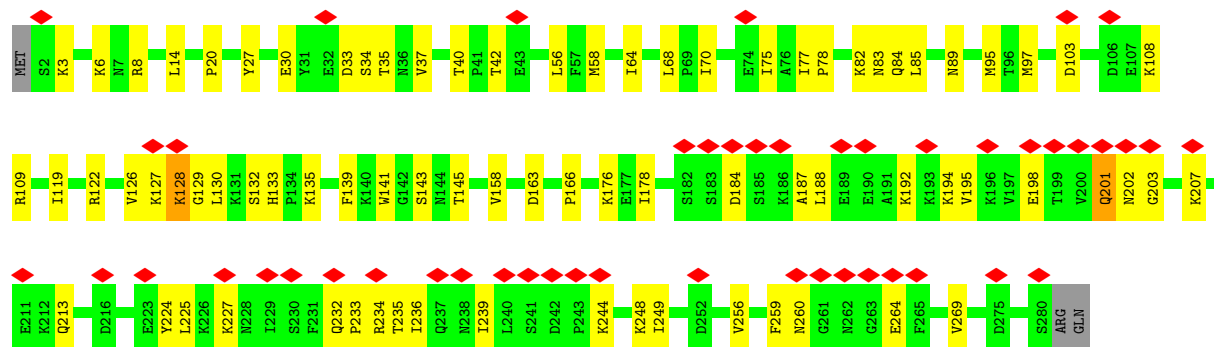




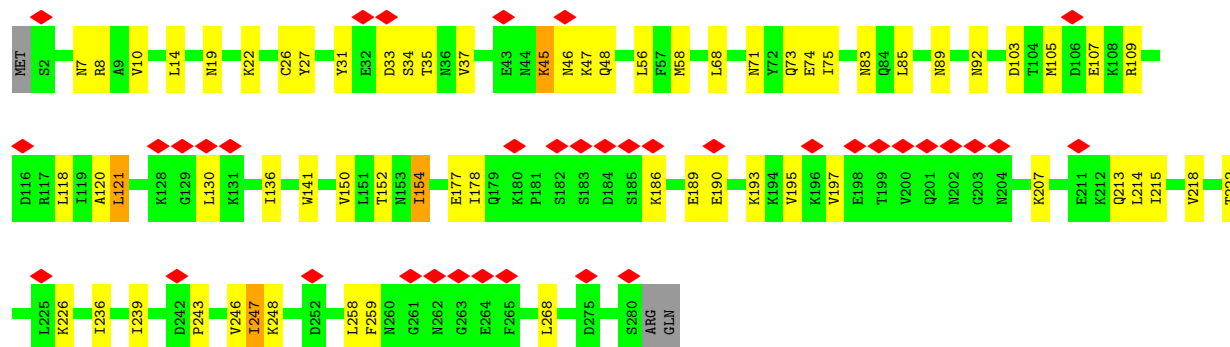
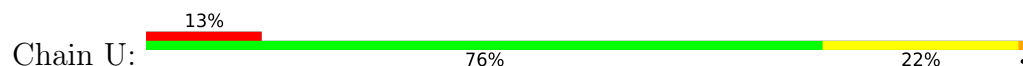
• Molecule 5: tube initiator



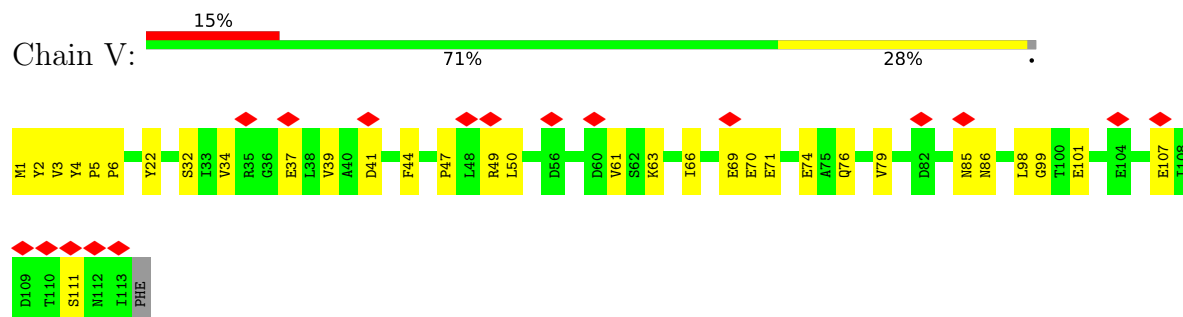
• Molecule 5: tube initiator



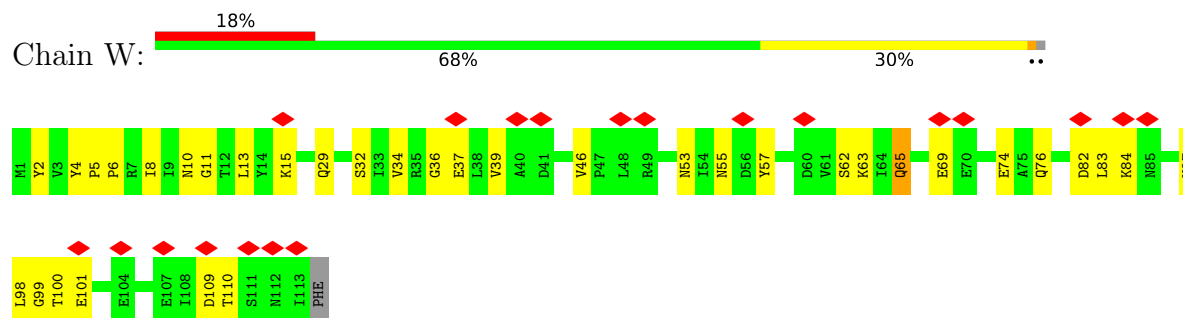
• Molecule 5: tube initiator



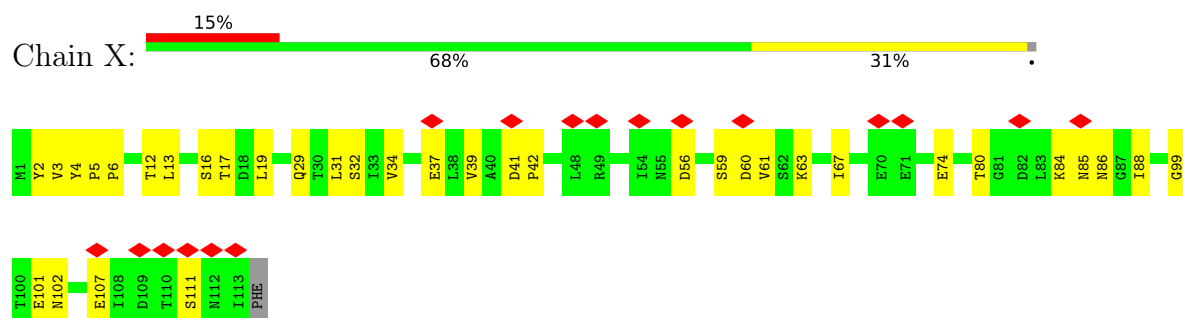
- Molecule 6: sheath initiator



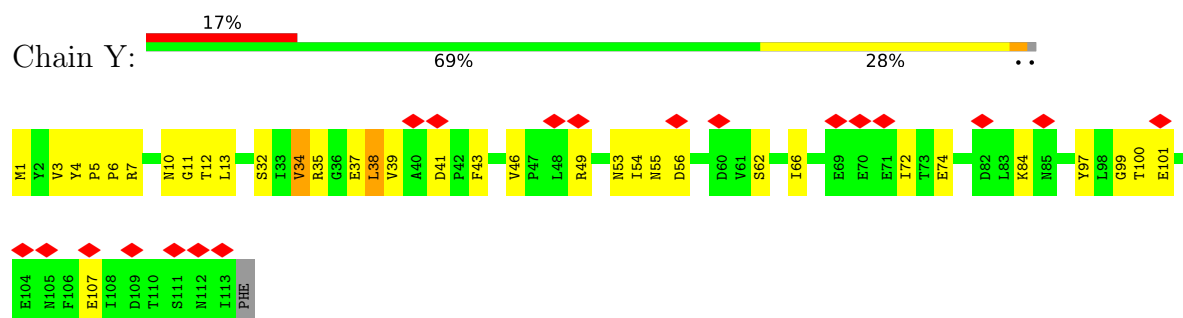
- Molecule 6: sheath initiator



- Molecule 6: sheath initiator

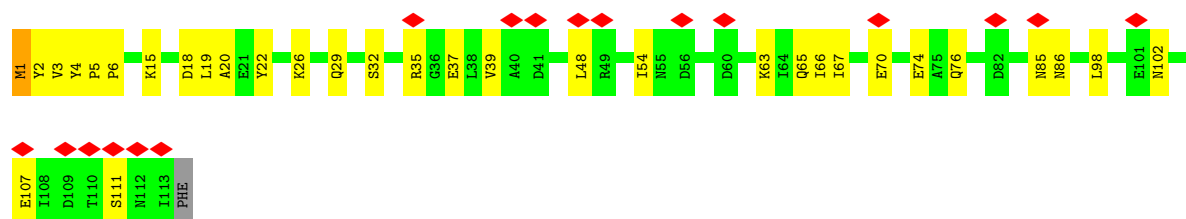


- Molecule 6: sheath initiator

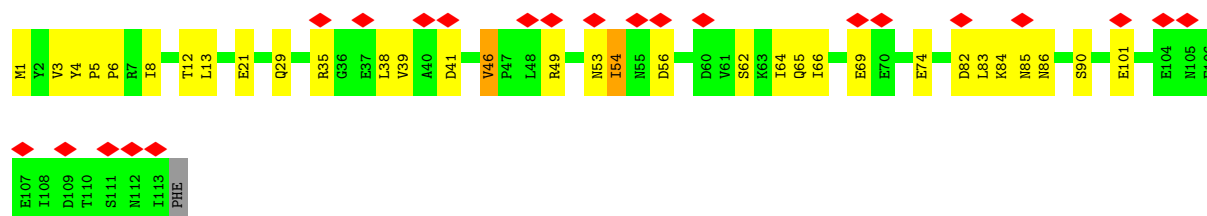


- Molecule 6: sheath initiator

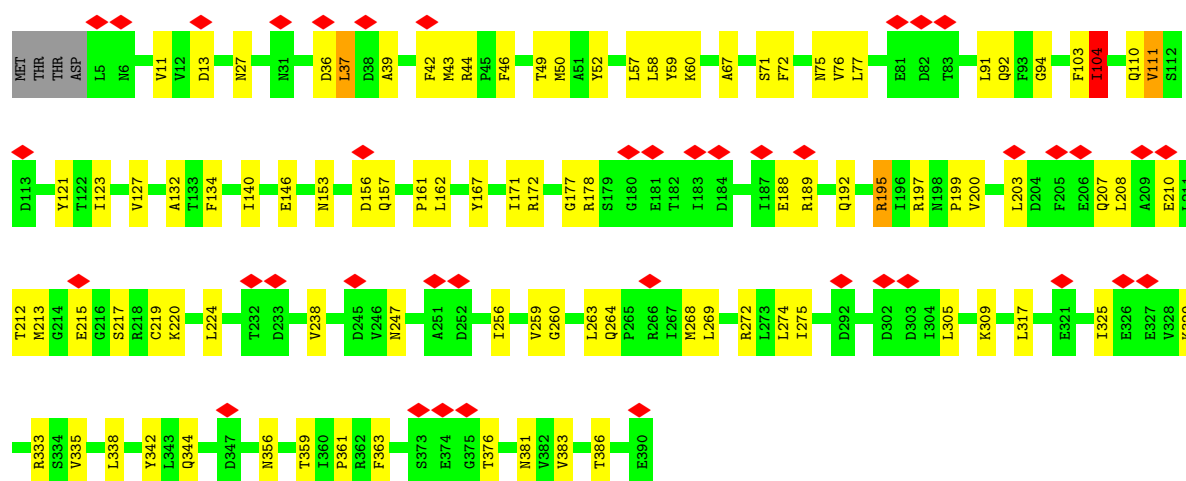
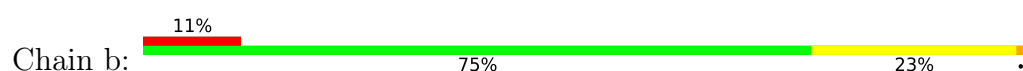




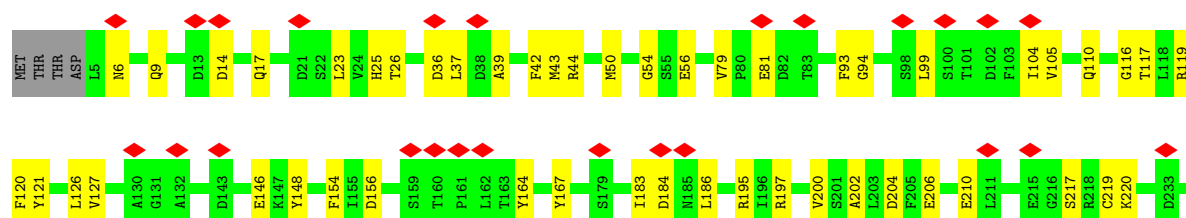
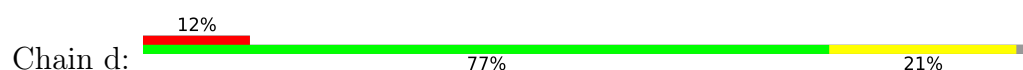
• Molecule 6: sheath initiator

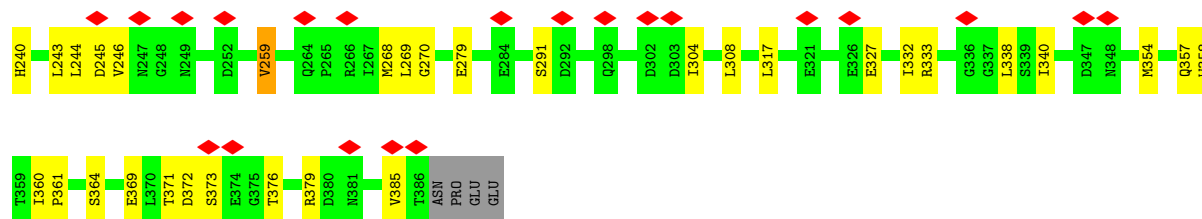


• Molecule 7: wedge protein gp31

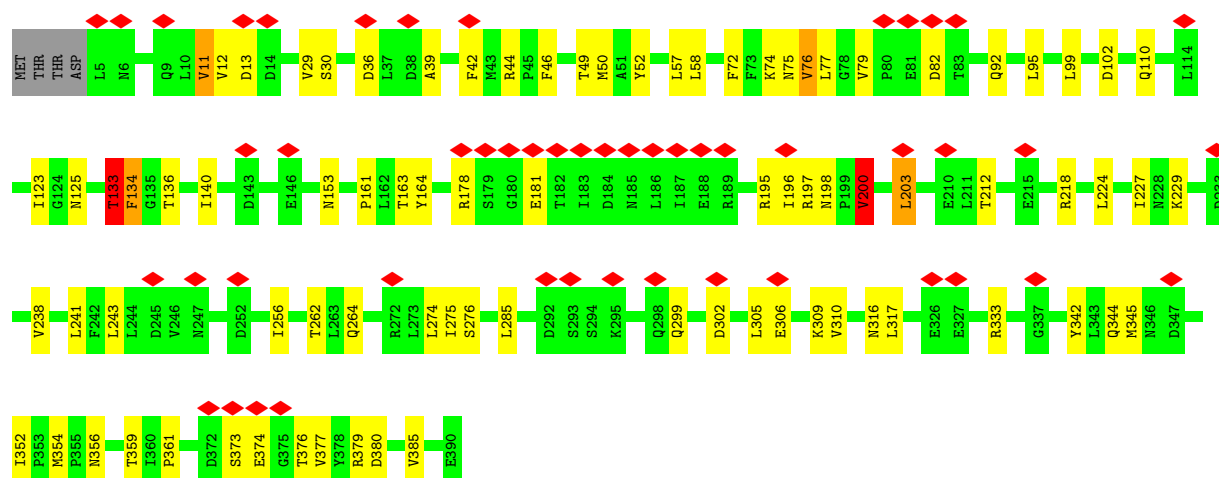
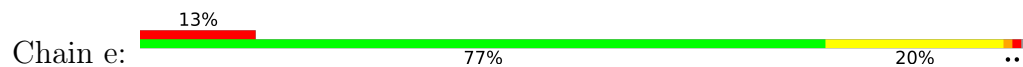


• Molecule 7: wedge protein gp31

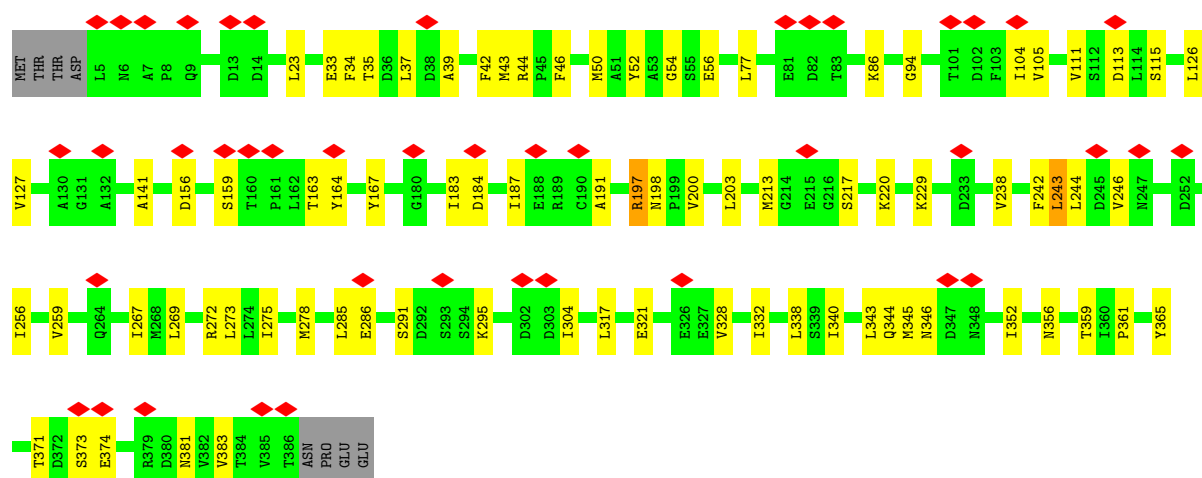
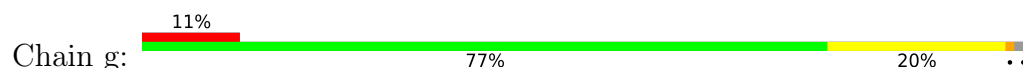




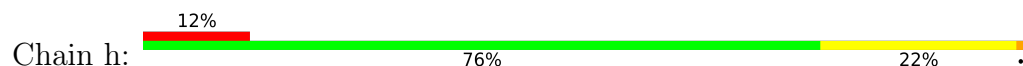
• Molecule 7: wedge protein gp31

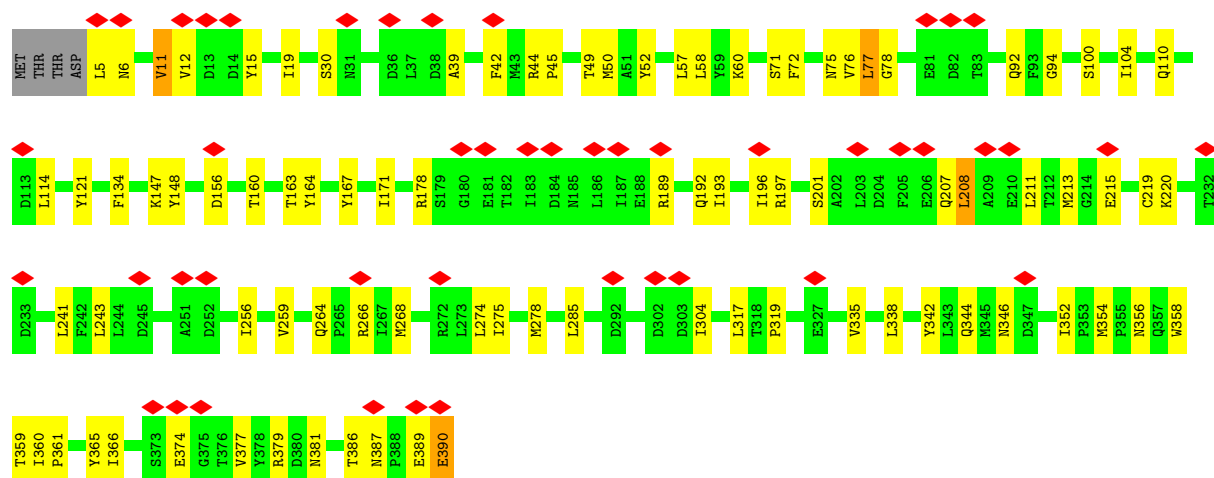


• Molecule 7: wedge protein gp31

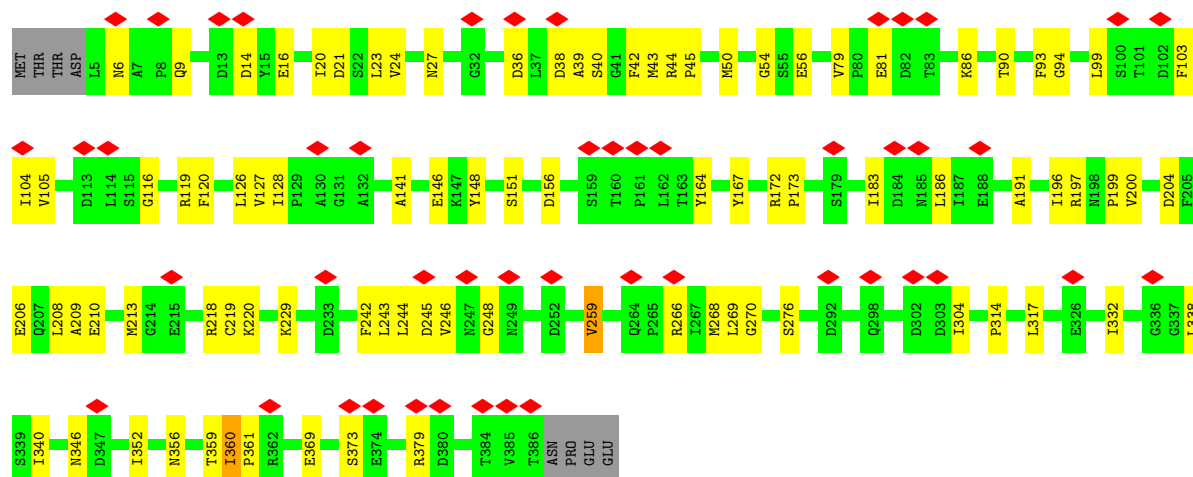
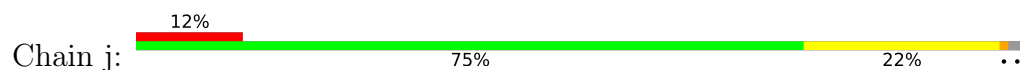


• Molecule 7: wedge protein gp31

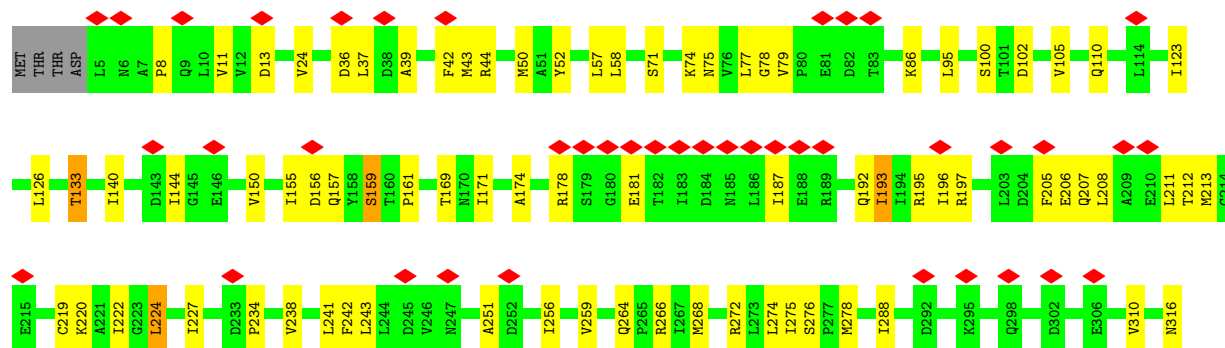
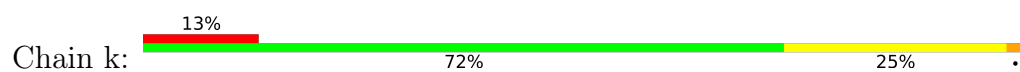


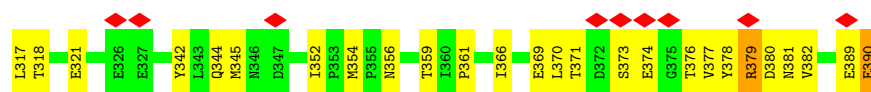


• Molecule 7: wedge protein gp31

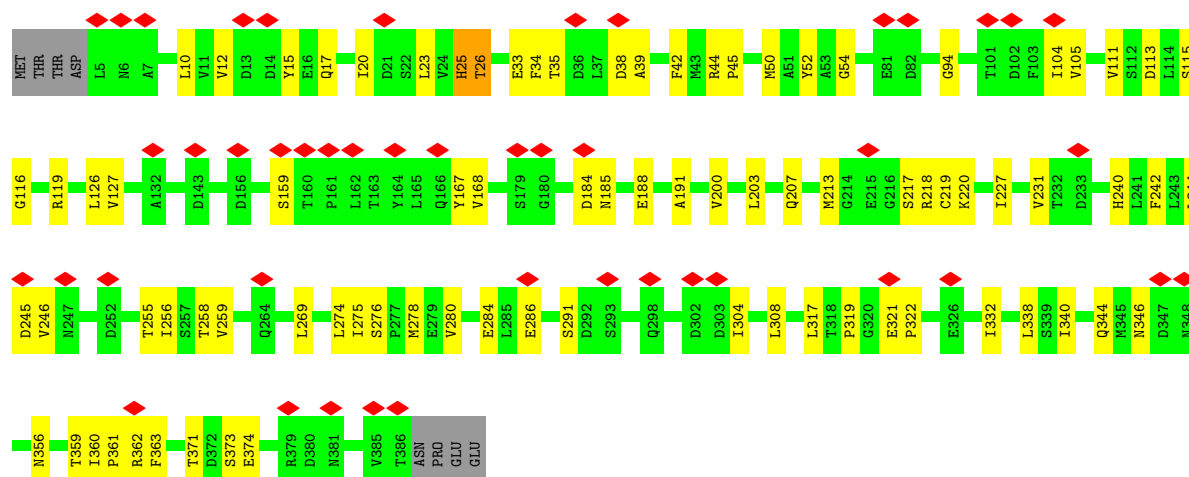
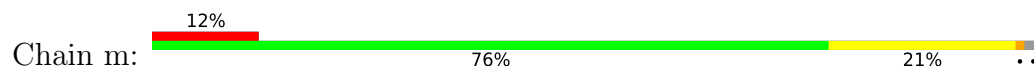


• Molecule 7: wedge protein gp31

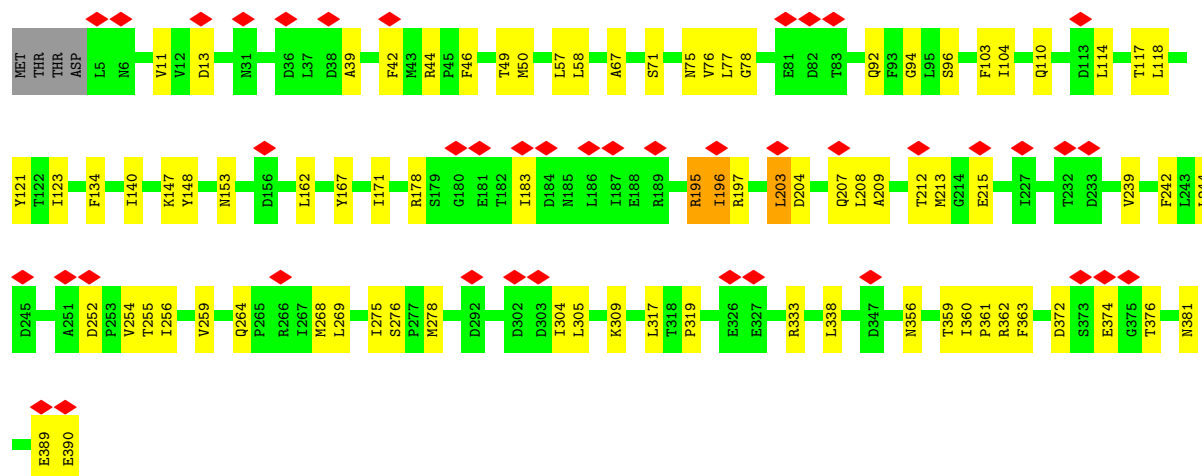
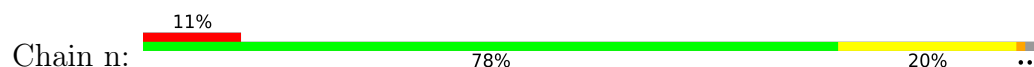




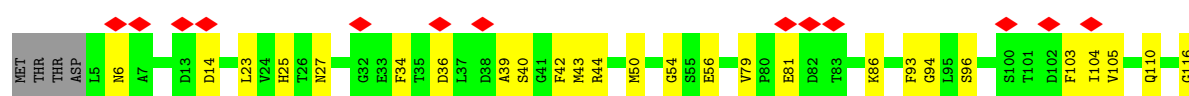
• Molecule 7: wedge protein gp31

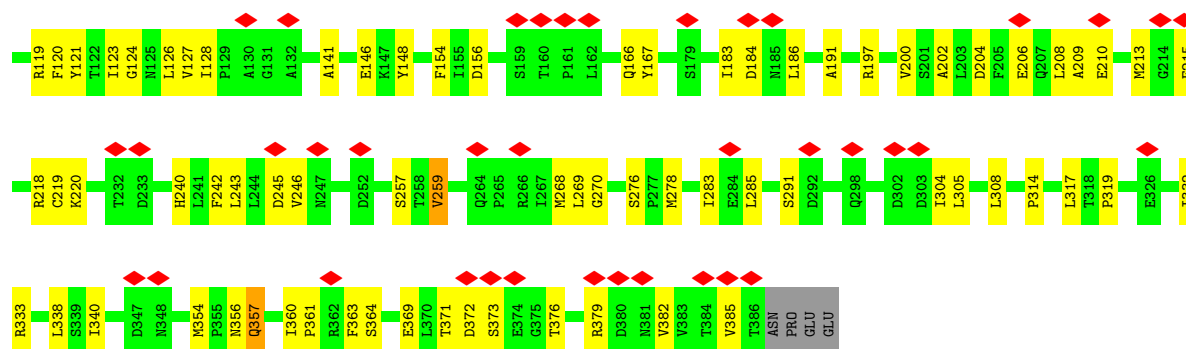


• Molecule 7: wedge protein gp31

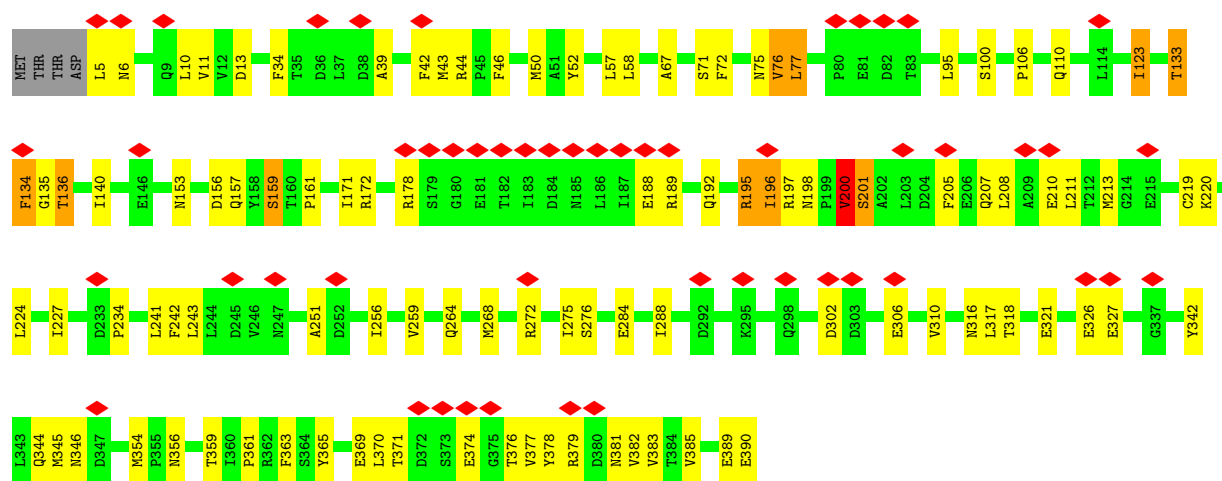
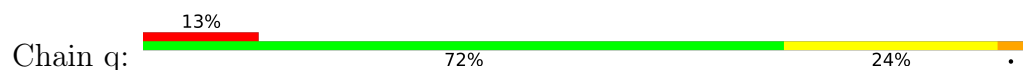


• Molecule 7: wedge protein gp31

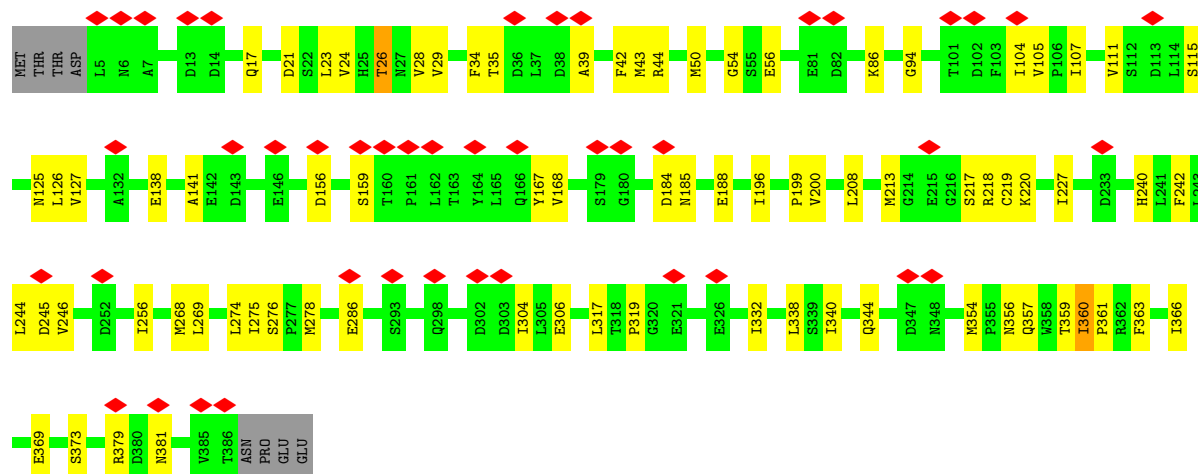
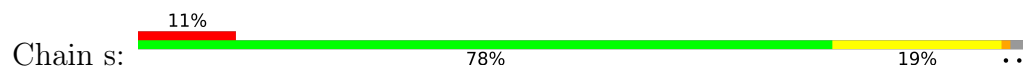




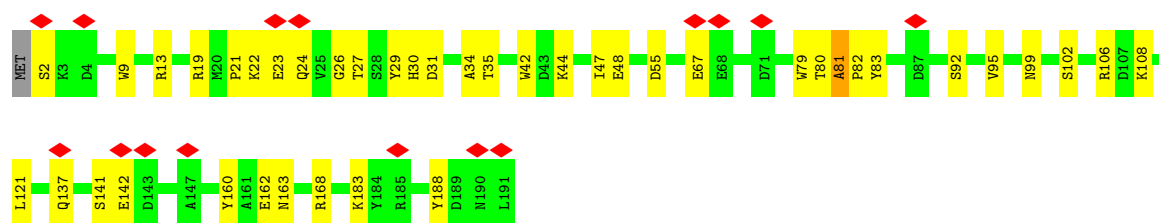
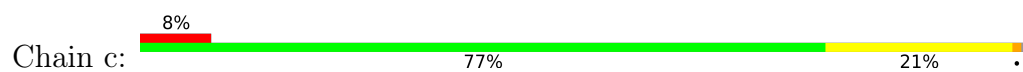
• Molecule 7: wedge protein gp31



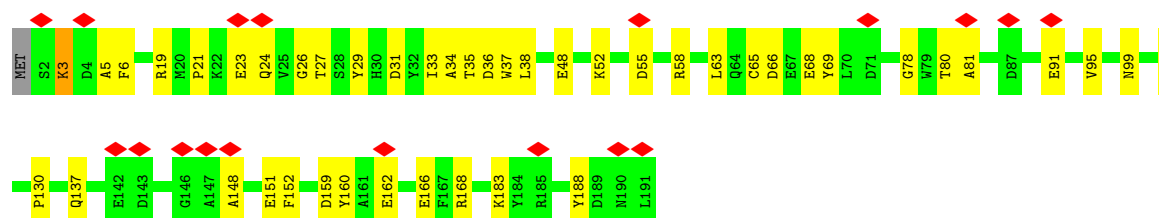
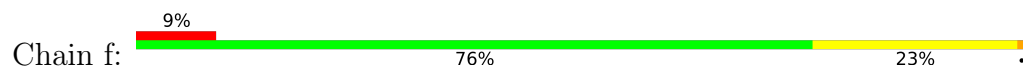
• Molecule 7: wedge protein gp31



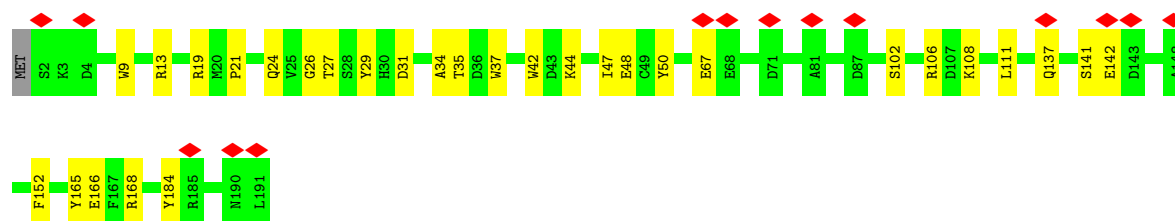
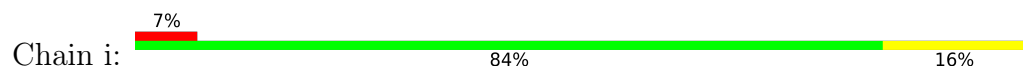
• Molecule 8: wedge protein gp32



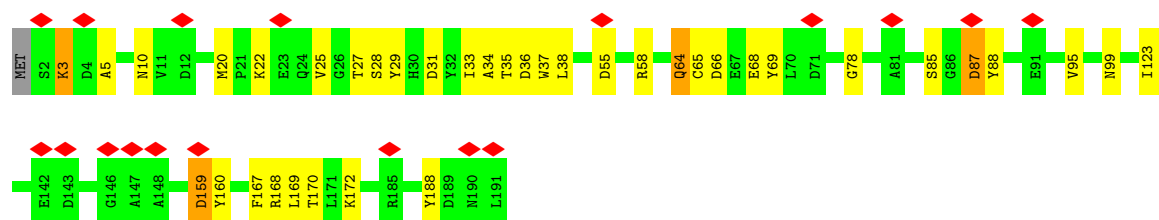
- Molecule 8: wedge protein gp32



- Molecule 8: wedge protein gp32



- Molecule 8: wedge protein gp32

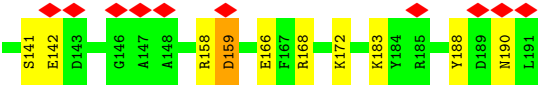
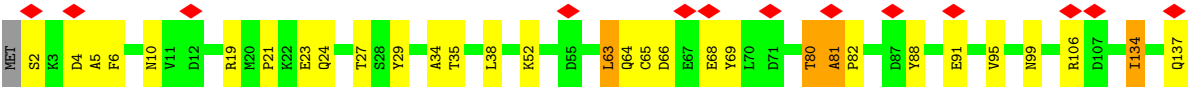
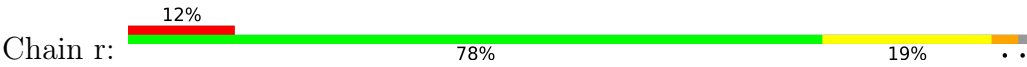


- Molecule 8: wedge protein gp32





• Molecule 8: wedge protein gp32



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	41062	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.033	Depositor
Minimum map value	-0.014	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.01	Depositor
Map size ($\text{\AA}$)	479.36002, 479.36002, 479.36002	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.07, 1.07, 1.07	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.17	0/6909	0.41	1/9362 (0.0%)
1	B	0.18	0/6909	0.47	8/9362 (0.1%)
1	C	0.20	0/6909	0.52	13/9362 (0.1%)
2	D	0.27	0/1926	0.61	6/2612 (0.2%)
2	E	0.25	0/1926	0.52	1/2612 (0.0%)
2	F	0.26	0/1926	0.60	6/2612 (0.2%)
3	G	0.68	0/190	1.01	1/257 (0.4%)
3	H	0.64	0/190	1.29	4/257 (1.6%)
3	I	0.64	0/190	0.95	1/257 (0.4%)
4	J	0.29	0/1189	0.87	11/1607 (0.7%)
4	K	0.28	0/1214	0.65	2/1640 (0.1%)
4	L	0.30	0/1189	0.70	3/1607 (0.2%)
4	M	0.30	0/1204	0.72	2/1628 (0.1%)
4	N	0.26	0/1189	0.60	1/1607 (0.1%)
4	O	0.32	0/1204	0.65	3/1628 (0.2%)
5	P	0.24	0/2259	0.51	2/3052 (0.1%)
5	Q	0.25	0/2259	0.49	2/3052 (0.1%)
5	R	0.26	0/2280	0.50	4/3078 (0.1%)
5	S	0.21	0/2259	0.49	4/3052 (0.1%)
5	T	0.24	0/2259	0.52	3/3052 (0.1%)
5	U	0.23	0/2259	0.56	6/3052 (0.2%)
6	V	0.19	0/924	0.47	0/1258
6	W	0.16	0/924	0.43	0/1258
6	X	0.18	0/924	0.43	0/1258
6	Y	0.30	0/924	0.62	3/1258 (0.2%)
6	Z	0.21	0/924	0.54	0/1258
6	a	0.17	0/924	0.42	0/1258
7	b	0.20	0/3006	0.42	1/4100 (0.0%)
7	d	0.19	0/2971	0.35	0/4053
7	e	0.26	0/3006	0.49	3/4100 (0.1%)
7	g	0.19	0/2971	0.36	0/4053
7	h	0.22	0/3006	0.43	0/4100
7	j	0.22	0/2971	0.42	3/4053 (0.1%)
7	k	0.22	0/3006	0.44	0/4100

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
7	m	0.20	0/2971	0.36	0/4053
7	n	0.21	0/3006	0.43	2/4100 (0.0%)
7	p	0.18	0/2971	0.33	0/4053
7	q	0.31	0/3006	0.55	5/4100 (0.1%)
7	s	0.21	0/2971	0.40	1/4053 (0.0%)
8	c	0.20	0/1632	0.37	0/2224
8	f	0.21	0/1632	0.43	2/2224 (0.1%)
8	i	0.20	0/1632	0.35	0/2224
8	l	0.20	0/1632	0.39	0/2224
8	o	0.24	0/1632	0.40	0/2224
8	r	0.20	0/1632	0.42	3/2224 (0.1%)
All	All	0.23	0/99037	0.49	107/134558 (0.1%)

There are no bond length outliers.

All (107) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	15	SER	N-CA-C	-12.18	98.90	113.88
1	C	792	LYS	N-CA-C	11.75	126.78	111.75
3	H	682	GLN	N-CA-C	-11.69	98.51	113.12
5	U	121	LEU	N-CA-C	-11.00	97.92	114.64
7	q	136	THR	N-CA-C	10.09	125.16	109.52
2	D	107	ALA	N-CA-C	-9.43	101.19	112.89
1	B	460	ILE	N-CA-C	9.36	120.56	111.67
4	J	13	ILE	N-CA-C	-9.14	104.24	113.10
4	J	45	ASP	N-CA-C	9.03	123.23	110.68
5	T	33	ASP	N-CA-C	-9.03	101.23	112.88
4	L	45	ASP	N-CA-C	8.82	122.94	110.68
7	j	24	VAL	N-CA-C	-8.66	100.14	112.35
1	B	612	ASP	N-CA-C	8.60	121.43	111.11
2	F	107	ALA	N-CA-C	-8.58	102.07	112.54
1	B	459	ALA	N-CA-C	8.27	123.73	112.90
1	C	231	PHE	N-CA-C	-7.95	97.75	108.24
4	J	15	SER	N-CA-C	-7.91	103.62	113.28
6	Y	41	ASP	CA-C-N	-7.65	111.96	120.45
6	Y	41	ASP	C-N-CA	-7.65	111.96	120.45
1	C	11	GLY	N-CA-C	-7.60	98.58	111.73
7	e	134	PHE	N-CA-C	7.50	120.61	108.76
2	F	108	ASN	CA-C-N	-7.48	112.97	120.98
2	F	108	ASN	C-N-CA	-7.48	112.97	120.98
4	J	78	ASP	N-CA-C	-7.48	100.38	109.72
1	C	12	ASN	N-CA-C	7.47	121.01	112.57

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	P	35	THR	CB-CA-C	-7.42	101.19	111.95
7	n	195	ARG	N-CA-C	7.28	118.81	108.54
4	M	152	ASP	N-CA-C	7.24	120.45	110.24
5	U	247	ILE	CB-CA-C	7.14	121.40	111.19
5	P	202	ASN	N-CA-C	-7.10	99.03	108.19
5	R	33	ASP	N-CA-C	-7.05	103.85	113.30
7	e	200	VAL	CB-CA-C	-7.00	104.05	110.63
5	U	121	LEU	N-CA-CB	6.91	122.05	111.06
5	T	232	GLN	CA-C-N	-6.86	113.24	120.03
5	T	232	GLN	C-N-CA	-6.86	113.24	120.03
5	S	19	ASN	CA-C-N	-6.77	113.82	120.52
5	S	19	ASN	C-N-CA	-6.77	113.82	120.52
4	N	15	SER	N-CA-C	-6.75	104.05	112.90
7	j	360	ILE	CA-C-N	-6.46	113.98	120.31
7	j	360	ILE	C-N-CA	-6.46	113.98	120.31
3	H	688	TYR	N-CA-C	6.41	119.85	109.40
4	O	131	SER	N-CA-C	-6.41	98.75	109.07
1	B	68	PHE	CB-CA-C	-6.36	98.59	110.36
7	q	196	ILE	CB-CA-C	6.29	118.47	111.80
7	q	135	GLY	N-CA-C	6.25	120.43	111.12
4	L	149	PHE	CB-CA-C	6.23	121.75	109.66
5	U	120	ALA	CB-CA-C	-6.21	102.01	112.00
5	U	19	ASN	CA-C-N	-6.20	114.35	120.98
5	U	19	ASN	C-N-CA	-6.20	114.35	120.98
1	C	792	LYS	CB-CA-C	-6.20	98.44	110.46
8	f	27	THR	N-CA-CB	6.18	120.94	110.49
5	S	36	ASN	CB-CA-C	-6.18	99.34	109.53
2	D	205	GLY	N-CA-C	6.16	119.10	112.33
7	q	197	ARG	N-CA-C	-6.15	98.23	108.32
8	r	81	ALA	N-CA-C	6.03	123.13	109.81
2	D	207	ASN	N-CA-C	-6.00	104.48	112.94
7	e	133	THR	N-CA-C	-5.99	104.36	112.26
6	Y	32	SER	N-CA-C	-5.97	105.82	114.12
7	q	77	LEU	N-CA-C	-5.94	106.58	113.88
1	B	69	LEU	N-CA-CB	5.85	118.70	110.98
5	R	180	LYS	CA-C-N	-5.83	113.93	119.76
5	R	180	LYS	C-N-CA	-5.83	113.93	119.76
1	B	69	LEU	N-CA-C	-5.74	106.06	114.39
5	R	129	GLY	N-CA-C	-5.72	99.62	113.18
2	D	100	TYR	N-CA-C	5.70	118.54	109.81
1	C	231	PHE	CB-CA-C	-5.68	100.41	112.78
4	J	14	GLU	N-CA-C	-5.68	106.02	113.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	Q	19	ASN	CA-C-N	-5.63	113.87	119.56
5	Q	19	ASN	C-N-CA	-5.63	113.87	119.56
1	C	232	ASN	N-CA-CB	-5.59	100.74	111.53
4	J	21	LEU	N-CA-C	-5.59	107.01	113.88
4	J	23	LYS	CA-C-N	-5.46	113.01	119.84
4	J	23	LYS	C-N-CA	-5.46	113.01	119.84
7	s	24	VAL	N-CA-C	-5.46	104.27	111.09
2	F	222	LEU	N-CA-C	-5.44	101.03	109.14
3	H	681	TRP	CB-CA-C	-5.39	99.87	110.11
1	C	458	ASN	N-CA-C	-5.38	99.76	108.52
8	r	80	THR	CB-CA-C	-5.37	100.81	109.89
4	L	46	ILE	N-CA-C	5.37	120.51	109.34
5	S	37	VAL	N-CA-C	5.37	114.47	106.85
8	r	80	THR	N-CA-C	5.34	117.08	108.32
2	E	224	GLY	N-CA-C	-5.33	100.55	113.18
4	J	46	ILE	N-CA-C	5.28	120.32	109.34
3	I	667	GLN	N-CA-C	-5.25	105.23	111.69
7	n	196	ILE	N-CA-C	-5.23	108.02	113.10
4	K	133	THR	N-CA-C	5.23	121.94	110.80
3	H	667	GLN	N-CA-C	-5.23	105.26	111.69
1	A	433	GLN	CB-CA-C	5.22	118.33	109.50
3	G	667	GLN	N-CA-C	-5.21	105.28	111.69
4	O	44	PHE	CA-C-N	-5.21	114.68	122.39
4	O	44	PHE	C-N-CA	-5.21	114.68	122.39
4	K	3	THR	N-CA-C	5.20	117.23	108.96
1	B	710	ILE	CA-C-N	-5.20	113.23	120.25
1	B	710	ILE	C-N-CA	-5.20	113.23	120.25
2	D	106	ASP	N-CA-C	-5.19	107.61	114.31
2	F	223	GLY	N-CA-C	5.14	125.36	113.18
1	C	232	ASN	CB-CA-C	-5.13	101.76	111.97
7	b	104	ILE	N-CA-C	5.12	115.23	107.75
8	f	81	ALA	N-CA-C	5.11	120.51	113.77
4	J	60	GLU	CB-CA-C	5.10	118.89	110.88
2	D	243	THR	N-CA-C	-5.10	105.63	111.14
1	C	12	ASN	N-CA-CB	-5.08	102.88	110.91
2	F	106	ASP	N-CA-C	-5.06	107.77	114.04
4	J	60	GLU	N-CA-C	-5.04	105.67	111.07
1	C	311	GLY	N-CA-C	-5.04	108.11	115.72
1	C	226	LYS	CA-C-N	-5.01	113.58	119.84
1	C	226	LYS	C-N-CA	-5.01	113.58	119.84

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	A	6783	0	6696	215	0
1	B	6783	0	6696	224	0
1	C	6783	0	6696	216	0
2	D	1899	0	1872	87	0
2	E	1899	0	1872	101	0
2	F	1899	0	1872	94	0
3	G	187	0	182	24	0
3	H	187	0	182	38	0
3	I	187	0	182	23	0
4	J	1173	0	1181	60	0
4	K	1198	0	1202	55	0
4	L	1173	0	1181	69	0
4	M	1188	0	1194	58	0
4	N	1173	0	1181	69	0
4	O	1188	0	1194	63	0
5	P	2217	0	2277	70	0
5	Q	2217	0	2277	66	0
5	R	2238	0	2298	61	0
5	S	2217	0	2277	72	0
5	T	2217	0	2277	69	0
5	U	2217	0	2277	55	0
6	V	907	0	905	44	0
6	W	907	0	905	55	0
6	X	907	0	905	45	0
6	Y	907	0	905	49	0
6	Z	907	0	905	41	0
6	a	907	0	905	39	0
7	b	2952	0	2951	112	0
7	d	2918	0	2926	76	0
7	e	2952	0	2951	85	0
7	g	2918	0	2926	66	0
7	h	2952	0	2951	101	0
7	j	2918	0	2926	70	0
7	k	2952	0	2951	112	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	m	2918	0	2926	58	0
7	n	2952	0	2951	90	0
7	p	2918	0	2926	85	0
7	q	2952	0	2951	89	0
7	s	2918	0	2926	47	0
8	c	1580	0	1512	37	0
8	f	1580	0	1512	38	0
8	i	1580	0	1512	32	0
8	l	1580	0	1512	29	0
8	o	1580	0	1512	41	0
8	r	1580	0	1512	46	0
All	All	97165	0	96830	2297	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (2297) 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:E:9:VAL:HG12	3:H:681:TRP:CD1	1.51	1.44
4:O:18:LEU:CD1	4:O:21:LEU:HD21	1.62	1.30
2:E:9:VAL:HG12	3:H:681:TRP:CG	1.70	1.23
7:n:49:THR:HG21	7:p:43:MET:CE	1.68	1.23
6:W:10:ASN:HA	7:p:154:PHE:CE2	1.72	1.23
4:J:18:LEU:HB2	7:n:212:THR:CG2	1.69	1.22
4:N:128:VAL:HG23	7:j:14:ASP:OD1	1.37	1.20
3:G:674:ALA:HB2	3:H:680:GLN:OE1	1.40	1.20
1:B:701:ILE:HG12	5:Q:75:ILE:HD11	1.22	1.19
6:Y:10:ASN:HA	7:d:154:PHE:CE2	1.78	1.19
7:e:49:THR:HG21	7:g:43:MET:CE	1.72	1.18
1:C:542:VAL:HG21	4:O:107:ASN:O	1.40	1.16
4:O:18:LEU:HD12	4:O:21:LEU:HD21	1.15	1.14
6:W:37:GLU:HB3	8:r:21:PRO:HB3	1.23	1.14
6:X:12:THR:HG22	7:b:36:ASP:HB2	1.28	1.14
6:X:37:GLU:HB3	8:c:21:PRO:HB3	1.30	1.14
1:B:168:ASN:HD22	7:h:381:ASN:ND2	1.46	1.13
4:M:40:ASP:HB3	6:Z:19:LEU:HD13	1.27	1.11
6:Y:12:THR:HG22	7:e:36:ASP:HB2	1.33	1.09
1:A:200:PRO:CB	7:b:171:ILE:HD12	1.83	1.09
6:V:37:GLU:HB3	8:o:21:PRO:HB3	1.35	1.08
1:A:638:GLN:HG3	7:n:104:ILE:HD12	1.35	1.08

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:701:ILE:HG12	5:U:75:ILE:CD1	1.82	1.07
1:B:592:GLY:HA3	1:B:613:ASN:HD22	1.07	1.07
2:E:9:VAL:CG1	3:H:681:TRP:CD1	2.37	1.06
1:A:553:VAL:HG11	4:J:110:THR:O	1.54	1.06
4:O:18:LEU:HD12	4:O:21:LEU:CD2	1.85	1.06
5:S:207:LYS:NZ	7:p:25:HIS:HB2	1.70	1.06
5:S:207:LYS:HZ3	7:p:25:HIS:HB2	0.94	1.05
7:n:49:THR:HG21	7:p:43:MET:HE1	1.09	1.05
1:A:200:PRO:HB3	7:b:171:ILE:HD12	1.38	1.04
4:K:31:LEU:CD2	7:q:71:SER:HB2	1.86	1.04
1:C:638:GLN:HG3	7:h:104:ILE:HD12	1.39	1.04
6:W:53:ASN:HD21	6:W:55:ASN:ND2	1.55	1.04
1:A:200:PRO:HB3	7:b:171:ILE:CD1	1.88	1.03
1:A:701:ILE:HG12	5:U:75:ILE:HD11	1.07	1.03
1:C:791:MET:HE3	1:C:881:GLU:CD	1.83	1.03
4:J:18:LEU:HB2	7:n:212:THR:HG22	1.36	1.02
1:C:553:VAL:HG11	4:N:110:THR:O	1.59	1.02
5:S:207:LYS:HZ3	7:p:25:HIS:CB	1.73	1.02
6:W:10:ASN:CA	7:p:154:PHE:CE2	2.42	1.02
7:b:46:PHE:O	7:b:49:THR:HG22	1.61	1.01
6:W:10:ASN:HA	7:p:154:PHE:CD2	1.95	1.01
2:E:9:VAL:CG1	3:H:681:TRP:CB	2.38	1.00
6:W:10:ASN:CA	7:p:154:PHE:HE2	1.74	1.00
4:K:3:THR:HB	7:q:276:SER:HB3	1.42	0.99
7:e:49:THR:HG21	7:g:43:MET:HE2	1.39	0.99
5:T:207:LYS:NZ	5:T:213:GLN:HE22	1.61	0.99
6:Y:53:ASN:HD21	6:Y:55:ASN:ND2	1.58	0.99
1:B:872:THR:HG21	7:e:153:ASN:OD1	1.62	0.99
1:A:168:ASN:HD22	7:b:381:ASN:ND2	1.59	0.99
2:F:9:VAL:HG12	3:G:681:TRP:CG	1.98	0.99
6:Y:10:ASN:CA	7:d:154:PHE:HE2	1.75	0.98
6:W:10:ASN:HA	7:p:154:PHE:HE2	1.22	0.98
6:W:34:VAL:CG2	8:r:24:GLN:HE21	1.77	0.98
1:B:701:ILE:HG12	5:Q:75:ILE:CD1	1.93	0.97
1:A:638:GLN:CG	7:n:104:ILE:HD12	1.94	0.96
1:B:553:VAL:HG11	4:L:110:THR:O	1.63	0.96
7:e:49:THR:HG21	7:g:43:MET:HE1	1.42	0.95
1:B:592:GLY:HA3	1:B:613:ASN:ND2	1.80	0.95
4:O:22:ILE:HD11	7:k:193:ILE:HG23	1.46	0.95
1:B:542:VAL:HG21	4:M:107:ASN:O	1.66	0.95
6:Y:10:ASN:CA	7:d:154:PHE:CE2	2.47	0.95

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:n:49:THR:CG2	7:p:43:MET:HE1	1.96	0.95
5:U:207:LYS:NZ	5:U:213:GLN:HE22	1.63	0.95
6:W:10:ASN:C	7:p:154:PHE:CE2	2.45	0.95
4:M:3:THR:HB	7:e:276:SER:HB3	1.46	0.95
1:C:496:THR:CG2	7:k:110:GLN:NE2	2.30	0.94
1:B:607:ILE:HD11	7:b:161:PRO:O	1.68	0.94
2:E:9:VAL:CG1	3:H:681:TRP:CG	2.50	0.93
1:B:486:THR:HG22	7:e:161:PRO:HG3	1.49	0.93
1:A:701:ILE:CG1	5:U:75:ILE:HD11	1.97	0.93
5:P:207:LYS:HZ1	5:P:213:GLN:NE2	1.65	0.93
3:H:677:ILE:HD11	3:I:677:ILE:HD11	1.49	0.93
7:e:46:PHE:O	7:e:49:THR:HG22	1.68	0.93
7:e:92:GLN:NE2	7:e:134:PHE:HZ	1.66	0.93
7:n:46:PHE:O	7:n:49:THR:HG22	1.68	0.93
6:W:34:VAL:HG22	8:r:24:GLN:HE21	1.31	0.93
6:Y:10:ASN:HA	7:d:154:PHE:HE2	1.23	0.93
6:Y:10:ASN:C	7:d:154:PHE:CE2	2.47	0.93
2:D:9:VAL:HG12	3:I:678:ASN:OD1	1.69	0.92
4:O:29:SER:CB	7:k:75:ASN:HD21	1.81	0.92
4:N:18:LEU:C	7:h:266:ARG:HH22	1.77	0.92
1:B:168:ASN:HD22	7:h:381:ASN:HD21	1.08	0.92
5:R:143:SER:HB3	6:Y:62:SER:OG	1.69	0.92
5:P:207:LYS:NZ	5:P:213:GLN:HE22	1.66	0.92
1:C:45:ASP:OD1	5:S:130:LEU:HD12	1.70	0.91
1:A:496:THR:CG2	7:q:110:GLN:NE2	2.34	0.91
1:B:78:THR:O	7:e:102:ASP:HB2	1.71	0.91
2:E:9:VAL:CG1	3:H:681:TRP:HB3	2.00	0.91
4:O:18:LEU:CD1	4:O:21:LEU:CD2	2.47	0.91
6:Y:10:ASN:HA	7:d:154:PHE:CD2	2.04	0.90
4:N:18:LEU:HD21	7:h:207:GLN:OE1	1.71	0.90
5:R:127:LYS:HE2	5:R:132:SER:OG	1.71	0.90
4:L:149:PHE:O	5:U:246:VAL:HG23	1.70	0.90
4:L:12:THR:HG22	4:L:14:GLU:OE1	1.71	0.90
1:C:496:THR:HG23	7:k:110:GLN:NE2	1.87	0.90
2:E:9:VAL:HG11	3:H:681:TRP:CB	2.02	0.89
2:F:9:VAL:CG1	3:G:681:TRP:CB	2.50	0.89
1:C:638:GLN:CG	7:h:104:ILE:HD12	2.03	0.89
4:O:18:LEU:HD11	4:O:21:LEU:HD21	1.50	0.89
4:O:29:SER:HB3	7:k:75:ASN:HD21	1.35	0.88
6:a:12:THR:CG2	7:k:36:ASP:HB2	2.02	0.88
1:A:553:VAL:CG1	4:J:110:THR:O	2.22	0.88

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:X:12:THR:HG21	7:b:36:ASP:OD2	1.73	0.88
6:a:13:LEU:HD21	8:l:38:LEU:HD11	1.55	0.87
4:M:40:ASP:CB	6:Z:19:LEU:HD13	2.04	0.87
5:P:207:LYS:HZ1	5:P:213:GLN:HE22	0.87	0.87
1:B:698:SER:OG	1:B:699:GLU:OE1	1.90	0.87
1:B:592:GLY:CA	1:B:613:ASN:HD22	1.88	0.86
1:B:607:ILE:CD1	7:b:161:PRO:O	2.23	0.86
6:W:13:LEU:HD21	8:r:38:LEU:HD11	1.57	0.86
6:W:53:ASN:HD21	6:W:55:ASN:HD21	1.19	0.86
1:A:542:VAL:HG21	4:K:107:ASN:O	1.75	0.86
6:W:37:GLU:CB	8:r:21:PRO:HB3	2.05	0.85
7:b:197:ARG:HB3	7:d:197:ARG:HG3	1.59	0.85
5:S:58:MET:HE1	5:S:103:ASP:H	1.40	0.85
1:A:496:THR:HG23	7:q:110:GLN:NE2	1.91	0.85
5:T:143:SER:HB3	6:a:62:SER:OG	1.76	0.85
6:Y:10:ASN:C	7:d:154:PHE:HE2	1.82	0.84
1:B:506:ASP:OD2	4:M:109:PRO:HB3	1.77	0.84
6:Y:12:THR:HG22	7:e:36:ASP:CB	2.06	0.84
1:C:553:VAL:CG1	4:N:110:THR:O	2.25	0.84
5:U:58:MET:HE1	5:U:103:ASP:H	1.41	0.84
1:B:200:PRO:CB	7:h:171:ILE:HG22	2.07	0.84
3:H:677:ILE:HD13	3:I:677:ILE:HG12	1.58	0.84
1:A:168:ASN:HD22	7:b:381:ASN:HD22	1.25	0.84
1:C:168:ASN:HD22	7:n:381:ASN:ND2	1.75	0.84
4:K:31:LEU:HD23	7:q:71:SER:HB2	1.58	0.84
5:Q:207:LYS:HE2	7:h:52:TYR:CE1	2.12	0.84
6:a:12:THR:HG22	7:k:36:ASP:CB	2.08	0.84
1:C:585:SER:OG	2:D:24:GLU:HG2	1.77	0.84
4:L:107:ASN:OD1	4:L:112:LYS:HE2	1.78	0.83
1:B:599:VAL:CG2	2:F:85:MET:HE1	2.07	0.83
4:L:4:GLN:NE2	7:b:256:ILE:CG2	2.41	0.83
4:L:31:LEU:CD2	7:b:71:SER:HB2	2.08	0.83
4:N:31:LEU:CD2	7:h:71:SER:HB2	2.07	0.83
4:N:18:LEU:HG	7:h:266:ARG:NH1	1.93	0.83
6:W:8:ILE:HD12	7:q:34:PHE:HD1	1.43	0.83
1:C:506:ASP:OD2	4:O:109:PRO:HB3	1.78	0.82
4:J:21:LEU:HD23	7:n:196:ILE:HD11	1.61	0.82
2:F:9:VAL:HG12	3:G:681:TRP:CD1	2.15	0.82
5:S:207:LYS:NZ	7:p:25:HIS:ND1	2.27	0.82
1:A:200:PRO:CG	7:b:171:ILE:HD12	2.10	0.82
1:C:45:ASP:OD1	5:S:130:LEU:CD1	2.27	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:585:SER:HB3	2:E:24:GLU:OE1	1.79	0.82
6:X:12:THR:HG22	7:b:36:ASP:CB	2.08	0.82
5:S:207:LYS:NZ	7:p:25:HIS:CB	2.35	0.82
1:A:638:GLN:HG3	7:n:104:ILE:CD1	2.09	0.81
6:Z:111:SER:HB2	7:g:115:SER:O	1.80	0.81
1:B:553:VAL:CG1	4:L:110:THR:O	2.29	0.81
5:U:207:LYS:HZ1	5:U:213:GLN:HE22	1.25	0.81
1:A:543:GLY:HA3	4:K:123:LEU:HD23	1.61	0.81
1:B:496:THR:CG2	7:e:110:GLN:NE2	2.44	0.81
5:Q:190:GLU:HA	5:Q:193:LYS:HE3	1.62	0.81
1:B:685:GLY:HA2	4:L:114:LEU:HB2	1.62	0.81
3:G:680:GLN:OE1	3:I:674:ALA:HB2	1.81	0.81
5:S:207:LYS:HZ1	7:p:25:HIS:CG	1.99	0.81
5:S:207:LYS:NZ	7:p:25:HIS:CG	2.49	0.80
4:J:16:GLU:OE1	5:P:234:ARG:HB3	1.81	0.80
1:A:32:LYS:HG2	2:E:1:MET:HG3	1.62	0.80
1:B:168:ASN:ND2	7:h:381:ASN:ND2	2.29	0.80
1:B:1:MET:HE1	5:R:133:HIS:NE2	1.96	0.80
7:b:49:THR:HG21	7:d:43:MET:HE2	1.64	0.80
7:h:197:ARG:HB3	7:j:197:ARG:HG3	1.63	0.80
2:F:9:VAL:HG21	3:G:677:ILE:HG22	1.64	0.79
4:J:31:LEU:CD2	7:n:71:SER:HB2	2.12	0.79
4:L:4:GLN:HE22	7:b:256:ILE:HB	1.47	0.79
1:B:1:MET:CE	5:R:133:HIS:NE2	2.46	0.79
4:M:40:ASP:HB3	6:Z:19:LEU:CD1	2.10	0.79
5:T:207:LYS:NZ	5:T:213:GLN:NE2	2.32	0.78
7:h:45:PRO:O	7:h:49:THR:HG23	1.83	0.78
6:W:10:ASN:C	7:p:154:PHE:HE2	1.87	0.78
6:V:34:VAL:HG21	8:o:23:GLU:CD	2.09	0.78
6:X:12:THR:CG2	7:b:36:ASP:OD2	2.30	0.78
1:B:496:THR:HG23	7:e:110:GLN:NE2	1.99	0.78
4:N:128:VAL:CG2	7:j:14:ASP:OD1	2.27	0.78
6:W:53:ASN:ND2	6:W:55:ASN:ND2	2.31	0.77
6:Y:53:ASN:ND2	6:Y:55:ASN:ND2	2.30	0.77
1:C:168:ASN:HD22	7:n:381:ASN:HD22	1.30	0.77
1:A:228:GLN:HB3	1:A:232:ASN:HA	1.67	0.77
6:a:3:VAL:O	7:m:42:PHE:CE1	2.38	0.77
7:b:49:THR:HG21	7:d:43:MET:CE	2.15	0.77
5:S:24:GLN:HE22	5:T:163:ASP:HA	1.49	0.77
6:X:32:SER:HB3	8:c:27:THR:O	1.84	0.77
7:q:374:GLU:OE1	7:q:374:GLU:N	2.18	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:430:LYS:HE3	4:M:149:PHE:CG	2.19	0.77
1:B:681:PRO:HB3	4:L:132:ASN:O	1.85	0.77
4:O:22:ILE:CD1	7:k:193:ILE:HG23	2.15	0.76
4:J:18:LEU:CB	7:n:212:THR:CG2	2.59	0.76
2:E:106:ASP:CG	7:h:164:TYR:OH	2.29	0.76
4:K:46:ILE:HG22	6:X:101:GLU:OE1	1.86	0.76
1:C:200:PRO:HB3	7:n:171:ILE:HG22	1.68	0.76
3:H:670:ALA:HB1	3:I:676:ILE:HG23	1.66	0.76
1:B:486:THR:CG2	7:e:161:PRO:HG3	2.16	0.76
1:B:204:ARG:HD3	7:h:92:GLN:NE2	2.01	0.76
1:C:79:ASN:HB3	7:n:114:LEU:CD2	2.16	0.75
6:X:37:GLU:CB	8:c:21:PRO:HB3	2.14	0.75
2:F:9:VAL:HG12	3:G:681:TRP:CB	2.15	0.75
5:U:207:LYS:NZ	5:U:213:GLN:NE2	2.33	0.75
7:k:374:GLU:OE1	7:k:374:GLU:N	2.20	0.75
4:O:27:ASP:OD2	7:k:74:LYS:HE3	1.86	0.75
8:r:80:THR:HG22	8:r:82:PRO:HD2	1.67	0.75
7:j:105:VAL:HB	7:j:126:LEU:HB3	1.68	0.75
1:C:791:MET:CE	1:C:881:GLU:CD	2.59	0.75
7:n:49:THR:HG21	7:p:43:MET:HE2	1.66	0.75
1:B:599:VAL:HG21	2:F:85:MET:HE1	1.67	0.75
4:N:80:THR:HG21	8:i:50:TYR:HE1	1.51	0.75
6:Y:12:THR:HG21	7:e:36:ASP:OD2	1.86	0.75
6:a:12:THR:CG2	7:k:36:ASP:CB	2.65	0.75
1:B:168:ASN:ND2	7:h:381:ASN:HD21	1.85	0.74
1:C:638:GLN:HG3	7:h:104:ILE:CD1	2.14	0.74
2:E:9:VAL:HG11	3:H:681:TRP:HB2	1.69	0.74
4:J:21:LEU:HD23	7:n:196:ILE:CD1	2.18	0.74
5:T:207:LYS:HZ1	5:T:213:GLN:HE22	1.33	0.74
1:A:7:LYS:HE3	1:A:9:LEU:HD21	1.70	0.74
2:F:211:LEU:HD13	2:F:221:ARG:HD3	1.69	0.74
1:C:79:ASN:HB3	7:n:114:LEU:HD23	1.68	0.74
1:C:564:VAL:HG21	1:C:679:THR:HB	1.70	0.74
4:J:44:PHE:HA	6:W:99:GLY:O	1.88	0.74
2:F:9:VAL:CG1	3:G:681:TRP:HB2	2.17	0.74
8:l:65:CYS:SG	8:l:66:ASP:N	2.61	0.74
7:j:373:SER:O	8:l:168:ARG:NH2	2.21	0.73
4:J:60:GLU:O	5:S:48:GLN:HG2	1.87	0.73
7:d:373:SER:O	8:f:168:ARG:NH2	2.21	0.73
4:J:18:LEU:HB2	7:n:212:THR:HG21	1.67	0.73
7:k:95:LEU:HB2	7:k:133:THR:HG22	1.69	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2:GLN:HB3	5:S:86:ASN:OD1	1.89	0.73
1:C:78:THR:O	7:k:102:ASP:HB2	1.87	0.73
7:b:27:ASN:HB2	7:b:37:LEU:HD11	1.69	0.73
1:B:22:ILE:CD1	5:T:77:ILE:HG13	2.18	0.73
7:q:243:LEU:HD21	7:q:259:VAL:HG21	1.70	0.72
3:H:677:ILE:CD1	3:I:677:ILE:HG12	2.19	0.72
5:Q:207:LYS:NZ	7:h:52:TYR:OH	2.22	0.72
3:H:681:TRP:CG	3:H:681:TRP:O	2.43	0.72
5:P:206:LYS:HE3	7:s:28:VAL:HG22	1.72	0.72
6:a:12:THR:HG23	7:k:36:ASP:HB2	1.70	0.72
6:a:74:GLU:OE2	6:a:74:GLU:N	2.22	0.72
2:F:191:THR:HG23	2:F:205:GLY:HA2	1.71	0.72
5:Q:44:ASN:HD22	5:Q:47:LYS:HE3	1.55	0.72
7:p:317:LEU:HD13	7:p:361:PRO:HG2	1.71	0.72
1:B:405:LYS:HZ1	2:E:81:GLN:NE2	1.88	0.72
3:G:673:ILE:HG12	3:I:673:ILE:HD13	1.72	0.72
6:W:74:GLU:OE2	6:W:74:GLU:N	2.22	0.72
6:Y:53:ASN:HD21	6:Y:55:ASN:HD21	1.38	0.72
6:a:6:PRO:O	8:l:34:ALA:HB3	1.90	0.72
4:L:128:VAL:HG23	7:d:14:ASP:OD1	1.90	0.71
1:A:200:PRO:HB3	7:b:171:ILE:HD11	1.71	0.71
4:O:31:LEU:CD2	7:k:71:SER:OG	2.37	0.71
6:Y:101:GLU:O	6:Y:101:GLU:CD	2.34	0.71
1:B:701:ILE:CG1	5:Q:75:ILE:HD11	2.12	0.71
7:e:374:GLU:N	7:e:374:GLU:OE2	2.23	0.71
7:m:244:LEU:HB2	7:m:278:MET:HE2	1.71	0.71
1:C:427:ILE:HG12	4:J:143:ILE:HG13	1.72	0.71
1:A:599:VAL:CG2	2:D:85:MET:HE1	2.20	0.71
4:L:107:ASN:OD1	4:L:112:LYS:CE	2.39	0.71
5:Q:66:TYR:CE1	5:Q:95:MET:HG3	2.25	0.71
5:R:64:ILE:HG12	5:R:97:MET:HG2	1.72	0.71
8:f:68:GLU:OE1	8:f:68:GLU:N	2.21	0.71
7:n:374:GLU:OE1	7:n:374:GLU:N	2.21	0.71
5:P:64:ILE:HG12	5:P:97:MET:HG2	1.73	0.71
6:V:71:GLU:HG3	7:p:40:SER:OG	1.90	0.71
5:Q:44:ASN:ND2	5:Q:47:LYS:HE3	2.05	0.71
7:p:105:VAL:HB	7:p:126:LEU:HB3	1.72	0.71
1:B:607:ILE:HD11	7:b:162:LEU:HA	1.71	0.71
4:N:22:ILE:HD11	7:h:193:ILE:HG22	1.72	0.71
8:r:65:CYS:SG	8:r:66:ASP:N	2.64	0.71
4:O:9:LYS:HB2	7:k:264:GLN:HB3	1.73	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:b:317:LEU:HD13	7:b:361:PRO:HG2	1.73	0.70
5:U:35:THR:HA	6:X:63:LYS:HD3	1.74	0.70
1:B:56:SER:CB	4:N:136:SER:OG	2.40	0.70
4:K:29:SER:CB	7:q:75:ASN:HD21	2.04	0.70
1:B:200:PRO:HB3	7:h:171:ILE:CG2	2.22	0.70
7:p:373:SER:O	8:r:168:ARG:NH2	2.23	0.70
6:a:6:PRO:HB2	8:l:34:ALA:HB3	1.74	0.70
7:d:105:VAL:HB	7:d:126:LEU:HB3	1.72	0.70
7:e:92:GLN:NE2	7:e:134:PHE:CZ	2.48	0.70
2:D:188:ALA:HB2	2:E:184:ILE:HG12	1.74	0.70
5:P:35:THR:HA	6:W:63:LYS:HD2	1.74	0.70
8:f:151:GLU:HG2	8:f:183:LYS:HZ2	1.57	0.70
7:b:199:PRO:HA	7:b:203:LEU:HD12	1.71	0.69
7:j:317:LEU:HD13	7:j:361:PRO:HG2	1.74	0.69
7:b:208:LEU:HD21	7:b:263:LEU:HD11	1.74	0.69
1:A:599:VAL:HG23	2:D:85:MET:HE1	1.75	0.69
6:W:32:SER:O	8:r:24:GLN:HG3	1.92	0.69
6:a:85:ASN:OD1	6:a:86:ASN:N	2.25	0.69
8:c:168:ARG:NH2	7:s:373:SER:O	2.25	0.69
7:m:373:SER:O	8:o:168:ARG:NH2	2.25	0.69
6:W:8:ILE:HD12	7:q:34:PHE:CD1	2.27	0.69
7:g:23:LEU:HD11	7:g:44:ARG:HD3	1.75	0.69
4:K:9:LYS:HB2	7:q:264:GLN:HB3	1.74	0.69
4:M:24:PRO:HG3	7:g:191:ALA:CB	2.23	0.69
5:T:187:ALA:HB1	7:m:17:GLN:HE22	1.58	0.69
7:j:39:ALA:HA	7:j:44:ARG:HG2	1.75	0.69
6:Z:85:ASN:OD1	6:Z:86:ASN:N	2.24	0.68
4:N:9:LYS:HB2	7:h:264:GLN:HB3	1.75	0.68
4:K:44:PHE:HA	6:X:99:GLY:O	1.94	0.68
4:O:18:LEU:O	4:O:18:LEU:HG	1.93	0.68
6:X:74:GLU:OE2	6:X:74:GLU:N	2.26	0.68
1:C:22:ILE:CD1	5:P:77:ILE:HG13	2.23	0.68
7:d:317:LEU:HD13	7:d:361:PRO:HG2	1.75	0.68
7:m:317:LEU:HD13	7:m:361:PRO:HG2	1.74	0.68
1:B:56:SER:HB2	4:N:136:SER:OG	1.94	0.68
1:C:496:THR:HG23	7:k:110:GLN:HE22	1.57	0.68
7:d:197:ARG:NH2	7:d:204:ASP:OD2	2.27	0.68
1:B:594:ARG:NH2	1:B:610:ASP:OD2	2.27	0.68
4:N:24:PRO:HG3	7:j:191:ALA:CB	2.24	0.68
6:Z:37:GLU:HB3	8:i:21:PRO:HB3	1.74	0.68
2:D:80:PRO:HG3	2:D:102:PRO:HG3	1.76	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:T:207:LYS:HZ3	5:T:213:GLN:HE22	1.37	0.68
1:A:280:GLU:HA	1:B:806:GLN:HE22	1.59	0.68
2:E:9:VAL:CG1	3:H:681:TRP:HD1	2.04	0.68
4:L:4:GLN:NE2	7:b:256:ILE:HG21	2.09	0.68
4:N:93:ASP:HB2	4:N:96:ALA:HB3	1.75	0.68
2:D:179:ARG:NH1	2:F:187:ASP:OD2	2.25	0.67
2:F:213:GLN:HG3	2:F:219:LYS:HB3	1.75	0.67
5:P:212:LYS:NZ	7:q:13:ASP:O	2.25	0.67
6:Y:12:THR:CG2	7:e:36:ASP:OD2	2.41	0.67
4:L:44:PHE:HA	6:Y:99:GLY:O	1.95	0.67
7:q:224:LEU:HD12	7:q:234:PRO:HB2	1.75	0.67
1:A:638:GLN:CD	7:n:104:ILE:HD12	2.19	0.67
8:f:65:CYS:SG	8:f:66:ASP:N	2.67	0.67
1:C:200:PRO:CB	7:n:171:ILE:HG22	2.24	0.67
4:L:4:GLN:HE21	7:b:256:ILE:HG21	1.59	0.67
2:E:187:ASP:OD1	2:F:179:ARG:NH1	2.27	0.67
6:W:76:GLN:HG3	6:W:98:LEU:HD21	1.76	0.67
1:A:543:GLY:CA	4:K:123:LEU:HD23	2.24	0.67
1:B:427:ILE:HG12	4:N:143:ILE:HG13	1.76	0.67
5:U:207:LYS:HZ1	5:U:213:GLN:NE2	1.91	0.67
6:X:6:PRO:HB2	8:c:34:ALA:HB3	1.77	0.67
5:Q:207:LYS:CE	7:h:52:TYR:CZ	2.78	0.67
3:H:677:ILE:HD11	3:I:677:ILE:CD1	2.24	0.67
5:S:136:ILE:HG23	5:S:178:ILE:HD11	1.77	0.66
6:Y:6:PRO:HB2	8:f:34:ALA:HB3	1.76	0.66
6:Z:74:GLU:OE1	6:Z:74:GLU:N	2.27	0.66
4:N:18:LEU:C	7:h:266:ARG:NH2	2.50	0.66
5:U:136:ILE:HG23	5:U:178:ILE:HD11	1.77	0.66
1:C:179:ASN:OD1	1:C:184:ASN:ND2	2.28	0.66
1:C:5:ILE:HG21	5:T:130:LEU:HG	1.78	0.66
4:O:27:ASP:CG	7:k:74:LYS:HE3	2.21	0.66
6:V:111:SER:HB3	7:m:115:SER:O	1.95	0.66
6:Y:37:GLU:HB3	8:f:21:PRO:HB3	1.78	0.66
6:Y:74:GLU:OE2	6:Y:74:GLU:N	2.23	0.66
1:B:168:ASN:HB2	7:h:381:ASN:HD22	1.59	0.66
6:a:65:GLN:O	6:a:69:GLU:HG3	1.96	0.66
7:s:286:GLU:HG3	7:s:344:GLN:HB2	1.76	0.66
1:B:791:MET:HB2	1:B:794:ARG:HG3	1.78	0.66
6:W:34:VAL:HG22	8:r:24:GLN:NE2	2.08	0.66
4:M:5:GLU:HG3	7:e:274:LEU:HD11	1.77	0.65
5:S:85:LEU:HD12	5:T:178:ILE:HG22	1.78	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:V:37:GLU:CB	8:o:21:PRO:HB3	2.22	0.65
1:B:516:ASN:ND2	2:E:64:ASN:ND2	2.44	0.65
1:B:607:ILE:HD11	7:b:162:LEU:CA	2.26	0.65
5:T:207:LYS:HZ1	5:T:213:GLN:NE2	1.92	0.65
8:r:80:THR:O	8:r:82:PRO:HD2	1.97	0.65
1:C:56:SER:HB2	4:J:136:SER:OG	1.97	0.65
4:N:80:THR:HG21	8:i:50:TYR:CE1	2.31	0.65
7:k:178:ARG:HH12	7:k:181:GLU:HB3	1.60	0.65
1:B:200:PRO:CB	7:h:171:ILE:CG2	2.74	0.65
1:B:204:ARG:HD3	7:h:92:GLN:HE22	1.60	0.65
4:N:18:LEU:HG	7:h:266:ARG:HH12	1.57	0.65
6:W:6:PRO:HB2	8:r:34:ALA:HB3	1.78	0.65
2:E:127:ASN:N	2:F:119:ASP:OD1	2.28	0.65
2:F:14:LEU:HA	3:H:681:TRP:HH2	1.62	0.65
5:Q:207:LYS:NZ	7:h:52:TYR:CZ	2.65	0.65
7:h:201:SER:OG	8:i:108:LYS:NZ	2.29	0.65
7:m:105:VAL:HB	7:m:126:LEU:HB3	1.79	0.65
1:B:179:ASN:OD1	1:B:184:ASN:ND2	2.29	0.65
1:C:204:ARG:HD3	7:n:92:GLN:NE2	2.11	0.65
1:C:292:THR:OG1	1:C:358:ARG:NH1	2.30	0.65
1:C:413:GLU:OE1	7:k:100:SER:HB3	1.96	0.65
7:g:286:GLU:HG3	7:g:344:GLN:HB2	1.79	0.65
8:r:80:THR:O	8:r:82:PRO:CD	2.44	0.65
1:A:18:GLY:HA2	5:R:78:PRO:O	1.97	0.65
4:L:6:PHE:CE2	7:b:260:GLY:HA3	2.32	0.65
7:h:387:ASN:HB3	7:h:390:GLU:HB3	1.77	0.65
1:C:56:SER:CB	4:J:136:SER:OG	2.45	0.65
4:L:36:GLN:NE2	4:L:117:ASP:OD2	2.30	0.65
4:L:93:ASP:HB2	4:L:96:ALA:HB3	1.79	0.65
6:W:97:TYR:HD2	6:W:100:THR:HG22	1.62	0.65
1:B:56:SER:HB2	4:N:136:SER:HG	1.62	0.65
1:C:94:THR:HG22	1:C:159:ARG:HH12	1.61	0.65
1:C:770:ARG:HB2	1:C:774:GLY:HA2	1.79	0.65
1:A:204:ARG:HD3	7:b:92:GLN:NE2	2.12	0.64
1:B:8:ILE:HG12	1:B:436:LEU:HD13	1.80	0.64
2:D:227:ASN:HA	2:F:218:ARG:HH12	1.61	0.64
1:A:358:ARG:HH12	1:A:382:LEU:HD22	1.62	0.64
1:A:604:GLY:HA2	2:D:85:MET:HE1	1.80	0.64
1:B:503:LEU:HD23	4:M:128:VAL:HG22	1.77	0.64
5:U:246:VAL:HG22	5:U:247:ILE:O	1.98	0.64
7:e:49:THR:CG2	7:g:43:MET:HE1	2.23	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:e:200:VAL:HG21	8:f:108:LYS:HG2	1.80	0.64
5:P:184:ASP:O	5:P:188:LEU:HB3	1.98	0.64
6:V:34:VAL:O	6:V:37:GLU:HG2	1.96	0.64
6:W:82:ASP:OD2	6:W:84:LYS:NZ	2.30	0.64
7:d:206:GLU:O	7:d:210:GLU:HG2	1.98	0.64
7:g:373:SER:O	8:i:168:ARG:NH2	2.30	0.64
1:A:681:PRO:HB3	4:J:132:ASN:O	1.96	0.64
1:B:94:THR:HG22	1:B:159:ARG:HH12	1.62	0.64
4:J:93:ASP:HB2	4:J:96:ALA:HB3	1.79	0.64
1:A:701:ILE:HD11	5:U:73:GLN:CB	2.28	0.64
1:B:79:ASN:HB3	7:h:114:LEU:HD23	1.78	0.64
2:E:66:ILE:HG22	2:E:100:TYR:HD2	1.62	0.64
4:O:5:GLU:OE2	7:k:272:ARG:CD	2.45	0.64
4:O:55:ASN:HB2	7:m:52:TYR:OH	1.97	0.64
1:B:578:GLN:HE21	4:K:151:PHE:H	1.46	0.64
1:B:585:SER:CB	2:E:24:GLU:OE1	2.46	0.64
3:H:670:ALA:HA	3:I:676:ILE:HD13	1.79	0.64
7:b:46:PHE:O	7:b:49:THR:CG2	2.43	0.64
1:B:128:TYR:HA	1:B:159:ARG:HB2	1.80	0.64
1:C:603:SER:HA	2:E:106:ASP:HB3	1.78	0.64
7:b:13:ASP:OD2	7:b:59:TYR:HA	1.98	0.64
7:b:156:ASP:OD1	7:b:157:GLN:NE2	2.31	0.64
1:A:602:ASP:HB3	2:F:47:ARG:HH21	1.62	0.64
1:A:801:ASP:OD1	1:A:879:HIS:ND1	2.30	0.64
2:F:209:GLU:HA	2:F:223:GLY:HA3	1.78	0.64
6:Z:32:SER:O	8:i:24:GLN:HG3	1.98	0.64
5:R:127:LYS:HG2	5:R:132:SER:HB3	1.80	0.64
7:h:208:LEU:HD11	7:h:241:LEU:HD13	1.79	0.64
1:A:42:PHE:CZ	5:R:84:GLN:HG2	2.33	0.63
1:C:18:GLY:HA2	5:P:78:PRO:O	1.97	0.63
1:C:194:GLN:HG3	1:C:199:LEU:HD12	1.79	0.63
3:H:670:ALA:HA	3:I:676:ILE:HG21	1.80	0.63
4:O:5:GLU:OE2	7:k:272:ARG:HD2	1.99	0.63
6:X:32:SER:O	8:c:24:GLN:HG3	1.97	0.63
7:k:242:PHE:HB3	7:k:278:MET:HG2	1.79	0.63
7:n:317:LEU:HD13	7:n:361:PRO:HG2	1.78	0.63
1:B:599:VAL:HG21	2:F:85:MET:CE	2.28	0.63
2:F:219:LYS:HG2	2:F:231:ASP:HB3	1.79	0.63
4:K:31:LEU:HD21	7:q:75:ASN:HD22	1.64	0.63
6:Y:62:SER:O	6:Y:66:ILE:HG13	1.98	0.63
6:a:3:VAL:O	7:m:42:PHE:CD1	2.51	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:h:317:LEU:HD13	7:h:361:PRO:HG2	1.80	0.63
1:A:200:PRO:HD3	7:b:153:ASN:HD21	1.63	0.63
2:D:75:GLN:HG3	2:E:122:VAL:HG13	1.79	0.63
1:A:638:GLN:CD	7:n:104:ILE:CD1	2.71	0.63
4:J:44:PHE:CZ	5:S:46:ASN:ND2	2.67	0.63
6:V:74:GLU:OE2	6:V:74:GLU:N	2.30	0.63
7:d:39:ALA:HA	7:d:44:ARG:HG2	1.79	0.63
7:g:105:VAL:HB	7:g:126:LEU:HB3	1.79	0.63
4:M:3:THR:CB	7:e:276:SER:HB3	2.26	0.63
5:U:248:LYS:HD2	5:U:259:PHE:CE1	2.34	0.63
8:f:65:CYS:SG	8:f:69:TYR:HB2	2.38	0.63
7:j:206:GLU:O	7:j:210:GLU:HG2	1.98	0.63
8:o:102:SER:HA	8:o:106:ARG:HH21	1.63	0.63
7:p:333:ARG:NH2	7:q:327:GLU:OE1	2.31	0.63
3:G:674:ALA:CB	3:H:680:GLN:OE1	2.32	0.63
4:M:3:THR:HG23	7:e:227:ILE:HD11	1.79	0.63
4:L:9:LYS:HB2	7:b:264:GLN:HB3	1.81	0.63
6:V:34:VAL:CB	8:o:23:GLU:OE1	2.46	0.63
7:q:171:ILE:HD12	7:q:172:ARG:HG3	1.79	0.63
1:A:601:ALA:HB1	2:F:99:TYR:OH	1.99	0.63
1:B:262:ASP:OD2	2:E:123:ARG:NH1	2.28	0.63
2:F:9:VAL:HG11	3:G:681:TRP:HB2	1.78	0.63
6:Z:29:GLN:HE22	7:j:45:PRO:HG2	1.64	0.63
8:f:95:VAL:O	8:f:99:ASN:ND2	2.32	0.63
1:A:56:SER:CB	4:L:136:SER:OG	2.47	0.63
1:C:194:GLN:O	7:n:153:ASN:ND2	2.25	0.63
1:A:496:THR:HG23	7:q:110:GLN:HE22	1.62	0.62
7:p:39:ALA:HA	7:p:44:ARG:HG2	1.81	0.62
7:p:116:GLY:O	7:p:119:ARG:NH1	2.32	0.62
1:A:22:ILE:CD1	5:R:77:ILE:HG13	2.29	0.62
1:B:473:ASN:HA	1:B:476:LEU:HD12	1.79	0.62
1:B:801:ASP:OD1	1:B:879:HIS:ND1	2.31	0.62
1:C:585:SER:OG	2:D:24:GLU:CG	2.45	0.62
4:L:31:LEU:HD21	7:b:75:ASN:HD22	1.64	0.62
8:i:102:SER:HA	8:i:106:ARG:HH21	1.63	0.62
1:A:631:PRO:HD2	2:F:92:ASP:HB3	1.80	0.62
1:B:630:VAL:CG2	2:E:29:ARG:CZ	2.78	0.62
1:C:630:VAL:CG2	2:D:29:ARG:CZ	2.77	0.62
1:A:94:THR:HG22	1:A:159:ARG:HH12	1.62	0.62
1:C:200:PRO:HB3	7:n:171:ILE:CG2	2.29	0.62
4:M:40:ASP:CB	6:Z:19:LEU:CD1	2.75	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:i:141:SER:OG	8:i:142:GLU:OE1	2.17	0.62
5:Q:44:ASN:HB3	5:Q:47:LYS:HG2	1.81	0.62
7:m:286:GLU:HG3	7:m:344:GLN:HB2	1.82	0.62
4:K:3:THR:CB	7:q:276:SER:HB3	2.23	0.62
4:K:139:LEU:HD13	4:L:143:ILE:HD11	1.80	0.62
6:Z:22:TYR:CE2	6:Z:26:LYS:HD2	2.35	0.62
4:K:31:LEU:HD21	7:q:71:SER:HB2	1.80	0.62
1:B:78:THR:O	7:e:102:ASP:CB	2.48	0.61
1:B:578:GLN:NE2	4:K:151:PHE:H	1.97	0.61
1:C:512:GLU:HG3	1:C:636:GLN:HE21	1.64	0.61
2:D:184:ILE:HG13	2:F:188:ALA:HB2	1.81	0.61
2:F:9:VAL:CG1	3:G:681:TRP:CG	2.78	0.61
4:M:5:GLU:HG3	7:e:274:LEU:CD1	2.29	0.61
4:N:22:ILE:CD1	7:h:193:ILE:HG22	2.29	0.61
5:S:28:LEU:HD11	5:S:173:MET:HE1	1.82	0.61
7:b:213:MET:HE3	7:b:217:SER:HB2	1.82	0.61
8:l:95:VAL:O	8:l:99:ASN:ND2	2.33	0.61
7:s:317:LEU:HD13	7:s:361:PRO:HG2	1.81	0.61
1:B:200:PRO:CG	7:h:171:ILE:HG22	2.29	0.61
1:C:801:ASP:OD1	1:C:879:HIS:ND1	2.33	0.61
2:F:9:VAL:CG1	3:G:681:TRP:HB3	2.28	0.61
6:a:12:THR:CG2	7:k:36:ASP:OD2	2.48	0.61
7:j:369:GLU:HG2	7:j:379:ARG:HG2	1.82	0.61
7:k:213:MET:HE1	7:k:243:LEU:HG	1.82	0.61
2:E:9:VAL:HG11	3:H:681:TRP:HB3	1.72	0.61
4:L:12:THR:CG2	4:L:14:GLU:OE1	2.47	0.61
5:P:249:ILE:HG12	5:P:256:VAL:HG22	1.82	0.61
6:W:82:ASP:OD1	6:W:83:LEU:N	2.33	0.61
7:s:105:VAL:HB	7:s:126:LEU:HB3	1.81	0.61
1:A:200:PRO:CB	7:b:171:ILE:CD1	2.60	0.61
1:B:551:ILE:HG22	1:B:647:ALA:HB3	1.83	0.61
8:c:67:GLU:OE1	8:c:67:GLU:N	2.33	0.61
7:d:243:LEU:HD11	7:d:259:VAL:HG11	1.81	0.61
1:B:18:GLY:HA2	5:T:78:PRO:O	2.01	0.61
2:D:72:SER:HB3	2:D:75:GLN:HE22	1.65	0.61
4:L:4:GLN:NE2	7:b:256:ILE:HB	2.16	0.61
5:T:30:GLU:HG3	5:T:135:LYS:HG2	1.82	0.61
6:Z:32:SER:HB3	8:i:27:THR:O	2.01	0.61
7:j:243:LEU:HD11	7:j:259:VAL:HG11	1.82	0.61
7:p:243:LEU:HD11	7:p:259:VAL:HG11	1.81	0.61
1:C:200:PRO:CG	7:n:171:ILE:HG22	2.31	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:48:ARG:HB3	2:E:79:LEU:HD21	1.83	0.61
4:L:5:GLU:OE1	7:b:272:ARG:HG3	2.00	0.61
4:N:31:LEU:HD21	7:h:75:ASN:HD22	1.65	0.61
6:a:49:ARG:NH2	6:a:56:ASP:OD1	2.33	0.61
7:b:195:ARG:HH12	8:c:80:THR:HG22	1.66	0.61
1:A:542:VAL:HG13	1:A:545:VAL:HG13	1.83	0.61
1:A:630:VAL:CG2	2:F:29:ARG:CZ	2.79	0.61
1:B:607:ILE:HD11	7:b:161:PRO:C	2.26	0.61
4:J:60:GLU:HB3	5:S:47:LYS:HB2	1.82	0.61
6:W:39:VAL:HG12	8:r:2:SER:HA	1.83	0.61
2:E:191:THR:HG23	2:E:205:GLY:HA2	1.82	0.60
4:K:42:ASP:N	4:K:42:ASP:OD1	2.32	0.60
1:C:401:LYS:O	1:C:405:LYS:HG3	2.02	0.60
4:J:31:LEU:HD21	7:n:75:ASN:HD22	1.66	0.60
5:S:37:VAL:HB	6:V:49:ARG:HD2	1.82	0.60
1:A:602:ASP:CG	2:F:67:ARG:HH21	2.07	0.60
4:O:18:LEU:HD23	7:k:266:ARG:HH21	1.65	0.60
6:Y:97:TYR:HD2	6:Y:100:THR:HG22	1.65	0.60
7:b:13:ASP:OD2	7:b:59:TYR:CA	2.49	0.60
2:D:24:GLU:HB2	2:F:19:MET:HG3	1.84	0.60
4:O:29:SER:CB	7:k:75:ASN:ND2	2.59	0.60
5:U:207:LYS:HZ3	5:U:213:GLN:HE22	1.48	0.60
6:a:1:MET:HG3	7:m:34:PHE:CE1	2.36	0.60
7:d:116:GLY:O	7:d:119:ARG:NH1	2.34	0.60
8:r:88:TYR:OH	8:r:172:LYS:NZ	2.35	0.60
5:Q:207:LYS:HE2	7:h:52:TYR:CZ	2.36	0.60
6:X:34:VAL:O	6:X:37:GLU:HG2	2.02	0.60
7:h:178:ARG:NE	7:h:215:GLU:OE2	2.35	0.60
1:B:1:MET:CE	5:R:133:HIS:CD2	2.84	0.60
1:B:54:SER:OG	4:N:134:GLU:OE1	2.20	0.60
1:C:42:PHE:HE1	5:P:75:ILE:HD12	1.67	0.60
6:Z:6:PRO:HB2	8:i:34:ALA:HB3	1.84	0.60
7:b:172:ARG:NH1	7:b:247:ASN:OD1	2.35	0.60
7:g:238:VAL:HG22	7:g:272:ARG:HB2	1.82	0.60
1:C:790:TYR:HD2	1:C:791:MET:O	1.85	0.60
6:V:32:SER:HB3	8:o:27:THR:O	2.02	0.60
1:C:661:SER:H	1:C:664:ASP:HB2	1.66	0.60
4:N:104:PHE:HB3	5:T:201:GLN:O	2.01	0.60
7:q:243:LEU:HD22	7:q:256:ILE:HD13	1.83	0.60
5:P:64:ILE:HG21	5:P:95:MET:HE3	1.84	0.59
5:P:207:LYS:NZ	5:P:213:GLN:NE2	2.38	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:r:65:CYS:SG	8:r:69:TYR:HB2	2.41	0.59
1:A:859:ARG:NH2	1:A:889:SER:OG	2.35	0.59
1:B:79:ASN:HB3	7:h:114:LEU:CD2	2.32	0.59
1:C:859:ARG:NH2	1:C:889:SER:OG	2.36	0.59
5:S:222:THR:HG22	5:S:226:LYS:HE2	1.84	0.59
6:X:107:GLU:OE2	6:X:107:GLU:N	2.33	0.59
6:a:12:THR:HG21	7:k:36:ASP:OD2	2.02	0.59
8:f:91:GLU:OE2	8:f:91:GLU:N	2.25	0.59
8:o:79:TRP:HB3	8:o:84:TRP:HB2	1.83	0.59
4:K:29:SER:OG	7:q:75:ASN:ND2	2.30	0.59
4:M:3:THR:HB	7:e:276:SER:CB	2.28	0.59
5:P:225:LEU:HD21	5:P:269:VAL:HG11	1.84	0.59
5:Q:35:THR:HA	6:Z:63:LYS:HD3	1.85	0.59
5:S:198:GLU:OE2	5:S:199:THR:N	2.34	0.59
7:e:224:LEU:HD21	8:f:183:LYS:HB2	1.85	0.59
7:g:243:LEU:HD21	7:g:259:VAL:HG11	1.84	0.59
1:B:859:ARG:NH2	1:B:889:SER:OG	2.36	0.59
1:C:539:MET:HB3	1:C:546:LEU:HD11	1.84	0.59
8:l:55:ASP:OD2	8:l:58:ARG:NH2	2.35	0.59
7:n:49:THR:HG23	7:n:50:MET:N	2.17	0.59
1:A:128:TYR:HA	1:A:159:ARG:HB2	1.85	0.59
1:A:204:ARG:HD3	7:b:92:GLN:HE22	1.66	0.59
1:B:770:ARG:HB2	1:B:774:GLY:HA2	1.84	0.59
1:C:6:ILE:HD12	1:C:17:LEU:HD22	1.83	0.59
2:D:170:GLN:NE2	2:E:162:GLU:OE1	2.35	0.59
4:L:134:GLU:OE2	4:L:137:LYS:HE2	2.03	0.59
1:C:614:LYS:NZ	1:C:624:PHE:O	2.35	0.59
3:H:670:ALA:HB2	3:I:676:ILE:HG12	1.83	0.59
4:K:94:GLN:NE2	5:P:127:LYS:HA	2.18	0.59
4:O:29:SER:OG	7:k:71:SER:HB2	2.02	0.59
5:P:213:GLN:NE2	7:q:52:TYR:HE1	2.00	0.59
7:p:197:ARG:NH2	7:p:204:ASP:OD2	2.36	0.59
8:r:63:LEU:HB2	8:r:64:GLN:NE2	2.18	0.59
1:A:442:ARG:O	4:K:101:ILE:HD12	2.03	0.59
1:B:6:ILE:HD12	1:B:17:LEU:HD22	1.84	0.59
2:E:40:ASN:HB3	2:E:51:LYS:HB2	1.85	0.59
5:Q:195:VAL:HG13	7:j:27:ASN:ND2	2.18	0.59
1:A:179:ASN:OD1	1:A:184:ASN:ND2	2.36	0.59
1:B:518:SER:OG	2:E:96:GLU:OE1	2.21	0.59
1:B:599:VAL:HG23	2:F:85:MET:HE1	1.82	0.59
3:H:677:ILE:CD1	3:I:677:ILE:CG1	2.80	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:47:GLU:OE1	6:X:102:ASN:OD1	2.21	0.59
4:M:9:LYS:HB2	7:e:264:GLN:HB3	1.83	0.59
7:e:195:ARG:NH1	8:f:78:GLY:O	2.33	0.59
1:A:685:GLY:HA2	4:J:114:LEU:HB2	1.85	0.58
1:C:128:TYR:HA	1:C:159:ARG:HB2	1.84	0.58
2:E:59:ASN:O	7:e:163:THR:HG21	2.03	0.58
6:a:3:VAL:HG23	6:a:5:PRO:HD2	1.85	0.58
8:i:166:GLU:OE2	8:i:166:GLU:N	2.33	0.58
7:p:23:LEU:HD11	7:p:44:ARG:HD3	1.85	0.58
6:V:6:PRO:HB2	8:o:34:ALA:HB3	1.85	0.58
6:X:31:LEU:O	8:c:24:GLN:NE2	2.36	0.58
8:c:9:TRP:NE1	7:d:56:GLU:OE1	2.34	0.58
8:r:80:THR:O	8:r:82:PRO:N	2.36	0.58
1:B:473:ASN:HB3	1:B:541:THR:HG21	1.84	0.58
2:E:188:ALA:HB2	2:F:184:ILE:HG12	1.85	0.58
5:T:225:LEU:HD21	5:T:269:VAL:HG11	1.84	0.58
1:A:614:LYS:NZ	1:A:624:PHE:O	2.36	0.58
1:B:22:ILE:HD11	5:T:77:ILE:HG13	1.84	0.58
5:T:207:LYS:HZ3	5:T:213:GLN:NE2	1.97	0.58
8:l:29:TYR:HB3	8:l:35:THR:HG21	1.85	0.58
7:q:208:LEU:HD11	7:q:259:VAL:HG13	1.85	0.58
8:r:95:VAL:O	8:r:99:ASN:ND2	2.36	0.58
1:A:272:THR:HG21	1:B:601:ALA:HB3	1.85	0.58
1:B:270:ASP:OD1	1:B:271:THR:N	2.36	0.58
1:C:551:ILE:HG22	1:C:647:ALA:HB3	1.84	0.58
4:O:22:ILE:CD1	7:k:193:ILE:CG2	2.81	0.58
6:W:65:GLN:O	6:W:69:GLU:HG2	2.03	0.58
6:Y:12:THR:CG2	7:e:36:ASP:HB2	2.22	0.58
8:c:141:SER:OG	8:c:142:GLU:OE1	2.20	0.58
7:d:81:GLU:HG3	7:d:186:LEU:HD22	1.85	0.58
1:A:200:PRO:CG	7:b:171:ILE:CD1	2.80	0.58
1:B:451:LEU:HG	4:M:125:LEU:HD23	1.85	0.58
1:C:204:ARG:HD3	7:n:92:GLN:HE22	1.68	0.58
6:V:34:VAL:HB	8:o:23:GLU:OE1	2.03	0.58
1:C:539:MET:HG2	1:C:548:ILE:HG12	1.85	0.58
6:X:3:VAL:HG23	6:X:5:PRO:HD2	1.85	0.58
1:B:569:LYS:HD3	5:Q:77:ILE:CD1	2.33	0.58
8:c:44:LYS:O	8:c:48:GLU:HG3	2.04	0.58
1:C:583:GLY:O	2:D:21:LYS:NZ	2.36	0.58
2:D:48:ARG:HB3	2:D:79:LEU:HD21	1.85	0.58
3:H:670:ALA:CB	3:I:676:ILE:HG12	2.34	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:V:22:TYR:HE2	7:p:36:ASP:OD2	1.87	0.58
6:W:32:SER:HB3	8:r:27:THR:O	2.03	0.58
2:E:22:ARG:HG2	2:F:26:LEU:HB3	1.86	0.58
8:c:79:TRP:HE3	8:c:83:TYR:O	1.86	0.58
1:A:197:ASN:ND2	7:b:171:ILE:O	2.28	0.57
5:R:225:LEU:HD21	5:R:269:VAL:HG11	1.85	0.57
6:V:32:SER:O	8:o:24:GLN:HG3	2.04	0.57
6:V:34:VAL:HG21	8:o:23:GLU:OE1	2.03	0.57
6:X:39:VAL:HG12	8:c:2:SER:HA	1.86	0.57
1:B:539:MET:HB3	1:B:546:LEU:HD11	1.86	0.57
7:n:178:ARG:NE	7:n:215:GLU:OE2	2.37	0.57
7:n:269:LEU:HD13	7:p:202:ALA:HB2	1.86	0.57
1:A:601:ALA:CB	2:F:99:TYR:OH	2.52	0.57
4:J:31:LEU:HD23	7:n:71:SER:HB2	1.86	0.57
7:h:60:LYS:NZ	7:j:9:GLN:O	2.36	0.57
7:q:317:LEU:HD13	7:q:361:PRO:HG2	1.86	0.57
1:C:406:ASN:O	1:C:410:GLU:HG2	2.03	0.57
4:L:31:LEU:O	7:d:183:ILE:HG12	2.05	0.57
5:U:35:THR:HA	6:X:63:LYS:CD	2.35	0.57
6:W:10:ASN:CA	7:p:154:PHE:CD2	2.76	0.57
7:d:369:GLU:HG2	7:d:379:ARG:HG2	1.87	0.57
1:C:2:GLN:CB	5:S:86:ASN:OD1	2.52	0.57
1:C:585:SER:HG	2:D:24:GLU:CD	2.11	0.57
2:F:48:ARG:HB3	2:F:79:LEU:HD21	1.86	0.57
6:W:34:VAL:O	6:W:37:GLU:HG2	2.05	0.57
6:Z:107:GLU:N	6:Z:107:GLU:OE2	2.33	0.57
8:f:55:ASP:OD2	8:f:58:ARG:NH2	2.36	0.57
7:m:113:ASP:OD1	7:m:115:SER:OG	2.22	0.57
7:p:209:ALA:O	7:p:213:MET:HG3	2.04	0.57
1:A:355:ARG:HB2	1:A:358:ARG:HG3	1.87	0.57
1:A:520:VAL:HG13	2:F:56:LEU:HD21	1.87	0.57
1:B:26:PHE:HB2	1:B:695:HIS:H	1.68	0.57
1:B:405:LYS:NZ	2:E:81:GLN:NE2	2.52	0.57
2:E:54:ASP:N	2:E:54:ASP:OD1	2.35	0.57
4:L:128:VAL:CG2	7:d:14:ASP:OD1	2.53	0.57
5:S:24:GLN:NE2	5:T:163:ASP:HA	2.19	0.57
5:U:207:LYS:HZ3	5:U:213:GLN:NE2	2.02	0.57
8:c:26:GLY:N	8:c:31:ASP:OD2	2.38	0.57
7:k:243:LEU:HD21	7:k:259:VAL:HG21	1.86	0.57
1:A:56:SER:HB2	4:L:136:SER:OG	2.05	0.57
1:A:87:VAL:HG13	1:A:95:VAL:HB	1.85	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:638:GLN:CG	7:n:104:ILE:CD1	2.75	0.57
5:Q:27:TYR:HB3	5:Q:56:LEU:HD23	1.87	0.57
7:g:356:ASN:OD1	7:g:359:THR:OG1	2.20	0.57
1:C:790:TYR:CD2	1:C:791:MET:O	2.56	0.57
2:D:62:GLU:HG2	7:k:161:PRO:HB2	1.86	0.57
2:F:66:ILE:HG22	2:F:100:TYR:HD2	1.69	0.57
4:J:31:LEU:HD21	7:n:75:ASN:ND2	2.20	0.57
4:O:18:LEU:HD22	7:k:212:THR:CG2	2.34	0.57
2:E:9:VAL:HG22	3:H:678:ASN:OD1	2.04	0.57
3:G:676:ILE:HG23	3:I:670:ALA:HB1	1.86	0.57
4:M:29:SER:CB	7:e:75:ASN:HD21	2.17	0.57
4:O:22:ILE:HD11	7:k:193:ILE:CG2	2.28	0.57
6:V:107:GLU:OE1	6:V:107:GLU:N	2.38	0.57
6:Y:34:VAL:HG22	8:f:24:GLN:HE21	1.69	0.57
7:d:146:GLU:HB3	7:e:42:PHE:HZ	1.69	0.57
7:j:116:GLY:O	7:j:119:ARG:NH1	2.37	0.57
2:D:14:LEU:HA	3:G:681:TRP:HH2	1.70	0.56
2:F:40:ASN:HB3	2:F:51:LYS:HB2	1.85	0.56
4:N:31:LEU:O	7:j:183:ILE:HG12	2.05	0.56
7:b:76:VAL:HG23	7:b:77:LEU:HD23	1.87	0.56
7:k:86:LYS:HG3	7:k:144:ILE:HG22	1.87	0.56
1:A:168:ASN:HD22	7:b:381:ASN:HD21	1.50	0.56
1:C:488:VAL:HB	7:k:159:SER:HB3	1.87	0.56
6:Y:3:VAL:HG23	6:Y:5:PRO:HD2	1.87	0.56
7:d:93:PHE:HE2	7:d:105:VAL:HG11	1.69	0.56
1:B:322:ALA:HB2	1:B:349:ASP:HB3	1.88	0.56
1:C:584:SER:HB2	2:D:24:GLU:OE1	2.04	0.56
2:D:192:ILE:HG12	2:E:184:ILE:HB	1.87	0.56
2:D:214:ASP:OD1	2:D:218:ARG:N	2.37	0.56
4:N:31:LEU:HD23	7:h:71:SER:HB2	1.84	0.56
4:N:104:PHE:CB	5:T:201:GLN:O	2.53	0.56
4:O:44:PHE:HA	6:V:99:GLY:O	2.05	0.56
5:S:14:LEU:O	5:T:109:ARG:NH1	2.38	0.56
5:T:64:ILE:HG12	5:T:97:MET:HG2	1.86	0.56
5:T:213:GLN:NE2	7:k:52:TYR:HE1	2.04	0.56
7:e:49:THR:HG23	7:e:50:MET:N	2.21	0.56
7:e:354:MET:HE1	7:e:361:PRO:HB3	1.87	0.56
7:h:219:CYS:SG	7:h:220:LYS:N	2.78	0.56
7:k:243:LEU:HD22	7:k:256:ILE:HD13	1.86	0.56
7:q:5:LEU:HG	7:q:6:ASN:OD1	2.05	0.56
5:S:85:LEU:HD11	5:T:176:LYS:HD3	1.86	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:m:39:ALA:HA	7:m:44:ARG:HG2	1.86	0.56
1:A:8:ILE:HG12	1:A:436:LEU:HD13	1.87	0.56
1:C:442:ARG:O	4:O:101:ILE:HD12	2.06	0.56
1:C:516:ASN:ND2	2:D:96:GLU:OE1	2.39	0.56
4:K:139:LEU:HD23	4:K:145:LYS:HD2	1.88	0.56
5:R:14:LEU:O	5:U:109:ARG:NH1	2.38	0.56
6:W:37:GLU:HB3	8:r:21:PRO:CB	2.15	0.56
6:X:3:VAL:O	7:d:42:PHE:CE1	2.59	0.56
7:d:327:GLU:OE1	7:e:333:ARG:NH1	2.36	0.56
1:A:322:ALA:HB2	1:A:349:ASP:HB3	1.86	0.56
1:A:542:VAL:CG2	4:K:107:ASN:O	2.51	0.56
1:C:355:ARG:HB2	1:C:358:ARG:HG3	1.88	0.56
8:f:19:ARG:NH2	7:g:56:GLU:OE2	2.27	0.56
7:j:81:GLU:HG3	7:j:186:LEU:HD22	1.88	0.56
7:s:244:LEU:HB2	7:s:278:MET:HE3	1.87	0.56
1:A:318:GLY:O	1:A:363:SER:OG	2.24	0.56
3:G:673:ILE:HG23	3:I:673:ILE:HG21	1.88	0.56
5:R:64:ILE:HG21	5:R:95:MET:HE2	1.88	0.56
8:l:88:TYR:OH	8:l:172:LYS:NZ	2.38	0.56
7:q:11:VAL:HG21	7:q:58:LEU:HD22	1.87	0.56
1:A:344:VAL:N	1:B:808:GLY:O	2.39	0.56
2:D:175:LYS:N	2:E:167:ASP:OD1	2.36	0.56
4:M:42:ASP:N	4:M:42:ASP:OD1	2.36	0.56
5:P:195:VAL:HG11	7:s:35:THR:HA	1.88	0.56
7:m:227:ILE:HG13	7:m:274:LEU:HD13	1.88	0.56
7:m:242:PHE:HB3	7:m:278:MET:HG3	1.87	0.56
1:A:484:ARG:NH1	1:A:516:ASN:OD1	2.32	0.56
2:D:198:SER:OG	2:E:206:GLY:O	2.22	0.56
4:L:6:PHE:CE2	7:b:275:ILE:HD12	2.40	0.56
2:E:240:ILE:HG23	2:F:231:ASP:HA	1.87	0.56
4:J:105:ILE:HB	5:P:202:ASN:OD1	2.05	0.56
4:K:95:LYS:HE3	5:P:126:VAL:HB	1.88	0.56
4:N:18:LEU:HG	4:N:18:LEU:O	2.05	0.56
6:W:34:VAL:HG11	8:r:23:GLU:OE1	2.05	0.56
7:k:192:GLN:NE2	7:k:206:GLU:OE1	2.39	0.56
1:A:405:LYS:NZ	2:F:81:GLN:OE1	2.38	0.55
1:A:600:ASP:OD2	1:A:603:SER:OG	2.23	0.55
1:A:770:ARG:HB2	1:A:774:GLY:HA2	1.86	0.55
1:C:322:ALA:HB2	1:C:349:ASP:HB3	1.87	0.55
2:F:64:ASN:ND2	2:F:96:GLU:OE1	2.39	0.55
4:J:43:LEU:HD13	4:J:90:LYS:HD3	1.87	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:V:3:VAL:HG23	6:V:5:PRO:HD2	1.89	0.55
6:Z:32:SER:C	8:i:24:GLN:HG3	2.31	0.55
7:b:269:LEU:HD13	7:d:202:ALA:HB2	1.88	0.55
7:k:345:MET:HE3	7:k:352:ILE:HD12	1.87	0.55
1:C:156:ASN:C	1:C:157:ILE:HD13	2.32	0.55
1:C:194:GLN:HG2	7:n:153:ASN:HB3	1.88	0.55
1:C:473:ASN:HB3	1:C:541:THR:HG21	1.88	0.55
2:F:9:VAL:CG1	3:G:681:TRP:CD1	2.87	0.55
2:F:14:LEU:CA	3:H:681:TRP:HH2	2.19	0.55
4:L:5:GLU:OE2	7:b:272:ARG:HG2	2.07	0.55
5:R:213:GLN:NE2	7:e:52:TYR:HE1	2.04	0.55
5:U:27:TYR:HB3	5:U:56:LEU:HD23	1.88	0.55
7:g:317:LEU:HD13	7:g:361:PRO:HG2	1.86	0.55
7:g:332:ILE:HB	7:g:340:ILE:HD11	1.88	0.55
7:m:360:ILE:HG12	7:m:361:PRO:HD2	1.88	0.55
1:B:59:GLN:H	1:B:63:ASP:HB2	1.71	0.55
1:C:22:ILE:HD11	5:P:77:ILE:HG13	1.87	0.55
2:D:40:ASN:HB3	2:D:51:LYS:HB2	1.88	0.55
7:e:11:VAL:HG21	7:e:58:LEU:HD22	1.88	0.55
1:A:701:ILE:HD11	5:U:73:GLN:HB3	1.87	0.55
1:B:1:MET:HE2	5:R:133:HIS:CD2	2.42	0.55
1:B:496:THR:HG23	7:e:110:GLN:HE22	1.69	0.55
1:C:42:PHE:CZ	5:P:84:GLN:HG2	2.41	0.55
4:O:94:GLN:HA	4:O:97:LEU:HD12	1.88	0.55
8:c:79:TRP:CE3	8:c:83:TYR:O	2.59	0.55
1:B:675:TYR:OH	4:L:112:LYS:HB3	2.07	0.55
4:L:31:LEU:HD21	7:b:75:ASN:ND2	2.21	0.55
5:T:64:ILE:HG21	5:T:95:MET:HE3	1.89	0.55
6:V:32:SER:C	8:o:24:GLN:HG3	2.31	0.55
6:V:71:GLU:CG	7:p:40:SER:OG	2.54	0.55
7:k:354:MET:HE1	7:k:361:PRO:HB3	1.89	0.55
7:m:213:MET:HE3	7:m:217:SER:HB2	1.89	0.55
7:q:76:VAL:HG23	7:q:76:VAL:O	2.07	0.55
1:C:673:ALA:HB1	1:C:687:SER:HB3	1.89	0.55
8:l:65:CYS:SG	8:l:69:TYR:HB2	2.47	0.55
7:p:81:GLU:HG3	7:p:186:LEU:HD22	1.87	0.55
2:F:232:LEU:HD11	2:F:237:MET:HB3	1.89	0.55
7:h:76:VAL:HG23	7:h:77:LEU:HD23	1.88	0.55
4:N:31:LEU:HD21	7:h:75:ASN:ND2	2.22	0.55
7:d:279:GLU:HG3	7:d:358:TRP:CD1	2.42	0.55
7:j:209:ALA:O	7:j:213:MET:HG3	2.07	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:10:ILE:O	1:C:11:GLY:C	2.50	0.55
8:o:141:SER:OG	8:o:142:GLU:OE1	2.20	0.55
1:C:585:SER:OG	2:D:24:GLU:OE1	2.25	0.55
1:C:791:MET:HE2	1:C:881:GLU:HG2	1.89	0.55
7:m:332:ILE:HB	7:m:340:ILE:HD11	1.89	0.55
1:A:585:SER:HA	1:A:588:ILE:HD12	1.89	0.54
1:B:1:MET:HE2	5:R:133:HIS:NE2	2.22	0.54
1:B:156:ASN:C	1:B:157:ILE:HD13	2.32	0.54
1:C:8:ILE:HG12	1:C:436:LEU:HD13	1.89	0.54
1:C:520:VAL:HG13	2:D:56:LEU:HD21	1.89	0.54
1:C:585:SER:HG	2:D:24:GLU:CG	2.21	0.54
3:G:680:GLN:OE1	3:I:674:ALA:CB	2.54	0.54
7:b:60:LYS:NZ	7:d:9:GLN:O	2.40	0.54
2:E:217:GLY:O	2:E:219:LYS:NZ	2.40	0.54
6:Y:6:PRO:O	8:f:34:ALA:HB3	2.07	0.54
8:l:159:ASP:OD1	8:l:159:ASP:N	2.40	0.54
7:n:46:PHE:O	7:n:49:THR:CG2	2.50	0.54
1:B:42:PHE:CZ	5:T:84:GLN:HG2	2.42	0.54
1:B:675:TYR:OH	4:L:112:LYS:CB	2.56	0.54
1:C:59:GLN:H	1:C:63:ASP:HB2	1.72	0.54
4:J:31:LEU:O	7:p:183:ILE:HG12	2.06	0.54
4:J:36:GLN:NE2	4:J:117:ASP:OD1	2.40	0.54
6:Y:49:ARG:NH2	6:Y:56:ASP:OD1	2.38	0.54
1:A:551:ILE:HG22	1:A:647:ALA:HB3	1.89	0.54
1:A:578:GLN:HE22	4:O:152:ASP:H	1.55	0.54
1:A:872:THR:HG21	7:q:153:ASN:OD1	2.06	0.54
4:N:25:ASN:ND2	7:h:78:GLY:HA3	2.22	0.54
4:O:31:LEU:HD12	4:O:32:THR:HG23	1.90	0.54
6:Y:1:MET:HG2	7:g:33:GLU:OE2	2.07	0.54
6:Y:3:VAL:O	7:g:42:PHE:CE1	2.61	0.54
1:A:844:LEU:HB2	1:A:879:HIS:HB3	1.88	0.54
1:B:152:GLN:HB2	1:B:157:ILE:HD11	1.90	0.54
4:N:32:THR:HB	4:N:35:LYS:HE2	1.90	0.54
7:b:192:GLN:NE2	7:b:210:GLU:OE2	2.36	0.54
7:b:356:ASN:OD1	7:b:359:THR:OG1	2.21	0.54
1:A:262:ASP:CG	2:F:111:ARG:HH12	2.16	0.54
1:B:631:PRO:HD2	2:E:92:ASP:HB3	1.90	0.54
2:E:9:VAL:HG21	3:H:677:ILE:HG22	1.90	0.54
2:E:216:GLN:OE1	2:E:218:ARG:NH1	2.40	0.54
7:j:16:GLU:H	7:j:16:GLU:CD	2.15	0.54
7:n:76:VAL:HG23	7:n:77:LEU:HD23	1.88	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:613:ASN:O	1:C:479:ARG:NH2	2.38	0.54
1:B:587:LYS:CD	2:D:4:ASP:HA	2.38	0.54
2:D:115:ASP:HB3	2:D:119:ASP:OD1	2.07	0.54
5:Q:128:LYS:HD3	5:Q:133:HIS:NE2	2.23	0.54
6:a:1:MET:SD	7:m:33:GLU:OE2	2.66	0.54
7:b:49:THR:HG23	7:b:50:MET:N	2.22	0.54
1:C:578:GLN:NE2	4:M:151:PHE:H	2.06	0.54
2:D:74:ASN:ND2	2:E:125:GLU:OE2	2.41	0.54
4:L:56:LYS:O	4:L:60:GLU:HG3	2.08	0.54
7:b:333:ARG:NH1	7:b:338:LEU:O	2.37	0.54
1:C:430:LYS:O	1:C:452:HIS:ND1	2.41	0.54
4:K:31:LEU:CD2	7:q:71:SER:CB	2.75	0.54
5:S:97:MET:HE1	5:S:173:MET:HE2	1.90	0.54
5:S:190:GLU:HA	5:S:193:LYS:HE3	1.89	0.54
7:e:57:LEU:HD13	7:g:54:GLY:HA3	1.88	0.54
1:A:32:LYS:CG	2:E:1:MET:HG3	2.38	0.53
1:A:662:GLN:O	1:A:666:GLU:HG2	2.08	0.53
1:B:445:ILE:HG13	4:M:101:ILE:HG21	1.89	0.53
4:M:24:PRO:HG3	7:g:191:ALA:HB2	1.89	0.53
4:N:60:GLU:O	5:Q:48:GLN:HG2	2.08	0.53
6:Z:3:VAL:HG23	6:Z:5:PRO:HD2	1.90	0.53
7:d:304:ILE:HD11	7:d:338:LEU:HD22	1.90	0.53
7:n:242:PHE:HB3	7:n:278:MET:HG3	1.91	0.53
1:A:506:ASP:HB3	1:A:547:GLN:HB3	1.89	0.53
1:B:1:MET:HE1	5:R:133:HIS:CE1	2.43	0.53
1:C:585:SER:OG	2:D:24:GLU:CD	2.51	0.53
2:F:54:ASP:OD1	2:F:54:ASP:N	2.39	0.53
4:M:70:ILE:HG22	4:M:92:PRO:HG2	1.90	0.53
5:U:31:TYR:C	5:U:33:ASP:H	2.16	0.53
6:V:111:SER:CB	7:m:115:SER:O	2.56	0.53
6:X:6:PRO:HG2	8:c:35:THR:OG1	2.07	0.53
7:k:227:ILE:H	7:k:227:ILE:HD12	1.73	0.53
1:A:604:GLY:HA2	2:D:85:MET:CE	2.38	0.53
4:L:31:LEU:HD23	7:b:71:SER:HB2	1.90	0.53
4:O:40:ASP:HA	4:O:43:LEU:HB2	1.89	0.53
5:P:275:ASP:OD2	7:s:29:VAL:HG22	2.07	0.53
7:k:317:LEU:HD13	7:k:361:PRO:HG2	1.91	0.53
1:B:355:ARG:HB2	1:B:358:ARG:HG3	1.90	0.53
1:B:481:LYS:NZ	1:B:500:GLN:OE1	2.40	0.53
4:M:14:GLU:O	7:e:262:THR:HG23	2.09	0.53
5:S:191:ALA:HA	5:S:194:LYS:HE3	1.89	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:p:369:GLU:HG2	7:p:379:ARG:HG2	1.91	0.53
8:r:159:ASP:OD1	8:r:159:ASP:N	2.41	0.53
7:b:52:TYR:HB2	7:d:25:HIS:HD2	1.73	0.53
7:e:243:LEU:HD22	7:e:256:ILE:HD13	1.90	0.53
7:e:317:LEU:HD13	7:e:361:PRO:HG2	1.90	0.53
4:L:4:GLN:NE2	7:b:256:ILE:CB	2.70	0.53
5:Q:207:LYS:CE	7:h:52:TYR:CE1	2.85	0.53
5:S:112:GLN:HG2	5:S:166:PRO:HD2	1.90	0.53
5:S:239:ILE:HD11	5:S:258:LEU:HB3	1.91	0.53
8:o:26:GLY:N	8:o:31:ASP:OD2	2.41	0.53
1:B:520:VAL:HG13	2:E:56:LEU:HD21	1.90	0.53
2:E:113:LYS:HE2	2:E:116:PRO:HA	1.91	0.53
4:N:18:LEU:CG	7:h:266:ARG:NH1	2.67	0.53
6:Y:4:TYR:HA	7:g:42:PHE:HD1	1.73	0.53
7:m:26:THR:HG23	7:m:34:PHE:HB3	1.91	0.53
7:q:57:LEU:HD13	7:s:54:GLY:HA3	1.91	0.53
7:q:268:MET:HA	7:s:200:VAL:HG22	1.89	0.53
1:B:73:ASP:O	7:e:125:ASN:ND2	2.31	0.53
4:J:18:LEU:CB	7:n:212:THR:HG21	2.32	0.53
4:J:128:VAL:HG23	7:p:14:ASP:OD1	2.09	0.53
4:K:43:LEU:HD13	4:K:90:LYS:HD2	1.91	0.53
4:L:147:VAL:HG11	5:U:214:LEU:HD13	1.91	0.53
5:T:195:VAL:HG11	7:m:35:THR:HA	1.91	0.53
6:W:6:PRO:HG2	8:r:35:THR:OG1	2.08	0.53
7:h:374:GLU:OE2	7:h:374:GLU:N	2.40	0.53
1:C:78:THR:O	7:k:102:ASP:CB	2.56	0.53
5:R:3:LYS:HA	5:R:6:LYS:HD3	1.91	0.53
7:e:356:ASN:OD1	7:e:359:THR:OG1	2.20	0.53
8:r:29:TYR:HB3	8:r:35:THR:HG21	1.90	0.53
8:r:68:GLU:H	8:r:68:GLU:CD	2.16	0.53
1:B:9:LEU:HD23	1:B:14:THR:HB	1.90	0.53
1:B:22:ILE:HD13	5:T:77:ILE:HG13	1.91	0.53
1:B:872:THR:HG21	7:e:153:ASN:CG	2.33	0.53
4:K:5:GLU:OE2	7:q:272:ARG:HD2	2.09	0.53
5:T:249:ILE:HG12	5:T:256:VAL:HG22	1.91	0.53
7:e:198:ASN:HD21	7:g:198:ASN:H	1.56	0.53
8:f:29:TYR:HB3	8:f:35:THR:HG21	1.91	0.53
8:i:44:LYS:O	8:i:48:GLU:HG3	2.09	0.53
8:o:95:VAL:O	8:o:99:ASN:ND2	2.42	0.53
7:q:156:ASP:OD1	7:q:157:GLN:NE2	2.39	0.53
1:A:816:SER:N	1:A:861:THR:O	2.43	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:318:GLY:O	1:B:363:SER:OG	2.25	0.52
1:C:42:PHE:CE1	5:P:75:ILE:HD12	2.43	0.52
2:D:54:ASP:OD1	2:D:54:ASP:N	2.36	0.52
2:D:201:PHE:HA	2:E:204:LEU:HD11	1.90	0.52
2:E:214:ASP:OD1	2:E:218:ARG:N	2.40	0.52
5:T:40:THR:OG1	5:T:42:THR:O	2.26	0.52
5:T:224:TYR:HD1	5:T:225:LEU:HD22	1.73	0.52
7:g:39:ALA:HA	7:g:44:ARG:HG2	1.91	0.52
8:l:68:GLU:H	8:l:68:GLU:CD	2.16	0.52
1:B:200:PRO:HG2	7:h:171:ILE:HG22	1.91	0.52
3:H:670:ALA:HB1	3:I:676:ILE:CG2	2.38	0.52
5:Q:31:TYR:C	5:Q:33:ASP:H	2.17	0.52
5:Q:71:ASN:ND2	5:Q:89:ASN:OD1	2.37	0.52
6:Z:66:ILE:O	6:Z:70:GLU:HG2	2.10	0.52
7:b:178:ARG:NE	7:b:215:GLU:OE2	2.42	0.52
8:r:91:GLU:OE2	8:r:91:GLU:N	2.20	0.52
1:A:449:SER:OG	4:K:125:LEU:HD22	2.09	0.52
4:N:31:LEU:HD23	4:N:31:LEU:H	1.74	0.52
7:b:104:ILE:HD13	7:b:127:VAL:HG22	1.92	0.52
8:c:29:TYR:HB3	8:c:35:THR:HG21	1.91	0.52
8:c:81:ALA:HB1	8:c:82:PRO:HD2	1.91	0.52
8:f:130:PRO:HD3	8:f:152:PHE:HA	1.89	0.52
7:k:13:ASP:OD1	7:k:13:ASP:O	2.28	0.52
1:A:149:PRO:HG2	1:A:157:ILE:HG21	1.92	0.52
1:A:539:MET:HB3	1:A:546:LEU:HD11	1.91	0.52
1:B:168:ASN:HD22	7:h:381:ASN:HD22	1.50	0.52
3:H:670:ALA:CA	3:I:676:ILE:HG21	2.40	0.52
4:N:18:LEU:CD2	7:h:266:ARG:NH1	2.73	0.52
5:Q:28:LEU:HD11	5:Q:173:MET:HE1	1.91	0.52
5:U:215:ILE:O	5:U:218:VAL:HG12	2.09	0.52
8:o:83:TYR:HA	8:o:176:LEU:HD13	1.92	0.52
1:B:585:SER:N	2:E:24:GLU:OE1	2.42	0.52
1:C:804:LEU:HD12	1:C:814:VAL:HG22	1.92	0.52
4:J:31:LEU:HD23	4:J:31:LEU:H	1.75	0.52
7:b:11:VAL:HG21	7:b:58:LEU:HD22	1.91	0.52
8:i:13:ARG:HH21	8:i:47:ILE:HG23	1.74	0.52
7:n:239:VAL:HG13	8:o:180:LEU:HD23	1.91	0.52
1:C:54:SER:HB2	4:J:134:GLU:OE1	2.09	0.52
2:D:162:GLU:HG3	2:E:154:ILE:HB	1.92	0.52
4:J:73:ASP:OD2	4:J:121:SER:OG	2.26	0.52
4:O:31:LEU:HD21	7:k:71:SER:OG	2.08	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:119:ILE:O	5:P:122:ARG:HG2	2.10	0.52
5:S:46:ASN:OD1	6:W:101:GLU:OE2	2.28	0.52
8:r:190:ASN:OD1	8:r:190:ASN:N	2.42	0.52
1:B:519:GLN:NE2	1:B:522:GLN:O	2.37	0.52
1:C:318:GLY:O	1:C:363:SER:OG	2.27	0.52
1:C:816:SER:N	1:C:861:THR:O	2.42	0.52
6:X:6:PRO:O	8:c:34:ALA:HB3	2.10	0.52
7:b:46:PHE:C	7:b:49:THR:HG22	2.34	0.52
7:e:46:PHE:O	7:e:49:THR:CG2	2.51	0.52
7:e:345:MET:HB3	7:e:352:ILE:HD11	1.92	0.52
7:m:356:ASN:OD1	7:m:359:THR:OG1	2.21	0.52
7:n:13:ASP:OD1	7:n:13:ASP:O	2.28	0.52
1:A:12:ASN:OD1	1:A:51:LYS:NZ	2.41	0.52
1:B:427:ILE:HG22	4:N:139:LEU:HB3	1.91	0.52
1:A:156:ASN:C	1:A:157:ILE:HD13	2.35	0.51
1:C:36:ASN:ND2	3:H:687:ASP:HA	2.26	0.51
1:C:312:GLU:OE2	7:q:134:PHE:HD2	1.93	0.51
1:C:451:LEU:HG	4:O:125:LEU:HD23	1.91	0.51
4:K:79:PRO:O	8:r:5:ALA:HB3	2.10	0.51
5:S:119:ILE:O	5:S:122:ARG:HG3	2.10	0.51
5:S:233:PRO:HD2	5:S:236:ILE:HG13	1.92	0.51
7:q:219:CYS:SG	7:q:220:LYS:N	2.83	0.51
7:q:318:THR:HB	7:q:321:GLU:HG3	1.91	0.51
1:B:431:GLY:O	4:M:146:VAL:N	2.41	0.51
7:h:57:LEU:HD13	7:j:54:GLY:HA3	1.91	0.51
7:s:39:ALA:HA	7:s:44:ARG:HG2	1.90	0.51
1:A:406:ASN:O	1:A:410:GLU:HG2	2.11	0.51
1:B:701:ILE:HD11	5:Q:73:GLN:CB	2.40	0.51
1:C:630:VAL:HG21	2:D:29:ARG:CZ	2.40	0.51
2:D:91:VAL:HG12	2:D:92:ASP:OD2	2.10	0.51
4:N:73:ASP:OD2	4:N:121:SER:OG	2.23	0.51
6:Z:15:LYS:NZ	7:h:42:PHE:CD1	2.72	0.51
7:d:245:ASP:OD1	7:d:246:VAL:N	2.40	0.51
7:j:197:ARG:NH2	7:j:204:ASP:OD2	2.43	0.51
7:q:284:GLU:OE2	7:q:346:ASN:ND2	2.44	0.51
7:s:26:THR:HG23	7:s:34:PHE:HB3	1.93	0.51
7:s:363:PHE:HZ	7:s:366:ILE:HB	1.76	0.51
1:B:595:MET:HE3	1:B:631:PRO:HG3	1.93	0.51
1:C:585:SER:N	2:D:24:GLU:OE1	2.38	0.51
2:D:136:ASP:OD1	2:D:137:SER:N	2.44	0.51
2:E:218:ARG:HD2	2:E:232:LEU:HD23	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:30:ILE:HG13	7:q:71:SER:HB3	1.93	0.51
4:O:18:LEU:HD11	4:O:21:LEU:CD2	2.30	0.51
4:O:55:ASN:OD1	7:m:52:TYR:CE1	2.64	0.51
5:P:109:ARG:NH1	5:U:14:LEU:O	2.42	0.51
5:R:249:ILE:HG12	5:R:256:VAL:HG22	1.93	0.51
7:h:50:MET:HE3	8:i:42:TRP:CD1	2.45	0.51
1:B:140:GLU:O	1:B:143:MET:HG2	2.11	0.51
1:C:22:ILE:HD13	5:P:77:ILE:HG13	1.91	0.51
1:C:181:SER:H	1:C:184:ASN:HB2	1.75	0.51
1:C:595:MET:HE3	1:C:631:PRO:HG3	1.92	0.51
4:J:101:ILE:HG22	4:J:103:LYS:NZ	2.25	0.51
4:K:31:LEU:HD21	7:q:75:ASN:ND2	2.25	0.51
4:M:13:ILE:HA	4:M:16:GLU:HB2	1.92	0.51
5:R:119:ILE:O	5:R:122:ARG:HG2	2.10	0.51
6:V:44:PHE:HE1	6:V:71:GLU:HG2	1.75	0.51
6:Z:6:PRO:HG2	8:i:35:THR:OG1	2.11	0.51
7:n:389:GLU:O	7:n:389:GLU:HG2	2.11	0.51
1:A:152:GLN:HB2	1:A:157:ILE:HD11	1.93	0.51
1:A:506:ASP:OD2	4:K:109:PRO:HB3	2.10	0.51
4:M:60:GLU:OE1	5:R:47:LYS:NZ	2.29	0.51
5:S:35:THR:HA	6:V:63:LYS:HD3	1.92	0.51
6:V:85:ASN:OD1	6:V:86:ASN:N	2.44	0.51
7:p:93:PHE:HE2	7:p:105:VAL:HG11	1.74	0.51
1:A:59:GLN:H	1:A:63:ASP:HB2	1.74	0.51
1:B:649:VAL:HG21	4:K:154:THR:HG21	1.91	0.51
1:C:312:GLU:OE2	7:q:134:PHE:HB2	2.10	0.51
4:K:3:THR:HG23	7:q:227:ILE:HD11	1.92	0.51
5:U:107:GLU:N	5:U:107:GLU:OE1	2.42	0.51
7:g:259:VAL:HG13	7:g:275:ILE:HD13	1.92	0.51
7:q:370:LEU:HD12	7:q:378:TYR:HD2	1.75	0.51
1:C:570:SER:HB2	1:C:657:GLU:HB3	1.92	0.51
1:C:638:GLN:CD	7:h:104:ILE:HD12	2.35	0.51
5:Q:97:MET:HE3	5:Q:173:MET:HG3	1.93	0.51
5:Q:207:LYS:CE	7:h:52:TYR:OH	2.59	0.51
5:R:85:LEU:HD12	5:U:178:ILE:HG22	1.92	0.51
5:S:27:TYR:HB3	5:S:56:LEU:HD23	1.92	0.51
5:T:184:ASP:OD2	5:T:192:LYS:NZ	2.35	0.51
7:k:241:LEU:HB2	7:k:275:ILE:HG12	1.92	0.51
1:C:401:LYS:HE2	1:C:405:LYS:HE2	1.93	0.51
2:D:71:VAL:HG11	2:E:71:VAL:HG23	1.91	0.51
2:E:75:GLN:HG3	2:F:122:VAL:HG22	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:221:ARG:HB3	2:E:226:PHE:HZ	1.76	0.51
6:W:84:LYS:HA	6:W:84:LYS:HE3	1.92	0.51
6:X:32:SER:CB	8:c:27:THR:O	2.57	0.51
7:e:39:ALA:O	7:e:44:ARG:HD3	2.11	0.51
7:k:208:LEU:HD11	7:k:259:VAL:HG13	1.92	0.51
7:k:242:PHE:HA	7:k:276:SER:O	2.11	0.51
7:q:326:GLU:OE2	7:q:326:GLU:N	2.29	0.51
1:C:43:ASP:OD2	1:C:49:ALA:N	2.44	0.51
3:G:676:ILE:CG2	3:I:670:ALA:HB1	2.41	0.51
5:T:119:ILE:O	5:T:122:ARG:HG2	2.11	0.51
8:i:67:GLU:OE1	8:i:67:GLU:N	2.43	0.51
7:p:364:SER:HB2	7:p:385:VAL:HG12	1.93	0.51
8:r:106:ARG:NH1	7:s:196:ILE:HD13	2.26	0.51
7:s:332:ILE:HB	7:s:340:ILE:HD11	1.92	0.51
1:C:872:THR:HG22	7:k:171:ILE:HG22	1.91	0.50
5:P:213:GLN:NE2	7:q:52:TYR:CE1	2.79	0.50
6:X:85:ASN:OD1	6:X:86:ASN:N	2.43	0.50
8:i:106:ARG:HH12	7:j:196:ILE:HD13	1.76	0.50
7:n:123:ILE:HD11	7:n:140:ILE:HB	1.92	0.50
7:p:304:ILE:HD11	7:p:338:LEU:HD22	1.92	0.50
3:H:677:ILE:CD1	3:I:677:ILE:CD1	2.88	0.50
5:Q:14:LEU:O	5:R:109:ARG:NH1	2.44	0.50
5:Q:109:ARG:NH1	5:T:14:LEU:O	2.45	0.50
5:R:95:MET:HE1	5:R:139:PHE:CD2	2.46	0.50
7:k:52:TYR:HB2	7:m:25:HIS:HD2	1.76	0.50
1:A:630:VAL:CG2	2:F:29:ARG:NH2	2.74	0.50
2:D:191:THR:OG1	2:D:205:GLY:HA2	2.10	0.50
6:V:2:TYR:OH	7:n:42:PHE:O	2.29	0.50
6:V:76:GLN:HG3	6:V:98:LEU:HD21	1.94	0.50
6:X:111:SER:HB3	7:s:115:SER:O	2.12	0.50
7:m:256:ILE:HD12	7:m:275:ILE:HG22	1.94	0.50
1:B:56:SER:HB3	4:N:136:SER:OG	2.10	0.50
1:B:826:GLY:O	1:B:831:MET:HB3	2.11	0.50
2:E:71:VAL:HG21	2:F:71:VAL:HG23	1.93	0.50
7:g:244:LEU:HB2	7:g:278:MET:HE2	1.93	0.50
2:F:162:GLU:N	2:F:162:GLU:OE2	2.43	0.50
4:O:29:SER:OG	7:k:71:SER:CB	2.60	0.50
6:V:6:PRO:O	8:o:34:ALA:HB3	2.12	0.50
6:Y:10:ASN:CA	7:d:154:PHE:CD2	2.85	0.50
6:Y:53:ASN:ND2	6:Y:55:ASN:HD21	2.04	0.50
6:Z:22:TYR:CE2	7:j:36:ASP:OD2	2.63	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:n:268:MET:HA	7:p:200:VAL:HG22	1.93	0.50
8:o:22:LYS:HG2	8:o:30:HIS:CD2	2.47	0.50
1:A:430:LYS:HE3	4:K:149:PHE:CG	2.46	0.50
1:A:629:ASP:OD1	2:D:30:ARG:NH2	2.44	0.50
1:A:808:GLY:O	1:C:344:VAL:N	2.44	0.50
2:D:72:SER:HB3	2:D:75:GLN:NE2	2.26	0.50
5:U:207:LYS:NZ	5:U:213:GLN:OE1	2.44	0.50
8:l:58:ARG:HD3	8:l:64:GLN:OE1	2.12	0.50
8:r:166:GLU:H	8:r:166:GLU:CD	2.20	0.50
1:A:599:VAL:CG2	2:D:85:MET:CE	2.88	0.50
1:B:630:VAL:HG21	2:E:29:ARG:CZ	2.42	0.50
2:F:20:VAL:HG23	2:F:23:SER:HB3	1.93	0.50
4:M:47:GLU:OE2	6:Z:102:ASN:ND2	2.45	0.50
5:P:227:LYS:O	5:P:227:LYS:HD3	2.12	0.50
5:T:233:PRO:HD2	5:T:236:ILE:HD13	1.94	0.50
6:V:22:TYR:CE2	7:p:36:ASP:OD2	2.63	0.50
6:Y:34:VAL:HG21	8:f:23:GLU:HB3	1.94	0.50
7:e:123:ILE:HD11	7:e:140:ILE:HB	1.93	0.50
7:h:192:GLN:O	7:h:196:ILE:HG12	2.12	0.50
7:j:94:GLY:HA3	7:j:167:TYR:CE2	2.46	0.50
7:p:245:ASP:OD1	7:p:246:VAL:N	2.42	0.50
1:B:661:SER:H	1:B:664:ASP:HB2	1.77	0.50
4:J:105:ILE:HG13	4:J:114:LEU:HD23	1.93	0.50
4:M:18:LEU:HG	7:e:212:THR:HG22	1.94	0.50
4:N:24:PRO:HG3	7:j:191:ALA:HB1	1.94	0.50
4:O:31:LEU:HD23	7:k:71:SER:OG	2.12	0.50
5:Q:10:VAL:HG13	5:R:58:MET:HG3	1.92	0.50
6:V:34:VAL:CG2	8:o:23:GLU:OE1	2.60	0.50
7:g:113:ASP:OD1	7:g:115:SER:OG	2.29	0.50
7:p:94:GLY:HA3	7:p:167:TYR:CE2	2.47	0.50
1:B:11:GLY:HA2	1:B:432:THR:HG21	1.94	0.50
1:B:204:ARG:HD2	7:h:134:PHE:CE2	2.47	0.50
1:B:816:SER:N	1:B:861:THR:O	2.45	0.50
1:C:405:LYS:NZ	2:D:84:GLN:HE21	2.09	0.50
2:E:52:ILE:HG12	2:E:66:ILE:HD12	1.94	0.50
5:P:193:LYS:HZ2	5:P:199:THR:HG22	1.77	0.50
5:Q:122:ARG:HG2	5:T:68:LEU:HD21	1.93	0.50
6:Z:29:GLN:HE22	7:j:45:PRO:CG	2.25	0.50
8:c:19:ARG:NH2	7:d:56:GLU:OE2	2.45	0.50
7:h:189:ARG:O	7:h:192:GLN:HG2	2.12	0.50
7:n:244:LEU:HB2	7:n:278:MET:HE2	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:413:GLU:OE1	7:q:100:SER:HB3	2.12	0.49
1:A:631:PRO:CD	2:F:92:ASP:HB3	2.42	0.49
1:C:78:THR:O	7:k:102:ASP:OD2	2.30	0.49
4:L:104:PHE:HB3	5:R:201:GLN:HG2	1.94	0.49
4:M:43:LEU:HD22	4:M:90:LYS:HB3	1.94	0.49
5:Q:35:THR:HB	6:Z:67:ILE:HD11	1.94	0.49
6:Y:13:LEU:HD11	8:f:38:LEU:CD1	2.42	0.49
7:b:123:ILE:HD11	7:b:140:ILE:HB	1.94	0.49
7:b:203:LEU:HD21	8:c:108:LYS:NZ	2.27	0.49
7:j:304:ILE:HD11	7:j:338:LEU:HD22	1.94	0.49
7:m:185:ASN:O	7:m:188:GLU:HG3	2.11	0.49
8:o:19:ARG:NH2	7:p:56:GLU:OE1	2.44	0.49
7:q:195:ARG:HH12	8:r:80:THR:HB	1.77	0.49
1:B:804:LEU:HD12	1:B:814:VAL:HG22	1.93	0.49
1:C:791:MET:HE3	1:C:881:GLU:OE2	2.09	0.49
4:N:43:LEU:HD13	4:N:90:LYS:HD3	1.94	0.49
5:Q:115:ILE:O	5:Q:119:ILE:HG12	2.12	0.49
6:Y:84:LYS:HA	6:Y:84:LYS:HE3	1.94	0.49
6:a:6:PRO:O	8:l:34:ALA:CB	2.60	0.49
7:k:195:ARG:NH1	8:l:78:GLY:O	2.37	0.49
7:m:111:VAL:HG11	7:m:168:VAL:HG11	1.94	0.49
7:m:280:VAL:HG21	7:m:362:ARG:HH21	1.77	0.49
1:C:430:LYS:HE3	4:O:149:PHE:CG	2.47	0.49
2:F:9:VAL:HG21	3:G:677:ILE:CG2	2.37	0.49
5:P:18:LYS:HE3	6:W:57:TYR:OH	2.12	0.49
5:P:224:TYR:HD1	5:P:225:LEU:HD22	1.77	0.49
6:W:53:ASN:ND2	6:W:55:ASN:HD21	1.96	0.49
7:b:103:PHE:HZ	7:b:162:LEU:HB3	1.76	0.49
8:c:22:LYS:HE3	8:c:30:HIS:NE2	2.26	0.49
7:h:268:MET:HA	7:j:200:VAL:HG22	1.94	0.49
7:j:93:PHE:HE2	7:j:105:VAL:HG11	1.74	0.49
7:p:146:GLU:HB3	7:q:42:PHE:HZ	1.76	0.49
7:s:219:CYS:SG	7:s:220:LYS:N	2.86	0.49
7:s:244:LEU:HD22	7:s:360:ILE:HG21	1.94	0.49
1:A:143:MET:HB2	1:A:180:TYR:O	2.12	0.49
1:B:280:GLU:HB2	1:B:395:PRO:HG3	1.93	0.49
4:J:103:LYS:NZ	4:J:116:SER:OG	2.41	0.49
7:g:220:LYS:HB3	7:g:242:PHE:HB2	1.95	0.49
6:V:6:PRO:HG2	8:o:35:THR:OG1	2.13	0.49
6:X:13:LEU:HB2	7:b:43:MET:SD	2.53	0.49
6:Y:1:MET:HA	7:g:34:PHE:CZ	2.47	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Z:22:TYR:HE2	7:j:36:ASP:OD2	1.95	0.49
7:g:365:TYR:HD1	7:g:383:VAL:HG22	1.77	0.49
8:i:26:GLY:N	8:i:31:ASP:OD2	2.45	0.49
7:q:213:MET:HE1	7:q:243:LEU:HG	1.95	0.49
1:A:599:VAL:HG21	2:D:85:MET:CE	2.42	0.49
1:B:170:ALA:HB2	1:B:188:LEU:HD13	1.93	0.49
1:C:170:ALA:HB2	1:C:188:LEU:HD13	1.95	0.49
1:C:228:GLN:HB3	1:C:231:PHE:O	2.12	0.49
2:F:221:ARG:HB3	2:F:229:THR:HB	1.93	0.49
4:M:55:ASN:HB2	7:g:52:TYR:OH	2.11	0.49
4:O:24:PRO:HG3	7:m:191:ALA:CB	2.43	0.49
5:S:124:PRO:HB2	5:S:132:SER:HB3	1.95	0.49
5:T:95:MET:HE1	5:T:139:PHE:CD2	2.48	0.49
6:Z:4:TYR:HA	7:j:42:PHE:HD2	1.76	0.49
6:a:12:THR:HG22	7:k:36:ASP:HB3	1.94	0.49
7:b:57:LEU:HD13	7:d:54:GLY:HA3	1.95	0.49
7:g:304:ILE:HD11	7:g:338:LEU:HD13	1.94	0.49
7:n:11:VAL:HG21	7:n:58:LEU:HD22	1.93	0.49
7:n:57:LEU:HD13	7:p:54:GLY:HA3	1.93	0.49
7:q:242:PHE:HA	7:q:276:SER:O	2.12	0.49
7:s:17:GLN:NE2	7:s:21:ASP:OD1	2.45	0.49
1:A:280:GLU:HA	1:B:806:GLN:NE2	2.24	0.49
1:A:281:TYR:O	1:B:807:ASN:ND2	2.42	0.49
1:B:68:PHE:O	4:M:135:PHE:HB2	2.13	0.49
4:L:31:LEU:HD23	4:L:31:LEU:H	1.77	0.49
8:f:91:GLU:H	8:f:91:GLU:CD	2.15	0.49
7:k:57:LEU:HD13	7:m:54:GLY:HA3	1.94	0.49
7:k:227:ILE:HD11	7:k:272:ARG:HH12	1.77	0.49
7:s:111:VAL:HG11	7:s:168:VAL:HG11	1.95	0.49
1:B:406:ASN:O	1:B:410:GLU:HG2	2.11	0.49
1:B:433:GLN:NE2	4:M:125:LEU:H	2.09	0.49
1:C:506:ASP:HB3	1:C:547:GLN:HB3	1.94	0.49
1:C:767:GLU:HB2	1:C:789:SER:HB3	1.95	0.49
2:D:215:SER:HB3	2:E:208:GLY:HA3	1.95	0.49
6:X:60:ASP:OD1	6:X:61:VAL:N	2.46	0.49
6:Y:13:LEU:HD21	8:f:38:LEU:HD11	1.94	0.49
6:a:82:ASP:OD1	6:a:90:SER:HB3	2.13	0.49
8:c:13:ARG:HH21	8:c:47:ILE:HG23	1.78	0.49
7:e:310:VAL:O	7:e:316:ASN:ND2	2.42	0.49
8:r:158:ARG:HA	8:r:188:TYR:CE1	2.48	0.49
7:s:94:GLY:HA3	7:s:167:TYR:CE2	2.48	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:430:LYS:O	1:A:452:HIS:ND1	2.46	0.49
1:B:43:ASP:OD2	1:B:49:ALA:N	2.46	0.49
1:C:228:GLN:HG3	1:C:232:ASN:HA	1.95	0.49
7:m:219:CYS:SG	7:m:220:LYS:N	2.85	0.49
1:B:622:ARG:HD2	7:q:106:PRO:HB3	1.95	0.49
4:N:128:VAL:HG23	7:j:14:ASP:CG	2.28	0.49
5:P:89:ASN:ND2	5:U:83:ASN:OD1	2.46	0.49
5:Q:40:THR:HG23	5:Q:52:PHE:HE1	1.77	0.49
7:h:346:ASN:HD22	7:h:352:ILE:HD12	1.76	0.49
7:j:99:LEU:HD21	7:j:164:TYR:CE2	2.48	0.49
7:s:104:ILE:HD12	7:s:127:VAL:HG22	1.94	0.49
2:D:178:VAL:HB	2:F:186:ILE:HD13	1.94	0.48
4:J:25:ASN:ND2	7:n:78:GLY:CA	2.76	0.48
4:O:55:ASN:OD1	7:m:52:TYR:CZ	2.66	0.48
5:R:213:GLN:NE2	7:e:52:TYR:CE1	2.81	0.48
7:k:219:CYS:SG	7:k:220:LYS:N	2.85	0.48
1:B:767:GLU:HB2	1:B:789:SER:HB3	1.94	0.48
2:D:122:VAL:HG22	2:F:75:GLN:HG3	1.94	0.48
4:N:18:LEU:O	7:h:266:ARG:NH2	2.35	0.48
5:U:243:PRO:CG	7:b:335:VAL:O	2.61	0.48
8:o:42:TRP:CE3	7:p:50:MET:HE1	2.48	0.48
2:E:19:MET:HA	2:E:19:MET:HE2	1.95	0.48
2:F:69:ILE:HD11	2:F:99:TYR:HB3	1.95	0.48
4:M:50:PRO:HG3	4:M:85:ILE:HD13	1.95	0.48
4:N:107:ASN:OD1	4:N:107:ASN:O	2.31	0.48
4:O:79:PRO:O	8:l:5:ALA:HB3	2.13	0.48
4:O:80:THR:O	8:l:10:ASN:ND2	2.45	0.48
7:e:305:LEU:O	7:e:309:LYS:HG3	2.13	0.48
7:g:94:GLY:HA3	7:g:167:TYR:CE2	2.48	0.48
7:k:39:ALA:O	7:k:44:ARG:HD3	2.13	0.48
7:k:105:VAL:HB	7:k:126:LEU:HB3	1.96	0.48
8:o:148:ALA:HB1	8:o:151:GLU:HB2	1.95	0.48
7:q:365:TYR:HE1	7:q:381:ASN:HB3	1.79	0.48
1:A:503:LEU:HD23	4:K:128:VAL:HG22	1.94	0.48
2:E:188:ALA:HA	2:F:180:SER:O	2.13	0.48
4:J:25:ASN:ND2	7:n:78:GLY:HA3	2.28	0.48
5:S:97:MET:HE3	5:S:173:MET:HG3	1.96	0.48
6:V:4:TYR:HA	7:p:42:PHE:HD1	1.78	0.48
7:g:328:VAL:HG21	7:g:345:MET:HE1	1.95	0.48
7:k:24:VAL:HA	7:k:37:LEU:HD23	1.96	0.48
7:k:207:GLN:C	7:k:208:LEU:HD22	2.38	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34:GLN:NE2	1:B:470:GLN:HG2	2.29	0.48
1:C:143:MET:HB2	1:C:180:TYR:O	2.14	0.48
4:K:30:ILE:HG21	7:q:67:ALA:HB1	1.94	0.48
4:N:29:SER:O	4:N:33:ARG:HD3	2.13	0.48
5:S:44:ASN:ND2	5:S:47:LYS:HE3	2.28	0.48
5:U:7:ASN:HB3	5:U:10:VAL:HG12	1.95	0.48
6:V:34:VAL:HG11	8:o:23:GLU:OE1	2.13	0.48
6:X:12:THR:HG22	7:b:36:ASP:OD2	2.13	0.48
7:g:213:MET:HE2	7:g:217:SER:HB2	1.96	0.48
7:k:288:ILE:HG12	7:k:369:GLU:HG2	1.95	0.48
7:s:256:ILE:HD12	7:s:275:ILE:HG22	1.95	0.48
1:B:26:PHE:CB	1:B:695:HIS:H	2.27	0.48
2:D:228:SER:H	2:F:218:ARG:NH2	2.11	0.48
4:K:20:LEU:H	4:K:20:LEU:HG	1.40	0.48
5:P:70:ILE:HG12	5:S:122:ARG:HB3	1.96	0.48
5:P:197:VAL:HG12	5:P:201:GLN:HE22	1.79	0.48
5:Q:34:SER:O	6:Z:63:LYS:HD3	2.13	0.48
5:U:34:SER:O	6:X:63:LYS:HD3	2.14	0.48
6:Y:35:ARG:HH12	6:Y:43:PHE:HD1	1.60	0.48
1:A:22:ILE:HD11	5:R:77:ILE:HG13	1.96	0.48
1:A:578:GLN:NE2	4:O:151:PHE:H	2.12	0.48
1:B:560:TYR:OH	1:B:664:ASP:OD1	2.28	0.48
1:C:427:ILE:HG22	4:J:139:LEU:HB3	1.95	0.48
4:L:18:LEU:HB3	7:b:212:THR:HG22	1.96	0.48
1:C:602:ASP:HB3	2:D:47:ARG:HH21	1.78	0.48
5:S:115:ILE:O	5:S:119:ILE:HD13	2.13	0.48
5:U:222:THR:HG22	5:U:226:LYS:HE3	1.95	0.48
6:X:4:TYR:HA	7:d:42:PHE:HD1	1.78	0.48
7:d:104:ILE:HD12	7:d:127:VAL:HG22	1.94	0.48
7:j:151:SER:HA	7:j:173:PRO:HB3	1.94	0.48
7:q:256:ILE:HD12	7:q:275:ILE:HG22	1.96	0.48
7:q:302:ASP:O	7:q:306:GLU:HG2	2.14	0.48
1:C:171:ARG:NH1	1:C:175:PRO:O	2.47	0.48
1:C:364:TYR:CZ	1:C:368:LYS:HD2	2.49	0.48
4:J:128:VAL:HG23	7:p:14:ASP:CG	2.38	0.48
4:N:38:ILE:H	4:N:38:ILE:HG12	1.36	0.48
5:P:178:ILE:HG22	5:U:85:LEU:HD12	1.95	0.48
5:R:224:TYR:HD1	5:R:225:LEU:HD22	1.79	0.48
7:d:332:ILE:HB	7:d:340:ILE:HD11	1.94	0.48
7:j:245:ASP:OD1	7:j:246:VAL:N	2.42	0.48
7:m:304:ILE:HD11	7:m:338:LEU:HD13	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:n:103:PHE:HZ	7:n:162:LEU:HB3	1.79	0.48
8:o:29:TYR:HB3	8:o:35:THR:HG21	1.96	0.48
1:A:663:SER:HA	5:P:186:LYS:HZ1	1.79	0.48
1:B:746:GLU:HG2	1:B:758:LYS:HE3	1.96	0.48
5:P:14:LEU:O	5:S:109:ARG:NH1	2.47	0.48
7:g:346:ASN:HD22	7:g:352:ILE:HD13	1.78	0.48
1:A:56:SER:HB3	4:L:136:SER:OG	2.13	0.47
1:A:449:SER:HB3	4:K:123:LEU:HD22	1.96	0.47
1:A:482:ASN:OD1	1:A:521:SER:N	2.43	0.47
1:A:602:ASP:HB3	2:F:47:ARG:NH2	2.29	0.47
1:C:409:ALA:O	1:C:413:GLU:HG3	2.13	0.47
5:U:35:THR:HB	6:X:67:ILE:HD11	1.95	0.47
5:U:207:LYS:NZ	5:U:213:GLN:CD	2.72	0.47
5:U:243:PRO:HG3	7:b:335:VAL:O	2.14	0.47
8:c:95:VAL:O	8:c:99:ASN:ND2	2.46	0.47
7:g:285:LEU:HD22	7:g:343:LEU:HD11	1.94	0.47
7:q:13:ASP:O	7:q:13:ASP:OD1	2.32	0.47
1:B:22:ILE:HB	1:B:40:THR:HG22	1.95	0.47
1:B:442:ARG:O	4:M:101:ILE:HD12	2.14	0.47
1:C:844:LEU:HB2	1:C:879:HIS:HB3	1.97	0.47
3:H:681:TRP:O	3:H:681:TRP:CD2	2.67	0.47
4:L:34:ASN:O	4:L:34:ASN:ND2	2.46	0.47
6:X:56:ASP:OD1	6:X:59:SER:OG	2.20	0.47
7:b:268:MET:HA	7:d:200:VAL:HG22	1.96	0.47
7:d:99:LEU:HD21	7:d:164:TYR:CE2	2.48	0.47
1:B:143:MET:HB2	1:B:180:TYR:O	2.14	0.47
5:P:204:ASN:HD22	5:P:252:ASP:HB3	1.80	0.47
8:o:13:ARG:HH21	8:o:47:ILE:HG23	1.80	0.47
7:q:95:LEU:HB2	7:q:133:THR:HG22	1.97	0.47
1:A:115:LYS:HB3	1:A:235:GLN:HE22	1.79	0.47
1:A:200:PRO:CD	7:b:153:ASN:HD21	2.27	0.47
1:A:230:GLN:HE21	1:A:230:GLN:HB2	1.56	0.47
1:A:602:ASP:OD1	2:F:67:ARG:NH2	2.31	0.47
1:B:344:VAL:HB	1:C:809:ASN:HA	1.97	0.47
1:B:567:ASN:O	1:B:658:LEU:HB2	2.14	0.47
1:C:32:LYS:HD2	2:F:1:MET:HG3	1.95	0.47
1:C:631:PRO:HD2	2:D:92:ASP:HB3	1.97	0.47
4:O:102:LYS:HD2	4:O:114:LEU:HD21	1.95	0.47
5:Q:124:PRO:HB2	5:Q:132:SER:HB3	1.96	0.47
7:k:192:GLN:O	7:k:196:ILE:HB	2.14	0.47
7:q:310:VAL:O	7:q:316:ASN:ND2	2.41	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:ARG:NH1	1:A:175:PRO:O	2.47	0.47
1:C:149:PRO:HG2	1:C:157:ILE:HG21	1.95	0.47
2:E:94:ASP:HB3	2:E:97:LYS:HG3	1.95	0.47
2:E:115:ASP:HB3	2:E:119:ASP:OD1	2.15	0.47
4:N:18:LEU:HG	7:h:266:ARG:CZ	2.44	0.47
4:O:44:PHE:HB2	4:O:91:VAL:O	2.15	0.47
6:X:41:ASP:OD2	7:d:44:ARG:NH1	2.48	0.47
6:Y:3:VAL:O	7:g:42:PHE:CD1	2.67	0.47
7:j:120:PHE:HE1	7:j:148:TYR:HD2	1.63	0.47
7:n:49:THR:CG2	7:n:50:MET:N	2.77	0.47
1:B:204:ARG:HB2	7:h:134:PHE:CE1	2.50	0.47
4:K:94:GLN:HE22	5:P:127:LYS:HA	1.80	0.47
5:P:20:PRO:HG3	5:S:163:ASP:OD2	2.13	0.47
5:Q:163:ASP:OD1	5:T:20:PRO:HG3	2.14	0.47
6:Z:2:TYR:HD2	7:j:43:MET:HE1	1.78	0.47
8:f:151:GLU:HG2	8:f:183:LYS:NZ	2.27	0.47
7:p:104:ILE:HD12	7:p:127:VAL:HG22	1.96	0.47
7:q:123:ILE:HD11	7:q:140:ILE:HB	1.95	0.47
1:A:140:GLU:O	1:A:143:MET:HG2	2.15	0.47
1:A:168:ASN:ND2	7:b:381:ASN:HD22	2.05	0.47
1:A:488:VAL:HB	7:q:159:SER:HB3	1.96	0.47
1:B:587:LYS:HD3	2:D:4:ASP:HA	1.97	0.47
1:B:646:GLY:HA2	4:K:154:THR:HB	1.97	0.47
1:C:79:ASN:C	7:n:114:LEU:HD22	2.40	0.47
1:C:323:HIS:HB2	1:C:347:ILE:HD12	1.96	0.47
1:C:461:ILE:HD12	5:P:86:ASN:HB3	1.97	0.47
1:C:638:GLN:CD	7:h:104:ILE:CD1	2.88	0.47
4:J:25:ASN:HD21	7:n:78:GLY:HA2	1.80	0.47
4:L:4:GLN:NE2	7:b:256:ILE:HG22	2.27	0.47
4:O:18:LEU:O	4:O:18:LEU:CG	2.62	0.47
4:O:120:GLN:N	4:O:120:GLN:OE1	2.47	0.47
5:Q:243:PRO:HG3	7:h:335:VAL:O	2.15	0.47
5:R:195:VAL:HG11	7:g:35:THR:HA	1.97	0.47
6:W:109:ASP:N	6:W:109:ASP:OD1	2.47	0.47
7:h:94:GLY:HA3	7:h:167:TYR:CE2	2.50	0.47
7:m:104:ILE:HD12	7:m:127:VAL:HG22	1.94	0.47
7:p:269:LEU:HD23	7:p:270:GLY:N	2.30	0.47
7:q:241:LEU:HB2	7:q:275:ILE:HG12	1.97	0.47
7:s:185:ASN:O	7:s:188:GLU:HG3	2.15	0.47
2:D:9:VAL:CG1	3:I:678:ASN:OD1	2.52	0.47
4:N:18:LEU:HD23	7:h:266:ARG:CZ	2.44	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:225:LEU:HD12	5:P:240:LEU:HD11	1.96	0.47
6:W:6:PRO:O	8:r:34:ALA:HB3	2.15	0.47
6:Y:5:PRO:HB2	6:Y:7:ARG:HE	1.79	0.47
7:g:213:MET:SD	7:g:243:LEU:HD22	2.55	0.47
1:A:206:ASP:OD2	1:A:209:ASN:ND2	2.39	0.47
1:A:538:GLY:HA3	1:A:551:ILE:HD11	1.97	0.47
2:F:136:ASP:OD1	2:F:137:SER:N	2.48	0.47
4:J:25:ASN:O	7:n:75:ASN:HA	2.15	0.47
5:S:66:TYR:CE1	5:S:95:MET:HG3	2.50	0.47
5:T:184:ASP:O	5:T:188:LEU:HB3	2.15	0.47
5:U:150:VAL:HG13	5:U:178:ILE:HD13	1.96	0.47
6:W:4:TYR:HA	7:s:42:PHE:HD2	1.80	0.47
6:W:4:TYR:CD1	6:W:29:GLN:HG3	2.49	0.47
6:Z:3:VAL:O	7:j:42:PHE:CE2	2.68	0.47
7:d:110:GLN:HG3	7:d:121:TYR:CE1	2.50	0.47
7:g:229:LYS:HE2	7:g:242:PHE:HE2	1.79	0.47
1:A:573:VAL:HG21	1:A:683:ILE:HD11	1.97	0.47
1:A:638:GLN:CD	7:n:104:ILE:HD11	2.40	0.47
1:C:755:THR:O	1:C:766:TYR:OH	2.30	0.47
2:E:75:GLN:HG3	2:F:122:VAL:HG13	1.96	0.47
5:Q:61:PRO:HB3	5:Q:97:MET:HG2	1.96	0.47
7:g:104:ILE:HD12	7:g:127:VAL:HG22	1.97	0.47
8:i:29:TYR:HB3	8:i:35:THR:HG21	1.97	0.47
7:q:50:MET:HE3	7:s:50:MET:HE2	1.96	0.47
7:q:188:GLU:OE2	8:r:80:THR:HG21	2.15	0.47
8:r:4:ASP:N	8:r:4:ASP:OD1	2.48	0.47
1:A:170:ALA:HB2	1:A:188:LEU:HD13	1.96	0.46
1:A:564:VAL:HG21	1:A:679:THR:HB	1.98	0.46
2:D:69:ILE:HD11	2:D:99:TYR:HB3	1.95	0.46
4:L:6:PHE:CD2	7:b:275:ILE:HD12	2.50	0.46
4:M:112:LYS:HB3	4:M:112:LYS:HE2	1.79	0.46
4:N:31:LEU:HD21	7:h:71:SER:HB2	1.96	0.46
5:U:8:ARG:HD3	5:U:8:ARG:HA	1.59	0.46
6:Y:12:THR:HG22	7:e:36:ASP:CG	2.40	0.46
6:a:12:THR:HG22	7:k:36:ASP:OD2	2.15	0.46
7:e:241:LEU:HB2	7:e:275:ILE:HG12	1.97	0.46
7:e:256:ILE:HD12	7:e:275:ILE:HG22	1.96	0.46
8:f:160:TYR:O	8:f:188:TYR:OH	2.22	0.46
7:j:242:PHE:HA	7:j:276:SER:O	2.15	0.46
7:k:256:ILE:HD12	7:k:275:ILE:HG22	1.96	0.46
7:s:242:PHE:HA	7:s:276:SER:O	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:471:SER:OG	1:A:473:ASN:OD1	2.29	0.46
1:C:78:THR:O	7:k:102:ASP:CG	2.58	0.46
1:C:264:GLN:HB2	1:C:399:ASN:HA	1.96	0.46
2:D:108:ASN:HD21	2:F:73:GLN:HA	1.80	0.46
4:L:81:LYS:HD3	4:L:81:LYS:HA	1.55	0.46
4:L:107:ASN:OD1	4:L:112:LYS:HD3	2.15	0.46
4:L:114:LEU:HD23	4:L:114:LEU:HA	1.82	0.46
4:M:24:PRO:CG	7:g:191:ALA:CB	2.93	0.46
5:T:27:TYR:HB3	5:T:56:LEU:HD23	1.97	0.46
5:U:239:ILE:HD12	5:U:258:LEU:HB3	1.97	0.46
7:b:342:TYR:CE2	7:b:344:GLN:HG3	2.50	0.46
7:d:94:GLY:HA3	7:d:167:TYR:CE2	2.51	0.46
7:h:207:GLN:C	7:h:208:LEU:HD23	2.40	0.46
8:i:42:TRP:CE3	7:j:50:MET:HE1	2.50	0.46
7:j:23:LEU:HD11	7:j:44:ARG:HD3	1.97	0.46
7:k:150:VAL:H	7:k:174:ALA:HB3	1.80	0.46
8:l:167:PHE:O	8:l:170:THR:HG22	2.14	0.46
7:m:94:GLY:HA3	7:m:167:TYR:CE2	2.50	0.46
7:q:39:ALA:O	7:q:44:ARG:HD3	2.14	0.46
1:B:503:LEU:CD2	4:M:128:VAL:HG22	2.44	0.46
1:C:496:THR:HG22	7:k:110:GLN:NE2	2.22	0.46
4:J:114:LEU:HD23	4:J:114:LEU:HA	1.83	0.46
4:K:65:SER:OG	6:W:39:VAL:O	2.22	0.46
5:P:122:ARG:HD3	5:U:68:LEU:HD21	1.96	0.46
5:Q:83:ASN:OD1	5:R:89:ASN:ND2	2.48	0.46
5:Q:178:ILE:HG22	5:T:85:LEU:HD12	1.97	0.46
6:V:39:VAL:HG12	8:o:2:SER:HA	1.98	0.46
7:b:39:ALA:O	7:b:44:ARG:HD3	2.14	0.46
7:b:256:ILE:HD12	7:b:275:ILE:HG22	1.96	0.46
7:d:120:PHE:HE1	7:d:148:TYR:HD2	1.63	0.46
7:d:357:GLN:OE1	7:d:357:GLN:N	2.47	0.46
7:h:365:TYR:HE1	7:h:381:ASN:HB3	1.80	0.46
7:j:269:LEU:HD23	7:j:270:GLY:N	2.30	0.46
7:m:244:LEU:HD22	7:m:360:ILE:HG21	1.96	0.46
8:o:10:ASN:HA	8:o:13:ARG:NH1	2.30	0.46
7:q:284:GLU:H	7:q:346:ASN:ND2	2.13	0.46
7:q:354:MET:HE1	7:q:361:PRO:HB3	1.97	0.46
7:s:304:ILE:HD11	7:s:338:LEU:HD13	1.96	0.46
1:A:6:ILE:HD12	1:A:17:LEU:HD22	1.96	0.46
1:A:22:ILE:HD13	5:R:77:ILE:HG13	1.96	0.46
1:A:71:ASN:HB3	4:K:133:THR:H	1.80	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:ASP:OD1	1:A:159:ARG:NH2	2.42	0.46
1:B:578:GLN:HE21	4:K:150:SER:HA	1.80	0.46
1:B:597:THR:HG22	2:F:55:PRO:HB3	1.98	0.46
2:F:164:ILE:HG22	2:F:166:GLY:H	1.81	0.46
6:V:66:ILE:O	6:V:70:GLU:HG2	2.15	0.46
6:W:8:ILE:CD1	7:q:34:PHE:CD1	2.98	0.46
7:g:217:SER:HB3	7:g:246:VAL:HG12	1.97	0.46
7:s:227:ILE:HG13	7:s:274:LEU:HD13	1.97	0.46
7:s:286:GLU:CG	7:s:344:GLN:HB2	2.45	0.46
1:A:204:ARG:HD2	7:b:134:PHE:CE2	2.50	0.46
1:A:660:THR:HB	1:A:702:PHE:HB3	1.97	0.46
1:B:578:GLN:HA	2:D:5:GLU:OE1	2.16	0.46
1:C:791:MET:CE	1:C:881:GLU:HG2	2.45	0.46
5:Q:28:LEU:O	5:Q:54:VAL:N	2.49	0.46
5:S:95:MET:HE3	5:S:97:MET:HE2	1.97	0.46
6:X:32:SER:C	8:c:24:GLN:HG3	2.41	0.46
6:a:6:PRO:HG2	8:l:35:THR:OG1	2.15	0.46
7:e:77:LEU:HB3	7:e:79:VAL:HG13	1.96	0.46
7:g:256:ILE:HD12	7:g:275:ILE:HG22	1.98	0.46
7:j:104:ILE:HD12	7:j:127:VAL:HG22	1.96	0.46
7:j:146:GLU:HB3	7:k:42:PHE:HZ	1.80	0.46
7:k:268:MET:HA	7:m:200:VAL:HG22	1.97	0.46
8:l:160:TYR:O	8:l:188:TYR:OH	2.23	0.46
7:n:305:LEU:O	7:n:309:LYS:HG3	2.15	0.46
7:p:208:LEU:HD12	7:p:208:LEU:HA	1.78	0.46
4:J:20:LEU:HD23	4:J:20:LEU:HA	1.83	0.46
4:K:80:THR:O	8:r:10:ASN:ND2	2.48	0.46
4:M:94:GLN:HE21	5:R:128:LYS:HA	1.80	0.46
5:P:95:MET:HE1	5:P:139:PHE:CD2	2.51	0.46
5:T:3:LYS:HA	5:T:6:LYS:HD3	1.97	0.46
7:e:50:MET:CE	7:g:46:PHE:HB3	2.45	0.46
8:f:159:ASP:OD1	8:f:159:ASP:N	2.48	0.46
7:s:43:MET:HE3	7:s:43:MET:HB3	1.72	0.46
1:A:409:ALA:O	1:A:413:GLU:HG3	2.16	0.46
1:A:781:LEU:HD23	1:A:781:LEU:HA	1.77	0.46
5:R:31:TYR:O	5:R:32:GLU:HB2	2.16	0.46
5:S:31:TYR:C	5:S:33:ASP:H	2.22	0.46
5:S:150:VAL:HG13	5:S:178:ILE:HD13	1.98	0.46
5:T:213:GLN:NE2	7:k:52:TYR:CE1	2.83	0.46
7:m:218:ARG:HE	7:m:319:PRO:HD3	1.81	0.46
7:n:94:GLY:HA3	7:n:167:TYR:CE2	2.51	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:s:23:LEU:HD11	7:s:44:ARG:HD3	1.97	0.46
1:A:344:VAL:HB	1:B:809:ASN:HA	1.96	0.46
1:C:482:ASN:OD1	1:C:521:SER:N	2.39	0.46
1:C:791:MET:CE	1:C:881:GLU:OE2	2.64	0.46
2:D:127:ASN:N	2:E:119:ASP:OD2	2.43	0.46
2:E:195:LYS:O	2:F:187:ASP:HA	2.15	0.46
5:T:227:LYS:O	5:T:227:LYS:HD3	2.15	0.46
6:W:36:GLY:O	8:r:2:SER:OG	2.27	0.46
7:d:360:ILE:HG12	7:d:361:PRO:HD2	1.98	0.46
7:e:218:ARG:HA	7:e:218:ARG:HD2	1.69	0.46
2:E:205:GLY:HA3	2:E:209:GLU:HG3	1.97	0.46
4:L:65:SER:HB3	6:X:42:PRO:HG3	1.98	0.46
4:O:115:ILE:HD12	4:O:118:ALA:HB2	1.98	0.46
7:b:94:GLY:HA3	7:b:167:TYR:CE2	2.50	0.46
7:h:342:TYR:CE2	7:h:344:GLN:HG3	2.51	0.46
8:i:152:PHE:CE1	8:i:184:TYR:HB3	2.50	0.46
7:n:256:ILE:HD12	7:n:275:ILE:HG22	1.98	0.46
7:p:206:GLU:O	7:p:210:GLU:HG2	2.16	0.46
7:p:219:CYS:SG	7:p:220:LYS:N	2.89	0.46
7:s:381:ASN:OD1	7:s:381:ASN:N	2.49	0.46
1:C:578:GLN:HE21	4:M:151:PHE:H	1.62	0.46
2:E:189:ASP:H	2:F:181:GLU:HA	1.80	0.46
2:F:9:VAL:HG13	3:G:681:TRP:HB3	1.97	0.46
4:N:141:ASP:C	4:N:141:ASP:OD1	2.59	0.46
4:O:13:ILE:H	4:O:13:ILE:HG12	1.50	0.46
5:Q:68:LEU:HD21	5:R:122:ARG:HD3	1.97	0.46
5:R:220:ARG:NH2	5:R:223:GLU:OE2	2.48	0.46
7:e:178:ARG:NH1	7:e:181:GLU:HG2	2.31	0.46
1:B:844:LEU:HB2	1:B:879:HIS:HB3	1.98	0.45
2:D:238:ALA:HB3	2:E:229:THR:HG22	1.97	0.45
3:H:673:ILE:HG12	3:I:673:ILE:HG12	1.98	0.45
5:P:30:GLU:HG3	5:P:135:LYS:HD3	1.97	0.45
5:U:118:LEU:HD13	5:U:154:ILE:HD11	1.97	0.45
8:c:160:TYR:O	8:c:188:TYR:OH	2.26	0.45
8:f:3:LYS:HE2	8:f:3:LYS:HB3	1.59	0.45
8:i:106:ARG:NH1	7:j:196:ILE:HD13	2.30	0.45
7:k:8:PRO:HG2	8:l:69:TYR:CZ	2.51	0.45
8:r:134:ILE:HB	8:r:137:GLN:OE1	2.16	0.45
7:s:199:PRO:HG3	7:s:208:LEU:HD22	1.97	0.45
1:A:643:ARG:NH1	4:O:153:ASN:HB2	2.31	0.45
1:B:364:TYR:CZ	1:B:368:LYS:HD2	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:846:MET:HE2	1:C:846:MET:HB2	1.80	0.45
4:J:46:ILE:HG22	6:W:101:GLU:HG3	1.98	0.45
5:Q:160:ARG:HB2	5:Q:168:LYS:HB3	1.97	0.45
6:Z:4:TYR:O	7:j:42:PHE:HE2	1.99	0.45
7:d:219:CYS:SG	7:d:220:LYS:N	2.88	0.45
7:g:23:LEU:HD13	7:g:37:LEU:HA	1.97	0.45
7:j:199:PRO:HG3	7:j:208:LEU:HD23	1.97	0.45
7:n:252:ASP:OD1	7:n:254:VAL:HG22	2.16	0.45
8:o:22:LYS:HE3	8:o:30:HIS:NE2	2.31	0.45
7:q:207:GLN:C	7:q:208:LEU:HD22	2.40	0.45
1:C:445:ILE:HG13	4:O:101:ILE:HG21	1.99	0.45
1:C:746:GLU:HG2	1:C:758:LYS:HE3	1.98	0.45
4:O:46:ILE:HG22	6:V:101:GLU:OE1	2.15	0.45
5:P:31:TYR:O	5:P:32:GLU:HB2	2.16	0.45
5:R:244:LYS:HB3	5:R:261:GLY:HA2	1.99	0.45
5:S:35:THR:O	6:V:47:PRO:HG3	2.16	0.45
5:T:207:LYS:NZ	5:T:213:GLN:CD	2.74	0.45
6:a:41:ASP:OD1	6:a:41:ASP:N	2.49	0.45
7:b:259:VAL:HG13	7:b:275:ILE:HD13	1.97	0.45
7:d:279:GLU:HG3	7:d:358:TRP:HD1	1.80	0.45
7:e:49:THR:CG2	7:e:50:MET:N	2.79	0.45
8:r:19:ARG:NH2	7:s:56:GLU:OE1	2.26	0.45
7:s:107:ILE:N	7:s:125:ASN:OD1	2.50	0.45
1:C:56:SER:HB2	4:J:136:SER:HG	1.80	0.45
5:T:207:LYS:NZ	5:T:213:GLN:OE1	2.50	0.45
6:Z:54:ILE:O	6:Z:54:ILE:HD12	2.16	0.45
7:q:356:ASN:OD1	7:q:359:THR:OG1	2.21	0.45
1:A:356:LEU:HD23	1:A:356:LEU:HA	1.79	0.45
2:D:105:ASN:HB2	2:D:106:ASP:H	1.58	0.45
4:K:31:LEU:HD23	4:K:31:LEU:H	1.82	0.45
4:L:107:ASN:OD1	4:L:112:LYS:CD	2.64	0.45
5:S:30:GLU:OE1	5:S:135:LYS:HE2	2.17	0.45
5:S:44:ASN:HD22	5:S:47:LYS:HE3	1.82	0.45
6:W:2:TYR:OH	7:q:42:PHE:O	2.32	0.45
6:Z:6:PRO:O	8:i:34:ALA:HB3	2.17	0.45
6:Z:76:GLN:HG3	6:Z:98:LEU:HD21	1.98	0.45
8:f:148:ALA:HB1	8:f:151:GLU:OE2	2.15	0.45
8:i:137:GLN:N	8:i:137:GLN:OE1	2.48	0.45
7:k:318:THR:HB	7:k:321:GLU:HG3	1.98	0.45
7:n:203:LEU:O	7:n:207:GLN:HG2	2.16	0.45
1:A:478:ARG:O	1:B:580:ASP:HB2	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:517:ILE:HD13	1:B:531:MET:HE1	1.98	0.45
1:B:620:ALA:HB3	1:B:624:PHE:HE2	1.81	0.45
1:C:1:MET:HE2	5:T:133:HIS:NE2	2.32	0.45
1:C:18:GLY:O	5:P:80:THR:CG2	2.64	0.45
4:K:133:THR:O	4:K:134:GLU:HB3	2.17	0.45
4:N:18:LEU:HB3	7:h:266:ARG:NH2	2.31	0.45
6:Z:1:MET:HE3	6:Z:1:MET:HB3	1.62	0.45
7:b:49:THR:HG21	7:d:43:MET:HE1	1.97	0.45
7:d:23:LEU:HD11	7:d:44:ARG:HD3	1.98	0.45
8:o:137:GLN:OE1	8:o:137:GLN:N	2.49	0.45
7:p:103:PHE:HB3	7:p:128:ILE:HB	1.98	0.45
1:A:132:SER:HB3	1:A:156:ASN:HB2	1.99	0.45
1:A:620:ALA:HB3	1:A:624:PHE:HE2	1.81	0.45
1:A:791:MET:HB2	1:A:794:ARG:HG3	1.97	0.45
1:B:429:ALA:CB	4:M:143:ILE:HG12	2.47	0.45
2:D:164:ILE:HG22	2:D:166:GLY:H	1.81	0.45
2:E:164:ILE:HG22	2:E:166:GLY:H	1.81	0.45
4:L:5:GLU:OE2	7:b:272:ARG:CG	2.65	0.45
4:O:27:ASP:O	4:O:32:THR:OG1	2.30	0.45
5:S:268:LEU:HD23	5:S:268:LEU:H	1.82	0.45
7:j:6:ASN:OD1	7:j:6:ASN:N	2.49	0.45
7:j:268:MET:HE2	7:j:268:MET:HB3	1.76	0.45
7:k:356:ASN:OD1	7:k:359:THR:OG1	2.22	0.45
1:B:323:HIS:HB2	1:B:347:ILE:HD12	1.98	0.45
1:B:506:ASP:HB3	1:B:547:GLN:HB3	1.99	0.45
1:B:846:MET:HE2	1:B:846:MET:HB2	1.80	0.45
1:C:45:ASP:OD1	5:S:130:LEU:HD11	2.14	0.45
1:C:270:ASP:N	1:C:270:ASP:OD1	2.48	0.45
4:M:27:ASP:CG	7:e:74:LYS:HE3	2.42	0.45
1:A:287:LEU:HD11	1:A:326:LEU:HD11	1.99	0.45
1:A:350:ARG:HD3	1:A:350:ARG:HA	1.81	0.45
1:B:747:ILE:HD11	1:B:802:PHE:CD1	2.52	0.45
1:C:769:TRP:CZ2	7:k:390:GLU:HA	2.52	0.45
1:C:794:ARG:HD3	7:k:379:ARG:HB2	1.98	0.45
4:J:46:ILE:HG22	6:W:101:GLU:CG	2.46	0.45
4:O:30:ILE:HD11	7:m:10:LEU:HD12	1.99	0.45
5:S:160:ARG:HB2	5:S:168:LYS:HB3	1.99	0.45
6:X:3:VAL:O	7:d:42:PHE:CD1	2.70	0.45
7:e:50:MET:HE1	7:g:46:PHE:HB3	1.98	0.45
7:g:163:THR:HG22	7:g:164:TYR:CD2	2.52	0.45
7:s:363:PHE:CZ	7:s:366:ILE:HB	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:LYS:H	1:A:76:LYS:HG3	1.49	0.45
1:A:364:TYR:CZ	1:A:368:LYS:HD2	2.51	0.45
1:A:663:SER:CA	5:P:186:LYS:HZ1	2.30	0.45
1:A:713:ALA:HB1	4:J:110:THR:HB	1.99	0.45
1:B:471:SER:OG	1:B:473:ASN:OD1	2.26	0.45
1:C:94:THR:OG1	1:C:106:ARG:HG2	2.17	0.45
4:J:103:LYS:CE	4:J:116:SER:OG	2.65	0.45
4:M:9:LYS:HD3	4:M:9:LYS:HA	1.39	0.45
4:N:13:ILE:HG23	5:T:234:ARG:CG	2.47	0.45
4:N:60:GLU:HB3	5:Q:47:LYS:HB2	1.99	0.45
5:P:159:THR:O	5:P:160:ARG:NH1	2.48	0.45
5:R:244:LYS:HB2	5:R:244:LYS:HE3	1.83	0.45
7:j:346:ASN:HD22	7:j:352:ILE:HD13	1.82	0.45
7:s:213:MET:HE3	7:s:217:SER:HB2	1.99	0.45
1:C:22:ILE:HB	1:C:40:THR:HG22	1.99	0.44
1:C:564:VAL:HG23	1:C:677:GLU:O	2.17	0.44
2:D:241:ASN:HB2	2:E:234:GLY:H	1.82	0.44
2:E:136:ASP:OD1	2:E:137:SER:N	2.50	0.44
2:E:186:ILE:HD13	2:F:178:VAL:HB	1.98	0.44
4:O:5:GLU:OE2	7:k:272:ARG:HD3	2.17	0.44
5:Q:207:LYS:NZ	7:j:21:ASP:HB3	2.32	0.44
7:b:200:VAL:O	7:b:203:LEU:HG	2.16	0.44
7:d:217:SER:OG	7:d:244:LEU:O	2.24	0.44
7:k:77:LEU:HB3	7:k:79:VAL:HG13	1.99	0.44
1:A:43:ASP:O	1:A:463:ASP:HB3	2.16	0.44
1:A:169:HIS:CE1	7:b:383:VAL:HB	2.52	0.44
1:B:7:LYS:HE3	1:B:9:LEU:HD21	2.00	0.44
1:B:736:SER:HB3	7:b:132:ALA:CB	2.47	0.44
2:E:211:LEU:HD11	2:E:219:LYS:HG2	1.99	0.44
4:L:20:LEU:HB2	4:L:23:LYS:HZ1	1.82	0.44
4:N:25:ASN:HD21	7:h:78:GLY:CA	2.30	0.44
5:Q:227:LYS:O	5:Q:227:LYS:HD2	2.17	0.44
5:T:58:MET:HE1	5:T:103:ASP:H	1.82	0.44
6:Z:29:GLN:NE2	7:j:45:PRO:HG2	2.32	0.44
6:a:21:GLU:H	6:a:21:GLU:HG2	1.62	0.44
8:c:137:GLN:N	8:c:137:GLN:OE1	2.50	0.44
7:g:286:GLU:CG	7:g:344:GLN:HB2	2.47	0.44
1:A:43:ASP:OD2	1:A:49:ALA:N	2.49	0.44
1:A:420:LYS:HA	1:B:612:ASP:HB2	1.99	0.44
1:A:489:THR:HA	1:A:513:MET:HA	1.99	0.44
1:A:543:GLY:O	4:K:125:LEU:HD11	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:VAL:HG13	1:B:95:VAL:HB	1.99	0.44
1:B:358:ARG:HH12	1:B:382:LEU:HD22	1.82	0.44
1:B:482:ASN:OD1	1:B:521:SER:N	2.37	0.44
1:C:749:SER:HB3	1:C:759:ILE:HD13	1.99	0.44
2:D:79:LEU:HB2	2:E:117:VAL:HA	1.98	0.44
4:M:3:THR:CG2	7:e:227:ILE:HD11	2.48	0.44
5:S:206:LYS:HE2	7:p:27:ASN:ND2	2.32	0.44
5:T:58:MET:CE	5:T:103:ASP:H	2.31	0.44
5:T:236:ILE:O	5:T:239:ILE:HG12	2.18	0.44
6:X:4:TYR:O	7:d:42:PHE:HE1	2.00	0.44
6:Y:13:LEU:HD11	8:f:38:LEU:HD11	1.98	0.44
6:a:38:LEU:HA	6:a:38:LEU:HD23	1.74	0.44
7:g:381:ASN:OD1	7:g:381:ASN:N	2.50	0.44
7:h:30:SER:HB3	8:i:37:TRP:CE2	2.52	0.44
1:B:474:TRP:HZ3	4:M:147:VAL:HG21	1.81	0.44
1:B:516:ASN:HD22	2:E:64:ASN:HD21	1.65	0.44
2:E:236:PRO:HG2	2:F:227:ASN:OD1	2.18	0.44
5:P:195:VAL:CG1	7:s:35:THR:HA	2.48	0.44
5:R:248:LYS:HD3	5:R:259:PHE:CE1	2.52	0.44
7:e:212:THR:HG21	7:e:262:THR:HG21	2.00	0.44
7:k:156:ASP:OD1	7:k:157:GLN:NE2	2.41	0.44
7:p:268:MET:HB3	7:p:268:MET:HE2	1.64	0.44
7:p:372:ASP:OD1	7:p:376:THR:N	2.51	0.44
1:B:781:LEU:HD23	1:B:781:LEU:HA	1.78	0.44
1:C:287:LEU:HD11	1:C:326:LEU:HD11	1.99	0.44
4:M:7:LEU:HD13	4:M:7:LEU:HA	1.79	0.44
4:O:29:SER:HB2	7:k:75:ASN:HD21	1.76	0.44
5:P:8:ARG:NH1	5:S:107:GLU:OE1	2.48	0.44
6:a:12:THR:CG2	7:k:36:ASP:CG	2.90	0.44
7:b:146:GLU:HG3	7:b:177:GLY:O	2.18	0.44
8:c:42:TRP:CE3	7:d:50:MET:HE1	2.52	0.44
7:g:197:ARG:HE	7:g:197:ARG:HB3	1.45	0.44
1:A:391:GLU:OE2	2:E:42:ASN:ND2	2.50	0.44
4:L:61:TYR:HE1	5:U:46:ASN:HB3	1.83	0.44
4:M:82:GLU:HB2	8:f:6:PHE:CG	2.52	0.44
5:Q:243:PRO:CG	7:h:335:VAL:O	2.65	0.44
5:S:75:ILE:HB	5:S:84:GLN:HB2	1.99	0.44
6:X:34:VAL:HG21	8:c:23:GLU:HG2	1.99	0.44
7:b:207:GLN:O	7:b:208:LEU:HD13	2.18	0.44
7:h:304:ILE:HD11	7:h:338:LEU:HD13	2.00	0.44
7:p:283:ILE:HB	7:p:363:PHE:HA	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:519:GLN:NE2	1:A:522:GLN:O	2.40	0.44
1:B:461:ILE:HD13	1:B:461:ILE:HA	1.86	0.44
1:B:516:ASN:ND2	2:E:64:ASN:HD21	2.12	0.44
2:D:126:GLY:C	2:F:134:LYS:HB2	2.43	0.44
5:R:19:ASN:HD22	5:R:20:PRO:HD2	1.82	0.44
6:W:11:GLY:N	7:p:154:PHE:CE2	2.84	0.44
7:n:255:THR:O	7:n:259:VAL:HG23	2.17	0.44
7:q:133:THR:HB	7:q:134:PHE:CD1	2.53	0.44
8:r:80:THR:C	8:r:82:PRO:HD2	2.41	0.44
1:A:22:ILE:HB	1:A:40:THR:HG22	1.98	0.44
1:A:26:PHE:O	1:A:694:ARG:HD3	2.18	0.44
1:C:5:ILE:HG12	1:C:439:SER:HB3	1.98	0.44
2:D:134:LYS:HB2	2:E:126:GLY:C	2.43	0.44
4:M:30:ILE:HD12	4:M:30:ILE:HA	1.63	0.44
5:P:160:ARG:HB2	5:P:168:LYS:HB3	2.00	0.44
5:R:160:ARG:HB2	5:R:168:LYS:HB3	1.98	0.44
5:R:193:LYS:HG3	5:R:198:GLU:OE2	2.17	0.44
5:S:10:VAL:HG13	5:T:58:MET:HG3	1.99	0.44
6:a:84:LYS:HD3	6:a:90:SER:HB2	2.00	0.44
7:n:304:ILE:HD11	7:n:338:LEU:HD13	1.99	0.44
1:B:171:ARG:NH1	1:B:175:PRO:O	2.51	0.44
1:B:496:THR:HG22	7:e:110:GLN:NE2	2.31	0.44
1:C:87:VAL:HG13	1:C:95:VAL:HB	2.00	0.44
1:C:140:GLU:O	1:C:143:MET:HG2	2.18	0.44
1:C:471:SER:OG	1:C:473:ASN:OD1	2.27	0.44
1:C:685:GLY:HA2	4:N:114:LEU:HB3	2.00	0.44
4:J:80:THR:HG22	8:o:5:ALA:HB1	2.00	0.44
4:N:31:LEU:CD2	7:h:71:SER:CB	2.89	0.44
7:n:50:MET:HE3	8:o:42:TRP:CD1	2.53	0.44
7:q:205:PHE:CE1	7:q:220:LYS:HA	2.53	0.44
1:C:597:THR:HG22	2:E:55:PRO:HB3	2.00	0.43
1:C:842:ARG:NH1	7:k:381:ASN:O	2.45	0.43
2:E:134:LYS:HB3	2:F:127:ASN:OD1	2.18	0.43
4:J:19:ASP:HB3	4:J:20:LEU:H	1.53	0.43
5:T:128:LYS:HB3	5:T:129:GLY:H	1.71	0.43
6:a:38:LEU:HD21	7:m:45:PRO:HB3	1.99	0.43
7:b:305:LEU:O	7:b:309:LYS:HG3	2.18	0.43
8:i:9:TRP:NE1	7:j:56:GLU:OE1	2.39	0.43
7:q:342:TYR:CE2	7:q:344:GLN:HG3	2.53	0.43
7:s:138:GLU:N	7:s:138:GLU:OE2	2.51	0.43
1:A:42:PHE:CE1	5:R:75:ILE:HD12	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:72:SER:OG	2:F:77:ASN:HB3	2.18	0.43
4:O:112:LYS:HB3	4:O:112:LYS:HE2	1.78	0.43
5:T:158:VAL:HG11	5:T:166:PRO:HB3	2.00	0.43
5:T:201:GLN:HE21	5:T:201:GLN:HB2	1.66	0.43
6:X:2:TYR:OH	7:b:42:PHE:O	2.31	0.43
7:b:49:THR:CG2	7:b:50:MET:N	2.81	0.43
7:d:156:ASP:OD1	7:d:156:ASP:N	2.50	0.43
7:e:82:ASP:OD2	7:e:181:GLU:N	2.51	0.43
8:f:33:ILE:HD12	8:f:36:ASP:HB3	2.00	0.43
8:f:166:GLU:CD	8:f:166:GLU:H	2.26	0.43
7:g:86:LYS:HE2	7:g:141:ALA:O	2.18	0.43
7:j:218:ARG:HD2	7:j:314:PRO:O	2.18	0.43
8:o:67:GLU:OE2	8:o:94:ARG:NH2	2.48	0.43
7:p:110:GLN:HG3	7:p:121:TYR:CE1	2.53	0.43
7:p:332:ILE:HB	7:p:340:ILE:HD11	1.99	0.43
7:p:333:ARG:HD2	7:p:333:ARG:O	2.18	0.43
7:q:243:LEU:HB3	7:q:251:ALA:HB2	1.99	0.43
1:A:767:GLU:HB2	1:A:789:SER:HB3	2.00	0.43
1:B:660:THR:HB	1:B:702:PHE:HB3	1.99	0.43
1:C:519:GLN:NE2	1:C:522:GLN:O	2.41	0.43
1:C:859:ARG:NH2	1:C:893:SER:OG	2.50	0.43
2:E:136:ASP:OD1	2:E:136:ASP:C	2.61	0.43
2:F:66:ILE:HG23	2:F:98:GLY:C	2.43	0.43
2:F:105:ASN:HB3	2:F:106:ASP:H	1.53	0.43
5:S:37:VAL:HG22	6:V:47:PRO:CB	2.48	0.43
6:X:12:THR:HG22	7:b:36:ASP:CG	2.44	0.43
7:g:374:GLU:CD	8:i:165:TYR:HD1	2.27	0.43
7:h:39:ALA:O	7:h:44:ARG:HD3	2.18	0.43
7:n:209:ALA:O	7:n:213:MET:HE2	2.19	0.43
7:n:356:ASN:OD1	7:n:359:THR:OG1	2.21	0.43
7:n:372:ASP:OD1	7:n:376:THR:N	2.51	0.43
7:p:356:ASN:HB2	7:p:357:GLN:H	1.69	0.43
1:C:23:ASP:C	1:C:23:ASP:OD1	2.61	0.43
2:D:202:ILE:HD12	2:E:204:LEU:HD12	2.00	0.43
2:E:74:ASN:ND2	2:F:125:GLU:OE2	2.51	0.43
4:L:31:LEU:HD21	7:b:71:SER:HB2	1.95	0.43
5:S:19:ASN:HD22	5:T:108:LYS:NZ	2.17	0.43
8:f:48:GLU:O	8:f:52:LYS:HG2	2.18	0.43
7:g:291:SER:N	7:g:371:THR:O	2.32	0.43
7:g:374:GLU:OE1	8:i:165:TYR:HA	2.18	0.43
7:j:229:LYS:HD3	7:j:242:PHE:HE1	1.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:l:33:ILE:HD12	8:l:36:ASP:HB3	1.99	0.43
7:m:23:LEU:HD11	7:m:44:ARG:HD3	2.00	0.43
7:m:242:PHE:HA	7:m:276:SER:O	2.19	0.43
7:n:319:PRO:HG3	7:n:360:ILE:HD13	2.01	0.43
1:A:19:GLN:HB3	1:A:20:GLU:OE1	2.19	0.43
1:B:5:ILE:HG12	1:B:439:SER:HB3	1.99	0.43
1:B:344:VAL:N	1:C:808:GLY:O	2.46	0.43
1:B:599:VAL:HB	1:B:606:LEU:HD13	2.00	0.43
1:C:358:ARG:HH12	1:C:382:LEU:HD22	1.84	0.43
5:R:158:VAL:HG11	5:R:166:PRO:HB3	2.00	0.43
6:Y:4:TYR:O	7:g:42:PHE:HE1	2.02	0.43
7:d:183:ILE:HD12	7:d:183:ILE:HA	1.89	0.43
7:k:123:ILE:HD11	7:k:140:ILE:HB	2.00	0.43
7:m:245:ASP:OD1	7:m:246:VAL:N	2.45	0.43
7:p:278:MET:HE1	7:p:319:PRO:HG2	2.01	0.43
8:r:141:SER:OG	8:r:142:GLU:OE1	2.37	0.43
1:A:97:ARG:HG2	1:A:97:ARG:HH11	1.84	0.43
1:A:746:GLU:HG2	1:A:758:LYS:HE3	2.00	0.43
1:B:26:PHE:O	1:B:694:ARG:HG3	2.18	0.43
1:C:407:GLN:OE1	7:n:96:SER:HB2	2.18	0.43
2:D:184:ILE:HB	2:F:192:ILE:HG12	2.01	0.43
4:L:104:PHE:CZ	4:L:117:ASP:HB2	2.54	0.43
4:N:81:LYS:HD3	4:N:81:LYS:HA	1.76	0.43
4:O:5:GLU:CD	7:k:272:ARG:HD2	2.43	0.43
5:R:192:LYS:HE2	5:R:192:LYS:HB3	1.78	0.43
5:U:247:ILE:HG22	5:U:258:LEU:HD13	2.00	0.43
7:b:72:PHE:O	7:b:76:VAL:HG22	2.19	0.43
7:j:90:THR:OG1	7:j:172:ARG:NH1	2.52	0.43
7:j:103:PHE:HB3	7:j:128:ILE:HB	2.00	0.43
7:k:222:ILE:HD12	7:k:242:PHE:CE2	2.54	0.43
7:n:362:ARG:HH12	7:n:390:GLU:HB3	1.83	0.43
7:p:120:PHE:HE1	7:p:148:TYR:HD2	1.67	0.43
1:A:23:ASP:C	1:A:23:ASP:OD1	2.62	0.43
1:A:486:THR:HG22	7:q:161:PRO:HG3	1.99	0.43
1:A:563:SER:OG	1:A:678:ASN:OD1	2.32	0.43
1:A:809:ASN:HA	1:C:344:VAL:HB	2.00	0.43
1:B:27:GLN:HB3	1:B:36:ASN:H	1.83	0.43
1:B:501:TYR:OH	1:B:524:ASP:OD2	2.37	0.43
1:C:30:GLU:HG3	1:C:540:ARG:HH11	1.83	0.43
1:C:32:LYS:HB3	3:H:688:TYR:CE2	2.53	0.43
1:C:791:MET:HE2	1:C:799:VAL:HB	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:57:PHE:HB3	2:D:61:ILE:HG12	2.01	0.43
4:M:79:PRO:O	8:f:5:ALA:HB3	2.18	0.43
4:M:139:LEU:HD23	4:M:145:LYS:HD2	2.00	0.43
4:N:114:LEU:HD12	4:N:114:LEU:HA	1.87	0.43
5:P:85:LEU:HB2	5:S:178:ILE:HG22	2.01	0.43
7:g:220:LYS:HD2	7:g:220:LYS:HA	1.79	0.43
7:m:374:GLU:HB3	8:o:165:TYR:HD1	1.83	0.43
7:q:200:VAL:HB	7:q:201:SER:H	1.60	0.43
7:q:224:LEU:HD13	8:r:183:LYS:HB2	2.00	0.43
1:A:30:GLU:OE1	1:A:540:ARG:NH1	2.52	0.43
1:A:807:ASN:ND2	1:C:281:TYR:O	2.51	0.43
1:C:206:ASP:OD2	1:C:209:ASN:ND2	2.41	0.43
1:C:791:MET:CE	1:C:881:GLU:CG	2.96	0.43
2:E:5:GLU:H	2:E:5:GLU:HG2	1.58	0.43
4:K:82:GLU:HB2	8:r:6:PHE:CG	2.54	0.43
4:N:35:LYS:HB2	4:N:35:LYS:HE3	1.80	0.43
5:R:83:ASN:HB2	5:U:92:ASN:OD1	2.19	0.43
5:U:190:GLU:H	5:U:190:GLU:HG3	1.70	0.43
6:W:4:TYR:HA	7:s:42:PHE:CD2	2.54	0.43
7:b:325:ILE:O	7:b:329:LYS:HG3	2.18	0.43
7:k:50:MET:HE3	7:m:50:MET:HE2	2.01	0.43
4:N:123:LEU:HD23	4:N:123:LEU:HA	1.82	0.43
4:O:23:LYS:O	7:k:78:GLY:HA3	2.19	0.43
7:j:219:CYS:SG	7:j:220:LYS:N	2.92	0.43
7:k:310:VAL:O	7:k:316:ASN:ND2	2.46	0.43
7:k:345:MET:HB3	7:k:352:ILE:HD11	2.00	0.43
8:l:28:SER:H	8:l:31:ASP:HB2	1.83	0.43
7:m:217:SER:HB3	7:m:246:VAL:HA	2.00	0.43
7:n:242:PHE:HA	7:n:276:SER:O	2.19	0.43
1:A:21:ILE:O	5:R:78:PRO:HD2	2.19	0.43
1:A:791:MET:HE3	1:A:791:MET:HB3	1.81	0.43
1:C:194:GLN:HG2	7:n:153:ASN:CB	2.49	0.43
4:L:70:ILE:HG22	4:L:92:PRO:HG2	2.00	0.43
4:L:134:GLU:OE2	4:L:137:LYS:CE	2.66	0.43
4:N:13:ILE:H	4:N:13:ILE:HG13	1.33	0.43
5:Q:31:TYR:HB2	5:Q:136:ILE:HG22	2.00	0.43
5:R:66:TYR:CE1	5:R:95:MET:HG3	2.54	0.43
5:T:244:LYS:HB2	5:T:244:LYS:HE3	1.83	0.43
6:X:4:TYR:CG	6:X:29:GLN:HB2	2.53	0.43
6:a:54:ILE:H	6:a:54:ILE:HG13	1.47	0.43
6:a:62:SER:O	6:a:66:ILE:HG12	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:d:43:MET:HE3	7:d:43:MET:HA	2.01	0.43
7:e:342:TYR:CE2	7:e:344:GLN:HG3	2.53	0.43
7:h:356:ASN:OD1	7:h:359:THR:OG1	2.26	0.43
7:j:156:ASP:N	7:j:156:ASP:OD1	2.51	0.43
8:l:85:SER:OG	8:l:87:ASP:OD2	2.27	0.43
1:A:54:SER:O	1:A:428:SER:OG	2.32	0.42
1:B:531:MET:HE2	1:B:531:MET:HA	2.01	0.42
1:C:313:ARG:H	1:C:313:ARG:HG2	1.60	0.42
2:E:219:LYS:NZ	2:E:231:ASP:OD2	2.51	0.42
5:Q:219:LYS:HE2	5:Q:219:LYS:HB2	1.77	0.42
5:R:186:LYS:HA	5:R:186:LYS:HD2	1.63	0.42
7:b:91:LEU:HD13	7:b:111:VAL:HG21	2.01	0.42
7:n:110:GLN:HG3	7:n:121:TYR:CE2	2.54	0.42
7:p:156:ASP:N	7:p:156:ASP:OD1	2.50	0.42
1:A:280:GLU:HB2	1:A:395:PRO:HG3	2.01	0.42
1:A:540:ARG:HB3	1:A:547:GLN:HG3	2.01	0.42
1:B:23:ASP:C	1:B:23:ASP:OD1	2.61	0.42
1:B:492:GLY:O	1:B:496:THR:HG23	2.18	0.42
1:B:646:GLY:CA	4:K:154:THR:HB	2.49	0.42
1:C:36:ASN:HD21	3:H:687:ASP:HA	1.84	0.42
1:C:634:GLN:NE2	1:C:639:TYR:O	2.49	0.42
2:D:14:LEU:HB2	3:G:681:TRP:CZ3	2.53	0.42
2:D:180:SER:O	2:F:188:ALA:HA	2.19	0.42
2:F:57:PHE:HB3	2:F:61:ILE:HG12	2.00	0.42
4:J:101:ILE:CG2	4:J:103:LYS:NZ	2.82	0.42
4:O:29:SER:HB3	7:k:75:ASN:ND2	2.17	0.42
5:R:27:TYR:HB3	5:R:56:LEU:HD23	2.01	0.42
6:Y:107:GLU:OE1	7:d:117:THR:HG23	2.19	0.42
6:Z:18:ASP:OD1	6:Z:18:ASP:C	2.62	0.42
7:d:372:ASP:OD1	7:d:376:THR:N	2.51	0.42
7:h:11:VAL:HG21	7:h:58:LEU:HD22	2.02	0.42
7:h:319:PRO:HG3	7:h:360:ILE:HD13	2.01	0.42
7:j:99:LEU:HD21	7:j:164:TYR:CD2	2.54	0.42
7:k:366:ILE:HG23	7:k:382:VAL:HB	2.01	0.42
1:A:496:THR:HG22	7:q:110:GLN:NE2	2.26	0.42
1:A:630:VAL:HG23	2:F:29:ARG:CZ	2.49	0.42
1:B:126:GLU:H	1:B:126:GLU:HG2	1.68	0.42
1:C:152:GLN:HB2	1:C:157:ILE:HD11	2.01	0.42
4:L:23:LYS:HA	4:L:24:PRO:HD3	1.93	0.42
4:L:29:SER:CB	7:b:75:ASN:HD21	2.31	0.42
4:M:126:ILE:HD12	4:M:126:ILE:HA	1.83	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:139:LEU:HD12	4:M:139:LEU:HA	1.89	0.42
5:Q:122:ARG:HB3	5:T:70:ILE:HG12	2.01	0.42
6:V:69:GLU:HA	6:V:69:GLU:OE2	2.19	0.42
7:b:189:ARG:O	7:b:192:GLN:HG2	2.18	0.42
8:f:26:GLY:N	8:f:31:ASP:OD2	2.44	0.42
7:h:278:MET:HG3	7:h:358:TRP:O	2.18	0.42
8:o:81:ALA:HB1	8:o:82:PRO:HD2	2.01	0.42
8:r:21:PRO:HG2	8:r:29:TYR:HD2	1.84	0.42
1:A:747:ILE:HD11	1:A:802:PHE:CD1	2.54	0.42
1:A:767:GLU:OE1	1:A:767:GLU:N	2.48	0.42
5:P:176:LYS:HD3	5:U:85:LEU:HD11	2.02	0.42
5:Q:92:ASN:OD1	5:T:83:ASN:HB2	2.19	0.42
5:S:19:ASN:HD22	5:T:108:LYS:HZ1	1.67	0.42
5:T:260:ASN:OD1	5:T:264:GLU:HG2	2.19	0.42
5:U:268:LEU:HD23	5:U:268:LEU:H	1.85	0.42
7:h:259:VAL:HG13	7:h:275:ILE:HD13	2.01	0.42
7:h:377:VAL:HG12	7:h:379:ARG:HD3	2.00	0.42
7:m:291:SER:N	7:m:371:THR:O	2.40	0.42
7:p:360:ILE:HG12	7:p:361:PRO:HD2	2.01	0.42
7:s:86:LYS:HE2	7:s:141:ALA:O	2.19	0.42
1:A:56:SER:HB2	4:L:136:SER:HG	1.84	0.42
1:A:319:ILE:HG22	1:A:345:VAL:HG12	2.00	0.42
1:A:461:ILE:HB	1:A:462:SER:H	1.71	0.42
1:A:630:VAL:HG23	2:F:29:ARG:NH1	2.34	0.42
1:B:749:SER:HA	1:B:802:PHE:HB3	2.00	0.42
1:C:43:ASP:O	1:C:463:ASP:HB3	2.19	0.42
1:C:405:LYS:HZ3	2:D:84:GLN:HE21	1.66	0.42
1:C:754:ARG:H	1:C:754:ARG:HG2	1.66	0.42
5:P:143:SER:HB3	6:W:62:SER:OG	2.19	0.42
5:Q:85:LEU:HD11	5:R:176:LYS:HD3	2.01	0.42
5:R:236:ILE:O	5:R:239:ILE:HG12	2.20	0.42
5:S:186:LYS:O	5:S:186:LYS:HD3	2.20	0.42
6:W:11:GLY:N	7:p:154:PHE:HE2	2.16	0.42
8:c:92:SER:HB3	8:c:121:LEU:HD23	2.02	0.42
8:c:102:SER:HA	8:c:106:ARG:HH21	1.84	0.42
7:h:243:LEU:HD21	7:h:259:VAL:HG11	2.02	0.42
7:h:285:LEU:O	7:h:366:ILE:HA	2.20	0.42
8:l:124:ASN:OD1	8:l:160:TYR:OH	2.37	0.42
7:m:113:ASP:OD1	7:m:115:SER:N	2.49	0.42
7:p:86:LYS:HE2	7:p:141:ALA:O	2.19	0.42
7:q:10:LEU:O	8:r:52:LYS:HE2	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:ARG:HB2	7:b:134:PHE:CE1	2.54	0.42
1:A:479:ARG:NH1	1:B:580:ASP:OD2	2.53	0.42
1:B:675:TYR:OH	4:L:112:LYS:HB2	2.20	0.42
1:C:106:ARG:HB3	1:C:254:TYR:CE2	2.55	0.42
1:C:204:ARG:HB2	7:n:134:PHE:CE1	2.55	0.42
1:C:819:SER:OG	1:C:859:ARG:N	2.53	0.42
1:C:831:MET:HA	1:C:843:LEU:O	2.19	0.42
1:C:845:HIS:HE1	7:k:390:GLU:OXT	2.02	0.42
5:U:58:MET:HE2	5:U:58:MET:HB3	1.91	0.42
6:X:19:LEU:HD23	6:X:19:LEU:HA	1.84	0.42
6:a:46:VAL:HG23	6:a:64:ILE:HG12	2.02	0.42
7:d:210:GLU:OE2	7:d:219:CYS:N	2.53	0.42
7:h:110:GLN:HG3	7:h:121:TYR:CE2	2.54	0.42
7:j:16:GLU:OE1	7:j:16:GLU:N	2.42	0.42
7:k:224:LEU:HD12	7:k:234:PRO:HB2	2.00	0.42
8:l:33:ILE:HG13	8:l:37:TRP:CE2	2.55	0.42
7:q:46:PHE:O	7:q:50:MET:HG2	2.20	0.42
1:A:32:LYS:HD2	2:E:1:MET:CG	2.50	0.42
1:A:579:THR:HG23	1:A:582:THR:HG22	2.02	0.42
1:B:64:LEU:HD21	4:N:143:ILE:CG2	2.49	0.42
1:B:264:GLN:HB2	1:B:399:ASN:HA	2.00	0.42
1:C:165:ILE:HG23	7:n:381:ASN:HB3	2.02	0.42
1:C:204:ARG:HD2	7:n:134:PHE:CE2	2.54	0.42
1:C:844:LEU:HD23	7:k:390:GLU:CD	2.45	0.42
2:D:237:MET:HE2	2:D:237:MET:HB2	1.86	0.42
2:F:36:SER:HB3	2:F:52:ILE:HB	2.00	0.42
4:J:9:LYS:HB2	7:n:264:GLN:HB3	2.02	0.42
4:J:139:LEU:HD12	4:J:139:LEU:HA	1.92	0.42
4:K:95:LYS:HE2	4:K:95:LYS:HB3	1.80	0.42
4:L:16:GLU:HA	4:L:19:ASP:HB2	2.02	0.42
5:P:3:LYS:HA	5:P:6:LYS:HD3	2.00	0.42
6:Y:1:MET:HE3	6:Y:1:MET:HB3	1.91	0.42
6:a:8:ILE:HD13	6:a:8:ILE:HA	1.95	0.42
7:g:267:ILE:HG21	7:g:273:LEU:HB2	2.01	0.42
7:j:38:ASP:OD1	7:j:38:ASP:N	2.46	0.42
7:m:116:GLY:O	7:m:119:ARG:NH1	2.53	0.42
1:A:461:ILE:O	1:A:462:SER:C	2.61	0.42
1:A:481:LYS:NZ	1:A:500:GLN:OE1	2.53	0.42
1:A:679:THR:OG1	1:A:680:LEU:N	2.49	0.42
1:B:165:ILE:HG23	7:h:381:ASN:CB	2.49	0.42
2:E:198:SER:OG	2:F:206:GLY:O	2.27	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:41:ARG:H	4:J:41:ARG:HG3	1.71	0.42
4:N:105:ILE:CG2	4:N:112:LYS:HD2	2.50	0.42
4:N:145:LYS:HB3	4:N:145:LYS:HE3	1.72	0.42
5:P:82:LYS:HD3	5:S:177:GLU:CD	2.45	0.42
5:P:83:ASN:HB2	5:S:92:ASN:OD1	2.19	0.42
5:R:246:VAL:HG22	5:R:259:PHE:HB2	2.02	0.42
5:S:199:THR:HG23	5:S:201:GLN:HG2	2.02	0.42
6:V:61:VAL:HG13	6:V:79:VAL:HG12	2.01	0.42
7:g:374:GLU:OE2	8:i:168:ARG:HB2	2.20	0.42
7:q:189:ARG:CZ	7:q:189:ARG:HB2	2.49	0.42
1:B:544:LYS:HB2	4:M:125:LEU:HD12	2.02	0.42
1:B:742:LEU:HB2	1:B:899:TRP:CD1	2.55	0.42
2:F:134:LYS:HA	2:F:134:LYS:HD3	1.92	0.42
4:K:70:ILE:HG22	4:K:92:PRO:HG2	2.02	0.42
4:N:44:PHE:HB2	4:N:91:VAL:O	2.19	0.42
5:P:244:LYS:HB2	5:P:244:LYS:HE3	1.82	0.42
5:U:45:LYS:HB3	5:U:45:LYS:HE3	1.33	0.42
6:V:34:VAL:CG1	8:o:23:GLU:OE1	2.67	0.42
7:e:198:ASN:O	7:e:200:VAL:HG22	2.19	0.42
7:k:243:LEU:C	7:k:278:MET:HG3	2.44	0.42
7:m:259:VAL:HG12	7:m:275:ILE:HD13	2.01	0.42
7:n:117:THR:HG23	7:n:118:LEU:HG	2.02	0.42
7:n:333:ARG:O	7:n:333:ARG:HG3	2.20	0.42
1:A:262:ASP:OD1	2:F:111:ARG:NH2	2.52	0.42
1:A:630:VAL:HG21	2:F:29:ARG:CZ	2.49	0.42
1:C:19:GLN:HB3	1:C:20:GLU:OE2	2.20	0.42
4:M:82:GLU:HB2	8:f:6:PHE:CD2	2.55	0.42
5:Q:47:LYS:HG3	5:Q:50:GLN:CG	2.50	0.42
6:Y:12:THR:HG22	7:e:36:ASP:OD2	2.20	0.42
7:b:238:VAL:HG13	7:b:274:LEU:HD23	2.02	0.42
7:d:93:PHE:HD2	7:d:105:VAL:HG21	1.84	0.42
7:e:72:PHE:O	7:e:76:VAL:HG13	2.19	0.42
7:e:95:LEU:HB2	7:e:133:THR:HG22	2.02	0.42
7:j:332:ILE:HB	7:j:340:ILE:HD11	2.02	0.42
7:p:93:PHE:HD2	7:p:105:VAL:HG21	1.84	0.42
1:A:661:SER:OG	1:A:664:ASP:OD2	2.36	0.41
1:A:872:THR:C	1:A:874:THR:H	2.28	0.41
1:B:39:PHE:CE1	1:B:467:PHE:HB2	2.55	0.41
1:B:872:THR:C	1:B:874:THR:H	2.27	0.41
1:C:40:THR:HG23	1:C:464:THR:HG23	2.02	0.41
1:C:165:ILE:HG23	7:n:381:ASN:CB	2.49	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:638:GLN:CG	7:h:104:ILE:CD1	2.85	0.41
1:C:747:ILE:HD11	1:C:802:PHE:CD1	2.55	0.41
4:L:6:PHE:HE2	7:b:275:ILE:HD12	1.84	0.41
4:L:106:VAL:HG12	4:L:113:GLN:HB2	2.02	0.41
4:M:27:ASP:OD1	7:e:74:LYS:HE3	2.20	0.41
5:P:114:LEU:HG	5:U:14:LEU:HD21	2.02	0.41
6:V:3:VAL:O	7:p:42:PHE:CE1	2.73	0.41
7:d:354:MET:HE2	7:d:361:PRO:HD3	2.02	0.41
7:k:43:MET:HE3	7:k:43:MET:HB3	1.77	0.41
7:k:211:LEU:C	7:k:213:MET:H	2.28	0.41
8:l:123:ILE:HD11	8:l:169:LEU:HD23	2.02	0.41
7:q:371:THR:HG22	7:q:377:VAL:HG13	2.02	0.41
1:B:538:GLY:HA3	1:B:551:ILE:HD11	2.02	0.41
2:D:22:ARG:HA	2:D:22:ARG:HD2	1.79	0.41
6:Z:4:TYR:HA	7:j:42:PHE:CD2	2.54	0.41
7:e:238:VAL:HG13	7:e:274:LEU:HD23	2.02	0.41
7:k:205:PHE:CE1	7:k:220:LYS:HA	2.55	0.41
1:A:323:HIS:HB2	1:A:347:ILE:HD12	2.02	0.41
1:B:1:MET:CE	5:R:133:HIS:HE2	2.30	0.41
1:C:501:TYR:OH	1:C:524:ASP:OD2	2.38	0.41
2:D:14:LEU:CA	3:G:681:TRP:HH2	2.32	0.41
5:P:85:LEU:HD12	5:S:178:ILE:HG22	2.02	0.41
7:b:110:GLN:HG3	7:b:121:TYR:CE2	2.56	0.41
7:b:188:GLU:C	7:b:188:GLU:OE1	2.64	0.41
7:b:203:LEU:HD21	8:c:108:LYS:HZ2	1.84	0.41
7:d:268:MET:HE2	7:d:268:MET:HB3	1.73	0.41
7:e:203:LEU:HD13	7:e:203:LEU:HA	1.77	0.41
7:m:12:VAL:HB	7:m:15:TYR:CE1	2.55	0.41
7:m:321:GLU:HG3	7:m:322:PRO:HD2	2.01	0.41
7:n:39:ALA:O	7:n:44:ARG:HD3	2.20	0.41
1:B:457:HIS:HD2	1:C:680:LEU:HD11	1.86	0.41
1:C:319:ILE:HG22	1:C:345:VAL:HG12	2.00	0.41
1:C:350:ARG:HD3	1:C:350:ARG:HA	1.78	0.41
1:C:791:MET:HE3	1:C:881:GLU:OE1	2.17	0.41
2:D:36:SER:HB3	2:D:52:ILE:HB	2.01	0.41
5:P:244:LYS:HB3	5:P:261:GLY:HA2	2.02	0.41
5:Q:184:ASP:O	5:Q:188:LEU:HB3	2.21	0.41
5:T:248:LYS:HD3	5:T:259:PHE:CD1	2.55	0.41
5:U:74:GLU:C	5:U:75:ILE:HD13	2.45	0.41
6:X:5:PRO:HA	6:X:6:PRO:HD3	1.94	0.41
7:j:86:LYS:HE2	7:j:141:ALA:O	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:j:208:LEU:HD21	7:j:266:ARG:HE	1.85	0.41
7:j:244:LEU:HD21	7:j:248:GLY:HA2	2.03	0.41
7:k:342:TYR:CE2	7:k:344:GLN:HG3	2.56	0.41
7:n:147:LYS:HE2	7:n:148:TYR:CE2	2.55	0.41
7:p:6:ASN:OD1	7:p:6:ASN:N	2.51	0.41
7:q:288:ILE:HA	7:q:369:GLU:HB3	2.02	0.41
7:q:354:MET:HE3	7:q:361:PRO:HD3	2.01	0.41
1:A:26:PHE:HB2	1:A:695:HIS:O	2.20	0.41
1:A:680:LEU:HD11	1:C:457:HIS:CD2	2.55	0.41
1:B:445:ILE:HG13	4:M:101:ILE:CG2	2.49	0.41
1:B:568:VAL:HA	1:B:658:LEU:HB2	2.03	0.41
1:B:666:GLU:HA	4:M:106:VAL:HG11	2.02	0.41
1:B:859:ARG:NH2	1:B:893:SER:OG	2.49	0.41
1:B:880:ILE:HG12	1:B:887:LEU:HD21	2.03	0.41
1:C:492:GLY:O	1:C:496:THR:HG23	2.20	0.41
2:D:136:ASP:OD1	2:D:136:ASP:C	2.63	0.41
2:E:60:LEU:HD23	2:E:60:LEU:HA	1.89	0.41
5:P:31:TYR:C	5:P:33:ASP:H	2.27	0.41
5:Q:22:LYS:HD3	5:Q:22:LYS:HA	1.39	0.41
5:Q:97:MET:HE3	5:Q:97:MET:HB2	1.81	0.41
5:Q:97:MET:HE1	5:Q:173:MET:HE2	2.03	0.41
5:U:71:ASN:ND2	5:U:89:ASN:OD1	2.50	0.41
7:e:163:THR:HG23	7:e:164:TYR:CD2	2.55	0.41
7:e:224:LEU:CD2	8:f:183:LYS:HB2	2.49	0.41
1:A:32:LYS:HB2	1:A:32:LYS:HE3	1.80	0.41
1:A:94:THR:OG1	1:A:106:ARG:HG2	2.21	0.41
1:A:270:ASP:OD1	1:A:270:ASP:N	2.50	0.41
1:A:742:LEU:HD23	1:A:742:LEU:HA	1.91	0.41
1:B:30:GLU:HG3	1:B:670:PRO:HB2	2.02	0.41
1:B:411:ASN:HD22	1:C:605:SER:HB3	1.85	0.41
1:C:670:PRO:HA	1:C:690:ILE:HB	2.01	0.41
1:C:769:TRP:HZ2	7:k:390:GLU:HA	1.84	0.41
4:J:29:SER:HB2	7:n:75:ASN:HD21	1.86	0.41
4:N:25:ASN:ND2	7:h:78:GLY:CA	2.84	0.41
5:Q:63:ASN:HB3	5:R:159:THR:HG22	2.03	0.41
5:Q:143:SER:OG	5:R:163:ASP:OD2	2.21	0.41
6:Y:38:LEU:HD23	6:Y:38:LEU:HA	1.76	0.41
7:d:308:LEU:HD23	7:d:308:LEU:HA	1.90	0.41
7:e:345:MET:HE3	7:e:345:MET:HB2	1.91	0.41
7:g:77:LEU:HD23	7:g:77:LEU:HA	1.87	0.41
7:k:208:LEU:HB3	7:k:213:MET:HE2	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:m:203:LEU:O	7:m:207:GLN:HG3	2.21	0.41
7:q:72:PHE:O	7:q:76:VAL:HG13	2.21	0.41
1:A:749:SER:HA	1:A:802:PHE:HB3	2.03	0.41
1:B:287:LEU:HD11	1:B:326:LEU:HD11	2.02	0.41
1:B:762:LEU:HD23	1:B:762:LEU:HA	1.90	0.41
2:E:106:ASP:OD2	7:h:164:TYR:OH	2.39	0.41
4:L:134:GLU:HG2	4:L:137:LYS:HG2	2.02	0.41
5:R:82:LYS:HD3	5:U:177:GLU:CD	2.45	0.41
6:V:1:MET:HA	7:p:34:PHE:CZ	2.55	0.41
6:W:15:LYS:HZ3	6:W:15:LYS:HG2	1.61	0.41
7:d:14:ASP:OD2	7:d:17:GLN:HB2	2.21	0.41
7:e:99:LEU:HD21	7:e:164:TYR:CD1	2.56	0.41
7:h:72:PHE:O	7:h:76:VAL:HG22	2.21	0.41
7:m:308:LEU:HD23	7:m:308:LEU:HA	1.88	0.41
7:p:43:MET:HE3	7:p:43:MET:HB3	1.72	0.41
7:q:178:ARG:NH1	7:q:178:ARG:HB2	2.35	0.41
7:s:156:ASP:OD1	7:s:156:ASP:N	2.52	0.41
7:s:245:ASP:OD1	7:s:246:VAL:N	2.44	0.41
1:B:54:SER:O	1:B:428:SER:OG	2.35	0.41
1:B:578:GLN:NE2	4:K:150:SER:HB2	2.36	0.41
2:E:9:VAL:HG13	3:H:681:TRP:HB3	1.97	0.41
4:J:30:ILE:HG21	7:n:67:ALA:HB1	2.03	0.41
4:K:3:THR:CG2	7:q:276:SER:HB3	2.50	0.41
4:L:30:ILE:HG21	7:b:67:ALA:HB1	2.02	0.41
5:P:35:THR:O	5:P:35:THR:OG1	2.26	0.41
5:S:38:LYS:HD2	5:S:52:PHE:CE2	2.55	0.41
6:W:5:PRO:HA	6:W:6:PRO:HD3	1.94	0.41
6:Z:4:TYR:CG	6:Z:29:GLN:HB2	2.55	0.41
7:e:299:GLN:HA	7:e:302:ASP:OD1	2.21	0.41
7:e:305:LEU:HD12	7:e:309:LYS:NZ	2.36	0.41
7:j:93:PHE:HD2	7:j:105:VAL:HG21	1.85	0.41
7:k:370:LEU:HD12	7:k:378:TYR:HD2	1.86	0.41
7:q:210:GLU:HG2	7:q:211:LEU:HG	2.03	0.41
1:B:200:PRO:HB2	7:h:171:ILE:HG22	1.96	0.41
1:B:630:VAL:HG23	2:E:29:ARG:NH1	2.36	0.41
1:B:755:THR:O	1:B:766:TYR:OH	2.28	0.41
1:C:13:ASP:OD1	1:C:52:TYR:OH	2.37	0.41
1:C:56:SER:HB3	4:J:136:SER:OG	2.18	0.41
1:C:620:ALA:HB3	1:C:624:PHE:HE2	1.85	0.41
1:C:781:LEU:HD23	1:C:781:LEU:HA	1.78	0.41
2:D:85:MET:HE3	2:D:85:MET:HB2	1.91	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:99:TYR:OH	2:F:35:LEU:HD11	2.21	0.41
2:F:5:GLU:H	2:F:5:GLU:HG2	1.62	0.41
2:F:18:LYS:HE2	2:F:18:LYS:HB2	1.55	0.41
2:F:136:ASP:OD1	2:F:136:ASP:C	2.63	0.41
3:G:677:ILE:HD13	3:H:677:ILE:HG12	2.02	0.41
4:J:24:PRO:HG3	7:p:191:ALA:CB	2.51	0.41
4:L:20:LEU:H	4:L:20:LEU:HG	1.43	0.41
4:L:22:ILE:HD13	7:d:195:ARG:HG2	2.03	0.41
4:M:27:ASP:O	4:M:32:THR:OG1	2.28	0.41
4:N:139:LEU:HD12	4:N:139:LEU:HA	1.94	0.41
4:O:7:LEU:HD13	4:O:7:LEU:HA	1.89	0.41
5:Q:40:THR:HG23	5:Q:52:PHE:CE1	2.56	0.41
5:Q:177:GLU:CD	5:T:82:LYS:HD3	2.46	0.41
5:U:186:LYS:O	5:U:190:GLU:HG3	2.20	0.41
6:Y:4:TYR:HA	7:g:42:PHE:CD1	2.54	0.41
6:a:4:TYR:HA	7:m:42:PHE:HD1	1.86	0.41
6:a:5:PRO:HA	6:a:6:PRO:HD3	1.95	0.41
7:d:333:ARG:O	7:d:333:ARG:HD2	2.20	0.41
7:e:285:LEU:HD23	7:e:345:MET:HG3	2.03	0.41
7:g:183:ILE:HD12	7:g:183:ILE:HA	1.90	0.41
7:h:354:MET:HE2	7:h:354:MET:HA	2.03	0.41
7:k:11:VAL:HG21	7:k:58:LEU:HD22	2.02	0.41
7:k:371:THR:HG22	7:k:377:VAL:HG13	2.02	0.41
7:m:284:GLU:H	7:m:346:ASN:ND2	2.19	0.41
8:o:144:THR:OG1	8:o:145:LEU:N	2.54	0.41
8:o:152:PHE:CE1	8:o:184:TYR:HB3	2.55	0.41
7:p:119:ARG:C	7:p:120:PHE:HD1	2.29	0.41
7:p:305:LEU:HD11	7:p:382:VAL:HG11	2.02	0.41
1:A:492:GLY:O	1:A:496:THR:HG23	2.21	0.41
1:A:501:TYR:OH	1:B:617:ALA:O	2.36	0.41
1:A:666:GLU:OE1	5:P:186:LYS:NZ	2.53	0.41
1:B:42:PHE:HE1	5:T:75:ILE:HD12	1.85	0.41
1:B:506:ASP:O	1:B:547:GLN:HA	2.20	0.41
2:E:113:LYS:HE3	2:E:119:ASP:O	2.21	0.41
3:H:673:ILE:HG12	3:I:673:ILE:HG23	2.03	0.41
5:P:236:ILE:O	5:P:239:ILE:HG12	2.21	0.41
5:Q:185:SER:HB2	5:Q:186:LYS:H	1.65	0.41
5:Q:228:ASN:O	5:Q:232:GLN:HG2	2.20	0.41
5:S:68:LEU:HD21	5:T:122:ARG:HD3	2.02	0.41
5:S:275:ASP:HB2	7:n:44:ARG:HH21	1.86	0.41
5:U:26:CYS:HB3	5:U:141:TRP:CG	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:V:50:LEU:HD23	6:V:50:LEU:HA	1.84	0.41
7:b:219:CYS:SG	7:b:220:LYS:N	2.94	0.41
7:e:75:ASN:HB3	7:g:187:ILE:HD13	2.03	0.41
7:h:256:ILE:HD12	7:h:275:ILE:HG22	2.02	0.41
7:k:243:LEU:HB3	7:k:251:ALA:HB2	2.03	0.41
8:o:68:GLU:H	8:o:68:GLU:HG2	1.65	0.41
7:p:291:SER:N	7:p:371:THR:O	2.49	0.41
1:A:32:LYS:HG2	2:E:1:MET:CG	2.41	0.40
1:A:473:ASN:HB3	1:A:541:THR:HG21	2.02	0.40
1:C:126:GLU:H	1:C:126:GLU:HG2	1.70	0.40
2:D:66:ILE:HG22	2:D:100:TYR:HD2	1.86	0.40
2:F:185:LEU:HD22	2:F:185:LEU:HA	1.94	0.40
4:J:70:ILE:HG22	4:J:92:PRO:HG2	2.02	0.40
4:N:70:ILE:HG22	4:N:92:PRO:HG2	2.03	0.40
5:Q:95:MET:HE3	5:Q:97:MET:HE2	2.03	0.40
5:R:123:GLU:HA	5:R:124:PRO:HD3	1.93	0.40
5:R:128:LYS:H	5:R:128:LYS:HG2	1.46	0.40
5:S:48:GLN:HG2	5:S:48:GLN:H	1.73	0.40
5:S:83:ASN:OD1	5:T:89:ASN:ND2	2.54	0.40
5:T:248:LYS:HD3	5:T:259:PHE:CE1	2.56	0.40
6:Y:11:GLY:N	7:d:154:PHE:HE2	2.17	0.40
6:Z:18:ASP:OD1	6:Z:20:ALA:N	2.48	0.40
7:d:6:ASN:N	7:d:6:ASN:OD1	2.51	0.40
7:g:43:MET:HE3	7:g:43:MET:HB3	1.81	0.40
8:l:3:LYS:HB3	8:l:3:LYS:HE2	1.62	0.40
7:p:285:LEU:HD13	7:p:308:LEU:HD13	2.03	0.40
7:q:43:MET:HE3	7:q:43:MET:HB3	1.77	0.40
1:A:42:PHE:HE1	5:R:75:ILE:HD12	1.86	0.40
1:A:578:GLN:HE21	4:O:151:PHE:H	1.67	0.40
1:B:747:ILE:HD11	1:B:802:PHE:CG	2.56	0.40
1:C:516:ASN:ND2	2:D:64:ASN:OD1	2.54	0.40
4:N:36:GLN:O	4:N:119:LYS:NZ	2.49	0.40
5:P:95:MET:HE1	5:P:139:PHE:CE2	2.56	0.40
5:S:26:CYS:HB3	5:S:141:TRP:CG	2.57	0.40
5:T:8:ARG:HD3	5:T:8:ARG:HA	1.65	0.40
6:X:84:LYS:HB2	6:X:88:ILE:HB	2.03	0.40
6:a:12:THR:HG22	7:k:36:ASP:CG	2.45	0.40
7:b:224:LEU:HD21	8:c:183:LYS:HB2	2.03	0.40
7:k:155:ILE:O	7:k:169:THR:HA	2.21	0.40
7:k:197:ARG:H	7:k:197:ARG:HG2	1.40	0.40
7:q:171:ILE:H	7:q:171:ILE:HG13	1.77	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:19:GLN:HB3	1:B:20:GLU:OE2	2.20	0.40
1:B:620:ALA:HB3	1:B:624:PHE:CE2	2.57	0.40
1:B:662:GLN:O	1:B:666:GLU:HG2	2.21	0.40
1:C:209:ASN:O	1:C:213:LYS:HG2	2.21	0.40
1:C:481:LYS:NZ	1:C:500:GLN:OE1	2.54	0.40
1:C:872:THR:C	1:C:874:THR:H	2.30	0.40
5:R:127:LYS:CG	5:R:132:SER:HB3	2.50	0.40
6:Z:5:PRO:HA	6:Z:6:PRO:HD3	1.93	0.40
6:a:4:TYR:CG	6:a:29:GLN:HB2	2.57	0.40
7:d:94:GLY:HA3	7:d:167:TYR:CZ	2.56	0.40
7:h:15:TYR:CZ	7:h:19:ILE:HD11	2.57	0.40
7:h:147:LYS:HE2	7:h:148:TYR:CE2	2.56	0.40
7:h:208:LEU:HD13	7:h:259:VAL:HG21	2.02	0.40
8:l:68:GLU:CD	8:l:68:GLU:N	2.78	0.40
7:n:46:PHE:C	7:n:49:THR:HG22	2.41	0.40
7:p:96:SER:HB3	7:p:166:GLN:HB2	2.02	0.40
7:s:218:ARG:HE	7:s:319:PRO:HD3	1.85	0.40
1:A:165:ILE:HG23	7:b:381:ASN:CB	2.52	0.40
1:A:578:GLN:NE2	4:O:152:ASP:H	2.19	0.40
1:B:408:ILE:CD1	2:E:107:ALA:HB2	2.51	0.40
1:C:356:LEU:HD23	1:C:356:LEU:HA	1.81	0.40
1:C:630:VAL:HG23	2:D:29:ARG:NH1	2.37	0.40
2:D:66:ILE:HG23	2:D:98:GLY:C	2.46	0.40
2:E:133:ASP:OD2	2:F:125:GLU:HA	2.22	0.40
4:L:9:LYS:HZ3	4:L:9:LYS:HG3	1.72	0.40
4:N:49:GLU:H	4:N:49:GLU:HG2	1.76	0.40
5:Q:164:GLY:HA3	5:T:141:TRP:O	2.22	0.40
5:Q:211:GLU:OE2	5:Q:211:GLU:N	2.55	0.40
6:a:101:GLU:O	6:a:101:GLU:HG3	2.22	0.40
8:c:19:ARG:HH22	7:d:56:GLU:CD	2.28	0.40
7:d:291:SER:N	7:d:371:THR:O	2.45	0.40
7:d:364:SER:HB2	7:d:385:VAL:HB	2.02	0.40
8:f:33:ILE:HG13	8:f:37:TRP:CE2	2.56	0.40
7:g:156:ASP:OD1	7:g:156:ASP:N	2.54	0.40
7:k:187:ILE:HD13	7:k:187:ILE:HA	1.88	0.40
7:k:238:VAL:HG13	7:k:274:LEU:HD23	2.02	0.40
7:p:123:ILE:HG13	7:p:124:GLY:N	2.36	0.40
7:p:218:ARG:HD2	7:p:314:PRO:O	2.20	0.40
1:A:668:LEU:HD12	1:A:668:LEU:HA	1.96	0.40
1:C:578:GLN:HA	2:F:5:GLU:OE2	2.22	0.40
2:D:134:LYS:HB3	2:E:127:ASN:OD1	2.20	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:187:ASP:HB3	2:E:179:ARG:HD2	2.03	0.40
4:J:123:LEU:HD23	4:J:123:LEU:HA	1.86	0.40
4:K:112:LYS:HE3	4:K:112:LYS:HB3	1.81	0.40
5:P:125:THR:OG1	5:P:133:HIS:O	2.30	0.40
5:S:35:THR:HA	6:V:63:LYS:CD	2.51	0.40
5:T:207:LYS:HZ3	5:T:213:GLN:CD	2.29	0.40
6:Z:48:LEU:HD12	6:Z:48:LEU:HA	1.87	0.40
8:c:162:GLU:OE2	8:c:163:ASN:ND2	2.40	0.40
7:d:269:LEU:HD23	7:d:270:GLY:N	2.36	0.40
8:f:137:GLN:N	8:f:137:GLN:OE1	2.55	0.40
7:g:113:ASP:OD1	7:g:115:SER:N	2.52	0.40
7:h:5:LEU:HD12	7:h:6:ASN:H	1.86	0.40
7:h:211:LEU:C	7:h:213:MET:H	2.29	0.40
8:i:19:ARG:HH22	7:j:56:GLU:CD	2.30	0.40
8:i:111:LEU:HA	7:j:269:LEU:HD12	2.03	0.40
7:m:255:THR:HA	7:m:258:THR:HG22	2.02	0.40
7:n:183:ILE:HD12	7:n:183:ILE:HA	1.93	0.40
7:p:242:PHE:HA	7:p:276:SER:O	2.21	0.40
7:s:268:MET:HE2	7:s:268:MET:HB3	1.96	0.40
7:s:369:GLU:HG2	7:s:379:ARG:HG3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	874/899 (97%)	837 (96%)	36 (4%)	1 (0%)	48	78
1	B	874/899 (97%)	841 (96%)	33 (4%)	0	100	100
1	C	874/899 (97%)	839 (96%)	35 (4%)	0	100	100
2	D	243/270 (90%)	236 (97%)	7 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	243/270 (90%)	232 (96%)	11 (4%)	0	100	100
2	F	243/270 (90%)	231 (95%)	12 (5%)	0	100	100
3	G	22/689 (3%)	22 (100%)	0	0	100	100
3	H	22/689 (3%)	22 (100%)	0	0	100	100
3	I	22/689 (3%)	22 (100%)	0	0	100	100
4	J	149/155 (96%)	143 (96%)	6 (4%)	0	100	100
4	K	152/155 (98%)	141 (93%)	9 (6%)	2 (1%)	9	37
4	L	149/155 (96%)	141 (95%)	8 (5%)	0	100	100
4	M	151/155 (97%)	146 (97%)	4 (3%)	1 (1%)	18	50
4	N	149/155 (96%)	143 (96%)	6 (4%)	0	100	100
4	O	151/155 (97%)	143 (95%)	8 (5%)	0	100	100
5	P	277/282 (98%)	264 (95%)	13 (5%)	0	100	100
5	Q	277/282 (98%)	269 (97%)	8 (3%)	0	100	100
5	R	279/282 (99%)	266 (95%)	11 (4%)	2 (1%)	18	50
5	S	277/282 (98%)	269 (97%)	8 (3%)	0	100	100
5	T	277/282 (98%)	259 (94%)	17 (6%)	1 (0%)	30	61
5	U	277/282 (98%)	267 (96%)	10 (4%)	0	100	100
6	V	111/114 (97%)	105 (95%)	6 (5%)	0	100	100
6	W	111/114 (97%)	104 (94%)	7 (6%)	0	100	100
6	X	111/114 (97%)	104 (94%)	7 (6%)	0	100	100
6	Y	111/114 (97%)	102 (92%)	9 (8%)	0	100	100
6	Z	111/114 (97%)	107 (96%)	4 (4%)	0	100	100
6	a	111/114 (97%)	105 (95%)	6 (5%)	0	100	100
7	b	384/390 (98%)	374 (97%)	10 (3%)	0	100	100
7	d	380/390 (97%)	377 (99%)	3 (1%)	0	100	100
7	e	384/390 (98%)	377 (98%)	7 (2%)	0	100	100
7	g	380/390 (97%)	377 (99%)	3 (1%)	0	100	100
7	h	384/390 (98%)	372 (97%)	12 (3%)	0	100	100
7	j	380/390 (97%)	376 (99%)	4 (1%)	0	100	100
7	k	384/390 (98%)	371 (97%)	13 (3%)	0	100	100
7	m	380/390 (97%)	377 (99%)	3 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	n	384/390 (98%)	376 (98%)	8 (2%)	0	100	100
7	p	380/390 (97%)	375 (99%)	5 (1%)	0	100	100
7	q	384/390 (98%)	373 (97%)	10 (3%)	1 (0%)	36	66
7	s	380/390 (97%)	376 (99%)	4 (1%)	0	100	100
8	c	188/191 (98%)	182 (97%)	5 (3%)	1 (0%)	24	56
8	f	188/191 (98%)	184 (98%)	4 (2%)	0	100	100
8	i	188/191 (98%)	183 (97%)	5 (3%)	0	100	100
8	l	188/191 (98%)	185 (98%)	3 (2%)	0	100	100
8	o	188/191 (98%)	181 (96%)	7 (4%)	0	100	100
8	r	188/191 (98%)	183 (97%)	4 (2%)	1 (0%)	24	56
All	All	12360/14706 (84%)	11959 (97%)	391 (3%)	10 (0%)	49	78

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	461	ILE
4	M	132	ASN
8	r	81	ALA
4	K	133	THR
8	c	81	ALA
5	T	203	GLY
5	R	129	GLY
5	R	127	LYS
7	q	200	VAL
4	K	132	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	A	743/760 (98%)	705 (95%)	38 (5%)	21	49
1	B	743/760 (98%)	713 (96%)	30 (4%)	28	54

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	743/760 (98%)	691 (93%)	52 (7%)	14	40
2	D	213/231 (92%)	198 (93%)	15 (7%)	14	40
2	E	213/231 (92%)	198 (93%)	15 (7%)	14	40
2	F	213/231 (92%)	199 (93%)	14 (7%)	15	42
3	G	19/545 (4%)	18 (95%)	1 (5%)	20	48
3	H	19/545 (4%)	16 (84%)	3 (16%)	2	13
3	I	19/545 (4%)	17 (90%)	2 (10%)	6	26
4	J	133/137 (97%)	110 (83%)	23 (17%)	2	10
4	K	136/137 (99%)	116 (85%)	20 (15%)	3	15
4	L	133/137 (97%)	108 (81%)	25 (19%)	1	8
4	M	135/137 (98%)	116 (86%)	19 (14%)	3	16
4	N	133/137 (97%)	115 (86%)	18 (14%)	4	18
4	O	135/137 (98%)	106 (78%)	29 (22%)	1	5
5	P	253/256 (99%)	241 (95%)	12 (5%)	23	51
5	Q	253/256 (99%)	239 (94%)	14 (6%)	19	47
5	R	255/256 (100%)	241 (94%)	14 (6%)	19	47
5	S	253/256 (99%)	245 (97%)	8 (3%)	34	59
5	T	253/256 (99%)	240 (95%)	13 (5%)	21	49
5	U	253/256 (99%)	238 (94%)	15 (6%)	18	45
6	V	102/103 (99%)	101 (99%)	1 (1%)	68	75
6	W	102/103 (99%)	99 (97%)	3 (3%)	37	61
6	X	102/103 (99%)	99 (97%)	3 (3%)	37	61
6	Y	102/103 (99%)	96 (94%)	6 (6%)	18	45
6	Z	102/103 (99%)	98 (96%)	4 (4%)	28	55
6	a	102/103 (99%)	96 (94%)	6 (6%)	18	45
7	b	329/333 (99%)	322 (98%)	7 (2%)	47	66
7	d	325/333 (98%)	318 (98%)	7 (2%)	45	65
7	e	329/333 (99%)	309 (94%)	20 (6%)	17	44
7	g	325/333 (98%)	314 (97%)	11 (3%)	32	58
7	h	329/333 (99%)	317 (96%)	12 (4%)	31	57
7	j	325/333 (98%)	318 (98%)	7 (2%)	45	65

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	k	329/333 (99%)	319 (97%)	10 (3%)	36	60
7	m	325/333 (98%)	315 (97%)	10 (3%)	35	60
7	n	329/333 (99%)	323 (98%)	6 (2%)	51	68
7	p	325/333 (98%)	317 (98%)	8 (2%)	42	63
7	q	329/333 (99%)	307 (93%)	22 (7%)	15	41
7	s	325/333 (98%)	314 (97%)	11 (3%)	32	58
8	c	169/170 (99%)	168 (99%)	1 (1%)	78	80
8	f	169/170 (99%)	165 (98%)	4 (2%)	43	64
8	i	169/170 (99%)	169 (100%)	0	100	100
8	l	169/170 (99%)	161 (95%)	8 (5%)	23	51
8	o	169/170 (99%)	164 (97%)	5 (3%)	36	60
8	r	169/170 (99%)	166 (98%)	3 (2%)	51	68
All	All	10800/12600 (86%)	10245 (95%)	555 (5%)	23	49

All (555) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	PHE
1	A	74	ASP
1	A	76	LYS
1	A	94	THR
1	A	226	LYS
1	A	230	GLN
1	A	232	ASN
1	A	233	GLN
1	A	234	VAL
1	A	312	GLU
1	A	433	GLN
1	A	434	ILE
1	A	435	THR
1	A	461	ILE
1	A	480	VAL
1	A	518	SER
1	A	545	VAL
1	A	561	THR
1	A	564	VAL
1	A	568	VAL
1	A	570	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	573	VAL
1	A	599	VAL
1	A	607	ILE
1	A	611	LYS
1	A	630	VAL
1	A	653	GLN
1	A	654	LEU
1	A	676	ILE
1	A	696	SER
1	A	710	ILE
1	A	712	VAL
1	A	766	TYR
1	A	792	LYS
1	A	794	ARG
1	A	796	ASN
1	A	802	PHE
1	A	831	MET
1	B	33	LYS
1	B	94	THR
1	B	292	THR
1	B	299	ASN
1	B	312	GLU
1	B	415	ILE
1	B	432	THR
1	B	455	THR
1	B	460	ILE
1	B	463	ASP
1	B	464	THR
1	B	480	VAL
1	B	518	SER
1	B	561	THR
1	B	566	ASP
1	B	573	VAL
1	B	588	ILE
1	B	599	VAL
1	B	603	SER
1	B	611	LYS
1	B	614	LYS
1	B	640	SER
1	B	643	ARG
1	B	712	VAL
1	B	766	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	791	MET
1	B	792	LYS
1	B	794	ARG
1	B	796	ASN
1	B	802	PHE
1	C	26	PHE
1	C	41	ILE
1	C	55	THR
1	C	74	ASP
1	C	94	THR
1	C	144	VAL
1	C	194	GLN
1	C	228	GLN
1	C	230	GLN
1	C	232	ASN
1	C	313	ARG
1	C	432	THR
1	C	460	ILE
1	C	461	ILE
1	C	518	SER
1	C	545	VAL
1	C	561	THR
1	C	568	VAL
1	C	588	ILE
1	C	599	VAL
1	C	600	ASP
1	C	602	ASP
1	C	603	SER
1	C	638	GLN
1	C	645	GLU
1	C	651	GLU
1	C	654	LEU
1	C	656	LEU
1	C	658	LEU
1	C	659	HIS
1	C	660	THR
1	C	665	LEU
1	C	668	LEU
1	C	672	THR
1	C	676	ILE
1	C	677	GLU
1	C	686	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	687	SER
1	C	690	ILE
1	C	692	SER
1	C	693	VAL
1	C	696	SER
1	C	699	GLU
1	C	701	ILE
1	C	702	PHE
1	C	710	ILE
1	C	712	VAL
1	C	766	TYR
1	C	792	LYS
1	C	794	ARG
1	C	796	ASN
1	C	802	PHE
2	D	23	SER
2	D	61	ILE
2	D	71	VAL
2	D	81	GLN
2	D	103	ILE
2	D	105	ASN
2	D	110	SER
2	D	184	ILE
2	D	185	LEU
2	D	237	MET
2	D	240	ILE
2	D	241	ASN
2	D	243	THR
2	D	244	SER
2	D	245	VAL
2	E	4	ASP
2	E	5	GLU
2	E	11	GLU
2	E	14	LEU
2	E	61	ILE
2	E	62	GLU
2	E	75	GLN
2	E	162	GLU
2	E	177	GLU
2	E	178	VAL
2	E	221	ARG
2	E	226	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	228	SER
2	E	243	THR
2	E	244	SER
2	F	1	MET
2	F	2	ILE
2	F	18	LYS
2	F	19	MET
2	F	21	LYS
2	F	61	ILE
2	F	62	GLU
2	F	75	GLN
2	F	185	LEU
2	F	235	LEU
2	F	237	MET
2	F	240	ILE
2	F	243	THR
2	F	244	SER
3	G	684	THR
3	H	673	ILE
3	H	684	THR
3	H	686	THR
3	I	680	GLN
3	I	684	THR
4	J	3	THR
4	J	4	GLN
4	J	7	LEU
4	J	8	SER
4	J	9	LYS
4	J	13	ILE
4	J	15	SER
4	J	16	GLU
4	J	17	LEU
4	J	18	LEU
4	J	21	LEU
4	J	22	ILE
4	J	23	LYS
4	J	81	LYS
4	J	84	ASP
4	J	95	LYS
4	J	102	LYS
4	J	105	ILE
4	J	106	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	J	138	THR
4	J	145	LYS
4	J	146	VAL
4	J	150	SER
4	K	3	THR
4	K	7	LEU
4	K	9	LYS
4	K	11	LYS
4	K	13	ILE
4	K	16	GLU
4	K	18	LEU
4	K	20	LEU
4	K	21	LEU
4	K	22	ILE
4	K	23	LYS
4	K	25	ASN
4	K	26	THR
4	K	27	ASP
4	K	42	ASP
4	K	56	LYS
4	K	60	GLU
4	K	131	SER
4	K	147	VAL
4	K	153	ASN
4	L	2	THR
4	L	3	THR
4	L	7	LEU
4	L	9	LYS
4	L	12	THR
4	L	13	ILE
4	L	15	SER
4	L	16	GLU
4	L	17	LEU
4	L	18	LEU
4	L	20	LEU
4	L	23	LYS
4	L	25	ASN
4	L	26	THR
4	L	27	ASP
4	L	41	ARG
4	L	81	LYS
4	L	83	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	L	84	ASP
4	L	139	LEU
4	L	143	ILE
4	L	145	LYS
4	L	146	VAL
4	L	147	VAL
4	L	150	SER
4	M	3	THR
4	M	4	GLN
4	M	7	LEU
4	M	9	LYS
4	M	13	ILE
4	M	14	GLU
4	M	16	GLU
4	M	18	LEU
4	M	25	ASN
4	M	26	THR
4	M	30	ILE
4	M	31	LEU
4	M	46	ILE
4	M	125	LEU
4	M	126	ILE
4	M	133	THR
4	M	149	PHE
4	M	150	SER
4	M	154	THR
4	N	4	GLN
4	N	5	GLU
4	N	7	LEU
4	N	8	SER
4	N	9	LYS
4	N	13	ILE
4	N	17	LEU
4	N	35	LYS
4	N	38	ILE
4	N	41	ARG
4	N	45	ASP
4	N	46	ILE
4	N	49	GLU
4	N	56	LYS
4	N	138	THR
4	N	145	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	N	146	VAL
4	N	147	VAL
4	O	3	THR
4	O	4	GLN
4	O	7	LEU
4	O	9	LYS
4	O	12	THR
4	O	13	ILE
4	O	14	GLU
4	O	15	SER
4	O	25	ASN
4	O	36	GLN
4	O	38	ILE
4	O	40	ASP
4	O	43	LEU
4	O	110	THR
4	O	122	ILE
4	O	125	LEU
4	O	126	ILE
4	O	128	VAL
4	O	133	THR
4	O	136	SER
4	O	137	LYS
4	O	139	LEU
4	O	140	LYS
4	O	145	LYS
4	O	146	VAL
4	O	147	VAL
4	O	152	ASP
4	O	153	ASN
4	O	154	THR
5	P	33	ASP
5	P	36	ASN
5	P	37	VAL
5	P	40	THR
5	P	127	LYS
5	P	128	LYS
5	P	130	LEU
5	P	145	THR
5	P	200	VAL
5	P	201	GLN
5	P	236	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	P	238	ASN
5	Q	22	LYS
5	Q	38	LYS
5	Q	39	GLN
5	Q	40	THR
5	Q	130	LEU
5	Q	132	SER
5	Q	145	THR
5	Q	189	GLU
5	Q	194	LYS
5	Q	199	THR
5	Q	247	ILE
5	Q	248	LYS
5	Q	249	ILE
5	Q	258	LEU
5	R	19	ASN
5	R	34	SER
5	R	38	LYS
5	R	40	THR
5	R	126	VAL
5	R	128	LYS
5	R	130	LEU
5	R	145	THR
5	R	185	SER
5	R	186	LYS
5	R	201	GLN
5	R	202	ASN
5	R	206	LYS
5	R	207	LYS
5	S	130	LEU
5	S	152	THR
5	S	154	ILE
5	S	205	LEU
5	S	218	VAL
5	S	246	VAL
5	S	247	ILE
5	S	248	LYS
5	T	34	SER
5	T	35	THR
5	T	37	VAL
5	T	126	VAL
5	T	127	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	T	128	LYS
5	T	132	SER
5	T	145	THR
5	T	194	LYS
5	T	198	GLU
5	T	201	GLN
5	T	202	ASN
5	T	235	THR
5	U	22	LYS
5	U	37	VAL
5	U	45	LYS
5	U	47	LYS
5	U	48	GLN
5	U	105	MET
5	U	121	LEU
5	U	130	LEU
5	U	152	THR
5	U	154	ILE
5	U	189	GLU
5	U	193	LYS
5	U	195	VAL
5	U	197	VAL
5	U	236	ILE
6	V	41	ASP
6	W	46	VAL
6	W	65	GLN
6	W	110	THR
6	X	16	SER
6	X	17	THR
6	X	80	THR
6	Y	34	VAL
6	Y	38	LEU
6	Y	39	VAL
6	Y	46	VAL
6	Y	54	ILE
6	Y	72	ILE
6	Z	1	MET
6	Z	35	ARG
6	Z	39	VAL
6	Z	65	GLN
6	a	35	ARG
6	a	39	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	a	46	VAL
6	a	53	ASN
6	a	54	ILE
6	a	83	LEU
7	b	37	LEU
7	b	104	ILE
7	b	111	VAL
7	b	195	ARG
7	b	363	PHE
7	b	376	THR
7	b	386	THR
8	c	55	ASP
7	d	26	THR
7	d	36	ASP
7	d	37	LEU
7	d	79	VAL
7	d	184	ASP
7	d	240	HIS
7	d	259	VAL
7	e	11	VAL
7	e	12	VAL
7	e	13	ASP
7	e	29	VAL
7	e	30	SER
7	e	76	VAL
7	e	133	THR
7	e	136	THR
7	e	196	ILE
7	e	197	ARG
7	e	200	VAL
7	e	203	LEU
7	e	229	LYS
7	e	306	GLU
7	e	373	SER
7	e	376	THR
7	e	377	VAL
7	e	379	ARG
7	e	380	ASP
7	e	385	VAL
8	f	3	LYS
8	f	63	LEU
8	f	80	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	f	162	GLU
7	g	50	MET
7	g	111	VAL
7	g	159	SER
7	g	184	ASP
7	g	197	ARG
7	g	200	VAL
7	g	203	LEU
7	g	243	LEU
7	g	269	LEU
7	g	295	LYS
7	g	321	GLU
7	h	11	VAL
7	h	12	VAL
7	h	77	LEU
7	h	100	SER
7	h	156	ASP
7	h	160	THR
7	h	163	THR
7	h	208	LEU
7	h	274	LEU
7	h	386	THR
7	h	389	GLU
7	h	390	GLU
7	j	20	ILE
7	j	40	SER
7	j	79	VAL
7	j	259	VAL
7	j	356	ASN
7	j	359	THR
7	j	360	ILE
7	k	133	THR
7	k	159	SER
7	k	193	ILE
7	k	224	LEU
7	k	373	SER
7	k	376	THR
7	k	379	ARG
7	k	380	ASP
7	k	389	GLU
7	k	390	GLU
8	l	3	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	l	20	MET
8	l	22	LYS
8	l	25	VAL
8	l	27	THR
8	l	64	GLN
8	l	87	ASP
8	l	159	ASP
7	m	20	ILE
7	m	25	HIS
7	m	26	THR
7	m	38	ASP
7	m	159	SER
7	m	184	ASP
7	m	231	VAL
7	m	240	HIS
7	m	269	LEU
7	m	363	PHE
7	n	195	ARG
7	n	197	ARG
7	n	203	LEU
7	n	204	ASP
7	n	208	LEU
7	n	363	PHE
8	o	7	THR
8	o	55	ASP
8	o	76	LEU
8	o	85	SER
8	o	87	ASP
7	p	79	VAL
7	p	184	ASP
7	p	215	GLU
7	p	240	HIS
7	p	257	SER
7	p	259	VAL
7	p	354	MET
7	p	357	GLN
7	q	76	VAL
7	q	77	LEU
7	q	123	ILE
7	q	133	THR
7	q	134	PHE
7	q	136	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	q	159	SER
7	q	192	GLN
7	q	195	ARG
7	q	196	ILE
7	q	198	ASN
7	q	200	VAL
7	q	201	SER
7	q	345	MET
7	q	363	PHE
7	q	376	THR
7	q	379	ARG
7	q	382	VAL
7	q	383	VAL
7	q	385	VAL
7	q	389	GLU
7	q	390	GLU
8	r	63	LEU
8	r	134	ILE
8	r	159	ASP
7	s	26	THR
7	s	159	SER
7	s	184	ASP
7	s	240	HIS
7	s	269	LEU
7	s	306	GLU
7	s	354	MET
7	s	356	ASN
7	s	357	GLN
7	s	359	THR
7	s	360	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (167) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	36	ASN
1	A	38	ASN
1	A	59	GLN
1	A	71	ASN
1	A	194	GLN
1	A	230	GLN
1	A	235	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	310	ASN
1	A	315	ASN
1	A	433	GLN
1	A	470	GLN
1	A	578	GLN
1	A	653	GLN
1	A	655	GLN
1	A	667	ASN
1	A	705	GLN
1	A	797	GLN
1	A	829	ASN
1	A	845	HIS
1	A	866	GLN
1	B	36	ASN
1	B	38	ASN
1	B	194	GLN
1	B	359	GLN
1	B	433	GLN
1	B	516	ASN
1	B	522	GLN
1	B	559	ASN
1	B	578	GLN
1	B	613	ASN
1	B	667	ASN
1	B	797	GLN
1	B	845	HIS
1	B	866	GLN
1	C	34	GLN
1	C	36	ASN
1	C	38	ASN
1	C	71	ASN
1	C	194	GLN
1	C	230	GLN
1	C	299	ASN
1	C	310	ASN
1	C	359	GLN
1	C	418	ASN
1	C	470	GLN
1	C	516	ASN
1	C	578	GLN
1	C	636	GLN
1	C	667	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	678	ASN
1	C	797	GLN
1	C	829	ASN
1	C	845	HIS
2	D	81	GLN
2	D	84	GLN
2	D	155	ASN
2	D	227	ASN
2	E	81	GLN
2	F	152	GLN
3	H	672	GLN
4	J	25	ASN
4	J	69	GLN
4	K	4	GLN
4	K	52	GLN
4	K	153	ASN
4	L	4	GLN
4	L	69	GLN
4	M	10	ASN
4	M	25	ASN
4	M	94	GLN
4	M	99	ASN
4	N	25	ASN
4	N	69	GLN
4	O	10	ASN
4	O	55	ASN
4	O	94	GLN
4	O	99	ASN
5	P	144	ASN
5	P	153	ASN
5	P	201	GLN
5	P	213	GLN
5	Q	19	ASN
5	Q	73	GLN
5	Q	99	ASN
5	Q	112	GLN
5	Q	204	ASN
5	R	153	ASN
5	R	202	ASN
5	R	213	GLN
5	S	19	ASN
5	S	24	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	S	46	ASN
5	S	99	ASN
5	S	204	ASN
5	S	228	ASN
5	S	262	ASN
5	T	153	ASN
5	T	201	GLN
5	T	213	GLN
5	T	228	ASN
5	U	36	ASN
5	U	46	ASN
5	U	213	GLN
5	U	228	ASN
5	U	262	ASN
6	V	10	ASN
6	W	29	GLN
6	W	55	ASN
6	W	85	ASN
6	W	105	ASN
6	X	102	ASN
6	Y	55	ASN
6	Y	58	GLN
6	Z	29	GLN
6	a	53	ASN
7	b	108	ASN
7	b	166	GLN
7	b	176	ASN
7	b	381	ASN
8	c	64	GLN
8	c	124	ASN
7	e	27	ASN
7	e	75	ASN
7	e	110	GLN
7	e	192	GLN
7	e	198	ASN
7	e	207	GLN
7	e	381	ASN
7	e	387	ASN
8	f	10	ASN
8	f	24	GLN
7	g	298	GLN
7	h	75	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	h	92	GLN
7	h	108	ASN
7	h	176	ASN
7	h	240	HIS
7	h	381	ASN
7	j	298	GLN
7	j	346	ASN
7	k	25	HIS
7	k	31	ASN
7	k	75	ASN
7	k	110	GLN
8	l	10	ASN
7	m	17	GLN
7	m	110	GLN
7	n	27	ASN
7	n	75	ASN
7	n	108	ASN
7	n	166	GLN
7	n	381	ASN
7	n	387	ASN
8	o	24	GLN
7	p	192	GLN
7	p	346	ASN
7	q	25	HIS
7	q	27	ASN
7	q	75	ASN
7	q	110	GLN
7	q	192	GLN
7	q	198	ASN
7	q	346	ASN
8	r	10	ASN
8	r	24	GLN
8	r	64	GLN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

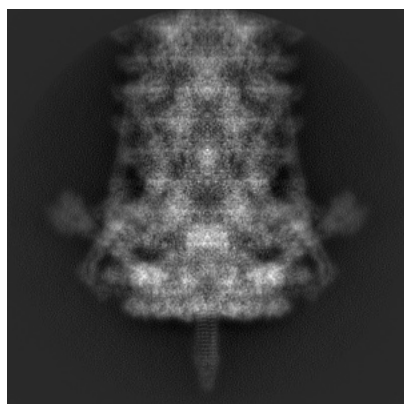
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37151. These allow visual inspection of the internal detail of the map and identification of artifacts.

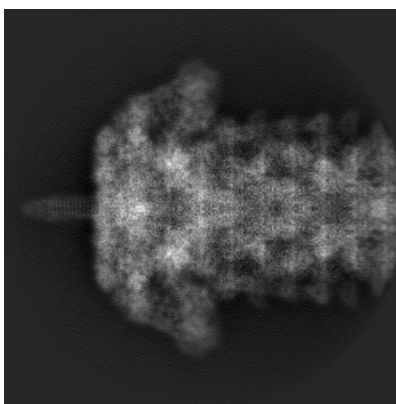
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

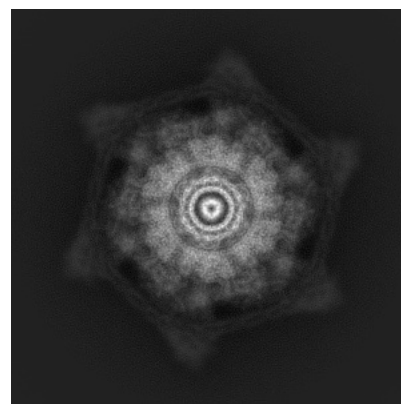
6.1.1 Primary map



X

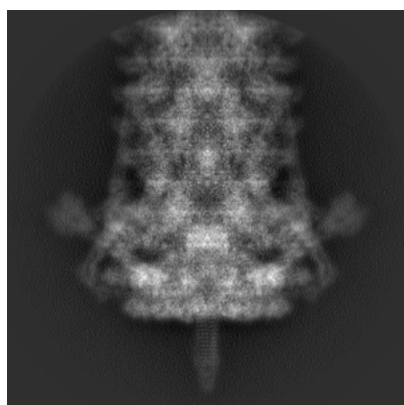


Y

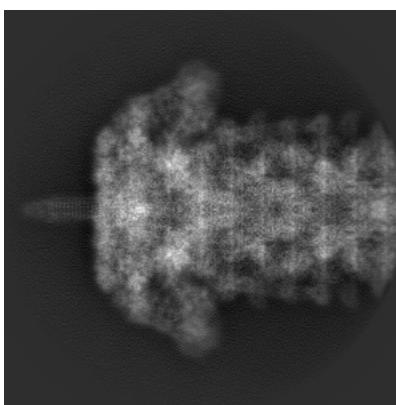


Z

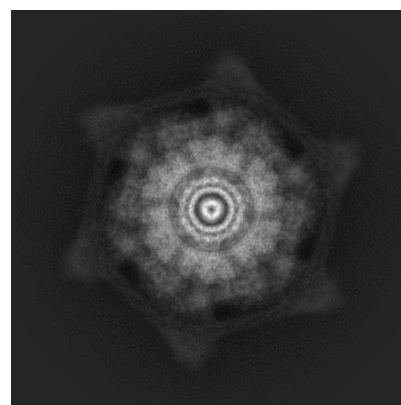
6.1.2 Raw map



X



Y

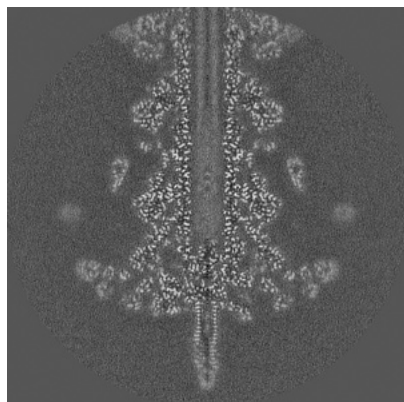


Z

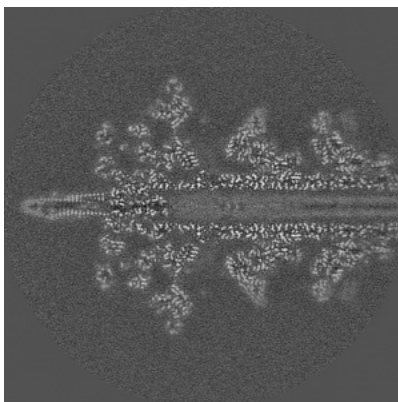
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

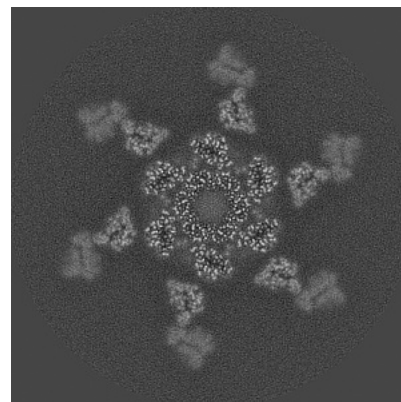
6.2.1 Primary map



X Index: 224

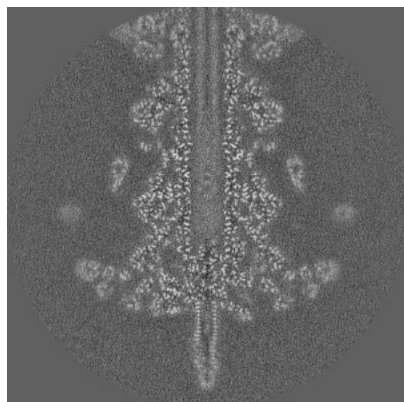


Y Index: 224

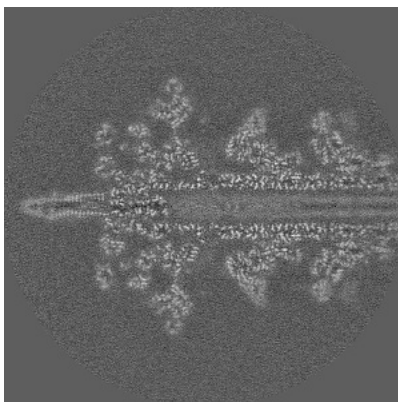


Z Index: 224

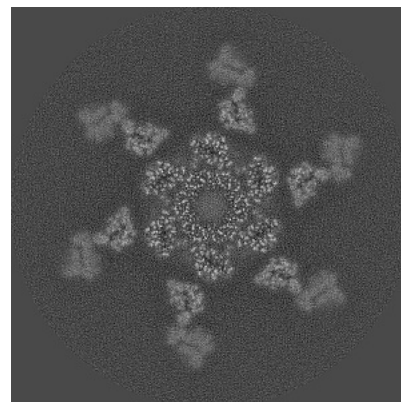
6.2.2 Raw map



X Index: 224



Y Index: 224

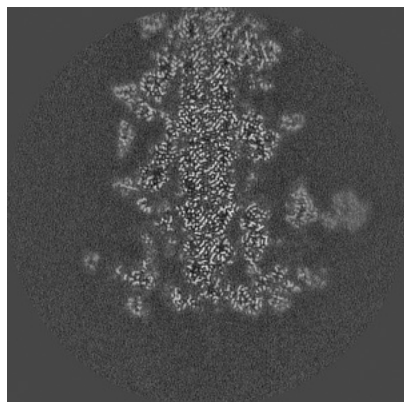


Z Index: 224

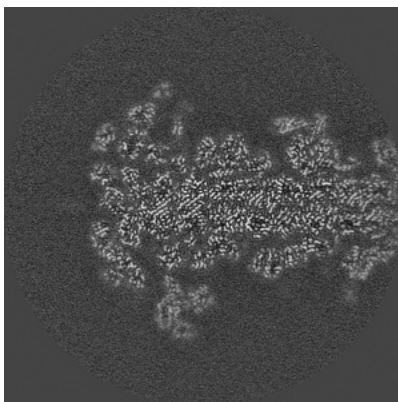
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

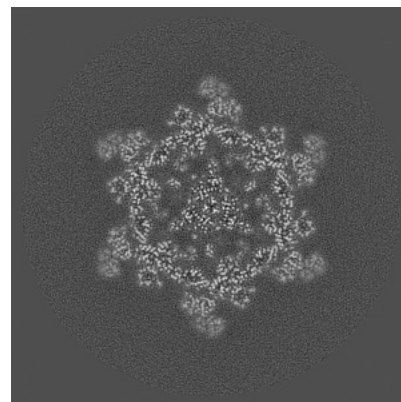
6.3.1 Primary map



X Index: 244

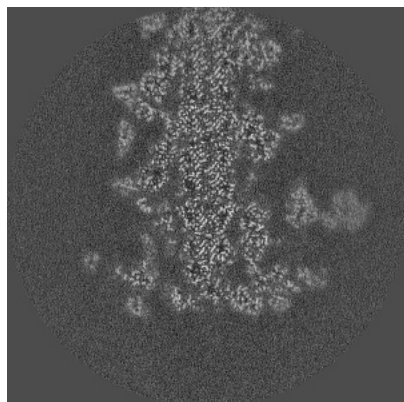


Y Index: 204

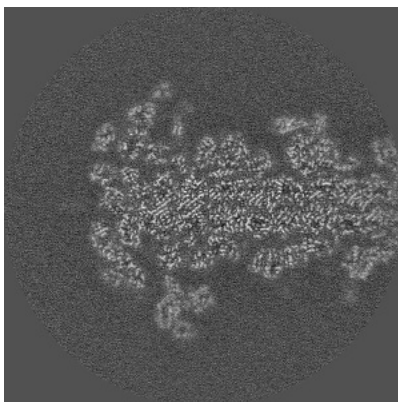


Z Index: 148

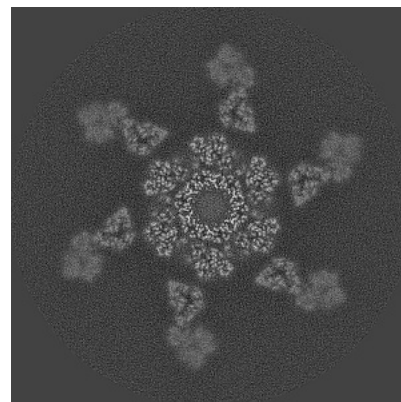
6.3.2 Raw map



X Index: 244



Y Index: 204

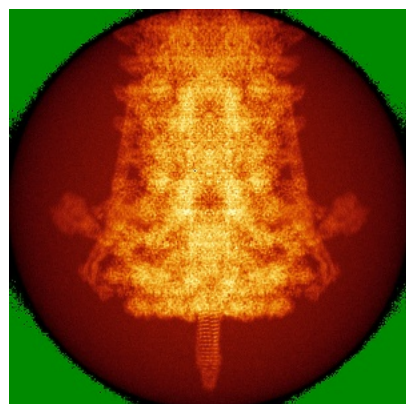


Z Index: 221

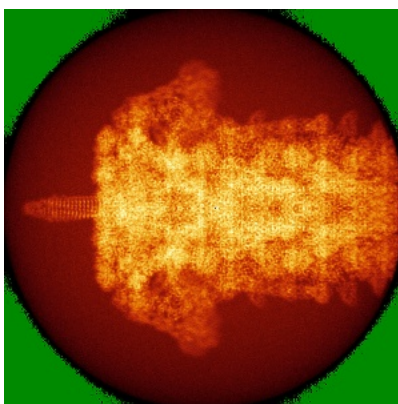
The images above show the largest variance slices of the map in three orthogonal directions.

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

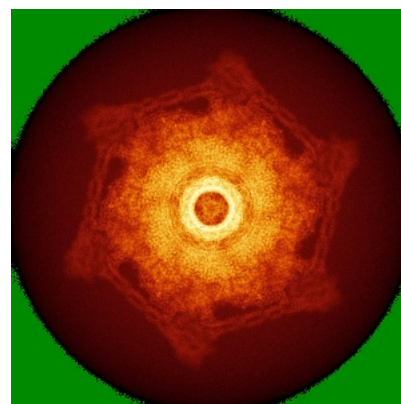
6.4.1 Primary map



X

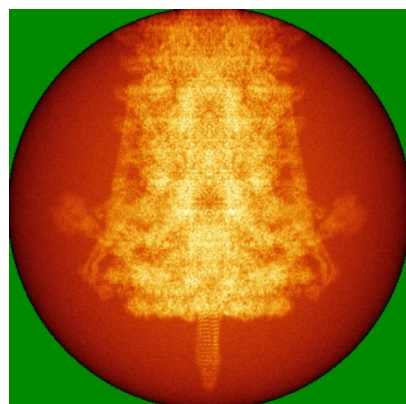


Y

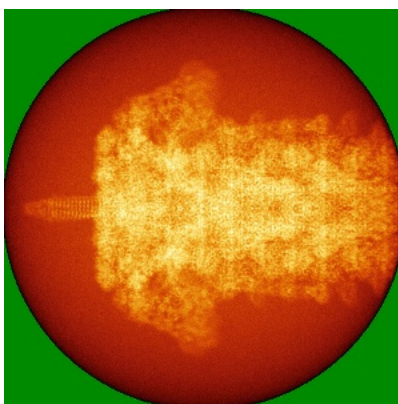


Z

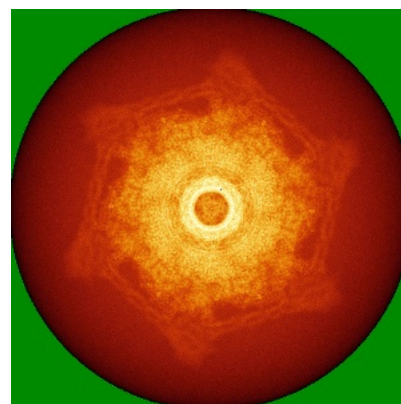
6.4.2 Raw map



X



Y

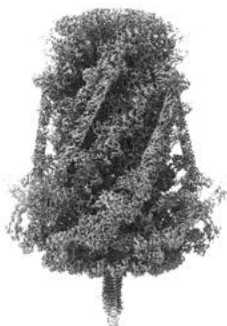


Z

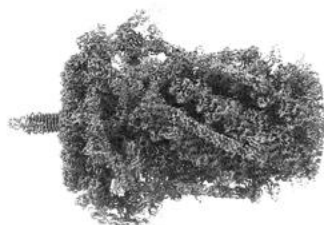
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

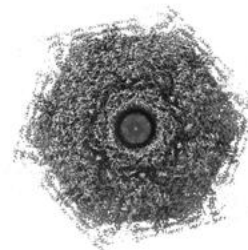
6.5.1 Primary map



X



Y



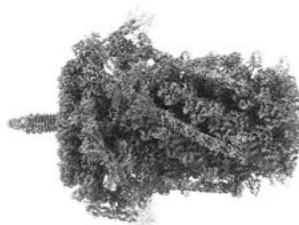
Z

The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

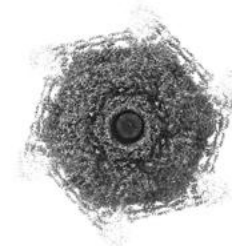
6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

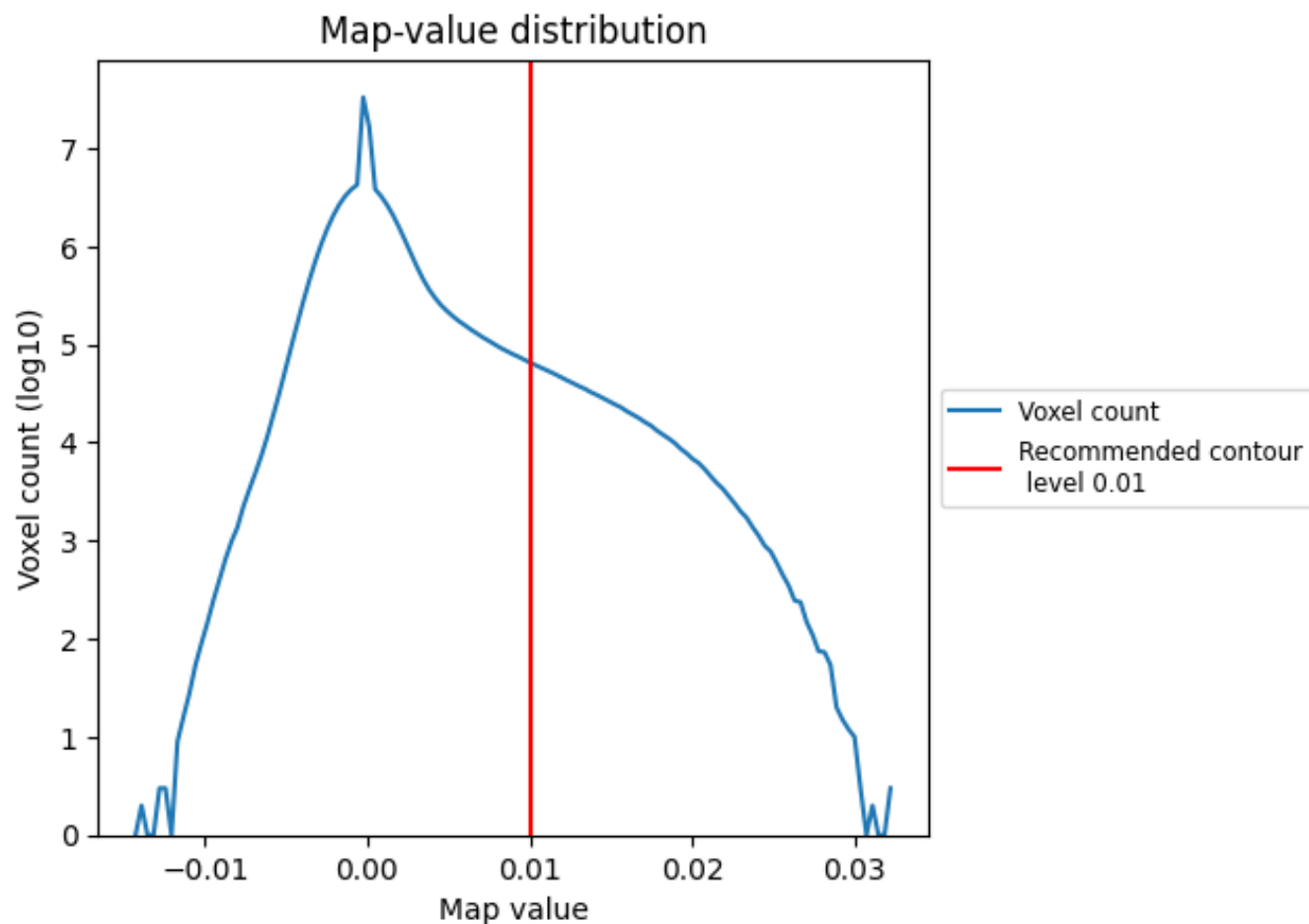
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

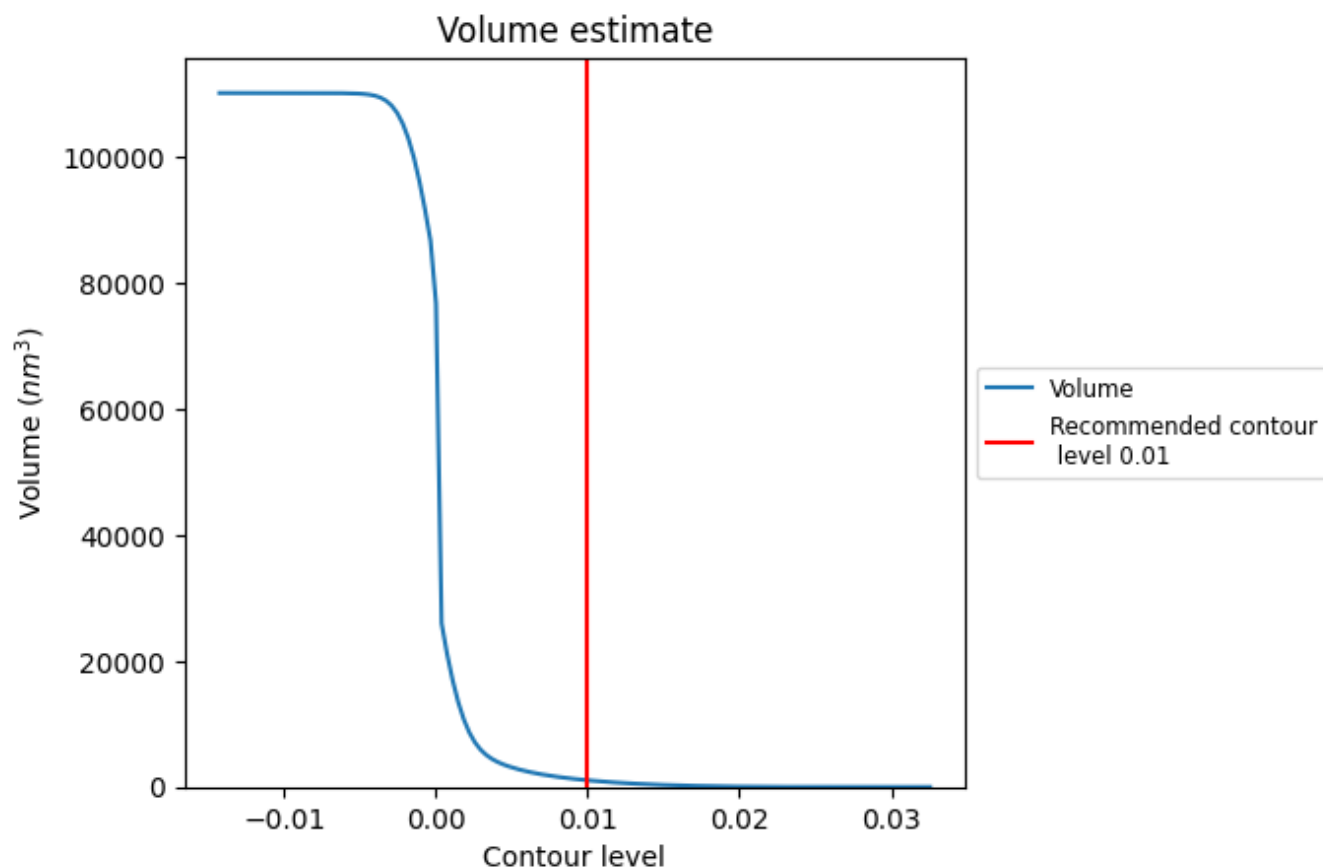
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

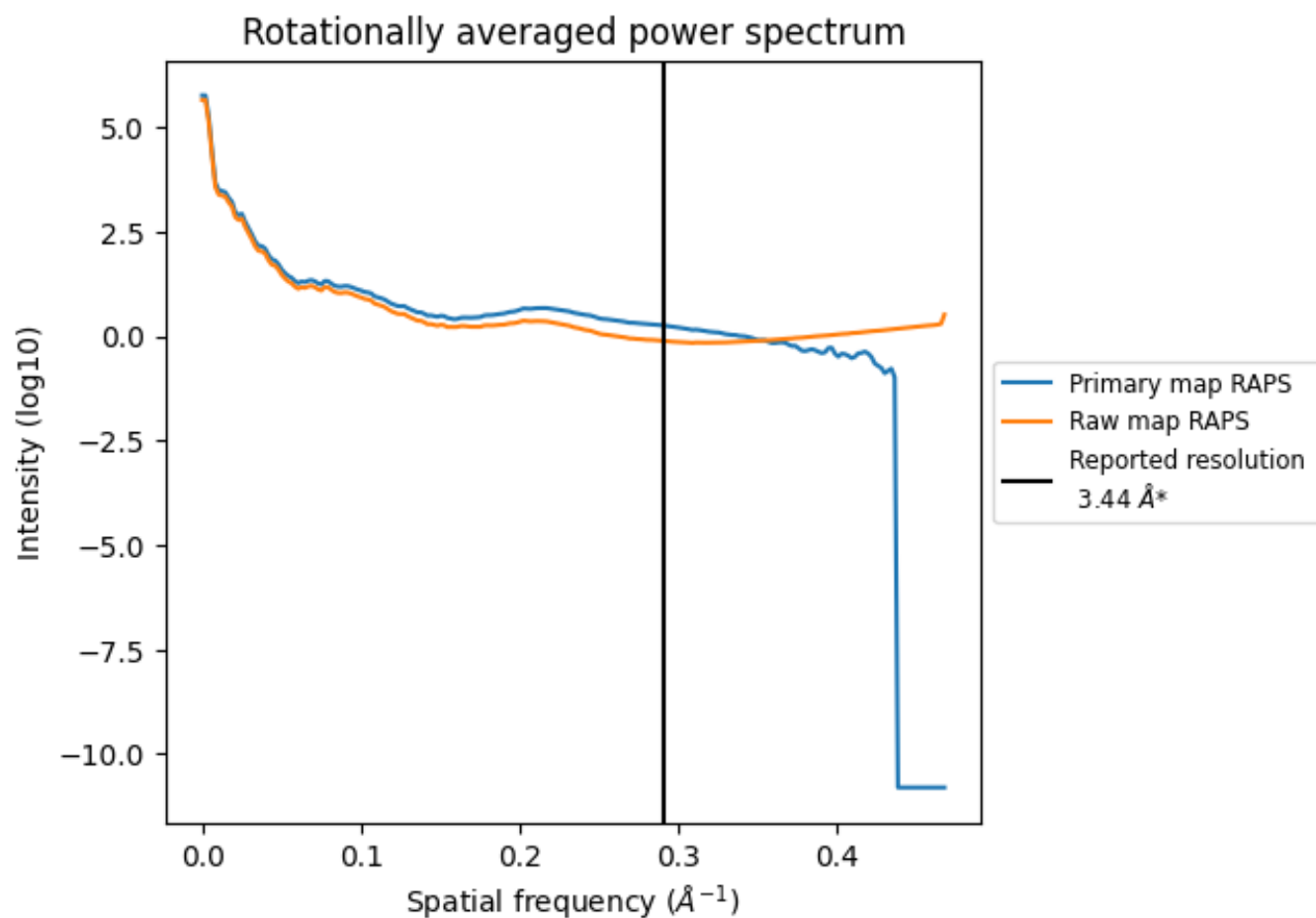
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1060 nm³; this corresponds to an approximate mass of 957 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 ⓘ

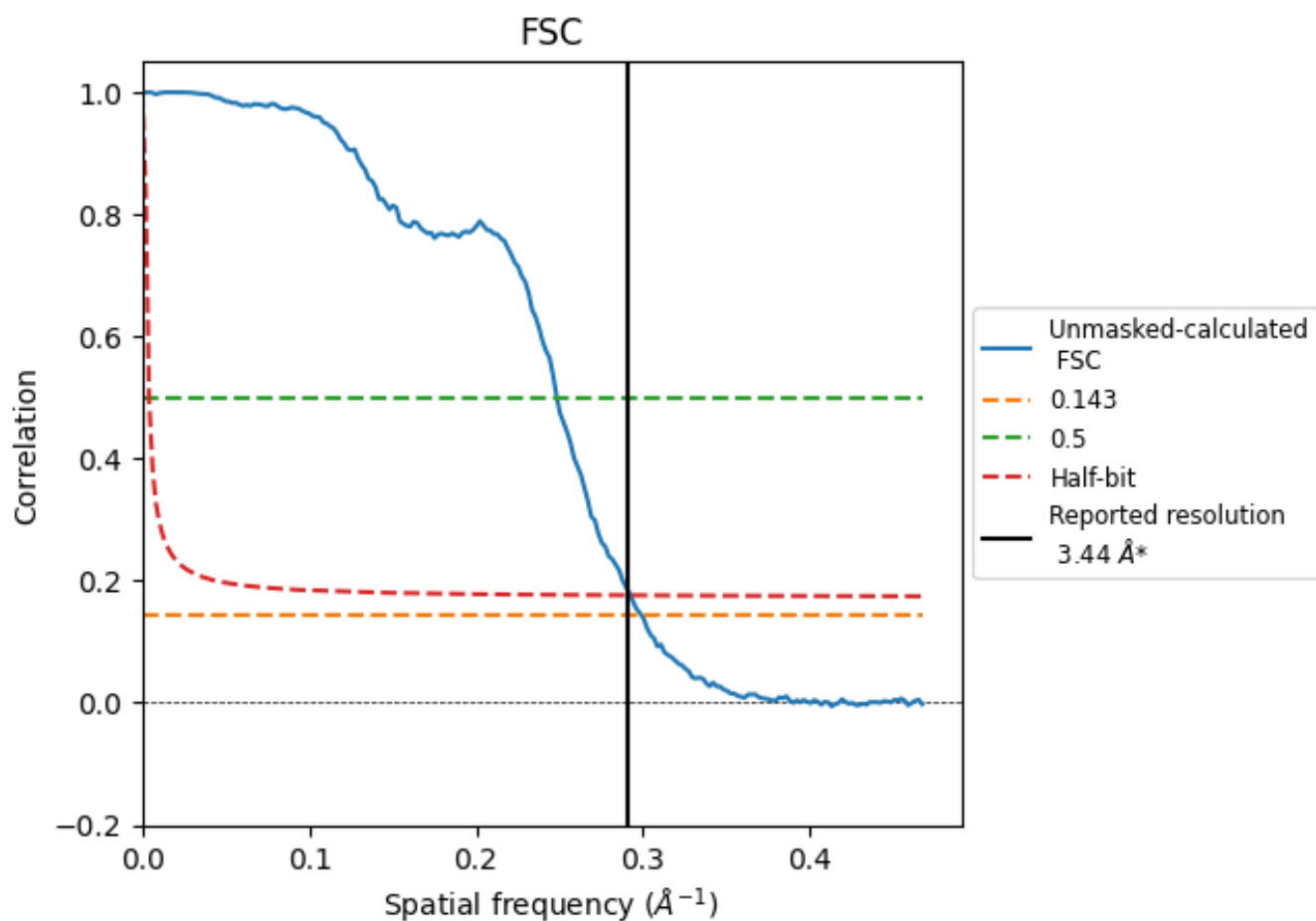


*Reported resolution corresponds to spatial frequency of 0.291 $\text{\AA}^{-1}$

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 0.291 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

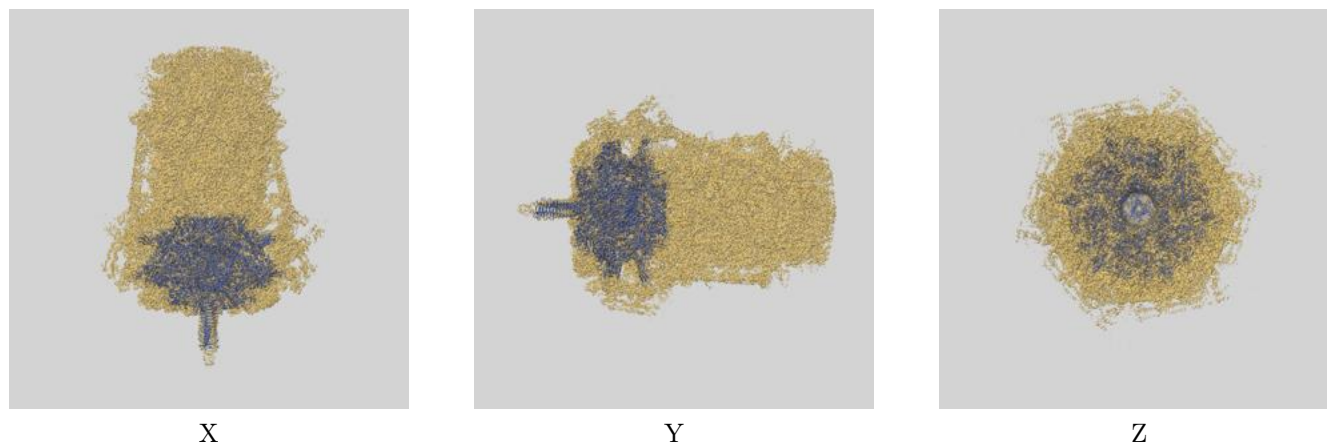
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.44	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.34	4.02	3.42

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

9 Map-model fit [i](#)

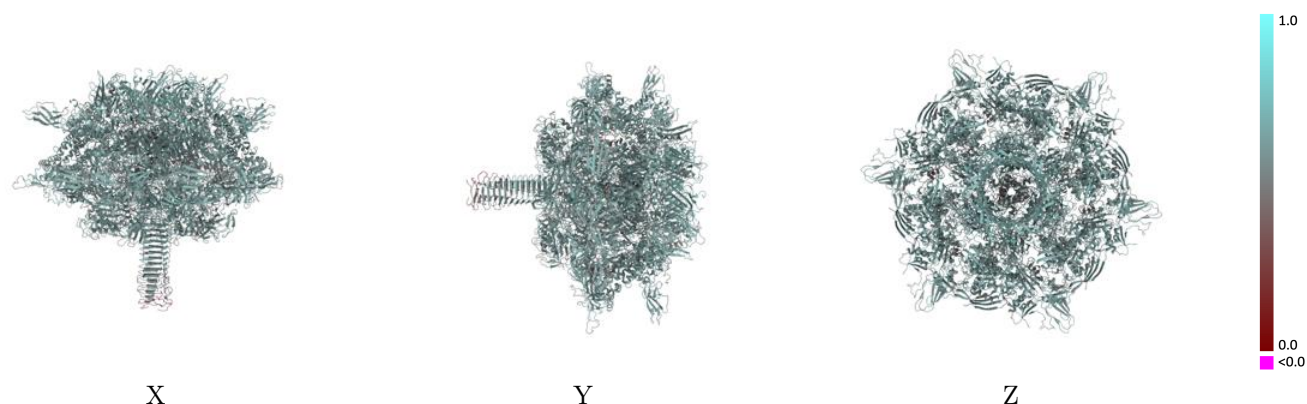
This section contains information regarding the fit between EMDB map EMD-37151 and PDB model 8KEA. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



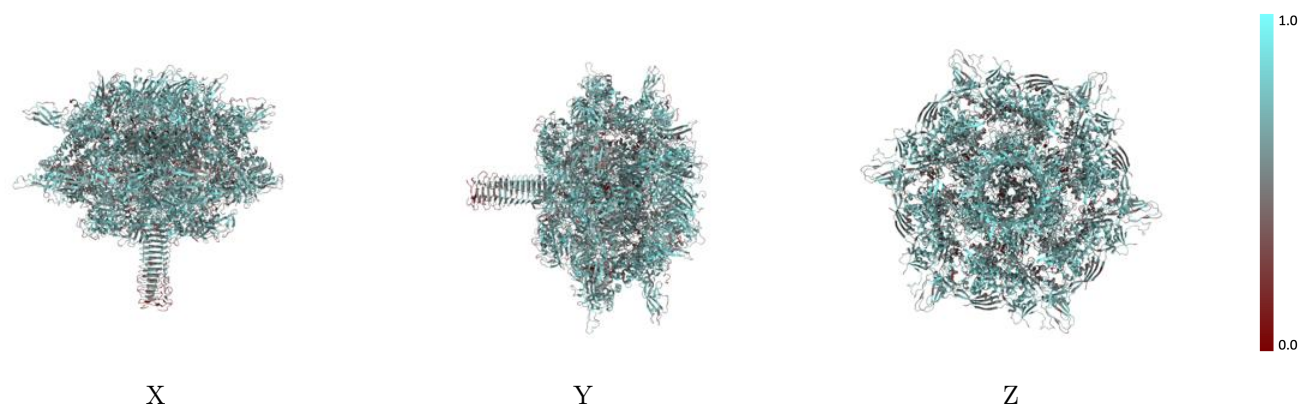
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



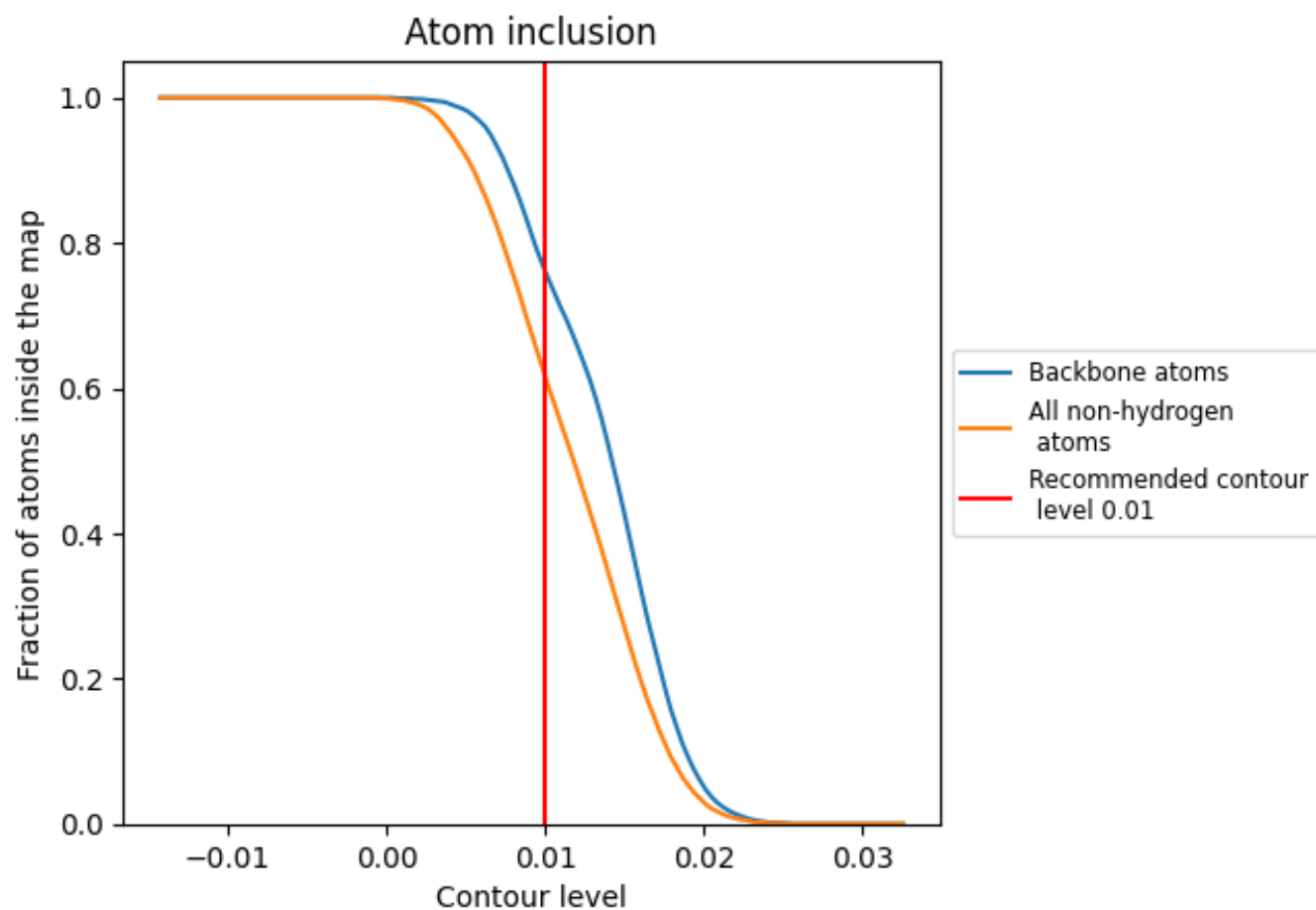
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.01).

9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 62% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6160	 0.5780
A	 0.6320	 0.5810
B	 0.6330	 0.5820
C	 0.6320	 0.5800
D	 0.6060	 0.5650
E	 0.6010	 0.5640
F	 0.6000	 0.5640
G	 0.4810	 0.4890
H	 0.4600	 0.4690
I	 0.4650	 0.4530
J	 0.4880	 0.5400
K	 0.5410	 0.5410
L	 0.4790	 0.5400
M	 0.5370	 0.5530
N	 0.4850	 0.5360
O	 0.5250	 0.5390
P	 0.6270	 0.5980
Q	 0.6190	 0.5930
R	 0.6240	 0.5940
S	 0.6230	 0.5960
T	 0.6270	 0.5950
U	 0.6240	 0.5950
V	 0.6130	 0.5750
W	 0.5960	 0.5670
X	 0.6240	 0.5670
Y	 0.5970	 0.5680
Z	 0.6030	 0.5640
a	 0.5930	 0.5640
b	 0.6290	 0.5820
c	 0.6900	 0.5900
d	 0.6080	 0.5830
e	 0.6090	 0.5790
f	 0.6760	 0.5870
g	 0.6130	 0.5760
h	 0.6320	 0.5820



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
i	 0.6940	 0.5910
j	 0.6100	 0.5830
k	 0.6040	 0.5730
l	 0.6860	 0.5910
m	 0.6050	 0.5780
n	 0.6370	 0.5860
o	 0.6850	 0.5870
p	 0.6070	 0.5820
q	 0.6050	 0.5700
r	 0.6810	 0.5920
s	 0.6070	 0.5760