



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:02 AM GMT

PDB ID : 2F16
Title : Crystal structure of the yeast 20S proteasome in complex with bortezomib
Authors : Groll, M.
Deposited on : 2005-11-14
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

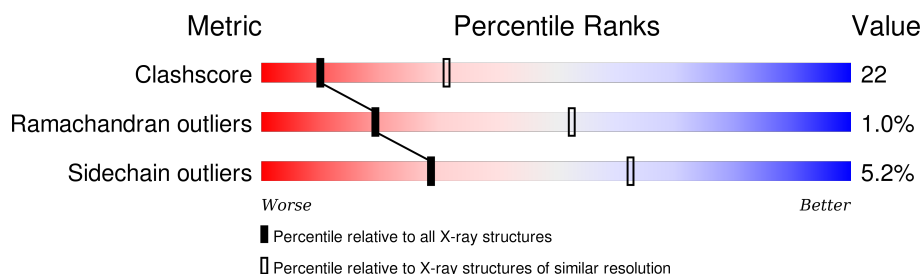
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)






















The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	250	
1	O	250	
2	B	244	
2	P	244	
3	C	241	
3	Q	241	
4	D	242	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	R	242	
5	E	233	
5	S	233	
6	F	244	
6	T	244	
7	G	243	
7	U	243	
8	H	222	
8	V	222	
9	I	204	
9	W	204	
10	J	198	
10	X	198	
11	K	212	
11	Y	212	
12	L	222	
12	Z	222	
13	1	233	
13	M	233	
14	2	196	
14	N	196	

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 50753 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Proteasome component Y7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	250	Total	C	N	O	S	0	0	0
			1915	1219	315	377	4			
1	O	250	Total	C	N	O	S	0	0	0
			1915	1219	315	377	4			

- Molecule 2 is a protein called Proteasome component Y13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	244	Total	C	N	O	S	0	0	0
			1905	1201	321	380	3			
2	P	244	Total	C	N	O	S	0	0	0
			1905	1201	321	380	3			

- Molecule 3 is a protein called Proteasome component PRE6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	241	Total	C	N	O	S	0	0	0
			1891	1181	331	375	4			
3	Q	241	Total	C	N	O	S	0	0	0
			1891	1181	331	375	4			

- Molecule 4 is a protein called Proteasome component PUP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	242	Total	C	N	O	S	0	0	0
			1862	1162	314	379	7			
4	R	242	Total	C	N	O	S	0	0	0
			1862	1162	314	379	7			

- Molecule 5 is a protein called Proteasome component PRE5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	233	Total	C	N	O	S	0	0	0
			1795	1129	312	350	4			
5	S	233	Total	C	N	O	S	0	0	0
			1795	1129	312	350	4			

- Molecule 6 is a protein called Proteasome component C1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	244	Total	C	N	O	S	0	0	0
			1897	1205	330	358	4			
6	T	244	Total	C	N	O	S	0	0	0
			1897	1205	330	358	4			

- Molecule 7 is a protein called Proteasome component C7-alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	243	Total	C	N	O	S	0	0	0
			1921	1221	322	370	8			
7	U	243	Total	C	N	O	S	0	0	0
			1921	1221	322	370	8			

- Molecule 8 is a protein called Proteasome component PUP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	222	Total	C	N	O	S	0	0	0
			1685	1061	293	324	7			
8	V	222	Total	C	N	O	S	0	0	0
			1685	1061	293	324	7			

- Molecule 9 is a protein called Proteasome component PUP3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	204	Total	C	N	O	S	0	0	0
			1581	1010	258	305	8			
9	W	204	Total	C	N	O	S	0	0	0
			1581	1010	258	305	8			

- Molecule 10 is a protein called Proteasome component C11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	198	Total	C	N	O	S	0	0	0
			1585	1005	269	305	6			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	X	198	Total	C	N	O	S	0	0	0
			1585	1005	269	305	6			

- Molecule 11 is a protein called Proteasome component PRE2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	212	Total	C	N	O	S	0	0	0
			1644	1045	280	312	7			
11	Y	212	Total	C	N	O	S	0	0	0
			1644	1045	280	312	7			

- Molecule 12 is a protein called Proteasome component C5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	222	Total	C	N	O	S	0	0	0
			1757	1115	303	335	4			
12	Z	222	Total	C	N	O	S	0	0	0
			1757	1115	303	335	4			

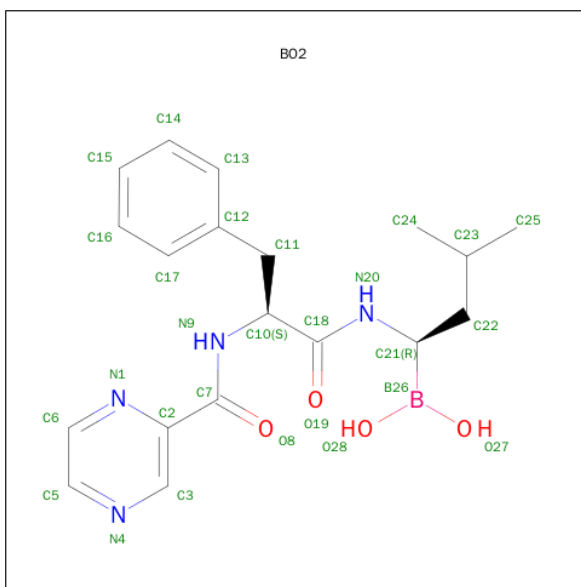
- Molecule 13 is a protein called Proteasome component PRE4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			
13	1	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			

- Molecule 14 is a protein called Proteasome component PRE3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	196	Total	C	N	O	S	0	0	0
			1512	955	250	300	7			
14	2	196	Total	C	N	O	S	0	0	0
			1512	955	250	300	7			

- Molecule 15 is N-[(1R)-1-(DIHYDROXYBORYL)-3-METHYLBUTYL]-N-(PYRAZIN-2-YLCARBONYL)-L-PHENYLALANINAMIDE (three-letter code: BO2) (formula: C₁₉H₂₅BN₄O₄).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	H	1	Total	B	C	N	O	0	0
			28	1	19	4	4		
15	K	1	Total	B	C	N	O	0	0
			28	1	19	4	4		
15	N	1	Total	B	C	N	O	0	0
			28	1	19	4	4		
15	V	1	Total	B	C	N	O	0	0
			28	1	19	4	4		
15	Y	1	Total	B	C	N	O	0	0
			28	1	19	4	4		
15	2	1	Total	B	C	N	O	0	0
			28	1	19	4	4		

- Molecule 16 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	46	Total	O	0	0
			46	46		
16	B	31	Total	O	0	0
			31	31		
16	C	33	Total	O	0	0
			33	33		
16	D	26	Total	O	0	0
			26	26		
16	E	14	Total	O	0	0
			14	14		
16	F	36	Total	O	0	0
			36	36		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	G	48	Total O 48 48	0	0
16	H	42	Total O 42 42	0	0
16	I	50	Total O 50 50	0	0
16	J	45	Total O 45 45	0	0
16	K	33	Total O 33 33	0	0
16	L	42	Total O 42 42	0	0
16	M	52	Total O 52 52	0	0
16	N	43	Total O 43 43	0	0
16	O	23	Total O 23 23	0	0
16	P	21	Total O 21 21	0	0
16	Q	21	Total O 21 21	0	0
16	R	20	Total O 20 20	0	0
16	S	16	Total O 16 16	0	0
16	T	32	Total O 32 32	0	0
16	U	56	Total O 56 56	0	0
16	V	34	Total O 34 34	0	0
16	W	46	Total O 46 46	0	0
16	X	39	Total O 39 39	0	0
16	Y	32	Total O 32 32	0	0
16	Z	42	Total O 42 42	0	0
16	1	63	Total O 63 63	0	0

Continued on next page...

Continued from previous page...

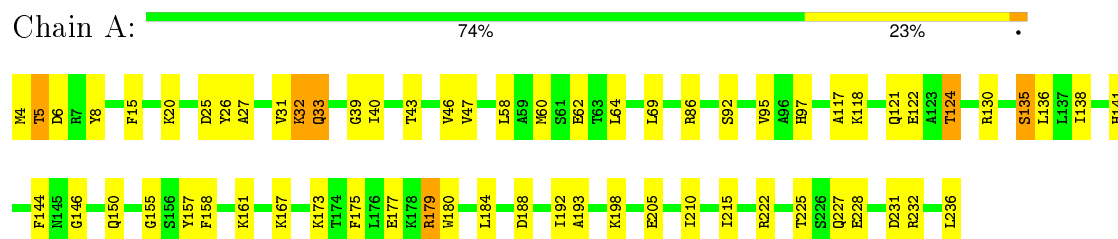
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	2	51	Total	O	0	0
			51	51		

3 Residue-property plots [i](#)

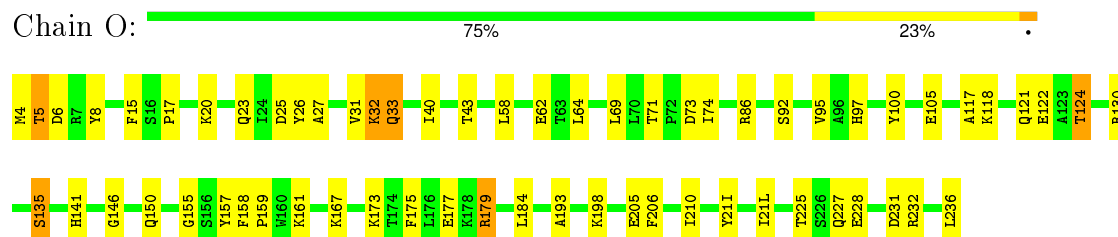
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

Note EDS was not executed.

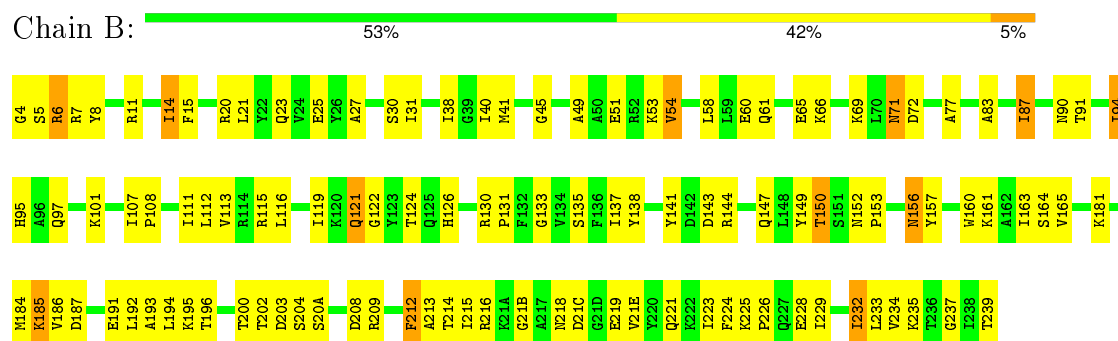
• Molecule 1: Proteasome component Y7



• Molecule 1: Proteasome component Y7

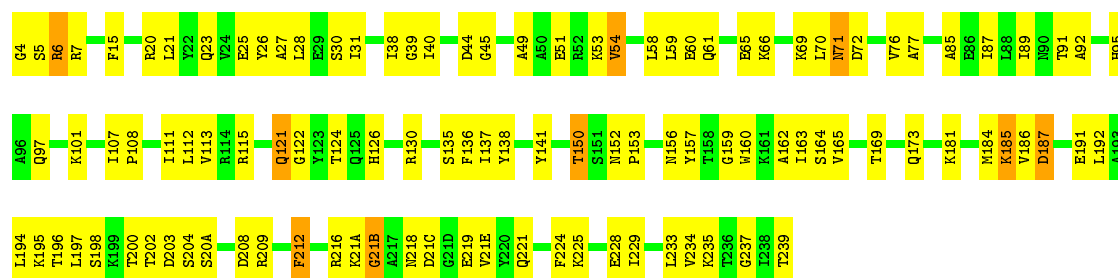


• Molecule 2: Proteasome component Y13



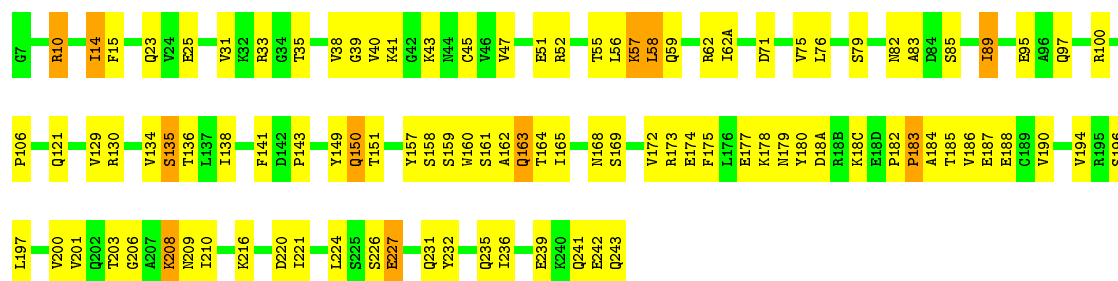
• Molecule 2: Proteasome component Y13





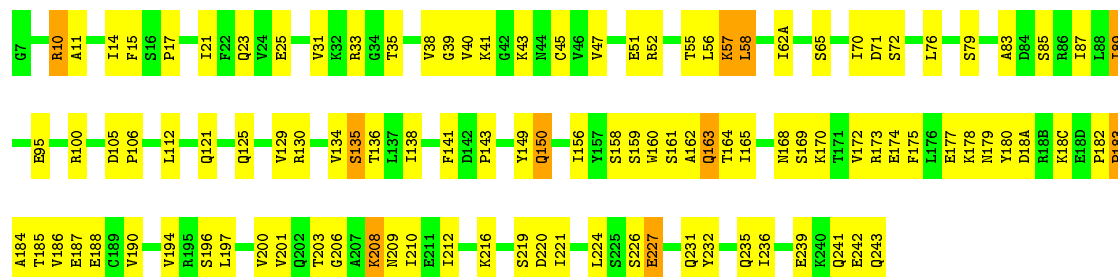
• Molecule 3: Proteasome component PRE6

Chain C: 58% 37% 5%



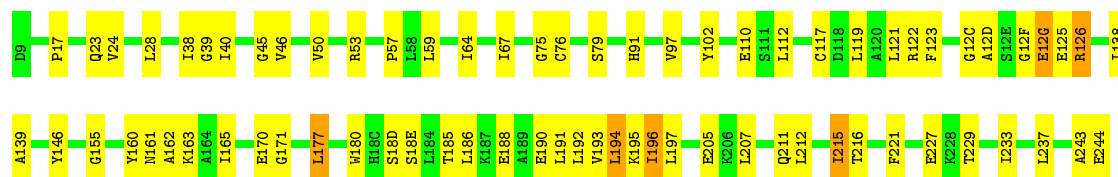
• Molecule 3: Proteasome component PRE6

Chain Q: 55% 41% 4%



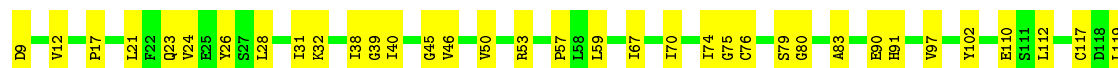
• Molecule 4: Proteasome component PUP2

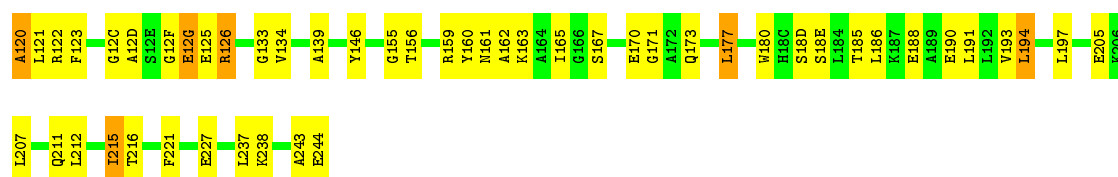
Chain D: 70% 28% 2%



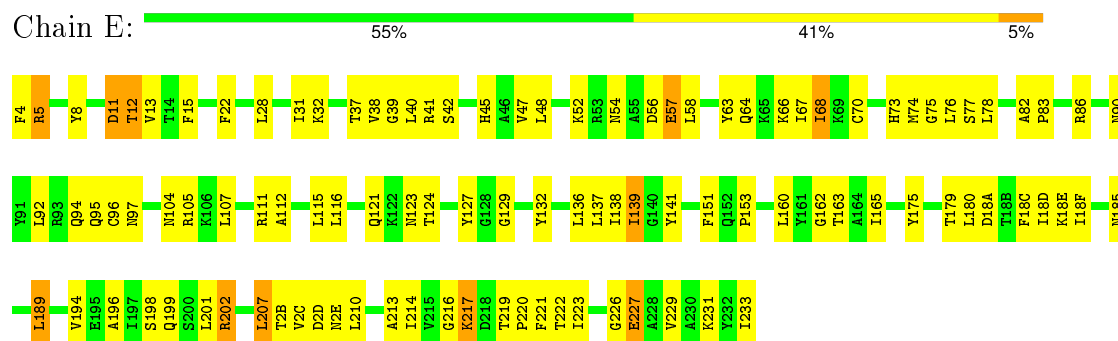
• Molecule 4: Proteasome component PUP2

Chain R: 65% 33% 2%

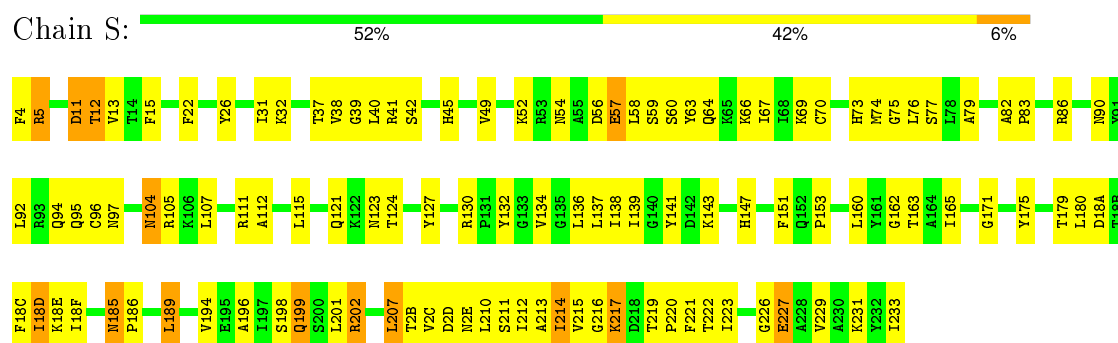




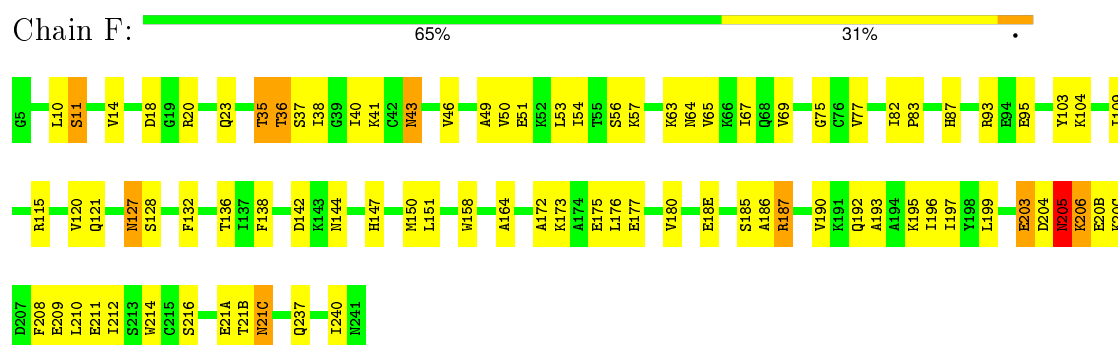
• Molecule 5: Proteasome component PRE5



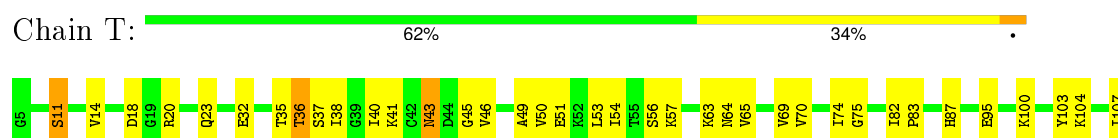
• Molecule 5: Proteasome component PRE5



• Molecule 6: Proteasome component C1

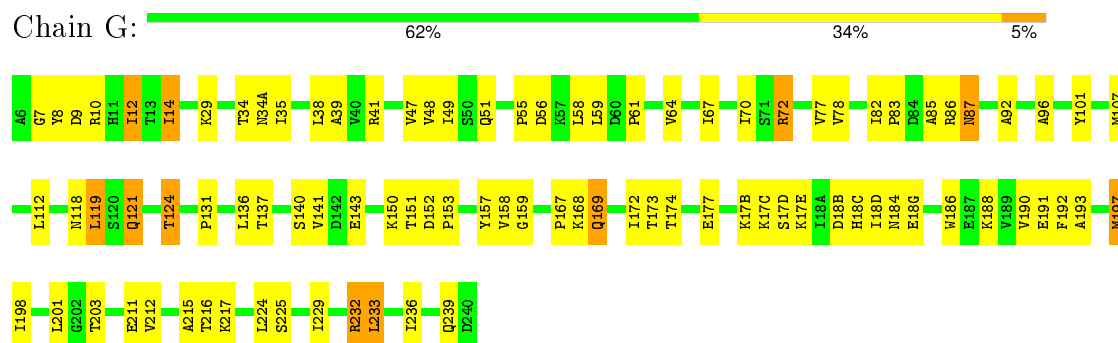


• Molecule 6: Proteasome component C1

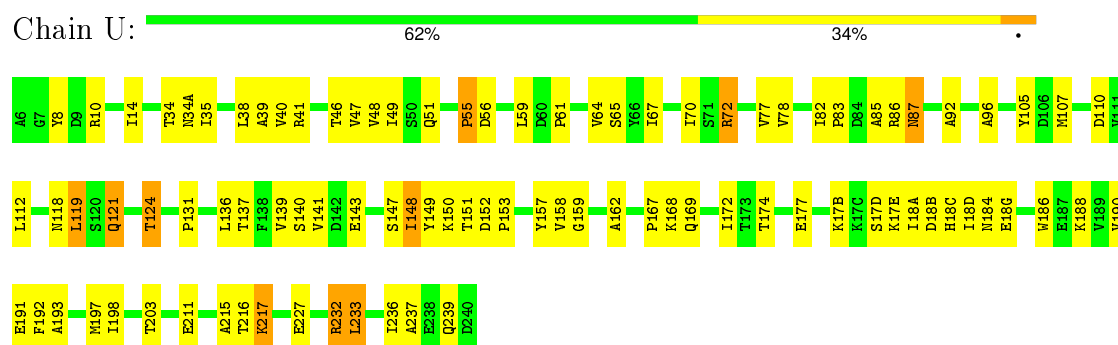




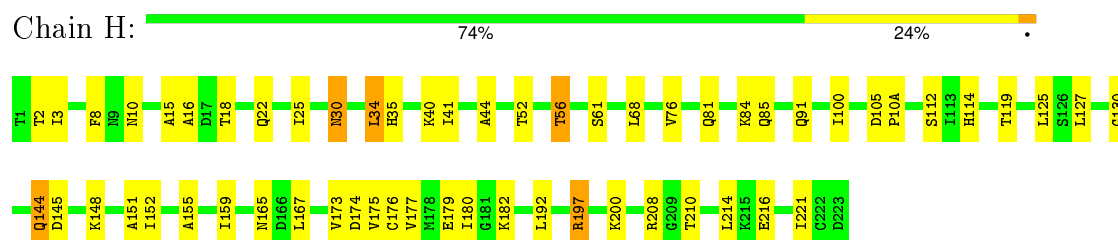
• Molecule 7: Proteasome component C7-alpha



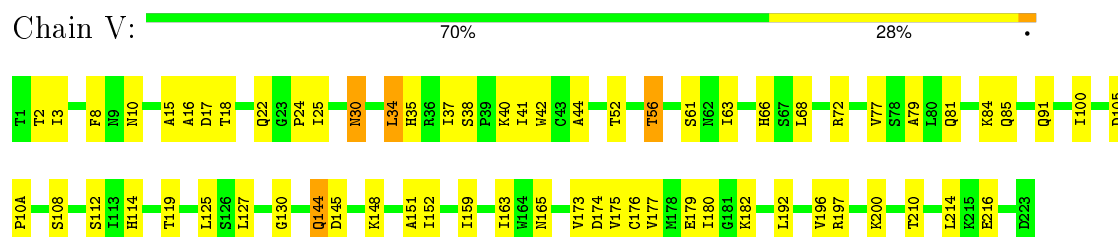
• Molecule 7: Proteasome component C7-alpha



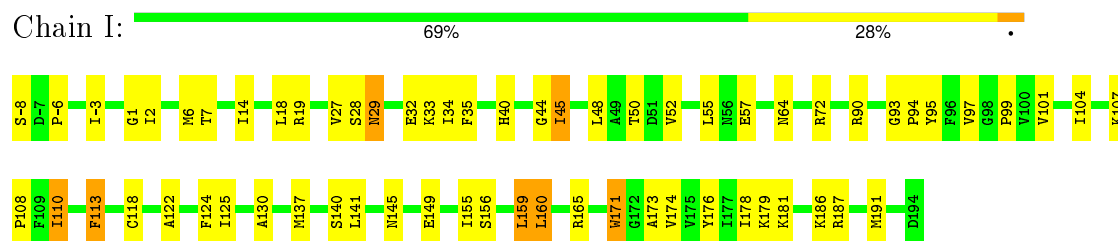
• Molecule 8: Proteasome component PUP1



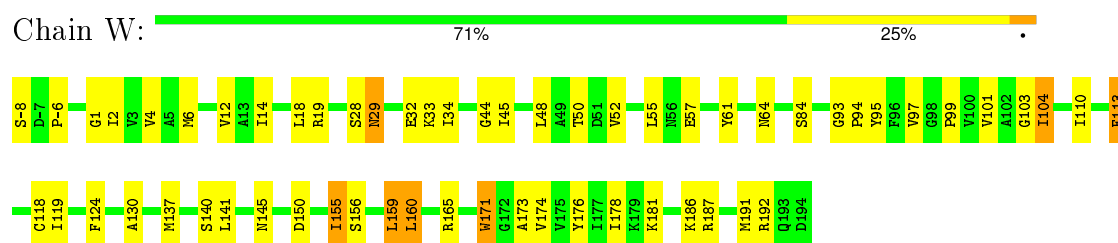
• Molecule 8: Proteasome component PUP1



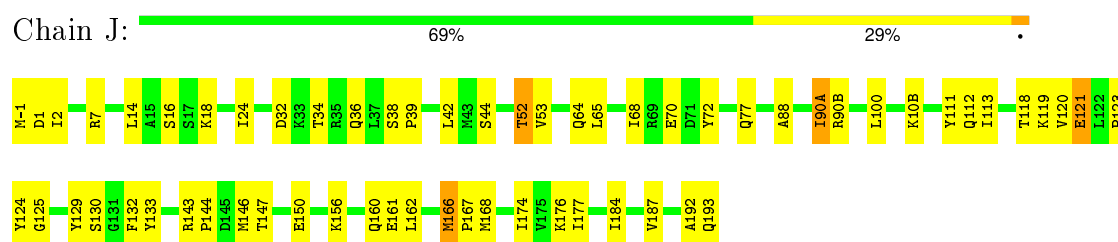
- Molecule 9: Proteasome component PUP3



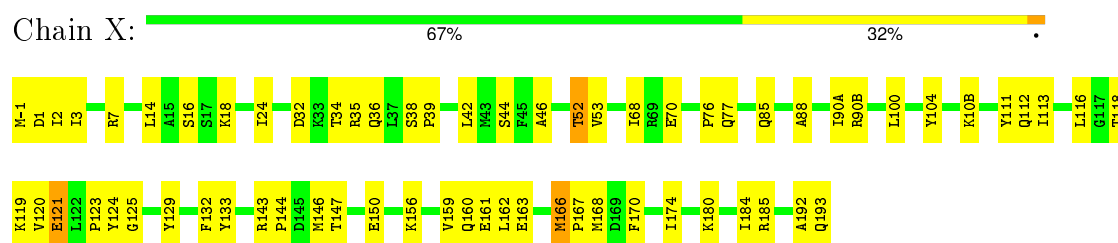
- Molecule 9: Proteasome component PUP3



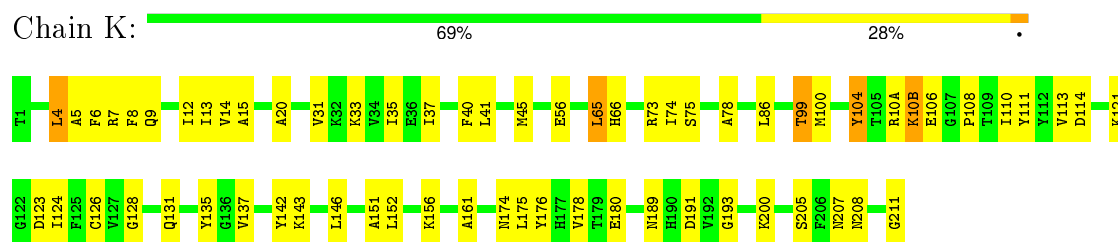
- Molecule 10: Proteasome component C11



- Molecule 10: Proteasome component C11

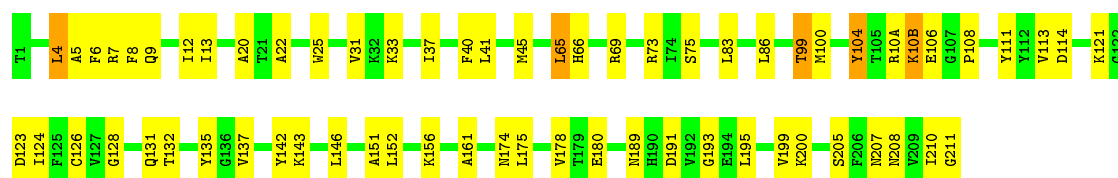


- Molecule 11: Proteasome component PRE2



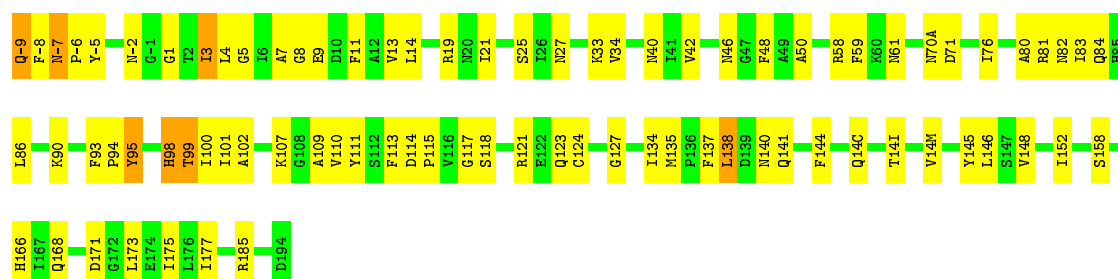
- Molecule 11: Proteasome component PRE2

Chain Y:  69% 28% .



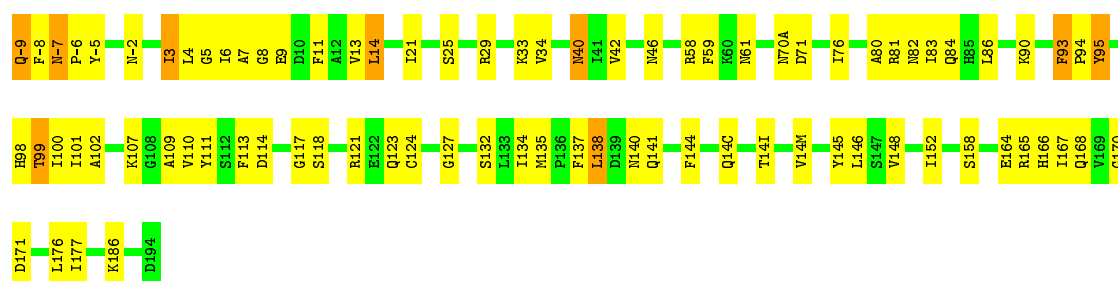
• Molecule 12: Proteasome component C5

Chain L:  63% 34% .



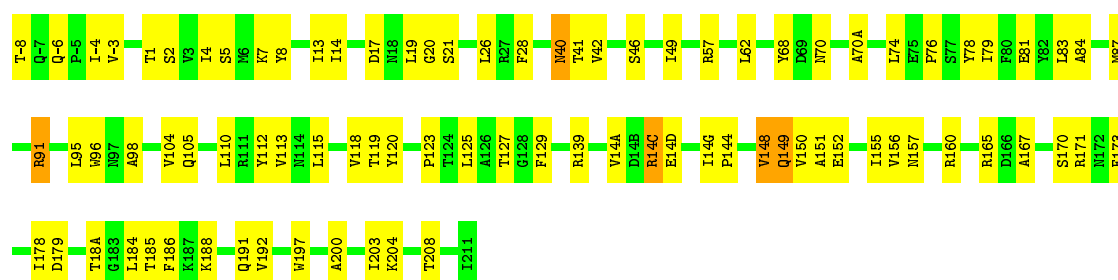
• Molecule 12: Proteasome component C5

Chain Z:  63% 33% .



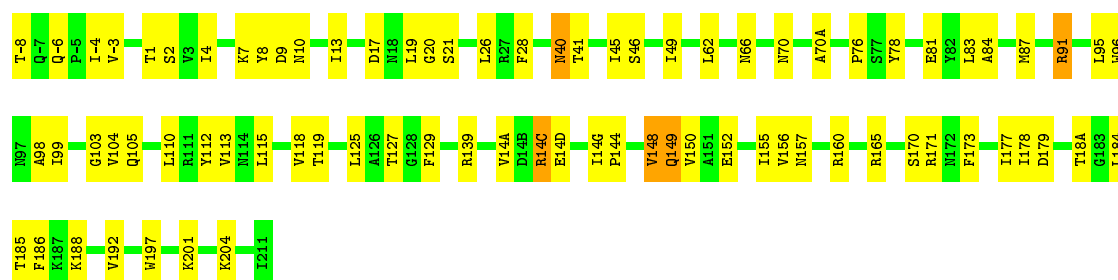
• Molecule 13: Proteasome component PRE4

Chain M:  63% 35% .



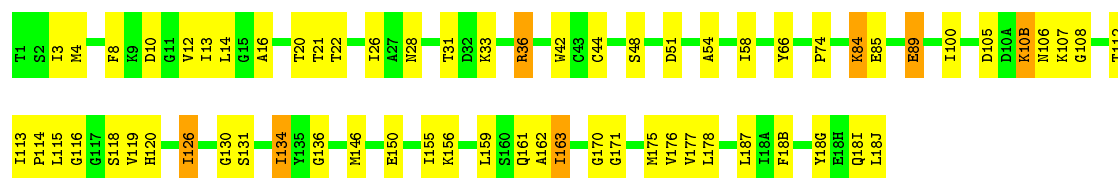
• Molecule 13: Proteasome component PRE4

Chain 1:  66% 32% .



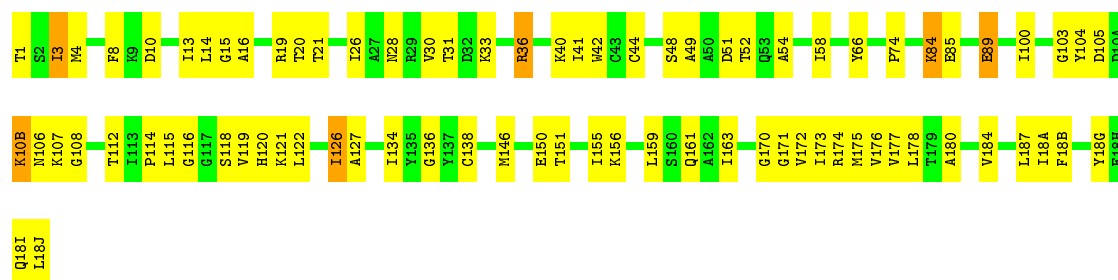
• Molecule 14: Proteasome component PRE3

Chain N: 67% 30% .



• Molecule 14: Proteasome component PRE3

Chain 2: 59% 38% .



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	136.18Å 300.72Å 144.66Å 90.00° 113.28° 90.00°	Depositor
Resolution (Å)	15.00 – 2.80	Depositor
% Data completeness (in resolution range)	96.4 (15.00-2.80)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.231 , 0.264	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	50753	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BO2

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	0.37	0/1952	0.62	0/2642
1	O	0.37	0/1952	0.62	0/2642
2	B	0.36	0/1935	0.64	0/2618
2	P	0.37	0/1935	0.63	0/2618
3	C	0.36	0/1920	0.62	0/2598
3	Q	0.35	0/1920	0.62	0/2598
4	D	0.35	0/1887	0.63	0/2541
4	R	0.36	0/1887	0.62	0/2541
5	E	0.37	0/1823	0.61	0/2463
5	S	0.38	0/1823	0.61	0/2463
6	F	0.37	0/1937	0.62	0/2614
6	T	0.37	0/1937	0.63	0/2614
7	G	0.40	0/1959	0.64	0/2652
7	U	0.39	0/1959	0.64	0/2652
8	H	0.38	0/1716	0.67	0/2326
8	V	0.36	0/1716	0.67	0/2326
9	I	0.39	0/1611	0.67	0/2174
9	W	0.40	0/1611	0.68	0/2174
10	J	0.38	0/1613	0.65	0/2173
10	X	0.37	0/1613	0.65	0/2173
11	K	0.41	0/1681	0.65	0/2274
11	Y	0.39	0/1681	0.65	0/2274
12	L	0.39	0/1795	0.67	1/2420 (0.0%)
12	Z	0.38	0/1795	0.67	1/2420 (0.0%)
13	1	0.41	0/1855	0.69	1/2514 (0.0%)
13	M	0.39	0/1855	0.67	1/2514 (0.0%)
14	2	0.41	0/1541	0.65	0/2087
14	N	0.41	0/1541	0.65	0/2087
All	All	0.38	0/50450	0.64	4/68192 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
13	1	95	LEU	N-CA-C	-5.76	95.45	111.00
13	M	95	LEU	N-CA-C	-5.66	95.72	111.00
12	L	95	TYR	N-CA-C	-5.23	96.89	111.00
12	Z	95	TYR	N-CA-C	-5.23	96.89	111.00

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	1915	0	1926	56	0
1	O	1915	0	1926	58	0
2	B	1905	0	1901	139	0
2	P	1905	0	1901	118	0
3	C	1891	0	1900	117	0
3	Q	1891	0	1900	122	0
4	D	1862	0	1836	71	0
4	R	1862	0	1836	84	0
5	E	1795	0	1797	120	0
5	S	1795	0	1797	128	0
6	F	1897	0	1886	88	0
6	T	1897	0	1886	87	0
7	G	1921	0	1910	90	0
7	U	1921	0	1910	104	0
8	H	1685	0	1687	59	0
8	V	1685	0	1687	62	0
9	I	1581	0	1574	76	0
9	W	1581	0	1574	65	0
10	J	1585	0	1590	77	0
10	X	1585	0	1590	76	0
11	K	1644	0	1594	74	0
11	Y	1644	0	1594	69	0
12	L	1757	0	1711	76	0
12	Z	1757	0	1711	80	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	1	1824	0	1832	83	0
13	M	1824	0	1832	79	0
14	2	1512	0	1480	92	0
14	N	1512	0	1480	71	0
15	2	28	0	25	8	0
15	H	28	0	25	2	0
15	K	28	0	25	0	0
15	N	28	0	25	5	0
15	V	28	0	25	2	0
15	Y	28	0	25	1	0
16	1	63	0	0	4	0
16	2	51	0	0	6	0
16	A	46	0	0	1	0
16	B	31	0	0	5	0
16	C	33	0	0	1	0
16	D	26	0	0	1	0
16	E	14	0	0	0	0
16	F	36	0	0	2	0
16	G	48	0	0	3	0
16	H	42	0	0	1	0
16	I	50	0	0	0	0
16	J	45	0	0	5	0
16	K	33	0	0	3	0
16	L	42	0	0	4	0
16	M	52	0	0	3	0
16	N	43	0	0	1	0
16	O	23	0	0	0	0
16	P	21	0	0	1	0
16	Q	21	0	0	5	0
16	R	20	0	0	2	0
16	S	16	0	0	3	0
16	T	32	0	0	2	0
16	U	56	0	0	5	0
16	V	34	0	0	2	0
16	W	46	0	0	2	0
16	X	39	0	0	4	0
16	Y	32	0	0	7	0
16	Z	42	0	0	3	0
All	All	50753	0	49398	2178	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 22.

All (2178) 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)
14:N:13:ILE:CD1	14:N:177:VAL:HG13	1.58	1.31
3:Q:197:LEU:HD13	3:Q:210:ILE:HD12	1.22	1.20
5:S:49:VAL:HG13	5:S:212:ILE:CD1	1.72	1.19
3:C:197:LEU:HD13	3:C:210:ILE:HD12	1.20	1.16
1:A:177:GLU:HG2	2:B:58:LEU:HD21	1.20	1.16
3:C:201:VAL:HG21	3:C:210:ILE:HD11	1.17	1.14
3:Q:201:VAL:HG21	3:Q:210:ILE:HD11	1.18	1.13
9:W:6:MET:HE3	9:W:155:ILE:HD13	1.18	1.13
4:R:162:ALA:HB3	5:S:58:LEU:HD23	1.30	1.12
11:Y:10(B):LYS:H	11:Y:10(B):LYS:HD2	1.06	1.11
8:H:15:ALA:CB	8:H:159:ILE:HD11	1.80	1.11
8:H:15:ALA:HB3	8:H:159:ILE:HD11	1.20	1.11
11:K:10(B):LYS:H	11:K:10(B):LYS:HD2	1.04	1.10
14:N:13:ILE:HD11	14:N:177:VAL:HG13	1.23	1.10
2:P:40:ILE:HD12	2:P:162:ALA:HB1	1.30	1.09
7:G:9:ASP:HA	7:G:14:ILE:HD11	1.32	1.08
14:N:136:GLY:HA2	14:2:161:GLN:HE21	1.17	1.08
2:B:108:PRO:HB2	2:B:111:ILE:HD13	1.31	1.07
14:N:161:GLN:HE21	14:2:136:GLY:HA2	1.14	1.06
2:B:124:THR:HG22	3:C:130:ARG:HH21	1.20	1.04
14:N:13:ILE:HD12	14:N:177:VAL:HG13	1.35	1.04
13:1:13:ILE:HD12	13:1:177:ILE:HG12	1.37	1.03
2:B:202:THR:HG22	2:B:204:SER:H	1.22	1.03
8:H:41:ILE:HD12	8:H:76:VAL:HG22	1.39	1.03
4:R:31:ILE:HD11	4:R:134:VAL:HA	1.39	1.02
13:1:45:ILE:HG12	13:1:99:ILE:HD12	1.40	1.01
2:P:202:THR:HG22	2:P:204:SER:H	1.22	1.01
6:F:38:ILE:HD12	6:F:40:ILE:HD11	1.44	0.99
7:G:96:ALA:HA	7:G:107:MET:HE2	1.44	0.99
8:V:38:SER:OG	8:V:41:ILE:HD13	1.63	0.98
1:A:15:PHE:H	2:B:23:GLN:HE22	1.08	0.98
5:E:68:ILE:HD11	5:E:78:LEU:HD23	1.43	0.98
13:M:200:ALA:HA	13:M:203:ILE:HD12	1.42	0.97
13:1:13:ILE:CD1	13:1:177:ILE:HG23	1.95	0.96
7:U:147:SER:C	7:U:148:ILE:HD12	1.85	0.96
3:C:163:GLN:HE21	3:C:164:THR:H	1.07	0.96
1:A:177:GLU:HG2	2:B:58:LEU:CD2	1.95	0.95
5:S:214:ILE:HD12	5:S:219:THR:HG21	1.49	0.95
12:L:3:ILE:HD12	12:L:46:ASN:HB2	1.48	0.95
4:D:229:THR:O	4:D:233:ILE:HD13	1.67	0.95

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:201:VAL:CG2	3:Q:210:ILE:HD11	1.98	0.94
2:B:15:PHE:H	3:C:23:GLN:HE22	1.14	0.94
3:C:163:GLN:NE2	3:C:164:THR:H	1.65	0.94
5:S:49:VAL:HG13	5:S:212:ILE:HD12	1.49	0.94
5:E:213:ALA:HB2	5:E:223:ILE:HD12	1.49	0.94
4:R:31:ILE:HD11	4:R:134:VAL:CA	1.98	0.94
12:Z:3:ILE:HD12	12:Z:46:ASN:HB2	1.50	0.94
3:Q:163:GLN:HE21	3:Q:164:THR:H	1.11	0.93
1:O:15:PHE:H	2:P:23:GLN:HE22	1.14	0.93
2:B:194:LEU:HD11	2:B:232:ILE:CD1	1.99	0.93
6:T:49:ALA:CB	6:T:197:ILE:HD11	1.99	0.93
13:M:-4:ILE:HD12	14:N:116:GLY:N	1.84	0.92
2:P:40:ILE:HD12	2:P:162:ALA:CB	1.98	0.92
3:C:201:VAL:CG2	3:C:210:ILE:HD11	1.98	0.92
3:Q:15:PHE:H	4:R:23:GLN:HE22	1.09	0.92
14:N:13:ILE:CD1	14:N:177:VAL:CG1	2.48	0.92
4:R:31:ILE:CD1	4:R:134:VAL:HA	1.99	0.92
6:T:49:ALA:HB1	6:T:197:ILE:HD11	1.52	0.92
7:U:96:ALA:HA	7:U:107:MET:HE2	1.52	0.92
11:Y:10(B):LYS:CD	11:Y:10(B):LYS:H	1.82	0.92
7:U:40:VAL:HB	7:U:18(D):ILE:HD11	1.49	0.91
2:B:194:LEU:HD11	2:B:232:ILE:HD12	1.53	0.91
3:Q:163:GLN:NE2	3:Q:164:THR:H	1.69	0.91
7:G:18(G):GLU:HG2	7:G:188:LYS:HB2	1.53	0.90
7:U:18(A):ILE:HD13	7:U:18(C):HIS:H	1.33	0.90
10:J:177:ILE:HD11	10:J:187:VAL:CG2	2.01	0.90
14:N:134:ILE:HD12	14:N:162:ALA:HB2	1.52	0.90
5:S:49:VAL:HG13	5:S:212:ILE:HD11	1.51	0.90
2:B:11:ARG:O	2:B:14:ILE:HD12	1.70	0.90
7:U:18(G):GLU:HG2	7:U:188:LYS:HB2	1.53	0.90
2:P:61:GLN:OE1	2:P:208:ASP:HA	1.71	0.90
2:P:40:ILE:CD1	2:P:162:ALA:HB1	2.02	0.90
13:M:157:ASN:HD22	13:M:160:ARG:HH11	0.97	0.90
2:P:71:ASN:ND2	2:P:72:ASP:H	1.68	0.90
11:K:10(B):LYS:H	11:K:10(B):LYS:CD	1.81	0.90
2:B:83:ALA:O	2:B:87:ILE:HD13	1.72	0.90
11:K:7:ARG:HG3	11:K:12:ILE:CD1	2.03	0.89
14:N:131:SER:HA	14:N:134:ILE:HD11	1.53	0.89
2:B:61:GLN:OE1	2:B:208:ASP:HA	1.72	0.89
2:B:71:ASN:ND2	2:B:72:ASP:H	1.70	0.89
13:1:157:ASN:HD22	13:1:160:ARG:HH11	0.95	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:165:ASN:HD22	13:1:139:ARG:HH11	1.20	0.89
5:S:213:ALA:HB2	5:S:223:ILE:HD12	1.52	0.88
2:B:71:ASN:HD22	2:B:72:ASP:H	1.19	0.88
5:E:48:LEU:HD11	5:E:139:ILE:HD12	1.55	0.88
2:P:71:ASN:HD22	2:P:72:ASP:H	1.18	0.88
13:M:139:ARG:HH11	8:V:165:ASN:HD22	1.17	0.88
11:K:10(B):LYS:N	11:K:10(B):LYS:HD2	1.89	0.87
1:O:130:ARG:HH21	7:U:124:THR:CG2	1.88	0.87
13:1:-4:ILE:HD12	14:2:116:GLY:N	1.88	0.87
14:2:21:THR:CG2	14:2:26:ILE:HD13	2.04	0.86
5:S:198:SER:HA	5:S:201:LEU:HG	1.57	0.86
3:C:201:VAL:HG21	3:C:210:ILE:CD1	2.03	0.86
5:E:139:ILE:HD11	5:E:221:PHE:HE2	1.40	0.85
3:C:15:PHE:H	4:D:23:GLN:HE22	1.25	0.85
5:S:207:LEU:HD23	5:S:207:LEU:H	1.40	0.85
10:X:2:ILE:C	10:X:3:ILE:HD12	1.96	0.85
3:C:163:GLN:HE21	3:C:164:THR:N	1.74	0.85
6:F:193:ALA:O	6:F:197:ILE:CD1	2.25	0.85
14:2:21:THR:HG22	14:2:26:ILE:HD13	1.58	0.84
6:T:95:GLU:HG2	6:T:115:ARG:HB3	1.59	0.84
3:Q:201:VAL:HG21	3:Q:210:ILE:CD1	2.04	0.84
1:O:124:THR:HG22	2:P:130:ARG:HH21	1.43	0.84
3:Q:185:THR:HG22	3:Q:187:GLU:H	1.42	0.84
4:R:97:VAL:HG21	11:Y:65:LEU:HD13	1.58	0.84
13:1:13:ILE:HD13	13:1:177:ILE:HG23	1.59	0.84
9:I:110:ILE:HD13	9:I:110:ILE:H	1.43	0.84
2:B:38:ILE:HD13	2:B:164:SER:HB3	1.58	0.84
3:Q:185:THR:HB	3:Q:188:GLU:HG2	1.59	0.83
7:U:67:ILE:HD12	7:U:211:GLU:HG2	1.60	0.83
2:B:90:ASN:O	2:B:94:ILE:HD13	1.78	0.83
5:E:207:LEU:HD23	5:E:207:LEU:H	1.42	0.83
4:D:229:THR:HG22	4:D:233:ILE:HD11	1.60	0.83
1:A:20:LYS:HE3	1:A:25:ASP:OD1	1.79	0.83
6:T:54:ILE:HD11	6:T:209:GLU:HB2	1.59	0.83
5:E:198:SER:HA	5:E:201:LEU:HG	1.58	0.83
5:E:28:LEU:HA	5:E:31:ILE:HD13	1.58	0.82
3:C:185:THR:HG22	3:C:187:GLU:H	1.43	0.82
5:E:15:PHE:H	6:F:23:GLN:HE22	1.27	0.82
6:F:54:ILE:HD11	6:F:209:GLU:HB2	1.59	0.82
14:N:13:ILE:HD12	14:N:177:VAL:HA	1.59	0.82
11:Y:143:LYS:HB2	11:Y:146:LEU:CD1	2.10	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:32:ASP:OD2	10:X:34:THR:HG22	1.79	0.82
14:N:13:ILE:HD11	14:N:177:VAL:CG1	2.06	0.82
3:C:185:THR:HB	3:C:188:GLU:HG2	1.59	0.82
9:I:44:GLY:C	9:I:45:ILE:HD12	1.99	0.82
16:Q:245:HOH:O	10:X:68:ILE:HD13	1.78	0.82
13:1:3:VAL:HG12	13:1:49:ILE:HD12	1.61	0.82
4:D:97:VAL:HG21	11:K:65:LEU:HD13	1.62	0.82
9:W:6:MET:CE	9:W:155:ILE:HD13	2.07	0.81
12:L:3:ILE:HD12	12:L:46:ASN:CB	2.10	0.81
11:K:7:ARG:HG3	11:K:12:ILE:HD11	1.61	0.81
2:B:116:LEU:HD23	2:B:119:ILE:HD12	1.61	0.81
2:B:124:THR:CG2	3:C:130:ARG:HH21	1.91	0.81
1:O:20:LYS:HE3	1:O:25:ASP:OD1	1.80	0.81
3:Q:65:SER:HB2	16:Q:247:HOH:O	1.78	0.81
5:E:75:GLY:O	5:E:139:ILE:HD13	1.80	0.81
8:H:15:ALA:CB	8:H:159:ILE:CD1	2.58	0.81
3:Q:163:GLN:HE21	3:Q:164:THR:N	1.77	0.81
11:K:143:LYS:HB2	11:K:146:LEU:CD1	2.10	0.81
13:M:-4:ILE:HD13	14:N:115:LEU:HB3	1.62	0.81
14:N:161:GLN:NE2	14:2:136:GLY:HA2	1.94	0.81
8:H:155:ALA:O	8:H:159:ILE:HD12	1.80	0.81
9:I:35:PHE:CE1	9:I:45:ILE:HD13	2.16	0.81
9:W:6:MET:HE3	9:W:155:ILE:CD1	2.09	0.80
13:1:45:ILE:HG23	13:1:99:ILE:CD1	2.11	0.80
7:G:67:ILE:HD12	7:G:211:GLU:HG2	1.61	0.80
13:1:13:ILE:CG2	13:1:155:ILE:HD12	2.12	0.80
1:O:71:THR:OG1	1:O:74:ILE:HD13	1.80	0.80
13:M:157:ASN:HD22	13:M:160:ARG:NH1	1.78	0.79
10:J:32:ASP:OD2	10:J:34:THR:HG22	1.82	0.79
6:F:95:GLU:HG2	6:F:115:ARG:HB3	1.61	0.79
2:B:97:GLN:HE22	9:I:64:ASN:HD22	1.30	0.79
13:M:14(C):ARG:HH11	13:M:14(C):ARG:HG3	1.46	0.79
12:Z:3:ILE:HD12	12:Z:46:ASN:CB	2.13	0.79
6:T:197:ILE:HD13	6:T:210:LEU:HD11	1.65	0.79
11:K:35:ILE:HD12	11:K:56:GLU:HB2	1.63	0.79
14:N:13:ILE:HD12	14:N:177:VAL:CG1	2.10	0.79
7:G:198:ILE:HG23	7:G:203:THR:O	1.82	0.79
8:H:40:LYS:O	8:H:41:ILE:HD13	1.82	0.79
6:F:193:ALA:O	6:F:197:ILE:HD12	1.83	0.79
2:P:124:THR:HG22	3:Q:130:ARG:HH21	1.47	0.78
2:P:71:ASN:HD22	2:P:72:ASP:N	1.81	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1:157:ASN:HD22	13:1:160:ARG:NH1	1.77	0.78
11:Y:99:THR:HG22	11:Y:113:VAL:HB	1.64	0.78
5:E:139:ILE:H	5:E:139:ILE:HD13	1.47	0.78
11:K:99:THR:HG22	11:K:113:VAL:HB	1.64	0.78
14:N:12:VAL:O	14:N:13:ILE:HD13	1.82	0.78
2:B:215:ILE:HD12	2:B:221:GLN:HG2	1.65	0.78
11:Y:33:LYS:HA	11:Y:45:MET:HE2	1.63	0.78
13:1:14(C):ARG:HG3	13:1:14(C):ARG:HH11	1.47	0.78
11:Y:10(B):LYS:N	11:Y:10(B):LYS:HD2	1.90	0.78
14:N:136:GLY:HA2	14:2:161:GLN:NE2	1.95	0.78
13:M:157:ASN:ND2	13:M:160:ARG:HH11	1.80	0.78
13:1:40:ASN:HD22	13:1:40:ASN:H	1.29	0.77
5:S:214:ILE:HD13	5:S:215:VAL:N	1.99	0.77
2:P:28:LEU:HA	2:P:31:ILE:HD12	1.66	0.77
9:W:45:ILE:HB	9:W:52:VAL:HG13	1.65	0.77
5:S:15:PHE:H	6:T:23:GLN:HE22	1.29	0.77
7:U:198:ILE:HG23	7:U:203:THR:O	1.83	0.77
13:1:76:PRO:HD2	13:1:105:GLN:OE1	1.84	0.77
12:L:3:ILE:HD13	12:L:127:GLY:O	1.84	0.77
11:K:35:ILE:HD12	11:K:56:GLU:CB	2.15	0.77
13:M:-4:ILE:CD1	14:N:115:LEU:HB3	2.14	0.77
2:B:194:LEU:CD1	2:B:232:ILE:CD1	2.63	0.76
13:M:167:ALA:HB2	14:2:26:ILE:HD11	1.68	0.76
6:T:74:ILE:HG12	6:T:109:ILE:CD1	2.15	0.76
1:A:124:THR:CG2	2:B:130:ARG:HH21	1.98	0.76
12:Z:4:LEU:HD11	12:Z:138:LEU:HD21	1.67	0.76
9:W:34:ILE:HD13	9:W:44:GLY:HA3	1.67	0.76
10:X:18:LYS:HD3	10:X:174:ILE:HG13	1.68	0.76
2:B:71:ASN:HD22	2:B:72:ASP:N	1.83	0.76
1:O:130:ARG:HH21	7:U:124:THR:HG22	1.50	0.76
13:M:40:ASN:H	13:M:40:ASN:HD22	1.28	0.76
1:O:124:THR:CG2	2:P:130:ARG:HH21	1.98	0.76
7:G:151:THR:HG22	7:G:157:TYR:HB2	1.67	0.76
3:Q:85:SER:O	3:Q:89:ILE:HD13	1.85	0.76
12:L:4:LEU:HD11	12:L:138:LEU:HD21	1.65	0.76
5:E:48:LEU:CD1	5:E:139:ILE:HD12	2.15	0.75
12:Z:3:ILE:HD13	12:Z:127:GLY:O	1.86	0.75
8:H:3:ILE:HD12	8:H:100:ILE:HG12	1.68	0.75
7:U:151:THR:HG22	7:U:157:TYR:HB2	1.67	0.75
13:1:157:ASN:ND2	13:1:160:ARG:HH11	1.79	0.75
9:I:34:ILE:HD13	9:I:44:GLY:HA3	1.67	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:35:PHE:HE1	9:I:45:ILE:HD13	1.50	0.75
10:J:133:TYR:HD1	16:Y:1425:HOH:O	1.69	0.75
5:S:211:SER:O	5:S:212:ILE:HD13	1.87	0.75
9:W:34:ILE:HD13	9:W:44:GLY:CA	2.15	0.75
7:U:41:ARG:HD3	7:U:148:ILE:HD13	1.68	0.75
11:K:33:LYS:HA	11:K:45:MET:HE2	1.67	0.75
7:U:41:ARG:HG2	7:U:148:ILE:HD11	1.67	0.74
7:G:233:LEU:O	7:G:236:ILE:HG13	1.87	0.74
4:R:12(D):ALA:HB3	4:R:126:ARG:HD3	1.69	0.74
3:C:164:THR:HG21	3:C:172:VAL:HG13	1.69	0.74
3:C:85:SER:O	3:C:89:ILE:HD13	1.87	0.74
7:G:18(G):GLU:HG2	7:G:188:LYS:CB	2.17	0.74
2:B:160:TRP:CE2	2:B:163:ILE:HD12	2.22	0.74
9:I:34:ILE:HD13	9:I:44:GLY:CA	2.17	0.74
12:Z:4:LEU:CD1	12:Z:138:LEU:HD21	2.17	0.74
12:L:4:LEU:CD1	12:L:138:LEU:HD21	2.17	0.74
8:V:3:ILE:HD12	8:V:100:ILE:HG12	1.70	0.74
7:U:18(A):ILE:HD13	7:U:18(C):HIS:O	1.86	0.74
2:B:15:PHE:H	3:C:23:GLN:NE2	1.86	0.74
2:P:160:TRP:CE2	2:P:163:ILE:HD12	2.23	0.74
13:1:13:ILE:HG22	13:1:155:ILE:HD12	1.70	0.74
4:D:229:THR:HG22	4:D:233:ILE:CD1	2.16	0.74
10:X:3:ILE:CD1	10:X:46:ALA:HB2	2.17	0.73
12:Z:-7:ASN:ND2	12:Z:-5:TYR:H	1.86	0.73
3:Q:40:VAL:HG12	3:Q:162:ALA:HB1	1.70	0.73
5:S:220:PRO:O	5:S:222:THR:HG23	1.88	0.73
7:U:59:LEU:O	7:U:61:PRO:HD3	1.88	0.73
3:Q:70:ILE:HD13	3:Q:112:LEU:HD11	1.69	0.73
8:V:40:LYS:C	8:V:41:ILE:HD12	2.09	0.73
7:U:18(A):ILE:O	7:U:18(A):ILE:HD12	1.88	0.73
9:I:45:ILE:N	9:I:45:ILE:HD12	2.04	0.73
11:K:37:ILE:HB	11:K:41:LEU:HB3	1.70	0.73
5:E:15:PHE:HB2	6:F:23:GLN:HE22	1.53	0.73
7:U:18(D):ILE:H	7:U:18(D):ILE:HD12	1.53	0.73
9:I:45:ILE:HB	9:I:52:VAL:HG13	1.70	0.73
10:J:90(A):ILE:O	10:J:90(A):ILE:HD13	1.89	0.73
2:P:39:GLY:O	2:P:40:ILE:HD13	1.89	0.73
3:Q:70:ILE:HD11	3:Q:76:LEU:HB2	1.70	0.73
9:I:7:THR:CG2	9:I:110:ILE:HD12	2.19	0.72
7:G:59:LEU:O	7:G:61:PRO:HD3	1.89	0.72
3:Q:164:THR:HG21	3:Q:172:VAL:HG13	1.69	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:9:ASP:HA	7:G:14:ILE:CD1	2.14	0.72
1:O:121:GLN:O	1:O:124:THR:HB	1.88	0.72
1:A:124:THR:HG22	2:B:130:ARG:HH21	1.53	0.72
14:2:112:THR:HG22	14:2:120:HIS:HB2	1.70	0.72
10:J:177:ILE:HD11	10:J:187:VAL:HG23	1.71	0.72
13:M:139:ARG:HH11	8:V:165:ASN:ND2	1.87	0.72
3:C:40:VAL:HG12	3:C:162:ALA:HB1	1.71	0.72
9:I:124:PHE:C	9:I:125:ILE:HD12	2.09	0.72
9:W:4:VAL:CG1	9:W:155:ILE:HD11	2.20	0.71
7:U:18(G):GLU:HG2	7:U:188:LYS:CB	2.19	0.71
13:1:-4:ILE:HD13	14:2:115:LEU:HB3	1.71	0.71
10:X:3:ILE:HD11	10:X:46:ALA:HB2	1.72	0.71
12:L:-7:ASN:ND2	12:L:-5:TYR:H	1.88	0.71
10:J:18:LYS:HD3	10:J:174:ILE:HG13	1.71	0.71
13:M:203:ILE:HD13	14:2:30:VAL:HG21	1.73	0.71
6:F:67:ILE:HD13	6:F:77:VAL:HB	1.72	0.71
2:P:185:LYS:HD3	2:P:186:VAL:N	2.05	0.71
8:V:159:ILE:O	8:V:163:ILE:HD13	1.90	0.71
4:R:161:ASN:N	5:S:58:LEU:O	2.21	0.71
6:T:193:ALA:O	6:T:197:ILE:HD12	1.90	0.71
8:H:15:ALA:HB1	8:H:159:ILE:CD1	2.20	0.71
4:D:12(D):ALA:HB3	4:D:126:ARG:HD3	1.70	0.71
7:G:172:ILE:HD11	7:G:201:LEU:HD21	1.72	0.71
2:B:121:GLN:O	2:B:124:THR:HB	1.90	0.71
5:E:220:PRO:O	5:E:222:THR:HG23	1.91	0.71
1:A:121:GLN:O	1:A:124:THR:HB	1.91	0.71
9:W:192:ARG:HG3	16:W:200:HOH:O	1.89	0.71
14:N:12:VAL:C	14:N:13:ILE:HD13	2.12	0.71
11:Y:37:ILE:HB	11:Y:41:LEU:HB3	1.73	0.70
2:B:185:LYS:HD3	2:B:186:VAL:N	2.06	0.70
13:1:4:ILE:HD11	13:1:155:ILE:HG23	1.73	0.70
7:U:18(A):ILE:CD1	7:U:18(C):HIS:O	2.39	0.70
7:U:40:VAL:HB	7:U:18(D):ILE:CD1	2.21	0.70
5:S:201:LEU:HD11	5:S:207:LEU:HD22	1.73	0.70
1:O:225:THR:OG1	1:O:228:GLU:HG3	1.90	0.70
14:2:19:ARG:CD	14:2:26:ILE:HD12	2.22	0.70
3:Q:33:ARG:HB2	3:Q:33:ARG:NH1	2.06	0.70
11:K:142:TYR:O	11:K:143:LYS:HD2	1.92	0.70
13:M:76:PRO:HD2	13:M:105:GLN:OE1	1.92	0.70
10:J:168:MET:HE1	10:X:167:PRO:HB2	1.74	0.70
7:U:227:GLU:HG2	16:U:292:HOH:O	1.92	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:217:LYS:HE3	7:U:217:LYS:HA	1.72	0.70
12:Z:59:PHE:CD1	12:Z:83:ILE:HD11	2.27	0.70
11:Y:10(A):ARG:HB3	11:Y:10(B):LYS:HE3	1.74	0.70
6:F:193:ALA:O	6:F:197:ILE:HD13	1.92	0.70
3:Q:163:GLN:HE22	3:Q:173:ARG:HE	1.40	0.70
11:K:10(A):ARG:HB3	11:K:10(B):LYS:HE3	1.72	0.69
6:T:49:ALA:HB1	6:T:197:ILE:CD1	2.21	0.69
1:A:225:THR:OG1	1:A:228:GLU:HG3	1.91	0.69
5:E:201:LEU:HD11	5:E:207:LEU:HD22	1.73	0.69
14:N:112:THR:HG22	14:N:120:HIS:HB2	1.74	0.69
11:Y:142:TYR:O	11:Y:143:LYS:HD2	1.93	0.69
6:F:37:SER:HB3	6:F:50:VAL:HG23	1.73	0.69
12:L:76:ILE:HD11	12:L:101:ILE:HD13	1.73	0.69
9:I:27:VAL:HG13	16:J:230:HOH:O	1.92	0.69
10:J:156:LYS:O	10:J:160:GLN:HG3	1.93	0.69
8:H:216:GLU:HG3	9:I:187:ARG:HG2	1.73	0.69
11:K:180:GLU:HB2	16:K:1426:HOH:O	1.93	0.69
1:O:86:ARG:HE	7:U:118:ASN:HD21	1.40	0.69
8:H:22:GLN:HG3	15:H:1400:BO2:H6	1.75	0.69
7:G:12:ILE:HD13	7:G:12:ILE:H	1.57	0.69
8:H:41:ILE:HD12	8:H:76:VAL:CG2	2.19	0.69
5:S:45:HIS:HD2	5:S:214:ILE:HD11	1.58	0.69
2:B:15:PHE:N	3:C:23:GLN:HE22	1.90	0.69
10:X:156:LYS:O	10:X:160:GLN:HG3	1.93	0.69
2:B:65:GLU:HG3	2:B:66:LYS:HG3	1.74	0.69
7:G:217:LYS:HA	7:G:217:LYS:HE3	1.73	0.69
6:T:37:SER:HB3	6:T:50:VAL:HG23	1.74	0.69
7:U:121:GLN:O	7:U:124:THR:HB	1.93	0.69
10:J:2:ILE:HD13	10:J:130:SER:OG	1.93	0.69
2:P:65:GLU:HG3	2:P:66:LYS:HG3	1.74	0.69
3:C:163:GLN:HE22	3:C:173:ARG:HE	1.41	0.68
13:1:19:LEU:HD21	13:1:26:LEU:HD22	1.75	0.68
5:E:15:PHE:HB2	6:F:23:GLN:NE2	2.08	0.68
6:F:35:THR:HG21	6:F:51:GLU:O	1.93	0.68
3:C:41:LYS:HG2	3:C:161:SER:O	1.93	0.68
1:O:73:ASP:C	1:O:74:ILE:HD12	2.14	0.68
8:V:37:ILE:CG2	8:V:63:ILE:HD12	2.24	0.68
3:Q:52:ARG:HB2	3:Q:209:ASN:HA	1.75	0.68
14:N:159:LEU:O	14:N:163:ILE:HD13	1.93	0.68
2:P:121:GLN:O	2:P:124:THR:HB	1.93	0.68
6:T:35:THR:HG21	6:T:51:GLU:O	1.94	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:175:PHE:O	3:C:179:ASN:HB2	1.94	0.68
8:V:22:GLN:HG3	15:V:1401:BO2:H6	1.75	0.68
9:W:155:ILE:O	9:W:155:ILE:HD12	1.93	0.68
14:2:134:ILE:HD13	14:2:138:CYS:SG	2.33	0.68
12:Z:99:THR:HG22	16:Z:202:HOH:O	1.94	0.68
2:B:6:ARG:HG2	3:C:10:ARG:HH21	1.59	0.68
3:C:33:ARG:HB2	3:C:33:ARG:NH1	2.08	0.67
2:P:6:ARG:HG2	3:Q:10:ARG:NH2	2.08	0.67
13:M:19:LEU:HD21	13:M:26:LEU:HD22	1.77	0.67
1:A:130:ARG:HH21	7:G:124:THR:CG2	2.06	0.67
9:I:97:VAL:HG23	9:I:99:PRO:HD3	1.75	0.67
9:W:4:VAL:HG13	9:W:155:ILE:HD11	1.75	0.67
8:V:35:HIS:HB3	8:V:56:THR:HG21	1.75	0.67
4:R:70:ILE:HD12	4:R:74:ILE:CG2	2.24	0.67
5:S:92:LEU:HD11	5:S:112:ALA:HB1	1.77	0.67
8:H:165:ASN:ND2	13:1:139:ARG:HH11	1.92	0.67
14:2:100:ILE:HD11	14:2:127:ALA:HB3	1.77	0.67
2:P:4:GLY:HA3	5:S:127:TYR:CE1	2.28	0.67
5:S:221:PHE:CE1	5:S:223:ILE:HD11	2.30	0.67
2:B:161:LYS:HG3	3:C:59:GLN:O	1.94	0.67
2:P:28:LEU:HD23	2:P:31:ILE:HD12	1.76	0.67
2:B:41:MET:HE3	16:B:240:HOH:O	1.94	0.67
13:M:74:LEU:HD13	13:M:79:ILE:HD11	1.75	0.67
10:J:167:PRO:HB2	10:X:168:MET:HE1	1.76	0.67
13:1:-4:ILE:CD1	14:2:115:LEU:HB3	2.24	0.67
3:C:106:PRO:HG2	3:C:143:PRO:CG	2.25	0.67
2:P:159:GLY:HA3	3:Q:62(A):ILE:CD1	2.25	0.67
5:S:226:GLY:O	5:S:229:VAL:HG22	1.95	0.67
4:R:160:TYR:CE2	5:S:59:SER:HB3	2.29	0.66
5:S:141:TYR:CE2	5:S:217:LYS:HA	2.29	0.66
5:E:213:ALA:HB2	5:E:223:ILE:CD1	2.25	0.66
9:W:97:VAL:HG23	9:W:99:PRO:HD3	1.76	0.66
12:L:59:PHE:CD1	12:L:83:ILE:HD11	2.29	0.66
8:H:200:LYS:HE3	9:I:140:SER:O	1.94	0.66
5:E:67:ILE:CD1	5:E:77:SER:HB3	2.26	0.66
3:C:226:SER:HB2	3:C:227:GLU:OE1	1.95	0.66
2:P:97:GLN:HE22	9:W:64:ASN:HD22	1.42	0.66
9:I:110:ILE:N	9:I:110:ILE:HD13	2.08	0.66
3:Q:226:SER:HB2	3:Q:227:GLU:OE1	1.96	0.66
8:H:35:HIS:HB3	8:H:56:THR:HG21	1.75	0.66
4:D:194:LEU:HD21	4:D:233:ILE:HD12	1.77	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:213:ALA:CB	5:E:223:ILE:HD12	2.22	0.66
14:2:13:ILE:HG12	14:2:177:VAL:HG13	1.77	0.66
13:M:41:THR:OG1	13:M:76:PRO:HG3	1.95	0.66
8:V:38:SER:HG	8:V:41:ILE:HD13	1.60	0.66
13:M:203:ILE:HD13	14:2:30:VAL:CG2	2.26	0.66
2:B:181:LYS:O	2:B:184:MET:HG3	1.95	0.66
5:S:221:PHE:CZ	5:S:223:ILE:HD11	2.30	0.66
3:C:52:ARG:HB2	3:C:209:ASN:HA	1.78	0.66
5:S:18(C):PHE:HA	5:S:18(F):ILE:HG12	1.78	0.66
4:D:229:THR:O	4:D:233:ILE:CD1	2.42	0.66
2:B:97:GLN:NE2	9:I:64:ASN:HD22	1.92	0.66
9:I:104:ILE:HD11	9:I:178:ILE:HG22	1.78	0.66
5:E:221:PHE:CE1	5:E:223:ILE:HD11	2.31	0.65
4:D:192:LEU:O	4:D:196:ILE:HD13	1.96	0.65
2:P:101:LYS:NZ	10:X:85:GLN:NE2	2.43	0.65
14:N:126:ILE:HD13	14:N:126:ILE:H	1.59	0.65
4:R:156:THR:HG22	5:S:83:PRO:HD3	1.77	0.65
3:Q:172:VAL:HG23	3:Q:196:SER:HB2	1.78	0.65
2:P:159:GLY:HA3	3:Q:62(A):ILE:HD11	1.79	0.65
3:C:206:GLY:HA3	3:C:209:ASN:HB2	1.78	0.65
14:2:126:ILE:H	14:2:126:ILE:HD13	1.62	0.65
6:F:237:GLN:O	6:F:240:ILE:HG22	1.96	0.65
3:Q:33:ARG:HH11	3:Q:33:ARG:CB	2.09	0.65
8:V:196:VAL:HG23	16:V:1418:HOH:O	1.95	0.65
6:T:237:GLN:O	6:T:240:ILE:HG22	1.95	0.65
8:H:167:LEU:HB3	12:Z:167:ILE:HD13	1.78	0.65
5:E:141:TYR:CE2	5:E:217:LYS:HA	2.31	0.65
5:E:139:ILE:HD11	5:E:221:PHE:CE2	2.28	0.65
3:Q:106:PRO:HG2	3:Q:143:PRO:CG	2.25	0.65
2:P:15:PHE:H	3:Q:23:GLN:HE22	1.43	0.65
13:1:-3:VAL:CG1	13:1:49:ILE:HD12	2.26	0.65
12:Z:76:ILE:HD11	12:Z:101:ILE:HD13	1.78	0.65
2:B:163:ILE:HG12	2:B:164:SER:H	1.61	0.65
12:L:148:VAL:O	12:L:152:ILE:HG12	1.95	0.65
2:B:147:GLN:HG2	3:C:62(A):ILE:HD13	1.78	0.65
5:S:18(D):ILE:HD13	5:S:18(D):ILE:O	1.96	0.65
5:E:221:PHE:CZ	5:E:223:ILE:HD11	2.31	0.65
2:B:213:ALA:HB2	2:B:223:ILE:HD13	1.79	0.65
8:V:216:GLU:HG3	9:W:187:ARG:HG2	1.79	0.65
6:F:69:VAL:HG12	16:F:248:HOH:O	1.97	0.65
3:C:14:ILE:H	3:C:14:ILE:HD13	1.61	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:8:TYR:CE2	7:G:12:ILE:HD12	2.32	0.65
2:B:232:ILE:O	2:B:232:ILE:HD13	1.96	0.65
7:G:96:ALA:CA	7:G:107:MET:HE2	2.25	0.64
13:1:41:THR:OG1	13:1:76:PRO:HG3	1.96	0.64
7:G:8:TYR:O	7:G:12:ILE:HD13	1.97	0.64
7:G:12:ILE:HG12	7:G:14:ILE:HD12	1.79	0.64
5:E:2(B):THR:H	5:E:2(E):ASN:HD22	1.44	0.64
9:I:104:ILE:HD13	9:I:181:LYS:N	2.12	0.64
5:E:226:GLY:O	5:E:229:VAL:HG22	1.97	0.64
9:I:33:LYS:O	9:I:44:GLY:HA2	1.98	0.64
9:I:45:ILE:N	9:I:45:ILE:CD1	2.61	0.64
6:T:173:LYS:O	6:T:177:GLU:HG3	1.97	0.64
4:D:45:GLY:HA2	4:D:146:TYR:CE1	2.32	0.64
5:S:74:MET:HE1	5:S:96:CYS:SG	2.38	0.64
2:P:163:ILE:HG12	2:P:164:SER:N	2.12	0.64
2:P:163:ILE:HG12	2:P:164:SER:H	1.61	0.64
10:J:-1:MET:HG2	10:J:1:ASP:H	1.62	0.64
10:X:10(B):LYS:NZ	10:X:10(B):LYS:HB2	2.13	0.64
4:D:196:ILE:N	4:D:196:ILE:CD1	2.60	0.64
6:F:173:LYS:O	6:F:177:GLU:HG3	1.97	0.64
2:B:186:VAL:HG21	2:B:216:ARG:HD3	1.80	0.64
11:K:7:ARG:HG3	11:K:12:ILE:HD13	1.78	0.64
10:J:68:ILE:HG12	16:J:227:HOH:O	1.98	0.64
14:N:146:MET:HE3	14:N:150:GLU:HB3	1.79	0.64
7:U:87:ASN:HD22	7:U:87:ASN:C	1.99	0.64
5:S:207:LEU:H	5:S:207:LEU:CD2	2.10	0.64
1:O:71:THR:OG1	1:O:74:ILE:CD1	2.46	0.64
1:A:130:ARG:HH21	7:G:124:THR:HG22	1.62	0.64
8:V:34:LEU:HB2	16:V:1415:HOH:O	1.98	0.64
7:U:34(A):ASN:HD22	7:U:167:PRO:HG2	1.63	0.64
2:B:163:ILE:HG12	2:B:164:SER:N	2.13	0.64
2:B:149:TYR:CZ	3:C:62(A):ILE:HD12	2.33	0.64
2:B:219:GLU:HG2	2:B:21(E):VAL:N	2.13	0.64
1:A:33:GLN:HA	1:A:33:GLN:HE21	1.63	0.64
5:S:75:GLY:HA3	5:S:221:PHE:CE2	2.32	0.63
12:Z:59:PHE:CG	12:Z:83:ILE:HD11	2.33	0.63
1:A:179:ARG:HB3	1:A:179:ARG:HH11	1.63	0.63
9:W:33:LYS:O	9:W:44:GLY:HA2	1.98	0.63
10:J:168:MET:HE3	10:X:168:MET:HE3	1.80	0.63
7:G:87:ASN:HD22	7:G:87:ASN:C	2.02	0.63
9:I:110:ILE:HD11	9:I:122:ALA:O	1.98	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:186:LEU:O	4:D:190:GLU:HG3	1.99	0.63
5:E:92:LEU:HD11	5:E:112:ALA:HB1	1.79	0.63
7:U:148:ILE:N	7:U:148:ILE:HD12	2.12	0.63
3:C:40:VAL:HG12	3:C:162:ALA:CB	2.28	0.63
3:Q:175:PHE:O	3:Q:179:ASN:HB2	1.97	0.63
6:F:20(B):GLU:HG3	6:F:20(C):LYS:HG3	1.80	0.63
2:P:219:GLU:HG2	2:P:21(E):VAL:N	2.12	0.63
7:G:151:THR:HG22	7:G:157:TYR:CB	2.29	0.63
3:C:33:ARG:CB	3:C:33:ARG:HH11	2.11	0.63
2:B:77:ALA:HB3	2:B:137:ILE:HB	1.80	0.63
7:U:39:ALA:HB2	7:U:48:VAL:HG12	1.81	0.63
14:2:175:MET:HB2	14:2:187:LEU:HB2	1.79	0.63
6:F:38:ILE:HG22	6:F:164:ALA:HB2	1.79	0.63
6:T:40:ILE:HD12	6:T:193:ALA:HB2	1.80	0.63
14:2:44:CYS:HB2	14:2:100:ILE:HB	1.80	0.63
11:Y:66:HIS:HA	16:Y:1433:HOH:O	1.97	0.63
11:Y:210:ILE:HD12	16:Y:1432:HOH:O	1.97	0.63
7:U:41:ARG:CG	7:U:148:ILE:CD1	2.77	0.63
4:R:186:LEU:O	4:R:190:GLU:HG3	1.99	0.63
11:Y:180:GLU:N	16:Y:1428:HOH:O	2.19	0.63
14:N:175:MET:HB2	14:N:187:LEU:HB2	1.79	0.63
13:1:13:ILE:CD1	13:1:177:ILE:HG12	2.21	0.63
5:E:67:ILE:HD13	5:E:77:SER:HB3	1.80	0.63
5:E:207:LEU:CD2	5:E:207:LEU:H	2.11	0.63
2:P:186:VAL:HG21	2:P:216:ARG:HD3	1.81	0.63
2:P:6:ARG:HD2	4:R:9:ASP:N	2.14	0.63
3:Q:41:LYS:HG2	3:Q:161:SER:O	1.98	0.63
2:P:181:LYS:O	2:P:184:MET:HG3	1.98	0.63
3:C:160:TRP:CE2	4:D:59:LEU:HD23	2.34	0.63
3:C:172:VAL:HG23	3:C:196:SER:HB2	1.80	0.63
3:Q:206:GLY:HA3	3:Q:209:ASN:HB2	1.79	0.63
7:G:121:GLN:O	7:G:124:THR:HB	1.98	0.63
12:L:59:PHE:CG	12:L:83:ILE:HD11	2.34	0.63
4:R:102:TYR:O	12:Z:81:ARG:HG3	1.98	0.63
3:Q:160:TRP:CE2	4:R:59:LEU:HD23	2.34	0.63
1:O:177:GLU:HG2	2:P:58:LEU:HD21	1.80	0.63
6:T:38:ILE:HG22	6:T:164:ALA:HB2	1.81	0.62
14:N:131:SER:HA	14:N:134:ILE:CD1	2.28	0.62
5:S:213:ALA:HB2	5:S:223:ILE:CD1	2.25	0.62
12:Z:83:ILE:HD13	12:Z:86:LEU:HD12	1.81	0.62
8:H:35:HIS:CB	8:H:56:THR:HG21	2.29	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:104:ILE:N	9:W:104:ILE:CD1	2.61	0.62
2:P:70:LEU:HD21	2:P:89:ILE:HD12	1.80	0.62
4:R:31:ILE:HD11	4:R:134:VAL:N	2.14	0.62
13:M:139:ARG:NH1	8:V:165:ASN:HD22	1.94	0.62
14:N:44:CYS:HB2	14:N:100:ILE:HB	1.80	0.62
8:V:35:HIS:CB	8:V:56:THR:HG21	2.28	0.62
2:B:219:GLU:HG2	2:B:21(E):VAL:H	1.64	0.62
2:P:76:VAL:HG21	2:P:89:ILE:HD11	1.81	0.62
13:M:4:ILE:HG13	13:M:155:ILE:HD12	1.81	0.62
4:D:102:TYR:O	12:L:81:ARG:HG3	1.99	0.62
1:O:27:ALA:O	1:O:31:VAL:HG23	1.99	0.62
4:R:177:LEU:HA	5:S:58:LEU:HD11	1.81	0.62
12:L:-9:GLN:HE21	13:M:-8:THR:HG21	1.64	0.62
7:G:34(A):ASN:HD22	7:G:167:PRO:HG2	1.64	0.62
8:H:173:VAL:HB	8:H:192:LEU:HB2	1.81	0.62
13:1:13:ILE:HD11	13:1:177:ILE:HG23	1.82	0.62
14:2:13:ILE:HD12	14:2:151:THR:CG2	2.30	0.62
5:S:143:LYS:HE3	16:1:254:HOH:O	1.99	0.62
3:Q:55:THR:HG22	3:Q:56:LEU:HD22	1.82	0.62
1:O:179:ARG:HH11	1:O:179:ARG:HB3	1.65	0.62
1:O:33:GLN:HE21	1:O:33:GLN:HA	1.63	0.62
7:U:41:ARG:CG	7:U:148:ILE:HD11	2.29	0.62
2:P:219:GLU:HG2	2:P:21(E):VAL:H	1.65	0.62
10:J:10(B):LYS:HB2	10:J:10(B):LYS:NZ	2.14	0.62
2:B:124:THR:HG22	3:C:130:ARG:NH2	2.03	0.62
5:S:2(B):THR:H	5:S:2(E):ASN:HD22	1.45	0.62
14:2:126:ILE:N	14:2:126:ILE:HD13	2.15	0.62
3:Q:41:LYS:HD3	3:Q:161:SER:HA	1.82	0.62
2:P:77:ALA:HB3	2:P:137:ILE:HB	1.80	0.62
8:H:10:ASN:OD1	8:H:180:ILE:HD12	1.98	0.62
12:L:33:LYS:HD2	12:L:46:ASN:ND2	2.15	0.62
5:E:75:GLY:HA3	5:E:221:PHE:CE2	2.34	0.62
5:E:15:PHE:H	6:F:23:GLN:NE2	1.98	0.62
3:Q:70:ILE:HD13	3:Q:112:LEU:CD1	2.29	0.62
2:P:6:ARG:HG2	3:Q:10:ARG:HH21	1.63	0.62
2:B:14:ILE:H	2:B:14:ILE:HD13	1.65	0.62
5:S:207:LEU:N	5:S:207:LEU:HD23	2.14	0.62
3:C:41:LYS:HD3	3:C:161:SER:HA	1.81	0.62
2:B:6:ARG:HG2	3:C:10:ARG:NH2	2.15	0.62
2:P:97:GLN:NE2	9:W:64:ASN:HD22	1.97	0.62
11:K:191:ASP:OD2	11:K:193:GLY:N	2.32	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:40:VAL:HG12	3:Q:162:ALA:CB	2.29	0.61
1:A:179:ARG:NH1	1:A:179:ARG:HB3	2.15	0.61
4:R:45:GLY:HA2	4:R:146:TYR:CE1	2.34	0.61
10:X:7:ARG:HG2	10:X:7:ARG:HH11	1.65	0.61
5:E:213:ALA:CB	5:E:223:ILE:CD1	2.78	0.61
10:J:133:TYR:HE1	16:X:221:HOH:O	1.83	0.61
7:G:39:ALA:HB2	7:G:48:VAL:HG12	1.81	0.61
7:G:86:ARG:HD2	16:G:257:HOH:O	2.00	0.61
6:T:35:THR:HG23	6:T:51:GLU:HB3	1.82	0.61
8:V:173:VAL:HB	8:V:192:LEU:HB2	1.83	0.61
4:R:67:ILE:HD12	4:R:211:GLN:HE21	1.65	0.61
3:C:35:THR:HB	3:C:51:GLU:HG3	1.82	0.61
7:U:107:MET:HE3	7:U:112:LEU:HB2	1.82	0.61
5:S:213:ALA:CB	5:S:223:ILE:CD1	2.78	0.61
13:M:167:ALA:HB2	14:2:26:ILE:CD1	2.30	0.61
12:Z:-6:PRO:O	13:1:91:ARG:NH1	2.32	0.61
7:U:151:THR:HG22	7:U:157:TYR:CB	2.31	0.61
2:B:141:TYR:CD1	2:B:21(E):VAL:HG21	2.34	0.61
3:C:55:THR:HG22	3:C:56:LEU:HD22	1.81	0.61
1:A:27:ALA:O	1:A:31:VAL:HG23	2.00	0.61
10:X:-1:MET:HG2	10:X:1:ASP:H	1.64	0.61
7:U:8:TYR:C	7:U:10:ARG:H	2.04	0.61
4:R:160:TYR:HA	5:S:59:SER:HA	1.83	0.61
5:S:74:MET:CE	5:S:96:CYS:SG	2.88	0.61
10:X:143:ARG:HG2	10:X:143:ARG:HH11	1.66	0.61
2:B:149:TYR:OH	3:C:62(A):ILE:HB	2.01	0.61
12:L:99:THR:HG23	12:L:113:PHE:HB2	1.82	0.61
9:I:6:MET:HE3	9:I:155:ILE:HG13	1.81	0.61
5:E:207:LEU:HD23	5:E:207:LEU:N	2.15	0.61
6:T:203:GLU:O	6:T:206:LYS:HD2	2.01	0.61
9:I:2:ILE:HG21	9:I:130:ALA:HB3	1.83	0.61
12:Z:114:ASP:HB2	12:Z:118:SER:HB3	1.83	0.60
14:2:107:LYS:HG2	14:2:108:GLY:H	1.64	0.60
12:L:114:ASP:HB2	12:L:118:SER:HB3	1.82	0.60
6:T:197:ILE:HD13	6:T:210:LEU:CD1	2.31	0.60
6:F:35:THR:HG23	6:F:51:GLU:HB3	1.82	0.60
12:Z:134:ILE:HD11	12:Z:158:SER:O	2.00	0.60
6:T:20(B):GLU:HG3	6:T:20(C):LYS:HG3	1.82	0.60
14:2:146:MET:HE3	14:2:150:GLU:HB3	1.80	0.60
5:E:139:ILE:CD1	5:E:139:ILE:H	2.13	0.60
8:V:112:SER:HB3	8:V:125:LEU:HD13	1.83	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1:-4:ILE:HD12	14:2:116:GLY:CA	2.32	0.60
14:2:49:ALA:HA	16:2:1423:HOH:O	1.99	0.60
10:X:133:TYR:CE2	10:X:166:MET:HG3	2.35	0.60
12:Z:7:ALA:HB2	12:Z:110:VAL:HG23	1.83	0.60
9:W:2:ILE:HG21	9:W:130:ALA:HB3	1.82	0.60
12:L:7:ALA:HB2	12:L:110:VAL:HG23	1.84	0.60
2:P:141:TYR:CD1	2:P:21(E):VAL:HG21	2.36	0.60
5:E:73:HIS:HE1	5:E:107:LEU:O	1.84	0.60
14:N:107:LYS:HG2	14:N:108:GLY:H	1.66	0.60
2:B:215:ILE:HD12	2:B:221:GLN:HA	1.84	0.60
7:G:212:VAL:HB	7:G:229:ILE:HD11	1.84	0.60
3:Q:35:THR:HB	3:Q:51:GLU:HG3	1.82	0.60
5:S:213:ALA:CB	5:S:223:ILE:HD12	2.28	0.60
7:U:41:ARG:HG2	7:U:148:ILE:CD1	2.31	0.60
3:Q:14:ILE:O	3:Q:21:ILE:HD13	2.01	0.60
11:K:104:TYR:CD1	11:K:180:GLU:HG3	2.36	0.60
1:O:179:ARG:NH1	1:O:179:ARG:HB3	2.16	0.60
6:T:69:VAL:HG12	16:T:261:HOH:O	2.02	0.60
12:L:98:HIS:HD2	16:L:199:HOH:O	1.82	0.60
7:U:35:ILE:HG23	7:U:51:GLN:HB2	1.84	0.60
9:I:48:LEU:HG	9:I:50:THR:HG22	1.84	0.60
7:G:131:PRO:HB3	16:G:244:HOH:O	2.00	0.60
5:E:210:LEU:HD22	5:E:233:ILE:HD11	1.84	0.60
7:U:18(D):ILE:HD12	7:U:18(D):ILE:N	2.16	0.60
11:Y:104:TYR:CD1	11:Y:180:GLU:HG3	2.36	0.60
8:V:200:LYS:HE3	9:W:140:SER:O	2.02	0.60
13:M:14(D):GLU:O	13:M:14(G):ILE:HG12	2.01	0.60
14:N:18(G):TYR:HA	14:N:18(J):LEU:HG	1.84	0.60
11:Y:7:ARG:HD2	11:Y:108:PRO:O	2.02	0.60
7:G:8:TYR:C	7:G:10:ARG:H	2.04	0.59
7:U:148:ILE:N	7:U:148:ILE:CD1	2.65	0.59
15:2:1405:BO2:H241	16:2:1423:HOH:O	2.02	0.59
14:N:126:ILE:HD13	14:N:126:ILE:N	2.16	0.59
5:S:73:HIS:HE1	5:S:107:LEU:O	1.85	0.59
2:B:101:LYS:HG3	9:I:57:GLU:HB3	1.84	0.59
11:K:208:ASN:HD21	9:W:29:ASN:HD21	1.50	0.59
4:D:12(G):GLU:HG2	4:D:125:GLU:H	1.66	0.59
14:N:8:PHE:CE1	14:N:10:ASP:HB2	2.37	0.59
4:R:159:ARG:HB3	5:S:60:SER:HB3	1.84	0.59
7:U:18(A):ILE:CD1	7:U:18(C):HIS:H	2.11	0.59
10:X:2:ILE:O	10:X:3:ILE:HD12	2.01	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:83:ILE:HD13	12:L:86:LEU:HD12	1.83	0.59
4:D:45:GLY:HA2	4:D:146:TYR:CD1	2.37	0.59
4:R:159:ARG:O	5:S:60:SER:N	2.35	0.59
12:L:134:ILE:HD11	12:L:158:SER:O	2.02	0.59
11:K:20:ALA:HB2	11:K:31:VAL:HG21	1.83	0.59
13:1:14(D):GLU:O	13:1:14(G):ILE:HG12	2.02	0.59
13:M:7:LYS:HG3	13:M:14(G):ILE:HD12	1.83	0.59
7:G:152:ASP:HB2	7:G:153:PRO:CD	2.33	0.59
11:Y:10(A):ARG:H	11:Y:10(B):LYS:HZ2	1.50	0.59
3:C:106:PRO:HG2	3:C:143:PRO:HG3	1.85	0.59
7:U:18(A):ILE:C	7:U:18(A):ILE:HD12	2.21	0.59
12:Z:3:ILE:HG13	12:Z:100:ILE:HD13	1.85	0.59
14:2:174:ARG:HG2	14:2:18(A):ILE:CD1	2.32	0.59
5:S:97:ASN:HD21	12:Z:61:ASN:HD21	1.48	0.59
13:M:-4:ILE:HD12	14:N:116:GLY:CA	2.32	0.59
3:Q:185:THR:HG22	3:Q:187:GLU:N	2.15	0.59
12:L:-6:PRO:O	13:M:91:ARG:NH1	2.32	0.59
4:D:67:ILE:HD12	4:D:211:GLN:HE21	1.67	0.59
1:O:58:LEU:HB3	7:U:162:ALA:O	2.03	0.59
7:U:96:ALA:CA	7:U:107:MET:HE2	2.31	0.59
8:V:114:HIS:CE1	15:2:1405:BO2:H5	2.38	0.59
1:A:4:MET:SD	1:A:5:THR:N	2.64	0.59
11:K:10(A):ARG:H	11:K:10(B):LYS:NZ	2.01	0.59
5:S:194:VAL:HG13	5:S:207:LEU:HD11	1.85	0.59
3:C:185:THR:HG22	3:C:187:GLU:N	2.16	0.59
4:R:12(G):GLU:HG2	4:R:125:GLU:H	1.67	0.59
14:2:8:PHE:CE1	14:2:10:ASP:HB2	2.38	0.59
2:B:185:LYS:HD2	2:B:187:ASP:H	1.66	0.59
11:Y:20:ALA:HB2	11:Y:31:VAL:HG21	1.84	0.59
7:G:186:TRP:O	7:G:190:VAL:HG23	2.03	0.59
8:H:112:SER:HB3	8:H:125:LEU:HD13	1.85	0.58
9:I:110:ILE:CD1	9:I:110:ILE:N	2.66	0.58
11:K:208:ASN:ND2	9:W:29:ASN:HD21	2.01	0.58
6:F:175:GLU:HB3	6:F:196:ILE:HD12	1.85	0.58
4:R:31:ILE:HD12	4:R:79:SER:O	2.03	0.58
10:J:2:ILE:CD1	10:J:130:SER:OG	2.51	0.58
1:O:159:PRO:O	2:P:59:LEU:HD12	2.03	0.58
13:1:179:ASP:HB3	13:1:18(A):THR:OG1	2.04	0.58
6:F:203:GLU:O	6:F:206:LYS:HD2	2.03	0.58
3:C:158:SER:HB2	4:D:59:LEU:HD21	1.83	0.58
1:A:69:LEU:C	1:A:69:LEU:HD23	2.23	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:2:40:LYS:O	14:2:41:ILE:HD13	2.03	0.58
9:I:29:ASN:HD21	11:Y:208:ASN:HD21	1.51	0.58
10:J:7:ARG:HG2	10:J:7:ARG:HH11	1.68	0.58
1:A:86:ARG:HE	7:G:118:ASN:HD21	1.49	0.58
4:D:59:LEU:HD11	4:D:64:ILE:HD11	1.85	0.58
7:U:152:ASP:HB2	7:U:153:PRO:CD	2.34	0.58
13:M:19:LEU:HB2	13:M:170:SER:HB2	1.86	0.58
9:I:104:ILE:CD1	9:I:178:ILE:HG22	2.33	0.58
13:1:7:LYS:HG3	13:1:14(G):ILE:HD12	1.84	0.58
9:W:48:LEU:HG	9:W:50:THR:HG22	1.85	0.58
4:R:177:LEU:HD22	5:S:58:LEU:HD13	1.85	0.58
14:2:19:ARG:HD3	14:2:26:ILE:CD1	2.34	0.58
2:P:185:LYS:HD2	2:P:187:ASP:H	1.67	0.58
10:J:-1:MET:HG2	10:J:1:ASP:N	2.18	0.58
2:B:152:ASN:HB2	2:B:153:PRO:HD2	1.85	0.58
8:V:148:LYS:O	8:V:152:ILE:HG12	2.03	0.58
2:P:38:ILE:HD12	2:P:197:LEU:HG	1.86	0.58
1:O:69:LEU:HD23	1:O:69:LEU:C	2.23	0.58
7:U:72:ARG:HB2	7:U:72:ARG:NH1	2.19	0.58
12:Z:-7:ASN:HD22	12:Z:-7:ASN:C	2.07	0.58
11:K:75:SER:HB2	11:K:106:GLU:OE2	2.04	0.58
11:K:10(A):ARG:HG2	11:K:10(A):ARG:HH11	1.69	0.58
2:B:214:THR:O	2:B:215:ILE:HD13	2.04	0.58
4:R:70:ILE:HD12	4:R:74:ILE:HG22	1.85	0.58
5:S:132:TYR:O	5:S:153:PRO:HB3	2.03	0.58
6:T:175:GLU:HB3	6:T:196:ILE:HD12	1.84	0.58
2:B:202:THR:HG22	2:B:204:SER:N	2.07	0.57
4:D:177:LEU:HD13	5:E:58:LEU:HD11	1.85	0.57
11:Y:191:ASP:OD2	11:Y:193:GLY:N	2.37	0.57
5:E:194:VAL:HG13	5:E:207:LEU:HD11	1.86	0.57
7:U:86:ARG:HD2	16:U:249:HOH:O	2.02	0.57
12:Z:99:THR:HG23	12:Z:113:PHE:HB2	1.85	0.57
2:P:121:GLN:HG3	3:Q:83:ALA:HB1	1.86	0.57
3:C:241:GLN:C	3:C:243:GLN:H	2.07	0.57
2:P:239:THR:HG22	2:P:239:THR:OXT	2.03	0.57
3:C:168:ASN:HB2	3:C:200:VAL:HG11	1.86	0.57
6:T:95:GLU:CG	6:T:115:ARG:HB3	2.34	0.57
5:E:207:LEU:HA	5:E:2(E):ASN:ND2	2.19	0.57
11:Y:143:LYS:HB2	11:Y:146:LEU:HD13	1.87	0.57
12:L:173:LEU:HG	12:L:175:ILE:HD11	1.86	0.57
12:L:42:VAL:HG23	12:L:102:ALA:HB3	1.87	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:139:ILE:HD12	5:S:215:VAL:HG12	1.87	0.57
3:Q:168:ASN:HB2	3:Q:200:VAL:HG11	1.85	0.57
3:Q:186:VAL:O	3:Q:190:VAL:HG23	2.04	0.57
13:M:14(C):ARG:CG	13:M:14(C):ARG:HH11	2.15	0.57
10:J:133:TYR:CE2	10:J:166:MET:HG3	2.39	0.57
2:P:225:LYS:HG3	2:P:228:GLU:OE1	2.04	0.57
7:U:186:TRP:O	7:U:190:VAL:HG23	2.04	0.57
2:P:152:ASN:HB2	2:P:153:PRO:HD2	1.86	0.57
8:V:37:ILE:HD13	8:V:56:THR:O	2.05	0.57
9:W:84:SER:OG	9:W:119:ILE:HD11	2.05	0.57
9:W:84:SER:CB	9:W:119:ILE:HD11	2.35	0.57
14:N:36:ARG:HG3	14:N:42:TRP:CE2	2.39	0.57
5:S:201:LEU:O	5:S:202:ARG:HB2	2.03	0.57
3:Q:33:ARG:HH11	3:Q:33:ARG:HB2	1.69	0.57
10:X:44:SER:OG	10:X:100:LEU:HB2	2.04	0.57
14:2:10(B):LYS:HD3	14:2:10(B):LYS:C	2.25	0.57
6:F:38:ILE:HG22	6:F:164:ALA:CB	2.34	0.57
9:W:12:VAL:HG22	9:W:104:ILE:HD11	1.87	0.57
14:2:172:VAL:HG21	14:2:18(A):ILE:HD11	1.87	0.57
14:2:18(G):TYR:HA	14:2:18(J):LEU:HG	1.85	0.57
12:Z:166:HIS:HD2	12:Z:168:GLN:H	1.53	0.57
7:G:35:ILE:HG23	7:G:51:GLN:HB2	1.87	0.57
4:D:229:THR:CG2	4:D:233:ILE:HD11	2.32	0.57
4:D:196:ILE:H	4:D:196:ILE:HD13	1.70	0.57
12:Z:114:ASP:HB3	12:Z:118:SER:H	1.70	0.57
6:F:120:VAL:HG21	6:F:151:LEU:HD21	1.87	0.57
3:Q:241:GLN:C	3:Q:243:GLN:H	2.07	0.57
5:S:214:ILE:CD1	5:S:219:THR:HG21	2.30	0.57
6:T:38:ILE:HD11	6:T:49:ALA:HB3	1.87	0.57
5:E:201:LEU:O	5:E:202:ARG:HB2	2.05	0.57
14:N:156:LYS:HG2	14:N:18(J):LEU:HD11	1.87	0.57
13:M:149:GLN:NE2	13:M:149:GLN:H	2.03	0.57
7:G:107:MET:HE3	7:G:112:LEU:HB2	1.87	0.56
14:2:19:ARG:HG3	14:2:26:ILE:HD12	1.87	0.56
5:S:207:LEU:HA	5:S:2(E):ASN:ND2	2.19	0.56
1:O:86:ARG:HE	7:U:118:ASN:ND2	2.03	0.56
4:R:45:GLY:HA2	4:R:146:TYR:CD1	2.40	0.56
3:Q:182:PRO:O	3:Q:184:ALA:N	2.38	0.56
13:1:103:GLY:HA2	13:1:178:ILE:HD13	1.86	0.56
14:2:176:VAL:HG12	14:2:178:LEU:HD13	1.87	0.56
11:Y:10(A):ARG:H	11:Y:10(B):LYS:NZ	2.02	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:41:ARG:CD	7:U:148:ILE:HD13	2.35	0.56
3:C:186:VAL:O	3:C:190:VAL:HG23	2.05	0.56
11:K:99:THR:CG2	11:K:113:VAL:HB	2.33	0.56
13:1:14(C):ARG:CG	13:1:14(C):ARG:HH11	2.17	0.56
3:C:14:ILE:HD13	3:C:14:ILE:N	2.19	0.56
4:R:50:VAL:HG22	4:R:67:ILE:HD11	1.86	0.56
4:D:50:VAL:HG22	4:D:67:ILE:HD11	1.87	0.56
14:2:36:ARG:HG3	14:2:42:TRP:CE2	2.40	0.56
11:K:40:PHE:CD2	11:K:73:ARG:HD2	2.40	0.56
12:Z:8:GLY:HA3	12:Z:11:PHE:CE2	2.40	0.56
4:R:177:LEU:HD22	5:S:58:LEU:CD1	2.35	0.56
5:E:15:PHE:N	6:F:23:GLN:HE22	2.01	0.56
4:D:12(D):ALA:HB3	4:D:126:ARG:CD	2.36	0.56
13:M:179:ASP:HB3	13:M:18(A):THR:OG1	2.05	0.56
11:Y:75:SER:HB2	11:Y:106:GLU:OE2	2.05	0.56
10:X:147:THR:OG1	10:X:150:GLU:HG3	2.05	0.56
11:Y:123:ASP:HB2	11:Y:124:ILE:HD12	1.86	0.56
14:N:10(B):LYS:HD3	14:N:10(B):LYS:C	2.26	0.56
14:N:13:ILE:HD12	14:N:177:VAL:CA	2.33	0.56
2:B:8:TYR:CD2	7:G:12:ILE:HD12	2.40	0.56
8:V:159:ILE:HG22	8:V:163:ILE:HD13	1.87	0.56
16:B:256:HOH:O	3:C:33:ARG:HD2	2.04	0.56
2:B:239:THR:OXT	2:B:239:THR:HG22	2.05	0.56
3:Q:57:LYS:HD2	3:Q:58:LEU:N	2.20	0.56
3:C:45:CYS:HA	3:C:141:PHE:HZ	1.70	0.56
11:Y:40:PHE:CD2	11:Y:73:ARG:HD2	2.41	0.56
7:G:72:ARG:NH1	7:G:72:ARG:HB2	2.20	0.56
7:G:172:ILE:HD11	7:G:201:LEU:CD2	2.35	0.56
10:X:-1:MET:HG2	10:X:1:ASP:N	2.20	0.56
3:C:57:LYS:HD2	3:C:58:LEU:N	2.21	0.56
10:J:44:SER:OG	10:J:100:LEU:HB2	2.05	0.56
12:L:8:GLY:HA3	12:L:11:PHE:CE2	2.40	0.56
6:F:11:SER:HB3	6:F:14:VAL:HG23	1.86	0.56
5:S:179:THR:O	5:S:179:THR:HG22	2.05	0.56
6:T:38:ILE:HG22	6:T:164:ALA:CB	2.36	0.56
13:1:19:LEU:HB2	13:1:170:SER:HB2	1.87	0.56
8:H:167:LEU:HD13	12:Z:167:ILE:CD1	2.36	0.56
5:E:73:HIS:CE1	5:E:74:MET:HE2	2.40	0.56
2:B:152:ASN:HB2	2:B:153:PRO:CD	2.36	0.56
7:U:140:SER:HA	7:U:215:ALA:HB1	1.88	0.56
3:C:216:LYS:HD2	3:C:220:ASP:OD1	2.06	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:149:TYR:CE1	3:Q:159:SER:HB3	2.41	0.56
11:Y:10(A):ARG:HH11	11:Y:10(A):ARG:HG2	1.70	0.56
12:L:-8:PHE:HB2	13:M:-8:THR:HG23	1.86	0.56
7:U:18(A):ILE:HD13	7:U:18(C):HIS:N	2.13	0.56
6:T:49:ALA:HB3	6:T:197:ILE:HD11	1.84	0.56
11:K:143:LYS:HB2	11:K:146:LEU:HD13	1.86	0.56
8:V:22:GLN:HG3	15:V:1401:BO2:C6	2.36	0.56
3:Q:106:PRO:HG2	3:Q:143:PRO:HG3	1.86	0.56
2:B:21:LEU:HD13	2:B:124:THR:HG23	1.87	0.56
2:B:21:LEU:O	2:B:25:GLU:HG2	2.06	0.56
12:L:3:ILE:HG13	12:L:100:ILE:HD13	1.88	0.56
15:2:1405:BO2:H21	16:2:1453:HOH:O	2.05	0.56
14:2:175:MET:HE3	14:2:18(B):PHE:CE2	2.41	0.56
7:G:77:VAL:CG1	7:G:137:THR:HB	2.36	0.56
10:J:143:ARG:HH11	10:J:143:ARG:HG2	1.71	0.56
4:R:53:ARG:HG2	4:R:53:ARG:O	2.05	0.56
6:T:210:LEU:HD11	6:T:212:ILE:HD11	1.87	0.56
14:N:130:GLY:O	14:N:134:ILE:HD13	2.05	0.56
9:I:1:GLY:HA3	9:I:33:LYS:HE2	1.87	0.56
7:G:140:SER:HA	7:G:215:ALA:HB1	1.87	0.56
6:T:11:SER:HB3	6:T:14:VAL:HG23	1.87	0.56
3:Q:216:LYS:HD2	3:Q:220:ASP:OD1	2.05	0.56
4:R:173:GLN:CG	5:S:56:ASP:OD2	2.54	0.56
9:W:150:ASP:HA	16:W:237:HOH:O	2.05	0.56
15:2:1405:BO2:H251	16:2:1423:HOH:O	2.06	0.55
12:L:-7:ASN:C	12:L:-7:ASN:HD22	2.09	0.55
14:2:14:LEU:O	14:2:175:MET:HA	2.05	0.55
9:W:29:ASN:HB3	9:W:171:TRP:CE3	2.41	0.55
10:J:144:PRO:CG	11:Y:207:ASN:ND2	2.70	0.55
14:N:20:THR:HG22	15:N:1404:BO2:H221	1.87	0.55
6:T:54:ILE:HG12	6:T:208:PHE:HA	1.88	0.55
11:K:123:ASP:HB2	11:K:124:ILE:HD12	1.87	0.55
7:U:168:LYS:HE3	16:U:277:HOH:O	2.05	0.55
3:Q:45:CYS:HA	3:Q:141:PHE:HZ	1.70	0.55
5:E:132:TYR:O	5:E:153:PRO:HB3	2.06	0.55
5:S:67:ILE:HG21	5:S:223:ILE:HD12	1.88	0.55
2:B:214:THR:C	2:B:215:ILE:HD13	2.26	0.55
13:1:40:ASN:HD22	13:1:40:ASN:N	1.94	0.55
4:R:12(D):ALA:HB3	4:R:126:ARG:CD	2.35	0.55
8:V:100:ILE:HD11	8:V:127:LEU:HG	1.87	0.55
6:F:54:ILE:HG12	6:F:208:PHE:HA	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:29:ASN:HB3	9:I:171:TRP:CE3	2.41	0.55
3:Q:159:SER:HB2	16:Q:261:HOH:O	2.06	0.55
13:M:184:LEU:HD23	13:M:185:THR:N	2.21	0.55
3:C:182:PRO:O	3:C:184:ALA:N	2.39	0.55
11:K:35:ILE:HD12	11:K:56:GLU:HB3	1.89	0.55
6:T:192:GLN:NE2	6:T:195:LYS:CE	2.69	0.55
2:B:225:LYS:HG3	2:B:228:GLU:OE1	2.06	0.55
2:B:121:GLN:CG	3:C:83:ALA:HB1	2.36	0.55
2:P:71:ASN:ND2	2:P:72:ASP:N	2.43	0.55
8:H:100:ILE:HD11	8:H:127:LEU:HG	1.87	0.55
7:U:72:ARG:HB2	7:U:72:ARG:HH11	1.72	0.55
10:X:14:LEU:HD12	10:X:42:LEU:HD23	1.89	0.55
9:W:174:VAL:HG21	9:W:186:LYS:HE3	1.88	0.55
10:J:147:THR:OG1	10:J:150:GLU:HG3	2.05	0.55
5:E:75:GLY:O	5:E:139:ILE:CD1	2.54	0.55
6:F:95:GLU:CG	6:F:115:ARG:HB3	2.35	0.55
3:Q:83:ALA:O	3:Q:87:ILE:HD12	2.07	0.55
10:J:24:ILE:HG13	10:X:133:TYR:OH	2.06	0.55
2:B:20:ARG:HH11	2:B:20:ARG:HG2	1.71	0.55
13:1:149:GLN:H	13:1:149:GLN:NE2	2.04	0.55
11:K:7:ARG:HD2	11:K:108:PRO:O	2.06	0.55
14:N:14:LEU:O	14:N:175:MET:HA	2.06	0.55
8:H:179:GLU:OE2	8:H:182:LYS:HE2	2.06	0.55
13:1:3:VAL:HG12	13:1:49:ILE:CD1	2.34	0.55
5:S:2(C):VAL:HG13	5:S:2(D):ASP:N	2.21	0.55
5:E:2(C):VAL:HG13	5:E:2(D):ASP:N	2.21	0.55
12:L:166:HIS:HD2	12:L:168:GLN:H	1.55	0.55
8:H:15:ALA:HB1	8:H:159:ILE:HD13	1.89	0.55
6:F:38:ILE:HD11	6:F:197:ILE:HD11	1.88	0.55
9:I:7:THR:HG21	9:I:110:ILE:HD12	1.86	0.55
12:Z:33:LYS:HD2	12:Z:46:ASN:ND2	2.22	0.54
11:Y:99:THR:CG2	11:Y:113:VAL:HB	2.36	0.54
6:F:203:GLU:C	6:F:205:ASN:H	2.10	0.54
14:2:20:THR:HG22	15:2:1405:BO2:H221	1.89	0.54
5:S:198:SER:HA	5:S:201:LEU:CG	2.34	0.54
7:G:224:LEU:HB2	7:G:229:ILE:HD11	1.90	0.54
14:2:174:ARG:HG2	14:2:18(A):ILE:HD12	1.90	0.54
1:O:159:PRO:HB2	2:P:60:GLU:HB3	1.89	0.54
14:2:156:LYS:HG2	14:2:18(J):LEU:HD11	1.88	0.54
7:G:158:VAL:HG22	7:G:159:GLY:N	2.22	0.54
8:V:179:GLU:OE2	8:V:182:LYS:HE2	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:169:SER:HA	3:C:172:VAL:CG1	2.37	0.54
9:I:29:ASN:HD21	11:Y:208:ASN:ND2	2.05	0.54
9:I:165:ARG:NH2	12:Z:135:MET:CE	2.70	0.54
5:S:86:ARG:HH11	5:S:86:ARG:HG3	1.72	0.54
5:E:179:THR:O	5:E:179:THR:HG22	2.07	0.54
1:O:232:ARG:HH11	1:O:232:ARG:HG3	1.73	0.54
1:O:118:LYS:HE2	1:O:122:GLU:OE1	2.07	0.54
2:P:21:LEU:HD13	2:P:124:THR:HG23	1.89	0.54
2:P:20:ARG:HH11	2:P:20:ARG:HG2	1.73	0.54
5:S:67:ILE:HG21	5:S:223:ILE:CD1	2.37	0.54
14:N:48:SER:HB3	14:N:51:ASP:HB2	1.90	0.54
11:Y:10(B):LYS:CD	11:Y:10(B):LYS:N	2.59	0.54
16:X:221:HOH:O	11:Y:132:THR:HG22	2.06	0.54
11:K:180:GLU:CB	16:K:1426:HOH:O	2.53	0.54
5:E:74:MET:CE	5:E:96:CYS:SG	2.95	0.54
2:P:202:THR:HG22	2:P:204:SER:N	2.07	0.54
7:U:107:MET:HE3	7:U:112:LEU:HD13	1.90	0.54
2:P:87:ILE:O	2:P:91:THR:HG23	2.08	0.54
6:T:51:GLU:OE1	6:T:53:LEU:HD21	2.08	0.54
6:F:192:GLN:O	6:F:196:ILE:HG12	2.08	0.54
5:E:58:LEU:HD12	5:E:58:LEU:N	2.23	0.54
13:1:184:LEU:HD23	13:1:185:THR:N	2.23	0.54
7:U:236:ILE:HG13	7:U:237:ALA:N	2.22	0.54
10:X:113:ILE:HG12	10:X:119:LYS:HG3	1.89	0.54
6:T:186:ALA:O	6:T:190:VAL:HG23	2.07	0.54
6:F:63:LYS:O	6:F:65:VAL:HG23	2.08	0.54
4:R:31:ILE:HD13	4:R:80:GLY:HA3	1.90	0.54
3:Q:177:GLU:OE2	4:R:57:PRO:HD2	2.08	0.54
2:B:14:ILE:H	2:B:14:ILE:CD1	2.20	0.54
8:H:22:GLN:HG3	15:H:1400:BO2:C6	2.36	0.54
5:E:210:LEU:HD22	5:E:233:ILE:CD1	2.37	0.54
7:U:77:VAL:CG1	7:U:137:THR:HB	2.37	0.54
6:F:109:ILE:CD1	6:F:142:ASP:HB3	2.37	0.54
1:A:232:ARG:HG3	1:A:232:ARG:HH11	1.72	0.54
4:R:207:LEU:C	4:R:207:LEU:HD23	2.28	0.54
5:E:86:ARG:HH11	5:E:86:ARG:HG3	1.73	0.54
3:Q:173:ARG:O	3:Q:177:GLU:HG3	2.08	0.54
14:2:163:ILE:HG23	14:2:170:GLY:HA2	1.88	0.54
1:A:97:HIS:HD2	8:H:61:SER:OG	1.91	0.54
14:N:176:VAL:HG12	14:N:178:LEU:HD13	1.89	0.54
5:E:198:SER:HA	5:E:201:LEU:CG	2.35	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:31:ILE:HD12	5:E:31:ILE:H	1.72	0.53
10:J:168:MET:HE1	10:X:167:PRO:CB	2.37	0.53
3:C:33:ARG:HB2	3:C:33:ARG:HH11	1.71	0.53
8:V:148:LYS:HE3	8:V:177:VAL:HG11	1.89	0.53
2:P:20:ARG:NH1	2:P:20:ARG:HG2	2.23	0.53
2:P:121:GLN:CD	3:Q:87:ILE:HD11	2.28	0.53
9:W:55:LEU:CD1	9:W:97:VAL:HG21	2.38	0.53
6:F:11:SER:HB3	6:F:14:VAL:CG2	2.38	0.53
4:D:40:ILE:HG13	4:D:193:VAL:CG2	2.38	0.53
5:E:2(C):VAL:O	5:E:226:GLY:HA2	2.09	0.53
14:N:175:MET:HE3	14:N:18(B):PHE:CE2	2.42	0.53
12:L:175:ILE:HD12	12:L:175:ILE:N	2.23	0.53
13:1:104:VAL:HG23	13:1:178:ILE:HG22	1.91	0.53
3:Q:221:ILE:N	3:Q:221:ILE:HD12	2.24	0.53
12:Z:148:VAL:O	12:Z:152:ILE:HG13	2.08	0.53
4:R:31:ILE:HD11	4:R:133:GLY:C	2.28	0.53
12:L:-7:ASN:HD22	12:L:-6:PRO:N	2.06	0.53
3:Q:52:ARG:HD2	3:Q:208:LYS:O	2.08	0.53
2:B:20:ARG:NH1	2:B:20:ARG:HG2	2.23	0.53
2:P:76:VAL:HG21	2:P:89:ILE:CD1	2.39	0.53
2:P:152:ASN:HB2	2:P:153:PRO:CD	2.38	0.53
2:P:31:ILE:HD11	2:P:153:PRO:HG2	1.90	0.53
13:M:40:ASN:HD22	13:M:40:ASN:N	1.93	0.53
6:T:203:GLU:C	6:T:205:ASN:H	2.10	0.53
12:L:135:MET:CE	9:W:165:ARG:NH2	2.72	0.53
5:E:95:GLN:HG3	5:E:115:LEU:HD13	1.91	0.53
3:Q:169:SER:HA	3:Q:172:VAL:CG1	2.38	0.53
11:K:156:LYS:HB2	11:K:175:LEU:HD11	1.90	0.53
4:R:38:ILE:HD12	4:R:197:LEU:HG	1.91	0.53
5:S:138:ILE:N	5:S:138:ILE:HD12	2.23	0.53
1:A:173:LYS:O	1:A:177:GLU:HG3	2.08	0.53
7:G:14:ILE:HD13	7:G:14:ILE:H	1.72	0.53
10:J:177:ILE:CD1	10:J:187:VAL:HG23	2.38	0.53
5:S:2(C):VAL:O	5:S:226:GLY:HA2	2.09	0.53
6:T:192:GLN:O	6:T:196:ILE:HG12	2.09	0.53
13:1:45:ILE:HG23	13:1:99:ILE:HD11	1.91	0.53
5:E:68:ILE:HD12	5:E:68:ILE:N	2.24	0.53
14:2:19:ARG:HD3	14:2:26:ILE:HD12	1.90	0.53
1:A:118:LYS:HE2	1:A:122:GLU:OE1	2.08	0.53
6:T:120:VAL:HG21	6:T:151:LEU:HD21	1.89	0.53
12:L:33:LYS:HD2	12:L:46:ASN:HD22	1.74	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:33:ARG:NH1	3:Q:33:ARG:CB	2.71	0.53
2:P:101:LYS:HZ2	10:X:85:GLN:NE2	2.05	0.53
8:H:8:PHE:HB3	8:H:151:ALA:HB2	1.91	0.53
5:E:18(D):ILE:HG23	5:E:18(E):LYS:HG3	1.89	0.53
9:W:1:GLY:HA3	9:W:33:LYS:HE2	1.90	0.53
10:J:168:MET:CE	10:X:168:MET:HE3	2.38	0.53
14:2:107:LYS:HG2	14:2:108:GLY:N	2.23	0.53
12:L:42:VAL:CG2	12:L:102:ALA:HB3	2.38	0.53
13:1:84:ALA:HA	13:1:113:VAL:HG21	1.91	0.53
5:S:12:THR:HG21	5:S:124:THR:HA	1.91	0.53
11:K:66:HIS:CG	11:K:74:ILE:HD13	2.43	0.53
12:Z:42:VAL:HG23	12:Z:102:ALA:HB3	1.90	0.53
2:B:121:GLN:HG3	3:C:83:ALA:HB1	1.90	0.52
7:U:18(A):ILE:CD1	7:U:18(A):ILE:C	2.77	0.52
9:I:174:VAL:HG21	9:I:186:LYS:HE3	1.90	0.52
4:D:207:LEU:HD23	4:D:207:LEU:C	2.28	0.52
12:Z:4:LEU:HD11	12:Z:6:ILE:HD11	1.92	0.52
2:P:137:ILE:HD11	2:P:165:VAL:HG22	1.89	0.52
6:T:82:ILE:HB	6:T:83:PRO:HD3	1.92	0.52
14:2:19:ARG:CG	14:2:26:ILE:HD12	2.39	0.52
11:K:174:ASN:HD21	11:K:189:ASN:HD22	1.58	0.52
8:V:108:SER:HB3	8:V:180:ILE:HD11	1.92	0.52
13:M:84:ALA:HA	13:M:113:VAL:HG21	1.90	0.52
14:N:113:ILE:N	14:N:113:ILE:HD12	2.24	0.52
5:S:58:LEU:N	5:S:58:LEU:HD12	2.23	0.52
2:B:87:ILE:O	2:B:91:THR:HG23	2.09	0.52
3:C:52:ARG:HD2	3:C:208:LYS:O	2.09	0.52
5:E:70:CYS:SG	5:E:92:LEU:HD23	2.49	0.52
6:F:186:ALA:O	6:F:190:VAL:HG23	2.09	0.52
1:A:215:ILE:N	1:A:215:ILE:HD12	2.24	0.52
6:T:63:LYS:O	6:T:65:VAL:HG23	2.08	0.52
5:E:227:GLU:CD	5:E:227:GLU:N	2.63	0.52
6:F:210:LEU:HD21	6:F:212:ILE:HD11	1.91	0.52
2:P:5:SER:O	2:P:7:ARG:N	2.43	0.52
7:G:72:ARG:HB2	7:G:72:ARG:HH11	1.74	0.52
7:U:233:LEU:O	7:U:236:ILE:HG12	2.09	0.52
6:F:158:TRP:CZ3	7:G:64:VAL:HA	2.45	0.52
12:L:109:ALA:HB2	12:L:121:ARG:NH2	2.24	0.52
12:L:93:PHE:N	12:L:94:PRO:HD3	2.24	0.52
4:D:12(D):ALA:HA	5:E:129:GLY:HA2	1.90	0.52
12:L:101:ILE:HD12	12:L:101:ILE:C	2.30	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:107:LYS:HG2	14:N:108:GLY:N	2.25	0.52
12:Z:93:PHE:N	12:Z:94:PRO:HD3	2.25	0.52
6:F:21(B):THR:O	6:F:21(C):ASN:HB2	2.10	0.52
7:U:158:VAL:HG22	7:U:159:GLY:N	2.24	0.52
13:M:-6:GLN:O	13:M:-6:GLN:HG3	2.09	0.52
2:P:27:ALA:O	2:P:30:SER:HB3	2.10	0.52
6:T:74:ILE:HG12	6:T:109:ILE:HD11	1.90	0.52
13:M:19:LEU:HD12	13:M:20:GLY:H	1.75	0.52
2:P:137:ILE:CD1	2:P:165:VAL:HG22	2.40	0.52
3:C:216:LYS:HB2	3:C:220:ASP:HB3	1.92	0.52
10:J:14:LEU:HD12	10:J:42:LEU:HD23	1.90	0.52
4:D:53:ARG:HG2	4:D:53:ARG:O	2.10	0.52
4:R:160:TYR:CE2	4:R:163:LYS:HD3	2.45	0.52
3:C:173:ARG:O	3:C:177:GLU:HG3	2.10	0.52
11:K:12:ILE:HD12	11:K:110:ILE:CG1	2.40	0.52
1:O:173:LYS:O	1:O:177:GLU:HG3	2.09	0.52
6:F:192:GLN:NE2	6:F:195:LYS:CE	2.73	0.52
4:D:177:LEU:HD22	5:E:58:LEU:CD1	2.40	0.52
4:D:38:ILE:HD12	4:D:197:LEU:HG	1.91	0.52
5:E:54:ASN:ND2	5:E:56:ASP:O	2.41	0.52
13:M:171:ARG:HG3	13:M:192:VAL:HB	1.92	0.52
6:F:127:ASN:HD22	6:F:127:ASN:N	2.07	0.52
2:B:111:ILE:N	2:B:111:ILE:HD12	2.25	0.52
5:S:207:LEU:HA	5:S:2(E):ASN:HD22	1.75	0.52
14:2:112:THR:CG2	14:2:120:HIS:HB2	2.38	0.52
7:U:87:ASN:ND2	7:U:87:ASN:C	2.62	0.52
12:Z:137:PHE:CE1	12:Z:141:GLN:HG3	2.45	0.52
5:S:52:LYS:CB	5:S:63:TYR:HB3	2.40	0.52
2:B:71:ASN:ND2	2:B:72:ASP:N	2.45	0.52
3:Q:76:LEU:HD12	3:Q:138:ILE:HG12	1.92	0.52
8:V:159:ILE:HG22	8:V:163:ILE:CD1	2.40	0.52
8:V:17:ASP:HB3	8:V:163:ILE:HD11	1.90	0.52
14:N:163:ILE:HG23	14:N:170:GLY:HA2	1.91	0.52
4:R:70:ILE:HD12	4:R:74:ILE:HG21	1.92	0.52
3:C:57:LYS:NZ	3:C:58:LEU:HA	2.25	0.52
6:F:51:GLU:OE1	6:F:53:LEU:HD21	2.10	0.51
2:B:234:VAL:HA	2:B:239:THR:HA	1.93	0.51
4:D:40:ILE:CD1	4:D:193:VAL:HG23	2.40	0.51
4:R:121:LEU:HB2	16:R:853:HOH:O	2.10	0.51
5:S:210:LEU:HD11	5:S:212:ILE:HD11	1.91	0.51
7:U:96:ALA:HA	7:U:107:MET:CE	2.33	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:-7:ASN:HD22	12:Z:-6:PRO:N	2.07	0.51
6:T:20(B):GLU:HG3	6:T:20(C):LYS:N	2.25	0.51
6:T:11:SER:HB3	6:T:14:VAL:CG2	2.40	0.51
10:J:52:THR:HG22	10:J:53:VAL:N	2.25	0.51
9:I:137:MET:HE3	9:I:141:LEU:HD11	1.92	0.51
13:1:-6:GLN:O	13:1:-6:GLN:HG3	2.09	0.51
5:S:82:ALA:HB3	5:S:83:PRO:HD3	1.92	0.51
9:W:19:ARG:HB2	9:W:171:TRP:HB2	1.92	0.51
8:H:148:LYS:O	8:H:152:ILE:HG13	2.09	0.51
10:J:113:ILE:HG12	10:J:119:LYS:HG3	1.92	0.51
13:1:110:LEU:HG	13:1:125:LEU:HD12	1.92	0.51
12:L:5:GLY:O	12:L:124:CYS:HA	2.11	0.51
8:V:8:PHE:HB3	8:V:151:ALA:HB2	1.92	0.51
5:E:67:ILE:HG21	5:E:223:ILE:CD1	2.41	0.51
10:J:177:ILE:HD11	10:J:187:VAL:HG22	1.90	0.51
5:S:18(D):ILE:HG23	5:S:18(E):LYS:HG3	1.91	0.51
7:G:87:ASN:ND2	7:G:87:ASN:C	2.64	0.51
12:L:-8:PHE:CB	13:M:-8:THR:HG23	2.40	0.51
11:K:207:ASN:ND2	10:X:144:PRO:CG	2.73	0.51
10:J:144:PRO:CG	11:Y:207:ASN:HD21	2.24	0.51
3:Q:216:LYS:HB2	3:Q:220:ASP:HB3	1.92	0.51
5:E:47:VAL:HG22	5:E:214:ILE:HD13	1.92	0.51
4:D:138:ILE:N	4:D:138:ILE:HD12	2.25	0.51
7:G:12:ILE:HD13	7:G:12:ILE:N	2.26	0.51
6:F:40:ILE:N	6:F:40:ILE:HD12	2.26	0.51
7:U:41:ARG:CG	7:U:148:ILE:HD13	2.41	0.51
3:C:227:GLU:OE1	3:C:227:GLU:N	2.42	0.51
2:B:27:ALA:O	2:B:30:SER:HB3	2.11	0.51
11:K:126:CYS:HB2	11:K:135:TYR:CE1	2.45	0.51
14:N:54:ALA:O	14:N:58:ILE:HG12	2.11	0.51
5:E:18(C):PHE:HA	5:E:18(F):ILE:HG13	1.92	0.51
2:P:51:GLU:OE2	2:P:209:ARG:NH2	2.44	0.51
12:Z:100:ILE:N	12:Z:100:ILE:HD12	2.26	0.51
7:G:18(G):GLU:CG	7:G:188:LYS:HB2	2.34	0.51
5:S:70:CYS:SG	5:S:92:LEU:HD23	2.49	0.51
5:S:73:HIS:CE1	5:S:74:MET:HE2	2.46	0.51
9:W:103:GLY:C	9:W:104:ILE:HD12	2.31	0.51
6:F:109:ILE:H	6:F:109:ILE:HD12	1.75	0.51
8:H:148:LYS:HE3	8:H:177:VAL:HG11	1.91	0.51
6:F:82:ILE:HB	6:F:83:PRO:HD3	1.91	0.51
12:L:137:PHE:CE1	12:L:141:GLN:HG3	2.45	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:227:GLU:N	5:S:227:GLU:CD	2.64	0.51
5:S:40:LEU:HD23	5:S:40:LEU:N	2.26	0.51
2:P:124:THR:CG2	3:Q:130:ARG:HH21	2.21	0.51
12:Z:42:VAL:CG2	12:Z:102:ALA:HB3	2.41	0.51
13:1:66:ASN:HB3	16:1:221:HOH:O	2.10	0.51
2:P:126:HIS:HB3	3:Q:129:VAL:HG12	1.92	0.51
5:S:49:VAL:CG1	5:S:212:ILE:HD12	2.32	0.51
7:U:18(G):GLU:CG	7:U:188:LYS:HB2	2.36	0.51
9:W:14:ILE:HG12	9:W:34:ILE:HD12	1.93	0.51
10:J:168:MET:CE	10:X:168:MET:CE	2.89	0.51
2:B:213:ALA:CB	2:B:223:ILE:HD13	2.40	0.51
6:T:192:GLN:NE2	6:T:195:LYS:HE3	2.26	0.51
6:T:175:GLU:OE1	6:T:199:LEU:HD23	2.11	0.51
14:2:10(B):LYS:HD3	14:2:10(B):LYS:O	2.10	0.51
10:X:18:LYS:CD	10:X:174:ILE:HG13	2.40	0.51
9:I:55:LEU:CD1	9:I:97:VAL:HG21	2.41	0.51
2:B:137:ILE:HD11	2:B:165:VAL:HG22	1.92	0.51
3:Q:57:LYS:NZ	3:Q:58:LEU:HA	2.25	0.51
11:K:66:HIS:CD2	11:K:74:ILE:HD13	2.46	0.51
6:T:63:LYS:O	6:T:65:VAL:N	2.44	0.51
11:Y:13:ILE:HD12	11:Y:152:LEU:HD23	1.93	0.51
14:2:48:SER:HB3	14:2:51:ASP:HB2	1.92	0.51
8:V:63:ILE:HD11	8:V:79:ALA:HA	1.93	0.51
2:B:27:ALA:O	2:B:31:ILE:HG12	2.12	0.51
7:U:131:PRO:HB3	16:U:261:HOH:O	2.10	0.51
12:Z:14(I):THR:HG21	12:Z:14(M):VAL:HB	1.93	0.51
12:L:90:LYS:HD3	12:L:95:TYR:CZ	2.46	0.51
10:X:10(B):LYS:HB2	10:X:10(B):LYS:HZ3	1.76	0.50
14:2:146:MET:CE	14:2:150:GLU:HB3	2.41	0.50
14:N:10(B):LYS:O	14:N:10(B):LYS:HD3	2.10	0.50
3:C:57:LYS:O	3:C:58:LEU:HB2	2.11	0.50
3:Q:220:ASP:C	3:Q:221:ILE:HD12	2.31	0.50
5:E:45:HIS:HB3	5:E:214:ILE:HD11	1.93	0.50
4:D:170:GLU:N	4:D:170:GLU:OE1	2.44	0.50
6:F:18:ASP:OD1	6:F:20:ARG:HD3	2.11	0.50
10:J:64:GLN:NE2	16:J:217:HOH:O	2.33	0.50
11:Y:156:LYS:HB2	11:Y:175:LEU:HD11	1.92	0.50
4:D:215:ILE:HD13	4:D:215:ILE:C	2.31	0.50
3:C:136:THR:O	3:C:150:GLN:HA	2.11	0.50
11:K:10(A):ARG:H	11:K:10(B):LYS:HZ2	1.56	0.50
14:N:112:THR:CG2	14:N:120:HIS:HB2	2.39	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:78:VAL:HG11	7:U:85:ALA:CB	2.41	0.50
7:U:136:LEU:O	7:U:150:LYS:HA	2.10	0.50
8:H:18:THR:HB	8:H:30:ASN:HA	1.94	0.50
9:I:110:ILE:HG12	9:I:125:ILE:CD1	2.42	0.50
2:P:31:ILE:HD11	2:P:153:PRO:CG	2.42	0.50
6:F:175:GLU:CB	6:F:196:ILE:HD12	2.42	0.50
13:M:17:ASP:HA	13:M:173:PHE:CB	2.42	0.50
4:R:215:ILE:HD13	4:R:215:ILE:C	2.31	0.50
13:1:13:ILE:CD1	13:1:177:ILE:CG2	2.82	0.50
6:F:67:ILE:HD13	6:F:77:VAL:CB	2.40	0.50
14:2:159:LEU:HB3	14:2:173:ILE:HD12	1.92	0.50
14:2:1:THR:HG22	14:2:3:ILE:HD12	1.93	0.50
9:W:113:PHE:HA	9:W:118:CYS:O	2.11	0.50
10:X:52:THR:CG2	10:X:53:VAL:N	2.75	0.50
3:C:149:TYR:CE1	3:C:159:SER:HB3	2.46	0.50
5:E:12:THR:HG21	5:E:124:THR:HA	1.92	0.50
13:M:14(A):VAL:O	13:M:14(A):VAL:HG23	2.12	0.50
12:Z:5:GLY:O	12:Z:124:CYS:HA	2.11	0.50
6:T:127:ASN:HD22	6:T:127:ASN:N	2.08	0.50
12:L:14(I):THR:HG21	12:L:14(M):VAL:HB	1.94	0.50
2:P:108:PRO:CG	2:P:111:ILE:HD12	2.41	0.50
1:A:150:GLN:O	1:A:157:TYR:HA	2.11	0.50
1:O:150:GLN:O	1:O:157:TYR:HA	2.11	0.50
5:E:40:LEU:HD23	5:E:40:LEU:N	2.27	0.50
13:1:14(A):VAL:O	13:1:14(A):VAL:HG23	2.12	0.50
6:F:38:ILE:HD11	6:F:197:ILE:CD1	2.42	0.50
13:M:104:VAL:HG23	13:M:178:ILE:HG22	1.94	0.50
10:X:113:ILE:HA	10:X:118:THR:O	2.12	0.50
10:J:52:THR:CG2	10:J:53:VAL:N	2.74	0.50
5:E:18(C):PHE:HA	5:E:18(F):ILE:CD1	2.42	0.50
9:W:101:VAL:O	9:W:110:ILE:HA	2.12	0.50
8:V:84:LYS:HG3	8:V:85:GLN:N	2.26	0.50
3:Q:156:ILE:HD13	4:R:83:ALA:HB2	1.92	0.50
12:L:84:GLN:HG3	12:L:117:GLY:O	2.12	0.50
14:N:22:THR:O	14:N:22:THR:HG22	2.11	0.50
1:O:4:MET:SD	1:O:5:THR:N	2.67	0.50
2:B:95:HIS:HB2	16:B:259:HOH:O	2.12	0.50
4:D:160:TYR:CE2	4:D:163:LYS:HD3	2.47	0.50
4:D:194:LEU:HD21	4:D:233:ILE:CD1	2.42	0.50
2:P:101:LYS:HZ2	10:X:85:GLN:HE21	1.59	0.50
6:F:20(B):GLU:HG3	6:F:20(C):LYS:N	2.26	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:124:ILE:N	11:K:124:ILE:HD12	2.26	0.50
12:L:13:VAL:HG12	12:L:177:ILE:HG13	1.93	0.50
8:H:81:GLN:O	8:H:85:GLN:HG3	2.12	0.50
5:S:39:GLY:O	5:S:162:GLY:HA2	2.12	0.50
4:R:185:THR:OG1	4:R:188:GLU:HG3	2.12	0.50
11:K:211:GLY:HA2	8:V:214:LEU:HD13	1.94	0.50
2:B:4:GLY:HA3	5:E:127:TYR:CE1	2.46	0.50
13:M:57:ARG:NE	16:M:245:HOH:O	2.44	0.50
12:Z:5:GLY:C	12:Z:6:ILE:HD12	2.31	0.50
12:Z:101:ILE:HD12	12:Z:101:ILE:C	2.32	0.50
4:R:75:GLY:HA3	4:R:221:PHE:CD2	2.46	0.50
6:T:175:GLU:CB	6:T:196:ILE:HD12	2.41	0.50
8:V:81:GLN:O	8:V:85:GLN:HG3	2.12	0.50
12:L:177:ILE:HD12	12:L:177:ILE:N	2.27	0.50
4:D:75:GLY:HA3	4:D:221:PHE:CD2	2.46	0.50
6:T:21(B):THR:O	6:T:21(C):ASN:HB2	2.11	0.50
5:E:97:ASN:HD21	12:L:61:ASN:HD21	1.59	0.50
8:V:41:ILE:N	8:V:41:ILE:HD12	2.27	0.49
12:L:100:ILE:HD12	12:L:100:ILE:N	2.26	0.49
13:1:19:LEU:HD12	13:1:20:GLY:H	1.77	0.49
2:B:147:GLN:HB3	3:C:62(A):ILE:HD13	1.94	0.49
7:G:78:VAL:HG11	7:G:85:ALA:CB	2.42	0.49
12:Z:109:ALA:HB2	12:Z:121:ARG:NH2	2.27	0.49
11:K:13:ILE:HD12	11:K:152:LEU:HD23	1.94	0.49
6:F:175:GLU:OE1	6:F:199:LEU:HD23	2.11	0.49
5:S:38:VAL:HG12	5:S:39:GLY:N	2.27	0.49
8:H:210:THR:CG2	12:Z:14(C):GLN:HG2	2.42	0.49
7:G:177:GLU:O	7:G:17(B):LYS:HG3	2.12	0.49
6:T:18:ASP:OD1	6:T:20:ARG:HD3	2.12	0.49
8:H:214:LEU:HD13	11:Y:211:GLY:HA2	1.92	0.49
3:Q:227:GLU:OE1	3:Q:227:GLU:N	2.44	0.49
11:Y:124:ILE:HD12	11:Y:124:ILE:N	2.26	0.49
14:2:3:ILE:HG22	14:2:16:ALA:CB	2.42	0.49
8:H:84:LYS:HG3	8:H:85:GLN:N	2.26	0.49
13:1:171:ARG:HG3	13:1:192:VAL:HB	1.95	0.49
14:N:84:LYS:HG3	14:N:119:VAL:HG22	1.94	0.49
5:E:52:LYS:CB	5:E:63:TYR:HB3	2.43	0.49
5:S:194:VAL:CG1	5:S:207:LEU:HD11	2.43	0.49
5:S:2(B):THR:OG1	5:S:2(E):ASN:HB3	2.13	0.49
10:X:2:ILE:HD13	10:X:170:PHE:CG	2.47	0.49
5:E:2(B):THR:OG1	5:E:2(E):ASN:HB3	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:215:ILE:CD1	2:B:221:GLN:HG2	2.38	0.49
2:P:101:LYS:HG3	9:W:57:GLU:HB3	1.94	0.49
14:2:1:THR:HG22	14:2:3:ILE:CD1	2.43	0.49
6:T:18:ASP:N	6:T:18:ASP:OD2	2.40	0.49
9:I:113:PHE:HA	9:I:118:CYS:O	2.11	0.49
7:G:136:LEU:O	7:G:150:LYS:HA	2.12	0.49
12:Z:177:ILE:N	12:Z:177:ILE:HD12	2.27	0.49
3:Q:136:THR:O	3:Q:150:GLN:HA	2.12	0.49
13:M:1:THR:HG22	16:M:214:HOH:O	2.12	0.49
2:B:53:LYS:HG2	2:B:54:VAL:HG23	1.94	0.49
1:O:32:LYS:HE2	1:O:32:LYS:HA	1.95	0.49
13:1:19:LEU:HD12	13:1:28:PHE:O	2.12	0.49
3:C:227:GLU:CD	3:C:227:GLU:H	2.16	0.49
5:S:52:LYS:HB2	5:S:63:TYR:HB3	1.92	0.49
2:P:95:HIS:HB2	16:P:243:HOH:O	2.13	0.49
5:E:38:VAL:HG12	5:E:39:GLY:N	2.28	0.49
10:J:90(B):ARG:HH11	10:J:90(B):ARG:HG2	1.78	0.49
2:B:107:ILE:HD11	2:B:111:ILE:HG22	1.95	0.49
2:B:51:GLU:OE2	2:B:202:THR:HG23	2.12	0.49
5:S:194:VAL:HG13	5:S:207:LEU:CD1	2.42	0.49
12:L:101:ILE:O	12:L:101:ILE:HD12	2.12	0.49
14:2:100:ILE:HD11	14:2:127:ALA:CB	2.40	0.49
2:P:4:GLY:HA3	5:S:127:TYR:CZ	2.47	0.49
12:L:135:MET:HE3	9:W:165:ARG:NH2	2.27	0.49
10:X:52:THR:HG22	10:X:53:VAL:N	2.28	0.49
5:S:11:ASP:OD1	5:S:13:VAL:HG12	2.12	0.49
6:F:56:SER:OG	6:F:57:LYS:N	2.45	0.49
13:1:17:ASP:HA	13:1:173:PHE:CB	2.42	0.49
1:A:32:LYS:HE2	1:A:32:LYS:HA	1.94	0.49
7:U:46:THR:HG23	7:U:148:ILE:HD11	1.95	0.49
2:B:185:LYS:HE2	2:B:187:ASP:OD1	2.13	0.49
13:M:19:LEU:HD12	13:M:28:PHE:O	2.13	0.49
2:P:234:VAL:HA	2:P:239:THR:HA	1.94	0.49
9:I:8:SER:O	9:I:6:PRO:HD3	2.12	0.49
10:J:111:TYR:CE1	10:J:121:GLU:HG3	2.48	0.49
11:Y:126:CYS:HB2	11:Y:135:TYR:CE1	2.47	0.49
5:E:116:LEU:CD1	5:E:138:ILE:HD11	2.42	0.49
10:X:90(A):ILE:CD1	10:X:116:LEU:HD23	2.42	0.49
4:D:233:ILE:N	4:D:233:ILE:HD12	2.28	0.49
5:S:201:LEU:HD11	5:S:207:LEU:CD2	2.42	0.49
5:E:207:LEU:HA	5:E:2(E):ASN:HD22	1.76	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:56:ASP:HB3	7:G:59:LEU:HG	1.95	0.49
12:L:76:ILE:HD11	12:L:101:ILE:CD1	2.42	0.49
12:Z:101:ILE:HD12	12:Z:101:ILE:O	2.13	0.49
2:B:137:ILE:CD1	2:B:165:VAL:HG22	2.42	0.49
9:W:104:ILE:CD1	9:W:178:ILE:HG22	2.43	0.49
8:V:18:THR:HB	8:V:30:ASN:HA	1.94	0.49
7:U:49:ILE:HD13	7:U:193:ALA:HB1	1.94	0.49
2:B:5:SER:O	2:B:7:ARG:N	2.45	0.49
14:2:21:THR:O	15:2:1405:BO2:H3	2.13	0.49
5:E:194:VAL:HG13	5:E:207:LEU:CD1	2.43	0.49
5:E:31:ILE:HD12	5:E:31:ILE:N	2.27	0.49
2:B:215:ILE:HD12	2:B:221:GLN:CG	2.39	0.49
13:M:40:ASN:ND2	13:M:40:ASN:N	2.61	0.49
14:2:155:ILE:HG22	14:2:175:MET:HE1	1.95	0.49
7:G:225:SER:O	7:G:229:ILE:HG12	2.12	0.49
14:2:163:ILE:CD1	14:2:173:ILE:HD11	2.43	0.49
12:L:14(C):GLN:HG2	8:V:210:THR:CG2	2.42	0.49
2:P:53:LYS:HG2	2:P:54:VAL:HG23	1.94	0.49
12:L:185:ARG:NH1	16:L:230:HOH:O	2.45	0.49
14:2:84:LYS:HG3	14:2:119:VAL:HG22	1.94	0.49
10:X:123:PRO:HB2	10:X:124:TYR:CD1	2.47	0.49
12:L:145:TYR:CD1	12:L:146:LEU:N	2.81	0.49
11:Y:86:LEU:C	11:Y:86:LEU:HD13	2.33	0.49
13:1:4:ILE:CD1	13:1:155:ILE:HG12	2.43	0.49
11:K:12:ILE:HD12	11:K:110:ILE:HD11	1.95	0.49
6:F:36:THR:HG22	6:F:51:GLU:OE2	2.13	0.49
5:S:54:ASN:ND2	5:S:56:ASP:O	2.42	0.49
6:F:63:LYS:O	6:F:65:VAL:N	2.45	0.49
4:D:112:LEU:C	4:D:112:LEU:HD13	2.33	0.49
12:L:3:ILE:CD1	12:L:46:ASN:CB	2.88	0.48
4:D:229:THR:C	4:D:233:ILE:HD13	2.31	0.48
11:K:7:ARG:CG	11:K:12:ILE:HD11	2.39	0.48
7:U:65:SER:OG	7:U:211:GLU:OE2	2.25	0.48
11:Y:123:ASP:CB	11:Y:124:ILE:HD12	2.43	0.48
11:Y:174:ASN:HD21	11:Y:189:ASN:HD22	1.60	0.48
6:T:176:LEU:O	6:T:180:VAL:HG23	2.13	0.48
13:M:178:ILE:CD1	13:M:184:LEU:HG	2.42	0.48
2:P:107:ILE:HD11	2:P:111:ILE:HG22	1.95	0.48
9:I:35:PHE:CD1	9:I:45:ILE:HD13	2.47	0.48
14:2:41:ILE:CD1	14:2:103:GLY:HA3	2.43	0.48
3:Q:57:LYS:O	3:Q:58:LEU:HB2	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:38:VAL:HG22	3:Q:39:GLY:N	2.27	0.48
6:T:56:SER:OG	6:T:57:LYS:N	2.44	0.48
13:M:197:TRP:CH2	14:2:171:GLY:HA2	2.48	0.48
6:T:35:THR:CG2	6:T:36:THR:N	2.77	0.48
4:D:196:ILE:N	4:D:196:ILE:HD13	2.27	0.48
5:E:210:LEU:CD2	5:E:233:ILE:HD11	2.44	0.48
14:2:174:ARG:NH1	14:2:18(A):ILE:HD13	2.28	0.48
4:D:185:THR:OG1	4:D:188:GLU:HG3	2.13	0.48
5:E:67:ILE:HG21	5:E:223:ILE:HD12	1.95	0.48
9:I:19:ARG:HB2	9:I:171:TRP:HB2	1.95	0.48
9:I:160:LEU:HD11	9:I:191:MET:HB3	1.96	0.48
10:X:161:GLU:OE2	10:X:161:GLU:HA	2.12	0.48
7:U:147:SER:O	7:U:148:ILE:HD12	2.11	0.48
3:C:163:GLN:HA	3:C:163:GLN:HE21	1.79	0.48
2:P:101:LYS:HZ1	10:X:85:GLN:NE2	2.09	0.48
5:S:52:LYS:HD2	5:S:63:TYR:O	2.13	0.48
9:W:18:LEU:CD2	9:W:32:GLU:HG2	2.43	0.48
14:2:54:ALA:O	14:2:58:ILE:HG13	2.13	0.48
5:S:175:TYR:CD2	5:S:196:ALA:HA	2.48	0.48
2:B:191:GLU:O	2:B:195:LYS:HG2	2.13	0.48
11:K:86:LEU:HD13	11:K:86:LEU:C	2.34	0.48
8:V:37:ILE:HG21	8:V:63:ILE:HD12	1.93	0.48
3:Q:156:ILE:CD1	4:R:83:ALA:HB2	2.44	0.48
3:Q:31:VAL:HG11	3:Q:135:SER:HB2	1.96	0.48
3:Q:235:GLN:O	3:Q:239:GLU:HG2	2.14	0.48
9:I:18:LEU:CD2	9:I:32:GLU:HG2	2.44	0.48
2:B:51:GLU:OE2	2:B:209:ARG:NH2	2.47	0.48
3:C:163:GLN:CA	3:C:163:GLN:HE21	2.27	0.48
5:S:214:ILE:HD13	5:S:214:ILE:C	2.33	0.48
10:J:177:ILE:CD1	10:J:187:VAL:CG2	2.86	0.48
3:Q:187:GLU:HG3	3:Q:232:TYR:OH	2.14	0.48
10:J:133:TYR:OH	10:X:24:ILE:HG13	2.14	0.48
2:B:185:LYS:CD	2:B:187:ASP:H	2.26	0.48
3:Q:227:GLU:H	3:Q:227:GLU:CD	2.17	0.48
9:I:178:ILE:N	9:I:178:ILE:HD12	2.29	0.48
9:I:156:SER:O	9:I:160:LEU:HB2	2.14	0.48
1:O:97:HIS:HD2	8:V:61:SER:OG	1.96	0.48
3:Q:14:ILE:C	3:Q:21:ILE:HD13	2.34	0.48
5:E:201:LEU:HD11	5:E:207:LEU:CD2	2.43	0.48
2:P:27:ALA:O	2:P:31:ILE:HG13	2.14	0.48
7:U:56:ASP:HB3	7:U:59:LEU:HG	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:147:GLN:CG	3:C:62(A):ILE:HD13	2.43	0.48
3:Q:55:THR:C	3:Q:56:LEU:HD22	2.34	0.48
1:A:222:ARG:HD2	16:A:275:HOH:O	2.13	0.48
12:Z:90:LYS:HD3	12:Z:95:TYR:CZ	2.48	0.48
5:E:175:TYR:CD2	5:E:196:ALA:HA	2.49	0.48
6:F:187:ARG:HG3	6:F:187:ARG:HH11	1.79	0.48
3:Q:79:SER:HB2	3:Q:165:ILE:HD12	1.96	0.48
4:D:121:LEU:HD23	4:D:123:PHE:HE1	1.79	0.48
5:E:82:ALA:HB3	5:E:83:PRO:HD3	1.95	0.48
5:S:66:LYS:O	5:S:77:SER:HA	2.13	0.48
8:H:208:ARG:CZ	9:I:149:GLU:HB2	2.44	0.48
2:P:51:GLU:OE2	2:P:202:THR:HG23	2.13	0.48
7:U:18(D):ILE:H	7:U:18(D):ILE:CD1	2.24	0.48
10:J:177:ILE:N	10:J:177:ILE:HD12	2.29	0.48
5:E:28:LEU:CA	5:E:31:ILE:HD13	2.37	0.48
2:B:69:LYS:HG3	2:B:221:GLN:OE1	2.14	0.48
2:P:185:LYS:HD3	2:P:186:VAL:H	1.79	0.48
9:W:178:ILE:N	9:W:178:ILE:HD12	2.29	0.48
10:X:143:ARG:HG2	10:X:143:ARG:NH1	2.29	0.48
11:K:207:ASN:ND2	10:X:144:PRO:HG3	2.28	0.48
7:U:78:VAL:HG11	7:U:85:ALA:HB2	1.96	0.48
5:E:4:PHE:CG	5:E:5:ARG:N	2.82	0.48
6:T:41:LYS:HA	6:T:46:VAL:HG12	1.96	0.48
3:C:38:VAL:HG22	3:C:39:GLY:N	2.29	0.48
6:T:172:ALA:O	6:T:176:LEU:HD23	2.14	0.47
3:Q:134:VAL:HG12	3:Q:135:SER:N	2.29	0.47
1:A:141:HIS:HA	1:A:146:GLY:O	2.14	0.47
3:C:79:SER:HB2	3:C:165:ILE:HD12	1.96	0.47
8:V:17:ASP:CB	8:V:163:ILE:HD11	2.44	0.47
14:N:155:ILE:HG22	14:N:175:MET:HE1	1.96	0.47
1:O:141:HIS:HA	1:O:146:GLY:O	2.14	0.47
3:C:235:GLN:O	3:C:239:GLU:HG2	2.14	0.47
5:S:4:PHE:CG	5:S:5:ARG:N	2.81	0.47
9:I:28:SER:CB	10:J:120:VAL:HG21	2.44	0.47
14:N:3:ILE:HG22	14:N:16:ALA:CB	2.43	0.47
1:O:62:GLU:CD	1:O:62:GLU:H	2.16	0.47
7:G:232:ARG:NE	7:G:232:ARG:HA	2.28	0.47
10:X:90(B):ARG:HG2	10:X:90(B):ARG:HH11	1.78	0.47
12:Z:145:TYR:CD1	12:Z:146:LEU:N	2.82	0.47
7:G:8:TYR:C	7:G:10:ARG:N	2.68	0.47
6:F:49:ALA:HB3	6:F:197:ILE:HD11	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1:-4:ILE:HD12	14:2:116:GLY:HA2	1.96	0.47
6:F:67:ILE:HD13	6:F:77:VAL:CG2	2.44	0.47
12:L:76:ILE:CD1	12:L:101:ILE:HD13	2.41	0.47
3:C:97:GLN:NE2	16:C:244:HOH:O	2.43	0.47
6:F:41:LYS:HA	6:F:46:VAL:HG12	1.96	0.47
7:G:49:ILE:HD13	7:G:193:ALA:HB1	1.95	0.47
1:A:40:ILE:HD12	1:A:193:ALA:HB2	1.96	0.47
7:U:177:GLU:O	7:U:17(B):LYS:HG3	2.15	0.47
6:F:176:LEU:O	6:F:180:VAL:HG23	2.14	0.47
9:W:160:LEU:HD11	9:W:191:MET:HB3	1.96	0.47
8:V:175:VAL:HG12	8:V:176:CYS:N	2.29	0.47
11:Y:4:LEU:O	11:Y:4:LEU:HD22	2.14	0.47
9:I:110:ILE:HG12	9:I:125:ILE:HD11	1.96	0.47
12:Z:4:LEU:HG	12:Z:6:ILE:CD1	2.45	0.47
5:E:74:MET:HE1	5:E:96:CYS:SG	2.53	0.47
7:G:77:VAL:HG12	7:G:137:THR:HB	1.97	0.47
14:2:3:ILE:HG22	14:2:16:ALA:HB2	1.96	0.47
5:S:69:LYS:HB3	16:S:237:HOH:O	2.14	0.47
1:A:60:MET:HE1	16:G:269:HOH:O	2.13	0.47
12:Z:9:GLU:O	12:Z:107:LYS:HA	2.14	0.47
9:I:14:ILE:HG12	9:I:34:ILE:HD12	1.96	0.47
1:O:71:THR:HG1	1:O:74:ILE:HD13	1.79	0.47
2:P:21:LEU:O	2:P:25:GLU:HG2	2.15	0.47
4:D:196:ILE:H	4:D:196:ILE:CD1	2.27	0.47
12:Z:167:ILE:HD12	12:Z:167:ILE:C	2.35	0.47
11:K:123:ASP:CB	11:K:124:ILE:HD12	2.43	0.47
6:F:127:ASN:HD22	6:F:128:SER:N	2.13	0.47
7:G:141:VAL:HG21	7:G:216:THR:HA	1.97	0.47
2:B:150:THR:O	2:B:157:TYR:HA	2.14	0.47
10:J:123:PRO:HB2	10:J:124:TYR:CD1	2.50	0.47
13:1:8:TYR:CZ	13:1:148:VAL:HG13	2.50	0.47
10:X:76:PRO:HD2	16:X:205:HOH:O	2.15	0.47
14:2:3:ILE:HD13	14:2:3:ILE:N	2.29	0.47
7:U:82:ILE:N	7:U:83:PRO:HD2	2.30	0.47
12:Z:-9:GLN:HE21	13:1:-8:THR:HG21	1.80	0.47
2:B:111:ILE:H	2:B:111:ILE:HD12	1.80	0.47
7:U:41:ARG:NH2	7:U:18(B):ASP:O	2.48	0.47
13:M:165:ARG:HA	14:2:26:ILE:HB	1.96	0.47
9:I:101:VAL:O	9:I:110:ILE:HA	2.14	0.47
9:I:6:MET:CE	9:I:155:ILE:HA	2.45	0.47
2:B:160:TRP:CD2	2:B:163:ILE:HD12	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1:40:ASN:ND2	13:1:40:ASN:N	2.62	0.47
10:J:167:PRO:CB	10:X:168:MET:HE1	2.42	0.47
3:C:33:ARG:CB	3:C:33:ARG:NH1	2.72	0.47
5:E:216:GLY:O	5:E:219:THR:N	2.47	0.47
12:L:114:ASP:HB3	12:L:118:SER:H	1.79	0.47
6:F:192:GLN:NE2	6:F:195:LYS:HE3	2.28	0.47
6:F:109:ILE:HD12	6:F:109:ILE:N	2.29	0.47
2:P:108:PRO:HG2	2:P:111:ILE:HD12	1.96	0.47
3:C:31:VAL:HG11	3:C:135:SER:HB2	1.95	0.47
5:S:136:LEU:HB2	5:S:151:PHE:HB3	1.96	0.47
13:M:112:TYR:HE1	13:M:127:THR:HG22	1.79	0.47
12:L:-2:ASN:HA	12:L:21:ILE:O	2.14	0.47
4:R:243:ALA:O	4:R:244:GLU:HG2	2.15	0.47
7:U:232:ARG:HA	7:U:232:ARG:NE	2.30	0.47
13:1:4:ILE:C	13:1:4:ILE:HD12	2.34	0.47
8:H:165:ASN:HD22	13:1:139:ARG:NH1	1.99	0.47
5:E:194:VAL:CG1	5:E:207:LEU:HD11	2.44	0.47
13:1:20:GLY:HA2	13:1:49:ILE:HD11	1.97	0.47
3:C:76:LEU:HD12	3:C:138:ILE:HG12	1.96	0.47
9:I:165:ARG:NH2	12:Z:135:MET:HE2	2.29	0.47
14:N:84:LYS:HG3	14:N:119:VAL:CG2	2.45	0.47
9:I:28:SER:HB2	10:J:120:VAL:HG21	1.96	0.47
3:C:134:VAL:HG12	3:C:135:SER:N	2.29	0.47
2:P:229:ILE:O	2:P:233:LEU:HB2	2.15	0.47
5:E:90:ASN:O	5:E:94:GLN:HG3	2.15	0.47
11:Y:10(A):ARG:HG2	11:Y:10(A):ARG:NH1	2.30	0.47
5:E:66:LYS:O	5:E:77:SER:HA	2.14	0.47
3:Q:163:GLN:HA	3:Q:163:GLN:HE21	1.80	0.47
6:F:35:THR:CG2	6:F:36:THR:N	2.77	0.47
9:I:137:MET:CE	9:I:141:LEU:HD11	2.44	0.47
7:G:78:VAL:HG11	7:G:85:ALA:HB2	1.97	0.47
11:K:111:TYR:CE1	11:K:121:LYS:HB2	2.50	0.47
1:O:122:GLU:C	1:O:124:THR:H	2.18	0.47
6:T:74:ILE:HG12	6:T:109:ILE:HD13	1.93	0.47
2:P:185:LYS:HE2	2:P:187:ASP:OD1	2.14	0.47
12:L:101:ILE:HD11	12:L:111:TYR:HB2	1.97	0.47
14:2:100:ILE:N	14:2:100:ILE:HD12	2.29	0.47
11:K:13:ILE:HG13	11:K:151:ALA:HB1	1.96	0.47
1:A:138:ILE:HD12	1:A:138:ILE:N	2.30	0.47
4:R:170:GLU:HG2	4:R:171:GLY:N	2.30	0.47
10:X:38:SER:HB2	10:X:39:PRO:HD2	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:40:ILE:HD12	1:O:193:ALA:HB2	1.95	0.47
5:S:45:HIS:HB2	5:S:189:LEU:HD12	1.97	0.46
10:X:90(A):ILE:HD11	10:X:116:LEU:HD23	1.96	0.46
1:O:92:SER:O	1:O:95:VAL:HG12	2.15	0.46
14:2:19:ARG:CD	14:2:26:ILE:CD1	2.92	0.46
3:Q:190:VAL:O	3:Q:194:VAL:HG23	2.14	0.46
2:P:121:GLN:CG	3:Q:83:ALA:HB1	2.45	0.46
10:J:144:PRO:HG3	11:Y:207:ASN:ND2	2.30	0.46
8:V:18:THR:HB	8:V:30:ASN:HD22	1.80	0.46
3:C:97:GLN:HG3	10:J:65:LEU:HB2	1.97	0.46
2:P:191:GLU:O	2:P:195:LYS:HG2	2.15	0.46
5:E:227:GLU:CD	5:E:227:GLU:H	2.17	0.46
7:U:141:VAL:HG21	7:U:216:THR:HA	1.97	0.46
2:B:144:ARG:NH1	10:J:72:TYR:HB2	2.30	0.46
2:P:235:LYS:N	2:P:235:LYS:HD3	2.30	0.46
6:F:87:HIS:HD2	6:F:132:PHE:CE2	2.33	0.46
13:M:110:LEU:HG	13:M:125:LEU:HD12	1.97	0.46
11:K:10(B):LYS:CD	11:K:10(B):LYS:N	2.58	0.46
14:2:116:GLY:HA3	16:2:1408:HOH:O	2.15	0.46
3:C:89:ILE:CD1	3:C:89:ILE:N	2.77	0.46
2:B:141:TYR:C	2:B:141:TYR:CD1	2.89	0.46
5:S:227:GLU:CD	5:S:227:GLU:H	2.17	0.46
6:F:18:ASP:N	6:F:18:ASP:OD2	2.42	0.46
13:1:46:SER:OG	13:1:98:ALA:HB3	2.16	0.46
8:H:2:THR:OG1	8:H:130:GLY:HA3	2.15	0.46
6:T:187:ARG:HH11	6:T:187:ARG:HG3	1.80	0.46
12:L:3:ILE:CD1	12:L:127:GLY:O	2.59	0.46
3:C:190:VAL:O	3:C:194:VAL:HG23	2.15	0.46
2:P:185:LYS:CD	2:P:187:ASP:H	2.28	0.46
6:T:50:VAL:HG22	6:T:51:GLU:N	2.30	0.46
10:X:147:THR:HG23	10:X:150:GLU:OE2	2.16	0.46
6:F:109:ILE:HG21	6:F:147:HIS:HB2	1.98	0.46
4:R:121:LEU:N	16:R:853:HOH:O	2.42	0.46
4:D:170:GLU:HG2	4:D:171:GLY:N	2.30	0.46
1:A:136:LEU:HB2	1:A:138:ILE:HD11	1.98	0.46
8:V:105:ASP:HB2	8:V:10(A):PRO:HD2	1.97	0.46
10:J:168:MET:HE3	10:X:168:MET:CE	2.44	0.46
3:C:55:THR:C	3:C:56:LEU:HD22	2.35	0.46
5:E:18(D):ILE:HG13	5:E:18(D):ILE:O	2.15	0.46
6:T:127:ASN:HD22	6:T:128:SER:N	2.13	0.46
2:P:235:LYS:C	2:P:237:GLY:H	2.19	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1:112:TYR:HE1	13:1:127:THR:HG22	1.80	0.46
2:B:196:THR:O	2:B:200:THR:HG23	2.16	0.46
12:Z:76:ILE:CD1	12:Z:101:ILE:HD13	2.45	0.46
14:2:107:LYS:CG	14:2:108:GLY:H	2.28	0.46
14:2:41:ILE:HD13	14:2:103:GLY:HA3	1.97	0.46
9:W:6:MET:CE	9:W:155:ILE:HA	2.45	0.46
11:Y:10(A):ARG:HB3	11:Y:10(B):LYS:CE	2.45	0.46
5:S:214:ILE:HD13	5:S:215:VAL:CA	2.45	0.46
10:J:18:LYS:CD	10:J:174:ILE:HG13	2.41	0.46
7:U:34:THR:O	7:U:35:ILE:HG13	2.15	0.46
2:B:224:PHE:N	2:B:224:PHE:CD2	2.84	0.46
6:F:50:VAL:HG22	6:F:51:GLU:N	2.30	0.46
6:F:36:THR:CG2	6:F:51:GLU:OE2	2.64	0.46
14:N:3:ILE:HG22	14:N:16:ALA:HB2	1.98	0.46
1:O:206:PHE:CD1	1:O:210:ILE:HD11	2.50	0.46
2:B:235:LYS:HD3	2:B:235:LYS:N	2.31	0.46
8:H:105:ASP:HB2	8:H:10(A):PRO:HD2	1.98	0.46
13:M:186:PHE:CE1	13:M:188:LYS:HG3	2.51	0.46
12:L:9:GLU:O	12:L:107:LYS:HA	2.16	0.46
5:S:95:GLN:HG3	5:S:115:LEU:HD13	1.97	0.46
5:E:11:ASP:OD1	5:E:13:VAL:HG12	2.16	0.46
3:Q:163:GLN:HE21	3:Q:163:GLN:CA	2.28	0.46
6:T:54:ILE:HG12	6:T:208:PHE:CA	2.45	0.46
11:K:180:GLU:N	16:K:1426:HOH:O	2.41	0.46
2:P:69:LYS:HG3	2:P:221:GLN:OE1	2.16	0.46
13:1:186:PHE:CE1	13:1:188:LYS:HG3	2.51	0.46
9:W:-8:SER:O	9:W:-6:PRO:HD3	2.16	0.46
4:D:117:CYS:HB3	4:D:155:GLY:O	2.15	0.46
3:C:197:LEU:HD13	3:C:210:ILE:CD1	2.15	0.45
2:P:160:TRP:CD2	2:P:163:ILE:HD12	2.51	0.45
8:H:52:THR:O	8:H:56:THR:HB	2.16	0.45
12:Z:101:ILE:HD11	12:Z:111:TYR:HB2	1.98	0.45
9:W:12:VAL:HG22	9:W:104:ILE:CD1	2.46	0.45
10:J:113:ILE:HA	10:J:118:THR:O	2.16	0.45
5:E:52:LYS:HD2	5:E:63:TYR:O	2.16	0.45
10:X:88:ALA:O	10:X:90(A):ILE:HG22	2.17	0.45
14:2:84:LYS:HG3	14:2:119:VAL:CG2	2.46	0.45
6:T:87:HIS:HD2	6:T:132:PHE:CE2	2.35	0.45
7:G:192:PHE:CD1	7:G:192:PHE:C	2.89	0.45
7:G:41:ARG:NH2	7:G:18(B):ASP:O	2.50	0.45
5:S:79:ALA:HA	16:S:235:HOH:O	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:GLU:H	1:A:62:GLU:CD	2.18	0.45
11:K:10(A):ARG:NH1	11:K:10(A):ARG:HG2	2.30	0.45
12:Z:99:THR:CG2	16:Z:202:HOH:O	2.59	0.45
9:I:55:LEU:HD21	9:I:95:TYR:CD1	2.51	0.45
7:U:8:TYR:C	7:U:10:ARG:N	2.68	0.45
4:R:121:LEU:HD23	4:R:123:PHE:HE1	1.81	0.45
9:W:156:SER:O	9:W:160:LEU:HB2	2.16	0.45
11:Y:4:LEU:C	11:Y:4:LEU:HD22	2.36	0.45
2:B:229:ILE:O	2:B:233:LEU:HB2	2.16	0.45
1:A:161:LYS:HE3	2:B:60:GLU:OE1	2.16	0.45
9:W:137:MET:CE	9:W:141:LEU:HD11	2.46	0.45
8:H:34:LEU:HB2	16:H:1425:HOH:O	2.15	0.45
5:S:111:ARG:HG2	5:S:111:ARG:HH11	1.81	0.45
8:H:155:ALA:O	8:H:159:ILE:CD1	2.60	0.45
14:2:4:MET:HB3	14:2:126:ILE:HG22	1.99	0.45
3:C:158:SER:CB	4:D:59:LEU:HD21	2.46	0.45
1:O:33:GLN:HE21	1:O:33:GLN:CA	2.23	0.45
5:E:39:GLY:O	5:E:162:GLY:HA2	2.15	0.45
7:G:49:ILE:HD13	7:G:193:ALA:CB	2.46	0.45
13:1:201:LYS:HA	16:1:255:HOH:O	2.16	0.45
8:V:2:THR:OG1	8:V:130:GLY:HA3	2.15	0.45
4:D:227:GLU:OE2	4:D:227:GLU:N	2.42	0.45
10:J:161:GLU:HA	10:J:161:GLU:OE2	2.16	0.45
7:G:96:ALA:HA	7:G:107:MET:CE	2.31	0.45
6:F:54:ILE:HG12	6:F:208:PHE:CA	2.46	0.45
9:W:55:LEU:HD11	9:W:97:VAL:HG21	1.97	0.45
14:N:146:MET:CE	14:N:150:GLU:HB3	2.43	0.45
5:S:31:ILE:HD11	5:S:153:PRO:CD	2.46	0.45
13:1:113:VAL:HA	13:1:118:VAL:O	2.17	0.45
12:Z:84:GLN:HG3	12:Z:117:GLY:O	2.16	0.45
4:R:117:CYS:HB3	4:R:155:GLY:O	2.16	0.45
10:X:159:VAL:O	10:X:163:GLU:HG3	2.17	0.45
1:A:205:GLU:OE2	1:A:205:GLU:HA	2.17	0.45
7:G:188:LYS:HD3	7:G:191:GLU:OE2	2.15	0.45
2:P:122:GLY:C	2:P:124:THR:H	2.20	0.45
6:T:109:ILE:HG21	6:T:147:HIS:HB2	1.98	0.45
3:Q:89:ILE:N	3:Q:89:ILE:CD1	2.80	0.45
11:Y:128:GLY:O	11:Y:131:GLN:HG2	2.16	0.45
8:V:3:ILE:HD11	8:V:127:LEU:HB2	1.98	0.45
6:T:36:THR:HG22	6:T:51:GLU:OE2	2.15	0.45
2:B:147:GLN:CB	3:C:62(A):ILE:HD13	2.47	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:7:ARG:NH1	10:X:7:ARG:HG2	2.30	0.45
8:H:175:VAL:HG12	8:H:176:CYS:N	2.31	0.45
10:X:111:TYR:CE1	10:X:121:GLU:HG3	2.51	0.45
1:O:205:GLU:HA	1:O:205:GLU:OE2	2.15	0.45
3:C:76:LEU:HD22	3:C:89:ILE:HD11	1.99	0.45
2:P:150:THR:O	2:P:157:TYR:HA	2.16	0.45
2:P:224:PHE:N	2:P:224:PHE:CD2	2.84	0.45
10:J:168:MET:HE2	10:X:168:MET:HE2	1.99	0.45
2:B:143:ASP:OD2	10:J:10(B):LYS:HE2	2.17	0.45
6:F:127:ASN:H	6:F:127:ASN:ND2	2.15	0.45
5:E:52:LYS:HB2	5:E:63:TYR:HB3	1.97	0.45
12:Z:13:VAL:HG12	12:Z:177:ILE:HG13	1.98	0.45
7:U:83:PRO:HG2	16:U:267:HOH:O	2.16	0.45
7:G:82:ILE:N	7:G:83:PRO:HD2	2.31	0.45
9:I:125:ILE:N	9:I:125:ILE:HD12	2.30	0.45
10:J:143:ARG:HA	10:J:144:PRO:HD3	1.87	0.45
3:Q:156:ILE:HD11	4:R:83:ALA:N	2.31	0.45
12:L:140:ASN:O	12:L:144:PHE:HA	2.17	0.45
11:Y:25:TRP:CH2	12:Z:132:SER:HA	2.52	0.45
1:O:6:ASP:OD2	1:O:8:TYR:HB2	2.17	0.45
3:C:232:TYR:O	3:C:236:ILE:HG13	2.17	0.45
2:P:141:TYR:C	2:P:141:TYR:CD1	2.89	0.45
14:N:33:LYS:HE2	15:N:1404:BO2:H222	1.99	0.45
7:U:49:ILE:HD13	7:U:193:ALA:CB	2.46	0.45
2:B:224:PHE:HD2	2:B:224:PHE:N	2.14	0.45
13:M:46:SER:OG	13:M:98:ALA:HB3	2.17	0.45
3:Q:18(A):ASP:OD2	3:Q:18(C):LYS:HG2	2.16	0.45
4:D:243:ALA:O	4:D:244:GLU:HG2	2.17	0.45
14:N:13:ILE:HD12	14:N:177:VAL:CB	2.46	0.45
4:R:160:TYR:HA	5:S:58:LEU:O	2.17	0.45
5:E:67:ILE:HD13	5:E:77:SER:CB	2.46	0.45
12:Z:6:ILE:N	12:Z:6:ILE:HD12	2.32	0.45
10:J:166:MET:HA	10:J:167:PRO:HD3	1.82	0.45
2:B:185:LYS:HD3	2:B:186:VAL:H	1.81	0.45
1:O:31:VAL:HG11	1:O:135:SER:HB2	1.98	0.45
10:J:147:THR:HG23	10:J:150:GLU:OE2	2.17	0.45
13:1:113:VAL:HG23	13:1:119:THR:HG22	1.98	0.45
9:I:113:PHE:CD2	9:I:113:PHE:N	2.85	0.45
2:P:224:PHE:N	2:P:224:PHE:HD2	2.15	0.45
13:1:70:ASN:ND2	13:1:70(A):ALA:HA	2.32	0.45
4:D:91:HIS:CG	4:D:119:LEU:HD11	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:112:GLN:HE21	10:X:125:GLY:HA3	1.83	0.45
6:T:103:TYR:O	6:T:104:LYS:HB3	2.17	0.45
3:Q:43:LYS:HG2	3:Q:43:LYS:O	2.15	0.45
2:B:194:LEU:CD1	2:B:232:ILE:HD13	2.45	0.44
1:A:122:GLU:C	1:A:124:THR:H	2.19	0.44
11:Y:37:ILE:HB	11:Y:41:LEU:CB	2.45	0.44
1:O:86:ARG:HH21	7:U:118:ASN:HD22	1.65	0.44
6:T:36:THR:CG2	6:T:51:GLU:OE2	2.65	0.44
4:R:112:LEU:C	4:R:112:LEU:HD13	2.38	0.44
9:I:104:ILE:CD1	9:I:179:LYS:C	2.85	0.44
7:G:18(B):ASP:O	7:G:18(C):HIS:HB3	2.17	0.44
6:F:103:TYR:O	6:F:104:LYS:HB3	2.17	0.44
2:B:94:ILE:CD1	2:B:94:ILE:N	2.80	0.44
5:E:216:GLY:O	5:E:217:LYS:C	2.56	0.44
1:A:86:ARG:HH21	7:G:118:ASN:HD22	1.65	0.44
1:A:86:ARG:HH21	7:G:118:ASN:ND2	2.16	0.44
11:Y:13:ILE:HG13	11:Y:151:ALA:HB1	1.97	0.44
5:S:77:SER:OG	5:S:137:LEU:HB2	2.17	0.44
2:B:235:LYS:C	2:B:237:GLY:H	2.20	0.44
11:K:200:LYS:HG3	11:K:205:SER:O	2.17	0.44
12:L:1:GLY:N	16:L:218:HOH:O	2.50	0.44
1:A:188:ASP:O	1:A:192:ILE:HG12	2.18	0.44
9:I:159:LEU:HD21	9:I:173:ALA:HB1	1.99	0.44
7:G:29:LYS:HD2	7:G:29:LYS:HA	1.75	0.44
14:N:13:ILE:CD1	14:N:177:VAL:HA	2.41	0.44
13:1:4:ILE:HD13	13:1:155:ILE:HG12	2.00	0.44
8:H:41:ILE:CD1	8:H:76:VAL:HG22	2.29	0.44
1:A:15:PHE:N	2:B:23:GLN:HE22	1.93	0.44
3:C:177:GLU:OE2	4:D:57:PRO:HD2	2.16	0.44
5:E:222:THR:C	5:E:223:ILE:HD13	2.38	0.44
3:C:187:GLU:HG3	3:C:232:TYR:OH	2.17	0.44
2:B:6:ARG:HG3	2:B:6:ARG:HH11	1.82	0.44
9:W:104:ILE:HD12	9:W:104:ILE:N	2.33	0.44
7:U:77:VAL:HG12	7:U:137:THR:HB	1.99	0.44
5:E:18(F):ILE:HG22	5:E:18(F):ILE:O	2.17	0.44
9:I:-6:PRO:HA	9:I:-3:ILE:HD12	2.00	0.44
4:R:170:GLU:OE1	4:R:170:GLU:N	2.46	0.44
12:Z:29:ARG:NH1	12:Z:171:ASP:OD1	2.45	0.44
11:K:128:GLY:O	11:K:131:GLN:HG2	2.17	0.44
5:E:136:LEU:HB2	5:E:151:PHE:HB3	1.98	0.44
10:J:36:GLN:HG3	10:J:184:ILE:HD12	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:38:LEU:HD12	7:G:38:LEU:C	2.37	0.44
7:U:188:LYS:HD3	7:U:191:GLU:OE2	2.18	0.44
14:2:21:THR:CG2	14:2:26:ILE:CD1	2.88	0.44
9:W:14:ILE:HG12	9:W:34:ILE:CD1	2.48	0.44
11:Y:12:ILE:HB	11:Y:178:VAL:HB	2.00	0.44
1:A:58:LEU:HD12	7:G:173:THR:HG23	2.00	0.44
1:A:117:ALA:HB1	1:A:155:GLY:O	2.17	0.44
9:I:176:TYR:HB3	9:I:178:ILE:HD11	2.00	0.44
9:W:104:ILE:HG21	9:W:181:LYS:HG2	2.00	0.44
7:G:34:THR:O	7:G:35:ILE:HG13	2.17	0.44
14:N:20:THR:OG1	14:N:28:ASN:HB3	2.18	0.44
14:2:1:THR:CG2	14:2:3:ILE:HD12	2.47	0.44
1:O:4:MET:CG	1:O:5:THR:H	2.31	0.44
2:B:126:HIS:HB3	3:C:129:VAL:HG12	1.98	0.44
10:J:129:TYR:O	10:J:132:PHE:HB2	2.17	0.44
1:A:43:THR:HG23	1:A:184:LEU:O	2.16	0.44
13:M:8:TYR:CZ	13:M:148:VAL:HG13	2.52	0.44
13:M:70:ASN:ND2	13:M:70(A):ALA:HA	2.33	0.44
7:U:119:LEU:HA	7:U:119:LEU:HD12	1.82	0.44
7:U:38:LEU:C	7:U:38:LEU:HD12	2.38	0.44
7:U:18(A):ILE:HD11	7:U:18(C):HIS:O	2.16	0.44
3:C:163:GLN:HA	3:C:163:GLN:NE2	2.33	0.44
3:Q:232:TYR:O	3:Q:236:ILE:HG13	2.17	0.44
7:U:143:GLU:HA	7:U:217:LYS:NZ	2.33	0.44
9:W:176:TYR:HB3	9:W:178:ILE:HD11	2.00	0.44
2:B:31:ILE:HD11	2:B:133:GLY:C	2.38	0.44
12:Z:123:GLN:HG3	12:Z:145:TYR:OH	2.18	0.44
2:P:196:THR:O	2:P:200:THR:HG23	2.17	0.44
13:M:13:ILE:HD12	13:M:151:ALA:HB1	2.00	0.44
14:N:66:TYR:CD2	14:N:74:PRO:HB3	2.53	0.44
12:L:113:PHE:CD1	12:L:113:PHE:N	2.85	0.44
8:V:159:ILE:O	8:V:163:ILE:CD1	2.64	0.44
6:T:53:LEU:HD11	6:T:205:ASN:OD1	2.18	0.44
2:B:49:ALA:HB2	2:B:212:PHE:CE1	2.53	0.44
13:1:1:THR:OG1	13:1:2:SER:N	2.48	0.44
6:T:158:TRP:CZ3	7:U:64:VAL:HA	2.52	0.44
1:A:6:ASP:OD2	1:A:8:TYR:HB2	2.18	0.44
14:N:105:ASP:OD2	14:N:106:ASN:N	2.46	0.44
10:J:88:ALA:O	10:J:90(A):ILE:HG22	2.17	0.44
10:J:143:ARG:HG2	10:J:143:ARG:NH1	2.32	0.44
8:V:84:LYS:HE2	8:V:119:THR:HG23	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:14(C):GLN:HG2	8:V:210:THR:HG21	2.00	0.44
4:D:122:ARG:HH11	4:D:122:ARG:HG2	1.82	0.44
4:D:233:ILE:N	4:D:233:ILE:CD1	2.80	0.44
13:1:14(C):ARG:CG	13:1:14(C):ARG:NH1	2.80	0.44
5:S:18(F):ILE:O	5:S:18(F):ILE:HG22	2.17	0.44
2:P:70:LEU:HD21	2:P:89:ILE:CD1	2.46	0.44
4:R:159:ARG:HB3	5:S:60:SER:CB	2.47	0.44
3:Q:57:LYS:HZ2	3:Q:58:LEU:HA	1.82	0.44
11:K:66:HIS:CE1	11:K:74:ILE:HD13	2.52	0.44
9:W:113:PHE:CD2	9:W:113:PHE:N	2.86	0.44
2:P:95:HIS:CD2	2:P:115:ARG:HG2	2.52	0.44
12:L:123:GLN:HG3	12:L:145:TYR:OH	2.18	0.44
6:F:187:ARG:HB2	16:F:262:HOH:O	2.17	0.44
12:Z:140:ASN:O	12:Z:144:PHE:HA	2.17	0.44
10:X:36:GLN:HG3	10:X:184:ILE:HD12	2.00	0.44
2:B:156:ASN:ND2	3:C:82:ASN:HB2	2.33	0.44
8:H:25:ILE:HD13	12:Z:165:ARG:O	2.18	0.44
11:K:137:VAL:HG21	11:K:161:ALA:HB2	2.00	0.44
3:C:43:LYS:HG2	3:C:43:LYS:O	2.18	0.44
5:E:111:ARG:HG2	5:E:111:ARG:HH11	1.82	0.44
10:J:38:SER:HB2	10:J:39:PRO:HD2	1.99	0.44
7:U:192:PHE:CD1	7:U:192:PHE:C	2.89	0.44
4:R:160:TYR:CZ	4:R:163:LYS:HD3	2.54	0.43
12:L:99:THR:C	12:L:100:ILE:HD12	2.38	0.43
7:U:107:MET:CE	7:U:112:LEU:HD13	2.48	0.43
9:I:6:MET:HG2	9:I:124:PHE:HB3	2.00	0.43
8:V:52:THR:O	8:V:56:THR:HB	2.18	0.43
12:Z:76:ILE:HD11	12:Z:101:ILE:CD1	2.44	0.43
11:K:123:ASP:C	11:K:124:ILE:HD12	2.38	0.43
4:D:39:GLY:O	4:D:162:ALA:HA	2.18	0.43
3:C:151:THR:HG22	3:C:157:TYR:HB3	2.00	0.43
3:C:18(A):ASP:OD2	3:C:18(C):LYS:HG2	2.18	0.43
9:W:93:GLY:N	9:W:94:PRO:CD	2.81	0.43
7:G:70:ILE:HD12	7:G:92:ALA:HB3	2.00	0.43
5:S:233:ILE:HG22	5:S:233:ILE:OXT	2.17	0.43
9:W:4:VAL:CG2	9:W:155:ILE:HD11	2.48	0.43
2:B:232:ILE:C	2:B:232:ILE:HD13	2.38	0.43
2:B:147:GLN:HB3	3:C:62(A):ILE:CD1	2.47	0.43
13:M:14(G):ILE:HB	13:M:144:PRO:CD	2.48	0.43
10:J:7:ARG:HG2	10:J:7:ARG:NH1	2.33	0.43
5:E:45:HIS:HB2	5:E:189:LEU:HD12	1.98	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:156:ILE:HD11	4:R:83:ALA:H	1.82	0.43
4:D:160:TYR:CZ	4:D:163:LYS:HD3	2.53	0.43
8:H:105:ASP:HB2	8:H:10(A):PRO:CD	2.48	0.43
3:Q:170:LYS:HB2	16:Q:255:HOH:O	2.17	0.43
3:Q:125:GLN:NE2	16:Q:258:HOH:O	2.51	0.43
1:O:21(I):TYR:HE2	1:O:21(L):ILE:HD13	1.83	0.43
1:O:23:GLN:NE2	7:U:14:ILE:HD12	2.32	0.43
12:Z:113:PHE:CD1	12:Z:113:PHE:N	2.86	0.43
3:Q:15:PHE:HA	3:Q:21:ILE:HD13	2.01	0.43
8:H:44:ALA:HB3	8:H:100:ILE:HB	2.00	0.43
8:H:3:ILE:HD11	8:H:127:LEU:HB2	1.99	0.43
8:V:3:ILE:HG22	8:V:16:ALA:HB2	2.01	0.43
12:Z:-7:ASN:ND2	12:Z:-7:ASN:C	2.71	0.43
13:M:14(G):ILE:N	13:M:144:PRO:HD2	2.33	0.43
12:Z:-2:ASN:HA	12:Z:21:ILE:O	2.17	0.43
5:E:160:LEU:HD12	5:E:163:THR:HG21	2.00	0.43
1:A:144:PHE:CD2	9:I:72:ARG:HD2	2.53	0.43
7:U:70:ILE:HD12	7:U:92:ALA:HB3	2.00	0.43
5:S:41:ARG:NH1	5:S:42:SER:O	2.51	0.43
3:Q:168:ASN:O	3:Q:172:VAL:HG12	2.19	0.43
2:B:194:LEU:HD12	2:B:232:ILE:CD1	2.47	0.43
5:S:15:PHE:H	6:T:23:GLN:NE2	2.08	0.43
1:O:161:LYS:HD2	2:P:58:LEU:HA	2.00	0.43
9:W:104:ILE:HD11	9:W:178:ILE:HG22	1.99	0.43
11:K:208:ASN:HD21	9:W:29:ASN:ND2	2.13	0.43
1:A:97:HIS:CD2	8:H:61:SER:OG	2.69	0.43
5:E:8:TYR:CE1	6:F:10:LEU:HD23	2.53	0.43
3:Q:17:PRO:HA	4:R:26:TYR:CD1	2.54	0.43
1:O:227:GLN:NE2	1:O:231:ASP:OD1	2.49	0.43
14:2:121:LYS:O	14:2:122:LEU:HD23	2.18	0.43
5:S:15:PHE:HB2	6:T:23:GLN:HE22	1.83	0.43
7:G:168:LYS:O	7:G:172:ILE:HG12	2.19	0.43
14:N:126:ILE:N	14:N:126:ILE:CD1	2.81	0.43
11:Y:180:GLU:HB2	16:Y:1428:HOH:O	2.18	0.43
13:1:14(G):ILE:N	13:1:144:PRO:HD2	2.33	0.43
1:A:86:ARG:HE	7:G:118:ASN:ND2	2.16	0.43
5:E:57:GLU:C	5:E:58:LEU:HD12	2.39	0.43
5:E:58:LEU:CD1	5:E:58:LEU:N	2.81	0.43
8:H:18:THR:HB	8:H:30:ASN:HD22	1.83	0.43
5:S:160:LEU:HD12	5:S:163:THR:HG21	2.00	0.43
5:E:41:ARG:NH1	5:E:42:SER:O	2.51	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:75:GLY:O	6:F:138:PHE:HA	2.19	0.43
3:C:224:LEU:HD12	3:C:224:LEU:N	2.34	0.43
7:G:107:MET:HE3	7:G:112:LEU:HD13	1.99	0.43
11:K:99:THR:HG22	11:K:113:VAL:O	2.18	0.43
5:S:2(C):VAL:HG22	5:S:226:GLY:HA2	2.00	0.43
7:U:39:ALA:HA	7:U:47:VAL:O	2.19	0.43
11:Y:6:PHE:HA	11:Y:123:ASP:O	2.18	0.43
9:W:137:MET:HE3	9:W:141:LEU:HD11	2.01	0.43
2:P:194:LEU:O	2:P:198:SER:HB2	2.19	0.43
9:I:107:LYS:HA	9:I:108:PRO:HD3	1.90	0.43
8:H:221:ILE:HD12	9:I:40:HIS:HA	2.01	0.43
3:Q:224:LEU:HD12	3:Q:224:LEU:N	2.34	0.43
5:S:216:GLY:O	5:S:217:LYS:C	2.56	0.43
4:D:194:LEU:HD22	4:D:212:LEU:HD11	2.01	0.43
5:E:233:ILE:OXT	5:E:233:ILE:HG22	2.19	0.43
5:S:90:ASN:O	5:S:94:GLN:HG3	2.17	0.43
13:1:83:LEU:O	13:1:87:MET:HG2	2.18	0.43
4:R:21:LEU:HD21	5:S:130:ARG:HD2	2.01	0.43
4:D:79:SER:HB3	4:D:165:ILE:HD12	2.01	0.43
7:G:17(C):LYS:HB2	7:G:17(C):LYS:HE3	1.78	0.43
5:S:123:ASN:N	5:S:123:ASN:HD22	2.17	0.43
4:R:79:SER:HB3	4:R:165:ILE:HD12	2.01	0.43
12:L:33:LYS:HE2	12:L:33:LYS:HB3	1.76	0.43
6:T:147:HIS:HD2	16:T:242:HOH:O	2.01	0.43
12:L:-7:ASN:ND2	12:L:-7:ASN:C	2.72	0.43
3:C:227:GLU:O	3:C:231:GLN:HG3	2.19	0.43
11:Y:123:ASP:C	11:Y:124:ILE:HD12	2.39	0.43
8:V:105:ASP:HB2	8:V:10(A):PRO:CD	2.47	0.43
5:S:147:HIS:HA	16:S:238:HOH:O	2.18	0.43
4:R:194:LEU:HD22	4:R:212:LEU:HD11	2.00	0.43
2:P:113:VAL:HG22	2:P:138:TYR:CD2	2.54	0.43
14:N:26:ILE:HB	13:1:165:ARG:HA	2.00	0.43
2:P:121:GLN:C	2:P:121:GLN:NE2	2.72	0.43
9:I:104:ILE:HG21	9:I:181:LYS:HG2	2.01	0.43
4:D:195:LYS:HB3	4:D:196:ILE:HD13	2.01	0.43
1:O:175:PHE:O	1:O:179:ARG:HG2	2.19	0.43
14:N:20:THR:HG23	14:N:31:THR:OG1	2.19	0.43
5:S:162:GLY:O	5:S:163:THR:HB	2.19	0.43
1:A:227:GLN:NE2	1:A:231:ASP:OD1	2.50	0.43
3:C:71:ASP:OD1	3:C:100:ARG:NH1	2.51	0.43
14:N:171:GLY:HA2	13:1:197:TRP:CH2	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:169:GLN:HE21	7:G:169:GLN:HB3	1.67	0.43
13:M:191:GLN:HE21	13:M:191:GLN:HB3	1.55	0.43
3:C:163:GLN:HE22	3:C:173:ARG:NE	2.13	0.43
3:C:168:ASN:O	3:C:172:VAL:HG12	2.19	0.43
14:2:20:THR:HG23	14:2:31:THR:OG1	2.19	0.43
3:Q:185:THR:HG22	3:Q:186:VAL:N	2.33	0.43
3:Q:227:GLU:O	3:Q:231:GLN:HG3	2.18	0.43
9:W:181:LYS:HE3	9:W:181:LYS:HB3	1.90	0.43
3:Q:72:SER:O	3:Q:221:ILE:HD13	2.19	0.43
6:T:127:ASN:ND2	6:T:127:ASN:H	2.16	0.43
3:C:95:GLU:OE2	3:C:95:GLU:HA	2.19	0.43
5:S:58:LEU:N	5:S:58:LEU:CD1	2.82	0.42
8:H:15:ALA:HA	8:H:174:ASP:O	2.18	0.42
11:K:12:ILE:HB	11:K:178:VAL:HB	2.01	0.42
2:B:97:GLN:NE2	16:B:246:HOH:O	2.52	0.42
12:L:-7:ASN:HD22	12:L:-6:PRO:CD	2.32	0.42
2:P:101:LYS:HZ1	10:X:85:GLN:HE22	1.66	0.42
14:N:4:MET:HB3	14:N:126:ILE:HG22	2.01	0.42
14:2:15:GLY:HA2	14:2:174:ARG:O	2.19	0.42
14:N:85:GLU:O	14:N:89:GLU:HB2	2.19	0.42
6:T:75:GLY:O	6:T:138:PHE:HA	2.18	0.42
8:H:144:GLN:O	8:H:145:ASP:HB2	2.19	0.42
9:I:93:GLY:N	9:I:94:PRO:CD	2.80	0.42
12:Z:14:LEU:HD13	12:Z:34:VAL:HG13	1.99	0.42
4:D:161:ASN:HB3	4:D:180:TRP:CE2	2.54	0.42
3:Q:163:GLN:HA	3:Q:163:GLN:NE2	2.34	0.42
10:J:34:THR:HG21	10:J:176:LYS:NZ	2.34	0.42
3:Q:76:LEU:HD22	3:Q:89:ILE:HD11	2.01	0.42
10:J:24:ILE:O	10:J:24:ILE:HG13	2.19	0.42
3:Q:106:PRO:HG2	3:Q:143:PRO:HG2	1.98	0.42
4:D:215:ILE:HD13	4:D:216:THR:N	2.34	0.42
5:S:5:ARG:HG3	5:S:22:PHE:CE1	2.54	0.42
12:Z:170:GLY:O	12:Z:171:ASP:HB2	2.20	0.42
1:O:21(L):ILE:HD11	8:V:42:TRP:HH2	1.84	0.42
14:2:66:TYR:CD2	14:2:74:PRO:HB3	2.53	0.42
5:E:139:ILE:CD1	5:E:139:ILE:N	2.78	0.42
13:M:-4:ILE:HD12	14:N:116:GLY:HA2	1.99	0.42
9:W:55:LEU:HD21	9:W:95:TYR:CD1	2.54	0.42
11:K:40:PHE:CG	11:K:73:ARG:CZ	3.03	0.42
11:K:6:PHE:HA	11:K:123:ASP:O	2.19	0.42
4:D:24:VAL:O	4:D:28:LEU:HD13	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:40:ASN:ND2	16:Z:220:HOH:O	2.39	0.42
5:E:105:ARG:HB2	13:M:78:TYR:CD1	2.54	0.42
2:P:44:ASP:N	2:P:44:ASP:OD2	2.53	0.42
4:R:39:GLY:O	4:R:162:ALA:HA	2.20	0.42
5:S:57:GLU:C	5:S:58:LEU:HD12	2.40	0.42
2:B:108:PRO:CB	2:B:111:ILE:HD13	2.23	0.42
4:R:31:ILE:CD1	4:R:80:GLY:HA3	2.49	0.42
5:E:48:LEU:CD1	5:E:139:ILE:CD1	2.92	0.42
13:1:40:ASN:ND2	13:1:40:ASN:H	2.07	0.42
10:J:168:MET:CE	10:X:168:MET:HG2	2.49	0.42
2:P:45:GLY:HA3	2:P:216:ARG:HG2	2.01	0.42
12:Z:-8:PHE:HB2	13:1:-8:THR:HG23	2.01	0.42
13:1:186:PHE:HE1	13:1:188:LYS:HG3	1.85	0.42
10:J:16:SER:HB2	16:J:206:HOH:O	2.18	0.42
2:B:112:LEU:C	2:B:112:LEU:HD23	2.40	0.42
9:W:6:MET:HG2	9:W:124:PHE:HB3	2.01	0.42
7:G:8:TYR:O	7:G:12:ILE:CD1	2.65	0.42
6:F:49:ALA:HA	6:F:211:GLU:O	2.18	0.42
12:Z:99:THR:C	12:Z:100:ILE:HD12	2.40	0.42
2:B:20:ARG:NH2	3:C:33:ARG:HE	2.16	0.42
1:A:33:GLN:HE21	1:A:33:GLN:CA	2.25	0.42
11:K:207:ASN:HD21	10:X:144:PRO:CG	2.32	0.42
6:F:127:ASN:HD22	6:F:127:ASN:H	1.66	0.42
4:R:121:LEU:HA	4:R:123:PHE:CE1	2.55	0.42
13:M:83:LEU:O	13:M:87:MET:HG2	2.20	0.42
13:1:150:VAL:HG21	16:1:233:HOH:O	2.18	0.42
13:M:5:SER:HB3	13:M:14:ILE:HG13	2.01	0.42
6:T:70:VAL:HG11	6:T:112:PHE:CE1	2.55	0.42
3:C:185:THR:HG22	3:C:186:VAL:N	2.33	0.42
1:O:86:ARG:NE	7:U:118:ASN:HD21	2.13	0.42
9:I:55:LEU:HD11	9:I:97:VAL:HG21	2.01	0.42
10:J:143:ARG:HB2	10:J:146:MET:HG3	2.01	0.42
14:2:159:LEU:CB	14:2:173:ILE:HD12	2.50	0.42
4:D:40:ILE:HD12	4:D:193:VAL:HG23	2.00	0.42
11:K:74:ILE:HD11	11:K:78:ALA:HB3	2.02	0.42
5:E:227:GLU:OE2	5:E:227:GLU:N	2.52	0.42
2:P:136:PHE:O	2:P:150:THR:HA	2.20	0.42
13:M:8:TYR:CE2	13:M:148:VAL:HG22	2.54	0.42
14:2:105:ASP:OD2	14:2:106:ASN:N	2.45	0.42
5:E:104:ASN:HB2	13:M:81:GLU:HG2	2.00	0.42
6:F:43:ASN:N	6:F:43:ASN:ND2	2.67	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1:152:GLU:O	13:1:156:VAL:HG23	2.19	0.42
8:V:15:ALA:HA	8:V:174:ASP:O	2.20	0.42
10:X:129:TYR:O	10:X:132:PHE:HB2	2.18	0.42
14:2:20:THR:OG1	14:2:28:ASN:HB3	2.19	0.42
10:X:166:MET:HA	10:X:167:PRO:HD3	1.81	0.42
6:F:53:LEU:HD11	6:F:205:ASN:OD1	2.20	0.42
8:H:167:LEU:HD13	12:Z:167:ILE:HD13	2.00	0.42
1:A:175:PHE:O	1:A:179:ARG:HG2	2.19	0.42
13:M:113:VAL:HG23	13:M:119:THR:HG22	2.01	0.42
7:G:101:TYR:OH	14:N:58:ILE:HD11	2.20	0.42
8:H:84:LYS:HE2	8:H:119:THR:HG23	2.02	0.42
3:Q:38:VAL:CG2	3:Q:39:GLY:N	2.83	0.42
5:E:5:ARG:HG3	5:E:22:PHE:CE1	2.55	0.42
12:L:21:ILE:HD12	12:L:21:ILE:C	2.39	0.42
9:W:28:SER:HB2	10:X:120:VAL:HG21	2.01	0.42
1:A:198:LYS:HE3	1:A:236:LEU:HD11	2.02	0.42
14:2:85:GLU:O	14:2:89:GLU:HB2	2.20	0.42
14:N:114:PRO:HD2	14:N:118:SER:O	2.20	0.42
5:E:123:ASN:HD22	5:E:123:ASN:N	2.18	0.42
4:R:161:ASN:HB3	4:R:180:TRP:CE2	2.55	0.42
8:H:3:ILE:HG22	8:H:16:ALA:HB2	2.02	0.42
12:Z:-7:ASN:HD22	12:Z:-6:PRO:CD	2.32	0.42
2:B:45:GLY:HA3	2:B:216:ARG:HG2	2.01	0.42
3:C:14:ILE:CD1	3:C:14:ILE:N	2.83	0.42
11:Y:180:GLU:CB	16:Y:1428:HOH:O	2.68	0.42
4:R:173:GLN:HG2	5:S:56:ASP:OD2	2.19	0.42
6:F:172:ALA:O	6:F:176:LEU:HD23	2.19	0.42
1:A:92:SER:O	1:A:95:VAL:HG12	2.20	0.42
2:B:113:VAL:HG22	2:B:138:TYR:CD2	2.54	0.42
5:S:37:THR:HG22	5:S:165:ILE:HG13	2.02	0.42
11:K:4:LEU:C	11:K:4:LEU:HD22	2.40	0.42
4:R:46:VAL:HG11	4:R:139:ALA:HB1	2.01	0.42
2:B:87:ILE:CD1	2:B:87:ILE:N	2.83	0.42
1:O:74:ILE:N	1:O:74:ILE:HD12	2.34	0.42
7:G:172:ILE:HD12	7:G:197:MET:CE	2.50	0.42
3:Q:33:ARG:HH11	3:Q:33:ARG:HB3	1.84	0.42
1:O:86:ARG:HH21	7:U:118:ASN:ND2	2.18	0.42
1:A:31:VAL:HG11	1:A:135:SER:HB2	2.01	0.42
13:M:123:PRO:HB3	13:M:14(G):ILE:HD11	2.02	0.42
9:I:29:ASN:ND2	11:Y:208:ASN:HD21	2.16	0.42
5:S:227:GLU:OE2	5:S:227:GLU:N	2.53	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:136:LEU:HD12	5:S:151:PHE:CD2	2.55	0.42
3:Q:18(A):ASP:OD1	3:Q:18(C):LYS:HB2	2.19	0.42
6:T:136:THR:O	6:T:150:MET:HA	2.20	0.42
6:T:43:ASN:ND2	6:T:185:SER:HA	2.34	0.42
5:S:104:ASN:HB2	13:1:81:GLU:HG2	2.01	0.42
11:Y:200:LYS:HG3	11:Y:205:SER:O	2.20	0.42
10:J:193:GLN:OXT	10:J:193:GLN:HG2	2.19	0.42
3:Q:95:GLU:OE2	3:Q:95:GLU:HA	2.19	0.42
13:M:115:LEU:HD23	13:M:115:LEU:N	2.35	0.42
13:1:-3:VAL:HA	13:1:21:SER:O	2.20	0.42
2:B:116:LEU:HA	2:B:119:ILE:HD12	2.01	0.42
14:N:163:ILE:N	14:N:163:ILE:CD1	2.82	0.42
4:R:70:ILE:HD13	4:R:112:LEU:HD11	2.02	0.42
3:C:106:PRO:HG2	3:C:143:PRO:HG2	1.99	0.42
14:2:13:ILE:HD12	14:2:151:THR:HG22	2.02	0.42
9:W:29:ASN:C	9:W:29:ASN:HD22	2.22	0.42
14:N:21:THR:O	15:N:1404:BO2:H3	2.19	0.42
6:T:127:ASN:H	6:T:127:ASN:HD22	1.67	0.42
4:D:121:LEU:HA	4:D:123:PHE:CE1	2.55	0.42
7:G:18(D):ILE:HD12	7:G:192:PHE:CE2	2.55	0.42
8:V:24:PRO:HG2	8:V:25:ILE:HD12	2.02	0.42
10:X:185:ARG:HH11	10:X:185:ARG:HG2	1.85	0.42
1:A:26:TYR:CD1	1:A:26:TYR:N	2.87	0.42
2:P:202:THR:HG22	2:P:203:ASP:N	2.35	0.41
6:T:95:GLU:HG3	6:T:115:ARG:HD2	2.02	0.41
4:D:192:LEU:HD12	4:D:196:ILE:HD11	2.02	0.41
10:J:144:PRO:HG2	11:Y:207:ASN:HD21	1.85	0.41
14:2:163:ILE:HD12	14:2:173:ILE:HD11	2.02	0.41
11:K:74:ILE:HD11	11:K:78:ALA:CB	2.50	0.41
13:M:-3:VAL:HA	13:M:21:SER:O	2.20	0.41
6:F:216:SER:HB3	6:F:21(A):GLU:HB2	2.01	0.41
6:F:136:THR:O	6:F:150:MET:HA	2.20	0.41
4:D:229:THR:HG22	4:D:233:ILE:HD13	2.01	0.41
12:Z:80:ALA:HA	12:Z:113:PHE:HZ	1.84	0.41
8:V:114:HIS:ND1	15:2:1405:BO2:H5	2.35	0.41
10:X:24:ILE:HG13	10:X:24:ILE:O	2.20	0.41
6:F:203:GLU:HA	6:F:203:GLU:OE1	2.20	0.41
7:G:143:GLU:HA	7:G:217:LYS:NZ	2.35	0.41
2:P:6:ARG:HG3	2:P:6:ARG:HH11	1.85	0.41
14:2:126:ILE:N	14:2:126:ILE:CD1	2.81	0.41
2:P:15:PHE:H	3:Q:23:GLN:NE2	2.15	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:177:GLU:HG2	2:P:58:LEU:CD2	2.48	0.41
10:X:143:ARG:HB2	10:X:146:MET:HG3	2.02	0.41
4:D:177:LEU:HD22	5:E:58:LEU:HD13	2.01	0.41
10:J:143:ARG:O	10:J:146:MET:HG3	2.20	0.41
8:H:114:HIS:CE1	15:N:1404:BO2:H5	2.55	0.41
10:J:112:GLN:HE21	10:J:125:GLY:HA3	1.84	0.41
1:O:43:THR:HG23	1:O:184:LEU:O	2.20	0.41
1:O:17:PRO:HA	2:P:26:TYR:CD1	2.55	0.41
8:V:72:ARG:HH11	8:V:72:ARG:HG3	1.85	0.41
9:I:90:ARG:HH11	9:I:90:ARG:HA	1.85	0.41
7:U:105:TYR:OH	8:V:66:HIS:HE1	2.04	0.41
11:K:10(A):ARG:HB3	11:K:10(B):LYS:CE	2.43	0.41
7:G:107:MET:CE	7:G:112:LEU:HD13	2.50	0.41
3:Q:163:GLN:HE22	3:Q:173:ARG:NE	2.13	0.41
3:Q:190:VAL:HG13	3:Q:212:ILE:HG21	2.02	0.41
9:I:110:ILE:CG1	9:I:125:ILE:HD13	2.50	0.41
13:M:14(C):ARG:CG	13:M:14(C):ARG:NH1	2.78	0.41
8:V:44:ALA:HB3	8:V:100:ILE:HB	2.02	0.41
13:1:14(G):ILE:HB	13:1:144:PRO:CD	2.50	0.41
1:A:46:VAL:HB	1:A:215:ILE:HD13	2.02	0.41
8:H:210:THR:HG21	12:Z:14(C):GLN:HG2	2.01	0.41
6:T:100:LYS:O	6:T:104:LYS:N	2.51	0.41
6:T:45:GLY:HA3	6:T:215:CYS:O	2.20	0.41
10:X:16:SER:HB2	16:X:227:HOH:O	2.20	0.41
12:L:27:ASN:HB3	13:M:120:TYR:CE1	2.55	0.41
11:K:14:VAL:HB	11:K:176:TYR:HB2	2.03	0.41
8:H:197:ARG:HG3	12:Z:164:GLU:CD	2.41	0.41
6:T:157:TYR:CD1	6:T:157:TYR:C	2.93	0.41
1:O:26:TYR:CD1	1:O:26:TYR:N	2.87	0.41
5:S:216:GLY:O	5:S:219:THR:N	2.47	0.41
5:E:77:SER:OG	5:E:137:LEU:HB2	2.21	0.41
7:G:152:ASP:HB2	7:G:153:PRO:HD2	2.03	0.41
13:M:113:VAL:HA	13:M:118:VAL:O	2.19	0.41
10:X:53:VAL:HB	16:Y:1427:HOH:O	2.19	0.41
12:L:19:ARG:NE	12:L:171:ASP:OD2	2.43	0.41
7:U:110:ASP:HB3	7:U:149:TYR:CZ	2.55	0.41
2:B:160:TRP:HA	3:C:59:GLN:HA	2.01	0.41
7:U:55:PRO:HG2	7:U:56:ASP:H	1.85	0.41
5:E:2(C):VAL:HG22	5:E:226:GLY:HA2	2.01	0.41
9:I:29:ASN:HD22	9:I:29:ASN:C	2.23	0.41
7:G:101:TYR:CE1	14:N:58:ILE:HD13	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:127:ASN:ND2	6:T:127:ASN:N	2.69	0.41
3:C:75:VAL:HG13	3:C:221:ILE:HD13	2.01	0.41
5:S:105:ARG:HB2	13:1:78:TYR:CE1	2.56	0.41
5:S:171:GLY:HA3	5:S:199:GLN:O	2.21	0.41
4:R:40:ILE:HG12	4:R:193:VAL:CG2	2.51	0.41
11:Y:111:TYR:CE1	11:Y:121:LYS:HB2	2.56	0.41
2:P:112:LEU:HD23	2:P:112:LEU:C	2.40	0.41
10:X:193:GLN:HG2	10:X:193:GLN:OXT	2.20	0.41
11:K:114:ASP:OD1	11:K:114:ASP:C	2.58	0.41
10:J:162:LEU:O	10:J:166:MET:HB2	2.20	0.41
9:W:104:ILE:N	9:W:104:ILE:HD13	2.36	0.41
3:C:35:THR:HB	3:C:51:GLU:CG	2.50	0.41
11:K:40:PHE:CE2	11:K:73:ARG:HD2	2.56	0.41
11:Y:40:PHE:CG	11:Y:73:ARG:CZ	3.04	0.41
4:R:215:ILE:HD13	4:R:216:THR:N	2.35	0.41
2:B:95:HIS:CD2	2:B:115:ARG:HG2	2.56	0.41
5:E:162:GLY:O	5:E:163:THR:HB	2.20	0.41
4:R:120:ALA:CB	4:R:155:GLY:HA2	2.50	0.41
7:G:17(D):SER:O	7:G:17(E):LYS:HB2	2.21	0.41
11:Y:137:VAL:HG21	11:Y:161:ALA:HB2	2.03	0.41
3:Q:71:ASP:OD1	3:Q:100:ARG:NH1	2.53	0.41
4:R:91:HIS:CG	4:R:119:LEU:HD11	2.56	0.41
2:B:40:ILE:HD12	2:B:193:ALA:HB2	2.01	0.41
3:C:201:VAL:HG11	3:C:210:ILE:HG12	2.02	0.41
11:Y:99:THR:HG22	11:Y:113:VAL:O	2.20	0.41
10:J:168:MET:HG2	10:X:168:MET:CE	2.51	0.41
10:X:143:ARG:O	10:X:146:MET:HG3	2.20	0.41
3:Q:219:SER:C	3:Q:221:ILE:HD12	2.41	0.41
14:2:48:SER:O	14:2:52:THR:HG23	2.20	0.41
3:Q:39:GLY:HA2	3:Q:47:VAL:O	2.20	0.41
1:A:161:LYS:HD3	1:A:180:TRP:CZ3	2.55	0.41
13:1:9:ASP:OD1	13:1:10:ASN:N	2.53	0.41
11:Y:195:LEU:O	11:Y:199:VAL:HG23	2.20	0.41
6:T:107:ILE:HA	6:T:108:PRO:HD3	1.84	0.41
2:B:122:GLY:C	2:B:124:THR:H	2.23	0.41
2:B:38:ILE:CD1	2:B:164:SER:HB3	2.39	0.41
2:B:130:ARG:HA	2:B:131:PRO:HD3	1.89	0.41
6:T:203:GLU:OE1	6:T:203:GLU:HA	2.21	0.41
3:Q:161:SER:HB3	3:Q:180:TYR:CE1	2.56	0.41
13:M:42:VAL:HG23	13:M:178:ILE:HD11	2.02	0.41
3:C:224:LEU:N	3:C:224:LEU:CD1	2.84	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:224:LEU:CD1	3:Q:224:LEU:N	2.84	0.41
11:K:4:LEU:O	11:K:4:LEU:HD22	2.21	0.41
7:U:110:ASP:HB3	7:U:149:TYR:CE2	2.56	0.41
14:2:184:VAL:HG21	16:2:1412:HOH:O	2.20	0.41
4:R:24:VAL:O	4:R:28:LEU:HD13	2.21	0.41
4:R:227:GLU:OE2	4:R:227:GLU:N	2.44	0.41
3:Q:201:VAL:HG11	3:Q:210:ILE:HG12	2.02	0.41
2:B:111:ILE:H	2:B:111:ILE:CD1	2.34	0.41
2:B:209:ARG:HH11	2:B:209:ARG:HG2	1.85	0.41
12:L:80:ALA:HA	12:L:113:PHE:HZ	1.86	0.41
12:Z:3:ILE:CD1	12:Z:46:ASN:CB	2.90	0.41
14:2:33:LYS:HE2	15:2:1405:BO2:H222	2.03	0.41
10:X:3:ILE:HD13	10:X:46:ALA:HB2	2.02	0.41
11:Y:65:LEU:HD12	11:Y:65:LEU:HA	1.93	0.41
10:X:162:LEU:O	10:X:166:MET:HB2	2.21	0.41
11:K:37:ILE:HB	11:K:41:LEU:CB	2.44	0.41
12:L:-7:ASN:HD22	12:L:-5:TYR:H	1.67	0.41
7:G:121:GLN:NE2	7:G:121:GLN:C	2.74	0.41
3:Q:105:ASP:OD2	3:Q:106:PRO:HD2	2.21	0.41
2:P:89:ILE:O	2:P:92:ALA:HB3	2.21	0.41
10:J:10(B):LYS:HB2	10:J:10(B):LYS:HZ2	1.82	0.41
4:R:67:ILE:HG22	4:R:221:PHE:HZ	1.86	0.41
6:F:175:GLU:OE2	6:F:175:GLU:HA	2.21	0.41
5:S:134:VAL:O	5:S:153:PRO:HG3	2.21	0.41
3:Q:241:GLN:C	3:Q:243:GLN:N	2.74	0.41
5:S:52:LYS:HB3	5:S:63:TYR:O	2.21	0.41
10:J:52:THR:HG22	10:J:53:VAL:H	1.86	0.41
12:L:90:LYS:HD3	12:L:95:TYR:CE1	2.56	0.41
6:F:176:LEU:HB3	7:G:58:LEU:HD21	2.02	0.41
11:Y:4:LEU:C	11:Y:4:LEU:CD2	2.89	0.41
6:T:43:ASN:ND2	6:T:43:ASN:N	2.68	0.41
13:M:-3:VAL:HG12	13:M:49:ILE:HG13	2.03	0.41
11:Y:22:ALA:HB2	15:Y:1403:BO2:H6	2.02	0.41
4:D:46:VAL:HG11	4:D:139:ALA:HB1	2.03	0.41
4:D:205:GLU:HA	4:D:205:GLU:OE2	2.21	0.41
7:G:119:LEU:HA	7:G:119:LEU:HD12	1.83	0.41
13:M:208:THR:HG22	8:V:77:VAL:HB	2.02	0.41
7:U:17(D):SER:O	7:U:17(E):LYS:HB2	2.21	0.41
6:T:32:GLU:HB3	6:T:169:ARG:NH2	2.36	0.41
5:E:37:THR:HG22	5:E:165:ILE:HG13	2.03	0.41
2:P:21(A):LYS:O	2:P:21(B):GLY:C	2.60	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:38:ILE:HD12	6:T:38:ILE:C	2.42	0.41
9:I:14:ILE:HG12	9:I:34:ILE:CD1	2.50	0.41
2:P:5:SER:O	2:P:6:ARG:C	2.59	0.41
4:D:192:LEU:HD12	4:D:196:ILE:CD1	2.50	0.41
3:Q:158:SER:HB2	4:R:59:LEU:HD21	2.03	0.41
7:G:224:LEU:HD12	7:G:229:ILE:CD1	2.51	0.41
5:S:97:ASN:HD21	12:Z:61:ASN:ND2	2.18	0.41
2:B:225:LYS:O	2:B:226:PRO:C	2.60	0.41
3:C:39:GLY:HA2	3:C:47:VAL:O	2.21	0.41
3:C:18(A):ASP:OD1	3:C:18(C):LYS:HB2	2.21	0.41
1:O:117:ALA:HB1	1:O:155:GLY:O	2.20	0.41
8:V:144:GLN:O	8:V:145:ASP:HB2	2.21	0.41
4:R:122:ARG:HH11	4:R:122:ARG:HG2	1.86	0.41
6:T:49:ALA:CB	6:T:212:ILE:HD13	2.51	0.40
5:S:75:GLY:HA3	5:S:221:PHE:CZ	2.56	0.40
9:W:29:ASN:H	9:W:29:ASN:ND2	2.19	0.40
6:T:175:GLU:OE2	6:T:175:GLU:HA	2.21	0.40
4:D:177:LEU:HD22	5:E:58:LEU:HD11	2.04	0.40
3:Q:182:PRO:O	3:Q:183:PRO:C	2.59	0.40
9:I:165:ARG:NH2	12:Z:135:MET:HE3	2.37	0.40
12:L:27:ASN:HB3	13:M:120:TYR:CZ	2.55	0.40
14:2:114:PRO:HD2	14:2:118:SER:O	2.20	0.40
12:L:48:PHE:CZ	12:L:50:ALA:HB3	2.56	0.40
9:W:159:LEU:HD21	9:W:173:ALA:HB1	2.03	0.40
10:X:35:ARG:HD3	10:X:35:ARG:HA	1.91	0.40
2:B:202:THR:HG22	2:B:203:ASP:N	2.36	0.40
7:U:18(B):ASP:O	7:U:18(C):HIS:HB3	2.21	0.40
3:C:33:ARG:HH11	3:C:33:ARG:HB3	1.84	0.40
10:X:143:ARG:HA	10:X:144:PRO:HD3	1.87	0.40
15:N:1404:BO2:H21	16:N:1440:HOH:O	2.20	0.40
3:C:182:PRO:O	3:C:183:PRO:C	2.59	0.40
1:A:232:ARG:NH1	1:A:232:ARG:HG3	2.35	0.40
6:F:127:ASN:N	6:F:127:ASN:ND2	2.68	0.40
13:M:186:PHE:HE1	13:M:188:LYS:HG3	1.85	0.40
1:O:100:TYR:HD1	1:O:105:GLU:O	2.02	0.40
6:F:93:ARG:HD3	13:M:68:TYR:CD2	2.56	0.40
12:Z:176:LEU:HG	12:Z:186:LYS:HG2	2.03	0.40
4:R:90:GLU:OE2	11:Y:69:ARG:NH1	2.54	0.40
6:T:49:ALA:HA	6:T:211:GLU:O	2.22	0.40
2:B:14:ILE:HD13	16:B:268:HOH:O	2.20	0.40
7:U:188:LYS:HA	7:U:188:LYS:HD3	1.91	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:3:ILE:CD1	8:H:100:ILE:HG12	2.44	0.40
8:V:3:ILE:HG22	8:V:16:ALA:CB	2.51	0.40
3:C:161:SER:HB3	3:C:180:TYR:CE1	2.56	0.40
4:R:59:LEU:HD13	4:R:59:LEU:C	2.42	0.40
7:U:139:VAL:O	7:U:140:SER:HB3	2.20	0.40
7:U:168:LYS:O	7:U:172:ILE:HG13	2.21	0.40
7:U:82:ILE:HG22	7:U:83:PRO:HD3	2.03	0.40
11:K:4:LEU:HD11	11:K:15:ALA:HB3	2.02	0.40
2:P:49:ALA:HB2	2:P:212:PHE:CE1	2.56	0.40
13:M:150:VAL:HG21	16:M:259:HOH:O	2.22	0.40
12:L:34:VAL:HB	16:L:227:HOH:O	2.19	0.40
14:2:104:TYR:OH	14:2:180:ALA:HB2	2.21	0.40
6:T:216:SER:HB3	6:T:21(A):GLU:HB2	2.02	0.40
1:A:39:GLY:HA2	1:A:47:VAL:O	2.22	0.40
4:D:17:PRO:HD2	16:D:266:HOH:O	2.21	0.40
4:R:205:GLU:OE2	4:R:205:GLU:HA	2.21	0.40
11:Y:114:ASP:C	11:Y:114:ASP:OD1	2.59	0.40
10:J:18:LYS:CG	10:J:174:ILE:HG13	2.52	0.40
6:F:67:ILE:CD1	6:F:77:VAL:HB	2.47	0.40
2:B:41:MET:HE1	3:C:62:ARG:NH2	2.36	0.40
2:P:85:ALA:O	2:P:89:ILE:HG12	2.21	0.40
3:Q:55:THR:O	3:Q:56:LEU:HD13	2.22	0.40
7:G:39:ALA:HA	7:G:47:VAL:O	2.20	0.40
8:V:10:ASN:O	8:V:180:ILE:HG12	2.21	0.40
10:X:52:THR:HG22	10:X:53:VAL:H	1.86	0.40
5:S:185:ASN:HA	5:S:186:PRO:HD2	1.96	0.40
13:1:115:LEU:N	13:1:115:LEU:HD23	2.36	0.40
6:F:197:ILE:HG21	6:F:210:LEU:HD13	2.02	0.40
11:Y:83:LEU:HD23	11:Y:99:THR:HG21	2.03	0.40
10:J:133:TYR:C	16:J:198:HOH:O	2.59	0.40
11:Y:131:GLN:HG3	11:Y:132:THR:N	2.37	0.40
9:I:29:ASN:ND2	9:I:29:ASN:H	2.20	0.40
12:Z:21:ILE:CD1	12:Z:168:GLN:HG2	2.51	0.40
11:Y:5:ALA:HA	11:Y:13:ILE:O	2.22	0.40
11:K:5:ALA:HA	11:K:13:ILE:O	2.21	0.40
6:F:87:HIS:HD2	6:F:132:PHE:HE2	1.69	0.40
5:E:136:LEU:HD12	5:E:151:PHE:CD2	2.57	0.40
6:F:43:ASN:ND2	6:F:185:SER:HA	2.36	0.40
5:S:105:ARG:HB2	13:1:78:TYR:CD1	2.57	0.40
4:R:17:PRO:HA	5:S:26:TYR:CD2	2.56	0.40
13:M:152:GLU:O	13:M:156:VAL:HG23	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:32:LYS:O	4:R:167:SER:HA	2.22	0.40
3:Q:11:ALA:CB	4:R:12:VAL:HG11	2.51	0.40
1:O:198:LYS:HE3	1:O:236:LEU:HD11	2.02	0.40
10:X:104:TYR:CD1	10:X:180:LYS:HA	2.57	0.40
2:P:169:THR:O	2:P:173:GLN:HB2	2.22	0.40
4:R:238:LYS:HE2	4:R:238:LYS:HB3	1.90	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 X-ray entries followed by that with respect to entries of similar resolution.

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	248/250 (99%)	236 (95%)	10 (4%)	2 (1%)	24	58
1	O	248/250 (99%)	235 (95%)	11 (4%)	2 (1%)	24	58
2	B	242/244 (99%)	221 (91%)	16 (7%)	5 (2%)	9	29
2	P	242/244 (99%)	220 (91%)	17 (7%)	5 (2%)	9	29
3	C	239/241 (99%)	219 (92%)	16 (7%)	4 (2%)	11	36
3	Q	239/241 (99%)	218 (91%)	17 (7%)	4 (2%)	11	36
4	D	240/242 (99%)	225 (94%)	11 (5%)	4 (2%)	11	36
4	R	240/242 (99%)	223 (93%)	12 (5%)	5 (2%)	9	29
5	E	231/233 (99%)	210 (91%)	15 (6%)	6 (3%)	7	22
5	S	231/233 (99%)	210 (91%)	15 (6%)	6 (3%)	7	22
6	F	242/244 (99%)	222 (92%)	17 (7%)	3 (1%)	16	47
6	T	242/244 (99%)	222 (92%)	17 (7%)	3 (1%)	16	47
7	G	241/243 (99%)	226 (94%)	12 (5%)	3 (1%)	16	47
7	U	241/243 (99%)	224 (93%)	15 (6%)	2 (1%)	24	58
8	H	220/222 (99%)	208 (94%)	11 (5%)	1 (0%)	34	69

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	V	220/222 (99%)	211 (96%)	8 (4%)	1 (0%)	34	69
9	I	202/204 (99%)	195 (96%)	6 (3%)	1 (0%)	34	69
9	W	202/204 (99%)	195 (96%)	6 (3%)	1 (0%)	34	69
10	J	196/198 (99%)	184 (94%)	11 (6%)	1 (0%)	34	69
10	X	196/198 (99%)	186 (95%)	9 (5%)	1 (0%)	34	69
11	K	210/212 (99%)	201 (96%)	9 (4%)	0	100	100
11	Y	210/212 (99%)	202 (96%)	8 (4%)	0	100	100
12	L	220/222 (99%)	205 (93%)	14 (6%)	1 (0%)	34	69
12	Z	220/222 (99%)	206 (94%)	12 (6%)	2 (1%)	21	55
13	1	231/233 (99%)	218 (94%)	13 (6%)	0	100	100
13	M	231/233 (99%)	218 (94%)	11 (5%)	2 (1%)	21	55
14	2	194/196 (99%)	184 (95%)	10 (5%)	0	100	100
14	N	194/196 (99%)	185 (95%)	9 (5%)	0	100	100
All	All	6312/6368 (99%)	5909 (94%)	338 (5%)	65 (1%)	19	52

All (65) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	20(A)	SER
3	C	58	LEU
4	D	12(G)	GLU
5	E	217	LYS
2	P	20(A)	SER
3	Q	58	LEU
4	R	12(G)	GLU
5	S	217	LYS
1	A	5	THR
2	B	6	ARG
2	B	54	VAL
2	B	21(B)	GLY
2	B	21(C)	ASP
3	C	183	PRO
5	E	5	ARG
5	E	202	ARG
6	F	64	ASN
6	F	205	ASN
9	I	145	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	O	5	THR
2	P	6	ARG
2	P	54	VAL
2	P	21(B)	GLY
2	P	21(C)	ASP
3	Q	183	PRO
5	S	5	ARG
5	S	202	ARG
6	T	64	ASN
6	T	205	ASN
9	W	145	ASN
3	C	203	THR
4	D	12(F)	GLY
5	E	64	GLN
5	E	18(A)	ASP
8	H	91	GLN
12	L	71	ASP
3	Q	203	THR
4	R	12(F)	GLY
5	S	64	GLN
5	S	18(A)	ASP
6	T	206	LYS
8	V	91	GLN
4	D	18(D)	SER
5	E	180	LEU
6	F	206	LYS
10	J	192	ALA
1	O	167	LYS
4	R	18(D)	SER
5	S	180	LEU
10	X	192	ALA
12	Z	71	ASP
1	A	167	LYS
3	C	242	GLU
4	D	12(C)	GLY
7	G	239	GLN
13	M	2	SER
13	M	96	TRP
4	R	120	ALA
4	R	12(C)	GLY
7	G	55	PRO
3	Q	242	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	U	55	PRO
7	U	239	GLN
12	Z	93	PHE
7	G	7	GLY

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 X-ray entries followed by that with respect to entries of similar resolution.

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	209/209 (100%)	201 (96%)	8 (4%)	40	74
1	O	209/209 (100%)	202 (97%)	7 (3%)	45	79
2	B	203/203 (100%)	190 (94%)	13 (6%)	22	52
2	P	203/203 (100%)	193 (95%)	10 (5%)	31	65
3	C	213/213 (100%)	200 (94%)	13 (6%)	23	55
3	Q	213/213 (100%)	201 (94%)	12 (6%)	26	59
4	D	198/198 (100%)	188 (95%)	10 (5%)	29	63
4	R	198/198 (100%)	189 (96%)	9 (4%)	34	68
5	E	192/192 (100%)	178 (93%)	14 (7%)	17	44
5	S	192/192 (100%)	177 (92%)	15 (8%)	16	41
6	F	201/201 (100%)	187 (93%)	14 (7%)	19	47
6	T	201/201 (100%)	188 (94%)	13 (6%)	21	52
7	G	207/207 (100%)	194 (94%)	13 (6%)	22	53
7	U	207/207 (100%)	194 (94%)	13 (6%)	22	53
8	H	181/181 (100%)	175 (97%)	6 (3%)	45	79
8	V	181/181 (100%)	175 (97%)	6 (3%)	45	79
9	I	172/172 (100%)	165 (96%)	7 (4%)	37	72
9	W	172/172 (100%)	164 (95%)	8 (5%)	32	67
10	J	175/175 (100%)	169 (97%)	6 (3%)	44	78
10	X	175/175 (100%)	170 (97%)	5 (3%)	50	83

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	K	169/169 (100%)	161 (95%)	8 (5%)	32	67
11	Y	169/169 (100%)	161 (95%)	8 (5%)	32	67
12	L	185/185 (100%)	172 (93%)	13 (7%)	19	47
12	Z	185/185 (100%)	173 (94%)	12 (6%)	21	52
13	1	199/199 (100%)	190 (96%)	9 (4%)	34	68
13	M	199/199 (100%)	191 (96%)	8 (4%)	38	73
14	2	162/162 (100%)	155 (96%)	7 (4%)	35	70
14	N	162/162 (100%)	154 (95%)	8 (5%)	31	65
All	All	5332/5332 (100%)	5057 (95%)	275 (5%)	29	62

All (275) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	LYS
1	A	33	GLN
1	A	64	LEU
1	A	124	THR
1	A	135	SER
1	A	158	PHE
1	A	179	ARG
1	A	210	ILE
2	B	14	ILE
2	B	71	ASN
2	B	87	ILE
2	B	94	ILE
2	B	121	GLN
2	B	135	SER
2	B	150	THR
2	B	156	ASN
2	B	185	LYS
2	B	192	LEU
2	B	212	PHE
2	B	218	ASN
2	B	232	ILE
3	C	10	ARG
3	C	14	ILE
3	C	25	GLU
3	C	57	LYS
3	C	89	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	121	GLN
3	C	135	SER
3	C	150	GLN
3	C	163	GLN
3	C	174	GLU
3	C	178	LYS
3	C	208	LYS
3	C	227	GLU
4	D	76	CYS
4	D	110	GLU
4	D	126	ARG
4	D	177	LEU
4	D	18(E)	SER
4	D	191	LEU
4	D	194	LEU
4	D	196	ILE
4	D	215	ILE
4	D	237	LEU
5	E	11	ASP
5	E	12	THR
5	E	32	LYS
5	E	57	GLU
5	E	68	ILE
5	E	76	LEU
5	E	121	GLN
5	E	139	ILE
5	E	185	ASN
5	E	189	LEU
5	E	199	GLN
5	E	207	LEU
5	E	227	GLU
5	E	231	LYS
6	F	11	SER
6	F	35	THR
6	F	36	THR
6	F	43	ASN
6	F	121	GLN
6	F	127	ASN
6	F	144	ASN
6	F	18(E)	GLU
6	F	187	ARG
6	F	203	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	F	204	ASP
6	F	205	ASN
6	F	214	TRP
6	F	21(C)	ASN
7	G	12	ILE
7	G	14	ILE
7	G	72	ARG
7	G	87	ASN
7	G	119	LEU
7	G	121	GLN
7	G	124	THR
7	G	169	GLN
7	G	174	THR
7	G	184	ASN
7	G	197	MET
7	G	232	ARG
7	G	233	LEU
8	H	30	ASN
8	H	34	LEU
8	H	56	THR
8	H	68	LEU
8	H	144	GLN
8	H	197	ARG
9	I	29	ASN
9	I	45	ILE
9	I	110	ILE
9	I	113	PHE
9	I	159	LEU
9	I	160	LEU
9	I	171	TRP
10	J	52	THR
10	J	70	GLU
10	J	77	GLN
10	J	90(A)	ILE
10	J	121	GLU
10	J	166	MET
11	K	4	LEU
11	K	8	PHE
11	K	9	GLN
11	K	65	LEU
11	K	99	THR
11	K	100	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	K	104	TYR
11	K	10(B)	LYS
12	L	-9	GLN
12	L	-7	ASN
12	L	3	ILE
12	L	14	LEU
12	L	25	SER
12	L	40	ASN
12	L	58	ARG
12	L	70(A)	ASN
12	L	82	ASN
12	L	98	HIS
12	L	99	THR
12	L	115	PRO
12	L	138	LEU
13	M	40	ASN
13	M	62	LEU
13	M	91	ARG
13	M	129	PHE
13	M	14(C)	ARG
13	M	148	VAL
13	M	149	GLN
13	M	204	LYS
14	N	36	ARG
14	N	84	LYS
14	N	89	GLU
14	N	10(B)	LYS
14	N	126	ILE
14	N	134	ILE
14	N	163	ILE
14	N	18(I)	GLN
1	O	32	LYS
1	O	33	GLN
1	O	64	LEU
1	O	124	THR
1	O	135	SER
1	O	158	PHE
1	O	179	ARG
2	P	71	ASN
2	P	121	GLN
2	P	135	SER
2	P	150	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	P	156	ASN
2	P	185	LYS
2	P	187	ASP
2	P	192	LEU
2	P	212	PHE
2	P	218	ASN
3	Q	10	ARG
3	Q	25	GLU
3	Q	57	LYS
3	Q	89	ILE
3	Q	121	GLN
3	Q	135	SER
3	Q	150	GLN
3	Q	163	GLN
3	Q	174	GLU
3	Q	178	LYS
3	Q	208	LYS
3	Q	227	GLU
4	R	76	CYS
4	R	110	GLU
4	R	126	ARG
4	R	177	LEU
4	R	18(E)	SER
4	R	191	LEU
4	R	194	LEU
4	R	215	ILE
4	R	237	LEU
5	S	11	ASP
5	S	12	THR
5	S	32	LYS
5	S	57	GLU
5	S	76	LEU
5	S	104	ASN
5	S	121	GLN
5	S	18(D)	ILE
5	S	185	ASN
5	S	189	LEU
5	S	199	GLN
5	S	207	LEU
5	S	214	ILE
5	S	227	GLU
5	S	231	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	T	11	SER
6	T	36	THR
6	T	43	ASN
6	T	121	GLN
6	T	127	ASN
6	T	144	ASN
6	T	18(E)	GLU
6	T	187	ARG
6	T	203	GLU
6	T	204	ASP
6	T	205	ASN
6	T	214	TRP
6	T	21(C)	ASN
7	U	72	ARG
7	U	87	ASN
7	U	119	LEU
7	U	121	GLN
7	U	124	THR
7	U	148	ILE
7	U	169	GLN
7	U	174	THR
7	U	184	ASN
7	U	197	MET
7	U	217	LYS
7	U	232	ARG
7	U	233	LEU
8	V	30	ASN
8	V	34	LEU
8	V	56	THR
8	V	68	LEU
8	V	144	GLN
8	V	197	ARG
9	W	29	ASN
9	W	61	TYR
9	W	104	ILE
9	W	113	PHE
9	W	155	ILE
9	W	159	LEU
9	W	160	LEU
9	W	171	TRP
10	X	52	THR
10	X	70	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	X	77	GLN
10	X	121	GLU
10	X	166	MET
11	Y	4	LEU
11	Y	8	PHE
11	Y	9	GLN
11	Y	65	LEU
11	Y	99	THR
11	Y	100	MET
11	Y	104	TYR
11	Y	10(B)	LYS
12	Z	-9	GLN
12	Z	-7	ASN
12	Z	3	ILE
12	Z	14	LEU
12	Z	25	SER
12	Z	40	ASN
12	Z	58	ARG
12	Z	70(A)	ASN
12	Z	82	ASN
12	Z	98	HIS
12	Z	99	THR
12	Z	138	LEU
13	1	40	ASN
13	1	62	LEU
13	1	91	ARG
13	1	96	TRP
13	1	129	PHE
13	1	14(C)	ARG
13	1	148	VAL
13	1	149	GLN
13	1	204	LYS
14	2	3	ILE
14	2	36	ARG
14	2	84	LYS
14	2	89	GLU
14	2	10(B)	LYS
14	2	126	ILE
14	2	18(I)	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (190) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	97	HIS
2	B	23	GLN
2	B	71	ASN
2	B	95	HIS
2	B	97	GLN
2	B	121	GLN
2	B	125	GLN
2	B	156	ASN
2	B	177	GLN
2	B	218	ASN
3	C	23	GLN
3	C	82	ASN
3	C	97	GLN
3	C	121	GLN
3	C	125	GLN
3	C	150	GLN
3	C	163	GLN
3	C	238	GLN
3	C	243	GLN
4	D	23	GLN
4	D	108	ASN
4	D	147	GLN
4	D	211	GLN
4	D	226	ASN
5	E	33	GLN
5	E	73	HIS
5	E	104	ASN
5	E	121	GLN
5	E	123	ASN
5	E	125	GLN
5	E	156	ASN
5	E	185	ASN
5	E	199	GLN
5	E	2(E)	ASN
6	F	23	GLN
6	F	43	ASN
6	F	90	ASN
6	F	121	GLN
6	F	127	ASN
6	F	192	GLN
7	G	34(A)	ASN
7	G	87	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	G	118	ASN
7	G	121	GLN
7	G	125	GLN
7	G	169	GLN
7	G	170	GLN
7	G	178	ASN
7	G	184	ASN
7	G	228	ASN
8	H	30	ASN
8	H	66	HIS
8	H	144	GLN
8	H	165	ASN
8	H	172	ASN
8	H	190	ASN
9	I	29	ASN
9	I	81	GLN
9	I	145	ASN
10	J	54	GLN
10	J	77	GLN
10	J	85	GLN
10	J	112	GLN
10	J	141	HIS
10	J	186	GLN
11	K	9	GLN
11	K	85	ASN
11	K	131	GLN
11	K	174	ASN
11	K	207	ASN
11	K	208	ASN
12	L	-9	GLN
12	L	-7	ASN
12	L	40	ASN
12	L	61	ASN
12	L	70(A)	ASN
12	L	82	ASN
12	L	85	HIS
12	L	98	HIS
12	L	14(B)	ASN
12	L	1(I)	ASN
13	M	-7	GLN
13	M	10	ASN
13	M	40	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	M	89	GLN
13	M	93	ASN
13	M	149	GLN
13	M	157	ASN
13	M	172	ASN
13	M	191	GLN
14	N	69	GLN
14	N	145	ASN
14	N	157	HIS
14	N	161	GLN
1	O	33	GLN
1	O	97	HIS
2	P	23	GLN
2	P	71	ASN
2	P	95	HIS
2	P	97	GLN
2	P	121	GLN
2	P	125	GLN
2	P	156	ASN
2	P	177	GLN
2	P	218	ASN
3	Q	23	GLN
3	Q	82	ASN
3	Q	121	GLN
3	Q	125	GLN
3	Q	150	GLN
3	Q	163	GLN
3	Q	238	GLN
3	Q	243	GLN
4	R	23	GLN
4	R	108	ASN
4	R	114	GLN
4	R	147	GLN
4	R	211	GLN
4	R	226	ASN
5	S	73	HIS
5	S	104	ASN
5	S	121	GLN
5	S	123	ASN
5	S	125	GLN
5	S	156	ASN
5	S	185	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	S	199	GLN
5	S	2(E)	ASN
6	T	23	GLN
6	T	43	ASN
6	T	90	ASN
6	T	121	GLN
6	T	127	ASN
6	T	147	HIS
6	T	192	GLN
7	U	34(A)	ASN
7	U	87	ASN
7	U	118	ASN
7	U	121	GLN
7	U	125	GLN
7	U	169	GLN
7	U	170	GLN
7	U	178	ASN
7	U	184	ASN
7	U	228	ASN
8	V	10	ASN
8	V	30	ASN
8	V	66	HIS
8	V	144	GLN
8	V	165	ASN
8	V	172	ASN
8	V	190	ASN
9	W	29	ASN
9	W	81	GLN
9	W	145	ASN
10	X	54	GLN
10	X	77	GLN
10	X	85	GLN
10	X	112	GLN
10	X	141	HIS
10	X	186	GLN
11	Y	85	ASN
11	Y	131	GLN
11	Y	174	ASN
11	Y	207	ASN
11	Y	208	ASN
12	Z	-9	GLN
12	Z	-7	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	Z	40	ASN
12	Z	61	ASN
12	Z	70(A)	ASN
12	Z	82	ASN
12	Z	85	HIS
12	Z	14(B)	ASN
12	Z	1(I)	ASN
12	Z	166	HIS
12	Z	168	GLN
13	1	10	ASN
13	1	40	ASN
13	1	89	GLN
13	1	93	ASN
13	1	149	GLN
13	1	157	ASN
13	1	172	ASN
13	1	191	GLN
14	2	69	GLN
14	2	145	ASN
14	2	157	HIS
14	2	161	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link

column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	BO2	2	1405	14	28,29,29	1.49	7 (25%)	31,38,38	2.07	11 (35%)
15	BO2	H	1400	8	28,29,29	1.42	5 (17%)	31,38,38	1.74	8 (25%)
15	BO2	K	1402	11	28,29,29	1.22	1 (3%)	31,38,38	1.89	11 (35%)
15	BO2	N	1404	14	28,29,29	1.55	8 (28%)	31,38,38	2.04	11 (35%)
15	BO2	V	1401	8	28,29,29	1.40	4 (14%)	31,38,38	1.82	9 (29%)
15	BO2	Y	1403	11	28,29,29	1.27	2 (7%)	31,38,38	1.83	10 (32%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	BO2	2	1405	14	-	0/22/28/28	0/2/2/2
15	BO2	H	1400	8	-	0/22/28/28	0/2/2/2
15	BO2	K	1402	11	-	0/22/28/28	0/2/2/2
15	BO2	N	1404	14	-	0/22/28/28	0/2/2/2
15	BO2	V	1401	8	-	0/22/28/28	0/2/2/2
15	BO2	Y	1403	11	-	0/22/28/28	0/2/2/2

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	V	1401	BO2	C17-C12	2.01	1.43	1.38
15	K	1402	BO2	C13-C12	2.01	1.43	1.38
15	H	1400	BO2	C16-C15	2.02	1.43	1.38
15	Y	1403	BO2	C17-C12	2.05	1.43	1.38
15	2	1405	BO2	C16-C15	2.06	1.43	1.38
15	2	1405	BO2	C16-C17	2.10	1.43	1.38
15	V	1401	BO2	C13-C12	2.15	1.43	1.38
15	2	1405	BO2	C14-C13	2.18	1.43	1.38
15	V	1401	BO2	C16-C17	2.24	1.43	1.38
15	N	1404	BO2	C16-C15	2.24	1.43	1.38
15	N	1404	BO2	C11-C10	2.25	1.59	1.54
15	N	1404	BO2	C16-C17	2.27	1.43	1.38
15	V	1401	BO2	C14-C13	2.30	1.43	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	N	1404	BO2	C11-C12	2.34	1.57	1.51
15	H	1400	BO2	C17-C12	2.35	1.43	1.38
15	2	1405	BO2	C11-C12	2.37	1.57	1.51
15	H	1400	BO2	C14-C13	2.38	1.43	1.38
15	2	1405	BO2	C15-C14	2.39	1.44	1.38
15	H	1400	BO2	C13-C12	2.41	1.43	1.38
15	Y	1403	BO2	C13-C12	2.45	1.44	1.38
15	N	1404	BO2	C15-C14	2.53	1.44	1.38
15	H	1400	BO2	C16-C17	2.54	1.44	1.38
15	2	1405	BO2	C13-C12	2.65	1.44	1.38
15	N	1404	BO2	C14-C13	2.72	1.44	1.38
15	N	1404	BO2	C13-C12	2.78	1.44	1.38
15	N	1404	BO2	C17-C12	2.93	1.45	1.38
15	2	1405	BO2	C17-C12	2.94	1.45	1.38

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	V	1401	BO2	C3-C2-N1	-3.49	117.44	121.68
15	H	1400	BO2	C3-C2-N1	-3.38	117.57	121.68
15	2	1405	BO2	C2-C3-N4	-3.21	118.71	122.11
15	N	1404	BO2	C5-C6-N1	-3.17	118.32	122.25
15	2	1405	BO2	C5-C6-N1	-3.17	118.32	122.25
15	N	1404	BO2	C2-C3-N4	-3.13	118.80	122.11
15	K	1402	BO2	C2-C3-N4	-3.02	118.91	122.11
15	K	1402	BO2	C5-C6-N1	-2.92	118.64	122.25
15	2	1405	BO2	C3-C2-N1	-2.91	118.14	121.68
15	N	1404	BO2	C3-C2-N1	-2.86	118.19	121.68
15	Y	1403	BO2	C2-C3-N4	-2.81	119.14	122.11
15	Y	1403	BO2	C11-C10-N9	-2.74	105.07	110.80
15	K	1402	BO2	C18-C10-N9	-2.74	103.55	111.26
15	Y	1403	BO2	C18-C10-N9	-2.71	103.62	111.26
15	2	1405	BO2	O8-C7-C2	-2.71	115.46	121.23
15	Y	1403	BO2	C5-C6-N1	-2.70	118.90	122.25
15	2	1405	BO2	C11-C10-N9	-2.69	105.17	110.80
15	K	1402	BO2	C11-C10-N9	-2.68	105.18	110.80
15	N	1404	BO2	O8-C7-C2	-2.64	115.62	121.23
15	H	1400	BO2	C6-C5-N4	-2.61	118.41	121.94
15	V	1401	BO2	C5-C6-N1	-2.54	119.10	122.25
15	N	1404	BO2	C11-C10-N9	-2.49	105.59	110.80
15	K	1402	BO2	C3-C2-N1	-2.48	118.65	121.68
15	V	1401	BO2	C6-C5-N4	-2.44	118.64	121.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	Y	1403	BO2	C3-C2-N1	-2.41	118.75	121.68
15	V	1401	BO2	O8-C7-C2	-2.40	116.12	121.23
15	N	1404	BO2	C6-C5-N4	-2.40	118.70	121.94
15	2	1405	BO2	C18-C10-N9	-2.38	104.56	111.26
15	Y	1403	BO2	C6-C5-N4	-2.37	118.73	121.94
15	N	1404	BO2	C18-C10-N9	-2.30	104.78	111.26
15	K	1402	BO2	C6-C5-N4	-2.30	118.83	121.94
15	2	1405	BO2	C6-C5-N4	-2.24	118.91	121.94
15	H	1400	BO2	O8-C7-C2	-2.17	116.60	121.23
15	H	1400	BO2	C5-C6-N1	-2.13	119.60	122.25
15	K	1402	BO2	O8-C7-C2	-2.10	116.77	121.23
15	V	1401	BO2	C2-C3-N4	-2.08	119.91	122.11
15	Y	1403	BO2	C2-C7-N9	2.33	120.29	115.10
15	K	1402	BO2	C2-C7-N9	2.41	120.46	115.10
15	H	1400	BO2	C5-N4-C3	2.79	121.97	116.84
15	Y	1403	BO2	C5-N4-C3	2.87	122.12	116.84
15	V	1401	BO2	C5-N4-C3	2.94	122.24	116.84
15	K	1402	BO2	C5-N4-C3	3.08	122.52	116.84
15	2	1405	BO2	C5-N4-C3	3.11	122.57	116.84
15	N	1404	BO2	C5-N4-C3	3.19	122.72	116.84
15	H	1400	BO2	C2-C7-N9	3.35	122.56	115.10
15	2	1405	BO2	C2-C7-N9	3.44	122.75	115.10
15	N	1404	BO2	C2-C7-N9	3.45	122.78	115.10
15	V	1401	BO2	C2-C7-N9	3.50	122.90	115.10
15	H	1400	BO2	C3-C2-C7	3.79	123.41	119.55
15	V	1401	BO2	C3-C2-C7	3.84	123.46	119.55
15	H	1400	BO2	C6-N1-C2	3.95	122.22	116.92
15	Y	1403	BO2	C6-N1-C2	4.06	122.37	116.92
15	K	1402	BO2	C6-N1-C2	4.12	122.45	116.92
15	V	1401	BO2	C6-N1-C2	4.28	122.67	116.92
15	Y	1403	BO2	C3-C2-C7	4.29	123.92	119.55
15	K	1402	BO2	C3-C2-C7	4.51	124.14	119.55
15	N	1404	BO2	C3-C2-C7	4.53	124.17	119.55
15	N	1404	BO2	C6-N1-C2	4.74	123.27	116.92
15	2	1405	BO2	C6-N1-C2	4.79	123.35	116.92
15	2	1405	BO2	C3-C2-C7	4.79	124.43	119.55

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	2	1405	BO2	8	0
15	H	1400	BO2	2	0
15	N	1404	BO2	5	0
15	V	1401	BO2	2	0
15	Y	1403	BO2	1	0

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 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.