



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:02 AM GMT

PDB ID : 3GPW  
Title : Crystal structure of the yeast 20S proteasome in complex with Salinosporamide derivatives: irreversible inhibitor ligand  
Authors : Groll, M.; Macherla, V.R.; Manam, R.R.; Arthur, K.A.M.; Potts, C.B.  
Deposited on : 2009-03-23  
Resolution : 2.50 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](mailto: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) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

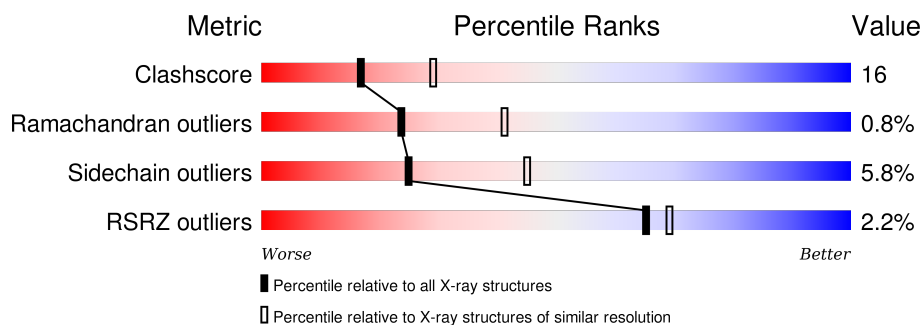
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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  $\geq 3$ , 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.

Mol	Chain	Length	Quality of chain
1	A	250	<div> <div></div> <div> <div></div> <div>77%</div> <div>21%</div> <div>.</div> </div> </div>
1	O	250	<div> <div>2%</div> <div> <div></div> <div>76%</div> <div>22%</div> <div>.</div> </div> </div>
2	B	244	<div> <div>2%</div> <div> <div></div> <div>61%</div> <div>33%</div> <div>6%</div> </div> </div>
2	P	244	<div> <div>4%</div> <div> <div></div> <div>61%</div> <div>32%</div> <div>7%</div> </div> </div>
3	C	241	<div> <div>4%</div> <div> <div></div> <div>59%</div> <div>36%</div> <div>5%</div> </div> </div>
3	Q	241	<div> <div>15%</div> <div> <div></div> <div>59%</div> <div>36%</div> <div>5%</div> </div> </div>
4	D	242	<div> <div>3%</div> <div> <div></div> <div>73%</div> <div>24%</div> <div>.</div> </div> </div>

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	R	242	 4% 71% 26% •
5	E	233	 3% 61% 33% 6%
5	S	233	 8% 59% 35% 6%
6	F	244	 % 66% 30% •
6	T	244	 2% 64% 32% •
7	G	243	 2% 68% 29% •
7	U	243	 % 67% 30% •
8	H	222	 65% 32% •
8	V	222	 63% 35% •
9	I	204	 74% 25% •
9	W	204	 74% 25% •
10	J	198	 2% 72% 25% •
10	X	198	 2% 70% 28% •
11	K	212	 74% 24% •
11	Y	212	 72% 25% •
12	L	222	 % 72% 25% •
12	Z	222	 % 72% 26% •
13	1	233	 69% 29% •
13	M	233	 70% 28% •
14	2	196	 65% 32% •
14	N	196	 69% 28% •

## 2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 51001 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			

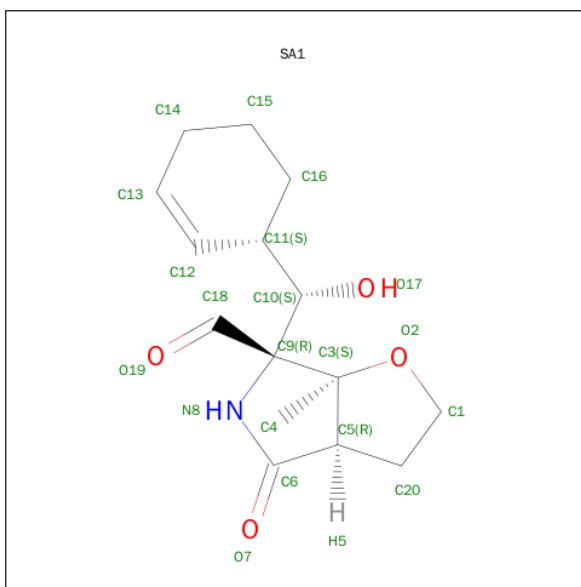
- Molecule 13 is a protein called Proteasome component PRE4.

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 (3AR,6R,6AS)-6-((S)-((S)-CYCLOHEX-2-ENYL)(HYDROXY)METHYL)-6A-METHYL-4-OXO-HEXAHYDRO-2H-FURO[3,2-C]PYRROLE-6-CARBALDEHYDE (three-letter code: SA1) (formula: C<sub>15</sub>H<sub>21</sub>NO<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	H	1	Total	C	N	O	0	0
			20	15	1	4		
15	K	1	Total	C	N	O	0	0
			20	15	1	4		
15	N	1	Total	C	N	O	0	0
			20	15	1	4		
15	V	1	Total	C	N	O	0	0
			20	15	1	4		
15	Y	1	Total	C	N	O	0	0
			20	15	1	4		
15	2	1	Total	C	N	O	0	0
			20	15	1	4		

- Molecule 16 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	57	Total	O	0	0
			57	57		
16	B	37	Total	O	0	0
			37	37		
16	C	42	Total	O	0	0
			42	42		
16	D	40	Total	O	0	0
			40	40		
16	E	23	Total	O	0	0
			23	23		
16	F	48	Total	O	0	0
			48	48		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	G	63	Total O 63 63	0	0
16	H	50	Total O 50 50	0	0
16	I	68	Total O 68 68	0	0
16	J	50	Total O 50 50	0	0
16	K	47	Total O 47 47	0	0
16	L	55	Total O 55 55	0	0
16	M	70	Total O 70 70	0	0
16	N	57	Total O 57 57	0	0
16	O	34	Total O 34 34	0	0
16	P	28	Total O 28 28	0	0
16	Q	28	Total O 28 28	0	0
16	R	30	Total O 30 30	0	0
16	S	20	Total O 20 20	0	0
16	T	40	Total O 40 40	0	0
16	U	60	Total O 60 60	0	0
16	V	49	Total O 49 49	0	0
16	W	60	Total O 60 60	0	0
16	X	47	Total O 47 47	0	0
16	Y	49	Total O 49 49	0	0
16	Z	53	Total O 53 53	0	0
16	1	72	Total O 72 72	0	0

*Continued on next page...*



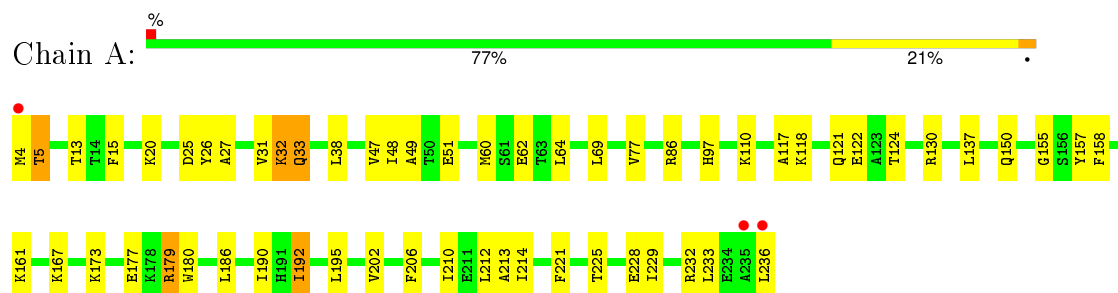
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	2	56	Total	O	0	0
			56	56		

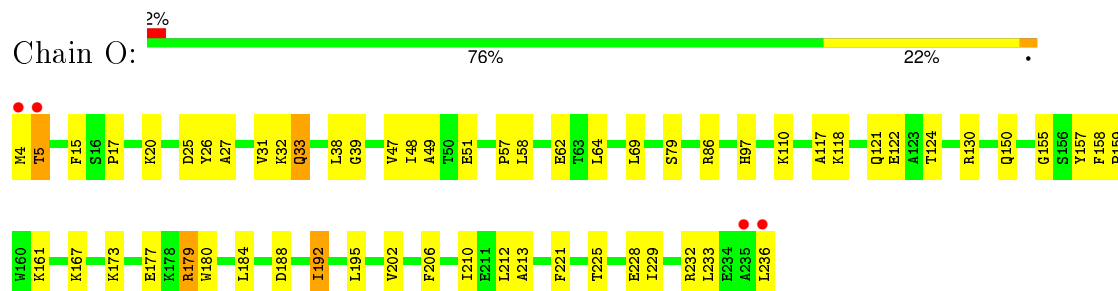
### 3 Residue-property plots [i](#)

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.

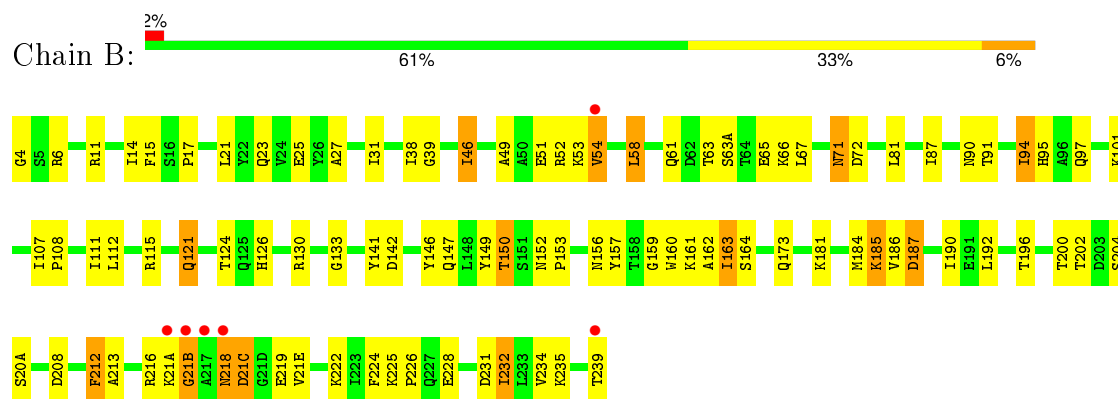
#### • Molecule 1: Proteasome component Y7



#### • Molecule 1: Proteasome component Y7

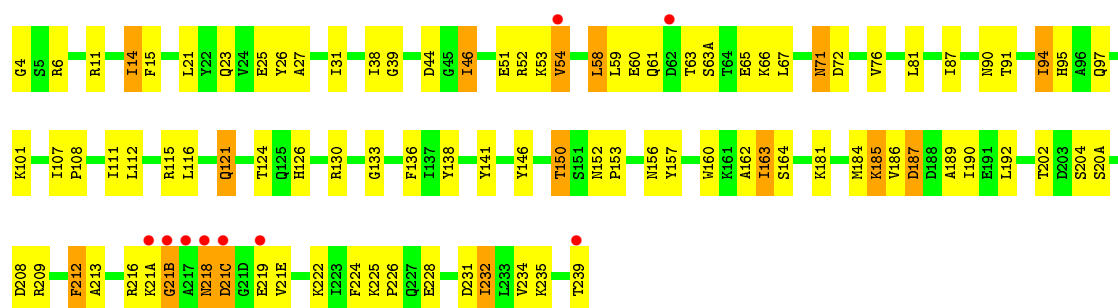


#### • Molecule 2: Proteasome component Y13

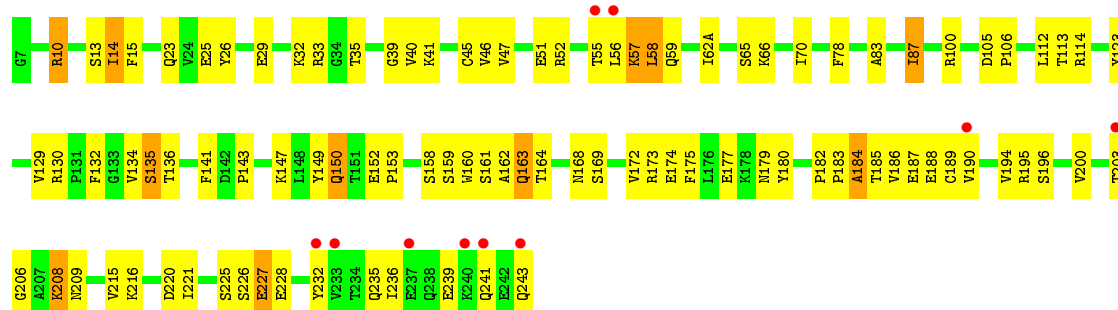


#### • Molecule 2: Proteasome component Y13

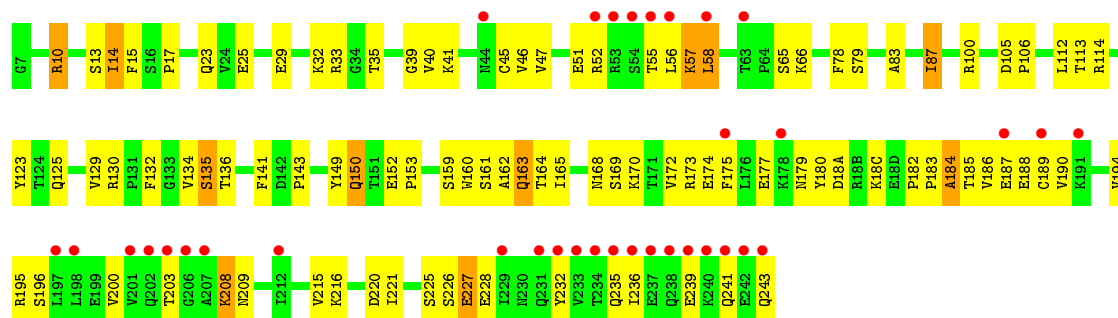




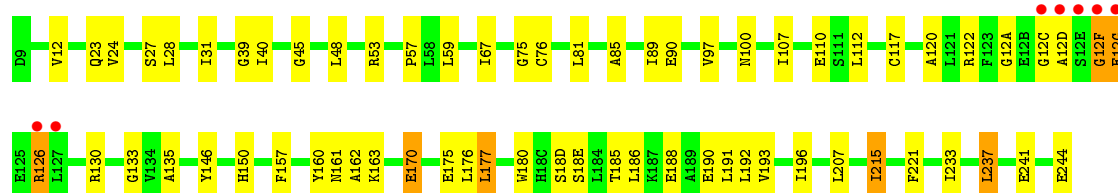
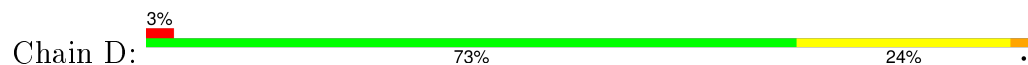
• Molecule 3: Proteasome component PRE6



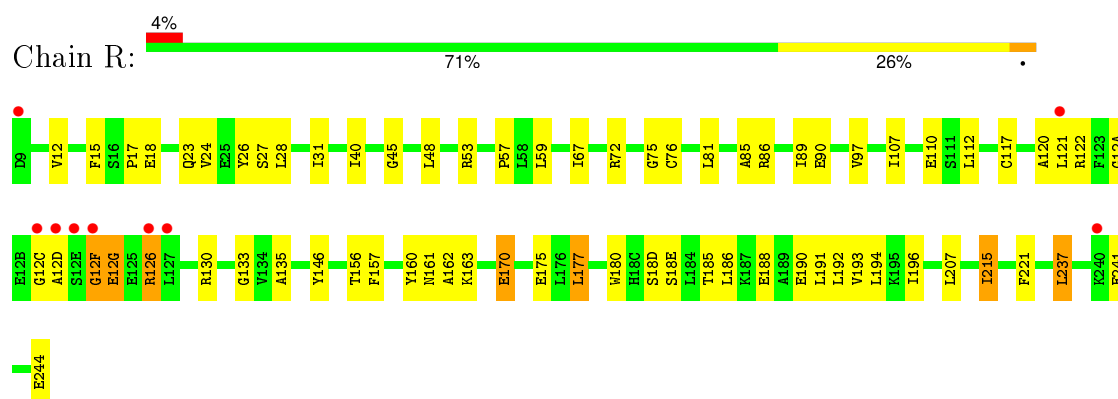
• Molecule 3: Proteasome component PRE6



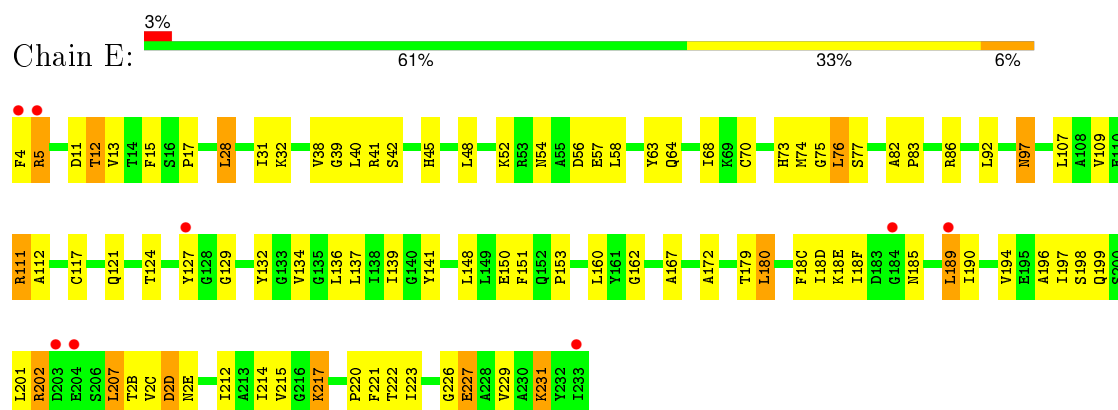
• Molecule 4: Proteasome component PUP2



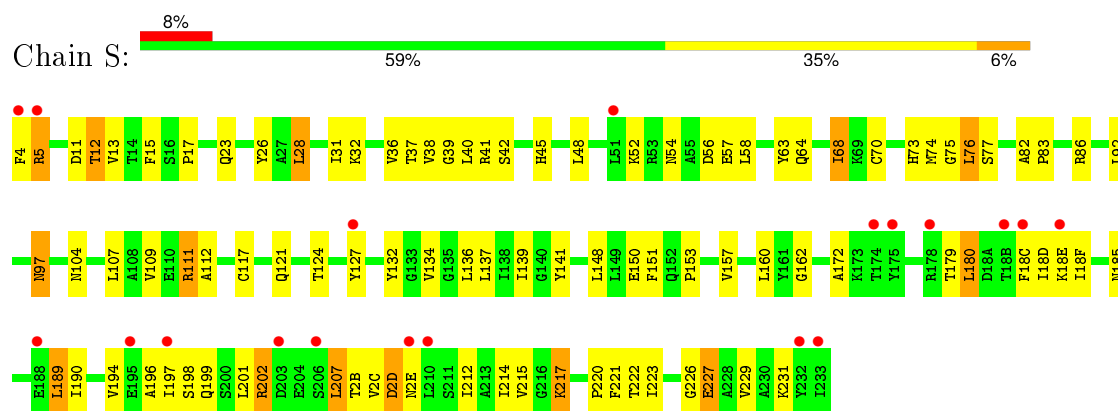
• Molecule 4: Proteasome component PUP2



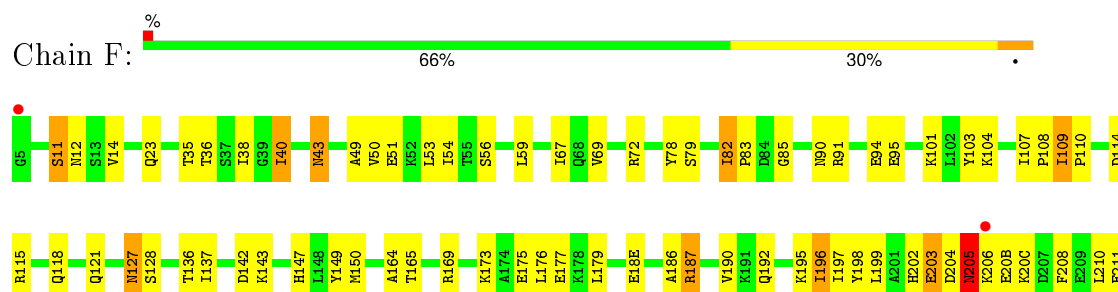
• Molecule 5: Proteasome component PRE5



• Molecule 5: Proteasome component PRE5

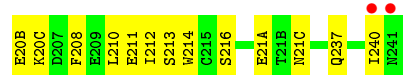
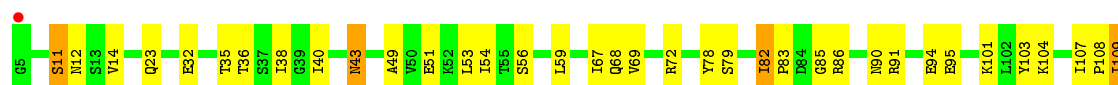


• Molecule 6: Proteasome component C1

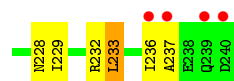
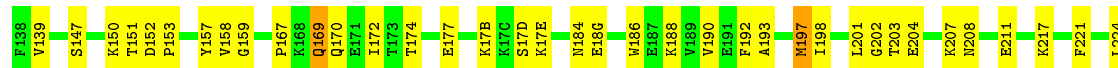
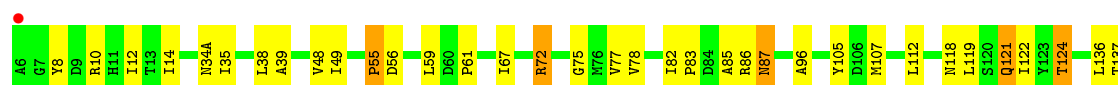




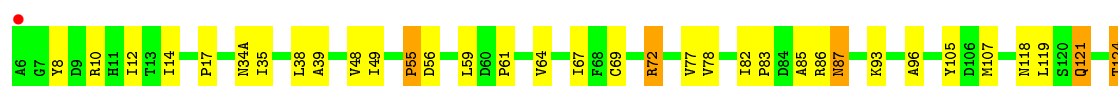
• Molecule 6: Proteasome component C1



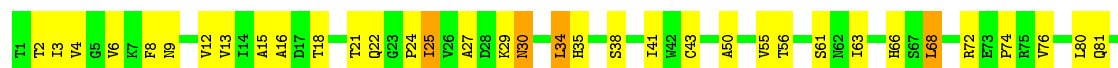
• Molecule 7: Proteasome component C7-alpha

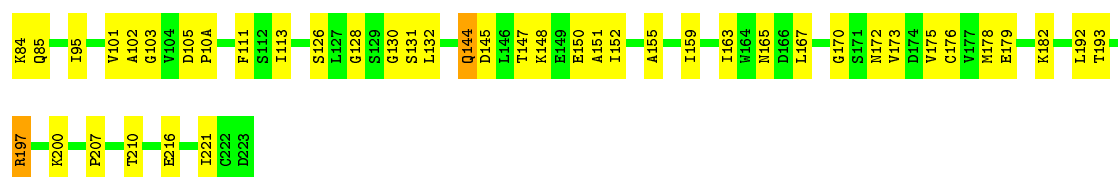


• Molecule 7: Proteasome component C7-alpha

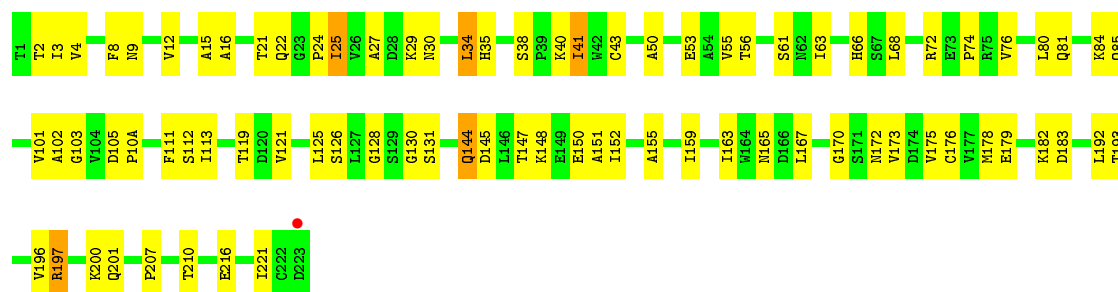


• Molecule 8: Proteasome component PUP1

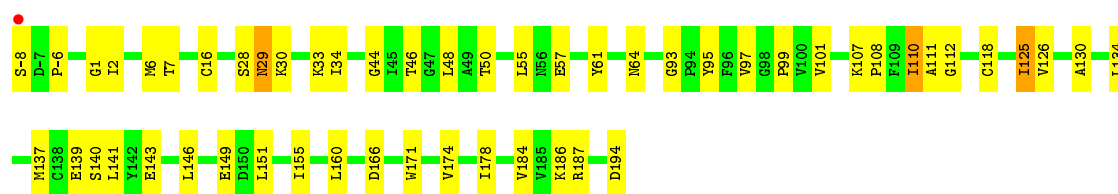




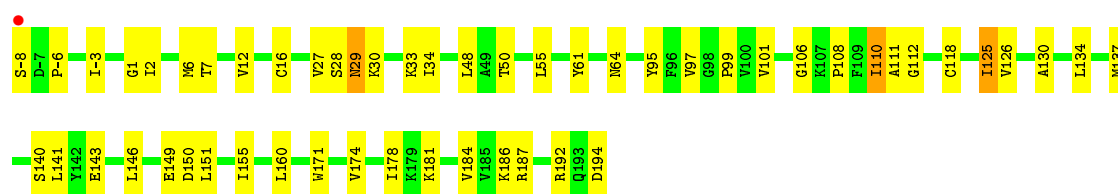
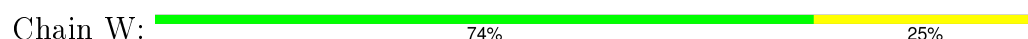
• Molecule 8: Proteasome component PUP1



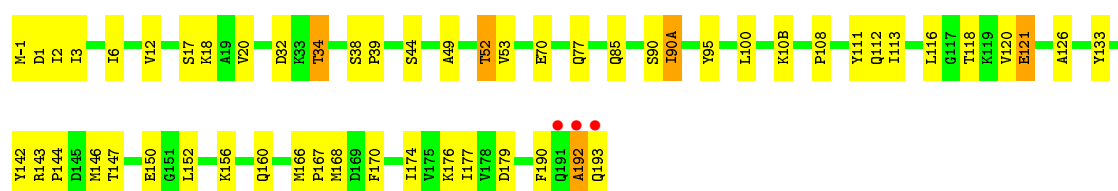
• Molecule 9: Proteasome component PUP3



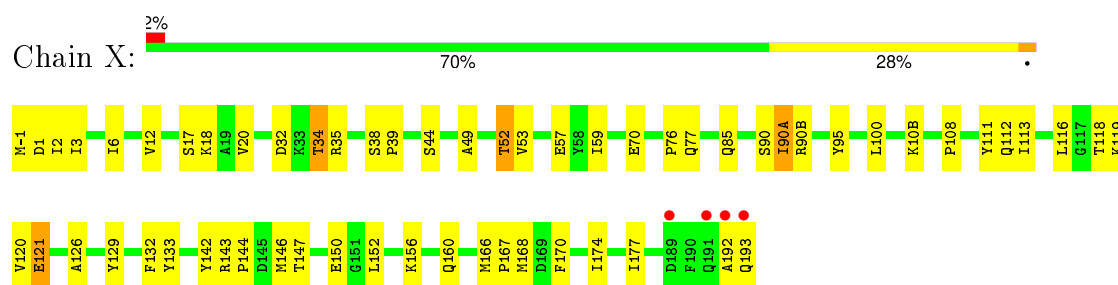
• Molecule 9: Proteasome component PUP3



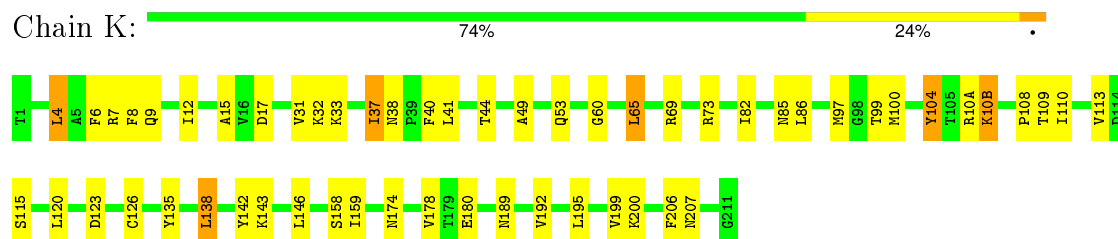
• Molecule 10: Proteasome component C11



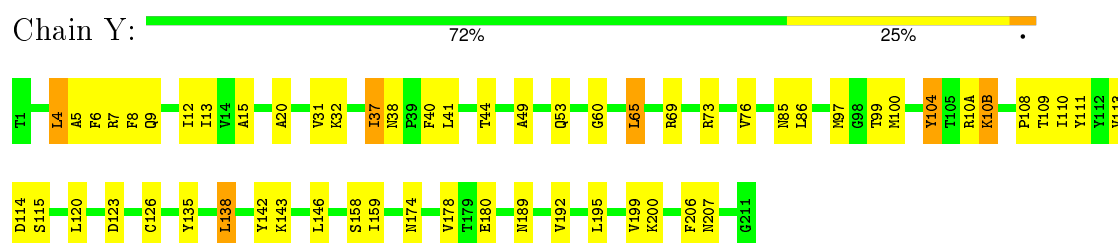
• Molecule 10: Proteasome component C11



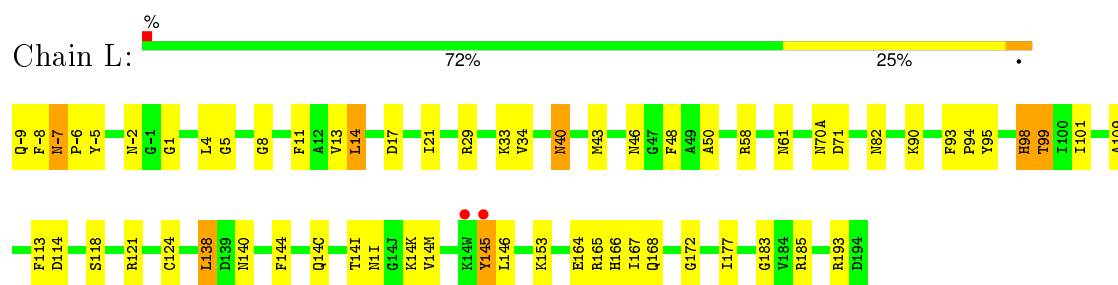
- Molecule 11: Proteasome component PRE2



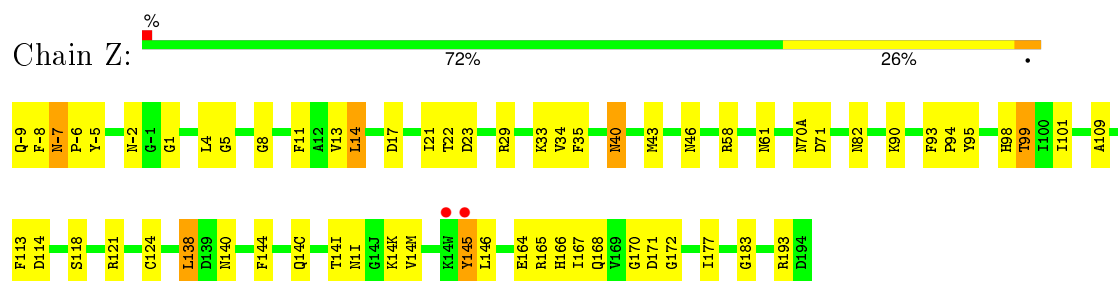
- Molecule 11: Proteasome component PRE2



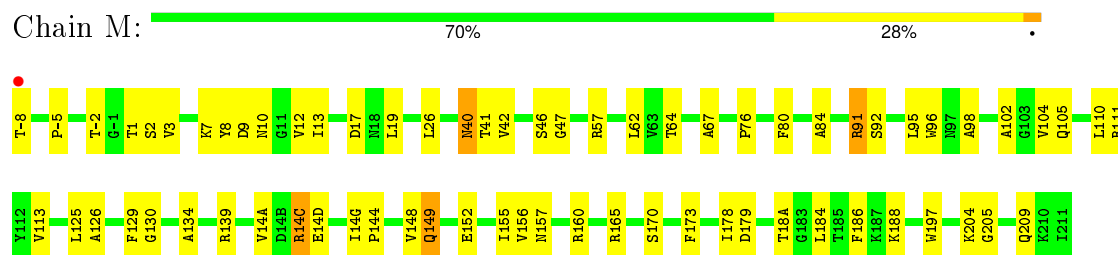
- Molecule 12: Proteasome component C5



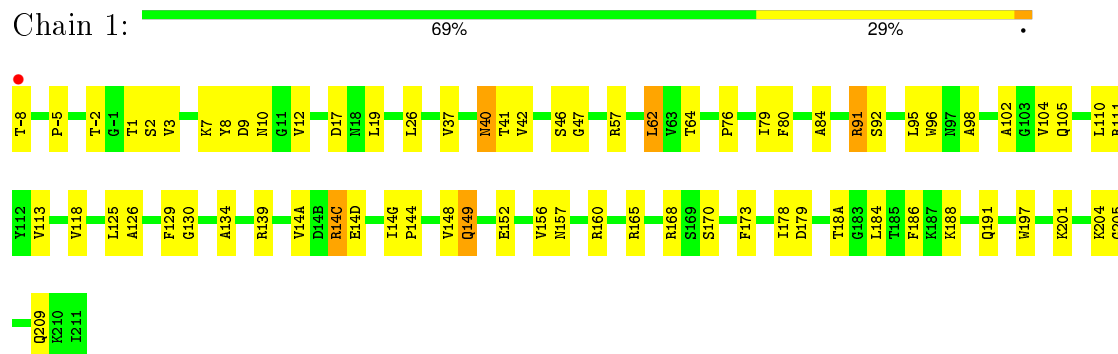
- Molecule 12: Proteasome component C5



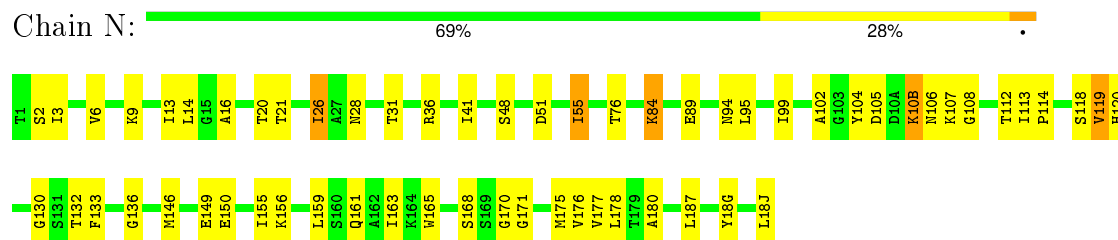
- Molecule 13: Proteasome component PRE4



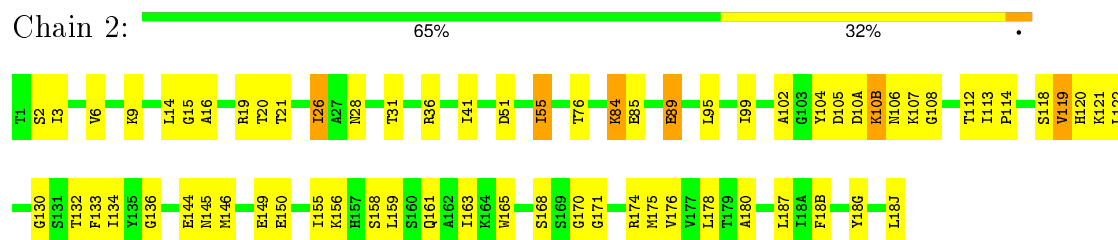
• Molecule 13: Proteasome component PRE4



• Molecule 14: Proteasome component PRE3



• Molecule 14: Proteasome component PRE3





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	135.24Å 301.45Å 144.42Å 90.00° 112.94° 90.00°	Depositor
Resolution (Å)	15.00 – 2.50 49.48 – 2.21	Depositor EDS
% Data completeness (in resolution range)	99.7 (15.00-2.50) 99.2 (49.48-2.21)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.90 (at 2.20Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.230 , 0.255 0.242 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	25.4	Xtriage
Anisotropy	0.792	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 53.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 526739 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	51001	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.44% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 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: SA1

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	0.36	0/1952	0.65	0/2642
1	O	0.38	0/1952	0.64	0/2642
2	B	0.37	0/1935	0.62	0/2618
2	P	0.38	0/1935	0.63	0/2618
3	C	0.35	0/1920	0.61	0/2598
3	Q	0.35	0/1920	0.61	0/2598
4	D	0.35	0/1887	0.61	0/2541
4	R	0.36	0/1887	0.61	0/2541
5	E	0.35	0/1823	0.61	0/2463
5	S	0.36	0/1823	0.60	0/2463
6	F	0.37	0/1937	0.61	0/2614
6	T	0.38	0/1937	0.62	0/2614
7	G	0.39	0/1959	0.62	0/2652
7	U	0.41	0/1959	0.62	0/2652
8	H	0.39	0/1716	0.68	0/2326
8	V	0.37	0/1716	0.68	0/2326
9	I	0.39	0/1611	0.66	0/2174
9	W	0.41	0/1611	0.67	0/2174
10	J	0.37	0/1613	0.65	0/2173
10	X	0.38	0/1613	0.65	0/2173
11	K	0.40	0/1681	0.65	0/2274
11	Y	0.38	0/1681	0.64	0/2274
12	L	0.38	0/1795	0.66	0/2420
12	Z	0.38	0/1795	0.66	0/2420
13	1	0.41	0/1855	0.69	1/2514 (0.0%)
13	M	0.39	0/1855	0.68	1/2514 (0.0%)
14	2	0.40	0/1541	0.66	0/2087
14	N	0.41	0/1541	0.66	0/2087
All	All	0.38	0/50450	0.64	2/68192 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	1	95	LEU	N-CA-C	-5.39	96.45	111.00
13	M	95	LEU	N-CA-C	-5.20	96.96	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	51	0
1	O	1915	0	1926	59	0
2	B	1905	0	1901	93	0
2	P	1905	0	1901	93	0
3	C	1891	0	1900	105	0
3	Q	1891	0	1900	97	0
4	D	1862	0	1836	47	0
4	R	1862	0	1836	49	0
5	E	1795	0	1797	83	0
5	S	1795	0	1797	92	0
6	F	1897	0	1886	71	0
6	T	1897	0	1886	74	0
7	G	1921	0	1910	69	0
7	U	1921	0	1910	74	0
8	H	1685	0	1687	65	0
8	V	1685	0	1687	64	0
9	I	1581	0	1574	41	0
9	W	1581	0	1574	43	0
10	J	1585	0	1590	52	0
10	X	1585	0	1590	59	0
11	K	1644	0	1594	52	0
11	Y	1644	0	1594	54	0
12	L	1757	0	1711	51	0
12	Z	1757	0	1711	50	0
13	1	1824	0	1832	63	0
13	M	1824	0	1832	54	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	2	1512	0	1480	61	0
14	N	1512	0	1480	57	0
15	2	20	0	20	4	0
15	H	20	0	20	1	0
15	K	20	0	20	1	0
15	N	20	0	20	4	0
15	V	20	0	20	1	0
15	Y	20	0	20	1	0
16	1	72	0	0	4	0
16	2	56	0	0	1	0
16	A	57	0	0	2	0
16	B	37	0	0	2	0
16	C	42	0	0	3	0
16	D	40	0	0	1	0
16	E	23	0	0	2	0
16	F	48	0	0	4	0
16	G	63	0	0	3	0
16	H	50	0	0	2	0
16	I	68	0	0	1	0
16	J	50	0	0	2	0
16	K	47	0	0	2	0
16	L	55	0	0	3	0
16	M	70	0	0	1	0
16	N	57	0	0	2	0
16	O	34	0	0	2	0
16	P	28	0	0	2	0
16	Q	28	0	0	3	0
16	R	30	0	0	3	0
16	S	20	0	0	0	0
16	T	40	0	0	2	0
16	U	60	0	0	3	0
16	V	49	0	0	4	0
16	W	60	0	0	2	0
16	X	47	0	0	3	0
16	Y	49	0	0	2	0
16	Z	53	0	0	2	0
All	All	51001	0	49368	1624	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 16.

All (1624) 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)
11:Y:10(B):LYS:HD2	11:Y:10(B):LYS:H	1.06	1.19
11:K:10(B):LYS:H	11:K:10(B):LYS:HD2	1.05	1.13
7:U:96:ALA:HA	7:U:107:MET:HE2	1.32	1.10
14:N:161:GLN:HE21	14:2:136:GLY:HA2	1.16	1.10
14:N:136:GLY:HA2	14:2:161:GLN:HE21	1.17	1.06
7:G:96:ALA:HA	7:G:107:MET:HE2	1.35	1.03
2:P:202:THR:HG22	2:P:204:SER:H	1.27	0.99
3:C:163:GLN:HE21	3:C:164:THR:H	1.08	0.97
3:Q:185:THR:HG22	3:Q:187:GLU:H	1.31	0.96
2:B:124:THR:HG22	3:C:130:ARG:HH21	1.29	0.95
3:Q:15:PHE:H	4:R:23:GLN:HE22	1.16	0.94
2:B:202:THR:HG22	2:B:204:SER:H	1.28	0.94
5:S:15:PHE:H	6:T:23:GLN:HE22	1.15	0.94
3:Q:185:THR:HB	3:Q:188:GLU:HG2	1.50	0.93
14:N:161:GLN:NE2	14:2:136:GLY:HA2	1.84	0.92
13:1:157:ASN:HD22	13:1:160:ARG:HH11	0.93	0.92
3:C:185:THR:HG22	3:C:187:GLU:H	1.32	0.92
12:L:43:MET:HB2	12:L:101:ILE:HG22	1.51	0.91
1:O:86:ARG:HE	7:U:118:ASN:HD21	1.18	0.91
13:1:157:ASN:HD22	13:1:160:ARG:NH1	1.68	0.91
4:D:97:VAL:HG21	11:K:65:LEU:HD13	1.52	0.91
3:Q:163:GLN:HE21	3:Q:164:THR:H	1.12	0.91
14:N:136:GLY:HA2	14:2:161:GLN:NE2	1.86	0.90
13:M:157:ASN:HD22	13:M:160:ARG:NH1	1.70	0.90
3:C:185:THR:HB	3:C:188:GLU:HG2	1.51	0.90
2:B:15:PHE:H	3:C:23:GLN:HE22	1.16	0.90
12:Z:43:MET:HB2	12:Z:101:ILE:HG22	1.51	0.89
13:1:157:ASN:ND2	13:1:160:ARG:HH11	1.69	0.89
13:M:157:ASN:HD22	13:M:160:ARG:HH11	0.97	0.89
2:P:124:THR:HG22	3:Q:130:ARG:HH21	1.37	0.88
1:O:124:THR:HG22	2:P:130:ARG:HH21	1.38	0.88
5:S:207:LEU:HD23	5:S:207:LEU:H	1.37	0.88
3:C:15:PHE:H	4:D:23:GLN:HE22	1.22	0.88
9:I:7:THR:HG23	9:I:110:ILE:HD13	1.55	0.87
9:W:7:THR:HG23	9:W:110:ILE:HD13	1.54	0.87
5:E:15:PHE:H	6:F:23:GLN:HE22	1.21	0.87
2:B:163:ILE:HG13	2:B:164:SER:H	1.39	0.87
5:E:207:LEU:HD23	5:E:207:LEU:H	1.38	0.87
11:Y:99:THR:HG22	11:Y:113:VAL:O	1.74	0.87
11:Y:10(B):LYS:N	11:Y:10(B):LYS:HD2	1.90	0.87
13:M:157:ASN:ND2	13:M:160:ARG:HH11	1.72	0.87
2:P:163:ILE:HG13	2:P:164:SER:H	1.38	0.87

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:99:THR:HG22	11:K:113:VAL:O	1.75	0.86
11:K:10(B):LYS:N	11:K:10(B):LYS:HD2	1.89	0.86
4:R:97:VAL:HG21	11:Y:65:LEU:HD13	1.58	0.86
14:N:20:THR:HG22	15:N:0:SA1:H12	1.57	0.86
1:O:15:PHE:H	2:P:23:GLN:HE22	1.20	0.86
14:2:20:THR:HG22	15:2:0:SA1:H12	1.58	0.85
3:C:163:GLN:NE2	3:C:164:THR:H	1.73	0.85
3:Q:195:ARG:HG3	3:Q:236:ILE:HD13	1.58	0.85
14:2:84:LYS:HG3	14:2:119:VAL:HG22	1.57	0.85
14:N:84:LYS:HG3	14:N:119:VAL:HG22	1.58	0.85
3:C:195:ARG:HG3	3:C:236:ILE:HD13	1.60	0.84
3:Q:163:GLN:NE2	3:Q:164:THR:H	1.75	0.83
1:A:124:THR:HG22	2:B:130:ARG:HH21	1.42	0.83
9:I:137:MET:HE3	9:I:141:LEU:HD11	1.61	0.83
6:T:95:GLU:HG2	6:T:115:ARG:HB3	1.59	0.82
9:W:137:MET:HE3	9:W:141:LEU:HD11	1.62	0.82
1:A:15:PHE:H	2:B:23:GLN:HE22	1.26	0.82
1:A:86:ARG:HE	7:G:118:ASN:HD21	1.27	0.82
1:O:130:ARG:HH21	7:U:124:THR:CG2	1.92	0.82
2:B:124:THR:CG2	3:C:130:ARG:HH21	1.92	0.81
9:W:192:ARG:HG3	16:W:202:HOH:O	1.80	0.81
6:T:36:THR:HG22	6:T:51:GLU:OE2	1.80	0.81
3:Q:33:ARG:HB2	3:Q:33:ARG:NH1	1.94	0.81
3:Q:65:SER:HB2	16:Q:303:HOH:O	1.80	0.81
3:Q:163:GLN:HE22	3:Q:173:ARG:HE	1.29	0.81
6:F:95:GLU:HG2	6:F:115:ARG:HB3	1.60	0.80
3:C:33:ARG:HB2	3:C:33:ARG:HH11	1.47	0.80
3:Q:33:ARG:HH11	3:Q:33:ARG:HB2	1.44	0.80
6:F:36:THR:HG22	6:F:51:GLU:OE2	1.81	0.80
3:C:163:GLN:HE21	3:C:164:THR:N	1.80	0.80
10:X:133:TYR:CE2	10:X:166:MET:HG3	2.17	0.79
3:Q:14:ILE:HD12	3:Q:14:ILE:H	1.48	0.79
3:C:33:ARG:HB2	3:C:33:ARG:NH1	1.97	0.79
2:P:61:GLN:OE1	2:P:208:ASP:HA	1.83	0.78
7:G:96:ALA:HA	7:G:107:MET:CE	2.14	0.78
4:R:177:LEU:HD22	5:S:58:LEU:HD13	1.65	0.78
7:U:96:ALA:HA	7:U:107:MET:CE	2.13	0.78
3:Q:100:ARG:HH11	3:Q:106:PRO:HB3	1.49	0.77
3:C:163:GLN:HE22	3:C:173:ARG:HE	1.32	0.77
3:Q:232:TYR:O	3:Q:236:ILE:HG13	1.84	0.77
11:K:10(B):LYS:H	11:K:10(B):LYS:CD	1.88	0.77

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:100:ARG:NH1	3:Q:106:PRO:HB3	1.98	0.77
3:C:232:TYR:O	3:C:236:ILE:HG13	1.84	0.77
2:P:126:HIS:HB3	3:Q:129:VAL:HG12	1.66	0.77
2:B:61:GLN:OE1	2:B:208:ASP:HA	1.84	0.77
9:I:6:MET:HE1	9:I:155:ILE:HA	1.66	0.77
7:G:217:LYS:HA	7:G:217:LYS:HE3	1.67	0.77
1:A:20:LYS:HE3	1:A:25:ASP:OD1	1.84	0.77
6:F:35:THR:HG21	6:F:51:GLU:O	1.85	0.76
1:O:20:LYS:HE3	1:O:25:ASP:OD1	1.85	0.76
3:Q:163:GLN:HE21	3:Q:164:THR:N	1.83	0.76
1:O:86:ARG:HH21	7:U:118:ASN:HD22	1.33	0.76
2:B:126:HIS:HB3	3:C:129:VAL:HG12	1.66	0.76
7:G:198:ILE:HG23	7:G:203:THR:O	1.85	0.76
3:C:106:PRO:HG2	3:C:143:PRO:CG	2.16	0.75
10:J:133:TYR:CE2	10:J:166:MET:HG3	2.20	0.75
7:U:217:LYS:HE3	7:U:217:LYS:HA	1.66	0.75
7:U:198:ILE:HG23	7:U:203:THR:O	1.86	0.75
6:T:35:THR:HG21	6:T:51:GLU:O	1.86	0.75
1:O:130:ARG:HH21	7:U:124:THR:HG22	1.51	0.75
5:S:18(C):PHE:HA	5:S:18(F):ILE:HG12	1.70	0.74
6:T:20(B):GLU:HG3	6:T:20(C):LYS:HG3	1.69	0.74
1:O:124:THR:CG2	2:P:130:ARG:HH21	2.00	0.74
5:E:201:LEU:HD11	5:E:207:LEU:HD22	1.69	0.74
1:A:130:ARG:HH21	7:G:124:THR:CG2	2.00	0.74
5:S:207:LEU:HA	5:S:2(E):ASN:ND2	2.03	0.74
5:S:201:LEU:HD11	5:S:207:LEU:HD22	1.69	0.73
3:C:100:ARG:NH1	3:C:106:PRO:HB3	2.02	0.73
3:Q:33:ARG:HH11	3:Q:33:ARG:CB	2.01	0.73
6:F:20(B):GLU:HG3	6:F:20(C):LYS:HG3	1.69	0.73
1:A:124:THR:CG2	2:B:130:ARG:HH21	2.02	0.73
12:L:33:LYS:HD2	12:L:46:ASN:HD22	1.53	0.73
13:1:14(C):ARG:HG3	13:1:14(C):ARG:HH11	1.53	0.73
5:E:18(C):PHE:HA	5:E:18(F):ILE:HG12	1.70	0.73
1:A:177:GLU:HG2	2:B:58:LEU:HD22	1.69	0.73
3:C:41:LYS:HG2	3:C:161:SER:O	1.89	0.73
2:P:163:ILE:HG13	2:P:164:SER:N	2.05	0.72
14:N:55:ILE:HD11	14:N:95:LEU:HD13	1.70	0.72
5:E:207:LEU:HA	5:E:2(E):ASN:ND2	2.05	0.72
1:A:130:ARG:HH21	7:G:124:THR:HG22	1.55	0.72
8:V:172:ASN:HD22	8:V:193:THR:HA	1.54	0.72
3:Q:106:PRO:HG2	3:Q:143:PRO:CG	2.18	0.72

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:106:PRO:HG2	3:C:143:PRO:HG3	1.72	0.72
13:M:40:ASN:H	13:M:40:ASN:HD22	1.35	0.72
5:S:12:THR:HG21	5:S:124:THR:HA	1.72	0.72
1:A:86:ARG:HH21	7:G:118:ASN:HD22	1.38	0.72
12:Z:-7:ASN:ND2	12:Z:-5:TYR:H	1.88	0.72
4:D:175:GLU:HG2	4:D:196:ILE:HD12	1.69	0.72
11:Y:10(B):LYS:CD	11:Y:10(B):LYS:H	1.89	0.71
4:R:175:GLU:HG2	4:R:196:ILE:HD12	1.71	0.71
9:I:6:MET:HE3	9:I:155:ILE:HG13	1.72	0.71
5:S:207:LEU:H	5:S:207:LEU:CD2	2.03	0.71
3:C:100:ARG:HH11	3:C:106:PRO:HB3	1.56	0.71
5:E:12:THR:HG21	5:E:124:THR:HA	1.71	0.71
1:O:86:ARG:HE	7:U:118:ASN:ND2	1.88	0.71
7:U:18(G):GLU:HG2	7:U:188:LYS:HB2	1.72	0.71
1:A:179:ARG:HB3	1:A:179:ARG:HH11	1.55	0.71
13:1:7:LYS:HG3	13:1:14(G):ILE:HD12	1.73	0.71
8:H:128:GLY:O	8:H:131:SER:HB2	1.89	0.71
2:B:190:ILE:CG2	2:B:232:ILE:HD11	2.20	0.71
8:V:128:GLY:O	8:V:131:SER:HB2	1.90	0.71
9:W:6:MET:HE3	9:W:155:ILE:HG13	1.73	0.71
5:E:28:LEU:HA	5:E:31:ILE:HD12	1.73	0.71
2:P:190:ILE:CG2	2:P:232:ILE:HD11	2.21	0.71
5:E:207:LEU:CD2	5:E:207:LEU:H	2.04	0.70
8:H:165:ASN:HD22	13:1:139:ARG:HH11	1.36	0.70
12:L:-7:ASN:ND2	12:L:-5:TYR:H	1.89	0.70
14:2:84:LYS:HG3	14:2:119:VAL:CG2	2.21	0.70
12:Z:166:HIS:HD2	12:Z:168:GLN:H	1.37	0.70
14:2:107:LYS:HG2	14:2:108:GLY:H	1.55	0.70
14:N:107:LYS:HG2	14:N:108:GLY:H	1.54	0.70
13:M:139:ARG:HH11	8:V:165:ASN:HD22	1.36	0.70
1:O:179:ARG:HH11	1:O:179:ARG:HB3	1.55	0.70
13:M:7:LYS:HG3	13:M:14(G):ILE:HD12	1.74	0.70
11:Y:142:TYR:O	11:Y:143:LYS:HD2	1.92	0.70
2:P:101:LYS:NZ	10:X:85:GLN:NE2	2.39	0.70
13:1:40:ASN:HD22	13:1:40:ASN:H	1.36	0.70
2:B:219:GLU:HG2	2:B:21(E):VAL:H	1.57	0.70
7:G:18(G):GLU:HG2	7:G:188:LYS:HB2	1.74	0.70
9:W:143:GLU:HG3	9:W:146:LEU:HD21	1.72	0.70
14:N:84:LYS:HG3	14:N:119:VAL:CG2	2.21	0.69
11:Y:143:LYS:HB2	11:Y:146:LEU:HD13	1.74	0.69
6:T:38:ILE:HG22	6:T:164:ALA:HB2	1.73	0.69

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:198:SER:HA	5:S:201:LEU:HG	1.74	0.69
6:T:186:ALA:O	6:T:190:VAL:HG23	1.91	0.69
4:D:177:LEU:HD22	5:E:58:LEU:HD13	1.74	0.69
5:S:28:LEU:HA	5:S:31:ILE:HD12	1.74	0.69
5:S:75:GLY:HA3	5:S:221:PHE:CE2	2.26	0.69
3:C:14:ILE:HD12	3:C:14:ILE:H	1.57	0.69
2:B:163:ILE:HG13	2:B:164:SER:N	2.06	0.69
12:L:166:HIS:HD2	12:L:168:GLN:H	1.39	0.69
12:Z:114:ASP:HB2	12:Z:118:SER:HB3	1.73	0.69
13:M:14(C):ARG:HH11	13:M:14(C):ARG:HG3	1.57	0.69
12:Z:33:LYS:HD2	12:Z:46:ASN:HD22	1.57	0.69
3:Q:106:PRO:HG2	3:Q:143:PRO:HG3	1.75	0.69
7:G:18(G):GLU:HG2	7:G:188:LYS:CB	2.22	0.69
3:C:65:SER:HB2	16:C:274:HOH:O	1.91	0.69
3:C:33:ARG:CB	3:C:33:ARG:HH11	2.04	0.69
5:E:198:SER:HA	5:E:201:LEU:HG	1.74	0.68
8:V:81:GLN:O	8:V:85:GLN:HG3	1.93	0.68
11:K:142:TYR:O	11:K:143:LYS:HD2	1.93	0.68
9:I:143:GLU:HG3	9:I:146:LEU:HD21	1.74	0.68
2:B:38:ILE:HD13	2:B:164:SER:HB3	1.76	0.68
7:U:18(G):GLU:HG2	7:U:188:LYS:CB	2.24	0.68
2:P:219:GLU:HG2	2:P:21(E):VAL:H	1.57	0.68
12:Z:14:LEU:HD13	12:Z:34:VAL:HG13	1.75	0.68
4:D:81:LEU:HD12	4:D:133:GLY:HA3	1.76	0.68
14:2:55:ILE:HD11	14:2:95:LEU:HD13	1.75	0.68
3:C:185:THR:HG22	3:C:187:GLU:N	2.07	0.68
3:Q:41:LYS:HG2	3:Q:161:SER:O	1.93	0.68
2:P:124:THR:CG2	3:Q:130:ARG:HH21	2.05	0.68
1:A:33:GLN:HA	1:A:33:GLN:HE21	1.59	0.68
2:B:15:PHE:H	3:C:23:GLN:NE2	1.90	0.67
5:E:75:GLY:HA3	5:E:221:PHE:CE2	2.29	0.67
9:W:6:MET:HE1	9:W:155:ILE:HA	1.75	0.67
8:V:196:VAL:HG23	16:V:652:HOH:O	1.93	0.67
1:O:159:PRO:O	2:P:59:LEU:HD12	1.94	0.67
12:L:114:ASP:HB2	12:L:118:SER:HB3	1.76	0.67
8:H:172:ASN:HD22	8:H:193:THR:HA	1.59	0.67
7:G:77:VAL:HG12	7:G:137:THR:HB	1.76	0.67
7:U:121:GLN:O	7:U:124:THR:HB	1.94	0.67
7:U:59:LEU:O	7:U:61:PRO:HD3	1.94	0.67
5:E:207:LEU:HA	5:E:2(E):ASN:HD22	1.60	0.66
4:R:81:LEU:HD12	4:R:133:GLY:HA3	1.77	0.66

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:52:LYS:HB3	5:S:63:TYR:HB3	1.77	0.66
2:B:219:GLU:HG2	2:B:21(E):VAL:N	2.11	0.66
3:Q:159:SER:HB2	16:Q:1140:HOH:O	1.96	0.66
11:K:143:LYS:HB2	11:K:146:LEU:HD13	1.76	0.66
6:F:186:ALA:O	6:F:190:VAL:HG23	1.94	0.66
7:U:227:GLU:HG2	16:U:1255:HOH:O	1.95	0.66
2:B:160:TRP:CE2	2:B:163:ILE:HD13	2.31	0.66
7:U:77:VAL:HG12	7:U:137:THR:HB	1.78	0.66
9:W:112:GLY:N	9:W:125:ILE:HD12	2.11	0.66
5:E:15:PHE:HB2	6:F:23:GLN:HE22	1.60	0.65
13:1:84:ALA:HA	13:1:113:VAL:HG21	1.77	0.65
7:G:121:GLN:O	7:G:124:THR:HB	1.96	0.65
12:L:14:LEU:HD13	12:L:34:VAL:HG13	1.76	0.65
6:F:69:VAL:HG12	16:F:319:HOH:O	1.95	0.65
9:W:27:VAL:HG13	16:X:622:HOH:O	1.95	0.65
6:F:38:ILE:HG22	6:F:164:ALA:HB2	1.78	0.65
6:F:237:GLN:O	6:F:240:ILE:HG22	1.97	0.65
6:T:237:GLN:O	6:T:240:ILE:HG22	1.96	0.65
3:Q:52:ARG:HB2	3:Q:209:ASN:HA	1.77	0.65
2:P:6:ARG:HG2	3:Q:10:ARG:HH21	1.62	0.65
2:P:15:PHE:H	3:Q:23:GLN:HE22	1.41	0.65
3:Q:185:THR:HG22	3:Q:187:GLU:N	2.06	0.65
5:S:207:LEU:N	5:S:207:LEU:HD23	2.12	0.65
5:E:52:LYS:HB3	5:E:63:TYR:HB3	1.77	0.65
1:O:121:GLN:O	1:O:124:THR:HB	1.97	0.65
5:S:207:LEU:HA	5:S:2(E):ASN:HD22	1.59	0.65
4:R:192:LEU:O	4:R:196:ILE:HG12	1.96	0.64
14:N:161:GLN:HE21	14:2:136:GLY:CA	2.03	0.64
2:B:121:GLN:O	2:B:124:THR:HB	1.98	0.64
3:C:160:TRP:CE2	4:D:59:LEU:HD23	2.32	0.64
12:L:8:GLY:HA3	12:L:11:PHE:CE2	2.33	0.64
5:E:167:ALA:HB3	16:E:1131:HOH:O	1.97	0.64
1:O:33:GLN:HE21	1:O:33:GLN:HA	1.60	0.64
5:S:2(B):THR:H	5:S:2(E):ASN:HD22	1.44	0.64
1:A:121:GLN:O	1:A:124:THR:HB	1.97	0.64
8:V:172:ASN:ND2	8:V:193:THR:HA	2.13	0.64
1:A:4:MET:SD	1:A:5:THR:N	2.62	0.64
4:D:12(D):ALA:HA	5:E:129:GLY:HA2	1.80	0.64
7:G:87:ASN:HD22	7:G:87:ASN:C	2.01	0.64
2:P:38:ILE:HD13	2:P:164:SER:HB3	1.78	0.64
5:S:132:TYR:O	5:S:153:PRO:HB3	1.97	0.64

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:219:GLU:HG2	2:P:21(E):VAL:N	2.11	0.64
3:C:52:ARG:HB2	3:C:209:ASN:HA	1.78	0.64
13:M:84:ALA:HA	13:M:113:VAL:HG21	1.80	0.64
2:P:160:TRP:CE2	2:P:163:ILE:HD13	2.32	0.64
3:C:46:VAL:O	3:C:215:VAL:HG12	1.98	0.64
2:P:121:GLN:O	2:P:124:THR:HB	1.96	0.64
5:E:2(B):THR:H	5:E:2(E):ASN:HD22	1.45	0.64
2:B:186:VAL:HG21	2:B:216:ARG:HD3	1.80	0.64
12:L:4:LEU:HD11	12:L:138:LEU:HD21	1.80	0.64
3:C:186:VAL:O	3:C:190:VAL:HG23	1.99	0.63
2:P:228:GLU:O	2:P:232:ILE:HG22	1.98	0.63
3:Q:215:VAL:HG23	3:Q:221:ILE:HG12	1.81	0.63
1:O:225:THR:OG1	1:O:228:GLU:HG3	1.98	0.63
3:C:195:ARG:CG	3:C:236:ILE:HD13	2.27	0.63
12:Z:4:LEU:HD11	12:Z:138:LEU:HD21	1.79	0.63
7:G:59:LEU:O	7:G:61:PRO:HD3	1.98	0.63
14:2:14:LEU:HD11	14:2:102:ALA:HB3	1.80	0.63
3:Q:164:THR:HG21	3:Q:172:VAL:HG13	1.80	0.63
1:A:86:ARG:HE	7:G:118:ASN:ND2	1.96	0.63
12:Z:8:GLY:HA3	12:Z:11:PHE:CE2	2.33	0.63
5:E:207:LEU:HD23	5:E:207:LEU:N	2.13	0.63
3:Q:195:ARG:CG	3:Q:236:ILE:HD13	2.25	0.63
3:Q:186:VAL:O	3:Q:190:VAL:HG23	1.99	0.63
3:Q:46:VAL:O	3:Q:215:VAL:HG12	1.98	0.63
8:H:81:GLN:O	8:H:85:GLN:HG3	1.98	0.63
5:E:226:GLY:O	5:E:229:VAL:HG22	1.99	0.63
14:N:14:LEU:HD11	14:N:102:ALA:HB3	1.78	0.63
10:X:143:ARG:O	10:X:146:MET:HG3	1.98	0.63
7:U:87:ASN:HD22	7:U:87:ASN:C	2.02	0.63
13:M:40:ASN:HD22	13:M:40:ASN:N	1.96	0.63
1:O:179:ARG:NH1	1:O:179:ARG:HB3	2.13	0.63
13:M:110:LEU:HG	13:M:125:LEU:HD12	1.80	0.63
4:D:192:LEU:O	4:D:196:ILE:HG12	1.98	0.63
2:B:65:GLU:HG3	2:B:66:LYS:HG3	1.79	0.63
3:C:215:VAL:HG23	3:C:221:ILE:HG12	1.81	0.63
10:X:156:LYS:O	10:X:160:GLN:HG3	1.98	0.62
2:P:107:ILE:HD11	2:P:111:ILE:HG22	1.80	0.62
7:G:34(A):ASN:HD22	7:G:167:PRO:HG2	1.63	0.62
9:I:28:SER:HB2	10:J:120:VAL:HG21	1.81	0.62
2:B:228:GLU:O	2:B:232:ILE:HG22	1.99	0.62
3:Q:168:ASN:HB2	3:Q:200:VAL:HG11	1.80	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:53:GLU:HB2	16:V:1327:HOH:O	1.99	0.62
5:S:226:GLY:O	5:S:229:VAL:HG22	1.99	0.62
13:1:157:ASN:HB3	16:1:558:HOH:O	1.98	0.62
2:P:186:VAL:HG21	2:P:216:ARG:HD3	1.80	0.62
8:H:35:HIS:HB2	8:H:56:THR:HG21	1.82	0.62
11:Y:85:ASN:ND2	16:Y:215:HOH:O	2.32	0.62
3:C:164:THR:HG21	3:C:172:VAL:HG13	1.80	0.62
1:A:225:THR:OG1	1:A:228:GLU:HG3	1.99	0.62
7:U:34(A):ASN:HD22	7:U:167:PRO:HG2	1.65	0.62
8:H:163:ILE:HG23	8:H:170:GLY:HA2	1.82	0.62
1:A:97:HIS:HD2	8:H:61:SER:OG	1.83	0.62
1:A:110:LYS:HG2	16:A:285:HOH:O	1.98	0.62
5:E:15:PHE:HB2	6:F:23:GLN:NE2	2.15	0.62
2:P:65:GLU:HG3	2:P:66:LYS:HG3	1.80	0.62
4:R:215:ILE:C	4:R:215:ILE:HD13	2.20	0.62
2:B:51:GLU:OE2	2:B:202:THR:HG23	2.00	0.62
14:N:146:MET:HE3	14:N:150:GLU:HB3	1.81	0.62
3:Q:160:TRP:CE2	4:R:59:LEU:HD23	2.35	0.62
1:A:179:ARG:HB3	1:A:179:ARG:NH1	2.13	0.62
10:J:147:THR:OG1	10:J:150:GLU:HG3	1.98	0.62
13:1:168:ARG:HB2	16:1:1064:HOH:O	2.00	0.62
12:L:90:LYS:HD3	12:L:95:TYR:CE1	2.35	0.62
13:1:104:VAL:HG23	13:1:178:ILE:HG22	1.81	0.61
3:C:168:ASN:HB2	3:C:200:VAL:HG11	1.81	0.61
13:1:40:ASN:HD22	13:1:40:ASN:N	1.96	0.61
4:R:12(D):ALA:HB3	4:R:126:ARG:HD3	1.82	0.61
8:V:38:SER:OG	8:V:41:ILE:HG13	2.00	0.61
13:1:76:PRO:HD2	13:1:105:GLN:OE1	2.00	0.61
6:T:95:GLU:CG	6:T:115:ARG:HB3	2.28	0.61
2:P:185:LYS:HD3	2:P:186:VAL:N	2.16	0.61
2:B:107:ILE:HD11	2:B:111:ILE:HG22	1.82	0.61
2:B:21:LEU:HD13	2:B:124:THR:HG23	1.82	0.61
5:E:31:ILE:HD11	5:E:153:PRO:HG2	1.83	0.61
9:W:28:SER:HB2	10:X:120:VAL:HG21	1.82	0.61
6:F:109:ILE:CD1	6:F:109:ILE:N	2.63	0.61
5:E:132:TYR:O	5:E:153:PRO:HB3	1.99	0.61
13:M:8:TYR:CE2	13:M:148:VAL:HG22	2.34	0.61
2:B:15:PHE:N	3:C:23:GLN:HE22	1.93	0.61
3:Q:195:ARG:HG3	3:Q:236:ILE:CD1	2.31	0.61
14:N:176:VAL:HG12	14:N:178:LEU:HD13	1.83	0.61
6:F:95:GLU:CG	6:F:115:ARG:HB3	2.31	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:143:LYS:HB2	11:Y:146:LEU:CD1	2.31	0.60
5:S:31:ILE:HD11	5:S:153:PRO:HG2	1.83	0.60
3:Q:177:GLU:OE2	4:R:57:PRO:HD2	2.02	0.60
8:V:35:HIS:HB2	8:V:56:THR:HG21	1.83	0.60
1:O:69:LEU:HD23	1:O:69:LEU:C	2.21	0.60
8:H:24:PRO:HG2	8:H:25:ILE:HD13	1.84	0.60
4:R:112:LEU:C	4:R:112:LEU:HD13	2.21	0.60
8:H:172:ASN:ND2	8:H:193:THR:HA	2.17	0.60
14:2:176:VAL:HG12	14:2:178:LEU:HD13	1.83	0.60
13:M:76:PRO:HD2	13:M:105:GLN:OE1	2.02	0.60
12:Z:114:ASP:CB	12:Z:118:SER:HB3	2.32	0.60
9:I:1:GLY:HA3	9:I:33:LYS:HE2	1.83	0.60
12:L:21:ILE:HD12	12:L:21:ILE:C	2.22	0.60
5:S:15:PHE:H	6:T:23:GLN:NE2	1.92	0.60
5:S:18(D):ILE:O	5:S:18(D):ILE:HG12	2.01	0.60
8:V:216:GLU:HG3	9:W:187:ARG:HG2	1.84	0.60
2:B:6:ARG:HB2	5:E:127:TYR:OH	2.01	0.60
7:U:38:LEU:HD23	7:U:197:MET:HE3	1.84	0.60
5:S:220:PRO:O	5:S:222:THR:HG23	2.02	0.59
6:T:38:ILE:HG22	6:T:164:ALA:CB	2.31	0.59
10:X:113:ILE:HA	10:X:118:THR:O	2.02	0.59
8:V:163:ILE:HG23	8:V:170:GLY:HA2	1.84	0.59
14:N:107:LYS:HG2	14:N:108:GLY:N	2.17	0.59
6:F:109:ILE:HG21	6:F:147:HIS:HB2	1.83	0.59
10:J:113:ILE:HA	10:J:118:THR:O	2.03	0.59
9:W:2:ILE:HG21	9:W:130:ALA:HB3	1.84	0.59
4:D:112:LEU:C	4:D:112:LEU:HD13	2.22	0.59
12:L:-7:ASN:HD22	12:L:-6:PRO:HD2	1.67	0.59
13:1:110:LEU:HG	13:1:125:LEU:HD12	1.83	0.59
5:S:15:PHE:HB2	6:T:23:GLN:HE22	1.67	0.59
2:B:185:LYS:HD3	2:B:186:VAL:N	2.18	0.59
10:X:147:THR:OG1	10:X:150:GLU:HG3	2.03	0.59
1:A:69:LEU:HD23	1:A:69:LEU:C	2.22	0.59
3:Q:172:VAL:HG23	3:Q:196:SER:HB2	1.84	0.59
8:V:4:VAL:HG12	8:V:126:SER:HB3	1.83	0.59
1:O:86:ARG:HH21	7:U:118:ASN:ND2	2.00	0.59
2:P:108:PRO:HB2	2:P:111:ILE:HD12	1.85	0.59
6:T:216:SER:HB3	6:T:21(A):GLU:HB2	1.85	0.59
8:H:216:GLU:HG3	9:I:187:ARG:HG2	1.85	0.59
3:Q:55:THR:HG22	3:Q:56:LEU:HD22	1.85	0.59
13:1:42:VAL:HG23	13:1:178:ILE:HD11	1.84	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:6:MET:CE	9:W:155:ILE:HA	2.33	0.58
12:Z:90:LYS:HD3	12:Z:95:TYR:CE1	2.38	0.58
6:F:198:TYR:HE2	6:F:237:GLN:HE21	1.50	0.58
13:M:42:VAL:HG23	13:M:178:ILE:HD11	1.85	0.58
13:M:149:GLN:NE2	13:M:149:GLN:H	2.01	0.58
2:P:51:GLU:OE2	2:P:202:THR:HG23	2.03	0.58
3:C:172:VAL:HG23	3:C:196:SER:HB2	1.84	0.58
2:P:21:LEU:HD13	2:P:124:THR:HG23	1.84	0.58
9:I:6:MET:CE	9:I:155:ILE:HA	2.34	0.58
10:X:152:LEU:HD13	10:X:193:GLN:HE22	1.67	0.58
11:K:143:LYS:HB2	11:K:146:LEU:CD1	2.33	0.58
2:B:108:PRO:HB2	2:B:111:ILE:HD12	1.85	0.58
7:U:67:ILE:CD1	7:U:211:GLU:HG2	2.34	0.58
5:E:220:PRO:O	5:E:222:THR:HG23	2.04	0.58
11:Y:10(A):ARG:HH11	11:Y:10(A):ARG:HG2	1.69	0.58
13:1:14(D):GLU:O	13:1:14(G):ILE:HG12	2.04	0.58
11:K:7:ARG:HG2	11:K:108:PRO:HB2	1.85	0.58
10:J:143:ARG:O	10:J:146:MET:HG3	2.03	0.58
10:X:44:SER:OG	10:X:100:LEU:HB2	2.03	0.58
4:R:162:ALA:HB3	5:S:58:LEU:HD23	1.84	0.58
4:D:175:GLU:CG	4:D:196:ILE:HD12	2.34	0.58
1:O:97:HIS:HD2	8:V:61:SER:OG	1.85	0.58
12:Z:-6:PRO:O	13:1:91:ARG:NH1	2.34	0.58
2:P:152:ASN:HB2	2:P:153:PRO:HD2	1.86	0.58
10:J:156:LYS:O	10:J:160:GLN:HG3	2.03	0.58
8:V:155:ALA:O	8:V:159:ILE:HD12	2.04	0.58
9:W:178:ILE:HG23	9:W:184:VAL:HG22	1.86	0.57
8:H:38:SER:OG	8:H:41:ILE:HG13	2.04	0.57
7:G:72:ARG:NH1	7:G:72:ARG:HB2	2.19	0.57
12:L:114:ASP:CB	12:L:118:SER:HB3	2.34	0.57
1:O:150:GLN:O	1:O:157:TYR:HA	2.04	0.57
11:Y:7:ARG:HG2	11:Y:108:PRO:HB2	1.85	0.57
6:T:109:ILE:CD1	6:T:109:ILE:N	2.66	0.57
5:E:18(D):ILE:O	5:E:18(D):ILE:HG12	2.02	0.57
4:D:12(D):ALA:HB3	4:D:126:ARG:HD3	1.84	0.57
2:P:181:LYS:O	2:P:184:MET:HG3	2.04	0.57
6:F:216:SER:HB3	6:F:21(A):GLU:HB2	1.85	0.57
3:C:35:THR:HB	3:C:51:GLU:HG3	1.85	0.57
10:J:168:MET:HG2	10:X:168:MET:CE	2.35	0.57
9:W:29:ASN:H	9:W:29:ASN:ND2	2.02	0.57
14:N:18(G):TYR:HA	14:N:18(J):LEU:HG	1.86	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:155:ALA:O	8:H:159:ILE:HD12	2.04	0.57
2:B:181:LYS:O	2:B:184:MET:HG3	2.03	0.57
14:N:20:THR:HG22	15:N:0:SA1:C12	2.33	0.57
3:Q:35:THR:HB	3:Q:51:GLU:HG3	1.86	0.57
1:O:118:LYS:HE2	1:O:122:GLU:OE1	2.04	0.57
5:S:15:PHE:HB2	6:T:23:GLN:NE2	2.19	0.57
5:E:15:PHE:H	6:F:23:GLN:NE2	1.95	0.57
14:2:107:LYS:HG2	14:2:108:GLY:N	2.18	0.57
6:F:38:ILE:HG22	6:F:164:ALA:CB	2.34	0.57
3:Q:235:GLN:O	3:Q:239:GLU:HG2	2.05	0.57
13:1:14(A):VAL:O	13:1:14(A):VAL:HG23	2.05	0.57
8:V:41:ILE:HD13	8:V:76:VAL:HG22	1.86	0.57
7:U:67:ILE:HD12	7:U:211:GLU:HG2	1.85	0.57
8:H:4:VAL:HG12	8:H:126:SER:HB3	1.85	0.57
5:S:92:LEU:HD11	5:S:112:ALA:HB1	1.85	0.57
9:I:112:GLY:N	9:I:125:ILE:HD12	2.19	0.57
12:Z:21:ILE:HD12	12:Z:21:ILE:C	2.25	0.57
5:E:92:LEU:HD11	5:E:112:ALA:HB1	1.86	0.57
1:O:184:LEU:HB2	16:O:486:HOH:O	2.03	0.57
3:Q:14:ILE:HD12	3:Q:14:ILE:N	2.19	0.57
11:K:207:ASN:HD21	10:X:144:PRO:CG	2.18	0.57
13:M:14(A):VAL:O	13:M:14(A):VAL:HG23	2.04	0.57
3:C:177:GLU:OE2	4:D:57:PRO:HD2	2.05	0.57
12:Z:-7:ASN:HD22	12:Z:-6:PRO:HD2	1.70	0.57
9:I:2:ILE:HG21	9:I:130:ALA:HB3	1.86	0.57
9:I:174:VAL:HG21	9:I:186:LYS:HE3	1.87	0.57
9:I:178:ILE:HG23	9:I:184:VAL:HG22	1.86	0.57
9:I:7:THR:CG2	9:I:110:ILE:HD13	2.33	0.56
3:Q:105:ASP:OD2	3:Q:106:PRO:HD2	2.04	0.56
13:1:41:THR:OG1	13:1:76:PRO:HG3	2.04	0.56
10:X:18:LYS:HD3	10:X:174:ILE:HG13	1.86	0.56
9:W:1:GLY:HA3	9:W:33:LYS:HE2	1.85	0.56
13:1:8:TYR:CE2	13:1:148:VAL:HG22	2.39	0.56
8:V:15:ALA:HB3	8:V:159:ILE:HD11	1.88	0.56
2:P:112:LEU:HD23	2:P:112:LEU:C	2.25	0.56
4:R:53:ARG:HG2	4:R:53:ARG:O	2.05	0.56
2:B:202:THR:HG22	2:B:204:SER:N	2.11	0.56
12:L:-6:PRO:O	13:M:91:ARG:NH1	2.35	0.56
13:M:104:VAL:HG23	13:M:178:ILE:HG22	1.86	0.56
3:C:57:LYS:O	3:C:58:LEU:HB2	2.05	0.56
7:U:72:ARG:HB2	7:U:72:ARG:NH1	2.20	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1:149:GLN:H	13:1:149:GLN:NE2	2.04	0.56
10:J:152:LEU:HD13	10:J:193:GLN:HE22	1.70	0.56
4:R:160:TYR:CE2	4:R:163:LYS:HD3	2.40	0.56
2:B:152:ASN:HB2	2:B:153:PRO:HD2	1.86	0.56
7:G:170:GLN:HE21	7:G:174:THR:HG23	1.70	0.56
3:Q:186:VAL:HG21	3:Q:216:LYS:HE2	1.87	0.56
3:C:195:ARG:HG3	3:C:236:ILE:CD1	2.35	0.56
2:P:101:LYS:HZ2	10:X:85:GLN:NE2	2.01	0.56
6:T:198:TYR:HE2	6:T:237:GLN:HE21	1.52	0.56
10:J:18:LYS:HD3	10:J:174:ILE:HG13	1.87	0.56
4:D:160:TYR:CE2	4:D:163:LYS:HD3	2.40	0.56
11:K:10(A):ARG:HG2	11:K:10(A):ARG:HH11	1.70	0.56
3:C:55:THR:HG22	3:C:56:LEU:HD22	1.86	0.56
12:L:165:ARG:NH2	8:V:29:LYS:HE2	2.20	0.56
2:B:27:ALA:O	2:B:31:ILE:HG12	2.06	0.56
1:O:4:MET:SD	1:O:5:THR:N	2.64	0.56
2:P:101:LYS:HZ1	10:X:85:GLN:NE2	2.02	0.56
7:G:77:VAL:CG1	7:G:137:THR:HB	2.35	0.56
10:X:38:SER:HB2	10:X:39:PRO:HD2	1.88	0.56
5:E:86:ARG:HH11	5:E:86:ARG:HG3	1.71	0.56
3:C:186:VAL:HG21	3:C:216:LYS:HE2	1.88	0.56
1:A:118:LYS:HE2	1:A:122:GLU:OE1	2.06	0.56
11:Y:97:MET:HG2	11:Y:115:SER:HB3	1.86	0.56
13:M:139:ARG:HH11	8:V:165:ASN:ND2	2.03	0.56
4:R:81:LEU:HB3	16:R:599:HOH:O	2.05	0.56
3:Q:170:LYS:HB2	16:Q:833:HOH:O	2.05	0.56
12:L:99:THR:HG23	12:L:113:PHE:HB2	1.88	0.56
7:G:105:TYR:OH	8:H:66:HIS:HE1	1.89	0.56
3:C:105:ASP:OD2	3:C:106:PRO:HD2	2.06	0.56
4:R:175:GLU:CG	4:R:196:ILE:HD12	2.35	0.56
13:M:14(D):GLU:O	13:M:14(G):ILE:HG12	2.06	0.56
2:P:6:ARG:HG2	3:Q:10:ARG:NH2	2.21	0.56
7:G:151:THR:HG22	7:G:157:TYR:CB	2.36	0.56
3:C:235:GLN:O	3:C:239:GLU:HG2	2.06	0.56
7:G:67:ILE:CD1	7:G:211:GLU:HG2	2.36	0.56
12:L:109:ALA:HB2	12:L:121:ARG:NH2	2.20	0.55
13:M:197:TRP:CH2	14:2:171:GLY:HA2	2.40	0.55
10:X:12:VAL:HG23	10:X:108:PRO:HB2	1.88	0.55
5:S:15:PHE:N	6:T:23:GLN:HE22	1.94	0.55
2:B:46:ILE:HD11	2:B:146:TYR:HB3	1.88	0.55
14:2:112:THR:HG22	14:2:120:HIS:HB2	1.89	0.55

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:194:VAL:O	5:S:197:ILE:HG22	2.06	0.55
14:N:171:GLY:HA2	13:1:197:TRP:CH2	2.41	0.55
3:Q:216:LYS:HB2	3:Q:220:ASP:HB3	1.89	0.55
11:K:4:LEU:HD13	11:K:15:ALA:O	2.07	0.55
3:C:227:GLU:OE1	3:C:227:GLU:N	2.39	0.55
14:2:18(G):TYR:HA	14:2:18(J):LEU:HG	1.87	0.55
5:S:97:ASN:HD21	12:Z:61:ASN:HD21	1.55	0.55
4:R:207:LEU:C	4:R:207:LEU:HD23	2.27	0.55
16:B:565:HOH:O	3:C:33:ARG:HD2	2.06	0.55
11:K:4:LEU:HD11	11:K:15:ALA:HB3	1.88	0.55
2:B:71:ASN:ND2	2:B:72:ASP:H	2.05	0.55
3:C:225:SER:OG	3:C:228:GLU:HG3	2.06	0.55
7:U:8:TYR:C	7:U:10:ARG:H	2.10	0.55
10:J:12:VAL:HG23	10:J:108:PRO:HB2	1.88	0.55
1:A:150:GLN:O	1:A:157:TYR:HA	2.06	0.55
2:P:95:HIS:CD2	2:P:115:ARG:HG2	2.41	0.55
13:M:17:ASP:HA	13:M:173:PHE:CB	2.37	0.55
7:U:151:THR:HG22	7:U:157:TYR:CB	2.37	0.55
7:U:151:THR:HG22	7:U:157:TYR:HB2	1.89	0.55
5:S:227:GLU:N	5:S:227:GLU:CD	2.60	0.55
14:N:136:GLY:CA	14:2:161:GLN:HE21	2.05	0.55
14:2:20:THR:OG1	14:2:28:ASN:HB3	2.07	0.55
8:V:148:LYS:O	8:V:152:ILE:HG13	2.06	0.55
7:G:87:ASN:ND2	7:G:87:ASN:C	2.60	0.55
6:T:109:ILE:HG21	6:T:147:HIS:HB2	1.87	0.55
11:K:97:MET:HG2	11:K:115:SER:HB3	1.88	0.55
13:M:41:THR:OG1	13:M:76:PRO:HG3	2.07	0.55
12:Z:99:THR:HG23	12:Z:113:PHE:HB2	1.89	0.55
2:P:239:THR:HG22	2:P:239:THR:OXT	2.07	0.55
5:E:97:ASN:HD21	12:L:61:ASN:HD21	1.55	0.55
10:X:76:PRO:HD2	16:X:275:HOH:O	2.07	0.55
9:I:29:ASN:H	9:I:29:ASN:ND2	2.04	0.55
5:S:86:ARG:HH11	5:S:86:ARG:HG3	1.71	0.55
2:P:202:THR:HG22	2:P:204:SER:N	2.10	0.54
4:D:186:LEU:O	4:D:190:GLU:HG3	2.07	0.54
5:E:194:VAL:O	5:E:197:ILE:HG22	2.07	0.54
10:J:168:MET:CE	10:X:168:MET:HG2	2.37	0.54
12:Z:1:GLY:HA3	12:Z:33:LYS:HZ2	1.72	0.54
11:Y:4:LEU:HD13	11:Y:15:ALA:O	2.07	0.54
11:Y:37:ILE:HD13	11:Y:37:ILE:H	1.72	0.54
7:G:38:LEU:HD23	7:G:197:MET:HE3	1.88	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:14(I):THR:HG21	12:Z:14(M):VAL:HB	1.89	0.54
2:B:95:HIS:CD2	2:B:115:ARG:HG2	2.42	0.54
14:2:20:THR:HG23	14:2:31:THR:OG1	2.07	0.54
5:S:18(D):ILE:HG23	5:S:18(E):LYS:HG3	1.88	0.54
2:P:71:ASN:ND2	2:P:72:ASP:H	2.06	0.54
7:U:77:VAL:CG1	7:U:137:THR:HB	2.37	0.54
4:R:186:LEU:O	4:R:190:GLU:HG3	2.07	0.54
14:2:20:THR:HG22	15:2:0:SA1:C12	2.34	0.54
7:G:203:THR:HG22	7:G:204:GLU:N	2.23	0.54
4:D:177:LEU:CD2	5:E:58:LEU:HD13	2.37	0.54
14:2:175:MET:HB2	14:2:187:LEU:HB2	1.88	0.54
7:G:8:TYR:C	7:G:10:ARG:H	2.09	0.54
10:J:38:SER:HB2	10:J:39:PRO:HD2	1.90	0.54
8:H:165:ASN:ND2	13:1:139:ARG:HH11	2.04	0.54
5:S:70:CYS:SG	5:S:92:LEU:HD23	2.47	0.54
8:H:179:GLU:OE2	8:H:182:LYS:HE2	2.07	0.54
7:G:151:THR:HG22	7:G:157:TYR:HB2	1.90	0.54
4:D:207:LEU:HD23	4:D:207:LEU:C	2.27	0.54
3:Q:225:SER:OG	3:Q:228:GLU:HG3	2.07	0.54
4:D:215:ILE:HD13	4:D:215:ILE:C	2.28	0.54
5:E:227:GLU:CD	5:E:227:GLU:N	2.60	0.54
10:J:-1:MET:HG2	10:J:1:ASP:H	1.73	0.54
14:2:41:ILE:HD13	14:2:76:THR:HA	1.89	0.54
10:J:44:SER:OG	10:J:100:LEU:HB2	2.08	0.54
12:L:14(C):GLN:HG2	8:V:210:THR:CG2	2.38	0.54
3:C:216:LYS:HB2	3:C:220:ASP:HB3	1.89	0.53
11:K:4:LEU:HD12	11:K:159:ILE:HD11	1.90	0.53
1:A:206:PHE:CD1	1:A:210:ILE:HD11	2.43	0.53
2:B:150:THR:O	2:B:157:TYR:HA	2.07	0.53
6:F:192:GLN:HE21	6:F:195:LYS:HE3	1.73	0.53
7:U:170:GLN:HE21	7:U:174:THR:HG23	1.72	0.53
3:Q:241:GLN:C	3:Q:243:GLN:H	2.12	0.53
4:D:53:ARG:HG2	4:D:53:ARG:O	2.08	0.53
5:S:134:VAL:O	5:S:153:PRO:HG3	2.08	0.53
10:X:100:LEU:CD2	10:X:112:GLN:HG3	2.38	0.53
5:E:18(D):ILE:HG23	5:E:18(E):LYS:HG3	1.88	0.53
6:T:136:THR:O	6:T:150:MET:HA	2.08	0.53
4:D:177:LEU:HD22	5:E:58:LEU:CD1	2.37	0.53
12:L:40:ASN:HD21	12:L:183:GLY:HA2	1.73	0.53
2:P:150:THR:O	2:P:157:TYR:HA	2.07	0.53
1:A:86:ARG:HH21	7:G:118:ASN:ND2	2.04	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:87:ASN:ND2	7:U:87:ASN:C	2.61	0.53
7:G:67:ILE:HD12	7:G:211:GLU:HG2	1.89	0.53
2:B:218:ASN:O	2:B:21(C):ASP:HB2	2.08	0.53
11:K:37:ILE:HB	11:K:41:LEU:HB2	1.90	0.53
10:X:2:ILE:O	10:X:3:ILE:HD13	2.08	0.53
1:A:173:LYS:O	1:A:177:GLU:HG3	2.09	0.53
3:Q:57:LYS:O	3:Q:58:LEU:HB2	2.07	0.53
2:B:152:ASN:HB2	2:B:153:PRO:CD	2.39	0.53
9:W:174:VAL:HG21	9:W:186:LYS:HE3	1.89	0.53
7:U:86:ARG:HD2	16:U:248:HOH:O	2.09	0.53
8:H:8:PHE:HB3	8:H:151:ALA:HB2	1.90	0.53
2:B:6:ARG:HG2	3:C:10:ARG:HH21	1.74	0.53
11:K:37:ILE:HD13	11:K:37:ILE:H	1.73	0.53
8:H:144:GLN:O	8:H:145:ASP:HB2	2.09	0.53
3:C:241:GLN:C	3:C:243:GLN:H	2.12	0.53
10:J:144:PRO:CG	11:Y:207:ASN:HD21	2.21	0.53
4:R:90:GLU:OE1	11:Y:69:ARG:HD2	2.09	0.53
8:H:113:ILE:N	8:H:113:ILE:HD12	2.24	0.53
3:Q:173:ARG:O	3:Q:177:GLU:HG3	2.09	0.53
12:L:-7:ASN:HD22	12:L:-6:PRO:CD	2.21	0.53
7:U:56:ASP:HB3	7:U:59:LEU:HG	1.90	0.53
2:P:27:ALA:O	2:P:31:ILE:HG12	2.09	0.53
10:X:10(B):LYS:NZ	10:X:10(B):LYS:HB2	2.24	0.53
2:P:121:GLN:CG	3:Q:83:ALA:HB1	2.39	0.53
9:W:6:MET:HB3	9:W:151:LEU:HD11	1.91	0.53
7:G:56:ASP:HB3	7:G:59:LEU:HG	1.90	0.53
14:N:175:MET:HB2	14:N:187:LEU:HB2	1.89	0.53
3:Q:182:PRO:O	3:Q:184:ALA:N	2.42	0.53
8:V:179:GLU:OE2	8:V:182:LYS:HE2	2.09	0.53
13:I:152:GLU:O	13:I:156:VAL:HG23	2.09	0.53
1:O:27:ALA:O	1:O:31:VAL:HG23	2.09	0.53
2:B:112:LEU:C	2:B:112:LEU:HD23	2.28	0.53
5:S:194:VAL:HG13	5:S:207:LEU:HD11	1.90	0.53
7:U:203:THR:HG22	7:U:204:GLU:N	2.24	0.53
2:P:186:VAL:O	2:P:190:ILE:HG13	2.09	0.53
3:C:226:SER:HB2	3:C:227:GLU:OE1	2.09	0.52
3:Q:227:GLU:N	3:Q:227:GLU:OE1	2.40	0.52
5:E:194:VAL:HG13	5:E:207:LEU:HD11	1.90	0.52
2:P:163:ILE:CG1	2:P:164:SER:N	2.71	0.52
8:H:221:ILE:HD11	9:I:184:VAL:HG21	1.90	0.52
5:S:227:GLU:CD	5:S:227:GLU:H	2.12	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:82:ILE:HB	6:T:83:PRO:HD3	1.91	0.52
8:V:12:VAL:HG11	8:V:102:ALA:HB1	1.90	0.52
2:B:161:LYS:HE3	3:C:59:GLN:O	2.09	0.52
8:H:34:LEU:HB2	16:H:540:HOH:O	2.10	0.52
3:Q:163:GLN:HE22	3:Q:173:ARG:NE	2.03	0.52
6:T:51:GLU:OE1	6:T:53:LEU:HD21	2.09	0.52
14:2:107:LYS:CG	14:2:108:GLY:H	2.21	0.52
3:C:46:VAL:HB	3:C:215:VAL:CG1	2.40	0.52
11:Y:4:LEU:HD12	11:Y:159:ILE:HD11	1.91	0.52
13:M:152:GLU:O	13:M:156:VAL:HG23	2.10	0.52
12:L:5:GLY:O	12:L:124:CYS:HA	2.08	0.52
14:N:26:ILE:HG13	13:1:165:ARG:C	2.30	0.52
14:2:163:ILE:HG23	14:2:170:GLY:HA2	1.90	0.52
2:P:218:ASN:O	2:P:21(C):ASP:HB2	2.09	0.52
7:U:105:TYR:OH	8:V:66:HIS:HE1	1.91	0.52
10:X:133:TYR:CZ	10:X:166:MET:HG3	2.43	0.52
7:G:18(G):GLU:HG2	7:G:188:LYS:HB3	1.91	0.52
8:V:4:VAL:HG12	8:V:126:SER:CB	2.39	0.52
14:N:156:LYS:HG2	14:N:18(J):LEU:HD11	1.92	0.52
6:F:203:GLU:HA	6:F:203:GLU:OE1	2.09	0.52
5:E:15:PHE:N	6:F:23:GLN:HE22	1.98	0.52
2:P:152:ASN:HB2	2:P:153:PRO:CD	2.39	0.52
5:S:97:ASN:ND2	12:Z:61:ASN:HD21	2.07	0.52
10:X:-1:MET:HG2	10:X:1:ASP:H	1.74	0.52
8:V:200:LYS:HE3	9:W:140:SER:O	2.09	0.52
8:V:80:LEU:HD22	8:V:111:PHE:CD2	2.45	0.52
14:N:163:ILE:HG23	14:N:170:GLY:HA2	1.92	0.52
3:C:14:ILE:H	3:C:14:ILE:CD1	2.21	0.52
3:Q:46:VAL:HB	3:Q:215:VAL:CG1	2.39	0.52
14:N:94:ASN:ND2	16:N:946:HOH:O	2.43	0.52
11:K:126:CYS:HB2	11:K:135:TYR:CE1	2.45	0.52
14:N:20:THR:OG1	14:N:28:ASN:HB3	2.09	0.52
1:A:177:GLU:HG2	2:B:58:LEU:CD2	2.39	0.52
11:Y:37:ILE:HB	11:Y:41:LEU:HB2	1.91	0.52
6:T:54:ILE:HG13	6:T:208:PHE:HA	1.91	0.52
1:O:48:ILE:HD11	1:O:213:ALA:HB3	1.92	0.52
5:E:97:ASN:ND2	12:L:61:ASN:HD21	2.07	0.52
7:U:78:VAL:HG11	7:U:85:ALA:CB	2.40	0.52
1:O:173:LYS:O	1:O:177:GLU:HG3	2.09	0.52
6:T:192:GLN:HE21	6:T:195:LYS:HE3	1.73	0.52
6:F:203:GLU:O	6:F:206:LYS:HD2	2.10	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:73:HIS:HE1	5:S:107:LEU:O	1.91	0.52
3:C:14:ILE:HD13	3:C:14:ILE:C	2.31	0.52
2:B:31:ILE:HD11	2:B:133:GLY:C	2.31	0.52
10:J:100:LEU:CD2	10:J:112:GLN:HG3	2.40	0.52
12:L:13:VAL:HG12	12:L:177:ILE:HG13	1.91	0.52
7:U:233:LEU:O	7:U:236:ILE:HG13	2.10	0.52
8:V:144:GLN:O	8:V:145:ASP:HB2	2.10	0.52
8:H:29:LYS:HE2	12:Z:165:ARG:NH2	2.25	0.52
6:F:78:TYR:CE1	6:F:85:GLY:HA3	2.45	0.52
6:T:101:LYS:HE2	13:1:57:ARG:NH2	2.25	0.52
1:O:49:ALA:HB2	1:O:212:LEU:HG	1.92	0.51
5:S:179:THR:O	5:S:179:THR:HG22	2.09	0.51
10:J:167:PRO:HB2	10:X:168:MET:HE1	1.92	0.51
4:R:161:ASN:HB3	4:R:180:TRP:CE2	2.46	0.51
12:L:33:LYS:HD2	12:L:46:ASN:ND2	2.23	0.51
8:V:15:ALA:HB3	8:V:159:ILE:CD1	2.40	0.51
10:J:-1:MET:HG2	10:J:1:ASP:N	2.26	0.51
3:Q:226:SER:HB2	3:Q:227:GLU:OE1	2.10	0.51
4:D:24:VAL:O	4:D:27:SER:HB3	2.10	0.51
2:B:239:THR:OXT	2:B:239:THR:HG22	2.10	0.51
5:E:54:ASN:ND2	5:E:56:ASP:O	2.41	0.51
8:V:8:PHE:HB3	8:V:151:ALA:HB2	1.91	0.51
5:E:82:ALA:HB3	5:E:83:PRO:HD3	1.92	0.51
13:M:9:ASP:OD1	13:M:10:ASN:N	2.43	0.51
14:2:146:MET:HE3	14:2:150:GLU:HB3	1.92	0.51
6:T:175:GLU:OE1	6:T:199:LEU:HD23	2.09	0.51
12:Z:93:PHE:N	12:Z:94:PRO:HD3	2.26	0.51
8:V:221:ILE:HD11	9:W:184:VAL:HG21	1.92	0.51
5:E:227:GLU:CD	5:E:227:GLU:H	2.12	0.51
2:P:31:ILE:HD11	2:P:133:GLY:C	2.30	0.51
2:B:97:GLN:HE22	9:I:64:ASN:HD22	1.57	0.51
1:O:206:PHE:CD1	1:O:210:ILE:HD11	2.46	0.51
2:B:149:TYR:OH	3:C:62(A):ILE:HB	2.09	0.51
8:H:148:LYS:O	8:H:152:ILE:HG13	2.10	0.51
6:F:210:LEU:HD21	6:F:212:ILE:HD11	1.93	0.51
10:J:10(B):LYS:HB2	10:J:10(B):LYS:NZ	2.25	0.51
4:D:31:ILE:HD13	4:D:135:ALA:HB2	1.92	0.51
3:Q:14:ILE:C	3:Q:14:ILE:HD13	2.30	0.51
13:M:139:ARG:NH1	8:V:165:ASN:HD22	2.08	0.51
9:W:143:GLU:CG	9:W:146:LEU:HD21	2.39	0.51
9:I:143:GLU:CG	9:I:146:LEU:HD21	2.40	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:155:ILE:HG22	14:N:175:MET:HE2	1.92	0.51
9:W:29:ASN:H	9:W:29:ASN:HD22	1.59	0.51
12:Z:14(I):THR:O	12:Z:14(K):LYS:HB2	2.10	0.51
8:H:210:THR:CG2	12:Z:14(C):GLN:HG2	2.40	0.51
6:T:203:GLU:O	6:T:206:LYS:HD2	2.10	0.51
2:P:87:ILE:O	2:P:91:THR:HG23	2.11	0.51
8:H:200:LYS:HE3	9:I:140:SER:O	2.09	0.51
13:1:17:ASP:HA	13:1:173:PHE:CB	2.40	0.51
7:G:55:PRO:HG2	7:G:56:ASP:H	1.74	0.51
12:L:14(I):THR:HG21	12:L:14(M):VAL:HB	1.92	0.51
5:S:38:VAL:HG12	5:S:39:GLY:N	2.24	0.51
10:X:111:TYR:CE1	10:X:121:GLU:HG3	2.46	0.51
8:V:113:ILE:HD12	8:V:113:ILE:N	2.25	0.51
1:A:27:ALA:O	1:A:31:VAL:HG23	2.11	0.51
16:F:1121:HOH:O	13:M:67:ALA:HB3	2.10	0.51
3:C:182:PRO:O	3:C:184:ALA:N	2.43	0.51
10:J:133:TYR:CZ	10:J:166:MET:HG3	2.45	0.51
13:M:91:ARG:HG3	13:M:92:SER:N	2.24	0.51
12:L:14(C):GLN:HG2	8:V:210:THR:HG21	1.93	0.51
6:F:173:LYS:O	6:F:177:GLU:HG3	2.11	0.51
8:H:12:VAL:HG11	8:H:102:ALA:HB1	1.92	0.51
5:E:201:LEU:HD11	5:E:207:LEU:CD2	2.40	0.51
11:K:109:THR:C	11:K:110:ILE:HD13	2.30	0.51
11:K:200:LYS:HE2	16:K:1088:HOH:O	2.11	0.51
5:E:38:VAL:HG12	5:E:39:GLY:N	2.25	0.51
7:U:228:ASN:HB3	16:U:242:HOH:O	2.09	0.51
13:M:80:PHE:CE1	13:M:111:ARG:HD3	2.46	0.51
5:E:179:THR:HG22	5:E:179:THR:O	2.11	0.51
6:T:187:ARG:HG3	6:T:187:ARG:HH11	1.76	0.51
11:Y:7:ARG:HD2	11:Y:108:PRO:O	2.10	0.51
2:B:81:LEU:HD23	2:B:133:GLY:HA3	1.92	0.51
2:B:90:ASN:O	2:B:94:ILE:HD12	2.11	0.51
10:J:111:TYR:CE1	10:J:121:GLU:HG3	2.45	0.51
3:C:87:ILE:N	3:C:87:ILE:HD13	2.26	0.51
1:A:33:GLN:HE21	1:A:33:GLN:CA	2.20	0.50
2:P:81:LEU:HD23	2:P:133:GLY:HA3	1.92	0.50
10:X:52:THR:CG2	10:X:53:VAL:N	2.73	0.50
13:1:19:LEU:HD21	13:1:26:LEU:HD22	1.93	0.50
7:U:55:PRO:HG2	7:U:56:ASP:H	1.76	0.50
13:1:9:ASP:OD1	13:1:10:ASN:N	2.44	0.50
14:2:114:PRO:HD2	14:2:118:SER:O	2.11	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:173:LYS:O	6:T:177:GLU:HG3	2.12	0.50
2:P:90:ASN:O	2:P:94:ILE:HD12	2.12	0.50
6:F:101:LYS:HE2	13:M:57:ARG:NH2	2.27	0.50
9:I:6:MET:HB3	9:I:151:LEU:HD11	1.93	0.50
5:E:134:VAL:O	5:E:153:PRO:HG3	2.11	0.50
6:F:109:ILE:HD12	6:F:109:ILE:N	2.25	0.50
10:X:147:THR:HG23	10:X:150:GLU:OE2	2.11	0.50
11:K:7:ARG:HD2	11:K:108:PRO:O	2.10	0.50
11:K:37:ILE:HD13	11:K:37:ILE:N	2.27	0.50
10:J:52:THR:CG2	10:J:53:VAL:N	2.74	0.50
13:1:80:PHE:CE1	13:1:111:ARG:HD3	2.46	0.50
4:R:31:ILE:HD13	4:R:135:ALA:HB2	1.92	0.50
1:A:161:LYS:HD3	1:A:180:TRP:CH2	2.45	0.50
14:N:114:PRO:HD2	14:N:118:SER:O	2.11	0.50
6:F:82:ILE:HB	6:F:83:PRO:HD3	1.93	0.50
2:B:190:ILE:HG23	2:B:212:PHE:CE2	2.47	0.50
8:H:4:VAL:HG12	8:H:126:SER:CB	2.41	0.50
2:P:95:HIS:HB2	16:P:249:HOH:O	2.10	0.50
6:T:192:GLN:HE21	6:T:195:LYS:CE	2.25	0.50
6:T:203:GLU:OE1	6:T:203:GLU:HA	2.11	0.50
11:K:200:LYS:HE3	11:K:206:PHE:O	2.11	0.50
6:F:127:ASN:HD22	6:F:127:ASN:C	2.13	0.50
5:S:77:SER:OG	5:S:137:LEU:HB2	2.11	0.50
14:N:20:THR:HG23	14:N:31:THR:OG1	2.12	0.50
8:H:15:ALA:HB3	8:H:159:ILE:HD11	1.93	0.50
5:S:82:ALA:HB3	5:S:83:PRO:HD3	1.93	0.50
11:K:85:ASN:ND2	16:K:697:HOH:O	2.44	0.50
3:C:40:VAL:HG12	3:C:162:ALA:HB1	1.93	0.50
8:H:21:THR:OG1	15:H:0:SA1:H202	2.11	0.50
5:E:4:PHE:CG	5:E:5:ARG:N	2.79	0.50
4:D:161:ASN:HB3	4:D:180:TRP:CE2	2.46	0.50
3:C:163:GLN:HE22	3:C:173:ARG:NE	2.07	0.50
5:S:201:LEU:HD11	5:S:207:LEU:CD2	2.39	0.50
12:L:93:PHE:N	12:L:94:PRO:HD3	2.25	0.50
11:K:207:ASN:ND2	10:X:144:PRO:CG	2.74	0.50
6:T:127:ASN:HD22	6:T:127:ASN:C	2.15	0.50
2:P:46:ILE:HD11	2:P:146:TYR:HB3	1.93	0.50
1:O:161:LYS:HD3	1:O:180:TRP:CH2	2.47	0.50
4:R:121:LEU:HB2	16:R:853:HOH:O	2.10	0.50
8:V:84:LYS:HG3	8:V:85:GLN:N	2.27	0.50
1:A:49:ALA:HB2	1:A:212:LEU:HG	1.94	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:2:113:ILE:N	14:2:113:ILE:HD12	2.27	0.50
14:2:161:GLN:HE22	14:2:165:TRP:HE1	1.59	0.50
3:C:173:ARG:O	3:C:177:GLU:HG3	2.11	0.50
14:2:21:THR:OG1	15:2:0:SA1:H202	2.12	0.50
10:X:-1:MET:HG2	10:X:1:ASP:N	2.26	0.50
14:N:112:THR:HG22	14:N:120:HIS:HB2	1.93	0.50
8:H:147:THR:OG1	8:H:150:GLU:HG3	2.12	0.50
16:C:1154:HOH:O	11:K:82:ILE:HG13	2.11	0.50
4:R:85:ALA:O	4:R:89:ILE:HG12	2.11	0.50
12:Z:5:GLY:O	12:Z:124:CYS:HA	2.12	0.50
6:F:51:GLU:OE1	6:F:53:LEU:HD21	2.11	0.50
11:Y:4:LEU:HD11	11:Y:15:ALA:HB3	1.94	0.50
6:F:136:THR:O	6:F:150:MET:HA	2.12	0.50
9:I:48:LEU:HG	9:I:50:THR:HG22	1.94	0.50
13:1:91:ARG:HG3	13:1:92:SER:N	2.25	0.49
6:F:192:GLN:HE21	6:F:195:LYS:CE	2.25	0.49
10:J:168:MET:HE1	10:X:167:PRO:HB2	1.93	0.49
7:U:18(G):GLU:HG2	7:U:188:LYS:HB3	1.94	0.49
2:B:190:ILE:HG22	2:B:232:ILE:HD11	1.93	0.49
2:P:101:LYS:HZ1	10:X:85:GLN:HE22	1.58	0.49
5:E:214:ILE:HG12	5:E:215:VAL:N	2.27	0.49
5:S:214:ILE:HG12	5:S:215:VAL:N	2.27	0.49
6:F:35:THR:HG23	6:F:51:GLU:HB3	1.95	0.49
10:J:168:MET:HG2	10:X:168:MET:HE3	1.93	0.49
1:O:159:PRO:HB2	2:P:60:GLU:HB3	1.92	0.49
6:T:147:HIS:HD2	16:T:242:HOH:O	1.96	0.49
9:I:29:ASN:ND2	9:I:30:LYS:HG3	2.27	0.49
6:T:49:ALA:HA	6:T:211:GLU:O	2.12	0.49
7:G:233:LEU:O	7:G:236:ILE:HG13	2.12	0.49
10:X:32:ASP:OD2	10:X:34:THR:HG22	2.12	0.49
5:S:141:TYR:CE2	5:S:217:LYS:HA	2.47	0.49
1:O:33:GLN:HE21	1:O:33:GLN:CA	2.20	0.49
12:L:14(I):THR:O	12:L:14(K):LYS:HB2	2.11	0.49
6:T:38:ILE:HG12	6:T:197:ILE:HD11	1.94	0.49
10:X:2:ILE:HD13	10:X:2:ILE:N	2.27	0.49
14:N:13:ILE:HD13	14:N:177:VAL:HG22	1.94	0.49
8:V:175:VAL:HG12	8:V:176:CYS:N	2.28	0.49
14:N:113:ILE:N	14:N:113:ILE:HD12	2.27	0.49
12:Z:109:ALA:HB2	12:Z:121:ARG:NH2	2.27	0.49
2:B:186:VAL:O	2:B:190:ILE:HG13	2.12	0.49
6:F:109:ILE:HD13	6:F:142:ASP:HB3	1.95	0.49

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:210:LEU:HD21	6:T:212:ILE:HD11	1.93	0.49
11:Y:138:LEU:HD13	11:Y:158:SER:OG	2.12	0.49
2:P:52:ARG:HH22	2:P:63(A):SER:HB3	1.78	0.49
11:Y:104:TYR:HB3	11:Y:180:GLU:HA	1.95	0.49
3:C:175:PHE:O	3:C:179:ASN:HB2	2.13	0.49
5:S:52:LYS:CB	5:S:63:TYR:HB3	2.41	0.49
6:F:175:GLU:OE1	6:F:199:LEU:HD23	2.13	0.49
14:2:14:LEU:O	14:2:175:MET:HA	2.13	0.49
12:L:-9:GLN:HE21	13:M:-8:THR:HG21	1.78	0.49
4:R:185:THR:OG1	4:R:188:GLU:HG3	2.13	0.49
1:A:48:ILE:HD11	1:A:213:ALA:HB3	1.93	0.49
3:C:161:SER:HB3	3:C:180:TYR:CE1	2.47	0.49
5:S:201:LEU:O	5:S:202:ARG:HB2	2.13	0.49
14:N:21:THR:OG1	15:N:0:SA1:H202	2.12	0.49
3:C:57:LYS:HD2	3:C:58:LEU:N	2.27	0.49
14:N:41:ILE:HD13	14:N:76:THR:HA	1.94	0.49
10:J:147:THR:HG23	10:J:150:GLU:OE2	2.13	0.49
14:2:156:LYS:HG2	14:2:18(J):LEU:HD11	1.93	0.49
12:Z:13:VAL:HG12	12:Z:177:ILE:HG13	1.94	0.49
11:Y:126:CYS:HB2	11:Y:135:TYR:CE1	2.48	0.49
6:F:54:ILE:HG13	6:F:208:PHE:HA	1.94	0.49
5:E:141:TYR:CE2	5:E:217:LYS:HA	2.48	0.49
7:U:236:ILE:HD12	7:U:237:ALA:N	2.28	0.48
13:1:19:LEU:HB2	13:1:170:SER:HB2	1.95	0.48
16:E:574:HOH:O	6:F:12:ASN:HB2	2.12	0.48
9:W:48:LEU:HG	9:W:50:THR:HG22	1.94	0.48
13:1:205:GLY:HA3	13:1:209:GLN:HB3	1.95	0.48
13:M:13:ILE:HB	13:M:155:ILE:HD12	1.94	0.48
6:F:187:ARG:HG3	6:F:187:ARG:HH11	1.78	0.48
3:Q:14:ILE:H	3:Q:14:ILE:CD1	2.24	0.48
2:B:232:ILE:HG12	2:B:232:ILE:O	2.13	0.48
3:Q:161:SER:HB3	3:Q:180:TYR:CE1	2.48	0.48
6:F:38:ILE:HG12	6:F:197:ILE:HD11	1.95	0.48
1:A:97:HIS:CD2	8:H:61:SER:OG	2.65	0.48
8:H:15:ALA:HB3	8:H:159:ILE:CD1	2.43	0.48
13:1:46:SER:OG	13:1:98:ALA:HB3	2.14	0.48
6:T:137:ILE:HA	6:T:149:TYR:O	2.12	0.48
11:K:138:LEU:HD13	11:K:158:SER:OG	2.12	0.48
2:B:121:GLN:CG	3:C:83:ALA:HB1	2.43	0.48
2:P:121:GLN:HG3	3:Q:83:ALA:HB1	1.95	0.48
2:P:190:ILE:HG22	2:P:232:ILE:HD11	1.94	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:41:ILE:HD13	8:H:76:VAL:HG22	1.94	0.48
9:I:29:ASN:H	9:I:29:ASN:HD22	1.61	0.48
7:G:49:ILE:HD13	7:G:193:ALA:HB1	1.95	0.48
3:Q:87:ILE:HD13	3:Q:87:ILE:N	2.28	0.48
1:O:32:LYS:HE2	1:O:32:LYS:HA	1.95	0.48
12:Z:-7:ASN:HD22	12:Z:-6:PRO:CD	2.25	0.48
3:Q:57:LYS:HD2	3:Q:58:LEU:N	2.29	0.48
4:R:24:VAL:O	4:R:27:SER:HB3	2.13	0.48
3:Q:40:VAL:HG12	3:Q:162:ALA:HB1	1.94	0.48
12:Z:40:ASN:HD21	12:Z:183:GLY:HA2	1.78	0.48
6:F:49:ALA:HA	6:F:211:GLU:O	2.13	0.48
14:2:10(B):LYS:C	14:2:10(B):LYS:HD3	2.34	0.48
6:T:12:ASN:O	6:T:12:ASN:OD1	2.30	0.48
3:Q:13:SER:O	4:R:130:ARG:HD3	2.14	0.48
4:D:122:ARG:HG2	4:D:122:ARG:HH11	1.78	0.48
11:K:99:THR:CG2	11:K:113:VAL:HB	2.44	0.48
8:V:173:VAL:HB	8:V:192:LEU:HB2	1.95	0.48
14:2:155:ILE:HG22	14:2:175:MET:HE1	1.94	0.48
14:N:14:LEU:O	14:N:175:MET:HA	2.13	0.48
12:L:90:LYS:HD3	12:L:95:TYR:CZ	2.48	0.48
2:B:213:ALA:HA	2:B:222:LYS:O	2.13	0.48
7:G:17(D):SER:O	7:G:17(E):LYS:HB2	2.13	0.48
13:M:1:THR:HG22	16:M:214:HOH:O	2.13	0.48
13:M:3:VAL:HG23	13:M:46:SER:HB3	1.95	0.48
2:B:52:ARG:HH22	2:B:63(A):SER:HB3	1.77	0.48
7:U:49:ILE:HD13	7:U:193:ALA:HB1	1.96	0.48
8:H:84:LYS:HG3	8:H:85:GLN:N	2.28	0.48
7:G:136:LEU:O	7:G:150:LYS:HA	2.13	0.48
5:S:4:PHE:CG	5:S:5:ARG:N	2.79	0.48
8:V:21:THR:OG1	15:V:0:SA1:H202	2.14	0.48
1:A:232:ARG:HG3	1:A:232:ARG:HH11	1.79	0.48
13:M:40:ASN:ND2	13:M:40:ASN:N	2.61	0.48
5:S:31:ILE:HD11	5:S:153:PRO:CG	2.43	0.48
6:F:199:LEU:HD12	6:F:240:ILE:HD13	1.95	0.48
6:T:199:LEU:HD12	6:T:240:ILE:HD13	1.96	0.48
11:Y:10(A):ARG:HG2	11:Y:10(A):ARG:NH1	2.28	0.48
11:K:10(A):ARG:HG2	11:K:10(A):ARG:NH1	2.29	0.48
7:G:82:ILE:HG22	7:G:83:PRO:HD3	1.94	0.48
8:V:24:PRO:HG2	8:V:25:ILE:HD13	1.95	0.48
3:C:158:SER:HB2	4:D:59:LEU:HD21	1.96	0.48
4:D:177:LEU:HD13	5:E:58:LEU:HD11	1.95	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:112:GLN:NE2	10:X:126:ALA:H	2.12	0.48
5:S:111:ARG:HH11	5:S:111:ARG:HG2	1.77	0.48
8:H:210:THR:HG21	12:Z:14(C):GLN:HG2	1.95	0.48
7:U:136:LEU:O	7:U:150:LYS:HA	2.12	0.48
10:J:168:MET:HE1	10:X:167:PRO:CB	2.43	0.48
2:P:101:LYS:HZ2	10:X:85:GLN:HE21	1.62	0.48
11:K:110:ILE:N	11:K:110:ILE:HD13	2.28	0.48
4:R:156:THR:HG22	5:S:83:PRO:HD3	1.96	0.48
6:T:67:ILE:HG13	6:T:211:GLU:OE1	2.14	0.48
7:U:82:ILE:HG22	7:U:83:PRO:HD3	1.95	0.48
14:2:3:ILE:HG22	14:2:16:ALA:CB	2.44	0.48
13:M:19:LEU:HD21	13:M:26:LEU:HD22	1.96	0.48
8:H:175:VAL:HG12	8:H:176:CYS:N	2.28	0.48
5:S:54:ASN:ND2	5:S:56:ASP:O	2.44	0.48
6:T:35:THR:HG23	6:T:51:GLU:HB3	1.95	0.47
7:U:172:ILE:HD12	7:U:197:MET:CE	2.44	0.47
4:D:112:LEU:O	4:D:112:LEU:HD13	2.14	0.47
6:F:203:GLU:C	6:F:205:ASN:H	2.17	0.47
6:T:179:LEU:HD11	6:T:192:GLN:HG3	1.95	0.47
12:Z:177:ILE:HD12	12:Z:177:ILE:N	2.28	0.47
13:M:165:ARG:HA	14:2:26:ILE:HG13	1.96	0.47
2:P:97:GLN:HE22	9:W:64:ASN:HD22	1.61	0.47
10:J:179:ASP:HB2	16:J:535:HOH:O	2.13	0.47
4:D:185:THR:OG1	4:D:188:GLU:HG3	2.13	0.47
3:C:168:ASN:CB	3:C:200:VAL:HG11	2.44	0.47
3:Q:190:VAL:O	3:Q:194:VAL:HG23	2.15	0.47
2:P:190:ILE:HG23	2:P:212:PHE:CE2	2.50	0.47
13:M:19:LEU:HB2	13:M:170:SER:HB2	1.96	0.47
4:R:12(F):GLY:O	4:R:12(G):GLU:HB2	2.14	0.47
2:P:4:GLY:HA3	5:S:127:TYR:CE1	2.49	0.47
6:F:40:ILE:HD13	6:F:176:LEU:HD11	1.96	0.47
1:O:232:ARG:HH11	1:O:232:ARG:HG3	1.78	0.47
2:B:160:TRP:CD2	2:B:163:ILE:HD13	2.49	0.47
7:G:118:ASN:O	7:G:122:ILE:HD12	2.14	0.47
3:C:14:ILE:HD12	3:C:14:ILE:N	2.26	0.47
1:A:161:LYS:HD3	1:A:180:TRP:CZ3	2.49	0.47
1:O:161:LYS:HD3	1:O:180:TRP:CZ3	2.49	0.47
7:G:236:ILE:HD12	7:G:237:ALA:N	2.29	0.47
2:B:101:LYS:HG3	9:I:57:GLU:HB3	1.96	0.47
3:C:14:ILE:HD13	3:C:14:ILE:O	2.14	0.47
3:Q:52:ARG:HD2	3:Q:208:LYS:O	2.14	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:78:TYR:CE1	6:T:85:GLY:HA3	2.49	0.47
10:J:2:ILE:O	10:J:3:ILE:HD13	2.14	0.47
11:K:40:PHE:HB3	11:K:73:ARG:NH2	2.29	0.47
12:Z:29:ARG:NH1	12:Z:193:ARG:HB3	2.30	0.47
1:O:86:ARG:NE	7:U:118:ASN:HD21	1.98	0.47
6:F:137:ILE:HA	6:F:149:TYR:O	2.14	0.47
10:J:10(B):LYS:HB2	10:J:10(B):LYS:HZ3	1.78	0.47
5:E:2(C):VAL:HG13	5:E:2(D):ASP:N	2.29	0.47
5:E:73:HIS:HE1	5:E:107:LEU:O	1.96	0.47
4:D:85:ALA:O	4:D:89:ILE:HG12	2.15	0.47
3:Q:168:ASN:CB	3:Q:200:VAL:HG11	2.44	0.47
2:B:163:ILE:CG1	2:B:164:SER:N	2.75	0.47
7:G:72:ARG:HH11	7:G:72:ARG:HB2	1.79	0.47
11:K:4:LEU:CD1	11:K:159:ILE:HD11	2.45	0.47
12:L:177:ILE:HD12	12:L:177:ILE:N	2.29	0.47
12:L:164:GLU:CD	8:V:197:ARG:HG3	2.35	0.47
6:F:72:ARG:HD2	13:M:64:THR:OG1	2.14	0.47
14:N:10(B):LYS:HD3	14:N:10(B):LYS:C	2.35	0.47
3:C:190:VAL:O	3:C:194:VAL:HG23	2.15	0.47
10:J:167:PRO:CB	10:X:168:MET:HE1	2.45	0.47
13:1:14(C):ARG:CG	13:1:14(C):ARG:HH11	2.26	0.47
3:C:14:ILE:CD1	3:C:14:ILE:N	2.78	0.47
12:Z:33:LYS:HD2	12:Z:46:ASN:ND2	2.25	0.47
5:E:52:LYS:CB	5:E:63:TYR:HB3	2.43	0.47
12:Z:90:LYS:HE3	12:Z:93:PHE:O	2.15	0.47
11:Y:37:ILE:HD13	11:Y:37:ILE:N	2.30	0.47
6:F:179:LEU:HD11	6:F:192:GLN:HG3	1.95	0.47
6:F:82:ILE:N	6:F:82:ILE:HD13	2.29	0.47
6:F:127:ASN:HD22	6:F:128:SER:N	2.12	0.47
2:B:87:ILE:O	2:B:91:THR:HG23	2.14	0.47
7:G:12:ILE:HG13	7:G:14:ILE:HG23	1.96	0.47
5:S:2(C):VAL:HG13	5:S:2(D):ASP:N	2.28	0.47
8:H:80:LEU:HD22	8:H:111:PHE:CD2	2.50	0.47
5:E:111:ARG:HG2	5:E:111:ARG:HH11	1.80	0.47
11:Y:109:THR:C	11:Y:110:ILE:HD13	2.35	0.47
2:B:124:THR:HG22	3:C:130:ARG:NH2	2.13	0.47
9:W:101:VAL:O	9:W:110:ILE:HA	2.15	0.47
14:2:175:MET:HE3	14:2:18(B):PHE:CE2	2.50	0.47
4:R:12(D):ALA:HB3	4:R:126:ARG:CD	2.44	0.47
5:S:64:GLN:NE2	5:S:82:ALA:HB2	2.29	0.47
11:K:104:TYR:HB3	11:K:180:GLU:HA	1.97	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:213:ALA:HA	2:P:222:LYS:O	2.14	0.47
8:H:197:ARG:HG3	12:Z:164:GLU:CD	2.34	0.47
5:E:201:LEU:O	5:E:202:ARG:HB2	2.15	0.47
8:V:172:ASN:HB3	8:V:192:LEU:O	2.15	0.47
3:Q:149:TYR:CE1	3:Q:159:SER:HB3	2.50	0.47
4:D:12(D):ALA:HB3	4:D:126:ARG:CD	2.45	0.47
8:H:167:LEU:HD22	12:Z:167:ILE:O	2.15	0.47
2:P:181:LYS:HG3	2:P:184:MET:HG3	1.96	0.47
3:Q:40:VAL:HG23	3:Q:189:CYS:SG	2.55	0.47
3:Q:134:VAL:HG12	3:Q:135:SER:N	2.29	0.47
7:G:207:LYS:HG3	7:G:208:ASN:OD1	2.14	0.47
10:J:17:SER:HB2	10:J:170:PHE:HB2	1.97	0.47
1:O:62:GLU:CD	1:O:62:GLU:H	2.18	0.47
5:E:31:ILE:HD11	5:E:153:PRO:CG	2.43	0.47
3:C:52:ARG:HD2	3:C:208:LYS:O	2.15	0.47
9:I:111:ALA:C	9:I:125:ILE:HD12	2.35	0.47
6:T:203:GLU:C	6:T:205:ASN:H	2.18	0.47
6:T:127:ASN:HD22	6:T:128:SER:N	2.13	0.47
12:L:145:TYR:CD1	12:L:146:LEU:N	2.83	0.47
3:Q:45:CYS:HA	3:Q:141:PHE:HZ	1.80	0.47
2:P:232:ILE:O	2:P:232:ILE:HG12	2.14	0.46
8:H:173:VAL:HB	8:H:192:LEU:HB2	1.96	0.46
13:1:3:VAL:HG23	13:1:46:SER:HB3	1.97	0.46
12:Z:-9:GLN:HE21	13:1:-8:THR:HG21	1.80	0.46
14:2:104:TYR:OH	14:2:180:ALA:HB2	2.15	0.46
7:U:207:LYS:HG3	7:U:208:ASN:OD1	2.14	0.46
4:D:40:ILE:HG12	4:D:193:VAL:CG2	2.44	0.46
10:J:90(A):ILE:HG12	10:J:116:LEU:HA	1.95	0.46
4:R:177:LEU:HD22	5:S:58:LEU:CD1	2.40	0.46
14:N:107:LYS:CG	14:N:108:GLY:H	2.20	0.46
13:1:42:VAL:CG2	13:1:178:ILE:HD11	2.44	0.46
10:X:100:LEU:HD21	10:X:112:GLN:HG3	1.97	0.46
7:U:72:ARG:HB2	7:U:72:ARG:HH11	1.79	0.46
13:1:-5:PRO:HD3	13:1:96:TRP:CE2	2.51	0.46
7:U:17(D):SER:O	7:U:17(E):LYS:HB2	2.13	0.46
11:Y:200:LYS:HE3	11:Y:206:PHE:O	2.15	0.46
11:Y:86:LEU:C	11:Y:86:LEU:HD13	2.35	0.46
13:1:40:ASN:ND2	13:1:40:ASN:N	2.63	0.46
4:R:112:LEU:O	4:R:112:LEU:HD13	2.14	0.46
2:B:181:LYS:HG3	2:B:184:MET:HG3	1.97	0.46
6:T:69:VAL:HG12	16:T:811:HOH:O	2.14	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:185:ARG:NH1	16:L:1161:HOH:O	2.36	0.46
5:S:41:ARG:NH1	5:S:42:SER:O	2.48	0.46
5:S:48:LEU:HG	5:S:139:ILE:HD13	1.96	0.46
1:A:32:LYS:HE2	1:A:32:LYS:HA	1.98	0.46
5:E:70:CYS:SG	5:E:92:LEU:HD23	2.55	0.46
7:G:172:ILE:HD12	7:G:197:MET:CE	2.45	0.46
5:S:160:LEU:CD2	6:T:59:LEU:HD12	2.46	0.46
3:C:134:VAL:HG12	3:C:135:SER:N	2.30	0.46
1:A:62:GLU:H	1:A:62:GLU:CD	2.19	0.46
10:X:166:MET:HA	10:X:167:PRO:HD3	1.79	0.46
14:N:159:LEU:O	14:N:163:ILE:HG13	2.15	0.46
6:T:169:ARG:O	6:T:173:LYS:HG3	2.16	0.46
6:F:12:ASN:O	6:F:12:ASN:OD1	2.33	0.46
3:Q:175:PHE:O	3:Q:179:ASN:HB2	2.15	0.46
1:A:233:LEU:O	1:A:236:LEU:HB2	2.16	0.46
11:K:174:ASN:HD21	11:K:189:ASN:HD22	1.63	0.46
12:Z:145:TYR:CD1	12:Z:146:LEU:N	2.83	0.46
2:B:231:ASP:O	2:B:235:LYS:HG2	2.15	0.46
13:M:205:GLY:HA3	13:M:209:GLN:HB3	1.97	0.46
4:D:12(F):GLY:O	4:D:12(G):GLU:HB2	2.14	0.46
2:B:224:PHE:N	2:B:224:PHE:CD2	2.84	0.46
9:W:29:ASN:ND2	9:W:30:LYS:HG3	2.30	0.46
11:K:4:LEU:HD12	11:K:159:ILE:CD1	2.46	0.46
4:D:45:GLY:HA2	4:D:146:TYR:CE1	2.51	0.46
13:1:1:THR:OG1	13:1:2:SER:N	2.48	0.46
10:X:17:SER:HB2	10:X:170:PHE:HB2	1.97	0.46
8:V:22:GLN:HG3	8:V:27:ALA:HB2	1.98	0.46
13:M:130:GLY:O	13:M:134:ALA:HB3	2.15	0.46
8:V:72:ARG:HH11	8:V:72:ARG:HG3	1.80	0.46
9:I:101:VAL:O	9:I:110:ILE:HA	2.16	0.46
3:C:106:PRO:HG2	3:C:143:PRO:HG2	1.95	0.46
8:H:128:GLY:O	8:H:131:SER:CB	2.62	0.46
2:P:101:LYS:NZ	10:X:85:GLN:HE22	2.12	0.46
8:V:3:ILE:HG22	8:V:16:ALA:CB	2.46	0.46
10:J:193:GLN:OXT	10:J:193:GLN:HG2	2.16	0.46
7:U:170:GLN:NE2	7:U:174:THR:HG23	2.31	0.46
13:M:46:SER:OG	13:M:98:ALA:HB3	2.16	0.46
7:G:82:ILE:CG2	7:G:83:PRO:HD3	2.45	0.46
5:S:136:LEU:HD12	5:S:151:PHE:CD2	2.51	0.46
13:1:186:PHE:CE1	13:1:188:LYS:HG3	2.51	0.46
3:C:13:SER:O	4:D:130:ARG:HD3	2.16	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:103:TYR:O	6:F:104:LYS:HB3	2.16	0.46
11:Y:31:VAL:HG11	15:Y:0:SA1:H13	1.97	0.46
7:G:192:PHE:CD1	7:G:192:PHE:C	2.88	0.46
13:1:14(C):ARG:NH1	13:1:14(C):ARG:HG3	2.28	0.46
1:O:233:LEU:O	1:O:236:LEU:HB2	2.16	0.46
2:P:231:ASP:O	2:P:235:LYS:HG2	2.16	0.46
7:G:39:ALA:HB2	7:G:48:VAL:HG12	1.98	0.46
12:Z:-7:ASN:HD22	12:Z:-7:ASN:C	2.19	0.46
5:S:75:GLY:HA3	5:S:221:PHE:CZ	2.51	0.46
10:X:113:ILE:HG12	10:X:119:LYS:HG3	1.97	0.46
10:J:12:VAL:CG2	10:J:108:PRO:HB2	2.46	0.46
11:Y:4:LEU:CD1	11:Y:159:ILE:HD11	2.45	0.46
7:U:82:ILE:N	7:U:83:PRO:HD2	2.31	0.46
3:C:66:LYS:HE2	3:C:78:PHE:CZ	2.51	0.46
6:T:172:ALA:O	6:T:176:LEU:CD2	2.64	0.46
3:C:45:CYS:HA	3:C:141:PHE:HZ	1.81	0.46
8:V:147:THR:OG1	8:V:150:GLU:HG3	2.15	0.46
1:A:51:GLU:OE1	1:A:202:VAL:HG22	2.16	0.46
2:P:121:GLN:C	2:P:121:GLN:NE2	2.70	0.46
11:Y:99:THR:CG2	11:Y:113:VAL:HB	2.46	0.46
13:M:42:VAL:CG2	13:M:178:ILE:HD11	2.45	0.46
5:S:160:LEU:HD23	6:T:59:LEU:HA	1.98	0.46
3:Q:66:LYS:HE2	3:Q:78:PHE:CZ	2.50	0.46
2:B:53:LYS:HG2	2:B:54:VAL:HG23	1.98	0.46
7:G:170:GLN:NE2	7:G:174:THR:HG23	2.31	0.45
11:Y:4:LEU:C	11:Y:4:LEU:HD22	2.35	0.45
10:J:144:PRO:CG	11:Y:207:ASN:ND2	2.79	0.45
3:C:40:VAL:HG23	3:C:189:CYS:SG	2.56	0.45
4:D:90:GLU:OE1	11:K:69:ARG:HD2	2.16	0.45
11:Y:49:ALA:O	11:Y:53:GLN:HB2	2.17	0.45
16:F:306:HOH:O	7:G:86:ARG:HD2	2.15	0.45
7:U:39:ALA:HB2	7:U:48:VAL:HG12	1.97	0.45
10:J:168:MET:HE3	10:X:168:MET:HG2	1.99	0.45
4:R:161:ASN:N	5:S:58:LEU:O	2.46	0.45
12:L:-7:ASN:C	12:L:-7:ASN:HD22	2.19	0.45
14:N:14:LEU:HD11	14:N:102:ALA:CB	2.47	0.45
8:V:3:ILE:HG22	8:V:16:ALA:HB2	1.98	0.45
1:O:97:HIS:CD2	8:V:61:SER:OG	2.68	0.45
6:T:82:ILE:N	6:T:82:ILE:HD13	2.31	0.45
6:T:192:GLN:O	6:T:196:ILE:HG13	2.17	0.45
8:H:63:ILE:HG23	8:H:74:PRO:HB3	1.98	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:63:ILE:HG23	8:V:74:PRO:HB3	1.98	0.45
11:K:195:LEU:O	11:K:199:VAL:HG23	2.16	0.45
7:U:192:PHE:CD1	7:U:192:PHE:C	2.88	0.45
7:G:224:LEU:HB3	7:G:228:ASN:HB2	1.99	0.45
3:C:158:SER:CB	4:D:59:LEU:HD21	2.46	0.45
5:E:41:ARG:NH1	5:E:42:SER:O	2.49	0.45
5:E:48:LEU:HG	5:E:139:ILE:HD13	1.97	0.45
14:2:144:GLU:HG2	16:2:1115:HOH:O	2.16	0.45
9:I:149:GLU:H	9:I:149:GLU:CD	2.20	0.45
8:H:172:ASN:HB3	8:H:192:LEU:O	2.16	0.45
12:Z:90:LYS:HD3	12:Z:95:TYR:CZ	2.51	0.45
10:J:38:SER:HA	16:J:301:HOH:O	2.16	0.45
14:2:146:MET:CE	14:2:150:GLU:HB3	2.46	0.45
4:R:40:ILE:HG12	4:R:193:VAL:CG2	2.45	0.45
3:C:185:THR:HG22	3:C:186:VAL:N	2.32	0.45
2:B:141:TYR:CD1	2:B:21(E):VAL:HG21	2.51	0.45
8:H:22:GLN:HG3	8:H:27:ALA:HB2	1.99	0.45
7:U:12:ILE:HG13	7:U:14:ILE:HG23	1.97	0.45
3:Q:136:THR:O	3:Q:150:GLN:HA	2.17	0.45
2:P:141:TYR:CD1	2:P:21(E):VAL:HG21	2.52	0.45
8:H:4:VAL:HG22	8:H:159:ILE:HD11	1.98	0.45
7:G:8:TYR:C	7:G:10:ARG:N	2.70	0.45
7:G:78:VAL:HG11	7:G:85:ALA:CB	2.47	0.45
8:H:50:ALA:HB2	9:I:118:CYS:HB2	1.98	0.45
7:U:152:ASP:HB2	7:U:153:PRO:CD	2.46	0.45
2:P:224:PHE:N	2:P:224:PHE:CD2	2.84	0.45
7:U:217:LYS:HA	7:U:217:LYS:CE	2.42	0.45
10:X:193:GLN:HG2	10:X:193:GLN:OXT	2.17	0.45
10:X:12:VAL:CG2	10:X:108:PRO:HB2	2.46	0.45
12:L:140:ASN:O	12:L:144:PHE:HA	2.17	0.45
5:E:160:LEU:HD23	6:F:59:LEU:HA	1.98	0.45
16:V:1181:HOH:O	9:W:150:ASP:HA	2.16	0.45
11:Y:4:LEU:HD12	11:Y:159:ILE:CD1	2.47	0.45
10:J:100:LEU:HD21	10:J:112:GLN:HG3	1.99	0.45
2:B:97:GLN:NE2	9:I:64:ASN:HD22	2.15	0.45
7:U:82:ILE:CG2	7:U:83:PRO:HD3	2.46	0.45
13:M:165:ARG:C	14:2:26:ILE:HG13	2.37	0.45
5:E:139:ILE:HG22	5:E:148:LEU:HD13	1.99	0.45
6:T:158:TRP:CZ3	7:U:64:VAL:HA	2.52	0.45
13:M:186:PHE:CE1	13:M:188:LYS:HG3	2.52	0.45
3:Q:112:LEU:HD13	3:Q:112:LEU:O	2.17	0.45

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:97:ASN:HD21	12:Z:61:ASN:ND2	2.15	0.45
13:M:179:ASP:HB3	13:M:18(A):THR:OG1	2.16	0.45
5:E:77:SER:OG	5:E:137:LEU:HB2	2.16	0.45
1:O:221:PHE:C	1:O:221:PHE:CD2	2.90	0.45
4:R:122:ARG:HH11	4:R:122:ARG:HG2	1.81	0.45
2:B:21:LEU:O	2:B:25:GLU:HG2	2.17	0.45
6:F:35:THR:CG2	6:F:51:GLU:O	2.60	0.45
4:R:177:LEU:CD2	5:S:58:LEU:HD13	2.42	0.45
1:A:60:MET:HE1	16:G:600:HOH:O	2.16	0.45
8:H:72:ARG:HH11	8:H:72:ARG:HG3	1.81	0.45
2:P:63:THR:HG22	2:P:63:THR:O	2.17	0.45
14:N:161:GLN:HE22	14:N:165:TRP:HE1	1.63	0.44
14:2:112:THR:CG2	14:2:120:HIS:HB2	2.47	0.44
6:F:192:GLN:O	6:F:196:ILE:HG13	2.16	0.44
2:B:224:PHE:HD2	2:B:224:PHE:N	2.14	0.44
2:P:224:PHE:N	2:P:224:PHE:HD2	2.15	0.44
4:R:15:PHE:HB2	5:S:23:GLN:OE1	2.17	0.44
8:H:132:LEU:HB2	16:H:347:HOH:O	2.16	0.44
6:T:11:SER:HB3	6:T:14:VAL:HG23	1.99	0.44
11:Y:40:PHE:HB3	11:Y:73:ARG:NH2	2.32	0.44
9:W:126:VAL:HG11	9:W:134:LEU:HB3	2.00	0.44
8:H:2:THR:OG1	8:H:130:GLY:HA3	2.17	0.44
5:E:40:LEU:HD23	5:E:40:LEU:N	2.32	0.44
2:B:38:ILE:HD13	2:B:164:SER:CB	2.45	0.44
5:E:194:VAL:CG1	5:E:207:LEU:HD11	2.47	0.44
12:L:166:HIS:CD2	12:L:168:GLN:H	2.28	0.44
8:H:3:ILE:HG22	8:H:16:ALA:CB	2.48	0.44
10:J:112:GLN:NE2	10:J:126:ALA:H	2.15	0.44
7:U:139:VAL:HA	7:U:147:SER:O	2.18	0.44
4:D:170:GLU:N	4:D:170:GLU:OE1	2.49	0.44
2:B:63:THR:HG22	2:B:63:THR:O	2.17	0.44
5:S:40:LEU:HD23	5:S:40:LEU:N	2.32	0.44
3:Q:185:THR:HG22	3:Q:186:VAL:N	2.32	0.44
14:2:106:ASN:O	14:2:107:LYS:HB3	2.17	0.44
14:N:146:MET:CE	14:N:150:GLU:HB3	2.47	0.44
5:E:97:ASN:HD22	5:E:97:ASN:HA	1.59	0.44
5:S:172:ALA:HB2	5:S:196:ALA:O	2.16	0.44
14:N:104:TYR:OH	14:N:180:ALA:HB2	2.17	0.44
6:T:72:ARG:HD2	13:1:64:THR:OG1	2.17	0.44
1:O:124:THR:HG22	2:P:130:ARG:NH2	2.20	0.44
10:J:168:MET:CE	10:X:168:MET:CE	2.96	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:4:LEU:C	11:K:4:LEU:HD22	2.38	0.44
7:U:224:LEU:HB3	7:U:228:ASN:HB2	1.99	0.44
7:G:82:ILE:N	7:G:83:PRO:HD2	2.32	0.44
13:M:-5:PRO:HD3	13:M:96:TRP:CE2	2.53	0.44
3:C:112:LEU:HD13	3:C:112:LEU:O	2.17	0.44
12:Z:140:ASN:O	12:Z:144:PHE:HA	2.16	0.44
1:A:117:ALA:HB1	1:A:155:GLY:O	2.17	0.44
2:P:39:GLY:O	2:P:162:ALA:HA	2.17	0.44
3:Q:169:SER:HA	3:Q:172:VAL:CG1	2.48	0.44
14:2:51:ASP:O	14:2:55:ILE:HG13	2.17	0.44
12:L:-2:ASN:HA	12:L:21:ILE:O	2.18	0.44
2:B:11:ARG:HD2	3:C:10:ARG:NH1	2.30	0.44
7:U:78:VAL:HG11	7:U:85:ALA:HB2	1.99	0.44
6:F:11:SER:HB3	6:F:14:VAL:HG23	1.98	0.44
12:L:98:HIS:HD2	16:L:198:HOH:O	2.00	0.44
2:B:39:GLY:O	2:B:162:ALA:HA	2.18	0.44
11:Y:6:PHE:HA	11:Y:123:ASP:O	2.17	0.44
3:Q:106:PRO:HG2	3:Q:143:PRO:HG2	1.96	0.44
13:1:14(G):ILE:HB	13:1:144:PRO:CD	2.47	0.44
14:N:6:VAL:CG2	14:N:155:ILE:HD11	2.47	0.44
7:U:172:ILE:HD11	7:U:201:LEU:HD21	2.00	0.44
9:W:178:ILE:HG23	9:W:184:VAL:CG2	2.48	0.44
6:F:169:ARG:O	6:F:173:LYS:HG3	2.16	0.44
14:2:3:ILE:HG22	14:2:16:ALA:HB2	1.98	0.44
9:I:46:THR:HA	16:I:199:HOH:O	2.18	0.44
3:C:136:THR:O	3:C:150:GLN:HA	2.17	0.44
7:G:177:GLU:O	7:G:17(B):LYS:HG3	2.18	0.44
11:Y:195:LEU:O	11:Y:199:VAL:HG23	2.18	0.44
9:W:137:MET:HE3	9:W:141:LEU:CD1	2.42	0.44
14:2:14:LEU:HD11	14:2:102:ALA:CB	2.48	0.44
14:2:6:VAL:CG2	14:2:155:ILE:HD11	2.47	0.44
8:V:2:THR:OG1	8:V:130:GLY:HA3	2.16	0.44
2:P:11:ARG:O	2:P:14:ILE:HD13	2.18	0.44
3:Q:152:GLU:HB2	3:Q:153:PRO:HD2	2.00	0.44
6:T:103:TYR:O	6:T:104:LYS:HB3	2.17	0.44
7:U:186:TRP:O	7:U:190:VAL:HG23	2.18	0.44
12:L:1:GLY:HA3	12:L:33:LYS:HZ2	1.81	0.44
13:M:14(G):ILE:HB	13:M:144:PRO:CD	2.47	0.44
3:Q:55:THR:C	3:Q:56:LEU:HD22	2.38	0.44
5:E:64:GLN:NE2	5:E:82:ALA:HB2	2.33	0.44
9:W:16:CYS:SG	9:W:34:ILE:HG12	2.57	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:185:LYS:HD2	2:P:187:ASP:H	1.82	0.44
1:O:47:VAL:HG23	1:O:212:LEU:HD21	2.00	0.44
14:N:2:SER:OG	14:N:130:GLY:HA3	2.18	0.44
7:G:152:ASP:HB2	7:G:153:PRO:CD	2.47	0.44
13:1:201:LYS:HA	16:1:731:HOH:O	2.17	0.44
11:K:31:VAL:HG11	15:K:0:SA1:H13	1.99	0.44
9:I:126:VAL:HG11	9:I:134:LEU:HB3	2.00	0.44
4:R:45:GLY:HA2	4:R:146:TYR:CE1	2.53	0.44
1:A:221:PHE:C	1:A:221:PHE:CD2	2.91	0.44
8:H:25:ILE:N	8:H:25:ILE:CD1	2.81	0.43
5:E:97:ASN:HD21	12:L:61:ASN:ND2	2.14	0.43
7:U:236:ILE:HD12	7:U:236:ILE:C	2.38	0.43
6:T:127:ASN:ND2	6:T:127:ASN:C	2.72	0.43
5:S:2(C):VAL:CG1	5:S:2(D):ASP:N	2.81	0.43
13:M:12:VAL:HG21	13:M:102:ALA:HB1	2.00	0.43
3:Q:163:GLN:HA	3:Q:163:GLN:HE21	1.83	0.43
5:E:194:VAL:HG13	5:E:207:LEU:CD1	2.48	0.43
14:N:105:ASP:HB3	14:N:106:ASN:HB2	2.00	0.43
6:T:240:ILE:HA	6:T:240:ILE:HD12	1.86	0.43
2:B:4:GLY:HA3	5:E:127:TYR:CE1	2.52	0.43
6:T:109:ILE:HD13	6:T:109:ILE:H	1.83	0.43
10:J:90:SER:HG	10:J:95:TYR:H	1.62	0.43
6:F:114:ASP:O	6:F:118:GLN:HG2	2.17	0.43
14:N:3:ILE:HG22	14:N:16:ALA:CB	2.48	0.43
3:C:39:GLY:HA2	3:C:47:VAL:O	2.18	0.43
5:S:194:VAL:CG1	5:S:207:LEU:HD11	2.48	0.43
14:N:106:ASN:O	14:N:107:LYS:HB3	2.18	0.43
7:G:172:ILE:HD11	7:G:201:LEU:HD21	2.00	0.43
5:S:148:LEU:HD23	5:S:162:GLY:HA2	2.00	0.43
13:1:3:VAL:O	13:1:126:ALA:HA	2.18	0.43
7:G:228:ASN:HB3	16:G:255:HOH:O	2.18	0.43
2:P:53:LYS:HG2	2:P:54:VAL:HG23	2.00	0.43
4:R:75:GLY:HA3	4:R:221:PHE:CD2	2.53	0.43
1:O:38:LEU:HD12	1:O:38:LEU:C	2.39	0.43
5:S:194:VAL:HG13	5:S:207:LEU:CD1	2.48	0.43
2:P:160:TRP:CD2	2:P:163:ILE:HD13	2.52	0.43
14:N:9:LYS:O	14:N:107:LYS:HD3	2.18	0.43
8:H:24:PRO:HG2	8:H:25:ILE:CD1	2.48	0.43
6:F:127:ASN:ND2	6:F:127:ASN:C	2.71	0.43
5:E:4:PHE:CE1	5:E:17:PRO:HD2	2.54	0.43
7:G:158:VAL:HG22	7:G:159:GLY:N	2.33	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:186:TRP:O	7:G:190:VAL:HG23	2.18	0.43
4:D:75:GLY:HA3	4:D:221:PHE:CD2	2.53	0.43
1:O:26:TYR:CD1	7:U:17:PRO:HA	2.53	0.43
2:P:44:ASP:N	2:P:44:ASP:OD2	2.51	0.43
6:T:43:ASN:HD22	6:T:43:ASN:N	2.16	0.43
9:W:149:GLU:H	9:W:149:GLU:CD	2.22	0.43
10:J:166:MET:HA	10:J:167:PRO:HD3	1.81	0.43
3:Q:14:ILE:O	3:Q:14:ILE:HD13	2.19	0.43
5:E:180:LEU:HA	5:E:18(C):PHE:CE2	2.54	0.43
6:T:109:ILE:HD13	6:T:109:ILE:N	2.33	0.43
5:E:2(C):VAL:CG1	5:E:2(D):ASP:N	2.82	0.43
12:Z:-8:PHE:CB	13:1:-8:THR:HG23	2.49	0.43
2:B:142:ASP:OD2	2:B:147:GLN:NE2	2.47	0.43
4:D:117:CYS:SG	4:D:157:PHE:HB3	2.59	0.43
4:D:12:VAL:CG2	4:D:12(A):GLY:HA2	2.48	0.43
13:M:184:LEU:C	13:M:184:LEU:HD23	2.38	0.43
7:U:203:THR:HG22	7:U:204:GLU:O	2.19	0.43
14:2:105:ASP:HB3	14:2:106:ASN:HB2	2.00	0.43
3:Q:215:VAL:O	3:Q:215:VAL:HG13	2.19	0.43
8:H:24:PRO:HA	12:Z:167:ILE:HD13	2.00	0.43
10:J:2:ILE:N	10:J:2:ILE:HD13	2.33	0.43
11:Y:20:ALA:HB2	11:Y:31:VAL:HG21	2.00	0.43
1:O:195:LEU:HD23	1:O:236:LEU:HD21	2.01	0.43
9:I:55:LEU:HD21	9:I:95:TYR:CD1	2.54	0.43
11:K:12:ILE:HB	11:K:178:VAL:HB	2.01	0.43
6:T:90:ASN:O	6:T:94:GLU:HG3	2.19	0.43
3:C:147:LYS:HE2	16:C:250:HOH:O	2.18	0.43
11:K:6:PHE:HA	11:K:123:ASP:O	2.19	0.43
10:X:90:SER:HG	10:X:95:TYR:H	1.64	0.43
4:R:194:LEU:HA	4:R:194:LEU:HD12	1.91	0.43
12:L:-7:ASN:HD22	12:L:-6:PRO:N	2.17	0.43
5:S:31:ILE:HD11	5:S:153:PRO:CD	2.48	0.43
12:L:90:LYS:HE3	12:L:93:PHE:O	2.17	0.43
3:C:58:LEU:HA	3:C:58:LEU:HD12	1.88	0.43
7:U:69:CYS:O	7:U:93:LYS:HE2	2.19	0.43
12:L:17:ASP:HA	12:L:172:GLY:O	2.19	0.43
2:B:225:LYS:O	2:B:226:PRO:C	2.57	0.43
11:K:192:VAL:HG11	9:W:194:ASP:HB3	1.99	0.43
8:H:6:VAL:O	8:H:13:VAL:HG12	2.18	0.43
3:C:163:GLN:HA	3:C:163:GLN:HE21	1.84	0.43
14:2:168:SER:HB3	15:2:0:SA1:H12A	2.00	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:168:MET:CE	10:X:168:MET:HE3	2.48	0.43
1:O:51:GLU:OE1	1:O:202:VAL:HG22	2.18	0.43
9:I:194:ASP:HB3	11:Y:192:VAL:HG11	2.00	0.43
5:S:11:ASP:OD1	5:S:13:VAL:HG12	2.19	0.43
14:N:133:PHE:HA	14:2:132:THR:O	2.18	0.43
5:E:136:LEU:HB2	5:E:151:PHE:HB3	2.01	0.43
13:1:184:LEU:C	13:1:184:LEU:HD23	2.39	0.43
9:W:192:ARG:HD2	16:W:1258:HOH:O	2.18	0.43
6:F:50:VAL:HG22	6:F:51:GLU:N	2.34	0.43
5:S:180:LEU:HA	5:S:18(C):PHE:CE2	2.54	0.43
12:Z:-2:ASN:HA	12:Z:21:ILE:O	2.18	0.43
13:1:12:VAL:HG21	13:1:102:ALA:HB1	2.01	0.43
13:1:37:VAL:HG11	13:1:79:ILE:HD12	2.01	0.43
6:T:114:ASP:O	6:T:118:GLN:HG2	2.18	0.43
6:T:79:SER:OG	6:T:165:THR:HG23	2.19	0.43
1:A:186:LEU:O	1:A:190:ILE:HG13	2.18	0.43
3:C:152:GLU:HB2	3:C:153:PRO:HD2	2.01	0.43
14:2:134:ILE:HG21	14:2:158:SER:O	2.19	0.43
4:R:170:GLU:OE1	4:R:170:GLU:N	2.51	0.43
3:Q:168:ASN:O	3:Q:172:VAL:HG12	2.19	0.43
1:A:177:GLU:CG	2:B:58:LEU:HD22	2.46	0.43
7:G:151:THR:HG22	7:G:157:TYR:HB3	2.00	0.43
12:L:153:LYS:HG2	8:V:201:GLN:HG3	2.01	0.43
3:Q:79:SER:OG	3:Q:165:ILE:HG13	2.19	0.43
11:K:86:LEU:HD13	11:K:86:LEU:C	2.40	0.43
9:W:111:ALA:C	9:W:125:ILE:HD12	2.40	0.42
1:A:86:ARG:HD3	16:A:401:HOH:O	2.18	0.42
5:E:75:GLY:HA3	5:E:221:PHE:CZ	2.53	0.42
7:G:34(A):ASN:HA	7:G:167:PRO:HG2	2.00	0.42
8:H:3:ILE:HG22	8:H:16:ALA:HB2	2.00	0.42
11:K:207:ASN:ND2	10:X:144:PRO:HG3	2.34	0.42
8:V:207:PRO:HG2	8:V:210:THR:OG1	2.19	0.42
5:E:136:LEU:HD12	5:E:151:PHE:CD2	2.54	0.42
7:G:139:VAL:HA	7:G:147:SER:O	2.19	0.42
11:K:49:ALA:O	11:K:53:GLN:HB2	2.18	0.42
12:Z:17:ASP:HA	12:Z:172:GLY:O	2.19	0.42
4:R:72:ARG:HG3	16:R:1302:HOH:O	2.18	0.42
11:K:38:ASN:OD1	11:K:38:ASN:C	2.57	0.42
2:B:185:LYS:HD2	2:B:187:ASP:H	1.83	0.42
1:O:179:ARG:HB3	1:O:192:ILE:HD13	2.01	0.42
10:X:142:TYR:O	10:X:143:ARG:HD3	2.19	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1:148:VAL:HG23	16:1:182:HOH:O	2.19	0.42
3:C:55:THR:C	3:C:56:LEU:HD22	2.40	0.42
11:Y:37:ILE:HG23	11:Y:60:GLY:HA2	2.02	0.42
1:A:47:VAL:HG23	1:A:212:LEU:HD21	2.01	0.42
9:I:107:LYS:HA	9:I:108:PRO:HD3	1.84	0.42
4:R:12:VAL:CG2	4:R:12(A):GLY:HA2	2.49	0.42
14:2:15:GLY:HA2	14:2:174:ARG:O	2.20	0.42
11:Y:38:ASN:OD1	11:Y:38:ASN:C	2.57	0.42
1:A:38:LEU:HD12	1:A:38:LEU:C	2.39	0.42
2:B:121:GLN:C	2:B:121:GLN:NE2	2.73	0.42
12:Z:-7:ASN:ND2	12:Z:-7:ASN:C	2.72	0.42
7:U:8:TYR:C	7:U:10:ARG:N	2.71	0.42
2:P:97:GLN:NE2	9:W:64:ASN:HD22	2.16	0.42
2:B:17:PRO:HA	3:C:26:TYR:CD1	2.55	0.42
5:S:74:MET:HE2	5:S:109:VAL:HG22	2.02	0.42
9:I:16:CYS:SG	9:I:34:ILE:HG12	2.59	0.42
6:T:107:ILE:HA	6:T:108:PRO:HD3	1.80	0.42
1:O:57:PRO:HG2	7:U:177:GLU:HG2	2.02	0.42
3:C:163:GLN:CA	3:C:163:GLN:HE21	2.32	0.42
6:F:240:ILE:HD12	6:F:240:ILE:HA	1.88	0.42
8:V:4:VAL:HG22	8:V:159:ILE:HD11	2.01	0.42
11:Y:159:ILE:HA	11:Y:159:ILE:HD13	1.91	0.42
2:B:234:VAL:HA	2:B:239:THR:HA	2.01	0.42
13:1:186:PHE:HE1	13:1:188:LYS:HG3	1.84	0.42
11:Y:5:ALA:HA	11:Y:13:ILE:O	2.20	0.42
13:1:-2:THR:HA	13:1:47:GLY:O	2.19	0.42
6:F:143:LYS:HB2	16:F:469:HOH:O	2.18	0.42
8:H:105:ASP:HB2	8:H:10(A):PRO:CD	2.49	0.42
2:P:51:GLU:OE2	2:P:209:ARG:NH2	2.51	0.42
8:V:128:GLY:O	8:V:131:SER:CB	2.63	0.42
3:C:227:GLU:CD	3:C:227:GLU:H	2.23	0.42
12:L:167:ILE:O	8:V:167:LEU:HD22	2.19	0.42
3:Q:17:PRO:HA	4:R:26:TYR:CD1	2.54	0.42
6:F:107:ILE:HA	6:F:108:PRO:HD3	1.78	0.42
13:1:179:ASP:HB3	13:1:18(A):THR:OG1	2.19	0.42
14:N:168:SER:HB3	15:N:0:SA1:H12A	2.02	0.42
8:H:3:ILE:O	8:H:126:SER:HA	2.20	0.42
12:Z:99:THR:CG2	16:Z:231:HOH:O	2.68	0.42
11:Y:37:ILE:CD1	11:Y:37:ILE:N	2.83	0.42
14:2:159:LEU:O	14:2:163:ILE:HG13	2.20	0.42
5:E:45:HIS:HB2	5:E:189:LEU:HD12	2.02	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:103:GLY:HA2	8:H:178:MET:SD	2.59	0.42
6:T:202:HIS:CG	6:T:202:HIS:O	2.73	0.42
14:N:51:ASP:O	14:N:55:ILE:HG13	2.19	0.42
14:N:26:ILE:HB	13:1:165:ARG:HA	2.00	0.42
5:S:107:LEU:HD11	5:S:111:ARG:HG2	2.02	0.42
8:H:207:PRO:HG2	8:H:210:THR:OG1	2.20	0.42
11:Y:12:ILE:HB	11:Y:178:VAL:HB	2.01	0.42
13:M:14(G):ILE:N	13:M:144:PRO:HD2	2.35	0.42
10:J:142:TYR:O	10:J:143:ARG:HD3	2.19	0.42
2:P:136:PHE:O	2:P:150:THR:HA	2.20	0.42
8:H:101:VAL:CG1	8:H:113:ILE:HD11	2.50	0.42
14:N:112:THR:CG2	14:N:120:HIS:HB2	2.48	0.42
8:H:68:LEU:HA	8:H:68:LEU:HD12	1.92	0.42
7:U:184:ASN:C	7:U:184:ASN:HD22	2.23	0.42
3:Q:14:ILE:N	3:Q:14:ILE:CD1	2.80	0.42
8:H:101:VAL:HG12	8:H:113:ILE:HD11	2.02	0.42
7:U:140:SER:HA	7:U:215:ALA:HB1	2.02	0.42
5:E:74:MET:HE2	5:E:109:VAL:HG22	2.01	0.42
11:Y:174:ASN:HD21	11:Y:189:ASN:HD22	1.67	0.42
3:Q:123:TYR:CD1	3:Q:132:PHE:HE1	2.38	0.42
3:C:29:GLU:OE2	3:C:32:LYS:HE2	2.20	0.42
1:A:26:TYR:N	1:A:26:TYR:CD1	2.87	0.42
3:C:169:SER:HA	3:C:172:VAL:CG1	2.49	0.42
9:W:7:THR:CG2	9:W:110:ILE:HD13	2.36	0.42
6:T:35:THR:CG2	6:T:36:THR:N	2.83	0.42
6:T:35:THR:CG2	6:T:51:GLU:O	2.61	0.42
2:B:141:TYR:C	2:B:141:TYR:CD1	2.93	0.42
14:2:176:VAL:HG12	14:2:178:LEU:CD1	2.48	0.42
8:V:101:VAL:HG12	8:V:113:ILE:HD11	2.02	0.42
8:H:197:ARG:NH2	9:I:139:GLU:HG3	2.35	0.42
4:D:150:HIS:O	4:D:157:PHE:HA	2.20	0.42
3:Q:39:GLY:HA2	3:Q:47:VAL:O	2.19	0.42
4:D:100:ASN:HB3	16:D:247:HOH:O	2.19	0.42
4:R:117:CYS:SG	4:R:157:PHE:HB3	2.60	0.42
14:N:26:ILE:HG13	13:1:165:ARG:HA	2.01	0.41
2:B:159:GLY:HA3	3:C:62(A):ILE:HG13	2.02	0.41
8:V:34:LEU:HB2	16:V:578:HOH:O	2.20	0.41
14:2:161:GLN:NE2	14:2:165:TRP:HE1	2.18	0.41
1:A:179:ARG:HB3	1:A:192:ILE:HD13	2.03	0.41
12:L:-7:ASN:ND2	12:L:-7:ASN:C	2.73	0.41
5:S:45:HIS:HB2	5:S:189:LEU:HD12	2.01	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:109:THR:HA	16:Y:595:HOH:O	2.19	0.41
8:V:112:SER:HB3	8:V:125:LEU:HD13	2.02	0.41
13:1:130:GLY:O	13:1:134:ALA:HB3	2.20	0.41
11:Y:32:LYS:N	11:Y:32:LYS:HD2	2.35	0.41
6:T:20(B):GLU:HG3	6:T:20(C):LYS:N	2.35	0.41
8:V:101:VAL:CG1	8:V:113:ILE:HD11	2.50	0.41
5:S:150:GLU:O	5:S:157:VAL:HA	2.21	0.41
1:A:77:VAL:HG12	1:A:137:LEU:HB2	2.02	0.41
1:O:117:ALA:HB1	1:O:155:GLY:O	2.20	0.41
4:D:237:LEU:HD22	4:D:241:GLU:HG3	2.02	0.41
5:S:76:LEU:HD23	5:S:76:LEU:C	2.40	0.41
10:X:129:TYR:O	10:X:132:PHE:HB2	2.21	0.41
11:K:32:LYS:N	11:K:32:LYS:HD2	2.35	0.41
11:Y:114:ASP:C	11:Y:114:ASP:OD1	2.59	0.41
4:R:86:ARG:HD3	4:R:86:ARG:HA	1.81	0.41
3:Q:163:GLN:HE21	3:Q:163:GLN:CA	2.32	0.41
14:N:48:SER:HB3	14:N:51:ASP:HB2	2.03	0.41
2:P:141:TYR:C	2:P:141:TYR:CD1	2.94	0.41
14:N:176:VAL:HG12	14:N:178:LEU:CD1	2.48	0.41
5:S:136:LEU:HB2	5:S:151:PHE:HB3	2.01	0.41
10:X:20:VAL:HG11	11:Y:120:LEU:HD11	2.01	0.41
3:C:149:TYR:CE1	3:C:159:SER:HB3	2.55	0.41
8:V:103:GLY:HA2	8:V:178:MET:SD	2.60	0.41
2:P:21(A):LYS:O	2:P:21(B):GLY:C	2.59	0.41
10:X:59:ILE:HD13	10:X:59:ILE:HA	1.93	0.41
2:P:184:MET:HE2	2:P:189:ALA:N	2.36	0.41
7:U:151:THR:HG22	7:U:157:TYR:HB3	2.02	0.41
5:S:148:LEU:CD2	5:S:162:GLY:HA2	2.51	0.41
8:V:113:ILE:HG13	8:V:119:THR:HG22	2.03	0.41
6:T:212:ILE:HG22	6:T:213:SER:N	2.36	0.41
6:F:67:ILE:HG13	6:F:211:GLU:OE1	2.21	0.41
5:S:4:PHE:CE1	5:S:17:PRO:HD2	2.55	0.41
5:E:148:LEU:HD23	5:E:162:GLY:HA2	2.02	0.41
3:Q:29:GLU:OE2	3:Q:32:LYS:HE2	2.20	0.41
12:L:29:ARG:NH1	12:L:193:ARG:HB3	2.35	0.41
9:W:55:LEU:HD21	9:W:95:TYR:CD1	2.54	0.41
4:R:17:PRO:HA	5:S:26:TYR:CG	2.55	0.41
11:K:44:THR:OG1	11:K:100:MET:HB2	2.20	0.41
1:O:58:LEU:HB3	7:U:162:ALA:O	2.21	0.41
11:Y:44:THR:OG1	11:Y:100:MET:HB2	2.21	0.41
8:V:105:ASP:HB2	8:V:10(A):PRO:CD	2.49	0.41

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:76:VAL:HG12	11:Y:111:TYR:HD2	1.86	0.41
6:F:91:ARG:O	6:F:95:GLU:HB2	2.21	0.41
2:B:190:ILE:CG2	2:B:232:ILE:CD1	2.96	0.41
13:1:113:VAL:HA	13:1:118:VAL:O	2.21	0.41
8:V:25:ILE:CD1	8:V:25:ILE:N	2.83	0.41
6:F:90:ASN:O	6:F:94:GLU:HG3	2.20	0.41
12:Z:22:THR:O	12:Z:23:ASP:HB2	2.20	0.41
9:W:-8:SER:O	9:W:-6:PRO:HD3	2.20	0.41
14:2:2:SER:OG	14:2:130:GLY:HA3	2.20	0.41
10:J:32:ASP:OD2	10:J:34:THR:HG22	2.21	0.41
4:R:18:GLU:OE2	4:R:18:GLU:N	2.53	0.41
7:G:107:MET:CE	7:G:112:LEU:HD13	2.51	0.41
1:O:86:ARG:NE	7:U:118:ASN:ND2	2.64	0.41
1:O:124:THR:CG2	1:O:124:THR:O	2.69	0.41
7:G:198:ILE:O	7:G:202:GLY:N	2.54	0.41
5:E:31:ILE:HD11	5:E:153:PRO:CD	2.50	0.41
8:H:165:ASN:HD22	13:1:139:ARG:NH1	2.09	0.41
3:Q:113:THR:HG21	3:Q:149:TYR:HB3	2.02	0.41
11:K:37:ILE:N	11:K:37:ILE:CD1	2.84	0.41
11:K:37:ILE:HG23	11:K:60:GLY:HA2	2.01	0.41
5:S:38:VAL:CG1	5:S:39:GLY:N	2.84	0.41
13:M:1:THR:OG1	13:M:2:SER:N	2.53	0.41
13:M:3:VAL:O	13:M:126:ALA:HA	2.20	0.41
2:B:224:PHE:HD2	2:B:224:PHE:H	1.67	0.41
6:F:79:SER:OG	6:F:165:THR:HG23	2.21	0.41
11:K:17:ASP:CG	11:K:33:LYS:HZ2	2.23	0.41
4:D:39:GLY:O	4:D:162:ALA:HA	2.21	0.41
6:F:43:ASN:N	6:F:43:ASN:HD22	2.18	0.41
5:E:76:LEU:HD23	5:E:76:LEU:C	2.41	0.41
2:P:38:ILE:HD13	2:P:164:SER:CB	2.47	0.41
14:N:105:ASP:HB2	16:N:775:HOH:O	2.20	0.41
8:V:3:ILE:O	8:V:126:SER:HA	2.21	0.41
2:P:234:VAL:HA	2:P:239:THR:HA	2.01	0.41
7:G:172:ILE:HD11	7:G:201:LEU:CD2	2.51	0.41
3:Q:227:GLU:H	3:Q:227:GLU:CD	2.24	0.41
6:T:32:GLU:HB3	6:T:169:ARG:NH2	2.36	0.41
12:L:-8:PHE:CB	13:M:-8:THR:HG23	2.51	0.41
11:Y:110:ILE:HD13	11:Y:110:ILE:N	2.36	0.41
10:J:190:PHE:C	10:J:192:ALA:H	2.24	0.41
5:E:172:ALA:HB2	5:E:196:ALA:O	2.21	0.41
9:I:-8:SER:O	9:I:-6:PRO:HD3	2.20	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:2:121:LYS:O	14:2:122:LEU:HD23	2.19	0.41
8:H:18:THR:HB	8:H:30:ASN:HA	2.03	0.41
5:E:11:ASP:OD1	5:E:13:VAL:HG12	2.20	0.41
13:1:191:GLN:HB3	13:1:191:GLN:HE21	1.63	0.41
3:C:168:ASN:O	3:C:172:VAL:HG12	2.21	0.41
9:W:110:ILE:HG13	9:W:125:ILE:HG13	2.03	0.41
1:A:13:THR:O	2:B:130:ARG:HD3	2.21	0.41
6:T:91:ARG:O	6:T:95:GLU:HB2	2.21	0.41
10:J:166:MET:CE	10:J:168:MET:HB2	2.51	0.41
7:G:203:THR:HG22	7:G:204:GLU:O	2.20	0.41
13:1:14(G):ILE:N	13:1:144:PRO:HD2	2.35	0.41
9:I:33:LYS:O	9:I:44:GLY:HA2	2.21	0.41
4:D:160:TYR:CZ	4:D:163:LYS:HD3	2.55	0.41
2:B:173:GLN:HG2	3:C:56:LEU:HD12	2.03	0.41
3:Q:58:LEU:HD12	3:Q:58:LEU:HA	1.87	0.41
1:O:39:GLY:HA2	1:O:47:VAL:O	2.20	0.41
5:S:137:LEU:CD2	5:S:150:GLU:HG3	2.51	0.41
1:O:161:LYS:N	2:P:58:LEU:O	2.53	0.41
7:G:236:ILE:HD12	7:G:236:ILE:C	2.41	0.41
14:2:19:ARG:CZ	14:2:26:ILE:CD1	2.99	0.41
2:B:101:LYS:NZ	10:J:85:GLN:NE2	2.69	0.41
5:S:172:ALA:CB	5:S:196:ALA:O	2.69	0.41
2:P:76:VAL:HG12	2:P:138:TYR:CD2	2.56	0.41
12:Z:35:PHE:HB3	16:Z:941:HOH:O	2.21	0.41
10:X:90(A):ILE:HG12	10:X:116:LEU:HA	2.02	0.41
14:N:132:THR:O	14:2:133:PHE:HA	2.21	0.41
12:L:48:PHE:CZ	12:L:50:ALA:HB3	2.56	0.41
14:2:85:GLU:O	14:2:89:GLU:HB2	2.21	0.41
5:E:231:LYS:HD2	5:E:231:LYS:H	1.86	0.41
3:Q:216:LYS:HD2	3:Q:220:ASP:OD1	2.21	0.41
2:B:121:GLN:HG3	3:C:83:ALA:HB1	2.02	0.41
3:C:216:LYS:HD2	3:C:220:ASP:OD1	2.21	0.41
2:P:21:LEU:O	2:P:25:GLU:HG2	2.21	0.41
7:G:122:ILE:HG13	16:G:642:HOH:O	2.21	0.41
6:T:36:THR:HB	6:T:168:GLY:H	1.86	0.41
14:2:9:LYS:O	14:2:107:LYS:HD3	2.20	0.41
1:O:31:VAL:HG13	1:O:79:SER:O	2.20	0.41
3:C:70:ILE:HG21	3:C:112:LEU:HD21	2.03	0.41
4:R:67:ILE:HG22	4:R:221:PHE:HZ	1.85	0.41
1:O:26:TYR:N	1:O:26:TYR:CD1	2.87	0.41
5:S:68:ILE:HB	5:S:76:LEU:CD2	2.51	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:113:THR:HG21	3:C:149:TYR:HB3	2.03	0.41
9:W:106:GLY:HA2	9:W:181:LYS:HD3	2.03	0.41
8:V:40:LYS:HE2	8:V:183:ASP:HA	2.03	0.41
3:C:123:TYR:CD1	3:C:132:PHE:HE1	2.38	0.41
2:B:21(A):LYS:O	2:B:21(B):GLY:C	2.58	0.41
1:O:17:PRO:HA	2:P:26:TYR:CD1	2.56	0.41
7:U:198:ILE:O	7:U:202:GLY:N	2.53	0.40
6:F:20(B):GLU:HG3	6:F:20(C):LYS:N	2.36	0.40
2:B:49:ALA:HB2	2:B:212:PHE:CE1	2.55	0.40
10:X:1:ASP:C	10:X:2:ILE:HD13	2.41	0.40
2:B:97:GLN:NE2	16:B:246:HOH:O	2.45	0.40
5:S:39:GLY:O	5:S:162:GLY:HA2	2.21	0.40
2:P:224:PHE:H	2:P:224:PHE:HD2	1.68	0.40
13:1:62:LEU:HD23	13:1:62:LEU:HA	1.88	0.40
6:T:142:ASP:C	6:T:142:ASP:OD2	2.59	0.40
3:Q:125:GLN:HG3	3:Q:125:GLN:O	2.21	0.40
6:F:202:HIS:O	6:F:202:HIS:CG	2.74	0.40
2:P:38:ILE:CD1	2:P:164:SER:HB3	2.50	0.40
12:L:1:GLY:N	16:L:755:HOH:O	2.54	0.40
3:C:41:LYS:HD3	3:C:160:TRP:O	2.21	0.40
1:O:188:ASP:O	1:O:192:ILE:HG13	2.21	0.40
6:F:109:ILE:H	6:F:109:ILE:CD1	2.35	0.40
6:F:109:ILE:N	6:F:110:PRO:CD	2.84	0.40
5:S:45:HIS:CD2	5:S:214:ILE:HD11	2.56	0.40
14:N:3:ILE:HG22	14:N:16:ALA:HB2	2.03	0.40
5:S:36:VAL:HG22	5:S:37:THR:N	2.37	0.40
5:E:190:ILE:CG2	5:E:212:ILE:HD13	2.51	0.40
9:W:97:VAL:HG23	9:W:99:PRO:HD3	2.04	0.40
5:S:190:ILE:CG2	5:S:212:ILE:HD13	2.51	0.40
7:G:169:GLN:HE21	7:G:169:GLN:HB3	1.72	0.40
2:P:121:GLN:NE2	16:P:462:HOH:O	2.55	0.40
10:J:168:MET:HE2	10:X:168:MET:HE2	2.04	0.40
3:C:206:GLY:HA3	3:C:209:ASN:HB2	2.03	0.40
9:I:130:ALA:HB2	9:I:166:ASP:HB2	2.03	0.40
9:I:178:ILE:HG23	9:I:184:VAL:CG2	2.49	0.40
1:O:4:MET:CG	1:O:5:THR:H	2.32	0.40
4:D:207:LEU:HD23	4:D:233:ILE:HD13	2.03	0.40
1:O:232:ARG:HG3	1:O:232:ARG:NH1	2.37	0.40
4:D:40:ILE:HD11	4:D:176:LEU:HD22	2.03	0.40
5:E:137:LEU:CD2	5:E:150:GLU:HG3	2.52	0.40
9:W:12:VAL:CG1	9:W:108:PRO:HB3	2.52	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:68:GLN:NE2	6:T:86:ARG:NH1	2.69	0.40
10:X:35:ARG:NH1	10:X:57:GLU:CG	2.85	0.40
9:I:97:VAL:HG23	9:I:99:PRO:HD3	2.03	0.40
12:Z:170:GLY:O	12:Z:171:ASP:HB2	2.22	0.40
7:U:158:VAL:HG22	7:U:159:GLY:N	2.36	0.40
6:F:109:ILE:HG22	6:F:149:TYR:CE2	2.56	0.40
7:U:172:ILE:HD11	7:U:201:LEU:CD2	2.51	0.40
14:2:144:GLU:O	14:2:145:ASN:HB2	2.21	0.40
10:J:34:THR:HG21	10:J:176:LYS:NZ	2.37	0.40
8:V:50:ALA:HB2	9:W:118:CYS:HB2	2.03	0.40
10:J:20:VAL:HG11	11:K:120:LEU:HD11	2.03	0.40
12:Z:-7:ASN:HD22	12:Z:-6:PRO:N	2.19	0.40
1:A:195:LEU:HD23	1:A:236:LEU:HD21	2.02	0.40
4:D:67:ILE:HG22	4:D:221:PHE:HZ	1.87	0.40
1:A:186:LEU:HD21	1:A:214:ILE:HD12	2.04	0.40
5:S:76:LEU:O	5:S:76:LEU:HD23	2.22	0.40
1:O:110:LYS:HG2	16:O:376:HOH:O	2.21	0.40
2:P:225:LYS:O	2:P:226:PRO:C	2.59	0.40
3:Q:18(A):ASP:OD2	3:Q:18(C):LYS:HG2	2.21	0.40
13:M:-2:THR:HA	13:M:47:GLY:O	2.22	0.40
10:X:90(B):ARG:NH1	16:X:266:HOH:O	2.43	0.40
4:R:237:LEU:HD22	4:R:241:GLU:HG3	2.03	0.40
7:G:75:GLY:HA3	7:G:221:PHE:CE2	2.57	0.40
2:B:196:THR:O	2:B:200:THR:HG23	2.22	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%)	233 (94%)	13 (5%)	2 (1%)	24 41

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	O	248/250 (99%)	232 (94%)	14 (6%)	2 (1%)	24	41
2	B	242/244 (99%)	221 (91%)	17 (7%)	4 (2%)	11	19
2	P	242/244 (99%)	220 (91%)	18 (7%)	4 (2%)	11	19
3	C	239/241 (99%)	220 (92%)	15 (6%)	4 (2%)	11	19
3	Q	239/241 (99%)	221 (92%)	14 (6%)	4 (2%)	11	19
4	D	240/242 (99%)	227 (95%)	8 (3%)	5 (2%)	9	14
4	R	240/242 (99%)	226 (94%)	9 (4%)	5 (2%)	9	14
5	E	231/233 (99%)	211 (91%)	16 (7%)	4 (2%)	11	19
5	S	231/233 (99%)	211 (91%)	16 (7%)	4 (2%)	11	19
6	F	242/244 (99%)	229 (95%)	12 (5%)	1 (0%)	39	61
6	T	242/244 (99%)	230 (95%)	10 (4%)	2 (1%)	24	41
7	G	241/243 (99%)	230 (95%)	10 (4%)	1 (0%)	39	61
7	U	241/243 (99%)	226 (94%)	13 (5%)	2 (1%)	24	41
8	H	220/222 (99%)	211 (96%)	8 (4%)	1 (0%)	34	55
8	V	220/222 (99%)	211 (96%)	8 (4%)	1 (0%)	34	55
9	I	202/204 (99%)	196 (97%)	5 (2%)	1 (0%)	34	55
9	W	202/204 (99%)	195 (96%)	7 (4%)	0	100	100
10	J	196/198 (99%)	187 (95%)	7 (4%)	2 (1%)	19	34
10	X	196/198 (99%)	187 (95%)	7 (4%)	2 (1%)	19	34
11	K	210/212 (99%)	204 (97%)	6 (3%)	0	100	100
11	Y	210/212 (99%)	205 (98%)	5 (2%)	0	100	100
12	L	220/222 (99%)	210 (96%)	9 (4%)	1 (0%)	34	55
12	Z	220/222 (99%)	211 (96%)	8 (4%)	1 (0%)	34	55
13	1	231/233 (99%)	220 (95%)	11 (5%)	0	100	100
13	M	231/233 (99%)	221 (96%)	10 (4%)	0	100	100
14	2	194/196 (99%)	187 (96%)	7 (4%)	0	100	100
14	N	194/196 (99%)	188 (97%)	6 (3%)	0	100	100
All	All	6312/6368 (99%)	5970 (95%)	289 (5%)	53 (1%)	24	41

All (53) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	58	LEU

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
4	D	12(G)	GLU
3	Q	58	LEU
4	R	12(G)	GLU
1	A	5	THR
2	B	54	VAL
2	B	21(B)	GLY
2	B	21(C)	ASP
3	C	183	PRO
3	C	203	THR
5	E	202	ARG
5	E	217	LYS
10	J	192	ALA
12	L	71	ASP
1	O	5	THR
2	P	54	VAL
2	P	21(B)	GLY
2	P	21(C)	ASP
3	Q	183	PRO
3	Q	184	ALA
3	Q	203	THR
5	S	202	ARG
5	S	217	LYS
8	V	9	ASN
10	X	192	ALA
12	Z	71	ASP
3	C	184	ALA
4	D	12(F)	GLY
4	D	18(D)	SER
5	E	5	ARG
8	H	9	ASN
2	P	20(A)	SER
4	R	12(F)	GLY
4	R	18(D)	SER
5	S	5	ARG
2	B	20(A)	SER
4	D	120	ALA
10	J	49	ALA
1	O	167	LYS
4	R	120	ALA
1	A	167	LYS
5	E	180	LEU
5	S	180	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
7	U	184	ASN
10	X	49	ALA
6	F	205	ASN
6	T	205	ASN
6	T	206	LYS
4	D	12(C)	GLY
4	R	12(C)	GLY
7	U	55	PRO
7	G	55	PRO
9	I	93	GLY

### 5.3.2 Protein sidechains [i](#)

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%)	202 (97%)	7 (3%)	45	73
1	O	209/209 (100%)	203 (97%)	6 (3%)	50	77
2	B	203/203 (100%)	187 (92%)	16 (8%)	15	28
2	P	203/203 (100%)	186 (92%)	17 (8%)	14	25
3	C	213/213 (100%)	201 (94%)	12 (6%)	26	47
3	Q	213/213 (100%)	201 (94%)	12 (6%)	26	47
4	D	198/198 (100%)	185 (93%)	13 (7%)	21	38
4	R	198/198 (100%)	185 (93%)	13 (7%)	21	38
5	E	192/192 (100%)	174 (91%)	18 (9%)	11	20
5	S	192/192 (100%)	173 (90%)	19 (10%)	10	18
6	F	201/201 (100%)	185 (92%)	16 (8%)	15	28
6	T	201/201 (100%)	186 (92%)	15 (8%)	17	31
7	G	207/207 (100%)	195 (94%)	12 (6%)	25	45
7	U	207/207 (100%)	195 (94%)	12 (6%)	25	45
8	H	181/181 (100%)	172 (95%)	9 (5%)	30	53
8	V	181/181 (100%)	171 (94%)	10 (6%)	27	48

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	I	172/172 (100%)	166 (96%)	6 (4%)	43	70
9	W	172/172 (100%)	165 (96%)	7 (4%)	37	63
10	J	175/175 (100%)	167 (95%)	8 (5%)	33	57
10	X	175/175 (100%)	167 (95%)	8 (5%)	33	57
11	K	169/169 (100%)	161 (95%)	8 (5%)	32	56
11	Y	169/169 (100%)	161 (95%)	8 (5%)	32	56
12	L	185/185 (100%)	174 (94%)	11 (6%)	24	44
12	Z	185/185 (100%)	174 (94%)	11 (6%)	24	44
13	1	199/199 (100%)	192 (96%)	7 (4%)	43	70
13	M	199/199 (100%)	192 (96%)	7 (4%)	43	70
14	2	162/162 (100%)	152 (94%)	10 (6%)	23	41
14	N	162/162 (100%)	153 (94%)	9 (6%)	26	47
All	All	5332/5332 (100%)	5025 (94%)	307 (6%)	25	45

All (307) 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	158	PHE
1	A	179	ARG
1	A	192	ILE
1	A	229	ILE
2	B	14	ILE
2	B	46	ILE
2	B	58	LEU
2	B	67	LEU
2	B	71	ASN
2	B	94	ILE
2	B	121	GLN
2	B	150	THR
2	B	156	ASN
2	B	163	ILE
2	B	185	LYS
2	B	187	ASP
2	B	192	LEU
2	B	212	PHE

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
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	87	ILE
3	C	114	ARG
3	C	135	SER
3	C	150	GLN
3	C	163	GLN
3	C	174	GLU
3	C	208	LYS
3	C	227	GLU
4	D	28	LEU
4	D	48	LEU
4	D	76	CYS
4	D	107	ILE
4	D	110	GLU
4	D	126	ARG
4	D	170	GLU
4	D	177	LEU
4	D	18(E)	SER
4	D	191	LEU
4	D	215	ILE
4	D	237	LEU
4	D	244	GLU
5	E	12	THR
5	E	28	LEU
5	E	32	LYS
5	E	57	GLU
5	E	68	ILE
5	E	76	LEU
5	E	97	ASN
5	E	111	ARG
5	E	117	CYS
5	E	121	GLN
5	E	185	ASN
5	E	189	LEU
5	E	199	GLN
5	E	207	LEU
5	E	2(D)	ASP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
5	E	223	ILE
5	E	227	GLU
5	E	231	LYS
6	F	11	SER
6	F	40	ILE
6	F	43	ASN
6	F	56	SER
6	F	82	ILE
6	F	109	ILE
6	F	121	GLN
6	F	127	ASN
6	F	18(E)	GLU
6	F	187	ARG
6	F	196	ILE
6	F	203	GLU
6	F	204	ASP
6	F	205	ASN
6	F	214	TRP
6	F	21(C)	ASN
7	G	35	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	184	ASN
7	G	197	MET
7	G	229	ILE
7	G	232	ARG
7	G	233	LEU
8	H	25	ILE
8	H	30	ASN
8	H	34	LEU
8	H	43	CYS
8	H	55	VAL
8	H	68	LEU
8	H	95	ILE
8	H	144	GLN
8	H	197	ARG
9	I	29	ASN
9	I	61	TYR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
9	I	110	ILE
9	I	125	ILE
9	I	160	LEU
9	I	171	TRP
10	J	6	ILE
10	J	34	THR
10	J	52	THR
10	J	70	GLU
10	J	77	GLN
10	J	90(A)	ILE
10	J	121	GLU
10	J	177	ILE
11	K	4	LEU
11	K	8	PHE
11	K	9	GLN
11	K	37	ILE
11	K	65	LEU
11	K	104	TYR
11	K	10(B)	LYS
11	K	138	LEU
12	L	-7	ASN
12	L	14	LEU
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	138	LEU
12	L	1(I)	ASN
12	L	145	TYR
13	M	40	ASN
13	M	62	LEU
13	M	91	ARG
13	M	129	PHE
13	M	14(C)	ARG
13	M	149	GLN
13	M	204	LYS
14	N	26	ILE
14	N	36	ARG
14	N	55	ILE
14	N	84	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
14	N	89	GLU
14	N	99	ILE
14	N	10(B)	LYS
14	N	119	VAL
14	N	149	GLU
1	O	33	GLN
1	O	64	LEU
1	O	158	PHE
1	O	179	ARG
1	O	192	ILE
1	O	229	ILE
2	P	14	ILE
2	P	46	ILE
2	P	58	LEU
2	P	67	LEU
2	P	71	ASN
2	P	94	ILE
2	P	116	LEU
2	P	121	GLN
2	P	150	THR
2	P	156	ASN
2	P	163	ILE
2	P	185	LYS
2	P	187	ASP
2	P	192	LEU
2	P	212	PHE
2	P	218	ASN
2	P	232	ILE
3	Q	10	ARG
3	Q	14	ILE
3	Q	25	GLU
3	Q	57	LYS
3	Q	87	ILE
3	Q	114	ARG
3	Q	135	SER
3	Q	150	GLN
3	Q	163	GLN
3	Q	174	GLU
3	Q	208	LYS
3	Q	227	GLU
4	R	28	LEU
4	R	48	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
4	R	76	CYS
4	R	107	ILE
4	R	110	GLU
4	R	126	ARG
4	R	170	GLU
4	R	177	LEU
4	R	18(E)	SER
4	R	191	LEU
4	R	215	ILE
4	R	237	LEU
4	R	244	GLU
5	S	12	THR
5	S	28	LEU
5	S	32	LYS
5	S	57	GLU
5	S	68	ILE
5	S	76	LEU
5	S	97	ASN
5	S	104	ASN
5	S	111	ARG
5	S	117	CYS
5	S	121	GLN
5	S	185	ASN
5	S	189	LEU
5	S	199	GLN
5	S	207	LEU
5	S	2(D)	ASP
5	S	223	ILE
5	S	227	GLU
5	S	231	LYS
6	T	11	SER
6	T	40	ILE
6	T	43	ASN
6	T	56	SER
6	T	82	ILE
6	T	109	ILE
6	T	121	GLN
6	T	127	ASN
6	T	18(E)	GLU
6	T	187	ARG
6	T	203	GLU
6	T	204	ASP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
6	T	205	ASN
6	T	214	TRP
6	T	21(C)	ASN
7	U	35	ILE
7	U	72	ARG
7	U	87	ASN
7	U	119	LEU
7	U	121	GLN
7	U	124	THR
7	U	169	GLN
7	U	184	ASN
7	U	197	MET
7	U	229	ILE
7	U	232	ARG
7	U	233	LEU
8	V	25	ILE
8	V	30	ASN
8	V	34	LEU
8	V	41	ILE
8	V	43	CYS
8	V	55	VAL
8	V	68	LEU
8	V	121	VAL
8	V	144	GLN
8	V	197	ARG
9	W	-3	ILE
9	W	29	ASN
9	W	61	TYR
9	W	110	ILE
9	W	125	ILE
9	W	160	LEU
9	W	171	TRP
10	X	6	ILE
10	X	34	THR
10	X	52	THR
10	X	70	GLU
10	X	77	GLN
10	X	90(A)	ILE
10	X	121	GLU
10	X	177	ILE
11	Y	4	LEU
11	Y	8	PHE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
11	Y	9	GLN
11	Y	37	ILE
11	Y	65	LEU
11	Y	104	TYR
11	Y	10(B)	LYS
11	Y	138	LEU
12	Z	-7	ASN
12	Z	14	LEU
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
12	Z	1(I)	ASN
12	Z	145	TYR
13	1	40	ASN
13	1	62	LEU
13	1	91	ARG
13	1	129	PHE
13	1	14(C)	ARG
13	1	149	GLN
13	1	204	LYS
14	2	26	ILE
14	2	36	ARG
14	2	55	ILE
14	2	84	LYS
14	2	89	GLU
14	2	99	ILE
14	2	10(A)	ASP
14	2	10(B)	LYS
14	2	119	VAL
14	2	149	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (195) 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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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	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	114	GLN
4	D	147	GLN
4	D	161	ASN
4	D	211	GLN
4	D	218	GLN
4	D	226	ASN
5	E	7	ASN
5	E	33	GLN
5	E	64	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

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
7	G	87	ASN
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
10	J	54	GLN
10	J	77	GLN
10	J	85	GLN
10	J	112	GLN
10	J	140	HIS
10	J	141	HIS
10	J	186	GLN
10	J	193	GLN
11	K	9	GLN
11	K	85	ASN
11	K	131	GLN
11	K	174	ASN
11	K	207	ASN
12	L	-9	GLN
12	L	-7	ASN
12	L	40	ASN
12	L	46	ASN
12	L	61	ASN
12	L	70(A)	ASN
12	L	82	ASN
12	L	98	HIS
12	L	14(B)	ASN
12	L	1(I)	ASN
12	L	166	HIS
13	M	10	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
13	M	40	ASN
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	94	ASN
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	161	ASN
4	R	211	GLN
4	R	218	GLN
4	R	226	ASN
5	S	7	ASN
5	S	64	GLN
5	S	73	HIS
5	S	104	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
5	S	121	GLN
5	S	125	GLN
5	S	156	ASN
5	S	185	ASN
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	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
10	X	54	GLN
10	X	77	GLN
10	X	85	GLN
10	X	112	GLN
10	X	140	HIS
10	X	141	HIS
10	X	186	GLN
10	X	193	GLN
11	Y	9	GLN
11	Y	85	ASN
11	Y	131	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
11	Y	174	ASN
11	Y	207	ASN
12	Z	-9	GLN
12	Z	-7	ASN
12	Z	40	ASN
12	Z	46	ASN
12	Z	61	ASN
12	Z	70(A)	ASN
12	Z	82	ASN
12	Z	14(B)	ASN
12	Z	1(I)	ASN
12	Z	166	HIS
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	145	ASN
14	2	157	HIS
14	2	161	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

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	SA1	2	0	14	18,22,22	1.27	1 (5%)	21,34,34	2.00	2 (9%)
15	SA1	H	0	8	18,22,22	1.50	3 (16%)	21,34,34	1.82	2 (9%)
15	SA1	K	0	11	18,22,22	1.29	1 (5%)	21,34,34	1.98	2 (9%)
15	SA1	N	0	14	18,22,22	1.29	1 (5%)	21,34,34	2.04	2 (9%)
15	SA1	V	0	8	18,22,22	1.36	2 (11%)	21,34,34	1.85	2 (9%)
15	SA1	Y	0	11	18,22,22	1.22	1 (5%)	21,34,34	1.94	2 (9%)

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	SA1	2	0	14	-	0/4/52/52	0/3/3/3
15	SA1	H	0	8	-	0/4/52/52	0/3/3/3
15	SA1	K	0	11	-	0/4/52/52	0/3/3/3
15	SA1	N	0	14	-	0/4/52/52	0/3/3/3
15	SA1	V	0	8	-	0/4/52/52	0/3/3/3
15	SA1	Y	0	11	-	0/4/52/52	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	V	0	SA1	O17-C10	2.18	1.47	1.42
15	H	0	SA1	O17-C10	2.19	1.47	1.42
15	N	0	SA1	C4-C3	3.07	1.57	1.51
15	2	0	SA1	C4-C3	3.09	1.57	1.51
15	H	0	SA1	O2-C3	3.13	1.48	1.45
15	Y	0	SA1	C4-C3	3.24	1.57	1.51
15	H	0	SA1	C4-C3	3.33	1.57	1.51
15	V	0	SA1	C4-C3	3.43	1.57	1.51
15	K	0	SA1	C4-C3	3.54	1.57	1.51

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	K	0	SA1	C3-C5-C6	-5.36	99.92	104.30
15	Y	0	SA1	C3-C5-C6	-5.08	100.15	104.30
15	2	0	SA1	C3-C5-C6	-4.92	100.28	104.30
15	N	0	SA1	C3-C5-C6	-4.87	100.32	104.30
15	H	0	SA1	C3-C5-C6	-4.59	100.55	104.30
15	V	0	SA1	C3-C5-C6	-4.51	100.61	104.30
15	H	0	SA1	C9-C10-C11	6.15	121.81	114.09
15	V	0	SA1	C9-C10-C11	6.55	122.31	114.09
15	K	0	SA1	C9-C10-C11	6.71	122.52	114.09
15	Y	0	SA1	C9-C10-C11	6.75	122.57	114.09
15	2	0	SA1	C9-C10-C11	6.99	122.87	114.09
15	N	0	SA1	C9-C10-C11	7.24	123.18	114.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	2	0	SA1	4	0
15	H	0	SA1	1	0
15	K	0	SA1	1	0
15	N	0	SA1	4	0
15	V	0	SA1	1	0
15	Y	0	SA1	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 ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	250/250 (100%)	-0.32	3 (1%) 81 83	21, 34, 63, 92	0
1	O	250/250 (100%)	-0.18	4 (1%) 74 78	24, 41, 69, 93	0
2	B	244/244 (100%)	-0.06	6 (2%) 61 65	19, 42, 77, 105	0
2	P	244/244 (100%)	0.04	9 (3%) 45 50	23, 43, 78, 105	0
3	C	241/241 (100%)	-0.06	10 (4%) 41 46	22, 43, 96, 110	0
3	Q	241/241 (100%)	0.41	35 (14%) 3 3	28, 49, 98, 109	0
4	D	242/242 (100%)	-0.06	7 (2%) 55 60	23, 43, 77, 108	0
4	R	242/242 (100%)	0.06	9 (3%) 45 50	27, 48, 79, 109	0
5	E	233/233 (100%)	0.01	8 (3%) 49 54	30, 47, 72, 98	0
5	S	233/233 (100%)	0.32	19 (8%) 14 15	29, 51, 77, 95	0
6	F	244/244 (100%)	-0.25	3 (1%) 81 83	20, 41, 76, 93	0
6	T	244/244 (100%)	-0.02	6 (2%) 61 65	22, 43, 78, 95	0
7	G	243/243 (100%)	-0.30	5 (2%) 67 71	19, 36, 62, 101	0
7	U	243/243 (100%)	-0.17	3 (1%) 81 83	19, 38, 62, 102	0
8	H	222/222 (100%)	-0.41	0 100 100	16, 31, 52, 81	0
8	V	222/222 (100%)	-0.42	1 (0%) 91 92	22, 35, 54, 83	0
9	I	204/204 (100%)	-0.46	1 (0%) 91 92	18, 32, 48, 65	0
9	W	204/204 (100%)	-0.27	1 (0%) 91 92	16, 31, 51, 66	0
10	J	198/198 (100%)	-0.35	3 (1%) 76 79	19, 35, 52, 107	0
10	X	198/198 (100%)	-0.35	4 (2%) 68 72	21, 35, 51, 108	0
11	K	212/212 (100%)	-0.48	0 100 100	16, 32, 50, 58	0
11	Y	212/212 (100%)	-0.42	0 100 100	19, 35, 53, 62	0
12	L	222/222 (100%)	-0.43	2 (0%) 85 88	17, 33, 55, 75	0
12	Z	222/222 (100%)	-0.40	2 (0%) 85 88	19, 34, 55, 75	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
13	1	233/233 (100%)	-0.47	1 (0%)	93	93	18, 33, 47, 50	0
13	M	233/233 (100%)	-0.44	1 (0%)	93	93	19, 34, 48, 55	0
14	2	196/196 (100%)	-0.41	0	100	100	18, 31, 51, 63	0
14	N	196/196 (100%)	-0.51	0	100	100	16, 29, 50, 65	0
All	All	6368/6368 (100%)	-0.22	143 (2%)	65	69	16, 38, 70, 110	0

All (143) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	R	12(F)	GLY	10.6
4	D	12(D)	ALA	10.4
4	R	12(D)	ALA	10.3
2	P	217	ALA	9.9
7	U	240	ASP	9.0
2	B	217	ALA	8.4
4	R	12(E)	SER	8.4
3	Q	236	ILE	8.2
4	D	12(C)	GLY	8.1
2	B	218	ASN	7.9
7	U	6	ALA	7.6
4	R	12(C)	GLY	6.8
3	C	55	THR	6.6
4	D	12(E)	SER	6.6
7	G	6	ALA	6.1
2	P	218	ASN	6.1
4	R	126	ARG	6.0
1	O	236	LEU	5.9
10	X	193	GLN	5.9
3	Q	56	LEU	5.8
5	E	4	PHE	5.5
5	S	5	ARG	5.4
10	X	192	ALA	5.2
5	S	233	ILE	5.2
10	J	192	ALA	5.2
3	C	56	LEU	4.9
5	S	4	PHE	4.9
1	O	4	MET	4.9
3	Q	243	GLN	4.8
7	G	240	ASP	4.7
5	S	206	SER	4.6
5	S	203	ASP	4.6

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	P	21(B)	GLY	4.6
4	D	127	LEU	4.5
6	F	5	GLY	4.5
10	J	193	GLN	4.4
4	D	126	ARG	4.4
1	O	235	ALA	4.4
2	B	54	VAL	4.3
3	Q	203	THR	4.1
3	Q	240	LYS	4.1
3	C	240	LYS	4.1
3	Q	63	THR	4.1
3	Q	242	GLU	4.0
3	Q	241	GLN	4.0
5	S	178	ARG	3.9
9	W	-8	SER	3.8
2	P	62	ASP	3.7
5	E	189	LEU	3.6
13	M	-8	THR	3.6
10	J	191	GLN	3.5
5	E	5	ARG	3.5
3	Q	206	GLY	3.4
2	B	21(B)	GLY	3.4
4	D	12(F)	GLY	3.4
2	P	21(C)	ASP	3.4
12	Z	145	TYR	3.4
2	P	219	GLU	3.3
5	S	210	LEU	3.3
3	Q	239	GLU	3.3
2	B	21(A)	LYS	3.3
5	E	203	ASP	3.3
2	P	239	THR	3.2
3	Q	229	ILE	3.2
3	Q	237	GLU	3.2
1	A	236	LEU	3.2
3	Q	197	LEU	3.2
3	C	237	GLU	3.1
4	D	12(G)	GLU	3.1
5	S	127	TYR	3.1
3	Q	235	GLN	3.1
12	Z	14(W)	LYS	3.0
3	Q	207	ALA	3.0
6	F	240	ILE	3.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	B	239	THR	3.0
3	Q	55	THR	3.0
6	T	5	GLY	3.0
4	R	127	LEU	3.0
3	Q	234	THR	3.0
1	A	4	MET	2.9
8	V	223	ASP	2.9
3	Q	233	VAL	2.9
1	O	5	THR	2.9
5	S	195	GLU	2.9
3	Q	191	LYS	2.8
5	E	233	ILE	2.8
5	S	197	ILE	2.8
5	S	232	TYR	2.8
7	G	237	ALA	2.8
3	Q	238	GLN	2.7
6	T	240	ILE	2.7
4	R	240	LYS	2.7
5	S	188	GLU	2.7
5	E	127	TYR	2.7
10	X	189	ASP	2.7
3	Q	212	ILE	2.7
12	L	145	TYR	2.6
7	G	239	GLN	2.6
3	C	190	VAL	2.6
3	Q	202	GLN	2.6
3	Q	53	ARG	2.5
5	E	204	GLU	2.5
2	P	21(A)	LYS	2.5
5	S	2(E)	ASN	2.5
7	U	239	GLN	2.5
5	E	184	GLY	2.4
13	1	-8	THR	2.4
3	Q	52	ARG	2.4
6	T	199	LEU	2.4
3	Q	231	GLN	2.4
3	Q	189	CYS	2.4
3	C	241	GLN	2.4
9	I	-8	SER	2.4
3	Q	187	GLU	2.4
4	R	9	ASP	2.3
5	S	174	THR	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
10	X	191	GLN	2.3
5	S	18(C)	PHE	2.3
3	Q	54	SER	2.3
3	Q	232	TYR	2.3
3	Q	198	LEU	2.3
6	T	18(B)	HIS	2.3
3	C	203	THR	2.3
3	Q	201	VAL	2.3
3	C	232	TYR	2.2
3	C	233	VAL	2.2
6	F	206	LYS	2.2
3	Q	58	LEU	2.2
5	S	18(E)	LYS	2.2
1	A	235	ALA	2.1
5	S	175	TYR	2.1
5	S	51	LEU	2.1
3	C	243	GLN	2.1
7	G	236	ILE	2.1
6	T	241	ASN	2.1
2	P	54	VAL	2.1
3	Q	44	ASN	2.1
3	Q	178	LYS	2.1
4	R	121	LEU	2.1
12	L	14(W)	LYS	2.0
3	Q	175	PHE	2.0
5	S	18(B)	THR	2.0
6	T	18(E)	GLU	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains.

The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
15	SA1	N	0	20/20	0.91	0.14	1.17	19,26,29,30	0
15	SA1	2	0	20/20	0.92	0.16	0.89	27,30,32,32	0
15	SA1	V	0	20/20	0.93	0.14	0.36	32,34,40,41	0
15	SA1	K	0	20/20	0.94	0.13	0.20	19,30,33,33	0
15	SA1	H	0	20/20	0.94	0.13	0.03	30,34,36,36	0
15	SA1	Y	0	20/20	0.95	0.12	-0.24	27,30,32,33	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.