



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 01:06 PM GMT

PDB ID : 3D29  
Title : Proteasome Inhibition by Fellutamide B  
Authors : Groll, M.; Hines, J.; Fahnestock, M.; Crews, M.C.  
Deposited on : 2008-05-07  
Resolution : 2.60 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

---

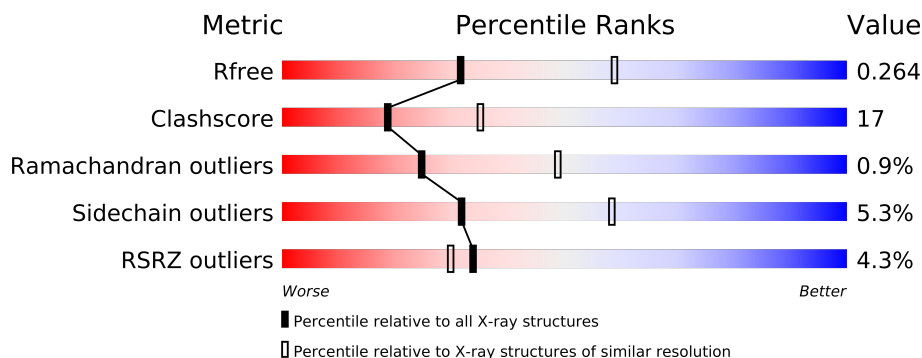
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.60 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.









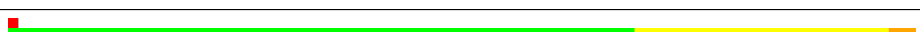
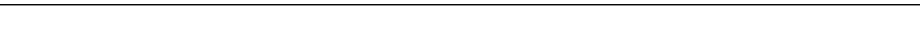
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	1718 (2.60-2.60)
Clashscore	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)
RSRZ outliers	66119	1718 (2.60-2.60)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	250	
1	O	250	
2	B	244	
2	P	244	
3	C	241	
3	Q	241	
4	D	242	
4	R	242	
5	E	233	
5	S	233	
6	F	244	
6	T	244	
7	G	243	
7	U	243	

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
8	H	222	
8	V	222	
9	I	204	
9	W	204	
10	J	198	
10	X	198	
11	K	212	
11	Y	212	
12	L	222	
12	Z	222	
13	1	233	
13	M	233	
14	2	196	
14	N	196	

## 2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 51114 atoms, of which 0 are hydrogen and 0 are deuterium.

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			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	237	GLU	-	EXPRESSION TAG	UNP P40303
C	238	GLN	-	EXPRESSION TAG	UNP P40303
C	239	GLU	-	EXPRESSION TAG	UNP P40303
C	240	LYS	-	EXPRESSION TAG	UNP P40303
C	241	GLN	-	EXPRESSION TAG	UNP P40303
C	242	GLU	-	EXPRESSION TAG	UNP P40303
C	243	GLN	-	EXPRESSION TAG	UNP P40303
Q	237	GLU	-	EXPRESSION TAG	UNP P40303

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
Q	238	GLN	-	EXPRESSION TAG	UNP P40303
Q	239	GLU	-	EXPRESSION TAG	UNP P40303
Q	240	LYS	-	EXPRESSION TAG	UNP P40303
Q	241	GLN	-	EXPRESSION TAG	UNP P40303
Q	242	GLU	-	EXPRESSION TAG	UNP P40303
Q	243	GLN	-	EXPRESSION TAG	UNP P40303

- 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			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	6	ALA	-	EXPRESSION TAG	UNP P21243
G	7	GLY	-	EXPRESSION TAG	UNP P21243
U	6	ALA	-	EXPRESSION TAG	UNP P21243
U	7	GLY	-	EXPRESSION TAG	UNP P21243

- Molecule 8 is a protein called Proteasome component PUP1 precursor.

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			
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 precursor.

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 precursor.

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

*Continued on next page...*

Continued from previous page...

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

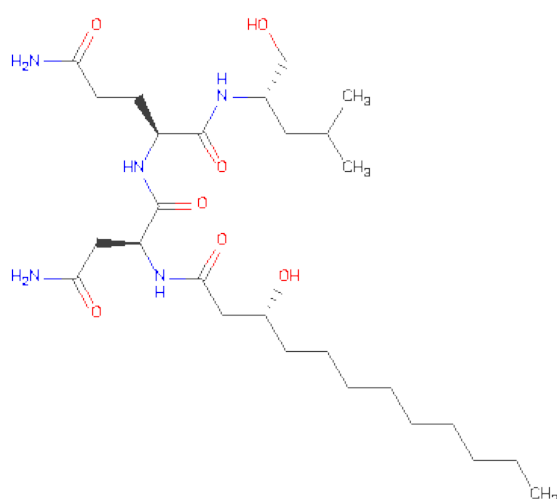
- Molecule 13 is a protein called Proteasome component PRE4 precursor.

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 precursor.

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

- Molecule 15 is N 2 -[(3R)-3-HYDROXYDODECANOYL]-L-ASPARAGINYL-N 1 -[(1S)-1-(HYDROXYMETHYL)-3-METHYLBUTYL]-L-GLUTAMAMIDE (three-letter code: FEB) (formula: C<sub>27</sub>H<sub>51</sub>N<sub>5</sub>O<sub>7</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	H	1	Total	C	N	O	0	0
			39	27	5	7		

Continued on next page...

*Continued from previous page...*

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	K	1	Total	C	N	O	0	0
			39	27	5	7		
15	N	1	Total	C	N	O	0	0
			39	27	5	7		
15	V	1	Total	C	N	O	0	0
			39	27	5	7		
15	Y	1	Total	C	N	O	0	0
			39	27	5	7		
15	2	1	Total	C	N	O	0	0
			39	27	5	7		

- Molecule 16 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	55	Total	O	0	0
			55	55		
16	B	36	Total	O	0	0
			36	36		
16	C	46	Total	O	0	0
			46	46		
16	D	42	Total	O	0	0
			42	42		
16	E	23	Total	O	0	0
			23	23		
16	F	46	Total	O	0	0
			46	46		
16	G	62	Total	O	0	0
			62	62		
16	H	51	Total	O	0	0
			51	51		
16	I	66	Total	O	0	0
			66	66		
16	J	53	Total	O	0	0
			53	53		
16	K	42	Total	O	0	0
			42	42		
16	L	56	Total	O	0	0
			56	56		
16	M	68	Total	O	0	0
			68	68		
16	N	59	Total	O	0	0
			59	59		

*Continued on next page...*



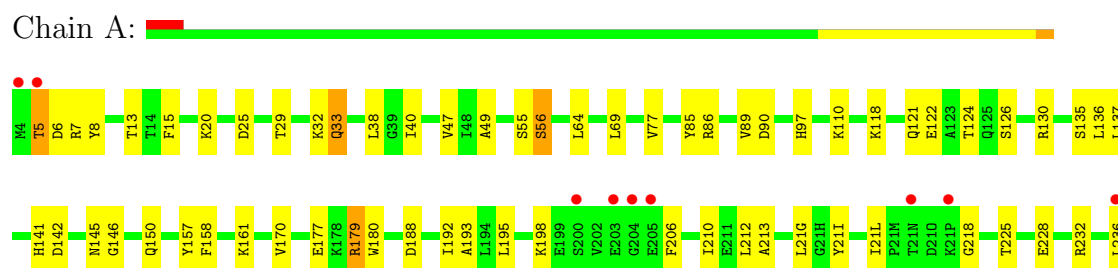
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	O	35	Total 35	O 35	0	0
16	P	29	Total 29	O 29	0	0
16	Q	26	Total 26	O 26	0	0
16	R	31	Total 31	O 31	0	0
16	S	20	Total 20	O 20	0	0
16	T	39	Total 39	O 39	0	0
16	U	61	Total 61	O 61	0	0
16	V	48	Total 48	O 48	0	0
16	W	59	Total 59	O 59	0	0
16	X	46	Total 46	O 46	0	0
16	Y	48	Total 48	O 48	0	0
16	Z	52	Total 52	O 52	0	0
16	1	74	Total 74	O 74	0	0
16	2	59	Total 59	O 59	0	0

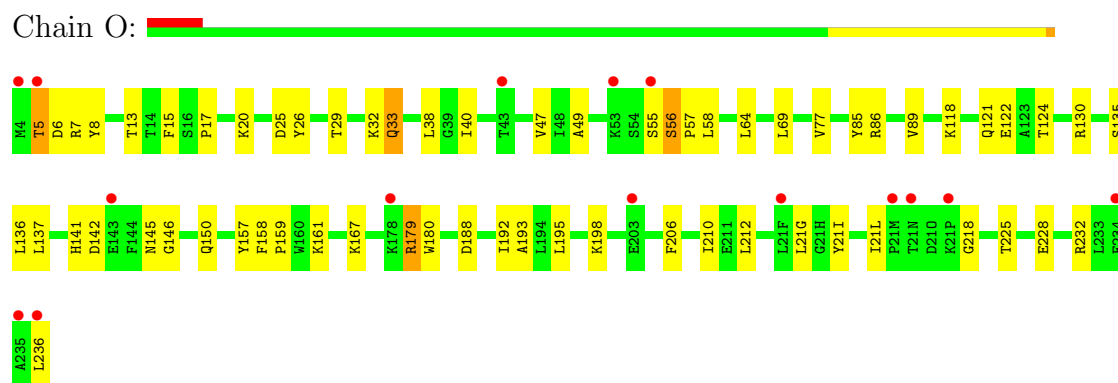
### 3 Residue-property plots

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.

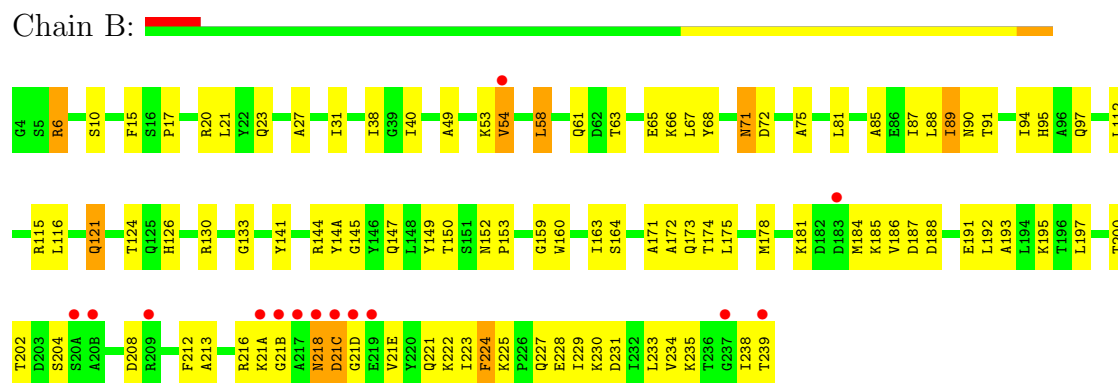
#### • Molecule 1: Proteasome component Y7



#### • Molecule 1: Proteasome component Y7

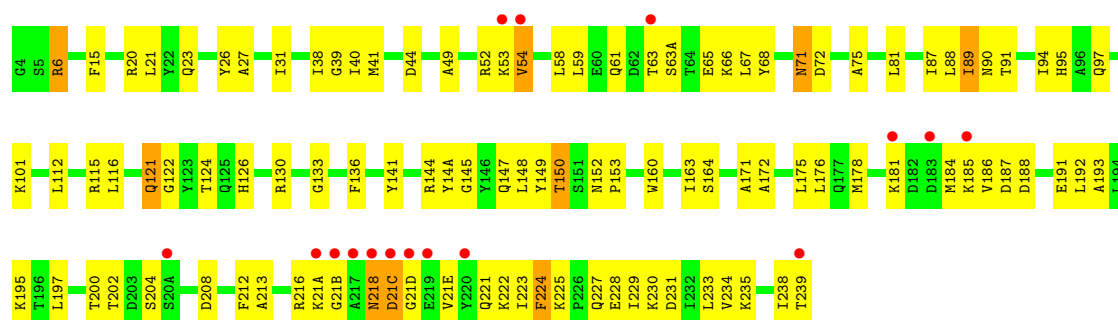


#### • Molecule 2: Proteasome component Y13

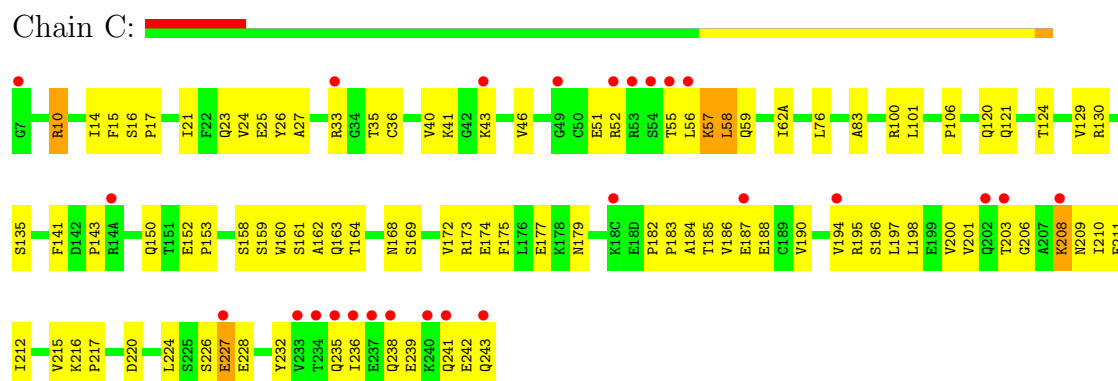


#### • Molecule 2: Proteasome component Y13

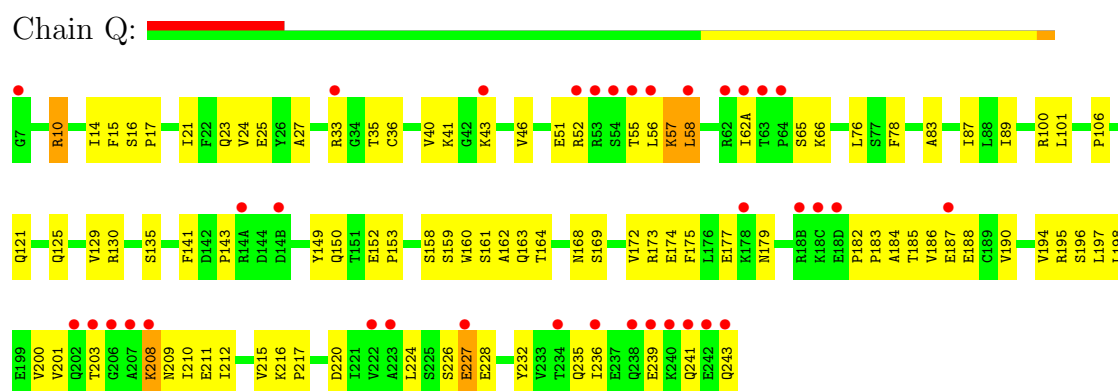




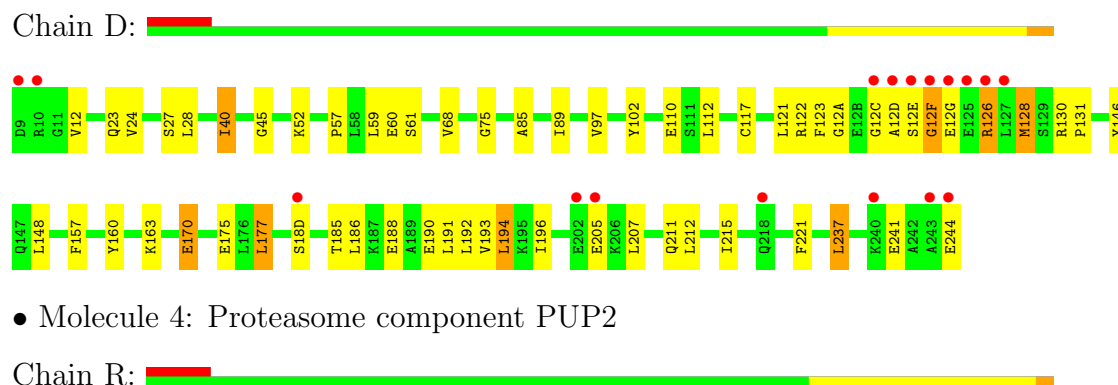
• Molecule 3: Proteasome component PRE6

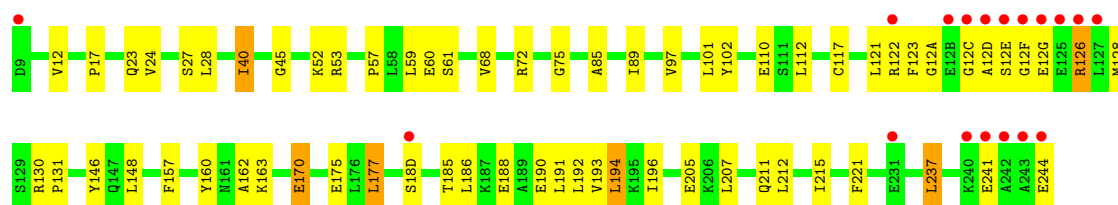


• Molecule 3: Proteasome component PRE6



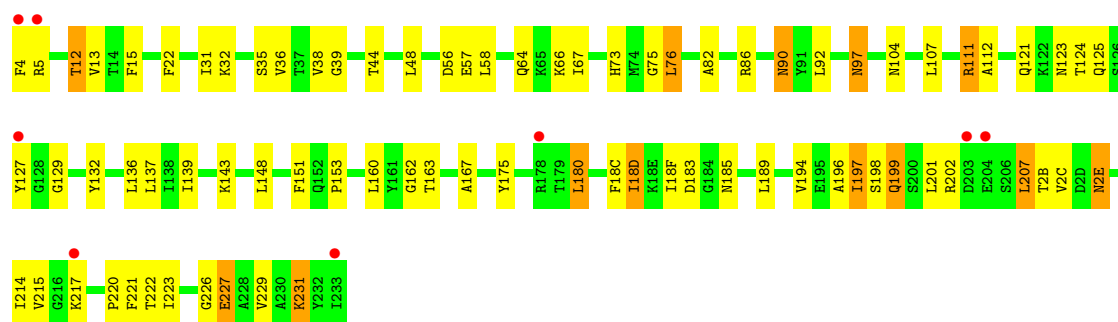
• Molecule 4: Proteasome component PUP2





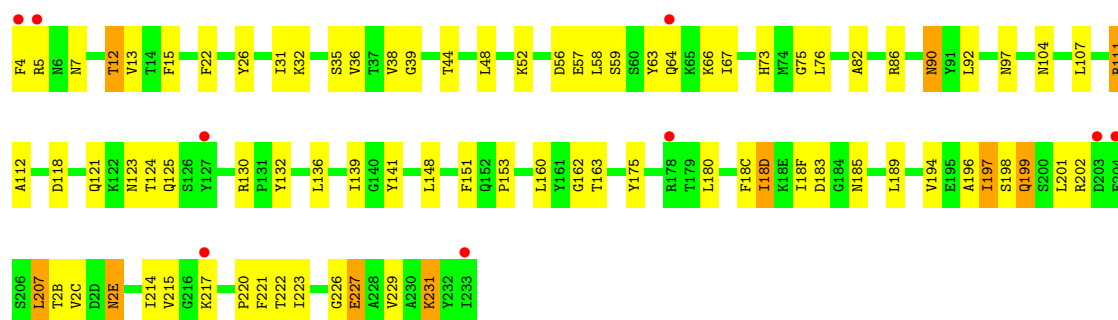
• Molecule 5: Proteasome component PRE5

Chain E:



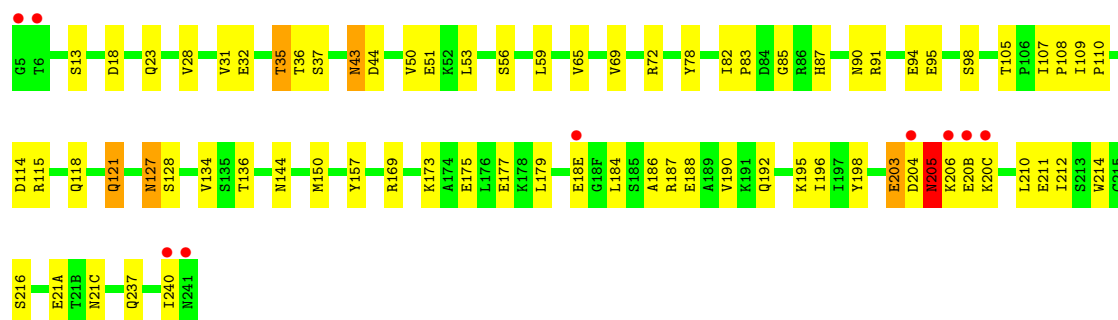
• Molecule 5: Proteasome component PRE5

Chain S:



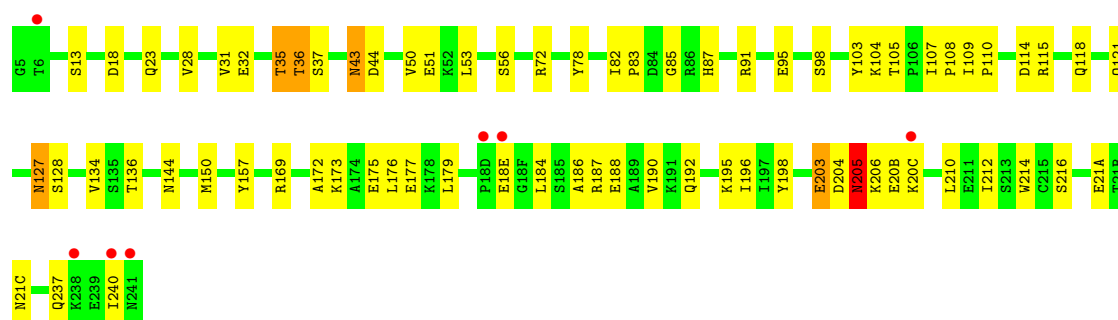
• Molecule 6: Proteasome component C1

Chain F:



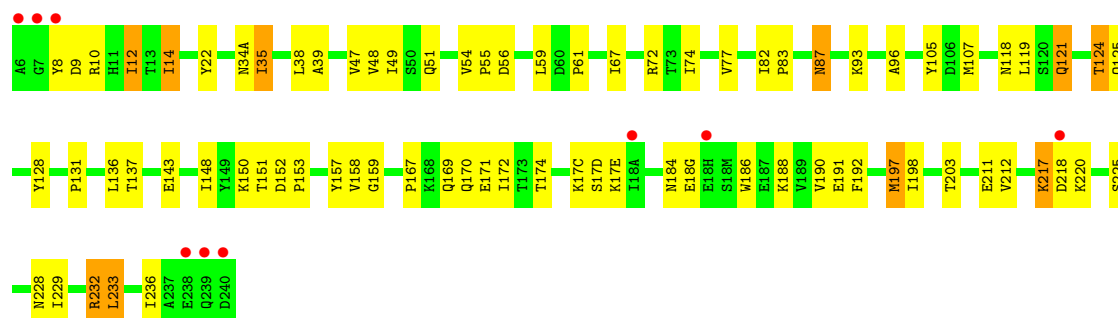
• Molecule 6: Proteasome component C1

Chain T:



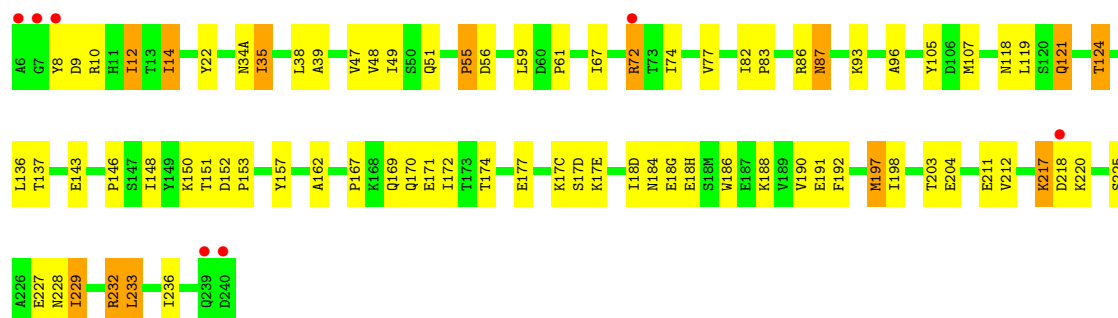
- Molecule 7: Proteasome component C7-alpha

Chain G:



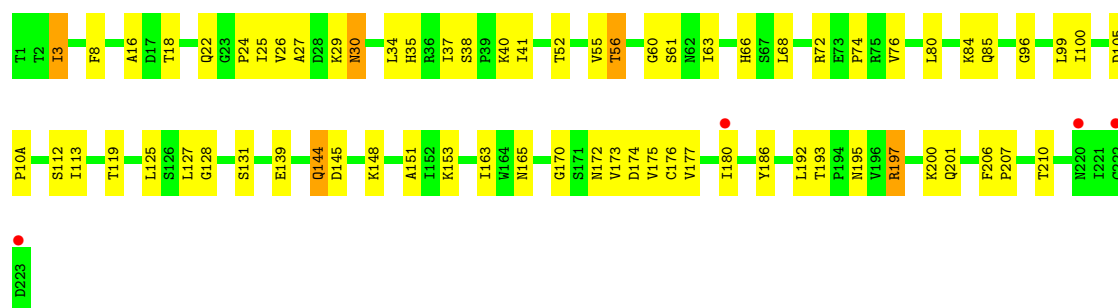
- Molecule 7: Proteasome component C7-alpha

Chain U:



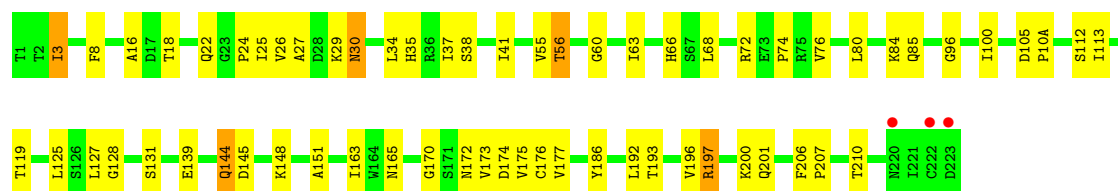
- Molecule 8: Proteasome component PUP1 precursor

Chain H: 



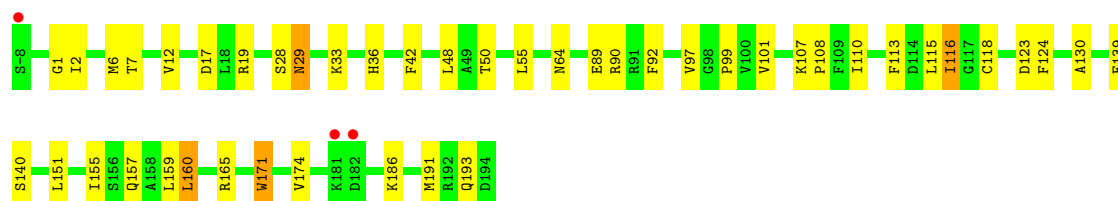
- Molecule 8: Proteasome component PUP1 precursor

Chain V:



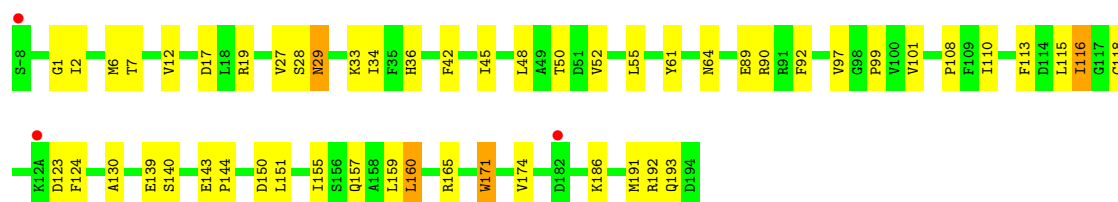
- Molecule 9: Proteasome component PUP3

Chain I:



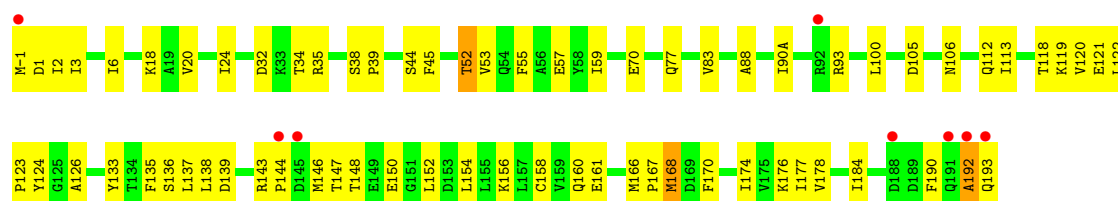
- Molecule 9: Proteasome component PUP3

Chain W:



- Molecule 10: Proteasome component C11

Chain J:



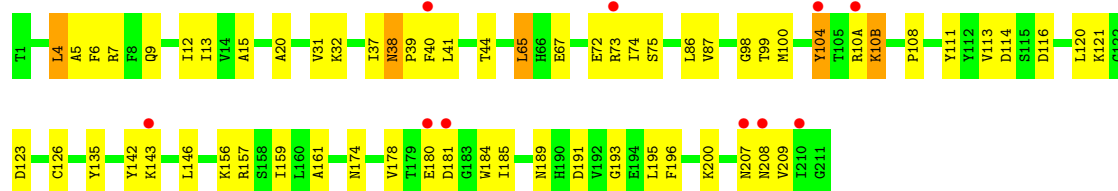
- Molecule 10: Proteasome component C11

Chain X:



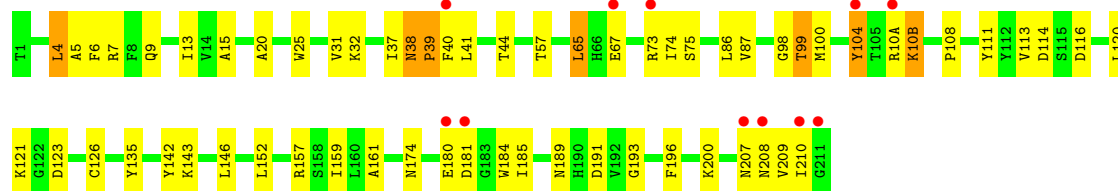
- Molecule 11: Proteasome component PRE2 precursor

Chain K:



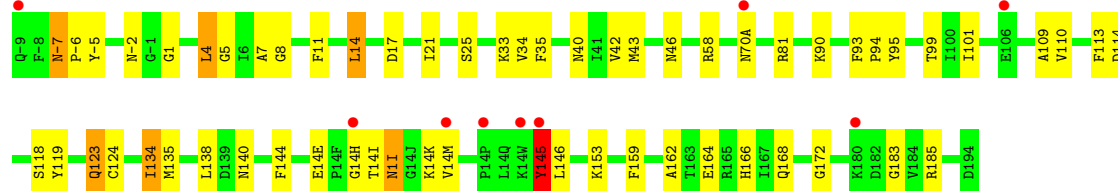
- Molecule 11: Proteasome component PRE2 precursor

Chain Y:



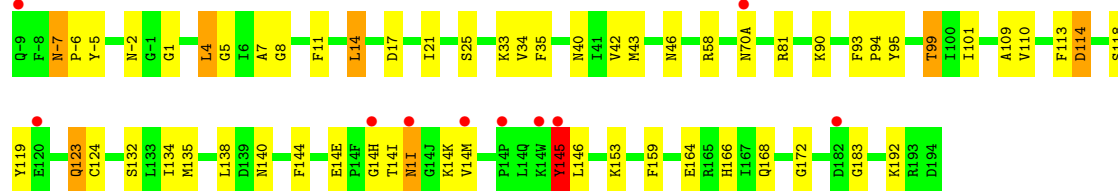
- Molecule 12: Proteasome component C5 precursor

Chain L:



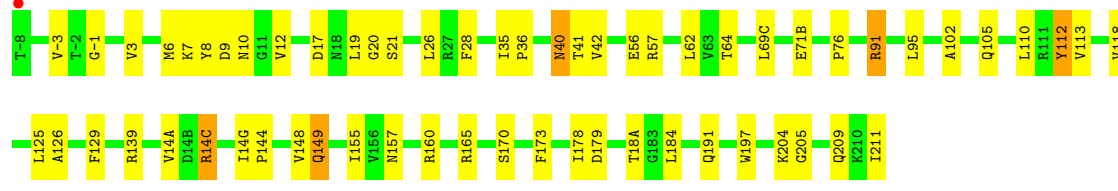
- Molecule 12: Proteasome component C5 precursor

Chain Z:

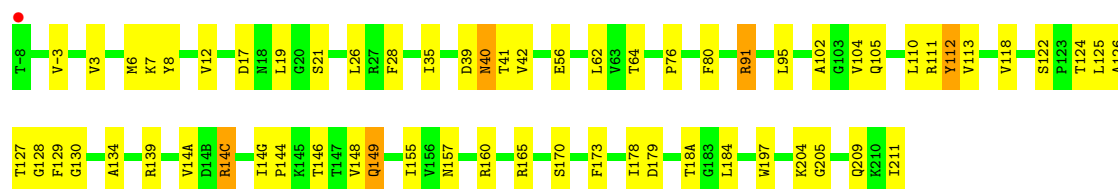


- Molecule 13: Proteasome component PRE4 precursor

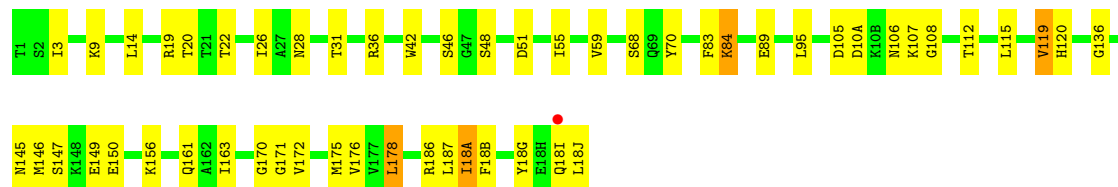
Chain M:



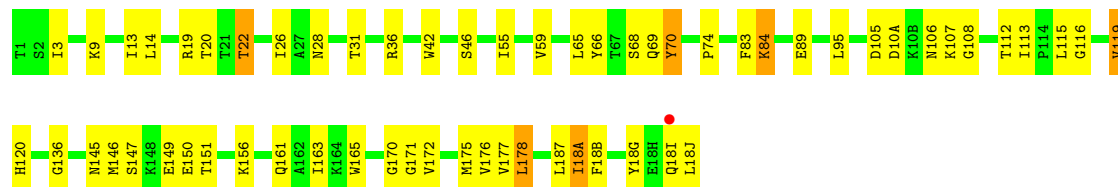
- Molecule 13: Proteasome component PRE4 precursor

Chain 1: 

- Molecule 14: Proteasome component PRE3 precursor

Chain N: 

- Molecule 14: Proteasome component PRE3 precursor

Chain 2: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	134.27Å 301.58Å 143.45Å 90.00° 112.70° 90.00°	Depositor
Resolution (Å)	15.00 – 2.60 19.99 – 2.56	Depositor EDS
% Data completeness (in resolution range)	98.2 (15.00-2.60) 98.0 (19.99-2.56)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.15 (at 2.56Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.240 , 0.266 0.239 , 0.264	Depositor DCC
$R_{free}$ test set	15649 reflections (4.98%)	DCC
Wilson B-factor (Å <sup>2</sup> )	47.3	Xtriage
Anisotropy	0.795	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 39.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	1 of 327957 reflections (0.000%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	51114	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.66% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

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

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	0.38	0/1952	0.63	0/2642
1	O	0.38	0/1952	0.63	0/2642
2	B	0.35	0/1935	0.62	0/2618
2	P	0.36	0/1935	0.62	0/2618
3	C	0.35	0/1920	0.60	0/2598
3	Q	0.35	0/1920	0.61	0/2598
4	D	0.35	0/1887	0.62	0/2541
4	R	0.35	0/1887	0.62	0/2541
5	E	0.36	0/1823	0.62	0/2463
5	S	0.36	0/1823	0.62	0/2463
6	F	0.38	0/1937	0.62	0/2614
6	T	0.39	0/1937	0.62	0/2614
7	G	0.42	0/1959	0.65	0/2652
7	U	0.41	0/1959	0.64	0/2652
8	H	0.39	0/1716	0.66	0/2326
8	V	0.39	0/1716	0.66	0/2326
9	I	0.40	0/1611	0.67	0/2174
9	W	0.41	0/1611	0.68	0/2174
10	J	0.39	0/1613	0.65	0/2173
10	X	0.39	0/1613	0.65	0/2173
11	K	0.42	0/1681	0.69	1/2274 (0.0%)
11	Y	0.43	0/1681	0.69	1/2274 (0.0%)
12	L	0.42	0/1795	0.70	1/2420 (0.0%)
12	Z	0.41	0/1795	0.69	1/2420 (0.0%)
13	1	0.40	0/1855	0.67	1/2514 (0.0%)
13	M	0.40	0/1855	0.67	1/2514 (0.0%)
14	2	0.41	0/1541	0.67	1/2087 (0.0%)
14	N	0.43	0/1541	0.67	0/2087
All	All	0.39	0/50450	0.65	7/68192 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying

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

Mol	Chain	#Chirality outliers	#Planarity outliers
12	L	0	1
12	Z	0	1
All	All	0	2

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	1	95	LEU	N-CA-C	-5.53	96.07	111.00
13	M	95	LEU	N-CA-C	-5.39	96.43	111.00
14	2	22	THR	N-CA-C	-5.16	97.07	111.00
11	K	98	GLY	N-CA-C	-5.16	100.21	113.10
11	Y	98	GLY	N-CA-C	-5.14	100.25	113.10
12	L	145	TYR	CA-CB-CG	-5.09	103.73	113.40
12	Z	145	TYR	CA-CB-CG	-5.09	103.73	113.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	L	145	TYR	Sidechain
12	Z	145	TYR	Sidechain

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1915	0	1926	59	0
1	O	1915	0	1926	58	0
2	B	1905	0	1901	97	0
2	P	1905	0	1901	91	0
3	C	1891	0	1900	107	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	Q	1891	0	1900	103	0
4	D	1862	0	1836	50	0
4	R	1862	0	1836	56	0
5	E	1795	0	1797	73	0
5	S	1795	0	1797	70	0
6	F	1897	0	1886	60	0
6	T	1897	0	1886	54	0
7	G	1921	0	1910	78	0
7	U	1921	0	1910	80	0
8	H	1685	0	1687	62	0
8	V	1685	0	1687	54	0
9	I	1581	0	1574	50	0
9	W	1581	0	1574	53	0
10	J	1585	0	1590	63	0
10	X	1585	0	1590	65	0
11	K	1644	0	1594	70	0
11	Y	1644	0	1594	71	0
12	L	1757	0	1711	52	0
12	Z	1757	0	1711	51	0
13	1	1824	0	1832	50	0
13	M	1824	0	1832	52	0
14	2	1512	0	1480	53	0
14	N	1512	0	1480	49	0
15	2	39	0	50	6	0
15	H	39	0	50	3	0
15	K	39	0	50	0	0
15	N	39	0	50	7	0
15	V	39	0	50	3	0
15	Y	39	0	50	0	0
16	1	74	0	0	4	0
16	2	59	0	0	1	0
16	A	55	0	0	4	0
16	B	36	0	0	1	0
16	C	46	0	0	1	0
16	D	42	0	0	2	0
16	E	23	0	0	1	0
16	F	46	0	0	2	0
16	G	62	0	0	3	0
16	H	51	0	0	3	0
16	I	66	0	0	2	0
16	J	53	0	0	3	0
16	K	42	0	0	6	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	L	56	0	0	4	0
16	M	68	0	0	6	0
16	N	59	0	0	2	0
16	O	35	0	0	0	0
16	P	29	0	0	2	0
16	Q	26	0	0	2	0
16	R	31	0	0	3	0
16	S	20	0	0	1	0
16	T	39	0	0	2	0
16	U	61	0	0	6	0
16	V	48	0	0	3	0
16	W	59	0	0	1	0
16	X	46	0	0	6	0
16	Y	48	0	0	13	0
16	Z	52	0	0	3	0
All	All	51114	0	49548	1656	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 17.

All (1656) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
11:K:10(B):LYS:H	11:K:10(B):LYS:HD2	1.10	1.16
8:V:3:ILE:HD11	8:V:127:LEU:HB2	1.33	1.10
8:H:3:ILE:HD11	8:H:127:LEU:HB2	1.33	1.10
3:Q:201:VAL:HG21	3:Q:210:ILE:HD11	1.10	1.09
11:Y:10(B):LYS:HD2	11:Y:10(B):LYS:H	1.11	1.09
3:C:201:VAL:HG21	3:C:210:ILE:HD11	1.10	1.06
4:D:175:GLU:HG2	4:D:196:ILE:HD12	1.36	1.06
7:U:9:ASP:HA	7:U:14:ILE:HD11	1.40	1.04
4:R:175:GLU:HG2	4:R:196:ILE:HD12	1.38	1.01
11:K:207:ASN:HD21	10:X:144:PRO:HG3	1.23	1.01
11:K:208:ASN:HD22	9:W:29:ASN:HD21	1.04	1.01
2:B:15:PHE:H	3:C:23:GLN:HE22	1.07	1.01
10:J:133:TYR:HD1	16:Y:232:HOH:O	1.44	1.00
13:M:157:ASN:HD22	13:M:160:ARG:HH11	1.10	0.99
7:G:9:ASP:HA	7:G:14:ILE:HD11	1.41	0.99
4:R:68:VAL:HG21	4:R:89:ILE:HD12	1.45	0.98
10:J:144:PRO:HG3	11:Y:207:ASN:HD21	1.25	0.98
10:J:133:TYR:HE1	16:X:225:HOH:O	1.45	0.97
3:C:100:ARG:NH1	3:C:106:PRO:HB3	1.80	0.97
1:A:15:PHE:H	2:B:23:GLN:HE22	1.11	0.96

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:D:68:VAL:HG21	4:D:89:ILE:HD12	1.47	0.96
3:C:163:GLN:NE2	3:C:164:THR:H	1.63	0.96
3:Q:100:ARG:NH1	3:Q:106:PRO:HB3	1.79	0.96
1:O:130:ARG:HH21	7:U:124:THR:HG22	1.27	0.96
2:P:202:THR:HG22	2:P:204:SER:H	1.29	0.95
7:U:96:ALA:HA	7:U:107:MET:HE2	1.44	0.95
2:B:202:THR:HG22	2:B:204:SER:H	1.31	0.95
11:K:207:ASN:ND2	10:X:144:PRO:HG3	1.82	0.95
3:Q:185:THR:HB	3:Q:188:GLU:HG2	1.49	0.95
3:Q:163:GLN:NE2	3:Q:164:THR:H	1.64	0.95
3:C:163:GLN:HE21	3:C:164:THR:N	1.66	0.94
12:Z:123:GLN:HG3	12:Z:145:TYR:OH	1.68	0.93
7:G:96:ALA:HA	7:G:107:MET:HE2	1.48	0.93
3:Q:163:GLN:HE21	3:Q:164:THR:N	1.67	0.93
1:O:124:THR:HG22	2:P:130:ARG:HH21	1.32	0.92
1:O:15:PHE:H	2:P:23:GLN:HE22	1.03	0.92
9:I:29:ASN:HD21	11:Y:208:ASN:HD22	1.01	0.92
3:C:185:THR:HB	3:C:188:GLU:HG2	1.50	0.92
10:J:144:PRO:HG3	11:Y:207:ASN:ND2	1.85	0.92
3:Q:15:PHE:H	4:R:23:GLN:HE22	1.13	0.92
2:B:124:THR:HG22	3:C:130:ARG:HH21	1.35	0.91
12:L:123:GLN:HG3	12:L:145:TYR:OH	1.67	0.91
9:I:29:ASN:HD21	11:Y:208:ASN:ND2	1.69	0.91
14:2:84:LYS:HG3	14:2:119:VAL:HG22	1.52	0.91
12:L:4:LEU:HD13	12:L:138:LEU:HD21	1.53	0.91
1:A:130:ARG:HH21	7:G:124:THR:HG22	1.37	0.90
13:1:157:ASN:HD22	13:1:160:ARG:HH11	1.11	0.90
14:N:84:LYS:HG3	14:N:119:VAL:HG22	1.51	0.90
11:Y:67:GLU:OE1	11:Y:73:ARG:HA	1.71	0.90
11:K:67:GLU:OE1	11:K:73:ARG:HA	1.72	0.89
5:S:2(B):THR:H	5:S:2(E):ASN:HD22	1.15	0.89
12:Z:4:LEU:HD13	12:Z:138:LEU:HD21	1.54	0.89
3:C:15:PHE:H	4:D:23:GLN:HE22	1.16	0.89
1:O:86:ARG:HE	7:U:118:ASN:HD21	1.19	0.88
5:E:2(B):THR:H	5:E:2(E):ASN:HD22	1.15	0.88
3:Q:201:VAL:CG2	3:Q:210:ILE:HD11	2.03	0.88
11:K:99:THR:HG22	11:K:113:VAL:O	1.74	0.88
11:K:208:ASN:ND2	9:W:29:ASN:HD21	1.71	0.87
13:M:139:ARG:HH11	8:V:165:ASN:HD22	1.22	0.87
5:S:207:LEU:HD23	5:S:207:LEU:H	1.39	0.87
1:O:130:ARG:HH21	7:U:124:THR:CG2	1.87	0.86
6:T:95:GLU:HG2	6:T:115:ARG:HB3	1.57	0.86

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:E:201:LEU:HD11	5:E:207:LEU:HD22	1.57	0.86
5:E:207:LEU:HD23	5:E:207:LEU:H	1.39	0.86
5:S:15:PHE:H	6:T:23:GLN:HE22	1.24	0.86
10:X:59:ILE:HD13	10:X:83:VAL:HG22	1.57	0.85
1:A:124:THR:HG22	2:B:130:ARG:HH21	1.42	0.85
10:J:59:ILE:HD13	10:J:83:VAL:HG22	1.58	0.85
6:F:95:GLU:HG2	6:F:115:ARG:HB3	1.57	0.84
13:1:157:ASN:HD22	13:1:160:ARG:NH1	1.75	0.84
8:H:165:ASN:HD22	13:1:139:ARG:HH11	1.19	0.84
2:P:15:PHE:H	3:Q:23:GLN:HE22	1.22	0.84
10:J:-1:MET:HG2	10:J:1:ASP:H	1.43	0.83
13:M:157:ASN:HD22	13:M:160:ARG:NH1	1.74	0.83
5:S:201:LEU:HD11	5:S:207:LEU:HD22	1.58	0.83
11:Y:210:ILE:HB	16:Y:248:HOH:O	1.78	0.83
3:C:201:VAL:CG2	3:C:210:ILE:HD11	2.03	0.83
7:U:170:GLN:HE21	7:U:174:THR:HG23	1.43	0.83
7:G:170:GLN:HE21	7:G:174:THR:HG23	1.44	0.83
2:P:124:THR:HG22	3:Q:130:ARG:HH21	1.44	0.82
14:N:161:GLN:HE21	14:2:136:GLY:HA2	1.44	0.82
11:Y:99:THR:HG22	11:Y:113:VAL:O	1.79	0.82
4:D:175:GLU:HG2	4:D:196:ILE:CD1	2.10	0.82
7:U:96:ALA:HA	7:U:107:MET:CE	2.08	0.82
7:G:96:ALA:HA	7:G:107:MET:CE	2.08	0.82
9:I:29:ASN:ND2	11:Y:208:ASN:HD22	1.77	0.81
5:E:15:PHE:H	6:F:23:GLN:HE22	1.28	0.81
14:N:136:GLY:HA2	14:2:161:GLN:HE21	1.46	0.81
8:V:163:ILE:HG23	8:V:170:GLY:HA2	1.62	0.80
3:Q:185:THR:HG22	3:Q:187:GLU:H	1.45	0.80
1:O:86:ARG:HE	7:U:118:ASN:ND2	1.77	0.80
1:A:130:ARG:HH21	7:G:124:THR:CG2	1.94	0.80
8:H:163:ILE:HG23	8:H:170:GLY:HA2	1.63	0.80
3:C:164:THR:HG21	3:C:172:VAL:HG13	1.65	0.79
3:C:185:THR:HG22	3:C:187:GLU:H	1.46	0.79
13:M:157:ASN:ND2	13:M:160:ARG:HH11	1.80	0.79
3:Q:164:THR:HG21	3:Q:172:VAL:HG13	1.65	0.79
2:P:202:THR:HG22	2:P:204:SER:N	1.98	0.79
1:O:124:THR:CG2	2:P:130:ARG:HH21	1.96	0.79
10:X:-1:MET:HG2	10:X:1:ASP:H	1.45	0.79
4:R:177:LEU:HD22	5:S:58:LEU:HD13	1.64	0.79
11:K:208:ASN:HD22	9:W:29:ASN:ND2	1.80	0.79
7:U:35:ILE:HG23	7:U:51:GLN:HB2	1.63	0.78
7:G:35:ILE:HG23	7:G:51:GLN:HB2	1.64	0.78

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
11:K:10(B):LYS:N	11:K:10(B):LYS:HD2	1.95	0.78
7:U:67:ILE:HD12	7:U:211:GLU:HG2	1.66	0.78
8:H:41:ILE:HD12	8:H:76:VAL:HG22	1.66	0.78
1:O:20:LYS:HE3	1:O:25:ASP:OD1	1.84	0.78
13:1:157:ASN:ND2	13:1:160:ARG:HH11	1.81	0.77
2:P:186:VAL:HG11	2:P:216:ARG:HD3	1.65	0.77
2:B:186:VAL:HG11	2:B:216:ARG:HD3	1.67	0.77
12:L:14:LEU:HD13	12:L:34:VAL:HG13	1.66	0.77
4:R:175:GLU:HG2	4:R:196:ILE:CD1	2.14	0.77
9:I:29:ASN:ND2	11:Y:208:ASN:ND2	2.32	0.77
14:N:136:GLY:HA2	14:2:161:GLN:NE2	1.99	0.77
12:Z:14:LEU:HD13	12:Z:34:VAL:HG13	1.67	0.76
1:A:20:LYS:HE3	1:A:25:ASP:OD1	1.85	0.76
6:F:35:THR:HG23	6:F:51:GLU:HB3	1.68	0.76
14:N:161:GLN:NE2	14:2:136:GLY:HA2	2.00	0.76
5:S:18(D):ILE:HD13	5:S:18(D):ILE:O	1.86	0.76
2:B:202:THR:HG22	2:B:204:SER:N	1.99	0.76
2:B:160:TRP:CE2	2:B:163:ILE:HD12	2.21	0.76
6:F:20(B):GLU:HG3	6:F:20(C):LYS:HG3	1.66	0.76
6:F:192:GLN:O	6:F:196:ILE:HG12	1.85	0.76
6:T:20(B):GLU:HG3	6:T:20(C):LYS:HG3	1.67	0.75
12:L:166:HIS:HD2	12:L:168:GLN:H	1.33	0.75
2:P:160:TRP:CE2	2:P:163:ILE:HD12	2.21	0.75
11:Y:143:LYS:O	11:Y:146:LEU:HD13	1.85	0.75
12:Z:166:HIS:HD2	12:Z:168:GLN:H	1.32	0.75
7:G:67:ILE:HD12	7:G:211:GLU:HG2	1.67	0.75
6:T:35:THR:HG23	6:T:51:GLU:HB3	1.68	0.75
1:A:86:ARG:HE	7:G:118:ASN:HD21	1.33	0.75
3:C:100:ARG:HH11	3:C:106:PRO:HB3	1.50	0.74
4:R:185:THR:OG1	4:R:188:GLU:HG3	1.87	0.74
4:R:52:LYS:HE3	4:R:211:GLN:HB2	1.68	0.74
4:D:177:LEU:HD22	5:E:58:LEU:HD13	1.68	0.74
13:1:42:VAL:HG23	13:1:178:ILE:HD11	1.70	0.74
14:2:36:ARG:HG3	14:2:42:TRP:CE2	2.23	0.74
11:K:208:ASN:ND2	9:W:29:ASN:ND2	2.35	0.74
6:T:36:THR:HG22	6:T:51:GLU:OE2	1.88	0.74
11:Y:10(B):LYS:HD2	11:Y:10(B):LYS:N	1.96	0.74
6:F:35:THR:HG21	6:F:51:GLU:O	1.88	0.73
6:F:36:THR:HG22	6:F:51:GLU:OE2	1.87	0.73
4:D:12(D):ALA:HB3	4:D:126:ARG:HD3	1.71	0.73
4:D:52:LYS:HE3	4:D:211:GLN:HB2	1.69	0.73
8:H:201:GLN:HG3	12:Z:153:LYS:HG2	1.71	0.73

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
11:K:10(B):LYS:H	11:K:10(B):LYS:CD	1.90	0.73
2:P:186:VAL:HG21	2:P:216:ARG:HD3	1.70	0.73
6:T:192:GLN:O	6:T:196:ILE:HG12	1.87	0.73
11:K:143:LYS:O	11:K:146:LEU:HD13	1.89	0.73
7:G:77:VAL:HG12	7:G:137:THR:HB	1.71	0.73
5:E:207:LEU:HA	5:E:2(E):ASN:ND2	2.03	0.73
4:D:97:VAL:HG21	11:K:65:LEU:HD13	1.70	0.73
2:B:185:LYS:HD3	2:B:186:VAL:N	2.04	0.72
8:V:172:ASN:HD22	8:V:193:THR:HA	1.54	0.72
6:T:237:GLN:O	6:T:240:ILE:HG22	1.89	0.72
13:M:42:VAL:HG23	13:M:178:ILE:HD11	1.71	0.72
1:A:124:THR:CG2	2:B:130:ARG:HH21	2.02	0.72
8:H:165:ASN:HD22	13:1:139:ARG:NH1	1.87	0.72
13:M:110:LEU:HG	13:M:125:LEU:HD12	1.71	0.72
5:S:207:LEU:HA	5:S:2(E):ASN:ND2	2.03	0.72
6:T:35:THR:HG21	6:T:51:GLU:O	1.89	0.72
12:Z:-7:ASN:ND2	12:Z:-5:TYR:H	1.88	0.72
8:H:172:ASN:HD22	8:H:193:THR:HA	1.55	0.72
3:Q:100:ARG:HH11	3:Q:106:PRO:HB3	1.52	0.72
2:B:186:VAL:HG21	2:B:216:ARG:HD3	1.71	0.72
14:N:36:ARG:HG3	14:N:42:TRP:CE2	2.23	0.72
5:E:18(D):ILE:O	5:E:18(D):ILE:HD13	1.89	0.72
7:U:217:LYS:HE3	7:U:217:LYS:HA	1.70	0.72
8:V:41:ILE:HD12	8:V:76:VAL:HG22	1.72	0.72
15:N:0:FEB:H14	15:N:0:FEB:H33	1.72	0.72
8:H:3:ILE:HD11	8:H:127:LEU:CB	2.18	0.72
3:Q:106:PRO:HG2	3:Q:143:PRO:HG3	1.72	0.71
4:D:185:THR:OG1	4:D:188:GLU:HG3	1.89	0.71
7:G:217:LYS:HA	7:G:217:LYS:HE3	1.71	0.71
13:1:110:LEU:HG	13:1:125:LEU:HD12	1.72	0.71
4:R:12(D):ALA:HB3	4:R:126:ARG:HD3	1.71	0.71
8:H:165:ASN:ND2	13:1:139:ARG:HH11	1.87	0.71
15:2:0:FEB:H14	15:2:0:FEB:H33	1.71	0.71
11:K:67:GLU:CD	11:K:73:ARG:HA	2.10	0.71
3:Q:185:THR:HG22	3:Q:187:GLU:N	2.05	0.71
3:Q:163:GLN:HE21	3:Q:164:THR:H	0.82	0.71
12:L:153:LYS:HG2	8:V:201:GLN:HG3	1.71	0.71
8:V:3:ILE:HD11	8:V:127:LEU:CB	2.19	0.71
13:M:57:ARG:NE	16:M:244:HOH:O	2.23	0.71
14:N:22:THR:HG22	15:N:0:FEB:N25	2.06	0.70
2:P:185:LYS:HD3	2:P:186:VAL:N	2.06	0.70
6:F:237:GLN:O	6:F:240:ILE:HG22	1.91	0.70

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
14:2:22:THR:HG22	15:2:0:FEB:N25	2.06	0.70
3:C:185:THR:HG22	3:C:187:GLU:N	2.05	0.70
11:Y:67:GLU:CD	11:Y:73:ARG:HA	2.11	0.70
3:C:106:PRO:HG2	3:C:143:PRO:HG3	1.72	0.69
14:N:84:LYS:HG3	14:N:119:VAL:CG2	2.21	0.69
2:P:61:GLN:OE1	2:P:208:ASP:HA	1.92	0.69
9:W:29:ASN:H	9:W:29:ASN:ND2	1.90	0.69
3:C:41:LYS:HG2	3:C:161:SER:O	1.91	0.69
5:E:207:LEU:CD2	5:E:207:LEU:H	2.06	0.69
10:J:146:MET:HE3	10:J:150:GLU:HB3	1.75	0.69
13:1:7:LYS:HG3	13:1:14(G):ILE:HD12	1.74	0.69
4:R:97:VAL:HG21	11:Y:65:LEU:HD13	1.73	0.69
5:S:207:LEU:H	5:S:207:LEU:CD2	2.06	0.69
2:B:121:GLN:O	2:B:124:THR:HB	1.93	0.69
13:M:139:ARG:HH11	8:V:165:ASN:ND2	1.90	0.69
1:O:179:ARG:HH11	1:O:179:ARG:HB3	1.56	0.68
2:B:15:PHE:H	3:C:23:GLN:NE2	1.88	0.68
14:2:22:THR:CG2	15:2:0:FEB:N25	2.57	0.68
11:Y:38:ASN:ND2	16:Y:258:HOH:O	2.25	0.68
12:L:-7:ASN:ND2	12:L:-5:TYR:H	1.92	0.68
3:Q:168:ASN:HB2	3:Q:200:VAL:HG11	1.74	0.68
11:Y:181:ASP:N	16:Y:240:HOH:O	2.18	0.68
1:A:179:ARG:HB3	1:A:179:ARG:HH11	1.57	0.68
4:R:192:LEU:O	4:R:196:ILE:HG12	1.95	0.67
7:U:77:VAL:HG12	7:U:137:THR:HB	1.75	0.67
10:J:52:THR:HG22	10:J:53:VAL:N	2.09	0.67
2:B:124:THR:CG2	3:C:130:ARG:HH21	2.04	0.67
3:C:216:LYS:HB2	3:C:220:ASP:HB3	1.77	0.67
9:I:2:ILE:HD13	9:I:159:LEU:CD1	2.24	0.67
9:I:6:MET:HE1	9:I:155:ILE:HA	1.76	0.67
2:B:97:GLN:HE22	9:I:64:ASN:HD22	1.41	0.67
13:M:139:ARG:NH1	8:V:165:ASN:HD22	1.91	0.67
10:J:112:GLN:NE2	16:J:234:HOH:O	2.26	0.67
14:2:84:LYS:HG3	14:2:119:VAL:CG2	2.23	0.67
3:C:168:ASN:HB2	3:C:200:VAL:HG11	1.77	0.67
1:O:86:ARG:HH21	7:U:118:ASN:HD22	1.43	0.67
2:B:149:TYR:OH	3:C:62(A):ILE:HB	1.95	0.67
2:P:97:GLN:HE22	9:W:64:ASN:HD22	1.41	0.67
1:A:21(G):LEU:HD13	1:A:218:GLY:HA2	1.75	0.67
14:2:20:THR:HG22	15:2:0:FEB:H8A	1.75	0.67
2:B:61:GLN:OE1	2:B:208:ASP:HA	1.94	0.67
11:K:4:LEU:HD12	11:K:159:ILE:HD11	1.76	0.67

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:G:87:ASN:HD22	7:G:87:ASN:C	1.98	0.67
9:I:2:ILE:HD13	9:I:159:LEU:HD11	1.75	0.66
7:G:77:VAL:CG1	7:G:137:THR:HB	2.26	0.66
7:U:87:ASN:HD22	7:U:87:ASN:C	1.99	0.66
14:N:22:THR:CG2	15:N:0:FEB:N25	2.58	0.66
5:S:227:GLU:CD	5:S:227:GLU:H	1.98	0.66
13:1:40:ASN:HD22	13:1:40:ASN:H	1.42	0.66
11:Y:10(B):LYS:CD	11:Y:10(B):LYS:H	1.91	0.66
3:Q:55:THR:HG22	3:Q:56:LEU:HD22	1.77	0.66
1:O:21(G):LEU:HD13	1:O:218:GLY:HA2	1.78	0.66
14:2:18(A):ILE:HD13	14:2:18(B):PHE:N	2.11	0.66
3:Q:41:LYS:HG2	3:Q:161:SER:O	1.95	0.66
10:X:52:THR:HG22	10:X:53:VAL:N	2.11	0.66
12:L:135:MET:CE	9:W:165:ARG:NH2	2.58	0.66
8:H:3:ILE:HD13	8:H:3:ILE:O	1.96	0.66
11:Y:4:LEU:HD12	11:Y:159:ILE:HD11	1.78	0.66
3:Q:106:PRO:HG2	3:Q:143:PRO:CG	2.25	0.66
9:W:2:ILE:HD13	9:W:159:LEU:CD1	2.26	0.66
9:W:2:ILE:HD13	9:W:159:LEU:HD11	1.76	0.66
13:M:7:LYS:HG3	13:M:14(G):ILE:HD12	1.77	0.65
3:Q:197:LEU:O	3:Q:201:VAL:HG23	1.95	0.65
10:X:146:MET:HE3	10:X:150:GLU:HB3	1.77	0.65
13:M:40:ASN:H	13:M:40:ASN:HD22	1.43	0.65
9:I:29:ASN:H	9:I:29:ASN:ND2	1.93	0.65
1:O:179:ARG:NH1	1:O:179:ARG:HB3	2.12	0.65
8:V:3:ILE:O	8:V:3:ILE:HD13	1.97	0.65
3:C:163:GLN:HE22	3:C:173:ARG:HE	1.45	0.65
11:K:73:ARG:NH2	11:K:104:TYR:O	2.30	0.65
3:C:106:PRO:HG2	3:C:143:PRO:CG	2.26	0.65
10:X:-1:MET:HG2	10:X:1:ASP:N	2.12	0.65
5:E:227:GLU:CD	5:E:227:GLU:H	1.98	0.65
10:J:6:ILE:HD11	10:J:154:LEU:HD23	1.79	0.65
5:S:132:TYR:O	5:S:153:PRO:HB3	1.98	0.65
2:B:160:TRP:HA	3:C:59:GLN:HA	1.78	0.64
3:Q:216:LYS:HB2	3:Q:220:ASP:HB3	1.78	0.64
8:H:24:PRO:HG2	8:H:25:ILE:HD12	1.78	0.64
7:U:121:GLN:O	7:U:124:THR:HB	1.97	0.64
10:J:-1:MET:HG2	10:J:1:ASP:N	2.10	0.64
3:C:55:THR:HG22	3:C:56:LEU:HD22	1.79	0.64
3:C:175:PHE:O	3:C:179:ASN:HB2	1.96	0.64
6:T:173:LYS:O	6:T:177:GLU:HG3	1.97	0.64
2:P:121:GLN:O	2:P:124:THR:HB	1.96	0.64

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:P:181:LYS:O	2:P:184:MET:HG3	1.96	0.64
14:N:20:THR:HG22	15:N:0:FEB:H8A	1.77	0.64
2:B:181:LYS:O	2:B:184:MET:HG3	1.98	0.64
7:G:198:ILE:HG23	7:G:203:THR:O	1.97	0.64
6:T:127:ASN:HD22	6:T:128:SER:N	1.96	0.64
12:Z:99:THR:HG23	16:Z:201:HOH:O	1.98	0.64
14:N:18(A):ILE:HD13	14:N:18(B):PHE:N	2.13	0.64
12:Z:109:ALA:HA	16:Z:205:HOH:O	1.97	0.64
13:1:42:VAL:CG2	13:1:178:ILE:HD11	2.28	0.64
6:T:179:LEU:HD21	6:T:192:GLN:HG2	1.80	0.64
10:J:133:TYR:OH	10:X:24:ILE:O	2.16	0.64
6:F:127:ASN:HD22	6:F:128:SER:N	1.95	0.64
8:V:24:PRO:HG2	8:V:25:ILE:HD12	1.78	0.64
9:W:6:MET:HE3	9:W:155:ILE:HG13	1.79	0.63
11:K:4:LEU:CD1	11:K:159:ILE:HD11	2.29	0.63
3:C:195:ARG:HG3	3:C:236:ILE:HD13	1.79	0.63
2:P:6:ARG:HG2	3:Q:10:ARG:HH21	1.64	0.63
7:U:55:PRO:HG2	7:U:56:ASP:H	1.64	0.63
7:G:55:PRO:HG2	7:G:56:ASP:H	1.63	0.63
11:Y:143:LYS:HB2	11:Y:146:LEU:CD1	2.28	0.63
3:C:41:LYS:HD3	3:C:161:SER:HA	1.80	0.63
9:I:165:ARG:NH2	12:Z:135:MET:CE	2.62	0.63
8:V:112:SER:HB3	8:V:125:LEU:HD13	1.80	0.63
3:Q:65:SER:HB2	16:Q:246:HOH:O	1.96	0.63
11:Y:73:ARG:NH2	11:Y:104:TYR:O	2.31	0.63
10:X:6:ILE:HD11	10:X:154:LEU:HD23	1.80	0.63
1:O:188:ASP:O	1:O:192:ILE:HG12	1.99	0.63
10:J:38:SER:HB2	10:J:39:PRO:HD2	1.81	0.63
3:Q:195:ARG:HG3	3:Q:236:ILE:HD13	1.79	0.63
3:Q:175:PHE:O	3:Q:179:ASN:HB2	1.99	0.63
1:A:188:ASP:O	1:A:192:ILE:HG12	1.98	0.63
3:C:197:LEU:O	3:C:201:VAL:HG23	1.98	0.62
10:X:38:SER:HB2	10:X:39:PRO:HD2	1.79	0.62
10:J:24:ILE:O	10:X:133:TYR:OH	2.17	0.62
1:A:86:ARG:HE	7:G:118:ASN:ND2	1.95	0.62
7:U:77:VAL:CG1	7:U:137:THR:HB	2.28	0.62
11:Y:67:GLU:OE2	16:Y:255:HOH:O	2.16	0.62
12:Z:43:MET:HB2	12:Z:101:ILE:HG22	1.79	0.62
5:E:2(B):THR:N	5:E:2(E):ASN:HD22	1.95	0.62
3:Q:190:VAL:O	3:Q:194:VAL:HG23	1.99	0.62
5:S:75:GLY:HA3	5:S:221:PHE:CE2	2.34	0.62
5:E:226:GLY:O	5:E:229:VAL:HG22	2.00	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
11:K:143:LYS:HB2	11:K:146:LEU:CD1	2.29	0.62
13:M:42:VAL:CG2	13:M:178:ILE:HD11	2.30	0.62
1:A:179:ARG:HB3	1:A:179:ARG:NH1	2.14	0.62
14:N:112:THR:HG22	14:N:120:HIS:HB2	1.81	0.62
3:C:190:VAL:O	3:C:194:VAL:HG23	2.00	0.62
6:F:173:LYS:O	6:F:177:GLU:HG3	1.99	0.62
3:Q:163:GLN:HE22	3:Q:173:ARG:HE	1.47	0.62
6:F:175:GLU:HB3	6:F:196:ILE:HD12	1.82	0.62
9:I:2:ILE:CD1	9:I:159:LEU:HD11	2.30	0.62
11:K:181:ASP:N	16:K:239:HOH:O	2.32	0.62
5:S:207:LEU:N	5:S:207:LEU:HD23	2.14	0.62
4:D:192:LEU:O	4:D:196:ILE:HG12	2.00	0.62
1:O:118:LYS:HE2	1:O:122:GLU:OE1	2.00	0.62
11:Y:40:PHE:HB3	11:Y:73:ARG:HH21	1.64	0.61
10:J:147:THR:OG1	10:J:150:GLU:HG3	2.00	0.61
13:1:12:VAL:HG21	13:1:102:ALA:HB1	1.82	0.61
1:A:110:LYS:HG2	16:A:245:HOH:O	2.00	0.61
11:K:40:PHE:HB3	11:K:73:ARG:HH21	1.65	0.61
1:A:118:LYS:HE2	1:A:122:GLU:OE1	2.00	0.61
4:R:237:LEU:HD22	4:R:241:GLU:HG3	1.82	0.61
10:X:156:LYS:O	10:X:160:GLN:HG3	2.01	0.61
11:K:44:THR:OG1	11:K:100:MET:HB2	2.00	0.61
10:J:55:PHE:CZ	10:J:59:ILE:HD11	2.36	0.61
14:2:112:THR:HG22	14:2:120:HIS:HB2	1.81	0.61
6:T:175:GLU:HB3	6:T:196:ILE:HD12	1.82	0.61
7:U:198:ILE:HG23	7:U:203:THR:O	2.01	0.61
2:B:202:THR:CG2	2:B:204:SER:H	2.10	0.61
4:D:186:LEU:O	4:D:190:GLU:HG3	2.01	0.61
11:Y:174:ASN:HD21	11:Y:189:ASN:HD22	1.49	0.61
12:L:109:ALA:HA	16:L:233:HOH:O	1.99	0.61
12:L:-7:ASN:HD22	12:L:-6:PRO:HD2	1.66	0.61
10:J:178:VAL:HG22	10:J:184:ILE:HG12	1.83	0.61
9:W:174:VAL:HG21	9:W:186:LYS:HE3	1.82	0.61
5:E:207:LEU:N	5:E:207:LEU:HD23	2.14	0.61
3:Q:41:LYS:HD3	3:Q:161:SER:HA	1.82	0.61
14:2:55:ILE:HD11	14:2:95:LEU:HD13	1.82	0.61
5:E:132:TYR:O	5:E:153:PRO:HB3	1.99	0.61
2:B:163:ILE:HG12	2:B:164:SER:N	2.15	0.61
2:B:126:HIS:HB3	3:C:129:VAL:HG12	1.83	0.61
13:1:148:VAL:HG23	16:1:228:HOH:O	2.01	0.61
11:Y:44:THR:OG1	11:Y:100:MET:HB2	2.01	0.61
5:E:12:THR:HG21	5:E:124:THR:HA	1.83	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:E:198:SER:HA	5:E:201:LEU:HG	1.83	0.60
2:P:163:ILE:HG12	2:P:164:SER:N	2.15	0.60
10:X:6:ILE:CD1	10:X:154:LEU:HD23	2.31	0.60
6:T:184:LEU:HD11	6:T:188:GLU:HB3	1.83	0.60
7:G:121:GLN:O	7:G:124:THR:HB	2.00	0.60
5:E:2(B):THR:OG1	5:E:2(E):ASN:HB3	2.00	0.60
10:J:146:MET:CE	10:J:150:GLU:HB3	2.31	0.60
10:J:6:ILE:CD1	10:J:154:LEU:HD23	2.31	0.60
3:Q:46:VAL:O	3:Q:215:VAL:HG12	2.01	0.60
16:P:250:HOH:O	3:Q:87:ILE:HD11	2.00	0.60
5:S:12:THR:HG21	5:S:124:THR:HA	1.83	0.60
2:P:202:THR:CG2	2:P:204:SER:H	2.10	0.60
9:I:1:GLY:HA3	9:I:33:LYS:HE2	1.83	0.60
4:D:112:LEU:C	4:D:112:LEU:HD13	2.21	0.60
14:N:55:ILE:HD11	14:N:95:LEU:HD13	1.84	0.60
4:D:237:LEU:HD22	4:D:241:GLU:HG3	1.82	0.60
9:W:2:ILE:HG21	9:W:130:ALA:HB3	1.84	0.60
10:J:20:VAL:HG11	11:K:120:LEU:HD11	1.83	0.60
6:F:184:LEU:HD11	6:F:188:GLU:HB3	1.84	0.60
8:V:80:LEU:HD12	8:V:113:ILE:HD11	1.83	0.60
6:F:179:LEU:HD21	6:F:192:GLN:HG2	1.83	0.60
11:K:4:LEU:HD12	11:K:159:ILE:CD1	2.32	0.60
13:M:12:VAL:HG21	13:M:102:ALA:HB1	1.82	0.60
1:A:177:GLU:HG2	2:B:58:LEU:HD22	1.83	0.60
3:C:15:PHE:CE1	3:C:21:ILE:HD11	2.37	0.60
8:V:113:ILE:HG12	8:V:119:THR:HG22	1.84	0.60
14:N:175:MET:HB2	14:N:187:LEU:HB2	1.83	0.60
2:P:126:HIS:HB3	3:Q:129:VAL:HG12	1.83	0.60
3:Q:197:LEU:HD13	3:Q:210:ILE:HD12	1.82	0.60
3:C:46:VAL:O	3:C:215:VAL:HG12	2.02	0.60
11:Y:104:TYR:CE1	11:Y:180:GLU:OE2	2.55	0.59
5:S:2(B):THR:OG1	5:S:2(E):ASN:HB3	2.02	0.59
7:U:67:ILE:CD1	7:U:211:GLU:HG2	2.31	0.59
10:X:146:MET:CE	10:X:150:GLU:HB3	2.32	0.59
14:2:22:THR:HG22	15:2:0:FEB:HN25	1.67	0.59
2:B:141:TYR:CD1	2:B:21(E):VAL:HG21	2.38	0.59
8:H:72:ARG:HH11	8:H:72:ARG:HG3	1.68	0.59
10:X:147:THR:OG1	10:X:150:GLU:HG3	2.00	0.59
7:G:39:ALA:HB2	7:G:48:VAL:HG12	1.83	0.59
9:I:174:VAL:HG21	9:I:186:LYS:HE3	1.84	0.59
11:Y:4:LEU:CD1	11:Y:159:ILE:HD11	2.33	0.59
9:W:2:ILE:CD1	9:W:159:LEU:HD11	2.32	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
12:L:43:MET:HB2	12:L:101:ILE:HG22	1.84	0.59
3:C:197:LEU:HD13	3:C:210:ILE:HD12	1.83	0.59
5:S:2(B):THR:N	5:S:2(E):ASN:HD22	1.95	0.59
3:C:141:PHE:CE1	3:C:217:PRO:HG3	2.37	0.59
6:T:186:ALA:O	6:T:190:VAL:HG23	2.02	0.59
13:1:14(C):ARG:HG3	13:1:14(C):ARG:HH11	1.67	0.59
9:W:48:LEU:HG	9:W:50:THR:HG22	1.84	0.59
10:X:161:GLU:OE2	10:X:161:GLU:HA	2.02	0.59
10:J:-1:MET:N	16:J:246:HOH:O	2.32	0.59
5:S:226:GLY:O	5:S:229:VAL:HG22	2.03	0.59
5:E:75:GLY:HA3	5:E:221:PHE:CE2	2.37	0.59
2:P:186:VAL:HG11	2:P:216:ARG:CD	2.33	0.59
8:V:84:LYS:HG3	8:V:85:GLN:N	2.17	0.59
3:Q:227:GLU:N	3:Q:227:GLU:OE1	2.36	0.59
8:V:172:ASN:ND2	8:V:193:THR:HA	2.17	0.59
3:C:186:VAL:O	3:C:190:VAL:HG23	2.03	0.59
11:K:174:ASN:HD21	11:K:189:ASN:HD22	1.49	0.59
3:C:163:GLN:HE21	3:C:164:THR:H	0.80	0.58
4:D:12(D):ALA:HB3	4:D:126:ARG:CD	2.33	0.58
3:Q:186:VAL:O	3:Q:190:VAL:HG23	2.03	0.58
8:H:128:GLY:O	8:H:131:SER:HB2	2.02	0.58
10:X:178:VAL:HG22	10:X:184:ILE:HG12	1.84	0.58
10:J:156:LYS:O	10:J:160:GLN:HG3	2.03	0.58
12:Z:-7:ASN:HD22	12:Z:-7:ASN:C	2.07	0.58
8:H:80:LEU:HD12	8:H:113:ILE:HD11	1.85	0.58
9:I:48:LEU:HG	9:I:50:THR:HG22	1.85	0.58
5:S:221:PHE:CE1	5:S:223:ILE:HD11	2.39	0.58
7:G:18(G):GLU:HG2	7:G:188:LYS:CB	2.34	0.58
13:M:35:ILE:HG12	13:M:56:GLU:CG	2.34	0.58
5:S:198:SER:HA	5:S:201:LEU:HG	1.84	0.58
13:1:76:PRO:HD2	13:1:105:GLN:OE1	2.04	0.58
3:Q:141:PHE:CE1	3:Q:217:PRO:HG3	2.39	0.58
10:X:44:SER:OG	10:X:100:LEU:HB2	2.04	0.58
7:U:39:ALA:HB2	7:U:48:VAL:HG12	1.84	0.58
1:A:86:ARG:HH21	7:G:118:ASN:HD22	1.49	0.58
8:H:172:ASN:ND2	8:H:193:THR:HA	2.18	0.58
14:N:107:LYS:HG2	14:N:108:GLY:N	2.18	0.58
13:1:149:GLN:H	13:1:149:GLN:NE2	2.02	0.58
14:N:22:THR:HG22	15:N:0:FEB:HN25	1.67	0.58
7:U:228:ASN:HB3	16:U:242:HOH:O	2.03	0.58
2:B:234:VAL:HA	2:B:239:THR:HA	1.85	0.58
4:R:121:LEU:HA	4:R:123:PHE:CE1	2.39	0.58

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:S:35:SER:HB3	5:S:66:LYS:HZ3	1.68	0.58
7:G:67:ILE:CD1	7:G:211:GLU:HG2	2.33	0.58
5:S:227:GLU:N	5:S:227:GLU:CD	2.57	0.58
5:E:175:TYR:CD2	5:E:196:ALA:HA	2.39	0.58
4:D:85:ALA:O	4:D:89:ILE:HG12	2.03	0.58
11:K:104:TYR:CE1	11:K:180:GLU:OE2	2.57	0.58
3:C:57:LYS:O	3:C:58:LEU:HB2	2.02	0.58
10:J:44:SER:OG	10:J:100:LEU:HB2	2.04	0.58
6:F:186:ALA:O	6:F:190:VAL:HG23	2.04	0.58
1:O:86:ARG:NE	7:U:118:ASN:HD21	1.98	0.58
2:P:185:LYS:HE2	2:P:187:ASP:OD1	2.04	0.58
12:Z:166:HIS:CD2	12:Z:168:GLN:H	2.19	0.58
5:S:175:TYR:CD2	5:S:196:ALA:HA	2.39	0.58
14:N:9:LYS:HA	14:N:145:ASN:HD22	1.69	0.57
3:Q:57:LYS:O	3:Q:58:LEU:HB2	2.04	0.57
13:M:149:GLN:NE2	13:M:149:GLN:H	2.02	0.57
2:P:124:THR:CG2	3:Q:130:ARG:HH21	2.14	0.57
2:B:185:LYS:HE2	2:B:187:ASP:OD1	2.04	0.57
9:I:2:ILE:HG21	9:I:130:ALA:HB3	1.85	0.57
1:O:21(L):ILE:N	1:O:21(L):ILE:HD12	2.19	0.57
2:B:71:ASN:ND2	2:B:72:ASP:H	2.02	0.57
3:C:227:GLU:OE1	3:C:227:GLU:N	2.37	0.57
2:B:15:PHE:N	3:C:23:GLN:HE22	1.89	0.57
5:E:221:PHE:CE1	5:E:223:ILE:HD11	2.40	0.57
8:H:113:ILE:HG12	8:H:119:THR:HG22	1.85	0.57
7:G:212:VAL:HG23	7:G:229:ILE:HD13	1.85	0.57
10:X:113:ILE:HG12	10:X:119:LYS:HG3	1.86	0.57
11:Y:114:ASP:OD1	11:Y:116:ASP:HB2	2.04	0.57
1:O:232:ARG:HG3	1:O:232:ARG:HH11	1.70	0.57
12:L:123:GLN:CG	12:L:145:TYR:OH	2.47	0.57
5:E:227:GLU:CD	5:E:227:GLU:N	2.57	0.57
12:L:135:MET:HE3	9:W:165:ARG:NH2	2.19	0.57
2:P:234:VAL:HA	2:P:239:THR:HA	1.85	0.57
14:2:175:MET:HB2	14:2:187:LEU:HB2	1.87	0.57
12:L:166:HIS:CD2	12:L:168:GLN:H	2.20	0.57
10:J:113:ILE:HG12	10:J:119:LYS:HG3	1.86	0.57
4:R:112:LEU:C	4:R:112:LEU:HD13	2.25	0.57
7:G:233:LEU:O	7:G:236:ILE:HG13	2.05	0.57
2:P:75:ALA:HB2	2:P:221:GLN:NE2	2.20	0.57
1:A:232:ARG:HG3	1:A:232:ARG:HH11	1.70	0.57
8:H:41:ILE:CD1	8:H:76:VAL:HG22	2.34	0.57
14:2:20:THR:OG1	14:2:28:ASN:HB3	2.04	0.57

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
8:V:84:LYS:HE2	8:V:119:THR:HG23	1.87	0.57
14:2:107:LYS:HG2	14:2:108:GLY:N	2.19	0.57
8:H:35:HIS:HB3	8:H:56:THR:HG21	1.87	0.57
8:H:112:SER:HB3	8:H:125:LEU:HD13	1.85	0.57
7:U:212:VAL:HG23	7:U:229:ILE:HD13	1.85	0.57
13:M:19:LEU:HD12	13:M:28:PHE:O	2.05	0.57
7:U:18(G):GLU:HG2	7:U:188:LYS:CB	2.35	0.57
8:H:200:LYS:HE3	9:I:140:SER:O	2.05	0.57
4:D:122:ARG:HG2	4:D:122:ARG:HH11	1.70	0.57
12:Z:123:GLN:CG	12:Z:145:TYR:OH	2.47	0.57
8:V:35:HIS:HB3	8:V:56:THR:HG21	1.87	0.57
2:B:75:ALA:HB2	2:B:221:GLN:NE2	2.20	0.57
8:V:128:GLY:O	8:V:131:SER:HB2	2.04	0.56
10:J:93:ARG:HH11	10:J:93:ARG:HG2	1.71	0.56
5:E:36:VAL:HG13	5:E:197:ILE:HD11	1.87	0.56
4:R:12(D):ALA:HB3	4:R:126:ARG:CD	2.34	0.56
5:E:167:ALA:HB3	16:E:253:HOH:O	2.06	0.56
11:K:40:PHE:HB3	11:K:73:ARG:NH2	2.20	0.56
6:F:175:GLU:HB3	6:F:196:ILE:CD1	2.36	0.56
2:P:71:ASN:ND2	2:P:72:ASP:H	2.02	0.56
8:V:8:PHE:HB3	8:V:151:ALA:HB2	1.87	0.56
12:L:90:LYS:HD3	12:L:95:TYR:CZ	2.41	0.56
8:V:72:ARG:HH11	8:V:72:ARG:HG3	1.69	0.56
13:1:35:ILE:HG12	13:1:56:GLU:CG	2.34	0.56
9:I:116:ILE:H	9:I:116:ILE:HD13	1.70	0.56
3:Q:15:PHE:CE1	3:Q:21:ILE:HD11	2.40	0.56
5:S:36:VAL:HG13	5:S:197:ILE:HD11	1.86	0.56
6:T:175:GLU:HB3	6:T:196:ILE:CD1	2.35	0.56
11:Y:4:LEU:HD12	11:Y:159:ILE:CD1	2.34	0.56
8:V:200:LYS:HE3	9:W:140:SER:O	2.05	0.56
2:P:81:LEU:HD23	2:P:133:GLY:HA3	1.87	0.56
5:S:220:PRO:O	5:S:222:THR:HG23	2.06	0.56
11:Y:6:PHE:HA	11:Y:123:ASP:O	2.05	0.56
9:W:29:ASN:ND2	9:W:29:ASN:N	2.51	0.56
9:I:29:ASN:N	9:I:29:ASN:ND2	2.53	0.56
12:Z:-7:ASN:HD22	12:Z:-6:PRO:HD2	1.70	0.56
7:U:143:GLU:HA	7:U:217:LYS:NZ	2.21	0.56
15:V:0:FEB:H26	9:W:115:LEU:HD21	1.88	0.56
5:E:86:ARG:O	5:E:90:ASN:HB2	2.05	0.56
2:B:224:PHE:HD2	2:B:224:PHE:H	1.54	0.56
10:X:55:PHE:CZ	10:X:59:ILE:HD11	2.39	0.56
8:H:84:LYS:HG3	8:H:85:GLN:N	2.18	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:D:40:ILE:HG13	4:D:193:VAL:CG2	2.35	0.56
9:W:1:GLY:HA3	9:W:33:LYS:HE2	1.86	0.56
3:C:35:THR:HB	3:C:51:GLU:HG3	1.87	0.56
2:B:49:ALA:HB2	2:B:212:PHE:CE1	2.41	0.56
4:R:186:LEU:O	4:R:190:GLU:HG3	2.06	0.56
4:D:121:LEU:HA	4:D:123:PHE:CE1	2.40	0.56
10:X:20:VAL:HG11	11:Y:120:LEU:HD11	1.88	0.56
13:M:76:PRO:HD2	13:M:105:GLN:OE1	2.06	0.56
2:P:21:LEU:HD13	2:P:124:THR:HG23	1.88	0.56
1:A:21(L):ILE:N	1:A:21(L):ILE:HD12	2.21	0.56
3:Q:52:ARG:HB2	3:Q:209:ASN:HA	1.87	0.56
14:2:9:LYS:HA	14:2:145:ASN:HD22	1.71	0.56
3:Q:35:THR:HB	3:Q:51:GLU:HG3	1.87	0.56
13:M:14(C):ARG:HH11	13:M:14(C):ARG:HG3	1.71	0.56
11:K:114:ASP:OD1	11:K:116:ASP:HB2	2.06	0.56
3:Q:224:LEU:N	3:Q:224:LEU:HD12	2.21	0.56
3:Q:173:ARG:O	3:Q:177:GLU:HG3	2.06	0.55
5:E:207:LEU:HA	5:E:2(E):ASN:HD21	1.70	0.55
6:T:95:GLU:CG	6:T:115:ARG:HB3	2.35	0.55
14:N:20:THR:OG1	14:N:28:ASN:HB3	2.06	0.55
5:S:86:ARG:O	5:S:90:ASN:HB2	2.06	0.55
11:K:6:PHE:HA	11:K:123:ASP:O	2.05	0.55
5:S:73:HIS:HE1	5:S:107:LEU:O	1.87	0.55
4:R:85:ALA:O	4:R:89:ILE:HG12	2.07	0.55
15:H:0:FEB:H26	9:I:115:LEU:HD21	1.89	0.55
13:1:113:VAL:HA	13:1:118:VAL:O	2.06	0.55
8:H:153:LYS:HD2	16:H:251:HOH:O	2.05	0.55
8:V:34:LEU:HB2	16:V:238:HOH:O	2.07	0.55
2:B:65:GLU:HG3	2:B:66:LYS:HG3	1.87	0.55
13:1:19:LEU:HD12	13:1:28:PHE:O	2.06	0.55
8:H:8:PHE:HB3	8:H:151:ALA:HB2	1.88	0.55
10:J:161:GLU:HA	10:J:161:GLU:OE2	2.06	0.55
6:F:175:GLU:CB	6:F:196:ILE:HD12	2.37	0.55
9:W:116:ILE:HD13	9:W:116:ILE:H	1.70	0.55
2:P:65:GLU:HG3	2:P:66:LYS:HG3	1.87	0.55
2:B:6:ARG:HG2	3:C:10:ARG:HH21	1.70	0.55
1:O:57:PRO:HG3	7:U:177:GLU:CD	2.26	0.55
11:Y:40:PHE:HB3	11:Y:73:ARG:NH2	2.20	0.55
11:Y:41:LEU:HB2	16:Y:258:HOH:O	2.05	0.55
10:X:34:THR:HG21	10:X:176:LYS:NZ	2.22	0.55
8:H:34:LEU:HB2	16:H:247:HOH:O	2.05	0.55
5:S:207:LEU:HA	5:S:2(E):ASN:HD21	1.70	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
11:K:142:TYR:O	11:K:143:LYS:HD2	2.07	0.55
8:H:84:LYS:HE2	8:H:119:THR:HG23	1.88	0.55
5:E:220:PRO:O	5:E:222:THR:HG23	2.07	0.55
2:P:141:TYR:CD1	2:P:21(E):VAL:HG21	2.40	0.55
2:P:6:ARG:HG2	3:Q:10:ARG:NH2	2.20	0.55
12:L:33:LYS:HD2	12:L:46:ASN:ND2	2.22	0.55
14:N:163:ILE:O	16:N:188:HOH:O	2.18	0.55
13:M:6:MET:HG2	13:M:155:ILE:HD11	1.88	0.55
4:D:12(F):GLY:HA3	16:D:267:HOH:O	2.07	0.55
3:C:15:PHE:CD1	3:C:21:ILE:HD11	2.42	0.55
5:S:15:PHE:H	6:T:23:GLN:NE2	1.98	0.55
2:P:160:TRP:CD2	2:P:163:ILE:HD12	2.42	0.55
11:K:20:ALA:HB2	11:K:31:VAL:HG21	1.88	0.55
12:L:7:ALA:HB2	12:L:110:VAL:HG23	1.87	0.55
13:M:157:ASN:ND2	16:M:279:HOH:O	2.39	0.55
2:B:21:LEU:HD13	2:B:124:THR:HG23	1.88	0.55
10:X:113:ILE:HA	10:X:118:THR:O	2.07	0.55
4:R:12:VAL:CG2	4:R:12(A):GLY:HA2	2.37	0.55
11:Y:191:ASP:OD2	11:Y:193:GLY:N	2.40	0.55
12:L:-7:ASN:C	12:L:-7:ASN:HD22	2.10	0.55
13:M:19:LEU:HD21	13:M:26:LEU:HD22	1.89	0.55
2:P:49:ALA:HB2	2:P:212:PHE:CE1	2.42	0.55
5:E:73:HIS:HE1	5:E:107:LEU:O	1.89	0.55
6:F:82:ILE:HB	6:F:83:PRO:HD3	1.88	0.55
2:B:186:VAL:HG11	2:B:216:ARG:CD	2.35	0.55
6:F:198:TYR:HE2	6:F:237:GLN:HE21	1.54	0.55
12:Z:90:LYS:HD3	12:Z:95:TYR:CZ	2.42	0.55
5:S:18(C):PHE:HA	5:S:18(F):ILE:HG13	1.89	0.55
8:H:3:ILE:CD1	8:H:127:LEU:O	2.55	0.54
3:Q:172:VAL:HG23	3:Q:196:SER:HB2	1.89	0.54
14:N:107:LYS:HG2	14:N:108:GLY:H	1.72	0.54
5:E:18(C):PHE:HA	5:E:18(F):ILE:HG13	1.89	0.54
16:L:199:HOH:O	9:W:192:ARG:HG3	2.07	0.54
1:O:150:GLN:O	1:O:157:TYR:HA	2.07	0.54
2:P:152:ASN:HB2	2:P:153:PRO:HD2	1.90	0.54
2:P:223:ILE:HD12	2:P:223:ILE:N	2.22	0.54
2:B:160:TRP:CD2	2:B:163:ILE:HD12	2.41	0.54
6:F:179:LEU:HD21	6:F:192:GLN:CG	2.37	0.54
6:T:175:GLU:CB	6:T:196:ILE:HD12	2.36	0.54
7:G:143:GLU:HA	7:G:217:LYS:NZ	2.22	0.54
12:L:40:ASN:HD21	12:L:183:GLY:HA2	1.72	0.54
12:Z:7:ALA:HB2	12:Z:110:VAL:HG23	1.88	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:223:ILE:N	2:B:223:ILE:HD12	2.22	0.54
14:2:176:VAL:HG12	14:2:178:LEU:HD13	1.89	0.54
6:F:20(B):GLU:HG3	6:F:20(C):LYS:N	2.23	0.54
6:T:179:LEU:HD21	6:T:192:GLN:CG	2.36	0.54
2:P:239:THR:HG22	2:P:239:THR:OXT	2.07	0.54
12:L:1:GLY:HA3	12:L:33:LYS:HZ2	1.72	0.54
14:N:176:VAL:HG12	14:N:178:LEU:HD13	1.89	0.54
1:O:161:LYS:HD3	1:O:180:TRP:CZ3	2.42	0.54
12:L:-7:ASN:HD22	12:L:-6:PRO:CD	2.20	0.54
11:K:191:ASP:OD2	11:K:193:GLY:N	2.40	0.54
16:I:224:HOH:O	10:J:122:LEU:HD13	2.06	0.54
1:O:141:HIS:HA	1:O:146:GLY:O	2.07	0.54
2:P:186:VAL:CG1	2:P:216:ARG:HD3	2.37	0.54
9:W:34:ILE:HB	16:W:215:HOH:O	2.08	0.54
2:B:81:LEU:HD23	2:B:133:GLY:HA3	1.89	0.54
7:U:14:ILE:HD13	7:U:14:ILE:H	1.73	0.54
5:S:15:PHE:HB2	6:T:23:GLN:HE22	1.73	0.54
13:M:113:VAL:HA	13:M:118:VAL:O	2.07	0.54
1:A:161:LYS:HD3	1:A:180:TRP:CZ3	2.42	0.54
10:J:52:THR:CG2	10:J:53:VAL:N	2.71	0.54
11:Y:20:ALA:HB2	11:Y:31:VAL:HG21	1.89	0.54
2:B:27:ALA:O	2:B:31:ILE:HG12	2.07	0.54
4:D:12:VAL:CG2	4:D:12(A):GLY:HA2	2.38	0.54
2:P:224:PHE:H	2:P:224:PHE:HD2	1.54	0.54
5:E:15:PHE:HB2	6:F:23:GLN:HE22	1.72	0.54
13:1:6:MET:HG2	13:1:155:ILE:HD11	1.89	0.54
9:W:29:ASN:H	9:W:29:ASN:HD22	1.55	0.54
3:C:172:VAL:HG23	3:C:196:SER:HB2	1.89	0.54
3:C:101:LEU:HD11	10:J:57:GLU:HB3	1.90	0.54
5:S:160:LEU:HD13	5:S:163:THR:HB	1.90	0.54
4:R:40:ILE:HG13	4:R:193:VAL:CG2	2.37	0.53
7:U:170:GLN:NE2	7:U:174:THR:HG23	2.20	0.53
10:J:52:THR:HG22	10:J:53:VAL:HG23	1.89	0.53
3:Q:216:LYS:HD2	3:Q:220:ASP:OD1	2.09	0.53
9:I:12:VAL:HG13	9:I:108:PRO:HB3	1.89	0.53
2:B:38:ILE:HD12	2:B:197:LEU:HG	1.90	0.53
9:I:165:ARG:NH2	12:Z:135:MET:HE3	2.21	0.53
2:B:239:THR:OXT	2:B:239:THR:HG22	2.09	0.53
5:E:86:ARG:HH11	5:E:86:ARG:HG3	1.72	0.53
1:A:141:HIS:HA	1:A:146:GLY:O	2.09	0.53
4:R:194:LEU:HD22	4:R:212:LEU:HD11	1.91	0.53
1:O:69:LEU:HD23	1:O:69:LEU:C	2.29	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:69:LEU:HD23	1:A:69:LEU:C	2.28	0.53
8:V:41:ILE:CD1	8:V:76:VAL:HG22	2.38	0.53
5:E:35:SER:HB3	5:E:66:LYS:NZ	2.23	0.53
7:G:151:THR:HG22	7:G:157:TYR:CB	2.38	0.53
2:B:152:ASN:HB2	2:B:153:PRO:CD	2.39	0.53
11:Y:142:TYR:O	11:Y:143:LYS:HD2	2.09	0.53
7:G:87:ASN:ND2	7:G:87:ASN:C	2.61	0.53
3:C:52:ARG:HB2	3:C:209:ASN:HA	1.90	0.53
16:D:273:HOH:O	5:E:86:ARG:HD3	2.08	0.53
7:U:9:ASP:HA	7:U:14:ILE:CD1	2.28	0.53
5:S:67:ILE:HG21	5:S:223:ILE:HD12	1.90	0.53
2:B:152:ASN:HB2	2:B:153:PRO:HD2	1.90	0.53
1:A:150:GLN:O	1:A:157:TYR:HA	2.08	0.53
11:Y:38:ASN:O	11:Y:40:PHE:N	2.42	0.53
7:U:87:ASN:ND2	7:U:87:ASN:C	2.61	0.53
5:S:86:ARG:HH11	5:S:86:ARG:HG3	1.74	0.53
2:P:38:ILE:HD12	2:P:197:LEU:HG	1.90	0.53
7:G:12:ILE:HD13	7:G:12:ILE:H	1.74	0.53
3:C:216:LYS:HD2	3:C:220:ASP:OD1	2.09	0.53
13:M:35:ILE:HG12	13:M:56:GLU:HG3	1.89	0.53
10:X:152:LEU:HD13	10:X:193:GLN:HE22	1.74	0.53
6:T:20(B):GLU:HG3	6:T:20(C):LYS:N	2.23	0.53
8:V:35:HIS:CB	8:V:56:THR:HG21	2.39	0.53
9:I:113:PHE:HA	9:I:118:CYS:O	2.08	0.53
14:2:156:LYS:HG2	14:2:18(J):LEU:HD11	1.91	0.53
5:E:15:PHE:H	6:F:23:GLN:NE2	2.03	0.53
6:T:192:GLN:NE2	6:T:195:LYS:HE3	2.23	0.53
10:X:32:ASP:OD2	10:X:34:THR:HG22	2.09	0.53
2:P:152:ASN:HB2	2:P:153:PRO:CD	2.38	0.53
3:Q:182:PRO:O	3:Q:184:ALA:N	2.42	0.53
9:W:12:VAL:HG13	9:W:108:PRO:HB3	1.90	0.53
7:U:233:LEU:O	7:U:236:ILE:HG13	2.08	0.53
7:U:8:TYR:C	7:U:10:ARG:H	2.13	0.53
4:D:170:GLU:N	4:D:170:GLU:OE1	2.41	0.53
4:R:205:GLU:OE2	4:R:205:GLU:HA	2.09	0.53
10:X:190:PHE:C	10:X:192:ALA:H	2.12	0.52
1:O:159:PRO:O	2:P:59:LEU:HD12	2.08	0.52
10:J:34:THR:HG21	10:J:176:LYS:NZ	2.24	0.52
3:C:241:GLN:C	3:C:243:GLN:H	2.13	0.52
3:Q:241:GLN:C	3:Q:243:GLN:H	2.13	0.52
3:Q:160:TRP:CE2	4:R:59:LEU:HD23	2.44	0.52
10:X:53:VAL:HB	16:Y:237:HOH:O	2.10	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
8:H:35:HIS:CB	8:H:56:THR:HG21	2.39	0.52
1:A:198:LYS:HE3	1:A:236:LEU:HD11	1.91	0.52
7:G:18(G):GLU:HG2	7:G:188:LYS:HB3	1.90	0.52
13:1:19:LEU:HD21	13:1:26:LEU:HD22	1.91	0.52
4:R:170:GLU:OE1	4:R:170:GLU:N	2.42	0.52
2:B:173:GLN:HG2	3:C:56:LEU:HD12	1.91	0.52
14:2:107:LYS:HG2	14:2:108:GLY:H	1.73	0.52
7:U:186:TRP:O	7:U:190:VAL:HG23	2.09	0.52
4:D:205:GLU:HA	4:D:205:GLU:OE2	2.08	0.52
2:B:186:VAL:CG1	2:B:216:ARG:HD3	2.38	0.52
3:C:224:LEU:N	3:C:224:LEU:HD12	2.24	0.52
2:B:17:PRO:HA	3:C:26:TYR:CD1	2.45	0.52
10:X:93:ARG:HG2	10:X:93:ARG:HH11	1.73	0.52
11:K:99:THR:CG2	11:K:113:VAL:HB	2.39	0.52
15:N:0:FEB:HN18	15:N:0:FEB:HN25	1.58	0.52
15:2:0:FEB:HN25	15:2:0:FEB:HN18	1.57	0.52
10:J:113:ILE:HA	10:J:118:THR:O	2.09	0.52
9:I:97:VAL:HG23	9:I:99:PRO:HD3	1.92	0.52
6:F:28:VAL:O	6:F:32:GLU:HG3	2.10	0.52
14:N:156:LYS:HG2	14:N:18(J):LEU:HD11	1.91	0.52
3:C:182:PRO:O	3:C:184:ALA:N	2.42	0.52
3:Q:177:GLU:OE2	4:R:57:PRO:HD2	2.10	0.52
9:I:6:MET:HB3	9:I:151:LEU:HD11	1.90	0.52
11:K:184:TRP:O	11:K:185:ILE:HD13	2.08	0.52
9:W:113:PHE:HA	9:W:118:CYS:O	2.08	0.52
10:X:135:PHE:HZ	16:X:216:HOH:O	1.91	0.52
13:M:184:LEU:HD23	13:M:184:LEU:C	2.30	0.52
8:V:3:ILE:HD13	8:V:127:LEU:H	1.73	0.52
3:Q:15:PHE:N	4:R:23:GLN:HE22	1.96	0.52
13:M:40:ASN:ND2	13:M:40:ASN:H	2.07	0.52
7:G:39:ALA:HB1	7:G:148:ILE:HD12	1.91	0.52
10:X:16:SER:HB2	16:X:233:HOH:O	2.08	0.52
2:B:21(A):LYS:HE2	2:B:21(D):GLY:O	2.10	0.52
7:G:38:LEU:C	7:G:38:LEU:HD12	2.30	0.52
3:Q:55:THR:O	3:Q:56:LEU:HD22	2.09	0.52
10:X:52:THR:CG2	10:X:53:VAL:N	2.72	0.52
9:W:6:MET:HB3	9:W:151:LEU:HD11	1.90	0.52
3:Q:36:CYS:N	3:Q:51:GLU:HG2	2.25	0.52
2:P:172:ALA:HB2	2:P:200:THR:HG21	1.91	0.52
14:N:146:MET:HE3	14:N:150:GLU:HB3	1.91	0.52
7:G:172:ILE:HD13	7:G:197:MET:CE	2.40	0.52
7:G:186:TRP:O	7:G:190:VAL:HG23	2.10	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
11:K:161:ALA:HB1	10:X:136:SER:HB2	1.92	0.52
14:N:106:ASN:O	14:N:107:LYS:HB3	2.09	0.52
9:W:19:ARG:HB2	9:W:171:TRP:HB2	1.92	0.52
2:P:21(A):LYS:HE2	2:P:21(D):GLY:O	2.10	0.52
7:G:14:ILE:HD13	7:G:14:ILE:H	1.74	0.51
1:O:121:GLN:O	1:O:124:THR:HB	2.10	0.51
14:2:106:ASN:O	14:2:107:LYS:HB3	2.08	0.51
4:R:24:VAL:O	4:R:27:SER:HB3	2.10	0.51
13:1:205:GLY:HA3	13:1:209:GLN:HB3	1.91	0.51
3:Q:100:ARG:HH12	3:Q:106:PRO:HB3	1.70	0.51
11:K:143:LYS:HB2	11:K:146:LEU:HD11	1.92	0.51
9:W:174:VAL:HG21	9:W:186:LYS:CE	2.41	0.51
5:S:35:SER:HB3	5:S:66:LYS:NZ	2.26	0.51
3:C:36:CYS:N	3:C:51:GLU:HG2	2.25	0.51
10:J:152:LEU:HD13	10:J:193:GLN:HE22	1.75	0.51
1:O:225:THR:OG1	1:O:228:GLU:HG3	2.10	0.51
7:G:8:TYR:C	7:G:10:ARG:H	2.12	0.51
2:P:27:ALA:O	2:P:31:ILE:HG12	2.09	0.51
9:I:6:MET:HE3	9:I:155:ILE:HG13	1.91	0.51
1:O:57:PRO:HG2	7:U:177:GLU:HG2	1.92	0.51
3:Q:15:PHE:CD1	3:Q:21:ILE:HD11	2.45	0.51
12:Z:-7:ASN:HD22	12:Z:-6:PRO:CD	2.23	0.51
5:E:160:LEU:HD13	5:E:163:THR:HB	1.92	0.51
8:H:3:ILE:HG12	8:H:100:ILE:HD12	1.92	0.51
7:G:12:ILE:HD11	7:G:14:ILE:HD12	1.92	0.51
11:Y:38:ASN:CG	16:Y:258:HOH:O	2.49	0.51
6:F:91:ARG:O	6:F:95:GLU:HB2	2.10	0.51
12:Z:-6:PRO:O	13:1:91:ARG:NH1	2.37	0.51
13:1:40:ASN:HD22	13:1:40:ASN:N	2.05	0.51
7:U:18(G):GLU:HG2	7:U:188:LYS:HB3	1.93	0.51
7:G:93:LYS:HD3	14:N:68:SER:HB3	1.90	0.51
2:B:231:ASP:O	2:B:235:LYS:HG2	2.11	0.51
8:V:22:GLN:HG3	8:V:27:ALA:HB2	1.92	0.51
8:H:3:ILE:HD13	8:H:127:LEU:H	1.76	0.51
11:K:38:ASN:O	11:K:40:PHE:N	2.43	0.51
7:G:170:GLN:NE2	7:G:174:THR:HG23	2.20	0.51
3:Q:168:ASN:CB	3:Q:200:VAL:HG11	2.41	0.51
10:J:190:PHE:C	10:J:192:ALA:H	2.13	0.51
8:H:173:VAL:HB	8:H:192:LEU:HB2	1.93	0.51
10:J:143:ARG:HB2	10:J:146:MET:HG3	1.92	0.51
3:C:160:TRP:CE2	4:D:59:LEU:HD23	2.46	0.51
12:Z:33:LYS:HD2	12:Z:46:ASN:ND2	2.26	0.51

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
15:V:0:FEB:H30A	9:W:92:PHE:HD2	1.76	0.51
13:M:8:TYR:CE2	13:M:148:VAL:HG22	2.45	0.51
4:R:122:ARG:HH11	4:R:122:ARG:HG2	1.75	0.51
2:B:172:ALA:HB2	2:B:200:THR:HG21	1.91	0.51
3:C:100:ARG:HH12	3:C:106:PRO:HB3	1.72	0.50
11:K:40:PHE:CB	11:K:73:ARG:NH2	2.74	0.50
11:Y:99:THR:CG2	11:Y:113:VAL:HB	2.41	0.50
5:E:67:ILE:HG21	5:E:223:ILE:HD12	1.93	0.50
6:F:32:GLU:HB3	6:F:169:ARG:NH2	2.26	0.50
9:W:97:VAL:HG23	9:W:99:PRO:HD3	1.93	0.50
14:2:3:ILE:HD13	14:2:46:SER:HB3	1.93	0.50
1:A:33:GLN:HE21	1:A:33:GLN:HA	1.76	0.50
7:U:38:LEU:C	7:U:38:LEU:HD12	2.32	0.50
3:C:173:ARG:O	3:C:177:GLU:HG3	2.11	0.50
6:T:91:ARG:O	6:T:95:GLU:HB2	2.11	0.50
11:Y:143:LYS:HB2	11:Y:146:LEU:HD11	1.92	0.50
10:X:52:THR:HG22	10:X:53:VAL:HG23	1.93	0.50
7:U:39:ALA:HB1	7:U:148:ILE:HD12	1.92	0.50
8:H:22:GLN:HG3	8:H:27:ALA:HB2	1.92	0.50
11:Y:7:ARG:HD2	11:Y:108:PRO:O	2.11	0.50
9:W:89:GLU:O	9:W:90:ARG:NH1	2.45	0.50
13:1:184:LEU:C	13:1:184:LEU:HD23	2.31	0.50
1:O:206:PHE:CD1	1:O:210:ILE:HD11	2.46	0.50
3:C:177:GLU:OE2	4:D:57:PRO:HD2	2.11	0.50
3:C:55:THR:O	3:C:56:LEU:HD22	2.12	0.50
13:M:205:GLY:HA3	13:M:209:GLN:HB3	1.92	0.50
5:E:201:LEU:HD11	5:E:207:LEU:CD2	2.37	0.50
11:Y:142:TYR:C	11:Y:143:LYS:HD2	2.32	0.50
11:K:142:TYR:C	11:K:143:LYS:HD2	2.31	0.50
13:1:40:ASN:ND2	13:1:40:ASN:H	2.06	0.50
5:S:31:ILE:HD11	5:S:153:PRO:HG2	1.93	0.50
3:C:211:GLU:C	3:C:212:ILE:HD12	2.32	0.50
6:T:82:ILE:HB	6:T:83:PRO:HD3	1.93	0.50
9:I:193:GLN:HG3	11:Y:196:PHE:CE1	2.46	0.50
8:V:148:LYS:HE3	8:V:177:VAL:HG11	1.92	0.50
11:Y:40:PHE:CB	11:Y:73:ARG:HH21	2.25	0.50
2:B:186:VAL:CG2	2:B:216:ARG:HD3	2.42	0.50
14:N:20:THR:HG23	14:N:31:THR:OG1	2.12	0.50
10:J:135:PHE:HZ	16:J:234:HOH:O	1.93	0.50
9:W:27:VAL:HG13	16:X:216:HOH:O	2.12	0.50
1:A:225:THR:OG1	1:A:228:GLU:HG3	2.12	0.50
9:I:89:GLU:O	9:I:90:ARG:NH1	2.45	0.50

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
10:J:123:PRO:HB2	10:J:124:TYR:CD1	2.47	0.50
4:D:194:LEU:HD22	4:D:212:LEU:HD11	1.93	0.50
10:X:123:PRO:HB2	10:X:124:TYR:CD1	2.46	0.50
6:T:192:GLN:NE2	6:T:195:LYS:CE	2.75	0.50
3:C:236:ILE:HA	3:C:239:GLU:HG2	1.93	0.50
7:G:172:ILE:CD1	7:G:197:MET:HE1	2.41	0.50
12:Z:40:ASN:HD21	12:Z:183:GLY:HA2	1.77	0.50
7:G:9:ASP:HA	7:G:14:ILE:CD1	2.28	0.50
11:Y:40:PHE:CB	11:Y:73:ARG:NH2	2.74	0.50
11:K:4:LEU:C	11:K:4:LEU:HD22	2.32	0.50
7:G:188:LYS:HD3	7:G:191:GLU:OE2	2.12	0.50
2:B:6:ARG:HB2	5:E:127:TYR:OH	2.12	0.50
14:N:18(G):TYR:HA	14:N:18(J):LEU:HG	1.94	0.50
2:B:88:LEU:HB3	2:B:116:LEU:HD21	1.94	0.50
4:D:24:VAL:O	4:D:27:SER:HB3	2.12	0.50
8:H:105:ASP:HB2	8:H:10(A):PRO:CD	2.41	0.50
10:X:143:ARG:HB2	10:X:146:MET:HG3	1.94	0.50
1:A:206:PHE:CD1	1:A:210:ILE:HD11	2.46	0.50
11:Y:157:ARG:HH11	11:Y:157:ARG:HG3	1.76	0.50
11:Y:38:ASN:OD1	11:Y:38:ASN:C	2.50	0.49
6:T:179:LEU:CD2	6:T:192:GLN:HG2	2.42	0.49
6:F:127:ASN:HD22	6:F:127:ASN:C	2.15	0.49
8:V:25:ILE:HD12	8:V:25:ILE:N	2.27	0.49
7:U:72:ARG:HG2	16:U:271:HOH:O	2.11	0.49
11:Y:184:TRP:O	11:Y:185:ILE:HD13	2.12	0.49
6:F:69:VAL:HG12	16:F:248:HOH:O	2.11	0.49
14:N:186:ARG:HD3	16:N:234:HOH:O	2.11	0.49
8:V:173:VAL:HB	8:V:192:LEU:HB2	1.94	0.49
2:P:186:VAL:HG21	2:P:216:ARG:CD	2.40	0.49
1:A:85:TYR:O	1:A:89:VAL:HG23	2.13	0.49
8:H:148:LYS:HE3	8:H:177:VAL:HG11	1.92	0.49
1:A:5:THR:O	1:A:7:ARG:HG2	2.13	0.49
4:R:207:LEU:C	4:R:207:LEU:HD23	2.32	0.49
11:K:208:ASN:HB3	16:K:237:HOH:O	2.12	0.49
9:I:29:ASN:HD22	9:I:29:ASN:H	1.59	0.49
1:A:121:GLN:O	1:A:124:THR:HB	2.12	0.49
10:X:2:ILE:HD13	10:X:170:PHE:CG	2.47	0.49
6:T:179:LEU:HD11	6:T:192:GLN:CG	2.43	0.49
2:B:147:GLN:HG2	3:C:62(A):ILE:HG21	1.95	0.49
9:I:174:VAL:HG21	9:I:186:LYS:CE	2.42	0.49
5:E:111:ARG:HG2	5:E:111:ARG:HH11	1.78	0.49
14:2:18(G):TYR:HA	14:2:18(J):LEU:HG	1.93	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:90:ASN:O	2:B:94:ILE:HD12	2.12	0.49
8:V:105:ASP:HB2	8:V:10(A):PRO:CD	2.42	0.49
7:U:12:ILE:H	7:U:12:ILE:HD13	1.76	0.49
4:D:112:LEU:O	4:D:112:LEU:HD13	2.13	0.49
2:B:224:PHE:N	2:B:224:PHE:CD2	2.81	0.49
3:C:212:ILE:HG22	3:C:224:LEU:HD13	1.95	0.49
4:D:75:GLY:HA3	4:D:221:PHE:CD2	2.47	0.49
9:I:19:ARG:HB2	9:I:171:TRP:HB2	1.94	0.49
6:T:72:ARG:HD2	13:1:64:THR:OG1	2.13	0.49
2:P:202:THR:CG2	2:P:204:SER:HB2	2.43	0.49
6:F:179:LEU:HD11	6:F:192:GLN:CG	2.42	0.49
13:1:35:ILE:HG12	13:1:56:GLU:HG3	1.93	0.49
7:U:151:THR:HG22	7:U:157:TYR:CB	2.42	0.49
6:F:136:THR:O	6:F:150:MET:HA	2.13	0.49
1:O:55:SER:O	1:O:56:SER:HB2	2.13	0.49
11:Y:135:TYR:HB2	16:Y:232:HOH:O	2.12	0.49
6:F:179:LEU:CD2	6:F:192:GLN:HG2	2.43	0.49
3:C:232:TYR:O	3:C:236:ILE:HG13	2.13	0.49
10:X:18:LYS:HD3	10:X:174:ILE:HG13	1.93	0.49
12:L:1(I):ASN:O	12:L:14(K):LYS:HG2	2.12	0.49
8:H:197:ARG:NH2	9:I:139:GLU:O	2.46	0.49
5:S:75:GLY:HA3	5:S:221:PHE:CZ	2.48	0.49
5:S:180:LEU:HA	5:S:18(C):PHE:CE2	2.48	0.49
10:X:190:PHE:HA	10:X:193:GLN:HB2	1.95	0.49
5:S:92:LEU:HD11	5:S:112:ALA:HB1	1.95	0.49
2:P:231:ASP:O	2:P:235:LYS:HG2	2.12	0.49
8:V:3:ILE:HG12	8:V:100:ILE:HD12	1.94	0.49
3:Q:169:SER:HA	3:Q:172:VAL:CG1	2.43	0.49
5:E:31:ILE:HD11	5:E:153:PRO:HG2	1.95	0.49
13:1:8:TYR:CE2	13:1:148:VAL:HG22	2.48	0.49
5:S:111:ARG:HH11	5:S:111:ARG:HG2	1.77	0.49
10:J:190:PHE:HA	10:J:193:GLN:HB2	1.95	0.49
10:X:185:ARG:NH1	16:X:222:HOH:O	2.41	0.49
1:O:198:LYS:HE3	1:O:236:LEU:HD11	1.94	0.49
4:D:12(E):SER:O	5:E:123:ASN:OD1	2.31	0.49
6:T:32:GLU:HB3	6:T:169:ARG:NH2	2.27	0.49
4:R:75:GLY:HA3	4:R:221:PHE:CD2	2.48	0.49
10:X:88:ALA:O	10:X:90(A):ILE:HG22	2.12	0.49
3:Q:14:ILE:C	3:Q:14:ILE:HD12	2.33	0.49
3:Q:33:ARG:HB2	3:Q:33:ARG:NH1	2.28	0.49
3:C:163:GLN:HE22	3:C:173:ARG:NE	2.11	0.48
2:P:163:ILE:HG12	2:P:164:SER:H	1.78	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
12:Z:-7:ASN:ND2	12:Z:-7:ASN:C	2.66	0.48
1:O:85:TYR:O	1:O:89:VAL:HG23	2.12	0.48
11:K:7:ARG:HD2	11:K:108:PRO:O	2.12	0.48
1:A:126:SER:HB3	16:A:253:HOH:O	2.12	0.48
6:F:53:LEU:HD11	6:F:205:ASN:OD1	2.13	0.48
5:E:143:LYS:HB2	16:M:258:HOH:O	2.11	0.48
6:F:20(B):GLU:CD	6:F:20(C):LYS:HE3	2.33	0.48
5:S:107:LEU:HD11	5:S:111:ARG:HG2	1.96	0.48
13:M:148:VAL:HG23	16:M:239:HOH:O	2.12	0.48
7:U:151:THR:HG22	7:U:157:TYR:HB2	1.95	0.48
8:V:175:VAL:HG12	8:V:176:CYS:N	2.28	0.48
12:Z:145:TYR:CD1	12:Z:146:LEU:N	2.81	0.48
5:E:107:LEU:HD11	5:E:111:ARG:HG2	1.95	0.48
11:K:196:PHE:CE1	9:W:193:GLN:HG3	2.48	0.48
10:J:18:LYS:HD3	10:J:174:ILE:HG13	1.95	0.48
10:J:45:PHE:CE1	10:J:52:THR:HG23	2.49	0.48
11:Y:4:LEU:C	11:Y:4:LEU:HD22	2.34	0.48
3:Q:236:ILE:HA	3:Q:239:GLU:HG2	1.93	0.48
2:B:238:ILE:O	2:B:239:THR:O	2.31	0.48
5:E:180:LEU:HA	5:E:18(C):PHE:CE2	2.49	0.48
6:T:136:THR:O	6:T:150:MET:HA	2.12	0.48
1:O:5:THR:O	1:O:7:ARG:HG2	2.14	0.48
11:K:86:LEU:HD13	11:K:86:LEU:C	2.34	0.48
12:L:145:TYR:CD1	12:L:146:LEU:N	2.80	0.48
11:K:38:ASN:OD1	11:K:38:ASN:C	2.51	0.48
6:T:28:VAL:O	6:T:32:GLU:HG3	2.14	0.48
12:Z:1(I):ASN:O	12:Z:14(K):LYS:HG2	2.14	0.48
3:C:169:SER:HA	3:C:172:VAL:CG1	2.43	0.48
6:F:192:GLN:NE2	6:F:195:LYS:HE3	2.28	0.48
4:D:177:LEU:CD2	5:E:58:LEU:HD13	2.41	0.48
2:P:224:PHE:N	2:P:224:PHE:CD2	2.81	0.48
2:B:17:PRO:HA	3:C:26:TYR:CE1	2.48	0.48
12:Z:114:ASP:HB2	12:Z:118:SER:N	2.28	0.48
1:O:47:VAL:HG23	1:O:212:LEU:HD21	1.94	0.48
4:R:45:GLY:HA2	4:R:146:TYR:CE1	2.47	0.48
4:D:45:GLY:HA2	4:D:146:TYR:CE1	2.48	0.48
1:O:33:GLN:HE21	1:O:33:GLN:HA	1.77	0.48
11:Y:86:LEU:C	11:Y:86:LEU:HD13	2.34	0.48
13:1:14(A):VAL:O	13:1:14(A):VAL:HG23	2.14	0.48
7:G:131:PRO:HB3	16:G:243:HOH:O	2.13	0.48
12:L:5:GLY:O	12:L:124:CYS:HA	2.13	0.48
6:T:20(B):GLU:CD	6:T:20(C):LYS:HE3	2.33	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:T:198:TYR:HE2	6:T:237:GLN:HE21	1.56	0.48
10:J:52:THR:HG22	10:J:53:VAL:H	1.78	0.48
7:U:227:GLU:HG2	16:U:295:HOH:O	2.14	0.48
2:P:88:LEU:HB3	2:P:116:LEU:HD21	1.96	0.48
1:A:55:SER:O	1:A:56:SER:HB2	2.13	0.48
10:J:2:ILE:HD13	10:J:170:PHE:CG	2.49	0.48
8:V:3:ILE:CD1	8:V:127:LEU:O	2.61	0.48
12:L:-7:ASN:C	12:L:-7:ASN:ND2	2.67	0.48
13:M:40:ASN:HD22	13:M:40:ASN:N	2.05	0.48
1:O:29:THR:O	1:O:33:GLN:HG2	2.14	0.48
6:T:53:LEU:HD11	6:T:205:ASN:OD1	2.14	0.48
3:C:33:ARG:NH1	3:C:33:ARG:HB2	2.29	0.48
11:K:10(B):LYS:CD	11:K:10(B):LYS:N	2.67	0.48
8:H:25:ILE:N	8:H:25:ILE:HD12	2.28	0.48
5:S:15:PHE:N	6:T:23:GLN:HE22	2.02	0.48
6:F:95:GLU:CG	6:F:115:ARG:HB3	2.35	0.48
12:L:-6:PRO:O	13:M:91:ARG:NH1	2.41	0.48
7:G:151:THR:HG22	7:G:157:TYR:HB2	1.96	0.48
3:Q:101:LEU:HD11	10:X:57:GLU:HB3	1.95	0.48
14:N:3:ILE:HD13	14:N:46:SER:HB3	1.96	0.48
2:P:101:LYS:NZ	10:X:85:GLN:NE2	2.62	0.48
7:G:228:ASN:HB3	16:G:253:HOH:O	2.14	0.48
4:D:177:LEU:HD22	5:E:58:LEU:CD1	2.40	0.47
10:X:52:THR:HG22	10:X:53:VAL:H	1.78	0.47
14:2:3:ILE:CD1	14:2:46:SER:HB3	2.43	0.47
3:Q:24:VAL:O	3:Q:27:ALA:HB3	2.13	0.47
8:H:26:VAL:HG11	8:H:29:LYS:HG2	1.94	0.47
12:L:-7:ASN:HD22	12:L:-6:PRO:N	2.12	0.47
1:A:21(G):LEU:HG	1:A:21(I):TYR:CE1	2.49	0.47
3:Q:232:TYR:O	3:Q:236:ILE:HG13	2.13	0.47
4:D:40:ILE:HG13	4:D:193:VAL:HG22	1.95	0.47
4:R:53:ARG:HD2	16:R:264:HOH:O	2.14	0.47
13:M:3:VAL:O	13:M:126:ALA:HA	2.14	0.47
2:B:163:ILE:HG12	2:B:164:SER:H	1.79	0.47
14:2:20:THR:HG23	14:2:31:THR:OG1	2.14	0.47
12:Z:99:THR:CG2	16:Z:201:HOH:O	2.61	0.47
7:G:212:VAL:HG23	7:G:229:ILE:CD1	2.45	0.47
3:Q:158:SER:HB2	4:R:59:LEU:HD21	1.96	0.47
3:C:158:SER:HB2	4:D:59:LEU:HD21	1.96	0.47
3:C:33:ARG:HH11	3:C:33:ARG:CB	2.27	0.47
5:E:15:PHE:N	6:F:23:GLN:HE22	2.06	0.47
4:R:177:LEU:HD22	5:S:58:LEU:CD1	2.41	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
12:Z:-7:ASN:HD22	12:Z:-6:PRO:N	2.11	0.47
10:X:45:PHE:CE1	10:X:52:THR:HG23	2.50	0.47
3:Q:211:GLU:C	3:Q:212:ILE:HD12	2.34	0.47
9:I:90:ARG:HD2	16:I:257:HOH:O	2.14	0.47
3:Q:33:ARG:HH11	3:Q:33:ARG:CB	2.26	0.47
13:1:128:GLY:N	16:1:281:HOH:O	2.46	0.47
3:C:24:VAL:O	3:C:27:ALA:HB3	2.14	0.47
5:S:201:LEU:HD11	5:S:207:LEU:CD2	2.38	0.47
7:U:188:LYS:HD3	7:U:191:GLU:OE2	2.14	0.47
15:H:0:FEB:H30A	9:I:92:PHE:HD2	1.80	0.47
4:R:45:GLY:HA2	4:R:146:TYR:CD1	2.50	0.47
12:L:114:ASP:HB2	12:L:118:SER:N	2.29	0.47
4:R:72:ARG:HG3	16:R:275:HOH:O	2.14	0.47
4:D:12(D):ALA:HA	5:E:129:GLY:HA2	1.96	0.47
6:T:127:ASN:HD22	6:T:127:ASN:C	2.17	0.47
2:B:224:PHE:HD2	2:B:224:PHE:N	2.12	0.47
7:U:10:ARG:HG2	7:U:22:TYR:CD2	2.50	0.47
8:V:197:ARG:NH2	9:W:139:GLU:O	2.46	0.47
4:R:160:TYR:CE2	5:S:59:SER:HB3	2.49	0.47
12:Z:93:PHE:N	12:Z:94:PRO:HD3	2.29	0.47
10:J:136:SER:HB2	11:Y:161:ALA:HB1	1.95	0.47
2:P:90:ASN:O	2:P:94:ILE:HD12	2.14	0.47
7:U:12:ILE:HD11	7:U:14:ILE:HD12	1.97	0.47
1:O:130:ARG:NH2	7:U:124:THR:HG22	2.11	0.47
2:P:186:VAL:CG2	2:P:216:ARG:HD3	2.40	0.47
2:B:186:VAL:HG21	2:B:216:ARG:CD	2.42	0.47
10:J:45:PHE:CD1	10:J:52:THR:HG23	2.50	0.47
5:E:35:SER:HB3	5:E:66:LYS:HZ3	1.80	0.47
6:F:72:ARG:HD2	13:M:64:THR:OG1	2.15	0.47
13:M:197:TRP:CH2	14:2:171:GLY:HA2	2.50	0.47
13:M:14(A):VAL:O	13:M:14(A):VAL:HG23	2.14	0.47
4:D:207:LEU:HD23	4:D:207:LEU:C	2.33	0.47
3:Q:40:VAL:HG12	3:Q:162:ALA:HB1	1.96	0.47
6:F:216:SER:HB3	6:F:21(A):GLU:HB2	1.96	0.47
3:C:14:ILE:HD12	3:C:14:ILE:C	2.35	0.47
2:B:202:THR:CG2	2:B:204:SER:HB2	2.45	0.47
3:Q:163:GLN:HG3	3:Q:164:THR:N	2.30	0.47
14:N:112:THR:CG2	14:N:120:HIS:HB2	2.44	0.47
14:2:107:LYS:CG	14:2:108:GLY:H	2.28	0.47
3:C:36:CYS:H	3:C:51:GLU:HG2	1.80	0.47
4:R:40:ILE:HG13	4:R:193:VAL:HG22	1.96	0.47
1:A:198:LYS:HE3	1:A:236:LEU:CD1	2.45	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:T:114:ASP:O	6:T:118:GLN:HG2	2.15	0.47
1:A:38:LEU:HD12	1:A:38:LEU:O	2.15	0.47
5:E:15:PHE:HB2	6:F:23:GLN:NE2	2.30	0.47
9:I:6:MET:CE	9:I:155:ILE:HA	2.44	0.47
3:Q:228:GLU:O	3:Q:232:TYR:HD1	1.97	0.47
1:A:177:GLU:CG	2:B:58:LEU:HD22	2.44	0.47
10:X:34:THR:HG21	10:X:176:LYS:HZ2	1.80	0.47
4:D:12(E):SER:HB2	5:E:123:ASN:OD1	2.15	0.47
8:V:37:ILE:HG23	8:V:60:GLY:HA2	1.97	0.47
8:H:3:ILE:HD12	8:H:127:LEU:O	2.15	0.47
3:Q:226:SER:HB2	3:Q:227:GLU:OE1	2.15	0.47
13:1:41:THR:OG1	13:1:76:PRO:HG3	2.15	0.47
15:V:0:FEB:H26A	9:W:116:ILE:HD12	1.96	0.47
2:P:224:PHE:N	2:P:224:PHE:HD2	2.12	0.47
3:Q:159:SER:O	4:R:59:LEU:HD22	2.15	0.47
12:L:140:ASN:O	12:L:144:PHE:HA	2.15	0.47
11:K:67:GLU:OE2	16:K:241:HOH:O	2.19	0.46
12:Z:5:GLY:O	12:Z:124:CYS:HA	2.15	0.46
2:B:97:GLN:NE2	9:I:64:ASN:HD22	2.12	0.46
7:U:18(G):GLU:HG2	7:U:188:LYS:HB2	1.96	0.46
10:J:168:MET:HE1	10:X:167:PRO:CB	2.45	0.46
7:U:74:ILE:HD13	16:U:287:HOH:O	2.15	0.46
2:P:229:ILE:O	2:P:233:LEU:HB2	2.15	0.46
8:H:175:VAL:HG12	8:H:176:CYS:N	2.31	0.46
8:H:38:SER:OG	8:H:41:ILE:HG12	2.16	0.46
5:E:75:GLY:HA3	5:E:221:PHE:CZ	2.50	0.46
13:M:19:LEU:HB2	13:M:170:SER:HB2	1.98	0.46
10:J:93:ARG:NH1	10:J:93:ARG:HG2	2.30	0.46
3:Q:36:CYS:H	3:Q:51:GLU:HG2	1.80	0.46
6:T:216:SER:HB3	6:T:21(A):GLU:HB2	1.97	0.46
5:E:92:LEU:HD11	5:E:112:ALA:HB1	1.96	0.46
7:U:59:LEU:O	7:U:61:PRO:HD3	2.15	0.46
7:U:17(C):LYS:HE3	7:U:17(C):LYS:HB2	1.75	0.46
3:Q:169:SER:HA	3:Q:172:VAL:HG12	1.98	0.46
5:S:15:PHE:HB2	6:T:23:GLN:NE2	2.30	0.46
3:Q:224:LEU:N	3:Q:224:LEU:CD1	2.77	0.46
1:O:40:ILE:HD12	1:O:193:ALA:HB2	1.96	0.46
12:L:93:PHE:N	12:L:94:PRO:HD3	2.30	0.46
9:W:6:MET:CE	9:W:155:ILE:HA	2.45	0.46
12:L:90:LYS:HD3	12:L:95:TYR:CE1	2.50	0.46
10:X:193:GLN:OXT	10:X:193:GLN:HG2	2.16	0.46
3:Q:159:SER:HB2	16:Q:264:HOH:O	2.16	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:E:48:LEU:HG	5:E:139:ILE:HD13	1.97	0.46
4:R:101:LEU:CD1	11:Y:57:THR:HG22	2.46	0.46
3:C:16:SER:HB2	3:C:17:PRO:HD2	1.96	0.46
11:Y:135:TYR:CB	16:Y:232:HOH:O	2.63	0.46
6:F:192:GLN:NE2	6:F:195:LYS:CE	2.79	0.46
8:V:105:ASP:HB2	8:V:10(A):PRO:HD2	1.98	0.46
13:M:17:ASP:HA	13:M:173:PHE:CB	2.45	0.46
2:B:144:ARG:HG2	2:B:144:ARG:O	2.16	0.46
11:Y:37:ILE:HB	11:Y:41:LEU:HB3	1.97	0.46
8:H:105:ASP:HB2	8:H:10(A):PRO:HD2	1.96	0.46
13:M:179:ASP:HB3	13:M:18(A):THR:OG1	2.15	0.46
3:Q:16:SER:HB2	3:Q:17:PRO:HD2	1.97	0.46
16:T:273:HOH:O	14:2:70:TYR:HE2	1.98	0.46
5:E:194:VAL:HG13	5:E:207:LEU:HD11	1.98	0.46
10:J:167:PRO:CB	10:X:168:MET:HE1	2.46	0.46
6:F:109:ILE:HB	6:F:110:PRO:HD3	1.97	0.46
6:F:121:GLN:NE2	16:F:258:HOH:O	2.48	0.46
2:P:63:THR:HG22	2:P:63:THR:O	2.16	0.46
1:A:13:THR:O	2:B:130:ARG:HD3	2.16	0.46
13:M:14(G):ILE:HB	13:M:144:PRO:CD	2.45	0.46
14:N:14:LEU:O	14:N:175:MET:HA	2.16	0.46
7:U:212:VAL:HG23	7:U:229:ILE:CD1	2.46	0.46
7:G:18(G):GLU:HG2	7:G:188:LYS:HB2	1.96	0.46
12:L:1:GLY:N	16:L:224:HOH:O	2.49	0.46
14:N:3:ILE:CD1	14:N:46:SER:HB3	2.46	0.46
7:U:83:PRO:HG2	16:U:265:HOH:O	2.15	0.46
10:X:14:LEU:HD12	10:X:42:LEU:HD23	1.98	0.46
13:1:179:ASP:HB3	13:1:18(A):THR:OG1	2.16	0.46
5:E:136:LEU:HB2	5:E:151:PHE:HB3	1.97	0.46
14:N:171:GLY:HA2	13:1:197:TRP:CH2	2.51	0.46
6:F:50:VAL:HG22	6:F:51:GLU:N	2.31	0.45
5:S:67:ILE:CG2	5:S:223:ILE:HD12	2.47	0.45
3:Q:141:PHE:CD1	3:Q:217:PRO:HG3	2.51	0.45
14:N:163:ILE:HG23	14:N:170:GLY:HA2	1.97	0.45
8:V:63:ILE:HD13	8:V:63:ILE:HA	1.85	0.45
5:S:48:LEU:HG	5:S:139:ILE:HD13	1.98	0.45
3:C:163:GLN:HG3	3:C:164:THR:N	2.30	0.45
9:I:55:LEU:CD1	9:I:97:VAL:HG21	2.46	0.45
3:C:224:LEU:N	3:C:224:LEU:CD1	2.80	0.45
8:H:63:ILE:HG23	8:H:74:PRO:HB3	1.98	0.45
6:T:78:TYR:CE1	6:T:85:GLY:HA3	2.51	0.45
2:B:229:ILE:O	2:B:233:LEU:HB2	2.15	0.45

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
11:K:5:ALA:HA	11:K:13:ILE:O	2.17	0.45
5:S:64:GLN:NE2	5:S:82:ALA:HB2	2.31	0.45
2:B:53:LYS:HG2	2:B:54:VAL:HG23	1.99	0.45
2:P:144:ARG:O	2:P:144:ARG:HG2	2.16	0.45
7:U:171:GLU:OE1	7:U:171:GLU:N	2.47	0.45
5:S:194:VAL:HG13	5:S:207:LEU:HD11	1.98	0.45
1:A:29:THR:O	1:A:33:GLN:HG2	2.15	0.45
8:H:144:GLN:O	8:H:145:ASP:HB2	2.16	0.45
6:F:210:LEU:HD21	6:F:212:ILE:HD11	1.98	0.45
2:B:191:GLU:O	2:B:195:LYS:HG2	2.16	0.45
4:R:68:VAL:CG2	4:R:89:ILE:HD12	2.33	0.45
7:G:96:ALA:CA	7:G:107:MET:CE	2.89	0.45
3:C:168:ASN:CB	3:C:200:VAL:HG11	2.43	0.45
3:C:141:PHE:CD1	3:C:217:PRO:HG3	2.51	0.45
3:Q:57:LYS:HG2	3:Q:208:LYS:NZ	2.32	0.45
6:F:203:GLU:C	6:F:205:ASN:H	2.19	0.45
12:Z:140:ASN:O	12:Z:144:PHE:HA	2.15	0.45
1:A:47:VAL:HG23	1:A:212:LEU:HD21	1.97	0.45
5:E:125:GLN:HE22	6:F:87:HIS:CD2	2.34	0.45
1:A:8:TYR:HD2	7:G:128:TYR:HB3	1.81	0.45
8:V:26:VAL:HG11	8:V:29:LYS:HG2	1.97	0.45
7:U:47:VAL:HG12	7:U:49:ILE:CD1	2.47	0.45
7:G:172:ILE:HD13	7:G:197:MET:HE1	1.98	0.45
6:T:203:GLU:C	6:T:205:ASN:H	2.19	0.45
8:V:63:ILE:HG23	8:V:74:PRO:HB3	1.99	0.45
7:G:218:ASP:O	7:G:220:LYS:HB2	2.16	0.45
7:U:146:PRO:HD2	16:U:299:HOH:O	2.16	0.45
10:J:88:ALA:O	10:J:90(A):ILE:HG22	2.16	0.45
12:L:4:LEU:HD23	12:L:159:PHE:CE1	2.52	0.45
8:V:38:SER:OG	8:V:41:ILE:HG12	2.16	0.45
1:A:21(L):ILE:HD11	8:H:186:TYR:CD2	2.52	0.45
1:O:21(G):LEU:HG	1:O:21(I):TYR:CE1	2.51	0.45
5:E:64:GLN:NE2	5:E:82:ALA:HB2	2.32	0.45
8:H:37:ILE:HG23	8:H:60:GLY:HA2	1.98	0.45
11:K:40:PHE:CB	11:K:73:ARG:HH21	2.25	0.45
11:K:99:THR:HG22	11:K:113:VAL:HB	1.99	0.45
2:P:97:GLN:NE2	9:W:64:ASN:HD22	2.12	0.45
8:V:196:VAL:HG23	16:V:242:HOH:O	2.16	0.45
13:M:-3:VAL:HA	13:M:21:SER:O	2.17	0.45
3:C:40:VAL:HG12	3:C:162:ALA:HB1	1.98	0.45
11:K:74:ILE:HG13	11:K:75:SER:N	2.30	0.45
7:G:105:TYR:OH	8:H:66:HIS:HE1	2.00	0.45

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
14:2:13:ILE:HG12	14:2:177:VAL:HG13	1.98	0.45
5:E:197:ILE:HG23	5:E:198:SER:N	2.32	0.45
10:J:193:GLN:OXT	10:J:193:GLN:HG2	2.16	0.45
12:L:14(E):GLU:HB2	12:L:14(M):VAL:HB	1.98	0.45
7:G:47:VAL:HG12	7:G:49:ILE:CD1	2.47	0.45
13:1:104:VAL:HG23	13:1:178:ILE:HG22	1.98	0.45
13:M:57:ARG:CD	16:M:244:HOH:O	2.64	0.45
13:1:14(G):ILE:HB	13:1:144:PRO:CD	2.46	0.45
10:X:45:PHE:CD1	10:X:52:THR:HG23	2.52	0.45
10:X:112:GLN:NE2	10:X:126:ALA:H	2.15	0.45
3:C:57:LYS:HG2	3:C:208:LYS:NZ	2.32	0.45
9:W:101:VAL:O	9:W:110:ILE:HA	2.17	0.45
6:F:43:ASN:HD22	6:F:44:ASP:N	2.15	0.45
13:1:146:THR:HA	16:1:233:HOH:O	2.17	0.45
12:L:4:LEU:HD23	12:L:159:PHE:HE1	1.82	0.45
3:C:228:GLU:O	3:C:232:TYR:HD1	1.99	0.45
4:R:112:LEU:O	4:R:112:LEU:HD13	2.16	0.45
5:S:111:ARG:NH1	5:S:111:ARG:HG2	2.32	0.45
7:G:151:THR:HG22	7:G:157:TYR:HB3	1.98	0.45
9:W:99:PRO:HB2	9:W:113:PHE:CD2	2.52	0.45
4:R:102:TYR:O	12:Z:81:ARG:HG3	2.16	0.45
12:Z:14(E):GLU:HB2	12:Z:14(M):VAL:HB	1.99	0.45
8:V:144:GLN:O	8:V:145:ASP:HB2	2.16	0.45
12:L:-2:ASN:HA	12:L:21:ILE:O	2.16	0.45
11:Y:74:ILE:HG13	11:Y:75:SER:N	2.32	0.45
13:1:-3:VAL:HA	13:1:21:SER:O	2.17	0.45
12:L:4:LEU:HD12	12:L:5:GLY:N	2.32	0.44
5:S:197:ILE:HG23	5:S:198:SER:N	2.31	0.44
10:J:-1:MET:CG	10:J:1:ASP:H	2.23	0.44
1:A:232:ARG:HG3	1:A:232:ARG:NH1	2.32	0.44
13:1:19:LEU:HB2	13:1:170:SER:HB2	1.98	0.44
12:Z:1:GLY:HA3	12:Z:33:LYS:NZ	2.32	0.44
1:A:38:LEU:HD12	1:A:38:LEU:C	2.37	0.44
5:S:125:GLN:HE22	6:T:87:HIS:CD2	2.34	0.44
7:U:218:ASP:O	7:U:220:LYS:HB2	2.17	0.44
7:G:34(A):ASN:HA	7:G:167:PRO:HG2	1.99	0.44
14:2:116:GLY:HA3	16:2:191:HOH:O	2.15	0.44
11:K:157:ARG:HH11	11:K:157:ARG:HG3	1.82	0.44
4:R:177:LEU:CD2	5:S:58:LEU:HD13	2.43	0.44
14:2:112:THR:CG2	14:2:120:HIS:HB2	2.46	0.44
3:C:226:SER:HB2	3:C:227:GLU:OE1	2.16	0.44
12:Z:1:GLY:HA3	12:Z:33:LYS:HZ2	1.81	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:Q:14:ILE:O	3:Q:14:ILE:HD12	2.17	0.44
12:Z:114:ASP:HB2	12:Z:118:SER:H	1.83	0.44
4:D:45:GLY:HA2	4:D:146:TYR:CD1	2.51	0.44
2:P:87:ILE:O	2:P:91:THR:HG23	2.16	0.44
6:F:78:TYR:CE1	6:F:85:GLY:HA3	2.52	0.44
2:P:218:ASN:O	2:P:21(C):ASP:HB2	2.18	0.44
7:U:172:ILE:HD13	7:U:197:MET:CE	2.47	0.44
10:J:112:GLN:NE2	10:J:126:ALA:H	2.15	0.44
13:M:19:LEU:HD12	13:M:20:GLY:H	1.83	0.44
9:W:55:LEU:CD1	9:W:97:VAL:HG21	2.46	0.44
1:O:198:LYS:HE3	1:O:236:LEU:CD1	2.47	0.44
14:2:146:MET:HB3	14:2:150:GLU:HB2	1.98	0.44
3:C:43:LYS:O	3:C:43:LYS:HG2	2.17	0.44
1:A:6:ASP:OD2	1:A:8:TYR:HB2	2.17	0.44
2:P:53:LYS:HG2	2:P:54:VAL:HG23	1.99	0.44
7:G:136:LEU:O	7:G:150:LYS:HA	2.17	0.44
1:O:17:PRO:HA	2:P:26:TYR:CD1	2.52	0.44
7:U:34(A):ASN:HA	7:U:167:PRO:HG2	2.00	0.44
7:G:59:LEU:O	7:G:61:PRO:HD3	2.16	0.44
1:O:38:LEU:HD12	1:O:38:LEU:O	2.18	0.44
11:Y:99:THR:HG22	11:Y:113:VAL:HB	1.99	0.44
2:B:85:ALA:O	2:B:89:ILE:HG13	2.18	0.44
5:S:44:THR:HG23	5:S:183:ASP:HB3	2.00	0.44
2:B:63:THR:HG22	2:B:63:THR:O	2.17	0.44
3:C:169:SER:HA	3:C:172:VAL:HG12	1.97	0.44
6:T:50:VAL:HG22	6:T:51:GLU:N	2.32	0.44
10:X:93:ARG:NH1	10:X:93:ARG:HG2	2.33	0.44
3:C:33:ARG:HG2	3:C:33:ARG:O	2.17	0.44
2:P:191:GLU:O	2:P:195:LYS:HG2	2.16	0.44
6:F:107:ILE:HA	6:F:108:PRO:HD3	1.88	0.44
14:2:36:ARG:HG3	14:2:42:TRP:CZ2	2.52	0.44
11:K:4:LEU:HD11	11:K:15:ALA:HB3	2.00	0.44
9:W:2:ILE:HD11	9:W:17:ASP:HB3	2.00	0.44
14:N:107:LYS:CG	14:N:108:GLY:H	2.28	0.44
4:D:122:ARG:NH1	4:D:122:ARG:HG2	2.32	0.44
2:B:6:ARG:HG2	3:C:10:ARG:NH2	2.33	0.44
12:Z:90:LYS:HD3	12:Z:95:TYR:CE1	2.52	0.44
9:W:7:THR:HG23	9:W:110:ILE:HD13	2.00	0.44
5:S:136:LEU:HB2	5:S:151:PHE:HB3	1.99	0.44
11:Y:200:LYS:HE2	16:Y:239:HOH:O	2.17	0.44
13:1:17:ASP:HA	13:1:173:PHE:CB	2.47	0.44
12:L:4:LEU:CD1	12:L:138:LEU:HD21	2.37	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:21(I):TYR:HE2	1:A:21(L):ILE:HD13	1.83	0.44
11:Y:5:ALA:HA	11:Y:13:ILE:O	2.18	0.44
2:B:171:ALA:O	2:B:175:LEU:HG	2.17	0.44
10:J:133:TYR:HE2	10:J:166:MET:SD	2.41	0.44
7:G:12:ILE:HD13	7:G:12:ILE:N	2.33	0.44
11:Y:208:ASN:O	11:Y:209:VAL:C	2.56	0.44
11:Y:40:PHE:CG	11:Y:73:ARG:NH2	2.86	0.44
11:K:67:GLU:HG2	11:K:72:GLU:O	2.18	0.44
2:P:186:VAL:CB	2:P:216:ARG:HD3	2.48	0.44
11:Y:4:LEU:HD11	11:Y:15:ALA:HB3	2.00	0.44
10:X:147:THR:HG23	10:X:150:GLU:OE2	2.18	0.44
5:E:44:THR:HG23	5:E:183:ASP:HB3	2.00	0.44
11:K:37:ILE:HB	11:K:41:LEU:HB3	1.98	0.44
6:T:109:ILE:HB	6:T:110:PRO:HD3	2.00	0.44
12:Z:-2:ASN:HA	12:Z:21:ILE:O	2.18	0.44
1:O:58:LEU:HB3	7:U:162:ALA:O	2.16	0.44
7:G:17(C):LYS:HE3	7:G:17(C):LYS:HB2	1.75	0.44
8:H:3:ILE:HG22	8:H:16:ALA:CB	2.47	0.43
4:R:162:ALA:HB3	5:S:58:LEU:HD23	1.99	0.43
3:C:235:GLN:O	3:C:239:GLU:HG2	2.18	0.43
2:B:126:HIS:HA	16:C:267:HOH:O	2.17	0.43
14:2:14:LEU:O	14:2:175:MET:HA	2.18	0.43
8:H:197:ARG:HG3	12:Z:164:GLU:CD	2.39	0.43
12:L:114:ASP:HB2	12:L:118:SER:H	1.83	0.43
2:P:95:HIS:CD2	2:P:115:ARG:HG2	2.53	0.43
2:B:112:LEU:C	2:B:112:LEU:HD23	2.39	0.43
11:K:32:LYS:N	11:K:32:LYS:HD2	2.33	0.43
3:Q:163:GLN:HE22	3:Q:173:ARG:NE	2.12	0.43
1:O:86:ARG:NE	7:U:118:ASN:ND2	2.55	0.43
9:I:1:GLY:HA2	9:I:17:ASP:OD1	2.18	0.43
13:1:40:ASN:ND2	13:1:40:ASN:N	2.65	0.43
7:G:188:LYS:HA	7:G:188:LYS:HD3	1.87	0.43
15:H:0:FEB:H26A	9:I:116:ILE:HD12	1.99	0.43
1:O:38:LEU:HD12	1:O:38:LEU:C	2.38	0.43
8:V:22:GLN:CG	8:V:27:ALA:HB2	2.48	0.43
6:T:210:LEU:HD21	6:T:212:ILE:HD11	2.00	0.43
9:I:160:LEU:HD12	9:I:191:MET:HE3	2.00	0.43
5:E:4:PHE:CG	5:E:5:ARG:N	2.86	0.43
13:1:3:VAL:O	13:1:126:ALA:HA	2.18	0.43
12:Z:17:ASP:HA	12:Z:172:GLY:O	2.18	0.43
6:T:172:ALA:O	6:T:176:LEU:HD23	2.18	0.43
14:2:59:VAL:HG11	14:2:83:PHE:CE2	2.54	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
10:J:138:LEU:HD21	10:J:158:CYS:SG	2.59	0.43
4:R:128:MET:HE3	4:R:130:ARG:O	2.19	0.43
11:Y:32:LYS:HD2	11:Y:32:LYS:N	2.32	0.43
6:T:37:SER:HB3	6:T:50:VAL:HG23	2.00	0.43
9:I:2:ILE:HD11	9:I:17:ASP:HB3	2.00	0.43
3:Q:235:GLN:O	3:Q:239:GLU:HG2	2.18	0.43
13:1:12:VAL:CG2	13:1:102:ALA:HB1	2.48	0.43
3:C:57:LYS:HG2	3:C:208:LYS:HZ3	1.83	0.43
3:Q:58:LEU:HD12	3:Q:58:LEU:HA	1.76	0.43
3:Q:33:ARG:HG2	3:Q:33:ARG:O	2.17	0.43
4:R:160:TYR:CE2	4:R:163:LYS:HD3	2.54	0.43
13:M:165:ARG:HA	14:2:26:ILE:HB	2.00	0.43
9:I:7:THR:HG23	9:I:110:ILE:HD13	2.00	0.43
8:H:18:THR:HB	8:H:30:ASN:HD22	1.84	0.43
16:V:264:HOH:O	9:W:150:ASP:HA	2.19	0.43
6:T:18:ASP:N	6:T:18:ASP:OD2	2.43	0.43
12:Z:4:LEU:HD23	12:Z:159:PHE:HE1	1.82	0.43
2:P:122:GLY:C	2:P:124:THR:H	2.22	0.43
3:Q:55:THR:C	3:Q:56:LEU:HD22	2.39	0.43
12:L:135:MET:HE2	9:W:165:ARG:NH2	2.31	0.43
2:B:184:MET:HE2	2:B:188:ASP:HB3	1.99	0.43
3:C:194:VAL:O	3:C:198:LEU:HG	2.17	0.43
13:1:148:VAL:CG2	16:1:228:HOH:O	2.62	0.43
1:O:232:ARG:HG3	1:O:232:ARG:NH1	2.32	0.43
14:2:105:ASP:OD2	14:2:106:ASN:N	2.45	0.43
1:A:170:VAL:HB	16:A:252:HOH:O	2.19	0.43
7:U:136:LEU:O	7:U:150:LYS:HA	2.17	0.43
6:T:107:ILE:HA	6:T:108:PRO:HD3	1.88	0.43
2:P:112:LEU:HD23	2:P:112:LEU:C	2.39	0.43
12:Z:4:LEU:HD12	12:Z:5:GLY:N	2.33	0.43
2:B:184:MET:CE	2:B:188:ASP:HB3	2.49	0.43
2:P:238:ILE:O	2:P:239:THR:O	2.37	0.43
10:J:32:ASP:OD2	10:J:34:THR:HG22	2.18	0.43
12:L:164:GLU:CD	8:V:197:ARG:HG3	2.39	0.43
6:F:90:ASN:O	6:F:94:GLU:HG3	2.19	0.43
2:P:68:TYR:CG	2:P:89:ILE:HD12	2.52	0.43
5:S:5:ARG:HG3	5:S:22:PHE:CZ	2.54	0.43
14:N:19:ARG:CZ	14:N:26:ILE:HD11	2.48	0.43
9:W:123:ASP:OD1	9:W:124:PHE:N	2.46	0.43
5:S:199:GLN:CA	5:S:199:GLN:HE21	2.32	0.43
10:J:133:TYR:CD1	16:Y:232:HOH:O	2.34	0.43
2:P:121:GLN:CG	3:Q:83:ALA:HB1	2.49	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:F:37:SER:HB3	6:F:50:VAL:HG23	2.00	0.43
14:2:146:MET:CE	14:2:150:GLU:HB3	2.49	0.43
2:B:227:GLN:OE1	2:B:230:LYS:HD3	2.19	0.43
3:C:152:GLU:HB2	3:C:153:PRO:HD2	2.00	0.43
10:X:138:LEU:HD21	10:X:158:CYS:SG	2.58	0.43
11:K:4:LEU:CD1	11:K:159:ILE:CD1	2.94	0.43
3:Q:149:TYR:CE1	3:Q:159:SER:HB3	2.54	0.43
3:Q:33:ARG:NH1	3:Q:33:ARG:CB	2.82	0.43
9:I:101:VAL:O	9:I:110:ILE:HA	2.19	0.43
5:S:4:PHE:CG	5:S:5:ARG:N	2.86	0.43
2:B:87:ILE:O	2:B:91:THR:HG23	2.18	0.43
8:V:207:PRO:HG2	8:V:210:THR:OG1	2.17	0.43
2:P:136:PHE:O	2:P:150:THR:HA	2.19	0.43
11:K:126:CYS:HB2	11:K:135:TYR:CE1	2.53	0.43
8:H:195:ASN:HB3	12:Z:192:LYS:HE3	2.01	0.43
11:K:208:ASN:O	11:K:209:VAL:C	2.57	0.43
7:G:12:ILE:CD1	7:G:14:ILE:HD12	2.49	0.43
11:K:40:PHE:CG	11:K:73:ARG:NH2	2.87	0.43
12:Z:4:LEU:HD23	12:Z:159:PHE:CE1	2.53	0.43
8:H:201:GLN:HG2	12:Z:153:LYS:HA	2.00	0.43
14:N:36:ARG:HG3	14:N:42:TRP:CZ2	2.54	0.43
11:K:184:TRP:C	11:K:185:ILE:HD13	2.38	0.43
14:N:146:MET:CE	14:N:150:GLU:HB3	2.49	0.43
2:B:218:ASN:O	2:B:21(C):ASP:HB2	2.19	0.43
13:1:112:TYR:HE1	13:1:127:THR:HG22	1.83	0.43
14:2:163:ILE:HG23	14:2:170:GLY:HA2	1.99	0.43
8:V:139:GLU:OE2	8:V:139:GLU:HA	2.19	0.43
1:O:6:ASP:OD2	1:O:8:TYR:HB2	2.18	0.43
2:B:95:HIS:CD2	2:B:115:ARG:HG2	2.53	0.43
7:U:96:ALA:CA	7:U:107:MET:CE	2.89	0.43
3:C:195:ARG:CG	3:C:236:ILE:HD13	2.46	0.43
7:G:8:TYR:C	7:G:10:ARG:N	2.73	0.43
1:O:77:VAL:HG12	1:O:137:LEU:HB2	2.00	0.43
3:Q:43:LYS:HG2	3:Q:43:LYS:O	2.19	0.43
11:Y:40:PHE:CG	11:Y:73:ARG:CZ	3.02	0.42
11:K:67:GLU:CB	16:K:241:HOH:O	2.67	0.42
2:P:184:MET:CE	2:P:188:ASP:HB3	2.49	0.42
14:2:36:ARG:HG3	14:2:42:TRP:NE1	2.33	0.42
1:O:21(I):TYR:HE2	1:O:21(L):ILE:HD13	1.84	0.42
14:N:59:VAL:HG11	14:N:83:PHE:CE2	2.54	0.42
3:C:206:GLY:HA3	3:C:209:ASN:HD22	1.84	0.42
8:H:22:GLN:CG	8:H:27:ALA:HB2	2.48	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
12:L:17:ASP:HA	12:L:172:GLY:O	2.19	0.42
8:V:3:ILE:HG22	8:V:16:ALA:CB	2.50	0.42
7:U:12:ILE:N	7:U:12:ILE:HD13	2.33	0.42
1:O:15:PHE:H	2:P:23:GLN:NE2	1.88	0.42
7:U:39:ALA:CB	7:U:148:ILE:HD12	2.49	0.42
3:C:58:LEU:HA	3:C:58:LEU:HD12	1.77	0.42
14:N:147:SER:OG	14:N:150:GLU:HG3	2.18	0.42
14:2:147:SER:OG	14:2:150:GLU:HG3	2.19	0.42
2:P:41:MET:HE2	16:P:244:HOH:O	2.19	0.42
12:L:185:ARG:NH1	16:L:242:HOH:O	2.51	0.42
2:P:227:GLN:OE1	2:P:230:LYS:HD3	2.18	0.42
11:K:111:TYR:CE1	11:K:121:LYS:HB2	2.55	0.42
3:Q:76:LEU:HD23	3:Q:76:LEU:C	2.40	0.42
2:B:40:ILE:HD12	2:B:193:ALA:HB2	2.01	0.42
6:F:31:VAL:HG22	6:F:134:VAL:HA	2.01	0.42
11:K:174:ASN:ND2	11:K:189:ASN:HD22	2.16	0.42
7:G:191:GLU:HG3	7:G:232:ARG:HG3	2.01	0.42
14:N:107:LYS:NZ	14:N:145:ASN:HD21	2.17	0.42
4:R:121:LEU:HA	4:R:123:PHE:HE1	1.84	0.42
7:U:225:SER:O	7:U:229:ILE:HG13	2.19	0.42
7:U:18(D):ILE:O	7:U:18(G):GLU:N	2.50	0.42
5:E:5:ARG:HG3	5:E:22:PHE:CZ	2.54	0.42
1:A:90:ASP:OD1	16:A:244:HOH:O	2.22	0.42
12:L:8:GLY:HA3	12:L:11:PHE:CE2	2.54	0.42
4:D:128:MET:HE3	4:D:130:ARG:O	2.19	0.42
4:D:148:LEU:HB3	4:D:160:TYR:O	2.19	0.42
13:M:191:GLN:HE21	13:M:191:GLN:HB3	1.61	0.42
5:E:67:ILE:CG2	5:E:223:ILE:HD12	2.49	0.42
2:P:141:TYR:CE2	2:P:145:GLY:HA2	2.55	0.42
14:N:146:MET:HB3	14:N:150:GLU:HB2	2.00	0.42
11:Y:39:PRO:HG3	16:Y:256:HOH:O	2.19	0.42
5:S:52:LYS:HB3	5:S:63:TYR:HB3	2.02	0.42
6:T:43:ASN:HD22	6:T:44:ASP:N	2.17	0.42
5:E:148:LEU:CD2	5:E:162:GLY:HA2	2.49	0.42
5:S:141:TYR:CE2	5:S:217:LYS:HA	2.55	0.42
7:G:74:ILE:HD13	16:G:246:HOH:O	2.20	0.42
6:T:157:TYR:CD1	6:T:157:TYR:C	2.92	0.42
1:A:130:ARG:HG2	7:G:125:GLN:HG3	2.02	0.42
3:Q:52:ARG:HD2	3:Q:208:LYS:O	2.19	0.42
7:U:191:GLU:HG3	7:U:232:ARG:HG3	2.02	0.42
3:C:33:ARG:NH1	3:C:33:ARG:CB	2.83	0.42
6:T:172:ALA:O	6:T:176:LEU:CD2	2.68	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:O:142:ASP:OD1	1:O:145:ASN:HB2	2.20	0.42
4:D:68:VAL:CG2	4:D:89:ILE:HD12	2.35	0.42
11:Y:174:ASN:ND2	11:Y:189:ASN:HD22	2.14	0.42
13:M:12:VAL:CG2	13:M:102:ALA:HB1	2.48	0.42
10:X:3:ILE:HD13	10:X:3:ILE:HA	1.90	0.42
13:M:41:THR:OG1	13:M:76:PRO:HG3	2.20	0.42
12:L:21:ILE:HD12	12:L:21:ILE:C	2.40	0.42
1:A:142:ASP:OD1	1:A:145:ASN:HB2	2.20	0.42
9:W:36:HIS:HB3	9:W:42:PHE:CD2	2.54	0.42
8:V:206:PHE:CZ	9:W:157:GLN:HG3	2.55	0.42
1:A:40:ILE:HD12	1:A:193:ALA:HB2	2.01	0.42
5:E:199:GLN:CA	5:E:199:GLN:HE21	2.32	0.42
3:Q:224:LEU:H	3:Q:224:LEU:CD1	2.32	0.42
5:E:111:ARG:NH1	5:E:111:ARG:HG2	2.33	0.42
9:I:99:PRO:HB2	9:I:113:PHE:CD2	2.55	0.42
4:R:59:LEU:HD13	4:R:59:LEU:C	2.40	0.42
12:Z:14(I):THR:HB	12:Z:14(M):VAL:HG23	2.01	0.42
9:I:123:ASP:OD1	9:I:124:PHE:N	2.50	0.42
1:A:97:HIS:HD2	8:H:61:SER:OG	2.03	0.42
4:D:102:TYR:O	12:L:81:ARG:HG3	2.20	0.42
3:Q:152:GLU:HB2	3:Q:153:PRO:HD2	2.00	0.42
8:H:139:GLU:HA	8:H:139:GLU:OE2	2.19	0.42
1:O:49:ALA:HB2	1:O:212:LEU:HG	2.00	0.42
4:D:160:TYR:CE2	4:D:163:LYS:HD3	2.55	0.42
6:T:31:VAL:HG22	6:T:134:VAL:HA	2.02	0.42
4:R:17:PRO:HA	5:S:26:TYR:CD1	2.54	0.42
7:U:93:LYS:HD3	14:2:68:SER:HB3	2.01	0.42
8:H:206:PHE:CZ	9:I:157:GLN:HG3	2.55	0.42
14:N:48:SER:HB3	14:N:51:ASP:HB2	2.02	0.42
2:B:213:ALA:HA	2:B:222:LYS:O	2.20	0.42
11:Y:126:CYS:HB2	11:Y:135:TYR:CE1	2.55	0.42
3:Q:194:VAL:O	3:Q:198:LEU:HG	2.19	0.42
3:Q:212:ILE:HG22	3:Q:224:LEU:HD13	2.00	0.42
12:L:1:GLY:HA3	12:L:33:LYS:NZ	2.34	0.42
2:P:52:ARG:HH22	2:P:63(A):SER:HB3	1.85	0.42
7:G:17(D):SER:O	7:G:17(E):LYS:HB2	2.20	0.42
8:V:18:THR:HB	8:V:30:ASN:HD22	1.85	0.42
7:U:17(D):SER:O	7:U:17(E):LYS:HB2	2.20	0.42
11:K:10(A):ARG:HG2	11:K:10(A):ARG:HH11	1.85	0.42
11:Y:10(A):ARG:HH11	11:Y:10(A):ARG:HG2	1.85	0.42
1:O:13:THR:O	2:P:130:ARG:HD3	2.19	0.42
2:B:186:VAL:CB	2:B:216:ARG:HD3	2.50	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
13:M:14(G):ILE:HB	13:M:144:PRO:HD3	2.02	0.42
2:B:184:MET:HE2	2:B:188:ASP:CB	2.50	0.42
14:N:55:ILE:O	14:N:59:VAL:HG23	2.20	0.42
10:J:190:PHE:C	10:J:192:ALA:N	2.74	0.42
5:E:44:THR:CG2	5:E:183:ASP:HB3	2.50	0.42
7:G:158:VAL:HG22	7:G:159:GLY:N	2.35	0.42
9:I:28:SER:HB2	10:J:120:VAL:HG21	2.01	0.42
2:P:213:ALA:HA	2:P:222:LYS:O	2.20	0.42
3:C:76:LEU:HD23	3:C:76:LEU:C	2.40	0.42
7:U:18(H):GLU:H	7:U:18(H):GLU:CD	2.23	0.42
5:S:7:ASN:HD22	5:S:7:ASN:HA	1.64	0.42
1:O:32:LYS:HE2	1:O:32:LYS:HA	2.01	0.42
14:2:113:ILE:HG12	14:2:119:VAL:HG13	2.01	0.41
2:B:141:TYR:CE2	2:B:145:GLY:HA2	2.54	0.41
7:G:225:SER:O	7:G:229:ILE:HG13	2.20	0.41
3:C:159:SER:O	4:D:59:LEU:HD22	2.20	0.41
7:U:34(A):ASN:HD22	7:U:167:PRO:HG2	1.84	0.41
14:2:19:ARG:CZ	14:2:26:ILE:HD11	2.50	0.41
5:S:148:LEU:CD2	5:S:162:GLY:HA2	2.49	0.41
2:P:149:TYR:OH	3:Q:62(A):ILE:HB	2.20	0.41
5:S:118:ASP:HA	16:S:234:HOH:O	2.20	0.41
9:W:28:SER:HB2	10:X:120:VAL:HG21	2.02	0.41
11:Y:143:LYS:HB2	11:Y:146:LEU:HD12	2.01	0.41
3:C:55:THR:C	3:C:56:LEU:HD22	2.41	0.41
7:U:212:VAL:CG2	7:U:229:ILE:HD13	2.49	0.41
1:A:212:LEU:HD23	1:A:213:ALA:N	2.35	0.41
2:B:68:TYR:CG	2:B:89:ILE:HD12	2.55	0.41
12:Z:21:ILE:HD12	12:Z:21:ILE:C	2.41	0.41
9:I:36:HIS:HB3	9:I:42:PHE:CD2	2.56	0.41
12:Z:113:PHE:CD2	12:Z:119:TYR:HB3	2.55	0.41
12:L:113:PHE:CD2	12:L:119:TYR:HB3	2.55	0.41
5:S:194:VAL:O	5:S:197:ILE:HG22	2.20	0.41
7:G:39:ALA:CB	7:G:148:ILE:HD12	2.49	0.41
3:C:52:ARG:HD2	3:C:208:LYS:O	2.20	0.41
8:H:52:THR:O	8:H:56:THR:HB	2.20	0.41
10:X:190:PHE:C	10:X:192:ALA:N	2.73	0.41
4:D:59:LEU:C	4:D:59:LEU:HD13	2.40	0.41
4:R:122:ARG:HG2	4:R:122:ARG:NH1	2.35	0.41
1:A:212:LEU:HD23	1:A:212:LEU:C	2.41	0.41
7:G:152:ASP:HB2	7:G:153:PRO:CD	2.51	0.41
2:B:225:LYS:N	2:B:228:GLU:OE1	2.48	0.41
12:L:35:PHE:O	12:L:42:VAL:HA	2.20	0.41

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:U:152:ASP:HB2	7:U:153:PRO:CD	2.49	0.41
5:E:214:ILE:HG12	5:E:215:VAL:N	2.35	0.41
10:X:98:ASN:HB3	10:X:127:HIS:CD2	2.55	0.41
8:H:40:LYS:HB2	16:H:238:HOH:O	2.20	0.41
5:E:97:ASN:HD22	5:E:97:ASN:HA	1.73	0.41
3:Q:186:VAL:HG21	3:Q:216:LYS:HE2	2.02	0.41
7:G:55:PRO:HG2	7:G:56:ASP:N	2.33	0.41
9:I:165:ARG:NH2	12:Z:135:MET:HE2	2.35	0.41
7:U:39:ALA:HA	7:U:47:VAL:O	2.21	0.41
2:B:71:ASN:HD22	2:B:72:ASP:H	1.69	0.41
7:G:212:VAL:CG2	7:G:229:ILE:HD13	2.50	0.41
2:B:20:ARG:NH1	2:B:20:ARG:HG2	2.35	0.41
4:R:148:LEU:HB3	4:R:160:TYR:O	2.21	0.41
5:E:125:GLN:HE22	6:F:87:HIS:HD2	1.68	0.41
13:1:112:TYR:CE1	13:1:127:THR:HG22	2.55	0.41
5:S:38:VAL:HG12	5:S:39:GLY:N	2.35	0.41
6:F:157:TYR:C	6:F:157:TYR:CD1	2.92	0.41
4:R:85:ALA:O	4:R:89:ILE:CG1	2.68	0.41
2:B:121:GLN:CG	3:C:83:ALA:HB1	2.50	0.41
12:L:14:LEU:HD13	12:L:34:VAL:CG1	2.44	0.41
6:F:35:THR:CG2	6:F:51:GLU:O	2.63	0.41
2:B:14(A):TYR:HB2	2:B:147:GLN:NE2	2.36	0.41
14:2:172:VAL:HB	14:2:18(A):ILE:HD11	2.02	0.41
10:J:154:LEU:HA	10:J:154:LEU:HD12	1.89	0.41
14:2:65:LEU:HG	14:2:69:GLN:HE21	1.85	0.41
10:J:148:THR:CG2	10:J:177:ILE:HD13	2.50	0.41
5:S:214:ILE:HG12	5:S:215:VAL:N	2.34	0.41
6:F:18:ASP:N	6:F:18:ASP:OD2	2.46	0.41
5:E:207:LEU:HA	5:E:2(E):ASN:HD22	1.84	0.41
3:Q:208:LYS:HD2	3:Q:208:LYS:O	2.21	0.41
14:2:107:LYS:CG	14:2:108:GLY:N	2.82	0.41
1:O:136:LEU:O	1:O:150:GLN:HA	2.21	0.41
3:C:14:ILE:HD12	3:C:14:ILE:O	2.19	0.41
7:U:172:ILE:CD1	7:U:197:MET:HE1	2.50	0.41
14:N:26:ILE:HB	13:1:165:ARG:HA	2.01	0.41
4:D:117:CYS:SG	4:D:157:PHE:HB3	2.60	0.41
13:1:122:SER:HB3	13:1:124:THR:O	2.20	0.41
11:K:200:LYS:HE2	16:K:244:HOH:O	2.21	0.41
14:2:66:TYR:CD2	14:2:74:PRO:HB3	2.55	0.41
7:U:192:PHE:CD1	7:U:192:PHE:C	2.93	0.41
11:K:40:PHE:CG	11:K:73:ARG:CZ	3.04	0.41
5:E:160:LEU:HD23	6:F:59:LEU:HA	2.03	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:G:34(A):ASN:HD22	7:G:167:PRO:HG2	1.86	0.41
2:P:40:ILE:HD12	2:P:193:ALA:HB2	2.02	0.41
2:P:225:LYS:N	2:P:228:GLU:OE1	2.49	0.41
13:M:69(C):LEU:HD13	13:M:71(B):GLU:HB2	2.03	0.41
9:W:61:TYR:C	9:W:61:TYR:CD1	2.94	0.41
13:M:112:TYR:C	13:M:112:TYR:CD2	2.94	0.41
6:F:179:LEU:HD11	6:F:192:GLN:HG3	2.02	0.41
10:J:147:THR:HG23	10:J:150:GLU:OE2	2.20	0.41
3:C:175:PHE:CZ	3:C:195:ARG:HB3	2.56	0.41
7:U:203:THR:HG22	7:U:204:GLU:O	2.21	0.41
3:C:215:VAL:O	3:C:215:VAL:HG13	2.20	0.41
10:J:3:ILE:HD12	10:J:44:SER:HB2	2.01	0.41
8:V:34:LEU:HD22	8:V:174:ASP:HB3	2.02	0.41
8:H:34:LEU:HD22	8:H:174:ASP:HB3	2.03	0.41
1:A:49:ALA:HB2	1:A:212:LEU:HG	2.03	0.41
1:A:77:VAL:HG12	1:A:137:LEU:HB2	2.02	0.41
3:C:238:GLN:O	3:C:242:GLU:HG3	2.21	0.41
3:Q:125:GLN:NE2	16:R:263:HOH:O	2.54	0.41
6:F:65:VAL:HA	6:F:211:GLU:OE2	2.20	0.41
7:G:82:ILE:CG2	7:G:83:PRO:HD3	2.51	0.41
11:Y:111:TYR:CE1	11:Y:121:LYS:HB2	2.55	0.41
11:K:156:LYS:HD3	11:K:195:LEU:HD11	2.03	0.41
14:2:161:GLN:NE2	14:2:165:TRP:HE1	2.18	0.41
14:N:36:ARG:HG3	14:N:42:TRP:NE1	2.34	0.41
13:M:40:ASN:ND2	13:M:40:ASN:N	2.64	0.41
3:Q:215:VAL:O	3:Q:215:VAL:HG13	2.20	0.41
3:C:57:LYS:HD2	3:C:58:LEU:N	2.35	0.41
14:2:107:LYS:NZ	14:2:145:ASN:HD21	2.18	0.41
1:A:195:LEU:HD23	1:A:236:LEU:HD21	2.03	0.41
7:G:10:ARG:HG2	7:G:22:TYR:CD2	2.55	0.41
3:C:158:SER:CB	4:D:59:LEU:HD21	2.51	0.41
7:U:82:ILE:CG2	7:U:83:PRO:HD3	2.51	0.41
7:G:47:VAL:CG1	7:G:49:ILE:CD1	2.99	0.41
12:L:14(I):THR:HB	12:L:14(M):VAL:HG23	2.02	0.41
11:K:12:ILE:HB	11:K:178:VAL:HB	2.03	0.41
8:H:207:PRO:HG2	8:H:210:THR:OG1	2.21	0.41
5:E:38:VAL:HG12	5:E:39:GLY:N	2.35	0.41
2:B:10:SER:HB2	16:B:248:HOH:O	2.21	0.41
4:R:117:CYS:SG	4:R:157:PHE:HB3	2.60	0.41
6:T:103:TYR:O	6:T:104:LYS:HB3	2.21	0.41
9:W:160:LEU:HD12	9:W:191:MET:HE3	2.03	0.41
7:U:105:TYR:OH	8:V:66:HIS:HE1	2.03	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:149:TYR:CZ	3:C:62(A):ILE:HB	2.56	0.41
10:X:3:ILE:O	10:X:126:ALA:HA	2.20	0.41
4:R:121:LEU:HD13	5:S:130:ARG:HH21	1.86	0.41
1:A:136:LEU:O	1:A:150:GLN:HA	2.21	0.41
10:X:136:SER:HA	10:X:139:ASP:HB2	2.03	0.41
8:H:63:ILE:HD13	8:H:63:ILE:HA	1.83	0.41
1:O:77:VAL:CG1	1:O:137:LEU:HB2	2.51	0.41
3:Q:76:LEU:HD22	3:Q:89:ILE:HG12	2.03	0.41
9:W:45:ILE:HB	9:W:52:VAL:HG13	2.03	0.41
3:C:120:GLN:O	3:C:124:THR:HG23	2.21	0.41
12:Z:8:GLY:HA3	12:Z:11:PHE:CE2	2.56	0.41
13:M:9:ASP:OD1	13:M:10:ASN:N	2.54	0.41
12:Z:35:PHE:O	12:Z:42:VAL:HA	2.21	0.41
2:P:14(A):TYR:HB2	2:P:147:GLN:NE2	2.36	0.41
7:G:171:GLU:OE1	7:G:171:GLU:N	2.47	0.41
1:O:26:TYR:CD1	1:O:26:TYR:N	2.88	0.41
14:2:161:GLN:HE22	14:2:165:TRP:HE1	1.69	0.40
9:W:6:MET:HE1	9:W:155:ILE:HA	2.03	0.40
3:Q:57:LYS:HD2	3:Q:58:LEU:N	2.36	0.40
4:D:121:LEU:HA	4:D:123:PHE:HE1	1.83	0.40
2:B:20:ARG:NH2	3:C:33:ARG:HE	2.19	0.40
1:A:77:VAL:CG1	1:A:137:LEU:HB2	2.52	0.40
12:L:134:ILE:HD11	12:L:162:ALA:HB2	2.03	0.40
13:1:80:PHE:CE1	13:1:111:ARG:HD3	2.56	0.40
3:Q:66:LYS:HE2	3:Q:78:PHE:CZ	2.57	0.40
2:B:174:THR:O	2:B:178:MET:HB2	2.21	0.40
2:P:39:GLY:O	2:P:148:LEU:HD21	2.21	0.40
2:P:176:LEU:C	2:P:178:MET:H	2.24	0.40
1:A:32:LYS:HE2	1:A:32:LYS:HA	2.03	0.40
7:G:192:PHE:CD1	7:G:192:PHE:C	2.94	0.40
13:M:-1:GLY:HA2	16:M:214:HOH:O	2.20	0.40
11:K:180:GLU:N	16:K:239:HOH:O	2.53	0.40
14:N:20:THR:HA	15:N:0:FEB:O12	2.21	0.40
9:I:2:ILE:O	9:I:2:ILE:HD12	2.21	0.40
5:E:221:PHE:HE1	5:E:223:ILE:HD11	1.84	0.40
4:D:123:PHE:CZ	4:D:131:PRO:HG3	2.56	0.40
14:2:13:ILE:HD12	14:2:151:THR:CG2	2.52	0.40
11:Y:13:ILE:HD12	11:Y:152:LEU:HD23	2.02	0.40
16:T:244:HOH:O	7:U:86:ARG:HD2	2.19	0.40
2:P:44:ASP:N	2:P:44:ASP:OD2	2.54	0.40
10:X:10(B):LYS:NZ	10:X:10(B):LYS:HB2	2.36	0.40
2:B:159:GLY:O	3:C:59:GLN:HB3	2.21	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
14:N:172:VAL:HB	14:N:18(A):ILE:HD11	2.04	0.40
3:Q:195:ARG:CG	3:Q:236:ILE:HD13	2.47	0.40
13:M:35:ILE:HA	13:M:36:PRO:HD3	1.93	0.40
10:X:3:ILE:HD12	10:X:44:SER:HB2	2.02	0.40
4:R:123:PHE:CZ	4:R:131:PRO:HG3	2.56	0.40
2:P:71:ASN:HD22	2:P:72:ASP:H	1.69	0.40
1:O:206:PHE:CE1	1:O:210:ILE:HD11	2.57	0.40
10:X:166:MET:HA	10:X:167:PRO:HD3	1.79	0.40
5:S:44:THR:CG2	5:S:183:ASP:HB3	2.50	0.40
8:H:3:ILE:CD1	8:H:3:ILE:H	2.35	0.40
11:K:143:LYS:HB2	11:K:146:LEU:HD12	2.03	0.40
1:O:21(L):ILE:HD11	8:V:186:TYR:CD2	2.57	0.40
7:G:54:VAL:HA	7:G:55:PRO:HD2	1.96	0.40
10:X:3:ILE:HB	16:X:234:HOH:O	2.20	0.40
14:N:105:ASP:OD2	14:N:106:ASN:N	2.46	0.40
4:R:121:LEU:HD23	4:R:123:PHE:HE1	1.87	0.40
9:I:107:LYS:HA	9:I:108:PRO:HD3	1.84	0.40
1:O:195:LEU:HD23	1:O:236:LEU:HD21	2.03	0.40
2:P:67:LEU:HD23	2:P:213:ALA:HB2	2.03	0.40
4:R:12(E):SER:O	5:S:123:ASN:OD1	2.39	0.40
11:Y:25:TRP:CH2	12:Z:132:SER:HA	2.57	0.40
6:F:114:ASP:O	6:F:118:GLN:HG2	2.21	0.40
5:E:76:LEU:HB2	5:E:137:LEU:O	2.21	0.40
2:P:171:ALA:O	2:P:175:LEU:HG	2.20	0.40
10:X:148:THR:CG2	10:X:177:ILE:HD13	2.51	0.40
2:P:185:LYS:O	2:P:188:ASP:HB2	2.22	0.40
6:F:179:LEU:HD11	6:F:192:GLN:HG2	2.04	0.40
2:P:163:ILE:CG1	2:P:164:SER:N	2.82	0.40
1:A:86:ARG:HH21	7:G:118:ASN:ND2	2.17	0.40
8:H:24:PRO:HG2	8:H:25:ILE:CD1	2.50	0.40
3:Q:175:PHE:CZ	3:Q:195:ARG:HB3	2.56	0.40
8:V:84:LYS:HE2	8:V:119:THR:CG2	2.49	0.40
12:L:43:MET:CB	12:L:101:ILE:HG22	2.51	0.40
8:H:84:LYS:HE2	8:H:119:THR:CG2	2.51	0.40
10:J:136:SER:HA	10:J:139:ASP:HB2	2.04	0.40
2:B:67:LEU:HD23	2:B:213:ALA:HB2	2.02	0.40
10:J:105:ASP:O	10:J:106:ASN:N	2.55	0.40
13:1:130:GLY:O	13:1:134:ALA:HB3	2.22	0.40
9:W:143:GLU:HA	9:W:144:PRO:HD3	1.89	0.40
2:P:20:ARG:NH1	2:P:20:ARG:HG2	2.37	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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%)	231 (93%)	15 (6%)	2 (1%)	27	53
1	O	248/250 (99%)	232 (94%)	13 (5%)	3 (1%)	19	39
2	B	242/244 (99%)	225 (93%)	13 (5%)	4 (2%)	14	26
2	P	242/244 (99%)	225 (93%)	13 (5%)	4 (2%)	14	26
3	C	239/241 (99%)	221 (92%)	15 (6%)	3 (1%)	18	35
3	Q	239/241 (99%)	221 (92%)	15 (6%)	3 (1%)	18	35
4	D	240/242 (99%)	221 (92%)	12 (5%)	7 (3%)	7	11
4	R	240/242 (99%)	221 (92%)	13 (5%)	6 (2%)	9	14
5	E	231/233 (99%)	214 (93%)	13 (6%)	4 (2%)	14	26
5	S	231/233 (99%)	213 (92%)	16 (7%)	2 (1%)	25	49
6	F	242/244 (99%)	230 (95%)	9 (4%)	3 (1%)	19	39
6	T	242/244 (99%)	230 (95%)	9 (4%)	3 (1%)	19	39
7	G	241/243 (99%)	229 (95%)	12 (5%)	0	100	100
7	U	241/243 (99%)	229 (95%)	11 (5%)	1 (0%)	43	72
8	H	220/222 (99%)	210 (96%)	8 (4%)	2 (1%)	25	49
8	V	220/222 (99%)	210 (96%)	9 (4%)	1 (0%)	38	67
9	I	202/204 (99%)	194 (96%)	8 (4%)	0	100	100
9	W	202/204 (99%)	193 (96%)	9 (4%)	0	100	100
10	J	196/198 (99%)	184 (94%)	11 (6%)	1 (0%)	38	67
10	X	196/198 (99%)	184 (94%)	11 (6%)	1 (0%)	38	67
11	K	210/212 (99%)	202 (96%)	7 (3%)	1 (0%)	38	67
11	Y	210/212 (99%)	202 (96%)	7 (3%)	1 (0%)	38	67
12	L	220/222 (99%)	209 (95%)	10 (4%)	1 (0%)	38	67
12	Z	220/222 (99%)	208 (94%)	11 (5%)	1 (0%)	38	67
13	1	231/233 (99%)	217 (94%)	14 (6%)	0	100	100
13	M	231/233 (99%)	217 (94%)	14 (6%)	0	100	100

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	2	194/196 (99%)	188 (97%)	6 (3%)	0	100	100
14	N	194/196 (99%)	188 (97%)	6 (3%)	0	100	100
All	All	6312/6368 (99%)	5948 (94%)	310 (5%)	54 (1%)	25	49

All (54) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	THR
1	A	56	SER
3	C	58	LEU
4	D	12(G)	GLU
10	J	192	ALA
1	O	5	THR
1	O	56	SER
3	Q	58	LEU
4	R	12(G)	GLU
10	X	192	ALA
2	B	54	VAL
2	B	21(B)	GLY
2	B	21(C)	ASP
3	C	183	PRO
3	C	203	THR
4	D	18(D)	SER
2	P	54	VAL
2	P	21(B)	GLY
2	P	21(C)	ASP
3	Q	183	PRO
3	Q	203	THR
4	R	18(D)	SER
4	D	12(F)	GLY
5	E	202	ARG
6	F	206	LYS
11	K	39	PRO
2	P	6	ARG
4	R	12(F)	GLY
5	S	202	ARG
6	T	206	LYS
11	Y	39	PRO
2	B	6	ARG
5	E	231	LYS
6	F	205	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
5	S	231	LYS
6	T	205	ASN
4	D	60	GLU
4	D	61	SER
4	R	60	GLU
4	R	61	SER
4	D	12(C)	GLY
4	D	128	MET
5	E	180	LEU
5	E	217	LYS
6	F	13	SER
1	O	167	LYS
4	R	12(C)	GLY
6	T	13	SER
8	V	96	GLY
8	H	180	ILE
12	L	14(H)	GLY
8	H	96	GLY
7	U	55	PRO
12	Z	14(H)	GLY

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	209/209 (100%)	204 (98%)	5 (2%)	61	87
1	O	209/209 (100%)	204 (98%)	5 (2%)	61	87
2	B	203/203 (100%)	195 (96%)	8 (4%)	43	74
2	P	203/203 (100%)	195 (96%)	8 (4%)	43	74
3	C	213/213 (100%)	204 (96%)	9 (4%)	40	71
3	Q	213/213 (100%)	204 (96%)	9 (4%)	40	71
4	D	198/198 (100%)	187 (94%)	11 (6%)	30	55
4	R	198/198 (100%)	187 (94%)	11 (6%)	30	55
5	E	192/192 (100%)	171 (89%)	21 (11%)	9	16
5	S	192/192 (100%)	171 (89%)	21 (11%)	9	16

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	201/201 (100%)	186 (92%)	15 (8%)	19	36
6	T	201/201 (100%)	185 (92%)	16 (8%)	17	33
7	G	207/207 (100%)	193 (93%)	14 (7%)	22	43
7	U	207/207 (100%)	192 (93%)	15 (7%)	21	39
8	H	181/181 (100%)	173 (96%)	8 (4%)	39	68
8	V	181/181 (100%)	174 (96%)	7 (4%)	43	74
9	I	172/172 (100%)	168 (98%)	4 (2%)	63	88
9	W	172/172 (100%)	168 (98%)	4 (2%)	63	88
10	J	175/175 (100%)	168 (96%)	7 (4%)	42	73
10	X	175/175 (100%)	168 (96%)	7 (4%)	42	73
11	K	169/169 (100%)	162 (96%)	7 (4%)	41	72
11	Y	169/169 (100%)	161 (95%)	8 (5%)	36	65
12	L	185/185 (100%)	174 (94%)	11 (6%)	28	52
12	Z	185/185 (100%)	173 (94%)	12 (6%)	24	46
13	1	199/199 (100%)	189 (95%)	10 (5%)	34	61
13	M	199/199 (100%)	190 (96%)	9 (4%)	38	67
14	2	162/162 (100%)	152 (94%)	10 (6%)	26	49
14	N	162/162 (100%)	152 (94%)	10 (6%)	26	49
All	All	5332/5332 (100%)	5050 (95%)	282 (5%)	32	58

All (282) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	64	LEU
1	A	135	SER
1	A	158	PHE
1	A	179	ARG
2	B	58	LEU
2	B	71	ASN
2	B	89	ILE
2	B	121	GLN
2	B	150	THR
2	B	192	LEU
2	B	218	ASN
2	B	224	PHE

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
3	C	10	ARG
3	C	25	GLU
3	C	57	LYS
3	C	121	GLN
3	C	135	SER
3	C	150	GLN
3	C	174	GLU
3	C	208	LYS
3	C	227	GLU
4	D	28	LEU
4	D	40	ILE
4	D	110	GLU
4	D	126	ARG
4	D	170	GLU
4	D	177	LEU
4	D	191	LEU
4	D	194	LEU
4	D	215	ILE
4	D	237	LEU
4	D	244	GLU
5	E	12	THR
5	E	13	VAL
5	E	32	LYS
5	E	56	ASP
5	E	57	GLU
5	E	76	LEU
5	E	90	ASN
5	E	97	ASN
5	E	104	ASN
5	E	111	ARG
5	E	121	GLN
5	E	18(D)	ILE
5	E	185	ASN
5	E	189	LEU
5	E	197	ILE
5	E	199	GLN
5	E	207	LEU
5	E	2(C)	VAL
5	E	2(E)	ASN
5	E	227	GLU
5	E	231	LYS
6	F	35	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
6	F	43	ASN
6	F	56	SER
6	F	98	SER
6	F	105	THR
6	F	121	GLN
6	F	127	ASN
6	F	144	ASN
6	F	18(E)	GLU
6	F	187	ARG
6	F	203	GLU
6	F	204	ASP
6	F	205	ASN
6	F	214	TRP
6	F	21(C)	ASN
7	G	12	ILE
7	G	14	ILE
7	G	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	217	LYS
7	G	232	ARG
7	G	233	LEU
8	H	3	ILE
8	H	30	ASN
8	H	55	VAL
8	H	56	THR
8	H	68	LEU
8	H	99	LEU
8	H	144	GLN
8	H	197	ARG
9	I	29	ASN
9	I	116	ILE
9	I	160	LEU
9	I	171	TRP
10	J	35	ARG
10	J	52	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
10	J	70	GLU
10	J	77	GLN
10	J	121	GLU
10	J	137	LEU
10	J	168	MET
11	K	4	LEU
11	K	9	GLN
11	K	38	ASN
11	K	65	LEU
11	K	87	VAL
11	K	104	TYR
11	K	10(B)	LYS
12	L	-7	ASN
12	L	4	LEU
12	L	14	LEU
12	L	25	SER
12	L	58	ARG
12	L	70(A)	ASN
12	L	99	THR
12	L	123	GLN
12	L	134	ILE
12	L	1(I)	ASN
12	L	145	TYR
13	M	40	ASN
13	M	62	LEU
13	M	91	ARG
13	M	112	TYR
13	M	129	PHE
13	M	14(C)	ARG
13	M	149	GLN
13	M	204	LYS
13	M	211	ILE
14	N	70	TYR
14	N	84	LYS
14	N	89	GLU
14	N	10(A)	ASP
14	N	115	LEU
14	N	119	VAL
14	N	149	GLU
14	N	178	LEU
14	N	18(A)	ILE
14	N	18(I)	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	O	33	GLN
1	O	64	LEU
1	O	135	SER
1	O	158	PHE
1	O	179	ARG
2	P	58	LEU
2	P	71	ASN
2	P	89	ILE
2	P	121	GLN
2	P	150	THR
2	P	192	LEU
2	P	218	ASN
2	P	224	PHE
3	Q	10	ARG
3	Q	25	GLU
3	Q	57	LYS
3	Q	121	GLN
3	Q	135	SER
3	Q	150	GLN
3	Q	174	GLU
3	Q	208	LYS
3	Q	227	GLU
4	R	28	LEU
4	R	40	ILE
4	R	110	GLU
4	R	126	ARG
4	R	170	GLU
4	R	177	LEU
4	R	191	LEU
4	R	194	LEU
4	R	215	ILE
4	R	237	LEU
4	R	244	GLU
5	S	12	THR
5	S	13	VAL
5	S	32	LYS
5	S	56	ASP
5	S	57	GLU
5	S	76	LEU
5	S	90	ASN
5	S	97	ASN
5	S	104	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
5	S	111	ARG
5	S	121	GLN
5	S	18(D)	ILE
5	S	185	ASN
5	S	189	LEU
5	S	197	ILE
5	S	199	GLN
5	S	207	LEU
5	S	2(C)	VAL
5	S	2(E)	ASN
5	S	227	GLU
5	S	231	LYS
6	T	35	THR
6	T	36	THR
6	T	43	ASN
6	T	56	SER
6	T	98	SER
6	T	105	THR
6	T	121	GLN
6	T	127	ASN
6	T	144	ASN
6	T	18(E)	GLU
6	T	187	ARG
6	T	203	GLU
6	T	204	ASP
6	T	205	ASN
6	T	214	TRP
6	T	21(C)	ASN
7	U	12	ILE
7	U	14	ILE
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	217	LYS
7	U	229	ILE
7	U	232	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
7	U	233	LEU
8	V	3	ILE
8	V	30	ASN
8	V	55	VAL
8	V	56	THR
8	V	68	LEU
8	V	144	GLN
8	V	197	ARG
9	W	29	ASN
9	W	116	ILE
9	W	160	LEU
9	W	171	TRP
10	X	35	ARG
10	X	52	THR
10	X	70	GLU
10	X	77	GLN
10	X	121	GLU
10	X	137	LEU
10	X	168	MET
11	Y	4	LEU
11	Y	9	GLN
11	Y	38	ASN
11	Y	65	LEU
11	Y	87	VAL
11	Y	99	THR
11	Y	104	TYR
11	Y	10(B)	LYS
12	Z	-7	ASN
12	Z	4	LEU
12	Z	14	LEU
12	Z	25	SER
12	Z	58	ARG
12	Z	70(A)	ASN
12	Z	99	THR
12	Z	114	ASP
12	Z	123	GLN
12	Z	134	ILE
12	Z	1(I)	ASN
12	Z	145	TYR
13	1	39	ASP
13	1	40	ASN
13	1	62	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
13	1	91	ARG
13	1	112	TYR
13	1	129	PHE
13	1	14(C)	ARG
13	1	149	GLN
13	1	204	LYS
13	1	211	ILE
14	2	70	TYR
14	2	84	LYS
14	2	89	GLU
14	2	10(A)	ASP
14	2	115	LEU
14	2	119	VAL
14	2	149	GLU
14	2	178	LEU
14	2	18(A)	ILE
14	2	18(I)	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (194) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	97	HIS
2	B	23	GLN
2	B	71	ASN
2	B	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	97	GLN
3	C	121	GLN
3	C	125	GLN
3	C	150	GLN
3	C	163	GLN
3	C	209	ASN
3	C	243	GLN
4	D	23	GLN
4	D	108	ASN
4	D	147	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
4	D	161	ASN
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	97	ASN
5	E	104	ASN
5	E	121	GLN
5	E	123	ASN
5	E	125	GLN
5	E	185	ASN
5	E	199	GLN
5	E	2(E)	ASN
6	F	23	GLN
6	F	43	ASN
6	F	90	ASN
6	F	121	GLN
6	F	127	ASN
6	F	192	GLN
7	G	34(A)	ASN
7	G	87	ASN
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	10	ASN
8	H	30	ASN
8	H	66	HIS
8	H	91	GLN
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	36	GLN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
10	J	54	GLN
10	J	77	GLN
10	J	85	GLN
10	J	112	GLN
10	J	140	HIS
10	J	186	GLN
10	J	193	GLN
11	K	9	GLN
11	K	53	GLN
11	K	66	HIS
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	61	ASN
12	L	67	HIS
12	L	70(A)	ASN
12	L	1(I)	ASN
12	L	166	HIS
13	M	10	ASN
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	69	GLN
14	N	145	ASN
14	N	161	GLN
1	O	33	GLN
1	O	97	HIS
2	P	23	GLN
2	P	71	ASN
2	P	97	GLN
2	P	121	GLN
2	P	125	GLN
2	P	156	ASN
2	P	177	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	P	218	ASN
3	Q	23	GLN
3	Q	97	GLN
3	Q	121	GLN
3	Q	125	GLN
3	Q	150	GLN
3	Q	163	GLN
3	Q	209	ASN
3	Q	243	GLN
4	R	23	GLN
4	R	108	ASN
4	R	147	GLN
4	R	161	ASN
4	R	218	GLN
4	R	226	ASN
5	S	7	ASN
5	S	33	GLN
5	S	64	GLN
5	S	73	HIS
5	S	97	ASN
5	S	104	ASN
5	S	121	GLN
5	S	123	ASN
5	S	125	GLN
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	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	170	GLN
7	U	178	ASN
7	U	184	ASN
7	U	228	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
8	V	10	ASN
8	V	30	ASN
8	V	66	HIS
8	V	91	GLN
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	36	GLN
10	X	54	GLN
10	X	77	GLN
10	X	85	GLN
10	X	112	GLN
10	X	140	HIS
10	X	186	GLN
10	X	193	GLN
11	Y	9	GLN
11	Y	53	GLN
11	Y	66	HIS
11	Y	85	ASN
11	Y	131	GLN
11	Y	174	ASN
11	Y	207	ASN
12	Z	-9	GLN
12	Z	-7	ASN
12	Z	40	ASN
12	Z	61	ASN
12	Z	67	HIS
12	Z	70(A)	ASN
12	Z	85	HIS
12	Z	1(I)	ASN
12	Z	166	HIS
13	1	-7	GLN
13	1	10	ASN
13	1	40	ASN
13	1	89	GLN
13	1	93	ASN
13	1	149	GLN
13	1	157	ASN
13	1	172	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
13	1	191	GLN
14	2	69	GLN
14	2	141	ASN
14	2	145	ASN
14	2	161	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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	FEB	2	0	14	38,38,38	1.44	5 (13%)	47,47,47	1.18	4 (8%)
15	FEB	H	0	8	38,38,38	0.80	0	47,47,47	0.95	1 (2%)
15	FEB	K	0	11	38,38,38	0.86	2 (5%)	47,47,47	0.78	0
15	FEB	N	0	14	38,38,38	1.42	3 (7%)	47,47,47	1.17	6 (12%)
15	FEB	V	0	8	38,38,38	0.79	0	47,47,47	0.96	1 (2%)
15	FEB	Y	0	11	38,38,38	0.86	1 (2%)	47,47,47	0.76	0

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	FEB	2	0	14	-	1/48/48/48	0/0/0/0
15	FEB	H	0	8	-	0/48/48/48	0/0/0/0
15	FEB	K	0	11	-	0/48/48/48	0/0/0/0
15	FEB	N	0	14	-	1/48/48/48	0/0/0/0
15	FEB	V	0	8	-	0/48/48/48	0/0/0/0
15	FEB	Y	0	11	-	0/48/48/48	0/0/0/0

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	2	0	FEB	C19-N18	5.47	1.58	1.45
15	N	0	FEB	C19-N18	5.37	1.57	1.45
15	N	0	FEB	C36-C27	2.89	1.61	1.52
15	2	0	FEB	C36-C27	2.88	1.61	1.52
15	2	0	FEB	O21-C20	2.46	1.28	1.23
15	2	0	FEB	C3-C2	2.29	1.56	1.52
15	N	0	FEB	O21-C20	2.25	1.27	1.23
15	2	0	FEB	C19-C20	2.18	1.58	1.52
15	K	0	FEB	C19-N18	2.17	1.50	1.45
15	K	0	FEB	C13-C10	2.06	1.58	1.53
15	Y	0	FEB	C19-N18	2.02	1.50	1.45

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	2	0	FEB	C19-N18-C38	3.03	129.65	121.53
15	V	0	FEB	C27-C36-C38	2.93	116.74	112.52
15	H	0	FEB	C27-C36-C38	2.92	116.73	112.52
15	2	0	FEB	C2-N1-C11	2.85	127.77	123.18
15	N	0	FEB	C19-N18-C38	2.84	129.16	121.53
15	N	0	FEB	C2-N1-C11	2.66	127.47	123.18
15	2	0	FEB	C10-N9-C20	2.61	127.40	121.63
15	N	0	FEB	C10-N9-C20	2.55	127.27	121.63
15	N	0	FEB	C27-C36-C38	2.45	116.05	112.52
15	2	0	FEB	C20-C19-N18	2.42	118.09	111.28
15	N	0	FEB	C20-C19-N18	2.23	117.55	111.28
15	N	0	FEB	C19-C20-N9	-2.04	112.06	116.81

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	N	0	FEB	O49-C38-N18-C19
15	2	0	FEB	O49-C38-N18-C19

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 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%)	-0.06	9 (3%)	41 37	34, 52, 85, 106	0
1	O	250/250 (100%)	-0.00	15 (6%)	21 18	35, 54, 85, 105	0
2	B	244/244 (100%)	0.20	14 (5%)	23 19	37, 56, 89, 116	0
2	P	244/244 (100%)	0.21	16 (6%)	18 15	40, 56, 89, 116	0
3	C	241/241 (100%)	0.44	26 (10%)	6 5	39, 61, 110, 124	0
3	Q	241/241 (100%)	0.56	36 (14%)	3 2	41, 62, 110, 124	0
4	D	242/242 (100%)	0.24	17 (7%)	16 13	43, 58, 94, 121	0
4	R	242/242 (100%)	0.31	18 (7%)	14 12	44, 59, 95, 122	0
5	E	233/233 (100%)	0.04	8 (3%)	43 39	42, 55, 82, 109	0
5	S	233/233 (100%)	-0.01	9 (3%)	37 33	41, 54, 82, 109	0
6	F	244/244 (100%)	-0.14	9 (3%)	39 35	36, 50, 89, 106	0
6	T	244/244 (100%)	-0.15	7 (2%)	49 46	34, 50, 89, 106	0
7	G	243/243 (100%)	-0.15	9 (3%)	39 35	33, 47, 75, 112	0
7	U	243/243 (100%)	-0.10	7 (2%)	49 46	33, 47, 75, 111	0
8	H	222/222 (100%)	-0.33	4 (1%)	65 64	30, 44, 62, 100	0
8	V	222/222 (100%)	-0.38	3 (1%)	72 72	29, 45, 63, 100	0
9	I	204/204 (100%)	-0.34	3 (1%)	70 71	35, 45, 63, 80	0
9	W	204/204 (100%)	-0.30	3 (1%)	70 71	36, 46, 64, 80	0
10	J	198/198 (100%)	-0.05	8 (4%)	36 32	38, 49, 69, 122	0
10	X	198/198 (100%)	-0.07	7 (3%)	42 38	38, 49, 69, 122	0
11	K	212/212 (100%)	-0.10	10 (4%)	30 27	34, 47, 72, 86	0
11	Y	212/212 (100%)	-0.11	11 (5%)	26 22	35, 47, 74, 86	0
12	L	222/222 (100%)	-0.16	9 (4%)	35 32	33, 48, 74, 89	0
12	Z	222/222 (100%)	-0.19	10 (4%)	32 28	34, 47, 74, 89	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%)	-0.44	1 (0%)	90 91	31, 43, 57, 61	0
13	M	233/233 (100%)	-0.37	1 (0%)	90 91	32, 43, 57, 63	0
14	2	196/196 (100%)	-0.38	1 (0%)	88 90	31, 41, 61, 81	0
14	N	196/196 (100%)	-0.37	1 (0%)	88 90	31, 40, 60, 81	0
All	All	6368/6368 (100%)	-0.07	272 (4%)	34 30	29, 50, 84, 124	0

All (272) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	55	THR	12.5
4	R	12(E)	SER	12.4
4	D	12(C)	GLY	11.0
7	U	240	ASP	9.8
10	X	192	ALA	9.5
10	J	192	ALA	9.4
4	R	12(C)	GLY	9.3
4	D	12(E)	SER	9.0
4	D	12(D)	ALA	9.0
7	G	240	ASP	8.6
4	R	12(F)	GLY	8.3
4	R	12(D)	ALA	8.2
3	Q	55	THR	8.1
2	B	54	VAL	7.6
2	B	218	ASN	7.6
6	F	5	GLY	7.3
2	B	217	ALA	7.3
3	C	56	LEU	7.2
7	G	6	ALA	6.9
4	D	12(F)	GLY	6.8
1	A	5	THR	6.6
2	P	218	ASN	6.3
1	O	5	THR	6.3
7	U	6	ALA	6.2
10	J	191	GLN	6.2
10	J	193	GLN	6.1
10	X	193	GLN	6.1
2	P	21(A)	LYS	6.1
1	A	4	MET	6.1
10	X	191	GLN	6.1
12	L	145	TYR	6.0
2	P	217	ALA	5.8

Continued on next page...



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	O	4	MET	5.8
11	Y	208	ASN	5.7
11	K	208	ASN	5.6
12	Z	145	TYR	5.5
3	Q	240	LYS	5.4
2	P	54	VAL	5.2
5	E	203	ASP	5.2
8	V	223	ASP	5.2
3	Q	243	GLN	5.2
3	Q	203	THR	5.1
5	S	4	PHE	5.0
4	R	126	ARG	5.0
3	Q	242	GLU	4.9
3	Q	56	LEU	4.9
5	S	203	ASP	4.9
8	H	223	ASP	4.9
2	P	21(C)	ASP	4.9
3	C	240	LYS	4.8
3	Q	54	SER	4.8
5	E	4	PHE	4.8
2	P	219	GLU	4.7
4	D	125	GLU	4.7
9	W	-8	SER	4.7
2	B	21(A)	LYS	4.7
1	O	53	LYS	4.6
4	R	242	ALA	4.5
9	I	-8	SER	4.4
3	Q	241	GLN	4.4
4	D	127	LEU	4.3
3	C	241	GLN	4.3
4	R	125	GLU	4.3
4	D	126	ARG	4.3
3	Q	64	PRO	4.2
12	L	14(P)	PRO	4.2
1	A	236	LEU	4.2
3	Q	207	ALA	4.2
4	R	243	ALA	4.2
6	T	240	ILE	4.2
5	S	5	ARG	4.2
11	Y	104	TYR	4.1
7	G	239	GLN	4.1
11	K	210	ILE	4.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
3	Q	63	THR	4.1
8	V	222	CYS	4.0
4	R	127	LEU	4.0
3	C	243	GLN	4.0
6	F	241	ASN	4.0
11	K	207	ASN	3.9
5	E	5	ARG	3.9
2	B	21(B)	GLY	3.8
12	L	14(H)	GLY	3.8
4	D	244	GLU	3.8
3	Q	236	ILE	3.8
6	F	204	ASP	3.8
11	Y	67	GLU	3.8
11	K	104	TYR	3.8
11	Y	210	ILE	3.7
3	Q	18(C)	LYS	3.7
11	Y	207	ASN	3.7
13	1	-8	THR	3.6
11	Y	181	ASP	3.6
8	H	220	ASN	3.6
2	P	21(B)	GLY	3.6
4	D	12(G)	GLU	3.6
4	R	12(G)	GLU	3.6
3	C	43	LYS	3.5
5	S	178	ARG	3.5
6	F	20(B)	GLU	3.5
1	O	21(P)	LYS	3.4
3	Q	202	GLN	3.4
12	Z	14(W)	LYS	3.4
2	B	21(C)	ASP	3.4
11	K	143	LYS	3.4
2	B	219	GLU	3.4
12	L	14(M)	VAL	3.4
4	D	243	ALA	3.4
3	Q	7	GLY	3.4
10	J	92	ARG	3.3
8	V	220	ASN	3.3
3	C	33	ARG	3.3
1	O	236	LEU	3.3
2	B	20(B)	ALA	3.3
7	U	8	TYR	3.3
11	Y	10(A)	ARG	3.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
12	Z	14(H)	GLY	3.3
7	G	7	GLY	3.2
2	P	53	LYS	3.2
4	R	9	ASP	3.2
8	H	222	CYS	3.2
5	S	127	TYR	3.2
5	S	217	LYS	3.2
12	L	14(W)	LYS	3.2
14	2	18(I)	GLN	3.2
3	C	203	THR	3.2
1	A	203	GLU	3.2
3	Q	53	ARG	3.2
2	P	185	LYS	3.2
2	P	183	ASP	3.2
6	F	240	ILE	3.2
6	T	241	ASN	3.2
11	K	40	PHE	3.1
3	Q	222	VAL	3.1
11	Y	180	GLU	3.1
3	C	237	GLU	3.1
13	M	-8	THR	3.1
1	O	235	ALA	3.1
10	J	-1	MET	3.1
2	P	239	THR	3.1
7	U	7	GLY	3.1
14	N	18(I)	GLN	3.1
3	Q	239	GLU	3.1
10	X	92	ARG	3.1
2	P	220	TYR	3.0
5	E	127	TYR	3.0
7	G	8	TYR	3.0
3	Q	178	LYS	3.0
3	Q	208	LYS	3.0
3	Q	223	ALA	3.0
7	U	218	ASP	3.0
3	C	52	ARG	3.0
9	W	182	ASP	3.0
3	C	208	LYS	3.0
7	G	18(A)	ILE	2.9
6	T	6	THR	2.9
12	Z	-9	GLN	2.9
7	G	218	ASP	2.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
6	F	206	LYS	2.9
12	Z	14(P)	PRO	2.9
6	T	18(E)	GLU	2.9
11	K	181	ASP	2.8
3	Q	14(B)	ASP	2.8
4	D	9	ASP	2.8
11	K	10(A)	ARG	2.8
3	C	238	GLN	2.8
4	D	218	GLN	2.8
2	B	239	THR	2.8
12	Z	14(M)	VAL	2.8
6	F	6	THR	2.8
3	Q	62	ARG	2.7
1	O	43	THR	2.7
5	S	204	GLU	2.7
9	I	181	LYS	2.7
4	R	244	GLU	2.7
11	K	73	ARG	2.7
1	O	21(F)	LEU	2.7
2	B	183	ASP	2.7
3	Q	238	GLN	2.7
3	Q	206	GLY	2.7
3	Q	62(A)	ILE	2.7
6	F	18(E)	GLU	2.6
12	L	70(A)	ASN	2.6
2	P	21(D)	GLY	2.6
5	E	233	ILE	2.6
3	C	194	VAL	2.6
2	B	21(D)	GLY	2.6
4	R	12(B)	GLU	2.6
3	Q	52	ARG	2.6
3	Q	18(D)	GLU	2.5
7	G	18(H)	GLU	2.5
3	C	53	ARG	2.5
1	A	21(N)	THR	2.5
5	E	204	GLU	2.5
6	T	20(C)	LYS	2.5
4	D	18(D)	SER	2.5
11	K	180	GLU	2.5
11	Y	73	ARG	2.5
5	S	233	ILE	2.5
7	U	239	GLN	2.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
10	X	188	ASP	2.4
4	R	241	GLU	2.4
12	Z	70(A)	ASN	2.4
2	P	181	LYS	2.4
2	P	20(A)	SER	2.4
1	O	143	GLU	2.4
3	C	18(C)	LYS	2.4
2	B	237	GLY	2.4
5	E	217	LYS	2.4
1	A	21(P)	LYS	2.4
3	Q	14(A)	ARG	2.3
3	Q	18(B)	ARG	2.3
3	Q	33	ARG	2.3
3	C	227	GLU	2.3
3	C	235	GLN	2.3
1	O	178	LYS	2.3
3	C	54	SER	2.3
3	C	233	VAL	2.3
10	X	168	MET	2.3
4	D	10	ARG	2.3
3	C	236	ILE	2.2
3	C	7	GLY	2.2
6	T	18(D)	PRO	2.2
7	U	72	ARG	2.2
3	C	202	GLN	2.2
12	Z	182	ASP	2.2
4	D	205	GLU	2.2
2	B	20(A)	SER	2.2
3	Q	43	LYS	2.2
10	J	145	ASP	2.2
12	Z	1(I)	ASN	2.2
12	Z	120	GLU	2.2
3	Q	58	LEU	2.2
3	Q	234	THR	2.2
9	W	12(A)	LYS	2.2
1	O	21(M)	PRO	2.2
9	I	182	ASP	2.2
7	G	238	GLU	2.2
12	L	-9	GLN	2.1
4	R	18(D)	SER	2.1
4	R	240	LYS	2.1
10	J	188	ASP	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	P	63	THR	2.1
8	H	180	ILE	2.1
3	C	234	THR	2.1
11	Y	211	GLY	2.1
4	D	240	LYS	2.1
10	X	-1	MET	2.1
1	A	205	GLU	2.1
3	Q	187	GLU	2.1
10	J	144	PRO	2.1
1	A	204	GLY	2.1
6	T	238	LYS	2.1
4	R	231	GLU	2.1
3	Q	227	GLU	2.1
6	F	20(C)	LYS	2.1
12	L	180	LYS	2.1
2	B	209	ARG	2.1
1	A	200	SER	2.1
1	O	55	SER	2.1
1	O	203	GLU	2.1
4	D	202	GLU	2.1
5	S	64	GLN	2.0
3	C	187	GLU	2.0
5	E	178	ARG	2.0
12	L	106	GLU	2.0
3	C	49	GLY	2.0
4	R	122	ARG	2.0
11	Y	40	PHE	2.0
1	O	21(N)	THR	2.0
1	O	234	GLU	2.0
3	C	14(A)	ARG	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands

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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
15	FEB	Y	0	39/39	0.20	-	34,43,56,58	0
15	FEB	H	0	39/39	0.18	-	38,45,58,63	0
15	FEB	N	0	39/39	0.22	-	40,49,60,61	0
15	FEB	K	0	39/39	0.18	-	32,40,55,56	0
15	FEB	V	0	39/39	0.20	-	39,45,58,63	0
15	FEB	2	0	39/39	0.27	-	39,50,60,65	0

## 6.5 Other polymers

There are no such residues in this entry.