



# Full wwPDB X-ray Structure Validation Report

Mar 31, 2014 – 06:09 PM BST

PDB ID : 3L2F  
Title : Glycocyamine kinase, beta-beta homodimer from marine worm *Namalycastis* sp., with transition state analog Mg(II)-ADP-NO<sub>3</sub>-glycocyamine.Part 1.  
Authors : Lim, K.; Pullalarevu, S.; Herzberg, O.  
Deposited on : 2009-12-15  
Resolution : 2.30 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>

---

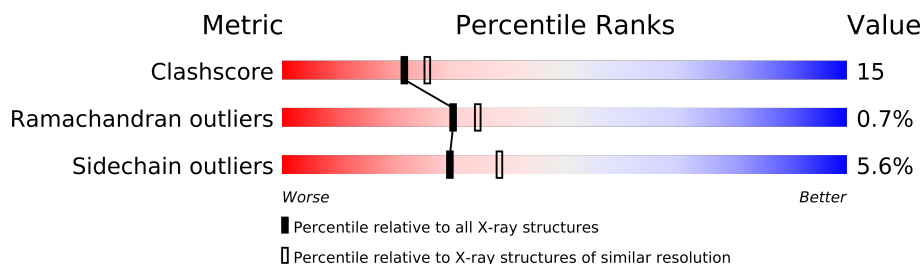
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : **NOT EXECUTED**  
Percentile statistics : 21963  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable23004

# 1 Overall quality at a glance

The reported resolution of this entry is 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)


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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	390	
1	B	390	
1	C	390	
1	D	390	
1	E	390	
1	F	390	
1	G	390	
1	H	390	
1	I	390	
1	J	390	
1	K	390	
1	L	390	
1	M	390	
1	N	390	
1	O	390	
1	P	390	
1	Q	390	

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	R	390	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
5	NO3	A	801	X	-
5	NO3	B	802	X	-
5	NO3	C	803	X	-
5	NO3	D	804	X	-
5	NO3	E	805	X	-
5	NO3	F	806	X	-
5	NO3	G	807	X	-
5	NO3	H	808	X	-
5	NO3	I	809	X	-
5	NO3	J	810	X	-
5	NO3	K	811	X	-
5	NO3	L	812	X	-
5	NO3	M	813	X	-
5	NO3	N	814	X	-
5	NO3	O	815	X	-
5	NO3	P	816	X	-
5	NO3	Q	817	X	-
5	NO3	R	818	X	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 56675 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 Glycocyamine kinase beta chain.

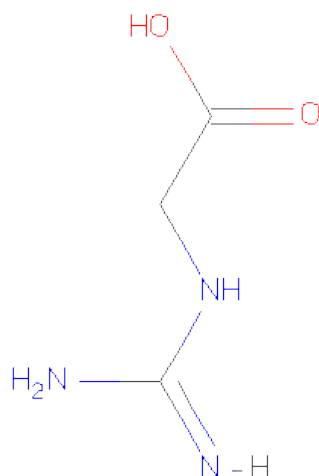
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	366	Total	C	N	O	S	0	0	0
			2901	1828	511	541	21			
1	B	387	Total	C	N	O	S	0	0	0
			3074	1939	543	571	21			
1	C	367	Total	C	N	O	S	0	0	0
			2910	1834	513	542	21			
1	D	382	Total	C	N	O	S	0	0	0
			3032	1912	537	562	21			
1	E	367	Total	C	N	O	S	0	0	0
			2910	1834	513	542	21			
1	F	385	Total	C	N	O	S	0	0	0
			3061	1930	541	569	21			
1	G	367	Total	C	N	O	S	0	0	0
			2910	1834	513	542	21			
1	H	384	Total	C	N	O	S	0	0	0
			3052	1925	539	567	21			
1	I	366	Total	C	N	O	S	0	0	0
			2901	1828	511	541	21			
1	J	385	Total	C	N	O	S	0	0	0
			3061	1930	541	569	21			
1	K	367	Total	C	N	O	S	0	0	0
			2910	1834	513	542	21			
1	L	384	Total	C	N	O	S	0	0	0
			3052	1925	539	567	21			
1	M	367	Total	C	N	O	S	0	0	0
			2910	1834	513	542	21			
1	N	382	Total	C	N	O	S	0	0	0
			3032	1912	537	562	21			
1	O	366	Total	C	N	O	S	0	0	0
			2901	1828	511	541	21			
1	P	381	Total	C	N	O	S	0	0	0
			3021	1903	536	561	21			

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	366	Total	C	N	O	S	0	0	0
			2901	1828	511	541	21			
1	R	379	Total	C	N	O	S	0	0	0
			3005	1892	533	559	21			

- Molecule 2 is GUANIDINO ACETATE (three-letter code: NMG) (formula:  $C_3H_7N_3O_2$ ).



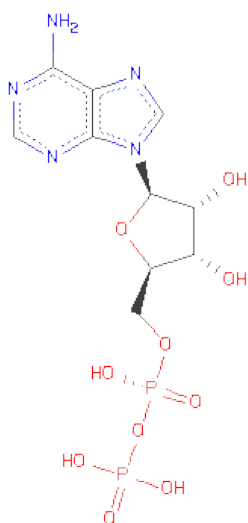
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			8	3	3	2		
2	B	1	Total	C	N	O	0	0
			8	3	3	2		
2	C	1	Total	C	N	O	0	0
			8	3	3	2		
2	D	1	Total	C	N	O	0	0
			8	3	3	2		
2	E	1	Total	C	N	O	0	0
			8	3	3	2		
2	F	1	Total	C	N	O	0	0
			8	3	3	2		
2	G	1	Total	C	N	O	0	0
			8	3	3	2		
2	H	1	Total	C	N	O	0	0
			8	3	3	2		
2	I	1	Total	C	N	O	0	0
			8	3	3	2		

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	J	1	Total	C	N	O	0	0
			8	3	3	2		
2	K	1	Total	C	N	O	0	0
			8	3	3	2		
2	L	1	Total	C	N	O	0	0
			8	3	3	2		
2	M	1	Total	C	N	O	0	0
			8	3	3	2		
2	N	1	Total	C	N	O	0	0
			8	3	3	2		
2	O	1	Total	C	N	O	0	0
			8	3	3	2		
2	P	1	Total	C	N	O	0	0
			8	3	3	2		
2	Q	1	Total	C	N	O	0	0
			8	3	3	2		
2	R	1	Total	C	N	O	0	0
			8	3	3	2		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

Continued on next page...

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	G	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	H	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	I	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	J	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	K	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	L	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	M	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	N	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	O	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	P	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	Q	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	R	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	P	1	Total	Mg	0	0
			1	1		
4	G	1	Total	Mg	0	0
			1	1		
4	J	1	Total	Mg	0	0
			1	1		

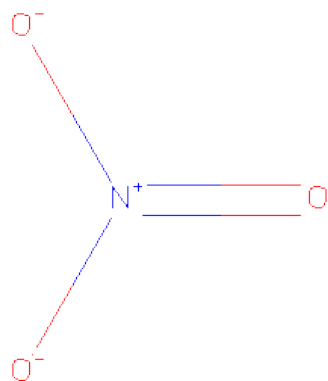
*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	Q	1	Total 1	Mg 1	0	0
4	D	1	Total 1	Mg 1	0	0
4	K	1	Total 1	Mg 1	0	0
4	E	1	Total 1	Mg 1	0	0
4	H	1	Total 1	Mg 1	0	0
4	B	1	Total 1	Mg 1	0	0
4	I	1	Total 1	Mg 1	0	0
4	C	1	Total 1	Mg 1	0	0
4	A	1	Total 1	Mg 1	0	0
4	N	1	Total 1	Mg 1	0	0
4	O	1	Total 1	Mg 1	0	0
4	R	1	Total 1	Mg 1	0	0
4	L	1	Total 1	Mg 1	0	0
4	F	1	Total 1	Mg 1	0	0
4	M	1	Total 1	Mg 1	0	0

- Molecule 5 is NITRATE ION (three-letter code: NO3) (formula: NO<sub>3</sub>).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	N	O	0	0
			4	1	3		
5	B	1	Total	N	O	0	0
			4	1	3		
5	C	1	Total	N	O	0	0
			4	1	3		
5	D	1	Total	N	O	0	0
			4	1	3		
5	E	1	Total	N	O	0	0
			4	1	3		
5	F	1	Total	N	O	0	0
			4	1	3		
5	G	1	Total	N	O	0	0
			4	1	3		
5	H	1	Total	N	O	0	0
			4	1	3		
5	I	1	Total	N	O	0	0
			4	1	3		
5	J	1	Total	N	O	0	0
			4	1	3		
5	K	1	Total	N	O	0	0
			4	1	3		
5	L	1	Total	N	O	0	0
			4	1	3		
5	M	1	Total	N	O	0	0
			4	1	3		
5	N	1	Total	N	O	0	0
			4	1	3		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	O	1	Total	N	O	0	0
			4	1	3		
5	P	1	Total	N	O	0	0
			4	1	3		
5	Q	1	Total	N	O	0	0
			4	1	3		
5	R	1	Total	N	O	0	0
			4	1	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	106	Total	O	0	0
			106	106		
6	B	138	Total	O	0	0
			138	138		
6	C	116	Total	O	0	0
			116	116		
6	D	149	Total	O	0	0
			149	149		
6	E	154	Total	O	0	0
			154	154		
6	F	116	Total	O	0	0
			116	116		
6	G	131	Total	O	0	0
			131	131		
6	H	88	Total	O	0	0
			88	88		
6	I	111	Total	O	0	0
			111	111		
6	J	136	Total	O	0	0
			136	136		
6	K	125	Total	O	0	0
			125	125		
6	L	157	Total	O	0	0
			157	157		
6	M	149	Total	O	0	0
			149	149		
6	N	116	Total	O	0	0
			116	116		
6	O	114	Total	O	0	0
			114	114		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	P	172	Total 172	O 172	0	0
6	Q	166	Total 166	O 166	0	0
6	R	167	Total 167	O 167	0	0

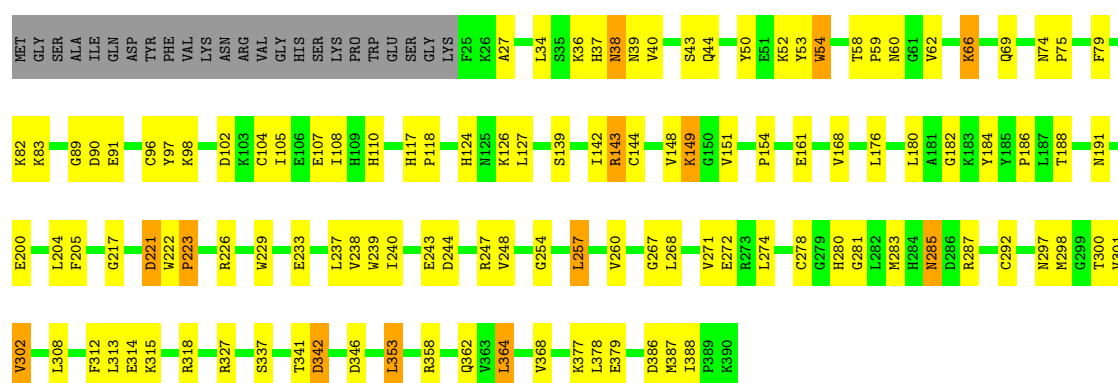
### 3 Residue-property plots

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.

Note EDS was not executed.

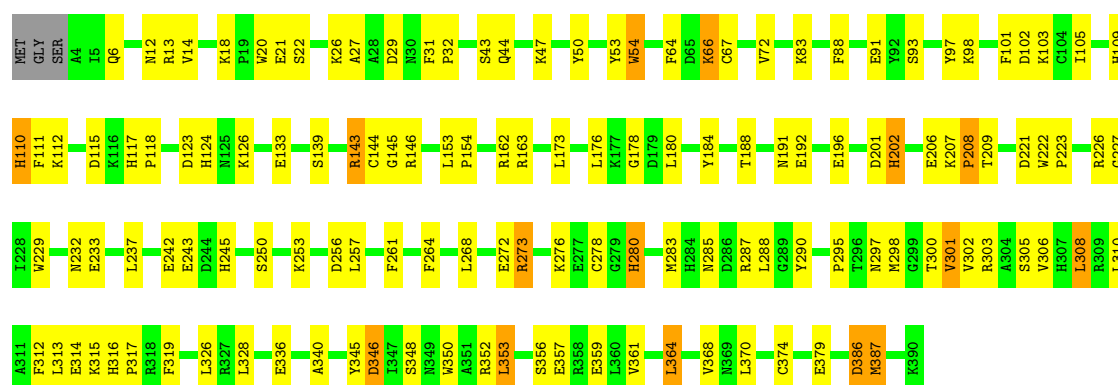
- Molecule 1: Glycocyamine kinase beta chain

Chain A:



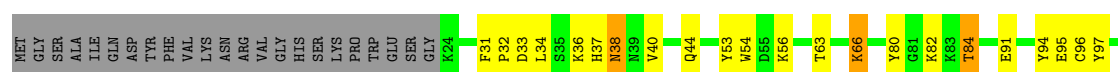
- Molecule 1: Glycocyamine kinase beta chain

Chain B:



- Molecule 1: Glycocyamine kinase beta chain

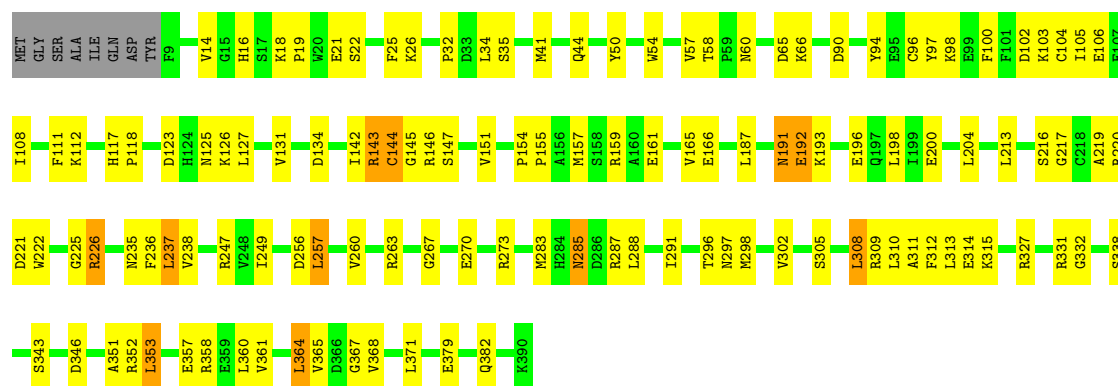
Chain C:





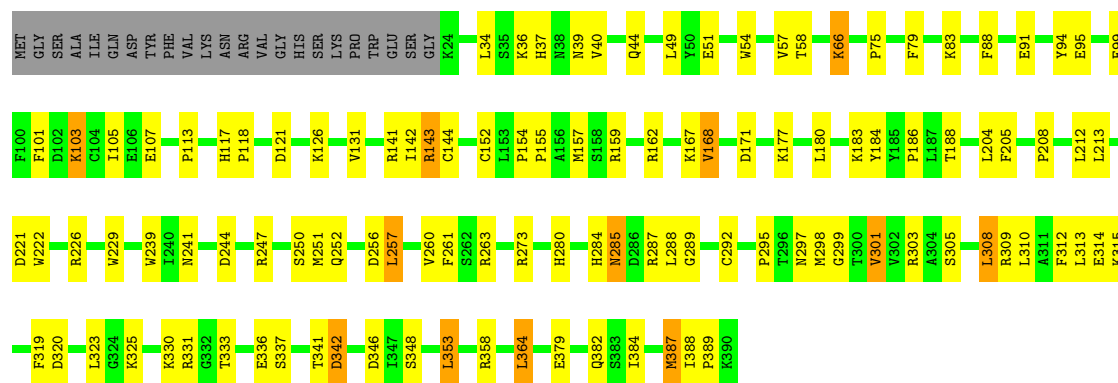
• Molecule 1: Glycocyamine kinase beta chain

Chain D:



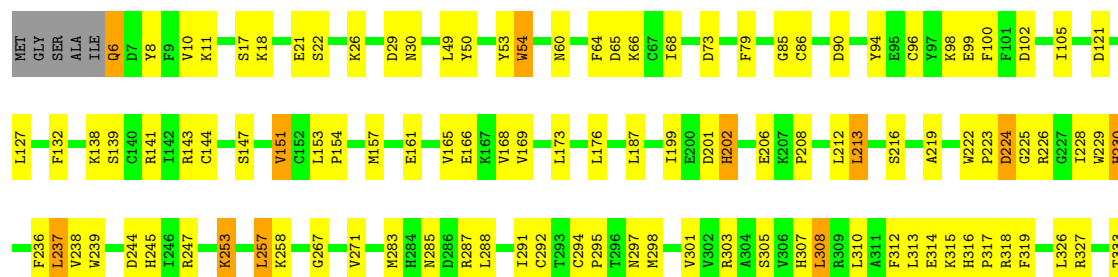
• Molecule 1: Glycocyamine kinase beta chain

Chain E:



• Molecule 1: Glycocyamine kinase beta chain

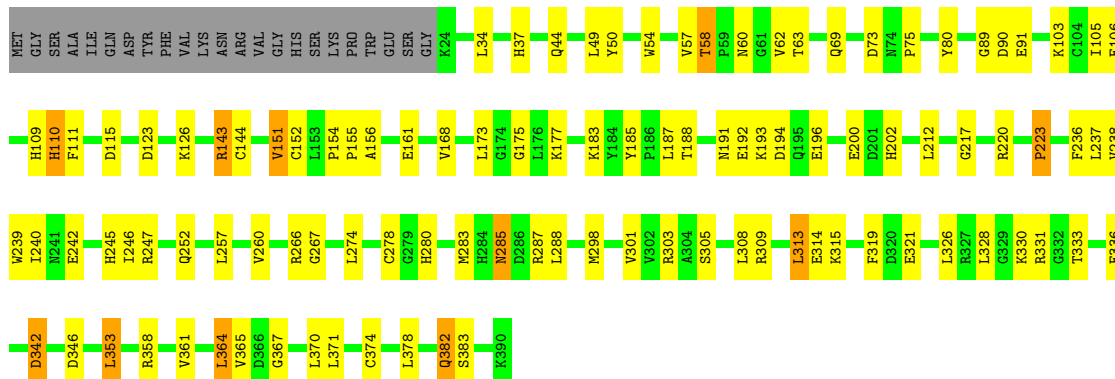
Chain F:





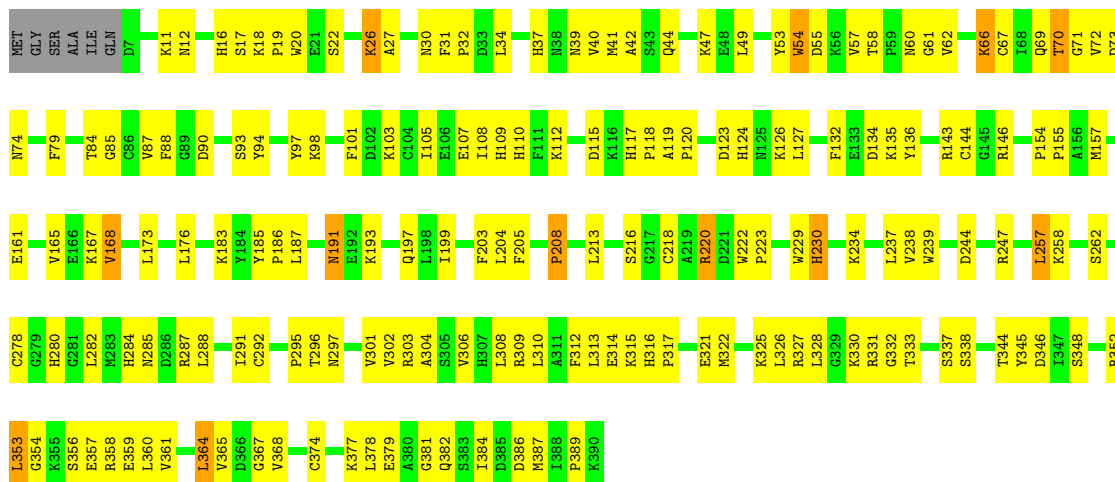
• Molecule 1: Glycocyamine kinase beta chain

Chain G:



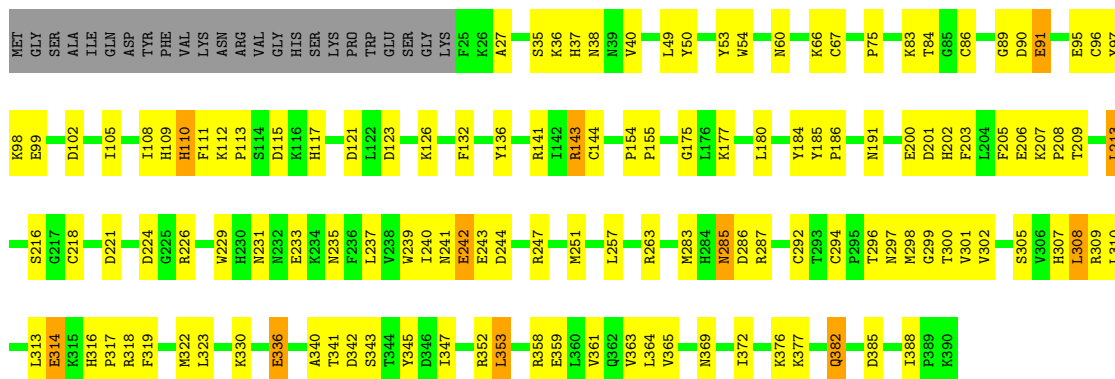
• Molecule 1: Glycocyamine kinase beta chain

Chain H:



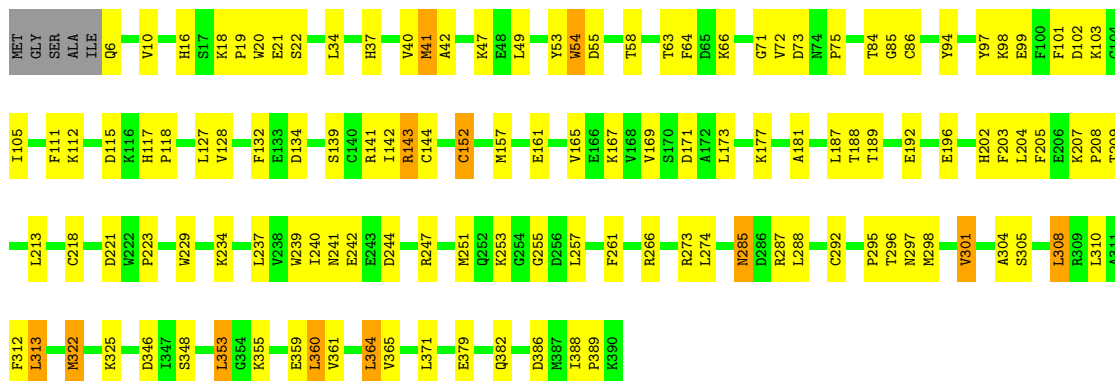
• Molecule 1: Glycocyamine kinase beta chain

Chain I:



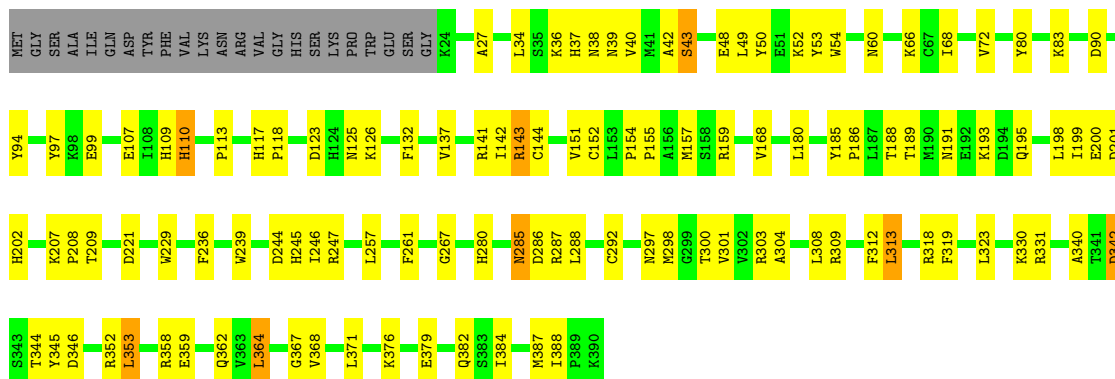
- Molecule 1: Glycocyamine kinase beta chain

Chain J:



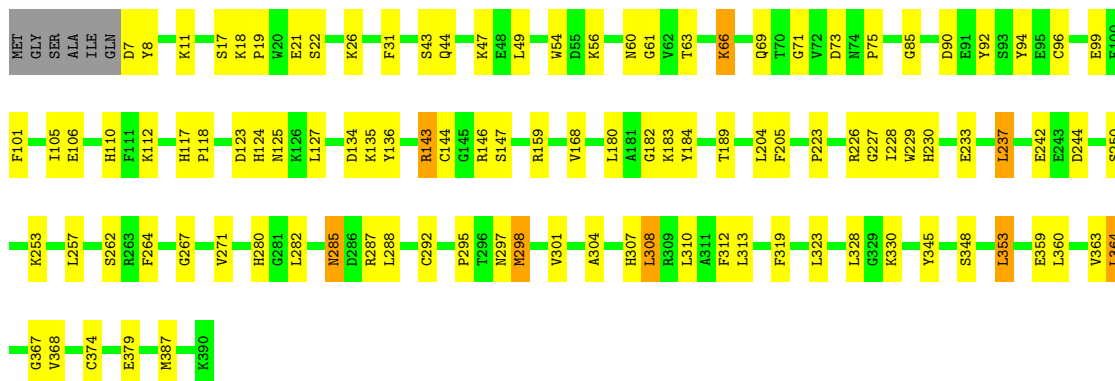
- Molecule 1: Glycocyamine kinase beta chain

Chain K:



- Molecule 1: Glycocyamine kinase beta chain

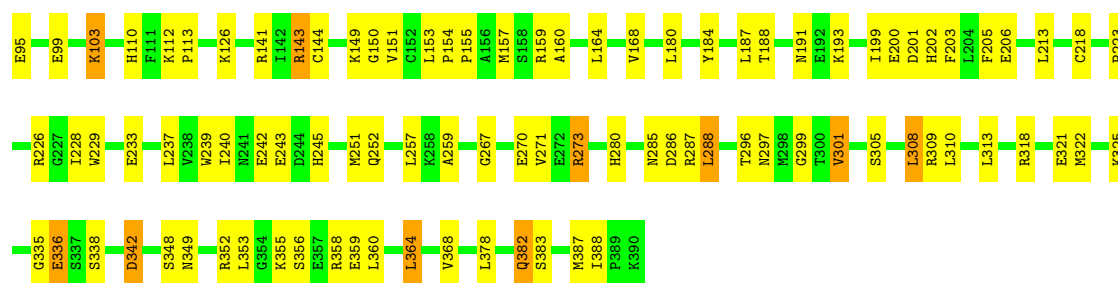
Chain L:



- Molecule 1: Glycocyamine kinase beta chain

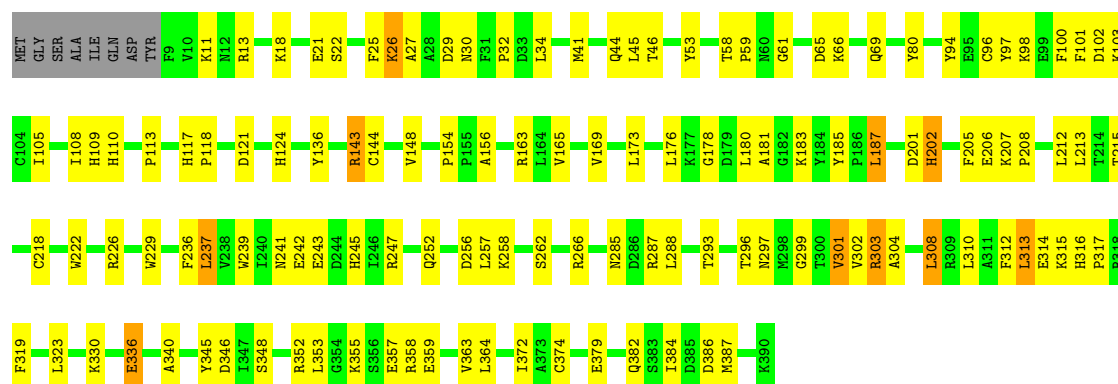
Chain M:





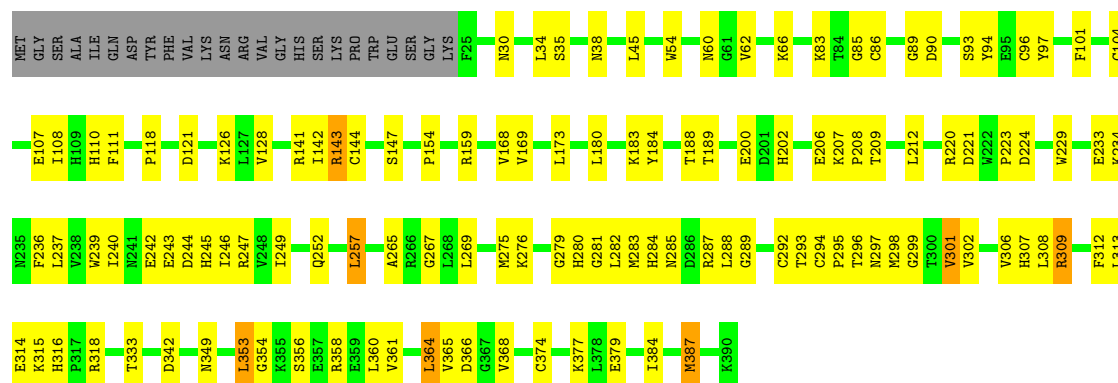
• Molecule 1: Glycocyamine kinase beta chain

Chain N:



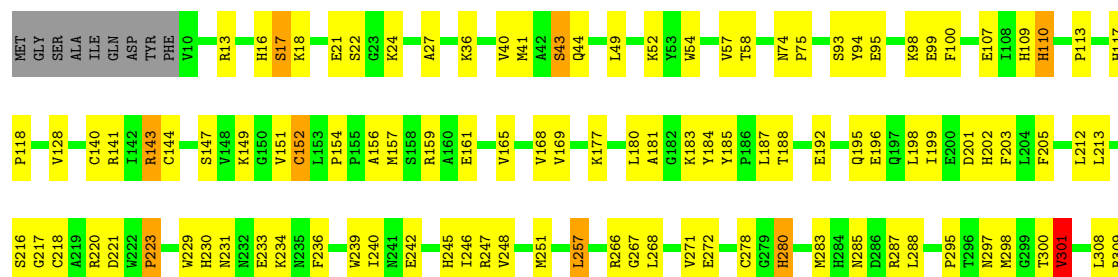
• Molecule 1: Glycocyamine kinase beta chain

Chain O:



• Molecule 1: Glycocyamine kinase beta chain

Chain P:

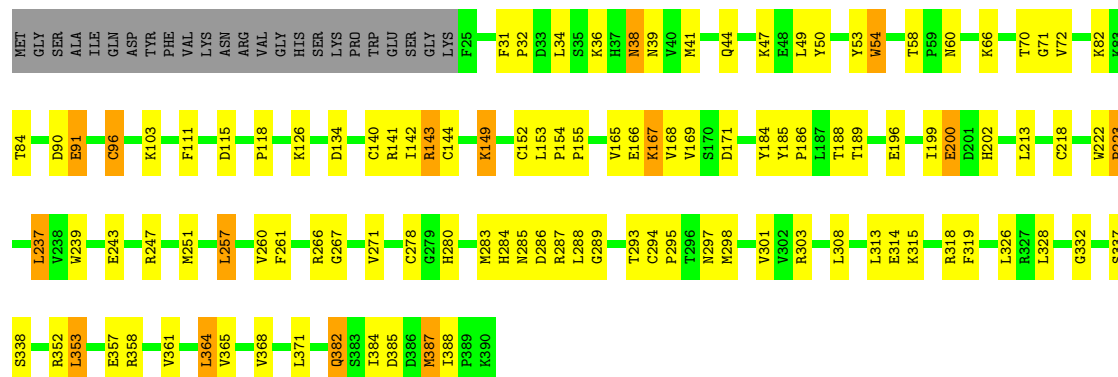






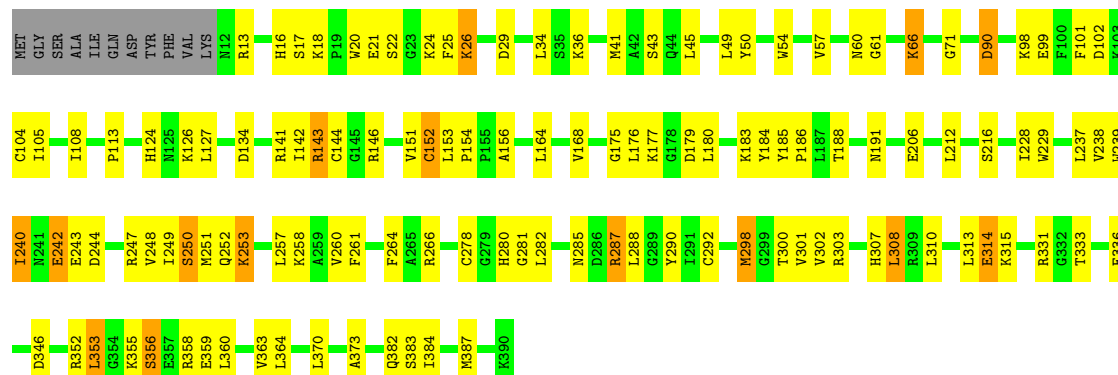
• Molecule 1: Glycocyamine kinase beta chain

Chain Q:



• Molecule 1: Glycocyamine kinase beta chain

Chain R:



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	243.11Å 114.27Å 259.90Å 90.00° 90.25° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.30)	Depositor
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.08 (at 2.29Å)	Xtriage
Refinement program	phenix	Depositor
R, $R_{free}$	0.197 , 0.263	Depositor
Wilson B-factor (Å <sup>2</sup> )	23.1	Xtriage
Anisotropy	0.184	Xtriage
Estimated twinning fraction	0.428 for h,-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	38 of 610844 reflections (0.006%)	Xtriage
Total number of atoms	56675	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 38.54 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 3.6323e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: NMG, MG, ADP, NO3

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	0.34	0/2963	0.51	0/3986
1	B	0.37	0/3142	0.55	0/4227
1	C	0.34	0/2972	0.53	0/3997
1	D	0.38	0/3099	0.55	0/4168
1	E	0.35	0/2972	0.52	0/3997
1	F	0.37	0/3129	0.56	0/4209
1	G	0.35	0/2972	0.53	1/3997 (0.0%)
1	H	0.35	0/3120	0.53	0/4197
1	I	0.34	0/2963	0.52	0/3986
1	J	0.37	0/3129	0.53	0/4209
1	K	0.35	0/2972	0.52	0/3997
1	L	0.38	0/3120	0.55	0/4197
1	M	0.35	0/2972	0.54	0/3997
1	N	0.37	0/3099	0.54	0/4168
1	O	0.34	0/2963	0.53	0/3986
1	P	0.39	0/3087	0.55	1/4152 (0.0%)
1	Q	0.35	0/2963	0.53	0/3986
1	R	0.38	0/3071	0.55	0/4131
All	All	0.36	0/54708	0.54	2/73587 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	353	LEU	CA-CB-CG	5.32	127.53	115.30
1	G	364	LEU	CA-CB-CG	5.26	127.40	115.30

There are no chirality outliers.

There are no planarity outliers.

## 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	2901	0	2866	94	0
1	B	3074	0	3034	107	0
1	C	2910	0	2879	88	0
1	D	3032	0	2997	81	0
1	E	2910	0	2879	83	0
1	F	3061	0	3018	96	0
1	G	2910	0	2879	78	0
1	H	3052	0	3010	141	0
1	I	2901	0	2866	89	0
1	J	3061	0	3018	85	0
1	K	2910	0	2879	89	0
1	L	3052	0	3010	79	0
1	M	2910	0	2879	81	0
1	N	3032	0	2997	93	0
1	O	2901	0	2866	93	0
1	P	3021	0	2988	108	0
1	Q	2901	0	2866	80	0
1	R	3005	0	2966	92	0
2	A	8	0	5	0	0
2	B	8	0	5	2	0
2	C	8	0	5	0	0
2	D	8	0	5	0	0
2	E	8	0	5	1	0
2	F	8	0	5	0	0
2	G	8	0	5	2	0
2	H	8	0	5	0	0
2	I	8	0	5	1	0
2	J	8	0	5	0	0
2	K	8	0	5	0	0
2	L	8	0	5	0	0
2	M	8	0	5	1	0
2	N	8	0	5	1	0
2	O	8	0	5	1	0
2	P	8	0	5	0	0
2	Q	8	0	5	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	R	8	0	5	0	0
3	A	27	0	12	1	0
3	B	27	0	12	2	0
3	C	27	0	12	1	0
3	D	27	0	12	0	0
3	E	27	0	12	4	0
3	F	27	0	12	7	0
3	G	27	0	12	2	0
3	H	27	0	12	3	0
3	I	27	0	12	3	0
3	J	27	0	12	3	0
3	K	27	0	12	5	0
3	L	27	0	12	1	0
3	M	27	0	12	2	0
3	N	27	0	12	1	0
3	O	27	0	12	4	0
3	P	27	0	12	5	0
3	Q	27	0	12	3	0
3	R	27	0	12	2	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
4	I	1	0	0	0	0
4	J	1	0	0	0	0
4	K	1	0	0	0	0
4	L	1	0	0	0	0
4	M	1	0	0	0	0
4	N	1	0	0	0	0
4	O	1	0	0	0	0
4	P	1	0	0	0	0
4	Q	1	0	0	0	0
4	R	1	0	0	0	0
5	A	4	0	0	0	0
5	B	4	0	0	0	0
5	C	4	0	0	0	0
5	D	4	0	0	1	0
5	E	4	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	4	0	0	0	0
5	G	4	0	0	0	0
5	H	4	0	0	0	0
5	I	4	0	0	0	0
5	J	4	0	0	0	0
5	K	4	0	0	0	0
5	L	4	0	0	0	0
5	M	4	0	0	0	0
5	N	4	0	0	0	0
5	O	4	0	0	1	0
5	P	4	0	0	0	0
5	Q	4	0	0	0	0
5	R	4	0	0	1	0
6	A	106	0	0	6	0
6	B	138	0	0	12	0
6	C	116	0	0	5	0
6	D	149	0	0	3	0
6	E	154	0	0	6	0
6	F	116	0	0	9	0
6	G	131	0	0	4	0
6	H	88	0	0	5	0
6	I	111	0	0	3	0
6	J	136	0	0	5	0
6	K	125	0	0	8	0
6	L	157	0	0	5	0
6	M	149	0	0	8	0
6	N	116	0	0	7	0
6	O	114	0	0	7	0
6	P	172	0	0	14	0
6	Q	166	0	0	9	0
6	R	167	0	0	5	0
All	All	56675	0	53203	1632	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 15.

All (1632) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:126:LYS:HB2	1:K:358:ARG:HD2	1.38	1.04
1:D:285:ASN:HB2	1:D:291:ILE:HD11	1.40	1.02
1:L:285:ASN:HD22	1:L:288:LEU:H	1.03	0.99
1:O:285:ASN:HD22	1:O:288:LEU:H	1.10	0.99

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:377:LYS:HG3	1:F:387:MET:HE1	1.45	0.98
1:A:297:ASN:HB3	1:A:301:VAL:HG13	1.45	0.95
1:L:285:ASN:ND2	1:L:288:LEU:H	1.66	0.93
1:Q:285:ASN:HD22	1:Q:288:LEU:H	1.17	0.92
1:H:285:ASN:HD22	1:H:288:LEU:N	1.68	0.92
1:F:295:PRO:O	1:F:298:MET:HE2	1.69	0.91
1:P:239:TRP:HB2	1:P:247:ARG:HB2	1.53	0.91
1:D:308:LEU:HD13	1:D:310:LEU:HD11	1.53	0.89
1:J:239:TRP:HB2	1:J:247:ARG:HB2	1.54	0.89
3:I:609:ADP:O2B	3:I:609:ADP:H5'2	1.72	0.88
1:H:285:ASN:ND2	1:H:288:LEU:H	1.73	0.87
1:M:126:LYS:HB2	1:M:358:ARG:HD2	1.57	0.87
1:A:36:LYS:HG3	6:A:1862:HOH:O	1.74	0.87
1:P:188:THR:HG22	1:P:223:PRO:HG2	1.57	0.86
1:H:285:ASN:HD22	1:H:288:LEU:H	0.89	0.85
1:P:357:GLU:O	1:P:361:VAL:HG23	1.77	0.85
1:G:89:GLY:HA2	1:G:155:PRO:HG2	1.56	0.84
1:R:314:GLU:HG2	1:R:315:LYS:HD2	1.58	0.83
1:P:278:CYS:HB3	1:P:280:HIS:CE1	2.13	0.83
1:F:285:ASN:HD22	1:F:288:LEU:H	1.24	0.83
1:G:192:GLU:O	1:G:196:GLU:HG3	1.79	0.83
1:E:297:ASN:HB3	1:E:301:VAL:HG13	1.59	0.82
1:R:144:CYS:HB3	1:R:302:VAL:HG22	1.60	0.82
1:A:285:ASN:ND2	1:A:287:ARG:H	1.78	0.81
1:G:50:TYR:O	1:G:54:TRP:HB3	1.81	0.81
1:A:40:VAL:HG13	1:A:107:GLU:OE1	1.81	0.80
1:P:18:LYS:O	1:P:21:GLU:HG2	1.81	0.80
1:I:285:ASN:HD22	1:I:287:ARG:H	1.25	0.80
1:L:244:ASP:OD1	1:L:292:CYS:HB3	1.82	0.79
1:K:239:TRP:HB2	1:K:247:ARG:HB2	1.64	0.79
1:Q:188:THR:HG22	1:Q:223:PRO:HG2	1.65	0.79
1:Q:313:LEU:HD22	1:Q:319:PHE:CD1	2.18	0.78
1:E:126:LYS:HB2	1:E:358:ARG:HD2	1.64	0.78
1:O:239:TRP:HB2	1:O:247:ARG:HB2	1.66	0.78
1:M:94:TYR:HD1	1:M:95:GLU:HG2	1.50	0.77
1:K:151:VAL:HG12	1:K:152:CYS:O	1.84	0.77
1:N:143:ARG:HG2	1:N:144:CYS:N	2.00	0.77
1:N:98:LYS:HE3	1:N:102:ASP:OD2	1.83	0.77
1:P:188:THR:HG23	6:P:2736:HOH:O	1.83	0.77
1:J:49:LEU:HD21	1:J:99:GLU:HG2	1.66	0.76
1:N:359:GLU:O	1:N:363:VAL:HG23	1.86	0.76
1:K:352:ARG:HG2	1:K:352:ARG:HH11	1.51	0.76

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:N:208:PRO:HG3	1:N:222:TRP:CE2	2.21	0.76
1:O:126:LYS:HB2	1:O:358:ARG:HD2	1.68	0.75
1:G:285:ASN:HD22	1:G:288:LEU:H	1.34	0.75
1:D:302:VAL:HG21	1:D:357:GLU:HG3	1.67	0.75
1:N:18:LYS:HB2	1:N:21:GLU:HG2	1.69	0.75
1:M:50:TYR:O	1:M:54:TRP:HB3	1.87	0.74
1:K:352:ARG:CG	1:K:352:ARG:HH11	2.00	0.74
1:F:237:LEU:HD12	1:F:237:LEU:N	2.02	0.74
1:Q:285:ASN:ND2	1:Q:287:ARG:H	1.85	0.74
1:E:239:TRP:HH2	3:E:605:ADP:H5'2	1.51	0.74
1:L:189:THR:HB	1:R:36:LYS:HG2	1.68	0.74
1:P:359:GLU:O	1:P:363:VAL:HG23	1.87	0.73
1:N:108:ILE:HD13	1:N:296:THR:HG22	1.70	0.73
1:A:39:ASN:HA	1:A:82:LYS:HE3	1.70	0.73
1:F:208:PRO:HG3	1:F:222:TRP:CE2	2.23	0.73
1:C:285:ASN:ND2	1:C:287:ARG:H	1.86	0.73
1:J:297:ASN:HB3	1:J:301:VAL:HG13	1.69	0.72
1:A:142:ILE:HG13	1:A:260:VAL:HG12	1.70	0.72
1:A:176:LEU:HD12	1:A:229:TRP:CH2	2.24	0.72
1:J:189:THR:O	1:P:36:LYS:HG2	1.89	0.72
1:P:213:LEU:HD12	1:P:218:CYS:HB2	1.72	0.72
1:M:285:ASN:ND2	1:M:287:ARG:H	1.88	0.72
1:H:88:PHE:HD2	1:H:93:SER:HB2	1.54	0.71
1:L:308:LEU:HD13	1:L:310:LEU:HD11	1.72	0.71
1:C:191:ASN:ND2	1:C:193:LYS:H	1.87	0.71
1:Q:168:VAL:HG13	1:Q:280:HIS:CE1	2.25	0.71
1:F:326:LEU:HD13	1:F:367:GLY:HA2	1.72	0.71
1:E:142:ILE:HD12	1:E:261:PHE:HA	1.72	0.71
1:H:313:LEU:HD12	1:H:374:CYS:HB2	1.73	0.71
1:O:285:ASN:HD22	1:O:288:LEU:N	1.87	0.71
1:A:312:PHE:CZ	1:A:379:GLU:HG3	2.26	0.71
1:C:318:ARG:HD3	1:C:388:ILE:HD13	1.71	0.71
1:A:34:LEU:HA	1:A:37:HIS:ND1	2.06	0.71
1:M:285:ASN:HD22	1:M:288:LEU:H	1.38	0.70
1:P:140:CYS:HB3	1:P:257:LEU:HD23	1.72	0.70
1:F:239:TRP:HB2	1:F:247:ARG:HB2	1.72	0.70
1:J:188:THR:HG22	1:J:223:PRO:HG2	1.73	0.70
1:I:285:ASN:ND2	1:I:287:ARG:H	1.89	0.70
1:K:66:LYS:HD3	1:K:66:LYS:O	1.91	0.70
1:G:126:LYS:HB2	1:G:358:ARG:HD2	1.73	0.70
1:P:143:ARG:HG2	1:P:144:CYS:N	2.05	0.70
1:H:304:ALA:O	1:H:348:SER:HB2	1.90	0.70

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:M:143:ARG:HG2	1:M:144:CYS:N	2.06	0.70
1:G:202:HIS:HB3	3:G:607:ADP:H1'	1.74	0.70
3:M:613:ADP:H5'1	3:M:613:ADP:O2B	1.91	0.70
1:Q:303:ARG:NH2	3:Q:617:ADP:O2A	2.23	0.70
1:I:98:LYS:HE3	1:I:102:ASP:OD2	1.92	0.70
1:E:336:GLU:OE2	2:E:505:NMG:NE	2.23	0.70
1:F:187:LEU:HD23	1:F:223:PRO:HB3	1.71	0.69
1:K:331:ARG:HB2	1:K:346:ASP:HB3	1.74	0.69
1:D:94:TYR:OH	1:D:98:LYS:HE3	1.92	0.69
1:M:286:ASP:HB2	6:M:1794:HOH:O	1.92	0.69
1:N:94:TYR:CE1	1:N:288:LEU:HD11	2.28	0.69
1:Q:278:CYS:HB3	1:Q:280:HIS:CE1	2.27	0.69
1:M:336:GLU:HB2	3:M:613:ADP:O1A	1.92	0.69
1:K:60:ASN:HB2	1:K:90:ASP:OD2	1.92	0.69
1:A:149:LYS:HB3	1:A:281:GLY:O	1.93	0.69
1:Q:126:LYS:HB2	1:Q:358:ARG:HD2	1.73	0.69
1:H:314:GLU:HG2	6:H:1841:HOH:O	1.93	0.68
1:F:8:TYR:HD2	1:F:11:LYS:HZ3	1.40	0.68
1:P:233:GLU:HB2	6:P:2502:HOH:O	1.91	0.68
3:P:616:ADP:H5'1	3:P:616:ADP:O2B	1.92	0.68
1:I:318:ARG:HD3	1:I:388:ILE:HD13	1.74	0.68
1:N:310:LEU:HD22	1:N:313:LEU:HB3	1.75	0.68
1:H:302:VAL:HG21	1:H:357:GLU:HG3	1.75	0.68
1:Q:213:LEU:HD12	1:Q:218:CYS:HB2	1.73	0.68
1:C:186:PRO:HG2	1:C:189:THR:OG1	1.93	0.68
1:M:285:ASN:HD21	1:M:287:ARG:HB2	1.58	0.68
1:G:151:VAL:HG22	1:G:161:GLU:HG2	1.75	0.68
1:B:154:PRO:HG2	1:B:243:GLU:O	1.93	0.68
1:Q:143:ARG:HG3	6:Q:1003:HOH:O	1.92	0.68
1:J:204:LEU:HD12	1:J:205:PHE:H	1.57	0.68
1:B:278:CYS:HB3	1:B:280:HIS:CE1	2.29	0.68
1:F:285:ASN:HB2	1:F:291:ILE:HD11	1.76	0.68
1:Q:385:ASP:HB3	6:Q:1286:HOH:O	1.93	0.68
1:G:37:HIS:CD2	1:G:75:PRO:HA	2.29	0.68
1:L:328:LEU:HD11	1:L:367:GLY:HA3	1.75	0.68
1:A:297:ASN:HB3	1:A:301:VAL:CG1	2.23	0.68
3:H:608:ADP:H5'1	3:H:608:ADP:O2B	1.92	0.68
1:F:239:TRP:HH2	3:F:606:ADP:H5'2	1.59	0.67
1:D:367:GLY:O	1:D:371:LEU:HG	1.95	0.67
1:D:98:LYS:HE2	1:D:102:ASP:OD2	1.94	0.67
1:A:188:THR:HG22	1:A:223:PRO:HG2	1.77	0.67
1:B:314:GLU:HG3	1:B:315:LYS:HD2	1.77	0.67

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:O:188:THR:HG23	6:O:1101:HOH:O	1.95	0.67
1:H:330:LYS:HE3	1:H:345:TYR:HE2	1.59	0.67
1:N:101:PHE:O	1:N:105:ILE:HG13	1.95	0.67
1:N:302:VAL:O	1:N:352:ARG:HD3	1.94	0.67
1:B:308:LEU:HD13	1:B:310:LEU:HD11	1.77	0.67
1:L:312:PHE:CE2	1:L:379:GLU:HA	2.30	0.67
1:F:236:PHE:C	1:F:237:LEU:HD12	2.16	0.67
1:A:34:LEU:HA	1:A:37:HIS:CE1	2.30	0.67
1:H:168:VAL:HG13	1:H:280:HIS:CE1	2.29	0.67
1:D:134:ASP:HB2	6:D:3218:HOH:O	1.95	0.67
1:D:314:GLU:HG3	1:D:315:LYS:HD2	1.76	0.66
1:J:161:GLU:O	1:J:165:VAL:HG23	1.94	0.66
1:E:284:HIS:CE1	1:E:289:GLY:HA2	2.29	0.66
1:H:108:ILE:HG21	1:H:296:THR:HG22	1.77	0.66
1:A:143:ARG:HG2	1:A:144:CYS:N	2.08	0.66
1:K:191:ASN:HD21	1:K:193:LYS:HB2	1.60	0.66
1:E:180:LEU:O	1:E:229:TRP:HH2	1.79	0.66
1:G:188:THR:HG23	6:G:1511:HOH:O	1.95	0.66
1:A:300:THR:OG1	1:A:302:VAL:HB	1.95	0.66
1:L:253:LYS:HE3	6:R:1027:HOH:O	1.95	0.66
1:J:322:MET:HG3	1:J:389:PRO:HD2	1.78	0.66
1:B:356:SER:OG	1:B:359:GLU:HG3	1.96	0.66
1:F:314:GLU:HG3	1:F:315:LYS:HD2	1.77	0.66
1:I:207:LYS:O	1:I:209:THR:HG23	1.96	0.65
1:R:384:ILE:HB	1:R:387:MET:HG3	1.76	0.65
1:B:364:LEU:O	1:B:368:VAL:HG23	1.96	0.65
1:C:280:HIS:HE1	6:C:2028:HOH:O	1.78	0.65
1:A:168:VAL:HG13	1:A:280:HIS:CE1	2.31	0.65
1:O:188:THR:HG22	1:O:223:PRO:HG2	1.77	0.65
1:O:60:ASN:HB2	1:O:90:ASP:OD2	1.96	0.65
1:B:313:LEU:CD2	1:B:319:PHE:CD1	2.80	0.65
1:R:285:ASN:HD22	1:R:288:LEU:H	1.45	0.65
1:H:364:LEU:O	1:H:368:VAL:HG23	1.97	0.65
1:B:98:LYS:HE3	1:B:102:ASP:OD2	1.96	0.65
1:F:285:ASN:ND2	1:F:287:ARG:H	1.95	0.65
1:R:175:GLY:O	1:R:177:LYS:HG2	1.97	0.65
1:G:44:GLN:OE1	1:G:103:LYS:HE3	1.96	0.65
1:C:285:ASN:HD22	1:C:288:LEU:H	1.44	0.65
1:D:104:CYS:O	1:D:108:ILE:HG13	1.96	0.65
1:N:247:ARG:HD2	6:N:1096:HOH:O	1.96	0.64
1:M:53:TYR:O	1:M:55:ASP:N	2.29	0.64
1:G:236:PHE:CE1	1:G:267:GLY:HA3	2.32	0.64

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:53:TYR:OH	1:K:99:GLU:HB3	1.97	0.64
1:C:297:ASN:HB3	1:C:301:VAL:HG13	1.79	0.64
1:E:314:GLU:HG3	1:E:315:LYS:HD2	1.78	0.64
1:I:50:TYR:O	1:I:54:TRP:HB3	1.97	0.64
1:R:331:ARG:NH1	1:R:336:GLU:HB2	2.12	0.64
1:G:188:THR:HG22	1:G:223:PRO:HG2	1.79	0.64
1:F:153:LEU:O	1:F:157:MET:HB3	1.97	0.64
1:F:313:LEU:HD22	1:F:319:PHE:CD1	2.32	0.64
1:F:26:LYS:N	1:F:29:ASP:OD2	2.25	0.64
1:G:105:ILE:HG12	1:G:298:MET:CE	2.27	0.64
1:M:321:GLU:O	1:M:325:LYS:HG3	1.98	0.64
1:P:113:PRO:HA	1:P:287:ARG:NH2	2.13	0.64
1:K:195:GLN:O	1:K:199:ILE:HG13	1.98	0.64
1:D:142:ILE:HD11	1:D:257:LEU:HD22	1.80	0.64
1:H:187:LEU:HD23	1:H:223:PRO:HB2	1.79	0.64
1:O:97:TYR:HB2	1:O:101:PHE:CE2	2.33	0.64
1:L:250:SER:HB3	1:L:264:PHE:HB2	1.79	0.64
1:D:166:GLU:OE1	1:D:225:GLY:HA2	1.98	0.64
1:H:328:LEU:HD11	1:H:367:GLY:HA3	1.79	0.64
1:R:239:TRP:HB2	1:R:247:ARG:HB2	1.79	0.64
1:K:313:LEU:HD12	1:K:371:LEU:O	1.98	0.63
1:B:188:THR:HG21	6:B:3077:HOH:O	1.98	0.63
1:O:297:ASN:O	1:O:301:VAL:HG13	1.98	0.63
1:I:239:TRP:HB2	1:I:247:ARG:HB2	1.79	0.63
1:E:121:ASP:OD2	1:E:358:ARG:HD3	1.99	0.63
1:N:213:LEU:HD12	1:N:218:CYS:HB2	1.79	0.63
1:D:143:ARG:HG2	1:D:144:CYS:N	2.13	0.63
1:R:287:ARG:HD3	6:R:3342:HOH:O	1.98	0.63
1:H:297:ASN:HB3	1:H:301:VAL:HG13	1.80	0.63
1:B:313:LEU:HD12	1:B:374:CYS:HB2	1.80	0.63
1:P:184:TYR:CE1	1:P:240:ILE:HD12	2.34	0.63
1:K:68:ILE:O	1:K:72:VAL:HG23	1.98	0.63
1:I:108:ILE:HG21	1:I:296:THR:HG22	1.81	0.63
1:H:94:TYR:CZ	1:H:288:LEU:HD11	2.35	0.62
1:R:331:ARG:HB2	1:R:346:ASP:HB3	1.81	0.62
1:N:330:LYS:HE3	1:N:345:TYR:CE2	2.34	0.62
1:F:244:ASP:OD1	1:F:292:CYS:HB3	1.98	0.62
1:K:236:PHE:CZ	1:K:267:GLY:HA3	2.33	0.62
1:E:384:ILE:O	1:E:388:ILE:HD12	2.00	0.62
1:K:52:LYS:NZ	1:K:99:GLU:OE2	2.32	0.62
1:G:321:GLU:HA	1:M:233:GLU:OE2	1.99	0.62
1:H:356:SER:OG	1:H:359:GLU:HG3	1.99	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:305:SER:HB3	1:B:348:SER:HB3	1.81	0.62
1:R:308:LEU:HD13	1:R:310:LEU:HD11	1.81	0.62
1:K:297:ASN:HB3	1:K:301:VAL:HG13	1.81	0.62
1:K:180:LEU:HD13	1:K:267:GLY:HA2	1.82	0.62
1:G:109:HIS:O	1:G:110:HIS:HB2	1.99	0.62
1:D:191:ASN:HD21	1:D:193:LYS:HB2	1.64	0.62
1:B:233:GLU:HG3	6:B:1233:HOH:O	1.99	0.62
1:I:91:GLU:HB2	1:I:283:MET:SD	2.40	0.62
1:H:374:CYS:O	1:H:378:LEU:HG	1.99	0.62
1:R:168:VAL:HG13	1:R:280:HIS:CE1	2.34	0.62
1:H:11:LYS:HA	1:H:61:GLY:CA	2.30	0.62
1:I:207:LYS:O	1:I:209:THR:N	2.33	0.61
1:A:151:VAL:CG1	1:A:161:GLU:HB3	2.29	0.61
1:D:161:GLU:O	1:D:165:VAL:HG23	1.99	0.61
1:G:69:GLN:HE21	1:G:73:ASP:CG	2.03	0.61
1:Q:285:ASN:ND2	1:Q:288:LEU:H	1.93	0.61
1:N:313:LEU:HD23	1:N:319:PHE:CD1	2.35	0.61
1:G:34:LEU:HA	1:G:37:HIS:ND1	2.15	0.61
1:R:331:ARG:HG3	6:R:1054:HOH:O	1.99	0.61
1:R:359:GLU:O	1:R:363:VAL:HG23	2.00	0.61
1:E:285:ASN:ND2	1:E:287:ARG:H	1.98	0.61
1:P:313:LEU:CD2	1:P:319:PHE:CD1	2.82	0.61
1:J:18:LYS:HB2	1:J:21:GLU:HG2	1.82	0.61
1:C:318:ARG:CD	1:C:388:ILE:HD13	2.30	0.61
1:O:314:GLU:HG2	1:O:315:LYS:HD2	1.81	0.61
1:R:124:HIS:O	1:R:258:LYS:HE3	2.01	0.61
1:D:352:ARG:HH11	1:D:352:ARG:HG2	1.66	0.61
1:P:358:ARG:HH21	1:P:359:GLU:HG3	1.66	0.61
1:H:123:ASP:OD2	1:H:126:LYS:HG2	2.01	0.61
1:G:143:ARG:HG2	1:G:144:CYS:N	2.16	0.61
1:G:212:LEU:HD23	2:G:507:NMG:NH1	2.16	0.61
1:B:184:TYR:CE1	1:B:227:GLY:HA3	2.34	0.61
1:R:98:LYS:HE3	1:R:102:ASP:OD2	2.01	0.61
1:P:247:ARG:HD2	6:P:1047:HOH:O	2.01	0.61
1:R:252:GLN:HG3	1:R:253:LYS:O	2.01	0.61
1:B:301:VAL:HG12	1:B:301:VAL:O	2.01	0.61
1:D:123:ASP:OD1	1:D:125:ASN:HB2	2.01	0.61
1:B:103:LYS:HG2	6:B:2488:HOH:O	2.01	0.61
1:O:361:VAL:O	1:O:365:VAL:HG23	2.00	0.61
1:P:154:PRO:HA	1:P:157:MET:HG2	1.83	0.61
1:N:44:GLN:HB3	1:N:103:LYS:HB2	1.83	0.61
1:E:152:CYS:SG	1:F:17:SER:HB3	2.41	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:239:TRP:HB2	1:H:247:ARG:HB2	1.82	0.60
1:H:292:CYS:HB2	1:H:297:ASN:O	1.99	0.60
1:K:113:PRO:HA	1:K:287:ARG:NH2	2.15	0.60
1:P:229:TRP:CE3	1:P:230:HIS:HA	2.36	0.60
1:J:188:THR:HG23	6:J:1879:HOH:O	2.00	0.60
1:B:310:LEU:O	1:B:314:GLU:HG2	2.01	0.60
1:M:267:GLY:O	1:M:271:VAL:HG23	2.01	0.60
1:F:50:TYR:O	1:F:54:TRP:HB3	2.01	0.60
1:Q:352:ARG:HG2	1:Q:352:ARG:HH11	1.64	0.60
1:M:297:ASN:HB3	1:M:301:VAL:HG13	1.83	0.60
1:Q:297:ASN:HB3	1:Q:301:VAL:HG13	1.83	0.60
1:C:63:THR:OG1	1:C:66:LYS:HB2	2.01	0.60
1:K:376:LYS:HB2	6:K:1597:HOH:O	2.01	0.60
1:I:184:TYR:CE1	1:I:240:ILE:HD12	2.36	0.60
1:D:236:PHE:CE1	1:D:267:GLY:HA3	2.37	0.60
1:H:47:LYS:HG3	6:H:1610:HOH:O	2.01	0.60
1:O:366:ASP:OD2	1:R:126:LYS:HD2	2.01	0.60
1:O:93:SER:O	1:O:101:PHE:HE2	1.84	0.60
1:R:184:TYR:CE1	1:R:240:ILE:HD12	2.37	0.60
1:A:126:LYS:HB2	1:A:358:ARG:HD2	1.84	0.60
1:N:165:VAL:O	1:N:169:VAL:HG23	2.01	0.60
1:G:191:ASN:HD21	1:G:193:LYS:HB2	1.65	0.60
1:K:330:LYS:HE3	1:K:345:TYR:CE2	2.35	0.60
1:B:109:HIS:O	1:B:110:HIS:HB2	2.01	0.60
1:O:184:TYR:CE1	1:O:240:ILE:HD12	2.37	0.60
1:J:167:LYS:HD3	1:J:171:ASP:OD2	2.00	0.60
1:K:143:ARG:HG2	1:K:144:CYS:N	2.15	0.60
1:A:53:TYR:CE2	1:A:97:TYR:HA	2.37	0.60
1:B:316:HIS:CD2	1:B:317:PRO:HD2	2.36	0.60
1:J:101:PHE:O	1:J:105:ILE:HG13	2.01	0.60
1:A:341:THR:HG23	6:A:1833:HOH:O	2.01	0.60
1:P:212:LEU:O	1:P:216:SER:HB3	2.01	0.60
1:H:71:GLY:HA3	1:H:85:GLY:O	2.02	0.60
1:L:18:LYS:HB2	1:L:21:GLU:HG2	1.83	0.60
1:H:191:ASN:HD21	1:H:193:LYS:HB2	1.67	0.60
1:B:297:ASN:HB3	1:B:301:VAL:HG13	1.82	0.59
1:Q:41:MET:HE3	1:Q:71:GLY:HA3	1.84	0.59
1:A:244:ASP:OD1	1:A:292:CYS:HB3	2.02	0.59
1:O:111:PHE:CE1	1:O:353:LEU:HD22	2.37	0.59
1:O:104:CYS:O	1:O:108:ILE:HG13	2.02	0.59
1:E:142:ILE:HG13	1:E:260:VAL:HG12	1.83	0.59
1:G:69:GLN:NE2	1:G:73:ASP:OD1	2.34	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:P:177:LYS:HA	1:P:181:ALA:HB2	1.83	0.59
1:Q:36:LYS:HG3	6:Q:1413:HOH:O	2.01	0.59
1:F:143:ARG:HG2	1:F:144:CYS:N	2.17	0.59
1:P:285:ASN:ND2	1:P:288:LEU:H	2.00	0.59
1:G:239:TRP:HB2	1:G:247:ARG:HB2	1.83	0.59
1:M:94:TYR:CD1	1:M:95:GLU:HG2	2.36	0.59
1:J:98:LYS:HE3	1:J:102:ASP:OD2	2.02	0.59
1:R:104:CYS:O	1:R:108:ILE:HG13	2.03	0.59
1:A:50:TYR:O	1:A:54:TRP:HB3	2.02	0.59
1:E:36:LYS:HE2	6:E:2285:HOH:O	2.02	0.59
1:P:151:VAL:HG12	1:P:152:CYS:O	2.02	0.59
1:B:188:THR:HG22	1:B:223:PRO:HG2	1.85	0.59
1:B:184:TYR:HE1	1:B:227:GLY:HA3	1.68	0.59
1:B:285:ASN:ND2	1:B:288:LEU:H	2.01	0.59
1:R:113:PRO:HA	1:R:287:ARG:NH2	2.17	0.59
1:I:297:ASN:HB3	1:I:301:VAL:HG13	1.84	0.59
1:O:224:ASP:HB2	6:O:2263:HOH:O	2.01	0.59
1:Q:144:CYS:HA	1:Q:301:VAL:O	2.03	0.59
1:N:124:HIS:O	1:N:258:LYS:HE3	2.02	0.59
1:K:298:MET:CE	1:K:353:LEU:HD12	2.32	0.59
1:C:252:GLN:NE2	1:C:256:ASP:HB3	2.17	0.59
1:A:285:ASN:HD22	1:A:287:ARG:N	2.01	0.58
1:C:217:GLY:HA2	6:C:2281:HOH:O	2.02	0.58
1:M:188:THR:HG23	6:M:2073:HOH:O	2.03	0.58
1:K:331:ARG:NH1	3:K:611:ADP:O2A	2.35	0.58
1:K:191:ASN:ND2	1:K:193:LYS:H	2.01	0.58
1:C:84:THR:HG23	1:C:108:ILE:HD11	1.85	0.58
1:N:285:ASN:HD22	1:N:288:LEU:H	1.50	0.58
1:C:53:TYR:CZ	1:C:97:TYR:HA	2.37	0.58
1:H:157:MET:HE2	1:H:161:GLU:HB3	1.86	0.58
1:F:229:TRP:CE3	1:F:230:HIS:HA	2.38	0.58
1:P:212:LEU:HB3	6:P:2271:HOH:O	2.03	0.58
1:Q:142:ILE:HD12	1:Q:261:PHE:HA	1.84	0.58
1:K:27:ALA:HB2	1:K:54:TRP:NE1	2.18	0.58
1:I:175:GLY:O	1:I:177:LYS:HE2	2.03	0.58
1:O:384:ILE:HB	1:O:387:MET:HG3	1.86	0.58
1:L:312:PHE:CE1	1:L:379:GLU:HG3	2.38	0.58
1:H:332:GLY:HA3	1:H:338:SER:O	2.04	0.58
1:C:168:VAL:HG13	1:C:280:HIS:CE1	2.38	0.58
1:I:95:GLU:HG3	6:I:2804:HOH:O	2.04	0.58
1:J:213:LEU:HD12	1:J:218:CYS:HB2	1.84	0.58
1:P:268:LEU:O	1:P:272:GLU:HG3	2.03	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:301:VAL:HG12	1:E:301:VAL:O	2.03	0.58
1:Q:196:GLU:O	1:Q:200:GLU:HB2	2.04	0.58
1:Q:60:ASN:HB2	1:Q:90:ASP:OD2	2.04	0.58
1:H:44:GLN:NE2	1:H:107:GLU:OE1	2.36	0.58
1:A:267:GLY:O	1:A:271:VAL:HG23	2.04	0.58
1:N:313:LEU:CD1	1:N:374:CYS:HB2	2.34	0.58
1:J:322:MET:HG3	1:J:388:ILE:HG23	1.85	0.58
1:J:295:PRO:O	1:J:298:MET:HG3	2.04	0.58
1:O:83:LYS:HE2	6:O:1356:HOH:O	2.04	0.58
1:J:192:GLU:O	1:J:196:GLU:HG3	2.04	0.57
1:I:141:ARG:HG3	1:I:251:MET:HB3	1.85	0.57
1:R:212:LEU:O	1:R:216:SER:HB3	2.04	0.57
1:G:336:GLU:OE2	2:G:507:NMG:NE	2.36	0.57
1:M:309:ARG:NH1	1:M:342:ASP:OD1	2.36	0.57
1:J:143:ARG:HG3	6:J:1077:HOH:O	2.04	0.57
1:H:313:LEU:O	1:H:313:LEU:HD23	2.04	0.57
1:M:305:SER:HB3	1:M:348:SER:HB3	1.86	0.57
1:C:38:ASN:ND2	1:C:82:LYS:HE3	2.18	0.57
1:R:34:LEU:HD11	1:R:45:LEU:HD23	1.87	0.57
1:P:13:ARG:HD3	1:P:156:ALA:O	2.04	0.57
1:N:310:LEU:HD22	1:N:313:LEU:CB	2.34	0.57
1:C:285:ASN:HD22	1:C:287:ARG:H	1.53	0.57
1:H:146:ARG:HD2	1:H:282:LEU:HD13	1.87	0.57
1:Q:141:ARG:HB2	1:Q:251:MET:HB3	1.87	0.57
1:H:88:PHE:CD2	1:H:93:SER:HB2	2.38	0.57
1:I:144:CYS:HA	1:I:301:VAL:O	2.05	0.57
1:I:323:LEU:HD13	1:I:330:LYS:HB2	1.86	0.57
1:H:176:LEU:HD12	1:H:229:TRP:CZ2	2.40	0.57
1:D:142:ILE:HD11	1:D:257:LEU:CD2	2.35	0.57
1:D:142:ILE:HG13	1:D:260:VAL:HG12	1.85	0.57
1:Q:167:LYS:HD3	1:Q:171:ASP:OD2	2.04	0.57
1:F:338:SER:O	1:F:339:LEU:HD23	2.04	0.57
1:K:364:LEU:HD22	1:K:368:VAL:HG23	1.86	0.57
1:E:184:TYR:CD2	1:E:186:PRO:HD3	2.39	0.57
1:G:374:CYS:O	1:G:378:LEU:HG	2.04	0.57
1:B:29:ASP:HA	6:B:3224:HOH:O	2.05	0.57
1:J:305:SER:HB3	1:J:348:SER:HB3	1.87	0.57
1:O:285:ASN:ND2	1:O:288:LEU:H	1.91	0.57
1:P:313:LEU:HD21	1:P:319:PHE:CD1	2.39	0.57
1:N:180:LEU:HD23	6:N:3082:HOH:O	2.04	0.57
1:O:309:ARG:NH1	1:O:342:ASP:OD1	2.37	0.57
1:E:57:VAL:HG12	1:E:58:THR:O	2.05	0.57

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:237:LEU:CD1	1:F:237:LEU:N	2.68	0.57
1:O:128:VAL:HG21	1:R:358:ARG:NH2	2.20	0.57
1:D:312:PHE:CZ	1:D:379:GLU:HG3	2.39	0.56
1:G:168:VAL:HG13	1:G:280:HIS:CE1	2.41	0.56
1:L:124:HIS:O	1:L:127:LEU:HB2	2.05	0.56
1:F:151:VAL:HA	6:F:2818:HOH:O	2.03	0.56
1:P:168:VAL:HG13	1:P:280:HIS:CE1	2.40	0.56
1:P:213:LEU:HD12	1:P:218:CYS:CB	2.35	0.56
1:C:169:VAL:O	1:C:173:LEU:HG	2.05	0.56
1:N:312:PHE:CZ	1:N:379:GLU:HG3	2.40	0.56
1:A:105:ILE:HG12	1:A:298:MET:HE1	1.87	0.56
1:I:60:ASN:HB2	1:I:90:ASP:OD2	2.06	0.56
1:O:316:HIS:CE1	1:O:318:ARG:HB2	2.41	0.56
1:D:159:ARG:NH1	1:D:221:ASP:OD1	2.39	0.56
1:H:384:ILE:HG22	1:H:387:MET:HE2	1.86	0.56
1:G:328:LEU:HD11	1:G:367:GLY:HA3	1.87	0.56
1:C:309:ARG:NH1	1:C:342:ASP:OD1	2.37	0.56
1:N:13:ARG:NH1	1:N:156:ALA:O	2.38	0.56
1:C:184:TYR:CE1	1:C:240:ILE:HD12	2.41	0.56
1:K:297:ASN:HA	1:K:352:ARG:HD2	1.87	0.56
1:C:161:GLU:O	1:C:164:LEU:HB3	2.05	0.56
1:E:247:ARG:NH1	3:E:605:ADP:O1B	2.39	0.56
1:G:37:HIS:HD2	1:G:75:PRO:HA	1.70	0.56
1:B:264:PHE:CZ	1:B:268:LEU:HD22	2.41	0.56
1:H:183:LYS:HB3	1:H:185:TYR:CZ	2.39	0.56
1:J:173:LEU:HD13	1:J:229:TRP:CG	2.41	0.56
1:J:47:LYS:HG3	6:J:2633:HOH:O	2.04	0.56
1:R:355:LYS:HB2	1:R:360:LEU:HD21	1.87	0.56
1:R:298:MET:HA	1:R:301:VAL:HG22	1.88	0.56
1:M:335:GLY:O	1:M:338:SER:OG	2.22	0.56
1:K:49:LEU:HD21	1:K:99:GLU:HG2	1.87	0.56
1:M:270:GLU:OE1	1:M:273:ARG:NH1	2.39	0.56
1:A:285:ASN:HD21	1:A:287:ARG:HB2	1.71	0.56
1:B:305:SER:CB	1:B:348:SER:HB3	2.36	0.56
1:Q:267:GLY:O	1:Q:271:VAL:HG23	2.05	0.56
1:M:154:PRO:HA	1:M:157:MET:SD	2.46	0.56
1:F:318:ARG:NH1	1:F:388:ILE:HD12	2.21	0.56
1:G:89:GLY:HA2	1:G:155:PRO:CG	2.31	0.56
1:A:285:ASN:HD22	1:A:287:ARG:H	1.47	0.56
1:L:292:CYS:SG	1:L:301:VAL:HG11	2.46	0.56
1:K:303:ARG:NE	3:K:611:ADP:O3B	2.34	0.56
1:K:364:LEU:HD22	1:K:368:VAL:CG2	2.36	0.56

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:201:ASP:O	1:B:202:HIS:HB2	2.06	0.56
1:I:298:MET:CE	1:I:353:LEU:HD12	2.36	0.56
3:O:615:ADP:O2B	3:O:615:ADP:H5'1	2.06	0.56
1:N:384:ILE:HB	1:N:387:MET:HG3	1.86	0.55
1:L:189:THR:HB	1:R:36:LYS:CG	2.37	0.55
1:G:298:MET:HE1	1:G:353:LEU:HD12	1.87	0.55
1:M:349:ASN:HD22	1:M:360:LEU:HD22	1.71	0.55
1:A:39:ASN:CA	1:A:82:LYS:HE3	2.35	0.55
1:L:295:PRO:O	1:L:298:MET:HG3	2.06	0.55
1:J:355:LYS:HB2	1:J:360:LEU:HD21	1.88	0.55
1:K:352:ARG:CG	1:K:352:ARG:NH1	2.63	0.55
1:H:306:VAL:HG13	1:H:364:LEU:HD11	1.87	0.55
1:N:312:PHE:CE1	1:N:379:GLU:HG3	2.41	0.55
1:P:192:GLU:O	1:P:196:GLU:HG3	2.07	0.55
1:F:212:LEU:HB3	6:F:2424:HOH:O	2.06	0.55
1:I:385:ASP:HA	1:I:388:ILE:HD12	1.87	0.55
1:H:187:LEU:HD23	1:H:223:PRO:CB	2.35	0.55
1:I:313:LEU:HD22	1:I:319:PHE:CD1	2.41	0.55
1:R:310:LEU:O	1:R:314:GLU:HB3	2.07	0.55
1:B:117:HIS:ND1	1:B:118:PRO:HD2	2.22	0.55
1:D:127:LEU:HD11	1:D:361:VAL:HG12	1.88	0.55
1:R:13:ARG:HD3	1:R:156:ALA:O	2.07	0.55
1:Q:298:MET:HE3	1:Q:353:LEU:HD12	1.87	0.55
1:G:274:LEU:O	1:G:278:CYS:SG	2.63	0.55
1:E:331:ARG:HB2	1:E:346:ASP:HB3	1.88	0.55
1:H:197:GLN:HB3	6:H:2456:HOH:O	2.05	0.55
1:G:285:ASN:ND2	1:G:288:LEU:H	2.03	0.55
1:J:187:LEU:HB3	1:J:223:PRO:HB2	1.89	0.55
1:Q:298:MET:HG2	6:Q:1831:HOH:O	2.06	0.55
1:L:168:VAL:HG13	1:L:280:HIS:CE1	2.41	0.55
1:H:203:PHE:CZ	1:H:234:LYS:HE2	2.41	0.55
1:I:143:ARG:HG3	6:I:1772:HOH:O	2.06	0.55
1:F:6:GLN:O	1:F:10:VAL:HG23	2.07	0.55
1:F:85:GLY:O	1:F:86:CYS:HB3	2.06	0.55
1:I:313:LEU:O	1:I:313:LEU:HD23	2.07	0.54
1:C:213:LEU:HD12	1:C:218:CYS:HB2	1.88	0.54
1:E:40:VAL:HG13	1:E:107:GLU:OE1	2.07	0.54
1:M:313:LEU:HD11	1:M:322:MET:HE1	1.89	0.54
1:A:148:VAL:O	1:A:283:MET:HE3	2.06	0.54
1:I:205:PHE:HB2	1:I:242:GLU:OE2	2.07	0.54
1:N:154:PRO:HG2	1:N:243:GLU:O	2.07	0.54
1:B:336:GLU:OE2	2:B:502:NMG:NE	2.34	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:O:30:ASN:OD1	1:P:159:ARG:HB2	2.07	0.54
1:M:205:PHE:HD2	1:M:239:TRP:CD2	2.25	0.54
1:P:141:ARG:HG3	1:P:251:MET:HB3	1.87	0.54
1:C:318:ARG:HD3	1:C:388:ILE:CD1	2.38	0.54
1:R:146:ARG:HD2	1:R:282:LEU:HD13	1.90	0.54
1:K:359:GLU:O	1:K:362:GLN:HB3	2.07	0.54
1:D:285:ASN:ND2	1:D:287:ARG:H	2.05	0.54
1:N:313:LEU:HD11	1:N:374:CYS:HB2	1.88	0.54
1:G:105:ILE:HG12	1:G:298:MET:HE2	1.88	0.54
1:N:213:LEU:HD12	1:N:218:CYS:CB	2.38	0.54
1:M:270:GLU:OE2	1:M:273:ARG:HD3	2.07	0.54
1:G:331:ARG:HB2	1:G:346:ASP:HB3	1.88	0.54
1:N:205:PHE:HB3	1:N:239:TRP:CZ3	2.42	0.54
1:G:266:ARG:HG3	6:G:2236:HOH:O	2.06	0.54
1:K:48:GLU:N	6:K:2251:HOH:O	2.38	0.54
1:I:35:SER:HB3	1:O:189:THR:OG1	2.07	0.54
1:N:187:LEU:HD22	1:N:226:ARG:HB3	1.89	0.54
1:C:94:TYR:CZ	1:C:288:LEU:HD11	2.43	0.54
1:K:285:ASN:ND2	1:K:287:ARG:H	2.06	0.54
1:O:108:ILE:HG21	1:O:296:THR:HG22	1.90	0.54
1:D:14:VAL:HG12	1:D:16:HIS:CD2	2.42	0.54
1:M:75:PRO:HD2	6:M:1483:HOH:O	2.06	0.54
1:H:314:GLU:HG2	1:H:315:LYS:HD2	1.90	0.54
1:H:193:LYS:HG3	1:M:193:LYS:HE3	1.89	0.54
1:N:314:GLU:HG3	1:N:315:LYS:HD2	1.90	0.54
1:P:95:GLU:HG3	6:P:3097:HOH:O	2.06	0.54
1:K:94:TYR:CZ	1:K:288:LEU:HD11	2.41	0.54
1:Q:39:ASN:C	1:Q:82:LYS:HE2	2.27	0.54
1:H:34:LEU:HD13	1:H:42:ALA:HA	1.90	0.54
1:K:50:TYR:O	1:K:54:TRP:HB3	2.07	0.54
1:C:126:LYS:HB2	1:C:358:ARG:HD2	1.89	0.54
1:O:141:ARG:HH21	1:O:249:ILE:HD13	1.72	0.54
1:D:154:PRO:HA	1:D:157:MET:SD	2.47	0.54
1:L:147:SER:HG	1:L:292:CYS:HA	1.73	0.54
1:F:303:ARG:NH2	3:F:606:ADP:O2A	2.41	0.54
3:F:606:ADP:H5'1	3:F:606:ADP:O2B	2.08	0.54
1:A:151:VAL:HG11	1:A:161:GLU:HB3	1.90	0.53
1:B:66:LYS:O	1:B:66:LYS:HD3	2.06	0.53
1:D:237:LEU:N	1:D:237:LEU:HD12	2.23	0.53
1:D:143:ARG:NH2	1:D:297:ASN:OD1	2.40	0.53
1:M:154:PRO:HG2	1:M:243:GLU:O	2.07	0.53
1:H:203:PHE:CE1	1:H:234:LYS:HB3	2.42	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:83:LYS:HD2	2:B:502:NMG:O1	2.09	0.53
1:F:121:ASP:HB3	1:F:356:SER:HB2	1.90	0.53
1:H:26:LYS:O	1:H:27:ALA:C	2.47	0.53
1:P:323:LEU:HD13	1:P:330:LYS:HB2	1.90	0.53
1:K:318:ARG:HD3	1:K:388:ILE:HD13	1.89	0.53
1:Q:285:ASN:ND2	1:Q:287:ARG:N	2.55	0.53
1:R:331:ARG:HH11	1:R:336:GLU:HB2	1.71	0.53
1:H:208:PRO:HD3	1:H:222:TRP:CZ2	2.43	0.53
1:Q:31:PHE:CD1	1:Q:32:PRO:HD2	2.44	0.53
1:D:105:ILE:HG12	1:D:298:MET:HE1	1.89	0.53
1:F:64:PHE:O	1:F:68:ILE:HG12	2.07	0.53
1:A:60:ASN:HB2	1:A:90:ASP:OD2	2.08	0.53
1:P:180:LEU:O	1:P:229:TRP:HH2	1.91	0.53
1:C:117:HIS:HE1	1:C:300:THR:HG23	1.73	0.53
1:B:346:ASP:OD1	1:B:346:ASP:C	2.47	0.53
1:H:330:LYS:HE3	1:H:345:TYR:CE2	2.42	0.53
1:N:303:ARG:HB2	1:N:352:ARG:NH1	2.24	0.53
1:E:285:ASN:HD22	1:E:287:ARG:H	1.57	0.53
1:L:319:PHE:O	1:L:323:LEU:HG	2.08	0.53
1:B:300:THR:HB	1:B:302:VAL:HG23	1.91	0.53
1:H:285:ASN:HB2	1:H:291:ILE:HD11	1.90	0.53
1:M:154:PRO:N	1:M:155:PRO:HD2	2.23	0.53
1:B:31:PHE:HD1	1:B:50:TYR:CD2	2.25	0.53
1:Q:285:ASN:HD22	1:Q:288:LEU:N	1.97	0.53
1:B:285:ASN:HD22	1:B:288:LEU:H	1.56	0.53
1:P:326:LEU:HD21	1:P:370:LEU:HD23	1.91	0.53
1:Q:284:HIS:CE1	1:Q:289:GLY:HA2	2.44	0.53
1:D:106:GLU:HG3	1:D:111:PHE:O	2.08	0.53
1:H:18:LYS:HB3	1:H:20:TRP:CE2	2.43	0.53
1:P:52:LYS:NZ	1:P:99:GLU:OE2	2.42	0.53
1:O:183:LYS:HG2	1:O:184:TYR:N	2.24	0.53
1:F:297:ASN:HB3	1:F:301:VAL:HG13	1.90	0.53
1:E:36:LYS:O	1:E:75:PRO:HB2	2.08	0.53
1:P:195:GLN:O	1:P:199:ILE:HG13	2.09	0.53
1:N:80:TYR:HB2	6:N:2884:HOH:O	2.09	0.53
1:B:143:ARG:HD2	3:B:602:ADP:O2B	2.09	0.53
1:I:226:ARG:HG3	1:I:241:ASN:O	2.09	0.53
1:H:94:TYR:CZ	1:H:98:LYS:HG3	2.44	0.53
1:K:66:LYS:NZ	1:K:155:PRO:O	2.41	0.53
1:H:44:GLN:OE1	1:H:44:GLN:HA	2.09	0.53
1:E:288:LEU:HD22	1:E:353:LEU:HD11	1.90	0.53
1:L:374:CYS:SG	1:L:387:MET:HE2	2.49	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:359:GLU:HG3	6:J:3116:HOH:O	2.08	0.53
1:L:285:ASN:ND2	1:L:287:ARG:H	2.06	0.53
1:M:285:ASN:ND2	1:M:287:ARG:N	2.56	0.53
1:D:32:PRO:HB2	1:D:34:LEU:HD21	1.90	0.53
1:L:159:ARG:HA	6:L:2389:HOH:O	2.09	0.53
1:D:351:ALA:O	1:D:360:LEU:HD22	2.08	0.53
1:M:159:ARG:HB2	1:N:30:ASN:OD1	2.09	0.53
1:C:250:SER:HB3	1:C:264:PHE:HB2	1.91	0.53
1:H:40:VAL:HB	1:H:84:THR:O	2.08	0.53
1:M:228:ILE:HG23	1:M:228:ILE:O	2.09	0.53
1:D:285:ASN:HD22	1:D:287:ARG:H	1.55	0.52
1:H:230:HIS:C	1:H:230:HIS:ND1	2.63	0.52
1:D:361:VAL:O	1:D:365:VAL:HG23	2.08	0.52
1:J:285:ASN:ND2	1:J:287:ARG:H	2.07	0.52
1:H:213:LEU:HD12	1:H:218:CYS:HB3	1.90	0.52
1:O:121:ASP:HB3	1:O:356:SER:HB2	1.91	0.52
1:P:310:LEU:HD13	1:P:313:LEU:HD22	1.92	0.52
1:O:298:MET:HE3	1:O:353:LEU:HD12	1.91	0.52
1:F:147:SER:HB2	1:F:283:MET:HB2	1.91	0.52
1:I:340:ALA:HB2	1:I:345:TYR:CE2	2.44	0.52
1:H:222:TRP:CD1	1:H:223:PRO:HB3	2.45	0.52
1:R:250:SER:OG	1:R:260:VAL:HG13	2.10	0.52
1:N:121:ASP:OD2	1:N:358:ARG:HD3	2.09	0.52
1:J:165:VAL:HB	1:J:241:ASN:HD21	1.75	0.52
1:O:60:ASN:O	1:P:17:SER:HA	2.10	0.52
1:J:18:LYS:HB3	1:J:20:TRP:CZ2	2.44	0.52
1:K:40:VAL:HG13	1:K:107:GLU:OE1	2.10	0.52
1:R:292:CYS:SG	1:R:301:VAL:HG11	2.49	0.52
1:K:143:ARG:HH22	1:K:297:ASN:CG	2.13	0.52
1:C:285:ASN:ND2	1:C:288:LEU:H	2.07	0.52
1:A:110:HIS:CD2	1:A:327:ARG:CZ	2.93	0.52
1:A:154:PRO:HG2	1:A:243:GLU:O	2.10	0.52
1:L:267:GLY:O	1:L:271:VAL:HG23	2.10	0.52
1:M:126:LYS:HG3	1:M:358:ARG:HH11	1.75	0.52
1:D:147:SER:HB2	1:D:283:MET:HB2	1.90	0.52
1:P:57:VAL:HG12	1:P:58:THR:O	2.10	0.52
1:A:79:PHE:CD2	1:A:337:SER:HA	2.45	0.52
1:E:325:LYS:HD3	1:E:389:PRO:HB2	1.92	0.52
1:M:359:GLU:HG2	1:P:128:VAL:CG2	2.40	0.52
1:A:257:LEU:HD11	1:A:364:LEU:HD12	1.91	0.52
1:A:38:ASN:HD22	1:A:38:ASN:C	2.13	0.52
1:G:285:ASN:ND2	1:G:287:ARG:H	2.07	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:109:HIS:O	1:H:110:HIS:HB2	2.09	0.52
1:C:56:LYS:NZ	6:C:2999:HOH:O	2.41	0.52
1:Q:165:VAL:O	1:Q:169:VAL:HG23	2.09	0.52
1:Q:326:LEU:O	1:Q:328:LEU:HG	2.09	0.52
1:J:204:LEU:HD12	1:J:205:PHE:N	2.25	0.52
1:B:242:GLU:CD	1:B:243:GLU:H	2.12	0.52
1:K:201:ASP:O	1:K:202:HIS:HB2	2.09	0.52
1:I:307:HIS:CD2	3:I:609:ADP:C6	2.98	0.52
1:E:44:GLN:HB3	1:E:103:LYS:HE2	1.92	0.52
1:N:65:ASP:O	1:N:69:GLN:HB2	2.10	0.52
1:P:351:ALA:C	1:P:352:ARG:HG2	2.30	0.52
1:L:297:ASN:HB3	1:L:301:VAL:HG13	1.92	0.52
1:F:228:ILE:HD11	1:F:237:LEU:HD23	1.92	0.52
1:N:285:ASN:HD22	1:N:288:LEU:CB	2.23	0.52
1:A:151:VAL:HG13	1:A:161:GLU:HB3	1.91	0.52
1:P:57:VAL:HG12	1:P:58:THR:N	2.24	0.52
1:K:34:LEU:HD13	1:K:42:ALA:HA	1.91	0.52
1:O:313:LEU:HD23	1:O:313:LEU:O	2.10	0.52
1:O:143:ARG:HG2	1:O:144:CYS:N	2.25	0.52
1:O:377:LYS:HG3	1:O:387:MET:CE	2.40	0.51
1:D:106:GLU:HG3	1:D:112:LYS:HA	1.92	0.51
1:M:164:LEU:HB2	6:M:2203:HOH:O	2.09	0.51
1:G:152:CYS:SG	1:H:17:SER:HB3	2.51	0.51
1:M:187:LEU:HB2	1:M:226:ARG:O	2.10	0.51
1:M:168:VAL:HG13	1:M:280:HIS:CE1	2.45	0.51
1:A:285:ASN:ND2	1:A:287:ARG:N	2.52	0.51
1:N:285:ASN:ND2	1:N:288:LEU:HD12	2.25	0.51
1:L:135:LYS:HD3	1:L:136:TYR:CE1	2.46	0.51
1:C:94:TYR:CD1	1:C:95:GLU:HG2	2.46	0.51
1:H:312:PHE:CE2	1:H:379:GLU:HA	2.45	0.51
1:N:32:PRO:HB2	1:N:34:LEU:HD21	1.92	0.51
1:H:203:PHE:CE2	1:H:234:LYS:HE2	2.46	0.51
1:P:49:LEU:HD21	1:P:99:GLU:HG2	1.92	0.51
1:M:359:GLU:HG2	1:P:128:VAL:HG22	1.91	0.51
1:D:270:GLU:OE2	1:D:270:GLU:HA	2.10	0.51
1:E:312:PHE:CZ	1:E:379:GLU:HG3	2.46	0.51
1:P:247:ARG:NH1	3:P:616:ADP:O1B	2.44	0.51
1:I:294:CYS:SG	1:I:296:THR:OG1	2.65	0.51
1:B:31:PHE:CE1	1:B:47:LYS:HA	2.46	0.51
1:D:41:MET:HG2	1:D:100:PHE:CZ	2.46	0.51
1:E:49:LEU:HD21	1:E:99:GLU:CD	2.31	0.51
1:R:141:ARG:HD2	1:R:251:MET:CE	2.40	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:364:LEU:O	1:C:368:VAL:HG23	2.11	0.51
1:A:142:ILE:HG13	1:A:260:VAL:CG1	2.40	0.51
1:K:36:LYS:HG3	6:K:2092:HOH:O	2.10	0.51
1:J:84:THR:HG22	1:J:86:CYS:H	1.76	0.51
1:P:94:TYR:OH	1:P:98:LYS:HE3	2.11	0.51
6:F:1110:HOH:O	1:I:177:LYS:HD3	2.10	0.51
1:F:212:LEU:HD12	1:F:216:SER:HB3	1.93	0.51
1:E:40:VAL:O	1:E:44:GLN:HG2	2.10	0.51
1:P:217:GLY:O	1:P:220:ARG:NE	2.44	0.51
1:J:63:THR:OG1	1:J:66:LYS:HB2	2.11	0.51
1:L:364:LEU:O	1:L:368:VAL:HG23	2.10	0.51
1:A:184:TYR:CE1	1:A:240:ILE:HD12	2.46	0.51
1:D:222:TRP:HA	1:D:226:ARG:HH12	1.76	0.51
1:M:199:ILE:HD13	1:M:206:GLU:HA	1.92	0.51
1:L:134:ASP:HB2	6:L:1793:HOH:O	2.10	0.51
1:D:19:PRO:O	1:D:25:PHE:HB2	2.11	0.51
1:H:112:LYS:O	1:H:115:ASP:HB2	2.11	0.51
1:N:285:ASN:ND2	1:N:288:LEU:H	2.09	0.51
1:K:285:ASN:HD22	1:K:287:ARG:H	1.59	0.51
1:I:205:PHE:CG	1:I:242:GLU:HG3	2.46	0.51
1:H:155:PRO:HB3	1:H:216:SER:O	2.11	0.51
1:I:314:GLU:OE1	1:I:343:SER:HA	2.11	0.51
1:K:142:ILE:HA	1:K:304:ALA:HA	1.92	0.51
1:J:6:GLN:O	1:J:10:VAL:HG23	2.10	0.51
1:A:66:LYS:O	1:A:66:LYS:HD3	2.11	0.51
1:B:357:GLU:O	1:B:361:VAL:HG23	2.11	0.51
1:E:177:LYS:HB3	1:L:43:SER:HA	1.92	0.51
1:N:285:ASN:HD22	1:N:288:LEU:N	2.08	0.50
1:I:36:LYS:HE2	1:O:189:THR:HB	1.93	0.50
1:F:98:LYS:HE3	1:F:102:ASP:OD2	2.11	0.50
1:G:220:ARG:HG2	1:H:69:GLN:NE2	2.25	0.50
1:L:285:ASN:HD22	1:L:288:LEU:N	1.88	0.50
1:R:278:CYS:HB3	1:R:280:HIS:CE1	2.47	0.50
1:P:298:MET:HE3	1:P:353:LEU:HD12	1.92	0.50
1:K:244:ASP:OD1	1:K:292:CYS:HB3	2.11	0.50
1:P:165:VAL:O	1:P:169:VAL:HG23	2.11	0.50
1:O:168:VAL:HG13	1:O:280:HIS:CE1	2.47	0.50
1:I:296:THR:O	1:I:352:ARG:HG3	2.11	0.50
1:E:384:ILE:HA	1:E:387:MET:HG3	1.92	0.50
1:R:18:LYS:HB2	1:R:21:GLU:CD	2.31	0.50
1:L:184:TYR:OH	1:L:227:GLY:HA3	2.11	0.50
1:P:143:ARG:NH1	3:P:616:ADP:O3B	2.45	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:322:MET:CG	1:J:389:PRO:HD2	2.41	0.50
1:J:18:LYS:HB3	1:J:20:TRP:CE2	2.47	0.50
1:Q:38:ASN:ND2	1:Q:82:LYS:HE3	2.26	0.50
1:D:235:ASN:HB2	1:D:263:ARG:NH1	2.27	0.50
1:I:66:LYS:NZ	1:I:216:SER:O	2.45	0.50
1:K:154:PRO:HA	1:K:157:MET:SD	2.52	0.50
1:K:126:LYS:HB2	1:K:358:ARG:CD	2.27	0.50
1:F:238:VAL:HA	1:F:247:ARG:O	2.12	0.50
1:B:26:LYS:N	1:B:29:ASP:OD2	2.33	0.50
1:M:160:ALA:HB1	1:N:25:PHE:CD1	2.46	0.50
1:A:217:GLY:HA2	6:A:1299:HOH:O	2.11	0.50
1:F:312:PHE:CZ	1:F:379:GLU:HG3	2.47	0.50
1:G:303:ARG:NH2	3:G:607:ADP:O2A	2.45	0.50
1:O:297:ASN:HB3	1:O:301:VAL:HG13	1.94	0.50
1:A:27:ALA:HB2	1:A:54:TRP:CD1	2.47	0.50
1:G:168:VAL:HG13	1:G:280:HIS:ND1	2.26	0.50
1:L:183:LYS:HD2	6:R:2851:HOH:O	2.11	0.50
1:P:149:LYS:HA	1:P:283:MET:HG3	1.93	0.50
1:H:134:ASP:HB2	6:H:1675:HOH:O	2.11	0.50
1:L:182:GLY:HA3	1:L:230:HIS:O	2.12	0.50
1:L:49:LEU:HD21	1:L:99:GLU:HG2	1.93	0.50
1:C:285:ASN:HD21	1:C:287:ARG:HB2	1.76	0.50
1:G:191:ASN:ND2	1:G:193:LYS:HB2	2.26	0.50
1:M:153:LEU:C	1:M:155:PRO:HD2	2.32	0.50
1:N:69:GLN:HG3	6:N:2516:HOH:O	2.12	0.50
1:C:340:ALA:HB2	1:C:345:TYR:CE2	2.47	0.50
1:H:185:TYR:HE1	1:H:230:HIS:CE1	2.30	0.50
6:M:2203:HOH:O	1:N:25:PHE:HE1	1.94	0.50
1:B:124:HIS:HA	1:B:261:PHE:CE2	2.47	0.50
1:E:34:LEU:HA	1:E:37:HIS:ND1	2.27	0.50
1:O:159:ARG:HD3	1:O:221:ASP:OD1	2.11	0.50
1:I:84:THR:N	2:I:509:NMG:O2	2.34	0.50
1:N:18:LYS:O	1:N:21:GLU:HG2	2.12	0.50
1:B:188:THR:CG2	1:B:223:PRO:HG2	2.42	0.50
1:C:152:CYS:HB2	1:C:161:GLU:OE1	2.12	0.50
1:E:101:PHE:O	1:E:105:ILE:HG13	2.12	0.50
1:N:113:PRO:HA	1:N:287:ARG:NH2	2.27	0.50
1:P:361:VAL:O	1:P:365:VAL:HG23	2.12	0.49
1:Q:188:THR:HG23	6:Q:1384:HOH:O	2.11	0.49
1:D:191:ASN:ND2	1:D:193:LYS:H	2.09	0.49
1:D:126:LYS:HB2	1:D:358:ARG:HD2	1.94	0.49
1:N:165:VAL:HG11	1:N:241:ASN:OD1	2.12	0.49

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:112:LYS:O	1:B:115:ASP:HB2	2.11	0.49
1:N:236:PHE:C	1:N:237:LEU:HG	2.32	0.49
1:H:183:LYS:HD3	1:H:185:TYR:HE2	1.78	0.49
1:R:179:ASP:CG	1:R:266:ARG:HH12	2.16	0.49
1:B:14:VAL:HG23	6:B:1357:HOH:O	2.11	0.49
1:E:320:ASP:OD1	1:E:330:LYS:NZ	2.43	0.49
1:R:352:ARG:HH11	1:R:352:ARG:HG2	1.77	0.49
1:K:303:ARG:NH2	3:K:611:ADP:O2A	2.45	0.49
1:H:199:ILE:HG13	1:H:204:LEU:HD23	1.94	0.49
1:G:187:LEU:HB3	1:G:223:PRO:HB2	1.94	0.49
1:L:56:LYS:HE2	1:L:96:CYS:SG	2.52	0.49
1:H:57:VAL:HG13	1:H:62:VAL:O	2.12	0.49
1:E:159:ARG:NH2	1:F:65:ASP:OD1	2.45	0.49
1:B:350:TRP:C	1:B:350:TRP:CD1	2.86	0.49
1:Q:237:LEU:N	1:Q:237:LEU:HD12	2.28	0.49
1:L:285:ASN:ND2	1:L:288:LEU:N	2.49	0.49
1:L:94:TYR:CZ	1:L:288:LEU:HD11	2.48	0.49
1:R:298:MET:CA	1:R:301:VAL:HG22	2.43	0.49
1:L:147:SER:OG	1:L:292:CYS:HA	2.13	0.49
1:Q:313:LEU:HD12	1:Q:371:LEU:O	2.12	0.49
1:Q:278:CYS:HB3	1:Q:280:HIS:HE1	1.75	0.49
1:A:278:CYS:HB3	1:A:280:HIS:CE1	2.48	0.49
1:A:105:ILE:HG12	1:A:298:MET:CE	2.42	0.49
1:M:356:SER:OG	1:M:359:GLU:HG3	2.13	0.49
1:C:310:LEU:O	1:C:314:GLU:HG2	2.12	0.49
1:B:18:LYS:HB3	1:B:20:TRP:CZ2	2.48	0.49
1:F:201:ASP:O	1:F:202:HIS:HB2	2.12	0.49
1:N:41:MET:HG2	1:N:100:PHE:HZ	1.77	0.49
1:M:112:LYS:HB3	1:M:113:PRO:HD2	1.95	0.49
1:M:180:LEU:O	1:M:229:TRP:HH2	1.95	0.49
1:C:285:ASN:HD22	1:C:287:ARG:N	2.11	0.49
1:M:286:ASP:HB3	6:M:2487:HOH:O	2.12	0.49
1:R:287:ARG:NH1	1:R:288:LEU:HD21	2.28	0.49
3:O:615:ADP:C5'	3:O:615:ADP:O2B	2.60	0.49
1:A:222:TRP:HA	1:A:226:ARG:NH1	2.27	0.49
1:Q:44:GLN:OE1	1:Q:103:LYS:HB3	2.12	0.49
1:C:159:ARG:NH2	1:D:65:ASP:OD1	2.34	0.49
1:G:183:LYS:HD3	1:G:185:TYR:CE2	2.48	0.49
1:B:176:LEU:HD12	1:B:229:TRP:CZ2	2.48	0.49
1:B:192:GLU:O	1:B:196:GLU:HG3	2.12	0.49
1:R:308:LEU:HD22	1:R:310:LEU:HG	1.95	0.49
1:J:53:TYR:OH	1:J:99:GLU:HB3	2.12	0.49

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:298:MET:HE1	1:I:353:LEU:HD12	1.94	0.49
1:A:314:GLU:HG3	1:A:315:LYS:HD2	1.93	0.49
1:F:168:VAL:HG12	1:F:169:VAL:N	2.27	0.49
1:I:37:HIS:CD2	1:I:75:PRO:HA	2.48	0.49
1:R:50:TYR:O	1:R:54:TRP:HB3	2.13	0.49
1:B:278:CYS:HB3	1:B:280:HIS:HE1	1.74	0.49
1:B:313:LEU:HD21	1:B:319:PHE:CD1	2.47	0.49
1:A:239:TRP:HB2	1:A:247:ARG:HB2	1.95	0.49
1:F:267:GLY:O	1:F:271:VAL:HG23	2.13	0.49
1:D:247:ARG:HB3	6:D:1350:HOH:O	2.12	0.49
1:A:346:ASP:OD1	1:A:346:ASP:C	2.51	0.49
1:C:191:ASN:HD21	1:C:193:LYS:H	1.58	0.48
1:P:159:ARG:HD3	1:P:221:ASP:OD1	2.13	0.48
1:B:143:ARG:HG2	1:B:144:CYS:N	2.27	0.48
1:C:137:VAL:HG13	1:C:306:VAL:HB	1.95	0.48
1:O:147:SER:HA	1:O:245:HIS:HB2	1.95	0.48
1:E:341:THR:O	1:E:342:ASP:CB	2.61	0.48
1:P:187:LEU:HB3	1:P:223:PRO:HB2	1.94	0.48
1:Q:222:TRP:CG	1:Q:223:PRO:HA	2.48	0.48
1:J:49:LEU:CD2	1:J:99:GLU:HG2	2.38	0.48
1:C:94:TYR:HD1	1:C:95:GLU:HG2	1.79	0.48
1:Q:247:ARG:NH1	3:Q:617:ADP:O1B	2.46	0.48
1:Q:361:VAL:O	1:Q:365:VAL:HG23	2.13	0.48
1:H:124:HIS:CE1	1:H:262:SER:HB2	2.48	0.48
1:I:83:LYS:HZ1	1:I:336:GLU:HG3	1.78	0.48
1:Q:152:CYS:SG	1:R:17:SER:HB3	2.53	0.48
1:L:180:LEU:O	1:L:229:TRP:HH2	1.95	0.48
1:P:213:LEU:HD13	6:P:2499:HOH:O	2.14	0.48
1:H:303:ARG:HG3	1:H:352:ARG:NH1	2.29	0.48
1:L:319:PHE:CE1	1:L:323:LEU:HD21	2.49	0.48
1:O:244:ASP:OD1	1:O:292:CYS:HB3	2.13	0.48
1:B:153:LEU:HB3	1:B:154:PRO:HD2	1.95	0.48
1:C:104:CYS:O	1:C:108:ILE:HG13	2.14	0.48
1:H:67:CYS:HB3	1:H:87:VAL:O	2.13	0.48
1:Q:318:ARG:CZ	1:Q:388:ILE:HD12	2.43	0.48
1:J:111:PHE:CG	1:J:353:LEU:HD13	2.48	0.48
1:N:262:SER:O	1:N:266:ARG:HB2	2.13	0.48
1:O:169:VAL:O	1:O:173:LEU:HG	2.13	0.48
1:E:168:VAL:HG22	1:E:280:HIS:CE1	2.48	0.48
1:F:30:ASN:ND2	1:F:50:TYR:OH	2.45	0.48
1:L:92:TYR:O	1:L:96:CYS:HB2	2.14	0.48
1:E:188:THR:HG23	6:E:1697:HOH:O	2.13	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:P:314:GLU:HG3	1:P:315:LYS:HD2	1.96	0.48
1:D:352:ARG:HH11	1:D:352:ARG:CG	2.26	0.48
1:C:312:PHE:CE1	1:C:379:GLU:HG3	2.49	0.48
1:K:110:HIS:HE1	6:K:3316:HOH:O	1.95	0.48
1:Q:314:GLU:HG3	1:Q:315:LYS:HD2	1.96	0.48
1:J:152:CYS:HB2	1:J:161:GLU:OE1	2.14	0.48
1:D:108:ILE:HG21	1:D:296:THR:HG22	1.94	0.48
1:H:18:LYS:HB3	1:H:20:TRP:CZ2	2.49	0.48
1:E:288:LEU:O	1:E:299:GLY:HA2	2.14	0.48
1:J:177:LYS:HA	1:J:181:ALA:HB2	1.96	0.48
1:Q:49:LEU:O	1:Q:53:TYR:HB2	2.13	0.48
1:R:183:LYS:O	1:R:185:TYR:CE1	2.67	0.48
1:D:305:SER:HB2	1:D:346:ASP:OD1	2.13	0.48
1:O:34:LEU:CD1	1:O:45:LEU:HD23	2.43	0.48
1:D:285:ASN:HD22	1:D:287:ARG:N	2.12	0.48
1:M:285:ASN:ND2	1:M:287:ARG:HB2	2.27	0.48
1:J:20:TRP:HB3	1:J:54:TRP:CE2	2.48	0.48
1:R:127:LEU:HB3	1:R:258:LYS:HD2	1.96	0.48
1:C:155:PRO:HD3	1:C:218:CYS:SG	2.54	0.48
1:K:207:LYS:O	1:K:209:THR:N	2.44	0.48
1:H:353:LEU:HD22	1:H:354:GLY:N	2.29	0.48
1:M:57:VAL:HG22	1:M:63:THR:HG22	1.96	0.48
1:P:328:LEU:HA	1:P:348:SER:O	2.14	0.48
1:I:361:VAL:O	1:I:365:VAL:HG23	2.14	0.48
1:G:75:PRO:HD2	6:G:2123:HOH:O	2.14	0.48
1:H:183:LYS:HD3	1:H:185:TYR:CE2	2.48	0.48
1:Q:364:LEU:HD22	1:Q:368:VAL:HG23	1.95	0.48
1:I:121:ASP:OD2	1:I:358:ARG:HD3	2.12	0.48
1:Q:84:THR:HG21	1:Q:295:PRO:HD2	1.95	0.48
1:E:208:PRO:HA	1:E:213:LEU:HD23	1.96	0.48
1:F:288:LEU:HD22	1:F:353:LEU:HD11	1.95	0.47
1:K:144:CYS:HA	1:K:301:VAL:O	2.14	0.47
1:A:39:ASN:HB2	1:A:83:LYS:O	2.14	0.47
1:H:303:ARG:HG3	1:H:352:ARG:HH12	1.79	0.47
1:F:314:GLU:OE1	1:F:345:TYR:OH	2.26	0.47
1:P:180:LEU:O	1:P:229:TRP:CH2	2.67	0.47
1:D:41:MET:HG2	1:D:100:PHE:HZ	1.79	0.47
1:C:159:ARG:O	1:C:163:ARG:HD2	2.14	0.47
1:B:312:PHE:CE1	1:B:379:GLU:HG3	2.49	0.47
1:C:180:LEU:O	1:C:229:TRP:HH2	1.96	0.47
1:H:204:LEU:HG	1:H:205:PHE:N	2.29	0.47
1:E:159:ARG:HG3	1:E:221:ASP:OD2	2.14	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:361:VAL:O	1:G:365:VAL:HG23	2.14	0.47
1:H:30:ASN:O	1:H:30:ASN:ND2	2.47	0.47
1:J:247:ARG:NH1	3:J:610:ADP:O1B	2.47	0.47
1:K:247:ARG:NH1	3:K:611:ADP:O1B	2.47	0.47
1:H:303:ARG:NH2	3:H:608:ADP:O2A	2.46	0.47
1:F:143:ARG:NH2	1:F:297:ASN:OD1	2.47	0.47
1:L:298:MET:HB2	1:L:353:LEU:HG	1.96	0.47
1:C:147:SER:HB2	1:C:283:MET:HB2	1.97	0.47
1:F:213:LEU:HD23	1:F:219:ALA:HB2	1.96	0.47
1:I:40:VAL:HG23	1:I:84:THR:HA	1.96	0.47
1:L:237:LEU:HD12	1:L:237:LEU:N	2.30	0.47
1:G:175:GLY:O	1:G:177:LYS:HE2	2.14	0.47
1:L:11:LYS:HA	1:L:61:GLY:HA3	1.97	0.47
1:I:359:GLU:O	1:I:363:VAL:HG23	2.14	0.47
1:D:155:PRO:HB3	1:D:216:SER:O	2.15	0.47
1:E:143:ARG:NH2	1:E:297:ASN:OD1	2.39	0.47
1:A:40:VAL:O	1:A:44:GLN:HG2	2.15	0.47
1:Q:143:ARG:HG2	1:Q:144:CYS:N	2.27	0.47
1:H:108:ILE:CG2	1:H:296:THR:HG22	2.43	0.47
1:H:208:PRO:HG3	1:H:222:TRP:CD1	2.48	0.47
1:F:79:PHE:HD1	1:F:339:LEU:CD2	2.27	0.47
1:H:321:GLU:HG2	1:H:325:LYS:HE3	1.96	0.47
1:O:312:PHE:CZ	1:O:379:GLU:HG3	2.49	0.47
1:K:123:ASP:OD1	1:K:125:ASN:HB2	2.14	0.47
1:I:27:ALA:HB2	1:I:54:TRP:NE1	2.30	0.47
1:C:300:THR:O	1:C:302:VAL:HG23	2.15	0.47
1:H:70:THR:O	1:H:74:ASN:ND2	2.47	0.47
1:P:201:ASP:HB3	1:P:203:PHE:CE2	2.50	0.47
1:O:285:ASN:HD21	1:O:287:ARG:HB2	1.80	0.47
1:H:285:ASN:ND2	1:H:288:LEU:N	2.46	0.47
1:P:143:ARG:HG3	6:P:1047:HOH:O	2.15	0.47
1:P:143:ARG:HA	1:P:248:VAL:O	2.14	0.47
1:E:239:TRP:HB2	1:E:247:ARG:HB2	1.96	0.47
1:M:49:LEU:HD22	1:M:53:TYR:CE1	2.49	0.47
1:H:208:PRO:HD3	1:H:222:TRP:CE2	2.50	0.47
1:A:341:THR:O	1:A:342:ASP:HB2	2.14	0.47
1:G:246:ILE:O	1:G:247:ARG:HD3	2.15	0.47
1:K:27:ALA:HB2	1:K:54:TRP:CD1	2.49	0.47
1:A:110:HIS:CD2	1:A:327:ARG:NH2	2.83	0.47
1:A:38:ASN:ND2	1:A:38:ASN:C	2.67	0.47
1:I:66:LYS:HE3	1:J:16:HIS:NE2	2.30	0.47
1:E:105:ILE:HG12	1:E:298:MET:HE1	1.97	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:109:HIS:O	1:K:110:HIS:HB2	2.14	0.47
1:P:377:LYS:HG2	6:P:2346:HOH:O	2.14	0.47
1:I:154:PRO:HG2	1:I:243:GLU:O	2.13	0.47
1:N:109:HIS:O	1:N:110:HIS:HB2	2.15	0.47
1:D:332:GLY:HA3	1:D:338:SER:O	2.13	0.47
1:Q:91:GLU:HB2	1:Q:283:MET:SD	2.54	0.47
1:E:167:LYS:HD3	1:E:171:ASP:OD2	2.14	0.47
1:B:105:ILE:HG12	1:B:298:MET:CE	2.45	0.47
1:R:248:VAL:C	1:R:249:ILE:HG13	2.34	0.47
1:M:213:LEU:HD12	1:M:218:CYS:HB3	1.97	0.47
1:F:53:TYR:OH	1:F:99:GLU:HB2	2.15	0.47
1:M:201:ASP:HB3	1:M:203:PHE:CE2	2.49	0.47
1:L:223:PRO:O	1:L:226:ARG:HD3	2.14	0.47
1:G:89:GLY:CA	1:G:155:PRO:HG2	2.37	0.47
1:R:300:THR:O	1:R:302:VAL:HG23	2.15	0.47
1:F:153:LEU:HB3	1:F:154:PRO:HD2	1.96	0.47
1:N:215:THR:HG21	6:N:3030:HOH:O	2.15	0.47
1:K:384:ILE:HB	1:K:387:MET:HG3	1.96	0.47
1:R:41:MET:CE	1:R:71:GLY:HA3	2.45	0.47
1:L:66:LYS:O	1:L:66:LYS:HD2	2.15	0.47
1:Q:285:ASN:HD21	1:Q:287:ARG:HB2	1.78	0.47
1:R:144:CYS:HA	1:R:301:VAL:O	2.14	0.47
1:J:18:LYS:O	1:J:21:GLU:HG2	2.15	0.47
1:H:316:HIS:CD2	1:H:317:PRO:HD2	2.50	0.47
1:H:135:LYS:HD3	1:H:136:TYR:CE1	2.49	0.47
1:B:256:ASP:HB3	6:B:2093:HOH:O	2.15	0.47
1:P:231:ASN:ND2	6:P:2502:HOH:O	2.48	0.47
1:R:164:LEU:O	1:R:168:VAL:HG23	2.15	0.47
1:F:294:CYS:HB3	1:F:297:ASN:HD22	1.79	0.47
1:C:314:GLU:HG3	1:C:315:LYS:HD2	1.97	0.47
1:L:106:GLU:OE2	1:L:112:LYS:HE2	2.14	0.47
1:F:285:ASN:HD22	1:F:288:LEU:N	2.02	0.46
1:Q:155:PRO:HG3	1:Q:293:THR:HG23	1.96	0.46
1:G:106:GLU:O	1:G:110:HIS:N	2.46	0.46
1:B:44:GLN:HB3	1:B:103:LYS:HE3	1.97	0.46
1:O:245:HIS:C	1:O:246:ILE:HG13	2.35	0.46
1:I:201:ASP:HB3	1:I:203:PHE:CE2	2.50	0.46
1:D:331:ARG:NH1	5:D:804:NO3:O2	2.47	0.46
1:N:18:LYS:HB2	1:N:21:GLU:CG	2.42	0.46
1:B:288:LEU:HD22	1:B:353:LEU:HD11	1.97	0.46
1:E:183:LYS:HG2	1:E:184:TYR:N	2.30	0.46
1:B:66:LYS:C	1:B:66:LYS:HD3	2.36	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:206:GLU:HG2	6:B:1423:HOH:O	2.16	0.46
1:O:207:LYS:O	1:O:209:THR:N	2.47	0.46
1:P:300:THR:C	1:P:301:VAL:HG23	2.36	0.46
1:I:112:LYS:HB3	1:I:113:PRO:HD2	1.96	0.46
1:G:80:TYR:CD2	1:G:330:LYS:HE2	2.50	0.46
1:O:236:PHE:CE1	1:O:267:GLY:HA3	2.50	0.46
1:P:24:LYS:NZ	6:P:2850:HOH:O	2.47	0.46
1:F:223:PRO:O	1:F:226:ARG:HB2	2.16	0.46
1:Q:352:ARG:HG2	1:Q:352:ARG:NH1	2.31	0.46
1:R:355:LYS:HB2	1:R:360:LEU:CD2	2.45	0.46
1:A:110:HIS:HD2	1:A:327:ARG:CZ	2.28	0.46
1:K:186:PRO:HG2	1:K:189:THR:OG1	2.15	0.46
1:Q:384:ILE:HA	1:Q:387:MET:HG3	1.98	0.46
1:J:203:PHE:CE2	1:J:234:LYS:HE2	2.50	0.46
1:L:31:PHE:CE1	1:L:47:LYS:HA	2.50	0.46
1:A:58:THR:HB	1:A:59:PRO:HD2	1.98	0.46
1:Q:382:GLN:HE21	1:Q:382:GLN:HB2	1.52	0.46
1:B:154:PRO:HD3	1:B:245:HIS:CD2	2.50	0.46
1:H:312:PHE:CD2	1:H:379:GLU:HA	2.51	0.46
1:M:184:TYR:CE1	1:M:240:ILE:HD12	2.50	0.46
1:B:139:SER:HB3	1:B:253:LYS:HA	1.97	0.46
1:A:313:LEU:HA	1:A:378:LEU:HD12	1.96	0.46
1:E:222:TRP:HA	1:E:226:ARG:NH1	2.30	0.46
1:N:45:LEU:HD12	1:N:46:THR:H	1.80	0.46
1:B:64:PHE:O	1:B:67:CYS:HB2	2.16	0.46
1:R:66:LYS:HD3	1:R:66:LYS:C	2.36	0.46
1:J:202:HIS:HB3	3:J:610:ADP:H1'	1.97	0.46
1:E:143:ARG:HG2	1:E:144:CYS:N	2.29	0.46
1:E:126:LYS:CB	1:E:358:ARG:HD2	2.39	0.46
1:G:173:LEU:HD11	1:G:238:VAL:HG11	1.97	0.46
1:O:128:VAL:HG21	1:R:358:ARG:HH21	1.81	0.46
1:A:247:ARG:NH1	3:A:601:ADP:O1B	2.49	0.46
1:G:175:GLY:HA2	1:G:177:LYS:NZ	2.31	0.46
1:L:307:HIS:CD2	3:L:612:ADP:C6	3.03	0.46
1:M:144:CYS:HA	1:M:301:VAL:O	2.15	0.46
1:H:377:LYS:HE2	1:H:387:MET:SD	2.56	0.46
1:O:202:HIS:HB3	3:O:615:ADP:H1'	1.98	0.46
1:B:302:VAL:O	1:B:352:ARG:HD3	2.16	0.46
1:H:312:PHE:CZ	1:H:379:GLU:HG3	2.50	0.46
1:N:252:GLN:NE2	1:N:256:ASP:HB3	2.30	0.46
1:H:11:LYS:HA	1:H:61:GLY:HA2	1.97	0.46
1:F:301:VAL:O	1:F:301:VAL:HG12	2.16	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:P:220:ARG:O	1:P:221:ASP:HB2	2.16	0.46
1:E:105:ILE:HG12	1:E:298:MET:CE	2.45	0.46
1:R:228:ILE:HD11	1:R:237:LEU:HD23	1.98	0.46
1:P:109:HIS:O	1:P:110:HIS:HB2	2.15	0.46
1:M:40:VAL:CG2	1:M:84:THR:HA	2.46	0.46
1:C:37:HIS:CE1	6:C:1718:HOH:O	2.68	0.46
1:R:49:LEU:HD21	1:R:99:GLU:HG2	1.98	0.46
1:G:237:LEU:N	1:G:237:LEU:HD12	2.31	0.46
1:Q:202:HIS:HB3	3:Q:617:ADP:H1'	1.97	0.46
1:F:153:LEU:HD23	1:F:245:HIS:CE1	2.51	0.46
1:C:91:GLU:OE2	1:C:149:LYS:HE2	2.15	0.46
1:B:105:ILE:CD1	1:B:298:MET:HE1	2.46	0.46
1:F:60:ASN:HD22	1:F:90:ASP:CB	2.29	0.46
1:R:188:THR:HG23	6:R:1289:HOH:O	2.16	0.46
1:M:26:LYS:N	1:M:29:ASP:OD2	2.44	0.46
1:L:60:ASN:HB2	1:L:90:ASP:OD2	2.16	0.46
1:O:377:LYS:HG3	1:O:387:MET:HE1	1.98	0.46
1:Q:196:GLU:HA	1:Q:199:ILE:HD12	1.98	0.46
1:L:123:ASP:OD1	1:L:125:ASN:HB2	2.16	0.46
1:I:117:HIS:HE1	1:I:300:THR:HG23	1.81	0.46
1:Q:50:TYR:O	1:Q:54:TRP:HB3	2.16	0.46
1:I:49:LEU:HD21	1:I:99:GLU:HG2	1.96	0.46
1:F:327:ARG:O	1:F:350:TRP:HB3	2.16	0.46
1:G:57:VAL:HG12	1:G:58:THR:N	2.31	0.46
1:E:273:ARG:NH2	6:E:3372:HOH:O	2.49	0.46
1:I:244:ASP:OD1	1:I:292:CYS:HB3	2.16	0.46
1:L:44:GLN:HA	1:L:44:GLN:OE1	2.16	0.46
1:M:288:LEU:O	1:M:299:GLY:HA2	2.17	0.45
1:H:297:ASN:HB3	1:H:301:VAL:CG1	2.44	0.45
1:O:298:MET:HB2	1:O:298:MET:HE2	1.39	0.45
1:R:179:ASP:OD1	1:R:180:LEU:HG	2.16	0.45
1:D:18:LYS:O	1:D:21:GLU:HG2	2.16	0.45
1:Q:47:LYS:HG3	6:Q:1798:HOH:O	2.16	0.45
1:G:252:GLN:HG2	1:G:260:VAL:CG2	2.47	0.45
1:C:359:GLU:O	1:C:363:VAL:HG23	2.16	0.45
1:C:318:ARG:NE	1:C:388:ILE:HD13	2.31	0.45
1:R:141:ARG:HD2	1:R:251:MET:HE3	1.98	0.45
1:B:18:LYS:HB2	1:B:21:GLU:HG2	1.98	0.45
1:L:330:LYS:HE3	1:L:345:TYR:CE2	2.51	0.45
1:R:24:LYS:HE3	1:R:25:PHE:CE2	2.52	0.45
1:H:53:TYR:CZ	1:H:97:TYR:HA	2.51	0.45
1:M:252:GLN:HE22	1:M:259:ALA:HB3	1.80	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:R:353:LEU:HD22	1:R:353:LEU:C	2.37	0.45
1:A:144:CYS:HA	1:A:301:VAL:O	2.16	0.45
1:P:141:ARG:HD3	3:P:616:ADP:C8	2.51	0.45
1:K:141:ARG:HD3	3:K:611:ADP:C8	2.51	0.45
1:R:285:ASN:HD22	1:R:288:LEU:N	2.13	0.45
1:O:94:TYR:HA	1:O:101:PHE:CD2	2.52	0.45
1:G:238:VAL:HA	1:G:247:ARG:O	2.16	0.45
1:I:298:MET:HE3	1:I:298:MET:HB2	1.82	0.45
1:G:80:TYR:CG	1:G:330:LYS:HE2	2.51	0.45
1:C:199:ILE:HG12	1:C:205:PHE:O	2.16	0.45
1:B:53:TYR:CZ	1:B:97:TYR:HA	2.51	0.45
1:P:117:HIS:ND1	1:P:118:PRO:HD2	2.32	0.45
1:C:222:TRP:CD1	1:C:223:PRO:HB3	2.51	0.45
1:E:212:LEU:HB3	6:E:3003:HOH:O	2.14	0.45
1:E:308:LEU:HD22	1:E:310:LEU:HG	1.98	0.45
1:H:322:MET:HG3	1:H:389:PRO:CD	2.46	0.45
1:A:124:HIS:H	1:A:124:HIS:CD2	2.34	0.45
1:I:224:ASP:OD1	1:I:224:ASP:C	2.55	0.45
1:D:309:ARG:O	1:D:310:LEU:HD23	2.16	0.45
1:O:188:THR:HG21	6:O:2652:HOH:O	2.17	0.45
1:C:38:ASN:HD21	1:C:82:LYS:HE3	1.80	0.45
1:P:297:ASN:HB3	1:P:301:VAL:CG1	2.46	0.45
1:G:58:THR:HG23	1:G:62:VAL:O	2.17	0.45
1:E:157:MET:HE1	1:E:162:ARG:HA	1.97	0.45
1:J:312:PHE:CZ	1:J:379:GLU:HG2	2.51	0.45
1:N:53:TYR:CZ	1:N:97:TYR:HA	2.51	0.45
1:J:253:LYS:HD2	1:P:317:PRO:HB2	1.99	0.45
1:E:244:ASP:OD1	1:E:292:CYS:HB3	2.15	0.45
1:O:288:LEU:O	1:O:299:GLY:HA2	2.17	0.45
1:A:182:GLY:N	1:A:229:TRP:CZ2	2.84	0.45
1:B:313:LEU:O	1:B:313:LEU:HD23	2.17	0.45
1:I:302:VAL:O	1:I:352:ARG:HD3	2.17	0.45
1:K:285:ASN:HD22	1:K:287:ARG:N	2.15	0.45
1:J:143:ARG:HG2	1:J:144:CYS:N	2.31	0.45
1:H:69:GLN:HE21	1:H:73:ASP:CG	2.20	0.45
1:Q:166:GLU:OE2	1:Q:184:TYR:OH	2.29	0.45
1:E:252:GLN:OE1	1:E:263:ARG:NH2	2.50	0.45
1:L:304:ALA:O	1:L:348:SER:HB2	2.16	0.45
1:P:266:ARG:NH2	6:P:1681:HOH:O	2.39	0.45
1:Q:239:TRP:CE3	1:Q:247:ARG:HG3	2.51	0.45
1:I:313:LEU:HD11	1:I:322:MET:HE1	1.99	0.45
1:D:151:VAL:HG11	1:D:165:VAL:CG2	2.47	0.45

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:309:ARG:NH1	1:I:342:ASP:OD1	2.49	0.45
1:J:273:ARG:NH2	1:J:274:LEU:HD21	2.32	0.45
1:O:285:ASN:ND2	1:O:288:LEU:HG	2.32	0.45
1:I:318:ARG:HD3	1:I:388:ILE:CD1	2.45	0.45
1:N:308:LEU:HD22	1:N:310:LEU:HG	1.98	0.45
1:H:377:LYS:HG3	1:H:387:MET:CE	2.47	0.45
1:K:142:ILE:HD12	1:K:261:PHE:HA	1.98	0.45
1:B:105:ILE:HG12	1:B:298:MET:HE1	1.97	0.45
1:B:207:LYS:O	1:B:209:THR:N	2.47	0.45
1:C:109:HIS:O	1:C:110:HIS:HB2	2.17	0.45
1:L:359:GLU:O	1:L:363:VAL:HG23	2.16	0.45
1:A:139:SER:HA	1:A:254:GLY:O	2.16	0.45
1:I:313:LEU:HD11	1:I:322:MET:CE	2.47	0.45
1:B:295:PRO:HA	1:B:298:MET:SD	2.57	0.45
1:I:123:ASP:HB3	1:I:126:LYS:HG3	1.99	0.45
1:L:63:THR:HB	6:L:1175:HOH:O	2.16	0.45
1:M:336:GLU:OE2	2:M:513:NMG:NE	2.49	0.45
1:R:285:ASN:ND2	1:R:288:LEU:HG	2.32	0.45
1:F:79:PHE:HD1	1:F:339:LEU:HD21	1.82	0.45
1:J:285:ASN:HD22	1:J:287:ARG:H	1.65	0.45
1:J:285:ASN:HD22	1:J:287:ARG:N	2.14	0.45
1:J:73:ASP:O	1:J:75:PRO:HD2	2.17	0.45
1:A:268:LEU:O	1:A:272:GLU:HG3	2.17	0.45
1:K:117:HIS:HA	1:K:118:PRO:HD2	1.80	0.45
1:R:60:ASN:HB2	1:R:90:ASP:OD2	2.16	0.45
1:E:305:SER:HB3	1:E:348:SER:HB3	1.99	0.45
1:B:273:ARG:O	1:B:276:LYS:HB3	2.16	0.45
1:J:361:VAL:O	1:J:365:VAL:HG23	2.17	0.45
1:E:141:ARG:HG3	1:E:251:MET:HB3	1.99	0.45
1:O:276:LYS:HG2	1:O:276:LYS:O	2.17	0.45
1:C:33:ASP:C	1:C:33:ASP:OD1	2.56	0.45
1:A:143:ARG:HA	1:A:248:VAL:O	2.17	0.44
1:P:278:CYS:HB3	1:P:280:HIS:HE1	1.76	0.44
1:A:285:ASN:C	1:A:285:ASN:HD22	2.21	0.44
1:N:302:VAL:HG21	1:N:357:GLU:HG3	1.99	0.44
1:I:108:ILE:CG2	1:I:296:THR:HG22	2.48	0.44
1:H:358:ARG:HB3	1:H:358:ARG:HE	1.58	0.44
1:O:387:MET:HG2	1:O:387:MET:H	1.44	0.44
1:B:303:ARG:HB2	1:B:352:ARG:NH1	2.32	0.44
1:O:144:CYS:HB3	1:O:302:VAL:HG22	1.98	0.44
1:A:184:TYR:CD2	1:A:186:PRO:HD3	2.52	0.44
1:N:212:LEU:HD23	2:N:514:NMG:NH1	2.32	0.44

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:71:GLY:HA3	1:J:85:GLY:O	2.16	0.44
1:R:101:PHE:O	1:R:105:ILE:HG13	2.16	0.44
1:L:69:GLN:NE2	1:L:73:ASP:OD1	2.50	0.44
1:O:265:ALA:O	1:O:269:LEU:HD12	2.17	0.44
1:N:117:HIS:HE1	1:N:355:LYS:O	1.99	0.44
1:F:308:LEU:HD22	1:F:310:LEU:HD21	1.99	0.44
1:J:37:HIS:NE2	1:J:72:VAL:O	2.45	0.44
1:D:314:GLU:CG	1:D:315:LYS:HD2	2.44	0.44
1:R:124:HIS:HA	1:R:261:PHE:CE2	2.52	0.44
1:M:188:THR:HG22	1:M:223:PRO:HG2	1.99	0.44
1:H:34:LEU:HD22	1:H:37:HIS:CD2	2.53	0.44
1:J:84:THR:OG1	1:J:296:THR:HG23	2.17	0.44
1:N:41:MET:HG2	1:N:100:PHE:CZ	2.52	0.44
1:H:346:ASP:OD1	1:H:346:ASP:C	2.56	0.44
1:E:117:HIS:ND1	1:E:118:PRO:HD2	2.32	0.44
1:N:26:LYS:HG3	1:N:29:ASP:OD2	2.17	0.44
1:D:364:LEU:HD22	1:D:368:VAL:HG23	1.98	0.44
1:F:223:PRO:O	1:F:224:ASP:C	2.56	0.44
1:H:278:CYS:HB3	1:H:280:HIS:CE1	2.52	0.44
1:L:18:LYS:HA	1:L:19:PRO:HD2	1.80	0.44
1:F:230:HIS:HD1	1:F:230:HIS:C	2.20	0.44
1:G:305:SER:HB2	1:G:346:ASP:OD1	2.18	0.44
1:P:295:PRO:O	1:P:298:MET:HE1	2.17	0.44
1:P:147:SER:HB2	1:P:283:MET:HB2	1.99	0.44
1:E:295:PRO:O	1:E:298:MET:HE2	2.18	0.44
1:G:313:LEU:HD22	1:G:319:PHE:CD1	2.52	0.44
1:R:26:LYS:HG3	1:R:29:ASP:OD2	2.17	0.44
1:O:62:VAL:HG11	1:O:89:GLY:HA3	2.00	0.44
1:E:204:LEU:HG	1:E:205:PHE:N	2.32	0.44
1:R:57:VAL:HG12	1:R:61:GLY:HA2	1.98	0.44
1:P:267:GLY:O	1:P:271:VAL:HG23	2.17	0.44
1:H:39:ASN:C	1:H:39:ASN:OD1	2.56	0.44
1:A:297:ASN:CB	1:A:301:VAL:HG13	2.32	0.44
1:F:105:ILE:HG12	1:F:298:MET:CE	2.47	0.44
1:H:247:ARG:NH1	3:H:608:ADP:O1B	2.48	0.44
1:J:325:LYS:HD3	1:J:389:PRO:HB2	1.99	0.44
1:O:307:HIS:CD2	3:O:615:ADP:C6	3.06	0.44
1:H:18:LYS:HA	1:H:19:PRO:HD2	1.86	0.44
1:J:312:PHE:CD1	1:J:379:GLU:HG3	2.52	0.44
1:N:316:HIS:HA	1:N:317:PRO:HD2	1.75	0.44
1:K:39:ASN:O	1:K:43:SER:HB2	2.17	0.44
1:J:308:LEU:HD13	1:J:310:LEU:HD11	2.00	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:169:VAL:HG12	1:J:240:ILE:HD11	1.99	0.44
1:I:213:LEU:O	1:I:213:LEU:HG	2.16	0.44
1:P:168:VAL:HG13	1:P:280:HIS:ND1	2.32	0.44
1:A:52:LYS:HE2	1:A:53:TYR:CE2	2.52	0.44
1:R:250:SER:HB3	1:R:264:PHE:HB2	2.00	0.44
1:H:69:GLN:O	1:H:72:VAL:N	2.48	0.44
1:J:40:VAL:O	1:J:41:MET:C	2.56	0.44
1:J:117:HIS:HA	1:J:118:PRO:HD2	1.80	0.44
1:O:154:PRO:HG2	1:O:243:GLU:O	2.18	0.44
1:N:136:TYR:CD2	1:N:372:ILE:HG23	2.53	0.44
1:E:95:GLU:HG3	6:E:2343:HOH:O	2.17	0.44
1:M:70:THR:O	1:M:74:ASN:ND2	2.49	0.44
1:F:139:SER:HB3	1:F:253:LYS:HA	2.00	0.44
1:Q:285:ASN:HD22	1:Q:287:ARG:N	2.16	0.44
1:F:105:ILE:HG12	1:F:298:MET:HE3	1.99	0.44
1:O:93:SER:O	1:O:101:PHE:CE2	2.66	0.44
1:H:326:LEU:O	1:H:327:ARG:HB2	2.18	0.44
1:O:243:GLU:O	1:O:243:GLU:HG2	2.17	0.44
1:F:258:LYS:HD2	6:F:2521:HOH:O	2.17	0.44
1:P:27:ALA:HB2	1:P:54:TRP:NE1	2.31	0.44
1:A:69:GLN:NE2	1:B:221:ASP:OD1	2.50	0.44
1:D:50:TYR:O	1:D:54:TRP:HB3	2.18	0.44
1:R:370:LEU:O	1:R:373:ALA:HB3	2.17	0.44
1:J:132:PHE:N	1:J:255:GLY:O	2.48	0.44
1:I:285:ASN:HD22	1:I:287:ARG:N	2.03	0.44
1:R:387:MET:H	1:R:387:MET:HG2	1.52	0.44
1:G:191:ASN:OD1	1:G:194:ASP:HB2	2.18	0.44
1:I:298:MET:HE3	1:I:353:LEU:HD12	2.00	0.44
1:P:40:VAL:O	1:P:43:SER:HB2	2.18	0.44
1:H:79:PHE:CD2	1:H:337:SER:HA	2.53	0.44
1:C:331:ARG:HB2	1:C:346:ASP:HB3	2.00	0.44
1:A:204:LEU:HG	1:A:205:PHE:N	2.33	0.44
1:E:303:ARG:NH2	3:E:605:ADP:O2A	2.50	0.44
1:R:285:ASN:HD22	1:R:288:LEU:HG	1.82	0.44
1:L:125:ASN:C	1:L:127:LEU:H	2.21	0.44
1:L:295:PRO:O	1:L:298:MET:CG	2.65	0.44
1:C:249:ILE:HG22	1:C:250:SER:N	2.33	0.44
1:C:112:LYS:HB3	1:C:113:PRO:CD	2.47	0.44
1:M:382:GLN:HB2	1:M:382:GLN:HE21	1.59	0.44
1:D:285:ASN:HB3	1:D:288:LEU:HB2	1.99	0.44
1:A:312:PHE:CE1	1:A:379:GLU:HG3	2.53	0.44
1:H:185:TYR:HA	1:H:186:PRO:HD3	1.72	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:M:313:LEU:HA	1:M:378:LEU:HD12	1.99	0.44
1:C:34:LEU:HA	1:C:37:HIS:CE1	2.53	0.44
1:I:111:PHE:CE1	1:I:115:ASP:HB3	2.53	0.44
1:D:327:ARG:HB3	6:D:1298:HOH:O	2.18	0.44
1:F:199:ILE:HD13	1:F:206:GLU:HA	2.00	0.44
1:Q:332:GLY:HA3	1:Q:338:SER:O	2.18	0.44
1:H:41:MET:SD	1:H:41:MET:C	2.96	0.44
1:R:356:SER:OG	1:R:359:GLU:HG3	2.17	0.43
1:O:220:ARG:HB3	1:O:221:ASP:OD2	2.17	0.43
1:E:221:ASP:N	1:F:73:ASP:OD1	2.50	0.43
1:P:41:MET:HG2	1:P:100:PHE:CZ	2.53	0.43
1:D:57:VAL:HG12	1:D:58:THR:O	2.18	0.43
1:O:142:ILE:HD11	1:O:257:LEU:CD2	2.47	0.43
1:G:382:GLN:HB2	1:G:382:GLN:HE21	1.53	0.43
1:R:244:ASP:OD1	1:R:292:CYS:HB3	2.18	0.43
1:P:18:LYS:HB2	1:P:21:GLU:CD	2.39	0.43
1:F:346:ASP:HB2	6:F:1526:HOH:O	2.18	0.43
1:F:239:TRP:CH2	3:F:606:ADP:H5'2	2.47	0.43
1:M:143:ARG:HG3	6:M:1918:HOH:O	2.18	0.43
1:K:285:ASN:C	1:K:285:ASN:HD22	2.22	0.43
1:H:34:LEU:HD22	1:H:37:HIS:CG	2.53	0.43
1:Q:140:CYS:HB2	1:Q:260:VAL:HG21	1.99	0.43
1:P:309:ARG:HA	1:P:344:THR:HA	2.00	0.43
1:M:364:LEU:HD22	1:M:368:VAL:HG23	1.99	0.43
1:J:142:ILE:HD12	1:J:261:PHE:HA	2.00	0.43
1:A:117:HIS:HA	1:A:118:PRO:HD2	1.78	0.43
1:K:330:LYS:HE3	1:K:345:TYR:HE2	1.84	0.43
1:Q:298:MET:CG	6:Q:1831:HOH:O	2.66	0.43
1:Q:384:ILE:CA	1:Q:387:MET:HG3	2.48	0.43
1:C:201:ASP:O	1:C:202:HIS:HB2	2.18	0.43
1:G:309:ARG:NH1	1:G:342:ASP:O	2.51	0.43
1:Q:153:LEU:HB3	1:Q:154:PRO:HD2	2.01	0.43
1:H:54:TRP:CD1	1:H:55:ASP:N	2.86	0.43
1:K:198:LEU:HD23	1:K:198:LEU:HA	1.86	0.43
1:A:180:LEU:O	1:A:229:TRP:HH2	2.01	0.43
1:F:314:GLU:CG	1:F:315:LYS:HD2	2.48	0.43
1:J:285:ASN:HD22	1:J:288:LEU:H	1.65	0.43
1:P:57:VAL:CG1	1:P:58:THR:N	2.81	0.43
1:K:188:THR:HG23	6:K:1331:HOH:O	2.17	0.43
1:H:154:PRO:O	1:H:220:ARG:NH2	2.51	0.43
1:B:88:PHE:HE2	1:B:101:PHE:CD2	2.37	0.43
1:L:143:ARG:HG3	6:L:1010:HOH:O	2.19	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:136:TYR:O	1:I:308:LEU:HD23	2.18	0.43
1:F:166:GLU:OE1	1:F:225:GLY:HA2	2.18	0.43
1:R:153:LEU:HB3	1:R:154:PRO:HD2	1.99	0.43
1:O:314:GLU:CG	1:O:315:LYS:HD2	2.47	0.43
1:R:142:ILE:HD12	1:R:261:PHE:HA	1.99	0.43
1:B:145:GLY:H	1:B:301:VAL:CG1	2.32	0.43
1:B:18:LYS:O	1:B:21:GLU:HG2	2.18	0.43
1:N:26:LYS:O	1:N:27:ALA:C	2.57	0.43
1:C:40:VAL:O	1:C:44:GLN:HG2	2.18	0.43
1:N:183:LYS:HD3	1:N:185:TYR:CE2	2.53	0.43
1:K:245:HIS:C	1:K:246:ILE:HG13	2.38	0.43
1:B:27:ALA:HB2	1:B:54:TRP:CE2	2.54	0.43
1:R:151:VAL:HG12	1:R:152:CYS:O	2.18	0.43
1:K:297:ASN:OD1	1:K:352:ARG:NE	2.49	0.43
1:N:340:ALA:HB2	1:N:345:TYR:CE2	2.54	0.43
1:H:126:LYS:O	1:H:358:ARG:HD2	2.18	0.43
1:P:285:ASN:HD22	1:P:288:LEU:H	1.65	0.43
1:M:157:MET:HE3	1:M:245:HIS:HE2	1.84	0.43
1:D:298:MET:CE	1:D:353:LEU:HD12	2.48	0.43
1:B:18:LYS:HB2	1:B:21:GLU:CD	2.39	0.43
1:I:341:THR:O	1:I:342:ASP:CB	2.66	0.43
1:B:88:PHE:HE2	1:B:101:PHE:CG	2.37	0.43
1:O:206:GLU:HB2	6:O:1465:HOH:O	2.17	0.43
1:K:312:PHE:CZ	1:K:379:GLU:HG3	2.54	0.43
1:M:31:PHE:O	1:N:163:ARG:NH2	2.43	0.43
1:A:176:LEU:HD23	1:A:274:LEU:HD11	2.01	0.43
1:N:285:ASN:HD22	1:N:288:LEU:HB2	1.83	0.43
1:H:327:ARG:O	1:H:328:LEU:HD23	2.19	0.43
3:B:602:ADP:H2'	6:B:1457:HOH:O	2.18	0.43
1:H:331:ARG:HB2	1:H:346:ASP:HB3	2.01	0.43
1:Q:154:PRO:HG2	1:Q:243:GLU:O	2.18	0.43
1:J:112:LYS:N	1:J:115:ASP:OD2	2.41	0.43
1:J:141:ARG:HG3	1:J:251:MET:HB3	2.01	0.43
1:G:60:ASN:HD22	1:G:90:ASP:HB2	1.83	0.43
1:C:94:TYR:CE2	1:C:288:LEU:HD11	2.54	0.43
1:M:335:GLY:O	1:M:336:GLU:C	2.57	0.43
1:C:185:TYR:HA	1:C:186:PRO:HD2	1.92	0.43
1:P:212:LEU:O	1:P:216:SER:CB	2.66	0.43
1:Q:91:GLU:OE2	1:Q:149:LYS:HE2	2.18	0.43
1:E:305:SER:CB	1:E:348:SER:HB3	2.48	0.43
1:R:307:HIS:CE1	3:R:618:ADP:C2	3.07	0.43
1:I:233:GLU:OE1	1:I:235:ASN:ND2	2.47	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:168:VAL:HG13	1:C:280:HIS:ND1	2.33	0.43
1:P:93:SER:O	1:P:94:TYR:C	2.57	0.43
1:K:117:HIS:CE1	1:K:300:THR:HG23	2.54	0.43
1:A:98:LYS:HG3	1:A:102:ASP:OD2	2.19	0.43
1:K:367:GLY:HA3	6:K:2460:HOH:O	2.17	0.43
1:C:31:PHE:HA	1:C:32:PRO:HD2	1.89	0.43
1:O:283:MET:HB2	6:O:2737:HOH:O	2.18	0.43
1:O:284:HIS:CE1	1:O:289:GLY:HA2	2.54	0.43
1:C:385:ASP:OD1	1:C:385:ASP:C	2.57	0.43
1:A:341:THR:O	1:A:342:ASP:CB	2.67	0.43
1:O:313:LEU:CD1	1:O:374:CYS:HB2	2.49	0.43
1:B:290:TYR:HB3	6:B:1089:HOH:O	2.19	0.43
1:L:146:ARG:HD2	1:L:282:LEU:HD13	2.00	0.43
1:I:67:CYS:O	1:I:86:CYS:HA	2.18	0.43
1:K:340:ALA:HB1	1:K:344:THR:O	2.19	0.43
1:O:281:GLY:O	1:O:282:LEU:HD23	2.19	0.43
3:I:609:ADP:O2B	3:I:609:ADP:C5'	2.55	0.42
1:R:384:ILE:CB	1:R:387:MET:HG3	2.45	0.42
1:E:57:VAL:HG12	1:E:58:THR:N	2.33	0.42
1:C:300:THR:OG1	1:C:302:VAL:HB	2.18	0.42
1:F:98:LYS:HG2	1:F:98:LYS:O	2.17	0.42
1:C:384:ILE:HA	1:C:387:MET:HG3	2.01	0.42
1:J:244:ASP:OD1	1:J:292:CYS:HB3	2.19	0.42
1:B:326:LEU:HD11	1:B:370:LEU:HD23	2.01	0.42
1:K:83:LYS:NZ	6:K:1333:HOH:O	2.52	0.42
1:R:143:ARG:CD	1:R:303:ARG:HB3	2.48	0.42
1:P:205:PHE:HD2	1:P:239:TRP:CD2	2.37	0.42
1:R:290:TYR:O	1:R:298:MET:HA	2.19	0.42
1:E:384:ILE:CA	1:E:387:MET:HG3	2.50	0.42
1:H:173:LEU:HD11	1:H:238:VAL:HG11	2.01	0.42
1:F:79:PHE:HA	1:F:339:LEU:HD21	2.01	0.42
1:J:94:TYR:CZ	1:J:288:LEU:HD11	2.54	0.42
1:K:34:LEU:HD22	1:K:37:HIS:CD2	2.54	0.42
1:A:247:ARG:HD2	6:A:1803:HOH:O	2.19	0.42
1:R:41:MET:HE2	1:R:71:GLY:HA3	2.02	0.42
1:M:149:LYS:HG3	1:M:150:GLY:N	2.35	0.42
1:I:316:HIS:HA	1:I:317:PRO:HD2	1.84	0.42
1:G:156:ALA:HB1	1:H:16:HIS:HA	2.00	0.42
1:L:117:HIS:HA	1:L:118:PRO:HD2	1.85	0.42
1:E:319:PHE:O	1:E:323:LEU:HG	2.19	0.42
1:Q:58:THR:HG22	1:Q:96:CYS:SG	2.59	0.42
1:O:349:ASN:HD22	1:O:360:LEU:HD22	1.84	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:316:HIS:HA	1:F:317:PRO:HD2	1.79	0.42
1:E:154:PRO:N	1:E:155:PRO:HD2	2.33	0.42
1:A:301:VAL:O	1:A:301:VAL:HG12	2.19	0.42
1:F:94:TYR:HE1	6:F:1575:HOH:O	2.03	0.42
1:K:331:ARG:HB2	1:K:346:ASP:CB	2.45	0.42
1:J:54:TRP:CD1	1:J:55:ASP:N	2.87	0.42
1:D:123:ASP:OD2	1:D:126:LYS:HG2	2.19	0.42
1:L:183:LYS:HG2	1:L:184:TYR:N	2.33	0.42
1:J:313:LEU:HD12	1:J:371:LEU:O	2.20	0.42
1:I:89:GLY:HA2	1:I:155:PRO:HG2	2.01	0.42
1:H:31:PHE:HA	1:H:32:PRO:HD3	1.87	0.42
1:M:318:ARG:HD3	1:M:388:ILE:CD1	2.49	0.42
1:B:173:LEU:HA	1:B:173:LEU:HD23	1.80	0.42
1:N:222:TRP:HA	1:N:226:ARG:NH1	2.35	0.42
1:L:250:SER:CB	1:L:264:PHE:HB2	2.45	0.42
1:P:313:LEU:HD23	1:P:319:PHE:CD1	2.53	0.42
1:L:124:HIS:ND1	1:L:262:SER:HB2	2.34	0.42
1:L:184:TYR:CZ	1:L:227:GLY:HA3	2.54	0.42
1:C:34:LEU:HA	1:C:37:HIS:ND1	2.35	0.42
1:J:34:LEU:HD13	1:J:42:ALA:HA	2.00	0.42
1:P:236:PHE:CZ	1:P:267:GLY:HA3	2.54	0.42
1:G:314:GLU:HG2	1:G:315:LYS:HD2	2.01	0.42
1:P:198:LEU:HD23	6:P:2747:HOH:O	2.19	0.42
1:P:74:ASN:HA	1:P:75:PRO:HD2	1.88	0.42
1:N:201:ASP:O	1:N:202:HIS:HB2	2.19	0.42
1:B:91:GLU:CD	1:B:283:MET:HG3	2.39	0.42
1:K:152:CYS:SG	1:L:17:SER:HB3	2.59	0.42
1:I:385:ASP:HB3	6:I:1448:HOH:O	2.19	0.42
1:F:143:ARG:HG3	6:F:1057:HOH:O	2.20	0.42
1:G:367:GLY:O	1:G:371:LEU:HG	2.19	0.42
1:C:91:GLU:HB2	1:C:283:MET:CE	2.49	0.42
1:H:119:ALA:HA	1:H:120:PRO:HD3	1.87	0.42
1:H:309:ARG:HA	1:H:344:THR:HA	2.01	0.42
1:G:240:ILE:HA	1:G:245:HIS:O	2.19	0.42
1:G:217:GLY:HA2	6:G:1468:HOH:O	2.20	0.42
1:H:60:ASN:HB2	1:H:90:ASP:OD2	2.19	0.42
1:I:305:SER:HA	1:I:347:ILE:O	2.18	0.42
1:H:361:VAL:O	1:H:365:VAL:HG23	2.20	0.42
1:B:146:ARG:NH2	1:B:272:GLU:OE1	2.49	0.42
1:F:138:LYS:HD2	6:F:2414:HOH:O	2.19	0.42
1:O:384:ILE:CB	1:O:387:MET:HG3	2.49	0.42
1:I:310:LEU:O	1:I:314:GLU:HB3	2.19	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:18:LYS:HB3	1:B:20:TRP:CE2	2.54	0.42
1:L:31:PHE:CZ	1:L:47:LYS:HG2	2.54	0.42
1:R:237:LEU:O	1:R:238:VAL:HG23	2.20	0.42
1:A:221:ASP:HA	1:B:72:VAL:HG12	2.02	0.42
1:A:377:LYS:HG3	1:A:387:MET:CE	2.50	0.42
1:I:185:TYR:HA	1:I:186:PRO:HD2	1.87	0.42
1:H:101:PHE:O	1:H:105:ILE:HG13	2.20	0.42
1:C:198:LEU:HA	1:C:198:LEU:HD23	1.91	0.42
1:N:144:CYS:HA	1:N:301:VAL:O	2.19	0.42
1:N:288:LEU:O	1:N:299:GLY:HA2	2.20	0.42
1:Q:155:PRO:HD3	1:Q:218:CYS:SG	2.59	0.42
1:L:312:PHE:CZ	1:L:379:GLU:HG3	2.55	0.42
1:H:193:LYS:HG3	1:M:193:LYS:CE	2.49	0.42
1:B:250:SER:CB	1:B:264:PHE:HB2	2.50	0.42
1:J:66:LYS:HD3	1:J:66:LYS:O	2.20	0.42
1:O:66:LYS:HE2	1:P:16:HIS:CD2	2.55	0.42
1:O:212:LEU:HD13	6:O:2268:HOH:O	2.19	0.42
1:I:180:LEU:O	1:I:229:TRP:HH2	2.02	0.42
1:F:287:ARG:NH1	6:F:1575:HOH:O	2.51	0.42
1:F:307:HIS:CD2	3:F:606:ADP:C6	3.07	0.42
1:E:180:LEU:O	1:E:229:TRP:CH2	2.67	0.42
1:I:105:ILE:HG12	1:I:298:MET:CE	2.50	0.42
1:I:36:LYS:HG2	1:O:189:THR:O	2.20	0.42
1:O:34:LEU:HD11	1:O:45:LEU:HD23	2.02	0.42
1:L:8:TYR:CD2	1:L:11:LYS:HE2	2.54	0.42
1:G:57:VAL:HG22	1:G:63:THR:HG22	2.02	0.42
1:M:31:PHE:CE1	1:M:47:LYS:HA	2.55	0.42
1:N:11:LYS:HA	1:N:61:GLY:HA2	2.01	0.42
1:F:127:LEU:HA	1:F:127:LEU:HD12	1.87	0.42
1:C:36:LYS:HA	6:C:1537:HOH:O	2.19	0.42
1:H:49:LEU:HD23	1:H:49:LEU:HA	1.92	0.42
1:N:108:ILE:HD13	1:N:296:THR:CG2	2.45	0.42
1:N:319:PHE:CZ	1:N:323:LEU:HD11	2.55	0.42
1:A:298:MET:CE	1:A:353:LEU:HD12	2.49	0.42
1:O:275:MET:HE3	1:O:280:HIS:HB2	2.02	0.42
1:M:355:LYS:NZ	6:M:1978:HOH:O	2.53	0.42
1:D:131:VAL:HG22	1:D:256:ASP:OD1	2.20	0.42
1:C:245:HIS:C	1:C:246:ILE:HG13	2.40	0.42
1:B:374:CYS:SG	1:B:387:MET:CE	3.08	0.42
1:H:144:CYS:HA	1:H:301:VAL:O	2.20	0.42
1:K:80:TYR:CZ	1:K:330:LYS:HE2	2.55	0.42
1:M:349:ASN:ND2	1:M:360:LEU:HD13	2.35	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:94:TYR:CZ	1:E:288:LEU:HD11	2.55	0.42
1:F:147:SER:HB2	1:F:283:MET:CB	2.50	0.42
1:K:36:LYS:HD3	1:Q:189:THR:O	2.20	0.42
1:E:88:PHE:HE2	1:E:101:PHE:CD2	2.38	0.42
1:B:12:ASN:O	1:B:14:VAL:N	2.52	0.42
1:O:292:CYS:HB3	1:O:293:THR:H	1.65	0.42
1:F:127:LEU:HD12	1:F:362:GLN:OE1	2.20	0.42
1:I:377:LYS:HE3	1:I:382:GLN:HB3	2.01	0.42
1:J:386:ASP:N	1:J:386:ASP:OD1	2.45	0.42
1:O:237:LEU:HD12	1:O:237:LEU:N	2.34	0.42
1:P:285:ASN:ND2	1:P:288:LEU:N	2.67	0.41
1:C:38:ASN:HD22	1:C:38:ASN:C	2.22	0.41
1:H:183:LYS:HB3	1:H:185:TYR:OH	2.19	0.41
1:I:109:HIS:O	1:I:110:HIS:HB2	2.20	0.41
1:R:176:LEU:HD12	1:R:229:TRP:CZ2	2.55	0.41
1:H:66:LYS:O	1:H:66:LYS:HD3	2.20	0.41
1:G:37:HIS:CD2	1:G:75:PRO:CA	3.01	0.41
1:J:213:LEU:HD12	1:J:218:CYS:CB	2.47	0.41
1:N:178:GLY:C	1:N:180:LEU:H	2.23	0.41
1:O:279:GLY:O	1:O:280:HIS:CD2	2.73	0.41
1:Q:357:GLU:O	1:Q:361:VAL:HG23	2.19	0.41
1:B:326:LEU:O	1:B:328:LEU:HG	2.20	0.41
1:H:127:LEU:HB3	1:H:258:LYS:HE3	2.02	0.41
1:D:198:LEU:HB3	1:D:204:LEU:HB2	2.02	0.41
1:C:80:TYR:CE2	1:C:339:LEU:HD22	2.55	0.41
1:Q:257:LEU:HD22	1:Q:257:LEU:O	2.20	0.41
1:H:287:ARG:NH2	1:H:288:LEU:HD21	2.35	0.41
1:M:53:TYR:O	1:M:56:LYS:N	2.47	0.41
1:M:53:TYR:OH	1:M:99:GLU:HB3	2.21	0.41
1:B:208:PRO:HD3	1:B:222:TRP:CZ2	2.55	0.41
1:N:180:LEU:O	1:N:229:TRP:HH2	2.03	0.41
1:H:12:ASN:OD1	1:H:18:LYS:HE3	2.21	0.41
1:I:201:ASP:O	1:I:202:HIS:HB2	2.20	0.41
1:P:297:ASN:HB3	1:P:301:VAL:HG13	2.02	0.41
1:B:93:SER:O	1:B:97:TYR:CD1	2.73	0.41
1:I:235:ASN:HB2	1:I:263:ARG:NH1	2.35	0.41
1:L:101:PHE:O	1:L:105:ILE:HG13	2.19	0.41
1:D:145:GLY:O	1:D:146:ARG:HD3	2.21	0.41
1:K:132:PHE:CB	1:K:137:VAL:HG21	2.51	0.41
1:L:71:GLY:HA3	1:L:85:GLY:O	2.20	0.41
1:H:117:HIS:HA	1:H:118:PRO:HD2	1.91	0.41
1:L:285:ASN:ND2	1:L:287:ARG:N	2.69	0.41

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:88:PHE:HE2	1:H:94:TYR:HA	1.84	0.41
1:P:202:HIS:HB3	3:P:616:ADP:H1'	2.02	0.41
1:M:99:GLU:O	1:M:103:LYS:HG3	2.21	0.41
1:H:356:SER:O	1:H:360:LEU:HG	2.20	0.41
1:R:184:TYR:CD2	1:R:186:PRO:HD3	2.55	0.41
1:D:270:GLU:OE2	1:D:273:ARG:HD3	2.19	0.41
1:M:201:ASP:O	1:M:202:HIS:HB2	2.20	0.41
1:C:377:LYS:HG3	1:C:387:MET:CE	2.51	0.41
1:R:143:ARG:HD3	1:R:303:ARG:HB3	2.02	0.41
1:Q:66:LYS:HE2	1:R:16:HIS:NE2	2.36	0.41
1:O:118:PRO:HD2	1:O:354:GLY:HA2	2.03	0.41
1:K:168:VAL:HG13	1:K:280:HIS:CE1	2.56	0.41
1:E:39:ASN:HB2	1:E:83:LYS:O	2.21	0.41
1:I:285:ASN:HD22	1:I:286:ASP:N	2.19	0.41
1:D:302:VAL:HG21	1:D:357:GLU:CG	2.43	0.41
1:F:141:ARG:HB3	1:F:305:SER:OG	2.20	0.41
1:C:144:CYS:HA	1:C:301:VAL:O	2.20	0.41
1:O:316:HIS:HE1	1:O:318:ARG:HB2	1.81	0.41
1:B:31:PHE:HE1	1:B:50:TYR:HB2	1.85	0.41
1:A:66:LYS:C	1:A:66:LYS:HD3	2.41	0.41
1:B:123:ASP:OD2	1:B:126:LYS:HG2	2.20	0.41
1:N:148:VAL:H	1:N:245:HIS:HD1	1.68	0.41
1:O:233:GLU:O	1:O:234:LYS:HB2	2.20	0.41
1:L:205:PHE:HB2	1:L:242:GLU:OE2	2.21	0.41
1:D:311:ALA:O	1:D:315:LYS:NZ	2.41	0.41
1:I:206:GLU:HG3	1:I:207:LYS:O	2.20	0.41
1:G:44:GLN:OE1	1:G:103:LYS:HB3	2.20	0.41
1:D:143:ARG:HB2	1:D:249:ILE:HG12	2.02	0.41
1:B:302:VAL:HG21	1:B:357:GLU:HG3	2.02	0.41
1:H:84:THR:HG21	1:H:295:PRO:HG2	2.03	0.41
1:L:228:ILE:HD11	1:L:237:LEU:HD23	2.02	0.41
1:F:139:SER:CB	1:F:253:LYS:HA	2.50	0.41
3:R:618:ADP:O1B	5:R:818:NO3:N	2.54	0.41
1:Q:111:PHE:CE1	1:Q:115:ASP:HB2	2.56	0.41
1:Q:70:THR:HG22	6:Q:1211:HOH:O	2.20	0.41
1:F:49:LEU:HD13	1:F:100:PHE:HB2	2.03	0.41
1:P:245:HIS:O	1:P:246:ILE:HG13	2.21	0.41
1:D:309:ARG:HA	1:D:343:SER:O	2.20	0.41
1:K:323:LEU:HD13	1:K:330:LYS:HB2	2.03	0.41
1:P:152:CYS:HB2	1:P:161:GLU:OE2	2.20	0.41
1:N:243:GLU:HB3	6:N:3399:HOH:O	2.20	0.41
1:A:38:ASN:HA	6:A:1248:HOH:O	2.21	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:O:313:LEU:HD11	1:O:374:CYS:HB2	2.01	0.41
1:K:185:TYR:HA	1:K:186:PRO:HD2	1.85	0.41
1:I:117:HIS:CE1	1:I:300:THR:HG23	2.56	0.41
1:C:384:ILE:CA	1:C:387:MET:HG3	2.51	0.41
1:R:176:LEU:HD12	1:R:229:TRP:CH2	2.56	0.41
1:A:318:ARG:HA	6:A:1506:HOH:O	2.20	0.41
1:G:91:GLU:HB2	1:G:283:MET:CE	2.51	0.41
1:M:141:ARG:HG3	1:M:251:MET:HB3	2.03	0.41
1:J:64:PHE:HB2	1:J:97:TYR:CE2	2.55	0.41
1:O:85:GLY:O	1:O:86:CYS:HB3	2.21	0.41
1:I:53:TYR:CZ	1:I:97:TYR:HA	2.55	0.41
1:G:326:LEU:HD21	1:G:370:LEU:HD23	2.01	0.41
1:A:104:CYS:O	1:A:108:ILE:HD12	2.20	0.41
1:M:308:LEU:HD13	1:M:310:LEU:HD11	2.03	0.41
1:G:111:PHE:CE1	1:G:115:ASP:HB3	2.55	0.41
1:G:49:LEU:HD23	1:G:49:LEU:HA	1.93	0.41
1:J:205:PHE:HD2	1:J:239:TRP:CG	2.38	0.41
1:G:154:PRO:N	1:G:155:PRO:HD2	2.35	0.41
1:N:143:ARG:NH2	1:N:297:ASN:OD1	2.38	0.41
1:N:208:PRO:HG3	1:N:222:TRP:NE1	2.36	0.41
1:F:346:ASP:OD2	3:F:606:ADP:C8	2.73	0.41
1:Q:247:ARG:NE	6:Q:3260:HOH:O	2.54	0.41
1:H:244:ASP:OD2	1:H:247:ARG:NE	2.52	0.41
1:H:161:GLU:O	1:H:165:VAL:HG23	2.21	0.41
1:C:117:HIS:HA	1:C:118:PRO:HD2	1.93	0.41
1:B:31:PHE:HA	1:B:32:PRO:HD2	1.72	0.41
1:R:18:LYS:HD3	1:R:20:TRP:CZ2	2.55	0.41
1:K:384:ILE:HA	1:K:387:MET:HG3	2.03	0.41
1:H:309:ARG:O	1:H:310:LEU:HD23	2.21	0.41
1:F:173:LEU:HD23	1:F:176:LEU:HD11	2.03	0.41
1:J:207:LYS:O	1:J:209:THR:N	2.53	0.41
1:A:127:LEU:HD12	1:A:362:GLN:OE1	2.21	0.41
1:L:360:LEU:HA	1:L:360:LEU:HD23	1.83	0.41
1:P:333:THR:O	1:P:333:THR:HG22	2.19	0.41
3:E:605:ADP:O2B	3:E:605:ADP:H5'1	2.20	0.41
1:C:111:PHE:HE2	1:C:287:ARG:NH2	2.19	0.41
1:P:234:LYS:N	6:P:2502:HOH:O	2.53	0.41
1:J:157:MET:HE1	1:J:165:VAL:HG21	2.03	0.41
1:K:53:TYR:CE2	1:K:97:TYR:HA	2.56	0.41
1:B:222:TRP:HA	1:B:223:PRO:HA	1.76	0.41
1:H:292:CYS:SG	1:H:301:VAL:HG11	2.60	0.41
1:J:18:LYS:HA	1:J:19:PRO:HD2	1.80	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:285:ASN:HD22	1:E:287:ARG:N	2.19	0.41
1:E:113:PRO:HA	1:E:287:ARG:NH2	2.35	0.41
1:C:208:PRO:HA	1:C:213:LEU:HD23	2.03	0.41
1:D:222:TRP:HA	1:D:226:ARG:NH1	2.34	0.41
1:E:295:PRO:O	1:E:298:MET:CE	2.69	0.41
1:F:201:ASP:O	1:F:202:HIS:CB	2.69	0.41
1:D:238:VAL:HA	1:D:247:ARG:O	2.21	0.41
1:B:290:TYR:O	1:B:298:MET:HA	2.21	0.41
1:P:377:LYS:HG3	1:P:387:MET:SD	2.60	0.41
1:P:43:SER:HB3	1:P:44:GLN:NE2	2.36	0.41
1:O:257:LEU:HD11	1:O:364:LEU:CD1	2.51	0.41
1:E:66:LYS:NZ	1:E:155:PRO:O	2.43	0.41
1:A:221:ASP:HA	1:B:72:VAL:CG1	2.51	0.41
1:A:318:ARG:HD3	1:A:388:ILE:CD1	2.51	0.41
1:N:336:GLU:HB3	3:N:614:ADP:O2A	2.21	0.41
1:E:79:PHE:CD2	1:E:337:SER:HA	2.55	0.41
1:K:159:ARG:HG3	1:K:221:ASP:OD2	2.20	0.41
1:O:180:LEU:O	1:O:229:TRP:HH2	2.04	0.41
1:K:342:ASP:N	6:K:3202:HOH:O	2.53	0.41
1:J:127:LEU:HG	1:J:128:VAL:N	2.36	0.41
1:D:96:CYS:C	1:D:97:TYR:CD2	2.95	0.41
1:N:206:GLU:HG3	1:N:207:LYS:O	2.21	0.41
2:O:515:NMG:NH1	5:O:815:NO3:O2	2.54	0.41
1:O:294:CYS:HA	1:O:295:PRO:HD3	1.93	0.41
1:R:242:GLU:CD	1:R:243:GLU:H	2.24	0.41
1:J:139:SER:OG	3:J:610:ADP:N1	2.44	0.41
1:M:285:ASN:HD22	1:M:287:ARG:N	2.18	0.41
1:F:314:GLU:HA	1:F:319:PHE:CD2	2.56	0.41
1:K:180:LEU:O	1:K:229:TRP:HH2	2.03	0.41
1:N:169:VAL:O	1:N:173:LEU:HG	2.20	0.41
1:R:212:LEU:HD12	1:R:216:SER:HB3	2.03	0.41
1:N:205:PHE:HB3	1:N:239:TRP:CH2	2.56	0.41
1:J:285:ASN:ND2	1:J:288:LEU:H	2.18	0.41
1:A:364:LEU:HD22	1:A:368:VAL:HG23	2.03	0.41
1:A:313:LEU:O	1:A:313:LEU:HD23	2.21	0.41
1:P:40:VAL:HG13	1:P:107:GLU:OE1	2.21	0.41
1:D:117:HIS:HA	1:D:118:PRO:HD2	1.87	0.41
1:J:304:ALA:CB	1:J:364:LEU:HD12	2.51	0.41
1:B:163:ARG:HG3	6:B:1314:HOH:O	2.21	0.41
1:A:62:VAL:HG11	1:A:89:GLY:HA3	2.01	0.41
1:F:132:PHE:HE1	1:F:257:LEU:HB2	1.86	0.41
1:F:229:TRP:C	1:F:229:TRP:CE3	2.94	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:205:PHE:HD2	1:C:239:TRP:CD2	2.39	0.40
1:J:34:LEU:HD21	1:J:72:VAL:HG22	2.02	0.40
1:G:370:LEU:O	1:G:370:LEU:HD12	2.21	0.40
1:D:217:GLY:O	1:D:220:ARG:NE	2.50	0.40
1:C:247:ARG:NH1	3:C:603:ADP:O1B	2.53	0.40
1:P:183:LYS:HD3	1:P:185:TYR:CE2	2.56	0.40
1:B:178:GLY:C	1:B:180:LEU:H	2.24	0.40
1:A:91:GLU:HG2	1:A:91:GLU:O	2.19	0.40
1:B:386:ASP:N	1:B:386:ASP:OD1	2.54	0.40
1:H:313:LEU:HA	1:H:378:LEU:CD1	2.50	0.40
1:F:141:ARG:HD2	3:F:606:ADP:C4	2.56	0.40
1:C:168:VAL:HG12	1:C:169:VAL:N	2.36	0.40
1:O:108:ILE:HD13	1:O:296:THR:HG22	2.04	0.40
1:E:36:LYS:HG2	6:E:2285:HOH:O	2.21	0.40
1:M:187:LEU:HB3	1:M:223:PRO:HB2	2.03	0.40
1:E:250:SER:OG	1:E:263:ARG:NH1	2.54	0.40
1:N:117:HIS:HA	1:N:118:PRO:HD2	1.86	0.40
1:C:44:GLN:OE1	1:C:103:LYS:HE3	2.22	0.40
1:I:372:ILE:HG22	1:I:376:LYS:HE2	2.03	0.40
1:D:192:GLU:O	1:D:196:GLU:HG3	2.21	0.40
1:B:133:GLU:HG3	6:B:2087:HOH:O	2.21	0.40
1:C:121:ASP:HB3	1:C:356:SER:HB2	2.03	0.40
1:E:131:VAL:HG22	1:E:256:ASP:OD1	2.21	0.40
1:I:205:PHE:CD1	1:I:242:GLU:HG3	2.56	0.40
1:G:175:GLY:HA2	1:G:177:LYS:HZ1	1.85	0.40
1:E:226:ARG:HG3	1:E:241:ASN:O	2.21	0.40
1:R:66:LYS:HD3	1:R:66:LYS:O	2.20	0.40
1:P:41:MET:HG2	1:P:100:PHE:HZ	1.86	0.40
1:C:384:ILE:HB	1:C:387:MET:HG3	2.03	0.40
1:A:74:ASN:HA	1:A:75:PRO:HD2	1.92	0.40
1:L:233:GLU:HG3	6:L:2661:HOH:O	2.21	0.40
1:N:304:ALA:O	1:N:348:SER:HB2	2.21	0.40
1:Q:34:LEU:HD21	1:Q:72:VAL:HG22	2.01	0.40
1:N:176:LEU:O	1:N:181:ALA:HA	2.20	0.40
1:M:296:THR:O	1:M:352:ARG:HD2	2.22	0.40
1:E:257:LEU:HD11	1:E:364:LEU:HD13	2.04	0.40
1:N:293:THR:HB	6:N:1021:HOH:O	2.22	0.40
1:D:200:GLU:HG2	1:D:200:GLU:O	2.21	0.40
1:E:382:GLN:HB2	1:E:382:GLN:HE21	1.69	0.40
1:N:374:CYS:HA	1:N:387:MET:HE2	2.03	0.40
1:L:312:PHE:CD2	1:L:379:GLU:HA	2.56	0.40
1:R:175:GLY:O	1:R:177:LYS:CG	2.67	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:111:PHE:CE1	1:B:353:LEU:HD22	2.56	0.40
1:H:183:LYS:NZ	6:H:3170:HOH:O	2.40	0.40
1:F:318:ARG:CZ	1:F:388:ILE:HD12	2.51	0.40
1:H:203:PHE:HE1	1:H:234:LYS:O	2.04	0.40
1:P:298:MET:HE2	1:P:298:MET:HB2	1.67	0.40
1:A:238:VAL:HA	1:A:247:ARG:O	2.22	0.40
1:Q:294:CYS:HA	1:Q:295:PRO:HD3	1.93	0.40
1:B:162:ARG:HH12	1:B:221:ASP:HB2	1.86	0.40
1:I:155:PRO:HD3	1:I:218:CYS:SG	2.61	0.40
1:F:18:LYS:O	1:F:21:GLU:HG2	2.21	0.40
1:H:132:PHE:HE1	1:H:257:LEU:HD12	1.86	0.40
1:B:340:ALA:HB2	1:B:345:TYR:CD2	2.56	0.40
1:J:134:ASP:HB2	6:J:1834:HOH:O	2.22	0.40
1:H:284:HIS:CD2	1:H:285:ASN:N	2.89	0.40
1:P:358:ARG:NH1	6:P:2539:HOH:O	2.55	0.40
1:B:313:LEU:C	1:B:313:LEU:HD23	2.42	0.40
1:K:313:LEU:HD22	1:K:319:PHE:CD1	2.56	0.40
1:H:297:ASN:CB	1:H:301:VAL:HG13	2.50	0.40
1:H:229:TRP:HB3	1:H:238:VAL:HB	2.03	0.40
1:B:143:ARG:HG3	6:B:1064:HOH:O	2.20	0.40
1:L:73:ASP:O	1:L:75:PRO:HD3	2.22	0.40
1:O:360:LEU:HD23	1:O:360:LEU:HA	1.84	0.40
1:L:204:LEU:HG	1:L:205:PHE:O	2.22	0.40
1:Q:185:TYR:HA	1:Q:186:PRO:HD2	1.88	0.40
1:F:161:GLU:O	1:F:165:VAL:HG23	2.22	0.40
1:D:44:GLN:OE1	1:D:103:LYS:HE3	2.22	0.40
1:D:60:ASN:HB2	1:D:90:ASP:OD2	2.21	0.40
1:I:132:PHE:HE2	1:I:369:ASN:OD1	2.03	0.40
1:D:213:LEU:CD2	1:D:219:ALA:HB2	2.51	0.40
1:O:306:VAL:HG21	1:O:368:VAL:HG21	2.03	0.40
1:N:58:THR:HB	1:N:59:PRO:HD2	2.03	0.40
1:N:346:ASP:C	1:N:346:ASP:OD1	2.59	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	364/390 (93%)	335 (92%)	29 (8%)	0	100	100
1	B	385/390 (99%)	360 (94%)	21 (6%)	4 (1%)	22	23
1	C	365/390 (94%)	338 (93%)	26 (7%)	1 (0%)	50	60
1	D	380/390 (97%)	359 (94%)	21 (6%)	0	100	100
1	E	365/390 (94%)	344 (94%)	19 (5%)	2 (0%)	38	45
1	F	383/390 (98%)	361 (94%)	20 (5%)	2 (0%)	38	45
1	G	365/390 (94%)	338 (93%)	23 (6%)	4 (1%)	21	21
1	H	382/390 (98%)	337 (88%)	41 (11%)	4 (1%)	22	23
1	I	364/390 (93%)	340 (93%)	21 (6%)	3 (1%)	27	30
1	J	383/390 (98%)	352 (92%)	27 (7%)	4 (1%)	22	23
1	K	365/390 (94%)	347 (95%)	17 (5%)	1 (0%)	50	60
1	L	382/390 (98%)	362 (95%)	20 (5%)	0	100	100
1	M	365/390 (94%)	336 (92%)	24 (7%)	5 (1%)	16	15
1	N	380/390 (97%)	351 (92%)	26 (7%)	3 (1%)	27	30
1	O	364/390 (93%)	342 (94%)	18 (5%)	4 (1%)	21	21
1	P	379/390 (97%)	355 (94%)	21 (6%)	3 (1%)	27	30
1	Q	364/390 (93%)	342 (94%)	21 (6%)	1 (0%)	50	60
1	R	377/390 (97%)	351 (93%)	22 (6%)	4 (1%)	21	21
All	All	6712/7020 (96%)	6250 (93%)	417 (6%)	45 (1%)	30	34

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	168	VAL
1	M	54	TRP
1	M	336	GLU
1	B	13	ARG
1	F	202	HIS
1	G	200	GLU
1	H	167	LYS
1	P	17	SER
1	G	123	ASP
1	G	301	VAL
1	J	242	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	M	242	GLU
1	O	208	PRO
1	P	242	GLU
1	B	202	HIS
1	K	208	PRO
1	O	35	SER
1	R	134	ASP
1	B	301	VAL
1	C	242	GLU
1	G	242	GLU
1	H	208	PRO
1	M	77	ASN
1	N	202	HIS
1	N	242	GLU
1	O	242	GLU
1	R	242	GLU
1	R	356	SER
1	E	301	VAL
1	E	342	ASP
1	F	224	ASP
1	I	231	ASN
1	J	41	MET
1	J	208	PRO
1	B	208	PRO
1	H	381	GLY
1	I	299	GLY
1	N	301	VAL
1	R	281	GLY
1	I	208	PRO
1	J	301	VAL
1	P	301	VAL
1	Q	118	PRO
1	M	301	VAL
1	O	301	VAL

### 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	315/335 (94%)	294 (93%)	21 (7%)	23	29
1	B	333/335 (99%)	311 (93%)	22 (7%)	24	29
1	C	316/335 (94%)	297 (94%)	19 (6%)	27	35
1	D	329/335 (98%)	311 (94%)	18 (6%)	30	39
1	E	316/335 (94%)	300 (95%)	16 (5%)	33	43
1	F	332/335 (99%)	314 (95%)	18 (5%)	31	40
1	G	316/335 (94%)	301 (95%)	15 (5%)	36	47
1	H	331/335 (99%)	312 (94%)	19 (6%)	29	37
1	I	315/335 (94%)	296 (94%)	19 (6%)	27	35
1	J	332/335 (99%)	313 (94%)	19 (6%)	29	37
1	K	316/335 (94%)	301 (95%)	15 (5%)	36	47
1	L	331/335 (99%)	315 (95%)	16 (5%)	35	46
1	M	316/335 (94%)	296 (94%)	20 (6%)	25	32
1	N	329/335 (98%)	313 (95%)	16 (5%)	35	45
1	O	315/335 (94%)	300 (95%)	15 (5%)	35	46
1	P	328/335 (98%)	314 (96%)	14 (4%)	40	52
1	Q	315/335 (94%)	295 (94%)	20 (6%)	25	32
1	R	326/335 (97%)	303 (93%)	23 (7%)	21	26
All	All	5811/6030 (96%)	5486 (94%)	325 (6%)	30	38

All (325) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ASN
1	A	43	SER
1	A	54	TRP
1	A	66	LYS
1	A	96	CYS
1	A	143	ARG
1	A	149	LYS
1	A	191	ASN
1	A	200	GLU
1	A	221	ASP
1	A	223	PRO
1	A	233	GLU
1	A	237	LEU
1	A	257	LEU

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	A	285	ASN
1	A	302	VAL
1	A	308	LEU
1	A	342	ASP
1	A	353	LEU
1	A	364	LEU
1	A	386	ASP
1	B	6	GLN
1	B	22	SER
1	B	43	SER
1	B	54	TRP
1	B	66	LYS
1	B	110	HIS
1	B	143	ARG
1	B	191	ASN
1	B	226	ARG
1	B	232	ASN
1	B	237	LEU
1	B	257	LEU
1	B	273	ARG
1	B	280	HIS
1	B	287	ARG
1	B	306	VAL
1	B	308	LEU
1	B	346	ASP
1	B	353	LEU
1	B	364	LEU
1	B	386	ASP
1	B	387	MET
1	C	38	ASN
1	C	54	TRP
1	C	66	LYS
1	C	84	THR
1	C	96	CYS
1	C	143	ARG
1	C	151	VAL
1	C	191	ASN
1	C	200	GLU
1	C	237	LEU
1	C	257	LEU
1	C	285	ASN
1	C	308	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	313	LEU
1	C	333	THR
1	C	341	THR
1	C	353	LEU
1	C	382	GLN
1	C	387	MET
1	D	22	SER
1	D	26	LYS
1	D	35	SER
1	D	66	LYS
1	D	143	ARG
1	D	144	CYS
1	D	187	LEU
1	D	191	ASN
1	D	192	GLU
1	D	226	ARG
1	D	237	LEU
1	D	257	LEU
1	D	285	ASN
1	D	308	LEU
1	D	313	LEU
1	D	353	LEU
1	D	364	LEU
1	D	382	GLN
1	E	51	GLU
1	E	54	TRP
1	E	66	LYS
1	E	91	GLU
1	E	103	LYS
1	E	143	ARG
1	E	168	VAL
1	E	257	LEU
1	E	285	ASN
1	E	308	LEU
1	E	309	ARG
1	E	313	LEU
1	E	333	THR
1	E	353	LEU
1	E	364	LEU
1	E	387	MET
1	F	6	GLN
1	F	22	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	F	54	TRP
1	F	66	LYS
1	F	96	CYS
1	F	151	VAL
1	F	213	LEU
1	F	230	HIS
1	F	237	LEU
1	F	253	LYS
1	F	257	LEU
1	F	308	LEU
1	F	333	THR
1	F	353	LEU
1	F	364	LEU
1	F	382	GLN
1	F	383	SER
1	F	386	ASP
1	G	58	THR
1	G	110	HIS
1	G	143	ARG
1	G	151	VAL
1	G	223	PRO
1	G	257	LEU
1	G	285	ASN
1	G	308	LEU
1	G	313	LEU
1	G	333	THR
1	G	342	ASP
1	G	353	LEU
1	G	364	LEU
1	G	382	GLN
1	G	383	SER
1	H	22	SER
1	H	26	LYS
1	H	54	TRP
1	H	58	THR
1	H	66	LYS
1	H	70	THR
1	H	103	LYS
1	H	143	ARG
1	H	191	ASN
1	H	220	ARG
1	H	230	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	H	237	LEU
1	H	257	LEU
1	H	308	LEU
1	H	333	THR
1	H	353	LEU
1	H	364	LEU
1	H	382	GLN
1	H	386	ASP
1	I	38	ASN
1	I	91	GLU
1	I	96	CYS
1	I	110	HIS
1	I	143	ARG
1	I	191	ASN
1	I	200	GLU
1	I	213	LEU
1	I	221	ASP
1	I	237	LEU
1	I	242	GLU
1	I	257	LEU
1	I	285	ASN
1	I	308	LEU
1	I	314	GLU
1	I	336	GLU
1	I	353	LEU
1	I	364	LEU
1	I	382	GLN
1	J	22	SER
1	J	54	TRP
1	J	58	THR
1	J	103	LYS
1	J	143	ARG
1	J	152	CYS
1	J	221	ASP
1	J	237	LEU
1	J	257	LEU
1	J	266	ARG
1	J	285	ASN
1	J	308	LEU
1	J	313	LEU
1	J	322	MET
1	J	346	ASP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	J	353	LEU
1	J	360	LEU
1	J	364	LEU
1	J	382	GLN
1	K	38	ASN
1	K	43	SER
1	K	110	HIS
1	K	143	ARG
1	K	200	GLU
1	K	257	LEU
1	K	285	ASN
1	K	286	ASP
1	K	308	LEU
1	K	309	ARG
1	K	313	LEU
1	K	342	ASP
1	K	353	LEU
1	K	364	LEU
1	K	382	GLN
1	L	7	ASP
1	L	22	SER
1	L	26	LYS
1	L	54	TRP
1	L	66	LYS
1	L	110	HIS
1	L	143	ARG
1	L	144	CYS
1	L	237	LEU
1	L	257	LEU
1	L	285	ASN
1	L	298	MET
1	L	308	LEU
1	L	313	LEU
1	L	353	LEU
1	L	364	LEU
1	M	38	ASN
1	M	54	TRP
1	M	66	LYS
1	M	103	LYS
1	M	110	HIS
1	M	143	ARG
1	M	151	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	M	191	ASN
1	M	200	GLU
1	M	237	LEU
1	M	257	LEU
1	M	273	ARG
1	M	288	LEU
1	M	308	LEU
1	M	342	ASP
1	M	353	LEU
1	M	364	LEU
1	M	382	GLN
1	M	383	SER
1	M	387	MET
1	N	22	SER
1	N	26	LYS
1	N	66	LYS
1	N	96	CYS
1	N	143	ARG
1	N	187	LEU
1	N	237	LEU
1	N	257	LEU
1	N	303	ARG
1	N	308	LEU
1	N	313	LEU
1	N	336	GLU
1	N	353	LEU
1	N	364	LEU
1	N	382	GLN
1	N	386	ASP
1	O	38	ASN
1	O	54	TRP
1	O	96	CYS
1	O	107	GLU
1	O	110	HIS
1	O	143	ARG
1	O	200	GLU
1	O	252	GLN
1	O	257	LEU
1	O	308	LEU
1	O	309	ARG
1	O	333	THR
1	O	353	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	O	364	LEU
1	O	387	MET
1	P	22	SER
1	P	43	SER
1	P	110	HIS
1	P	143	ARG
1	P	152	CYS
1	P	223	PRO
1	P	257	LEU
1	P	280	HIS
1	P	301	VAL
1	P	308	LEU
1	P	353	LEU
1	P	364	LEU
1	P	382	GLN
1	P	383	SER
1	Q	38	ASN
1	Q	54	TRP
1	Q	91	GLU
1	Q	96	CYS
1	Q	134	ASP
1	Q	143	ARG
1	Q	149	LYS
1	Q	167	LYS
1	Q	200	GLU
1	Q	223	PRO
1	Q	237	LEU
1	Q	257	LEU
1	Q	266	ARG
1	Q	286	ASP
1	Q	308	LEU
1	Q	337	SER
1	Q	353	LEU
1	Q	364	LEU
1	Q	382	GLN
1	Q	387	MET
1	R	22	SER
1	R	26	LYS
1	R	43	SER
1	R	66	LYS
1	R	90	ASP
1	R	143	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	R	152	CYS
1	R	191	ASN
1	R	206	GLU
1	R	240	ILE
1	R	250	SER
1	R	253	LYS
1	R	257	LEU
1	R	287	ARG
1	R	298	MET
1	R	308	LEU
1	R	313	LEU
1	R	314	GLU
1	R	333	THR
1	R	353	LEU
1	R	364	LEU
1	R	382	GLN
1	R	383	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (89) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	110	HIS
1	A	124	HIS
1	A	191	ASN
1	A	285	ASN
1	A	382	GLN
1	B	195	GLN
1	B	197	GLN
1	B	280	HIS
1	B	285	ASN
1	C	38	ASN
1	C	110	HIS
1	C	191	ASN
1	C	195	GLN
1	C	280	HIS
1	C	284	HIS
1	C	285	ASN
1	C	382	GLN
1	D	191	ASN
1	D	195	GLN
1	D	285	ASN
1	E	284	HIS

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	E	285	ASN
1	F	6	GLN
1	F	60	ASN
1	F	195	GLN
1	F	285	ASN
1	F	307	HIS
1	G	60	ASN
1	G	195	GLN
1	G	284	HIS
1	G	285	ASN
1	G	382	GLN
1	H	16	HIS
1	H	69	GLN
1	H	77	ASN
1	H	124	HIS
1	H	195	GLN
1	H	280	HIS
1	H	284	HIS
1	H	285	ASN
1	H	316	HIS
1	I	195	GLN
1	I	285	ASN
1	I	307	HIS
1	I	382	GLN
1	J	124	HIS
1	J	195	GLN
1	J	284	HIS
1	J	285	ASN
1	K	38	ASN
1	K	74	ASN
1	K	110	HIS
1	K	191	ASN
1	K	285	ASN
1	K	382	GLN
1	L	69	GLN
1	L	195	GLN
1	L	284	HIS
1	L	285	ASN
1	L	369	ASN
1	M	195	GLN
1	M	285	ASN
1	M	382	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	N	195	GLN
1	N	285	ASN
1	N	382	GLN
1	O	38	ASN
1	O	60	ASN
1	O	124	HIS
1	O	197	GLN
1	O	280	HIS
1	O	284	HIS
1	O	285	ASN
1	O	369	ASN
1	O	382	GLN
1	P	124	HIS
1	P	195	GLN
1	P	280	HIS
1	P	285	ASN
1	P	382	GLN
1	Q	38	ASN
1	Q	195	GLN
1	Q	280	HIS
1	Q	284	HIS
1	Q	285	ASN
1	Q	382	GLN
1	R	195	GLN
1	R	280	HIS
1	R	285	ASN

### 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 ⓘ

Of 72 ligands modelled in this entry, 18 are monoatomic - leaving 54 for Mogul analysis.

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$
2	NMG	A	501	-	7,7,7	0.68	0	8,8,8	1.74	1 (12%)
3	ADP	A	601	4	29,29,29	1.11	2 (6%)	45,45,45	1.69	6 (13%)
5	NO3	A	801	4	3,3,3	3.23	3 (100%)	3,3,3	0.13	0
2	NMG	B	502	-	7,7,7	0.77	0	8,8,8	2.14	2 (25%)
3	ADP	B	602	4	29,29,29	1.12	2 (6%)	45,45,45	1.92	9 (20%)
5	NO3	B	802	4	3,3,3	3.11	3 (100%)	3,3,3	0.18	0
2	NMG	C	503	-	7,7,7	0.72	0	8,8,8	1.63	1 (12%)
3	ADP	C	603	4	29,29,29	1.19	2 (6%)	45,45,45	1.70	6 (13%)
5	NO3	C	803	4	3,3,3	3.29	3 (100%)	3,3,3	0.25	0
2	NMG	D	504	-	7,7,7	0.66	0	8,8,8	1.57	2 (25%)
3	ADP	D	604	4	29,29,29	1.20	2 (6%)	45,45,45	1.68	6 (13%)
5	NO3	D	804	4	3,3,3	3.22	3 (100%)	3,3,3	0.15	0
2	NMG	E	505	-	7,7,7	0.72	0	8,8,8	1.98	2 (25%)
3	ADP	E	605	4	29,29,29	1.16	3 (10%)	45,45,45	1.68	5 (11%)
5	NO3	E	805	4	3,3,3	3.32	3 (100%)	3,3,3	0.06	0
2	NMG	F	506	-	7,7,7	0.96	0	8,8,8	1.79	1 (12%)
3	ADP	F	606	4	29,29,29	1.16	2 (6%)	45,45,45	1.77	7 (15%)
5	NO3	F	806	4	3,3,3	3.20	3 (100%)	3,3,3	0.21	0
2	NMG	G	507	-	7,7,7	0.65	0	8,8,8	1.42	1 (12%)
3	ADP	G	607	4	29,29,29	1.16	2 (6%)	45,45,45	1.93	9 (20%)
5	NO3	G	807	4	3,3,3	3.36	3 (100%)	3,3,3	0.22	0
2	NMG	H	508	-	7,7,7	0.68	0	8,8,8	1.59	1 (12%)
3	ADP	H	608	4	29,29,29	1.11	2 (6%)	45,45,45	1.64	7 (15%)
5	NO3	H	808	4	3,3,3	3.20	3 (100%)	3,3,3	0.11	0
2	NMG	I	509	-	7,7,7	0.72	0	8,8,8	1.74	1 (12%)
3	ADP	I	609	4	29,29,29	1.26	2 (6%)	45,45,45	1.76	8 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NO3	I	809	4	3,3,3	3.34	3 (100%)	3,3,3	0.05	0
2	NMG	J	510	-	7,7,7	0.67	0	8,8,8	1.64	2 (25%)
3	ADP	J	610	4	29,29,29	1.20	2 (6%)	45,45,45	1.88	8 (17%)
5	NO3	J	810	4	3,3,3	3.27	3 (100%)	3,3,3	0.14	0
2	NMG	K	511	-	7,7,7	0.67	0	8,8,8	1.22	1 (12%)
3	ADP	K	611	4	29,29,29	1.12	2 (6%)	45,45,45	1.95	9 (20%)
5	NO3	K	811	4	3,3,3	3.26	3 (100%)	3,3,3	0.17	0
2	NMG	L	512	-	7,7,7	0.71	0	8,8,8	1.70	1 (12%)
3	ADP	L	612	4	29,29,29	1.17	2 (6%)	45,45,45	1.63	7 (15%)
5	NO3	L	812	4	3,3,3	3.24	3 (100%)	3,3,3	0.24	0
2	NMG	M	513	-	7,7,7	0.82	0	8,8,8	1.56	1 (12%)
3	ADP	M	613	4	29,29,29	1.21	2 (6%)	45,45,45	1.89	10 (22%)
5	NO3	M	813	4	3,3,3	3.25	3 (100%)	3,3,3	0.16	0
2	NMG	N	514	-	7,7,7	0.68	0	8,8,8	1.71	1 (12%)
3	ADP	N	614	4	29,29,29	1.18	2 (6%)	45,45,45	1.87	8 (17%)
5	NO3	N	814	4	3,3,3	3.32	3 (100%)	3,3,3	0.27	0
2	NMG	O	515	-	7,7,7	0.71	0	8,8,8	1.45	1 (12%)
3	ADP	O	615	4	29,29,29	1.09	2 (6%)	45,45,45	1.71	6 (13%)
5	NO3	O	815	4	3,3,3	3.16	3 (100%)	3,3,3	0.16	0
2	NMG	P	516	-	7,7,7	0.67	0	8,8,8	1.59	1 (12%)
3	ADP	P	616	4	29,29,29	1.06	2 (6%)	45,45,45	1.91	8 (17%)
5	NO3	P	816	4	3,3,3	3.16	3 (100%)	3,3,3	0.13	0
2	NMG	Q	517	-	7,7,7	0.72	0	8,8,8	2.29	1 (12%)
3	ADP	Q	617	4	29,29,29	1.13	2 (6%)	45,45,45	1.89	9 (20%)
5	NO3	Q	817	4	3,3,3	3.28	3 (100%)	3,3,3	0.25	0
2	NMG	R	518	-	7,7,7	0.68	0	8,8,8	2.13	1 (12%)
3	ADP	R	618	4	29,29,29	1.09	2 (6%)	45,45,45	1.73	8 (17%)
5	NO3	R	818	4	3,3,3	3.33	3 (100%)	3,3,3	0.22	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
2	NMG	A	501	-	-	0/5/5/5	0/0/0/0

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	A	601	4	-	0/16/32/32	0/1/3/3
5	NO3	A	801	4	-	0/0/0/0	0/0/0/0
2	NMG	B	502	-	-	0/5/5/5	0/0/0/0
3	ADP	B	602	4	-	0/16/32/32	0/1/3/3
5	NO3	B	802	4	-	0/0/0/0	0/0/0/0
2	NMG	C	503	-	-	0/5/5/5	0/0/0/0
3	ADP	C	603	4	-	0/16/32/32	0/1/3/3
5	NO3	C	803	4	-	0/0/0/0	0/0/0/0
2	NMG	D	504	-	-	0/5/5/5	0/0/0/0
3	ADP	D	604	4	-	0/16/32/32	0/1/3/3
5	NO3	D	804	4	-	0/0/0/0	0/0/0/0
2	NMG	E	505	-	-	0/5/5/5	0/0/0/0
3	ADP	E	605	4	-	0/16/32/32	0/1/3/3
5	NO3	E	805	4	-	0/0/0/0	0/0/0/0
2	NMG	F	506	-	-	0/5/5/5	0/0/0/0
3	ADP	F	606	4	-	0/16/32/32	0/1/3/3
5	NO3	F	806	4	-	0/0/0/0	0/0/0/0
2	NMG	G	507	-	-	0/5/5/5	0/0/0/0
3	ADP	G	607	4	-	0/16/32/32	0/1/3/3
5	NO3	G	807	4	-	0/0/0/0	0/0/0/0
2	NMG	H	508	-	-	0/5/5/5	0/0/0/0
3	ADP	H	608	4	-	0/16/32/32	0/1/3/3
5	NO3	H	808	4	-	0/0/0/0	0/0/0/0
2	NMG	I	509	-	-	0/5/5/5	0/0/0/0
3	ADP	I	609	4	-	0/16/32/32	0/1/3/3
5	NO3	I	809	4	-	0/0/0/0	0/0/0/0
2	NMG	J	510	-	-	0/5/5/5	0/0/0/0
3	ADP	J	610	4	-	0/16/32/32	0/1/3/3
5	NO3	J	810	4	-	0/0/0/0	0/0/0/0
2	NMG	K	511	-	-	0/5/5/5	0/0/0/0
3	ADP	K	611	4	-	0/16/32/32	0/1/3/3
5	NO3	K	811	4	-	0/0/0/0	0/0/0/0
2	NMG	L	512	-	-	0/5/5/5	0/0/0/0
3	ADP	L	612	4	-	0/16/32/32	0/1/3/3
5	NO3	L	812	4	-	0/0/0/0	0/0/0/0
2	NMG	M	513	-	-	0/5/5/5	0/0/0/0
3	ADP	M	613	4	-	0/16/32/32	0/1/3/3
5	NO3	M	813	4	-	0/0/0/0	0/0/0/0
2	NMG	N	514	-	-	0/5/5/5	0/0/0/0
3	ADP	N	614	4	-	0/16/32/32	0/1/3/3
5	NO3	N	814	4	-	0/0/0/0	0/0/0/0
2	NMG	O	515	-	-	0/5/5/5	0/0/0/0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	O	615	4	-	0/16/32/32	0/1/3/3
5	NO3	O	815	4	-	0/0/0/0	0/0/0/0
2	NMG	P	516	-	-	0/5/5/5	0/0/0/0
3	ADP	P	616	4	-	0/16/32/32	0/1/3/3
5	NO3	P	816	4	-	0/0/0/0	0/0/0/0
2	NMG	Q	517	-	-	0/5/5/5	0/0/0/0
3	ADP	Q	617	4	-	0/16/32/32	0/1/3/3
5	NO3	Q	817	4	-	0/0/0/0	0/0/0/0
2	NMG	R	518	-	-	0/5/5/5	0/0/0/0
3	ADP	R	618	4	-	0/16/32/32	0/1/3/3
5	NO3	R	818	4	-	0/0/0/0	0/0/0/0

All (91) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	809	NO3	O1-N	4.08	1.41	1.24
5	E	805	NO3	O1-N	4.04	1.41	1.24
5	G	807	NO3	O1-N	4.02	1.41	1.24
5	R	818	NO3	O1-N	4.02	1.41	1.24
5	L	812	NO3	O1-N	3.90	1.40	1.24
5	K	811	NO3	O1-N	3.87	1.40	1.24
5	Q	817	NO3	O1-N	3.84	1.40	1.24
5	C	803	NO3	O1-N	3.83	1.40	1.24
5	A	801	NO3	O1-N	3.83	1.40	1.24
5	J	810	NO3	O1-N	3.82	1.40	1.24
5	H	808	NO3	O1-N	3.80	1.40	1.24
5	D	804	NO3	O1-N	3.80	1.40	1.24
5	N	814	NO3	O1-N	3.79	1.40	1.24
5	F	806	NO3	O1-N	3.79	1.40	1.24
5	O	815	NO3	O1-N	3.78	1.40	1.24
5	P	816	NO3	O1-N	3.78	1.40	1.24
3	I	609	ADP	C4-N9	-3.77	1.32	1.37
5	M	813	NO3	O1-N	3.75	1.40	1.24
3	G	607	ADP	C4-N9	-3.70	1.32	1.37
5	B	802	NO3	O1-N	3.65	1.39	1.24
3	M	613	ADP	C4-N9	-3.44	1.32	1.37
3	J	610	ADP	C4-N9	-3.36	1.32	1.37
3	M	613	ADP	C5-C4	3.35	1.48	1.40
3	L	612	ADP	C5-C4	3.29	1.47	1.40
3	Q	617	ADP	C4-N9	-3.28	1.33	1.37
3	R	618	ADP	C5-C4	3.27	1.47	1.40
3	D	604	ADP	C5-C4	3.26	1.47	1.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	ADP	C4-N9	-3.24	1.33	1.37
3	H	608	ADP	C5-C4	3.20	1.47	1.40
3	N	614	ADP	C5-C4	3.19	1.47	1.40
3	E	605	ADP	C5-C4	3.18	1.47	1.40
3	F	606	ADP	C5-C4	3.18	1.47	1.40
3	A	601	ADP	C5-C4	3.18	1.47	1.40
3	D	604	ADP	C4-N9	-3.18	1.33	1.37
3	O	615	ADP	C5-C4	3.15	1.47	1.40
3	C	603	ADP	C4-N9	-3.14	1.33	1.37
3	R	618	ADP	C4-N9	-3.14	1.33	1.37
3	P	616	ADP	C5-C4	3.14	1.47	1.40
5	N	814	NO3	O2-N	3.11	1.41	1.25
3	C	603	ADP	C5-C4	3.08	1.47	1.40
3	I	609	ADP	C5-C4	3.08	1.47	1.40
5	G	807	NO3	O3-N	3.06	1.41	1.25
5	R	818	NO3	O2-N	3.03	1.41	1.25
5	M	813	NO3	O3-N	3.02	1.41	1.25
5	J	810	NO3	O3-N	3.02	1.41	1.25
5	Q	817	NO3	O2-N	3.01	1.41	1.25
5	C	803	NO3	O3-N	3.01	1.41	1.25
5	N	814	NO3	O3-N	3.00	1.41	1.25
5	K	811	NO3	O3-N	3.00	1.41	1.25
3	O	615	ADP	C4-N9	-2.99	1.33	1.37
3	L	612	ADP	C4-N9	-2.98	1.33	1.37
5	C	803	NO3	O2-N	2.98	1.41	1.25
3	Q	617	ADP	C5-C4	2.98	1.47	1.40
5	L	812	NO3	O2-N	2.97	1.41	1.25
3	B	602	ADP	C5-C4	2.95	1.47	1.40
3	N	614	ADP	C4-N9	-2.95	1.33	1.37
5	D	804	NO3	O3-N	2.94	1.40	1.25
5	A	801	NO3	O2-N	2.94	1.40	1.25
5	F	806	NO3	O2-N	2.92	1.40	1.25
5	Q	817	NO3	O3-N	2.91	1.40	1.25
5	I	809	NO3	O2-N	2.91	1.40	1.25
3	K	611	ADP	C4-N9	-2.90	1.33	1.37
5	M	813	NO3	O2-N	2.90	1.40	1.25
5	E	805	NO3	O2-N	2.90	1.40	1.25
5	I	809	NO3	O3-N	2.89	1.40	1.25
5	B	802	NO3	O3-N	2.89	1.40	1.25
3	J	610	ADP	C5-C4	2.88	1.47	1.40
5	E	805	NO3	O3-N	2.88	1.40	1.25
5	J	810	NO3	O2-N	2.88	1.40	1.25

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	808	NO3	O3-N	2.88	1.40	1.25
5	G	807	NO3	O2-N	2.88	1.40	1.25
3	K	611	ADP	C5-C4	2.85	1.46	1.40
5	P	816	NO3	O2-N	2.85	1.40	1.25
5	O	815	NO3	O2-N	2.84	1.40	1.25
5	D	804	NO3	O2-N	2.84	1.40	1.25
5	H	808	NO3	O2-N	2.83	1.40	1.25
5	K	811	NO3	O2-N	2.82	1.40	1.25
5	A	801	NO3	O3-N	2.82	1.40	1.25
5	R	818	NO3	O3-N	2.81	1.40	1.25
5	F	806	NO3	O3-N	2.79	1.40	1.25
5	O	815	NO3	O3-N	2.77	1.40	1.25
5	P	816	NO3	O3-N	2.75	1.39	1.25
5	L	812	NO3	O3-N	2.74	1.39	1.25
5	B	802	NO3	O2-N	2.72	1.39	1.25
3	H	608	ADP	C4-N9	-2.66	1.33	1.37
3	F	606	ADP	C4-N9	-2.66	1.33	1.37
3	G	607	ADP	C5-C4	2.65	1.46	1.40
3	P	616	ADP	C4-N9	-2.63	1.33	1.37
3	A	601	ADP	C4-N9	-2.56	1.34	1.37
3	E	605	ADP	C4-N9	-2.50	1.34	1.37
3	E	605	ADP	O4'-C1'	2.09	1.44	1.41

All (158) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	616	ADP	N3-C2-N1	-7.99	122.03	128.71
3	K	611	ADP	N3-C2-N1	-7.81	122.18	128.71
3	J	610	ADP	N3-C2-N1	-6.99	122.86	128.71
3	B	602	ADP	N3-C2-N1	-6.96	122.89	128.71
3	M	613	ADP	N3-C2-N1	-6.80	123.02	128.71
3	F	606	ADP	N3-C2-N1	-6.64	123.15	128.71
3	G	607	ADP	N3-C2-N1	-6.49	123.28	128.71
3	Q	617	ADP	N3-C2-N1	-6.48	123.29	128.71
3	D	604	ADP	N3-C2-N1	-6.44	123.33	128.71
3	O	615	ADP	N3-C2-N1	-6.36	123.39	128.71
3	C	603	ADP	N3-C2-N1	-6.22	123.51	128.71
3	E	605	ADP	N3-C2-N1	-6.20	123.52	128.71
3	N	614	ADP	N3-C2-N1	-6.19	123.53	128.71
3	R	618	ADP	N3-C2-N1	-6.19	123.53	128.71
3	I	609	ADP	N3-C2-N1	-6.18	123.54	128.71
3	L	612	ADP	N3-C2-N1	-6.02	123.68	128.71

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Q	517	NMG	CD-NE-CZ	6.01	130.02	121.34
3	A	601	ADP	N3-C2-N1	-6.00	123.69	128.71
2	R	518	NMG	CD-NE-CZ	5.59	129.42	121.34
3	H	608	ADP	N3-C2-N1	-5.34	124.24	128.71
3	K	611	ADP	N3-C4-N9	5.27	134.95	125.43
2	B	502	NMG	CD-NE-CZ	5.27	128.96	121.34
3	H	608	ADP	N3-C4-N9	5.26	134.93	125.43
3	G	607	ADP	O4'-C1'-N9	5.25	113.33	108.44
3	Q	617	ADP	O4'-C1'-N9	5.22	113.30	108.44
3	F	606	ADP	N3-C4-N9	5.15	134.72	125.43
3	O	615	ADP	N3-C4-N9	5.14	134.71	125.43
3	E	605	ADP	N3-C4-N9	5.11	134.66	125.43
3	A	601	ADP	N3-C4-N9	5.10	134.64	125.43
3	J	610	ADP	N3-C4-N9	5.01	134.47	125.43
2	E	505	NMG	CD-NE-CZ	4.98	128.53	121.34
3	D	604	ADP	N3-C4-N9	4.95	134.37	125.43
3	C	603	ADP	N3-C4-N9	4.87	134.23	125.43
3	M	613	ADP	N3-C4-N9	4.82	134.14	125.43
3	N	614	ADP	N3-C4-N9	4.77	134.04	125.43
3	P	616	ADP	N3-C4-N9	4.73	133.97	125.43
3	B	602	ADP	N3-C4-N9	4.70	133.91	125.43
3	L	612	ADP	N3-C4-N9	4.64	133.80	125.43
3	R	618	ADP	N3-C4-N9	4.63	133.79	125.43
3	Q	617	ADP	N3-C4-N9	4.51	133.58	125.43
2	A	501	NMG	CD-NE-CZ	4.48	127.81	121.34
3	G	607	ADP	N3-C4-N9	4.45	133.46	125.43
2	F	506	NMG	CD-NE-CZ	4.44	127.76	121.34
2	N	514	NMG	CD-NE-CZ	4.37	127.65	121.34
2	I	509	NMG	CD-NE-CZ	4.28	127.52	121.34
3	I	609	ADP	N3-C4-N9	4.24	133.08	125.43
3	N	614	ADP	C4-C5-N7	-4.24	105.89	109.52
3	M	613	ADP	O4'-C1'-N9	4.19	112.34	108.44
3	N	614	ADP	O4'-C1'-N9	4.16	112.31	108.44
3	J	610	ADP	C8-N9-C4	4.06	110.00	106.90
2	C	503	NMG	CD-NE-CZ	4.03	127.17	121.34
2	L	512	NMG	CD-NE-CZ	4.02	127.15	121.34
3	K	611	ADP	O4'-C1'-N9	4.01	112.17	108.44
2	H	508	NMG	CD-NE-CZ	3.93	127.01	121.34
3	B	602	ADP	C8-N9-C4	3.93	109.90	106.90
3	B	602	ADP	O4'-C1'-N9	3.82	111.99	108.44
2	M	513	NMG	CD-NE-CZ	3.80	126.83	121.34
2	J	510	NMG	CD-NE-CZ	3.78	126.81	121.34

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	516	NMG	CD-NE-CZ	3.77	126.78	121.34
3	Q	617	ADP	C4-C5-N7	-3.73	106.33	109.52
3	H	608	ADP	C4-C5-N7	-3.67	106.38	109.52
3	M	613	ADP	C8-N9-C4	3.56	109.62	106.90
2	D	504	NMG	CD-NE-CZ	3.49	126.38	121.34
3	R	618	ADP	C4-C5-N7	-3.46	106.56	109.52
3	G	607	ADP	C4-C5-N7	-3.46	106.56	109.52
2	O	515	NMG	CD-NE-CZ	3.44	126.30	121.34
3	G	607	ADP	C8-N9-C4	3.42	109.51	106.90
3	I	609	ADP	C4-C5-N7	-3.40	106.61	109.52
3	P	616	ADP	C4-C5-N7	-3.40	106.61	109.52
3	D	604	ADP	C4-C5-N7	-3.38	106.63	109.52
3	F	606	ADP	C4-C5-N7	-3.36	106.65	109.52
3	K	611	ADP	C8-N9-C4	3.31	109.43	106.90
3	A	601	ADP	C4-C5-N7	-3.30	106.70	109.52
3	F	606	ADP	C5-C4-N3	-3.17	118.81	125.70
3	E	605	ADP	C5-C4-N3	-3.15	118.84	125.70
3	B	602	ADP	C4-C5-N7	-3.15	106.83	109.52
3	I	609	ADP	O4'-C1'-N9	3.14	111.36	108.44
3	H	608	ADP	C5-C4-N3	-3.11	118.93	125.70
3	F	606	ADP	O4'-C1'-N9	3.11	111.33	108.44
3	C	603	ADP	C4-C5-N7	-3.05	106.91	109.52
2	G	507	NMG	CD-NE-CZ	3.04	125.73	121.34
3	N	614	ADP	C5-C4-N3	-3.00	119.16	125.70
3	N	614	ADP	PA-O3A-PB	-3.00	122.89	131.68
3	E	605	ADP	C4-C5-N7	-2.98	106.97	109.52
3	D	604	ADP	C5-C4-N3	-2.96	119.26	125.70
3	A	601	ADP	C5-C4-N3	-2.95	119.27	125.70
3	O	615	ADP	C5-C4-N3	-2.93	119.32	125.70
3	C	603	ADP	C5-C4-N3	-2.90	119.38	125.70
3	M	613	ADP	O3A-PA-O5'	2.87	116.25	103.41
3	O	615	ADP	C8-N9-C4	2.85	109.08	106.90
3	K	611	ADP	C5-C4-N3	-2.84	119.51	125.70
3	P	616	ADP	C5-C4-N3	-2.83	119.53	125.70
3	O	615	ADP	C4-C5-N7	-2.80	107.13	109.52
3	R	618	ADP	C5-C4-N3	-2.78	119.65	125.70
3	I	609	ADP	C1'-N9-C4	-2.77	121.84	126.64
3	I	609	ADP	C8-N9-C4	2.75	109.00	106.90
3	L	612	ADP	C4-C5-N7	-2.74	107.17	109.52
3	Q	617	ADP	C8-N9-C4	2.71	108.97	106.90
3	P	616	ADP	C2-N3-C4	2.69	121.66	114.01
3	H	608	ADP	C8-N9-C4	2.65	108.92	106.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	612	ADP	C5-C4-N3	-2.64	119.94	125.70
2	K	511	NMG	CD-NE-CZ	2.64	125.16	121.34
3	J	610	ADP	C4-C5-N7	-2.63	107.27	109.52
3	G	607	ADP	C1'-N9-C4	-2.59	122.15	126.64
3	Q	617	ADP	C5-C4-N3	-2.59	120.06	125.70
3	K	611	ADP	C2-N3-C4	2.59	121.37	114.01
3	F	606	ADP	C2-N3-C4	2.55	121.27	114.01
3	J	610	ADP	C5-C4-N3	-2.55	120.15	125.70
3	G	607	ADP	C5-C4-N3	-2.52	120.22	125.70
3	R	618	ADP	C8-N9-C4	2.49	108.80	106.90
3	N	614	ADP	C8-N9-C4	2.47	108.78	106.90
3	B	602	ADP	C5-C4-N3	-2.47	120.32	125.70
3	B	602	ADP	C1'-N9-C4	-2.47	122.38	126.64
3	K	611	ADP	C4-C5-N7	-2.45	107.43	109.52
3	M	613	ADP	C1'-N9-C4	-2.43	122.43	126.64
3	I	609	ADP	C5-C4-N3	-2.43	120.40	125.70
3	M	613	ADP	C5-C4-N3	-2.43	120.41	125.70
3	A	601	ADP	C8-N9-C4	2.43	108.75	106.90
3	R	618	ADP	O4'-C1'-N9	2.43	110.70	108.44
3	M	613	ADP	C4-C5-N7	-2.41	107.46	109.52
3	C	603	ADP	C2-N3-C4	2.41	120.87	114.01
3	D	604	ADP	C8-N9-C4	2.40	108.73	106.90
3	E	605	ADP	C2-N3-C4	2.39	120.82	114.01
3	H	608	ADP	PA-O3A-PB	-2.35	124.78	131.68
3	L	612	ADP	C8-N9-C4	2.35	108.70	106.90
3	N	614	ADP	C2-N3-C4	2.33	120.63	114.01
3	O	615	ADP	C2-N3-C4	2.31	120.59	114.01
3	C	603	ADP	C8-N9-C4	2.31	108.66	106.90
3	M	613	ADP	C2-N1-C6	2.30	122.92	118.77
3	P	616	ADP	C8-N9-C4	2.29	108.65	106.90
3	B	602	ADP	C2-N3-C4	2.27	120.47	114.01
3	P	616	ADP	C2-N1-C6	2.25	122.83	118.77
3	D	604	ADP	C2-N3-C4	2.25	120.42	114.01
3	A	601	ADP	C2-N3-C4	2.24	120.38	114.01
3	G	607	ADP	C2-N3-C4	2.22	120.34	114.01
3	I	609	ADP	C2-N1-C6	2.22	122.77	118.77
2	D	504	NMG	CG-CD-NE	-2.21	107.53	112.83
2	B	502	NMG	CG-CD-NE	-2.21	107.55	112.83
3	P	616	ADP	C3'-C2'-C1'	2.18	104.31	100.91
3	L	612	ADP	C2-N3-C4	2.17	120.19	114.01
3	H	608	ADP	C2-N3-C4	2.17	120.19	114.01
3	Q	617	ADP	C2-N3-C4	2.17	120.18	114.01

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	611	ADP	O3B-PB-O2B	2.17	116.04	107.61
3	J	610	ADP	C2-N3-C4	2.16	120.15	114.01
3	R	618	ADP	C2-N3-C4	2.15	120.12	114.01
3	J	610	ADP	C2-N1-C6	2.13	122.61	118.77
3	B	602	ADP	C2'-C1'-N9	-2.13	107.81	113.27
3	Q	617	ADP	C2-N1-C6	2.11	122.58	118.77
3	G	607	ADP	PA-O3A-PB	-2.11	125.51	131.68
2	J	510	NMG	CG-CD-NE	-2.10	107.79	112.83
2	E	505	NMG	O1-CG-CD	2.10	120.60	112.98
3	F	606	ADP	C8-N9-C4	2.08	108.48	106.90
3	R	618	ADP	C2-N1-C6	2.07	122.51	118.77
3	L	612	ADP	C1'-N9-C4	-2.07	123.07	126.64
3	K	611	ADP	PA-O3A-PB	-2.06	125.64	131.68
3	M	613	ADP	C2-N3-C4	2.04	119.83	114.01
3	J	610	ADP	O4'-C1'-N9	2.03	110.33	108.44
3	Q	617	ADP	PA-O3A-PB	-2.00	125.81	131.68

There are no chirality outliers.

There are no torsion outliers.

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 ⓘ

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

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

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

### 6.3 Carbohydrates ⓘ

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

### 6.4 Ligands ⓘ

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

### 6.5 Other polymers ⓘ

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