



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 02:10 am GMT

PDB ID : 5C97  
Title : Insulin regulated aminopeptidase  
Authors : Mpakali, A.; Saridakis, E.; Harlos, K.; Zhao, Y.; Stratikos, E.  
Deposited on : 2015-06-26  
Resolution : 3.37 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

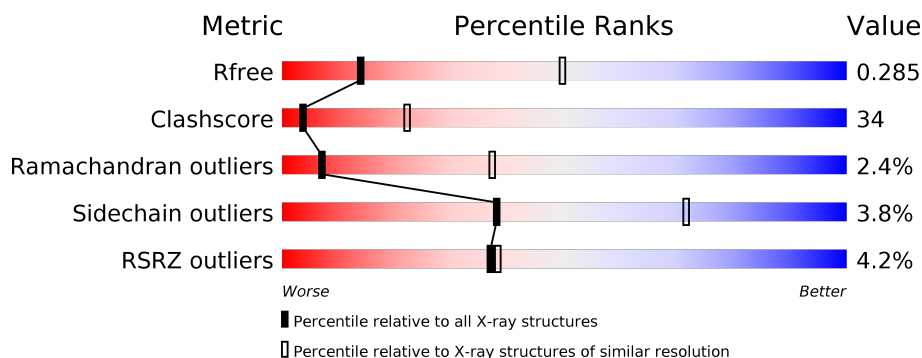
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.37 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	1241 (3.46-3.30)
Clashscore	112137	1319 (3.46-3.30)
Ramachandran outliers	110173	1298 (3.46-3.30)
Sidechain outliers	110143	1297 (3.46-3.30)
RSRZ outliers	101464	1251 (3.46-3.30)

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	912	<div> <div>3%</div> <div>51%</div> <div>39%</div> <div>6%</div> </div>
1	B	912	<div> <div>5%</div> <div>40%</div> <div>46%</div> <div>7%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	A	1106	-	-	-	X
3	NAG	A	1113	-	-	X	-
3	NAG	B	1107	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14098 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Leucyl-cystinyl aminopeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	860	Total	C	N	O	S	0	2	0
			6937	4487	1125	1298	27			
1	B	851	Total	C	N	O	S	0	1	0
			6808	4410	1097	1276	25			

There are 82 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	124	MET	-	initiating methionine	UNP Q9UIQ6
A	125	GLY	-	expression tag	UNP Q9UIQ6
A	126	ILE	-	expression tag	UNP Q9UIQ6
A	127	LEU	-	expression tag	UNP Q9UIQ6
A	128	PRO	-	expression tag	UNP Q9UIQ6
A	129	SER	-	expression tag	UNP Q9UIQ6
A	130	PRO	-	expression tag	UNP Q9UIQ6
A	131	GLY	-	expression tag	UNP Q9UIQ6
A	132	ASN	-	expression tag	UNP Q9UIQ6
A	133	PRO	-	expression tag	UNP Q9UIQ6
A	134	ALA	-	expression tag	UNP Q9UIQ6
A	135	LEU	-	expression tag	UNP Q9UIQ6
A	136	LEU	-	expression tag	UNP Q9UIQ6
A	137	SER	-	expression tag	UNP Q9UIQ6
A	138	LEU	-	expression tag	UNP Q9UIQ6
A	139	VAL	-	expression tag	UNP Q9UIQ6
A	140	SER	-	expression tag	UNP Q9UIQ6
A	141	LEU	-	expression tag	UNP Q9UIQ6
A	142	LEU	-	expression tag	UNP Q9UIQ6
A	143	SER	-	expression tag	UNP Q9UIQ6
A	144	VAL	-	expression tag	UNP Q9UIQ6
A	145	LEU	-	expression tag	UNP Q9UIQ6
A	146	LEU	-	expression tag	UNP Q9UIQ6
A	147	MET	-	expression tag	UNP Q9UIQ6
A	148	GLY	-	expression tag	UNP Q9UIQ6

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
A	149	CYS	-	expression tag	UNP Q9UIQ6
A	150	VAL	-	expression tag	UNP Q9UIQ6
A	151	ALA	-	expression tag	UNP Q9UIQ6
A	152	GLU	-	expression tag	UNP Q9UIQ6
A	153	THR	-	expression tag	UNP Q9UIQ6
A	154	GLY	-	expression tag	UNP Q9UIQ6
A	1026	ARG	-	expression tag	UNP Q9UIQ6
A	1027	THR	-	expression tag	UNP Q9UIQ6
A	1028	GLU	-	expression tag	UNP Q9UIQ6
A	1029	THR	-	expression tag	UNP Q9UIQ6
A	1030	SER	-	expression tag	UNP Q9UIQ6
A	1031	GLN	-	expression tag	UNP Q9UIQ6
A	1032	VAL	-	expression tag	UNP Q9UIQ6
A	1033	ALA	-	expression tag	UNP Q9UIQ6
A	1034	PRO	-	expression tag	UNP Q9UIQ6
A	1035	ALA	-	expression tag	UNP Q9UIQ6
B	124	MET	-	initiating methionine	UNP Q9UIQ6
B	125	GLY	-	expression tag	UNP Q9UIQ6
B	126	ILE	-	expression tag	UNP Q9UIQ6
B	127	LEU	-	expression tag	UNP Q9UIQ6
B	128	PRO	-	expression tag	UNP Q9UIQ6
B	129	SER	-	expression tag	UNP Q9UIQ6
B	130	PRO	-	expression tag	UNP Q9UIQ6
B	131	GLY	-	expression tag	UNP Q9UIQ6
B	132	ASN	-	expression tag	UNP Q9UIQ6
B	133	PRO	-	expression tag	UNP Q9UIQ6
B	134	ALA	-	expression tag	UNP Q9UIQ6
B	135	LEU	-	expression tag	UNP Q9UIQ6
B	136	LEU	-	expression tag	UNP Q9UIQ6
B	137	SER	-	expression tag	UNP Q9UIQ6
B	138	LEU	-	expression tag	UNP Q9UIQ6
B	139	VAL	-	expression tag	UNP Q9UIQ6
B	140	SER	-	expression tag	UNP Q9UIQ6
B	141	LEU	-	expression tag	UNP Q9UIQ6
B	142	LEU	-	expression tag	UNP Q9UIQ6
B	143	SER	-	expression tag	UNP Q9UIQ6
B	144	VAL	-	expression tag	UNP Q9UIQ6
B	145	LEU	-	expression tag	UNP Q9UIQ6
B	146	LEU	-	expression tag	UNP Q9UIQ6
B	147	MET	-	expression tag	UNP Q9UIQ6
B	148	GLY	-	expression tag	UNP Q9UIQ6
B	149	CYS	-	expression tag	UNP Q9UIQ6

*Continued on next page...*

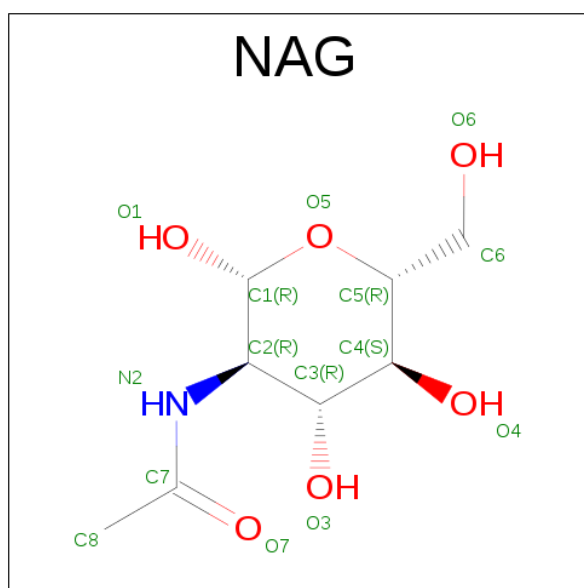
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	150	VAL	-	expression tag	UNP Q9UIQ6
B	151	ALA	-	expression tag	UNP Q9UIQ6
B	152	GLU	-	expression tag	UNP Q9UIQ6
B	153	THR	-	expression tag	UNP Q9UIQ6
B	154	GLY	-	expression tag	UNP Q9UIQ6
B	1026	ARG	-	expression tag	UNP Q9UIQ6
B	1027	THR	-	expression tag	UNP Q9UIQ6
B	1028	GLU	-	expression tag	UNP Q9UIQ6
B	1029	THR	-	expression tag	UNP Q9UIQ6
B	1030	SER	-	expression tag	UNP Q9UIQ6
B	1031	GLN	-	expression tag	UNP Q9UIQ6
B	1032	VAL	-	expression tag	UNP Q9UIQ6
B	1033	ALA	-	expression tag	UNP Q9UIQ6
B	1034	PRO	-	expression tag	UNP Q9UIQ6
B	1035	ALA	-	expression tag	UNP Q9UIQ6

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Zn 1 1	0	0
2	A	1	Total Zn 1 1	0	0

- Molecule 3 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		

Continued on next page...

*Continued from previous page...*

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	O	0	0
			1	1		





Chain B:  5% 40% 46% 7%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	69.00Å 260.15Å 73.36Å 90.00° 111.61° 90.00°	Depositor
Resolution (Å)	68.20 – 3.37 68.20 – 3.37	Depositor EDS
% Data completeness (in resolution range)	99.6 (68.20-3.37) 99.7 (68.20-3.37)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.86 (at 3.33Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, $R_{free}$	0.216 , 0.285 0.217 , 0.285	Depositor DCC
$R_{free}$ test set	1613 reflections (4.78%)	DCC
Wilson B-factor (Å <sup>2</sup> )	131.8	Xtriage
Anisotropy	0.395	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 75.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	14098	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	129.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.76% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.65	3/7115 (0.0%)	0.96	17/9660 (0.2%)
1	B	0.66	4/6979 (0.1%)	1.06	36/9486 (0.4%)
All	All	0.66	7/14094 (0.0%)	1.01	53/19146 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	11
1	B	0	16
All	All	0	27

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	627	GLU	CG-CD	-7.17	1.41	1.51
1	B	1024	TRP	CE3-CZ3	-6.41	1.27	1.38
1	B	797	LYS	CD-CE	6.17	1.66	1.51
1	A	433	TRP	CB-CG	-5.69	1.40	1.50
1	B	748	ARG	CB-CG	5.45	1.67	1.52
1	A	191	ARG	CG-CD	5.35	1.65	1.51
1	B	750	PHE	CA-C	5.28	1.66	1.52

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	377	LEU	CA-CB-CG	11.58	141.94	115.30
1	A	663	ARG	NE-CZ-NH1	10.70	125.65	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	663	ARG	NE-CZ-NH2	-9.93	115.33	120.30
1	B	369	LEU	CA-CB-CG	9.37	136.84	115.30
1	B	628	LEU	CA-CB-CG	9.24	136.55	115.30
1	A	627	GLU	N-CA-C	8.64	134.32	111.00
1	A	191	ARG	CA-CB-CG	8.30	131.65	113.40
1	B	1012	GLN	CA-CB-CG	8.21	131.45	113.40
1	B	612	LEU	CA-CB-CG	8.14	134.03	115.30
1	B	748	ARG	CG-CD-NE	8.14	128.90	111.80
1	B	751	ASP	CB-CG-OD1	7.99	125.49	118.30
1	B	451	SER	C-N-CA	-7.87	102.02	121.70
1	B	547	LEU	CB-CG-CD1	-7.85	97.66	111.00
1	B	746	LEU	CB-CG-CD2	7.75	124.17	111.00
1	B	452	MET	CG-SD-CE	7.67	112.47	100.20
1	A	628	LEU	CA-CB-CG	7.57	132.70	115.30
1	B	574	LEU	CA-CB-CG	7.46	132.47	115.30
1	B	665	TYR	N-CA-C	7.46	131.14	111.00
1	B	861	THR	N-CA-C	7.44	131.09	111.00
1	A	547	LEU	CB-CG-CD1	-7.23	98.70	111.00
1	B	1015	GLU	CB-CA-C	-7.13	96.14	110.40
1	B	1015	GLU	CA-CB-CG	7.12	129.07	113.40
1	B	457	LEU	CA-CB-CG	6.97	131.33	115.30
1	B	563	LEU	CA-CB-CG	6.80	130.94	115.30
1	B	797	LYS	CD-CE-NZ	6.66	127.02	111.70
1	B	577	HIS	CB-CA-C	-6.56	97.28	110.40
1	A	664	ASN	CB-CA-C	-6.25	97.90	110.40
1	B	751	ASP	CB-CG-OD2	-6.20	112.72	118.30
1	A	623	LYS	N-CA-C	6.17	127.67	111.00
1	B	1012	GLN	CB-CA-C	6.17	122.74	110.40
1	B	1012	GLN	N-CA-C	-6.14	94.42	111.00
1	B	600	THR	N-CA-C	5.92	126.98	111.00
1	B	556	LEU	CA-CB-CG	-5.85	101.85	115.30
1	B	369	LEU	CB-CG-CD2	5.80	120.86	111.00
1	A	433	TRP	CA-CB-CG	-5.78	102.72	113.70
1	A	748	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	A	405	GLN	C-N-CA	5.61	135.73	121.70
1	A	627	GLU	OE1-CD-OE2	5.59	130.01	123.30
1	A	638	ASN	N-CA-C	5.57	126.03	111.00
1	A	773	ASP	CB-CG-OD1	5.51	123.26	118.30
1	B	399	LYS	CA-CB-CG	5.49	125.48	113.40
1	B	613	GLN	CA-CB-CG	5.46	125.42	113.40
1	B	1015	GLU	CB-CG-CD	-5.35	99.75	114.20
1	B	455	ARG	CB-CG-CD	5.34	125.50	111.60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	424	ASP	CB-CG-OD2	-5.34	113.49	118.30
1	B	455	ARG	CB-CA-C	-5.30	99.79	110.40
1	B	805	GLN	CB-CA-C	-5.19	100.02	110.40
1	B	665	TYR	CB-CA-C	-5.15	100.10	110.40
1	B	451	SER	CA-C-N	5.13	128.48	117.20
1	B	367	LYS	CB-CA-C	5.11	120.63	110.40
1	B	608	LYS	CD-CE-NZ	-5.07	100.03	111.70
1	A	627	GLU	CB-CA-C	-5.06	100.28	110.40
1	A	402	GLU	CA-CB-CG	5.01	124.43	113.40

There are no chirality outliers.

All (27) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1018	LEU	Peptide
1	A	1019	LYS	Peptide
1	A	220	THR	Peptide
1	A	230	LYS	Peptide
1	A	284	ASN	Peptide
1	A	404	PHE	Peptide
1	A	626	LYS	Peptide
1	A	627	GLU	Peptide
1	A	638	ASN	Peptide
1	A	662	GLY	Peptide
1	A	730	ASN	Sidechain
1	B	191	ARG	Peptide
1	B	265	ALA	Peptide
1	B	399	LYS	Peptide
1	B	452	MET	Peptide
1	B	486	ASN	Sidechain
1	B	521	LYS	Peptide
1	B	608	LYS	Peptide
1	B	669	GLN	Peptide
1	B	697	ASN	Sidechain
1	B	743	LYS	Peptide
1	B	746	LEU	Peptide
1	B	747	LYS	Peptide
1	B	748	ARG	Peptide
1	B	797	LYS	Peptide
1	B	860	MET	Peptide
1	B	861	THR	Peptide

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6937	0	6760	412	1
1	B	6808	0	6593	534	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	182	0	166	20	0
3	B	168	0	153	8	1
4	A	1	0	0	0	0
All	All	14098	0	13672	952	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 34.

All (952) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:574:LEU:CD1	3:A:1113:NAG:H81	1.57	1.33
1:A:574:LEU:HD11	3:A:1113:NAG:C8	1.65	1.26
1:A:367:LYS:HD2	1:A:368:ASN:H	1.02	1.17
1:B:518:THR:O	1:B:521:LYS:HB2	1.49	1.12
1:B:695:ASN:HB3	1:B:726:LYS:HD2	1.31	1.10
1:A:405:GLN:HB2	1:A:406:ASN:HD22	1.16	1.10
1:B:627:GLU:HA	1:B:682:ASN:HB2	1.25	1.08
1:A:191:ARG:HH22	1:A:320:ILE:HB	1.12	1.08
1:A:405:GLN:HG3	1:A:406:ASN:H	0.99	1.07
1:A:574:LEU:HD12	3:A:1113:NAG:H81	1.34	1.07
1:B:1021:LEU:HA	1:B:1024:TRP:HE1	1.16	1.07
1:B:521:LYS:HG3	1:B:547:LEU:HD11	1.37	1.06
1:B:521:LYS:NZ	1:B:699:TYR:OH	1.89	1.06
1:B:518:THR:HG22	1:B:521:LYS:HE2	1.38	1.05
1:A:405:GLN:CG	1:A:406:ASN:H	1.68	1.05
1:B:660:THR:HB	1:B:687:VAL:HG11	1.38	1.05
1:B:735:ILE:HG12	1:B:749:ALA:HA	1.33	1.05
1:A:430:MET:HG2	1:A:431:GLU:H	1.23	1.04
1:B:748:ARG:CD	1:B:750:PHE:HB2	1.87	1.03
1:A:574:LEU:HD11	3:A:1113:NAG:H81	1.23	1.02

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1113:NAG:H62	3:A:1114:NAG:C7	1.91	1.01
1:B:563:LEU:HG	1:B:567:VAL:HG21	1.43	1.00
1:B:920:ARG:HH21	1:B:923:LYS:HE2	1.24	0.99
1:B:452:MET:SD	1:B:455:ARG:N	2.36	0.96
1:A:405:GLN:HG3	1:A:407:TYR:H	1.31	0.95
1:A:191:ARG:NH2	1:A:320:ILE:HB	1.80	0.95
1:B:608:LYS:HE2	1:B:612:LEU:HB3	1.49	0.95
1:A:182:HIS:H	1:A:191:ARG:HB2	1.32	0.94
1:B:622:GLN:HE21	1:B:705:ALA:HB2	1.30	0.94
1:A:574:LEU:HD11	3:A:1113:NAG:H83	1.50	0.94
1:B:748:ARG:HE	1:B:1024:TRP:HZ3	1.13	0.93
1:B:748:ARG:HB3	1:B:751:ASP:H	1.31	0.93
1:A:265:ALA:HA	3:A:1106:NAG:H82	1.49	0.92
1:A:574:LEU:CD1	3:A:1113:NAG:C8	2.35	0.92
1:A:405:GLN:HG3	1:A:406:ASN:N	1.83	0.92
1:B:452:MET:CE	1:B:455:ARG:HG2	2.00	0.91
1:A:182:HIS:N	1:A:191:ARG:HB2	1.85	0.91
1:B:455:ARG:HA	1:B:458:VAL:HG12	1.52	0.91
1:A:560:LYS:O	1:A:560:LYS:HD2	1.72	0.89
1:B:190:PHE:O	1:B:191:ARG:NH1	2.05	0.89
1:B:191:ARG:HG3	1:B:264:SER:HA	1.54	0.89
1:B:709:TRP:O	1:B:713:ILE:N	2.05	0.89
1:B:797:LYS:HG2	1:B:800:GLN:HA	1.55	0.88
1:B:637:LEU:HD22	1:B:1009:LEU:HD22	1.53	0.88
1:A:367:LYS:HD2	1:A:368:ASN:N	1.88	0.88
1:A:891:ASN:OD1	1:A:923:LYS:NZ	2.07	0.87
1:B:1021:LEU:HA	1:B:1024:TRP:NE1	1.89	0.87
1:A:184:ASN:HB2	3:A:1102:NAG:N2	1.90	0.87
1:B:861:THR:HG21	1:B:864:PHE:HB2	1.55	0.86
1:A:367:LYS:CD	1:A:368:ASN:H	1.87	0.86
1:B:560:LYS:HE3	1:B:568:PHE:HB3	1.58	0.85
1:A:403:PHE:O	1:A:405:GLN:HG2	1.77	0.85
1:B:748:ARG:HD2	1:B:750:PHE:HB2	1.58	0.85
1:A:388:GLY:O	1:A:391:HIS:ND1	2.11	0.84
1:B:653:HIS:CD2	1:B:675:ASP:HB2	2.12	0.84
1:B:857:THR:HA	1:B:860:MET:HB2	1.57	0.83
1:A:477:MET:SD	1:A:486:ASN:ND2	2.50	0.83
1:B:191:ARG:NH1	1:B:265:ALA:O	2.12	0.83
1:A:747:LYS:HE3	1:A:1019:LYS:HE3	1.59	0.82
1:A:521:LYS:O	1:A:521:LYS:HD2	1.79	0.82
1:B:637:LEU:HD13	1:B:1009:LEU:HD13	1.61	0.82

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:692:VAL:HB	1:B:702:VAL:HG11	1.61	0.82
1:B:762:THR:HG22	1:B:819:LEU:HB2	1.61	0.82
1:B:433:TRP:HE1	1:B:469:GLN:HA	1.45	0.82
1:A:747:LYS:HZ2	1:A:1024:TRP:HB3	1.44	0.81
1:B:430:MET:HG3	1:B:432:ASN:H	1.45	0.81
1:B:521:LYS:CG	1:B:547:LEU:HD11	2.10	0.81
1:B:602:ASP:OD1	1:B:603:VAL:N	2.14	0.81
1:A:405:GLN:HB2	1:A:406:ASN:ND2	1.94	0.80
1:A:433:TRP:HE1	1:A:469:GLN:HA	1.44	0.80
1:B:985:ALA:O	1:B:989:ASN:ND2	2.15	0.80
1:B:632:GLN:NE2	1:B:652:TRP:O	2.14	0.80
1:B:748:ARG:HD2	1:B:750:PHE:CB	2.12	0.80
1:B:748:ARG:NE	1:B:1024:TRP:HZ3	1.80	0.79
1:B:748:ARG:HB3	1:B:751:ASP:N	1.98	0.79
1:B:977:LYS:HG2	1:B:1011:ILE:HD13	1.64	0.78
1:B:191:ARG:CG	1:B:264:SER:HA	2.13	0.78
1:B:281:ASP:HB3	1:B:285:GLU:H	1.49	0.78
1:B:430:MET:HB3	1:B:437:THR:OG1	1.83	0.78
1:B:1015:GLU:HB3	1:B:1016:LYS:HG3	1.66	0.77
1:B:369:LEU:HG	1:B:387:ILE:HG21	1.66	0.77
1:B:486:ASN:N	1:B:486:ASN:HD22	1.81	0.77
1:B:367:LYS:NZ	1:B:384:PRO:O	2.18	0.77
1:B:627:GLU:HA	1:B:682:ASN:CB	2.13	0.77
1:A:1017:ASN:O	1:A:1019:LYS:HB2	1.84	0.77
1:B:623:LYS:HG3	1:B:628:LEU:HD23	1.67	0.77
1:B:795:VAL:HA	1:B:798:LEU:HD12	1.65	0.76
1:A:184:ASN:HB2	3:A:1102:NAG:HN2	1.50	0.76
1:A:634:ARG:HG2	1:A:652:TRP:HH2	1.50	0.76
1:A:270:SER:OG	1:A:271:TYR:N	2.14	0.76
3:A:1113:NAG:O6	3:A:1114:NAG:O7	2.02	0.76
1:A:861:THR:O	1:A:865:LYS:HD2	1.86	0.76
1:A:966:ILE:O	1:A:970:SER:OG	2.02	0.76
1:A:220:THR:HG21	1:A:231:GLN:HA	1.67	0.76
1:B:336:SER:OG	1:B:346:ASP:HA	1.85	0.76
1:A:451:SER:OG	1:A:454:ASP:OD1	2.02	0.75
1:B:653:HIS:HD2	1:B:675:ASP:HB2	1.49	0.75
1:B:891:ASN:OD1	1:B:923:LYS:NZ	2.20	0.75
1:B:563:LEU:HG	1:B:567:VAL:CG2	2.15	0.75
1:A:625:GLY:N	1:A:627:GLU:OE1	2.19	0.75
1:B:745:PRO:C	1:B:747:LYS:H	1.90	0.75
1:A:1016:LYS:HE3	1:A:1016:LYS:HA	1.68	0.75

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:399:LYS:HB2	1:B:402:GLU:HB2	1.66	0.75
1:B:595:GLU:HA	1:B:599:GLN:HA	1.67	0.75
1:B:920:ARG:NH2	1:B:923:LYS:HE2	2.00	0.75
1:A:294:PHE:HA	1:A:298:ALA:HB3	1.67	0.74
1:B:401:LEU:HG	1:B:405:GLN:HE21	1.50	0.74
3:A:1113:NAG:C6	3:A:1114:NAG:O7	2.35	0.74
1:A:626:LYS:C	1:A:627:GLU:HG2	2.06	0.74
3:A:1113:NAG:C6	3:A:1114:NAG:C7	2.65	0.74
1:B:796:PHE:CE2	1:B:797:LYS:HD2	2.21	0.74
1:A:172:VAL:HG21	1:A:207:ILE:HD13	1.69	0.74
1:A:207:ILE:HG13	1:A:245:ILE:HD11	1.68	0.74
1:B:623:LYS:HD3	1:B:624:LYS:N	2.03	0.74
1:A:220:THR:HG23	1:A:221:PHE:H	1.53	0.74
1:A:511:PHE:HE2	1:A:557:LEU:HD22	1.53	0.74
1:B:623:LYS:HE2	1:B:627:GLU:C	2.09	0.73
1:A:1020:SER:HB2	1:A:1023:TRP:CD1	2.23	0.73
1:A:660:THR:HB	1:A:687:VAL:HG11	1.69	0.73
1:B:691:LYS:HD3	1:B:731:LEU:HD21	1.69	0.73
1:B:684:THR:OG1	1:B:685:GLU:OE1	2.06	0.73
1:B:710:GLU:HA	1:B:713:ILE:HB	1.70	0.73
1:A:218:ARG:N	1:A:262:GLU:OE1	2.20	0.72
1:A:389:GLN:OE1	1:A:446:ASP:HB2	1.89	0.72
1:A:623:LYS:HD3	1:A:628:LEU:HA	1.72	0.72
1:B:183:PRO:HA	1:B:190:PHE:HA	1.71	0.72
1:B:977:LYS:HZ1	1:B:980:LEU:HD22	1.55	0.72
1:B:385:GLU:CD	1:B:385:GLU:H	1.93	0.71
1:B:521:LYS:HB3	1:B:522:ASP:HB2	1.72	0.71
1:A:482:ASP:OD1	1:A:586:SER:HB2	1.88	0.71
1:B:178:GLU:OE1	1:B:195:THR:OG1	2.07	0.71
1:A:215:ASN:HB3	1:A:264:SER:HB2	1.70	0.71
1:B:861:THR:HG21	1:B:864:PHE:CB	2.21	0.71
1:B:367:LYS:HG2	1:B:387:ILE:HD11	1.71	0.71
1:B:427:ALA:O	1:B:439:ARG:NH1	2.24	0.71
1:A:725:ASP:OD1	1:A:726:LYS:NZ	2.18	0.70
1:A:307:ASP:HA	1:A:356:THR:HG21	1.73	0.70
1:B:977:LYS:NZ	1:B:980:LEU:HD22	2.06	0.70
1:B:604:LYS:HD2	1:B:607:MET:HG2	1.72	0.70
1:B:966:ILE:O	1:B:970:SER:OG	2.09	0.70
1:A:597:THR:CB	1:A:601:LEU:HG	2.21	0.70
1:A:521:LYS:HG3	1:A:547:LEU:CD1	2.22	0.70
1:A:630:ILE:HG21	1:A:656:LEU:HD11	1.73	0.70

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:746:LEU:HB3	1:A:1019:LYS:HE2	1.74	0.70
1:A:406:ASN:O	1:A:409:GLU:HG3	1.91	0.69
1:A:634:ARG:HG2	1:A:652:TRP:CH2	2.26	0.69
1:A:728:ARG:HD2	1:A:755:TYR:OH	1.93	0.69
1:B:486:ASN:ND2	1:B:486:ASN:N	2.40	0.69
1:B:746:LEU:HD22	1:B:1020:SER:OG	1.93	0.69
1:B:567:VAL:HG23	1:B:568:PHE:N	2.08	0.69
1:B:748:ARG:HD3	1:B:750:PHE:HB2	1.73	0.69
1:B:214:HIS:NE2	1:B:301:SER:O	2.25	0.68
3:A:1113:NAG:H62	3:A:1114:NAG:O7	1.91	0.68
1:A:622:GLN:O	1:A:623:LYS:NZ	2.25	0.68
1:B:768:ALA:O	1:B:772:THR:OG1	2.11	0.68
1:B:626:LYS:O	1:B:683:LEU:N	2.23	0.68
1:B:856:PRO:HB2	1:B:859:VAL:HG22	1.75	0.68
1:B:452:MET:HE3	1:B:455:ARG:HG2	1.75	0.68
1:A:964:GLN:OE1	1:A:965:ASN:HB2	1.93	0.68
1:B:861:THR:OG1	1:B:863:VAL:N	2.26	0.68
1:A:396:THR:HA	1:A:399:LYS:NZ	2.09	0.68
1:A:622:GLN:HG3	1:A:705:ALA:HB2	1.75	0.68
1:A:626:LYS:H	1:A:627:GLU:CD	1.97	0.68
1:B:797:LYS:HG2	1:B:800:GLN:CA	2.22	0.68
1:B:212:THR:O	1:B:214:HIS:N	2.23	0.68
1:A:595:GLU:OE2	3:A:1114:NAG:O6	2.13	0.67
1:B:369:LEU:HG	1:B:387:ILE:CG2	2.24	0.67
1:A:696:MET:CG	1:A:730:ASN:HD22	2.06	0.67
1:B:451:SER:O	1:B:452:MET:HE1	1.94	0.67
1:B:452:MET:SD	1:B:455:ARG:HG2	2.34	0.67
1:B:748:ARG:CZ	1:B:750:PHE:HB3	2.24	0.67
1:B:954:GLN:HG2	1:B:955:LYS:HD2	1.75	0.67
1:A:405:GLN:HG3	1:A:407:TYR:N	2.06	0.67
1:A:713:ILE:HD13	1:A:752:LEU:HA	1.77	0.67
1:B:399:LYS:HA	1:B:402:GLU:H	1.58	0.67
1:B:484:TRP:HB3	1:B:548:SER:HB3	1.76	0.66
1:A:623:LYS:CD	1:A:628:LEU:HD12	2.26	0.66
1:A:853:GLN:NE2	1:A:854:SER:O	2.27	0.66
1:A:748:ARG:HG2	1:A:748:ARG:HH11	1.60	0.66
1:A:706:ASP:O	1:A:710:GLU:HG3	1.95	0.66
1:A:560:LYS:HB2	1:A:568:PHE:CG	2.31	0.66
1:B:718:ILE:HD12	1:B:719:ASN:HB3	1.78	0.66
1:A:166:ILE:HG22	1:A:240:HIS:NE2	2.10	0.66
1:B:167:ARG:HG3	1:B:167:ARG:HH11	1.59	0.66

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:689:TRP:CD1	1:B:715:GLN:HG3	2.30	0.66
1:A:629:PHE:HB3	1:A:631:GLN:HE22	1.59	0.66
1:B:748:ARG:HD2	1:B:750:PHE:C	2.17	0.66
1:B:750:PHE:O	1:B:753:ILE:HG22	1.95	0.66
1:A:1017:ASN:C	1:A:1019:LYS:HB2	2.16	0.65
1:B:343:LEU:HD23	1:B:344:VAL:N	2.12	0.65
1:A:403:PHE:C	1:A:405:GLN:HG2	2.16	0.65
1:A:710:GLU:HA	1:A:713:ILE:HG22	1.78	0.65
1:A:696:MET:HG3	1:A:730:ASN:ND2	2.11	0.65
1:A:626:LYS:N	1:A:627:GLU:OE1	2.29	0.65
1:B:510:ASP:OD1	1:B:511:PHE:N	2.29	0.65
1:B:623:LYS:HE2	1:B:627:GLU:CA	2.26	0.65
1:A:182:HIS:HB2	1:A:191:ARG:CZ	2.26	0.65
1:B:322:ASP:OD2	3:B:1103:NAG:O6	2.14	0.65
1:B:608:LYS:CE	1:B:612:LEU:HB3	2.25	0.65
1:B:525:ASN:OD1	1:B:614:LYS:NZ	2.29	0.65
1:B:608:LYS:HD3	1:B:612:LEU:H	1.62	0.65
1:B:695:ASN:HB3	1:B:726:LYS:CD	2.20	0.65
1:B:282:GLU:HG2	1:B:385:GLU:HG2	1.78	0.65
1:A:663:ARG:HG2	1:A:664:ASN:OD1	1.97	0.64
1:B:161:PHE:HE1	1:B:163:TRP:O	1.79	0.64
1:A:747:LYS:NZ	1:A:1024:TRP:HB3	2.12	0.64
1:B:748:ARG:NE	1:B:1024:TRP:CZ3	2.52	0.64
1:B:256:ASN:C	1:B:257:TYR:HD1	2.00	0.64
1:B:541:GLU:HA	1:B:544:PHE:HD1	1.60	0.64
1:B:796:PHE:CZ	1:B:832:LEU:HB3	2.33	0.64
1:B:977:LYS:NZ	1:B:1008:GLN:HA	2.13	0.64
1:A:224:ALA:O	1:A:226:SER:N	2.30	0.64
1:A:560:LYS:C	1:A:560:LYS:HD2	2.16	0.64
1:B:596:VAL:HG12	1:B:598:ASN:H	1.61	0.64
1:A:182:HIS:HB2	1:A:191:ARG:CG	2.27	0.64
1:A:166:ILE:HG22	1:A:240:HIS:CD2	2.33	0.64
1:B:510:ASP:O	1:B:513:ASP:HB3	1.97	0.64
1:B:478:LYS:HD2	1:B:585:GLN:HG3	1.78	0.64
1:A:445:TYR:OH	1:A:455:ARG:HD2	1.97	0.64
1:B:329:SER:OG	1:B:330:ASN:N	2.29	0.64
1:A:182:HIS:HB2	1:A:191:ARG:HG3	1.78	0.64
1:A:755:TYR:OH	1:A:759:GLU:OE1	2.15	0.64
1:A:445:TYR:CZ	1:A:455:ARG:HD2	2.33	0.64
1:A:623:LYS:HZ2	1:A:629:PHE:N	1.96	0.64
1:B:265:ALA:HB3	3:B:1107:NAG:H82	1.80	0.64

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:PHE:N	1:A:351:SER:OG	2.30	0.63
1:B:459:THR:HG22	1:B:498:LEU:HD11	1.79	0.63
1:B:174:PRO:HA	1:B:198:VAL:HG12	1.79	0.63
1:B:738:LEU:HB3	1:B:743:LYS:CB	2.28	0.63
1:B:735:ILE:CG1	1:B:749:ALA:HA	2.19	0.63
1:B:1012:GLN:O	1:B:1014:MET:N	2.31	0.63
1:B:748:ARG:NE	1:B:750:PHE:HB2	2.13	0.63
1:A:220:THR:OG1	1:A:232:ALA:N	2.29	0.63
1:B:411:GLN:HG3	3:B:1112:NAG:H82	1.81	0.63
1:B:187:SER:OG	1:B:188:MET:N	2.28	0.63
1:B:477:MET:SD	1:B:478:LYS:N	2.71	0.63
1:B:861:THR:HG22	1:B:892:LYS:HD3	1.81	0.63
1:A:949:TRP:O	1:A:953:VAL:HG23	1.98	0.63
1:B:578:ASN:HD22	3:B:1113:NAG:C7	2.09	0.63
1:A:1015:GLU:C	1:A:1016:LYS:HD2	2.18	0.63
1:A:433:TRP:HE1	1:A:469:GLN:CA	2.12	0.63
1:A:560:LYS:HB2	1:A:568:PHE:CD1	2.33	0.63
1:B:541:GLU:HA	1:B:544:PHE:CD1	2.33	0.63
1:B:215:ASN:ND2	1:B:264:SER:HB3	2.14	0.63
1:A:762:THR:HB	1:A:819:LEU:HB2	1.81	0.62
1:B:590:TRP:HB3	1:B:604:LYS:CB	2.29	0.62
1:B:872:LYS:HD2	1:B:875:SER:HB2	1.81	0.62
1:A:426:GLU:OE1	1:A:426:GLU:N	2.33	0.62
1:B:788:ALA:O	1:B:791:LEU:HB3	1.99	0.62
1:A:663:ARG:HD3	1:A:664:ASN:HD21	1.65	0.62
1:B:745:PRO:O	1:B:747:LYS:N	2.32	0.62
1:B:762:THR:CG2	1:B:819:LEU:HB2	2.28	0.62
1:B:373:VAL:HG22	1:B:374:ASN:H	1.65	0.62
1:A:726:LYS:HD3	1:A:726:LYS:N	2.14	0.62
1:B:623:LYS:HG2	1:B:628:LEU:HA	1.82	0.62
1:A:402:GLU:C	1:A:405:GLN:HB3	2.20	0.62
1:A:624:LYS:C	1:A:627:GLU:OE1	2.38	0.62
1:A:430:MET:HG2	1:A:431:GLU:N	2.04	0.62
1:B:696:MET:SD	1:B:730:ASN:ND2	2.72	0.62
1:B:1023:TRP:CE3	1:B:1024:TRP:HB3	2.35	0.61
1:A:1020:SER:HB2	1:A:1023:TRP:HD1	1.66	0.61
1:A:184:ASN:CB	3:A:1102:NAG:N2	2.62	0.61
1:B:560:LYS:HE3	1:B:568:PHE:CD1	2.36	0.61
1:A:809:THR:HG22	1:A:810:ASP:H	1.65	0.61
1:B:256:ASN:O	1:B:257:TYR:HD1	1.82	0.61
1:B:627:GLU:CA	1:B:682:ASN:HB2	2.16	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:920:ARG:HH22	1:A:922:GLN:CD	2.04	0.61
1:B:609:THR:HG21	1:B:653:HIS:ND1	2.15	0.61
1:A:367:LYS:HG3	1:A:387:ILE:HG12	1.82	0.61
1:B:451:SER:O	1:B:452:MET:CE	2.48	0.61
1:A:211:SER:HB2	1:A:304:PRO:HB3	1.83	0.61
1:B:457:LEU:HA	1:B:460:LYS:HB3	1.82	0.61
1:B:880:LYS:O	1:B:884:ILE:HG22	2.01	0.61
1:B:321:ARG:N	1:B:343:LEU:HD21	2.16	0.61
1:B:559:LEU:HD23	1:B:568:PHE:HE2	1.66	0.61
1:B:560:LYS:HE3	1:B:568:PHE:CB	2.29	0.61
1:B:282:GLU:HG2	1:B:385:GLU:CG	2.31	0.61
1:B:621:VAL:HG21	1:B:692:VAL:HG21	1.83	0.61
1:B:811:GLU:O	1:B:820:ARG:NH2	2.31	0.61
1:B:560:LYS:CE	1:B:568:PHE:HB3	2.29	0.60
1:A:161:PHE:CE1	1:A:163:TRP:HB3	2.35	0.60
1:B:294:PHE:HA	1:B:298:ALA:HB3	1.83	0.60
1:B:748:ARG:CD	1:B:750:PHE:CB	2.67	0.60
1:A:984:GLN:O	1:A:988:GLU:HG2	2.01	0.60
1:B:536:SER:OG	1:B:537:SER:N	2.33	0.60
1:B:562:TYR:CG	1:B:655:PRO:HB3	2.36	0.60
1:B:853:GLN:OE1	1:B:854:SER:N	2.34	0.60
1:B:433:TRP:NE1	1:B:469:GLN:HA	2.16	0.60
1:B:562:TYR:CD1	1:B:655:PRO:HB3	2.35	0.60
1:B:178:GLU:HA	1:B:316:ILE:O	2.01	0.60
1:B:373:VAL:HG22	1:B:374:ASN:N	2.17	0.60
1:B:861:THR:N	1:B:892:LYS:HD3	2.17	0.60
1:A:180:SER:OG	1:A:193:SER:HB3	2.02	0.60
1:A:861:THR:HG22	1:A:865:LYS:HE3	1.83	0.60
1:A:781:LYS:HD2	1:A:938:HIS:CG	2.37	0.60
1:B:695:ASN:HB2	1:B:697:ASN:OD1	2.02	0.60
1:B:942:TRP:NE1	1:B:946:LYS:HE2	2.17	0.60
1:A:220:THR:CG2	1:A:231:GLN:HA	2.32	0.59
1:B:455:ARG:O	1:B:459:THR:N	2.22	0.59
1:A:405:GLN:CG	1:A:406:ASN:N	2.48	0.59
1:A:623:LYS:HZ2	1:A:629:PHE:H	1.49	0.59
1:B:980:LEU:HG	1:B:984:GLN:NE2	2.17	0.59
1:B:445:TYR:CE1	1:B:450:SER:HB2	2.37	0.59
1:B:521:LYS:CD	1:B:522:ASP:HB2	2.32	0.59
1:B:623:LYS:HD3	1:B:623:LYS:C	2.21	0.59
1:B:860:MET:O	1:B:861:THR:HB	1.94	0.59
1:A:283:SER:O	1:A:284:ASN:HB2	2.01	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:623:LYS:HG2	1:A:627:GLU:CD	2.22	0.59
1:A:438:PHE:HE2	1:A:461:ILE:HG22	1.68	0.59
1:B:277:PHE:HZ	1:B:423:PRO:HD2	1.66	0.59
1:B:564:SER:O	1:B:567:VAL:HG22	2.03	0.59
1:A:432:ASN:HB2	1:A:435:LEU:O	2.02	0.59
1:B:296:PRO:HB2	1:B:297:LEU:HD12	1.84	0.59
1:B:746:LEU:HG	1:B:747:LYS:N	2.17	0.59
1:A:182:HIS:HB2	1:A:191:ARG:NE	2.17	0.59
1:B:748:ARG:NH1	1:B:750:PHE:HB3	2.16	0.59
1:B:746:LEU:HD22	1:B:1020:SER:CB	2.33	0.59
1:A:284:ASN:HB3	1:A:285:GLU:HB2	1.84	0.59
1:B:281:ASP:OD1	1:B:282:GLU:N	2.36	0.59
1:B:499:GLU:OE1	1:B:508:TYR:HB3	2.03	0.59
1:B:180:SER:HB3	1:B:193:SER:HB3	1.84	0.58
1:B:608:LYS:NZ	1:B:613:GLN:HG3	2.18	0.58
1:B:843:PHE:HB2	1:B:863:VAL:HG13	1.85	0.58
1:A:165:GLN:OE1	1:A:165:GLN:N	2.36	0.58
1:A:587:ASP:HA	1:A:590:TRP:CD1	2.38	0.58
1:A:696:MET:CG	1:A:730:ASN:ND2	2.66	0.58
1:B:954:GLN:HG2	1:B:955:LYS:CD	2.33	0.58
1:A:787:LEU:HD22	1:A:1025:LEU:HD23	1.85	0.58
1:A:623:LYS:NZ	1:A:629:PHE:H	2.02	0.58
1:A:368:ASN:OD1	3:A:1107:NAG:C2	2.47	0.58
1:B:862:THR:O	1:B:865:LYS:HB2	2.04	0.58
1:B:540:ILE:O	1:B:543:MET:HB2	2.04	0.57
1:B:784:TYR:CE2	1:B:1018:LEU:HD11	2.39	0.57
1:B:991:SER:HB2	1:B:994:THR:H	1.69	0.57
1:A:237:TYR:HE2	1:A:240:HIS:HD1	1.52	0.57
1:A:840:MET:HE1	1:A:867:GLY:HA2	1.85	0.57
1:A:182:HIS:H	1:A:191:ARG:CB	2.12	0.57
1:B:430:MET:SD	1:B:431:GLU:N	2.77	0.57
1:A:935:PHE:HB3	1:A:936:PRO:HD3	1.86	0.57
1:A:623:LYS:HG2	1:A:627:GLU:CG	2.34	0.57
1:A:220:THR:HG23	1:A:221:PHE:N	2.20	0.57
1:A:773:ASP:OD1	1:A:777:ASN:ND2	2.38	0.57
1:B:196:ILE:N	1:B:259:LEU:O	2.30	0.57
1:A:234:ILE:HD12	1:A:234:ILE:O	2.05	0.57
1:A:255:HIS:HB2	1:A:257:TYR:CE1	2.40	0.57
1:A:664:ASN:O	1:A:665:TYR:HB2	2.04	0.57
1:A:783:GLY:O	1:A:785:MET:N	2.34	0.57
1:A:735:ILE:HG12	1:A:749:ALA:HA	1.87	0.57

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:412:TYR:CZ	1:B:414:LEU:HB2	2.40	0.57
1:A:886:SER:O	1:A:890:LYS:HG3	2.04	0.56
1:B:320:ILE:HG23	1:B:343:LEU:HD22	1.86	0.56
1:A:521:LYS:HG3	1:A:547:LEU:HD11	1.86	0.56
1:A:781:LYS:HE2	1:A:973:LEU:HD13	1.87	0.56
1:A:281:ASP:HB3	1:A:285:GLU:H	1.70	0.56
1:B:1005:GLU:O	1:B:1009:LEU:HG	2.04	0.56
1:B:176:ARG:O	1:B:197:SER:OG	2.22	0.56
1:A:508:TYR:CE1	1:A:509:GLU:HG3	2.41	0.56
1:B:789:SER:O	1:B:793:THR:HG23	2.05	0.56
1:B:977:LYS:HZ3	1:B:1008:GLN:HA	1.69	0.56
1:B:555:LEU:HD21	1:B:610:TRP:HB3	1.88	0.56
1:B:312:LYS:NZ	1:B:476:THR:OG1	2.38	0.56
1:A:182:HIS:CB	1:A:191:ARG:HB2	2.35	0.56
1:A:219:VAL:HG22	1:A:261:ILE:HA	1.87	0.56
1:B:704:TYR:HB3	1:B:708:ASP:CB	2.36	0.56
1:A:182:HIS:O	1:A:190:PHE:HA	2.06	0.56
1:A:456:LYS:O	1:A:460:LYS:HG2	2.06	0.56
1:B:992:GLU:OE1	1:B:992:GLU:N	2.38	0.56
1:A:747:LYS:NZ	1:A:1021:LEU:HA	2.21	0.55
1:A:479:TRP:HZ3	1:A:534:VAL:O	1.89	0.55
1:B:1012:GLN:C	1:B:1015:GLU:HG3	2.25	0.55
1:B:204:THR:OG1	1:B:206:ASN:OD1	2.18	0.55
1:A:515:ARG:NH2	1:A:696:MET:O	2.35	0.55
1:A:368:ASN:C	1:A:368:ASN:HD22	2.10	0.55
3:B:1105:NAG:O6	3:B:1106:NAG:C7	2.54	0.55
1:B:592:SER:OG	3:B:1113:NAG:H81	2.07	0.55
1:A:992:GLU:N	1:A:992:GLU:OE1	2.38	0.55
1:A:368:ASN:C	1:A:368:ASN:ND2	2.60	0.55
1:B:651:LEU:HD21	1:B:676:LYS:HA	1.89	0.55
1:B:1005:GLU:HA	1:B:1008:GLN:OE1	2.07	0.55
1:B:332:PRO:HG3	1:B:416:LYS:HB3	1.88	0.55
1:A:784:TYR:CZ	1:A:1018:LEU:HD21	2.41	0.55
1:B:455:ARG:CA	1:B:458:VAL:HG12	2.33	0.55
1:B:792:VAL:O	1:B:796:PHE:N	2.38	0.55
1:A:469:GLN:HB2	1:A:470:TRP:CE3	2.42	0.55
1:B:442:THR:O	1:B:458:VAL:HG23	2.06	0.55
1:B:951:LYS:HE3	1:B:955:LYS:HD3	1.89	0.55
1:B:570:HIS:HA	1:B:573:VAL:HB	1.88	0.55
1:A:713:ILE:HD12	1:A:713:ILE:O	2.07	0.54
1:B:704:TYR:O	1:B:709:TRP:HZ3	1.90	0.54

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:861:THR:HG21	1:B:864:PHE:CG	2.41	0.54
1:B:884:ILE:HD12	1:B:885:GLY:H	1.71	0.54
1:A:228:GLN:OE1	1:A:229:GLU:N	2.33	0.54
1:A:433:TRP:NE1	1:A:469:GLN:HA	2.20	0.54
1:A:405:GLN:CG	1:A:407:TYR:H	2.15	0.54
1:B:468:HIS:O	1:B:473:ASN:ND2	2.40	0.54
1:B:881:TYR:O	1:B:890:LYS:HE2	2.06	0.54
1:A:281:ASP:OD1	1:A:282:GLU:N	2.38	0.54
1:B:411:GLN:CG	3:B:1112:NAG:H82	2.37	0.54
1:B:797:LYS:NZ	1:B:800:GLN:HG3	2.22	0.54
1:B:1009:LEU:O	1:B:1013:TRP:N	2.31	0.54
1:B:216:ILE:HA	1:B:263:TYR:HA	1.89	0.54
1:B:680:VAL:O	1:B:681:ILE:HD12	2.08	0.54
1:A:454:ASP:N	1:A:454:ASP:OD1	2.33	0.54
1:A:849:SER:O	1:A:852:THR:N	2.24	0.54
1:B:521:LYS:NZ	1:B:699:TYR:HH	1.99	0.54
1:B:214:HIS:HE1	1:B:300:ARG:O	1.91	0.54
1:B:564:SER:OG	1:B:565:GLU:N	2.40	0.54
1:B:797:LYS:NZ	1:B:800:GLN:O	2.40	0.54
1:B:859:VAL:O	1:B:861:THR:HA	2.08	0.54
1:A:564:SER:HB3	1:A:567:VAL:HG23	1.90	0.54
1:A:747:LYS:HE2	1:A:1021:LEU:HD23	1.89	0.54
1:A:992:GLU:HA	1:A:995:PHE:HB3	1.90	0.54
1:B:1021:LEU:HD23	1:B:1024:TRP:HE1	1.73	0.54
1:B:380:ILE:HG21	1:B:390:VAL:HB	1.89	0.54
1:B:503:LYS:HG3	1:B:503:LYS:O	2.08	0.54
1:B:189:THR:HG23	1:B:265:ALA:HA	1.90	0.54
1:B:255:HIS:HB2	1:B:257:TYR:CE1	2.43	0.54
1:B:401:LEU:O	1:B:405:GLN:HG3	2.08	0.54
1:B:521:LYS:HG3	1:B:547:LEU:CD1	2.24	0.54
1:A:232:ALA:HB2	1:A:248:PRO:HD3	1.89	0.53
1:B:389:GLN:HG2	1:B:446:ASP:HB2	1.89	0.53
1:A:763:ALA:HB3	1:A:764:PRO:HD3	1.89	0.53
1:B:720:PRO:HB2	1:B:728:ARG:HD3	1.91	0.53
1:B:861:THR:HG1	1:B:863:VAL:HB	1.73	0.53
1:A:191:ARG:CZ	1:A:320:ILE:HD13	2.39	0.53
1:B:495:TYR:O	1:B:499:GLU:HG3	2.07	0.53
1:B:516:PHE:HE2	1:B:767:GLU:HG3	1.74	0.53
1:A:182:HIS:CB	1:A:191:ARG:HG3	2.39	0.53
1:B:183:PRO:HB3	1:B:190:PHE:HB3	1.90	0.53
1:B:651:LEU:HD11	1:B:677:LYS:N	2.24	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:825:GLU:HG2	1:B:862:THR:OG1	2.08	0.53
1:A:179:LEU:HD21	1:A:181:LEU:HD11	1.91	0.53
1:A:366:MET:SD	1:A:381:TYR:HB3	2.49	0.53
1:A:534:VAL:O	1:A:535:GLN:HG3	2.09	0.53
1:A:802:GLN:O	1:A:806:GLN:HG2	2.08	0.53
1:B:886:SER:O	1:B:890:LYS:HB2	2.09	0.53
1:A:331:MET:HG3	1:A:351:SER:HA	1.90	0.53
1:B:521:LYS:HD2	1:B:522:ASP:HB2	1.90	0.53
1:B:955:LYS:N	1:B:955:LYS:HD2	2.24	0.53
1:A:358:LEU:HD11	1:A:473:ASN:HA	1.91	0.53
1:B:195:THR:HA	1:B:260:LYS:HA	1.89	0.52
1:B:518:THR:O	1:B:521:LYS:HE3	2.09	0.52
1:B:984:GLN:HG3	1:B:1004:LEU:HD22	1.91	0.52
1:A:881:TYR:CE1	1:A:890:LYS:HB3	2.44	0.52
1:A:657:SER:HB2	1:A:694:ILE:HG13	1.90	0.52
1:B:234:ILE:O	1:B:235:LEU:HD23	2.08	0.52
1:B:538:GLU:O	1:B:541:GLU:HG2	2.09	0.52
1:B:796:PHE:CD1	1:B:832:LEU:HD13	2.44	0.52
1:A:320:ILE:HG23	1:A:344:VAL:O	2.09	0.52
1:B:401:LEU:HG	1:B:405:GLN:NE2	2.19	0.52
1:B:762:THR:HG21	1:B:815:SER:O	2.09	0.52
1:A:1024:TRP:CG	1:A:1025:LEU:N	2.76	0.52
1:B:714:HIS:O	1:B:718:ILE:HG23	2.09	0.52
1:B:748:ARG:NH1	1:B:750:PHE:O	2.42	0.52
1:A:782:LEU:HD11	1:A:1014:MET:HG3	1.91	0.52
1:B:545:ASP:C	1:B:547:LEU:H	2.12	0.52
1:B:295:GLU:OE2	1:B:544:PHE:CZ	2.63	0.52
1:A:801:ASN:O	1:A:805:GLN:HG3	2.10	0.52
1:B:1012:GLN:O	1:B:1015:GLU:HG3	2.10	0.52
1:B:317:ILE:HD11	1:B:329:SER:HB2	1.91	0.52
1:A:717:LYS:NZ	1:A:751:ASP:OD1	2.32	0.52
1:B:443:LEU:HA	1:B:458:VAL:HG23	1.91	0.52
1:A:859:VAL:O	1:A:863:VAL:HG23	2.11	0.51
1:B:630:ILE:HG21	1:B:656:LEU:HD11	1.92	0.51
1:B:797:LYS:HZ2	1:B:800:GLN:HG3	1.73	0.51
1:A:168:LEU:HD13	1:A:306:PHE:HD1	1.76	0.51
1:A:394:LEU:O	1:A:398:VAL:HG23	2.09	0.51
1:A:796:PHE:HB2	1:A:832:LEU:HD13	1.93	0.51
1:B:626:LYS:HE2	1:B:684:THR:O	2.10	0.51
1:B:747:LYS:O	1:B:748:ARG:HB2	2.09	0.51
1:A:628:LEU:HD11	1:A:690:VAL:HG21	1.92	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:322:ASP:OD1	1:B:323:GLU:N	2.42	0.51
1:B:376:THR:HA	1:B:415:LYS:O	2.10	0.51
1:A:521:LYS:HG3	1:A:547:LEU:HD12	1.92	0.51
1:A:320:ILE:HG13	1:A:345:GLN:CB	2.40	0.51
1:B:452:MET:SD	1:B:452:MET:C	2.87	0.51
1:B:630:ILE:HG22	1:B:674:LEU:HD22	1.92	0.51
1:A:376:THR:HG21	1:A:412:TYR:CD2	2.45	0.51
1:A:521:LYS:HE3	1:A:547:LEU:HD13	1.92	0.51
1:B:748:ARG:CB	1:B:751:ASP:H	2.15	0.51
1:B:761:HIS:O	1:B:764:PRO:HD2	2.10	0.51
1:B:861:THR:HG22	1:B:892:LYS:CD	2.40	0.51
1:A:403:PHE:CB	1:A:501:ILE:HD11	2.40	0.51
1:B:205:TRP:CZ3	1:B:249:GLU:HA	2.45	0.51
1:A:1017:ASN:HA	1:A:1019:LYS:HG3	1.92	0.51
1:A:747:LYS:HE3	1:A:1019:LYS:CE	2.36	0.51
1:B:472:GLY:HA2	1:B:486:ASN:OD1	2.10	0.51
1:A:457:LEU:O	1:A:461:ILE:HG13	2.11	0.51
1:A:634:ARG:CG	1:A:652:TRP:HH2	2.21	0.51
1:B:192:GLY:O	1:B:193:SER:HB2	2.10	0.51
1:B:596:VAL:HG21	1:B:601:LEU:HB2	1.92	0.51
1:B:321:ARG:HD2	1:B:322:ASP:O	2.11	0.51
1:B:561:THR:HG21	1:B:697:ASN:ND2	2.26	0.51
1:B:745:PRO:C	1:B:747:LYS:N	2.58	0.51
1:B:748:ARG:HD2	1:B:750:PHE:CA	2.41	0.51
1:A:207:ILE:HB	1:A:245:ILE:HG12	1.93	0.50
1:A:519:MET:HG2	1:A:699:TYR:CE1	2.46	0.50
1:B:469:GLN:HB2	1:B:470:TRP:CE3	2.46	0.50
1:B:596:VAL:CG1	1:B:597:THR:N	2.74	0.50
1:A:220:THR:CG2	1:A:221:PHE:N	2.74	0.50
1:A:951:LYS:O	1:A:955:LYS:HD2	2.11	0.50
1:B:181:LEU:HB2	1:B:319:ILE:HG22	1.93	0.50
1:B:808:TRP:CZ2	1:B:824:LEU:HD22	2.46	0.50
1:B:925:SER:HB3	1:B:962:THR:HG23	1.93	0.50
1:A:980:LEU:HD22	1:A:1008:GLN:HG3	1.92	0.50
1:B:748:ARG:NE	1:B:750:PHE:CB	2.74	0.50
1:B:786:ASP:OD1	1:B:786:ASP:N	2.45	0.50
1:A:245:ILE:HG13	1:A:245:ILE:O	2.11	0.50
1:A:445:TYR:CE1	1:A:450:SER:HB2	2.46	0.50
1:A:997:LEU:HB3	1:A:999:CYS:SG	2.52	0.50
1:B:1012:GLN:HA	1:B:1015:GLU:HG3	1.94	0.50
1:A:180:SER:HB3	1:A:318:LYS:HE3	1.93	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:LEU:HD12	1:B:161:PHE:H	1.76	0.50
1:B:773:ASP:HA	1:B:776:TYR:HB3	1.93	0.50
1:A:673:LEU:O	1:A:673:LEU:HD23	2.11	0.50
1:A:696:MET:SD	1:A:730:ASN:ND2	2.85	0.50
1:A:874:TRP:CD2	1:A:905:LYS:HD3	2.47	0.50
1:A:386:LYS:C	1:A:388:GLY:H	2.14	0.50
1:B:1007:ILE:HG22	1:B:1011:ILE:HD12	1.93	0.50
1:B:617:PRO:HB3	1:B:652:TRP:CE3	2.47	0.50
1:B:748:ARG:HG3	1:B:751:ASP:CG	2.32	0.50
1:A:623:LYS:HG2	1:A:627:GLU:HG3	1.93	0.50
1:A:887:GLU:HA	1:A:890:LYS:HD2	1.92	0.50
1:A:745:PRO:HG2	1:A:748:ARG:HG3	1.94	0.50
1:B:191:ARG:HG3	1:B:263:TYR:O	2.12	0.50
1:B:560:LYS:HE3	1:B:568:PHE:CG	2.46	0.50
1:B:661:GLU:C	1:B:687:VAL:HG22	2.31	0.50
1:A:1024:TRP:CZ3	1:A:1025:LEU:HD13	2.47	0.49
1:A:336:SER:OG	1:A:346:ASP:OD1	2.13	0.49
1:A:809:THR:HB	1:A:811:GLU:HG2	1.94	0.49
1:A:218:ARG:O	1:A:262:GLU:HB3	2.12	0.49
1:A:438:PHE:CD1	1:A:443:LEU:HD11	2.48	0.49
1:A:517:LYS:HE3	1:A:770:PHE:CZ	2.47	0.49
1:B:281:ASP:CG	1:B:283:SER:H	2.15	0.49
1:B:604:LYS:CD	1:B:607:MET:HG2	2.42	0.49
1:A:220:THR:O	1:A:229:GLU:OE2	2.30	0.49
1:A:544:PHE:HA	1:A:549:TYR:OH	2.11	0.49
1:A:889:GLU:HA	1:A:892:LYS:HG3	1.95	0.49
1:B:1023:TRP:CZ3	1:B:1024:TRP:HB3	2.48	0.49
1:B:748:ARG:NH2	1:B:794:ARG:CZ	2.75	0.49
1:B:802:GLN:O	1:B:806:GLN:HG2	2.11	0.49
1:A:328:LEU:HD11	1:A:381:TYR:CD2	2.47	0.49
1:B:432:ASN:HB2	1:B:435:LEU:O	2.12	0.49
1:B:512:LEU:HD22	1:B:726:LYS:HB2	1.95	0.49
1:B:735:ILE:HD13	1:B:752:LEU:HB2	1.93	0.49
1:A:205:TRP:CZ3	1:A:250:ALA:HB2	2.46	0.49
1:B:352:VAL:HG21	1:B:581:TYR:CE2	2.47	0.49
1:A:403:PHE:CG	1:A:403:PHE:O	2.65	0.49
1:A:549:TYR:N	1:A:549:TYR:CD1	2.80	0.49
1:A:662:GLY:HA3	1:A:685:GLU:CD	2.33	0.49
1:B:746:LEU:HD22	1:B:1020:SER:HB2	1.94	0.49
1:B:860:MET:O	1:B:860:MET:HG2	2.12	0.49
1:A:446:ASP:OD1	1:A:446:ASP:C	2.51	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1012:GLN:CA	1:B:1015:GLU:HG3	2.43	0.49
1:B:315:PHE:N	1:B:351:SER:OG	2.46	0.49
1:B:385:GLU:N	1:B:385:GLU:OE1	2.43	0.49
1:B:704:TYR:HB3	1:B:708:ASP:HB2	1.94	0.49
1:B:934[B]:HIS:CD2	1:B:936:PRO:HD2	2.48	0.49
1:B:367:LYS:HD3	1:B:384:PRO:HA	1.93	0.49
1:B:427:ALA:HB3	1:B:439:ARG:HG2	1.93	0.49
1:B:825:GLU:CD	1:B:862:THR:HA	2.33	0.49
1:A:239:TYR:HD2	1:A:240:HIS:CE1	2.31	0.49
1:A:445:TYR:CE1	1:A:455:ARG:HG2	2.48	0.49
1:B:176:ARG:HB2	1:B:314:THR:OG1	2.12	0.49
1:B:575:TYR:HD2	1:B:576:LEU:HD12	1.77	0.49
1:A:621:VAL:HG21	1:A:692:VAL:HG21	1.95	0.49
1:B:389:GLN:HB2	1:B:444:LEU:HB3	1.95	0.49
1:B:567:VAL:HG23	1:B:568:PHE:H	1.78	0.49
1:B:608:LYS:O	1:B:608:LYS:HG3	2.13	0.49
1:B:631:GLN:HG2	1:B:633:GLU:OE2	2.13	0.49
1:A:412:TYR:CE2	1:A:417:LEU:HB2	2.48	0.48
1:A:817:ARG:HG2	1:A:820:ARG:HH21	1.77	0.48
1:B:578:ASN:ND2	3:B:1113:NAG:O7	2.46	0.48
1:A:279:TYR:HE2	1:A:383:VAL:HG21	1.77	0.48
1:A:613:GLN:OE1	1:A:650:TYR:HA	2.13	0.48
1:B:164:ALA:C	1:B:165:GLN:HG2	2.34	0.48
1:B:399:LYS:HE3	1:B:402:GLU:OE1	2.13	0.48
1:B:402:GLU:HA	1:B:405:GLN:OE1	2.13	0.48
1:B:608:LYS:HZ1	1:B:613:GLN:HG3	1.78	0.48
1:A:957:PRO:HG2	1:A:960:SER:HB3	1.94	0.48
1:A:534:VAL:HG13	1:A:539:GLN:HB3	1.94	0.48
1:A:551:LYS:HE3	1:A:699:TYR:HE2	1.78	0.48
1:A:742:GLY:O	1:A:744:VAL:N	2.46	0.48
1:B:567:VAL:CG2	1:B:568:PHE:N	2.76	0.48
1:B:708:ASP:O	1:B:711:ALA:HB3	2.14	0.48
1:B:1001:GLN:HA	1:B:1004:LEU:HD12	1.94	0.48
1:B:977:LYS:CG	1:B:1011:ILE:HG21	2.44	0.48
1:B:713:ILE:HG22	1:B:717:LYS:NZ	2.28	0.48
1:B:379:SER:OG	1:B:418:ASP:OD1	2.32	0.48
1:A:551:LYS:HE3	1:A:699:TYR:CE2	2.48	0.48
1:A:256:ASN:N	1:A:256:ASN:OD1	2.44	0.48
1:A:470:TRP:HE3	1:A:470:TRP:H	1.62	0.48
1:A:713:ILE:CD1	1:A:752:LEU:HA	2.43	0.48
1:B:1012:GLN:O	1:B:1015:GLU:N	2.47	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:220:THR:O	1:B:259:LEU:HD12	2.13	0.48
1:A:217:SER:HB2	1:A:262:GLU:CD	2.33	0.48
1:B:367:LYS:HG2	1:B:387:ILE:CD1	2.41	0.48
1:B:160:LEU:HD12	1:B:161:PHE:N	2.29	0.47
1:A:907:TYR:HA	1:A:910:MET:HE2	1.96	0.47
1:B:203:VAL:HG22	1:B:250:ALA:HB1	1.96	0.47
1:B:324:GLN:HG3	1:B:325:TYR:CD1	2.49	0.47
1:B:510:ASP:O	1:B:514:ALA:N	2.45	0.47
1:B:748:ARG:HG3	1:B:751:ASP:OD1	2.14	0.47
1:A:951:LYS:CD	1:A:951:LYS:N	2.77	0.47
1:B:174:PRO:HD2	1:B:311:PHE:HD2	1.79	0.47
1:B:379:SER:OG	1:B:381:TYR:HE1	1.97	0.47
1:B:400:LEU:HG	1:B:502:PHE:HE1	1.80	0.47
1:B:945:VAL:HG21	1:B:970:SER:OG	2.13	0.47
1:A:623:LYS:HZ2	1:A:628:LEU:HA	1.79	0.47
1:B:324:GLN:HE21	1:B:325:TYR:HE1	1.60	0.47
1:B:1009:LEU:O	1:B:1013:TRP:HB2	2.15	0.47
1:B:408:PHE:O	1:B:410:ILE:N	2.43	0.47
1:A:546:SER:O	1:A:550:PHE:HD2	1.97	0.47
1:A:594:ASN:O	1:A:600:THR:HG22	2.15	0.47
1:B:976:THR:C	1:B:1011:ILE:HD11	2.35	0.47
1:B:394:LEU:O	1:B:398:VAL:HG23	2.15	0.47
1:A:396:THR:HA	1:A:399:LYS:HZ2	1.78	0.47
1:B:977:LYS:HZ1	1:B:1008:GLN:HG3	1.78	0.47
1:B:536:SER:HB3	1:B:539:GLN:OE1	2.14	0.47
1:A:617:PRO:HB3	1:A:652:TRP:CE3	2.49	0.47
1:B:172:VAL:HG23	1:B:306:PHE:HE2	1.80	0.47
1:B:691:LYS:NZ	1:B:693:ASN:O	2.47	0.47
1:B:861:THR:OG1	1:B:864:PHE:N	2.46	0.47
1:B:994:THR:HA	1:B:997:LEU:HD11	1.97	0.47
1:B:547:LEU:HD12	1:B:547:LEU:HA	1.62	0.47
1:B:978:THR:OG1	1:B:979:HIS:N	2.48	0.47
1:B:994:THR:O	1:B:997:LEU:HD12	2.15	0.47
1:A:274:PHE:HD1	1:A:292:THR:HG22	1.80	0.47
1:B:572:VAL:HG13	1:B:576:LEU:HD13	1.96	0.47
1:A:222:MET:HG3	1:A:229:GLU:OE1	2.14	0.46
1:A:560:LYS:NZ	1:A:565:GLU:HB3	2.30	0.46
1:B:1012:GLN:O	1:B:1013:TRP:C	2.53	0.46
1:B:825:GLU:O	1:B:829:THR:OG1	2.19	0.46
1:A:1016:LYS:CE	1:A:1016:LYS:HA	2.37	0.46
1:B:237:TYR:HE2	1:B:240:HIS:ND1	2.13	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:245:ILE:HD13	1:B:259:LEU:HD21	1.97	0.46
1:B:884:ILE:HG13	1:B:886:SER:H	1.79	0.46
1:B:425:PHE:CD2	1:B:920:ARG:NH1	2.84	0.46
1:A:1021:LEU:HD22	1:A:1025:LEU:HD22	1.97	0.46
1:B:462:ILE:O	1:B:466:LEU:HB2	2.16	0.46
1:B:620:THR:OG1	1:B:622:GLN:OE1	2.27	0.46
1:B:693:ASN:ND2	1:B:696:MET:HA	2.29	0.46
1:B:748:ARG:CZ	1:B:750:PHE:CB	2.92	0.46
1:A:389:GLN:HG3	1:A:389:GLN:O	2.16	0.46
1:A:807:THR:O	1:A:820:ARG:HD3	2.15	0.46
1:B:191:ARG:NE	1:B:263:TYR:CD2	2.83	0.46
1:B:312:LYS:HG2	1:B:353:LYS:HB3	1.97	0.46
1:B:484:TRP:HZ2	1:B:531:SER:HB2	1.80	0.46
1:A:580:SER:O	1:A:581[B]:TYR:CG	2.68	0.46
1:A:660:THR:CB	1:A:687:VAL:HG11	2.41	0.46
1:B:688:LEU:O	1:B:711:ALA:HB1	2.16	0.46
1:B:718:ILE:HG13	1:B:719:ASN:N	2.29	0.46
1:B:718:ILE:HG13	1:B:719:ASN:H	1.80	0.46
1:A:233:GLU:O	1:A:246:VAL:HG22	2.14	0.46
1:A:623:LYS:HG2	1:A:627:GLU:OE2	2.16	0.46
1:B:256:ASN:C	1:B:257:TYR:CD1	2.86	0.46
1:A:310:ALA:HA	1:A:583:SER:OG	2.16	0.46
1:A:476:THR:O	1:A:584:ILE:HG13	2.16	0.46
1:A:747:LYS:HZ3	1:A:1024:TRP:HE3	1.64	0.46
1:B:257:TYR:N	1:B:257:TYR:CD1	2.84	0.46
1:B:405:GLN:HA	1:B:470:TRP:CZ2	2.51	0.46
1:A:747:LYS:NZ	1:A:1020:SER:O	2.49	0.46
1:A:320:ILE:HD11	1:A:345:GLN:OE1	2.16	0.46
1:B:460:LYS:HD2	1:B:494:GLU:CB	2.45	0.46
1:A:175:LEU:O	1:A:175:LEU:HD12	2.16	0.46
1:A:623:LYS:CD	1:A:628:LEU:HA	2.42	0.46
1:A:906:LEU:HD22	1:A:931:VAL:HG22	1.97	0.46
1:B:804:GLN:OE1	1:B:805:GLN:HG3	2.16	0.46
1:B:847:MET:HB2	1:B:847:MET:HE3	1.88	0.46
1:A:219:VAL:O	1:A:220:THR:OG1	2.26	0.46
1:A:604:LYS:HD3	1:A:604:LYS:HA	1.73	0.46
1:A:951:LYS:HB3	1:A:955:LYS:NZ	2.31	0.46
1:B:748:ARG:CZ	1:B:1024:TRP:HZ3	2.29	0.45
1:B:233:GLU:OE1	1:B:234:ILE:N	2.49	0.45
1:B:194:VAL:O	1:B:260:LYS:HA	2.16	0.45
1:B:715:GLN:HA	1:B:718:ILE:HG12	1.98	0.45

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:960:SER:O	1:B:963:ILE:HG22	2.16	0.45
1:B:977:LYS:HE2	1:B:1011:ILE:HB	1.98	0.45
1:B:994:THR:HA	1:B:997:LEU:CD1	2.46	0.45
1:A:396:THR:HA	1:A:399:LYS:HZ1	1.82	0.45
1:A:630:ILE:HG21	1:A:656:LEU:CD1	2.46	0.45
1:B:179:LEU:HA	1:B:193:SER:O	2.16	0.45
1:B:423:PRO:HA	1:B:440:GLU:OE1	2.16	0.45
1:B:559:LEU:HD23	1:B:568:PHE:CE2	2.48	0.45
1:B:595:GLU:O	1:B:596:VAL:O	2.33	0.45
1:B:601:LEU:HD12	1:B:601:LEU:HA	1.71	0.45
1:B:861:THR:OG1	1:B:863:VAL:HB	2.16	0.45
1:B:916:GLY:HA2	1:B:919:PHE:O	2.16	0.45
1:A:236:GLU:HA	1:A:243:ILE:HA	1.98	0.45
1:A:387:ILE:O	1:A:390:VAL:HG22	2.16	0.45
1:A:623:LYS:HE3	1:A:628:LEU:HD12	1.97	0.45
1:A:886:SER:OG	1:A:889:GLU:HG3	2.16	0.45
1:B:214:HIS:CE1	1:B:300:ARG:O	2.69	0.45
1:B:341:ASP:OD1	1:B:342:GLY:N	2.49	0.45
1:B:372:ASP:OD1	1:B:372:ASP:N	2.41	0.45
1:B:387:ILE:HG23	1:B:390:VAL:HG21	1.99	0.45
1:B:590:TRP:HB3	1:B:604:LYS:HG3	1.99	0.45
1:A:262:GLU:CD	1:A:262:GLU:C	2.75	0.45
1:A:410:ILE:HD11	1:A:577:HIS:CD2	2.52	0.45
1:B:521:LYS:CE	1:B:522:ASP:HB2	2.45	0.45
1:B:563:LEU:CG	1:B:567:VAL:HG21	2.30	0.45
1:A:986:PHE:CZ	1:A:990:GLN:NE2	2.84	0.45
1:B:1017:ASN:O	1:B:1021:LEU:HG	2.17	0.45
1:B:281:ASP:CG	1:B:282:GLU:N	2.69	0.45
1:B:271:TYR:OH	1:B:426:GLU:OE1	2.13	0.45
1:B:623:LYS:HE2	1:B:627:GLU:N	2.32	0.45
1:B:725:ASP:O	1:B:764:PRO:HG3	2.16	0.45
1:B:996:ARG:HA	1:B:1001:GLN:OE1	2.16	0.45
1:B:172:VAL:HG21	1:B:207:ILE:HG23	1.99	0.45
1:B:545:ASP:OD2	1:B:547:LEU:HB3	2.17	0.45
1:B:796:PHE:CE1	1:B:832:LEU:HB3	2.51	0.45
1:A:211:SER:N	1:A:241:GLY:O	2.38	0.45
1:B:190:PHE:HD1	1:B:267:ILE:HG12	1.81	0.45
1:B:445:TYR:OH	1:B:447:SER:HA	2.16	0.45
1:B:466:LEU:O	1:B:469:GLN:HG2	2.17	0.45
1:A:360:ALA:HB2	1:A:432:ASN:OD1	2.17	0.45
1:A:495:TYR:HE1	1:A:510:ASP:HB2	1.82	0.45

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:556:LEU:O	1:A:560:LYS:HB3	2.17	0.45
1:A:653:HIS:HD2	1:A:675:ASP:CB	2.30	0.45
1:B:1000:VAL:O	1:B:1004:LEU:HG	2.16	0.45
1:B:352:VAL:HG21	1:B:581:TYR:HE2	1.82	0.45
1:B:796:PHE:CG	1:B:832:LEU:HD13	2.52	0.45
1:B:949:TRP:O	1:B:953:VAL:HG13	2.16	0.45
1:A:295:GLU:HB3	1:A:430:MET:SD	2.57	0.45
1:A:209:LEU:HG	1:A:305:CYS:C	2.38	0.45
1:A:728:ARG:NH1	1:A:759:GLU:OE2	2.50	0.44
1:B:637:LEU:CD2	1:B:1009:LEU:HD22	2.35	0.44
1:B:433:TRP:HE1	1:B:469:GLN:CA	2.22	0.44
1:B:460:LYS:NZ	1:B:491:THR:O	2.50	0.44
1:B:604:LYS:HD3	1:B:604:LYS:HA	1.70	0.44
1:B:606:MET:HG3	1:B:653:HIS:HB2	1.99	0.44
1:A:1016:LYS:HD2	1:A:1016:LYS:N	2.30	0.44
1:A:368:ASN:HD22	1:A:369:LEU:N	2.15	0.44
1:B:368:ASN:O	1:B:369:LEU:HD23	2.17	0.44
1:B:367:LYS:HZ3	1:B:387:ILE:HG13	1.82	0.44
1:B:713:ILE:HG22	1:B:717:LYS:HZ2	1.80	0.44
1:A:163:TRP:HB2	1:A:208:ILE:HD13	1.98	0.44
1:A:320:ILE:HG13	1:A:345:GLN:HA	2.00	0.44
1:B:975:SER:C	1:B:1011:ILE:HG13	2.37	0.44
1:B:176:ARG:NE	1:B:350:GLU:OE1	2.50	0.44
1:B:177:TYR:CD2	1:B:196:ILE:HG12	2.52	0.44
1:B:412:TYR:HA	1:B:413:PRO:HD3	1.62	0.44
1:B:742:GLY:O	1:B:744:VAL:N	2.45	0.44
1:A:329:SER:OG	1:A:330:ASN:N	2.51	0.44
1:A:825:GLU:HB3	1:A:862:THR:OG1	2.18	0.44
1:A:961:TYR:O	1:A:964:GLN:OE1	2.35	0.44
1:B:203:VAL:HA	1:B:251:LEU:O	2.17	0.44
1:A:182:HIS:CA	1:A:191:ARG:HB2	2.46	0.44
1:A:438:PHE:CE2	1:A:461:ILE:HG22	2.51	0.44
1:B:609:THR:HG21	1:B:653:HIS:CE1	2.53	0.44
1:A:884:ILE:O	1:A:890:LYS:HE2	2.18	0.44
1:B:215:ASN:O	1:B:264:SER:N	2.51	0.44
1:B:486:ASN:ND2	1:B:486:ASN:H	2.14	0.44
1:B:500:LYS:HE3	1:B:500:LYS:HB2	1.70	0.44
1:A:163:TRP:CD2	1:A:169:PRO:HG3	2.52	0.44
1:A:182:HIS:CB	1:A:191:ARG:CZ	2.95	0.44
1:A:403:PHE:CG	1:A:501:ILE:HD11	2.53	0.44
1:A:616:PHE:HE2	1:A:701:ILE:HG13	1.82	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:912:SER:HB3	1:B:917:ASP:HB2	1.99	0.44
1:A:331:MET:CE	1:A:352:VAL:H	2.31	0.44
1:A:408:PHE:CD2	1:A:470:TRP:CG	3.05	0.44
1:B:343:LEU:C	1:B:343:LEU:HD23	2.38	0.44
1:B:913:SER:OG	1:B:924:LEU:HB2	2.18	0.44
1:B:954:GLN:C	1:B:955:LYS:HD2	2.38	0.44
1:A:403:PHE:C	1:A:405:GLN:CG	2.86	0.43
1:A:455:ARG:HA	1:A:458:VAL:HG12	1.98	0.43
1:B:445:TYR:CZ	1:B:447:SER:HA	2.53	0.43
1:A:1021:LEU:HB3	1:A:1025:LEU:HD23	1.99	0.43
1:A:476:THR:HG22	1:A:477:MET:N	2.33	0.43
1:A:623:LYS:HE2	1:A:623:LYS:HB2	1.66	0.43
1:B:1008:GLN:O	1:B:1012:GLN:HB3	2.18	0.43
1:B:183:PRO:HA	1:B:190:PHE:CA	2.44	0.43
1:B:512:LEU:HA	1:B:512:LEU:HD12	1.75	0.43
1:B:685:GLU:N	1:B:685:GLU:OE1	2.51	0.43
1:B:861:THR:CG2	1:B:864:PHE:HB2	2.38	0.43
1:B:921:THR:HG22	1:B:956:PHE:HZ	1.84	0.43
1:A:281:ASP:CB	1:A:285:GLU:H	2.32	0.43
1:A:386:LYS:C	1:A:388:GLY:N	2.72	0.43
1:A:399:LYS:NZ	1:A:399:LYS:HB2	2.31	0.43
1:A:683:LEU:HD13	1:A:685:GLU:O	2.18	0.43
1:A:703:HIS:HE1	1:A:744:VAL:HG23	1.83	0.43
1:A:881:TYR:HE1	1:A:890:LYS:O	2.01	0.43
1:B:709:TRP:CZ2	1:B:744:VAL:HG22	2.53	0.43
1:B:797:LYS:HG2	1:B:800:GLN:CB	2.48	0.43
1:B:861:THR:HG22	1:B:892:LYS:CG	2.48	0.43
1:B:190:PHE:O	1:B:191:ARG:HG2	2.19	0.43
1:B:196:ILE:HG22	1:B:198:VAL:HG13	2.00	0.43
1:B:402:GLU:HA	1:B:405:GLN:CD	2.38	0.43
1:B:748:ARG:NH2	1:B:794:ARG:NH2	2.66	0.43
1:B:861:THR:O	1:B:861:THR:HG23	2.17	0.43
1:A:161:PHE:HE1	1:A:163:TRP:HB3	1.80	0.43
1:A:405:GLN:CB	1:A:406:ASN:HD22	2.07	0.43
1:A:647:ASP:OD1	1:A:648:THR:N	2.51	0.43
1:A:696:MET:CB	1:A:730:ASN:HD22	2.32	0.43
1:B:653:HIS:HB3	1:B:673:LEU:HD11	2.00	0.43
1:B:792:VAL:HG13	1:B:826:PHE:CZ	2.54	0.43
1:A:160:LEU:HA	1:A:160:LEU:HD12	1.82	0.43
1:A:217:SER:H	1:A:262:GLU:CD	2.19	0.43
1:B:501:ILE:HG13	1:B:502:PHE:CD1	2.54	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:518:THR:C	1:B:521:LYS:HE3	2.39	0.43
1:A:163:TRP:CE3	1:A:169:PRO:HG3	2.53	0.43
1:A:963:ILE:HD12	1:A:963:ILE:HA	1.79	0.43
1:B:195:THR:HA	1:B:259:LEU:O	2.19	0.43
1:A:403:PHE:CD2	1:A:403:PHE:O	2.72	0.43
1:A:607:MET:O	1:A:611:THR:HG23	2.19	0.43
1:A:778:LEU:HA	1:A:778:LEU:HD23	1.87	0.43
1:A:964:GLN:CD	1:A:965:ASN:HB2	2.40	0.43
1:B:549:TYR:N	1:B:549:TYR:CD1	2.87	0.43
1:B:951:LYS:HA	1:B:951:LYS:HD3	1.86	0.43
1:A:422:ILE:HA	1:A:423:PRO:HD3	1.65	0.42
1:A:512:LEU:HA	1:A:512:LEU:HD12	1.52	0.42
1:B:748:ARG:HH22	1:B:794:ARG:NE	2.17	0.42
1:A:315:PHE:O	1:A:350:GLU:HA	2.19	0.42
1:A:466:LEU:HD12	1:A:466:LEU:HA	1.88	0.42
1:B:479:TRP:CG	1:B:480:TRP:N	2.87	0.42
1:B:727:ASP:OD1	1:B:728:ARG:N	2.52	0.42
1:A:511:PHE:CE2	1:A:557:LEU:HD22	2.43	0.42
1:A:626:LYS:N	1:A:686:GLU:OE2	2.52	0.42
1:A:653:HIS:HD2	1:A:675:ASP:HB2	1.85	0.42
1:A:783:GLY:O	1:A:785:MET:HG3	2.19	0.42
1:B:327:ALA:HB3	1:B:346:ASP:OD2	2.18	0.42
1:B:400:LEU:HD23	1:B:501:ILE:HD11	2.01	0.42
1:B:403:PHE:C	1:B:403:PHE:CD1	2.92	0.42
1:B:522:ASP:OD1	1:B:527:SER:OG	2.36	0.42
1:A:209:LEU:HD12	1:A:306:PHE:CE2	2.53	0.42
1:A:433:TRP:HE1	1:A:469:GLN:CB	2.32	0.42
1:A:440:GLU:CG	1:A:444:LEU:HD11	2.50	0.42
1:A:956:PHE:HA	1:A:957:PRO:HD2	1.94	0.42
1:B:367:LYS:NZ	1:B:387:ILE:HG13	2.34	0.42
1:B:680:VAL:C	1:B:681:ILE:HD12	2.39	0.42
1:A:480:TRP:CE3	1:A:483:LEU:HD12	2.54	0.42
1:A:495:TYR:CD1	1:A:511:PHE:HB2	2.54	0.42
1:A:788:ALA:O	1:A:791:LEU:HB3	2.20	0.42
1:A:965:ASN:O	1:A:969:GLY:N	2.40	0.42
1:B:1012:GLN:O	1:B:1015:GLU:CG	2.67	0.42
1:B:596:VAL:HG13	1:B:597:THR:H	1.84	0.42
1:A:747:LYS:HZ1	1:A:1021:LEU:HA	1.83	0.42
1:A:376:THR:HG21	1:A:412:TYR:CE2	2.54	0.42
1:A:569:GLN:O	1:A:572:VAL:HB	2.19	0.42
1:B:978:THR:HG23	1:B:978:THR:H	1.59	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1009:LEU:HD23	1:A:1009:LEU:HA	1.85	0.42
1:A:215:ASN:H	3:A:1106:NAG:H81	1.83	0.42
1:A:320:ILE:HG13	1:A:345:GLN:HB2	2.00	0.42
1:A:619:VAL:HB	1:A:702:VAL:HG22	2.00	0.42
1:A:623:LYS:HZ2	1:A:628:LEU:CA	2.33	0.42
1:A:633:GLU:CG	1:A:634:ARG:N	2.83	0.42
1:A:776:TYR:C	1:A:776:TYR:CD1	2.92	0.42
1:B:920:ARG:CZ	1:B:922:GLN:HE21	2.32	0.42
1:A:219:VAL:O	1:A:220:THR:CB	2.66	0.42
1:A:710:GLU:HA	1:A:713:ILE:CG2	2.48	0.42
1:B:452:MET:SD	1:B:455:ARG:CG	3.06	0.42
1:A:168:LEU:HA	1:A:168:LEU:HD23	1.84	0.42
1:A:306:PHE:HB3	1:A:311:PHE:CD2	2.54	0.42
1:A:653:HIS:CD2	1:A:675:ASP:HB2	2.54	0.42
1:B:747:LYS:O	1:B:748:ARG:CB	2.67	0.42
1:B:980:LEU:O	1:B:984:GLN:NE2	2.52	0.42
1:A:367:LYS:CE	1:A:368:ASN:O	2.68	0.42
1:A:435:LEU:HA	1:A:435:LEU:HD12	1.84	0.42
1:A:403:PHE:HB2	1:A:501:ILE:HD11	2.02	0.42
1:B:419:LEU:HG	1:B:438:PHE:HE1	1.84	0.42
1:B:796:PHE:CZ	1:B:797:LYS:HD2	2.54	0.42
1:B:952:LEU:HD22	1:B:966:ILE:HD13	2.02	0.42
1:A:538:GLU:O	1:A:542:GLU:HB3	2.20	0.41
1:A:809:THR:HG21	1:A:811:GLU:OE2	2.19	0.41
1:B:977:LYS:NZ	1:B:1011:ILE:HD13	2.35	0.41
1:A:869:LYS:NZ	1:A:899:SER:O	2.39	0.41
1:A:929:ARG:NH2	1:A:965:ASN:ND2	2.68	0.41
1:B:797:LYS:HB3	1:B:800:GLN:HB2	2.02	0.41
1:A:217:SER:OG	3:A:1104:NAG:H81	2.19	0.41
1:A:824:LEU:HA	1:A:824:LEU:HD23	1.79	0.41
1:B:1021:LEU:HD23	1:B:1024:TRP:NE1	2.34	0.41
1:B:383:VAL:CG2	1:B:384:PRO:HD2	2.50	0.41
1:B:628:LEU:O	1:B:630:ILE:HG12	2.21	0.41
1:B:738:LEU:O	1:B:741:LEU:N	2.54	0.41
1:A:791:LEU:HA	1:A:1025:LEU:HD11	2.01	0.41
1:B:631:GLN:HG3	1:B:677:LYS:O	2.21	0.41
1:B:653:HIS:HA	1:B:675:ASP:HA	2.02	0.41
1:B:715:GLN:CD	1:B:718:ILE:HG12	2.39	0.41
1:B:743:LYS:CB	1:B:744:VAL:HB	2.51	0.41
1:A:894:LEU:HD21	1:A:927:ILE:HG13	2.02	0.41
1:B:392:TYR:CE1	1:B:455:ARG:CZ	3.04	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:896:ALA:O	1:B:899:SER:N	2.41	0.41
1:B:485:LEU:HA	1:B:485:LEU:HD12	1.83	0.41
1:B:626:LYS:HG3	1:B:685:GLU:O	2.20	0.41
1:B:779:LEU:CB	1:B:788:ALA:HB2	2.50	0.41
1:B:872:LYS:HD2	1:B:875:SER:CB	2.49	0.41
1:A:578:ASN:ND2	1:A:579:HIS:HE1	2.19	0.41
1:B:399:LYS:HB2	1:B:399:LYS:HE3	1.89	0.41
1:B:452:MET:HG3	1:B:452:MET:O	2.20	0.41
1:B:545:ASP:C	1:B:547:LEU:N	2.74	0.41
1:B:689:TRP:HB3	1:B:715:GLN:HG3	2.03	0.41
1:A:169:PRO:HG2	1:A:208:ILE:HD12	2.03	0.41
1:A:825:GLU:O	1:A:829:THR:OG1	2.21	0.41
1:A:441:GLU:OE2	1:A:887:GLU:HG2	2.20	0.41
1:A:961:TYR:CG	1:A:961:TYR:O	2.73	0.41
1:A:938:HIS:CE1	1:A:974:PHE:CE1	3.08	0.41
1:B:210:HIS:ND1	1:B:307:ASP:HB3	2.35	0.41
1:B:320:ILE:HG23	1:B:343:LEU:CD2	2.51	0.41
1:B:433:TRP:CE2	1:B:473:ASN:HB2	2.56	0.41
1:B:521:LYS:HE3	1:B:521:LYS:HB2	1.57	0.41
1:A:746:LEU:HD23	1:A:1021:LEU:HD21	2.02	0.41
1:A:480:TRP:HE3	1:A:483:LEU:HD12	1.86	0.41
1:B:408:PHE:HZ	1:B:493:MET:HG3	1.86	0.41
1:B:617:PRO:HA	1:B:633:GLU:O	2.21	0.41
1:B:609:THR:CG2	1:B:653:HIS:ND1	2.83	0.41
1:B:784:TYR:N	1:B:784:TYR:CD1	2.89	0.41
1:A:230:LYS:HE2	1:A:230:LYS:HB2	1.91	0.41
1:A:218:ARG:NH1	1:A:262:GLU:HB2	2.35	0.41
1:A:316:ILE:HG13	1:A:316:ILE:O	2.21	0.41
1:A:381:TYR:OH	3:A:1107:NAG:H82	2.20	0.41
1:A:416:LYS:HD2	1:A:418:ASP:OD2	2.20	0.41
1:A:578:ASN:ND2	1:A:579:HIS:CE1	2.89	0.41
1:A:626:LYS:H	1:A:627:GLU:CG	2.34	0.41
1:B:207:ILE:HD13	1:B:259:LEU:HD22	2.03	0.41
1:B:567:VAL:HG13	1:B:567:VAL:H	1.50	0.41
1:B:594:ASN:O	1:B:600:THR:N	2.47	0.41
1:A:623:LYS:CE	1:A:628:LEU:HD12	2.51	0.41
1:A:696:MET:HB2	1:A:730:ASN:HD22	1.86	0.41
1:A:846:TRP:CD1	1:A:855:LEU:HG	2.56	0.41
1:B:387:ILE:HG21	1:B:387:ILE:HD13	1.67	0.41
1:B:404:PHE:CE1	1:B:497:SER:HB3	2.56	0.41
1:B:623:LYS:HE2	1:B:627:GLU:CB	2.51	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:456:LYS:HE3	1:B:818:GLU:OE2	2.20	0.41
1:B:845:ASP:O	1:B:848:ALA:HB3	2.21	0.41
1:A:270:SER:O	1:A:271:TYR:CG	2.73	0.40
1:A:321:ARG:HG3	1:A:321:ARG:H	1.70	0.40
1:A:405:GLN:HG3	1:A:406:ASN:CA	2.48	0.40
1:A:657:SER:HB2	1:A:694:ILE:CG1	2.51	0.40
1:A:752:LEU:O	1:A:755:TYR:HB3	2.21	0.40
1:A:279:TYR:CE2	1:A:383:VAL:HG21	2.55	0.40
1:A:811:GLU:O	1:A:820:ARG:NH2	2.48	0.40
1:A:992:GLU:O	1:A:996:ARG:HG3	2.21	0.40
1:B:817:ARG:NE	1:B:858:ASP:OD2	2.54	0.40
1:B:980:LEU:HD22	1:B:1008:GLN:HG3	2.03	0.40
1:A:214:HIS:CE1	1:A:304:PRO:HD3	2.55	0.40
1:A:331:MET:HE3	1:A:352:VAL:H	1.86	0.40
1:A:841:LYS:HE3	1:A:841:LYS:HB3	1.63	0.40
1:B:608:LYS:HZ3	1:B:613:GLN:HG3	1.85	0.40
1:A:847:MET:HG3	1:A:876:PHE:CG	2.57	0.40
1:A:877:LEU:HD22	1:A:893:ILE:HG12	2.04	0.40
1:B:420:VAL:HG13	1:B:437:THR:HG22	2.03	0.40
1:B:569:GLN:O	1:B:573:VAL:HG23	2.21	0.40
1:B:608:LYS:CD	1:B:612:LEU:H	2.32	0.40
1:B:797:LYS:HB3	1:B:800:GLN:OE1	2.22	0.40
1:A:352:VAL:HG22	1:A:353:LYS:H	1.86	0.40
1:B:191:ARG:HA	1:B:191:ARG:HD3	1.19	0.40
1:B:509:GLU:HG2	1:B:763:ALA:HB2	2.02	0.40
1:B:520:LYS:HD2	1:B:737:GLU:OE2	2.22	0.40
1:B:748:ARG:HD2	1:B:751:ASP:N	2.37	0.40
1:B:753:ILE:HA	1:B:753:ILE:HD12	1.83	0.40
1:B:943:ASP:O	1:B:947:GLU:HG2	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:LYS:CD	3:B:1106:NAG:O7[1_554]	1.77	0.43

## 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	858/912 (94%)	760 (89%)	84 (10%)	14 (2%)	11	45
1	B	844/912 (92%)	743 (88%)	74 (9%)	27 (3%)	5	31
All	All	1702/1824 (93%)	1503 (88%)	158 (9%)	41 (2%)	7	37

All (41) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	224	ALA
1	A	270	SER
1	A	284	ASN
1	A	626	LYS
1	A	627	GLU
1	A	638	ASN
1	A	664	ASN
1	A	718	ILE
1	A	743	LYS
1	A	1020	SER
1	B	265	ALA
1	B	409	GLU
1	B	536	SER
1	B	596	VAL
1	B	670	SER
1	B	743	LYS
1	B	744	VAL
1	B	746	LEU
1	B	748	ARG
1	B	861	THR
1	B	1015	GLU
1	A	385	GLU
1	B	193	SER
1	B	213	GLY
1	B	373	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	521	LYS
1	B	1013	TRP
1	A	599	GLN
1	A	1019	LYS
1	B	223	SER
1	B	599	GLN
1	A	663	ARG
1	B	600	THR
1	B	535	GLN
1	B	627	GLU
1	B	628	LEU
1	B	1012	GLN
1	B	507	SER
1	B	719	ASN
1	B	1022	THR
1	B	296	PRO

### 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	756/813 (93%)	728 (96%)	28 (4%)	39	72
1	B	736/813 (90%)	707 (96%)	29 (4%)	37	71
All	All	1492/1626 (92%)	1435 (96%)	57 (4%)	38	71

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	220	THR
1	A	228	GLN
1	A	256	ASN
1	A	262	GLU
1	A	368	ASN
1	A	373	VAL
1	A	377	LEU

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	A	420	VAL
1	A	433	TRP
1	A	454	ASP
1	A	477	MET
1	A	499	GLU
1	A	560	LYS
1	A	579	HIS
1	A	623	LYS
1	A	631	GLN
1	A	657	SER
1	A	664	ASN
1	A	673	LEU
1	A	713	ILE
1	A	743	LYS
1	A	755	TYR
1	A	762	THR
1	A	773	ASP
1	A	821	SER
1	A	962	THR
1	A	984	GLN
1	A	990	GLN
1	B	176	ARG
1	B	252	LEU
1	B	262	GLU
1	B	399	LYS
1	B	405	GLN
1	B	420	VAL
1	B	426	GLU
1	B	431	GLU
1	B	433	TRP
1	B	457	LEU
1	B	486	ASN
1	B	500	LYS
1	B	530	ILE
1	B	535	GLN
1	B	536	SER
1	B	549	TYR
1	B	622	GLN
1	B	623	LYS
1	B	666	SER
1	B	682	ASN
1	B	744	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	746	LEU
1	B	755	TYR
1	B	794	ARG
1	B	861	THR
1	B	923	LYS
1	B	953	VAL
1	B	984	GLN
1	B	992	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	206	ASN
1	A	405	GLN
1	A	406	ASN
1	A	577	HIS
1	A	579	HIS
1	A	631	GLN
1	A	664	ASN
1	A	730	ASN
1	A	733	ASN
1	A	734	ASN
1	A	938	HIS
1	B	255	HIS
1	B	324	GLN
1	B	405	GLN
1	B	406	ASN
1	B	486	ASN
1	B	715	GLN
1	B	730	ASN
1	B	922	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 27 ligands modelled in this entry, 2 are monoatomic - leaving 25 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
3	NAG	A	1102	1,3	14,14,15	1.09	1 (7%)	15,19,21	1.33	2 (13%)
3	NAG	A	1103	3	14,14,15	0.37	0	15,19,21	0.59	0
3	NAG	A	1104	1	14,14,15	0.78	1 (7%)	15,19,21	0.93	1 (6%)
3	NAG	A	1105	1	14,14,15	0.47	0	15,19,21	0.85	1 (6%)
3	NAG	A	1106	1	14,14,15	0.22	0	15,19,21	0.64	0
3	NAG	A	1107	1,3	14,14,15	1.19	1 (7%)	15,19,21	1.06	1 (6%)
3	NAG	A	1108	3	14,14,15	0.55	0	15,19,21	0.63	0
3	NAG	A	1109	1	14,14,15	0.46	0	15,19,21	1.12	1 (6%)
3	NAG	A	1110	1	14,14,15	0.75	1 (7%)	15,19,21	1.05	1 (6%)
3	NAG	A	1111	1	14,14,15	0.52	0	15,19,21	0.76	1 (6%)
3	NAG	A	1112	1	14,14,15	1.26	1 (7%)	15,19,21	1.47	1 (6%)
3	NAG	A	1113	1	14,14,15	0.56	0	15,19,21	0.94	2 (13%)
3	NAG	A	1114	-	14,14,15	0.69	0	15,19,21	0.66	0
3	NAG	B	1102	1,3	14,14,15	0.30	0	15,19,21	0.53	0
3	NAG	B	1103	3	14,14,15	0.25	0	15,19,21	0.55	0
3	NAG	B	1104	1	14,14,15	0.95	1 (7%)	15,19,21	0.57	0
3	NAG	B	1105	1,3	14,14,15	1.87	4 (28%)	15,19,21	2.17	4 (26%)
3	NAG	B	1106	3	14,14,15	0.33	0	15,19,21	0.56	0
3	NAG	B	1107	1	14,14,15	0.52	0	15,19,21	0.54	0
3	NAG	B	1108	1,3	14,14,15	0.94	2 (14%)	15,19,21	0.75	1 (6%)
3	NAG	B	1109	3	14,14,15	0.40	0	15,19,21	0.56	0
3	NAG	B	1110	1	14,14,15	0.66	1 (7%)	15,19,21	0.70	0
3	NAG	B	1111	1	14,14,15	0.49	0	15,19,21	0.60	0
3	NAG	B	1112	1	14,14,15	0.35	0	15,19,21	0.63	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	B	1113	1	14,14,15	0.86	1 (7%)	15,19,21	0.66	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
3	NAG	A	1102	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	1103	3	-	0/6/23/26	0/1/1/1
3	NAG	A	1104	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1105	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1106	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1107	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	1108	3	-	0/6/23/26	0/1/1/1
3	NAG	A	1109	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1110	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1111	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1112	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1113	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1114	-	-	0/6/23/26	0/1/1/1
3	NAG	B	1102	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	1103	3	-	0/6/23/26	0/1/1/1
3	NAG	B	1104	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1105	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	1106	3	-	0/6/23/26	0/1/1/1
3	NAG	B	1107	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1108	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	1109	3	-	0/6/23/26	0/1/1/1
3	NAG	B	1110	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1111	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1112	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1113	1	-	0/6/23/26	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1107	NAG	O5-C1	-3.73	1.37	1.43
3	B	1105	NAG	O5-C1	-2.89	1.39	1.43
3	B	1105	NAG	C2-N2	2.12	1.50	1.46
3	B	1110	NAG	O5-C1	2.12	1.47	1.43
3	B	1105	NAG	C3-C2	2.24	1.57	1.52

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1108	NAG	O5-C1	2.31	1.47	1.43
3	B	1104	NAG	C1-C2	2.52	1.55	1.52
3	A	1102	NAG	C1-C2	2.53	1.55	1.52
3	B	1108	NAG	C1-C2	2.56	1.56	1.52
3	B	1113	NAG	O5-C1	2.60	1.48	1.43
3	A	1104	NAG	O5-C1	2.64	1.48	1.43
3	A	1110	NAG	O5-C1	2.65	1.48	1.43
3	A	1112	NAG	O5-C1	4.56	1.51	1.43
3	B	1105	NAG	C1-C2	5.25	1.59	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1105	NAG	C1-O5-C5	-5.50	104.58	112.17
3	B	1105	NAG	C1-C2-N2	-4.13	103.44	110.49
3	A	1107	NAG	C1-O5-C5	-3.27	107.65	112.17
3	B	1105	NAG	O5-C1-C2	-3.04	107.25	111.47
3	A	1102	NAG	O5-C1-C2	-2.73	107.67	111.47
3	A	1113	NAG	C1-O5-C5	-2.18	109.16	112.17
3	B	1105	NAG	C4-C3-C2	2.04	114.00	111.02
3	B	1108	NAG	C1-O5-C5	2.24	115.25	112.17
3	A	1113	NAG	C1-C2-N2	2.27	114.37	110.49
3	A	1111	NAG	C1-O5-C5	2.29	115.33	112.17
3	A	1105	NAG	C1-O5-C5	2.33	115.38	112.17
3	A	1102	NAG	O3-C3-C4	2.95	116.78	110.36
3	A	1104	NAG	C1-O5-C5	3.23	116.61	112.17
3	A	1110	NAG	C1-O5-C5	3.51	117.01	112.17
3	A	1109	NAG	C1-O5-C5	3.77	117.36	112.17
3	A	1112	NAG	C1-O5-C5	5.49	119.73	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1102	NAG	3	0
3	A	1104	NAG	1	0
3	A	1106	NAG	2	0
3	A	1107	NAG	2	0
3	A	1113	NAG	11	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1114	NAG	6	0
3	B	1103	NAG	1	0
3	B	1105	NAG	1	0
3	B	1106	NAG	1	1
3	B	1107	NAG	1	0
3	B	1112	NAG	2	0
3	B	1113	NAG	3	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	860/912 (94%)	0.10	28 (3%) 47 48	77, 117, 159, 184	0
1	B	851/912 (93%)	0.11	44 (5%) 28 29	83, 141, 167, 189	0
All	All	1711/1824 (93%)	0.10	72 (4%) 37 38	77, 131, 162, 189	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	251	LEU	5.9
1	B	221	PHE	5.2
1	B	621	VAL	5.0
1	B	658	TYR	4.2
1	B	619	VAL	3.9
1	A	646	SER	3.7
1	B	363	VAL	3.7
1	B	327	ALA	3.6
1	B	261	ILE	3.5
1	A	259	LEU	3.5
1	B	618	LEU	3.5
1	B	361	PHE	3.4
1	A	251	LEU	3.4
1	B	701	ILE	3.3
1	B	328	LEU	3.3
1	A	436	LEU	3.3
1	A	160	LEU	3.3
1	B	534	VAL	3.3
1	B	319	ILE	3.2
1	A	200	ALA	3.2
1	B	702	VAL	3.2
1	B	688	LEU	3.0
1	A	1025	LEU	3.0
1	B	756	LEU	3.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	480	TRP	2.9
1	A	419	LEU	2.9
1	B	470	TRP	2.8
1	A	181	LEU	2.8
1	B	259	LEU	2.8
1	B	362	ILE	2.7
1	B	185	LEU	2.7
1	B	290	ALA	2.6
1	A	319	ILE	2.6
1	A	261	ILE	2.6
1	B	407	TYR	2.6
1	A	245	ILE	2.5
1	A	206	ASN	2.5
1	A	540	ILE	2.5
1	A	435	LEU	2.4
1	A	361	PHE	2.4
1	B	245	ILE	2.4
1	A	221	PHE	2.4
1	A	185	LEU	2.4
1	B	668	TYR	2.4
1	B	687	VAL	2.3
1	A	205	TRP	2.2
1	A	378	VAL	2.2
1	B	628	LEU	2.2
1	B	408	PHE	2.2
1	B	530	ILE	2.2
1	B	181	LEU	2.2
1	B	274	PHE	2.2
1	B	540	ILE	2.2
1	B	802	GLN	2.2
1	A	480	TRP	2.2
1	B	346	ASP	2.1
1	A	207	ILE	2.1
1	A	443	LEU	2.1
1	B	692	VAL	2.1
1	A	183	PRO	2.1
1	A	362	ILE	2.1
1	B	219	VAL	2.1
1	B	614	LYS	2.1
1	B	414	LEU	2.1
1	B	443	LEU	2.1
1	B	296	PRO	2.0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	862	THR	2.0
1	A	619	VAL	2.0
1	A	387	ILE	2.0
1	B	474	LEU	2.0
1	A	397	THR	2.0
1	B	731	LEU	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	NAG	A	1106	14/15	0.30	0.34	4.65	146,164,179,183	0
3	NAG	B	1107	14/15	0.78	0.24	3.90	144,155,160,163	0
2	ZN	A	1101	1/1	0.96	0.28	1.67	83,83,83,83	1
3	NAG	A	1113	14/15	0.66	0.28	0.77	121,136,145,146	0
2	ZN	B	1101	1/1	0.95	0.20	0.21	143,143,143,143	0
3	NAG	B	1102	14/15	0.84	0.20	-0.02	157,163,171,173	0
3	NAG	B	1113	14/15	0.77	0.19	-0.07	143,153,171,182	0
3	NAG	A	1102	14/15	0.81	0.18	-0.71	135,147,158,159	0
3	NAG	A	1105	14/15	0.90	0.15	-1.11	147,162,165,170	0
3	NAG	B	1105	14/15	0.91	0.09	-1.29	151,163,175,181	0
3	NAG	B	1109	14/15	0.84	0.26	-	155,181,185,185	0
3	NAG	B	1103	14/15	0.82	0.22	-	169,174,178,178	0
3	NAG	A	1112	14/15	0.84	0.23	-	157,172,178,180	0
3	NAG	B	1112	14/15	0.82	0.18	-	166,184,188,195	0
3	NAG	A	1110	14/15	0.84	0.25	-	127,139,149,152	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	A	1103	14/15	0.89	0.17	-	160,168,175,176	0
3	NAG	A	1109	14/15	0.80	0.20	-	144,166,176,184	0
3	NAG	A	1104	14/15	0.79	0.20	-	160,165,175,176	0
3	NAG	A	1108	14/15	0.90	0.12	-	166,182,196,202	0
3	NAG	B	1106	14/15	0.78	0.17	-	158,165,174,176	0
3	NAG	B	1110	14/15	0.78	0.30	-	166,174,187,189	0
3	NAG	A	1107	14/15	0.93	0.15	-	146,153,162,173	0
3	NAG	A	1114	14/15	0.72	0.21	-	123,136,144,170	0
3	NAG	B	1108	14/15	0.88	0.13	-	145,160,172,173	0
3	NAG	B	1111	14/15	0.74	0.31	-	150,163,166,167	0
3	NAG	A	1111	14/15	0.87	0.26	-	114,132,145,145	0
3	NAG	B	1104	14/15	0.75	0.22	-	162,180,186,189	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.