



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 18, 2017 – 11:20 AM EST

PDB ID : 5TRM  
Title : Crystal structure of human GCN5 histone acetyltransferase domain  
Authors : Guo, Y.R.; Tao, Y.J.  
Deposited on : 2016-10-26  
Resolution : 2.90 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  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030736  
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) : rb-20030736

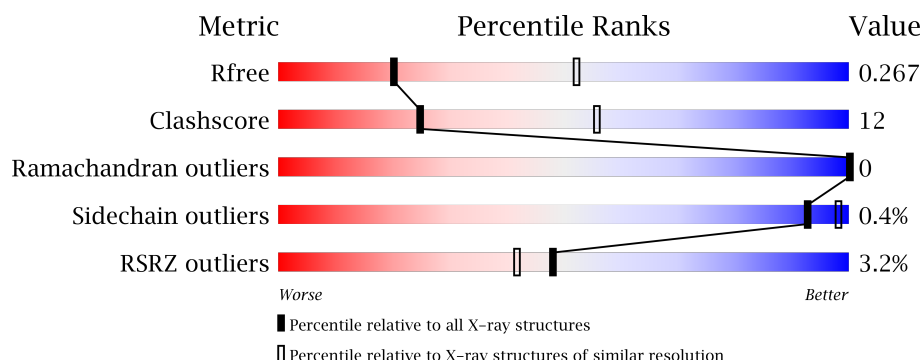
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	1586 (2.90-2.90)
Clashscore	112137	1807 (2.90-2.90)
Ramachandran outliers	110173	1768 (2.90-2.90)
Sidechain outliers	110143	1770 (2.90-2.90)
RSRZ outliers	101464	1596 (2.90-2.90)

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	168	<div> <div>0.1%</div> <div>76%</div> <div>20%</div> <div>0.1%</div> </div>
1	B	168	<div> <div>79%</div> <div>17%</div> <div>0.1%</div> </div>
1	C	168	<div> <div>0.1%</div> <div>82%</div> <div>13%</div> <div>5%</div> </div>
1	D	168	<div> <div>2%</div> <div>74%</div> <div>21%</div> <div>0.1%</div> </div>
1	E	168	<div> <div>3%</div> <div>76%</div> <div>21%</div> <div>0.1%</div> </div>

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	168	
1	G	168	
1	H	168	
1	I	168	
1	J	168	
1	K	168	
1	L	168	
1	M	168	
1	N	168	
1	O	168	
1	P	168	
1	Q	168	
1	R	168	
1	S	168	
1	T	168	
1	U	168	
1	V	168	
1	W	168	
1	X	168	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 31738 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 Histone acetyltransferase KAT2A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	162	Total	C	N	O	S	0	0	0
			1331	872	226	226	7			
1	W	160	Total	C	N	O	S	0	0	0
			1318	863	224	224	7			
1	V	161	Total	C	N	O	S	0	0	0
			1323	866	225	225	7			
1	U	164	Total	C	N	O	S	0	0	0
			1344	880	228	229	7			
1	T	160	Total	C	N	O	S	0	0	0
			1317	863	224	223	7			
1	S	161	Total	C	N	O	S	0	0	0
			1323	866	225	225	7			
1	R	162	Total	C	N	O	S	0	0	0
			1330	871	226	226	7			
1	Q	156	Total	C	N	O	S	0	0	0
			1284	839	220	218	7			
1	P	161	Total	C	N	O	S	0	0	0
			1323	866	225	225	7			
1	O	161	Total	C	N	O	S	0	0	0
			1323	866	225	225	7			
1	N	163	Total	C	N	O	S	0	0	0
			1335	874	227	227	7			
1	M	160	Total	C	N	O	S	0	0	0
			1315	860	224	224	7			
1	L	157	Total	C	N	O	S	0	0	0
			1296	850	220	219	7			
1	K	160	Total	C	N	O	S	0	0	0
			1318	863	224	224	7			
1	J	163	Total	C	N	O	S	0	0	0
			1335	874	227	227	7			
1	F	162	Total	C	N	O	S	0	0	0
			1330	871	226	226	7			

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	159	Total	C	N	O	S	0	0	0
			1312	860	223	222	7			
1	B	161	Total	C	N	O	S	0	0	0
			1326	869	225	225	7			
1	D	161	Total	C	N	O	S	0	0	0
			1323	866	225	225	7			
1	E	163	Total	C	N	O	S	0	0	0
			1332	871	227	227	7			
1	G	164	Total	C	N	O	S	0	0	0
			1340	877	228	228	7			
1	H	160	Total	C	N	O	S	0	0	0
			1314	861	223	223	7			
1	I	162	Total	C	N	O	S	0	0	0
			1331	872	226	226	7			
1	X	160	Total	C	N	O	S	0	0	0
			1315	860	224	224	7			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	495	GLY	-	expression tag	UNP Q92830
A	496	SER	-	expression tag	UNP Q92830
W	495	GLY	-	expression tag	UNP Q92830
W	496	SER	-	expression tag	UNP Q92830
V	495	GLY	-	expression tag	UNP Q92830
V	496	SER	-	expression tag	UNP Q92830
U	495	GLY	-	expression tag	UNP Q92830
U	496	SER	-	expression tag	UNP Q92830
T	495	GLY	-	expression tag	UNP Q92830
T	496	SER	-	expression tag	UNP Q92830
S	495	GLY	-	expression tag	UNP Q92830
S	496	SER	-	expression tag	UNP Q92830
R	495	GLY	-	expression tag	UNP Q92830
R	496	SER	-	expression tag	UNP Q92830
Q	495	GLY	-	expression tag	UNP Q92830
Q	496	SER	-	expression tag	UNP Q92830
P	495	GLY	-	expression tag	UNP Q92830
P	496	SER	-	expression tag	UNP Q92830
O	495	GLY	-	expression tag	UNP Q92830
O	496	SER	-	expression tag	UNP Q92830
N	495	GLY	-	expression tag	UNP Q92830
N	496	SER	-	expression tag	UNP Q92830
M	495	GLY	-	expression tag	UNP Q92830

*Continued on next page...*

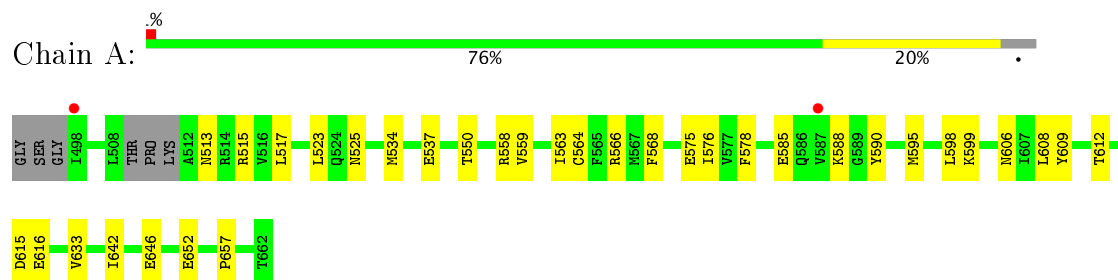
*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
M	496	SER	-	expression tag	UNP Q92830
L	495	GLY	-	expression tag	UNP Q92830
L	496	SER	-	expression tag	UNP Q92830
K	495	GLY	-	expression tag	UNP Q92830
K	496	SER	-	expression tag	UNP Q92830
J	495	GLY	-	expression tag	UNP Q92830
J	496	SER	-	expression tag	UNP Q92830
F	495	GLY	-	expression tag	UNP Q92830
F	496	SER	-	expression tag	UNP Q92830
C	495	GLY	-	expression tag	UNP Q92830
C	496	SER	-	expression tag	UNP Q92830
B	495	GLY	-	expression tag	UNP Q92830
B	496	SER	-	expression tag	UNP Q92830
D	495	GLY	-	expression tag	UNP Q92830
D	496	SER	-	expression tag	UNP Q92830
E	495	GLY	-	expression tag	UNP Q92830
E	496	SER	-	expression tag	UNP Q92830
G	495	GLY	-	expression tag	UNP Q92830
G	496	SER	-	expression tag	UNP Q92830
H	495	GLY	-	expression tag	UNP Q92830
H	496	SER	-	expression tag	UNP Q92830
I	495	GLY	-	expression tag	UNP Q92830
I	496	SER	-	expression tag	UNP Q92830
X	495	GLY	-	expression tag	UNP Q92830
X	496	SER	-	expression tag	UNP Q92830

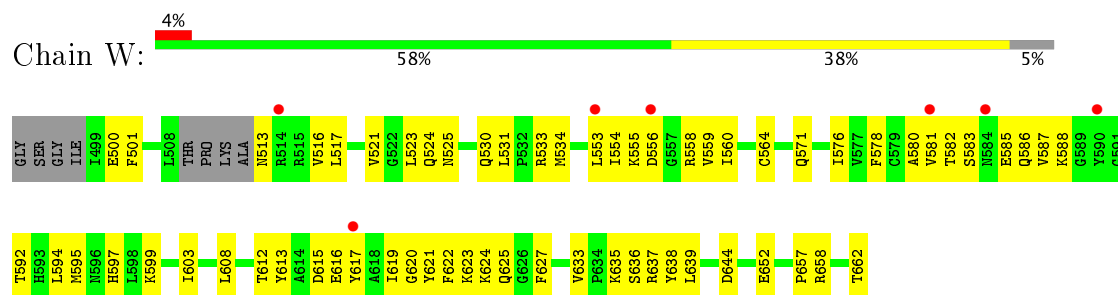
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

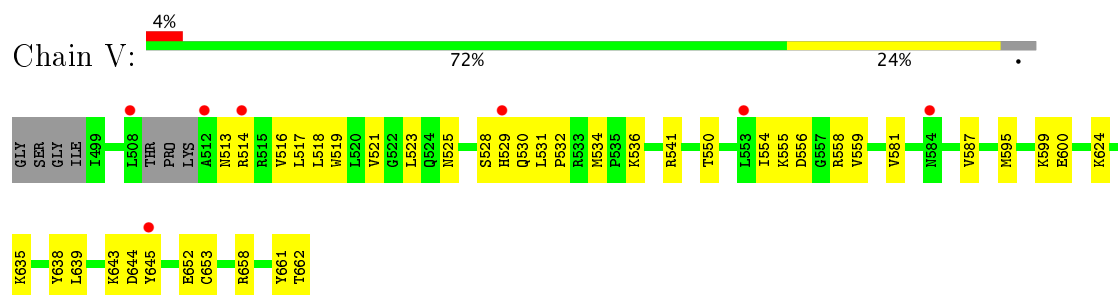
#### • Molecule 1: Histone acetyltransferase KAT2A



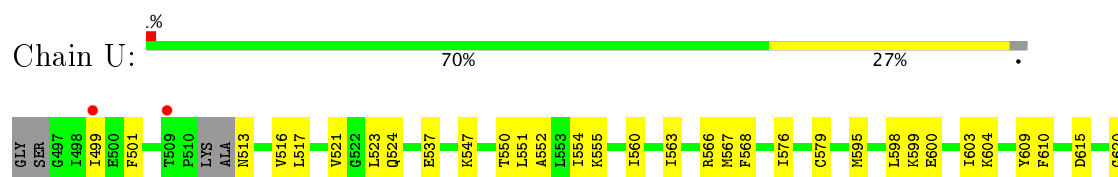
#### • Molecule 1: Histone acetyltransferase KAT2A



#### • Molecule 1: Histone acetyltransferase KAT2A

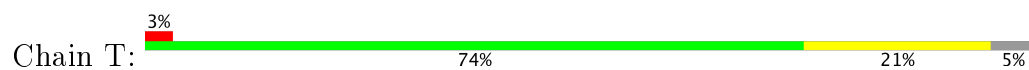


#### • Molecule 1: Histone acetyltransferase KAT2A

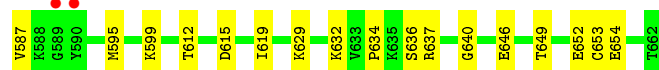
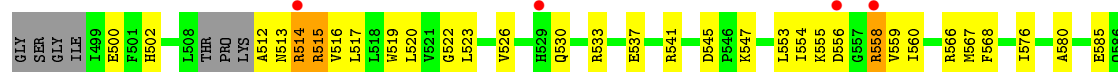




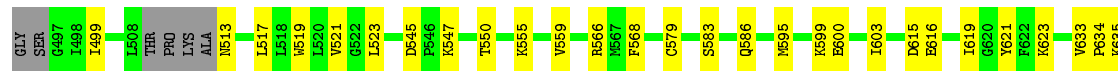
• Molecule 1: Histone acetyltransferase KAT2A



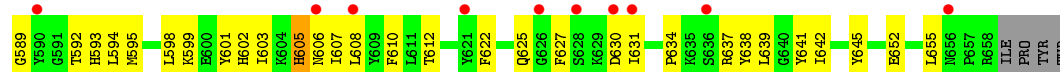
• Molecule 1: Histone acetyltransferase KAT2A



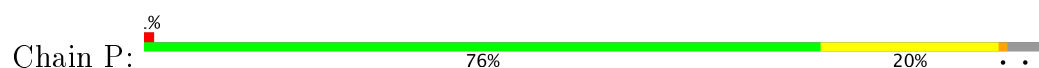
• Molecule 1: Histone acetyltransferase KAT2A



• Molecule 1: Histone acetyltransferase KAT2A

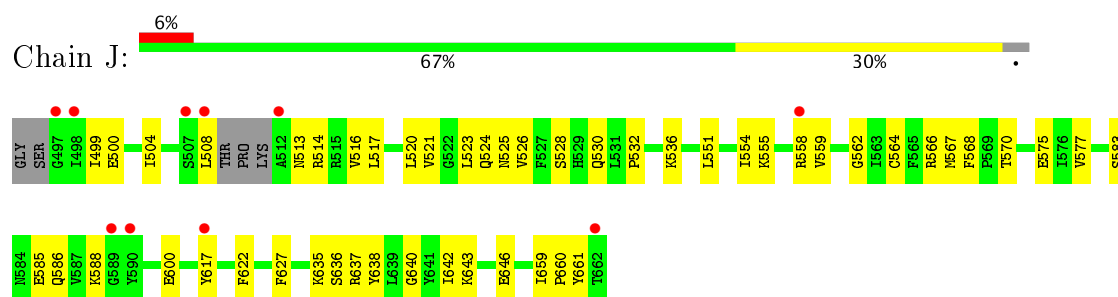


• Molecule 1: Histone acetyltransferase KAT2A

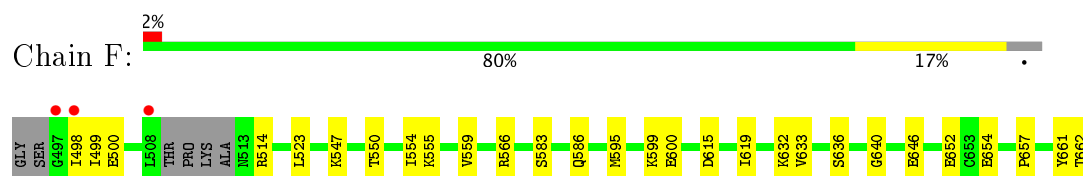




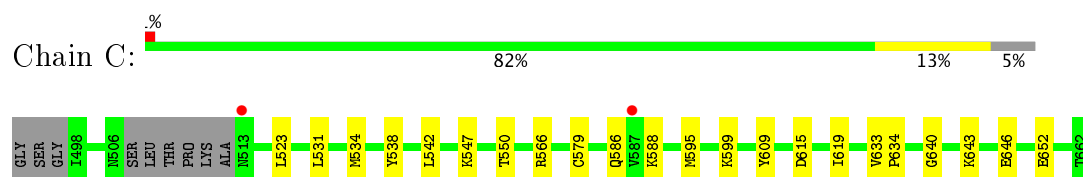




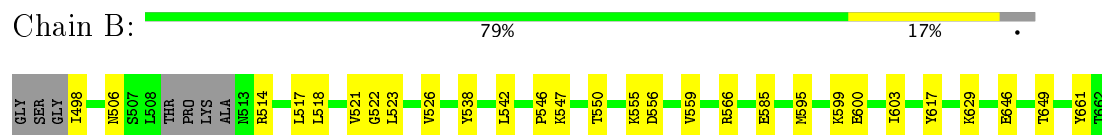
- Molecule 1: Histone acetyltransferase KAT2A



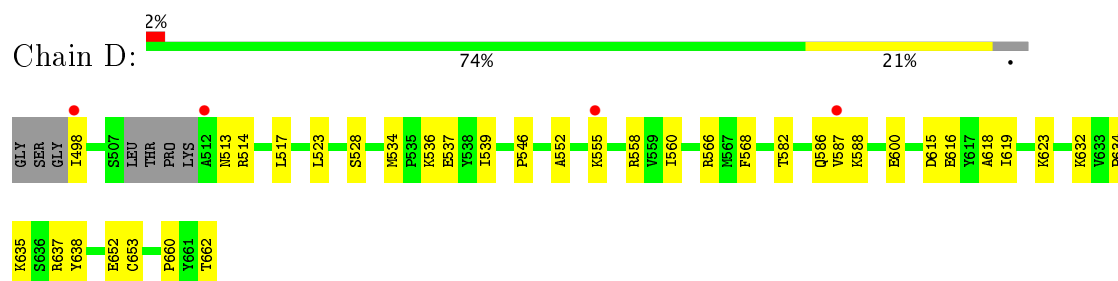
- Molecule 1: Histone acetyltransferase KAT2A



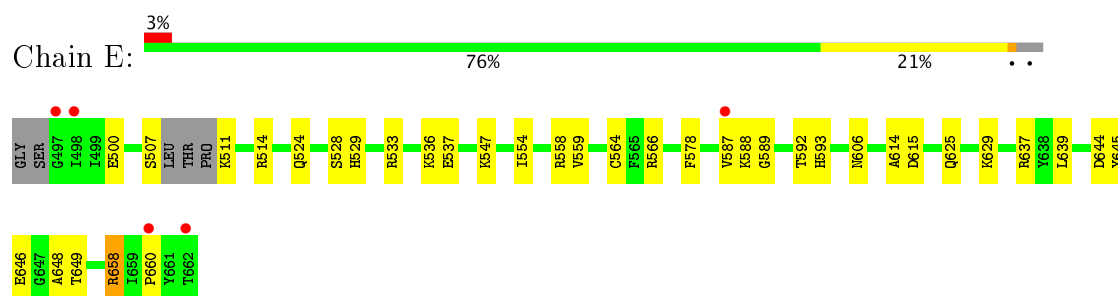
- Molecule 1: Histone acetyltransferase KAT2A



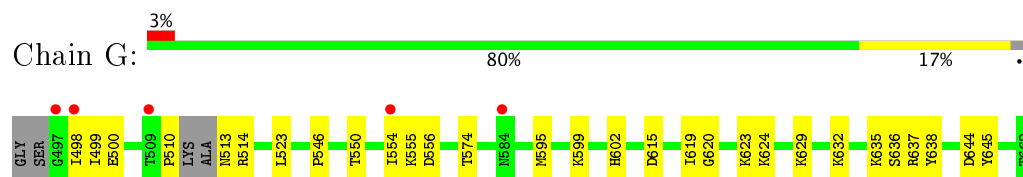
- Molecule 1: Histone acetyltransferase KAT2A



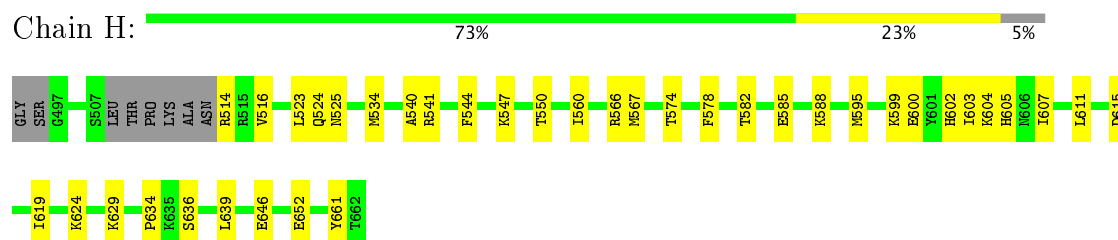
- Molecule 1: Histone acetyltransferase KAT2A



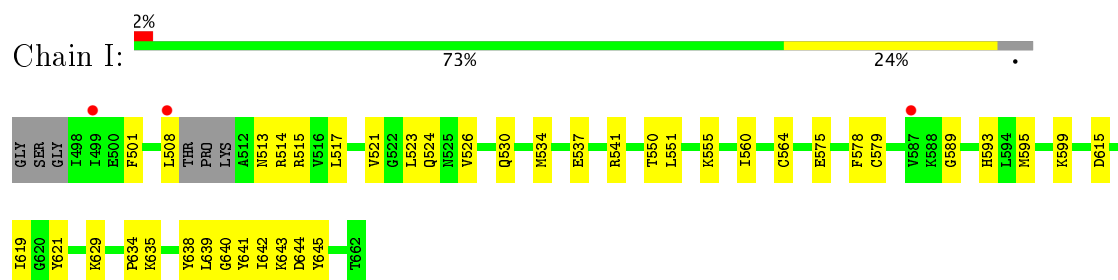
- Molecule 1: Histone acetyltransferase KAT2A



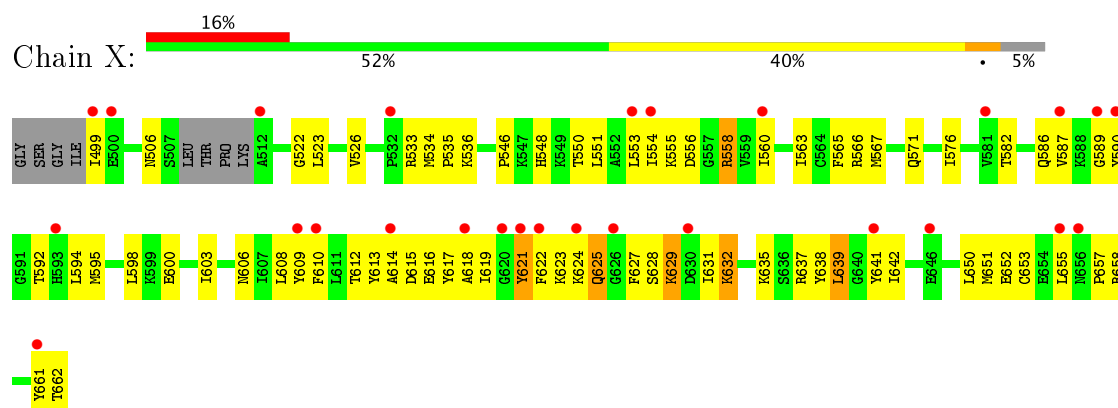
- Molecule 1: Histone acetyltransferase KAT2A



- Molecule 1: Histone acetyltransferase KAT2A



- Molecule 1: Histone acetyltransferase KAT2A



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	173.47Å 173.47Å 347.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.18 – 2.90 49.58 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.6 (48.18-2.90) 96.3 (49.58-2.90)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.49 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.10 _2152	Depositor
R, $R_{free}$	0.215 , 0.273 0.211 , 0.267	Depositor DCC
$R_{free}$ test set	5593 reflections (4.94%)	DCC
Wilson B-factor (Å <sup>2</sup> )	41.3	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 40.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	31738	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.73% 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](#)

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	0.44	0/1366	0.54	0/1842
1	B	0.49	0/1361	0.55	0/1835
1	C	0.48	1/1347 (0.1%)	0.54	0/1816
1	D	0.41	0/1358	0.57	0/1831
1	E	0.40	0/1367	0.56	0/1843
1	F	0.46	0/1365	0.52	0/1840
1	G	0.43	0/1375	0.57	1/1854 (0.1%)
1	H	0.48	0/1349	0.52	0/1818
1	I	0.42	0/1366	0.51	0/1842
1	J	0.43	0/1370	0.59	1/1847 (0.1%)
1	K	0.41	0/1353	0.51	0/1824
1	L	0.47	2/1331 (0.2%)	0.56	0/1794
1	M	0.41	0/1350	0.55	0/1820
1	N	0.42	0/1370	0.52	0/1847
1	O	0.42	0/1358	0.54	0/1831
1	P	0.47	1/1358 (0.1%)	0.52	0/1831
1	Q	0.40	0/1317	0.60	0/1773
1	R	0.52	0/1365	0.54	0/1840
1	S	0.54	2/1358 (0.1%)	0.71	5/1831 (0.3%)
1	T	0.38	0/1352	0.51	0/1823
1	U	0.48	0/1380	0.52	0/1862
1	V	0.42	0/1358	0.55	0/1831
1	W	0.51	2/1353 (0.1%)	0.58	0/1824
1	X	0.54	1/1350 (0.1%)	0.76	3/1820 (0.2%)
All	All	0.45	9/32577 (0.0%)	0.56	10/43919 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	J	0	1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	#Chirality outliers	#Planarity outliers
1	L	0	3
1	Q	0	1
1	X	0	2
All	All	0	7

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	W	616	GLU	CD-OE1	-9.27	1.15	1.25
1	W	616	GLU	CD-OE2	-8.24	1.16	1.25
1	X	621	TYR	CG-CD1	6.46	1.47	1.39
1	L	533	ARG	C-N	-6.34	1.19	1.34
1	S	514	ARG	CZ-NH1	6.13	1.41	1.33
1	C	579	CYS	CB-SG	-5.79	1.72	1.81
1	P	579	CYS	CB-SG	-5.60	1.72	1.81
1	L	579	CYS	CB-SG	-5.56	1.72	1.81
1	S	515	ARG	NE-CZ	-5.30	1.26	1.33

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	515	ARG	NE-CZ-NH2	-10.92	114.84	120.30
1	X	624	LYS	CD-CE-NZ	-7.12	95.34	111.70
1	S	515	ARG	NH1-CZ-NH2	6.66	126.72	119.40
1	S	558	ARG	NE-CZ-NH2	6.59	123.60	120.30
1	S	514	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	G	510	PRO	N-CA-CB	6.33	110.90	103.30
1	S	558	ARG	NE-CZ-NH1	-6.28	117.16	120.30
1	J	508	LEU	CA-CB-CG	5.88	128.82	115.30
1	X	639	LEU	CB-CG-CD1	-5.37	101.87	111.00
1	X	621	TYR	CA-CB-CG	5.21	123.31	113.40

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	J	646	GLU	Peptide
1	L	645	TYR	Peptide
1	L	646	GLU	Peptide
1	L	649	THR	Peptide
1	Q	605	HIS	Peptide

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
1	X	625	GLN	Peptide
1	X	632	LYS	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	1331	0	1347	26	0
1	B	1326	0	1342	17	3
1	C	1312	0	1326	14	1
1	D	1323	0	1336	39	0
1	E	1332	0	1341	40	0
1	F	1330	0	1345	17	1
1	G	1340	0	1348	28	1
1	H	1314	0	1328	35	3
1	I	1331	0	1347	34	2
1	J	1335	0	1348	46	0
1	K	1318	0	1331	14	0
1	L	1296	0	1308	58	0
1	M	1315	0	1325	28	0
1	N	1335	0	1350	14	0
1	O	1323	0	1336	23	1
1	P	1323	0	1336	27	0
1	Q	1284	0	1297	87	0
1	R	1330	0	1345	32	0
1	S	1323	0	1336	40	2
1	T	1317	0	1331	25	0
1	U	1344	0	1359	38	1
1	V	1323	0	1336	42	0
1	W	1318	0	1331	62	0
1	X	1315	0	1325	104	0
All	All	31738	0	32054	780	8

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 12.

All (780) 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:J:558:ARG:NH2	1:D:660:PRO:CB	1.69	1.52
1:V:514:ARG:HH12	1:V:518:LEU:CG	1.39	1.35
1:Q:571:GLN:HG2	1:Q:573:PHE:CE2	1.60	1.34
1:J:558:ARG:NH2	1:D:660:PRO:CG	1.95	1.30
1:J:558:ARG:NH2	1:D:660:PRO:HB2	1.29	1.29
1:L:500:GLU:OE2	1:L:502:HIS:CE1	1.88	1.25
1:Q:571:GLN:NE2	1:Q:637:ARG:O	1.73	1.22
1:V:514:ARG:NH1	1:V:518:LEU:HG	1.54	1.22
1:Q:571:GLN:CG	1:Q:573:PHE:CE2	2.26	1.19
1:Q:571:GLN:NE2	1:Q:637:ARG:C	1.97	1.16
1:X:555:LYS:NZ	1:X:556:ASP:OD2	1.82	1.12
1:V:514:ARG:HH12	1:V:518:LEU:HG	0.99	1.09
1:J:558:ARG:NH2	1:D:660:PRO:HG2	1.62	1.09
1:Q:571:GLN:CG	1:Q:573:PHE:HE2	1.65	1.08
1:R:600:GLU:OE2	1:R:661:TYR:HB2	1.54	1.07
1:D:546:PRO:HD3	1:G:514:ARG:NH2	1.68	1.05
1:O:555:LYS:NZ	1:O:585:GLU:OE2	1.86	1.05
1:R:600:GLU:OE2	1:R:661:TYR:CB	2.05	1.04
1:Q:571:GLN:CD	1:Q:573:PHE:CZ	2.32	1.03
1:V:514:ARG:HH12	1:V:518:LEU:CD1	1.71	1.02
1:Q:571:GLN:CD	1:Q:573:PHE:CE2	2.31	1.02
1:L:500:GLU:OE2	1:L:502:HIS:CD2	2.14	1.01
1:V:514:ARG:NH1	1:V:518:LEU:CG	2.17	1.01
1:R:600:GLU:OE2	1:R:661:TYR:CD2	2.12	1.01
1:L:500:GLU:CD	1:L:502:HIS:CE1	2.34	1.01
1:L:500:GLU:OE2	1:L:502:HIS:CG	2.14	1.01
1:V:514:ARG:NH1	1:V:518:LEU:CD1	2.25	0.99
1:Q:571:GLN:NE2	1:Q:573:PHE:CZ	2.31	0.98
1:L:500:GLU:OE2	1:L:502:HIS:ND1	1.96	0.98
1:L:500:GLU:OE2	1:L:502:HIS:NE2	1.97	0.96
1:S:632:LYS:NZ	1:S:654:GLU:OE1	1.98	0.96
1:Q:571:GLN:HE22	1:Q:637:ARG:C	1.64	0.96
1:X:613:TYR:CE2	1:X:650:LEU:HD12	2.00	0.96
1:O:658:ARG:HD2	1:X:535:PRO:HD2	1.48	0.95
1:P:606:ASN:OD1	1:J:643:LYS:NZ	1.99	0.95
1:D:546:PRO:HD3	1:G:514:ARG:HH22	1.28	0.94
1:L:544:PHE:O	1:F:514:ARG:NH1	2.00	0.94
1:K:632:LYS:NZ	1:K:654:GLU:OE1	2.00	0.92
1:D:586:GLN:O	1:D:588:LYS:HE2	1.68	0.92
1:W:530:GLN:NE2	1:W:581:VAL:O	2.02	0.92
1:X:571:GLN:HB3	1:X:637:ARG:HH11	1.35	0.92
1:X:576:ILE:HG13	1:X:612:THR:HG23	1.52	0.91

Continued on next page...



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:600:GLU:HG2	1:R:661:TYR:HB2	1.51	0.91
1:L:528:SER:OG	1:L:536:LYS:HG2	1.69	0.91
1:W:533:ARG:NH2	1:W:617:TYR:OH	2.04	0.91
1:Q:571:GLN:NE2	1:Q:573:PHE:CE2	2.38	0.91
1:W:533:ARG:NH1	1:W:615:ASP:OD1	2.03	0.91
1:E:536:LYS:HZ1	1:H:525:ASN:HD22	1.18	0.90
1:M:632:LYS:NZ	1:M:654:GLU:OE2	2.05	0.90
1:Q:641:TYR:HE1	1:G:637:ARG:HH12	1.07	0.89
1:W:501:PHE:CE1	1:W:553:LEU:HD23	2.06	0.89
1:T:639:LEU:O	1:X:637:ARG:NH2	2.06	0.89
1:B:514:ARG:NH1	1:B:518:LEU:HD11	1.87	0.89
1:I:639:LEU:HD23	1:I:640:GLY:N	1.88	0.89
1:R:600:GLU:CG	1:R:661:TYR:HB2	2.02	0.88
1:Q:571:GLN:HG2	1:Q:573:PHE:HE2	1.06	0.87
1:E:536:LYS:HZ3	1:H:525:ASN:HB3	1.38	0.87
1:X:556:ASP:O	1:X:558:ARG:NH1	2.07	0.86
1:Q:606:ASN:HA	1:L:643:LYS:HZ3	1.41	0.85
1:L:619:ILE:HG22	1:L:623:LYS:HE3	1.58	0.85
1:V:530:GLN:NE2	1:V:581:VAL:O	2.10	0.85
1:E:536:LYS:HZ1	1:H:525:ASN:ND2	1.76	0.84
1:J:528:SER:O	1:J:536:LYS:NZ	2.10	0.84
1:V:658:ARG:NH1	1:D:534:MET:SD	2.51	0.84
1:E:536:LYS:NZ	1:H:525:ASN:HB3	1.92	0.84
1:O:658:ARG:HD2	1:X:535:PRO:CD	2.07	0.83
1:R:600:GLU:OE2	1:R:661:TYR:HD2	1.58	0.82
1:W:620:GLY:HA2	1:W:623:LYS:HZ1	1.43	0.81
1:R:600:GLU:CD	1:R:661:TYR:HB2	2.00	0.80
1:B:514:ARG:HH12	1:B:518:LEU:HD11	1.43	0.80
1:X:566:ARG:NH1	1:X:567:MET:O	2.13	0.80
1:R:600:GLU:OE2	1:R:661:TYR:CG	2.34	0.80
1:Q:571:GLN:HE22	1:Q:638:TYR:HA	1.47	0.79
1:R:600:GLU:OE2	1:R:661:TYR:N	2.14	0.79
1:X:576:ILE:HG13	1:X:612:THR:CG2	2.11	0.79
1:U:644:ASP:OD2	1:U:645:TYR:N	2.16	0.79
1:L:533:ARG:NH1	1:L:615:ASP:OD1	2.15	0.79
1:T:530:GLN:NE2	1:T:581:VAL:O	2.16	0.79
1:D:546:PRO:CD	1:G:514:ARG:HH22	1.95	0.78
1:V:521:VAL:O	1:V:525:ASN:ND2	2.16	0.78
1:N:531:LEU:CD2	1:N:617:TYR:OH	2.31	0.78
1:K:583:SER:HA	1:K:586:GLN:HG3	1.64	0.78
1:Q:641:TYR:CE1	1:G:637:ARG:NH1	2.52	0.78

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:556:ASP:HB2	1:X:558:ARG:NH1	1.99	0.78
1:Q:571:GLN:NE2	1:Q:573:PHE:HZ	1.78	0.77
1:X:606:ASN:OD1	1:X:606:ASN:O	2.02	0.77
1:X:622:PHE:HD1	1:X:627:PHE:HZ	1.31	0.77
1:E:536:LYS:NZ	1:H:525:ASN:ND2	2.33	0.77
1:O:637:ARG:NH1	1:X:639:LEU:O	2.14	0.76
1:X:622:PHE:CD1	1:X:627:PHE:HZ	2.02	0.76
1:V:514:ARG:NH1	1:V:518:LEU:HD11	2.00	0.75
1:H:600:GLU:HG2	1:H:661:TYR:HB2	1.69	0.74
1:X:613:TYR:CE2	1:X:650:LEU:CD1	2.69	0.74
1:W:619:ILE:O	1:W:623:LYS:NZ	2.18	0.74
1:D:546:PRO:CD	1:G:514:ARG:NH2	2.49	0.74
1:W:571:GLN:O	1:W:637:ARG:NH2	2.12	0.74
1:A:525:ASN:HD21	1:U:524:GLN:HE22	1.35	0.74
1:S:566:ARG:HG2	1:S:566:ARG:HH11	1.53	0.73
1:D:600:GLU:OE2	1:D:660:PRO:HA	1.88	0.73
1:Q:603:ILE:HG12	1:Q:655:LEU:HD21	1.71	0.73
1:M:531:LEU:HD22	1:M:533:ARG:NH2	2.04	0.73
1:B:600:GLU:HG2	1:B:661:TYR:HB2	1.70	0.72
1:N:600:GLU:OE2	1:N:662:THR:OG1	2.06	0.72
1:J:558:ARG:NH2	1:D:660:PRO:HB3	1.99	0.72
1:M:530:GLN:NE2	1:M:581:VAL:O	2.23	0.71
1:Q:606:ASN:HA	1:L:643:LYS:NZ	2.04	0.71
1:X:571:GLN:HB3	1:X:637:ARG:NH1	2.06	0.71
1:D:600:GLU:HG3	1:D:662:THR:HB	1.73	0.70
1:E:558:ARG:HD3	1:E:559:VAL:H	1.55	0.70
1:N:531:LEU:HD21	1:N:617:TYR:OH	1.92	0.70
1:W:500:GLU:H	1:W:554:ILE:HG22	1.56	0.70
1:Q:571:GLN:HG2	1:Q:573:PHE:CD2	2.27	0.69
1:L:570:THR:OG1	1:L:571:GLN:NE2	2.24	0.69
1:X:619:ILE:HG22	1:X:623:LYS:HZ2	1.57	0.69
1:L:500:GLU:CD	1:L:502:HIS:ND1	2.43	0.69
1:O:644:ASP:OD1	1:O:645:TYR:N	2.25	0.69
1:E:536:LYS:NZ	1:H:525:ASN:CB	2.55	0.69
1:E:524:GLN:O	1:E:528:SER:OG	2.09	0.69
1:A:646:GLU:OE1	1:A:646:GLU:N	2.23	0.69
1:S:523:LEU:HD12	1:S:559:VAL:HG11	1.74	0.69
1:Q:571:GLN:HE22	1:Q:638:TYR:CA	2.05	0.69
1:E:536:LYS:NZ	1:H:525:ASN:HD22	1.90	0.68
1:L:637:ARG:CZ	1:I:641:TYR:HE1	2.06	0.68
1:P:656:ASN:O	1:P:659:ILE:HG22	1.94	0.67

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:603:ILE:HD13	1:X:657:PRO:HA	1.76	0.67
1:X:657:PRO:HB2	1:X:658:ARG:NH1	2.09	0.67
1:W:592:THR:HG21	1:W:624:LYS:CE	2.25	0.67
1:L:606:ASN:HD21	1:I:643:LYS:HZ2	1.39	0.67
1:Q:641:TYR:HE1	1:G:637:ARG:NH1	1.87	0.67
1:V:558:ARG:NH2	1:O:662:THR:O	2.24	0.66
1:L:658:ARG:HE	1:I:534:MET:HE3	1.60	0.66
1:L:606:ASN:HD21	1:I:643:LYS:NZ	1.92	0.66
1:Q:571:GLN:NE2	1:Q:573:PHE:HE2	1.93	0.66
1:D:514:ARG:NH1	1:G:546:PRO:HD3	2.11	0.66
1:H:514:ARG:HD2	1:H:516:VAL:HG22	1.76	0.66
1:J:521:VAL:O	1:J:525:ASN:ND2	2.29	0.66
1:Q:571:GLN:CD	1:Q:573:PHE:HZ	1.92	0.66
1:V:600:GLU:HG3	1:V:662:THR:HG23	1.78	0.66
1:T:558:ARG:HG3	1:S:537:GLU:HG2	1.78	0.66
1:M:531:LEU:HD22	1:M:533:ARG:HH21	1.61	0.65
1:Q:573:PHE:C	1:Q:607:ILE:HD11	2.15	0.65
1:L:616:GLU:OE2	1:L:648:ALA:HB2	1.96	0.65
1:W:619:ILE:C	1:W:623:LYS:NZ	2.50	0.65
1:X:603:ILE:HG13	1:X:655:LEU:HD23	1.78	0.65
1:Q:589:GLY:O	1:Q:593:HIS:ND1	2.28	0.65
1:U:639:LEU:O	1:R:637:ARG:NH1	2.22	0.65
1:U:566:ARG:NH1	1:U:567:MET:O	2.30	0.65
1:X:615:ASP:O	1:X:618:ALA:N	2.18	0.65
1:J:528:SER:HB2	1:J:536:LYS:HZ3	1.62	0.64
1:X:613:TYR:CZ	1:X:650:LEU:HD13	2.32	0.64
1:N:524:GLN:OE1	1:N:525:ASN:ND2	2.30	0.64
1:X:618:ALA:O	1:X:622:PHE:N	2.29	0.64
1:V:645:TYR:CE2	1:E:658:ARG:NH1	2.65	0.64
1:L:646:GLU:OE2	1:L:646:GLU:O	2.15	0.64
1:J:600:GLU:HG2	1:J:661:TYR:HB2	1.79	0.64
1:T:613:TYR:HB2	1:T:645:TYR:HD1	1.63	0.64
1:W:555:LYS:O	1:W:558:ARG:N	2.29	0.64
1:V:514:ARG:CZ	1:V:518:LEU:HD11	2.28	0.63
1:V:639:LEU:O	1:E:637:ARG:NH2	2.24	0.63
1:W:619:ILE:C	1:W:623:LYS:HZ3	2.00	0.63
1:U:633:VAL:HG23	1:U:652:GLU:OE2	1.97	0.63
1:Q:634:PRO:HD2	1:Q:637:ARG:NH2	2.13	0.63
1:Q:555:LYS:NZ	1:Q:585:GLU:OE2	2.26	0.63
1:X:553:LEU:HG	1:X:594:LEU:HD13	1.79	0.62
1:F:636:SER:HA	1:C:634:PRO:HG2	1.79	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:513:ASN:OD1	1:S:514:ARG:N	2.33	0.62
1:X:613:TYR:CZ	1:X:650:LEU:CD1	2.82	0.62
1:T:541:ARG:HD3	1:S:558:ARG:HH22	1.63	0.62
1:X:627:PHE:HB3	1:X:653:CYS:CA	2.29	0.62
1:Q:571:GLN:NE2	1:Q:638:TYR:N	2.47	0.62
1:F:500:GLU:HB2	1:F:554:ILE:HB	1.81	0.62
1:W:554:ILE:HG13	1:W:558:ARG:O	1.99	0.62
1:X:613:TYR:HE2	1:X:642:ILE:HD13	1.64	0.62
1:X:628:SER:C	1:X:651:MET:HE2	2.21	0.62
1:U:566:ARG:HD3	1:U:568:PHE:CZ	2.34	0.61
1:U:513:ASN:HB3	1:U:516:VAL:HB	1.82	0.61
1:X:631:ILE:HB	1:X:652:GLU:OE2	2.00	0.61
1:X:629:LYS:HA	1:X:651:MET:HG2	1.82	0.61
1:G:644:ASP:OD1	1:G:645:TYR:N	2.33	0.61
1:P:608:LEU:HD11	1:J:643:LYS:HD3	1.82	0.61
1:U:576:ILE:CG2	1:U:579:CYS:SG	2.88	0.61
1:S:555:LYS:HG3	1:S:556:ASP:N	2.16	0.61
1:Q:553:LEU:HB2	1:Q:594:LEU:HD21	1.81	0.61
1:W:592:THR:CG2	1:W:624:LYS:HE2	2.30	0.61
1:X:571:GLN:O	1:X:637:ARG:NH1	2.33	0.61
1:W:637:ARG:NH1	1:E:639:LEU:O	2.26	0.61
1:J:528:SER:HB2	1:J:536:LYS:NZ	2.16	0.61
1:T:553:LEU:HG	1:T:560:ILE:HG23	1.83	0.61
1:L:576:ILE:HB	1:L:612:THR:HB	1.83	0.61
1:S:595:MET:HG3	1:S:599:LYS:HE3	1.83	0.61
1:W:599:LYS:NZ	1:W:625:GLN:O	2.33	0.61
1:X:592:THR:HG23	1:X:625:GLN:NE2	2.16	0.61
1:F:633:VAL:HG23	1:F:652:GLU:OE2	2.00	0.61
1:X:556:ASP:CB	1:X:558:ARG:NH1	2.63	0.61
1:X:627:PHE:HB3	1:X:653:CYS:HA	1.82	0.61
1:S:515:ARG:HD2	1:S:519:TRP:CZ2	2.35	0.60
1:L:632:LYS:O	1:I:639:LEU:HD13	2.01	0.60
1:M:639:LEU:O	1:J:637:ARG:NH1	2.28	0.60
1:R:600:GLU:CD	1:R:661:TYR:H	2.04	0.60
1:V:523:LEU:HG	1:V:559:VAL:HG11	1.82	0.60
1:W:592:THR:CG2	1:W:624:LYS:CE	2.79	0.60
1:K:558:ARG:HD3	1:K:559:VAL:H	1.65	0.60
1:X:613:TYR:CD2	1:X:650:LEU:HD12	2.35	0.60
1:W:620:GLY:HA2	1:W:623:LYS:NZ	2.16	0.60
1:U:566:ARG:HH11	1:U:566:ARG:HG2	1.67	0.60
1:P:513:ASN:HB3	1:P:516:VAL:HG22	1.84	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:555:LYS:HD3	1:S:560:ILE:HD13	1.84	0.60
1:X:560:ILE:O	1:X:582:THR:HG23	2.02	0.60
1:R:595:MET:HG3	1:R:599:LYS:HE3	1.83	0.60
1:X:657:PRO:HD2	1:X:658:ARG:HH12	1.67	0.60
1:A:615:ASP:OD1	1:A:616:GLU:N	2.35	0.59
1:F:632:LYS:NZ	1:F:654:GLU:OE2	2.23	0.59
1:F:600:GLU:HG2	1:F:661:TYR:HB2	1.84	0.59
1:L:632:LYS:O	1:I:639:LEU:CD1	2.50	0.59
1:W:556:ASP:HB2	1:W:558:ARG:HG2	1.83	0.59
1:O:499:ILE:HD13	1:O:555:LYS:HA	1.84	0.59
1:R:499:ILE:HD11	1:R:555:LYS:HD3	1.84	0.59
1:E:660:PRO:HB3	1:X:558:ARG:HH21	1.68	0.59
1:E:533:ARG:HD3	1:E:646:GLU:OE2	2.03	0.59
1:O:658:ARG:HD3	1:X:534:MET:HG2	1.83	0.59
1:C:531:LEU:HD13	1:C:534:MET:HE1	1.84	0.59
1:M:512:ALA:N	1:I:508:LEU:HD13	2.18	0.58
1:E:589:GLY:O	1:E:593:HIS:ND1	2.32	0.58
1:L:537:GLU:OE2	1:L:537:GLU:N	2.25	0.58
1:Q:571:GLN:HE21	1:Q:637:ARG:C	2.03	0.58
1:X:622:PHE:HB3	1:X:627:PHE:CE1	2.38	0.58
1:M:641:TYR:OH	1:J:570:THR:O	2.12	0.58
1:S:555:LYS:HG3	1:S:556:ASP:H	1.67	0.58
1:P:514:ARG:HG3	1:P:515:ARG:H	1.68	0.58
1:X:600:GLU:OE2	1:X:662:THR:HG23	2.04	0.58
1:I:589:GLY:O	1:I:593:HIS:ND1	2.32	0.58
1:X:619:ILE:HG22	1:X:623:LYS:NZ	2.18	0.58
1:D:513:ASN:O	1:D:517:LEU:HG	2.03	0.58
1:F:523:LEU:HD13	1:F:550:THR:HG21	1.86	0.58
1:H:523:LEU:HD13	1:H:550:THR:HG21	1.86	0.58
1:E:536:LYS:HZ1	1:H:525:ASN:CB	2.17	0.58
1:I:523:LEU:HD13	1:I:550:THR:HG21	1.85	0.58
1:T:541:ARG:CD	1:S:558:ARG:HH22	2.17	0.58
1:V:523:LEU:HD22	1:V:550:THR:HG21	1.85	0.57
1:L:619:ILE:CG2	1:L:623:LYS:HE3	2.31	0.57
1:O:608:LEU:HD13	1:O:657:PRO:HG3	1.85	0.57
1:Q:536:LYS:HZ3	1:O:529:HIS:CE1	2.23	0.57
1:W:592:THR:HG21	1:W:624:LYS:HE2	1.87	0.57
1:E:500:GLU:HB2	1:E:554:ILE:HB	1.85	0.57
1:A:558:ARG:HD3	1:A:559:VAL:H	1.69	0.57
1:I:555:LYS:HD2	1:I:560:ILE:HD13	1.87	0.57
1:M:555:LYS:NZ	1:M:585:GLU:OE2	2.32	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:528:SER:HG	1:L:536:LYS:HG2	1.68	0.57
1:P:659:ILE:HG21	1:P:661:TYR:CZ	2.40	0.57
1:B:517:LEU:O	1:B:521:VAL:HG23	2.05	0.57
1:J:617:TYR:N	1:J:617:TYR:HD2	2.03	0.57
1:Q:571:GLN:HE22	1:Q:638:TYR:N	2.01	0.56
1:X:616:GLU:HA	1:X:619:ILE:HG12	1.86	0.56
1:Q:571:GLN:NE2	1:Q:637:ARG:HB3	2.19	0.56
1:S:566:ARG:HD3	1:S:568:PHE:CZ	2.38	0.56
1:T:585:GLU:OE1	1:T:588:LYS:NZ	2.28	0.56
1:X:556:ASP:CB	1:X:558:ARG:HH12	2.18	0.56
1:Q:571:GLN:NE2	1:Q:638:TYR:HA	2.16	0.56
1:W:619:ILE:HG23	1:W:623:LYS:NZ	2.20	0.56
1:T:641:TYR:OH	1:X:571:GLN:HA	2.05	0.56
1:Q:571:GLN:CD	1:Q:637:ARG:O	2.43	0.56
1:U:634:PRO:HG2	1:S:636:SER:HA	1.87	0.56
1:W:592:THR:HG21	1:W:624:LYS:HE3	1.87	0.56
1:I:526:VAL:O	1:I:530:GLN:HG2	2.04	0.56
1:Q:553:LEU:CD1	1:Q:594:LEU:HG	2.35	0.56
1:S:512:ALA:HA	1:S:516:VAL:HG21	1.86	0.56
1:Q:641:TYR:OH	1:G:637:ARG:NH1	2.39	0.56
1:N:595:MET:HG3	1:N:599:LYS:HE3	1.88	0.56
1:U:523:LEU:HD11	1:U:552:ALA:HB2	1.86	0.56
1:W:639:LEU:O	1:D:637:ARG:NH1	2.22	0.56
1:D:587:VAL:O	1:D:588:LYS:NZ	2.36	0.56
1:C:538:TYR:CZ	1:C:542:LEU:HD11	2.41	0.56
1:Q:553:LEU:HD12	1:Q:594:LEU:HG	1.86	0.56
1:V:514:ARG:NH2	1:V:518:LEU:HD11	2.20	0.56
1:X:563:ILE:HG12	1:X:598:LEU:HD22	1.87	0.56
1:B:629:LYS:HE3	1:B:649:THR:HG21	1.88	0.55
1:L:500:GLU:OE1	1:L:502:HIS:ND1	2.39	0.55
1:P:659:ILE:HG23	1:P:659:ILE:O	2.06	0.55
1:T:656:ASN:HD22	1:T:657:PRO:HD2	1.71	0.55
1:V:531:LEU:HD22	1:V:534:MET:HB2	1.86	0.55
1:W:603:ILE:HG22	1:W:608:LEU:HD22	1.87	0.55
1:I:639:LEU:C	1:I:639:LEU:HD23	2.26	0.55
1:L:645:TYR:HB2	1:L:647:GLY:N	2.22	0.55
1:R:566:ARG:HD3	1:R:568:PHE:CZ	2.41	0.55
1:B:595:MET:HG2	1:B:599:LYS:HE3	1.89	0.55
1:R:513:ASN:O	1:R:517:LEU:HD13	2.06	0.55
1:W:585:GLU:OE2	1:W:588:LYS:NZ	2.40	0.55
1:W:619:ILE:HG23	1:W:623:LYS:HZ2	1.72	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:659:ILE:HD11	1:J:661:TYR:CZ	2.41	0.55
1:W:620:GLY:CA	1:W:623:LYS:HZ1	2.18	0.55
1:H:574:THR:HG21	1:H:602:HIS:NE2	2.21	0.55
1:N:587:VAL:HG12	1:N:587:VAL:O	2.07	0.55
1:Q:571:GLN:HG3	1:Q:637:ARG:HB3	1.88	0.55
1:R:600:GLU:OE2	1:R:661:TYR:CA	2.54	0.55
1:U:636:SER:HA	1:R:634:PRO:HG2	1.89	0.55
1:G:500:GLU:HB2	1:G:554:ILE:HB	1.88	0.55
1:Q:573:PHE:CA	1:Q:607:ILE:HD11	2.37	0.55
1:X:565:PHE:HB3	1:X:576:ILE:HG22	1.88	0.55
1:U:547:LYS:HE3	1:U:566:ARG:HH21	1.72	0.54
1:W:501:PHE:CE1	1:W:553:LEU:CD2	2.85	0.54
1:X:608:LEU:C	1:X:609:TYR:HD2	2.10	0.54
1:X:613:TYR:CE2	1:X:642:ILE:HD13	2.42	0.54
1:L:583:SER:HA	1:L:586:GLN:HG3	1.89	0.54
1:O:637:ARG:NH2	1:X:641:TYR:CZ	2.75	0.54
1:X:576:ILE:CG1	1:X:612:THR:HG23	2.33	0.54
1:D:528:SER:OG	1:D:536:LYS:HG2	2.07	0.54
1:Q:576:ILE:O	1:Q:612:THR:HG23	2.07	0.54
1:D:586:GLN:O	1:D:588:LYS:CE	2.51	0.54
1:Q:566:ARG:NH1	1:Q:567:MET:O	2.40	0.54
1:E:533:ARG:CD	1:E:646:GLU:OE2	2.55	0.54
1:J:499:ILE:HG22	1:J:555:LYS:HB2	1.89	0.54
1:W:517:LEU:HD11	1:J:517:LEU:HD11	1.89	0.54
1:L:538:TYR:CZ	1:L:542:LEU:HD11	2.43	0.54
1:O:587:VAL:HG12	1:O:587:VAL:O	2.07	0.54
1:Q:563:ILE:HG21	1:Q:598:LEU:HD22	1.89	0.54
1:L:523:LEU:HD13	1:L:550:THR:HG21	1.90	0.53
1:L:615:ASP:O	1:L:619:ILE:HG12	2.08	0.53
1:S:500:GLU:OE2	1:S:502:HIS:NE2	2.39	0.53
1:X:622:PHE:HD1	1:X:627:PHE:CZ	2.20	0.53
1:E:547:LYS:O	1:E:566:ARG:HG3	2.09	0.53
1:T:516:VAL:O	1:T:520:LEU:HD12	2.08	0.53
1:Q:622:PHE:HB3	1:Q:627:PHE:HB2	1.91	0.53
1:Q:630:ASP:OD2	1:Q:630:ASP:O	2.25	0.53
1:R:523:LEU:HD13	1:R:550:THR:HG21	1.90	0.53
1:W:592:THR:CG2	1:W:624:LYS:HE3	2.39	0.53
1:W:657:PRO:HD2	1:W:658:ARG:HH21	1.74	0.53
1:O:658:ARG:CD	1:X:535:PRO:HD2	2.31	0.53
1:X:600:GLU:OE1	1:X:661:TYR:N	2.41	0.53
1:R:636:SER:HA	1:H:634:PRO:HG2	1.90	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:579:CYS:SG	1:O:621:TYR:CE2	3.00	0.53
1:U:620:GLY:O	1:U:624:LYS:HG3	2.09	0.53
1:V:525:ASN:O	1:V:529:HIS:ND1	2.42	0.53
1:W:586:GLN:HG3	1:W:587:VAL:HG13	1.89	0.53
1:D:566:ARG:HD3	1:D:568:PHE:CZ	2.44	0.53
1:X:614:ALA:HB3	1:X:619:ILE:HD11	1.90	0.53
1:B:599:LYS:O	1:B:603:ILE:HG23	2.08	0.53
1:U:523:LEU:HD13	1:U:550:THR:HG21	1.91	0.53
1:B:506:ASN:O	1:B:546:PRO:HA	2.09	0.53
1:E:592:THR:HG22	1:E:625:GLN:OE1	2.10	0.53
1:P:523:LEU:HD13	1:P:550:THR:HG21	1.91	0.52
1:H:574:THR:HG21	1:H:602:HIS:CD2	2.44	0.52
1:Q:547:LYS:O	1:Q:547:LYS:HG3	2.07	0.52
1:X:657:PRO:CD	1:X:658:ARG:HH12	2.22	0.52
1:F:583:SER:HA	1:F:586:GLN:HG3	1.91	0.52
1:P:528:SER:OG	1:P:536:LYS:HG2	2.09	0.52
1:V:519:TRP:O	1:V:523:LEU:HD12	2.09	0.52
1:S:519:TRP:O	1:S:523:LEU:HD13	2.10	0.52
1:U:595:MET:HG3	1:U:599:LYS:HE3	1.91	0.52
1:I:615:ASP:O	1:I:619:ILE:HG13	2.09	0.52
1:T:606:ASN:ND2	1:K:566:ARG:NH1	2.58	0.52
1:Q:588:LYS:HG3	1:Q:588:LYS:O	2.08	0.52
1:X:548:HIS:CD2	1:X:566:ARG:HB2	2.43	0.52
1:E:615:ASP:OD2	1:E:646:GLU:OE1	2.27	0.52
1:J:564:CYS:O	1:J:577:VAL:HG22	2.09	0.52
1:Q:576:ILE:HB	1:Q:612:THR:OG1	2.10	0.52
1:X:614:ALA:HB3	1:X:619:ILE:CD1	2.40	0.52
1:L:619:ILE:O	1:L:623:LYS:HG2	2.10	0.52
1:S:566:ARG:NH1	1:S:566:ARG:HG2	2.23	0.52
1:K:555:LYS:NZ	1:K:585:GLU:OE2	2.42	0.52
1:Q:571:GLN:HE21	1:Q:637:ARG:HB3	1.74	0.52
1:W:582:THR:CG2	1:W:585:GLU:HG2	2.40	0.52
1:J:617:TYR:N	1:J:617:TYR:CD2	2.78	0.52
1:E:558:ARG:HD3	1:E:559:VAL:N	2.24	0.52
1:X:603:ILE:HD11	1:X:655:LEU:HB3	1.92	0.52
1:W:620:GLY:CA	1:W:623:LYS:NZ	2.74	0.51
1:B:547:LYS:O	1:B:566:ARG:HG3	2.10	0.51
1:D:566:ARG:HG2	1:D:566:ARG:HH11	1.75	0.51
1:J:513:ASN:HB3	1:J:516:VAL:HG22	1.92	0.51
1:O:658:ARG:HD2	1:X:535:PRO:HD3	1.91	0.51
1:V:644:ASP:OD1	1:V:645:TYR:N	2.44	0.51

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:634:PRO:HD3	1:I:639:LEU:HD22	1.93	0.51
1:J:504:ILE:HD11	1:J:523:LEU:HD11	1.91	0.51
1:L:637:ARG:CZ	1:L:637:ARG:HB2	2.40	0.51
1:V:644:ASP:O	1:V:645:TYR:HD2	1.94	0.51
1:X:622:PHE:CD1	1:X:627:PHE:CZ	2.92	0.51
1:F:640:GLY:HA2	1:C:609:TYR:CE1	2.46	0.51
1:V:587:VAL:HG12	1:V:587:VAL:O	2.11	0.51
1:W:553:LEU:HB2	1:W:594:LEU:HD21	1.91	0.51
1:Q:522:GLY:O	1:Q:526:VAL:HG23	2.10	0.51
1:W:576:ILE:HB	1:W:612:THR:HB	1.93	0.51
1:X:555:LYS:HB2	1:X:560:ILE:HD11	1.91	0.51
1:H:547:LYS:O	1:H:566:ARG:HG3	2.11	0.51
1:J:500:GLU:OE2	1:J:554:ILE:HD11	2.10	0.51
1:L:601:TYR:HA	1:L:604:LYS:HE2	1.92	0.51
1:P:659:ILE:CG2	1:P:659:ILE:O	2.59	0.51
1:E:536:LYS:NZ	1:H:525:ASN:CG	2.64	0.51
1:J:566:ARG:NH1	1:J:567:MET:O	2.44	0.51
1:S:500:GLU:O	1:S:554:ILE:HG22	2.10	0.51
1:U:566:ARG:NH1	1:U:566:ARG:HG2	2.26	0.51
1:A:523:LEU:HD13	1:A:550:THR:HG21	1.91	0.51
1:B:522:GLY:O	1:B:526:VAL:HG23	2.11	0.51
1:J:520:LEU:HA	1:J:523:LEU:HD12	1.92	0.50
1:M:528:SER:OG	1:M:536:LYS:HG2	2.12	0.50
1:S:629:LYS:HE3	1:S:649:THR:HG21	1.93	0.50
1:D:635:LYS:HA	1:D:638:TYR:CE2	2.46	0.50
1:J:583:SER:HA	1:J:586:GLN:HG3	1.92	0.50
1:L:603:ILE:HD13	1:L:657:PRO:HA	1.93	0.50
1:N:636:SER:HA	1:M:634:PRO:HG2	1.94	0.50
1:Q:641:TYR:CZ	1:G:637:ARG:NH1	2.80	0.50
1:W:525:ASN:HD21	1:J:524:GLN:HE22	1.59	0.50
1:W:501:PHE:CD1	1:W:553:LEU:HD23	2.46	0.50
1:J:566:ARG:HD3	1:J:568:PHE:CZ	2.46	0.50
1:Q:631:ILE:HA	1:Q:652:GLU:OE2	2.11	0.50
1:W:622:PHE:HB3	1:W:627:PHE:HB2	1.93	0.50
1:X:610:PHE:O	1:X:652:GLU:HA	2.11	0.50
1:I:644:ASP:OD1	1:I:645:TYR:N	2.45	0.50
1:L:566:ARG:NH1	1:L:567:MET:O	2.33	0.50
1:W:582:THR:HG23	1:W:585:GLU:HG2	1.94	0.50
1:X:523:LEU:HD13	1:X:550:THR:HG21	1.94	0.50
1:U:537:GLU:H	1:U:537:GLU:CD	2.15	0.50
1:M:531:LEU:CD2	1:M:533:ARG:NH2	2.73	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:528:SER:OG	1:N:536:LYS:HG2	2.12	0.50
1:D:534:MET:HB2	1:D:539:ILE:HD11	1.94	0.50
1:W:523:LEU:HG	1:W:559:VAL:HG11	1.93	0.50
1:A:575:GLU:HB2	1:A:642:ILE:HG22	1.94	0.49
1:A:608:LEU:HD13	1:C:643:LYS:HB2	1.94	0.49
1:P:513:ASN:OD1	1:P:514:ARG:N	2.45	0.49
1:D:514:ARG:HH12	1:G:546:PRO:HD3	1.75	0.49
1:W:633:VAL:HG23	1:W:652:GLU:OE2	2.13	0.49
1:A:513:ASN:ND2	1:A:515:ARG:HB3	2.28	0.49
1:C:531:LEU:HD13	1:C:534:MET:CE	2.41	0.49
1:J:575:GLU:HB2	1:J:642:ILE:HG22	1.94	0.49
1:J:600:GLU:OE2	1:J:661:TYR:N	2.45	0.49
1:S:545:ASP:OD1	1:S:547:LYS:N	2.45	0.49
1:A:609:TYR:CE1	1:C:640:GLY:HA2	2.48	0.49
1:S:637:ARG:NH2	1:H:639:LEU:O	2.36	0.49
1:J:622:PHE:HB3	1:J:627:PHE:HB2	1.94	0.49
1:R:619:ILE:HG22	1:R:623:LYS:HE2	1.94	0.49
1:S:554:ILE:HG13	1:S:558:ARG:O	2.11	0.49
1:U:609:TYR:CE2	1:S:640:GLY:HA2	2.48	0.49
1:H:567:MET:HA	1:H:574:THR:HG22	1.93	0.49
1:K:558:ARG:HD3	1:K:559:VAL:N	2.26	0.49
1:T:633:VAL:HG23	1:T:652:GLU:OE2	2.12	0.49
1:E:629:LYS:HE3	1:E:649:THR:HG21	1.94	0.49
1:M:530:GLN:HE22	1:M:586:GLN:HE21	1.59	0.49
1:B:555:LYS:NZ	1:B:585:GLU:OE2	2.45	0.49
1:H:541:ARG:HH11	1:H:541:ARG:HG2	1.77	0.49
1:O:584:ASN:ND2	1:O:585:GLU:OE2	2.45	0.49
1:S:566:ARG:NH1	1:S:567:MET:O	2.46	0.49
1:V:643:LYS:HZ2	1:E:606:ASN:ND2	2.09	0.49
1:H:574:THR:HG23	1:H:607:ILE:HG21	1.94	0.49
1:M:595:MET:HG3	1:M:599:LYS:HE3	1.95	0.49
1:Q:605:HIS:O	1:Q:607:ILE:HG22	2.13	0.49
1:B:498:ILE:HG22	1:B:556:ASP:OD1	2.12	0.48
1:J:635:LYS:HA	1:J:638:TYR:CE2	2.48	0.48
1:O:513:ASN:OD1	1:O:516:VAL:HG22	2.13	0.48
1:R:635:LYS:CG	1:R:639:LEU:HD12	2.43	0.48
1:W:513:ASN:ND2	1:W:516:VAL:HG13	2.29	0.48
1:I:513:ASN:HD21	1:I:515:ARG:HH21	1.61	0.48
1:J:524:GLN:O	1:J:528:SER:OG	2.22	0.48
1:S:516:VAL:O	1:S:520:LEU:HG	2.13	0.48
1:X:589:GLY:C	1:X:590:TYR:HD1	2.16	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:499:ILE:HD11	1:G:555:LYS:HE3	1.96	0.48
1:A:525:ASN:HD21	1:U:524:GLN:NE2	2.09	0.48
1:S:520:LEU:HA	1:S:523:LEU:HD22	1.95	0.48
1:X:553:LEU:HB3	1:X:560:ILE:HB	1.96	0.48
1:D:615:ASP:O	1:D:619:ILE:HG13	2.14	0.48
1:F:615:ASP:O	1:F:619:ILE:HG13	2.13	0.48
1:X:595:MET:HE1	1:X:598:LEU:HD23	1.96	0.48
1:X:619:ILE:HA	1:X:622:PHE:HB2	1.96	0.48
1:M:555:LYS:HB2	1:M:560:ILE:HD13	1.95	0.48
1:P:595:MET:HG3	1:P:599:LYS:HE3	1.96	0.48
1:C:523:LEU:HD13	1:C:550:THR:HG21	1.94	0.48
1:Q:602:HIS:ND1	1:Q:610:PHE:HE2	2.12	0.48
1:H:534:MET:HE1	1:H:578:PHE:HE1	1.79	0.47
1:C:615:ASP:O	1:C:619:ILE:HG13	2.14	0.47
1:I:595:MET:HG3	1:I:599:LYS:HE3	1.95	0.47
1:R:579:CYS:SG	1:R:621:TYR:CE2	3.07	0.47
1:T:518:LEU:HD21	1:S:541:ARG:HG2	1.96	0.47
1:V:528:SER:O	1:V:532:PRO:HA	2.14	0.47
1:X:555:LYS:CB	1:X:560:ILE:HD11	2.45	0.47
1:L:534:MET:HE3	1:L:538:TYR:HD2	1.79	0.47
1:R:545:ASP:OD2	1:R:547:LYS:N	2.46	0.47
1:I:501:PHE:HB3	1:I:551:LEU:HD11	1.97	0.47
1:Q:501:PHE:HB3	1:Q:551:LEU:HD11	1.96	0.47
1:Q:583:SER:HA	1:Q:586:GLN:CD	2.34	0.47
1:T:500:GLU:OE1	1:T:502:HIS:NE2	2.46	0.47
1:T:536:LYS:HG3	1:T:537:GLU:OE1	2.15	0.47
1:T:576:ILE:HB	1:T:612:THR:HB	1.96	0.47
1:T:613:TYR:HB2	1:T:645:TYR:CD1	2.48	0.47
1:W:560:ILE:O	1:W:582:THR:HG22	2.15	0.47
1:X:628:SER:O	1:X:651:MET:HE2	2.14	0.47
1:Q:571:GLN:NE2	1:Q:638:TYR:CA	2.74	0.47
1:U:600:GLU:O	1:U:604:LYS:HG2	2.14	0.47
1:W:530:GLN:HG3	1:W:580:ALA:HB1	1.97	0.47
1:X:586:GLN:HG2	1:X:587:VAL:N	2.30	0.47
1:H:534:MET:HE1	1:H:578:PHE:CE1	2.49	0.47
1:Q:595:MET:HG3	1:Q:599:LYS:HE3	1.96	0.47
1:V:529:HIS:CD2	1:X:536:LYS:HE2	2.48	0.47
1:D:587:VAL:HB	1:D:588:LYS:NZ	2.29	0.47
1:Q:639:LEU:O	1:G:637:ARG:NH2	2.47	0.47
1:B:523:LEU:HG	1:B:559:VAL:HG11	1.97	0.47
1:I:579:CYS:SG	1:I:621:TYR:CE2	3.08	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:515:ARG:HD2	1:K:519:TRP:CZ2	2.50	0.47
1:R:603:ILE:HD11	1:R:655:LEU:HB3	1.96	0.47
1:H:524:GLN:HG3	1:H:540:ALA:HA	1.97	0.47
1:U:644:ASP:OD2	1:U:644:ASP:C	2.53	0.47
1:V:595:MET:HG3	1:V:599:LYS:HE3	1.96	0.47
1:K:553:LEU:HB2	1:K:594:LEU:HD21	1.96	0.46
1:N:635:LYS:HA	1:N:638:TYR:CE2	2.50	0.46
1:A:633:VAL:HG23	1:A:652:GLU:OE2	2.15	0.46
1:G:619:ILE:HG22	1:G:623:LYS:HE3	1.96	0.46
1:I:517:LEU:O	1:I:521:VAL:HG23	2.14	0.46
1:I:639:LEU:HD23	1:I:640:GLY:H	1.77	0.46
1:Q:571:GLN:CD	1:Q:573:PHE:HE2	1.91	0.46
1:T:587:VAL:O	1:T:587:VAL:HG12	2.15	0.46
1:H:585:GLU:OE1	1:H:588:LYS:NZ	2.33	0.46
1:W:623:LYS:HD3	1:W:623:LYS:H	1.81	0.46
1:A:517:LEU:HD11	1:U:517:LEU:HD21	1.97	0.46
1:M:563:ILE:HG21	1:M:598:LEU:HD22	1.97	0.46
1:U:639:LEU:HD22	1:R:633:VAL:HA	1.96	0.46
1:X:635:LYS:HD3	1:X:639:LEU:HD11	1.96	0.46
1:X:619:ILE:HD12	1:X:651:MET:SD	2.55	0.46
1:P:534:MET:HB2	1:P:539:ILE:HD11	1.96	0.46
1:U:610:PHE:HB2	1:U:653:CYS:HB3	1.97	0.46
1:B:538:TYR:CZ	1:B:542:LEU:HD11	2.50	0.46
1:L:585:GLU:HA	1:L:588:LYS:HE3	1.98	0.46
1:R:583:SER:HA	1:R:586:GLN:HG3	1.96	0.46
1:D:537:GLU:OE1	1:D:537:GLU:N	2.39	0.46
1:G:636:SER:HA	1:I:634:PRO:HG2	1.98	0.46
1:L:595:MET:HG3	1:L:599:LYS:HE3	1.97	0.46
1:P:600:GLU:HG3	1:P:662:THR:OG1	2.16	0.46
1:V:645:TYR:OH	1:E:658:ARG:NH2	2.49	0.46
1:V:555:LYS:HG2	1:V:556:ASP:OD2	2.16	0.46
1:X:635:LYS:HA	1:X:638:TYR:CE2	2.51	0.46
1:E:558:ARG:HA	1:E:558:ARG:NE	2.31	0.46
1:I:537:GLU:CD	1:I:537:GLU:H	2.19	0.46
1:X:586:GLN:HG2	1:X:587:VAL:HG13	1.98	0.46
1:X:576:ILE:O	1:X:612:THR:HG22	2.16	0.46
1:E:536:LYS:HZ3	1:H:525:ASN:CB	2.15	0.45
1:K:635:LYS:HA	1:K:638:TYR:CE2	2.51	0.45
1:M:584:ASN:ND2	1:M:585:GLU:HG2	2.32	0.45
1:W:621:TYR:O	1:W:625:GLN:HG2	2.15	0.45
1:A:558:ARG:NE	1:A:558:ARG:HA	2.31	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:620:GLY:O	1:G:624:LYS:HG2	2.16	0.45
1:J:514:ARG:H	1:J:514:ARG:HG2	1.45	0.45
1:Q:571:GLN:OE1	1:Q:641:TYR:CD1	2.69	0.45
1:V:513:ASN:O	1:V:517:LEU:HD12	2.15	0.45
1:A:576:ILE:HB	1:A:612:THR:HB	1.98	0.45
1:O:538:TYR:CZ	1:O:542:LEU:HD11	2.50	0.45
1:D:587:VAL:O	1:D:588:LYS:CE	2.65	0.45
1:P:634:PRO:HG2	1:J:636:SER:HA	1.99	0.45
1:T:595:MET:HG3	1:T:599:LYS:HE3	1.99	0.45
1:G:615:ASP:N	1:G:615:ASP:OD1	2.49	0.45
1:P:609:TYR:CE2	1:J:640:GLY:HA2	2.52	0.45
1:Q:567:MET:HA	1:Q:574:THR:HG23	1.97	0.45
1:A:566:ARG:HD3	1:A:568:PHE:CE2	2.51	0.45
1:A:564:CYS:HB3	1:A:578:PHE:HB2	1.99	0.45
1:F:657:PRO:HB2	1:B:538:TYR:CE1	2.52	0.45
1:X:553:LEU:O	1:X:560:ILE:N	2.47	0.45
1:A:585:GLU:OE1	1:A:588:LYS:NZ	2.40	0.45
1:W:636:SER:HA	1:D:634:PRO:HG2	1.98	0.45
1:M:656:ASN:HB3	1:M:659:ILE:HG12	1.99	0.45
1:Q:526:VAL:HA	1:Q:529:HIS:ND1	2.32	0.45
1:X:627:PHE:HB3	1:X:653:CYS:CB	2.45	0.45
1:V:600:GLU:HG2	1:V:661:TYR:HB2	1.98	0.45
1:C:595:MET:HG3	1:C:599:LYS:HE3	1.99	0.45
1:E:537:GLU:H	1:E:537:GLU:CD	2.20	0.45
1:W:525:ASN:HD21	1:J:524:GLN:NE2	2.15	0.45
1:V:635:LYS:HA	1:V:638:TYR:CE2	2.52	0.45
1:X:614:ALA:HB1	1:X:622:PHE:CD2	2.51	0.45
1:J:554:ILE:HG22	1:J:559:VAL:HG22	1.97	0.45
1:M:523:LEU:HD13	1:M:550:THR:HG21	1.98	0.45
1:X:631:ILE:O	1:X:632:LYS:HD2	2.17	0.45
1:A:534:MET:HB3	1:A:534:MET:HE3	1.57	0.44
1:D:560:ILE:O	1:D:582:THR:HG22	2.17	0.44
1:O:635:LYS:HA	1:O:638:TYR:CE2	2.53	0.44
1:V:517:LEU:O	1:V:521:VAL:HG23	2.16	0.44
1:E:644:ASP:OD1	1:E:645:TYR:N	2.50	0.44
1:S:517:LEU:HA	1:S:517:LEU:HD12	1.71	0.44
1:T:658:ARG:O	1:T:660:PRO:HD3	2.17	0.44
1:W:585:GLU:HA	1:W:588:LYS:NZ	2.32	0.44
1:D:498:ILE:O	1:D:555:LYS:HG3	2.16	0.44
1:F:600:GLU:HG3	1:F:662:THR:HG23	1.99	0.44
1:J:600:GLU:CG	1:J:661:TYR:HB2	2.47	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:518:LEU:HD21	1:I:541:ARG:HG3	1.99	0.44
1:P:514:ARG:HG3	1:P:515:ARG:N	2.31	0.44
1:S:537:GLU:O	1:S:541:ARG:HG3	2.17	0.44
1:E:587:VAL:O	1:E:587:VAL:HG12	2.17	0.44
1:R:615:ASP:O	1:R:619:ILE:HG13	2.17	0.44
1:R:635:LYS:HA	1:R:638:TYR:CE2	2.53	0.44
1:R:659:ILE:HD13	1:R:659:ILE:HA	1.85	0.44
1:X:533:ARG:HH12	1:X:617:TYR:HD2	1.64	0.44
1:X:658:ARG:N	1:X:658:ARG:HH11	2.15	0.44
1:F:547:LYS:O	1:F:566:ARG:HG3	2.18	0.44
1:R:519:TRP:CD1	1:R:559:VAL:HG23	2.53	0.44
1:X:618:ALA:O	1:X:621:TYR:HB3	2.18	0.44
1:B:523:LEU:HD13	1:B:550:THR:HG21	2.00	0.44
1:E:514:ARG:O	1:E:514:ARG:HG2	2.17	0.44
1:E:614:ALA:O	1:E:648:ALA:HB1	2.18	0.44
1:F:498:ILE:O	1:F:555:LYS:HA	2.17	0.44
1:G:637:ARG:O	1:G:637:ARG:HG3	2.17	0.44
1:I:508:LEU:H	1:I:508:LEU:HG	1.65	0.44
1:W:558:ARG:NH2	1:P:662:THR:O	2.51	0.44
1:X:613:TYR:CE1	1:X:650:LEU:HB2	2.53	0.44
1:L:517:LEU:HD13	1:L:517:LEU:HA	1.87	0.44
1:P:566:ARG:HD3	1:P:568:PHE:CE2	2.52	0.44
1:N:629:LYS:HE3	1:N:649:THR:HG21	2.00	0.44
1:Q:526:VAL:HG13	1:Q:529:HIS:HE1	1.83	0.44
1:Q:571:GLN:HE21	1:Q:637:ARG:CB	2.31	0.44
1:Q:602:HIS:HB3	1:Q:607:ILE:HG23	2.00	0.44
1:W:586:GLN:HG3	1:W:587:VAL:N	2.32	0.44
1:A:563:ILE:HG21	1:A:598:LEU:HD22	2.00	0.44
1:M:551:LEU:O	1:M:562:GLY:HA2	2.18	0.44
1:P:566:ARG:HH11	1:P:566:ARG:HG2	1.83	0.44
1:U:517:LEU:O	1:U:521:VAL:HG23	2.17	0.44
1:E:536:LYS:HZ1	1:H:525:ASN:CG	2.21	0.43
1:G:574:THR:HG1	1:G:602:HIS:CD2	2.36	0.43
1:L:535:PRO:HB3	1:L:537:GLU:OE2	2.18	0.43
1:O:615:ASP:O	1:O:619:ILE:HG13	2.18	0.43
1:S:530:GLN:HG3	1:S:580:ALA:HB1	1.99	0.43
1:L:575:GLU:HB2	1:L:642:ILE:HG22	2.00	0.43
1:P:657:PRO:HG2	1:J:643:LYS:HD2	2.00	0.43
1:Q:607:ILE:O	1:Q:608:LEU:HD23	2.17	0.43
1:A:608:LEU:HD22	1:A:657:PRO:HG3	2.00	0.43
1:J:530:GLN:C	1:J:532:PRO:HD3	2.38	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:575:GLU:HB2	1:O:642:ILE:HG22	2.00	0.43
1:S:558:ARG:O	1:S:559:VAL:HG23	2.19	0.43
1:X:534:MET:HB3	1:X:534:MET:HE3	1.88	0.43
1:X:613:TYR:CD1	1:X:650:LEU:HB2	2.53	0.43
1:X:657:PRO:CB	1:X:658:ARG:NH1	2.80	0.43
1:A:588:LYS:HE3	1:A:590:TYR:CE2	2.53	0.43
1:Q:571:GLN:CG	1:Q:637:ARG:HB3	2.49	0.43
1:C:586:GLN:O	1:C:588:LYS:HG3	2.18	0.43
1:D:616:GLU:H	1:D:616:GLU:HG3	1.64	0.43
1:G:595:MET:HG3	1:G:599:LYS:HE3	2.00	0.43
1:L:504:ILE:HG13	1:L:520:LEU:HD21	2.01	0.43
1:Q:536:LYS:NZ	1:O:529:HIS:CE1	2.86	0.43
1:E:564:CYS:HB3	1:E:578:PHE:HB2	2.01	0.43
1:M:546:PRO:HD3	1:I:514:ARG:NH2	2.34	0.43
1:M:525:ASN:HD21	1:I:524:GLN:HE22	1.66	0.43
1:U:499:ILE:HA	1:U:554:ILE:O	2.19	0.43
1:X:639:LEU:HD12	1:X:639:LEU:H	1.83	0.43
1:H:611:LEU:HD23	1:H:652:GLU:HB2	1.99	0.43
1:L:537:GLU:H	1:L:537:GLU:CD	2.11	0.43
1:L:604:LYS:O	1:I:541:ARG:HD3	2.19	0.43
1:A:595:MET:HG3	1:A:599:LYS:HE3	2.01	0.43
1:I:639:LEU:C	1:I:639:LEU:CD2	2.86	0.43
1:S:587:VAL:O	1:S:587:VAL:HG12	2.18	0.43
1:W:595:MET:HG3	1:W:599:LYS:HE3	2.01	0.43
1:A:537:GLU:CD	1:A:537:GLU:H	2.23	0.43
1:G:513:ASN:OD1	1:G:514:ARG:N	2.51	0.43
1:T:606:ASN:HD22	1:K:566:ARG:NH1	2.17	0.43
1:K:564:CYS:HB3	1:K:578:PHE:HB2	1.99	0.43
1:K:619:ILE:HG22	1:K:623:LYS:HE2	2.01	0.43
1:X:522:GLY:O	1:X:526:VAL:HG23	2.19	0.43
1:D:566:ARG:HG2	1:D:566:ARG:NH1	2.34	0.43
1:L:574:THR:HG1	1:L:602:HIS:CD2	2.36	0.43
1:Q:607:ILE:C	1:Q:608:LEU:HD23	2.39	0.43
1:V:519:TRP:CE2	1:V:554:ILE:HD13	2.54	0.43
1:C:547:LYS:HD3	1:C:566:ARG:NH2	2.34	0.42
1:U:555:LYS:HD2	1:U:560:ILE:HD13	2.00	0.42
1:E:507:SER:OG	1:E:511:LYS:O	2.37	0.42
1:P:585:GLU:HA	1:P:588:LYS:HE2	2.01	0.42
1:V:513:ASN:HB3	1:V:516:VAL:HG22	2.01	0.42
1:G:498:ILE:HG23	1:G:556:ASP:H	1.84	0.42
1:Q:517:LEU:HD11	1:O:517:LEU:HD11	2.01	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:523:LEU:HD11	1:D:552:ALA:HB2	2.02	0.42
1:P:636:SER:HA	1:N:634:PRO:HG2	2.00	0.42
1:T:604:LYS:HB2	1:T:604:LYS:NZ	2.34	0.42
1:D:652:GLU:HG2	1:D:653:CYS:N	2.34	0.42
1:J:523:LEU:HA	1:J:526:VAL:HG22	2.00	0.42
1:Q:564:CYS:HB3	1:Q:578:PHE:HB2	2.01	0.42
1:Q:608:LEU:HA	1:Q:655:LEU:HD22	2.02	0.42
1:S:652:GLU:HG2	1:S:653:CYS:N	2.34	0.42
1:W:597:HIS:HA	1:W:662:THR:HG21	2.02	0.42
1:X:595:MET:CE	1:X:598:LEU:HD23	2.50	0.42
1:L:522:GLY:O	1:L:526:VAL:HG23	2.19	0.42
1:V:514:ARG:HH22	1:V:518:LEU:HD11	1.85	0.42
1:W:582:THR:OG1	1:W:583:SER:N	2.53	0.42
1:W:592:THR:HG22	1:W:624:LYS:CE	2.49	0.42
1:N:659:ILE:HD12	1:N:659:ILE:HG23	1.86	0.42
1:S:615:ASP:O	1:S:619:ILE:HG13	2.19	0.42
1:T:566:ARG:HB3	1:T:575:GLU:HB3	2.02	0.42
1:L:632:LYS:O	1:I:639:LEU:HD11	2.20	0.42
1:M:534:MET:HB2	1:M:539:ILE:HD11	2.00	0.42
1:Q:592:THR:HG22	1:Q:625:GLN:OE1	2.20	0.42
1:A:525:ASN:ND2	1:U:524:GLN:HE22	2.11	0.42
1:U:576:ILE:HG21	1:U:579:CYS:SG	2.59	0.42
1:W:635:LYS:HA	1:W:638:TYR:CE2	2.54	0.42
1:X:619:ILE:CG2	1:X:623:LYS:HZ2	2.31	0.42
1:X:613:TYR:CZ	1:X:650:LEU:HD12	2.49	0.42
1:H:604:LYS:HE3	1:H:605:HIS:CD2	2.54	0.42
1:J:585:GLU:OE1	1:J:588:LYS:NZ	2.37	0.42
1:L:614:ALA:O	1:L:619:ILE:HD11	2.20	0.42
1:M:566:ARG:HD3	1:M:568:PHE:CZ	2.55	0.42
1:Q:526:VAL:HG13	1:Q:529:HIS:CE1	2.55	0.42
1:R:517:LEU:O	1:R:521:VAL:HG23	2.20	0.42
1:U:563:ILE:HG21	1:U:598:LEU:HD22	2.01	0.42
1:U:656:ASN:HB3	1:U:659:ILE:HG13	2.02	0.42
1:D:587:VAL:C	1:D:588:LYS:HE2	2.40	0.41
1:E:529:HIS:HD1	1:E:529:HIS:C	2.22	0.41
1:L:657:PRO:C	1:L:659:ILE:H	2.22	0.41
1:M:585:GLU:OE1	1:M:588:LYS:NZ	2.43	0.41
1:P:633:VAL:HG23	1:P:652:GLU:OE2	2.20	0.41
1:T:608:LEU:HD13	1:T:657:PRO:HD3	2.02	0.41
1:C:633:VAL:HG23	1:C:652:GLU:OE2	2.20	0.41
1:Q:639:LEU:HD21	1:G:632:LYS:HE2	2.01	0.41

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:514:ARG:NH1	1:H:544:PHE:O	2.53	0.41
1:V:528:SER:OG	1:V:536:LYS:HG2	2.19	0.41
1:X:499:ILE:HA	1:X:554:ILE:O	2.20	0.41
1:G:624:LYS:HA	1:G:624:LYS:HD3	1.92	0.41
1:U:643:LYS:HG3	1:U:643:LYS:H	1.62	0.41
1:X:551:LEU:HB3	1:X:563:ILE:CG2	2.50	0.41
1:G:523:LEU:HD13	1:G:550:THR:HG21	2.03	0.41
1:M:555:LYS:NZ	1:M:585:GLU:CD	2.73	0.41
1:N:659:ILE:HA	1:N:659:ILE:HD13	1.78	0.41
1:S:522:GLY:O	1:S:526:VAL:HG23	2.20	0.41
1:V:645:TYR:HE2	1:E:658:ARG:HH22	1.68	0.41
1:I:635:LYS:HA	1:I:638:TYR:CE2	2.56	0.41
1:Q:575:GLU:HB2	1:Q:642:ILE:HG22	2.01	0.41
1:S:634:PRO:HG2	1:H:636:SER:HA	2.01	0.41
1:U:615:ASP:OD1	1:U:615:ASP:N	2.39	0.41
1:W:530:GLN:O	1:W:531:LEU:HD12	2.20	0.41
1:L:649:THR:OG1	1:L:651:MET:HG3	2.21	0.41
1:M:522:GLY:O	1:M:526:VAL:HG23	2.20	0.41
1:H:603:ILE:HD13	1:H:603:ILE:HA	1.81	0.41
1:Q:516:VAL:O	1:Q:520:LEU:HG	2.21	0.41
1:Q:571:GLN:NE2	1:Q:637:ARG:CB	2.84	0.41
1:W:560:ILE:HD12	1:W:585:GLU:HG3	2.03	0.41
1:X:642:ILE:HD12	1:X:642:ILE:O	2.20	0.41
1:A:606:ASN:OD1	1:C:547:LYS:HD2	2.21	0.41
1:L:643:LYS:HA	1:L:643:LYS:HD2	1.42	0.41
1:N:516:VAL:HA	1:N:519:TRP:HB2	2.03	0.41
1:P:566:ARG:HD3	1:P:568:PHE:CZ	2.56	0.41
1:Q:627:PHE:HA	1:Q:652:GLU:O	2.21	0.41
1:S:576:ILE:HB	1:S:612:THR:HB	2.03	0.41
1:U:603:ILE:HD11	1:U:661:TYR:HE2	1.86	0.41
1:W:521:VAL:HG22	1:J:521:VAL:HG12	2.03	0.41
1:X:553:LEU:HD12	1:X:594:LEU:HD22	2.03	0.41
1:F:595:MET:HG3	1:F:599:LYS:HE3	2.01	0.41
1:I:564:CYS:HB3	1:I:578:PHE:HB2	2.03	0.41
1:P:545:ASP:HA	1:P:546:PRO:HD3	1.94	0.41
1:R:616:GLU:HG3	1:R:616:GLU:H	1.70	0.41
1:X:595:MET:HE3	1:X:598:LEU:HB3	2.01	0.41
1:X:614:ALA:CB	1:X:622:PHE:CD2	3.04	0.41
1:X:631:ILE:HB	1:X:652:GLU:HB3	2.02	0.41
1:Q:553:LEU:HD23	1:Q:560:ILE:HG13	2.03	0.41
1:E:587:VAL:C	1:E:588:LYS:HG3	2.42	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:560:ILE:O	1:H:582:THR:HG22	2.21	0.41
1:J:551:LEU:O	1:J:562:GLY:HA2	2.20	0.41
1:L:549:LYS:HZ2	1:L:567:MET:HE3	1.85	0.41
1:M:499:ILE:HA	1:M:554:ILE:O	2.21	0.41
1:Q:547:LYS:O	1:Q:547:LYS:CG	2.69	0.41
1:U:499:ILE:HG22	1:U:555:LYS:HB2	2.03	0.41
1:D:615:ASP:OD1	1:D:618:ALA:N	2.53	0.40
1:Q:599:LYS:O	1:Q:603:ILE:HG13	2.21	0.40
1:S:560:ILE:HB	1:S:585:GLU:HG3	2.03	0.40
1:V:652:GLU:HG2	1:V:653:CYS:N	2.35	0.40
1:X:506:ASN:O	1:X:546:PRO:HA	2.21	0.40
1:D:619:ILE:O	1:D:623:LYS:HG3	2.21	0.40
1:K:608:LEU:HD13	1:K:657:PRO:HG3	2.04	0.40
1:Q:601:TYR:O	1:Q:605:HIS:HB2	2.22	0.40
1:Q:622:PHE:HB3	1:Q:627:PHE:CB	2.52	0.40
1:V:541:ARG:HD2	1:V:541:ARG:HH11	1.77	0.40
1:V:624:LYS:HE3	1:V:624:LYS:HB3	1.90	0.40
1:X:657:PRO:CG	1:X:658:ARG:HH12	2.33	0.40
1:H:615:ASP:O	1:H:619:ILE:HG13	2.20	0.40
1:K:617:TYR:CD1	1:K:617:TYR:N	2.89	0.40
1:L:513:ASN:OD1	1:L:514:ARG:N	2.53	0.40
1:L:611:LEU:HD22	1:L:650:LEU:HD11	2.03	0.40
1:Q:563:ILE:HG13	1:Q:594:LEU:HD13	2.04	0.40
1:Q:547:LYS:HG3	1:Q:566:ARG:CZ	2.51	0.40
1:A:558:ARG:HD2	1:U:537:GLU:HG3	2.03	0.40
1:W:564:CYS:HB3	1:W:578:PHE:HB2	2.04	0.40
1:D:632:LYS:H	1:D:632:LYS:HG2	1.65	0.40
1:F:499:ILE:HA	1:F:554:ILE:O	2.22	0.40
1:G:635:LYS:HA	1:G:638:TYR:CE2	2.55	0.40
1:I:575:GLU:HB2	1:I:642:ILE:HG22	2.03	0.40
1:L:635:LYS:C	1:L:637:ARG:H	2.25	0.40
1:S:553:LEU:HG	1:S:560:ILE:HG13	2.02	0.40
1:U:501:PHE:HB3	1:U:551:LEU:HD11	2.04	0.40
1:B:547:LYS:HD3	1:B:566:ARG:NH2	2.36	0.40
1:F:523:LEU:HG	1:F:559:VAL:HG11	2.03	0.40
1:H:595:MET:O	1:H:599:LYS:HG3	2.21	0.40
1:H:624:LYS:HA	1:H:624:LYS:HD2	1.75	0.40
1:J:600:GLU:OE2	1:J:660:PRO:HA	2.21	0.40
1:P:499:ILE:HD11	1:P:555:LYS:HE3	2.03	0.40
1:W:613:TYR:CE2	1:W:644:ASP:HA	2.56	0.40
1:X:635:LYS:HA	1:X:638:TYR:CD2	2.57	0.40

All (8) 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:B:629:LYS:NZ	1:H:646:GLU:OE2[4_554]	1.95	0.25
1:C:646:GLU:OE2	1:G:629:LYS:NZ[4_454]	2.00	0.20
1:S:646:GLU:OE1	1:I:629:LYS:NZ[8_655]	2.07	0.13
1:B:617:TYR:OH	1:H:615:ASP:OD1[4_554]	2.07	0.13
1:U:629:LYS:NZ	1:F:646:GLU:OE2[5_545]	2.10	0.10
1:B:646:GLU:OE1	1:H:629:LYS:NZ[4_554]	2.11	0.09
1:O:533:ARG:NH2	1:O:615:ASP:OD2[8_665]	2.16	0.04
1:S:533:ARG:NH2	1:I:615:ASP:OD2[8_655]	2.17	0.03

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	158/168 (94%)	156 (99%)	2 (1%)	0	100	100
1	B	157/168 (94%)	154 (98%)	3 (2%)	0	100	100
1	C	155/168 (92%)	149 (96%)	6 (4%)	0	100	100
1	D	157/168 (94%)	152 (97%)	5 (3%)	0	100	100
1	E	159/168 (95%)	152 (96%)	7 (4%)	0	100	100
1	F	158/168 (94%)	154 (98%)	4 (2%)	0	100	100
1	G	160/168 (95%)	154 (96%)	6 (4%)	0	100	100
1	H	156/168 (93%)	151 (97%)	5 (3%)	0	100	100
1	I	158/168 (94%)	155 (98%)	3 (2%)	0	100	100
1	J	159/168 (95%)	151 (95%)	8 (5%)	0	100	100
1	K	156/168 (93%)	152 (97%)	4 (3%)	0	100	100
1	L	153/168 (91%)	148 (97%)	5 (3%)	0	100	100
1	M	156/168 (93%)	152 (97%)	4 (3%)	0	100	100
1	N	159/168 (95%)	157 (99%)	2 (1%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	O	157/168 (94%)	153 (98%)	4 (2%)	0	100	100
1	P	157/168 (94%)	151 (96%)	6 (4%)	0	100	100
1	Q	152/168 (90%)	142 (93%)	10 (7%)	0	100	100
1	R	158/168 (94%)	155 (98%)	3 (2%)	0	100	100
1	S	157/168 (94%)	149 (95%)	8 (5%)	0	100	100
1	T	156/168 (93%)	154 (99%)	2 (1%)	0	100	100
1	U	160/168 (95%)	157 (98%)	3 (2%)	0	100	100
1	V	157/168 (94%)	151 (96%)	6 (4%)	0	100	100
1	W	156/168 (93%)	150 (96%)	6 (4%)	0	100	100
1	X	156/168 (93%)	147 (94%)	9 (6%)	0	100	100
All	All	3767/4032 (93%)	3646 (97%)	121 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	143/147 (97%)	143 (100%)	0	100	100
1	B	143/147 (97%)	143 (100%)	0	100	100
1	C	141/147 (96%)	141 (100%)	0	100	100
1	D	142/147 (97%)	141 (99%)	1 (1%)	87	97
1	E	142/147 (97%)	141 (99%)	1 (1%)	87	97
1	F	143/147 (97%)	143 (100%)	0	100	100
1	G	143/147 (97%)	143 (100%)	0	100	100
1	H	141/147 (96%)	141 (100%)	0	100	100
1	I	143/147 (97%)	143 (100%)	0	100	100
1	J	143/147 (97%)	143 (100%)	0	100	100
1	K	142/147 (97%)	142 (100%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	139/147 (95%)	137 (99%)	2 (1%)	71	91
1	M	141/147 (96%)	141 (100%)	0	100	100
1	N	143/147 (97%)	143 (100%)	0	100	100
1	O	142/147 (97%)	140 (99%)	2 (1%)	71	91
1	P	142/147 (97%)	141 (99%)	1 (1%)	87	97
1	Q	138/147 (94%)	137 (99%)	1 (1%)	87	97
1	R	143/147 (97%)	143 (100%)	0	100	100
1	S	142/147 (97%)	142 (100%)	0	100	100
1	T	141/147 (96%)	141 (100%)	0	100	100
1	U	145/147 (99%)	145 (100%)	0	100	100
1	V	142/147 (97%)	142 (100%)	0	100	100
1	W	142/147 (97%)	140 (99%)	2 (1%)	71	91
1	X	141/147 (96%)	139 (99%)	2 (1%)	71	91
All	All	3407/3528 (97%)	3395 (100%)	12 (0%)	93	98

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	W	524	GLN
1	W	534	MET
1	Q	645	TYR
1	P	515	ARG
1	O	524	GLN
1	O	645	TYR
1	L	566	ARG
1	L	637	ARG
1	D	558	ARG
1	E	658	ARG
1	X	558	ARG
1	X	629	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	513	ASN
1	A	525	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	530	GLN
1	A	586	GLN
1	W	525	ASN
1	T	525	ASN
1	T	602	HIS
1	T	606	ASN
1	T	656	ASN
1	S	525	ASN
1	S	571	GLN
1	S	596	ASN
1	R	502	HIS
1	Q	571	GLN
1	O	530	GLN
1	M	525	ASN
1	M	530	GLN
1	M	584	ASN
1	L	571	GLN
1	L	606	ASN
1	D	525	ASN
1	E	525	ASN
1	E	586	GLN
1	E	606	ASN
1	G	525	ASN
1	G	571	GLN
1	H	525	ASN
1	H	586	GLN
1	I	586	GLN
1	X	502	HIS
1	X	593	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	L	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	L	533:ARG	C	534:MET	N	1.19

## 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	162/168 (96%)	-0.23	2 (1%) 79 77	7, 19, 54, 72	0
1	B	161/168 (95%)	-0.34	0 100 100	7, 15, 42, 82	0
1	C	159/168 (94%)	-0.21	2 (1%) 77 76	7, 19, 50, 91	0
1	D	161/168 (95%)	-0.04	4 (2%) 58 53	15, 30, 62, 96	0
1	E	163/168 (97%)	-0.00	5 (3%) 49 43	10, 26, 59, 84	0
1	F	162/168 (96%)	-0.21	3 (1%) 67 64	8, 20, 47, 76	0
1	G	164/168 (97%)	-0.13	5 (3%) 51 44	13, 26, 56, 104	0
1	H	160/168 (95%)	-0.33	0 100 100	6, 15, 36, 53	0
1	I	162/168 (96%)	-0.14	3 (1%) 67 64	11, 28, 56, 83	0
1	J	163/168 (97%)	0.14	10 (6%) 22 17	7, 33, 74, 113	0
1	K	160/168 (95%)	-0.10	4 (2%) 58 53	10, 24, 54, 77	0
1	L	157/168 (93%)	0.37	7 (4%) 34 29	14, 39, 70, 93	0
1	M	160/168 (95%)	-0.16	2 (1%) 77 76	10, 23, 54, 80	0
1	N	163/168 (97%)	-0.15	2 (1%) 79 77	7, 22, 59, 79	0
1	O	161/168 (95%)	-0.09	3 (1%) 67 64	15, 30, 63, 105	0
1	P	161/168 (95%)	-0.23	1 (0%) 89 88	7, 16, 49, 61	0
1	Q	156/168 (92%)	0.71	16 (10%) 7 5	23, 57, 83, 102	0
1	R	162/168 (96%)	-0.27	0 100 100	6, 14, 34, 80	0
1	S	161/168 (95%)	0.01	6 (3%) 42 37	9, 30, 68, 107	0
1	T	160/168 (95%)	0.21	5 (3%) 49 43	18, 41, 67, 87	0
1	U	164/168 (97%)	-0.25	2 (1%) 79 77	7, 16, 44, 107	0
1	V	161/168 (95%)	0.10	7 (4%) 36 31	13, 31, 67, 85	0
1	W	160/168 (95%)	0.29	7 (4%) 35 30	21, 42, 81, 96	0
1	X	160/168 (95%)	0.94	27 (16%) 2 1	33, 73, 105, 114	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
All	All	3863/4032 (95%)	-0.01	123 (3%)	48	42	6, 27, 73, 114	0

All (123) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Q	656	ASN	6.5
1	Q	573	PHE	5.6
1	U	509	THR	5.1
1	L	660	PRO	4.5
1	K	498	ILE	4.4
1	E	497	GLY	4.3
1	V	508	LEU	4.1
1	C	513	ASN	4.0
1	E	587	VAL	4.0
1	S	558	ARG	4.0
1	Q	606	ASN	3.9
1	X	589	GLY	3.8
1	F	508	LEU	3.8
1	X	655	LEU	3.7
1	A	587	VAL	3.7
1	Q	572	GLY	3.6
1	X	609	TYR	3.4
1	L	662	THR	3.2
1	T	498	ILE	3.2
1	Q	590	TYR	3.2
1	J	508	LEU	3.1
1	N	498	ILE	3.1
1	X	587	VAL	3.1
1	X	626	GLY	3.1
1	G	584	ASN	3.1
1	O	587	VAL	3.1
1	V	645	TYR	3.1
1	X	618	ALA	3.0
1	K	587	VAL	3.0
1	V	584	ASN	3.0
1	V	514	ARG	2.9
1	V	512	ALA	2.9
1	G	497	GLY	2.9
1	J	590	TYR	2.9
1	X	590	TYR	2.9
1	E	498	ILE	2.8
1	E	662	THR	2.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	J	589	GLY	2.8
1	L	499	ILE	2.8
1	G	509	THR	2.8
1	Q	608	LEU	2.8
1	X	620	GLY	2.8
1	W	581	VAL	2.7
1	L	584	ASN	2.7
1	W	617	TYR	2.7
1	O	507	SER	2.6
1	I	508	LEU	2.6
1	K	584	ASN	2.6
1	Q	630	ASP	2.6
1	E	660	PRO	2.6
1	M	512	ALA	2.6
1	J	512	ALA	2.6
1	X	622	PHE	2.6
1	Q	529	HIS	2.6
1	X	553	LEU	2.6
1	X	512	ALA	2.5
1	Q	628	SER	2.5
1	X	499	ILE	2.5
1	Q	636	SER	2.5
1	X	614	ALA	2.5
1	D	498	ILE	2.5
1	X	560	ILE	2.5
1	C	587	VAL	2.4
1	K	589	GLY	2.4
1	S	514	ARG	2.4
1	X	500	GLU	2.4
1	Q	631	ILE	2.4
1	M	662	THR	2.4
1	S	556	ASP	2.4
1	D	512	ALA	2.4
1	L	570	THR	2.4
1	J	497	GLY	2.3
1	Q	556	ASP	2.3
1	D	555	LYS	2.3
1	W	584	ASN	2.3
1	X	593	HIS	2.3
1	S	590	TYR	2.3
1	L	590	TYR	2.3
1	I	499	ILE	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	J	558	ARG	2.3
1	I	587	VAL	2.3
1	X	661	TYR	2.3
1	Q	587	VAL	2.2
1	X	641	TYR	2.2
1	G	554	ILE	2.2
1	Q	571	GLN	2.2
1	X	610	PHE	2.2
1	S	589	GLY	2.2
1	J	507	SER	2.2
1	X	624	LYS	2.2
1	V	553	LEU	2.2
1	V	529	HIS	2.2
1	X	581	VAL	2.2
1	A	498	ILE	2.1
1	J	498	ILE	2.1
1	F	498	ILE	2.1
1	S	529	HIS	2.1
1	X	621	TYR	2.1
1	X	630	ASP	2.1
1	Q	626	GLY	2.1
1	F	497	GLY	2.1
1	U	499	ILE	2.1
1	X	554	ILE	2.1
1	N	662	THR	2.1
1	X	646	GLU	2.1
1	T	555	LYS	2.1
1	D	587	VAL	2.1
1	T	616	GLU	2.1
1	O	590	TYR	2.1
1	J	662	THR	2.1
1	X	656	ASN	2.1
1	W	590	TYR	2.1
1	W	514	ARG	2.1
1	T	584	ASN	2.1
1	W	553	LEU	2.1
1	Q	621	TYR	2.1
1	X	532	PRO	2.1
1	T	587	VAL	2.0
1	J	617	TYR	2.0
1	W	556	ASP	2.0
1	L	572	GLY	2.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	G	498	ILE	2.0
1	P	662	THR	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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.