



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:23 AM UTC

PDB ID : 5TRM / pdb_00005trm
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

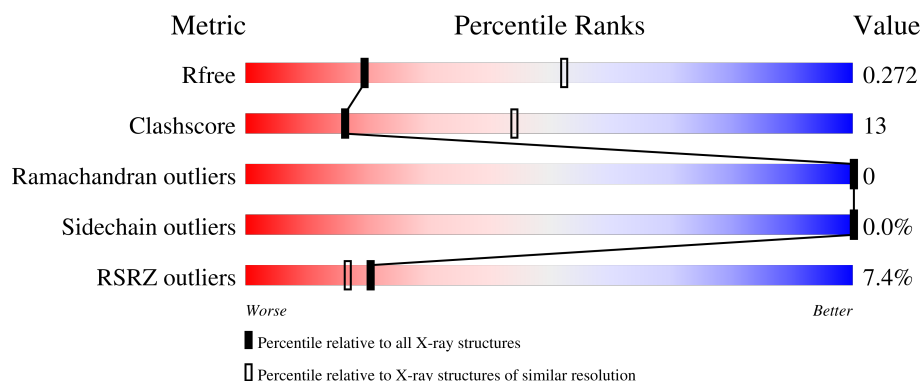
1 Overall quality at a glance

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}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	4% 74% 22% .
1	B	168	3% 77% 19% .
1	C	168	% 82% 12% 5%
1	D	168	5% 74% 21% .
1	E	168	7% 75% 22% .

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...

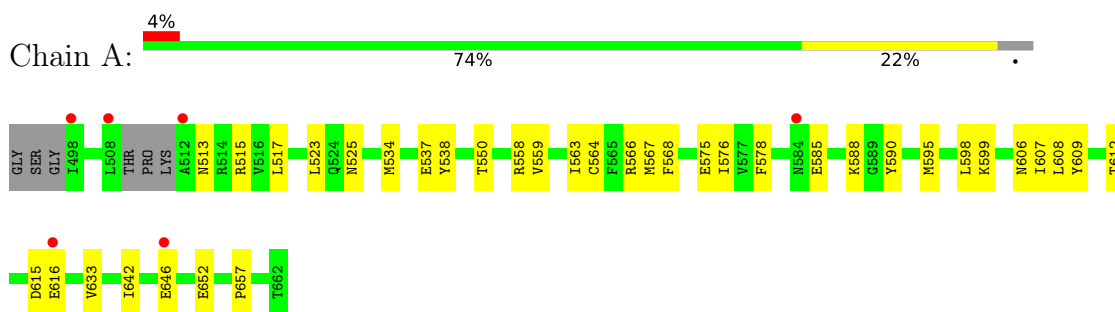
Continued from previous page...

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

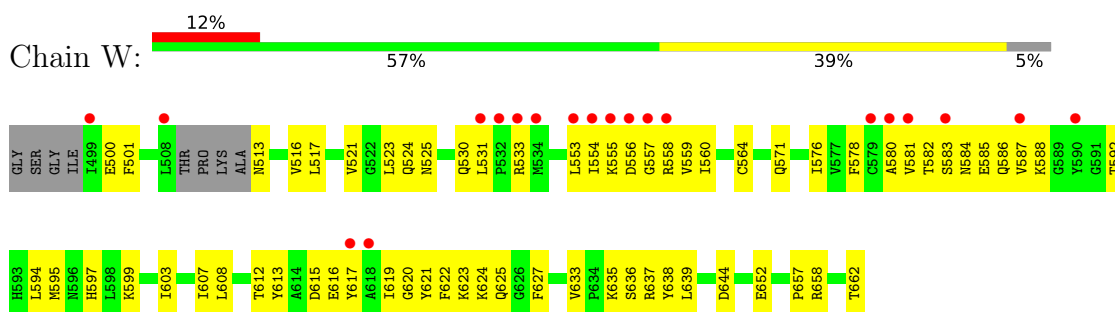
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

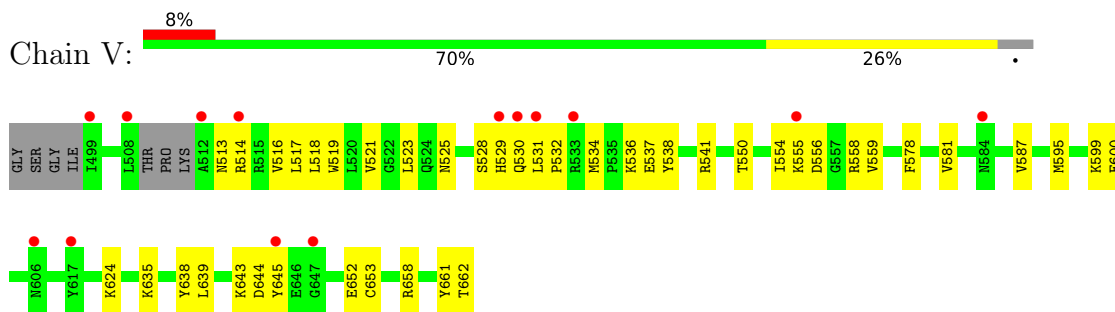
- Molecule 1: Histone acetyltransferase KAT2A



- Molecule 1: Histone acetyltransferase KAT2A



- Molecule 1: Histone acetyltransferase KAT2A

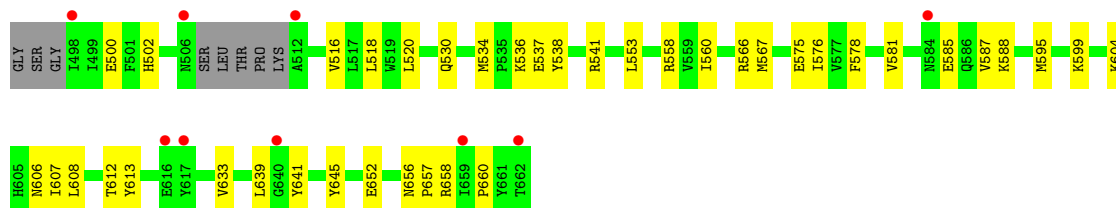


- Molecule 1: Histone acetyltransferase KAT2A

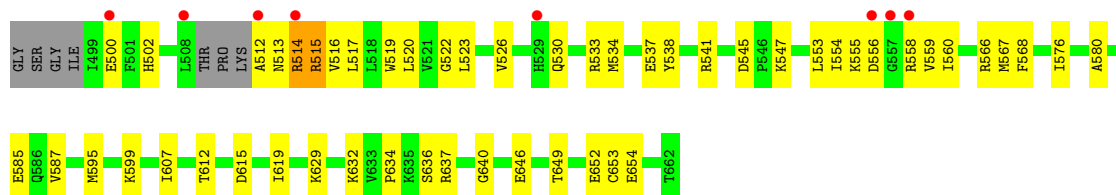




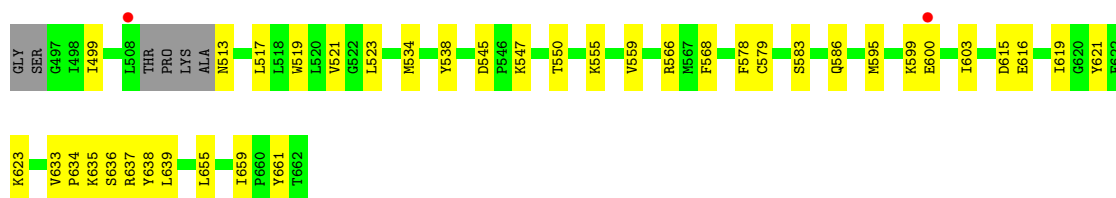
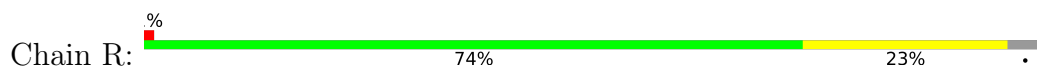
• Molecule 1: Histone acetyltransferase KAT2A



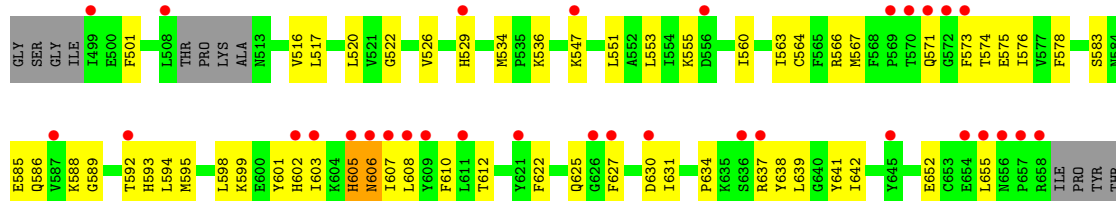
• Molecule 1: Histone acetyltransferase KAT2A



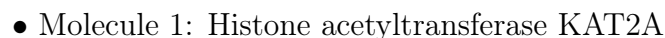
• Molecule 1: Histone acetyltransferase KAT2A



• Molecule 1: Histone acetyltransferase KAT2A



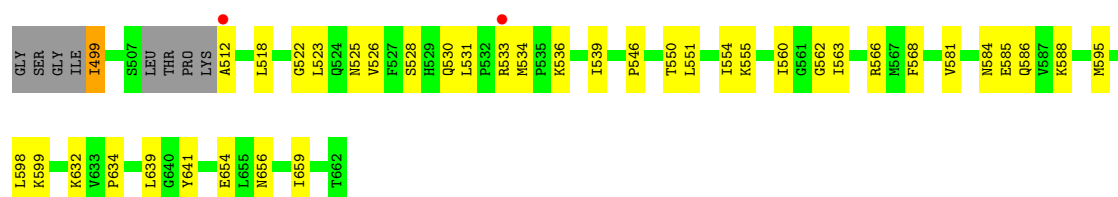
Chain P: 75% 21% 4%



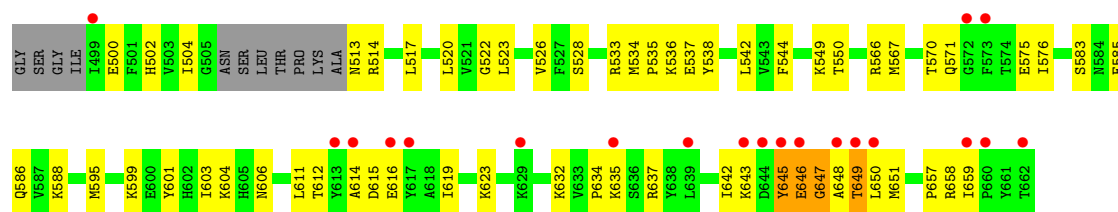
Chain N: 5% 85% 12%



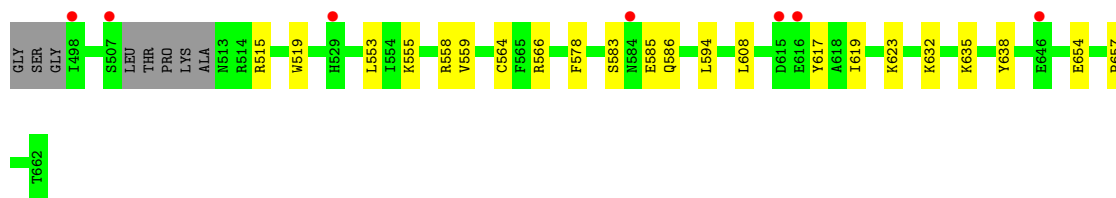
Chain M: %



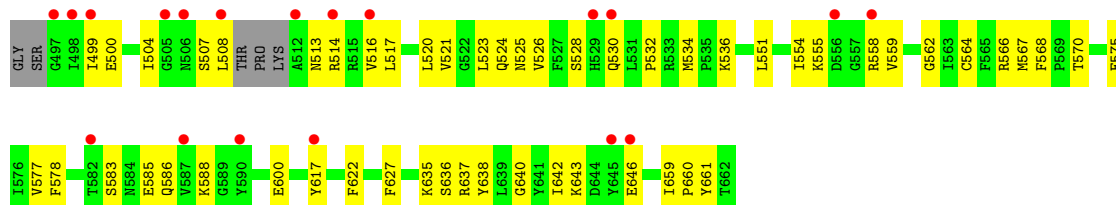
Chain L: 12% 58% 33% 7%



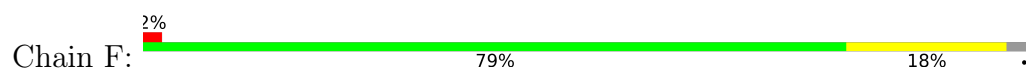
Chain K: 4% 82% 13% 5%



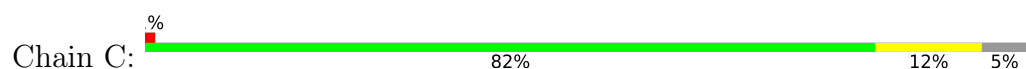
- Molecule 1: Histone acetyltransferase KAT2A



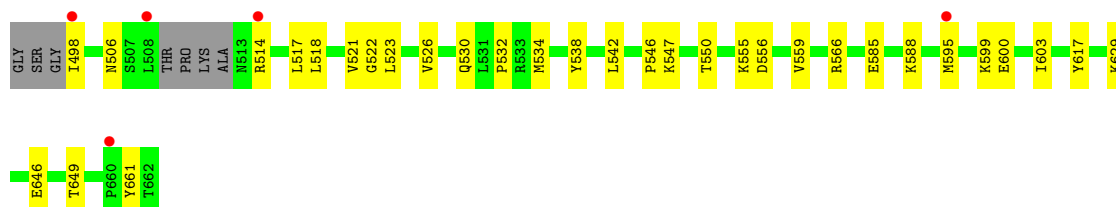
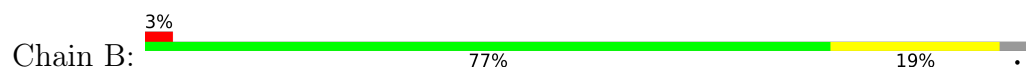
- Molecule 1: Histone acetyltransferase KAT2A



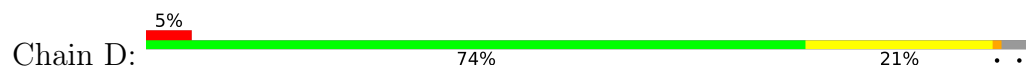
- Molecule 1: Histone acetyltransferase KAT2A

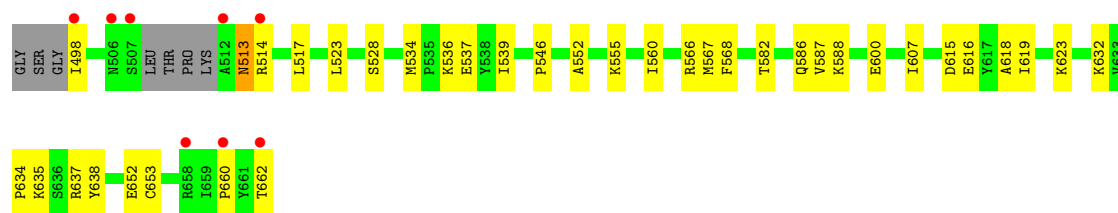


- Molecule 1: Histone acetyltransferase KAT2A

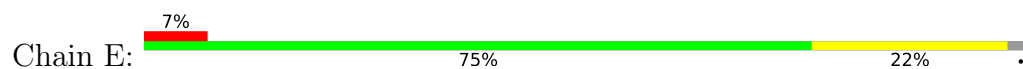


- Molecule 1: Histone acetyltransferase KAT2A

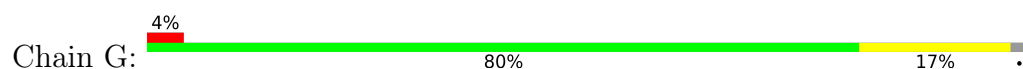




• Molecule 1: Histone acetyltransferase KAT2A



• Molecule 1: Histone acetyltransferase KAT2A



• Molecule 1: Histone acetyltransferase KAT2A

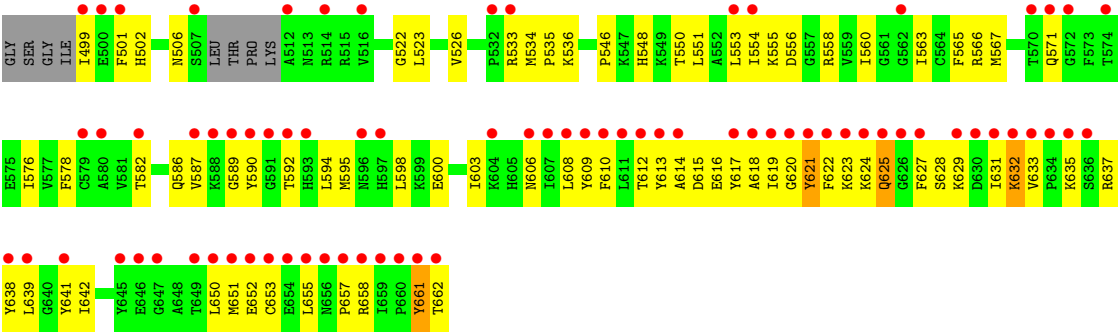


• Molecule 1: Histone acetyltransferase KAT2A



• 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, α , β , γ	173.47Å 173.47Å 347.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.18 – 2.90 48.18 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.6 (48.18-2.90) 96.3 (48.18-2.90)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.03 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.10_2152	Depositor
R, R_{free}	0.215 , 0.273 0.215 , 0.272	Depositor DCC
R_{free} test set	5807 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	41.2	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 37.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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 ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.78% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

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	0.37	0/1366	0.48	0/1842
1	B	0.41	0/1361	0.48	0/1835
1	C	0.40	0/1347	0.50	0/1816
1	D	0.33	0/1358	0.56	3/1831 (0.2%)
1	E	0.35	0/1367	0.51	0/1843
1	F	0.37	0/1365	0.48	0/1840
1	G	0.35	0/1375	0.49	1/1854 (0.1%)
1	H	0.40	0/1349	0.47	0/1818
1	I	0.35	0/1366	0.43	0/1842
1	J	0.34	0/1370	0.52	0/1847
1	K	0.32	0/1353	0.44	0/1824
1	L	0.38	0/1331	0.53	1/1794 (0.1%)
1	M	0.34	0/1350	0.49	1/1820 (0.1%)
1	N	0.34	0/1370	0.45	0/1847
1	O	0.35	0/1358	0.48	0/1831
1	P	0.38	0/1358	0.46	0/1831
1	Q	0.31	0/1317	0.59	2/1773 (0.1%)
1	R	0.45	0/1365	0.48	0/1840
1	S	0.49	2/1358 (0.1%)	0.60	1/1831 (0.1%)
1	T	0.28	0/1352	0.44	0/1823
1	U	0.40	0/1380	0.45	0/1862
1	V	0.34	0/1358	0.51	0/1831
1	W	0.37	1/1353 (0.1%)	0.55	0/1824
1	X	0.47	0/1350	0.83	6/1820 (0.3%)
All	All	0.37	3/32577 (0.0%)	0.52	15/43919 (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 (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S	515	ARG	NE-CZ	-6.26	1.26	1.33
1	S	514	ARG	CZ-NH1	5.91	1.41	1.32
1	W	616	GLU	CD-OE1	-5.21	1.15	1.25

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	633	VAL	N-CA-C	-8.56	99.63	108.96
1	X	620	GLY	CA-C-N	-7.43	110.53	120.63
1	X	620	GLY	C-N-CA	-7.43	110.53	120.63
1	G	510	PRO	N-CA-CB	7.18	110.90	103.00
1	Q	606	ASN	CA-C-N	-6.07	113.83	121.96
1	Q	606	ASN	C-N-CA	-6.07	113.83	121.96
1	D	513	ASN	CA-C-N	-5.85	113.02	121.98
1	D	513	ASN	C-N-CA	-5.85	113.02	121.98
1	S	515	ARG	NH1-CZ-NH2	5.71	126.72	119.30
1	D	513	ASN	N-CA-C	-5.43	101.60	108.45
1	M	499	ILE	N-CA-CB	-5.35	102.41	111.50
1	L	647	GLY	N-CA-C	-5.30	100.61	113.18
1	X	621	TYR	CA-CB-CG	5.23	123.31	113.90
1	X	624	LYS	CD-CE-NZ	-5.18	95.34	111.90
1	X	661	TYR	N-CA-C	-5.02	107.18	113.15

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
1	X	625	GLN	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
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	30	0
1	B	1326	0	1342	21	3
1	C	1312	0	1326	14	1
1	D	1323	0	1336	40	0
1	E	1332	0	1341	41	0
1	F	1330	0	1345	18	1
1	G	1340	0	1348	28	1
1	H	1314	0	1328	34	3
1	I	1331	0	1347	36	2
1	J	1335	0	1348	50	0
1	K	1318	0	1331	15	0
1	L	1296	0	1309	62	0
1	M	1315	0	1325	28	0
1	N	1335	0	1350	15	0
1	O	1323	0	1336	24	1
1	P	1323	0	1336	28	0
1	Q	1284	0	1297	90	0
1	R	1330	0	1345	35	0
1	S	1323	0	1336	44	2
1	T	1317	0	1331	30	0
1	U	1344	0	1359	39	1
1	V	1323	0	1336	48	0
1	W	1318	0	1331	65	0
1	X	1315	0	1325	108	0
All	All	31738	0	32055	831	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 13.

All (831) 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:NE2	1:Q:637:ARG:C	1.97	1.21
1:Q:571:GLN:CG	1:Q:573:PHE:CE2	2.26	1.19
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:CD	1:Q:573:PHE:CZ	2.32	1.08
1:Q:571:GLN:CD	1:Q:573:PHE:CE2	2.31	1.08
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:L:500:GLU:CD	1:L:502:HIS:CE1	2.34	1.05
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:V:514:ARG:HH12	1:V:518:LEU:CD1	1.71	1.02
1:V:514:ARG:NH1	1:V:518:LEU:CG	2.17	1.01
1:L:500:GLU:OE2	1:L:502:HIS:CD2	2.14	1.01
1:R:600:GLU:OE2	1:R:661:TYR:CD2	2.12	1.01
1:Q:571:GLN:HE22	1:Q:637:ARG:C	1.64	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:S:632:LYS:NZ	1:S:654:GLU:OE1	1.98	0.96
1:L:500:GLU:OE2	1:L:502:HIS:NE2	1.97	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:W:533:ARG:NH2	1:W:617:TYR:OH	2.04	0.91
1:L:528:SER:OG	1:L:536:LYS:HG2	1.69	0.91
1:W:533:ARG:NH1	1:W:615:ASP:OD1	2.03	0.91
1:Q:571:GLN:NE2	1:Q:573:PHE:CE2	2.38	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:W:620:GLY:HA2	1:W:623:LYS:HZ1	1.38	0.87
1:X:556:ASP:O	1:X:558:ARG:NH1	2.07	0.86
1:R:600:GLU:CD	1:R:661:TYR:HB2	2.00	0.85
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:J:528:SER:O	1:J:536:LYS:NZ	2.10	0.84
1:E:536:LYS:HZ1	1:H:525:ASN:ND2	1.76	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: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:T:530:GLN:NE2	1:T:581:VAL:O	2.16	0.79
1:L:533:ARG:NH1	1:L:615:ASP:OD1	2.15	0.79
1:V:521:VAL:O	1:V:525:ASN:ND2	2.16	0.78
1:D:546:PRO:CD	1:G:514:ARG:HH22	1.95	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: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:X:619:ILE:HG22	1:X:623:LYS:HZ2	1.53	0.74
1:L:500:GLU:CD	1:L:502:HIS:ND1	2.43	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:W:619:ILE:O	1:W:623:LYS:NZ	2.18	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:W:500:GLU:H	1:W:554:ILE:HG22	1.56	0.70
1:Q:573:PHE:C	1:Q:607:ILE:HD11	2.15	0.70
1:N:531:LEU:HD21	1:N:617:TYR:OH	1.92	0.70
1:W:619:ILE:C	1:W:623:LYS:NZ	2.50	0.69
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:Q:571:GLN:CD	1:Q:573:PHE:HZ	1.92	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:619:ILE:C	1:W:623:LYS:HZ3	2.00	0.68
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
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: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:Q:571:GLN:NE2	1:Q:573:PHE:HE2	1.93	0.66
1:L:606:ASN:HD21	1:I:643:LYS:NZ	1.92	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: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:L:616:GLU:OE2	1:L:648:ALA:HB2	1.96	0.65
1:R:600:GLU:CD	1:R:661:TYR:H	2.04	0.65
1:X:603:ILE:HG13	1:X:655:LEU:HD23	1.78	0.65
1:U:639:LEU:O	1:R:637:ARG:NH1	2.22	0.65
1:Q:589:GLY:O	1:Q:593:HIS:ND1	2.28	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:X:623:LYS:HG2	1:X:651:MET:HE1	1.79	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:D:567:MET:HE2	1:D:607:ILE:HD12	1.79	0.64
1:V:645:TYR:CE2	1:E:658:ARG:NH1	2.65	0.64
1:L:646:GLU:O	1:L:646:GLU:OE2	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: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:Q:571:GLN:HE21	1:Q:637:ARG:C	2.03	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:W:554:ILE:HG13	1:W:558:ARG:O	1.99	0.62
1:F:500:GLU:HB2	1:F:554:ILE:HB	1.81	0.62
1:X:613:TYR:HE2	1:X:642:ILE:HD13	1.64	0.62
1:U:566:ARG:HD3	1:U:568:PHE:CZ	2.34	0.61
1:V:534:MET:HE1	1:V:578:PHE:CE1	2.36	0.61
1:U:513:ASN:HB3	1:U:516:VAL:HB	1.82	0.61
1:X:629:LYS:HA	1:X:651:MET:HG2	1.82	0.61
1:X:631:ILE:HB	1:X:652:GLU:OE2	2.00	0.61
1:U:576:ILE:CG2	1:U:579:CYS:SG	2.88	0.61
1:P:608:LEU:HD11	1:J:643:LYS:HD3	1.82	0.61
1:G:644:ASP:OD1	1:G:645:TYR:N	2.33	0.61
1:H:531:LEU:HD13	1:H:534:MET:HE2	1.83	0.61
1:X:534:MET:HE1	1:X:578:PHE:CE1	2.35	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:Q:571:GLN:CD	1:Q:637:ARG:O	2.43	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:T:553:LEU:HG	1:T:560:ILE:HG23	1.83	0.61
1:J:528:SER:HB2	1:J:536:LYS:NZ	2.16	0.61
1:S:595:MET:HG3	1:S:599:LYS:HE3	1.83	0.61
1:L:576:ILE:HB	1:L:612:THR:HB	1.83	0.61
1:X:592:THR:HG23	1:X:625:GLN:NE2	2.16	0.61
1:W:620:GLY:CA	1:W:623:LYS:HZ1	2.12	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:W:599:LYS:NZ	1:W:625:GLN:O	2.33	0.60
1:S:515:ARG:HD2	1:S:519:TRP:CZ2	2.35	0.60
1:M:639:LEU:O	1:J:637:ARG:NH1	2.28	0.60
1:L:632:LYS:O	1:I:639:LEU:HD13	2.01	0.60
1:W:592:THR:CG2	1:W:624:LYS:CE	2.79	0.60
1:V:523:LEU:HG	1:V:559:VAL:HG11	1.82	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:X:534:MET:HE1	1:X:578:PHE:HE1	1.67	0.60
1:I:639:LEU:HD23	1:I:639:LEU:C	2.26	0.60
1:U:566:ARG:HH11	1:U:566:ARG:HG2	1.67	0.60
1:S:555:LYS:HD3	1:S:560:ILE:HD13	1.84	0.60
1:P:513:ASN:HB3	1:P:516:VAL:HG22	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:A:534:MET:HE1	1:A:578:PHE:HE1	1.67	0.59
1:W:619:ILE:HG23	1:W:623:LYS:HZ2	1.67	0.59
1:L:632:LYS:O	1:I:639:LEU:CD1	2.50	0.59
1:F:600:GLU:HG2	1:F:661:TYR:HB2	1.84	0.59
1:W:556:ASP:HB2	1:W:558:ARG:HG2	1.83	0.59
1:X:608:LEU:C	1:X:609:TYR:HD2	2.10	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:O:658:ARG:HD3	1:X:534:MET:HG2	1.83	0.59
1:E:533:ARG:HD3	1:E:646:GLU:OE2	2.03	0.59
1:G:567:MET:HE2	1:G:607:ILE:HD12	1.85	0.59
1:M:512:ALA:N	1:I:508:LEU:HD13	2.18	0.58
1:L:537:GLU:OE2	1:L:537:GLU:N	2.25	0.58
1:E:589:GLY:O	1:E:593:HIS:ND1	2.32	0.58
1:X:622:PHE:HB3	1:X:627:PHE:CE1	2.38	0.58
1:S:555:LYS:HG3	1:S:556:ASP:H	1.67	0.58
1:M:641:TYR:OH	1:J:570:THR:O	2.12	0.58
1:V:534:MET:HE3	1:V:538:TYR:HD2	1.69	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:F:523:LEU:HD13	1:F:550:THR:HG21	1.86	0.58
1:D:513:ASN:O	1:D:517:LEU:HG	2.03	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:608:LEU:HD13	1:O:657:PRO:HG3	1.85	0.57
1:L:619:ILE:CG2	1:L:623:LYS:HE3	2.31	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:M:555:LYS:NZ	1:M:585:GLU:OE2	2.32	0.57
1:I:555:LYS:HD2	1:I:560:ILE:HD13	1.87	0.57
1:P:659:ILE:HG21	1:P:661:TYR:CZ	2.40	0.57
1:J:617:TYR:HD2	1:J:617:TYR:N	2.03	0.57
1:C:531:LEU:HD13	1:C:534:MET:HE1	1.87	0.57
1:B:517:LEU:O	1:B:521:VAL:HG23	2.05	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:T:585:GLU:OE1	1:T:588:LYS:NZ	2.28	0.56
1:S:566:ARG:HD3	1:S:568:PHE:CZ	2.38	0.56
1:Q:571:GLN:NE2	1:Q:637:ARG:HB3	2.19	0.56
1:X:556:ASP:CB	1:X:558:ARG:HH12	2.18	0.56
1:W:619:ILE:HG23	1:W:623:LYS:NZ	2.20	0.56
1:U:634:PRO:HG2	1:S:636:SER:HA	1.87	0.56
1:T:641:TYR:OH	1:X:571:GLN:HA	2.05	0.56
1:Q:571:GLN:NE2	1:Q:638:TYR:HA	2.16	0.56
1:W:592:THR:HG21	1:W:624:LYS:HE3	1.87	0.56
1:Q:553:LEU:CD1	1:Q:594:LEU:HG	2.35	0.56
1:I:526:VAL:O	1:I:530:GLN:HG2	2.04	0.56
1:X:629:LYS:N	1:X:651:MET:HE3	2.21	0.56
1:S:512:ALA:HA	1:S:516:VAL:HG21	1.86	0.56
1:W:639:LEU:O	1:D:637:ARG:NH1	2.22	0.56
1:U:523:LEU:HD11	1:U:552:ALA:HB2	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:D:587:VAL:O	1:D:588:LYS:NZ	2.36	0.56
1:V:514:ARG:NH2	1:V:518:LEU:HD11	2.20	0.56
1:Q:553:LEU:HD12	1:Q:594:LEU:HG	1.86	0.56
1:C:538:TYR:CZ	1:C:542:LEU:HD11	2.41	0.56
1:X:563:ILE:HG12	1:X:598:LEU:HD22	1.87	0.56
1:E:536:LYS:NZ	1:H:525:ASN:CG	2.64	0.56
1:V:531:LEU:HD22	1:V:534:MET:HB2	1.86	0.55
1:T:656:ASN:HD22	1:T:657:PRO:HD2	1.71	0.55
1:P:659:ILE:HG23	1:P:659:ILE:O	2.06	0.55
1:L:500:GLU:OE1	1:L:502:HIS:ND1	2.39	0.55
1:B:629:LYS:HE3	1:B:649:THR:HG21	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:603:ILE:HG22	1:W:608:LEU:HD22	1.87	0.55
1:A:534:MET:HE1	1:A:578:PHE:CE1	2.41	0.55
1:R:566:ARG:HD3	1:R:568:PHE:CZ	2.41	0.55
1:L:645:TYR:HB2	1:L:647:GLY:N	2.22	0.55
1:S:567:MET:HE2	1:S:607:ILE:HD12	1.87	0.55
1:B:595:MET:HG2	1:B:599:LYS:HE3	1.89	0.55
1:W:585:GLU:OE2	1:W:588:LYS:NZ	2.40	0.55
1:R:513:ASN:O	1:R:517:LEU:HD13	2.06	0.55
1:J:659:ILE:HD11	1:J:661:TYR:CZ	2.41	0.55
1:F:632:LYS:NZ	1:F:654:GLU:OE2	2.23	0.55
1:U:636:SER:HA	1:R:634:PRO:HG2	1.89	0.55
1:R:600:GLU:OE2	1:R:661:TYR:CA	2.54	0.55
1:Q:571:GLN:HG3	1:Q:637:ARG:HB3	1.88	0.55
1:N:587:VAL:HG12	1:N:587:VAL:O	2.07	0.55
1:H:574:THR:HG21	1:H:602:HIS:NE2	2.21	0.55
1:G:500:GLU:HB2	1:G:554:ILE:HB	1.88	0.55
1:U:537:GLU:CD	1:U:537:GLU:H	2.15	0.55
1:X:565:PHE:HB3	1:X:576:ILE:HG22	1.88	0.55
1:W:501:PHE:CE1	1:W:553:LEU:CD2	2.85	0.54
1:U:547:LYS:HE3	1:U:566:ARG:HH21	1.72	0.54
1:X:613:TYR:CE2	1:X:642:ILE:HD13	2.42	0.54
1:O:637:ARG:NH2	1:X:641:TYR:CZ	2.75	0.54
1:L:583:SER:HA	1:L:586:GLN:HG3	1.89	0.54
1:X:576:ILE:CG1	1:X:612:THR:HG23	2.33	0.54
1:Q:576:ILE:O	1:Q:612:THR:HG23	2.07	0.54
1:D:528:SER:OG	1:D:536:LYS:HG2	2.07	0.54
1:Q:573:PHE:CA	1:Q:607:ILE:HD11	2.37	0.54
1:W:620:GLY:HA2	1:W:623:LYS:NZ	2.16	0.54
1:Q:566:ARG:NH1	1:Q:567:MET:O	2.40	0.54
1:D:586:GLN:O	1:D:588:LYS:CE	2.51	0.54
1:W:517:LEU:HD11	1:J:517:LEU:HD11	1.89	0.54
1:J:499:ILE:HG22	1:J:555:LYS:HB2	1.89	0.54
1:E:533:ARG:CD	1:E:646:GLU:OE2	2.55	0.54
1:Q:563:ILE:HG21	1:Q:598:LEU:HD22	1.89	0.54
1:O:587:VAL:O	1:O:587:VAL:HG12	2.07	0.54
1:L:538:TYR:CZ	1:L:542:LEU:HD11	2.43	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:516:VAL:O	1:T:520:LEU:HD12	2.08	0.53
1:X:589:GLY:C	1:X:590:TYR:HD1	2.16	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:V:534:MET:HE1	1:V:578:PHE:CZ	2.43	0.53
1:R:523:LEU:HD13	1:R:550:THR:HG21	1.90	0.53
1:Q:622:PHE:HB3	1:Q:627:PHE:HB2	1.91	0.53
1:Q:630:ASP:O	1:Q:630:ASP:OD2	2.25	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
1:O:579:CYS:SG	1:O:621:TYR:CE2	3.00	0.53
1:W:586:GLN:HG3	1:W:587:VAL:HG13	1.89	0.53
1:V:525:ASN:O	1:V:529:HIS:ND1	2.42	0.53
1:U:620:GLY:O	1:U:624:LYS:HG3	2.09	0.53
1:L:606:ASN:HD21	1:I:643:LYS:HZ2	1.55	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:U:523:LEU:HD13	1:U:550:THR:HG21	1.91	0.53
1:B:599:LYS:O	1:B:603:ILE:HG23	2.08	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:Q:547:LYS:HG3	1:Q:547:LYS:O	2.07	0.52
1:Q:583:SER:HA	1:Q:586:GLN:CD	2.34	0.52
1:H:574:THR:HG21	1:H:602:HIS:CD2	2.44	0.52
1:X:657:PRO:CD	1:X:658:ARG:HH12	2.22	0.52
1:V:519:TRP:O	1:V:523:LEU:HD12	2.09	0.52
1:P:528:SER:OG	1:P:536:LYS:HG2	2.09	0.52
1:L:534:MET:HE3	1:L:538:TYR:HD2	1.74	0.52
1:F:583:SER:HA	1:F:586:GLN:HG3	1.91	0.52
1:U:595:MET:HG3	1:U:599:LYS:HE3	1.91	0.52
1:S:519:TRP:O	1:S:523:LEU:HD13	2.10	0.52
1:T:606:ASN:ND2	1:K:566:ARG:NH1	2.58	0.52
1:Q:588:LYS:O	1:Q:588:LYS:HG3	2.08	0.52
1:I:615:ASP:O	1:I:619:ILE:HG13	2.09	0.52
1:X:548:HIS:CD2	1:X:566:ARG:HB2	2.43	0.52
1:Q:576:ILE:HB	1:Q:612:THR:OG1	2.10	0.52
1:J:564:CYS:O	1:J:577:VAL:HG22	2.09	0.52
1:E:615:ASP:OD2	1:E:646:GLU:OE1	2.27	0.52
1:X:614:ALA:HB3	1:X:619:ILE:CD1	2.40	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:566:ARG:HG2	1:S:566:ARG:NH1	2.23	0.52
1:L:619:ILE:O	1:L:623:LYS:HG2	2.10	0.52
1:W:582:THR:CG2	1:W:585:GLU:HG2	2.40	0.52
1:Q:571:GLN:HE21	1:Q:637:ARG:HB3	1.74	0.52
1:K:555:LYS:NZ	1:K:585:GLU:OE2	2.42	0.52
1:U:531:LEU:HD13	1:U:534:MET:HE3	1.92	0.52
1:J:617:TYR:N	1:J:617:TYR:CD2	2.78	0.52
1:T:534:MET:HE3	1:T:538:TYR:HE1	1.75	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:V:644:ASP:OD1	1:V:645:TYR:N	2.44	0.51
1:O:658:ARG:HD2	1:X:535:PRO:HD3	1.91	0.51
1:J:513:ASN:HB3	1:J:516:VAL:HG22	1.92	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:V:644:ASP:O	1:V:645:TYR:HD2	1.94	0.51
1:U:644:ASP:OD2	1:U:644:ASP:C	2.53	0.51
1:L:634:PRO:HD3	1:I:639:LEU:HD22	1.93	0.51
1:L:637:ARG:CZ	1:L:637:ARG:HB2	2.40	0.51
1:J:504:ILE:HD11	1:J:523:LEU:HD11	1.91	0.51
1:X:622:PHE:CD1	1:X:627:PHE:CZ	2.92	0.51
1:W:553:LEU:HB2	1:W:594:LEU:HD21	1.91	0.51
1:V:587:VAL:HG12	1:V:587:VAL:O	2.11	0.51
1:F:640:GLY:HA2	1:C:609:TYR:CE1	2.46	0.51
1:W:576:ILE:HB	1:W:612:THR:HB	1.93	0.51
1:Q:522:GLY:O	1:Q:526:VAL:HG23	2.10	0.51
1:Q:571:GLN:CD	1:Q:573:PHE:HE2	1.91	0.51
1:L:549:LYS:HZ2	1:L:567:MET:HE3	1.76	0.51
1:W:620:GLY:CA	1:W:623:LYS:NZ	2.74	0.51
1:X:555:LYS:HB2	1:X:560:ILE:HD11	1.91	0.51
1:P:659:ILE:O	1:P:659:ILE:CG2	2.59	0.51
1:L:601:TYR:HA	1:L:604:LYS:HE2	1.92	0.51
1:J:500:GLU:OE2	1:J:554:ILE:HD11	2.10	0.51
1:H:547:LYS:O	1:H:566:ARG:HG3	2.11	0.51
1:U:566:ARG:NH1	1:U:566:ARG:HG2	2.26	0.51
1:S:500:GLU:O	1:S:554:ILE:HG22	2.10	0.51
1:J:566:ARG:NH1	1:J:567:MET:O	2.44	0.51
1:X:595:MET:HE1	1:X:598:LEU:HD23	1.93	0.51
1:A:523:LEU:HD13	1:A:550:THR:HG21	1.91	0.51
1:V:534:MET:HE3	1:V:538:TYR:CD2	2.45	0.51
1:B:522:GLY:O	1:B:526:VAL:HG23	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:629:LYS:HE3	1:S:649:THR:HG21	1.93	0.50
1:M:528:SER:OG	1:M:536:LYS:HG2	2.12	0.50
1:J:520:LEU:HA	1:J:523:LEU:HD12	1.92	0.50
1:N:636:SER:HA	1:M:634:PRO:HG2	1.94	0.50
1:L:603:ILE:HD13	1:L:657:PRO:HA	1.93	0.50
1:J:583:SER:HA	1:J:586:GLN:HG3	1.92	0.50
1:D:635:LYS:HA	1:D:638:TYR:CE2	2.46	0.50
1:W:501:PHE:CD1	1:W:553:LEU:HD23	2.46	0.50
1:W:525:ASN:HD21	1:J:524:GLN:HE22	1.59	0.50
1:Q:641:TYR:CZ	1:G:637:ARG:NH1	2.80	0.50
1:I:537:GLU:CD	1:I:537:GLU:H	2.19	0.50
1:W:622:PHE:HB3	1:W:627:PHE:HB2	1.93	0.50
1:Q:631:ILE:HA	1:Q:652:GLU:OE2	2.11	0.50
1:J:566:ARG:HD3	1:J:568:PHE:CZ	2.46	0.50
1:X:610:PHE:O	1:X:652:GLU:HA	2.11	0.50
1:L:566:ARG:NH1	1:L:567:MET:O	2.33	0.50
1:I:644:ASP:OD1	1:I:645:TYR:N	2.45	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:L:534:MET:HE3	1:L:538:TYR:CD2	2.47	0.50
1:N:528:SER:OG	1:N:536:LYS:HG2	2.12	0.50
1:M:531:LEU:CD2	1:M:533:ARG:NH2	2.73	0.50
1:W:523:LEU:HG	1:W:559:VAL:HG11	1.93	0.50
1:D:534:MET:HB2	1:D:539:ILE:HD11	1.94	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:W:633:VAL:HG23	1:W:652:GLU:OE2	2.13	0.49
1:D:514:ARG:HH12	1:G:546:PRO:HD3	1.75	0.49
1:E:537:GLU:CD	1:E:537:GLU:H	2.20	0.49
1:A:513:ASN:ND2	1:A:515:ARG:HB3	2.28	0.49
1:T:534:MET:HE1	1:T:578:PHE:HE1	1.77	0.49
1:S:545:ASP:OD1	1:S:547:LYS:N	2.45	0.49
1:R:534:MET:HE3	1:R:538:TYR:CD2	2.47	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:C:531:LEU:HD13	1:C:534:MET:CE	2.41	0.49
1:A:609:TYR:CE1	1:C:640:GLY:HA2	2.48	0.49
1:U:609:TYR:CE2	1:S:640:GLY:HA2	2.48	0.49
1:S:554:ILE:HG13	1:S:558:ARG:O	2.11	0.49
1:S:637:ARG:NH2	1:H:639:LEU:O	2.36	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:619:ILE:HG22	1:R:623:LYS:HE2	1.94	0.49
1:J:622:PHE:HB3	1:J:627:PHE:HB2	1.94	0.49
1:A:534:MET:HE3	1:A:538:TYR:HD2	1.77	0.49
1:T:633:VAL:HG23	1:T:652:GLU:OE2	2.12	0.49
1:K:558:ARG:HD3	1:K:559:VAL:N	2.26	0.49
1:H:567:MET:HA	1:H:574:THR:HG22	1.93	0.49
1:M:530:GLN:HE22	1:M:586:GLN:HE21	1.59	0.49
1:E:629:LYS:HE3	1:E:649:THR:HG21	1.94	0.49
1:S:566:ARG:NH1	1:S:567:MET:O	2.46	0.49
1:O:584:ASN:ND2	1:O:585:GLU:OE2	2.45	0.49
1:J:530:GLN:C	1:J:532:PRO:HD3	2.38	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: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:Q:605:HIS:O	1:Q:607:ILE:HG22	2.13	0.49
1:M:595:MET:HG3	1:M:599:LYS:HE3	1.95	0.49
1:W:513:ASN:ND2	1:W:516:VAL:HG13	2.29	0.48
1:R:635:LYS:CG	1:R:639:LEU:HD12	2.43	0.48
1:O:513:ASN:OD1	1:O:516:VAL:HG22	2.13	0.48
1:J:635:LYS:HA	1:J:638:TYR:CE2	2.48	0.48
1:B:498:ILE:HG22	1:B:556:ASP:OD1	2.12	0.48
1:S:516:VAL:O	1:S:520:LEU:HG	2.13	0.48
1:J:524:GLN:O	1:J:528:SER:OG	2.22	0.48
1:I:513:ASN:HD21	1:I:515:ARG:HH21	1.61	0.48
1:G:499:ILE:HD11	1:G:555:LYS:HE3	1.96	0.48
1:E:536:LYS:HZ1	1:H:525:ASN:CG	2.21	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:F:615:ASP:O	1:F:619:ILE:HG13	2.13	0.48
1:D:615:ASP:O	1:D:619:ILE:HG13	2.14	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:Q:602:HIS:ND1	1:Q:610:PHE:HE2	2.12	0.48
1:Q:607:ILE:C	1:Q:608:LEU:HD23	2.39	0.48
1:C:523:LEU:HD13	1:C:550:THR:HG21	1.94	0.48
1:L:537:GLU:H	1:L:537:GLU:CD	2.11	0.48
1:L:657:PRO:C	1:L:659:ILE:H	2.22	0.48
1:A:537:GLU:CD	1:A:537:GLU:H	2.23	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:528:SER:O	1:V:532:PRO:HA	2.14	0.47
1:T:518:LEU:HD21	1:S:541:ARG:HG2	1.96	0.47
1:R:579:CYS:SG	1:R:621:TYR:CE2	3.07	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:I:639:LEU:C	1:I:639:LEU:CD2	2.86	0.47
1:X:555:LYS:CB	1:X:560:ILE:HD11	2.45	0.47
1:R:545:ASP:OD2	1:R:547:LYS:N	2.46	0.47
1:Q:501:PHE:HB3	1:Q:551:LEU:HD11	1.96	0.47
1:I:501:PHE:HB3	1:I:551:LEU:HD11	1.97	0.47
1:W:560:ILE:O	1:W:582:THR:HG22	2.15	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:L:623:LYS:HD3	1:L:651:MET:HE1	1.96	0.47
1:W:530:GLN:HG3	1:W:580:ALA:HB1	1.97	0.47
1:V:529:HIS:CD2	1:X:536:LYS:HE2	2.48	0.47
1:U:600:GLU:O	1:U:604:LYS:HG2	2.14	0.47
1:Q:571:GLN:NE2	1:Q:638:TYR:CA	2.74	0.47
1:Q:595:MET:HG3	1:Q:599:LYS:HE3	1.96	0.47
1:X:586:GLN:HG2	1:X:587:VAL:N	2.30	0.47
1:Q:639:LEU:O	1:G:637:ARG:NH2	2.47	0.47
1:D:587:VAL:HB	1:D:588:LYS:NZ	2.29	0.47
1:R:603:ILE:HD11	1:R:655:LEU:HB3	1.96	0.47
1:K:515:ARG:HD2	1:K:519:TRP:CZ2	2.50	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
1:V:595:MET:HG3	1:V:599:LYS:HE3	1.96	0.47
1:H:524:GLN:HG3	1:H:540:ALA:HA	1.97	0.47
1:N:635:LYS:HA	1:N:638:TYR:CE2	2.50	0.46
1:K:553:LEU:HB2	1:K:594:LEU:HD21	1.96	0.46
1:A:633:VAL:HG23	1:A:652:GLU:OE2	2.15	0.46
1:L:658:ARG:HE	1:I:534:MET:HE3	1.79	0.46
1:F:567:MET:HE2	1:F:607:ILE:HD12	1.96	0.46
1:G:619:ILE:HG22	1:G:623:LYS:HE3	1.96	0.46
1:H:585:GLU:OE1	1:H:588:LYS:NZ	2.33	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:W:623:LYS:HD3	1:W:623:LYS:H	1.81	0.46
1:B:534:MET:HE3	1:B:538:TYR:HD2	1.79	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:529:HIS:C	1:E:529:HIS:HD1	2.22	0.46
1:A:517:LEU:HD11	1:U:517:LEU:HD21	1.97	0.46
1:U:639:LEU:HD22	1:R:633:VAL:HA	1.96	0.46
1:M:563:ILE:HG21	1:M:598:LEU:HD22	1.97	0.46
1:D:587:VAL:C	1:D:588:LYS:HE2	2.40	0.46
1:X:619:ILE:HD12	1:X:651:MET:SD	2.55	0.46
1:X:635:LYS:HD3	1:X:639:LEU:HD11	1.96	0.46
1:U:610:PHE:HB2	1:U:653:CYS:HB3	1.97	0.46
1:P:534:MET:HB2	1:P:539:ILE:HD11	1.96	0.46
1:M:555:LYS:NZ	1:M:585:GLU:CD	2.73	0.46
1:T:587:VAL:O	1:T:587:VAL:HG12	2.15	0.46
1:L:585:GLU:HA	1:L:588:LYS:HE3	1.98	0.46
1:B:538:TYR:CZ	1:B:542:LEU:HD11	2.50	0.46
1:R:583:SER:HA	1:R:586:GLN:HG3	1.96	0.46
1:V:645:TYR:OH	1:E:658:ARG:NH2	2.49	0.46
1:P:600:GLU:HG3	1:P:662:THR:OG1	2.16	0.46
1:L:595:MET:HG3	1:L:599:LYS:HE3	1.97	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: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:L:606:ASN:HD21	1:I:643:LYS:HZ1	1.63	0.46
1:E:558:ARG:NE	1:E:558:ARG:HA	2.31	0.46
1:X:576:ILE:O	1:X:612:THR:HG22	2.16	0.46
1:X:586:GLN:HG2	1:X:587:VAL:HG13	1.98	0.46
1:W:621:TYR:O	1:W:625:GLN:HG2	2.15	0.45
1:M:584:ASN:ND2	1:M:585:GLU:HG2	2.32	0.45
1:K:635:LYS:HA	1:K:638:TYR:CE2	2.51	0.45
1:E:536:LYS:HZ3	1:H:525:ASN:CB	2.15	0.45
1:A:558:ARG:HA	1:A:558:ARG:NE	2.31	0.45
1:V:513:ASN:O	1:V:517:LEU:HD12	2.15	0.45
1:Q:571:GLN:OE1	1:Q:641:TYR:CD1	2.69	0.45
1:J:514:ARG:H	1:J:514:ARG:HG2	1.45	0.45
1:G:620:GLY:O	1:G:624:LYS:HG2	2.16	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:X:628:SER:C	1:X:651:MET:HE3	2.41	0.45
1:T:595:MET:HG3	1:T:599:LYS:HE3	1.99	0.45
1:P:634:PRO:HG2	1:J:636:SER:HA	1.99	0.45
1:D:587:VAL:O	1:D:588:LYS:CE	2.65	0.45
1:Q:567:MET:HA	1:Q:574:THR:HG23	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:609:TYR:CE2	1:J:640:GLY:HA2	2.52	0.45
1:B:534:MET:HE3	1:B:538:TYR:CD2	2.51	0.45
1:G:615:ASP:OD1	1:G:615:ASP:N	2.49	0.45
1:A:564:CYS:HB3	1:A:578:PHE:HB2	1.99	0.45
1:A:566:ARG:HD3	1:A:568:PHE:CE2	2.51	0.45
1:F:657:PRO:HB2	1:B:538:TYR:CE1	2.52	0.45
1:E:587:VAL:C	1:E:588:LYS:HG3	2.42	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:Q:526:VAL:HA	1:Q:529:HIS:ND1	2.32	0.45
1:P:574:THR:HG21	1:P:602:HIS:HE2	1.82	0.45
1:M:656:ASN:HB3	1:M:659:ILE:HG12	1.99	0.45
1:L:635:LYS:C	1:L:637:ARG:H	2.25	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: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:T:516:VAL:C	1:T:520:LEU:HD12	2.42	0.45
1:C:595:MET:HG3	1:C:599:LYS:HE3	1.99	0.45
1:X:614:ALA:HB1	1:X:622:PHE:CD2	2.51	0.45
1:V:537:GLU:H	1:V:537:GLU:CD	2.25	0.45
1:M:523:LEU:HD13	1:M:550:THR:HG21	1.98	0.45
1:J:554:ILE:HG22	1:J:559:VAL:HG22	1.97	0.45
1:X:631:ILE:O	1:X:632:LYS:HD2	2.17	0.45
1:V:517:LEU:O	1:V:521:VAL:HG23	2.16	0.44
1:O:635:LYS:HA	1:O:638:TYR:CE2	2.53	0.44
1:D:560:ILE:O	1:D:582:THR:HG22	2.17	0.44
1:W:585:GLU:HA	1:W:588:LYS:NZ	2.32	0.44
1:T:658:ARG:O	1:T:660:PRO:HD3	2.17	0.44
1:S:517:LEU:HA	1:S:517:LEU:HD12	1.71	0.44
1:E:644:ASP:OD1	1:E:645:TYR:N	2.50	0.44
1:S:537:GLU:O	1:S:541:ARG:HG3	2.17	0.44
1:P:514:ARG:HG3	1:P:515:ARG:N	2.31	0.44
1:M:518:LEU:HD21	1:I:541:ARG:HG3	1.99	0.44
1:J:600:GLU:CG	1:J:661:TYR:HB2	2.47	0.44
1:F:600:GLU:HG3	1:F:662:THR:HG23	1.99	0.44
1:D:498:ILE:O	1:D:555:LYS:HG3	2.16	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:587:VAL:HG12	1:E:587:VAL:O	2.17	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:R:519:TRP:CD1	1:R:559:VAL:HG23	2.53	0.44
1:Q:536:LYS:NZ	1:O:529:HIS:CE1	2.86	0.44
1:F:547:LYS:O	1:F:566:ARG:HG3	2.18	0.44
1:X:618:ALA:O	1:X:621:TYR:HB3	2.18	0.44
1:W:558:ARG:NH2	1:P:662:THR:O	2.51	0.44
1:T:534:MET:HE3	1:T:538:TYR:CE1	2.53	0.44
1:F:498:ILE:O	1:F:555:LYS:HA	2.17	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: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:X:613:TYR:CE1	1:X:650:LEU:HB2	2.53	0.44
1:P:566:ARG:HD3	1:P:568:PHE:CE2	2.52	0.44
1:L:517:LEU:HD13	1:L:517:LEU:HA	1.87	0.44
1:W:586:GLN:HG3	1:W:587:VAL:N	2.32	0.44
1:Q:526:VAL:HG13	1:Q:529:HIS:HE1	1.83	0.44
1:Q:536:LYS:HZ3	1:O:529:HIS:CE1	2.36	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:N:629:LYS:HE3	1:N:649:THR:HG21	2.00	0.44
1:B:530:GLN:C	1:B:532:PRO:HD3	2.43	0.44
1:X:628:SER:C	1:X:651:MET:CE	2.90	0.44
1:A:563:ILE:HG21	1:A:598:LEU:HD22	2.00	0.44
1:U:517:LEU:O	1:U:521:VAL:HG23	2.17	0.44
1:P:566:ARG:HH11	1:P:566:ARG:HG2	1.83	0.44
1:M:551:LEU:O	1:M:562:GLY:HA2	2.18	0.44
1:S:530:GLN:HG3	1:S:580:ALA:HB1	1.99	0.43
1:O:615:ASP:O	1:O:619:ILE:HG13	2.18	0.43
1:L:535:PRO:HB3	1:L:537:GLU:OE2	2.18	0.43
1:I:534:MET:HE2	1:I:538:TYR:CE2	2.52	0.43
1:Q:607:ILE:O	1:Q:608:LEU:HD23	2.17	0.43
1:P:657:PRO:HG2	1:J:643:LYS:HD2	2.00	0.43
1:L:575:GLU:HB2	1:L:642:ILE:HG22	2.00	0.43
1:A:608:LEU:HD22	1:A:657:PRO:HG3	2.00	0.43
1:S:558:ARG:O	1:S:559:VAL:HG23	2.19	0.43
1:O:575:GLU:HB2	1:O:642:ILE:HG22	2.00	0.43
1:O:651:MET:HE2	1:O:651:MET:HB3	1.93	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:599:LYS:NZ	1:E:625:GLN:O	2.46	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:L:504:ILE:HG13	1:L:520:LEU:HD21	2.01	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:U:499:ILE:HA	1:U:554:ILE:O	2.19	0.43
1:M:525:ASN:HD21	1:I:524:GLN:HE22	1.66	0.43
1:M:546:PRO:HD3	1:I:514:ARG:NH2	2.34	0.43
1:E:564:CYS:HB3	1:E:578:PHE:HB2	2.01	0.43
1:X:639:LEU:H	1:X:639:LEU:HD12	1.83	0.43
1:Q:534:MET:HE1	1:Q:578:PHE:HE1	1.83	0.43
1:L:604:LYS:O	1:I:541:ARG:HD3	2.19	0.43
1:H:611:LEU:HD23	1:H:652:GLU:HB2	1.99	0.43
1:A:595:MET:HG3	1:A:599:LYS:HE3	2.01	0.43
1:W:595:MET:HG3	1:W:599:LYS:HE3	2.01	0.43
1:S:587:VAL:HG12	1:S:587:VAL:O	2.18	0.43
1:Q:606:ASN:C	1:L:643:LYS:HZ1	2.26	0.43
1:T:606:ASN:HD22	1:K:566:ARG:NH1	2.17	0.43
1:Q:589:GLY:C	1:Q:593:HIS:HD1	2.25	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:G:513:ASN:OD1	1:G:514:ARG:N	2.51	0.43
1:X:501:PHE:C	1:X:502:HIS:HD2	2.26	0.43
1:X:522:GLY:O	1:X:526:VAL:HG23	2.19	0.43
1:V:519:TRP:CE2	1:V:554:ILE:HD13	2.54	0.43
1:D:566:ARG:HG2	1:D:566:ARG:NH1	2.34	0.43
1:A:534:MET:HE3	1:A:538:TYR:CD2	2.53	0.42
1:V:531:LEU:C	1:V:531:LEU:HD23	2.43	0.42
1:U:555:LYS:HD2	1:U:560:ILE:HD13	2.00	0.42
1:R:534:MET:HE1	1:R:578:PHE:CE1	2.53	0.42
1:C:547:LYS:HD3	1:C:566:ARG:NH2	2.34	0.42
1:V:513:ASN:HB3	1:V:516:VAL:HG22	2.01	0.42
1:P:585:GLU:HA	1:P:588:LYS:HE2	2.01	0.42
1:E:507:SER:OG	1:E:511:LYS:O	2.37	0.42
1:Q:517:LEU:HD11	1:O:517:LEU:HD11	2.01	0.42
1:G:498:ILE:HG23	1:G:556:ASP:H	1.84	0.42
1:T:604:LYS:HB2	1:T:604:LYS:NZ	2.34	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:636:SER:HA	1:N:634:PRO:HG2	2.00	0.42
1:D:523:LEU:HD11	1:D:552:ALA:HB2	2.02	0.42
1:Q:564:CYS:HB3	1:Q:578:PHE:HB2	2.01	0.42
1:K:555:LYS:NZ	1:K:585:GLU:CD	2.77	0.42
1:J:523:LEU:HA	1:J:526:VAL:HG22	2.00	0.42
1:D:652:GLU:HG2	1:D:653:CYS:N	2.34	0.42
1:W:597:HIS:HA	1:W:662:THR:HG21	2.02	0.42
1:S:652:GLU:HG2	1:S:653:CYS:N	2.34	0.42
1:Q:608:LEU:HA	1:Q:655:LEU:HD22	2.02	0.42
1:X:595:MET:CE	1:X:598:LEU:HD23	2.50	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:V:514:ARG:HH22	1:V:518:LEU:HD11	1.85	0.42
1:L:522:GLY:O	1:L:526:VAL:HG23	2.19	0.42
1:T:566:ARG:HB3	1:T:575:GLU:HB3	2.02	0.42
1:S:615:ASP:O	1:S:619:ILE:HG13	2.19	0.42
1:N:659:ILE:HD12	1:N:659:ILE:HG23	1.86	0.42
1:B:585:GLU:OE1	1:B:588:LYS:NZ	2.47	0.42
1:A:525:ASN:ND2	1:U:524:GLN:HE22	2.11	0.42
1:W:635:LYS:HA	1:W:638:TYR:CE2	2.54	0.42
1:U:576:ILE:HG21	1:U:579:CYS:SG	2.59	0.42
1:R:534:MET:HE3	1:R:538:TYR:HD2	1.85	0.42
1:Q:592:THR:HG22	1:Q:625:GLN:OE1	2.20	0.42
1:M:534:MET:HB2	1:M:539:ILE:HD11	2.00	0.42
1:L:632:LYS:O	1:I:639:LEU:HD11	2.20	0.42
1:L:645:TYR:C	1:L:647:GLY:H	2.28	0.42
1:X:613:TYR:CZ	1:X:650:LEU:HD12	2.49	0.42
1:W:607:ILE:C	1:W:608:LEU:HD23	2.45	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:R:517:LEU:O	1:R:521:VAL:HG23	2.20	0.42
1:Q:526:VAL:HG13	1:Q:529:HIS:CE1	2.55	0.42
1:M:566:ARG:HD3	1:M:568:PHE:CZ	2.55	0.42
1:L:614:ALA:O	1:L:619:ILE:HD11	2.20	0.42
1:J:534:MET:HE1	1:J:578:PHE:CE1	2.55	0.42
1:J:585:GLU:OE1	1:J:588:LYS:NZ	2.37	0.42
1:H:604:LYS:HE3	1:H:605:HIS:CD2	2.54	0.42
1:W:555:LYS:C	1:W:557:GLY:N	2.78	0.41
1:T:608:LEU:HD13	1:T:657:PRO:HD3	2.02	0.41
1:P:633:VAL:HG23	1:P:652:GLU:OE2	2.20	0.41
1:M:585:GLU:OE1	1:M:588:LYS:NZ	2.43	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:528:SER:OG	1:V:536:LYS:HG2	2.19	0.41
1:Q:639:LEU:HD21	1:G:632:LYS:HE2	2.01	0.41
1:C:633:VAL:HG23	1:C:652:GLU:OE2	2.20	0.41
1:E:514:ARG:NH1	1:H:544:PHE:O	2.53	0.41
1:X:499:ILE:HA	1:X:554:ILE:O	2.20	0.41
1:U:643:LYS:H	1:U:643:LYS:HG3	1.62	0.41
1:S:534:MET:HE3	1:S:538:TYR:HD2	1.84	0.41
1:G:624:LYS:HA	1:G:624:LYS:HD3	1.92	0.41
1:X:551:LEU:HB3	1:X:563:ILE:CG2	2.50	0.41
1:V:645:TYR:HE2	1:E:658:ARG:HH22	1.68	0.41
1:T:567:MET:HE2	1:T:607:ILE:HD12	2.02	0.41
1:S:522:GLY:O	1:S:526:VAL:HG23	2.20	0.41
1:N:659:ILE:HA	1:N:659:ILE:HD13	1.78	0.41
1:G:523:LEU:HD13	1:G:550:THR:HG21	2.03	0.41
1:W:530:GLN:O	1:W:531:LEU:HD12	2.20	0.41
1:W:584:ASN:C	1:W:586:GLN:H	2.29	0.41
1:U:615:ASP:OD1	1:U:615:ASP:N	2.39	0.41
1:S:634:PRO:HG2	1:H:636:SER:HA	2.01	0.41
1:Q:575:GLU:HB2	1:Q:642:ILE:HG22	2.01	0.41
1:I:635:LYS:HA	1:I:638:TYR:CE2	2.56	0.41
1:M:522:GLY:O	1:M:526:VAL:HG23	2.20	0.41
1:L:647:GLY:O	1:L:648:ALA:C	2.63	0.41
1:L:649:THR:OG1	1:L:651:MET:HG3	2.21	0.41
1:W:560:ILE:HD12	1:W:585:GLU:HG3	2.03	0.41
1:S:534:MET:HE3	1:S:538:TYR:CD2	2.55	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:N:534:MET:HE3	1:N:534:MET:HB2	1.81	0.41
1:H:603:ILE:HD13	1:H:603:ILE:HA	1.81	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:W:521:VAL:HG22	1:J:521:VAL:HG12	2.03	0.41
1:U:603:ILE:HD11	1:U:661:TYR:HE2	1.86	0.41
1:S:500:GLU:CD	1:S:502:HIS:HE2	2.29	0.41
1:S:576:ILE:HB	1:S:612:THR:HB	2.03	0.41
1:Q:627:PHE:HA	1:Q:652:GLU:O	2.21	0.41
1:P:566:ARG:HD3	1:P:568:PHE:CZ	2.56	0.41
1:N:516:VAL:HA	1:N:519:TRP:HB2	2.03	0.41
1:L:643:LYS:HA	1:L:643:LYS:HD2	1.42	0.41
1:X:553:LEU:HD12	1:X:594:LEU:HD22	2.03	0.41
1:R:616:GLU:H	1:R:616:GLU:HG3	1.70	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:553:LEU:HD23	1:Q:560:ILE:HG13	2.03	0.41
1:P:545:ASP:HA	1:P:546:PRO:HD3	1.94	0.41
1:J:517:LEU:C	1:J:517:LEU:HD23	2.46	0.41
1:J:534:MET:HE1	1:J:578:PHE:HE1	1.85	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: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:A:567:MET:HE2	1:A:607:ILE:HD12	2.02	0.41
1:U:499:ILE:HG22	1:U:555:LYS:HB2	2.03	0.41
1:Q:547:LYS:O	1:Q:547:LYS:CG	2.69	0.41
1:M:499:ILE:HA	1:M:554:ILE:O	2.21	0.41
1:J:551:LEU:O	1:J:562:GLY:HA2	2.20	0.41
1:H:560:ILE:O	1:H:582:THR:HG22	2.21	0.41
1:X:595:MET:HE3	1:X:598:LEU:HB3	2.01	0.41
1:V:652:GLU:HG2	1:V:653:CYS:N	2.35	0.40
1:S:560:ILE:HB	1:S:585:GLU:HG3	2.03	0.40
1:Q:599:LYS:O	1:Q:603:ILE:HG13	2.21	0.40
1:D:615:ASP:OD1	1:D:618:ALA:N	2.53	0.40
1:X:506:ASN:O	1:X:546:PRO:HA	2.21	0.40
1:V:541:ARG:HH11	1:V:541:ARG:HD2	1.77	0.40
1:V:624:LYS:HB3	1:V:624:LYS:HE3	1.90	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:K:608:LEU:HD13	1:K:657:PRO:HG3	2.04	0.40
1:D:619:ILE:O	1:D:623:LYS:HG3	2.21	0.40
1:X:657:PRO:CG	1:X:658:ARG:HH12	2.33	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:Q:547:LYS:HG3	1:Q:566:ARG:CZ	2.51	0.40
1:Q:563:ILE:HG13	1:Q:594:LEU:HD13	2.04	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:K:617:TYR:N	1:K:617:TYR:CD1	2.89	0.40
1:H:615:ASP:O	1:H:619:ILE:HG13	2.20	0.40
1:X:619:ILE:CG2	1:X:623:LYS:HZ2	2.27	0.40
1:U:501:PHE:HB3	1:U:551:LEU:HD11	2.04	0.40
1:S:553:LEU:HG	1:S:560:ILE:HG13	2.02	0.40
1:F:499:ILE:HA	1:F:554:ILE:O	2.22	0.40
1:D:632:LYS:H	1:D:632:LYS:HG2	1.65	0.40
1:G:635:LYS:HA	1:G:638:TYR:CE2	2.55	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:575:GLU:HB2	1:I:642:ILE:HG22	2.03	0.40
1:W:613:TYR:CE2	1:W:644:ASP:HA	2.56	0.40
1:P:499:ILE:HD11	1:P:555:LYS:HE3	2.03	0.40
1:J:507:SER:C	1:J:508:LEU:HD23	2.46	0.40
1:J:600:GLU:OE2	1:J:660:PRO:HA	2.21	0.40
1:F:523:LEU:HG	1:F:559:VAL:HG11	2.03	0.40
1:B:547:LYS:HD3	1:B:566:ARG:NH2	2.36	0.40
1:H:595:MET:O	1:H:599:LYS:HG3	2.21	0.40
1:H:624:LYS:HD2	1:H:624:LYS:HA	1.75	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 ⓘ

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	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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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%)	142 (100%)	0	100	100
1	E	142/147 (97%)	142 (100%)	0	100	100
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
1	L	139/147 (95%)	139 (100%)	0	100	100
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%)	142 (100%)	0	100	100
1	P	142/147 (97%)	142 (100%)	0	100	100
1	Q	138/147 (94%)	138 (100%)	0	100	100
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%)	141 (99%)	1 (1%)	76	92
1	X	141/147 (96%)	141 (100%)	0	100	100
All	All	3407/3528 (97%)	3406 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	W	524	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	513	ASN
1	A	525	ASN
1	A	529	HIS
1	A	530	GLN
1	A	586	GLN
1	A	625	GLN
1	W	525	ASN
1	W	593	HIS
1	V	571	GLN
1	U	502	HIS
1	U	625	GLN
1	T	530	GLN
1	T	571	GLN
1	T	656	ASN
1	S	571	GLN
1	S	596	ASN
1	R	502	HIS
1	R	625	GLN
1	Q	529	HIS
1	Q	571	GLN
1	P	530	GLN
1	O	530	GLN
1	O	625	GLN
1	N	506	ASN
1	M	525	ASN
1	M	530	GLN
1	M	584	ASN
1	L	571	GLN
1	L	605	HIS
1	L	606	ASN
1	J	502	HIS
1	J	596	ASN
1	J	606	ASN
1	C	525	ASN
1	B	502	HIS
1	B	625	GLN
1	D	525	ASN
1	D	530	GLN
1	D	597	HIS
1	E	525	ASN
1	E	586	GLN
1	E	606	ASN
1	G	525	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	625	GLN
1	H	525	ASN
1	H	530	GLN
1	H	586	GLN
1	H	605	HIS
1	I	586	GLN
1	X	593	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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, 95th 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 ²)	Q<0.9
1	A	162/168 (96%)	-0.11	6 (3%) 45 37	7, 19, 54, 72	0
1	B	161/168 (95%)	-0.20	5 (3%) 51 42	7, 15, 42, 82	0
1	C	159/168 (94%)	-0.09	2 (1%) 75 67	7, 19, 50, 91	0
1	D	161/168 (95%)	0.16	8 (4%) 34 27	15, 30, 62, 96	0
1	E	163/168 (97%)	0.13	11 (6%) 24 19	10, 26, 59, 84	0
1	F	162/168 (96%)	-0.07	3 (1%) 66 58	8, 20, 47, 76	0
1	G	164/168 (97%)	0.10	7 (4%) 40 31	13, 26, 56, 104	0
1	H	160/168 (95%)	-0.27	1 (0%) 85 81	6, 15, 36, 53	0
1	I	162/168 (96%)	0.12	7 (4%) 40 31	11, 28, 56, 83	0
1	J	163/168 (97%)	0.53	19 (11%) 9 8	7, 33, 74, 113	0
1	K	160/168 (95%)	-0.01	7 (4%) 39 30	10, 24, 54, 77	0
1	L	157/168 (93%)	0.71	20 (12%) 8 6	14, 39, 70, 93	0
1	M	160/168 (95%)	-0.04	2 (1%) 75 67	10, 23, 54, 80	0
1	N	163/168 (97%)	-0.05	9 (5%) 30 24	7, 22, 59, 79	0
1	O	161/168 (95%)	0.09	7 (4%) 40 31	15, 30, 63, 105	0
1	P	161/168 (95%)	-0.19	2 (1%) 76 69	7, 16, 49, 61	0
1	Q	156/168 (92%)	1.37	32 (20%) 2 2	23, 57, 83, 102	0
1	R	162/168 (96%)	-0.18	2 (1%) 76 69	6, 14, 34, 80	0
1	S	161/168 (95%)	0.33	8 (4%) 34 27	9, 30, 68, 107	0
1	T	160/168 (95%)	0.44	9 (5%) 30 23	18, 41, 67, 87	0
1	U	164/168 (97%)	-0.18	8 (4%) 35 27	7, 16, 44, 107	0
1	V	161/168 (95%)	0.38	14 (8%) 16 13	13, 31, 67, 85	0
1	W	160/168 (95%)	0.64	20 (12%) 8 7	21, 42, 81, 96	0
1	X	160/168 (95%)	2.00	77 (48%) 0 0	33, 73, 105, 114	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	3863/4032 (95%)	0.23	286 (7%) 20 17	6, 27, 73, 114	0

All (286) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Q	573	PHE	5.9
1	O	508	LEU	5.9
1	U	510	PRO	5.9
1	S	508	LEU	5.6
1	X	572	GLY	5.5
1	X	618	ALA	5.3
1	G	510	PRO	5.3
1	W	617	TYR	5.3
1	T	512	ALA	5.2
1	V	645	TYR	5.2
1	E	497	GLY	5.1
1	O	512	ALA	5.1
1	Q	656	ASN	5.0
1	I	508	LEU	5.0
1	X	622	PHE	4.9
1	J	617	TYR	4.8
1	Q	572	GLY	4.8
1	Q	570	THR	4.7
1	M	512	ALA	4.7
1	J	512	ALA	4.7
1	Q	569	PRO	4.7
1	X	641	TYR	4.6
1	Q	508	LEU	4.6
1	Q	606	ASN	4.6
1	Q	571	GLN	4.5
1	J	508	LEU	4.5
1	X	659	ILE	4.5
1	X	611	LEU	4.3
1	N	512	ALA	4.3
1	N	508	LEU	4.3
1	L	660	PRO	4.2
1	L	649	THR	4.2
1	I	498	ILE	4.2
1	A	508	LEU	4.1
1	R	508	LEU	4.1
1	S	558	ARG	4.1
1	T	498	ILE	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	507	SER	4.0
1	X	657	PRO	4.0
1	A	512	ALA	4.0
1	V	512	ALA	4.0
1	T	506	ASN	4.0
1	X	512	ALA	4.0
1	X	606	ASN	4.0
1	X	650	LEU	4.0
1	D	512	ALA	3.9
1	F	508	LEU	3.9
1	S	512	ALA	3.9
1	X	645	TYR	3.9
1	P	508	LEU	3.8
1	B	508	LEU	3.8
1	X	656	ASN	3.8
1	Q	529	HIS	3.7
1	X	655	LEU	3.7
1	Q	658	ARG	3.7
1	X	533	ARG	3.7
1	X	588	LYS	3.7
1	Q	645	TYR	3.7
1	X	654	GLU	3.6
1	S	529	HIS	3.6
1	X	632	LYS	3.6
1	X	661	TYR	3.6
1	G	508	LEU	3.6
1	X	646	GLU	3.6
1	X	625	GLN	3.6
1	V	514	ARG	3.6
1	X	658	ARG	3.6
1	D	498	ILE	3.6
1	X	635	LYS	3.5
1	W	508	LEU	3.5
1	X	587	VAL	3.5
1	W	531	LEU	3.5
1	V	499	ILE	3.5
1	I	533	ARG	3.5
1	L	645	TYR	3.5
1	X	570	THR	3.5
1	Q	607	ILE	3.4
1	L	572	GLY	3.4
1	X	608	LEU	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	J	497	GLY	3.4
1	R	600	GLU	3.4
1	X	614	ALA	3.4
1	L	659	ILE	3.4
1	L	639	LEU	3.4
1	X	597	HIS	3.4
1	G	497	GLY	3.3
1	J	587	VAL	3.3
1	X	532	PRO	3.3
1	X	499	ILE	3.3
1	X	627	PHE	3.2
1	X	623	LYS	3.2
1	X	633	VAL	3.2
1	V	508	LEU	3.2
1	I	512	ALA	3.2
1	T	640	GLY	3.2
1	U	579	CYS	3.2
1	X	609	TYR	3.2
1	X	593	HIS	3.2
1	X	651	MET	3.2
1	Q	636	SER	3.1
1	X	639	LEU	3.1
1	V	647	GLY	3.1
1	X	626	GLY	3.1
1	Q	605	HIS	3.1
1	K	498	ILE	3.1
1	X	660	PRO	3.1
1	X	621	TYR	3.0
1	X	507	SER	3.0
1	X	554	ILE	3.0
1	B	660	PRO	3.0
1	Q	621	TYR	3.0
1	V	555	LYS	3.0
1	O	507	SER	3.0
1	L	643	LYS	3.0
1	X	613	TYR	3.0
1	X	617	TYR	3.0
1	S	514	ARG	2.9
1	V	617	TYR	2.9
1	U	497	GLY	2.9
1	Q	630	ASP	2.9
1	C	513	ASN	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	U	509	THR	2.9
1	U	643	LYS	2.9
1	X	620	GLY	2.9
1	X	638	TYR	2.9
1	X	610	PHE	2.9
1	W	499	ILE	2.9
1	Q	603	ILE	2.9
1	J	498	ILE	2.9
1	G	584	ASN	2.9
1	X	604	LYS	2.9
1	X	624	LYS	2.9
1	X	629	LYS	2.9
1	Q	602	HIS	2.9
1	O	658	ARG	2.9
1	Q	657	PRO	2.9
1	X	500	GLU	2.8
1	Q	637	ARG	2.8
1	D	514	ARG	2.8
1	E	507	SER	2.8
1	E	646	GLU	2.8
1	X	596	ASN	2.8
1	V	531	LEU	2.8
1	Q	626	GLY	2.8
1	J	505	GLY	2.8
1	Q	547	LYS	2.8
1	J	590	TYR	2.8
1	L	614	ALA	2.8
1	V	529	HIS	2.8
1	E	615	ASP	2.8
1	W	533	ARG	2.8
1	Q	655	LEU	2.8
1	A	646	GLU	2.7
1	W	554	ILE	2.7
1	X	662	THR	2.7
1	O	529	HIS	2.7
1	W	557	GLY	2.7
1	X	580	ALA	2.7
1	X	653	CYS	2.7
1	S	557	GLY	2.7
1	J	558	ARG	2.7
1	E	647	GLY	2.7
1	Q	587	VAL	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	L	648	ALA	2.7
1	M	533	ARG	2.7
1	Q	556	ASP	2.7
1	J	646	GLU	2.7
1	W	583	SER	2.7
1	J	499	ILE	2.6
1	X	619	ILE	2.6
1	X	589	GLY	2.6
1	T	617	TYR	2.6
1	F	514	ARG	2.6
1	D	506	ASN	2.6
1	J	645	TYR	2.6
1	X	634	PRO	2.6
1	E	558	ARG	2.6
1	X	647	GLY	2.6
1	X	652	GLU	2.6
1	N	514	ARG	2.5
1	X	553	LEU	2.5
1	N	498	ILE	2.5
1	B	595	MET	2.5
1	X	571	GLN	2.5
1	G	509	THR	2.5
1	E	658	ARG	2.5
1	O	555	LYS	2.5
1	W	553	LEU	2.5
1	W	590	TYR	2.5
1	T	662	THR	2.5
1	Q	608	LEU	2.5
1	X	607	ILE	2.5
1	Q	609	TYR	2.5
1	X	501	PHE	2.5
1	J	530	GLN	2.5
1	V	606	ASN	2.5
1	K	507	SER	2.4
1	V	530	GLN	2.4
1	W	556	ASP	2.4
1	T	616	GLU	2.4
1	K	616	GLU	2.4
1	K	646	GLU	2.4
1	E	617	TYR	2.4
1	Q	499	ILE	2.4
1	X	514	ARG	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	L	646	GLU	2.4
1	X	612	THR	2.4
1	Q	611	LEU	2.4
1	A	584	ASN	2.4
1	K	584	ASN	2.4
1	W	587	VAL	2.4
1	X	579	CYS	2.4
1	X	649	THR	2.4
1	B	514	ARG	2.3
1	Q	627	PHE	2.3
1	E	648	ALA	2.3
1	X	582	THR	2.3
1	X	592	THR	2.3
1	X	591	GLY	2.3
1	I	534	MET	2.3
1	X	630	ASP	2.3
1	C	498	ILE	2.3
1	X	636	SER	2.3
1	J	582	THR	2.3
1	D	662	THR	2.3
1	V	584	ASN	2.3
1	N	617	TYR	2.3
1	D	660	PRO	2.3
1	E	511	LYS	2.2
1	G	498	ILE	2.2
1	W	532	PRO	2.2
1	W	581	VAL	2.2
1	L	635	LYS	2.2
1	T	659	ILE	2.2
1	W	579	CYS	2.2
1	L	662	THR	2.2
1	W	555	LYS	2.2
1	W	618	ALA	2.2
1	L	616	GLU	2.2
1	J	529	HIS	2.2
1	S	556	ASP	2.2
1	L	629	LYS	2.2
1	L	650	LEU	2.2
1	W	580	ALA	2.2
1	A	498	ILE	2.2
1	W	558	ARG	2.2
1	O	587	VAL	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	W	534	MET	2.2
1	X	590	TYR	2.2
1	G	646	GLU	2.2
1	L	499	ILE	2.1
1	B	498	ILE	2.1
1	X	574	THR	2.1
1	N	507	SER	2.1
1	V	533	ARG	2.1
1	D	658	ARG	2.1
1	U	498	ILE	2.1
1	K	529	HIS	2.1
1	J	556	ASP	2.1
1	Q	654	GLU	2.1
1	U	513	ASN	2.1
1	J	506	ASN	2.1
1	J	516	VAL	2.1
1	A	616	GLU	2.1
1	L	617	TYR	2.1
1	H	507	SER	2.1
1	F	513	ASN	2.1
1	N	556	ASP	2.1
1	N	558	ARG	2.1
1	X	631	ILE	2.1
1	S	500	GLU	2.1
1	L	613	TYR	2.1
1	I	645	TYR	2.1
1	I	532	PRO	2.0
1	U	584	ASN	2.0
1	J	514	ARG	2.0
1	X	562	GLY	2.0
1	P	499	ILE	2.0
1	K	615	ASP	2.0
1	X	516	VAL	2.0
1	T	584	ASN	2.0
1	L	573	PHE	2.0
1	N	499	ILE	2.0
1	E	498	ILE	2.0
1	Q	592	THR	2.0
1	L	644	ASP	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 oligosaccharides 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.