wwPDB X-ray Structure Validation Summary Report (i)

Sep 23, 2023 – 05:30 PM EDT

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 wwPDB X-ray Structure Validation Summary 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 (i) 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 (i)) were used in the production of this report:

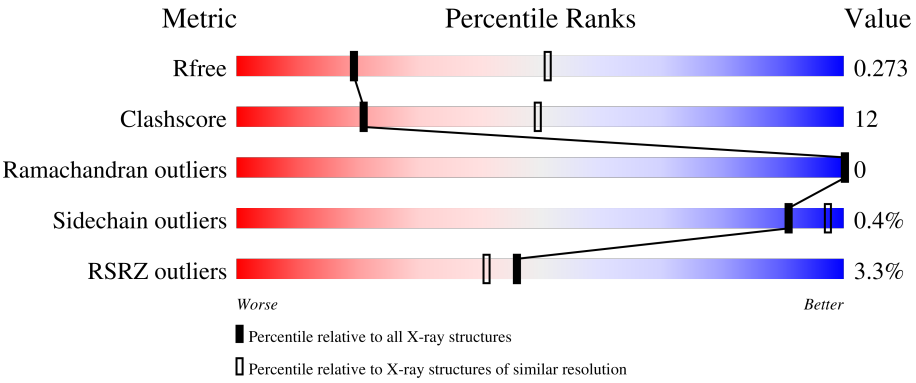
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (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 <=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	76% 20%
1	B	168	79% 17%
1	C	168	82% 13% 5%
1	D	168	74% 21%
1	E	168	76% 21%

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Mol	Chain	Length	Quality of chain
1	F	168	2% 80% 17%
1	G	168	3% 80% 17%
1	H	168	% 73% 23% 5%
1	I	168	2% 73% 24%
1	J	168	6% 67% 30%
1	K	168	2% 82% 13% 5%
1	L	168	4% 56% 34% 7%
1	M	168	% 72% 23% 5%
1	N	168	2% 85% 12%
1	O	168	2% 79% 16%
1	P	168	% 76% 20%
1	Q	168	10% 59% 33% 7%
1	R	168	76% 21%
1	S	168	4% 67% 27%
1	T	168	3% 74% 21% 5%
1	U	168	% 70% 27%
1	V	168	4% 72% 24%
1	W	168	4% 58% 38% 5%
1	X	168	17% 52% 40% 5%

2 Entry composition (i)

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			

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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

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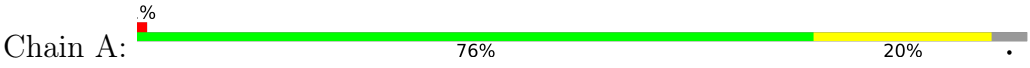
Chain	Residue	Modelled	Actual	Comment	Reference
M	496	SER	-	expression tag	UNP Q92830
L	495	GLY	-	expression tag	UNP Q92830
L	496	SER	-	expression tag	UNP Q92830
K	495	GLY	-	expression tag	UNP Q92830
K	496	SER	-	expression tag	UNP Q92830
J	495	GLY	-	expression tag	UNP Q92830
J	496	SER	-	expression tag	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

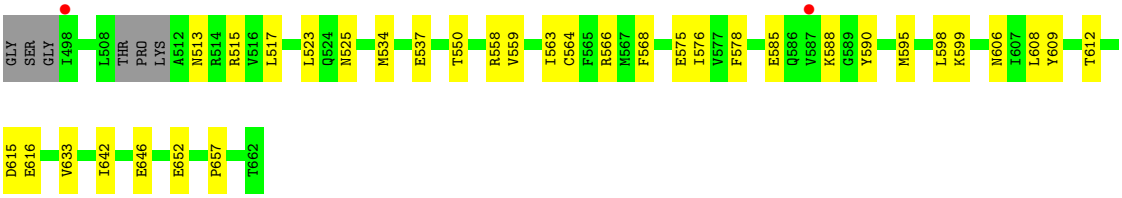
3 Residue-property plots (i)

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

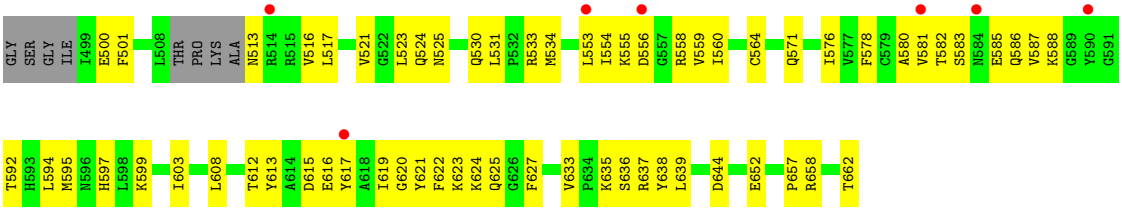
Chain A:





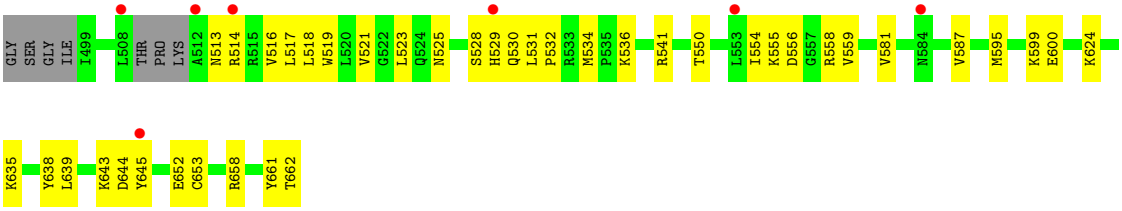
• Molecule 1: Histone acetyltransferase KAT2A

Chain W:



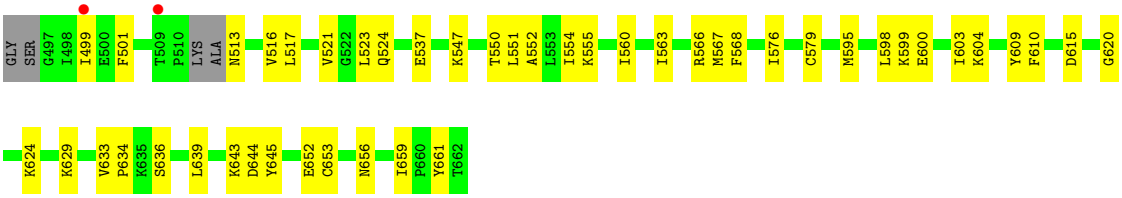
• Molecule 1: Histone acetyltransferase KAT2A

Chain V:

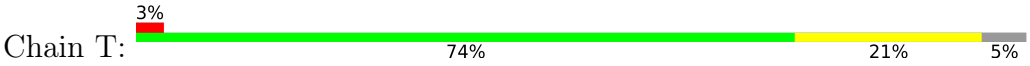


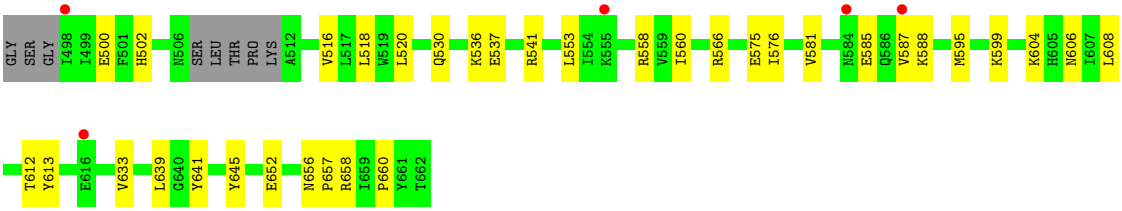
• Molecule 1: Histone acetyltransferase KAT2A

Chain U:

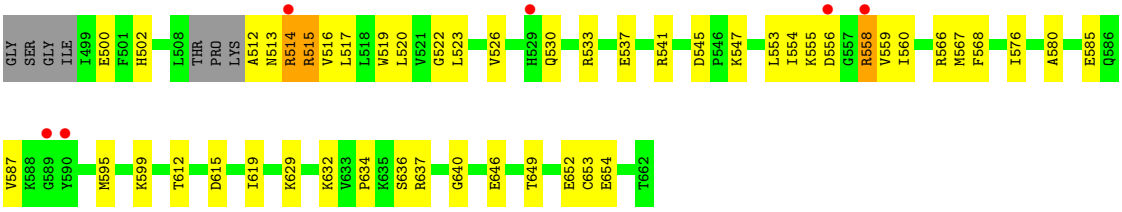


• Molecule 1: Histone acetyltransferase KAT2A

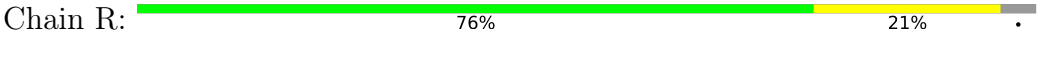


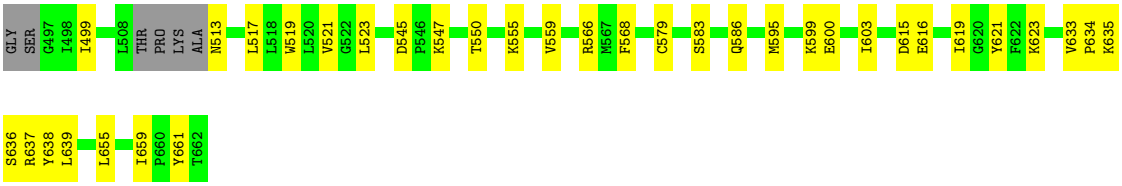


• Molecule 1: Histone acetyltransferase KAT2A

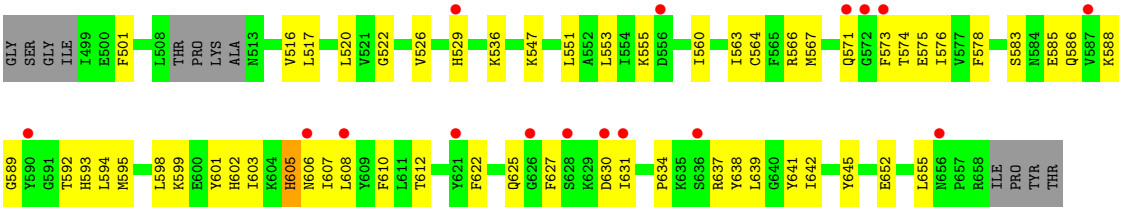


• Molecule 1: Histone acetyltransferase KAT2A



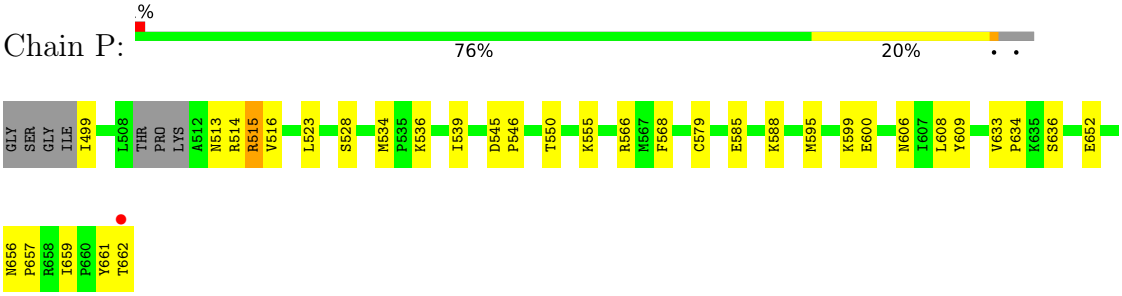


• Molecule 1: Histone acetyltransferase KAT2A



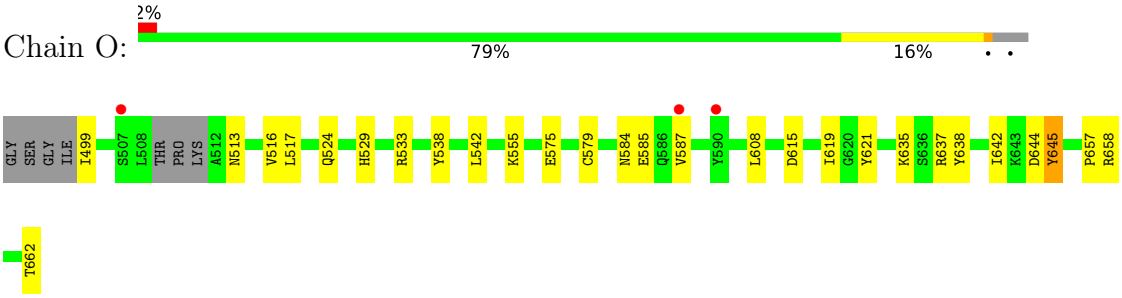
• Molecule 1: Histone acetyltransferase KAT2A

Chain P:



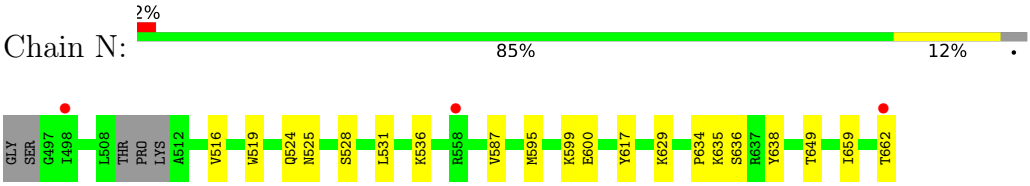
• Molecule 1: Histone acetyltransferase KAT2A

Chain O:



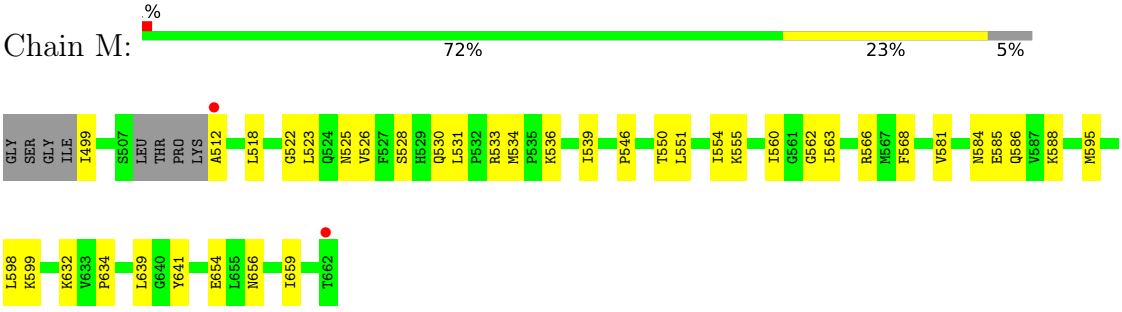
• Molecule 1: Histone acetyltransferase KAT2A

Chain N:



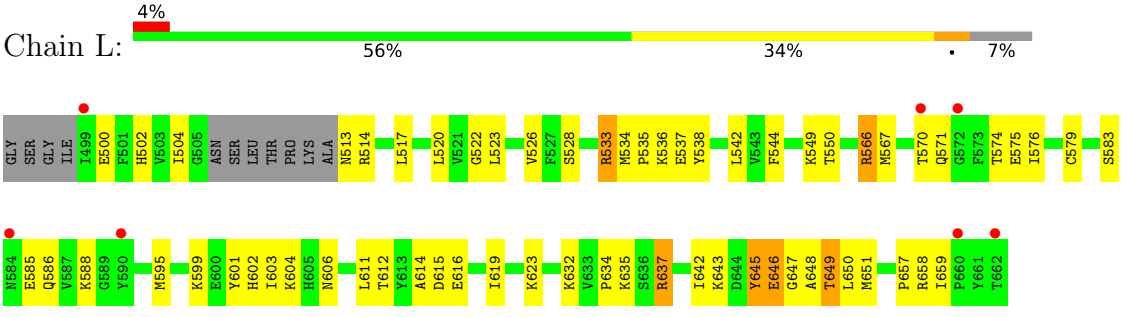
• Molecule 1: Histone acetyltransferase KAT2A

Chain M:



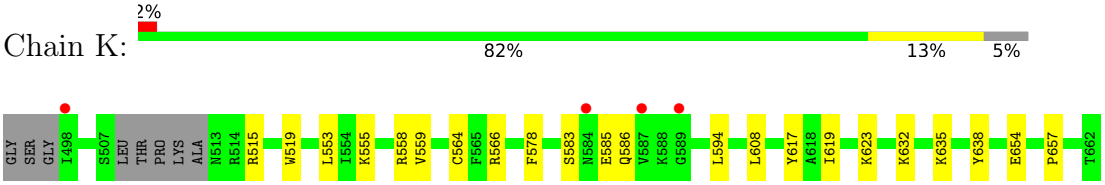
• Molecule 1: Histone acetyltransferase KAT2A

Chain L:



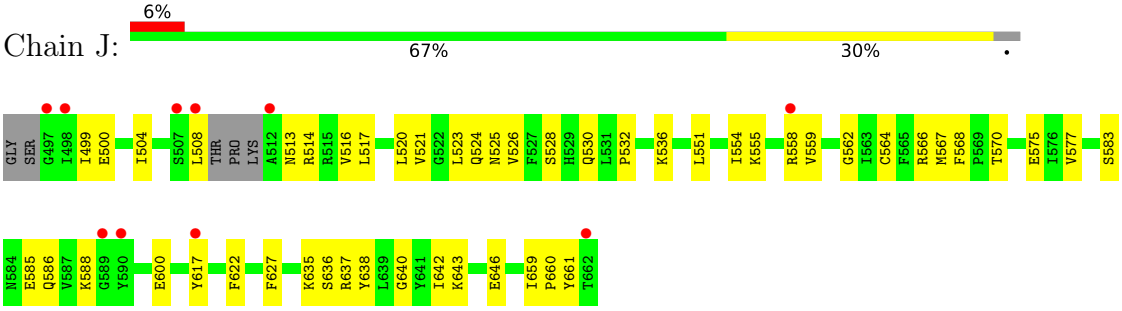
• Molecule 1: Histone acetyltransferase KAT2A

Chain K:



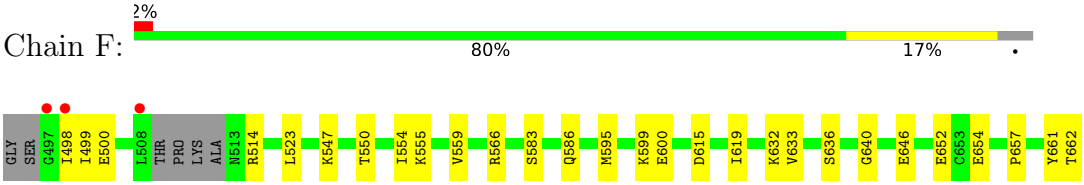
• Molecule 1: Histone acetyltransferase KAT2A

Chain J:



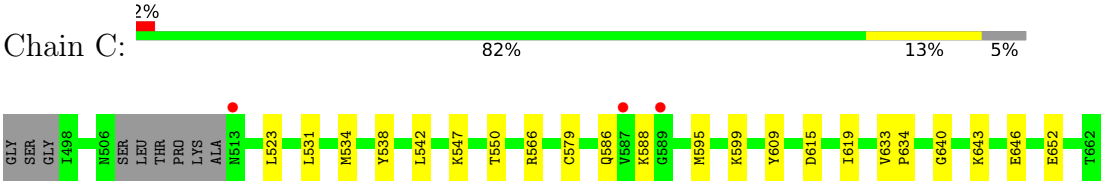
• Molecule 1: Histone acetyltransferase KAT2A

Chain F:



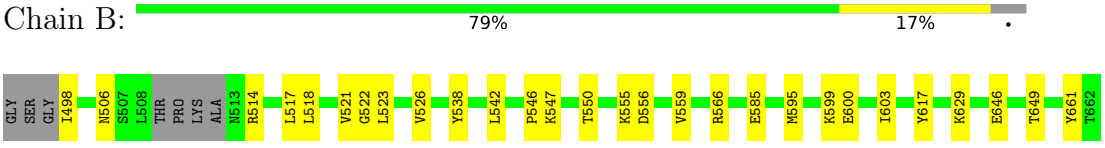
• Molecule 1: Histone acetyltransferase KAT2A

Chain C:



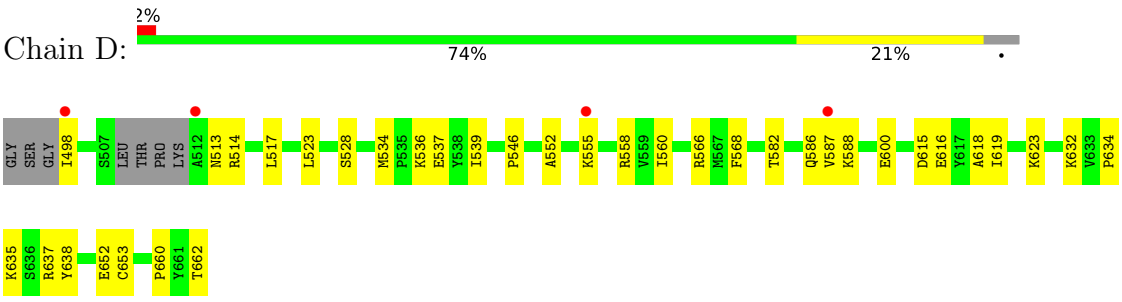
• Molecule 1: Histone acetyltransferase KAT2A

Chain B:



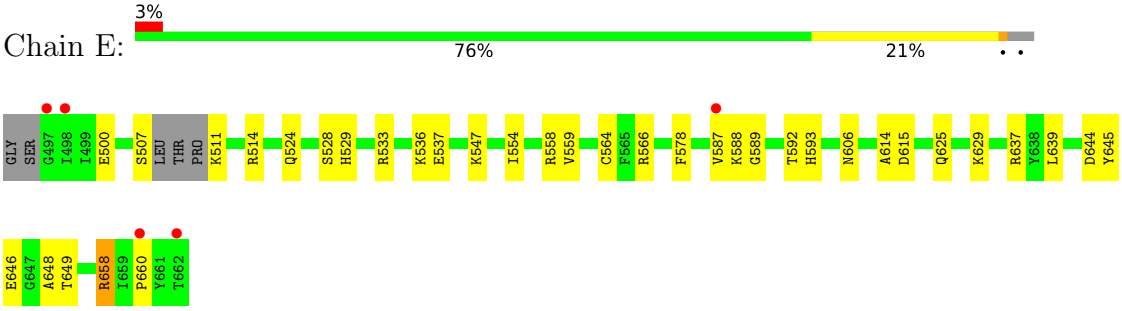
• Molecule 1: Histone acetyltransferase KAT2A

Chain D:



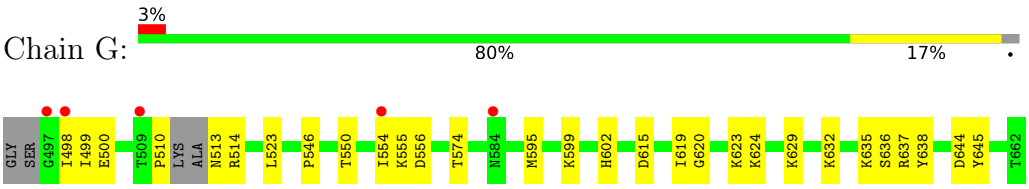
• Molecule 1: Histone acetyltransferase KAT2A

Chain E:



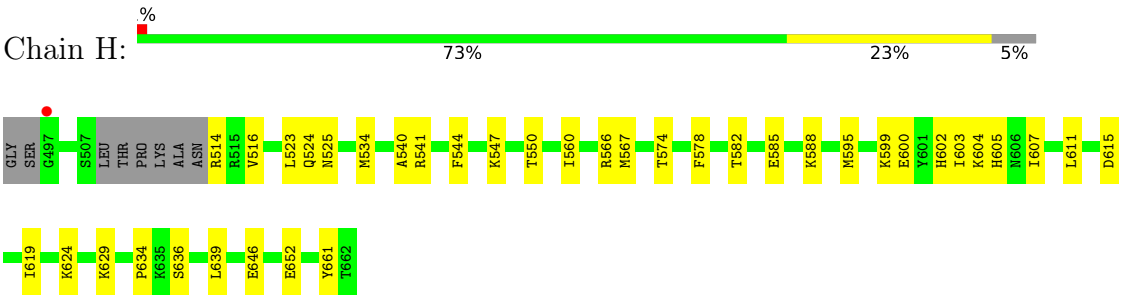
• Molecule 1: Histone acetyltransferase KAT2A

Chain G:



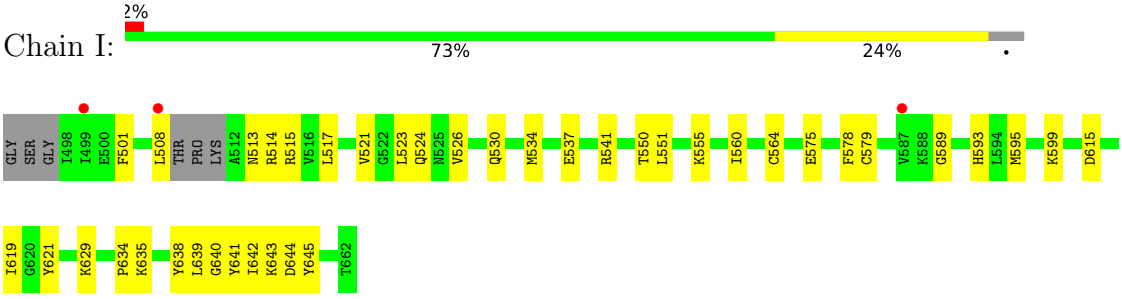
• Molecule 1: Histone acetyltransferase KAT2A

Chain H:



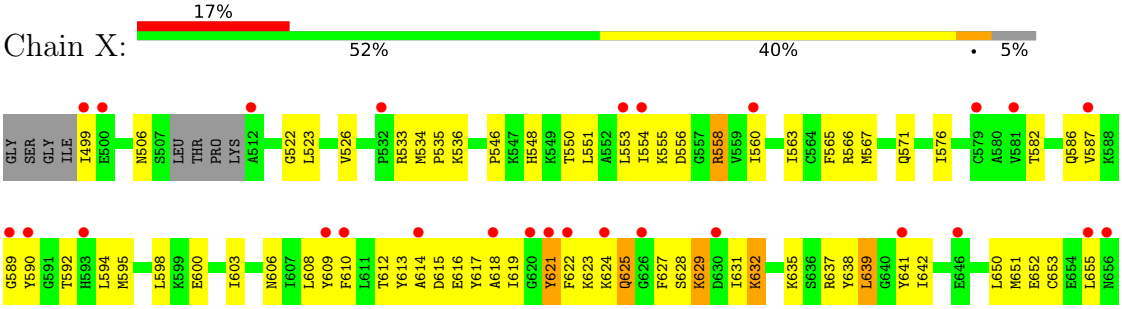
• Molecule 1: Histone acetyltransferase KAT2A

Chain I:



• Molecule 1: Histone acetyltransferase KAT2A

Chain X:




P657
R658
Y661
T662

4 Data and refinement statistics (i)

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 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
$< I/\sigma(I) >$ [1]	3.03 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.10_2152	Depositor
R, R_{free}	0.215 , 0.273 0.215 , 0.273	Depositor DCC
R_{free} test set	5807 reflections (4.95%)	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 , 40.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.44	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

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

The worst 5 of 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

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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

There are no chirality outliers.

5 of 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

5.2 Too-close contacts (i)

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.

The worst 5 of 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

The worst 5 of 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

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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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 (i)

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%)	84	95
1	E	142/147 (97%)	141 (99%)	1 (1%)	84	95
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%)	137 (99%)	2 (1%)	67	89
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%)	67	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	P	142/147 (97%)	141 (99%)	1 (1%)	84 95
1	Q	138/147 (94%)	137 (99%)	1 (1%)	84 95
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%)	67 89
1	X	141/147 (96%)	139 (99%)	2 (1%)	67 89
All	All	3407/3528 (97%)	3395 (100%)	12 (0%)	91 97

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	637	ARG
1	D	558	ARG
1	X	629	LYS
1	E	658	ARG
1	P	515	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
1	O	530	GLN
1	H	586	GLN
1	M	584	ASN
1	X	502	HIS
1	G	525	ASN

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 monosaccharides 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^{th} 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%)	-0.23	2 (1%) 79 79	7, 19, 54, 72	0
1	B	161/168 (95%)	-0.35	0 100 100	7, 15, 42, 82	0
1	C	159/168 (94%)	-0.20	3 (1%) 66 65	7, 19, 50, 91	0
1	D	161/168 (95%)	-0.04	4 (2%) 57 55	15, 30, 62, 96	0
1	E	163/168 (97%)	-0.00	5 (3%) 49 44	10, 26, 59, 84	0
1	F	162/168 (96%)	-0.21	3 (1%) 66 65	8, 20, 47, 76	0
1	G	164/168 (97%)	-0.13	5 (3%) 50 45	13, 26, 56, 104	0
1	H	160/168 (95%)	-0.33	1 (0%) 89 89	6, 15, 36, 53	0
1	I	162/168 (96%)	-0.14	3 (1%) 66 65	11, 28, 56, 83	0
1	J	163/168 (97%)	0.14	10 (6%) 21 17	7, 33, 74, 113	0
1	K	160/168 (95%)	-0.10	4 (2%) 57 55	10, 24, 54, 77	0
1	L	157/168 (93%)	0.37	7 (4%) 33 29	14, 39, 70, 93	0
1	M	160/168 (95%)	-0.16	2 (1%) 77 77	10, 23, 54, 80	0
1	N	163/168 (97%)	-0.15	3 (1%) 68 67	7, 22, 59, 79	0
1	O	161/168 (95%)	-0.09	3 (1%) 66 65	15, 30, 63, 105	0
1	P	161/168 (95%)	-0.23	1 (0%) 89 89	7, 16, 49, 61	0
1	Q	156/168 (92%)	0.71	16 (10%) 6 5	23, 57, 83, 102	0
1	R	162/168 (96%)	-0.28	0 100 100	6, 14, 34, 80	0
1	S	161/168 (95%)	0.01	6 (3%) 41 37	9, 30, 68, 107	0
1	T	160/168 (95%)	0.21	5 (3%) 49 44	18, 41, 67, 87	0
1	U	164/168 (97%)	-0.24	2 (1%) 79 79	7, 16, 44, 107	0
1	V	161/168 (95%)	0.11	7 (4%) 35 31	13, 31, 67, 85	0
1	W	160/168 (95%)	0.30	7 (4%) 34 30	21, 42, 81, 96	0
1	X	160/168 (95%)	0.94	28 (17%) 1 1	33, 73, 105, 114	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
All	All	3863/4032 (95%)	-0.01	127 (3%)	46	41	6, 27, 73, 114	0

The worst 5 of 127 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	4.3

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 monosaccharides 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.