



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 4, 2022 – 12:32 PM EDT

PDB ID : 4TT4
Title : Crystal structure of ATAD2A bromodomain complexed with H3(1-21)K14Ac peptide
Authors : Poncet-Montange, G.; Zhan, Y.; Bardenhagen, J.; Petrocchi, A.; Leo, E.; Shi, X.; Lee, G.; Leonard, P.; Geck Do, M.; Cardozo, M.; Palmer, W.; Andersen, J.; Jones, P.; Ladbury, J.
Deposited on : 2014-06-19
Resolution : 2.70 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : **FAILED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.27

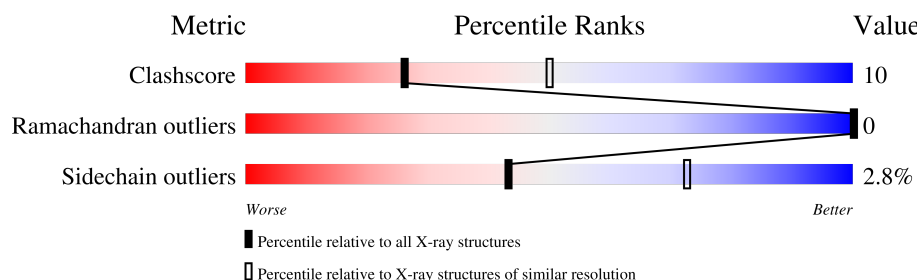
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)

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 $\leq 5\%$.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	130	91% 8% .
1	B	130	87% 13%
2	P	5	40% 40% 20%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ALY	P	101	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 2309 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 ATPase family AAA domain-containing protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	130	Total	C	N	O	S	0	0	0
			1084	679	189	211	5			
1	B	130	Total	C	N	O	S	0	1	0
			1091	684	191	211	5			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	979	SER	-	expression tag	UNP Q6PL18
A	980	MET	-	expression tag	UNP Q6PL18
B	979	SER	-	expression tag	UNP Q6PL18
B	980	MET	-	expression tag	UNP Q6PL18

- Molecule 2 is a protein called Histone H3(1-21)K4Ac.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	P	5	Total	C	N	O	0	0	0
			33	19	6	8			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		
4	B	1	Total	Cl	0	0
			1	1		

- Molecule 5 is water.


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	39	Total	O	0	0
			39	39		
5	B	38	Total	O	0	0
			38	38		
5	P	2	Total	O	0	0
			2	2		

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. 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. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.


Note EDS failed to run properly.

- Molecule 1: ATPase family AAA domain-containing protein 2

Chain A:  91% 8% .



- Molecule 1: ATPase family AAA domain-containing protein 2

Chain B:  87% 13%



- Molecule 2: Histone H3(1-21)K4Ac

Chain P:  40% 40% 20%



4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	108.16Å 115.68Å 77.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	79.01 – 2.70	Depositor
% Data completeness (in resolution range)	99.7 (79.01-2.70)	Depositor
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.84 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.215 , 0.240	Depositor
Wilson B-factor (Å ²)	41.5	Xtriage
Anisotropy	0.370	Xtriage
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
Total number of atoms	2309	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.28% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ALY, SO4, CL

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	0/1102	0.65	1/1487 (0.1%)
1	B	0.48	0/1113	0.58	0/1502
2	P	0.20	0/20	0.68	0/25
All	All	0.46	0/2235	0.62	1/3014 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1067	ARG	NE-CZ-NH1	5.01	122.80	120.30

There are no chirality outliers.

There are no planarity outliers.

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	1084	0	1072	7	0
1	B	1091	0	1079	36	0
2	P	33	0	30	33	0
3	A	10	0	0	0	0
3	B	10	0	0	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	39	0	0	2	0
5	B	38	0	0	3	0
5	P	2	0	0	0	0
All	All	2309	0	2181	46	0

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 10.

All (46) 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:B:1005:ARG:HH12	2:P:101:ALY:C	1.70	1.05
1:B:1005:ARG:HH22	2:P:101:ALY:C	1.71	1.02
1:B:1088:ILE:HG13	2:P:11:THR:CG2	1.92	0.98
1:B:1087:ALA:HB3	2:P:11:THR:OG1	1.65	0.96
1:B:1088:ILE:HG13	2:P:11:THR:HG21	1.48	0.95
1:B:1087:ALA:CB	2:P:11:THR:OG1	2.15	0.94
1:B:1084:THR:O	2:P:11:THR:HG21	1.70	0.90
2:P:11:THR:HG22	2:P:11:THR:O	1.70	0.87
1:B:1005:ARG:NH1	2:P:101:ALY:C	2.39	0.85
1:B:1005:ARG:NH2	2:P:101:ALY:C	2.40	0.83
1:B:1084:THR:HG23	2:P:11:THR:CG2	2.18	0.72
1:B:1088:ILE:HG13	2:P:11:THR:CB	2.22	0.70
1:B:1082:ARG:NH1	5:B:1301:HOH:O	2.24	0.69
1:B:1005:ARG:HH12	2:P:101:ALY:CA	2.09	0.66
1:B:1005:ARG:CZ	2:P:101:ALY:C	2.77	0.63
2:P:11:THR:CG2	2:P:11:THR:O	2.42	0.63
1:B:1005:ARG:NH1	2:P:101:ALY:HD2	2.14	0.62
1:B:1005:ARG:HH12	2:P:101:ALY:HD2	1.66	0.60
1:A:1016:ASP:OD1	1:A:1017:GLU:N	2.35	0.59
1:B:1084:THR:OG1	2:P:101:ALY:O	2.22	0.58
1:B:1087:ALA:CB	2:P:11:THR:HG1	2.17	0.55
1:B:1087:ALA:C	2:P:11:THR:OG1	2.45	0.55
1:A:1107:SER:HB2	2:P:101:ALY:HG3	1.89	0.53
1:B:1087:ALA:HB1	2:P:11:THR:OG1	2.08	0.53
1:B:1088:ILE:HG13	2:P:11:THR:HB	1.90	0.53
1:B:987:ARG:NH1	3:B:1201:SO4:O4	2.42	0.52
1:B:1084:THR:HG23	2:P:11:THR:HG23	1.91	0.52
1:B:1087:ALA:HB1	2:P:11:THR:HG1	1.74	0.52
1:B:1088:ILE:CG1	2:P:11:THR:HB	2.39	0.51
1:B:979:SER:N	5:B:1302:HOH:O	2.44	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1005:ARG:HH12	2:P:101:ALY:HCA	1.76	0.49
2:P:13:GLY:O	2:P:101:ALY:HB3	2.13	0.49
1:A:1036:SER:HA	5:A:1307:HOH:O	2.14	0.48
1:A:1099:GLN:O	1:A:1103:GLU:HG3	2.15	0.47
1:B:1099:GLN:O	1:B:1103:GLU:HG3	2.15	0.47
1:A:987:ARG:HD2	5:A:1314:HOH:O	2.14	0.47
1:B:1090:LYS:NZ	5:B:1303:HOH:O	2.48	0.46
1:B:1093:LEU:HD21	1:B:1098:GLU:HB2	1.98	0.45
1:B:1088:ILE:CG1	2:P:11:THR:CG2	2.81	0.44
1:B:1084:THR:HG23	2:P:11:THR:HG22	1.96	0.44
1:A:1093:LEU:HD21	1:A:1098:GLU:HB2	2.00	0.43
1:B:1084:THR:CG2	2:P:11:THR:CG2	2.92	0.43
1:A:1016:ASP:O	1:A:1017:GLU:C	2.58	0.42
1:B:1005:ARG:HD2	2:P:101:ALY:HH31	2.02	0.41
1:B:1016:ASP:O	1:B:1017:GLU:C	2.59	0.41
1:B:1088:ILE:N	2:P:11:THR:OG1	2.55	0.40

There are no symmetry-related clashes.

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	128/130 (98%)	127 (99%)	1 (1%)	0	100	100
1	B	129/130 (99%)	127 (98%)	2 (2%)	0	100	100
2	P	3/5 (60%)	1 (33%)	2 (67%)	0	100	100
All	All	260/265 (98%)	255 (98%)	5 (2%)	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	123/123 (100%)	120 (98%)	3 (2%)	49	77
1	B	124/123 (101%)	121 (98%)	3 (2%)	49	77
2	P	2/2 (100%)	1 (50%)	1 (50%)	0	0
All	All	249/248 (100%)	242 (97%)	7 (3%)	43	73

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1061	LEU
1	A	1067	ARG
1	A	1089	ILE
1	B	1022	VAL
1	B	1077	ARG
1	B	1089	ILE
2	P	11	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1041	HIS
1	B	1041	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

6.4 Ligands

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers

EDS failed to run properly - this section is therefore empty.