

Full wwPDB X-ray Structure Validation Report (i)

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PDB ID : 4TYL

> Title : Fragment-Based Screening of the Bromodomain of ATAD2

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2014-07-08 Deposited on

1.85 Å(reported) Resolution

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 (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 (1)) were used in the production of this report:

MolProbity 4.02b-467

> 1.8.5 (274361), CSD as541be (2020) Mogul

Xtriage (Phenix) 1.13

EDS 2.36

20191225.v01 (using entries in the PDB archive December 25th 2019) Percentile statistics

> Refmac 5.8.0158

CCP4 7.0.044 (Gargrove)

Ideal geometry (proteins) Engh & Huber (2001) Ideal geometry (DNA, RNA) Parkinson et al. (1996)

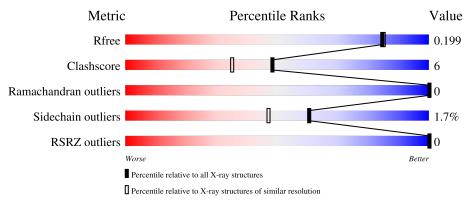
Validation Pipeline (wwPDB-VP) 2.36

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 1.85 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.



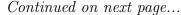
Metric	Whole archive $(\# \mathrm{Entries})$	${f Similar\ resolution} \ (\#{f Entries},\ resolution\ range(\AA))$		
R_{free}	130704	2469 (1.86-1.86)		
Clashscore	141614	2625 (1.86-1.86)		
Ramachandran outliers	138981	2592 (1.86-1.86)		
Sidechain outliers	138945	2592 (1.86-1.86)		
RSRZ outliers	127900	2436 (1.86-1.86)		

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	130	91%	8% •			

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CL	A	1202	-	-	X	-





Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CL	A	1205	-	-	X	-



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 1360 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.

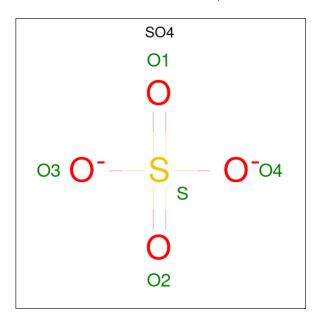
• Molecule 1 is a protein called ATPase family AAA domain-containing protein 2.

Mo	l Chai	n Re	sidues	Atoms			ZeroOcc	AltConf	Trace		
1	A		130	Total 1086	C 685	N 190	O 207	S 4	11	5	0

There are 2 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

• Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



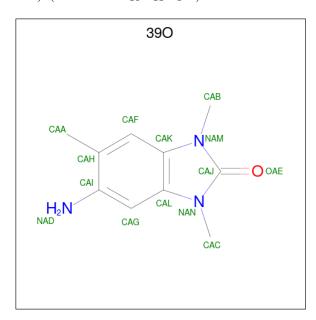
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 5	O 4	S 1	0	0

• Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	4	Total Cl 4 4	0	0

 \bullet Molecule 4 is 5-amino-1,3,6-trimethyl-1,3-dihydro-2H-benzimidazol-2-one (three-letter code: 39O) (formula: $\rm C_{10}H_{13}N_3O$).



1	VIOI	Chain	Residues		Lton	ns		ZeroOcc	AltConf
	4	A	1	Total	C 10	N	0	0	0

• Molecule 5 is water.

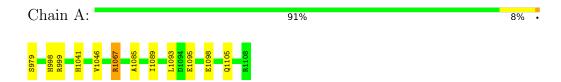
\mathbf{Mol}	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	251	Total O 251 251	0	0



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: ATPase family AAA domain-containing protein 2





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants	79.49Å 79.49Å 137.51Å	Donositor
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.18 - 1.85	Depositor
rtesolution (A)	38.18 - 1.85	EDS
% Data completeness	99.9 (38.18-1.85)	Depositor
(in resolution range)	95.9 (38.18-1.85)	EDS
R_{merge}	0.06	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) > 1$	3.14 (at 1.85Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
D D.	0.161 , 0.197	Depositor
R, R_{free}	0.163 , 0.199	DCC
R_{free} test set	2000 reflections (8.83%)	wwPDB-VP
Wilson B-factor (Å ²)	26.8	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.35 , 59.8	EDS
L-test for twinning ²	$< L >=0.50, < L^2>=0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	1360	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 6.42% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

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: 39O, CL, SO4

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		
		Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
	1	A	0.85	0/1125	0.79	$1/1522 \ (0.1\%)$	

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	${f Z}$	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
1	A	999	ARG	NE-CZ-NH2	-5.21	117.69	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	1086	0	1061	8	1
2	A	5	0	0	0	0
3	A	4	0	0	5	0
4	A	14	0	13	0	0
5	A	251	0	0	10	3
All	All	1360	0	1074	13	4

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 6.



All (13) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	Clash overlap (Å)
3:A:1205:CL:CL	5:A:1395:HOH:O	2.09	1.06
3:A:1204:CL:CL	5:A:1366:HOH:O	2.09	1.05
3:A:1202:CL:CL	5:A:1352:HOH:O	2.15	1.01
3:A:1202:CL:CL	5:A:1365:HOH:O	2.19	0.98
3:A:1205:CL:CL	5:A:1387:HOH:O	2.25	0.92
1:A:1095:GLU:OE1	5:A:1543:HOH:O	2.16	0.61
1:A:979:SER:N	5:A:1544:HOH:O	2.34	0.59
1:A:1085:ALA:O	1:A:1089[B]:ILE:HG12	2.06	0.56
1:A:1046[B]:VAL:HG21	1:A:1093:LEU:HD22	1.89	0.54
1:A:998[A]:HIS:CG	5:A:1502:HOH:O	2.69	0.45
1:A:998[A]:HIS:CD2	5:A:1502:HOH:O	2.73	0.41
1:A:998[A]:HIS:CD2	5:A:1340:HOH:O	2.72	0.41
1:A:1093:LEU:HD21	1:A:1098:GLU:HB2	2.03	0.40

All (4) 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	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	Clash overlap (Å)	
5:A:1361:HOH:O	5:A:1377:HOH:O[8_545]	2.02	0.18	
5:A:1340:HOH:O	5:A:1359:HOH:O[12_544]	2.05	0.15	
1:A:1041:HIS:NE2	1:A:1067[B]:ARG:NH2[6_554]	2.12	0.08	
5:A:1341:HOH:O	5:A:1374:HOH:O[6_554]	2.18	0.02	

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	Analysed Favoured Allo		Outliers	Percentiles
1	A	133/130 (102%)	133 (100%)	0	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	Analysed Rotameric		Percentiles	
1	A	121/123 (98%)	118 (98%)	3 (2%)	47 31	

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1067[A]	ARG
1	A	1067[B]	ARG
1	A	1105	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond



length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with |Z| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

	Mol	Type Chain		Dag	Link	Bond lengths			Bond angles		
	MIOI	Type	Chain	Res	Link	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
Ī	2	SO4	A	1201	-	4,4,4	0.34	0	6,6,6	0.57	0
	4	39O	A	1203	-	15,15,15	1.86	4 (26%)	22,23,23	1.82	7 (31%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	39O	A	1203	-	-	-	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	Observed(A)	$\operatorname{Ideal}(ext{\AA})$
4	A	1203	39O	CAJ-NAN	-4.37	1.33	1.37
4	A	1203	39O	CAF-CAK	3.38	1.45	1.39
4	A	1203	39O	CAG-CAL	2.84	1.44	1.39
4	A	1203	39O	CAI-NAD	2.16	1.45	1.37

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
4	A	1203	39O	CAL-NAN-CAJ	-4.43	107.65	110.25
4	A	1203	39O	CAC-NAN-CAJ	3.23	126.50	123.37
4	A	1203	39O	CAB-NAM-CAJ	3.12	126.40	123.37
4	A	1203	39O	CAK-NAM-CAJ	-3.08	108.44	110.25
4	A	1203	39O	OAE-CAJ-NAM	-2.52	124.56	127.02
4	A	1203	39O	CAG-CAL-NAN	2.11	133.45	129.21
4	A	1203	39O	NAN-CAJ-NAM	2.02	109.31	106.03

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 (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, 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>	$\#\text{RSRZ}{>}2$	$OWAB(A^2)$	Q < 0.9
1	A	130/130 (100%)	-0.63	0 100 100	18, 27, 64, 87	0

There are no RSRZ outliers to report.

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)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
3	CL	A	1205	1/1	0.65	0.16	92,92,92,92	1
3	CL	A	1206	1/1	0.75	0.10	91,91,91,91	0
3	CL	A	1204	1/1	0.95	0.13	40,40,40,40	0
4	39O	A	1203	14/14	0.95	0.18	27,50,61,64	0
3	CL	A	1202	1/1	0.96	0.08	62,62,62,62	0
2	SO4	A	1201	5/5	0.97	0.17	38,40,56,69	0



6.5 Other polymers (i)

There are no such residues in this entry.

