

Full wwPDB X-ray Structure Validation Report (i)

Sep 22, 2022 – 12:00 pm BST

PDB ID : 7QYE

Title: BAZ2A bromodomain in complex with acetylpyrrole derivative compound 78

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Deposited on : 2022-01-28

Resolution : 1.65 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 (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

Mogul : 1.8.4, CSD as541be (2020)

Xtriage (Phenix) : 1.13

EDS : 2.30

buster-report : 1.1.7 (2018)

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

Refmac : 5.8.0267

CCP4 : 7.1.010 (Gargrove)

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

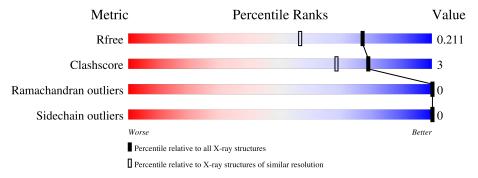
Validation Pipeline (wwPDB-VP) : 2.30

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 1.65 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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
R_{free}	130704	1827 (1.66-1.66)
Clashscore	141614	1931 (1.66-1.66)
Ramachandran outliers	138981	1891 (1.66-1.66)
Sidechain outliers	138945	1891 (1.66-1.66)

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%

Mol	Chain	Length	Quality of chain
1	A	105	96%



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 1083 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 Bromodomain adjacent to zinc finger domain protein 2A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	A	105	Total 899	C 567	N 158	O 166	S	0	6	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1794	SER	-	expression tag	UNP Q9UIF9
A	1795	MET	-	expression tag	UNP Q9UIF9
A	1845	HIS	GLU	engineered mutation	UNP Q9UIF9
A	1848	SER	LEU	engineered mutation	UNP Q9UIF9

• Molecule 2 is 1-[4-cyclopentyl-2-methyl-5-(2-piperazin-1-yl-1,3-thiazol-4-yl)-1 {H}-pyr rol-3-yl]ethanone (three-letter code: GQF) (formula: $C_{19}H_{26}N_4OS$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf			
9	Λ	1	Total	С	N	О	S	0	0	
$\begin{array}{ c c c c c }\hline Z & A \\ \hline \end{array}$	A	A 1		19	4	1	1	0		
9	2 4	1	Total	С	N	О	S	0	0	
2 A	A	1	25	19	4	1	1	0	0	

$\bullet\,$ Molecule 3 is water.

\mathbf{M}	ol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	3	A	134	Total O 134 134	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. 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.

• Molecule 1: Bromodomain adjacent to zinc finger domain protein 2A

Chain A: 96%





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	$37.46\text{\AA} 35.02\text{Å} 37.65\text{Å}$	Depositor
a, b, c, α , β , γ	90.00° 92.47° 90.00°	Depositor
Resolution (Å)	37.61 - 1.65	Depositor
rtesolution (A)	37.61 - 1.65	EDS
% Data completeness	99.6 (37.61-1.65)	Depositor
(in resolution range)	99.8 (37.61-1.65)	EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	3.56 (at 1.65Å)	Xtriage
Refinement program	PHENIX 1.11.1	Depositor
R, R_{free}	0.181 , 0.209	Depositor
, and the second	0.184 , 0.211	DCC
R_{free} test set	481 reflections (4.05%)	wwPDB-VP
Wilson B-factor (Å ²)	15.8	Xtriage
Anisotropy	0.834	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	(Not available), (Not available)	EDS
L-test for twinning ²	$< L > = 0.49, < L^2> = 0.32$	Xtriage
	0.000 for l,k,-h	
Estimated twinning fraction	0.041 for h,-k,-l	Xtriage
	0.024 for l,-k,h	
F_o, F_c correlation	0.95	EDS
Total number of atoms	1083	wwPDB-VP
Average B, all atoms (\mathring{A}^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 15.32% 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: GQF

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).

Mal	Chain	Bond	$\mathbf{lengths}$	Bond angles		
MIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.35	0/940	0.52	0/1263	

There are no bond length outliers.

There are no bond angle outliers.

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	899	0	861	4	0
2	A	50	0	0	1	0
3	A	134	0	0	2	0
All	All	1083	0	861	5	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 3.

All (5) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1 Atom-2		$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$\begin{array}{c} \text{Clash} \\ \text{overlap } (\text{\AA}) \end{array}$
1:A:1816:TRP:CG	1:A:1817:PRO:HD3	2.45	0.51

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Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	Clash overlap (Å)
1:A:1888[A]:ARG:NH1	3:A:2002:HOH:O	2.38	0.49
1:A:1849[B]:ARG:NH1	3:A:2005:HOH:O	2.48	0.47
2:A:1902:GQF:C11	2:A:1902:GQF:N19	2.78	0.47
1:A:1816:TRP:CD2	1:A:1817:PRO:HD3	2.52	0.45

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	Percer	ntiles
1	A	109/105 (104%)	109 (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 Rotameric Outliers		Percentiles	
1	A	100/94 (106%)	100 (100%)	0	100 100

There are no protein residues with a non-rotameric sidechain to report.

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)

2 ligands are modelled in this entry.

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	Res	Link	В	ond leng	gths	В	ond ang	cles
MIOI	туре	Chain	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GQF	A	1901	-	23,28,28	3.33	12 (52%)	20,40,40	1.21	2 (10%)
2	GQF	A	1902	-	23,28,28	3.39	11 (47%)	20,40,40	1.85	4 (20%)

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.

\mathbf{Mol}	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GQF	A	1901	-	-	1/2/31/31	0/4/4/4
2	GQF	A	1902	-	-	2/2/31/31	0/4/4/4

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	Observed(A)	$Ideal(\AA)$
2	A	1902	GQF	C18-N20	11.26	1.50	1.32

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Mol	Chain	Res	Type	Atoms	\mathbf{Z}	Observed(A)	Ideal(Å)
2	A	1901	GQF	C18-N20	10.55	1.48	1.32
2	A	1902	GQF	C14-C10	-4.64	1.37	1.54
2	A	1901	GQF	C14-C10	-4.49	1.37	1.54
2	A	1901	GQF	C06-C05	4.45	1.57	1.50
2	A	1901	GQF	C16-S17	-4.14	1.64	1.70
2	A	1902	GQF	C16-S17	-4.12	1.64	1.70
2	A	1902	GQF	C06-C05	4.02	1.57	1.50
2	A	1901	GQF	C09-C10	3.82	1.61	1.51
2	A	1902	GQF	C09-C10	3.69	1.61	1.51
2	A	1902	GQF	C13-C14	3.69	1.67	1.51
2	A	1901	GQF	C13-C14	3.65	1.67	1.51
2	A	1901	GQF	C08-C15	3.22	1.53	1.49
2	A	1902	GQF	C08-C15	3.12	1.53	1.49
2	A	1901	GQF	C25-N20	3.03	1.51	1.46
2	A	1902	GQF	C15-N19	2.87	1.46	1.37
2	A	1901	GQF	C15-N19	2.86	1.46	1.37
2	A	1902	GQF	C25-N20	2.79	1.51	1.46
2	A	1902	GQF	C21-N20	2.26	1.50	1.46
2	A	1901	GQF	C04-C02	2.23	1.55	1.49
2	A	1901	GQF	C12-C11	2.14	1.60	1.51
2	A	1901	GQF	C21-N20	2.12	1.50	1.46
2	A	1902	GQF	C12-C11	2.11	1.60	1.51

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
2	A	1902	GQF	C14-C10-C09	4.23	122.52	115.08
2	A	1902	GQF	C11-C10-C09	-4.00	108.04	115.08
2	A	1902	GQF	C04-C09-C10	-3.59	122.38	129.63
2	A	1901	GQF	C11-C10-C09	-3.48	108.95	115.08
2	A	1902	GQF	C14-C10-C11	2.71	107.23	102.43
2	A	1901	GQF	C14-C10-C11	2.04	106.03	102.43

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1901	GQF	S17-C18-N20-C25
2	A	1902	GQF	S17-C18-N20-C21
2	A	1902	GQF	S17-C18-N20-C25

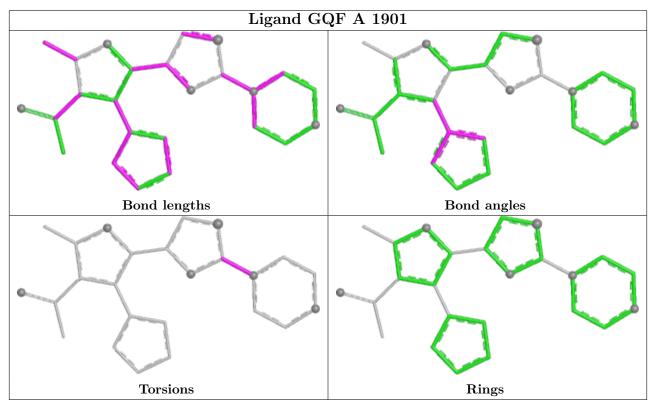
There are no ring outliers.



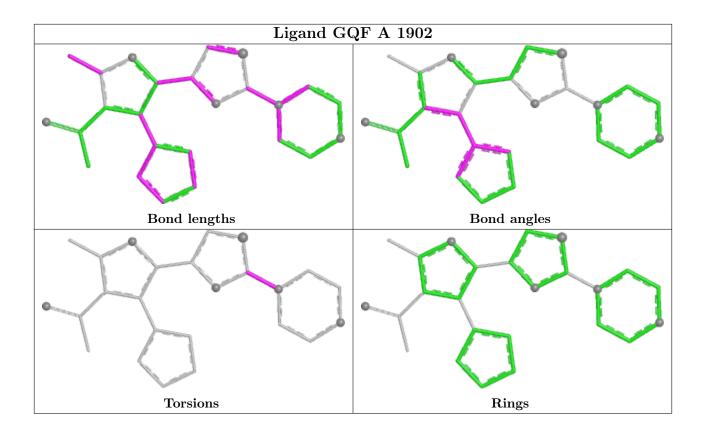
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1902	GQF	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







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)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

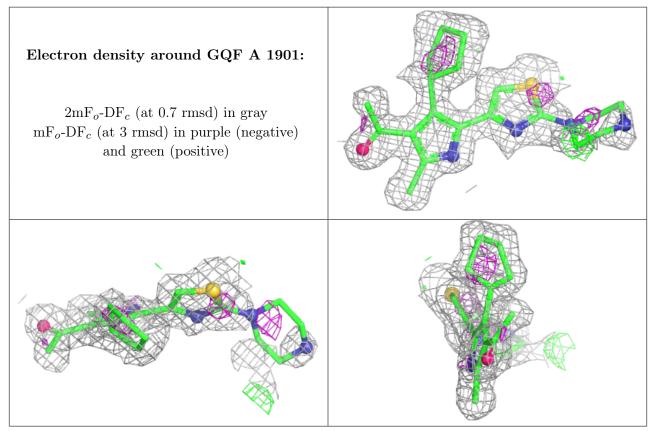
6.3 Carbohydrates (i)

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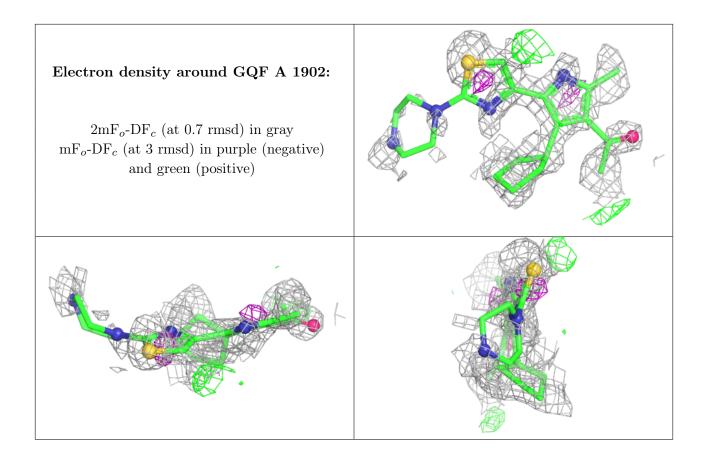
6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.







6.5 Other polymers (i)

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