

wwPDB X-ray Structure Validation Summary Report (i)

Nov 1, 2021 – 01:08 pm GMT

PDB ID	:	7APW
Title	:	The Fk1 domain of FKBP51 in complex with (1S,5S,6R)-10-(benzo[d]thiazol-
		6-ylsulfonyl)-5-(methoxymethyl)-3-(pyridin-2-ylethyl)-3,10-diazabicyclo[4.3.1]
		decan-2-one
Authors	:	Voll, A.M.; Kolos, J.M.; Pomplun, S.; Riess, B.; Purder, P.; Merz, S.; Bracher,
		A.; Meyners, C.; Krewald, V.; Hausch, F.
Deposited on	:	2020-10-20
Resolution	:	0.89 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 following versions of software and data (see references (1)) were used in the production of this report:

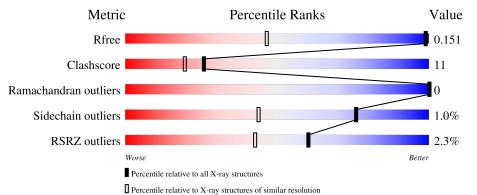
Xtriage (Phenix) EDS buster-report Percentile statistics Refmac	:::::::::::::::::::::::::::::::::::::::	20191225.v01 (using entries in the PDB archive December 25th 2019) 5.8.0267 7.1.010 (Gargrove) Engh & Huber (2001)
0 0 0 0	:	0
1 · · · · · · · · · · · · · · · · · · ·		-

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 0.89 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	$1061 \ (1.04-0.76)$
Clashscore	141614	1132(1.04-0.76)
Ramachandran outliers	138981	1055 (1.04-0.76)
Sidechain outliers	138945	1056 (1.04-0.76)
RSRZ outliers	127900	1028 (1.04-0.76)

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	А	128	83%	14%	



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 2593 atoms, of which 1167 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.

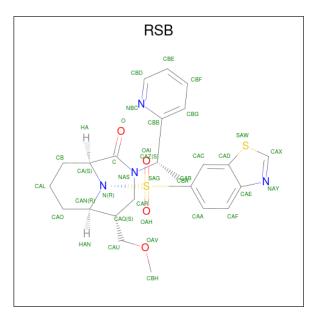
• Molecule 1 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
1	А	128	Total 2242	C 700	Н 1139	N 195	O 204	${S \over 4}$	24	14	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	13	GLY	-	expression tag	UNP Q13451
А	14	ALA	-	expression tag	UNP Q13451
А	15	PRO	-	expression tag	UNP Q13451
А	19	THR	ALA	engineered mutation	UNP Q13451

• Molecule 2 is (1S,5S,6R)-10-(benzo[d]thiazol-6-ylsulfonyl)-5-(methoxymethyl)-3-(py ridin-2-ylethyl)-3,10-diazabicyclo[4.3.1]decan-2-one (three-letter code: RSB) (formula: C₂₄H₂₈N₄O₄S₂) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf		
2	А	1	Total 62	C 24	Н 28	N 4	0 4	$\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$	0	0

• Molecule 3 is water.

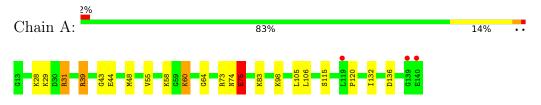
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	А	278	Total O 289 28) 9	0	11



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: Peptidyl-prolyl cis-trans isomerase FKBP5





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	Depositor
Resolution (Å)	$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	Depositor EDS
% Data completeness	90.4 (30.00-0.89) 90.4 (28.74.0.80)	Depositor EDS
$\frac{\text{(in resolution range)}}{R_{merge}}$	<u>90.4 (28.74-0.89)</u> 0.11	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.66 (at 0.89 Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	Depositor DCC
R_{free} test set	4541 reflections $(4.98%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	8.4	Xtriage
Anisotropy	0.281	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	(Not available), (Not available)	EDS
L-test for $twinning^2$	$< L > = 0.49, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.013 for -h,l,k	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	2593	wwPDB-VP
Average B, all atoms $(Å^2)$	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 7.13% of the height of the origin peak. No significant pseudotranslation is detected.

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.



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: RSB

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	Bo	nd lengths	Bo	nd angles
IVIOI	Mol Chain		# Z > 5	RMSZ	# Z > 5
1	А	1.24	16/1124~(1.4%)	1.12	9/1503~(0.6%)

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	А	0	1

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	Ideal(Å)
1	А	58	LYS	CB-CG	-8.22	1.30	1.52
1	А	48	MET	CG-SD	7.29	2.00	1.81
1	А	75[A]	GLU	CD-OE1	-6.37	1.18	1.25
1	А	75[B]	GLU	CD-OE1	-6.37	1.18	1.25
1	А	60	LYS	CA-CB	6.36	1.68	1.53

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	48	MET	CG-SD-CE	6.04	109.86	100.20
1	А	75[A]	GLU	OE1-CD-OE2	-6.00	116.10	123.30
1	А	75[B]	GLU	OE1-CD-OE2	-6.00	116.10	123.30
1	А	106	LEU	CB-CG-CD2	5.98	121.16	111.00
1	А	39[A]	ARG	NE-CZ-NH1	-5.84	117.38	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:



M	Iol	Chain	Res	Type	Group
	1	А	75[A]	GLU	Sidechain

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	А	1103	1139	1118	24	1
2	А	34	28	0	0	0
3	А	289	0	0	20	1
All	All	1426	1167	1118	24	1

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 11.

The worst 5 of 24 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:A:31[B]:ARG:NH2	3:A:304:HOH:O	1.56	1.27	
1:A:29[B]:LYS:HE2	3:A:316:HOH:O	1.15	1.25	
1:A:75[B]:GLU:OE1	3:A:303:HOH:O	1.56	1.24	
1:A:31[A]:ARG:NH2	3:A:304:HOH:O	1.83	1.07	
1:A:29[A]:LYS:CE	3:A:359:HOH:O	2.08	1.00	

All (1) 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:A:39[B]:ARG:HH22	3:A:456:HOH:O[4_445]	1.56	0.04

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	А	140/128~(109%)	139~(99%)	1 (1%)	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	А	119/106~(112%)	118~(99%)	1 (1%)	81 50	

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

Mol	Chain	Res	Type
1	А	120	PRO

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)

1 ligand is 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	Bo	ond leng	ths	B	ond ang	les	
	101	Type	Ullalli	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
	2	RSB	А	201	-	35,38,38	1.39	5 (14%)	34,56,56	1.54	6 (17%)

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
2	RSB	А	201	-	-	3/23/53/53	0/3/5/5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(Å)
2	А	201	RSB	CAD-SAW	-3.84	1.71	1.74
2	А	201	RSB	CAC-CAD	2.99	1.44	1.38
2	А	201	RSB	CAR-NAS	2.98	1.48	1.46
2	А	201	RSB	CAF-CAE	-2.85	1.36	1.41
2	А	201	RSB	CAF-CAA	2.09	1.41	1.36

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
2	А	201	RSB	CAR-NAS-C	4.00	126.14	122.11
2	А	201	RSB	CBF-CBG-CBB	-3.52	114.83	118.89
2	А	201	RSB	CAB-CAC-CAD	-3.02	116.60	120.44
2	А	201	RSB	CAD-CAE-NAY	2.79	114.08	107.87
2	А	201	RSB	CAF-CAE-NAY	-2.54	123.76	130.80

There are no chirality outliers.

All (3) torsion outliers are listed below:

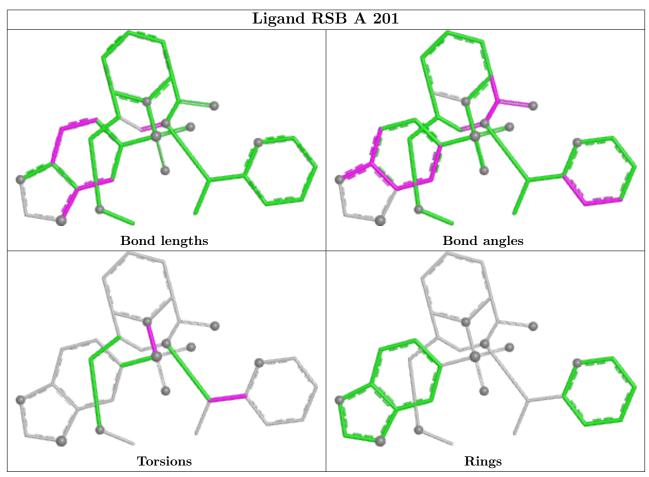


Mol	Chain	Res	Type	Atoms		
2	А	201	RSB	CBA-CAZ-CBB-NBC		
2	А	201	RSB	CA-N-SAG-OAH		
2	А	201	RSB	CA-N-SAG-CAB		

There are no ring outliers.

No monomer is involved in short contacts.

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 sufficient 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)

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	А	128/128 (100%)	-0.36	3 (2%) 60	43	5, 8, 22, 45	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	140	GLU	3.7
1	А	119	LEU	2.4
1	А	139	GLY	2.1

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)

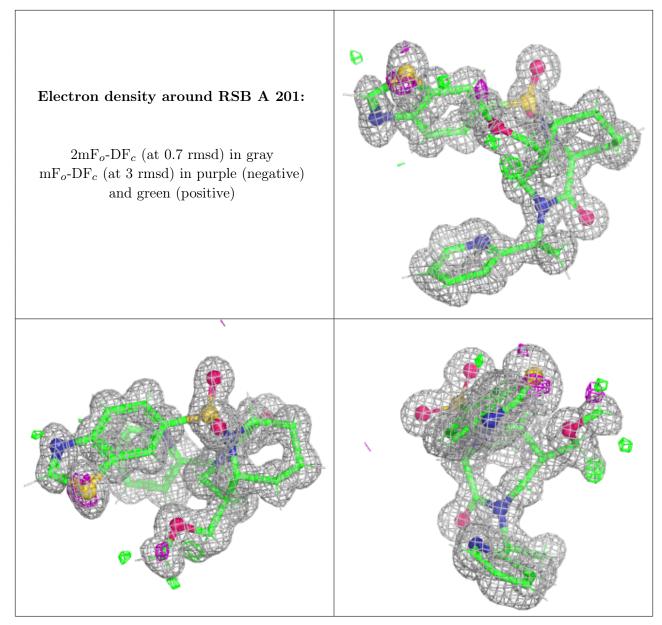
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
2	RSB	А	201	34/34	0.99	0.06	6,9,15,24	0

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)

There are no such residues in this entry.

