

# Full wwPDB X-ray Structure Validation Report (i)

#### Jun 3, 2024 – 03:24 PM JST

PDB ID	:	8JNZ
Title	:	Human ADP-ribosyltransferase 1 (PARP1) catalytic domain bound to a
		pyrazolopyrimidine carboxamide inhibitor
Authors	:	Wang, X.Y.; Wang, C.Y.; Zhou, J.; Xu, B.L.
Deposited on		
Resolution	:	2.84  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:

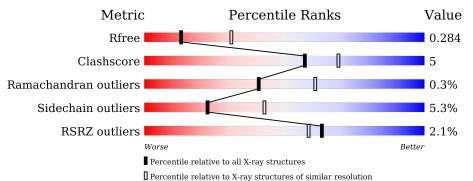
Xtriage (Phenix) EDS buster-report Percentile statistics Refmac CCP4 Ideal geometry (proteins) Ideal geometry (DNA, RNA)	: : : : :	20191225.v01 (using entries in the PDB archive December 25th 2019) 5.8.0158 7.0.044 (Gargrove) Engh & Huber (2001) Parkinson et al. (1996)
Ideal geometry (DNA, RNA) Validation Pipeline (wwPDB-VP)		Parkinson et al. (1996) 2.36.2

# 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 2.84 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	$\begin{array}{l} \textbf{Whole archive} \\ (\#\textbf{Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R <sub>free</sub>	130704	1031 (2.86-2.82)
Clashscore	141614	1078 (2.86-2.82)
Ramachandran outliers	138981	1050 (2.86-2.82)
Sidechain outliers	138945	1051 (2.86-2.82)
RSRZ outliers	127900	1019 (2.86-2.82)

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	354	88%	11%	••
1	В	354	79%	19%	••



## 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 5585 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.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	Δ	352	Total	С	Ν	0	$\mathbf{S}$	0	0	0
	I A	- 552	2767	1759	467	529	12			
1	D	352	Total	С	Ν	0	S	0	0	0
	ГВ	392	2767	1759	467	529	12	0	U	U

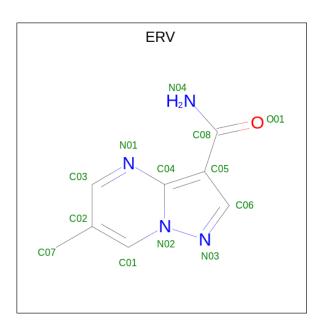
• Molecule 1 is a protein called Poly [ADP-ribose] polymerase 1, processed C-terminus.

Chain	Residue	Modelled	Actual	Comment	Reference
А	658	GLY	-	expression tag	UNP P09874
А	659	PRO	-	expression tag	UNP P09874
А	660	MET	-	expression tag	UNP P09874
А	661	THR	-	expression tag	UNP P09874
А	762	ALA	VAL	variant	UNP P09874
В	658	GLY	-	expression tag	UNP P09874
В	659	PRO	-	expression tag	UNP P09874
В	660	MET	-	expression tag	UNP P09874
В	661	THR	-	expression tag	UNP P09874
В	762	ALA	VAL	variant	UNP P09874

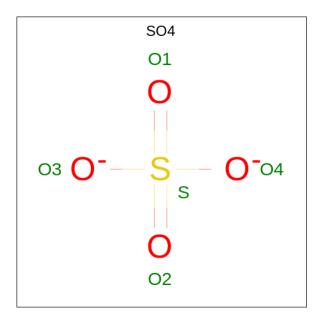
There are 10 discrepancies between the modelled and reference sequences:

• Molecule 2 is 6-methylpyrazolo[1,5-a]pyrimidine-3-carboxamide (three-letter code: ERV) (formula:  $C_8H_8N_4O$ ) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	Total         C         N         O           13         8         4         1	0	0
2	В	1	Total         C         N         O           13         8         4         1	0	0



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
3	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0

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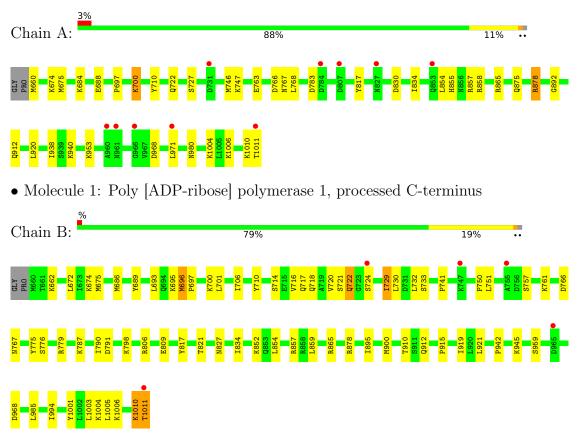
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
3	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
3	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	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: Poly [ADP-ribose] polymerase 1, processed C-terminus





## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	48.52Å 91.81Å 162.94Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	44.19 – 2.84	Depositor
Resolution (A)	46.75 - 2.84	EDS
% Data completeness	99.8 (44.19-2.84)	Depositor
(in resolution range)	99.8 (46.75 - 2.84)	EDS
R <sub>merge</sub>	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	$4.89 (at 2.86 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
D D.	0.219 , $0.278$	Depositor
$R, R_{free}$	0.226 , $0.284$	DCC
$R_{free}$ test set	876 reflections $(4.92%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	44.4	Xtriage
Anisotropy	0.126	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.36 , $41.6$	EDS
L-test for twinning <sup>2</sup>	$ \langle L  \rangle = 0.50, \langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	5585	wwPDB-VP
Average B, all atoms $(Å^2)$	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.66% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical 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.



<sup>&</sup>lt;sup>1</sup>Intensities 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: SO4, ERV

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		
	Unam	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	0.24	0/2819	0.46	0/3803	
1	В	0.24	0/2819	0.45	0/3803	
All	All	0.24	0/5638	0.45	0/7606	

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	А	2767	0	2807	19	0
1	В	2767	0	2807	37	0
2	А	13	0	0	0	0
2	В	13	0	0	0	0
3	А	15	0	0	1	0
3	В	10	0	0	0	0
All	All	5585	0	5614	55	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 5.

All (55) close contacts within the same asymmetric unit are listed below, sorted by their clash



magnitude.

Atom-1	Atom-2	Interatomic	Clash
Atom-1	At0111-2	distance (Å)	overlap (Å)
1:B:674:LYS:HG3	1:B:790:ILE:HD11	1.72	0.72
1:B:730:LEU:HA	1:B:751:LEU:HD21	1.76	0.67
1:B:689:TYR:OH	1:B:767:ASN:ND2	2.29	0.65
1:B:809:GLU:N	1:B:809:GLU:OE2	2.31	0.62
1:A:675:MET:HE1	1:A:1004:LYS:HD2	1.84	0.60
1:B:834:ILE:HD11	1:B:1006:LYS:HB2	1.83	0.59
1:B:701:LEU:HD22	1:B:706:ILE:HD11	1.86	0.57
1:A:834:ILE:HD11	1:A:1006:LYS:HB2	1.88	0.55
1:B:912:GLN:HE22	1:B:1011:THR:HG22	1.72	0.55
1:A:697:PRO:HG2	1:A:700:LYS:HE2	1.90	0.54
1:A:684:LYS:O	1:A:688:GLU:HG2	2.10	0.52
1:B:859:LEU:HG	1:B:921:LEU:HD22	1.92	0.51
1:A:858:ARG:NH2	3:A:1103:SO4:S	2.84	0.51
1:B:919:ILE:HG22	1:B:1003:LEU:HB2	1.93	0.51
1:B:686:MET:HB3	1:B:693:LEU:HD11	1.93	0.50
1:B:821:THR:HB	1:B:900:MET:HA	1.93	0.50
1:B:697:PRO:HD2	1:B:700:LYS:HG3	1.93	0.50
1:A:875:GLN:HB2	1:A:878:ARG:HD2	1.94	0.49
1:A:854:LEU:HD12	1:A:855:HIS:H	1.79	0.48
1:A:674:LYS:HB3	1:A:674:LYS:HE2	1.67	0.48
1:B:710:TYR:OH	1:B:766:ASP:OD1	2.30	0.48
1:A:767:ASN:HD22	1:A:865:ARG:HE	1.60	0.47
1:A:722:GLN:HG2	1:B:985:LEU:HG	1.96	0.47
1:B:761:LYS:HD3	1:B:761:LYS:HA	1.75	0.47
1:B:716:VAL:HG22	1:B:732:LEU:HB3	1.97	0.47
1:A:854:LEU:HD12	1:A:855:HIS:N	2.29	0.47
1:B:675:MET:HE1	1:B:1004:LYS:HD2	1.95	0.47
1:B:716:VAL:O	1:B:720:VAL:HG23	2.16	0.46
1:B:942:PRO:HG2	1:B:945:LYS:HG3	1.97	0.46
1:B:714:SER:O	1:B:717:GLN:HG2	2.15	0.45
1:B:895:ILE:HD11	1:B:994:ILE:HG22	1.98	0.45
1:A:854:LEU:O	1:A:857:ARG:HD3	2.16	0.45
1:B:695:LYS:HE2	1:B:695:LYS:HB3	1.69	0.44
1:B:775:TYR:CZ	1:B:779:ARG:HG3	2.52	0.44
1:B:910:THR:HG23	1:B:915:PRO:HA	1.99	0.44
1:B:809:GLU:H	1:B:809:GLU:CD	2.16	0.43
1:B:854:LEU:O	1:B:857:ARG:HD3	2.19	0.43
1:B:672:LEU:HA	1:B:675:MET:HE3	2.01	0.43
1:B:696:MET:HE1	1:B:701:LEU:HG	2.01	0.43
1:B:787:LYS:HE2	1:B:787:LYS:HB3	1.82	0.43
1:A:920:LEU:HD23	1:A:920:LEU:HA	1.93	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:696:MET:HG2	1:B:741:PRO:HD2	2.02	0.42
1:B:767:ASN:ND2	1:B:865:ARG:HD2	2.34	0.42
1:B:798:LYS:HB2	1:B:798:LYS:HE2	1.73	0.42
1:A:697:PRO:CG	1:A:700:LYS:HE2	2.49	0.42
1:B:729:ILE:HD13	1:B:729:ILE:HA	1.76	0.41
1:B:827:ASN:O	1:B:1010:LYS:HE3	2.21	0.41
1:B:921:LEU:HB2	1:B:1001:TYR:HB2	2.02	0.41
1:B:718:GLN:O	1:B:722:GLN:HG2	2.21	0.41
1:A:710:TYR:OH	1:A:766:ASP:OD1	2.26	0.41
1:A:892:GLY:HA3	1:A:938:ILE:O	2.20	0.41
1:A:768:LEU:HD23	1:A:768:LEU:HA	1.95	0.40
1:A:1010:LYS:HG3	1:A:1011:THR:HG22	2.03	0.40
1:B:696:MET:CG	1:B:741:PRO:HD2	2.51	0.40
1:A:953:LYS:HB2	1:A:953:LYS:HE2	1.77	0.40

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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	Percent	iles
1	А	350/354~(99%)	341 (97%)	9~(3%)	0	100 1	00
1	В	350/354~(99%)	343 (98%)	5 (1%)	2(1%)	25 4	6
All	All	700/708~(99%)	684 (98%)	14~(2%)	2~(0%)	41 6	1

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	В	750	PRO
1	В	722	GLN



#### 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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric Outliers		Percentiles		
1	А	309/310~(100%)	294~(95%)	15~(5%)	25 47		
1	В	309/310~(100%)	291~(94%)	18 (6%)	20 38		
All	All	618/620~(100%)	585~(95%)	33 (5%)	22 43		

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	660	MET
1	А	700	LYS
1	A	727	SER
1	A	746	MET
1	А	747	LYS
1	A	763	GLU
1	А	783	ASP
1	А	817	TYR
1	A A	830	ASP
1	А	878	ARG
1	А	912	GLN
1	А	940	LYS
1	А	968	ASP
1	А	971	LEU
1	А	980	ASN
1	В	662	LYS
1	В	696	MET
1	В	721	SER
1	В	724	SER
1	В	729	ILE
1	В	733	SER
1	В	757	SER
1	В	776	SER
1	В	791	ASP
1	В	806	ARG
1	В	817	TYR
1	В	852	LYS

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Mol	Chain	Res	Type
1	В	878	ARG
1	В	959	SER
1	В	968	ASP
1	В	1005	LEU
1	В	1010	LYS
1	В	1011	THR

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such side chains are listed below:

Mol	Chain	Res	Type
1	А	694	GLN
1	В	767	ASN
1	В	928	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)

7 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	ol Type Chain Res		Link	Bond lengths			Bond angles			
10101	Iol Type Chain	Unam	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
2	ERV	А	1101	-	$9,\!14,\!14$	1.04	0	10,20,20	0.81	0
2	ERV	В	1101	-	$9,\!14,\!14$	1.05	0	10,20,20	0.80	0
3	SO4	А	1104	-	$4,\!4,\!4$	0.14	0	$6,\!6,\!6$	0.06	0
3	SO4	В	1102	-	$4,\!4,\!4$	0.14	0	$6,\!6,\!6$	0.05	0
3	SO4	А	1103	-	$4,\!4,\!4$	0.14	0	$6,\!6,\!6$	0.05	0
3	SO4	В	1103	-	$4,\!4,\!4$	0.14	0	$6,\!6,\!6$	0.05	0
3	SO4	А	1102	-	$4,\!4,\!4$	0.14	0	$6,\!6,\!6$	0.05	0

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	ERV	В	1101	-	-	0/1/4/4	0/2/2/2
2	ERV	А	1101	-	-	0/1/4/4	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

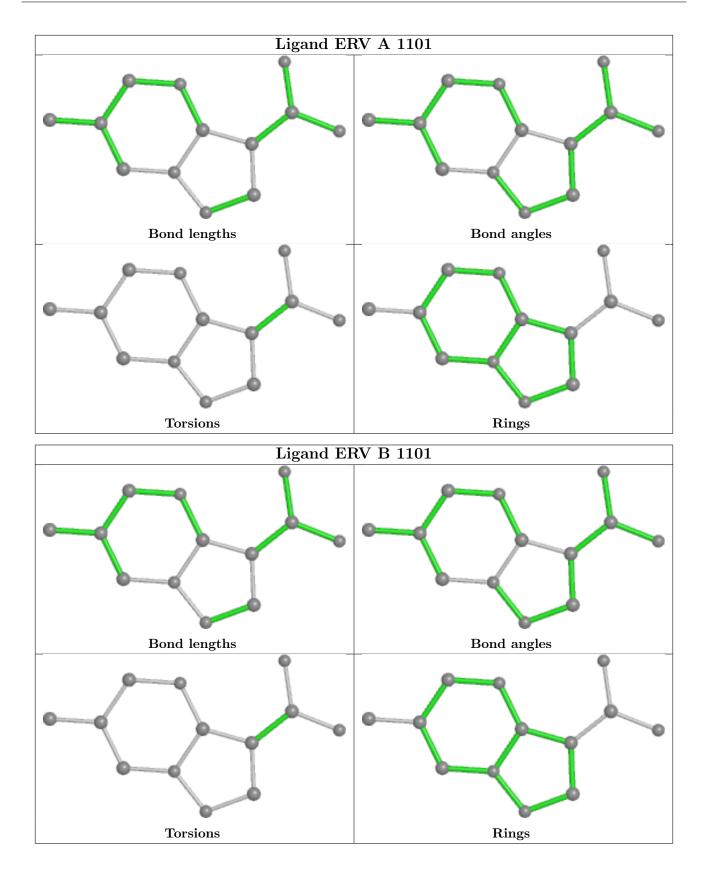
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	$\mathbf{Res}$	Type	Clashes	Symm-Clashes
3	А	1103	SO4	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 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	$\langle RSRZ \rangle$	# RSRZ > 2	$OWAB(Å^2)$	Q<0.9
1	А	352/354~(99%)	0.24	10 (2%) 53 47	25, 41, 62, 83	0
1	В	352/354~(99%)	0.11	5 (1%) 75 71	21, 35, 66, 104	0
All	All	704/708~(99%)	0.17	15 (2%) 63 58	21, 39, 63, 104	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	1011	THR	7.9
1	А	960	ALA	3.1
1	В	1011	THR	3.1
1	А	784	ASP	2.9
1	А	966	GLY	2.7
1	А	971	LEU	2.6
1	В	724	SER	2.6
1	В	755	ALA	2.5
1	А	853	GLN	2.5
1	А	827	ASN	2.4
1	В	965	ASP	2.2
1	А	807	ASP	2.2
1	А	731	ASP	2.2
1	В	747	LYS	2.1
1	А	961	ASN	2.0

## 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.

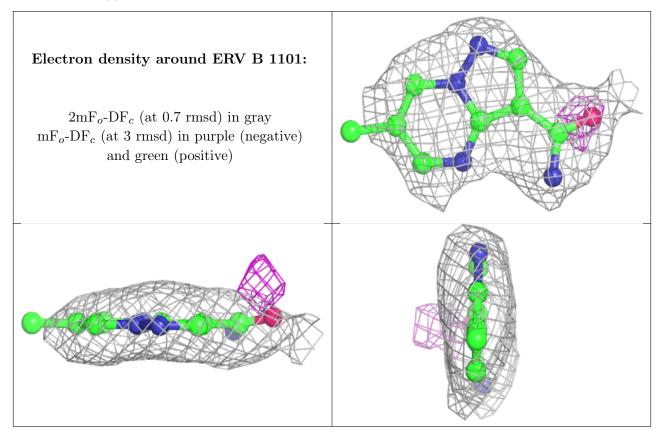


## 6.4 Ligands (i)

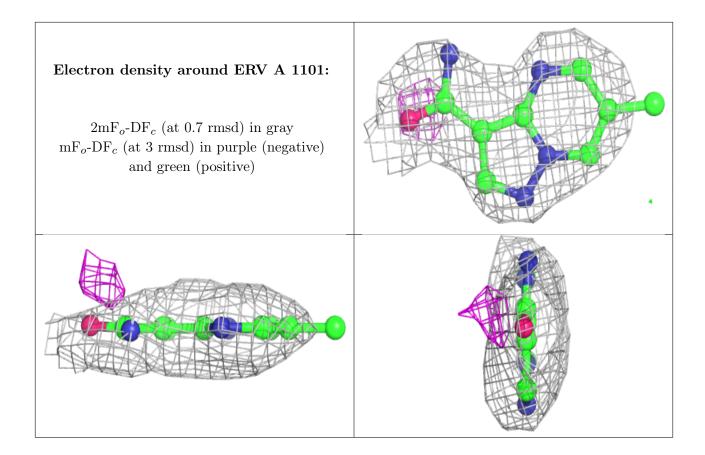
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median,  $95^{th}$  percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	SO4	А	1104	5/5	0.91	0.25	$55,\!57,\!64,\!75$	0
3	SO4	В	1103	5/5	0.91	0.32	59,69,80,86	0
3	SO4	А	1103	5/5	0.93	0.27	65,74,79,91	0
2	ERV	В	1101	13/13	0.94	0.21	22,32,37,39	0
2	ERV	А	1101	13/13	0.95	0.26	32,35,41,42	0
3	SO4	В	1102	5/5	0.97	0.16	35,36,40,41	0
3	SO4	А	1102	5/5	0.98	0.16	47,48,51,53	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.

