

Full wwPDB X-ray Structure Validation Report (i)

Nov 6, 2023 – 02:21 PM EST

PDB ID : 8S98

Title : Crystal structure of the TYK2 pseudokinase domain in complex with com-

pound 8

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Deposited on : 2023-03-27

Resolution : 1.87 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 : 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13

EDS : 2.36

buster-report : 1.1.7 (2018)

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

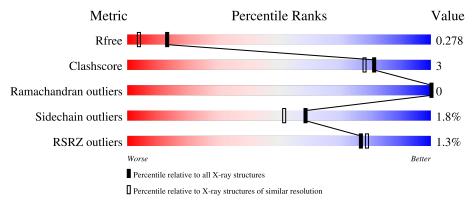
Refmac : 5.8.0158

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 1.87 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	$\begin{array}{c} \text{Whole archive} \\ (\#\text{Entries}) \end{array}$	$egin{aligned} ext{Similar resolution} \ (\# ext{Entries, resolution range}(ext{Å})) \end{aligned}$		
R_{free}	130704	9470 (1.90-1.86)		
Clashscore	141614	10282 (1.90-1.86)		
Ramachandran outliers	138981	10152 (1.90-1.86)		
Sidechain outliers	138945	10152 (1.90-1.86)		
RSRZ outliers	127900	9303 (1.90-1.86)		

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	295	80%	6%	13%
1	В	295	82%	5%	12%

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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



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Mol	Chain	Length	Quality of chain		
1	С	295	80%	8%	12%



2 Entry composition (i)

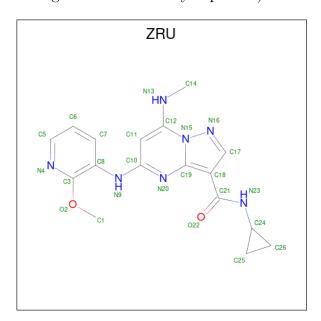
There are 3 unique types of molecules in this entry. The entry contains 6885 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Non-receptor tyrosine-protein kinase TYK2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	۸	256	Total	С	N	О	S	0	1	0
1	A	250	2025	1283	363	369	10	0		
1	В	259	Total	С	N	О	S	0	5	0
1	Б	259	2081	1315	376	379	11	0		
1	С	261	Total	С	N	О	S	0	5	0
1		201	2075	1316	370	378	11	U		

• Molecule 2 is (8S)-N-cyclopropyl-5-[(2-methoxypyridin-3-yl)amino]-7-(methylamino)pyrazol o[1,5-a]pyrimidine-3-carboxamide (three-letter code: ZRU) (formula: $C_{17}H_{19}N_7O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 26			0	0
2	В	1	Total 26	C 17		0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	С	1	Total 26	C 17	N 7	O 2	0	0

• Molecule 3 is water.

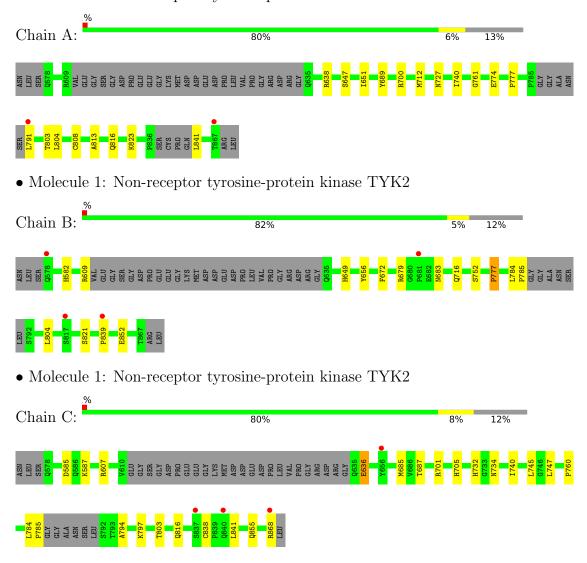
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	199	Total O 199 199	0	0
3	В	221	Total O 222 222	0	1
3	С	205	Total O 205 205	0	0



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: Non-receptor tyrosine-protein kinase TYK2





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	48.11Å 112.60Å 156.86Å	Donositon
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.47 - 1.87	Depositor
Resolution (A)	47.42 - 1.87	EDS
% Data completeness	95.2 (47.47-1.87)	Depositor
(in resolution range)	95.2 (47.42-1.87)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$< I/\sigma(I) > 1$	2.31 (at 1.87Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
D D	0.225 , 0.274	Depositor
R, R_{free}	0.230 , 0.278	DCC
R_{free} test set	2213 reflections (3.25%)	wwPDB-VP
Wilson B-factor (Å ²)	18.7	Xtriage
Anisotropy	0.753	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.35, 43.0	EDS
L-test for twinning ²	$ < L > = 0.49, < L^2> = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6885	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 14.61% 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.



 $^{^1 {\}rm Intensities}$ 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: CSO, ZRU

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	Clasia.	Boı	nd lengths	Bond angles		
Mol Chain		RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.80	2/2062~(0.1%)	0.95	1/2795 (0.0%)	
1	В	0.78	0/2121	0.94	$1/2876 \ (0.0\%)$	
1	С	0.83	1/2114 (0.0%)	0.93	0/2868	
All	All	0.81	$3/6297 \ (0.0\%)$	0.94	2/8539 (0.0%)	

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\text{\AA})$	Ideal(Å)
1	С	636	GLU	CD-OE1	-7.89	1.17	1.25
1	A	774	GLU	CD-OE1	-6.38	1.18	1.25
1	A	761	GLY	C-O	5.54	1.32	1.23

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
1	A	700	ARG	NE-CZ-NH1	6.23	123.42	120.30
1	В	777	PRO	N-CA-CB	-5.86	96.15	102.60

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	2025	0	2004	13	0
1	В	2081	0	2051	7	0
1	С	2075	0	2041	14	0
2	A	26	0	0	0	0
2	В	26	0	0	0	0
2	С	26	0	0	0	0
3	A	199	0	0	3	0
3	В	222	0	0	3	0
3	С	205	0	0	3	0
All	All	6885	0	6096	32	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 (32) 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:C:855[A]:GLN:OE1	3:C:1001:HOH:O	1.55	1.23
1:B:716[B]:GLN:NE2	3:B:1001:HOH:O	1.72	1.17
1:A:791:LEU:N	3:A:1001:HOH:O	2.25	0.70
1:C:816:GLN:HG3	3:C:1193:HOH:O	1.96	0.66
1:C:732:HIS:CE1	1:C:760:PRO:HB3	2.36	0.60
1:C:585:ASP:OD1	1:C:587:LYS:HG2	2.03	0.57
1:A:816:GLN:HE22	1:A:823:LYS:NZ	2.04	0.55
1:A:712:MET:CE	1:A:841:LEU:HD11	2.38	0.54
1:A:816:GLN:HG3	3:A:1162:HOH:O	2.08	0.53
1:A:712:MET:HE1	1:A:841:LEU:HD11	1.92	0.52
1:C:607:ARG:HB3	1:C:636:GLU:HG3	1.90	0.52
1:B:609:ARG:HG3	1:B:609:ARG:HH11	1.76	0.51
1:A:816:GLN:NE2	1:A:816:GLN:HA	2.26	0.50
1:A:808:CSO:SG	1:A:841:LEU:HD12	2.52	0.50
1:C:685:MET:HG2	1:C:687:THR:CG2	2.42	0.49
1:C:784:LEU:HB3	1:C:785:PRO:HD3	1.95	0.47
1:A:638:ARG:HD3	1:A:689:TYR:CE1	2.50	0.47
1:B:784:LEU:HB3	1:B:785:PRO:HD3	1.97	0.46
1:B:672:PHE:CE1	1:C:701:ARG:CZ	3.00	0.45
1:A:816:GLN:HE22	1:A:823:LYS:HZ3	1.62	0.45
1:C:838:CYS:HB3	3:C:1174:HOH:O	2.17	0.44
1:C:794:ALA:HA	1:C:797:LYS:HD2	1.99	0.44
3:B:1078:HOH:O	1:C:745:LEU:HD21	2.18	0.43
1:B:582[B]:HIS:CD2	1:C:705:HIS:NE2	2.87	0.42
1:A:740[A]:ILE:HD11	1:A:803:THR:HG21	2.01	0.42

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COHABABACA		DIEUIUU	DUIUE
0 0 1000100000			

Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	${\rm distance}({\rm \AA})$	overlap (Å)
1:B:656:TYR:OH	1:B:683:ASN:ND2	2.51	0.42
1:A:727:ASN:ND2	3:A:1013:HOH:O	2.53	0.41
1:C:747:LEU:HD23	1:C:747:LEU:HA	1.91	0.41
1:C:740:ILE:HD11	1:C:803:THR:HG21	2.01	0.41
1:A:647:SER:HB3	1:A:651:ILE:HB	2.03	0.41
1:A:813:ALA:HB3	1:A:816:GLN:HG2	2.03	0.40
1:B:852:GLU:N	3:B:1006:HOH:O	2.39	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	Perce	ntiles
1	A	248/295~(84%)	243 (98%)	5 (2%)	0	100	100
1	В	257/295~(87%)	249 (97%)	8 (3%)	0	100	100
1	С	259/295 (88%)	252 (97%)	7 (3%)	0	100	100
All	All	764/885 (86%)	744 (97%)	20 (3%)	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	ed Rotameric Outliers		Percentiles		
1	A	218/253~(86%)	216 (99%)	2 (1%)	78 76		
1	В	224/253 (88%)	217 (97%)	7 (3%)	40 29		
1	С	221/253 (87%)	218 (99%)	3 (1%)	67 62		
All	All	663/759 (87%)	651 (98%)	12 (2%)	59 52		

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	777	PRO
1	A	804	LEU
1	В	649	HIS
1	В	679	ARG
1	В	752	SER
1	В	777	PRO
1	В	804	LEU
1	В	821	SER
1	В	839	PRO
1	С	734	ASN
1	С	841	LEU
1	С	868	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	597	GLN
1	A	602	ASN
1	A	664	GLN
1	A	727	ASN
1	A	734	ASN
1	A	816	GLN
1	A	855	GLN
1	В	597	GLN
1	В	664	GLN
1	В	683	ASN
1	В	734	ASN
1	В	830	GLN
1	С	602	ASN
1	С	727	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)

3 non-standard protein/DNA/RNA residues 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		Be	ond leng	gths	В	ond ang	gles
MIOI	туре	Chain	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CSO	A	808	1	3,6,7	0.74	0	0,6,8	-	-
1	CSO	С	808	1	3,6,7	0.71	0	0,6,8	-	-
1	CSO	В	808	1	3,6,7	0.71	0	0,6,8	-	-

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
1	CSO	A	808	1	-	0/1/5/7	-
1	CSO	С	808	1	-	0/1/5/7	-
1	CSO	В	808	1	-	0/1/5/7	-

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	Res	Type	Clashes	Symm-Clashes
1	A	808	CSO	1	0



5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

3 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	Bond lengths			Bond angles			
MIOI	Type	Chain	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
2	ZRU	С	901	-	23,29,29	2.05	4 (17%)	29,41,41	1.72	9 (31%)
2	ZRU	В	901	-	23,29,29	1.97	3 (13%)	29,41,41	1.64	7 (24%)
2	ZRU	A	901	-	23,29,29	1.93	3 (13%)	29,41,41	2.39	8 (27%)

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	ZRU	С	901	-	-	0/14/18/18	0/4/4/4
2	ZRU	В	901	-	-	2/14/18/18	0/4/4/4
2	ZRU	A	901	-	-	2/14/18/18	0/4/4/4

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	$Ideal(\AA)$
2	В	901	ZRU	C18-C21	-7.46	1.37	1.50
2	A	901	ZRU	C18-C21	-7.22	1.38	1.50
2	С	901	ZRU	C18-C21	-7.18	1.38	1.50
2	С	901	ZRU	C14-N13	3.31	1.50	1.45
2	В	901	ZRU	C14-N13	2.90	1.50	1.45
2	С	901	ZRU	C25-C24	2.57	1.54	1.48
2	С	901	ZRU	C5-N4	2.42	1.39	1.34
2	A	901	ZRU	C14-N13	2.34	1.49	1.45

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Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(\mathbf{\mathring{A}})$	$\operatorname{Ideal}(\text{\AA})$
2	В	901	ZRU	C5-N4	2.18	1.39	1.34
2	A	901	ZRU	C5-N4	2.16	1.39	1.34

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$Ideal(^{o})$
2	A	901	ZRU	C26-C24-N23	-5.80	110.29	118.61
2	A	901	ZRU	C14-N13-C12	-5.29	118.18	123.37
2	A	901	ZRU	C10-N20-C19	4.79	121.95	117.59
2	A	901	ZRU	C25-C24-N23	-4.55	112.08	118.61
2	В	901	ZRU	C25-C24-N23	-4.24	112.53	118.61
2	С	901	ZRU	C10-N20-C19	3.52	120.79	117.59
2	С	901	ZRU	C25-C24-N23	-3.47	113.63	118.61
2	С	901	ZRU	C26-C24-N23	-3.46	113.64	118.61
2	A	901	ZRU	C1-O2-C3	3.35	120.54	117.21
2	В	901	ZRU	C14-N13-C12	-3.05	120.38	123.37
2	С	901	ZRU	C11-C10-N20	-2.91	118.58	123.91
2	A	901	ZRU	C11-C10-N20	-2.82	118.75	123.91
2	В	901	ZRU	C26-C24-N23	-2.79	114.61	118.61
2	A	901	ZRU	C8-C3-N4	-2.66	121.46	124.61
2	В	901	ZRU	C11-C10-N20	-2.66	119.04	123.91
2	A	901	ZRU	C26-C25-C24	-2.36	57.85	59.84
2	В	901	ZRU	C8-C3-N4	-2.30	121.90	124.61
2	С	901	ZRU	C8-C3-N4	-2.29	121.90	124.61
2	С	901	ZRU	C7-C8-C3	2.27	119.06	116.80
2	В	901	ZRU	C10-N20-C19	2.26	119.64	117.59
2	В	901	ZRU	C7-C8-C3	2.20	119.00	116.80
2	С	901	ZRU	C12-C11-C10	2.09	119.98	118.43
2	С	901	ZRU	C1-O2-C3	-2.02	115.21	117.21
2	С	901	ZRU	C14-N13-C12	-2.01	121.40	123.37

There are no chirality outliers.

All (4) torsion outliers are listed below:

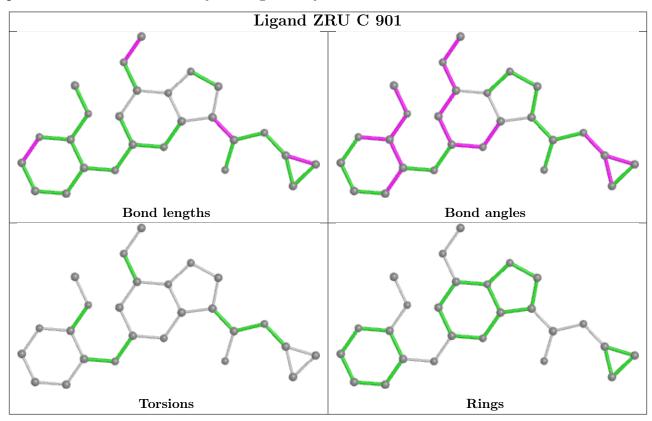
Mol	Chain	Res	Type	Atoms
2	A	901	ZRU	C11-C12-N13-C14
2	A	901	ZRU	N15-C12-N13-C14
2	В	901	ZRU	C8-C3-O2-C1
2	В	901	ZRU	N4-C3-O2-C1

There are no ring outliers.

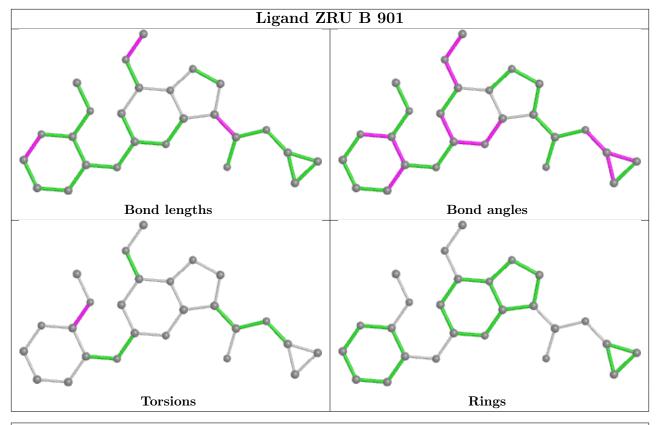


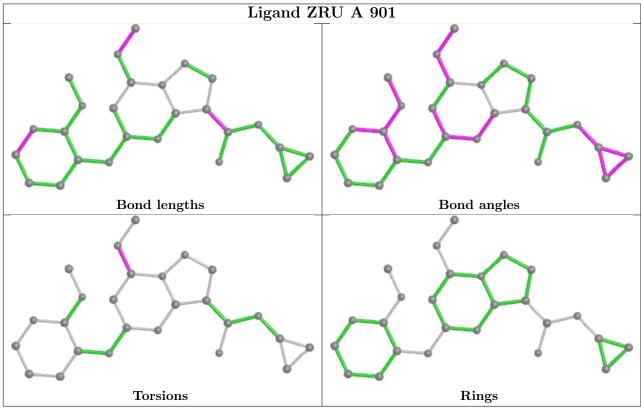
No monomer is involved in short contacts.

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 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)

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>	# RSRZ > 2	$OWAB(Å^2)$	Q<0.9
1	A	$255/295\ (86\%)$	0.12	2 (0%) 86 87	13, 21, 38, 49	0
1	В	258/295 (87%)	0.21	4 (1%) 72 74	12, 22, 38, 48	0
1	С	260/295 (88%)	0.11	4 (1%) 73 75	13, 22, 37, 60	0
All	All	773/885 (87%)	0.14	10 (1%) 77 79	12, 21, 38, 60	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	817	SER	4.0
1	В	681	PRO	3.5
1	В	578	GLN	3.4
1	С	837	SER	3.3
1	A	791	LEU	3.3
1	С	868	ARG	2.6
1	С	840	GLN	2.5
1	С	656	TYR	2.5
1	A	867	THR	2.3
1	В	839	PRO	2.1

6.2 Non-standard residues in protein, DNA, RNA chains (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
1	CSO	A	808	7/8	0.82	0.13	21,24,28,28	0
1	CSO	В	808	7/8	0.90	0.12	23,26,29,29	0
1	CSO	С	808	7/8	0.92	0.10	22,25,26,27	0



6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

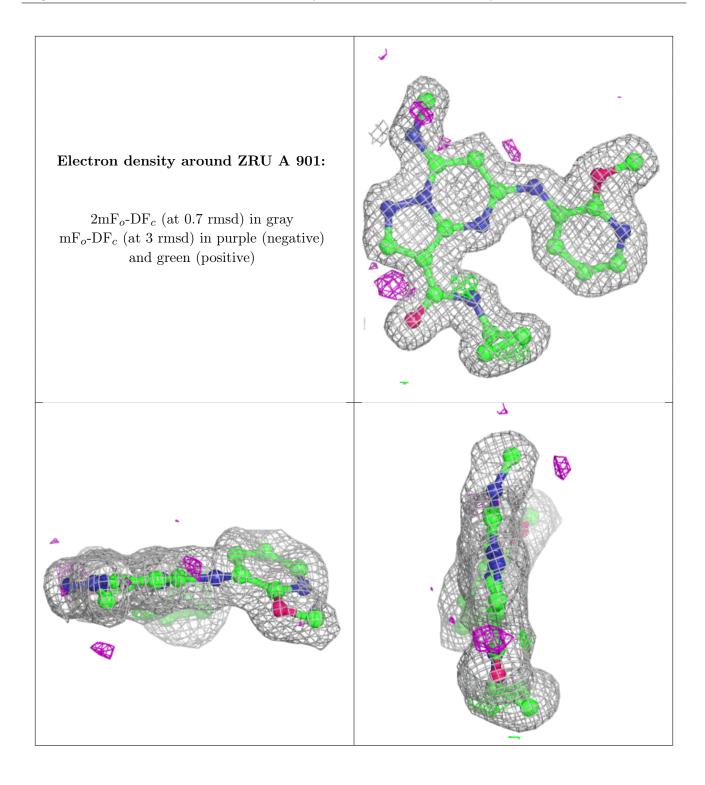
6.4 Ligands (i)

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
2	ZRU	A	901	26/26	0.92	0.11	12,14,15,15	0
2	ZRU	В	901	26/26	0.93	0.11	12,13,17,17	0
2	ZRU	С	901	26/26	0.93	0.10	12,15,17,17	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.

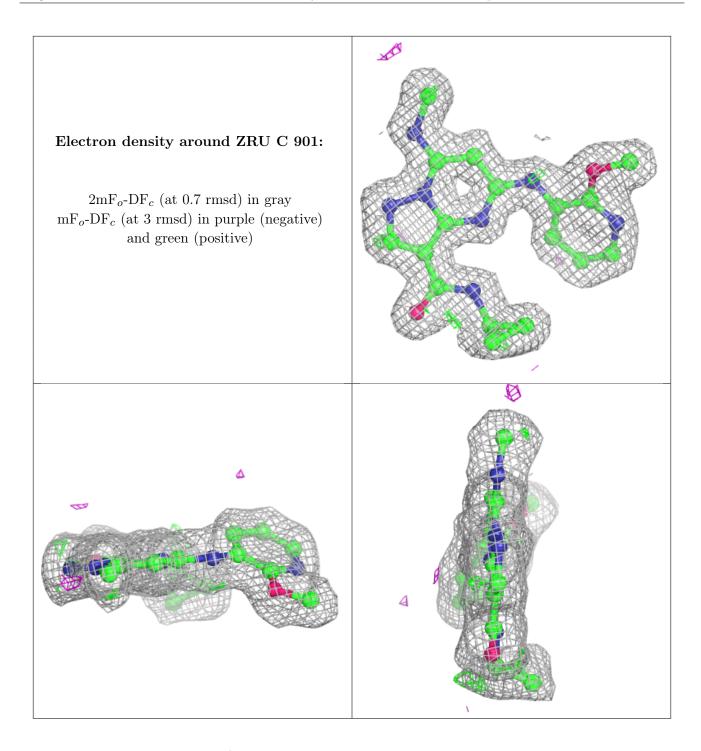






Electron density around ZRU B 901: $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray $\mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)





6.5 Other polymers (i)

There are no such residues in this entry.

