



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 6, 2021 – 07:05 pm GMT

PDB ID : 7AAC  
Title : Crystal structure of the catalytic domain of human PARP1 in complex with veliparib  
Authors : Schimpl, M.; Ogden, T.E.H.; Yang, J.-C.; Easton, L.E.; Underwood, E.; Rawlins, P.B.; Johannes, J.W.; Embrey, K.J.; Neuhaus, D.  
Deposited on : 2020-09-04  
Resolution : 1.59 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](mailto: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 ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) 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 : 2.16  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
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) : 2.16

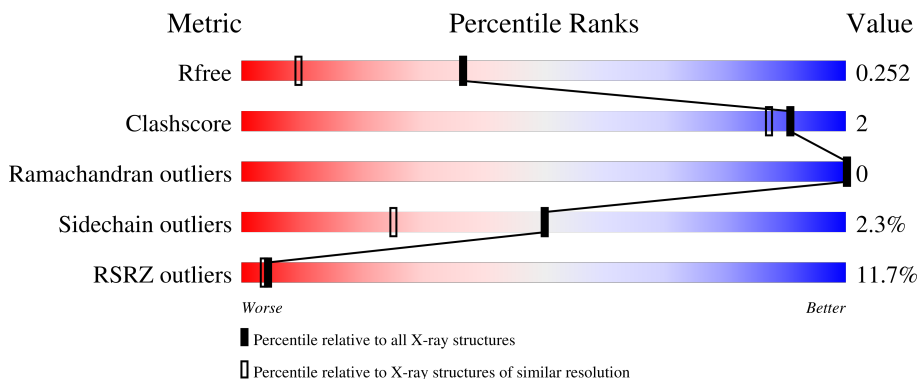
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.59 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 (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	352	 7% 93% 5% ..
1	B	352	 16% 94% 5% .

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6013 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.

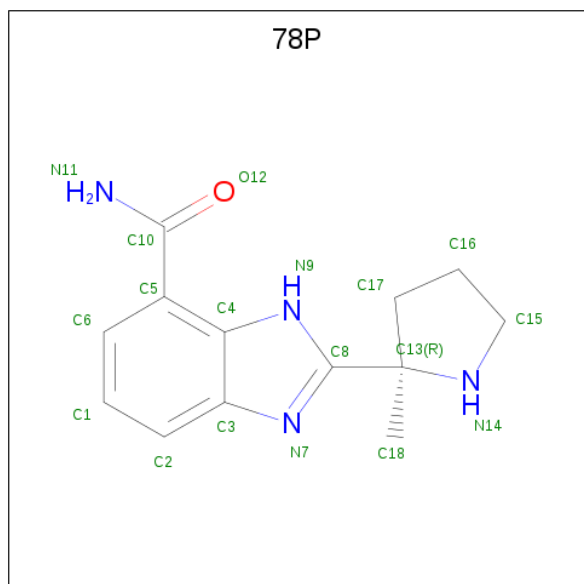
- Molecule 1 is a protein called Poly [ADP-ribose] polymerase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	350	Total 2740	C 1744	N 462	O 522	S 12	0	1	0
1	B	350	Total 2745	C 1748	N 463	O 522	S 12	0	1	0

There are 6 discrepancies between the modelled and reference sequences:

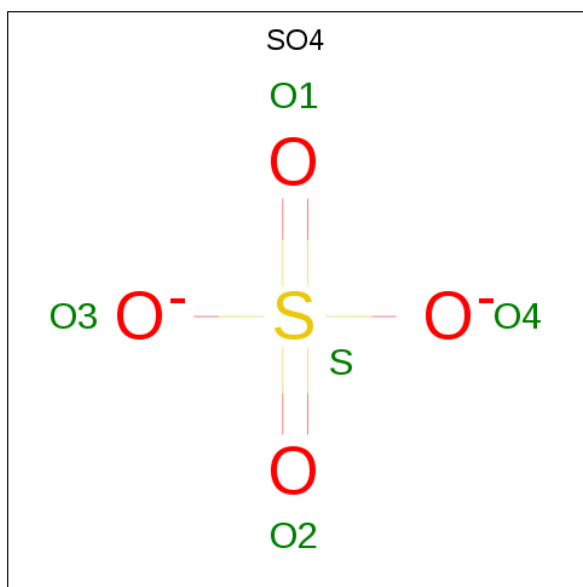
Chain	Residue	Modelled	Actual	Comment	Reference
A	660	GLY	-	expression tag	UNP P09874
A	661	SER	-	expression tag	UNP P09874
A	762	ALA	VAL	engineered mutation	UNP P09874
B	660	GLY	-	expression tag	UNP P09874
B	661	SER	-	expression tag	UNP P09874
B	762	ALA	VAL	engineered mutation	UNP P09874

- Molecule 2 is (2R)-2-(7-carbamoyl-1H-benzimidazol-2-yl)-2-methylpyrrolidinium (three-letter code: 78P) (formula: C<sub>13</sub>H<sub>16</sub>N<sub>4</sub>O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			18	13	4	1		
2	B	1	Total	C	N	O	0	0
			18	13	4	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

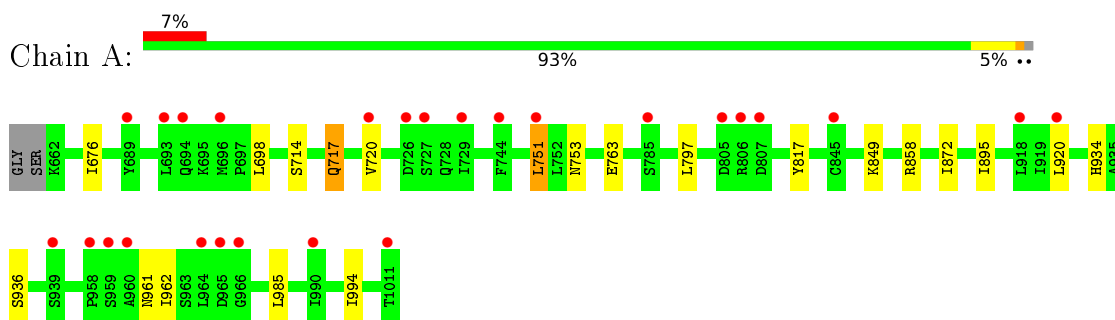
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	275	Total	O	0	0
			275	275		
4	B	207	Total	O	0	0
			207	207		

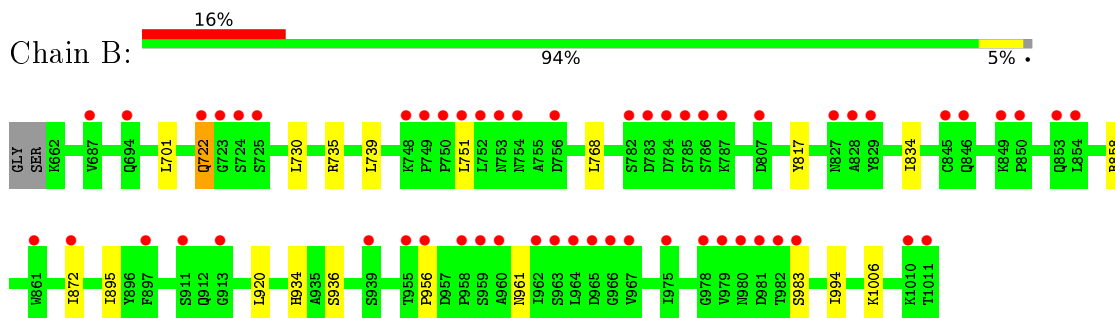
### 3 Residue-property plots [i](#)

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



- Molecule 1: Poly [ADP-ribose] polymerase 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	48.22Å 91.63Å 162.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.80 – 1.59 31.01 – 1.59	Depositor EDS
% Data completeness (in resolution range)	68.6 (31.80-1.59) 69.0 (31.01-1.59)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.12 (at 1.59Å)	Xtrriage
Refinement program	BUSTER 2.11.6	Depositor
R, $R_{free}$	0.210 , 0.242 0.220 , 0.252	Depositor DCC
$R_{free}$ test set	3298 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	16.2	Xtrriage
Anisotropy	0.138	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 43.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6013	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.67% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<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.

## 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: 78P, 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	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.50	0/2795	0.61	0/3775
1	B	0.49	0/2800	0.62	0/3780
All	All	0.50	0/5595	0.61	0/7555

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	2740	0	2768	10	0
1	B	2745	0	2781	9	0
2	A	18	0	16	1	0
2	B	18	0	16	1	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	275	0	0	1	0
4	B	207	0	0	2	0
All	All	6013	0	5581	19	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 2.

All (19) 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:763:GLU:HG2	4:A:1359:HOH:O	1.89	0.71
1:A:934:HIS:HD2	4:B:1274:HOH:O	1.79	0.64
1:B:956:PRO:HB3	4:B:1252:HOH:O	2.05	0.55
1:B:834:ILE:HD11	1:B:1006:LYS:HB2	1.88	0.55
1:A:872:ILE:HG21	1:A:920:LEU:HD11	1.91	0.53
2:B:1101:78P:H9	2:B:1101:78P:H111	1.57	0.53
2:A:1101:78P:H111	2:A:1101:78P:H9	1.58	0.52
1:A:895:ILE:HD11	1:A:994:ILE:HG22	1.93	0.51
1:B:895:ILE:HD11	1:B:994:ILE:HG22	1.93	0.50
1:B:934:HIS:CD2	1:B:983:SER:HB3	2.47	0.49
1:A:751:LEU:HD22	1:A:753:ASN:HB3	1.96	0.48
1:B:872:ILE:HG21	1:B:920:LEU:HD11	1.94	0.47
1:A:985:LEU:HD21	1:B:722:GLN:HG3	1.97	0.46
1:B:730:LEU:HD11	1:B:751:LEU:HD21	1.97	0.45
1:A:676:ILE:HD11	1:A:797:LEU:HD11	1.98	0.44
1:B:701:LEU:HD11	1:B:768:LEU:HD22	2.01	0.43
1:A:936:SER:HA	1:B:936:SER:HA	2.02	0.42
1:A:717:GLN:HA	1:A:720:VAL:HG22	2.02	0.41
1:A:714:SER:O	1:A:717:GLN:HG3	2.21	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	Percentiles	
1	A	349/352 (99%)	348 (100%)	1 (0%)	0	100	100
1	B	349/352 (99%)	348 (100%)	1 (0%)	0	100	100
All	All	698/704 (99%)	696 (100%)	2 (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	304/308 (99%)	296 (97%)	8 (3%)	46	21
1	B	305/308 (99%)	299 (98%)	6 (2%)	55	31
All	All	609/616 (99%)	595 (98%)	14 (2%)	50	25

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	698	LEU
1	A	717	GLN
1	A	751	LEU
1	A	817	TYR
1	A	849	LYS
1	A	858	ARG
1	A	961	ASN
1	A	962	ILE
1	B	722	GLN
1	B	735	ARG
1	B	739	LEU
1	B	817	TYR
1	B	858	ARG
1	B	961	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	759	GLN
1	A	906	ASN
1	A	934	HIS
1	A	961	ASN
1	B	722	GLN
1	B	728	GLN
1	B	734	ASN
1	B	759	GLN

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Mol	Chain	Res	Type
1	B	906	ASN
1	B	961	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](#)

4 ligands are modelled in this entry.

There are no bond length outliers.

There are no bond angle outliers.

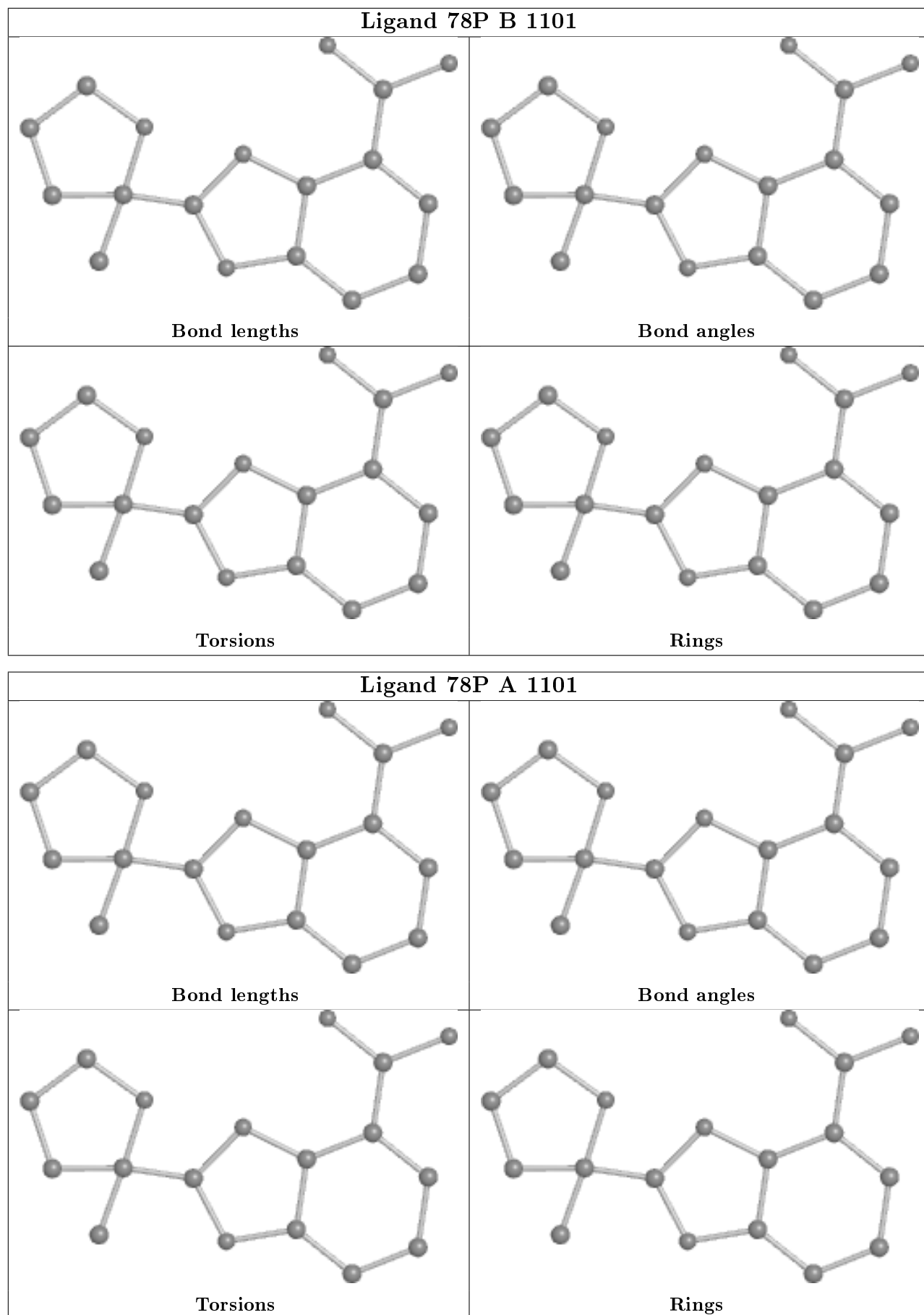
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 than 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

### 6.1 Protein, DNA and RNA chains

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	350/352 (99%)	0.68	26 (7%) 14 13	5, 18, 38, 67	0
1	B	350/352 (99%)	1.06	56 (16%) 1 1	8, 24, 49, 84	0
All	All	700/704 (99%)	0.87	82 (11%) 4 4	5, 21, 47, 84	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1011	THR	9.2
1	A	807	ASP	7.5
1	B	978	GLY	6.5
1	B	966	GLY	6.3
1	B	827	ASN	6.3
1	B	981	ASP	6.2
1	B	854	LEU	5.8
1	B	785	SER	5.4
1	B	979	VAL	5.3
1	B	980	ASN	5.0
1	A	726	ASP	4.9
1	B	958	PRO	4.7
1	B	845	CYS	4.5
1	B	723	GLY	4.5
1	B	853	GLN	4.2
1	B	783	ASP	4.1
1	A	964	LEU	4.0
1	B	724	SER	3.8
1	B	965	ASP	3.7
1	B	1010	LYS	3.7
1	B	784	ASP	3.6
1	B	975	ILE	3.6
1	B	849	LYS	3.6
1	A	751	LEU	3.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	751	LEU	3.5
1	B	846	GLN	3.4
1	A	1011	THR	3.4
1	B	748	LYS	3.4
1	B	959	SER	3.3
1	B	964	LEU	3.2
1	B	756	ASP	3.2
1	B	967	VAL	3.2
1	A	720	VAL	3.1
1	B	960	ALA	3.1
1	A	958	PRO	3.1
1	A	845	CYS	3.0
1	B	962	ILE	2.9
1	B	939	SER	2.9
1	B	850	PRO	2.9
1	A	689	TYR	2.9
1	B	786	SER	2.9
1	A	965	ASP	2.7
1	B	687	VAL	2.6
1	B	913	GLY	2.6
1	B	753	ASN	2.6
1	B	956	PRO	2.6
1	B	787	LYS	2.6
1	A	920	LEU	2.6
1	B	807	ASP	2.5
1	A	939	SER	2.5
1	B	829	TYR	2.5
1	B	982	THR	2.5
1	A	727	SER	2.4
1	B	861	TRP	2.4
1	A	785	SER	2.4
1	B	963	SER	2.4
1	A	918	LEU	2.4
1	A	806	ARG	2.4
1	A	960	ALA	2.4
1	B	694	GLN	2.4
1	A	744	PHE	2.3
1	B	725	SER	2.3
1	B	872	ILE	2.3
1	B	897	PHE	2.2
1	A	693	LEU	2.2
1	A	696	MET	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	694	GLN	2.2
1	A	805	ASP	2.2
1	B	749	PRO	2.2
1	A	966	GLY	2.1
1	A	729	ILE	2.1
1	B	754	ASN	2.1
1	B	782	SER	2.1
1	B	828	ALA	2.1
1	B	750	PRO	2.1
1	B	752	LEU	2.1
1	B	955	THR	2.1
1	B	911	SER	2.1
1	B	722	GLN	2.1
1	A	959	SER	2.0
1	A	990	ILE	2.0
1	B	983	SER	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.

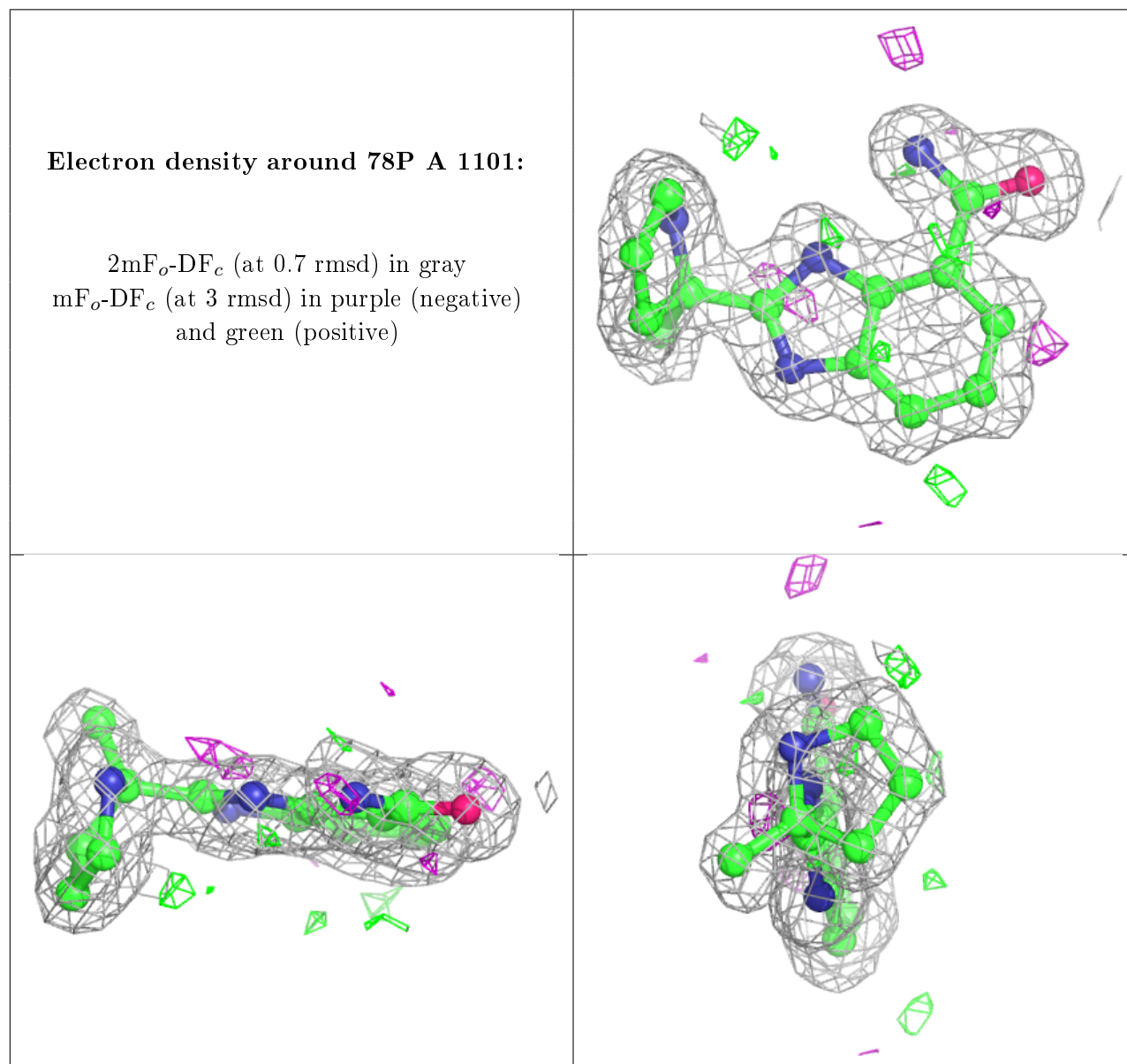
## 6.4 Ligands [i](#)

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<sup>th</sup> 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.

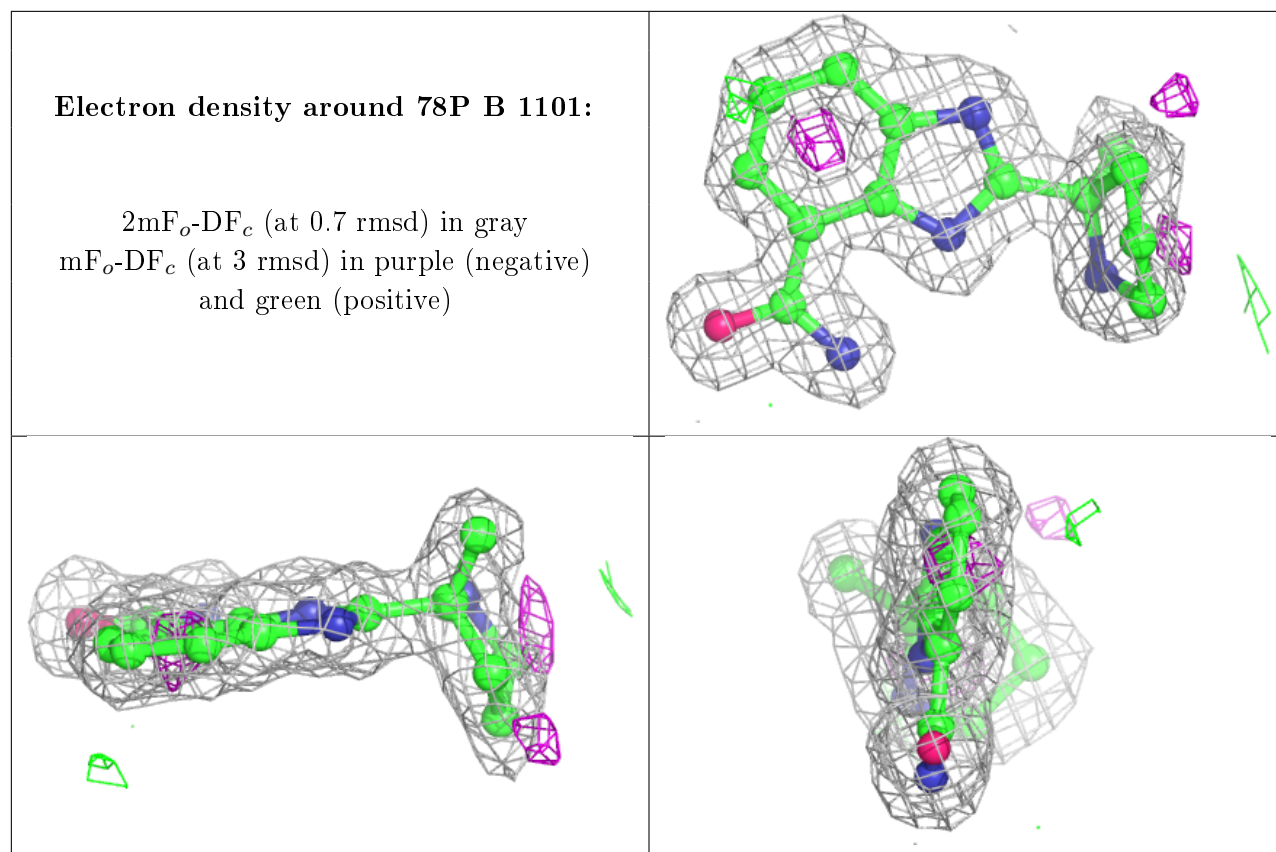
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	78P	A	1101	18/18	0.95	0.11	7,8,17,19	0
2	78P	B	1101	18/18	0.96	0.10	3,9,19,20	0
3	SO4	B	1102	5/5	0.96	0.08	21,27,28,31	0
3	SO4	A	1102	5/5	0.96	0.10	13,19,23,23	0

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.