



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 29, 2024 – 12:49 PM EDT

PDB ID : 4Q9Z  
Title : Human Protein Kinase C Theta in Complex with Compound35 ((1R)-9-(AZE  
TIDIN-3-YLAMINO)-1,8-DIMETHYL-3,5-DIHYDRO[1,2,4]TRIAZINO[3,4-  
C][1,4]BENZOXAZIN-2(1H)-ONE)  
Authors : Argiriadi, M.A.; George, D.M.  
Deposited on : 2014-05-02  
Resolution : 2.60 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

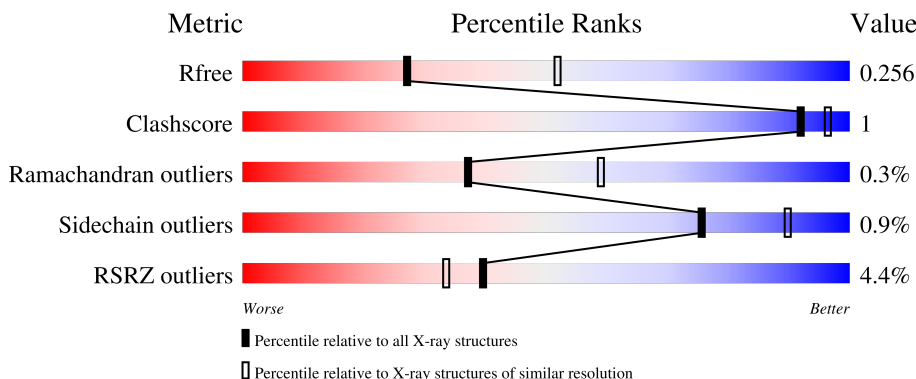
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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))
$R_{free}$	164625	3775 (2.60-2.60)
Clashscore	180529	4181 (2.60-2.60)
Ramachandran outliers	177936	4129 (2.60-2.60)
Sidechain outliers	177891	4129 (2.60-2.60)
RSRZ outliers	164620	3775 (2.60-2.60)

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	334	
1	B	334	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5453 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.

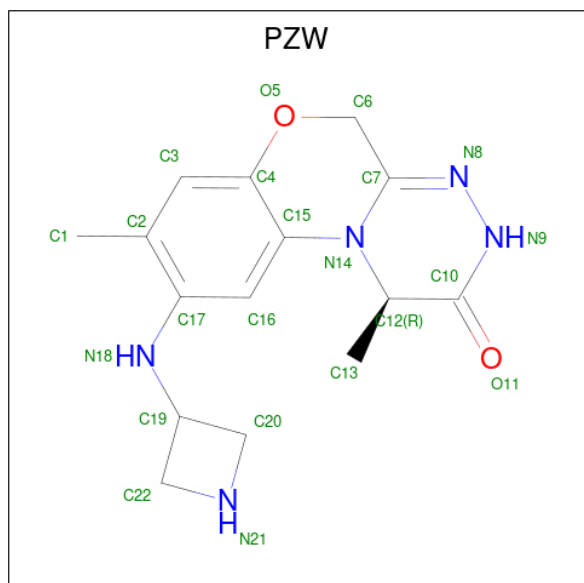
- Molecule 1 is a protein called HUMAN PROTEIN KINASE C THETA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	333	Total	C	N	O	P	S	87	1	0
			2780	1795	463	499	2	21			
1	B	309	Total	C	N	O	P	S	180	0	0
			2572	1668	427	457	1	19			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	381	GLU	ILE	engineered mutation	UNP Q04759
A	538	GLU	THR	engineered mutation	UNP Q04759
A	707	HIS	-	expression tag	UNP Q04759
B	381	GLU	ILE	engineered mutation	UNP Q04759
B	538	GLU	THR	engineered mutation	UNP Q04759
B	707	HIS	-	expression tag	UNP Q04759

- Molecule 2 is (1R)-9-(azetidin-3-ylamino)-1,8-dimethyl-3,5-dihydro[1,2,4]triazino[3,4-c][1,4]benzoxazin-2(1H)-one (three-letter code: PZW) (formula: C<sub>15</sub>H<sub>19</sub>N<sub>5</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			22	15	5	2		
2	B	1	Total	C	N	O	0	0
			22	15	5	2		

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	50	Total	O	0	0
			50	50		
4	B	6	Total	O	0	0
			6	6		

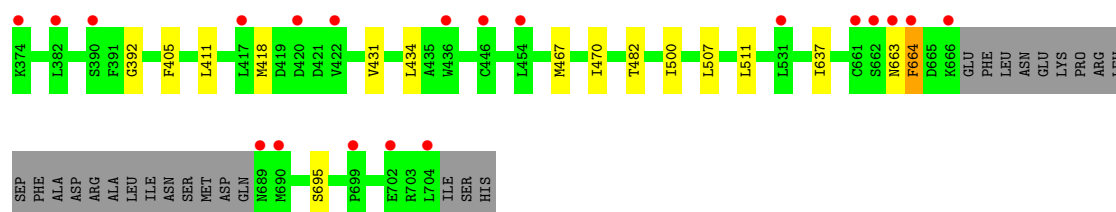
### 3 Residue-property plots [i](#)

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: HUMAN PROTEIN KINASE C THETA



- Molecule 1: HUMAN PROTEIN KINASE C THETA



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	76.95Å 78.58Å 146.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	73.48 – 2.60 73.48 – 2.60	Depositor EDS
% Data completeness (in resolution range)	96.2 (73.48-2.60) 96.2 (73.48-2.60)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.52 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.219 , 0.256 0.218 , 0.256	Depositor DCC
$R_{free}$ test set	921 reflections (3.41%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	58.5	Xtriage
Anisotropy	0.433	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 43.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.027 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5453	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.18% 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: PZW, SEP, NA

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	0.44	1/2831 (0.0%)	0.56	0/3802
1	B	0.45	0/2629	0.57	2/3530 (0.1%)
All	All	0.45	1/5460 (0.0%)	0.56	2/7332 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	652	ARG	CG-CD	-6.17	1.36	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	434	LEU	CB-CG-CD1	5.76	120.80	111.00
1	B	418	MET	CG-SD-CE	5.38	108.81	100.20

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	2780	0	2725	10	0
1	B	2572	0	2530	6	0
2	A	22	0	19	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	22	0	19	1	0
3	A	1	0	0	0	0
4	A	50	0	0	0	0
4	B	6	0	0	0	0
All	All	5453	0	5293	15	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 1.

All (15) 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:418[B]:MET:HE2	1:A:418[B]:MET:HA	1.18	1.16
1:A:418[B]:MET:HA	1:A:418[B]:MET:CE	1.89	1.02
1:B:431:VAL:HG22	1:B:500:ILE:HD13	1.78	0.65
1:A:418[B]:MET:CE	1:A:418[B]:MET:CA	2.71	0.64
1:A:417:LEU:HD21	1:B:405:PHE:CE1	2.46	0.51
1:A:507:LEU:HD23	1:A:568:LEU:HD11	1.95	0.48
1:B:511:LEU:HD21	2:B:801:PZW:H20	1.98	0.46
1:B:482:THR:HG22	1:B:637:ILE:HD11	1.97	0.45
1:A:701:MET:HA	1:A:701:MET:HE2	1.99	0.44
1:A:414:ASP:HB2	1:A:682:LEU:HD23	2.00	0.42
1:A:465:ASP:HB3	1:A:511:LEU:HD23	2.00	0.42
1:A:434:LEU:HD22	1:A:500:ILE:HD11	2.01	0.42
1:A:382:LEU:HD22	1:A:395:PHE:CB	2.50	0.41
1:B:392:GLY:HA3	1:B:411:LEU:HD23	2.02	0.41
1:B:467:MET:HE2	1:B:507:LEU:HB2	2.04	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	330/334 (99%)	316 (96%)	14 (4%)	0	100	100
1	B	304/334 (91%)	289 (95%)	13 (4%)	2 (1%)	19	38
All	All	634/668 (95%)	605 (95%)	27 (4%)	2 (0%)	37	59

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	663	ASN
1	B	664	PHE

### 5.3.2 Protein sidechains ⓘ

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	301/301 (100%)	298 (99%)	3 (1%)	73	88
1	B	279/301 (93%)	277 (99%)	2 (1%)	81	93
All	All	580/602 (96%)	575 (99%)	5 (1%)	75	90

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	412	LYS
1	A	429	LYS
1	A	538	GLU
1	B	470	ILE
1	B	664	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	403	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	SEP	A	676	1	8,9,10	1.58	1 (12%)	7,12,14	1.42	1 (14%)
1	SEP	A	695	1	8,9,10	1.61	1 (12%)	7,12,14	1.22	1 (14%)
1	SEP	B	695	1	8,9,10	1.63	1 (12%)	7,12,14	0.81	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
1	SEP	A	676	1	-	0/6/8/10	-
1	SEP	A	695	1	-	0/6/8/10	-
1	SEP	B	695	1	-	0/6/8/10	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	695	SEP	P-O1P	3.57	1.61	1.50
1	A	695	SEP	P-O1P	3.53	1.61	1.50
1	A	676	SEP	P-O1P	3.45	1.61	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	676	SEP	OG-CB-CA	3.24	111.30	108.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	695	SEP	OG-CB-CA	2.72	110.79	108.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

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		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	PZW	A	801	-	21,25,25	1.18	2 (9%)	23,37,37	1.77	3 (13%)
2	PZW	B	801	-	21,25,25	1.28	3 (14%)	23,37,37	1.77	2 (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
2	PZW	A	801	-	-	0/4/36/36	0/4/4/4
2	PZW	B	801	-	-	0/4/36/36	0/4/4/4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	PZW	O5-C4	-2.94	1.34	1.37
2	B	801	PZW	O5-C4	-2.71	1.34	1.37
2	B	801	PZW	C17-N18	2.48	1.43	1.37
2	B	801	PZW	C10-N9	2.37	1.36	1.34
2	A	801	PZW	C7-N14	2.09	1.41	1.37

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	PZW	C10-N9-N8	-6.76	121.27	126.95
2	A	801	PZW	C10-N9-N8	-6.58	121.42	126.95
2	A	801	PZW	C17-N18-C19	-2.71	120.15	124.60
2	B	801	PZW	C17-N18-C19	-2.49	120.51	124.60
2	A	801	PZW	C13-C12-N14	-2.01	109.32	111.43

There are no chirality outliers.

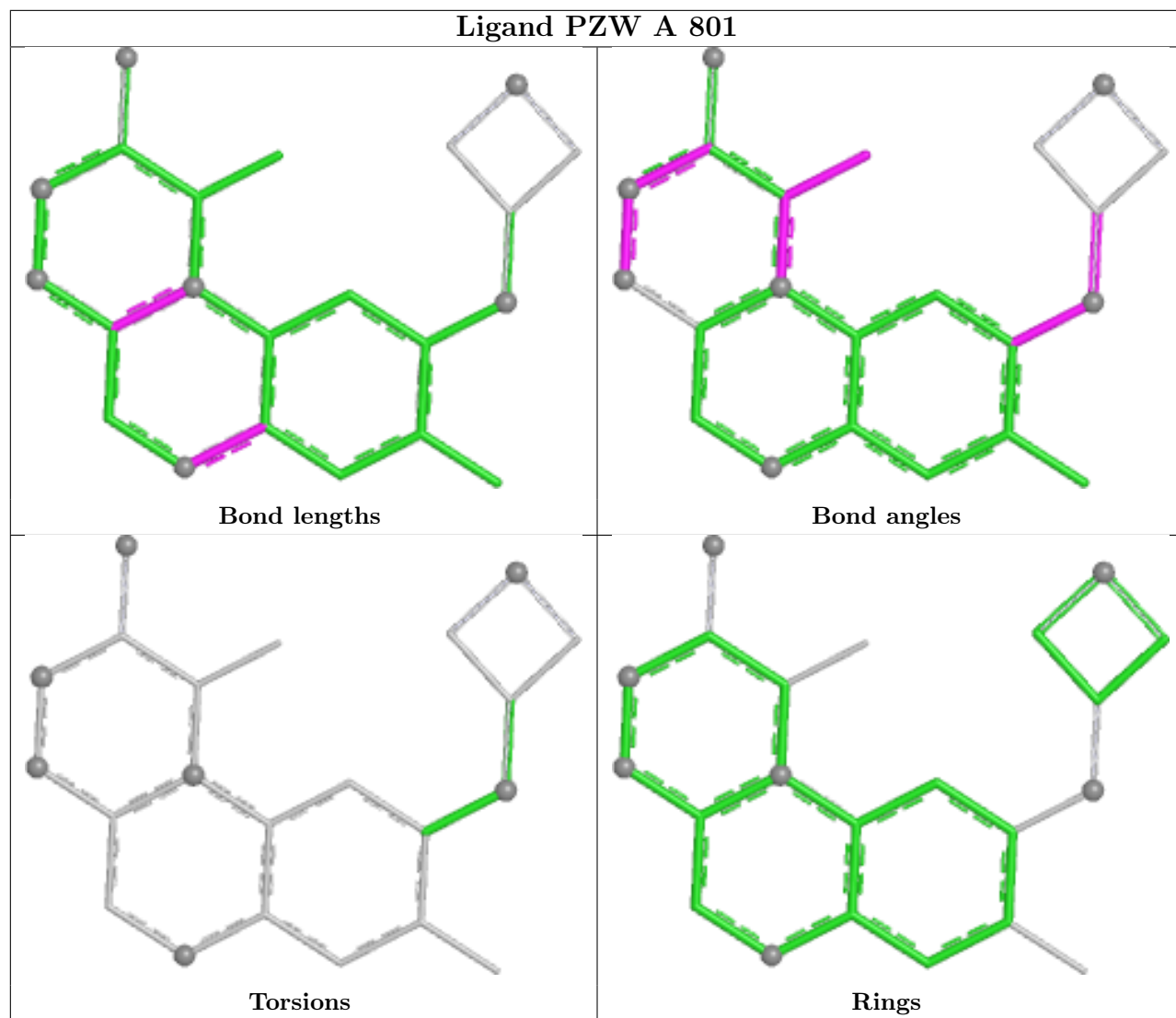
There are no torsion outliers.

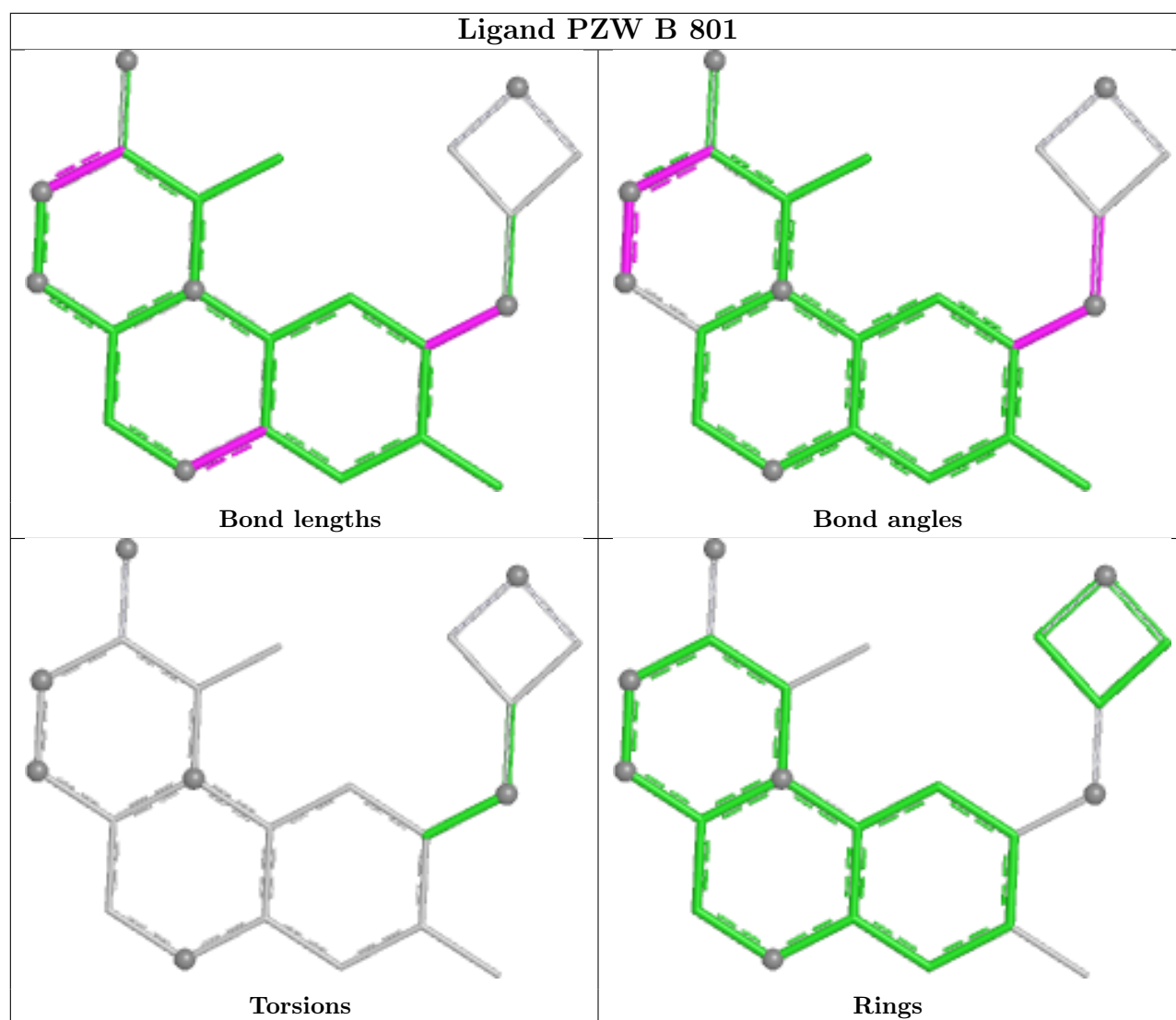
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	801	PZW	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 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	331/334 (99%)	0.02	8 (2%) 59 54	26, 49, 85, 132	30 (9%)
1	B	308/334 (92%)	0.44	20 (6%) 26 21	27, 66, 99, 145	57 (18%)
All	All	639/668 (95%)	0.22	28 (4%) 39 33	26, 58, 95, 145	87 (13%)

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	689	ASN	4.8
1	B	663	ASN	4.6
1	B	531	LEU	3.7
1	B	390	SER	3.5
1	B	664	PHE	3.5
1	B	666	LYS	3.3
1	B	699	PRO	3.2
1	B	704	LEU	3.2
1	B	662	SER	3.1
1	B	690	MET	2.9
1	A	707	HIS	2.9
1	B	420	ASP	2.9
1	B	436	TRP	2.8
1	A	436	TRP	2.7
1	A	668	PHE	2.7
1	B	454	LEU	2.7
1	A	704	LEU	2.5
1	A	700	GLY	2.5
1	B	661	CYS	2.4
1	B	446	CYS	2.3
1	B	422	VAL	2.3
1	B	417	LEU	2.3
1	B	374	LYS	2.2
1	B	702	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	382	LEU	2.1
1	A	672	LYS	2.1
1	A	388	LYS	2.1
1	A	705	ILE	2.0

## 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<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(Å <sup>2</sup> )	Q<0.9
1	SEP	B	695	10/11	0.86	0.10	106,108,113,114	0
1	SEP	A	695	10/11	0.92	0.09	63,67,72,74	0
1	SEP	A	676	10/11	0.93	0.10	60,65,70,70	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<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.

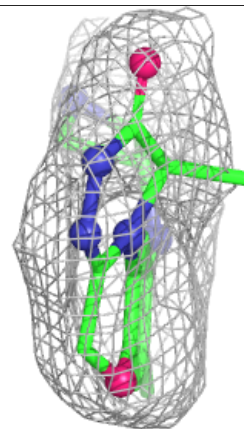
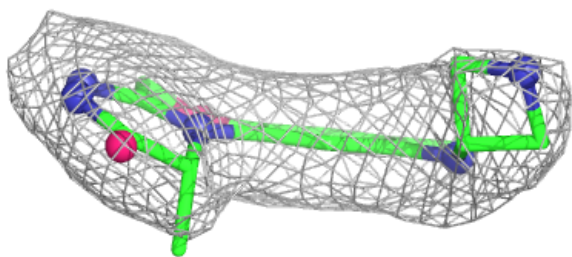
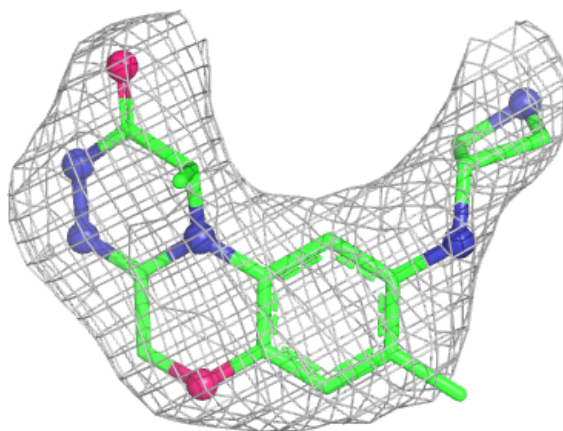
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	NA	A	802	1/1	0.88	0.17	61,61,61,61	0
2	PZW	B	801	22/22	0.92	0.12	63,70,75,76	0
2	PZW	A	801	22/22	0.95	0.12	49,54,63,65	0

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.



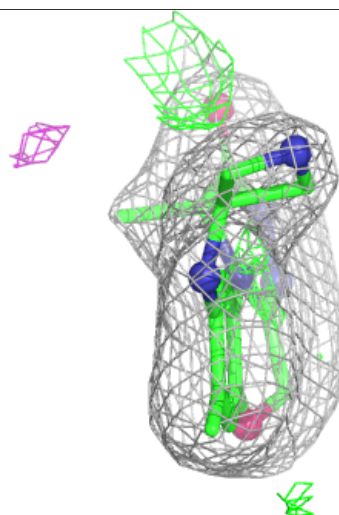
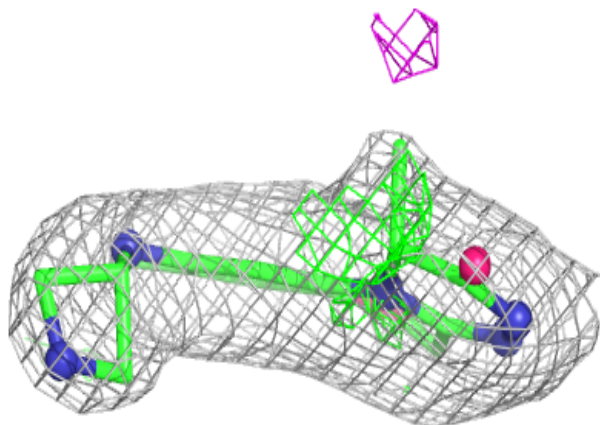
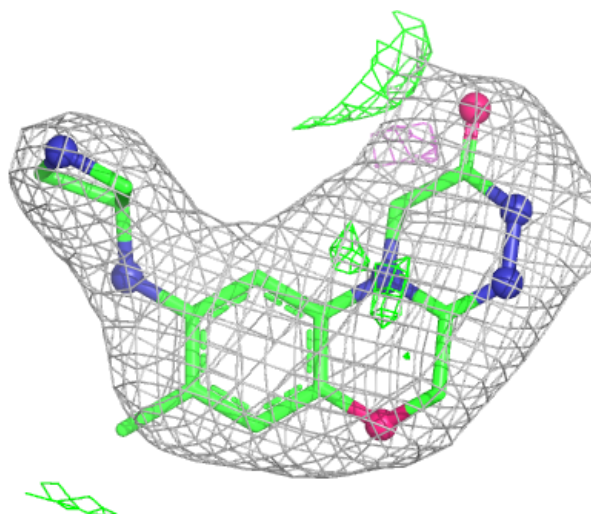
**Electron density around PZW B 801:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around PZW A 801:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.