

Full wwPDB X-ray Structure Validation Report (i)

May 18, 2020 – 12:54 am BST

PDB ID : 3KCK

Title : A Novel Chemotype of Kinase Inhibitors Authors : Zuccola, H.J.; Wang, T.; Ledeboer, M.W.

Deposited on : 2009-10-21

Resolution : 2.20 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 following versions of software and data (see references (1)) were used in the production of this report:

 $Mol Probity \quad : \quad 4.02b\text{--}467$

Mogul : 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13 EDS : 2.11

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)

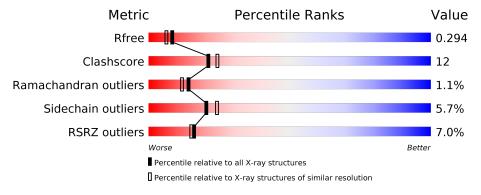
Validation Pipeline (wwPDB-VP) : 2.11

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 2.20 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	$\begin{array}{c} \text{Whole archive} \\ (\#\text{Entries}) \end{array}$	$\begin{array}{c} {\rm Similar resolution} \\ (\#{\rm Entries, resolution range(\AA)}) \end{array}$
R_{free}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 on 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			
			6%			
1	A	313	69%	20%	• 8%	



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 2506 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 Tyrosine-protein kinase JAK2.

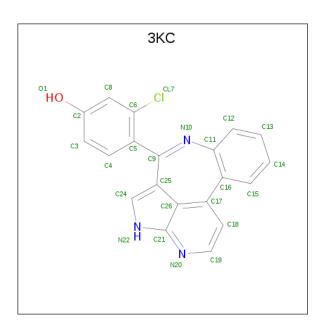
AltConf	Trace
1	0
	1

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	820	MET	-	EXPRESSION TAG	UNP O60674
A	821	GLY	-	EXPRESSION TAG	UNP O60674
A	822	SER	-	EXPRESSION TAG	UNP O60674
A	823	SER	-	EXPRESSION TAG	UNP O60674
A	824	HIS	-	EXPRESSION TAG	UNP O60674
A	825	HIS	-	EXPRESSION TAG	UNP O60674
A	826	HIS	-	EXPRESSION TAG	UNP O60674
A	827	HIS	-	EXPRESSION TAG	UNP O60674
A	828	HIS	-	EXPRESSION TAG	UNP O60674
A	829	HIS	-	EXPRESSION TAG	UNP O60674
A	830	SER	_	EXPRESSION TAG	UNP O60674
A	831	SER	_	EXPRESSION TAG	UNP O60674
A	832	GLY	-	EXPRESSION TAG	UNP O60674
A	833	LEU	-	EXPRESSION TAG	UNP O60674
A	834	VAL	-	EXPRESSION TAG	UNP O60674
A	835	PRO	-	EXPRESSION TAG	UNP O60674
A	836	ARG	-	EXPRESSION TAG	UNP O60674
A	837	GLY	=	EXPRESSION TAG	UNP O60674
A	838	SER	-	EXPRESSION TAG	UNP O60674
A	839	HIS	-	EXPRESSION TAG	UNP O60674
A	840	ASN	-	EXPRESSION TAG	UNP O60674
A	841	MET		EXPRESSION TAG	UNP O60674

• Molecule 2 is 3-chloro-4-(4H-3,4,7-triazadibenzo[cd,f]azulen-6-yl)phenol (three-letter code: 3KC) (formula: C₂₀H₁₂ClN₃O).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf		
9	Λ	1	Total	С	Cl	N	О	0	0
2	А	1	25	20	1	3	1	U	

• Molecule 3 is water.

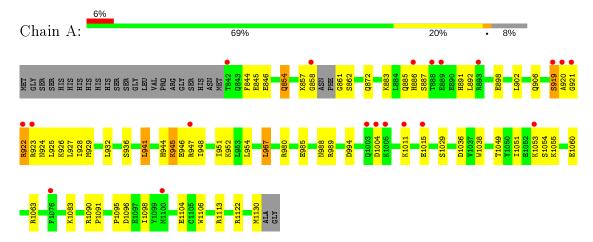
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	98	Total O 98 98	0	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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: Tyrosine-protein kinase JAK2





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants	95.16Å 100.80Å 67.62Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 - 2.20	Depositor
Resolution (A)	31.68 - 2.20	EDS
% Data completeness	98.9 (20.00-2.20)	Depositor
(in resolution range)	98.9 (31.68-2.20)	EDS
R_{merge}	0.09	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) > 1$	$3.09 \; ({\rm at} \; 2.20 {\rm \AA})$	Xtriage
Refinement program	REFMAC	Depositor
D D.	0.225 , 0.296	Depositor
R, R_{free}	0.223 , 0.294	DCC
R_{free} test set	1293 reflections (7.76%)	wwPDB-VP
Wilson B-factor (Å ²)	30.1	Xtriage
Anisotropy	0.412	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.38, 45.2	EDS
L-test for twinning ²	$ < L > = 0.51, < L^2> = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	2506	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 6.03% 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.



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: PTR, 3KC

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		
MIOI	Chain	RMSZ	# Z >5	RMSZ	# Z > 5	
1	A	1.00	0/2403	0.99	7/3230 (0.2%)	

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(^o)$	$\operatorname{Ideal}({}^o)$
1	A	936[A]	SER	CA-CB-OG	10.60	139.81	111.20
1	A	936[B]	SER	CA-CB-OG	10.60	139.81	111.20
1	A	1036	ASP	CB-CG-OD1	8.08	125.57	118.30
1	A	1113	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	A	980	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	A	1036	ASP	CB-CG-OD2	-5.77	113.11	118.30
1	A	967	LEU	CB-CG-CD2	-5.22	102.13	111.00

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	2383	0	2362	58	0
2	A	25	0	12	1	0
3	A	98	0	0	33	0
All	All	2506	0	2374	58	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 12.

All (58) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic	Clash
		$\operatorname{distance}\left(\mathrm{\AA}\right)$	overlap (Å)
1:A:919:SER:HB2	3:A:65:HOH:O	1.38	1.24
1:A:919:SER:HA	3:A:42:HOH:O	1.43	1.14
1:A:854:GLN:HG3	3:A:52:HOH:O	1.60	1.02
1:A:929:MET:CG	3:A:29:HOH:O	2.15	0.95
1:A:927:LEU:HD11	3:A:29:HOH:O	1.67	0.94
1:A:1130:MET:SD	3:A:70:HOH:O	2.28	0.92
1:A:1060:GLU:OE1	3:A:25:HOH:O	1.89	0.89
1:A:1095:PRO:HG2	1:A:1098:ILE:HD12	1.61	0.82
1:A:1122:ARG:HD3	3:A:87:HOH:O	1.82	0.79
1:A:929:MET:HG2	3:A:29:HOH:O	1.78	0.75
1:A:923:ARG:O	3:A:43:HOH:O	2.05	0.73
1:A:1122:ARG:NH1	3:A:87:HOH:O	2.08	0.71
1:A:902:LEU:HD23	3:A:29:HOH:O	1.90	0.71
1:A:924:ASN:HA	3:A:4:HOH:O	1.93	0.67
1:A:845:GLU:OE1	3:A:78:HOH:O	2.14	0.66
1:A:929:MET:HG3	3:A:29:HOH:O	1.91	0.64
1:A:1090:ARG:NH1	3:A:90:HOH:O	2.30	0.64
1:A:923:ARG:HD3	3:A:43:HOH:O	1.99	0.62
1:A:1083:LYS:HG3	3:A:41:HOH:O	1.99	0.61
1:A:922:ARG:NH2	1:A:924:ASN:CB	2.63	0.61
1:A:1104:GLU:CD	1:A:1122:ARG:HH12	2.04	0.61
1:A:857:LYS:HD2	1:A:862:SER:HB2	1.83	0.60
1:A:885:GLN:HA	3:A:84:HOH:O	2.01	0.59
1:A:922:ARG:NH2	1:A:924:ASN:HB2	2.17	0.59
1:A:844:PHE:CG	1:A:928:ILE:HD13	2.38	0.59
1:A:1090:ARG:HD2	3:A:13:HOH:O	2.02	0.58
1:A:1095:PRO:HG2	1:A:1098:ILE:CD1	2.32	0.56
1:A:1122:ARG:CD	3:A:87:HOH:O	2.47	0.55
1:A:951:ILE:HG13	3:A:70:HOH:O	2.07	0.54
1:A:922:ARG:NH2	1:A:924:ASN:CG	2.62	0.53
1:A:1055:LYS:HE3	3:A:83:HOH:O	2.09	0.52
1:A:898:GLU:OE2	2:A:1:3KC:O1	2.21	0.52
1:A:1049:THR:HG22	1:A:1091:PRO:HB3	1.91	0.52
1:A:891:HIS:CD2	3:A:95:HOH:O	2.63	0.52
1:A:1053:LYS:HG3	1:A:1054:SER:N	2.26	0.51
1:A:920:ALA:HA	3:A:57:HOH:O	2.12	0.50
1:A:941:LEU:HD23	1:A:948:ILE:HD12	1.92	0.50

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A + 0 roo 1	A 4 a ma 2	Interatomic	Clash
Atom-1	Atom-2	${f distance} ({f \AA})$	overlap (Å)
1:A:946:GLU:HG3	3:A:50:HOH:O	2.11	0.49
1:A:1095:PRO:CG	1:A:1098:ILE:HD12	2.38	0.49
1:A:1004:ASP:OD2	1:A:1004:ASP:N	2.43	0.48
1:A:1038:TRP:CE3	1:A:1106:TRP:HA	2.49	0.48
1:A:861:GLY:N	3:A:67:HOH:O	2.47	0.46
1:A:1063:ARG:HD3	3:A:14:HOH:O	2.16	0.46
1:A:944:HIS:O	1:A:947:ARG:HG3	2.15	0.45
1:A:1051:ILE:O	1:A:1051:ILE:HG22	2.16	0.45
1:A:952:LYS:NZ	1:A:988:ASN:OD1	2.49	0.45
1:A:858:GLY:HA3	3:A:98:HOH:O	2.16	0.44
1:A:924:ASN:CA	3:A:4:HOH:O	2.61	0.44
1:A:944:HIS:HA	1:A:947:ARG:NH2	2.33	0.43
1:A:857:LYS:HD2	1:A:862:SER:CB	2.48	0.42
1:A:932:LEU:HD22	1:A:985:GLU:HG3	2.01	0.42
1:A:1011:LYS:HG3	3:A:54:HOH:O	2.21	0.41
1:A:919:SER:CB	3:A:65:HOH:O	2.25	0.41
1:A:883:LYS:HB3	1:A:926:LYS:HG2	2.03	0.40
1:A:872:GLN:HG2	3:A:21:HOH:O	2.22	0.40
1:A:944:HIS:O	1:A:945:LYS:C	2.59	0.40
1:A:944:HIS:HB2	1:A:948:ILE:HD11	2.03	0.40
1:A:954:LEU:HA	1:A:954:LEU:HD23	1.87	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	$282/313 \ (90\%)$	269 (95%)	10 (4%)	3 (1%)	14 12

All (3) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	A	945	LYS
1	A	921	GLY
1	A	994	ASP

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	$262/282 \ (93\%)$	247 (94%)	15 (6%)	20 24

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	846	GLU
1	A	854	GLN
1	A	886	HIS
1	A	887	SER
1	A	892	LEU
1	A	906	GLN
1	A	919	SER
1	A	922	ARG
1	A	925	LEU
1	A	941	LEU
1	A	967	LEU
1	A	989	ARG
1	A	1015	GLU
1	A	1029	SER
1	A	1096	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	\mathbf{Type}
1	A	906	GLN
1	A	950	HIS
1	A	1084	ASN
1	A	1085	ASN

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Mol	Chain	Res	Type
1	A	1108	ASN
1	A	1112	GLN
1	A	1129	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)

2 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	PTR	A	1008	1	15,16,17	1.90	1 (6%)	19,22,24	1.03	1 (5%)
1	PTR	A	1007	1	15,16,17	2.05	2 (13%)	19,22,24	0.76	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	\mathbf{Res}	Link	Chirals	Torsions	Rings
1	PTR	A	1008	1	-	0/10/11/13	0/1/1/1
1	PTR	A	1007	1	-	0/10/11/13	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(\mathbf{\mathring{A}})$	$\operatorname{Ideal}(ext{\AA})$
1	A	1008	PTR	OH-CZ	-7.16	1.24	1.40
1	A	1007	PTR	OH-CZ	-7.00	1.24	1.40
1	A	1007	PTR	P-OH	2.27	1.62	1.59



All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^o)$	$\mathbf{Ideal}(^{o})$
1	A	1008	PTR	O2P-P-OH	2.51	113.08	105.24

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 carbohydrates 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).

1/4	Mol	Type	Chain	Pog	Link	Bond lengths			Bond angles		
MIOI	UI			nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	2	3KC	A	1	-	25,29,29	2.15	6 (24%)	24,43,43	2.71	8 (33%)

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	${f Res}$	Link	Chirals	Torsions	Rings
2	3KC	A	1	_	-	0/0/4/4	0/4/5/5

All (6) bond length outliers are listed below:

10101	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	ideai(A)
2	A	1	3KC	C25-C26	7.66	1.48	1.42

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$\alpha \cdots$	· ·	•	
Continued	trom	mromanne	maaa
-	110116	DICUIUU	Du_iu_{C}

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	${ m Observed}({ m \AA})$	$\operatorname{Ideal}(ext{\AA})$
2	A	1	3KC	C18-C19	3.42	1.41	1.36
2	A	1	3KC	C6-CL7	-2.94	1.66	1.73
2	A	1	3KC	C24-C25	-2.66	1.35	1.40
2	A	1	3KC	C21-N22	2.15	1.38	1.34
2	A	1	3KC	C8-C6	-2.07	1.35	1.38

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
2	A	1	3KC	C8-C6-C5	8.36	127.85	121.91
2	A	1	3KC	C19-N20-C21	6.20	124.24	116.60
2	A	1	3KC	C4-C5-C6	-3.31	113.97	117.63
2	A	1	3KC	C5-C6-CL7	-3.23	116.13	120.75
2	A	1	3KC	C19-C18-C17	-2.83	117.33	119.77
2	A	1	3KC	C18-C19-N20	-2.79	122.04	125.10
2	A	1	3KC	C4-C5-C9	2.46	123.20	120.14
2	A	1	3KC	C12-C11-C16	-2.06	117.22	120.05

There are no chirality outliers.

There are no torsion outliers.

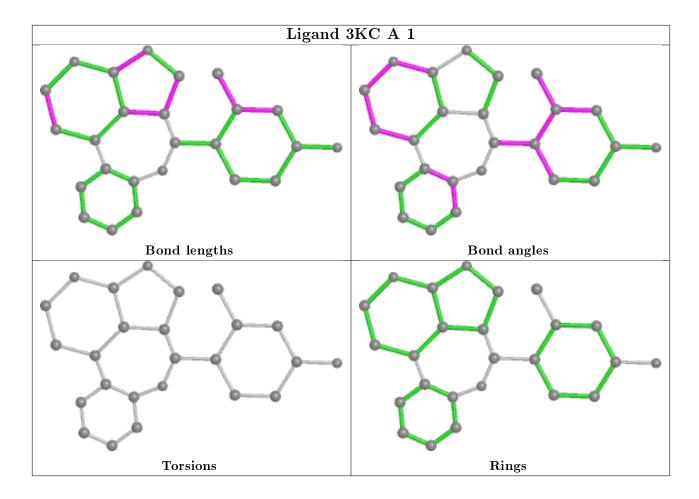
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	3KC	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 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 $>$	$\#\mathrm{RSRZ}{>}2$	$OWAB(Å^2)$	Q < 0.9
1	A	285/313 (91%)	0.24	20 (7%) 16 15	15, 26, 50, 68	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	920	ALA	13.0
1	A	922	ARG	8.3
1	A	921	GLY	5.0
1	A	1003	GLN	4.4
1	A	1004	ASP	4.4
1	A	919	SER	3.4
1	A	889	GLU	3.3
1	A	923	ARG	3.1
1	A	886	HIS	2.8
1	A	947	ARG	2.7
1	A	858	GLY	2.7
1	A	1100	MET	2.6
1	A	1005	LYS	2.3
1	A	1053	LYS	2.3
1	A	842	THR	2.3
1	A	1076	PHE	2.3
1	A	1015	GLU	2.2
1	A	893	ARG	2.1
1	A	1011	LYS	2.1
1	A	888	THR	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, 95th 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	${f B-factors}({f \AA}^2)$	Q<0.9
1	PTR	A	1007	16/17	0.81	0.21	27,38,54,54	0
1	PTR	A	1008	16/17	0.90	0.17	26,33,50,51	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

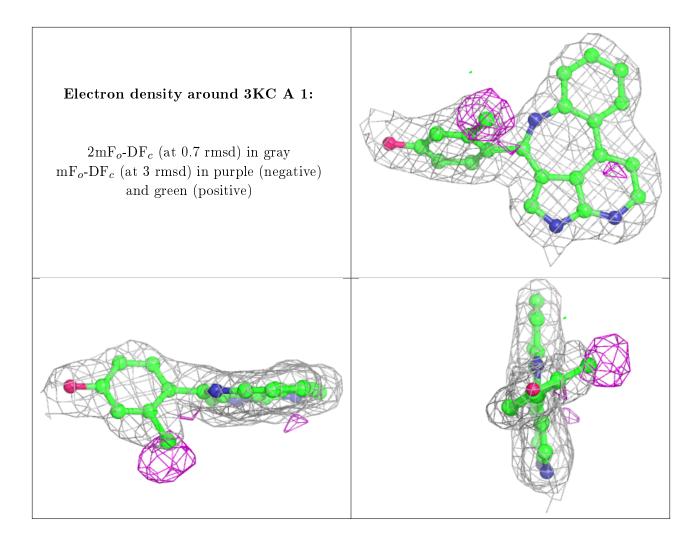
6.4 Ligands (i)

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	${f B\text{-factors}}({f \AA}^2)$	Q < 0.9
2	3KC	A	1	25/25	0.88	0.15	18,23,30,50	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.

