

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

### Aug 9, 2020 – 11:43 PM BST

PDB ID : 6RSB

Title : Structure based optimization of JAK1-ATP binding pocket Inhibitors in the

aminopyrazole class

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Deposited on : 2019-05-21

Resolution : 1.80 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:

MolProbity : 4.02b-467

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

Xtriage (Phenix) : 1.13

EDS : 2.13.1

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)

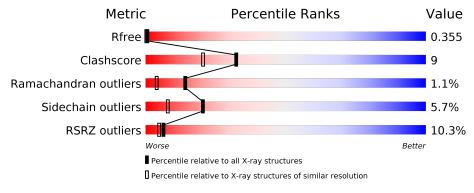
Validation Pipeline (wwPDB-VP) : 2.13.1

# 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 1.80 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 $(\# \mathrm{Entries})$	$\begin{array}{c} {\rm Similar \; resolution} \\ (\#{\rm Entries, \; resolution \; range(\AA)}) \end{array}$
$R_{free}$	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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					
1	A	302	10% 74%	18%	•• 5%			
	11		9%	1070				
1	В	302	73%	16%	• 7%			



# 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 5014 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 JAK1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace		
1	A	286		C 1477			P 2	S 15	0	0	0
1	В	281	Total 2291	C 1461	N 388		P 2	S 15	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	853	GLY	_	expression tag	UNP P23458
В	853	GLY	-	expression tag	UNP P23458

• Molecule 2 is 1-[(3 {R},4 {R})-4-(cyanomethyl)-1-[[4-(cyclohexen-1-yl)phenyl]methyl]-3-fl uoranyl-piperidin-4-yl]-3-(cyclopropylcarbonylamino)pyrazole-4-carboxamide (three-letter code: KGZ) (formula: C<sub>28</sub>H<sub>33</sub>FN<sub>6</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf			
9	Λ	1	Total	С	F	Ν	О	0	0	
2	2 A	1	37	28	1	6	2	0		
9	D	1	Total	С	F	Ν	О	0	0	
2	Б	1	37	28	1	6	2	U	0	

# $\bullet\,$ Molecule 3 is water.

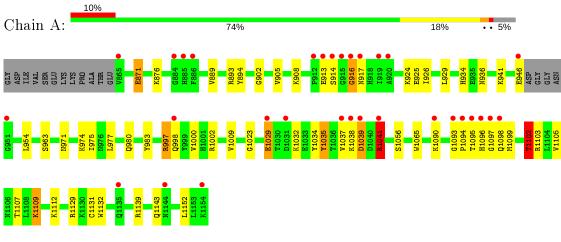
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	165	Total O 165 165	0	0
3	В	162	Total O 162 162	0	0



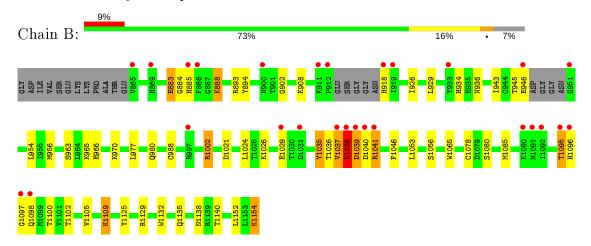
# 3 Residue-property plots (i)

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: Tyrosine-protein kinase JAK1



• Molecule 1: Tyrosine-protein kinase JAK1





# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	42.98Å 89.11Å 174.64Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	87.32 - 1.80	Depositor
resolution (A)	87.32 - 1.80	EDS
% Data completeness	98.4 (87.32-1.80)	Depositor
(in resolution range)	98.4 (87.32-1.80)	EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.59 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
P. P.	0.309 , $0.354$	Depositor
$R, R_{free}$	0.312 , $0.355$	DCC
$R_{free}$ test set	3053 reflections $(4.91%)$	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	11.7	Xtriage
Anisotropy	0.461	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.39 , 40.9	EDS
L-test for twinning <sup>2</sup>	$ < L >=0.53, < L^2>=0.37$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	5014	wwPDB-VP
Average B, all atoms $(Å^2)$	10.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The analyses of the Patterson function reveals a significant off-origin peak that is 52.42 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.8740e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

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



<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: KGZ, PTR

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	Chain	Boı	nd lengths	Bond angles		
Mol Chain		RMSZ	# Z  > 5	RMSZ	# Z >5	
1	A	0.91	$4/2338 \ (0.2\%)$	1.04	6/3147 (0.2%)	
1	В	0.93	3/2306 (0.1%)	1.06	3/3103 (0.1%)	
All	All	0.92	7/4644 (0.2%)	1.05	9/6250 (0.1%)	

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	В	0	3
All	All	0	5

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}( ext{\AA})$
1	В	956	MET	C-O	7.10	1.36	1.23
1	A	1029	GLU	C-O	6.98	1.36	1.23
1	В	1029	GLU	C-O	6.30	1.35	1.23
1	A	1097	GLY	C-O	6.08	1.33	1.23
1	A	871	GLU	CD-OE1	5.70	1.31	1.25
1	В	988	CYS	C-O	5.44	1.33	1.23
1	A	1099	MET	CG-SD	5.02	1.94	1.81

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^o)$
1	В	1002	ARG	NE-CZ-NH2	-10.52	115.04	120.30
1	В	1002	ARG	NE-CZ-NH1	8.21	124.40	120.30

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Mol	Chain	Res	Type	Atoms	${f Z}$	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^o)$
1	A	1002	ARG	NE-CZ-NH2	-6.44	117.08	120.30
1	A	1129	ARG	NE-CZ-NH2	-6.34	117.13	120.30
1	A	1002	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	A	983	TYR	CB-CG-CD1	6.15	124.69	121.00
1	A	1102	THR	CB-CA-C	-6.04	95.28	111.60
1	A	893	ARG	NE-CZ-NH2	-5.37	117.61	120.30
1	В	1002	ARG	CD-NE-CZ	5.05	130.67	123.60

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1039	ASP	Peptide
1	A	916	GLY	Peptide
1	В	1038	LYS	Peptide
1	В	1039	ASP	Peptide
1	В	1040	ASP	Peptide

### 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	2322	0	2310	37	0
1	В	2291	0	2286	59	0
2	A	37	0	0	0	0
2	В	37	0	0	0	0
3	A	165	0	0	3	0
3	В	162	0	0	6	0
All	All	5014	0	4596	82	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 9.

All (82) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



		Interatomic	Clash
Atom-1	Atom-2	${f distance} ({f \AA})$	overlap (Å)
1:A:1096:HIS:HB2	1:B:1041:ARG:HA	1.36	1.05
1:B:1037:VAL:CB	1:B:1038:LYS:HA	1.90	1.02
1:B:1037:VAL:HB	1:B:1038:LYS:CA	1.89	1.02
1:A:1103:ARG:HH12	1:B:1038:LYS:HB2	1.24	1.01
1:B:1037:VAL:HB	1:B:1038:LYS:HA	0.98	0.97
1:B:1096:HIS:CD2	1:B:1098:GLN:HB2	2.00	0.96
1:B:885:HIS:O	1:B:885:HIS:ND1	2.09	0.84
1:B:934:HIS:HD2	1:B:936:ASN:H	1.25	0.83
1:B:977:LEU:HA	1:B:980:GLN:HE21	1.43	0.82
1:A:977:LEU:HA	1:A:980:GLN:HE21	1.45	0.81
1:A:1103:ARG:NH1	1:B:1038:LYS:HB2	1.97	0.80
1:A:1041:ARG:O	1:B:1096:HIS:CD2	2.34	0.79
1:A:1103:ARG:HH12	1:B:1038:LYS:CB	1.95	0.79
1:A:1103:ARG:NH1	1:B:1038:LYS:CB	2.48	0.76
1:A:946:GLU:HA	3:A:1334:HOH:O	1.89	0.72
1:A:1094:PRO:O	1:A:1095:THR:OG1	2.07	0.72
1:B:918:HIS:N	3:B:1302:HOH:O	2.23	0.71
1:B:966:GLU:OE1	3:B:1301:HOH:O	2.09	0.70
1:A:934:HIS:HD2	1:A:936:ASN:H	1.35	0.70
1:A:1105:VAL:O	1:A:1109:LYS:HG3	1.92	0.69
1:B:934:HIS:CD2	1:B:936:ASN:H	2.08	0.68
1:B:965:LYS:HD2	1:B:1078:CYS:HB3	1.76	0.68
1:B:1096:HIS:ND1	1:B:1096:HIS:O	2.29	0.65
1:B:946:GLU:OE2	1:B:946:GLU:HA	1.98	0.64
1:A:1029:GLU:OE2	1:A:1032:LYS:HG3	1.97	0.63
1:B:1105:VAL:O	1:B:1109:LYS:HG3	1.98	0.62
1:A:1103:ARG:NH1	1:B:1038:LYS:HB3	2.15	0.61
1:B:1097:GLY:HA2	1:B:1100:THR:HB	1.83	0.60
1:B:888:LYS:N	1:B:888:LYS:HD2	2.17	0.60
1:A:934:HIS:CD2	1:A:936:ASN:H	2.19	0.60
1:B:963:SER:OG	1:B:966:GLU:OE1	2.09	0.60
1:A:1096:HIS:HB2	1:B:1041:ARG:CA	2.24	0.60
1:A:1096:HIS:HD2	1:B:1041:ARG:HB2	1.66	0.59
1:B:1026:LYS:HE2	3:B:1389:HOH:O	2.02	0.59
1:B:943:ILE:HD12	1:B:945:THR:HG23	1.84	0.58
1:B:943:ILE:HD12	1:B:945:THR:CG2	2.34	0.57
1:A:1094:PRO:C	1:A:1095:THR:OG1	2.44	0.56
1:B:1036:THR:HG22	1:B:1038:LYS:CG	2.37	0.55
1:B:888:LYS:H	1:B:888:LYS:HD2	1.73	0.54
1:B:1097:GLY:HA2	1:B:1100:THR:CB	2.38	0.54
1:B:1002:ARG:HD3	1:B:1024:LEU:O	2.08	0.53
1:A:1096:HIS:CG	1:B:1041:ARG:O	2.61	0.52

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Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	${ m distance}({ m \AA})$	overlap $( ext{Å})$
1:B:888:LYS:N	1:B:888:LYS:CD	2.72	0.52
1:B:883:GLU:OE1	1:B:884:GLY:N	2.43	0.52
1:B:1096:HIS:CG	1:B:1096:HIS:O	2.63	0.51
1:B:1095:THR:CG2	1:B:1096:HIS:N	2.74	0.50
1:A:1000:VAL:CG2	3:A:1367:HOH:O	2.60	0.49
1:B:1095:THR:HG22	1:B:1096:HIS:H	1.77	0.49
1:A:889:VAL:HG22	1:A:908:LYS:HB2	1.95	0.49
1:A:1035:PTR:HE1	1:A:1037:VAL:HG22	1.95	0.49
1:A:1107:THR:HG22	1:A:1112:LYS:HB2	1.96	0.47
1:A:1096:HIS:CD2	1:B:1041:ARG:O	2.67	0.47
1:A:1065:TRP:CE3	1:A:1132:TRP:HA	2.50	0.46
1:A:1041:ARG:HA	1:B:1096:HIS:CG	2.50	0.46
1:B:977:LEU:HA	1:B:980:GLN:NE2	2.22	0.46
1:A:894:TYR:O	1:A:902:GLY:HA3	2.15	0.46
1:B:1035:PTR:HE1	1:B:1037:VAL:HA	1.97	0.46
1:A:1096:HIS:CD2	1:B:1041:ARG:HB2	2.49	0.46
1:B:1065:TRP:CE3	1:B:1132:TRP:HA	2.50	0.46
1:B:894:TYR:O	1:B:902:GLY:HA3	2.16	0.46
1:A:925:GLU:OE1	1:A:1023:GLY:HA2	2.16	0.45
1:B:1135:GLN:HE21	1:B:1135:GLN:HA	1.82	0.45
1:A:1131:CYS:O	1:A:1139:ARG:HD3	2.17	0.45
1:B:1154:LYS:HA	1:B:1154:LYS:NZ	2.32	0.45
1:A:1102:THR:HG21	1:B:1053:LEU:O	2.18	0.44
1:B:1046:PHE:CD2	1:B:1085:MET:HG3	2.52	0.44
1:B:970:LYS:HE3	3:B:1445:HOH:O	2.17	0.44
1:A:971:ASN:O	1:A:975:ILE:HG12	2.17	0.44
1:B:893:ARG:NH2	3:B:1321:HOH:O	2.51	0.43
1:A:963:SER:HA	1:A:1009:VAL:O	2.18	0.43
1:A:905:VAL:HG12	1:A:941:LYS:HE2	2.01	0.42
1:A:926:ILE:HG12	1:A:954:LEU:HB2	2.00	0.42
1:A:997:ARG:O	1:A:998:GLN:HB2	2.18	0.42
1:B:908:LYS:NZ	1:B:1021:ASP:OD1	2.45	0.42
1:B:1026:LYS:HG3	1:B:1035:PTR:CE1	2.50	0.42
1:B:1097:GLY:N	1:B:1100:THR:OG1	2.52	0.42
1:A:1000:VAL:HG22	3:A:1367:HOH:O	2.19	0.42
1:B:1140:THR:HA	3:B:1342:HOH:O	2.20	0.42
1:B:926:ILE:HG12	1:B:954:LEU:HB2	2.02	0.41
1:A:1093:GLY:O	1:A:1095:THR:OG1	2.39	0.41
1:B:1138:ASN:HD22	1:B:1138:ASN:HA	1.65	0.40
1:B:1125:TYR:CZ	1:B:1129:ARG:HD3	2.57	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	${f Analysed}$	Favoured Allowed		Outliers	Percentiles	
1	A	$280/302 \ (93\%)$	267 (95%)	8 (3%)	5 (2%)	8 2	
1	В	273/302~(90%)	261 (96%)	11 (4%)	1 (0%)	34 21	
All	All	553/604 (92%)	528 (96%)	19 (3%)	6 (1%)	14 4	

### All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	913	GLU
1	A	917	ASN
1	A	1041	ARG
1	A	914	SER
1	A	916	GLY
1	В	1037	VAL

### 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	255/267~(96%)	239 (94%)	16 (6%)	18 6		
1	В	$252/267 \ (94\%)$	239 (95%)	13 (5%)	23 10		
All	All	507/534 (95%)	478 (94%)	29 (6%)	20 8		

All (29) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	A	871	GLU
1	A	876	LYS
1	A	924	LYS
1	A A	929	LEU
1	A	974	LYS
1	A A	997	ARG
1	A	1038	LYS
1	A A A	1039	ASP
1	A	1041	ARG
1		1056	SER
1	A	1090	LYS
1	A	1098	GLN
1	A A	1102	THR
1		1109	LYS
1	A	1143	GLN
1	A	1152	LEU
1	В	883	GLU
1	В	888	LYS
1	В	929	LEU
1	В	1038	LYS
1	В	1039	ASP
1	В	1041	ARG
1	В	1056	SER
1	В	1080	SER
1	В	1095	THR
1	В	1102	THR
1	В	1109	LYS
1	В	1152	LEU
1	В	1154	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	934	HIS
1	A	936	ASN
1	A	973	ASN
1	A	980	GLN
1	A	1098	GLN
1	A	1143	GLN
1	В	934	HIS
1	В	936	ASN
1	В	980	GLN
1	В	998	GLN

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Mol	Chain	Res	Type
1	В	1135	GLN
1	В	1138	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)

4 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	Dog	Res Link	Bond lengths		Bond angles			
Mol   Type   Ch	Chain	Chain Res	Counts		RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2	
1	PTR	В	1035	1	15,16,17	0.66	0	19,22,24	1.16	3 (15%)
1	PTR	A	1035	1	15,16,17	0.79	0	19,22,24	1.93	4 (21%)
1	PTR	В	1034	1	15,16,17	0.75	0	19,22,24	0.71	0
1	PTR	A	1034	1	15,16,17	0.78	0	19,22,24	0.97	2 (10%)

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	${ m Res}$	Link	Chirals	Torsions	Rings
1	PTR	В	1035	1	-	0/10/11/13	0/1/1/1
1	PTR	A	1035	1	-	2/10/11/13	0/1/1/1
1	PTR	В	1034	1	-	0/10/11/13	0/1/1/1
1	PTR	A	1034	1	-	0/10/11/13	0/1/1/1

There are no bond length outliers.

All (9) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^o)$
1	A	1035	PTR	OH-CZ-CE1	-4.44	106.02	119.23
1	A	1035	PTR	OH-CZ-CE2	3.94	130.95	119.23
1	A	1035	PTR	O2P-P-OH	3.46	116.05	105.24
1	A	1035	PTR	OH-P-O1P	-2.91	98.32	109.31
1	В	1035	PTR	O3P-P-OH	2.71	113.72	105.24
1	A	1034	PTR	OH-CZ-CE1	2.30	126.06	119.23
1	A	1034	PTR	OH-CZ-CE2	-2.21	112.65	119.23
1	В	1035	PTR	OH-CZ-CE1	-2.10	112.99	119.23
1	В	1035	PTR	OH-CZ-CE2	2.02	125.23	119.23

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1035	PTR	CZ-OH-P-O1P
1	A	1035	PTR	CZ-OH-P-O3P

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	$\operatorname{Res}$	Type	Clashes	Symm-Clashes
1	В	1035	PTR	2	0
1	A	1035	PTR	1	0

# 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry (i)

2 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	Во	ond leng	$ ag{ths}$	В	ond ang	les
MIOI	Iol Type Cha		nes	LIIIK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	KGZ	A	1201	-	36,41,41	0.75	1 (2%)	41,59,59	1.98	7 (17%)
2	KGZ	В	1201	-	36,41,41	0.69	1 (2%)	41,59,59	1.93	5 (12%)

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	KGZ	A	1201	-	-	8/20/56/56	0/5/5/5
2	KGZ	В	1201	-	-	3/20/56/56	0/5/5/5

### All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	${f Observed(\AA)}$	$\operatorname{Ideal}( ext{\AA})$
2	В	1201	KGZ	C9-C8	-2.54	1.47	1.51
2	A	1201	KGZ	C5-C7	-2.30	1.38	1.41

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	${\bf Observed}({}^o)$	$\operatorname{Ideal}(^{o})$
2	В	1201	KGZ	C4-N2-C3	10.11	131.87	124.18
2	A	1201	KGZ	C4-N2-C3	10.07	131.84	124.18
2	В	1201	KGZ	C2-C1-N1	-3.85	173.01	178.11
2	A	1201	KGZ	C4-N2-N5	-3.75	109.44	111.69
2	В	1201	KGZ	C28-C3-N2	2.90	113.20	109.06
2	A	1201	KGZ	C10-C9-C8	2.88	119.90	117.21
2	A	1201	KGZ	C2-C1-N1	-2.55	174.73	178.11
2	В	1201	KGZ	C12-C3-N2	-2.48	106.63	109.35
2	A	1201	KGZ	C2-C3-N2	2.47	113.42	109.92
2	В	1201	KGZ	C2-C3-N2	2.42	113.35	109.92
2	A	1201	KGZ	O2-C8-C9	2.18	124.96	122.12
2	A	1201	KGZ	C11-C9-C8	2.15	119.22	117.21

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1201	KGZ	O2-C8-C9-C11
2	A	1201	KGZ	O2-C8-C9-C10

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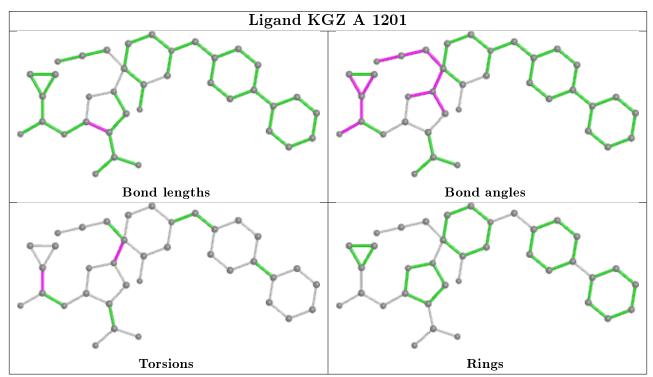
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Mol	Chain	Res	Type	Atoms
2	A	1201	KGZ	C2-C3-N2-C4
2	A	1201	KGZ	C12-C3-N2-N5
2	A	1201	KGZ	C2-C3-N2-N5
2	В	1201	KGZ	C2-C3-N2-C4
2	В	1201	KGZ	C12-C3-N2-N5
2	A	1201	KGZ	N4-C8-C9-C11
2	A	1201	KGZ	N4-C8-C9-C10
2	A	1201	KGZ	C12-C3-N2-C4
2	В	1201	KGZ	C12-C3-N2-C4

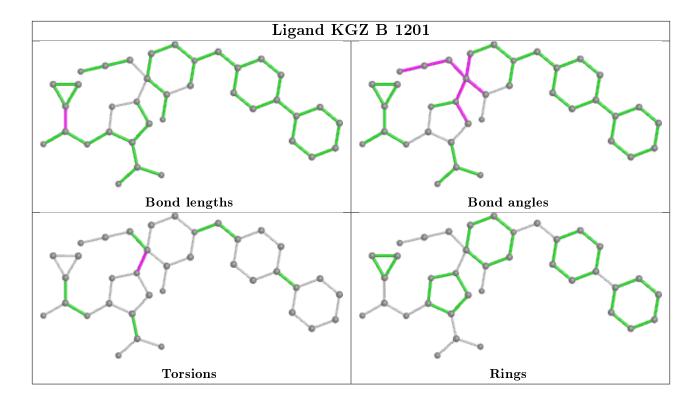
There are no ring outliers.

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 $>$	$\#\mathrm{RSRZ}{>}2$		$\mathbf{OWAB}(\mathbf{\mathring{A}}^2)$	Q < 0.9
1	A	$284/302 \ (94\%)$	1.10	31 (10%) 5	4	4, 8, 23, 44	0
1	В	279/302 (92%)	1.01	27 (9%) 7	6	4, 8, 19, 36	0
All	All	563/604 (93%)	1.05	58 (10%) 6	5	4, 8, 21, 44	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1094	PRO	11.2
1	В	1037	VAL	8.9
1	A	1093	GLY	8.4
1	A	916	GLY	7.9
1	В	1097	GLY	7.7
1	A	1097	GLY	6.5
1	В	1096	HIS	5.0
1	В	885	HIS	5.0
1	A	913	GLU	4.6
1	A	1031	ASP	4.6
1	A	946	GLU	4.6
1	A	1041	ARG	4.5
1	В	1041	ARG	4.4
1	A	1039	ASP	4.2
1	В	933	TYR	4.1
1	A	865	VAL	4.1
1	A	914	SER	4.1
1	A	1154	LYS	4.0
1	В	912	PRO	3.9
1	A	919	ILE	3.7
1	A	917	ASN	3.6
1	A	1096	HIS	3.6
1	В	1039	ASP	3.4
1	В	1090	LYS	3.4

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Mol	Chain	Res	Type	RSRZ	
1	В	919	ILE	3.4	
1	В	1031	ASP	3.4	
1	A	920	ALA	3.3	
1	A	885	HIS	3.3	
1	A	915	GLY	3.2	
1	A	998	GLN	3.2	
1	В	1098	GLN	3.2	
1	В	1095	THR	3.1	
1	A	1095	THR	3.1	
1	В	951	GLY	3.1	
1	A	951	GLY	2.9	
1	В	900	ASN	2.9	
1	A	912	PRO	2.8	
1	A	1037	VAL	2.7	
1	В	946	GLU	2.7	
1	A	884	GLY	2.7	
1	A	886	PHE	2.6	
1	A	1090	LYS	2.6	
1	В	911	LYS	2.6	
1	В	1040	ASP	2.5	
1	В	886	PHE	2.5	
1	A	1029	GLU	2.4	
1	В	1029	GLU	2.4	
1	В	869	HIS	2.4	
1	A	1098	GLN	2.3	
1	В	865	VAL	2.3	
1	В	918	HIS	2.2	
1	A	1038	LYS	2.2	
1	A	1144	ASN	2.2	
1	В	1092	ILE	2.2	
1	В	1091	MET	2.1	
1	В	997	ARG	2.1	
1	1 A		GLN	2.1	
1	В	1038	LYS	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	$ m ig  B ext{-factors}(\AA^2)$	Q<0.9
1	PTR	В	1034	16/17	0.74	0.21	16,18,23,24	0
1	PTR	В	1035	16/17	0.76	0.22	14,21,27,29	0
1	PTR	A	1035	16/17	0.78	0.16	11,14,19,19	0
1	PTR	A	1034	16/17	0.81	0.20	11,15,22,22	0

# 6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

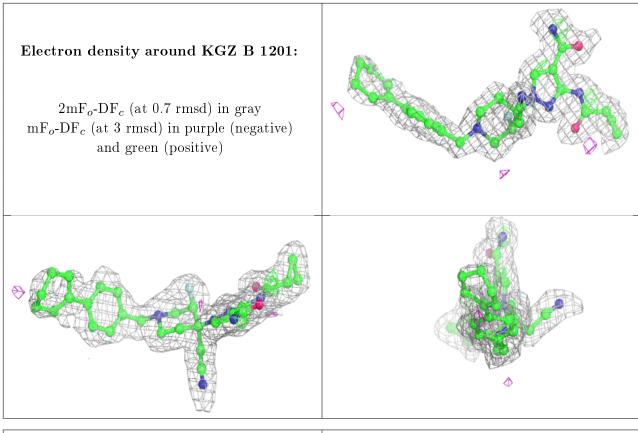
# 6.4 Ligands (i)

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	${f B-factors}({f \AA}^2)$	Q<0.9
2	KGZ	В	1201	37/37	0.90	0.19	8,13,29,30	0
2	KGZ	A	1201	37/37	0.92	0.20	8,12,27,28	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 KGZ A 1201: 2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative) and green (positive)



# 6.5 Other polymers (i)

There are no such residues in this entry.

