



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 1, 2026 – 10:16 AM EDT

PDB ID : 10PJ / pdb\_000010pj  
Title : JAK2 kinase (JH1 domain) in complex with povorcitinib  
Authors : Epling, L.B.; Fenalti, G.  
Deposited on : 2026-01-30  
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.

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 : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

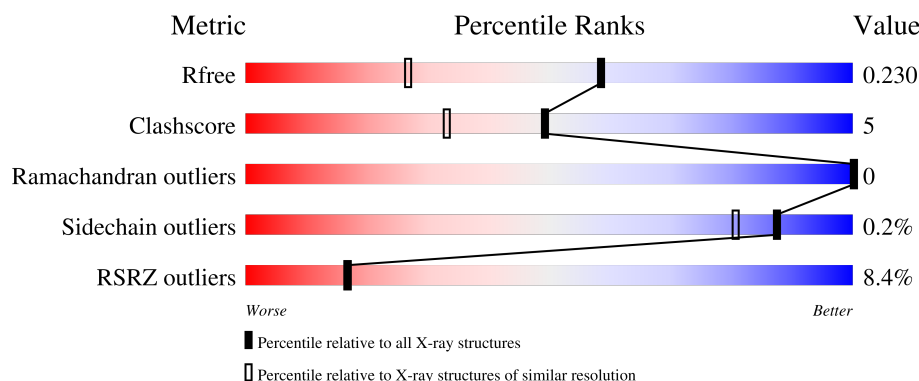
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	180053	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (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	316	<div> <div>8%</div> <div>86%</div> <div>9%</div> <div>5%</div> </div>
1	B	316	<div> <div>8%</div> <div>82%</div> <div>13%</div> <div>• 5%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5949 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.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	300	Total	C	N	O	P	S	0	17	0
			2575	1649	440	465	2	19			
1	B	300	Total	C	N	O	P	S	0	17	0
			2576	1650	438	466	2	20			

There are 46 discrepancies between the modelled and reference sequences:

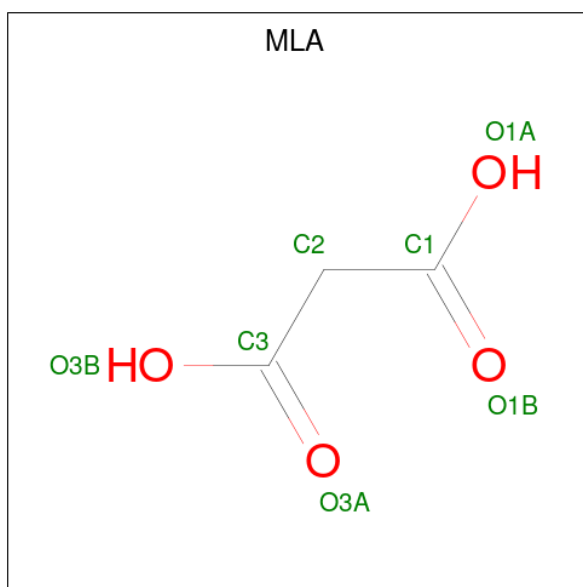
Chain	Residue	Modelled	Actual	Comment	Reference
A	817	MET	-	initiating methionine	UNP O60674
A	818	HIS	-	expression tag	UNP O60674
A	819	HIS	-	expression tag	UNP O60674
A	820	HIS	-	expression tag	UNP O60674
A	821	HIS	-	expression tag	UNP O60674
A	822	HIS	-	expression tag	UNP O60674
A	823	HIS	-	expression tag	UNP O60674
A	824	SER	-	expression tag	UNP O60674
A	825	SER	-	expression tag	UNP O60674
A	826	GLY	-	expression tag	UNP O60674
A	827	VAL	-	expression tag	UNP O60674
A	828	ASP	-	expression tag	UNP O60674
A	829	LEU	-	expression tag	UNP O60674
A	830	GLY	-	expression tag	UNP O60674
A	831	THR	-	expression tag	UNP O60674
A	832	GLU	-	expression tag	UNP O60674
A	833	ASN	-	expression tag	UNP O60674
A	834	LEU	-	expression tag	UNP O60674
A	835	TYR	-	expression tag	UNP O60674
A	836	PHE	-	expression tag	UNP O60674
A	837	GLN	-	expression tag	UNP O60674
A	838	SER	-	expression tag	UNP O60674
A	839	MET	-	expression tag	UNP O60674
B	817	MET	-	initiating methionine	UNP O60674
B	818	HIS	-	expression tag	UNP O60674

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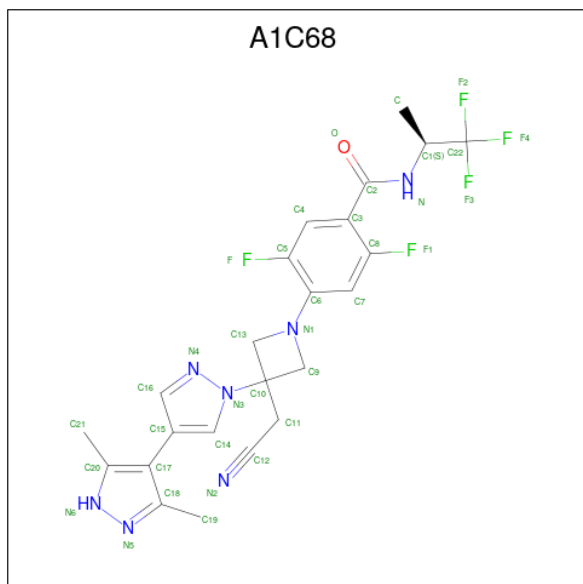
Chain	Residue	Modelled	Actual	Comment	Reference
B	819	HIS	-	expression tag	UNP O60674
B	820	HIS	-	expression tag	UNP O60674
B	821	HIS	-	expression tag	UNP O60674
B	822	HIS	-	expression tag	UNP O60674
B	823	HIS	-	expression tag	UNP O60674
B	824	SER	-	expression tag	UNP O60674
B	825	SER	-	expression tag	UNP O60674
B	826	GLY	-	expression tag	UNP O60674
B	827	VAL	-	expression tag	UNP O60674
B	828	ASP	-	expression tag	UNP O60674
B	829	LEU	-	expression tag	UNP O60674
B	830	GLY	-	expression tag	UNP O60674
B	831	THR	-	expression tag	UNP O60674
B	832	GLU	-	expression tag	UNP O60674
B	833	ASN	-	expression tag	UNP O60674
B	834	LEU	-	expression tag	UNP O60674
B	835	TYR	-	expression tag	UNP O60674
B	836	PHE	-	expression tag	UNP O60674
B	837	GLN	-	expression tag	UNP O60674
B	838	SER	-	expression tag	UNP O60674
B	839	MET	-	expression tag	UNP O60674

- Molecule 2 is MALONIC ACID (CCD ID: MLA) (formula:  $C_3H_4O_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			7	3	4		

- Molecule 3 is 4-{3-(cyanomethyl)-3-[(4M)-3',5'-dimethyl-1H,1'H-[4,4'-bipyrazol]-1-yl]azetid-1-yl}-2,5-difluoro-N-[(2S)-1,1,1-trifluoropropan-2-yl]benzamide (CCD ID: A1C68) (formula: C<sub>23</sub>H<sub>22</sub>F<sub>5</sub>N<sub>7</sub>O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	1
			56	35	10	9	2		
3	B	1	Total	C	F	N	O	0	1
			56	35	10	9	2		

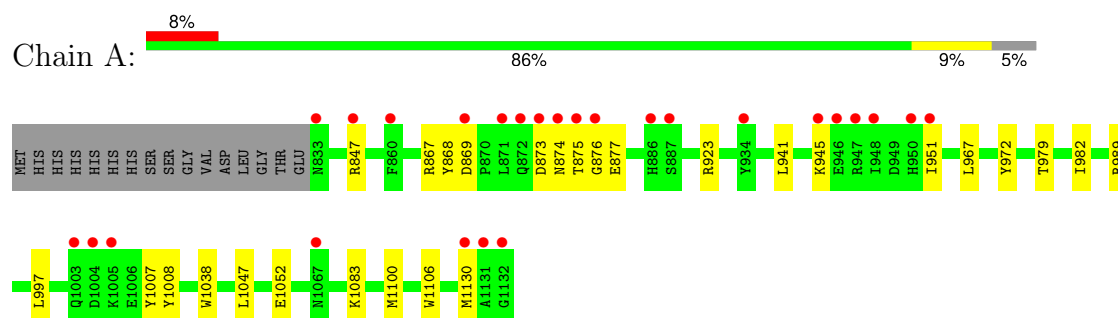
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	351	Total	O	0	1
			352	352		
4	B	325	Total	O	0	2
			327	327		

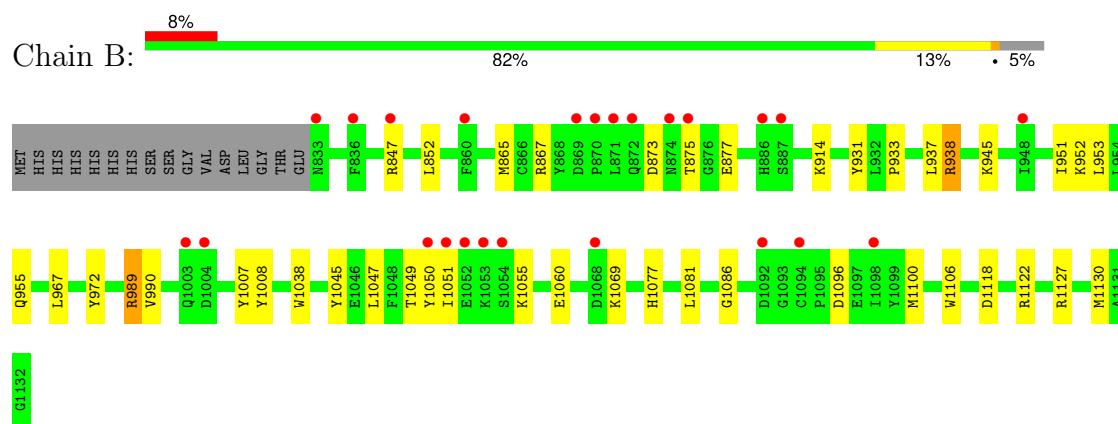
### 3 Residue-property plots [i](#)

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 JAK2



#### • Molecule 1: Tyrosine-protein kinase JAK2



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	99.61Å 69.13Å 110.33Å 90.00° 99.52° 90.00°	Depositor
Resolution (Å)	33.78 – 1.59 33.78 – 1.59	Depositor EDS
% Data completeness (in resolution range)	93.0 (33.78-1.59) 93.1 (33.78-1.59)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.40 (at 1.58Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, $R_{free}$	0.201 , 0.231 0.200 , 0.230	Depositor DCC
$R_{free}$ test set	4612 reflections (4.62%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	13.7	Xtriage
Anisotropy	0.607	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 44.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5949	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	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 90.16 % 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 2.5738e-08. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PTR, A1C68, MLA

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	0.59	0/2648	0.79	0/3563
1	B	0.61	0/2649	0.81	1/3562 (0.0%)
All	All	0.60	0/5297	0.80	1/7125 (0.0%)

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	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	989	ARG	CA-CB-CG	-6.28	101.53	114.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	923	ARG	Sidechain
1	B	938	ARG	Sidechain



## 5.2 Too-close contacts ⓘ

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	2575	0	2601	23	0
1	B	2576	0	2603	33	0
2	A	7	0	2	0	0
3	A	56	0	0	0	0
3	B	56	0	0	0	0
4	A	352	0	0	8	0
4	B	327	0	0	5	0
All	All	5949	0	5206	56	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 5.

All (56) 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:B:945:LYS:O	1:B:945:LYS:HD2	1.67	0.93
1:A:867[B]:ARG:HH22	1:A:875:THR:HA	1.42	0.85
1:B:938:ARG:NH1	1:B:1051:ILE:HG21	1.93	0.84
1:B:1100[A]:MET:HG3	4:B:2108:HOH:O	1.87	0.73
1:A:867[B]:ARG:NH2	1:A:875:THR:HA	2.03	0.71
1:A:1100[A]:MET:HG3	4:A:1416:HOH:O	1.92	0.69
1:A:967[B]:LEU:HD12	1:A:972:TYR:HB2	1.76	0.67
1:B:873:ASP:OD1	1:B:875:THR:HG22	1.95	0.66
1:B:938:ARG:CZ	1:B:1051:ILE:HG21	2.26	0.66
1:B:951:ILE:HD11	1:B:1130[A]:MET:SD	2.36	0.65
1:B:989:ARG:HG2	1:B:990:VAL:N	2.15	0.61
1:B:945:LYS:HD2	1:B:945:LYS:C	2.26	0.60
1:A:867[B]:ARG:HH12	1:A:874:ASN:C	2.10	0.60
1:B:1081:LEU:HD22	1:B:1086:GLY:HA3	1.84	0.59
1:B:1045:TYR:O	1:B:1049:THR:HG23	2.02	0.59
1:B:1055:LYS:HE3	1:B:1055:LYS:HA	1.85	0.59
1:A:873:ASP:OD1	1:A:875:THR:HG22	2.04	0.57
1:B:967[B]:LEU:HD12	1:B:972:TYR:HB2	1.88	0.56
1:A:951:ILE:HG23	4:A:1630:HOH:O	2.06	0.56
1:A:941:LEU:HD11	1:A:1047:LEU:HD23	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1130:MET:HE1	4:A:1451:HOH:O	2.06	0.55
1:B:967[A]:LEU:HG	1:B:972:TYR:HB2	1.89	0.54
1:A:847:ARG:HG2	4:A:1634:HOH:O	2.09	0.52
1:A:967[A]:LEU:HG	1:A:972:TYR:HB2	1.92	0.51
1:B:1038:TRP:CE3	1:B:1106:TRP:HA	2.46	0.50
1:B:1069:LYS:HE2	1:B:1077:HIS:CE1	2.46	0.49
1:B:937:LEU:HD21	1:B:1047:LEU:HD21	1.94	0.49
1:A:979:THR:HA	1:A:982[B]:ILE:HD12	1.96	0.47
1:A:875:THR:HG21	4:A:1460:HOH:O	2.15	0.47
1:A:951:ILE:HG21	1:A:1130:MET:HG2	1.97	0.47
1:B:875:THR:HG21	4:B:2163:HOH:O	2.16	0.46
1:B:1118:ASP:O	1:B:1122[B]:ARG:HG2	2.15	0.46
1:A:877:GLU:HG2	4:A:1424:HOH:O	2.16	0.44
1:B:877:GLU:OE2	1:B:914:LYS:HE2	2.17	0.44
1:B:1096:ASP:O	1:B:1100[B]:MET:HG2	2.17	0.44
1:A:945:LYS:HE3	1:A:1052:GLU:OE2	2.18	0.43
1:A:997[B]:LEU:HD13	4:A:1405:HOH:O	2.18	0.43
1:B:852:LEU:HD11	1:B:867:ARG:HB2	2.00	0.43
1:B:952:LYS:HD2	1:B:952:LYS:HA	1.70	0.43
1:A:868:TYR:O	1:A:876:GLY:HA3	2.19	0.42
1:B:847:ARG:HD2	4:B:2334:HOH:O	2.19	0.42
1:B:1045:TYR:CZ	1:B:1049:THR:HG21	2.54	0.42
1:B:955[B]:GLN:HG2	1:B:1127:ARG:NH2	2.35	0.42
1:B:1049:THR:C	1:B:1051:ILE:N	2.78	0.42
1:B:865:MET:HE2	1:B:931:TYR:CZ	2.55	0.42
1:B:1045:TYR:CE2	1:B:1049:THR:HG21	2.55	0.41
1:B:1051:ILE:HG22	4:B:2201:HOH:O	2.18	0.41
1:B:938:ARG:NH1	1:B:1051:ILE:CG2	2.76	0.41
1:B:1055:LYS:HE3	1:B:1060:GLU:OE2	2.21	0.41
1:B:931:TYR:CE2	1:B:933:PRO:HA	2.55	0.41
1:A:1038:TRP:CE3	1:A:1106:TRP:HA	2.56	0.41
1:B:953:LEU:HD11	1:B:1050:TYR:CZ	2.56	0.40
1:A:1083:LYS:NZ	4:A:1408:HOH:O	2.53	0.40
1:A:876:GLY:HA2	4:B:2153:HOH:O	2.20	0.40
1:A:941:LEU:O	1:A:945:LYS:HB3	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	313/316 (99%)	308 (98%)	5 (2%)	0	100	100
1	B	313/316 (99%)	307 (98%)	6 (2%)	0	100	100
All	All	626/632 (99%)	615 (98%)	11 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	287/286 (100%)	286 (100%)	1 (0%)	86	78
1	B	288/286 (101%)	288 (100%)	0	100	100
All	All	575/572 (100%)	574 (100%)	1 (0%)	87	81

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	989	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	853	GLN
1	A	854	GLN

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Mol	Chain	Res	Type
1	A	1077	HIS
1	A	1109	ASN
1	B	859	ASN
1	B	886	HIS
1	B	891	HIS
1	B	906	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
1	PTR	A	1007	1	15,16,17	2.56	2 (13%)	17,22,24	1.35	2 (11%)
1	PTR	B	1007	1	15,16,17	2.61	2 (13%)	17,22,24	1.37	2 (11%)
1	PTR	A	1008	1	15,16,17	2.29	2 (13%)	17,22,24	1.66	6 (35%)
1	PTR	B	1008	1	15,16,17	2.32	2 (13%)	17,22,24	1.74	3 (17%)

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	PTR	A	1007	1	-	0/10/11/13	0/1/1/1
1	PTR	B	1007	1	-	0/10/11/13	0/1/1/1
1	PTR	A	1008	1	-	0/10/11/13	0/1/1/1
1	PTR	B	1008	1	-	0/10/11/13	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1007	PTR	P-OH	9.47	1.77	1.59
1	A	1007	PTR	P-OH	9.09	1.76	1.59
1	B	1008	PTR	P-OH	8.10	1.74	1.59
1	A	1008	PTR	P-OH	7.66	1.74	1.59
1	A	1008	PTR	OH-CZ	-3.03	1.33	1.40
1	B	1008	PTR	OH-CZ	-3.01	1.33	1.40
1	A	1007	PTR	OH-CZ	-2.99	1.33	1.40
1	B	1007	PTR	OH-CZ	-2.55	1.34	1.40

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1007	PTR	O2P-P-OH	-3.63	94.59	105.32
1	B	1008	PTR	O2P-P-OH	-3.57	94.78	105.32
1	B	1007	PTR	O2P-P-OH	-3.10	96.15	105.32
1	A	1008	PTR	O2P-P-OH	-2.92	96.68	105.32
1	B	1008	PTR	O3P-P-O2P	2.51	117.22	107.80
1	A	1007	PTR	O3P-P-O2P	2.50	117.17	107.80
1	A	1008	PTR	OH-P-O1P	-2.48	101.19	109.48
1	A	1008	PTR	O3P-P-O2P	2.45	116.99	107.80
1	A	1008	PTR	CB-CG-CD1	2.33	125.24	120.90
1	B	1007	PTR	O3P-P-O2P	2.20	116.04	107.80
1	A	1008	PTR	CB-CG-CD2	-2.17	116.86	120.90
1	A	1008	PTR	OH-CZ-CE1	2.09	125.49	119.22
1	B	1008	PTR	CE2-CZ-CE1	-2.06	117.16	120.16

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](#)

5 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		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	MLA	A	1301	-	6,6,6	1.92	3 (50%)	7,7,7	1.33	1 (14%)
3	A1C68	A	1302[B]	-	37,39,39	1.93	9 (24%)	47,60,60	1.30	5 (10%)
3	A1C68	B	2001[B]	-	37,39,39	1.81	12 (32%)	47,60,60	1.17	5 (10%)
3	A1C68	B	2001[A]	-	37,39,39	1.72	9 (24%)	47,60,60	1.69	12 (25%)
3	A1C68	A	1302[A]	-	37,39,39	2.04	11 (29%)	47,60,60	1.43	5 (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	Res	Link	Chirals	Torsions	Rings
2	MLA	A	1301	-	-	0/4/4/4	-
3	A1C68	A	1302[B]	-	-	7/30/42/42	0/4/4/4
3	A1C68	B	2001[B]	-	-	6/30/42/42	0/4/4/4
3	A1C68	B	2001[A]	-	-	7/30/42/42	0/4/4/4
3	A1C68	A	1302[A]	-	-	7/30/42/42	0/4/4/4

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1302[A]	A1C68	C14-N3	5.82	1.40	1.35
3	A	1302[B]	A1C68	C14-N3	5.82	1.40	1.35
3	B	2001[A]	A1C68	C9-N1	4.67	1.54	1.48
3	A	1302[A]	A1C68	C13-C10	4.16	1.58	1.55
3	B	2001[B]	A1C68	C13-N1	3.99	1.53	1.48
3	A	1302[A]	A1C68	C10-N3	-3.79	1.42	1.48
3	A	1302[B]	A1C68	C10-N3	-3.79	1.42	1.48
3	A	1302[B]	A1C68	C2-N	3.78	1.43	1.34
3	A	1302[A]	A1C68	C9-N1	3.70	1.53	1.48
3	B	2001[B]	A1C68	C2-N	3.67	1.42	1.34
3	B	2001[A]	A1C68	C10-N3	-3.23	1.43	1.48
3	B	2001[B]	A1C68	C10-N3	-3.23	1.43	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2001[A]	A1C68	C2-N	3.18	1.41	1.34
3	B	2001[A]	A1C68	C7-C8	3.13	1.43	1.37
3	A	1302[A]	A1C68	C17-C15	-3.07	1.42	1.48
3	A	1302[B]	A1C68	C17-C15	-3.07	1.42	1.48
3	B	2001[B]	A1C68	C4-C3	-3.06	1.35	1.39
3	B	2001[A]	A1C68	C13-N1	3.05	1.52	1.48
3	A	1302[A]	A1C68	C2-N	3.03	1.41	1.34
3	B	2001[B]	A1C68	C3-C8	3.03	1.42	1.38
3	A	1302[B]	A1C68	C13-N1	2.97	1.52	1.48
3	B	2001[A]	A1C68	C17-C15	-2.96	1.42	1.48
3	B	2001[B]	A1C68	C17-C15	-2.96	1.42	1.48
3	A	1302[B]	A1C68	C3-C8	2.93	1.42	1.38
3	A	1302[A]	A1C68	C20-N6	2.91	1.40	1.34
3	A	1302[B]	A1C68	C20-N6	2.91	1.40	1.34
3	A	1302[A]	A1C68	C17-C18	2.68	1.48	1.43
3	A	1302[B]	A1C68	C17-C18	2.68	1.48	1.43
3	A	1302[A]	A1C68	C7-C8	2.65	1.42	1.37
2	A	1301	MLA	C2-C3	2.56	1.55	1.51
3	B	2001[B]	A1C68	C7-C8	2.55	1.42	1.37
3	B	2001[B]	A1C68	C9-C10	2.45	1.57	1.55
3	A	1302[B]	A1C68	C4-C3	-2.31	1.36	1.39
2	A	1301	MLA	C2-C1	2.30	1.54	1.51
3	B	2001[A]	A1C68	C17-C18	2.22	1.47	1.43
3	B	2001[B]	A1C68	C17-C18	2.22	1.47	1.43
3	B	2001[A]	A1C68	C13-C10	2.20	1.57	1.55
3	A	1302[A]	A1C68	O-C2	-2.19	1.18	1.23
3	B	2001[A]	A1C68	C20-N6	2.11	1.38	1.34
3	B	2001[B]	A1C68	C20-N6	2.11	1.38	1.34
3	B	2001[B]	A1C68	C9-N1	2.10	1.51	1.48
3	B	2001[B]	A1C68	F-C5	-2.09	1.29	1.35
2	A	1301	MLA	O1A-C1	-2.07	1.24	1.30
3	A	1302[A]	A1C68	F-C5	-2.01	1.30	1.35

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2001[A]	A1C68	C22-C1-N	-6.22	103.66	110.25
3	A	1302[A]	A1C68	C22-C1-N	-4.63	105.34	110.25
3	A	1302[A]	A1C68	C15-C14-N3	-3.57	104.46	107.75
3	A	1302[B]	A1C68	C15-C14-N3	-3.57	104.46	107.75
3	B	2001[A]	A1C68	C-C1-N	3.51	115.99	109.19
3	A	1302[B]	A1C68	C3-C2-N	-3.12	109.89	116.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2001[A]	A1C68	O-C2-C3	3.11	126.73	121.03
3	A	1302[A]	A1C68	O-C2-C3	3.00	126.54	121.03
3	B	2001[B]	A1C68	C3-C2-N	-2.89	110.40	116.67
3	B	2001[A]	A1C68	C15-C14-N3	-2.88	105.09	107.75
3	B	2001[B]	A1C68	C15-C14-N3	-2.88	105.09	107.75
3	B	2001[A]	A1C68	F-C5-C6	2.41	120.67	118.37
3	B	2001[A]	A1C68	C7-C6-C5	2.38	119.01	116.53
3	A	1302[B]	A1C68	C7-C6-C5	2.36	119.00	116.53
3	B	2001[A]	A1C68	C15-C16-N4	-2.32	110.25	112.09
3	B	2001[B]	A1C68	C15-C16-N4	-2.32	110.25	112.09
3	B	2001[A]	A1C68	C7-C8-C3	-2.28	120.96	123.48
3	A	1302[B]	A1C68	O-C2-C3	2.23	125.12	121.03
2	A	1301	MLA	O1B-C1-C2	-2.15	115.99	122.11
3	B	2001[A]	A1C68	C9-N1-C13	-2.13	90.30	93.99
3	A	1302[A]	A1C68	C-C1-N	2.11	113.28	109.19
3	B	2001[A]	A1C68	F1-C8-C3	2.11	123.18	119.62
3	B	2001[B]	A1C68	O-C2-C3	2.09	124.86	121.03
3	B	2001[A]	A1C68	C14-C15-C16	2.08	106.06	104.22
3	B	2001[B]	A1C68	C14-C15-C16	2.08	106.06	104.22
3	A	1302[B]	A1C68	F3-C22-C1	2.08	115.01	112.11
3	A	1302[A]	A1C68	F4-C22-F3	-2.04	102.44	106.87
3	B	2001[A]	A1C68	C4-C3-C8	2.03	119.35	116.83

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1302[A]	A1C68	C16-C15-C17-C20
3	A	1302[B]	A1C68	C16-C15-C17-C20
3	B	2001[A]	A1C68	C16-C15-C17-C20
3	B	2001[A]	A1C68	C16-C15-C17-C18
3	B	2001[B]	A1C68	C16-C15-C17-C20
3	B	2001[B]	A1C68	C16-C15-C17-C18
3	A	1302[A]	A1C68	N-C2-C3-C8
3	A	1302[B]	A1C68	N-C2-C3-C8
3	B	2001[A]	A1C68	N-C2-C3-C8
3	B	2001[B]	A1C68	N-C2-C3-C8
3	A	1302[B]	A1C68	O-C2-C3-C8
3	B	2001[B]	A1C68	O-C2-C3-C8
3	A	1302[A]	A1C68	O-C2-C3-C8
3	B	2001[A]	A1C68	O-C2-C3-C8
3	A	1302[B]	A1C68	C7-C6-N1-C13

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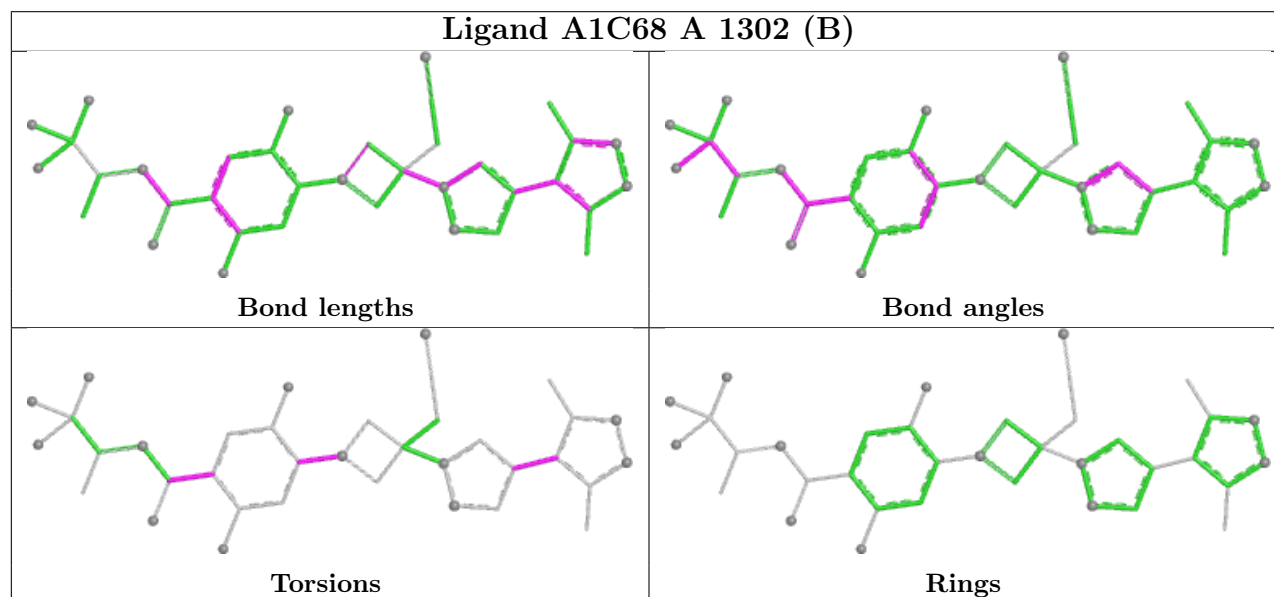
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Mol	Chain	Res	Type	Atoms
3	A	1302[A]	A1C68	C14-C15-C17-C20
3	A	1302[B]	A1C68	C14-C15-C17-C20
3	B	2001[A]	A1C68	C14-C15-C17-C20
3	B	2001[B]	A1C68	C14-C15-C17-C20
3	B	2001[B]	A1C68	C7-C6-N1-C13
3	B	2001[A]	A1C68	O-C2-C3-C4
3	A	1302[A]	A1C68	O-C2-C3-C4
3	B	2001[A]	A1C68	N-C2-C3-C4
3	A	1302[A]	A1C68	N-C2-C3-C4
3	A	1302[B]	A1C68	O-C2-C3-C4
3	A	1302[A]	A1C68	C16-C15-C17-C18
3	A	1302[B]	A1C68	C16-C15-C17-C18

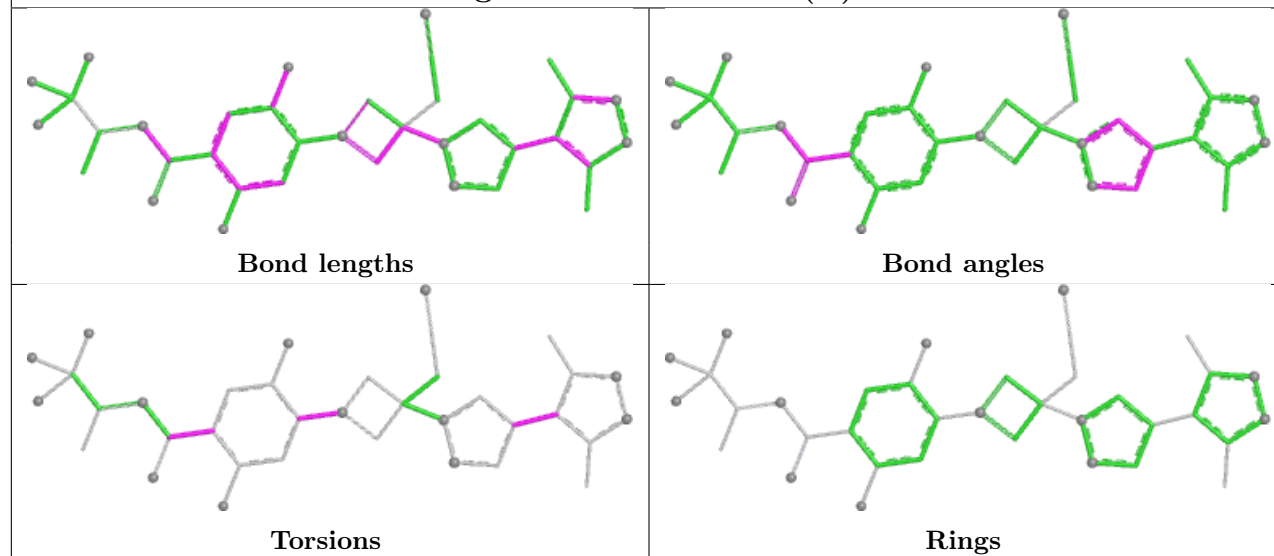
There are no ring outliers.

No monomer is involved in short contacts.

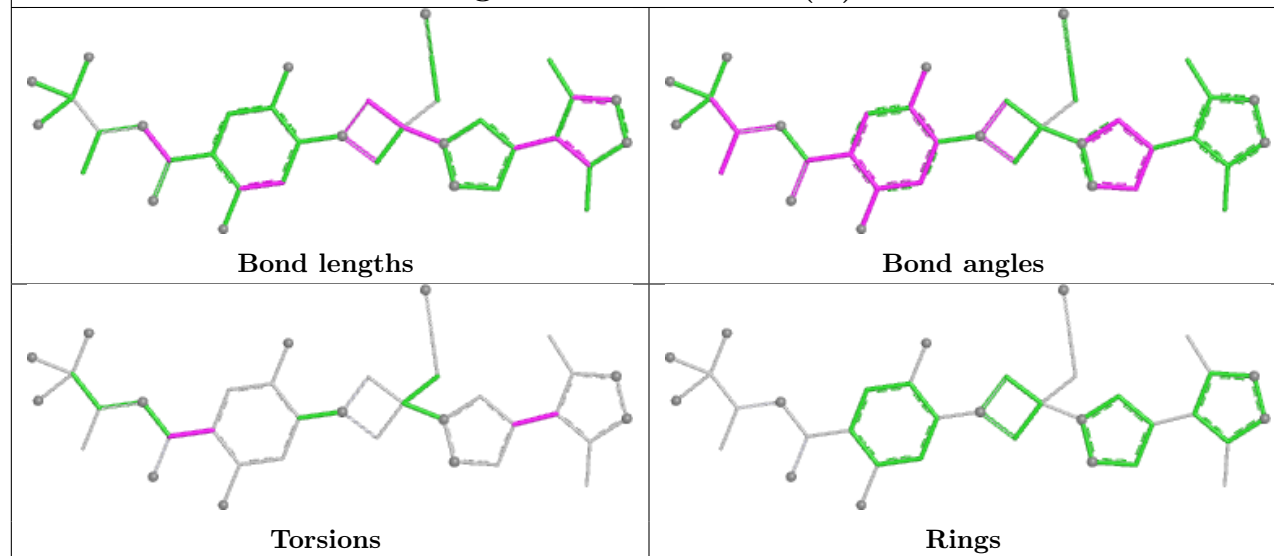
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

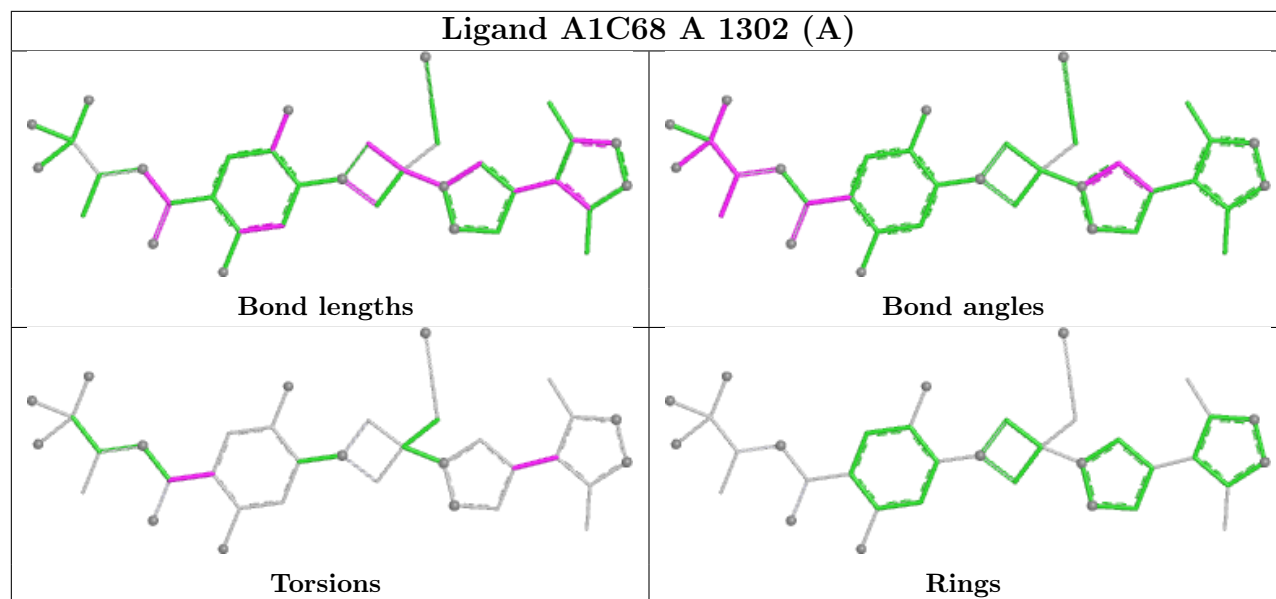


## Ligand A1C68 B 2001 (B)



## Ligand A1C68 B 2001 (A)





## 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	298/316 (94%)	0.46	26 (8%) 16 16	5, 15, 38, 54	17 (5%)
1	B	298/316 (94%)	0.43	24 (8%) 18 18	5, 16, 39, 50	17 (5%)
All	All	596/632 (94%)	0.45	50 (8%) 17 17	5, 16, 38, 54	34 (5%)

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1050	TYR	5.7
1	A	951	ILE	5.4
1	A	875	THR	5.3
1	A	871	LEU	5.2
1	A	1131	ALA	5.1
1	A	876	GLY	4.4
1	B	875	THR	4.1
1	A	872	GLN	3.9
1	A	1130	MET	3.6
1	B	860[A]	PHE	3.3
1	A	887	SER	3.3
1	B	1052	GLU	3.2
1	B	1051	ILE	3.2
1	B	886	HIS	3.1
1	B	1054	SER	3.1
1	B	1053	LYS	2.9
1	A	869[A]	ASP	2.9
1	A	874	ASN	2.8
1	A	950[A]	HIS	2.8
1	B	869	ASP	2.8
1	A	886	HIS	2.7
1	A	873	ASP	2.7
1	B	870	PRO	2.7
1	B	833	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	872	GLN	2.6
1	B	871	LEU	2.5
1	A	945	LYS	2.4
1	A	934	TYR	2.4
1	A	833	ASN	2.4
1	B	874	ASN	2.4
1	A	1132	GLY	2.4
1	A	1005	LYS	2.3
1	A	946	GLU	2.3
1	A	1004	ASP	2.3
1	B	836	PHE	2.3
1	B	847	ARG	2.3
1	B	887	SER	2.3
1	B	1068	ASP	2.2
1	A	860[A]	PHE	2.2
1	B	1003	GLN	2.2
1	B	1098	ILE	2.2
1	A	1003	GLN	2.1
1	A	847	ARG	2.1
1	B	948	ILE	2.1
1	A	947	ARG	2.1
1	B	1092	ASP	2.1
1	A	948	ILE	2.1
1	A	1067	ASN	2.1
1	B	1004	ASP	2.0
1	B	1094	CYS	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( $\text{\AA}^2$ )	Q<0.9
1	PTR	A	1007	16/17	0.90	0.12	18,31,57,59	0
1	PTR	A	1008	16/17	0.91	0.12	16,25,45,48	0
1	PTR	B	1007	16/17	0.91	0.11	18,27,57,60	0
1	PTR	B	1008	16/17	0.91	0.12	16,25,47,49	0

## 6.3 Carbohydrates [i](#)

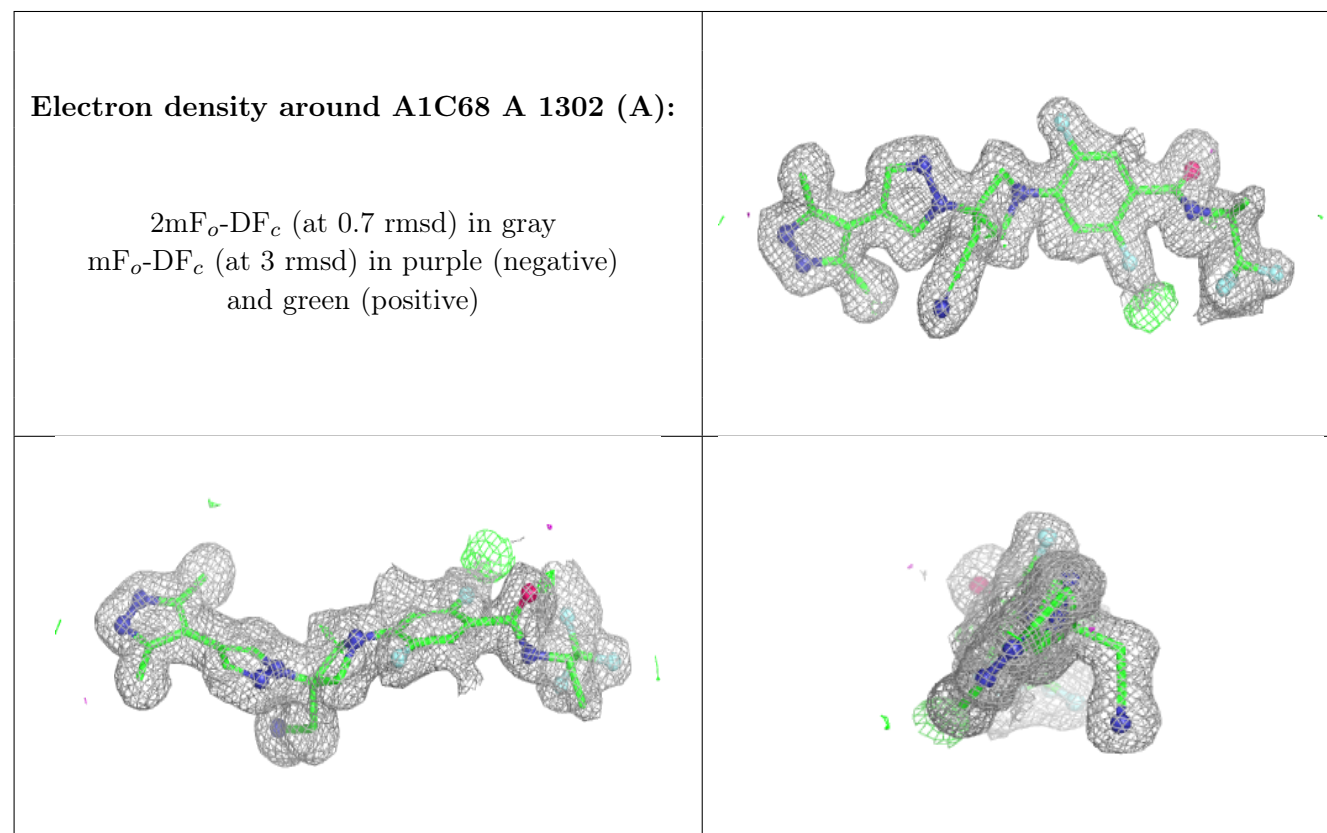
There are no oligosaccharides in this entry.

## 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.

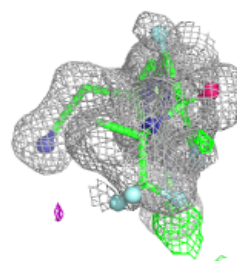
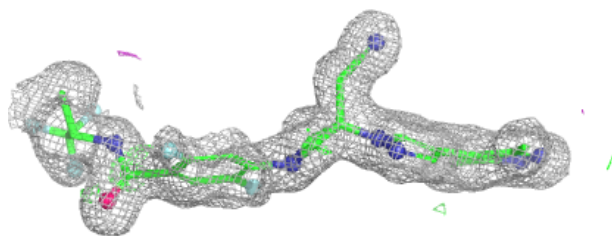
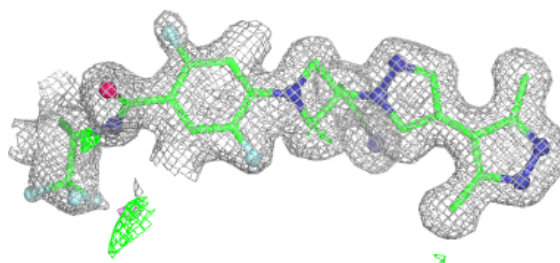
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	MLA	A	1301	7/7	0.92	0.20	15,17,23,23	0
3	A1C68	A	1302[A]	36/36	0.96	0.07	9,13,22,23	20
3	A1C68	A	1302[B]	36/36	0.96	0.07	9,13,21,24	20
3	A1C68	B	2001[A]	36/36	0.97	0.06	8,13,24,28	20
3	A1C68	B	2001[B]	36/36	0.97	0.06	8,13,21,22	20

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.

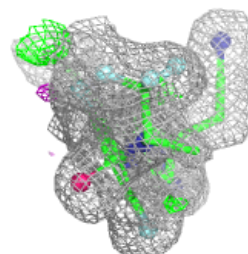
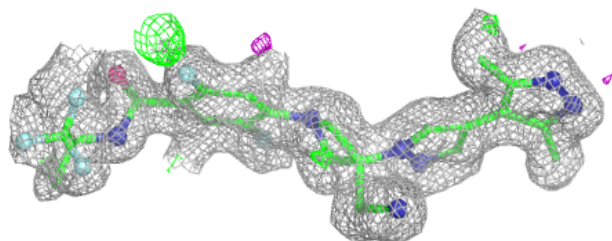
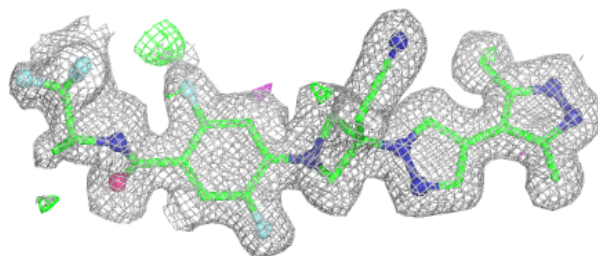


**Electron density around A1C68 A 1302 (B):**

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

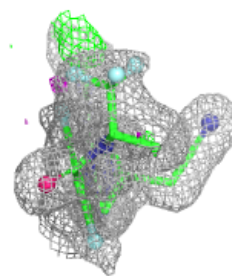
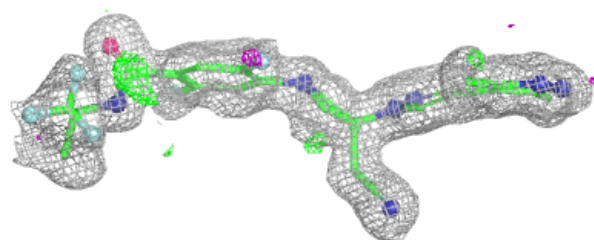
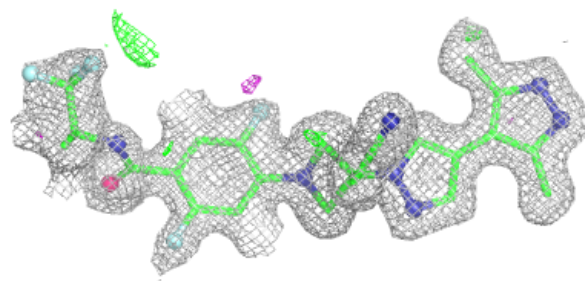
**Electron density around A1C68 B 2001 (A):**

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



**Electron density around A1C68 B 2001 (B):**

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



## 6.5 Other polymers ⓘ

There are no such residues in this entry.