



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 01:25 PM UTC

PDB ID : 8BX6 / pdb_00008bx6
Title : Crystal structure of JAK2 JH1 in complex with cerdulatinib
Authors : Haikarainen, T.
Deposited on : 2022-12-08
Resolution : 1.50 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 ⓘ symbol.

The types of validation reports are described at

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

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

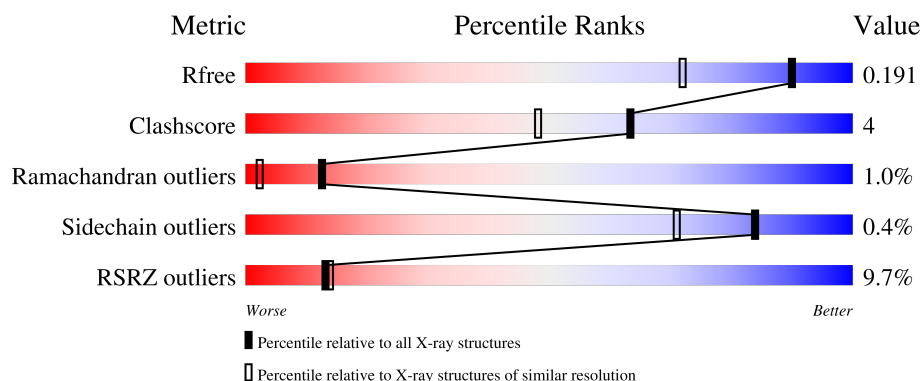
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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	4037 (1.50-1.50)
Clashscore	190562	4235 (1.50-1.50)
Ramachandran outliers	187476	4153 (1.50-1.50)
Sidechain outliers	187428	4150 (1.50-1.50)
RSRZ outliers	180081	4039 (1.50-1.50)

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 ≥ 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	9% 87% 7% • 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5251 atoms, of which 2479 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.

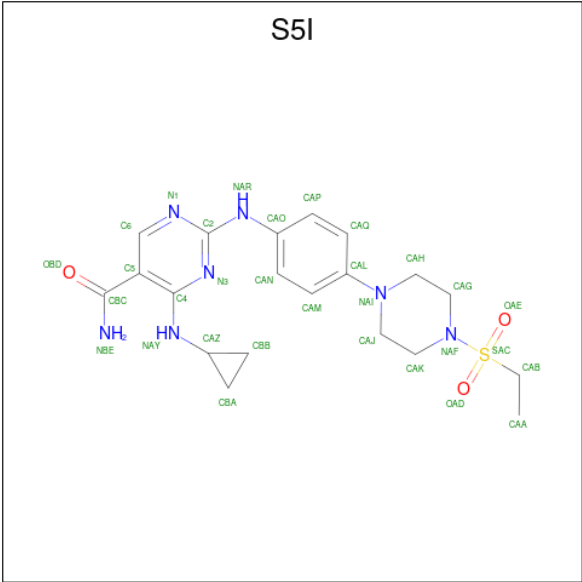
- Molecule 1 is a protein called Tyrosine-protein kinase JAK2.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	A	300	Total	C	H	N	O	P	S	0	9	0
			4953	1598	2452	421	465	2	15			

There are 23 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

- Molecule 2 is Cerdulatinib (CCD ID: S5I) (formula: C₂₀H₂₇N₇O₃S) (labeled as "Ligand of Interest" by depositor).



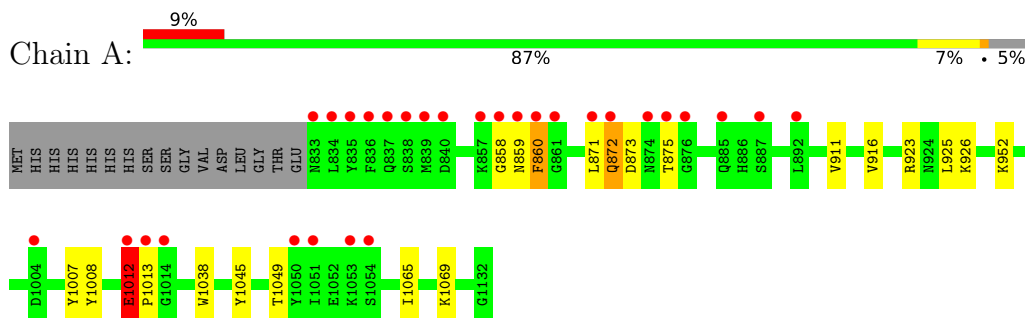
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	S	0	0
			58	20	27	7	3	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	231	Total	O	0	9
			240	240		

i

- Molecule 1: Tyrosine-protein kinase JAK2



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	107.89Å 69.23Å 50.27Å 90.00° 99.33° 90.00°	Depositor
Resolution (Å)	58.04 – 1.50 58.04 – 1.50	Depositor EDS
% Data completeness (in resolution range)	99.4 (58.04-1.50) 99.5 (58.04-1.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.32 (at 1.50Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.173 , 0.202 (Not available) , 0.191	Depositor DCC
R_{free} test set	2944 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	19.1	Xtriage
Anisotropy	0.390	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.45 , 40.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	5251	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.17% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: PTR, S5I

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	0.70	0/2548	0.78	0/3435

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1012	GLU	Peptide
1	A	923	ARG	Sidechain

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	2501	2452	2470	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	31	27	0	0	0
3	A	240	0	0	0	0
All	All	2772	2479	2470	20	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 4.

All (20) 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:916:VAL:HG13	1:A:925:LEU:CD1	2.31	0.60
1:A:911[A]:VAL:HG11	1:A:983:LEU:HD12	1.84	0.58
1:A:916:VAL:CG1	1:A:925:LEU:CD1	2.81	0.57
1:A:871:LEU:O	1:A:873:ASP:N	2.41	0.53
1:A:858:GLY:O	1:A:859:ASN:C	2.55	0.50
1:A:871:LEU:O	1:A:872:GLN:C	2.57	0.47
1:A:916:VAL:HG11	1:A:925:LEU:HD13	1.96	0.47
1:A:925:LEU:HD12	1:A:926:LYS:N	2.29	0.47
1:A:859:ASN:O	1:A:860:PHE:CD1	2.70	0.45
1:A:916:VAL:HG13	1:A:925:LEU:HD12	1.99	0.44
1:A:964:MET:SD	1:A:967[B]:LEU:HD12	2.58	0.43
1:A:1045:TYR:O	1:A:1049:THR:HG23	2.18	0.43
1:A:916:VAL:HG11	1:A:925:LEU:CD1	2.47	0.43
1:A:1065[A]:ILE:HG22	1:A:1069:LYS:HD2	1.99	0.43
1:A:860:PHE:O	1:A:860:PHE:CG	2.72	0.42
1:A:873:ASP:OD1	1:A:875:THR:OG1	2.35	0.41
1:A:1012:GLU:O	1:A:1013:PRO:C	2.63	0.41
1:A:916:VAL:CG1	1:A:925:LEU:HD13	2.51	0.41
1:A:1038:TRP:CD1	1:A:1038:TRP:C	3.00	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	305/316 (96%)	292 (96%)	10 (3%)	3 (1%)	12	2

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	872	GLN
1	A	1012	GLU
1	A	860	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	273/286 (96%)	271 (99%)	2 (1%)	76	57

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	967[A]	LEU
1	A	967[B]	LEU

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

Mol	Chain	Res	Type
1	A	853	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	1.38	1 (6%)	17,22,24	0.78	1 (5%)
1	PTR	A	1007	1	15,16,17	1.33	1 (6%)	17,22,24	0.69	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	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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1008	PTR	OH-CZ	-4.40	1.30	1.40
1	A	1007	PTR	OH-CZ	-4.16	1.31	1.40

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1008	PTR	P-OH-CZ	2.55	132.95	123.88

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](#)

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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	S5I	A	1201	-	34,34,34	3.82	16 (47%)	47,49,49	3.60	22 (46%)

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	S5I	A	1201	-	-	5/25/37/37	0/4/4/4

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1201	S5I	CAB-SAC	8.84	1.83	1.76
2	A	1201	S5I	SAC-NAF	7.72	1.73	1.63
2	A	1201	S5I	CAN-CAM	7.58	1.51	1.38
2	A	1201	S5I	CAP-CAO	7.40	1.51	1.39
2	A	1201	S5I	C4-NAY	6.67	1.45	1.35
2	A	1201	S5I	CAQ-CAL	6.26	1.51	1.39
2	A	1201	S5I	CBC-NBE	4.96	1.42	1.33
2	A	1201	S5I	CAN-CAO	-4.79	1.31	1.39
2	A	1201	S5I	C5-C4	-4.60	1.36	1.42
2	A	1201	S5I	OAD-SAC	3.75	1.47	1.43
2	A	1201	S5I	C5-CBC	3.55	1.54	1.50
2	A	1201	S5I	OAE-SAC	3.44	1.47	1.43
2	A	1201	S5I	CAQ-CAP	-3.27	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1201	S5I	C2-NAR	3.13	1.43	1.36
2	A	1201	S5I	CAM-CAL	-2.90	1.33	1.39
2	A	1201	S5I	CAL-NAI	2.32	1.45	1.38

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1201	S5I	OAE-SAC-OAD	-17.73	101.13	118.99
2	A	1201	S5I	CAK-NAF-CAG	7.10	120.28	112.12
2	A	1201	S5I	C6-C5-C4	5.25	119.94	114.67
2	A	1201	S5I	CAJ-NAI-CAH	4.65	122.03	111.57
2	A	1201	S5I	C4-NAY-CAZ	-4.58	116.45	124.18
2	A	1201	S5I	CAP-CAO-CAN	4.56	125.09	119.04
2	A	1201	S5I	C5-C6-N1	-3.73	119.07	124.32
2	A	1201	S5I	N1-C2-N3	-3.62	122.92	126.42
2	A	1201	S5I	OAD-SAC-NAF	3.49	110.68	107.28
2	A	1201	S5I	OAE-SAC-NAF	3.07	110.27	107.28
2	A	1201	S5I	CBA-CAZ-NAY	-3.07	111.67	118.06
2	A	1201	S5I	OAE-SAC-CAB	2.96	112.77	108.27
2	A	1201	S5I	CAQ-CAP-CAO	-2.63	117.28	120.30
2	A	1201	S5I	CAH-CAG-NAF	2.44	111.56	108.97
2	A	1201	S5I	CAM-CAN-CAO	-2.42	117.52	120.30
2	A	1201	S5I	CAM-CAL-NAI	-2.40	118.05	121.39
2	A	1201	S5I	CAQ-CAL-NAI	-2.33	118.16	121.39
2	A	1201	S5I	CAN-CAO-NAR	-2.30	112.81	120.61
2	A	1201	S5I	CAQ-CAL-CAM	2.26	123.49	119.18
2	A	1201	S5I	OAD-SAC-CAB	2.12	111.50	108.27
2	A	1201	S5I	OBD-CBC-C5	2.11	122.72	120.24
2	A	1201	S5I	NAR-C2-N3	2.08	124.03	116.90

There are no chirality outliers.

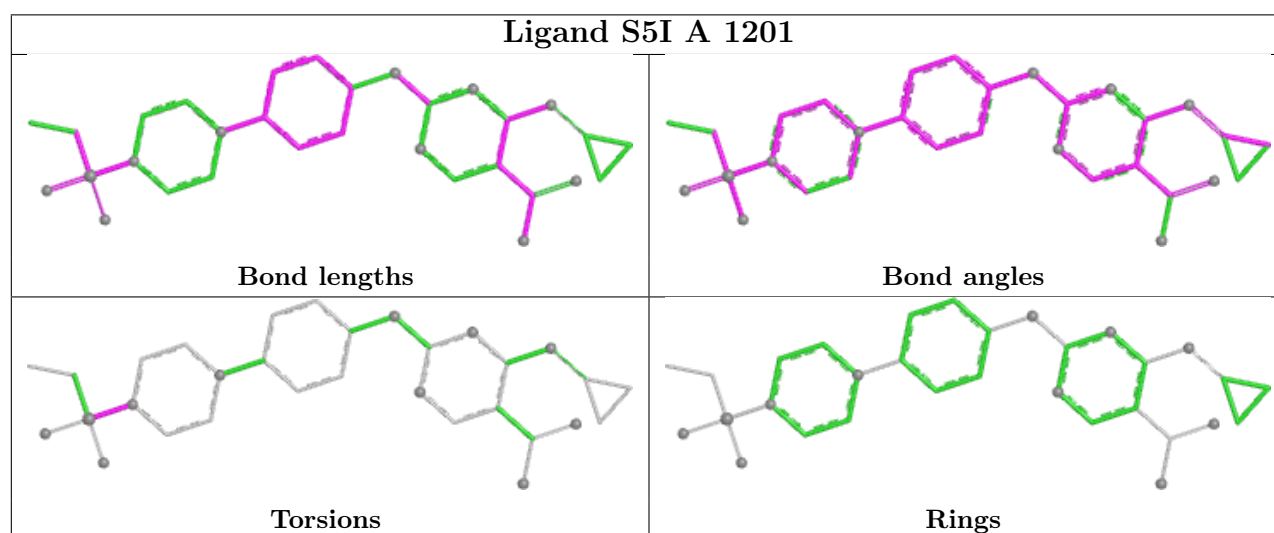
All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1201	S5I	CAG-NAF-SAC-CAB
2	A	1201	S5I	CAG-NAF-SAC-OAE
2	A	1201	S5I	CAK-NAF-SAC-CAB
2	A	1201	S5I	CAG-NAF-SAC-OAD
2	A	1201	S5I	CAK-NAF-SAC-OAE

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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 ²)	Q<0.9
1	A	298/316 (94%)	0.34	29 (9%) 13 14	11, 25, 60, 76	9 (3%)

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	860	PHE	8.3
1	A	859	ASN	5.8
1	A	1013	PRO	4.7
1	A	1050	TYR	4.3
1	A	875	THR	4.0
1	A	857	LYS	4.0
1	A	872	GLN	4.0
1	A	1051	ILE	3.9
1	A	858	GLY	3.8
1	A	839	MET	3.5
1	A	876	GLY	3.5
1	A	834	LEU	3.4
1	A	838	SER	3.2
1	A	836	PHE	3.0
1	A	833	ASN	2.9
1	A	861	GLY	2.9
1	A	887	SER	2.9
1	A	1053	LYS	2.9
1	A	892	LEU	2.8
1	A	871	LEU	2.8
1	A	1054	SER	2.7
1	A	885	GLN	2.5
1	A	1004	ASP	2.5
1	A	837	GLN	2.5
1	A	840	ASP	2.4
1	A	1012	GLU	2.3
1	A	1014	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	874	ASN	2.3
1	A	835	TYR	2.2

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	B-factors($\text{\AA}^2$)	Q<0.9
1	PTR	A	1007	16/17	0.92	0.10	24,35,62,68	0
1	PTR	A	1008	16/17	0.93	0.10	21,28,50,56	0

6.3 Carbohydrates [i](#)

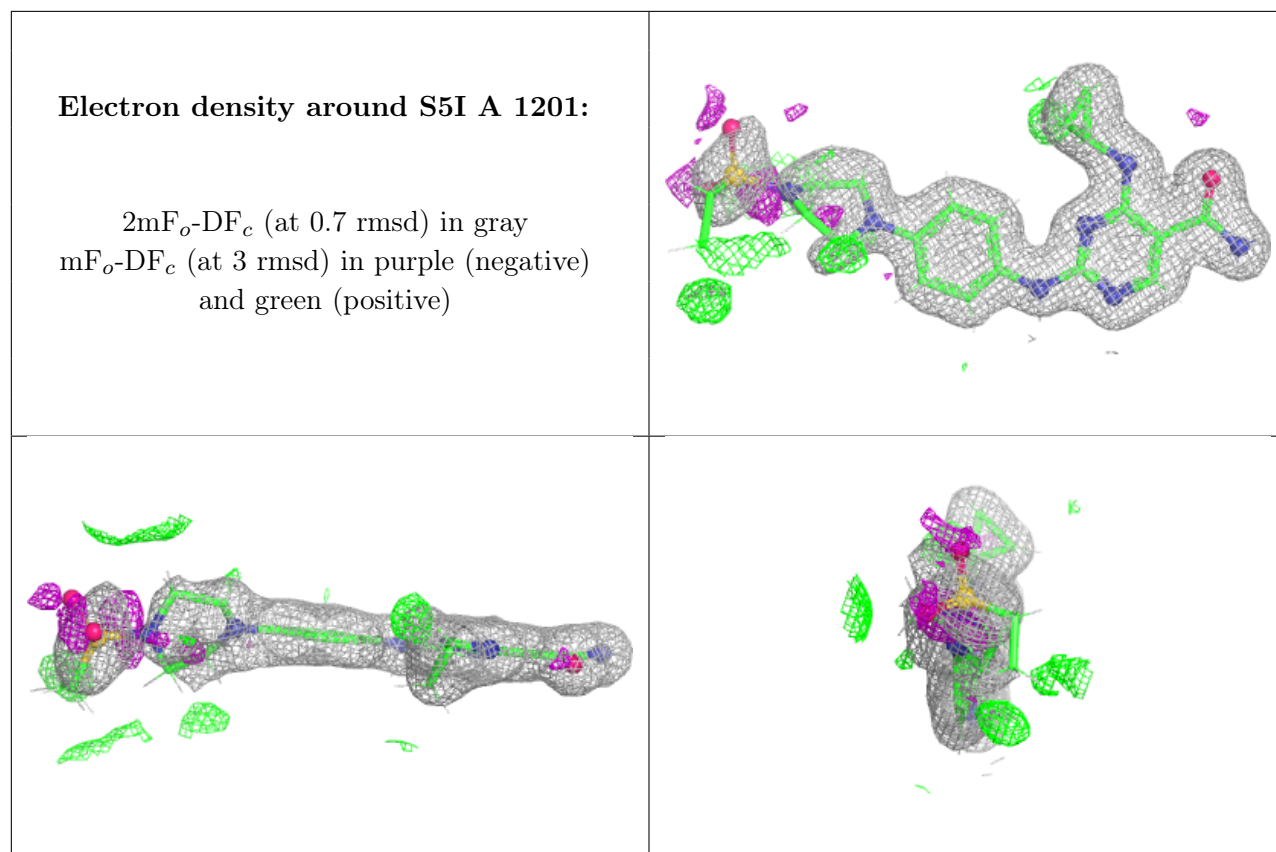
There are no oligosaccharides in this entry.

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, 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	B-factors($\text{\AA}^2$)	Q<0.9
2	S5I	A	1201	31/31	0.92	0.14	19,32,94,96	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.