



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:31 AM UTC

PDB ID : 5TQ5 / pdb_00005tq5
Title : Design and Synthesis of a pan-JAK Kinase Inhibitor Clinical Candidate (PF-06263276) Suitable for Inhaled and Topical Delivery for the Treatment of Inflammatory Diseases of the Lungs and Skin
Authors : Chrencik, J.; Jones, P.
Deposited on : 2016-10-23
Resolution : 2.30 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

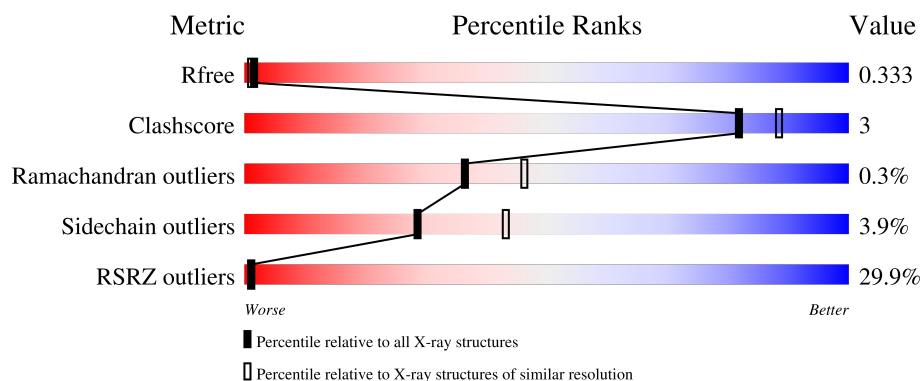
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	298	29% 87% 9% ..

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 2432 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.

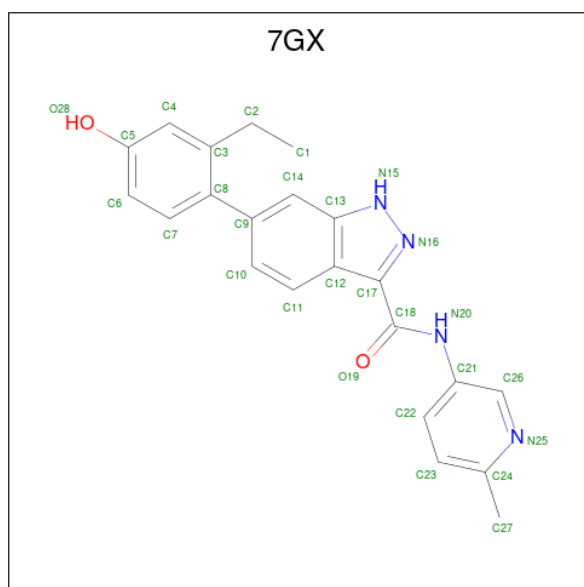
- Molecule 1 is a protein called Tyrosine-protein kinase JAK2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	291	Total	C	N	O	S	0	0	0
			2370	1508	408	441	13			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	835	GLY	-	expression tag	UNP O60674
A	836	SER	-	expression tag	UNP O60674
A	1073	SER	MET	engineered mutation	UNP O60674
A	1076	THR	PHE	engineered mutation	UNP O60674

- Molecule 2 is 6-(2-ethyl-4-hydroxyphenyl)-N-(6-methylpyridin-3-yl)-1H-indazole-3-carboxamide (CCD ID: 7GX) (formula: C₂₂H₂₀N₄O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			28	22	4	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	34	Total 34	O 34	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	37.00Å 45.11Å 52.81Å 104.11° 110.08° 94.73°	Depositor
Resolution (Å)	27.31 – 2.30 27.31 – 2.30	Depositor EDS
% Data completeness (in resolution range)	92.6 (27.31-2.30) 92.6 (27.31-2.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	50.00 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.279 , 0.332 0.281 , 0.333	Depositor DCC
R_{free} test set	663 reflections (5.27%)	wwPDB-VP
Wilson B-factor (Å ²)	13.3	Xtriage
Anisotropy	0.209	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 33.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.57$, $\langle L^2 \rangle = 0.42$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	2432	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.04% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 7GX

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	0.73	0/2422	0.95	1/3268 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	857	LYS	N-CA-C	5.07	116.78	109.07

There are no chirality outliers.

There are no planarity outliers.

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	2370	0	2326	12	0
2	A	28	0	0	0	0
3	A	34	0	0	0	0
All	All	2432	0	2326	12	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 3.

All (12) 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:907:HIS:HB3	1:A:910:ILE:HD13	1.71	0.72
1:A:911:VAL:HG21	1:A:983:LEU:HD12	1.78	0.65
1:A:909:ASN:C	1:A:910:ILE:HD12	2.29	0.58
1:A:850:LYS:HE3	1:A:872:GLN:HE21	1.73	0.53
1:A:942:GLN:HG3	1:A:1051:ILE:HB	1.92	0.51
1:A:937:LEU:HD21	1:A:1047:LEU:HD21	1.95	0.49
1:A:914:LYS:HD2	1:A:929:MET:C	2.40	0.46
1:A:869:ASP:OD2	1:A:872:GLN:HA	2.16	0.46
1:A:1018:ILE:HD12	1:A:1078:LEU:HD22	1.99	0.45
1:A:917:CYS:HB3	1:A:926:LYS:HB2	1.98	0.44
1:A:965:GLU:OE2	1:A:1117:ARG:NH1	2.52	0.43
1:A:979:THR:HA	1:A:982:ILE:HD12	2.02	0.42

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	289/298 (97%)	282 (98%)	6 (2%)	1 (0%)	36	46

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
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	258/271 (95%)	248 (96%)	10 (4%)	28	43

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	872	GLN
1	A	897	ARG
1	A	903	LYS
1	A	906	GLN
1	A	910	ILE
1	A	967	LEU
1	A	980	ARG
1	A	1005	LYS
1	A	1092	ASP
1	A	1117	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	872	GLN
1	A	906	GLN
1	A	1070	GLN
1	A	1108	ASN
1	A	1111	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](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	7GX	A	4000	-	31,31,31	0.39	0	42,44,44	0.81	2 (4%)

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	7GX	A	4000	-	-	2/14/14/14	0/4/4/4

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4000	7GX	C12-C17-N16	-3.67	108.28	111.17
2	A	4000	7GX	C17-N16-N15	2.15	107.64	106.07

There are no chirality outliers.

All (2) torsion outliers are listed below:

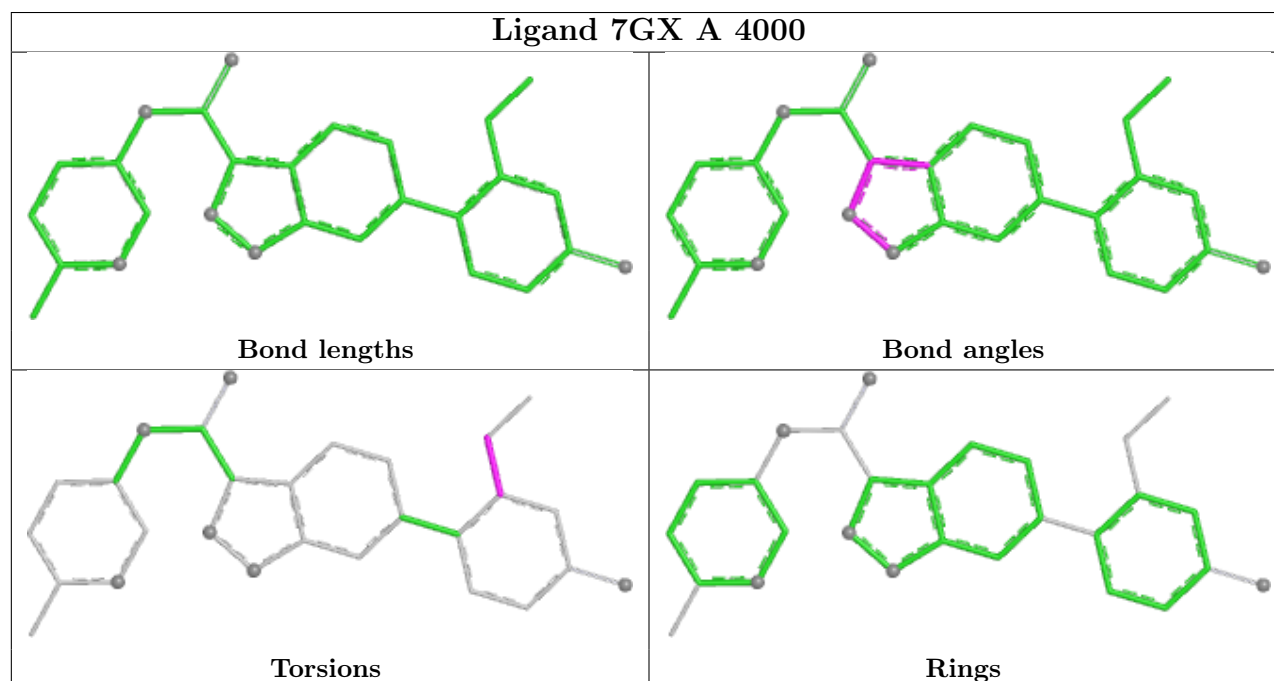
Mol	Chain	Res	Type	Atoms
2	A	4000	7GX	C1-C2-C3-C4
2	A	4000	7GX	C1-C2-C3-C8

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	291/298 (97%)	1.73	87 (29%) 1 1	4, 15, 38, 66	2 (0%)

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	842	THR	8.4
1	A	841	PRO	6.6
1	A	858	GLY	6.6
1	A	860	PHE	6.4
1	A	1092	ASP	6.2
1	A	1014	GLY	5.7
1	A	859	ASN	5.5
1	A	1011	LYS	5.2
1	A	843	GLN	5.1
1	A	1012	GLU	4.8
1	A	1013	PRO	4.8
1	A	886	HIS	4.7
1	A	918	TYR	4.4
1	A	861	GLY	4.2
1	A	885	GLN	4.1
1	A	888	THR	4.1
1	A	854	GLN	4.0
1	A	1122	ARG	4.0
1	A	1066	GLY	4.0
1	A	1010	VAL	4.0
1	A	1070	GLN	3.8
1	A	895	PHE	3.8
1	A	853	GLN	3.7
1	A	891	HIS	3.7
1	A	856	GLY	3.6
1	A	1068	ASP	3.6
1	A	1069	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	1071	GLY	3.5
1	A	1063	ARG	3.4
1	A	1029	SER	3.4
1	A	893	ARG	3.3
1	A	962	LYS	3.3
1	A	924	ASN	3.2
1	A	1004	ASP	3.2
1	A	1008	TYR	3.2
1	A	947	ARG	3.2
1	A	1000	VAL	3.2
1	A	1067	ASN	3.2
1	A	1118	ASP	3.1
1	A	1007	TYR	3.0
1	A	1051	ILE	3.0
1	A	942	GLN	3.0
1	A	1006	GLU	2.9
1	A	1015	GLU	2.9
1	A	844	PHE	2.9
1	A	906	GLN	2.9
1	A	887	SER	2.8
1	A	899	ILE	2.7
1	A	1057	PRO	2.7
1	A	894	ASP	2.7
1	A	1059	ALA	2.7
1	A	1131	ALA	2.6
1	A	890	GLU	2.6
1	A	855	LEU	2.6
1	A	892	LEU	2.6
1	A	1020	TRP	2.5
1	A	857	LYS	2.5
1	A	1084	ASN	2.5
1	A	1073	SER	2.4
1	A	966	TYR	2.4
1	A	1072	GLN	2.4
1	A	1065	ILE	2.4
1	A	1001	LEU	2.4
1	A	1083	LYS	2.4
1	A	988	ASN	2.3
1	A	884	LEU	2.3
1	A	980	ARG	2.3
1	A	1058	PRO	2.3
1	A	920	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	923	ARG	2.2
1	A	944	HIS	2.2
1	A	1054	SER	2.2
1	A	1129	ASN	2.2
1	A	1009	LYS	2.2
1	A	896	GLU	2.2
1	A	872	GLN	2.2
1	A	1079	ILE	2.1
1	A	1074	ILE	2.1
1	A	989	ARG	2.1
1	A	1100	MET	2.1
1	A	889	GLU	2.1
1	A	900	GLU	2.1
1	A	1121	LEU	2.1
1	A	879	VAL	2.1
1	A	958	SER	2.1
1	A	1018	ILE	2.1
1	A	1112	GLN	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

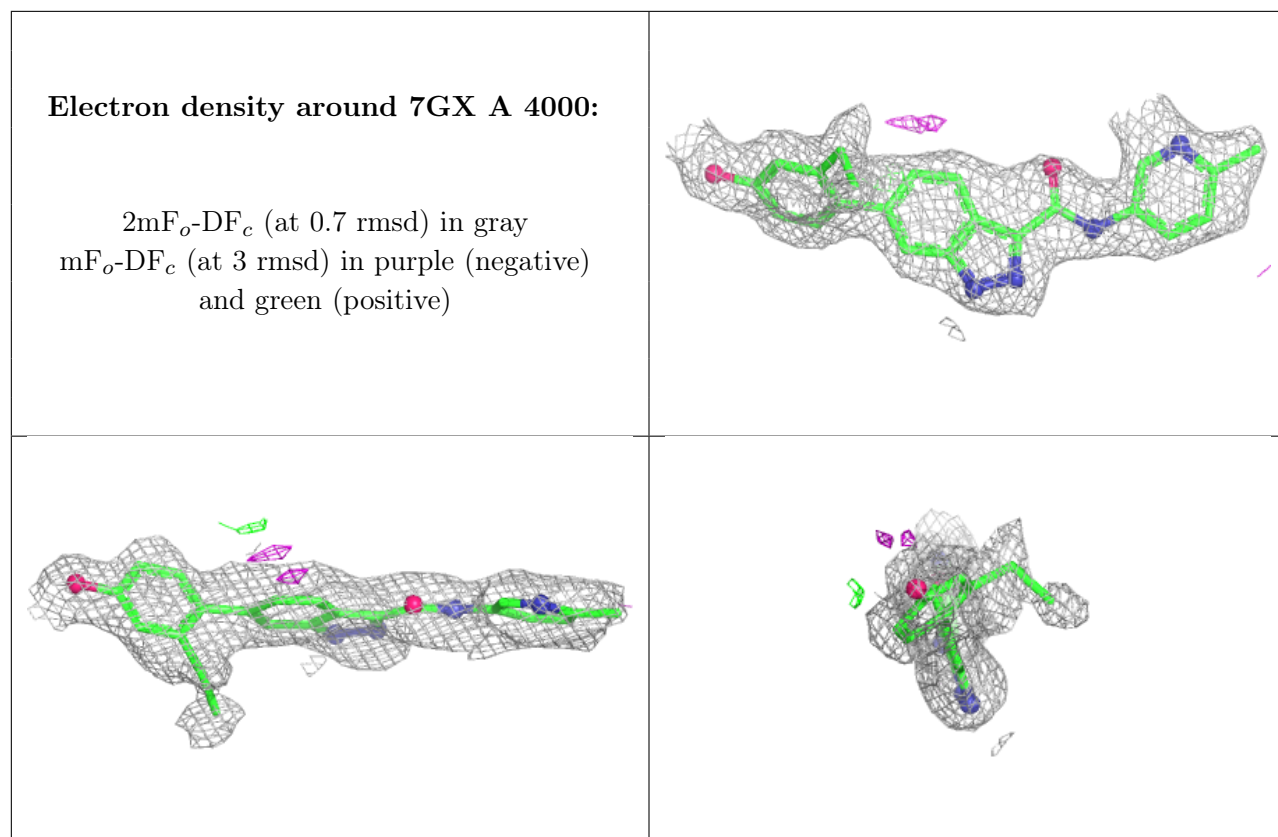
There are no oligosaccharides in this entry.

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	7GX	A	4000	28/28	0.82	0.15	13,14,17,18	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.