



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:03 PM UTC

PDB ID : 8FF8 / pdb_00008ff8
Title : CRYSTAL STRUCTURE OF GLYCOGEN SYNTHASE KINASE 3 BETA COMPLEXED WITH 2-[(4-CYANOPHENYL)AMINO]-N-(4-PHENYLPYRIDIN-3-YL)PYRIMIDINE-4-CARBOXAMIDE
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Deposited on : 2022-12-08
Resolution : 2.33 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

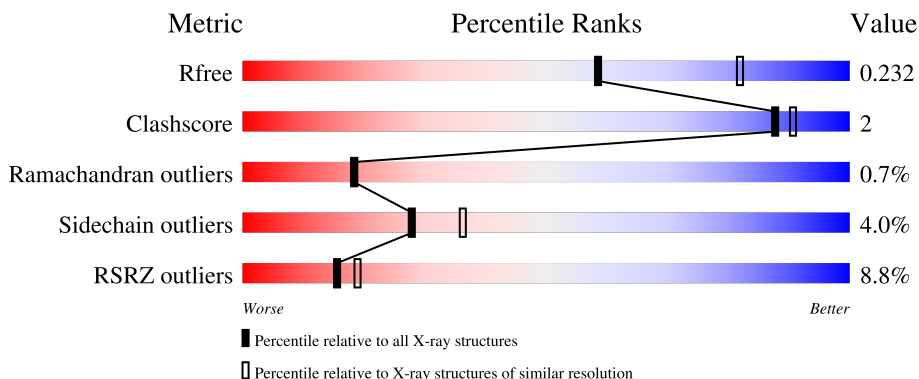
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.33 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	3031 (2.36-2.32)
Clashscore	190562	3127 (2.36-2.32)
Ramachandran outliers	187476	3095 (2.36-2.32)
Sidechain outliers	187428	3095 (2.36-2.32)
RSRZ outliers	180081	3033 (2.36-2.32)

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	441	 6% 72% 6% 21%
1	B	441	 8% 73% 5% 22%

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 5654 atoms, of which 32 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 Glycogen synthase kinase-3 beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	347	2674	1733	442	488	11	0	0	0
1	B	346	2661	1722	438	490	11	0	0	0

There are 42 discrepancies between the modelled and reference sequences:

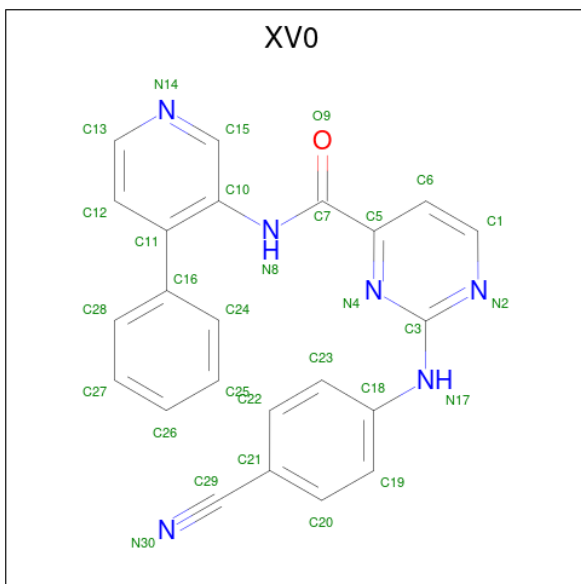
Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	initiating methionine	UNP P49841
A	-19	HIS	-	expression tag	UNP P49841
A	-18	SER	-	expression tag	UNP P49841
A	-17	SER	-	expression tag	UNP P49841
A	-16	HIS	-	expression tag	UNP P49841
A	-15	HIS	-	expression tag	UNP P49841
A	-14	HIS	-	expression tag	UNP P49841
A	-13	HIS	-	expression tag	UNP P49841
A	-12	HIS	-	expression tag	UNP P49841
A	-11	HIS	-	expression tag	UNP P49841
A	-10	SER	-	expression tag	UNP P49841
A	-9	SER	-	expression tag	UNP P49841
A	-8	GLY	-	expression tag	UNP P49841
A	-7	GLU	-	expression tag	UNP P49841
A	-6	ASN	-	expression tag	UNP P49841
A	-5	LEU	-	expression tag	UNP P49841
A	-4	TYR	-	expression tag	UNP P49841
A	-3	PHE	-	expression tag	UNP P49841
A	-2	GLN	-	expression tag	UNP P49841
A	-1	GLY	-	expression tag	UNP P49841
A	0	HIS	-	expression tag	UNP P49841
B	-20	MET	-	initiating methionine	UNP P49841
B	-19	HIS	-	expression tag	UNP P49841
B	-18	SER	-	expression tag	UNP P49841
B	-17	SER	-	expression tag	UNP P49841

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	HIS	-	expression tag	UNP P49841
B	-15	HIS	-	expression tag	UNP P49841
B	-14	HIS	-	expression tag	UNP P49841
B	-13	HIS	-	expression tag	UNP P49841
B	-12	HIS	-	expression tag	UNP P49841
B	-11	HIS	-	expression tag	UNP P49841
B	-10	SER	-	expression tag	UNP P49841
B	-9	SER	-	expression tag	UNP P49841
B	-8	GLY	-	expression tag	UNP P49841
B	-7	GLU	-	expression tag	UNP P49841
B	-6	ASN	-	expression tag	UNP P49841
B	-5	LEU	-	expression tag	UNP P49841
B	-4	TYR	-	expression tag	UNP P49841
B	-3	PHE	-	expression tag	UNP P49841
B	-2	GLN	-	expression tag	UNP P49841
B	-1	GLY	-	expression tag	UNP P49841
B	0	HIS	-	expression tag	UNP P49841

- Molecule 2 is 2-(4-cyanoanilino)-N-(4-phenylpyridin-3-yl)pyrimidine-4-carboxamide (CCD ID: XV0) (formula: C₂₃H₁₆N₆O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	H	N			O
2	A	1	Total	C	H	N	O	16	0
			46	23	16	6	1		
2	B	1	Total	C	H	N	O	16	0
			46	23	16	6	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	136	Total 136	O 136	0	0
3	B	91	Total 91	O 91	0	0

4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	82.84Å 84.08Å 177.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	88.89 – 2.33 88.89 – 2.33	Depositor EDS
% Data completeness (in resolution range)	92.6 (88.89-2.33) 92.5 (88.89-2.33)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.69 (at 2.32Å)	Xtrriage
Refinement program	BUSTER	Depositor
R, R_{free}	0.197 , 0.217 0.208 , 0.232	Depositor DCC
R_{free} test set	2440 reflections (4.51%)	wwPDB-VP
Wilson B-factor (Å ²)	40.5	Xtrriage
Anisotropy	0.949	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 45.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.028 for k,h,-l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5654	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% 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: XV0

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	0.76	0/2744	0.96	0/3756
1	B	0.72	0/2730	0.96	2/3740 (0.1%)
All	All	0.74	0/5474	0.96	2/7496 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	232	THR	N-CA-CB	-5.39	102.72	110.65
1	B	64	ASN	CA-CB-CG	5.19	117.79	112.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2674	0	2586	13	0
1	B	2661	0	2556	8	0
2	A	30	16	0	0	0
2	B	30	16	0	0	0
3	A	136	0	0	2	0
3	B	91	0	0	0	0
All	All	5622	32	5142	21	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 2.

All (21) 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:381:HIS:HD2	3:A:708:HOH:O	1.86	0.58
1:B:212:PRO:HB3	1:B:232:THR:HG23	1.89	0.54
1:B:162:MET:HE2	1:B:247:LEU:HB2	1.92	0.50
1:A:162:MET:HE2	1:A:247:LEU:HB2	1.95	0.48
1:A:304:VAL:HG22	1:A:305:PHE:CD2	2.48	0.47
1:A:301:TRP:HA	1:A:304:VAL:HG13	1.95	0.47
1:A:155:VAL:HG12	1:A:159:LYS:HE3	1.96	0.46
1:B:155:VAL:HG12	1:B:159:LYS:HE3	1.98	0.46
1:A:218:CYS:O	1:A:223:ARG:HD3	2.16	0.46
1:B:42:ALA:HB1	1:B:114:TYR:HB3	1.98	0.45
1:A:162:MET:HG3	1:A:247:LEU:HD13	1.98	0.45
1:A:62:ILE:HD13	1:A:72:GLN:HB2	1.99	0.44
1:A:226:GLU:HB3	1:A:284:MET:HB3	1.98	0.44
1:A:42:ALA:HB1	1:A:114:TYR:HB3	1.99	0.44
1:A:381:HIS:CD2	3:A:708:HOH:O	2.67	0.42
1:B:162:MET:HG3	1:B:247:LEU:HD13	2.01	0.42
1:A:304:VAL:HG22	1:A:305:PHE:CE2	2.55	0.42
1:B:373:LEU:O	1:B:377:LEU:HD22	2.20	0.41
1:B:224:ALA:HA	1:B:241:TRP:CD1	2.56	0.41
1:B:373:LEU:HB3	1:B:377:LEU:CD2	2.51	0.40
1:A:224:ALA:HA	1:A:241:TRP:CD1	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	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	345/441 (78%)	334 (97%)	8 (2%)	3 (1%)	14 13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	342/441 (78%)	330 (96%)	10 (3%)	2 (1%)	21	22
All	All	687/882 (78%)	664 (97%)	18 (3%)	5 (1%)	18	18

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	298	ALA
1	A	221	TYR
1	A	298	ALA
1	B	221	TYR
1	A	285	ASN

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	278/383 (73%)	269 (97%)	9 (3%)	34	44
1	B	278/383 (73%)	265 (95%)	13 (5%)	23	30
All	All	556/766 (73%)	534 (96%)	22 (4%)	28	36

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	SER
1	A	101	MET
1	A	126	VAL
1	A	189	LEU
1	A	263	VAL
1	A	266	LEU
1	A	284	MET
1	A	304	VAL
1	A	375	THR
1	B	46	GLN
1	B	55	SER

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Mol	Chain	Res	Type
1	B	64	ASN
1	B	81	LEU
1	B	101	MET
1	B	232	THR
1	B	263	VAL
1	B	266	LEU
1	B	290	GLU
1	B	343	LEU
1	B	354	ARG
1	B	375	THR
1	B	377	LEU

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

Mol	Chain	Res	Type
1	A	72	GLN
1	A	99	GLN
1	A	295	GLN
1	B	72	GLN
1	B	99	GLN
1	B	129	ASN
1	B	295	GLN

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 [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	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	XV0	A	501	-	33,33,33	0.20	0	43,44,44	0.54	0
2	XV0	B	501	-	33,33,33	0.20	0	43,44,44	0.53	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
2	XV0	A	501	-	-	0/18/18/18	0/4/4/4
2	XV0	B	501	-	-	0/18/18/18	0/4/4/4

There are no bond length outliers.

There are no bond angle outliers.

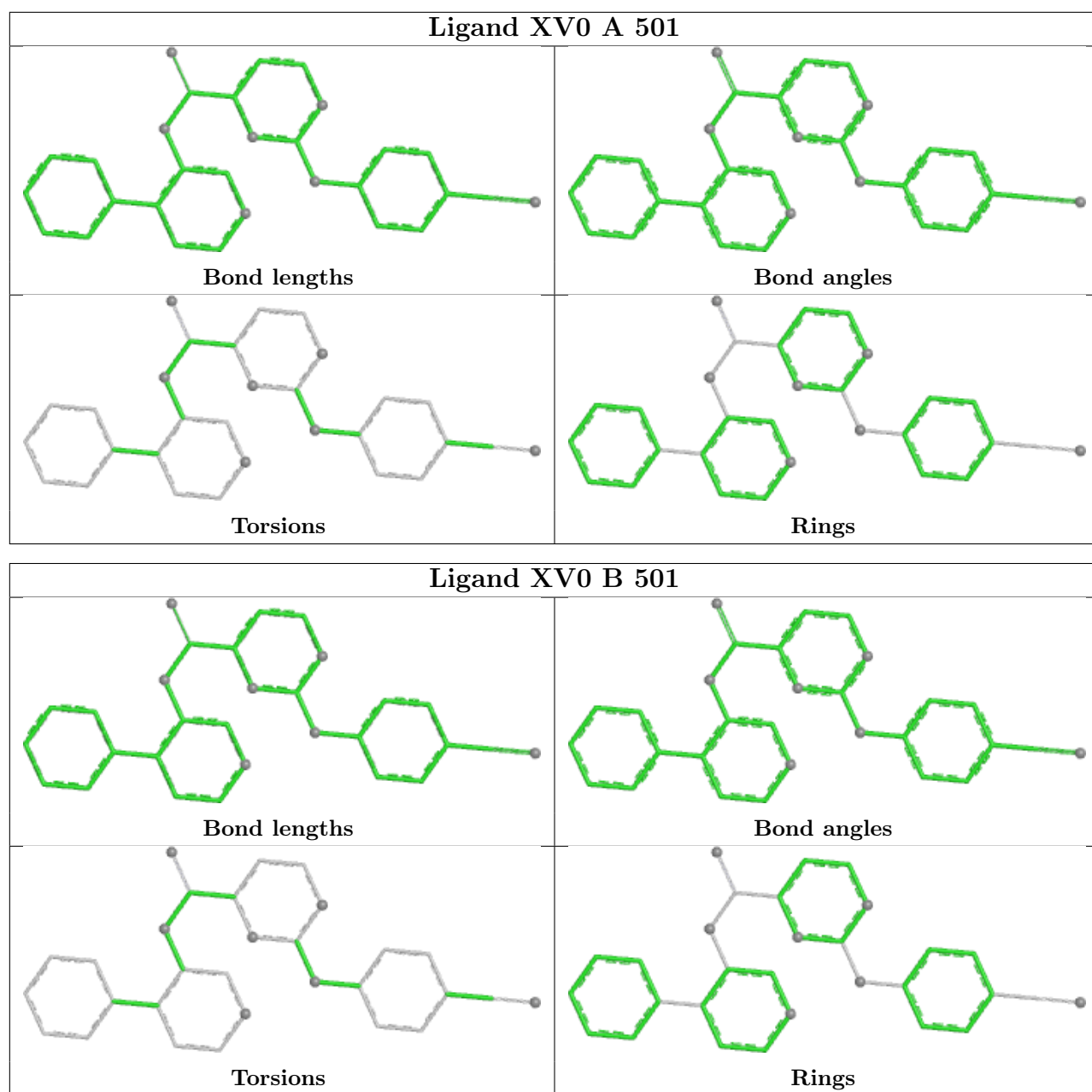
There are no chirality outliers.

There are no torsion outliers.

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	347/441 (78%)	0.52	25 (7%) 21 25	30, 47, 73, 85	0
1	B	346/441 (78%)	0.67	36 (10%) 11 14	33, 52, 77, 95	0
All	All	693/882 (78%)	0.60	61 (8%) 15 19	30, 49, 75, 95	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	298	ALA	5.7
1	B	298	ALA	5.5
1	A	299	HIS	5.2
1	B	299	HIS	5.1
1	B	124	ASP	4.4
1	B	119	SER	4.0
1	B	50	ARG	3.9
1	B	296	ILE	3.9
1	B	300	PRO	3.9
1	A	302	THR	3.7
1	A	119	SER	3.7
1	A	121	GLU	3.5
1	A	48	PRO	3.5
1	B	301	TRP	3.5
1	A	297	LYS	3.4
1	A	124	ASP	3.4
1	A	120	GLY	3.3
1	B	48	PRO	3.3
1	A	300	PRO	3.2
1	B	353	GLY	3.2
1	B	51	PRO	3.1
1	B	77	ASP	3.1
1	B	36	LYS	3.0
1	A	283	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	301	TRP	3.0
1	B	302	THR	2.9
1	B	297	LYS	2.9
1	A	66	SER	2.9
1	A	382	ALA	2.9
1	A	287	ASN	2.9
1	B	308	ARG	2.7
1	B	286	PRO	2.7
1	A	93	PHE	2.7
1	A	279	GLU	2.6
1	A	77	ASP	2.6
1	B	64	ASN	2.6
1	A	36	LYS	2.5
1	B	306	ARG	2.5
1	A	306	ARG	2.4
1	B	304	VAL	2.4
1	B	45	GLY	2.4
1	B	91	LYS	2.3
1	B	93	PHE	2.3
1	B	290	GLU	2.3
1	A	286	PRO	2.3
1	B	148	ARG	2.3
1	A	91	LYS	2.3
1	B	76	CYS	2.2
1	B	49	ASP	2.2
1	B	279	GLU	2.2
1	B	60	LYS	2.2
1	B	147	SER	2.2
1	B	352	ASN	2.1
1	B	385	GLN	2.1
1	B	145	HIS	2.1
1	A	123	LYS	2.1
1	B	114	TYR	2.1
1	B	294	PRO	2.1
1	A	289	THR	2.0
1	B	293	PHE	2.0
1	A	278	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates [i](#)

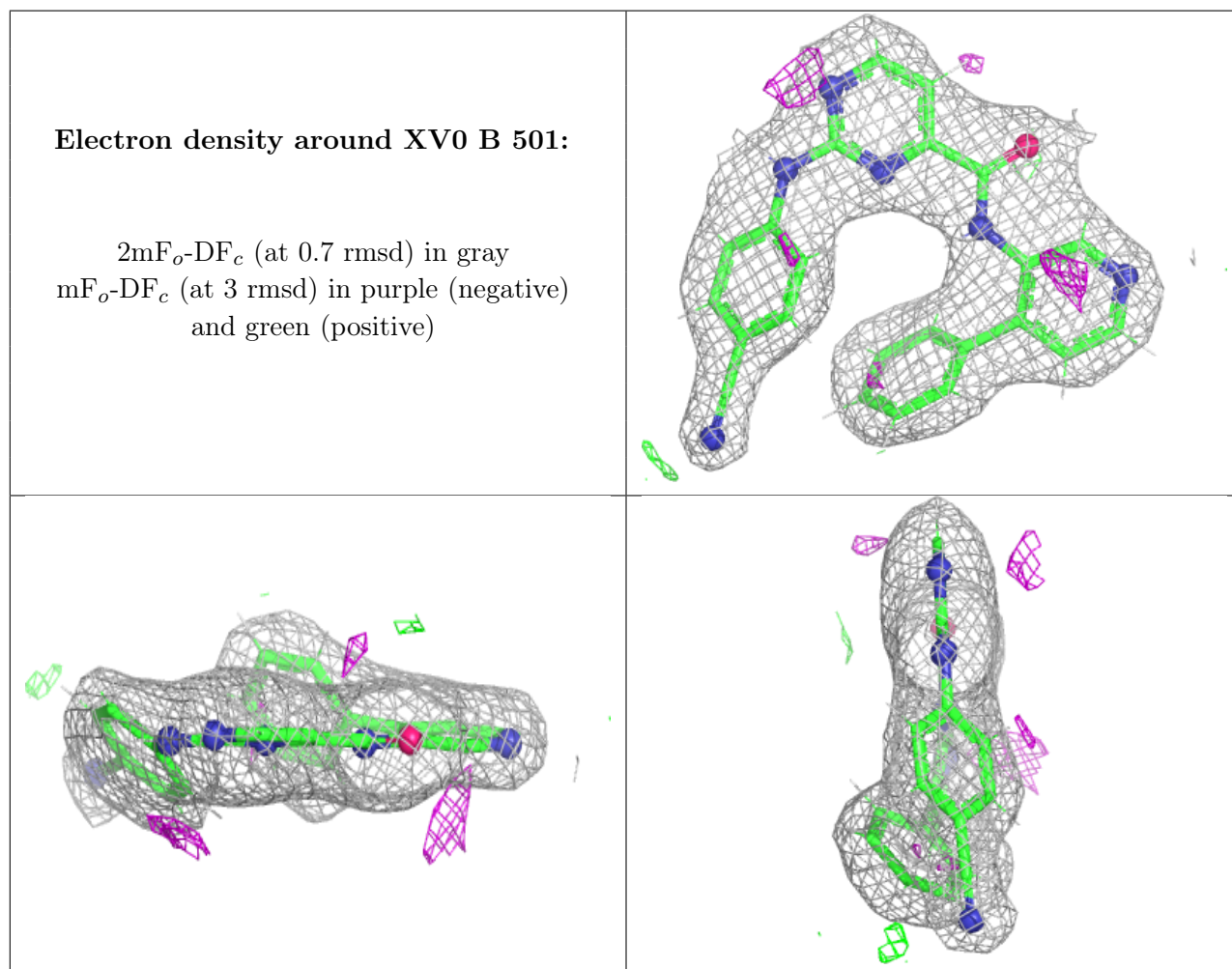
There are no oligosaccharides in this entry.

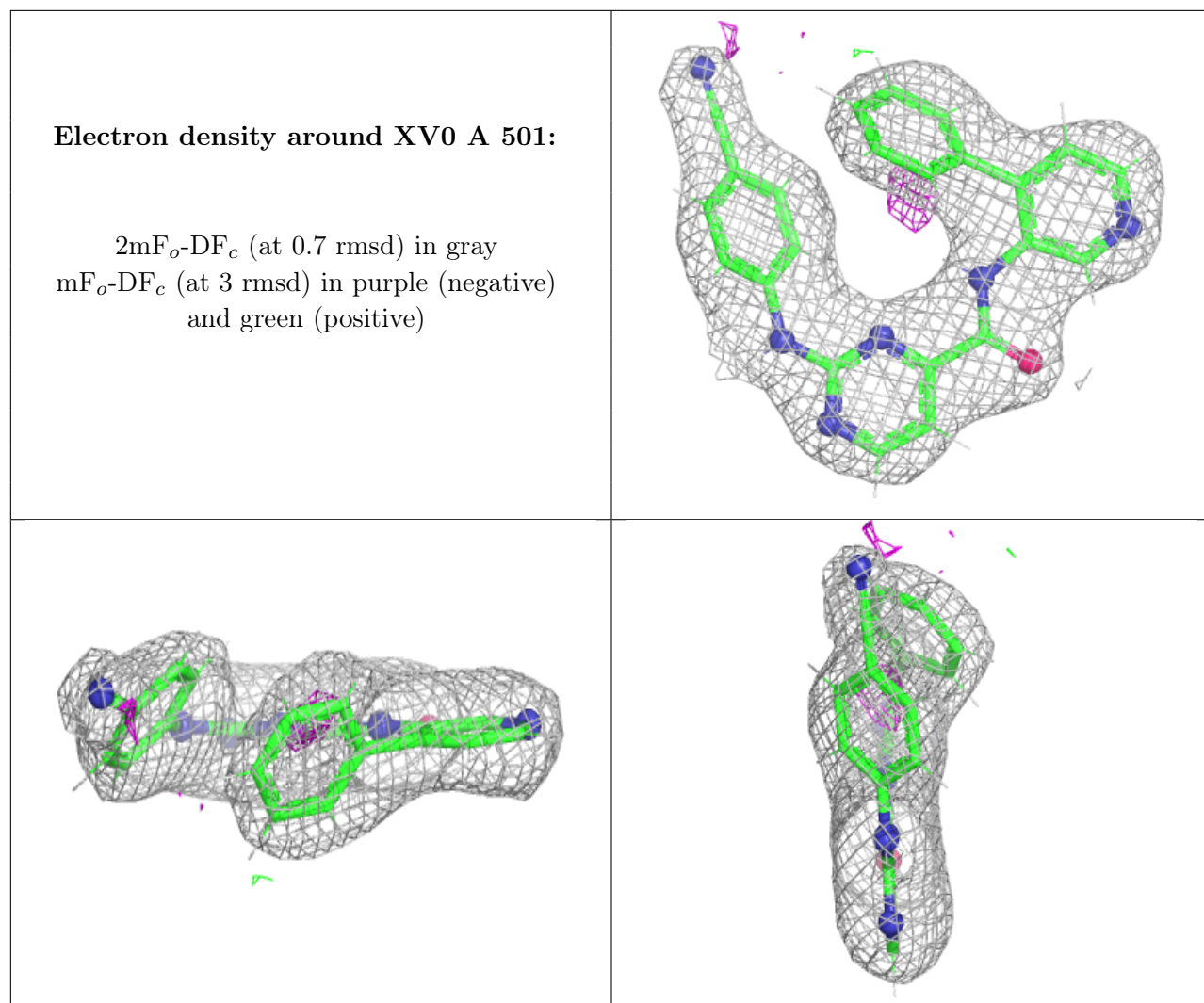
6.4 Ligands [i](#)

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(Å ²)	Q<0.9
2	XV0	B	501	30/30	0.94	0.09	44,46,55,56	16
2	XV0	A	501	30/30	0.95	0.09	42,49,60,60	16

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.