



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 04:59 AM UTC

PDB ID : 5F94 / pdb_00005f94
Title : Crystal structure of GSK3b in complex with Compound 15: 2-[(cyclopropylcarbonyl)amino]-N-(4-methoxypyridin-3-yl)pyridine-4-carboxamide
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Deposited on : 2015-12-09
Resolution : 2.51 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
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

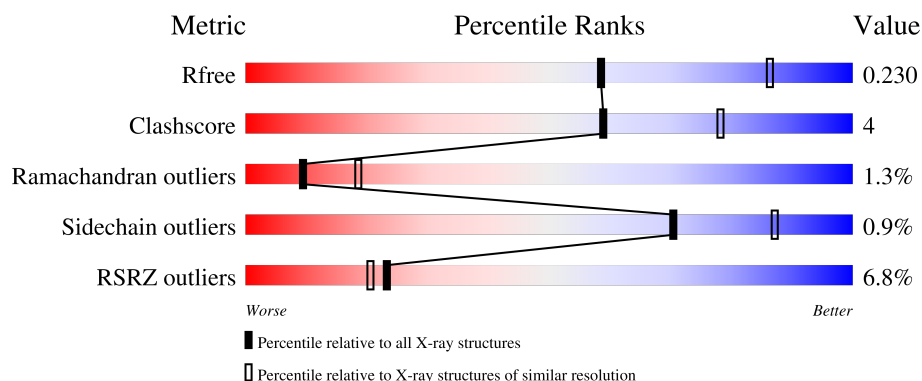
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.51 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	350	7% 89% 9% ..
1	B	350	7% 87% 13%

2 Entry composition [i](#)

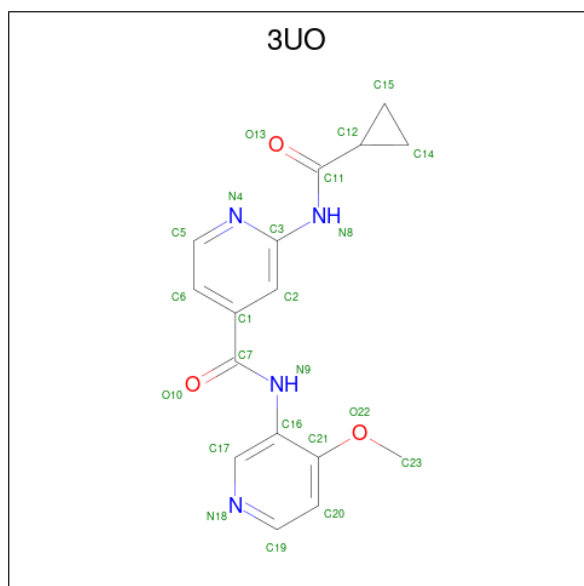
There are 3 unique types of molecules in this entry. The entry contains 5318 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Glycogen synthase kinase-3 beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	346	Total	C	N	O	S	0	0	0
			2628	1705	435	477	11			
1	B	349	Total	C	N	O	S	0	1	0
			2606	1692	429	473	12			

- Molecule 2 is 2-[(cyclopropylcarbonyl)amino]-N-(4-methoxypyridin-3-yl)pyridine-4-carboxamide (CCD ID: 3UO) (formula: C₁₆H₁₆N₄O₃).

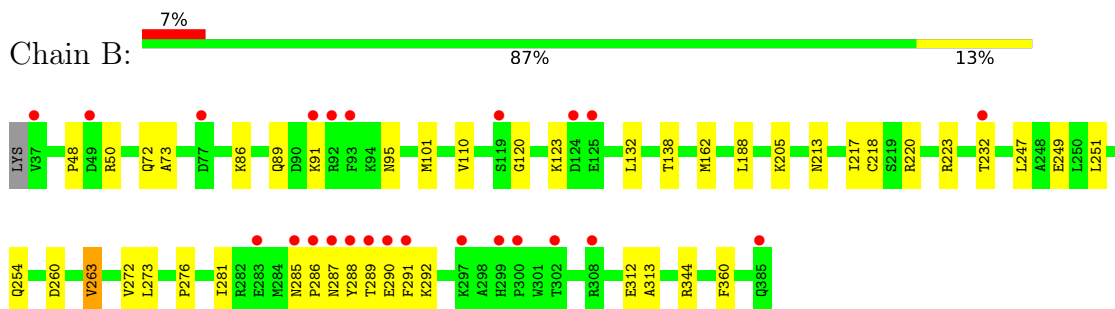
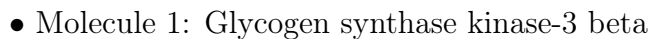


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			23	16	4	3		
2	B	1	Total	C	N	O	0	0
			23	16	4	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	28	Total 28	O 28	0	0
3	B	10	Total 10	O 10	0	0

- Molecule 1: Glycogen synthase kinase-3 beta



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	83.00Å 82.91Å 177.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.34 – 2.51 44.34 – 2.51	Depositor EDS
% Data completeness (in resolution range)	99.7 (44.34-2.51) 89.3 (44.34-2.51)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.99 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.189 , 0.226 0.199 , 0.230	Depositor DCC
R_{free} test set	2147 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	48.2	Xtriage
Anisotropy	0.843	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 54.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.027 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5318	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.49% 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: 3UO

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	0/2697	0.88	4/3694 (0.1%)
1	B	0.53	0/2677	0.87	0/3673
All	All	0.56	0/5374	0.88	4/7367 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	285	ASN	N-CA-C	6.66	119.29	109.50
1	A	371	PRO	N-CA-C	5.62	117.56	110.70
1	A	288	TYR	N-CA-C	-5.33	106.65	112.72
1	A	91	LYS	N-CA-C	-5.19	96.46	111.00

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	2628	0	2530	21	0
1	B	2606	0	2475	26	0
2	A	23	0	16	1	0
2	B	23	0	16	0	0
3	A	28	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	10	0	0	0	0
All	All	5318	0	5037	45	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 (45) 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:220:ARG:HD3	1:B:220:ARG:HD3	1.76	0.66
1:B:89:GLN:HG3	1:B:95:ASN:HB2	1.78	0.65
1:A:162:MET:HE2	1:A:247:LEU:HB2	1.81	0.62
1:B:162:MET:HE2	1:B:247:LEU:HB2	1.81	0.61
1:B:86:LYS:NZ	1:B:120:GLY:HA3	2.18	0.57
1:A:113:ARG:HD2	1:A:133:ASP:OD1	2.04	0.56
1:B:138:THR:HG22	1:B:188:LEU:HD23	1.89	0.54
1:A:319:ARG:HB3	1:A:329:LEU:HG	1.90	0.52
1:A:301:TRP:HH2	1:A:321:LEU:HD12	1.75	0.51
1:A:220:ARG:NH2	1:A:260:ASP:OD1	2.44	0.50
1:B:162:MET:HG3	1:B:247:LEU:HD13	1.94	0.49
1:B:48:PRO:O	1:B:50:ARG:N	2.46	0.49
1:B:290:GLU:C	1:B:292:LYS:H	2.21	0.49
1:B:86:LYS:HZ3	1:B:120:GLY:HA3	1.77	0.48
1:B:312:GLU:H	1:B:312:GLU:CD	2.20	0.48
1:B:220:ARG:NH1	1:B:260:ASP:OD1	2.47	0.48
1:A:133:ASP:O	2:A:401:3UO:H2	2.14	0.48
1:A:286:PRO:HG2	1:A:288:TYR:CE1	2.49	0.48
1:B:101:MET:HE1	1:B:110:VAL:HG13	1.96	0.47
1:B:249:GLU:HG3	1:B:254:GLN:C	2.40	0.47
1:A:180:ARG:HD2	1:A:217:ILE:HG12	1.97	0.47
1:B:205:LYS:NZ	1:B:213:ASN:HD22	2.13	0.47
1:B:218:CYS:HB3	1:B:223:ARG:HG2	1.98	0.46
1:A:173:HIS:CE1	1:A:236:SER:HB3	2.51	0.46
1:B:89:GLN:CG	1:B:95:ASN:HB2	2.46	0.45
1:A:72:GLN:HG2	1:A:73:ALA:N	2.31	0.45
1:B:286:PRO:HG2	1:B:288:TYR:HE1	1.81	0.45
1:A:217:ILE:HG22	1:B:263:VAL:HG21	1.99	0.45
1:A:301:TRP:CH2	1:A:321:LEU:HD12	2.53	0.44
1:B:281:ILE:O	1:B:285:ASN:N	2.41	0.44
1:B:72:GLN:HG2	1:B:73:ALA:N	2.32	0.43
1:B:272:VAL:HG12	1:B:273:LEU:HD23	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:MET:HG3	1:A:247:LEU:HD13	2.01	0.43
1:A:276:PRO:HB2	1:A:281:ILE:HG13	2.00	0.43
1:A:285:ASN:HA	1:A:286:PRO:HD2	1.86	0.43
1:A:286:PRO:HG2	1:A:288:TYR:CD1	2.54	0.43
1:B:286:PRO:HG2	1:B:288:TYR:CE1	2.55	0.42
1:A:98:LEU:HD13	1:A:130:LEU:HD21	2.02	0.42
1:B:276:PRO:HB2	1:B:281:ILE:HG13	2.01	0.42
1:B:285:ASN:HA	1:B:286:PRO:HD2	1.88	0.42
1:B:251:LEU:HD11	1:B:313:ALA:HB1	2.01	0.42
1:A:324:THR:HA	1:A:325:PRO:HD3	1.95	0.41
1:B:344:ARG:HG2	1:B:360:PHE:CE1	2.55	0.41
1:A:96:ARG:NH1	1:A:205:LYS:HD2	2.35	0.41
1:A:310:PRO:HA	1:A:311:PRO:HD2	1.86	0.41

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	344/350 (98%)	322 (94%)	18 (5%)	4 (1%)	10	20
1	B	348/350 (99%)	323 (93%)	20 (6%)	5 (1%)	9	17
All	All	692/700 (99%)	645 (93%)	38 (6%)	9 (1%)	9	18

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	91	LYS
1	B	287	ASN
1	A	123	LYS
1	B	91	LYS
1	B	123	LYS

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Mol	Chain	Res	Type
1	A	287	ASN
1	A	221	TYR
1	B	291	PHE
1	B	289	THR

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	270/312 (86%)	269 (100%)	1 (0%)	84	93
1	B	262/312 (84%)	258 (98%)	4 (2%)	57	80
All	All	532/624 (85%)	527 (99%)	5 (1%)	70	87

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	217	ILE
1	B	132	LEU
1	B	217	ILE
1	B	232	THR
1	B	263	VAL

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	52	GLN
1	A	254	GLN
1	A	365	GLN
1	A	381	HIS
1	B	72	GLN
1	B	213	ASN
1	B	365	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	3UO	B	401	-	25,25,25	0.23	0	33,34,34	0.53	0
2	3UO	A	401	-	25,25,25	0.25	0	33,34,34	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	3UO	B	401	-	-	0/18/20/20	0/3/3/3
2	3UO	A	401	-	-	0/18/20/20	0/3/3/3

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	3UO	1	0

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	346/350 (98%)	0.20	23 (6%) 24 21	45, 64, 107, 137	0
1	B	349/350 (99%)	0.34	24 (6%) 23 20	43, 69, 116, 181	1 (0%)
All	All	695/700 (99%)	0.27	47 (6%) 23 20	43, 66, 113, 181	1 (0%)

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	291	PHE	5.6
1	A	287	ASN	4.5
1	B	289	THR	4.3
1	B	287	ASN	4.0
1	B	385	GLN	4.0
1	A	91	LYS	3.7
1	A	286	PRO	3.6
1	A	93	PHE	3.5
1	B	299	HIS	3.4
1	B	119	SER	3.2
1	B	290	GLU	3.1
1	B	124	ASP	3.1
1	A	121	GLU	3.0
1	A	119	SER	3.0
1	A	298	ALA	3.0
1	A	308	ARG	2.8
1	B	93	PHE	2.7
1	A	283	GLU	2.7
1	B	283	GLU	2.7
1	A	300	PRO	2.7
1	B	125	GLU	2.7
1	B	49	ASP	2.7
1	B	286	PRO	2.6
1	B	285	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	290	GLU	2.6
1	A	299	HIS	2.6
1	A	306	ARG	2.6
1	B	300	PRO	2.5
1	A	120	GLY	2.4
1	B	77	ASP	2.4
1	B	92	ARG	2.4
1	A	125	GLU	2.3
1	A	92	ARG	2.3
1	B	308	ARG	2.3
1	B	297	LYS	2.3
1	B	37	VAL	2.3
1	A	302	THR	2.3
1	A	381	HIS	2.3
1	B	288	TYR	2.3
1	A	105	ASP	2.2
1	A	123	LYS	2.2
1	B	91	LYS	2.2
1	A	285	ASN	2.2
1	B	302	THR	2.1
1	A	284	MET	2.1
1	A	295	GLN	2.1
1	B	232	THR	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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	3UO	B	401	23/23	0.91	0.12	47,60,80,96	0
2	3UO	A	401	23/23	0.94	0.10	49,62,70,74	0

6.5 Other polymers [i](#)

There are no such residues in this entry.