



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 02:03 am GMT

PDB ID : 1R0E  
Title : Glycogen synthase kinase-3 beta in complex with 3-indolyl-4-arylmaleimide inhibitor  
Authors : Allard, J.; Nikolcheva, T.; Gong, L.; Wang, J.; Dunten, P.; Avnur, Z.; Waters, R.; Sun, Q.; Skinner, B.  
Deposited on : 2003-09-20  
Resolution : 2.25 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

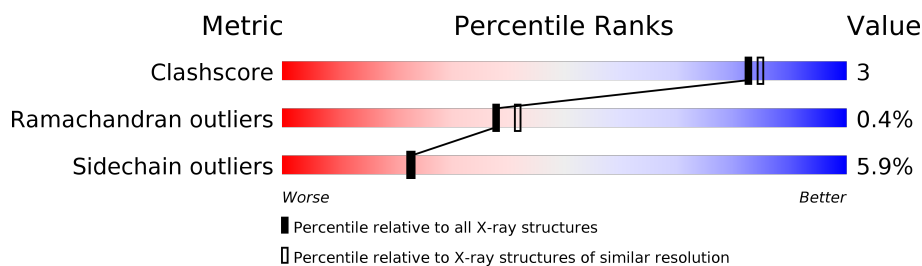
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.25 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))
Clashscore	112137	1178 (2.26-2.26)
Ramachandran outliers	110173	1145 (2.26-2.26)
Sidechain outliers	110143	1146 (2.26-2.26)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	391	
1	B	391	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5791 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.

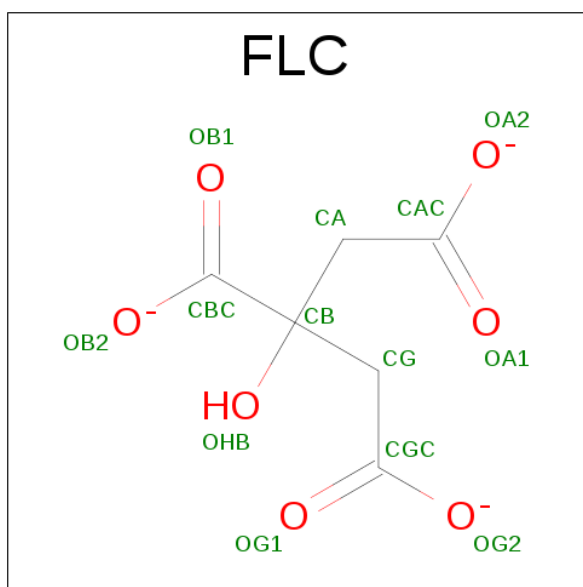
- Molecule 1 is a protein called Glycogen synthase kinase-3 beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	344	Total	C	N	O	S	0	2	0
			2760	1777	474	498	11			
1	B	344	Total	C	N	O	S	0	2	0
			2760	1777	474	498	11			

There are 10 discrepancies between the modelled and reference sequences:

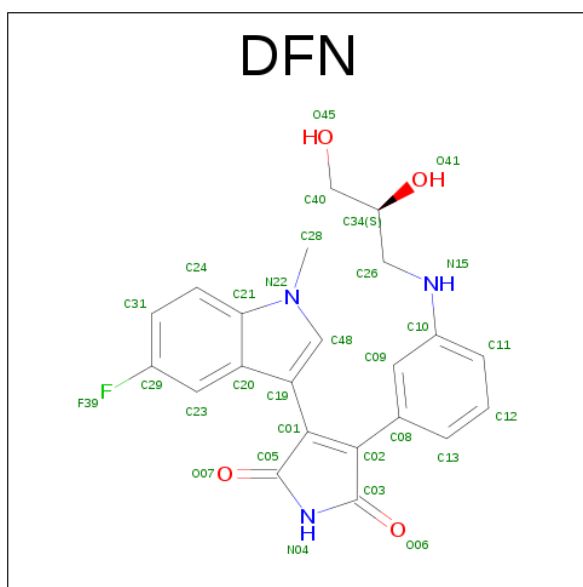
Chain	Residue	Modelled	Actual	Comment	Reference
A	30	GLY	-	CLONING ARTIFACT	UNP P49841
A	31	ALA	-	CLONING ARTIFACT	UNP P49841
A	32	MET	-	CLONING ARTIFACT	UNP P49841
A	33	SER	-	CLONING ARTIFACT	UNP P49841
A	34	LEU	-	CLONING ARTIFACT	UNP P49841
B	30	GLY	-	CLONING ARTIFACT	UNP P49841
B	31	ALA	-	CLONING ARTIFACT	UNP P49841
B	32	MET	-	CLONING ARTIFACT	UNP P49841
B	33	SER	-	CLONING ARTIFACT	UNP P49841
B	34	LEU	-	CLONING ARTIFACT	UNP P49841

- Molecule 2 is CITRATE ANION (three-letter code: FLC) (formula: C<sub>6</sub>H<sub>5</sub>O<sub>7</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			13	6	7		
2	A	1	Total	C	O	0	0
			13	6	7		

- Molecule 3 is 3-[3-(2,3-DIHYDROXY-PROPYLAMINO)-PHENYL]-4-(5-FLUORO-1-METHYL-1H-INDOL-3-YL)-PYRROLE-2,5-DIONE (three-letter code: DFN) (formula: C<sub>22</sub>H<sub>20</sub>FN<sub>3</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	0
			30	22	1	3	4		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	F	N	O	0	0
			30	22	1	3	4		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	90	Total	O	0	0
			90	90		
4	B	95	Total	O	0	0
			95	95		



Note EDS was not executed.

- Chain A:
- 
- 76% 11% 12%
- GLY MET SER LEU S45 K36 V40 Q46 D49 K60 F67 I84 K85 L88 Q89 D90 E97 M101 D105 F116 S119 GLY GLU LYS LYS ASP E125 L130 R144 V155 K159 D192 R209 I217 Q218 Y221 Y222 R223
- T232 D233 T238 D239 D260 V263 D264 R278 E290 P294 Q295 I296 K303 V304 F305 R306 I314 R319 L329 D341 S369 N370 P371 P372 R383 ILE GLN ALA ALA ALA ALA THR PRO THR ASN ALA THR ALA ALA ASP ALA ASN THR GLY ASP

- Chain B:
- 
- Sequence logo for Chain B. The y-axis represents information content in bits (0.00 to 0.25). The x-axis lists amino acids. A color scale at the top indicates conservation levels: green (75%), yellow (11%), and red (12%).
- | Position | Amino Acid | Information Content (bits) |
|----------|------------|----------------------------|
| 1        | ASP        | 0.01                       |
| 2        | THR        | 0.01                       |
| 3        | THR        | 0.01                       |
| 4        | GLY        | 0.01                       |
| 5        | GLY        | 0.01                       |
| 6        | ARG        | 0.01                       |
| 7        | GLY        | 0.01                       |
| 8        | GLN        | 0.01                       |
| 9        | THR        | 0.01                       |
| 10       | ASN        | 0.01                       |
| 11       | ASN        | 0.01                       |
| 12       | ALA        | 0.01                       |
| 13       | ALA        | 0.01                       |
| 14       | SER        | 0.01                       |
| 15       | ALA        | 0.01                       |
| 16       | ALA        | 0.01                       |
| 17       | ALA        | 0.01                       |
| 18       | ALA        | 0.01                       |
| 19       | ALA        | 0.01                       |
| 20       | ALA        | 0.01                       |
| 21       | ALA        | 0.01                       |
| 22       | ALA        | 0.01                       |
| 23       | ALA        | 0.01                       |
| 24       | ALA        | 0.01                       |
| 25       | ALA        | 0.01                       |
| 26       | ALA        | 0.01                       |
| 27       | ALA        | 0.01                       |
| 28       | ALA        | 0.01                       |
| 29       | ALA        | 0.01                       |
| 30       | ALA        | 0.01                       |
| 31       | ALA        | 0.01                       |
| 32       | ALA        | 0.01                       |
| 33       | ALA        | 0.01                       |
| 34       | ALA        | 0.01                       |
| 35       | ALA        | 0.01                       |
| 36       | ALA        | 0.01                       |
| 37       | ALA        | 0.01                       |
| 38       | ALA        | 0.01                       |
| 39       | ALA        | 0.01                       |
| 40       | ALA        | 0.01                       |

## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	83.96Å 84.01Å 180.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	91.29 – 2.25	Depositor
% Data completeness (in resolution range)	98.4 (91.29-2.25)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.223 , 0.252	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5791	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FLC, DFN

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	0.57	1/2839 (0.0%)	0.75	8/3865 (0.2%)
1	B	0.57	1/2839 (0.0%)	0.75	7/3865 (0.2%)
All	All	0.57	2/5678 (0.0%)	0.75	15/7730 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	218	CYS	CB-SG	-5.33	1.73	1.81
1	B	218	CYS	CB-SG	-5.02	1.73	1.81

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	105	ASP	CB-CG-OD2	6.72	124.34	118.30
1	A	260	ASP	CB-CG-OD2	6.52	124.17	118.30
1	B	233	ASP	CB-CG-OD2	6.45	124.11	118.30
1	A	264	ASP	CB-CG-OD2	6.02	123.71	118.30
1	A	49	ASP	CB-CG-OD2	5.91	123.62	118.30

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	2760	0	2772	16	0
1	B	2760	0	2772	17	0
2	A	13	0	5	0	0
2	B	13	0	5	0	0
3	A	30	0	20	1	0
3	B	30	0	20	0	0
4	A	90	0	0	0	0
4	B	95	0	0	0	0
All	All	5791	0	5594	32	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.

The worst 5 of 32 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:217:ILE:O	1:B:218:CYS:HB2	1.84	0.78
1:A:218:CYS:HB3	1:A:223:ARG:HG2	1.69	0.72
1:B:218:CYS:HB3	1:B:223:ARG:HG2	1.73	0.70
1:A:217:ILE:O	1:A:218:CYS:HB2	1.90	0.69
1:A:67:PHE:O	1:A:85:LYS:HE3	1.96	0.65

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	342/391 (88%)	329 (96%)	12 (4%)	1 (0%)	44	50
1	B	342/391 (88%)	328 (96%)	12 (4%)	2 (1%)	28	29
All	All	684/782 (88%)	657 (96%)	24 (4%)	3 (0%)	38	42

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	221	TYR
1	B	221	TYR
1	B	49	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	307/338 (91%)	290 (94%)	17 (6%)	25	26
1	B	307/338 (91%)	288 (94%)	19 (6%)	21	20
All	All	614/676 (91%)	578 (94%)	36 (6%)	23	23

5 of 36 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	370	ASN
1	B	72	GLN
1	B	369	SER
1	B	46	GLN
1	B	88	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	370	ASN
1	B	381	HIS
1	B	72	GLN
1	A	72	GLN
1	B	370	ASN

### 5.3.3 RNA [i](#)

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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

4 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	FLC	A	701	-	3,12,12	0.89	0	3,17,17	1.25	1 (33%)
3	DFN	A	702	-	30,33,33	1.14	2 (6%)	34,48,48	0.92	0
3	DFN	B	501	-	30,33,33	1.19	3 (10%)	34,48,48	0.91	0
2	FLC	B	601	-	3,12,12	0.85	0	3,17,17	0.97	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	FLC	A	701	-	-	0/6/16/16	0/0/0/0
3	DFN	A	702	-	-	0/11/31/31	0/4/4/4
3	DFN	B	501	-	-	0/11/31/31	0/4/4/4
2	FLC	B	601	-	-	0/6/16/16	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	501	DFN	C19-C01	-2.86	1.44	1.50
3	A	702	DFN	C19-C01	-2.82	1.44	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	501	DFN	C19-C20	2.37	1.44	1.42
3	B	501	DFN	C23-C29	2.46	1.40	1.36
3	A	702	DFN	C23-C29	2.54	1.40	1.36

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	FLC	CB-CA-CAC	-2.10	111.67	114.95

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
3	A	702	DFN	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.