



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 1ZYC / pdb_00001zyc
Title : Crystal Structure of eIF2alpha Protein Kinase GCN2: Wild-Type in Apo Form.
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Deposited on : 2005-06-09
Resolution : 3.00 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

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
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

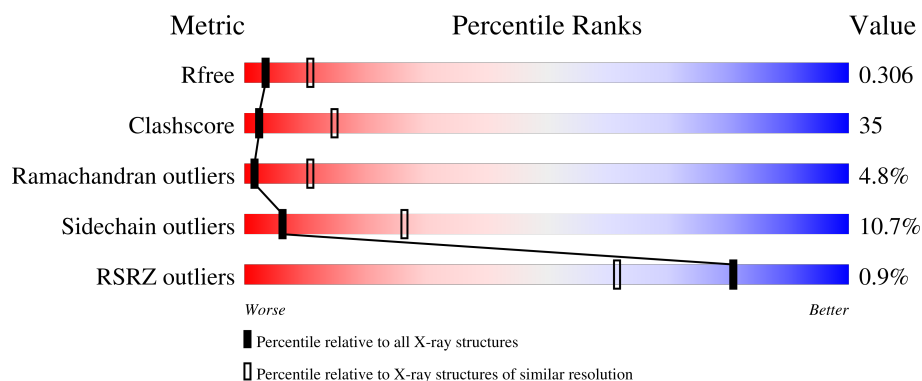
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	303	37%40%8%14%
1	B	303	% 38%36%9%16%
1	C	303	% 35%44%10%11%
1	D	303	% 32%41%11%16%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8601 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 Serine/threonine-protein kinase GCN2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	261	Total	C	N	O	S	5	0	0
			2153	1378	375	391	9			
1	B	254	Total	C	N	O	S	0	0	0
			2091	1341	364	377	9			
1	C	271	Total	C	N	O	S	0	0	0
			2235	1435	388	403	9			
1	D	256	Total	C	N	O	S	0	0	0
			2108	1352	366	381	9			

There are 8 discrepancies between the modelled and reference sequences:

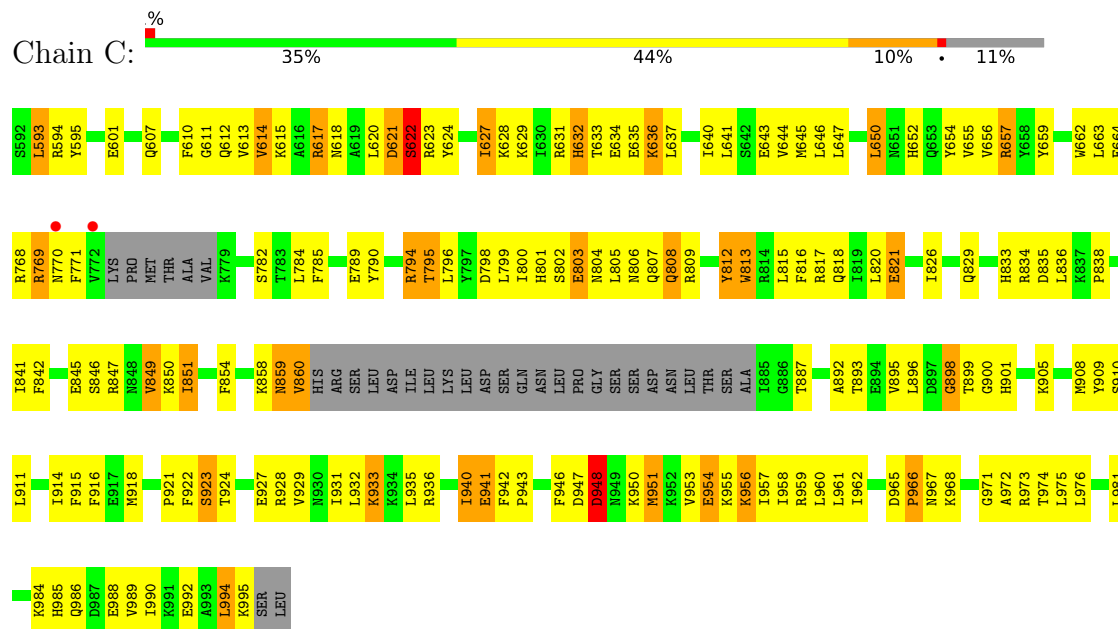
Chain	Residue	Modelled	Actual	Comment	Reference
A	592	SER	-	cloning artifact	UNP P15442
A	593	LEU	-	cloning artifact	UNP P15442
B	592	SER	-	cloning artifact	UNP P15442
B	593	LEU	-	cloning artifact	UNP P15442
C	592	SER	-	cloning artifact	UNP P15442
C	593	LEU	-	cloning artifact	UNP P15442
D	592	SER	-	cloning artifact	UNP P15442
D	593	LEU	-	cloning artifact	UNP P15442

- Molecule 2 is water.

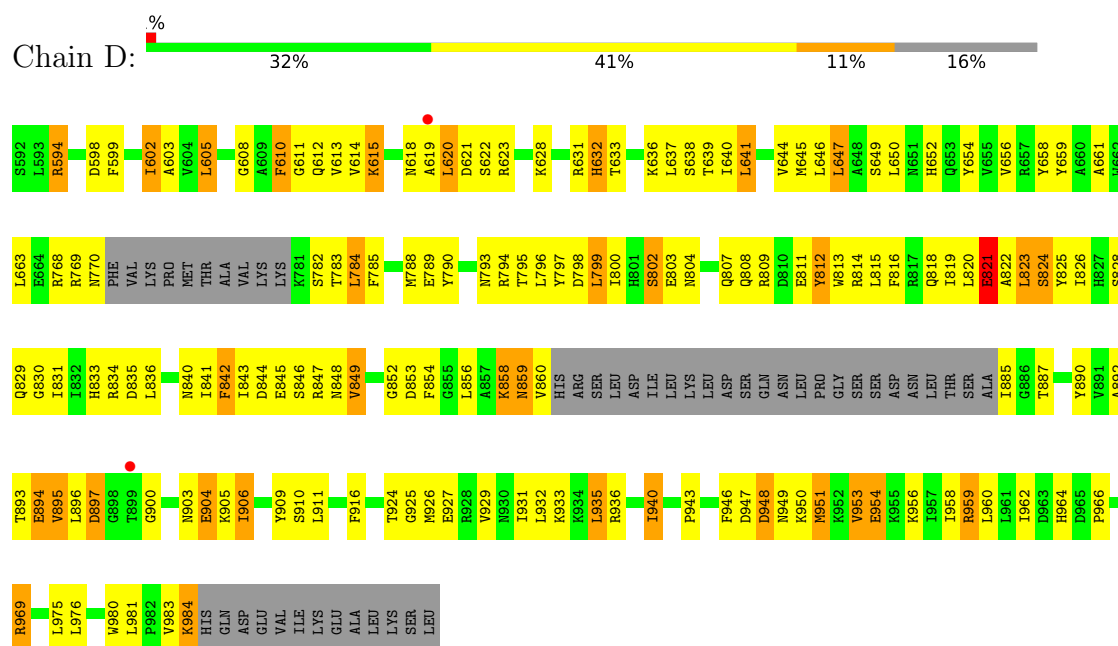
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	O	0	0
			3	3		
2	B	6	Total	O	0	0
			6	6		
2	C	5	Total	O	0	0
			5	5		

GLN
ASP
GLU
VAL
ILE
LYS
GLU
ALA
LYS
SER
LEU

● Molecule 1: Serine/threonine-protein kinase GCN2



● Molecule 1: Serine/threonine-protein kinase GCN2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	79.89Å 95.70Å 175.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.99 – 3.00 41.99 – 3.00	Depositor EDS
% Data completeness (in resolution range)	94.6 (41.99-3.00) 94.5 (41.99-3.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.37 (at 2.81Å)	Xtriage
Refinement program	CNX 2000.1	Depositor
R, R_{free}	0.234 , 0.299 (Not available) , 0.306	Depositor DCC
R_{free} test set	652 reflections (2.09%)	wwPDB-VP
Wilson B-factor (Å ²)	81.8	Xtriage
Anisotropy	0.487	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 72.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8601	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.32% 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](#)

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	1/2196 (0.0%)	1.06	11/2956 (0.4%)
1	B	0.55	1/2132 (0.0%)	1.15	16/2869 (0.6%)
1	C	0.54	0/2279	1.01	11/3066 (0.4%)
1	D	0.56	0/2150	1.03	13/2895 (0.4%)
All	All	0.56	2/8757 (0.0%)	1.06	51/11786 (0.4%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	632	HIS	CA-C	6.09	1.60	1.52
1	A	941	GLU	CA-C	5.83	1.59	1.52

The worst 5 of 51 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	633	THR	N-CA-C	17.94	141.84	108.65
1	A	659	TYR	N-CA-C	9.75	121.98	111.36
1	C	898	GLY	N-CA-C	-9.36	90.99	113.18
1	B	888	ALA	N-CA-C	-8.50	102.82	113.02
1	D	900	GLY	N-CA-C	-8.41	103.71	115.32

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	2153	0	2160	148	0
1	B	2091	0	2104	157	0
1	C	2235	0	2259	165	0
1	D	2108	0	2122	155	0
2	A	3	0	0	0	0
2	B	6	0	0	1	0
2	C	5	0	0	0	0
All	All	8601	0	8645	604	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 35.

The worst 5 of 604 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:D:924:THR:HG22	1:D:926:MET:H	1.09	1.14
1:B:769:ARG:HH11	1:B:769:ARG:HB3	1.22	1.00
1:B:769:ARG:HB3	1:B:769:ARG:NH1	1.78	0.97
1:D:858:LYS:H	1:D:858:LYS:HD2	1.34	0.92
1:C:657:ARG:HB2	1:C:789:GLU:HB2	1.52	0.92

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	255/303 (84%)	201 (79%)	42 (16%)	12 (5%)	2	11
1	B	246/303 (81%)	191 (78%)	46 (19%)	9 (4%)	2	15
1	C	265/303 (88%)	200 (76%)	51 (19%)	14 (5%)	1	9
1	D	250/303 (82%)	202 (81%)	34 (14%)	14 (6%)	1	8
All	All	1016/1212 (84%)	794 (78%)	173 (17%)	49 (5%)	2	11

5 of 49 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	858	LYS
1	C	770	ASN
1	D	904	GLU
1	A	639	THR
1	A	937	SER

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	179/272 (66%)	164 (92%)	15 (8%)	10	37
1	B	227/272 (84%)	198 (87%)	29 (13%)	4	19
1	C	243/272 (89%)	216 (89%)	27 (11%)	6	25
1	D	229/272 (84%)	206 (90%)	23 (10%)	7	29
All	All	878/1088 (81%)	784 (89%)	94 (11%)	6	26

5 of 94 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	813	TRP
1	D	605	LEU
1	C	841	ILE
1	C	911	LEU
1	D	647	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	787	GLN
1	D	806	ASN
1	D	930	ASN
1	B	807	GLN
1	B	804	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 [i](#)

There are no ligands in this entry.

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](#)

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	261/303 (86%)	-0.32	1 (0%) 88 76	41, 71, 112, 125	2 (0%)
1	B	254/303 (83%)	-0.21	4 (1%) 70 47	40, 78, 116, 132	0
1	C	271/303 (89%)	-0.32	2 (0%) 84 66	41, 76, 110, 117	0
1	D	256/303 (84%)	-0.37	2 (0%) 82 64	37, 67, 106, 118	0
All	All	1042/1212 (85%)	-0.30	9 (0%) 81 61	37, 73, 111, 132	2 (0%)

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	989	VAL	2.8
1	D	619	ALA	2.6
1	D	899	THR	2.4
1	C	772	VAL	2.3
1	C	770	ASN	2.3

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.