



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 15, 2026 – 01:22 PM UTC

PDB ID : 3GRC / pdb_00003grc
Title : Crystal structure of a sensor protein from Polaromonas sp. JS666
Authors : Palani, K.; Kumaran, D.; Burley, S.K.; Swaminathan, S.; New York SGX
Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2009-03-25
Resolution : 2.21 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
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

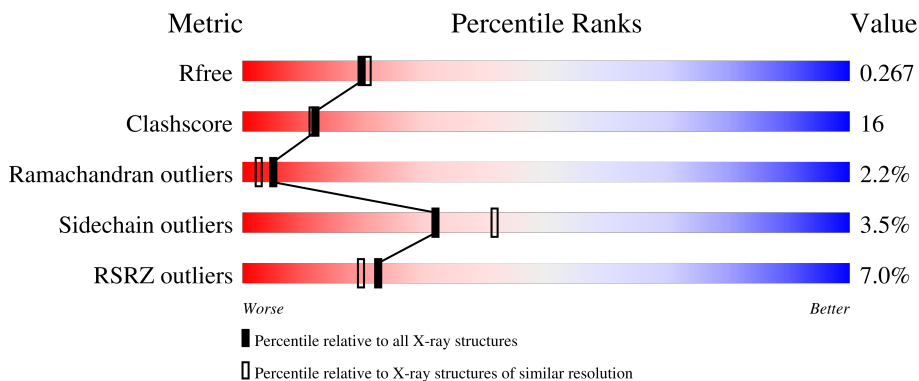
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.21 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	7682 (2.24-2.20)
Clashscore	190562	8402 (2.24-2.20)
Ramachandran outliers	187476	8303 (2.24-2.20)
Sidechain outliers	187428	8304 (2.24-2.20)
RSRZ outliers	180081	7683 (2.24-2.20)

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	140	 3% 65% 19% 6% 11%
1	B	140	 4% 60% 25% • 12%
1	C	140	 6% 61% 21% 7% 11%
1	D	140	 11% 55% 31% •• 11%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 4083 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 Sensor protein, Kinase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	125	976	606	178	187	1	4	0	0	0
1	B	123	963	598	176	185	1	3	0	0	0
1	C	125	976	606	178	187	1	4	0	0	0
1	D	125	976	606	178	187	1	4	0	0	0

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	542	MSE	-	expression tag	UNP Q121U0
A	543	SER	-	expression tag	UNP Q121U0
A	544	LEU	-	expression tag	UNP Q121U0
A	674	GLU	-	expression tag	UNP Q121U0
A	675	GLY	-	expression tag	UNP Q121U0
A	676	HIS	-	expression tag	UNP Q121U0
A	677	HIS	-	expression tag	UNP Q121U0
A	678	HIS	-	expression tag	UNP Q121U0
A	679	HIS	-	expression tag	UNP Q121U0
A	680	HIS	-	expression tag	UNP Q121U0
A	681	HIS	-	expression tag	UNP Q121U0
B	542	MSE	-	expression tag	UNP Q121U0
B	543	SER	-	expression tag	UNP Q121U0
B	544	LEU	-	expression tag	UNP Q121U0
B	674	GLU	-	expression tag	UNP Q121U0
B	675	GLY	-	expression tag	UNP Q121U0
B	676	HIS	-	expression tag	UNP Q121U0
B	677	HIS	-	expression tag	UNP Q121U0
B	678	HIS	-	expression tag	UNP Q121U0
B	679	HIS	-	expression tag	UNP Q121U0
B	680	HIS	-	expression tag	UNP Q121U0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	681	HIS	-	expression tag	UNP Q121U0
C	542	MSE	-	expression tag	UNP Q121U0
C	543	SER	-	expression tag	UNP Q121U0
C	544	LEU	-	expression tag	UNP Q121U0
C	674	GLU	-	expression tag	UNP Q121U0
C	675	GLY	-	expression tag	UNP Q121U0
C	676	HIS	-	expression tag	UNP Q121U0
C	677	HIS	-	expression tag	UNP Q121U0
C	678	HIS	-	expression tag	UNP Q121U0
C	679	HIS	-	expression tag	UNP Q121U0
C	680	HIS	-	expression tag	UNP Q121U0
C	681	HIS	-	expression tag	UNP Q121U0
D	542	MSE	-	expression tag	UNP Q121U0
D	543	SER	-	expression tag	UNP Q121U0
D	544	LEU	-	expression tag	UNP Q121U0
D	674	GLU	-	expression tag	UNP Q121U0
D	675	GLY	-	expression tag	UNP Q121U0
D	676	HIS	-	expression tag	UNP Q121U0
D	677	HIS	-	expression tag	UNP Q121U0
D	678	HIS	-	expression tag	UNP Q121U0
D	679	HIS	-	expression tag	UNP Q121U0
D	680	HIS	-	expression tag	UNP Q121U0
D	681	HIS	-	expression tag	UNP Q121U0

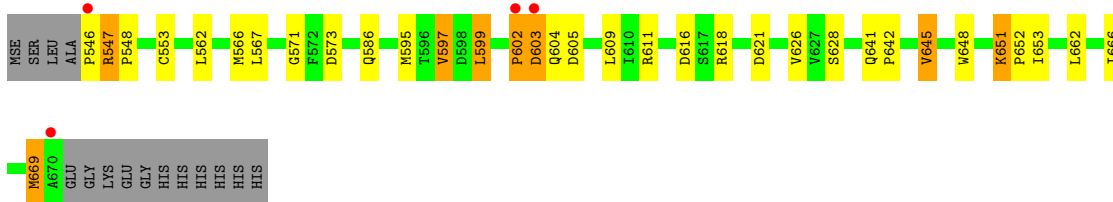
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	50	Total O 50 50	0	0
2	B	51	Total O 51 51	0	0
2	C	42	Total O 42 42	0	0
2	D	49	Total O 49 49	0	0

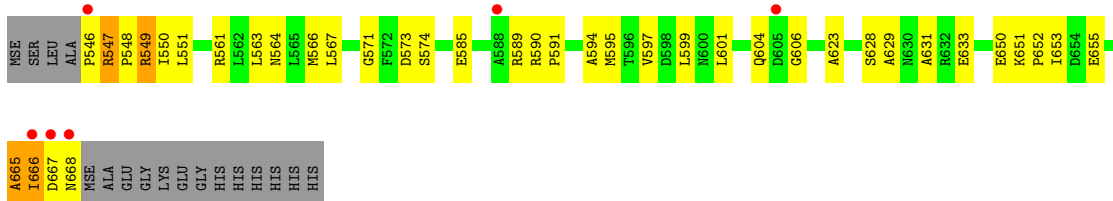
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

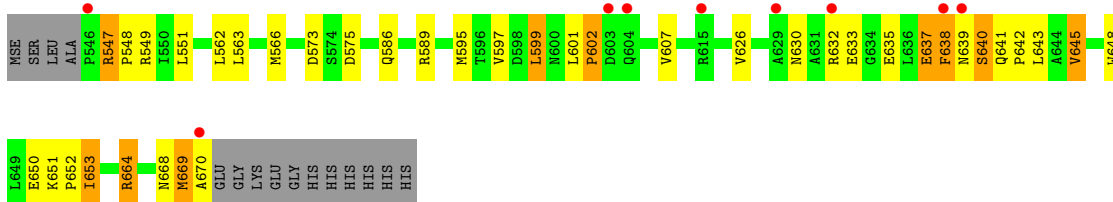
- Molecule 1: Sensor protein, Kinase



- Molecule 1: Sensor protein, Kinase

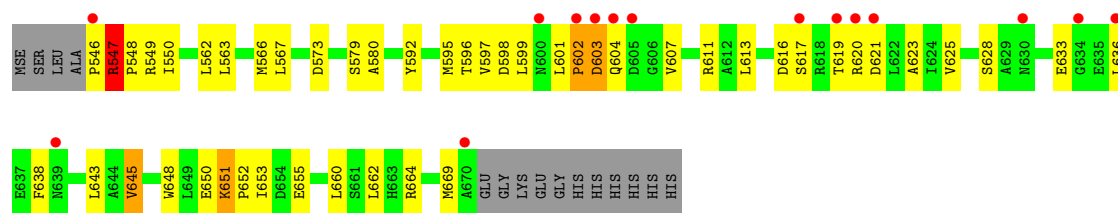


- Molecule 1: Sensor protein, Kinase



- Molecule 1: Sensor protein, Kinase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	64.36Å 87.81Å 103.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.44 – 2.21 40.44 – 2.21	Depositor EDS
% Data completeness (in resolution range)	95.9 (40.44-2.21) 96.2 (40.44-2.21)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.50 (at 2.20Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.221 , 0.265 0.221 , 0.267	Depositor DCC
R_{free} test set	1426 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å ²)	29.7	Xtrriage
Anisotropy	0.464	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 39.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4083	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.97 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.1150e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	0.52	0/985	1.03	5/1329 (0.4%)
1	B	0.54	0/973	1.01	7/1315 (0.5%)
1	C	0.51	0/985	1.06	4/1329 (0.3%)
1	D	0.48	0/985	0.96	4/1329 (0.3%)
All	All	0.51	0/3928	1.02	20/5302 (0.4%)

There are no bond length outliers.

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	573	ASP	N-CA-C	-7.50	99.42	110.52
1	A	573	ASP	N-CA-C	-7.18	99.89	110.52
1	B	665	ALA	N-CA-C	-7.09	100.57	110.35
1	D	653	ILE	N-CA-C	7.07	118.14	109.30
1	B	653	ILE	N-CA-C	6.96	118.03	108.84

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	976	0	988	27	0
1	B	963	0	974	28	0
1	C	976	0	988	30	0
1	D	976	0	988	38	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	50	0	0	1	0
2	B	51	0	0	0	0
2	C	42	0	0	0	0
2	D	49	0	0	1	0
All	All	4083	0	3938	123	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 16.

The worst 5 of 123 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:551:LEU:HD23	1:B:595:MSE:HE2	1.49	0.93
1:A:595:MSE:HE1	1:A:609:LEU:HD21	1.48	0.93
1:B:585:GLU:HG2	1:B:589:ARG:HH12	1.35	0.91
1:D:547:ARG:HB3	1:D:548:PRO:HD3	1.53	0.89
1:C:551:LEU:HD23	1:C:595:MSE:HE2	1.60	0.84

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	123/140 (88%)	119 (97%)	1 (1%)	3 (2%)	4	2
1	B	121/140 (86%)	118 (98%)	1 (1%)	2 (2%)	7	5
1	C	123/140 (88%)	112 (91%)	8 (6%)	3 (2%)	4	2
1	D	123/140 (88%)	118 (96%)	2 (2%)	3 (2%)	4	2
All	All	490/560 (88%)	467 (95%)	12 (2%)	11 (2%)	5	3

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	603	ASP
1	D	603	ASP
1	A	547	ARG
1	C	640	SER
1	D	602	PRO

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	107/114 (94%)	104 (97%)	3 (3%)	38	50
1	B	106/114 (93%)	105 (99%)	1 (1%)	70	82
1	C	107/114 (94%)	101 (94%)	6 (6%)	19	22
1	D	107/114 (94%)	102 (95%)	5 (5%)	23	29
All	All	427/456 (94%)	412 (96%)	15 (4%)	32	41

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	650	GLU
1	D	645	VAL
1	C	664	ARG
1	D	650	GLU
1	D	599	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	586	GLN
1	D	604	GLN
1	D	630	ASN
1	B	564	ASN
1	B	600	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	121/140 (86%)	0.06	4 (3%) 49 46	12, 30, 54, 60	0
1	B	120/140 (85%)	0.06	6 (5%) 34 31	15, 27, 53, 72	0
1	C	121/140 (86%)	0.45	9 (7%) 20 18	13, 34, 58, 66	0
1	D	121/140 (86%)	0.55	15 (12%) 8 6	14, 38, 66, 77	0
All	All	483/560 (86%)	0.28	34 (7%) 22 19	12, 32, 59, 77	0

The worst 5 of 34 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	638	PHE	5.2
1	C	670	ALA	5.2
1	D	603	ASP	4.8
1	B	546	PRO	4.8
1	D	546	PRO	4.6

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.