



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 04:16 PM UTC

PDB ID : 3IFR / pdb_00003ifr
Title : The crystal structure of xylulose kinase from *Rhodospirillum rubrum*
Authors : Zhang, Z.; Burley, S.K.; Swaminathan, S.; New York SGX Research Center
for Structural Genomics (NYSGXRC)
Deposited on : 2009-07-24
Resolution : 2.30 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

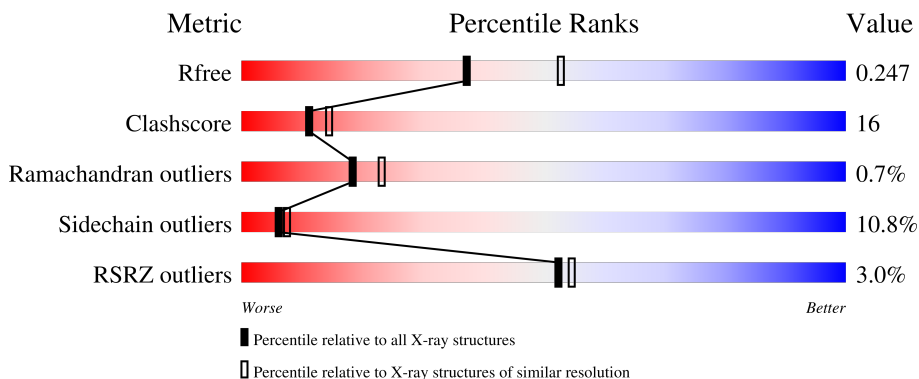
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	508	2% 66% 25% 5% .
1	B	508	3% 67% 21% 6% 6%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7532 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 Carbohydrate kinase, FGGY.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	488	Total	C	N	O	S	Se	0	0	0
			3624	2301	638	675	5	5			
1	B	480	Total	C	N	O	S	Se	0	0	0
			3564	2263	629	662	5	5			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	expression tag	UNP Q2RUX7
A	2	SER	-	expression tag	UNP Q2RUX7
A	3	LEU	-	expression tag	UNP Q2RUX7
A	501	GLU	-	expression tag	UNP Q2RUX7
A	502	GLY	-	expression tag	UNP Q2RUX7
A	503	HIS	-	expression tag	UNP Q2RUX7
A	504	HIS	-	expression tag	UNP Q2RUX7
A	505	HIS	-	expression tag	UNP Q2RUX7
A	506	HIS	-	expression tag	UNP Q2RUX7
A	507	HIS	-	expression tag	UNP Q2RUX7
A	508	HIS	-	expression tag	UNP Q2RUX7
B	1	MSE	-	expression tag	UNP Q2RUX7
B	2	SER	-	expression tag	UNP Q2RUX7
B	3	LEU	-	expression tag	UNP Q2RUX7
B	501	GLU	-	expression tag	UNP Q2RUX7
B	502	GLY	-	expression tag	UNP Q2RUX7
B	503	HIS	-	expression tag	UNP Q2RUX7
B	504	HIS	-	expression tag	UNP Q2RUX7
B	505	HIS	-	expression tag	UNP Q2RUX7
B	506	HIS	-	expression tag	UNP Q2RUX7
B	507	HIS	-	expression tag	UNP Q2RUX7
B	508	HIS	-	expression tag	UNP Q2RUX7

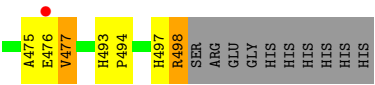
- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	170	Total	O	0	0
			170	170		
3	B	169	Total	O	0	0
			169	169		



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	129.09Å 149.81Å 54.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	64.55 – 2.30 64.55 – 2.30	Depositor EDS
% Data completeness (in resolution range)	95.8 (64.55-2.30) 98.4 (64.55-2.30)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.05 (at 2.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.206 , 0.260 0.204 , 0.247	Depositor DCC
R_{free} test set	2405 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	27.7	Xtriage
Anisotropy	0.678	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 36.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7532	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.59% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4

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	0.99	6/3707 (0.2%)	1.12	5/5065 (0.1%)
1	B	1.02	5/3644 (0.1%)	1.13	15/4975 (0.3%)
All	All	1.00	11/7351 (0.1%)	1.12	20/10040 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	244	ALA	C-O	-6.61	1.16	1.24
1	B	246	HIS	C-O	-6.43	1.16	1.24
1	A	476	GLU	C-O	-6.38	1.16	1.24
1	A	243	ALA	C-O	-5.91	1.17	1.24
1	B	244	ALA	C-O	-5.89	1.16	1.23

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	245	ASP	N-CA-C	7.05	119.58	111.11
1	A	42	SER	CA-C-N	6.42	125.99	119.19
1	A	42	SER	C-N-CA	6.42	125.99	119.19
1	B	42	SER	CA-C-N	5.75	125.37	119.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	42	SER	C-N-CA	5.75	125.37	119.56

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	455	TRP	Peptide
1	B	455	TRP	Peptide

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	3624	0	3580	121	0
1	B	3564	0	3516	112	0
2	A	5	0	0	0	0
3	A	170	0	0	6	0
3	B	169	0	0	12	0
All	All	7532	0	7096	233	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 233 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:301:MSE:HE2	1:B:390:HIS:CE1	1.80	1.16
1:B:95:ARG:HD2	1:B:95:ARG:O	1.61	1.01
1:B:261:VAL:HG22	1:B:273:VAL:HG22	1.40	1.00
1:B:458:VAL:HG12	1:B:458:VAL:O	1.59	0.98
1:A:426:ARG:HG3	1:A:426:ARG:HH11	1.30	0.97

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	484/508 (95%)	463 (96%)	18 (4%)	3 (1%)	21	27
1	B	472/508 (93%)	450 (95%)	18 (4%)	4 (1%)	16	20
All	All	956/1016 (94%)	913 (96%)	36 (4%)	7 (1%)	18	23

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	198	ASP
1	A	456	ASP
1	B	456	ASP
1	B	451	ASP
1	B	450	GLY

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	363/374 (97%)	321 (88%)	42 (12%)	5	6
1	B	356/374 (95%)	320 (90%)	36 (10%)	7	9
All	All	719/748 (96%)	641 (89%)	78 (11%)	6	7

5 of 78 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	202	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	457	ASP
1	B	255	ILE
1	B	333	GLU
1	B	476	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	289	HIS
1	B	425	GLN
1	B	497	HIS
1	B	433	ASN
1	B	390	HIS

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](#)

1 ligand is 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	PO4	A	509	-	4,4,4	0.77	0	6,6,6	0.76	0

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.

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	483/508 (95%)	0.09	12 (2%) 58 60	15, 25, 40, 54	0
1	B	475/508 (93%)	0.15	17 (3%) 46 48	16, 26, 40, 51	0
All	All	958/1016 (94%)	0.12	29 (3%) 52 54	15, 25, 40, 54	0

The worst 5 of 29 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	358	PHE	5.3
1	B	26	LEU	4.5
1	A	356	ASP	4.0
1	B	453	LEU	3.6
1	A	359	ALA	3.6

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](#)

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($\text{\AA}^2$)	Q<0.9
2	PO4	A	509	5/5	0.55	0.28	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.