



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 27, 2024 – 10:21 PM EDT

PDB ID : 1ZKD  
Title : X-Ray structure of the putative protein Q6N1P6 from Rhodopseudomonas palustris at the resolution 2.1 Å , Northeast Structural Genomics Consortium target RpR58  
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Deposited on : 2005-05-02  
Resolution : 2.10 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<https://www.wwpdb.org/validation/2017/FAQs#types>.

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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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)

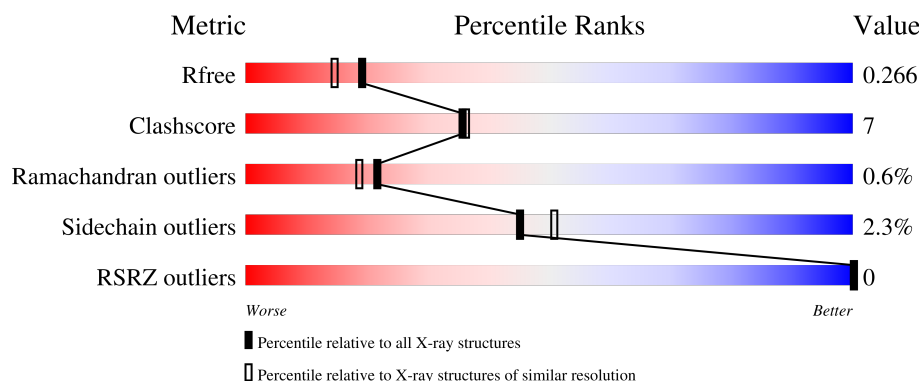
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*



The reported resolution of this entry is 2.10 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))
$R_{free}$	164625	6234 (2.10-2.10)
Clashscore	180529	6893 (2.10-2.10)
Ramachandran outliers	177936	6839 (2.10-2.10)
Sidechain outliers	177891	6840 (2.10-2.10)
RSRZ outliers	164620	6234 (2.10-2.10)

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  $\geq 3$ , 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	387	 78% 14% 8%
1	B	387	 75% 17% 8%

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5740 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 DUF185.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	357	Total	C	N	O	S	Se	0	0	0
			2740	1745	483	503	1	8			
1	B	356	Total	C	N	O	S	Se	0	0	0
			2729	1739	479	502	1	8			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	21	MSE	MET	modified residue	UNP Q6N1P6
A	27	MSE	MET	modified residue	UNP Q6N1P6
A	60	MSE	MET	modified residue	UNP Q6N1P6
A	94	MSE	MET	modified residue	UNP Q6N1P6
A	95	MSE	MET	modified residue	UNP Q6N1P6
A	317	MSE	MET	modified residue	UNP Q6N1P6
A	343	MSE	MET	modified residue	UNP Q6N1P6
A	346	MSE	MET	modified residue	UNP Q6N1P6
A	380	LEU	-	cloning artifact	UNP Q6N1P6
A	381	GLU	-	cloning artifact	UNP Q6N1P6
A	382	HIS	-	cloning artifact	UNP Q6N1P6
A	383	HIS	-	cloning artifact	UNP Q6N1P6
A	384	HIS	-	cloning artifact	UNP Q6N1P6
A	385	HIS	-	cloning artifact	UNP Q6N1P6
A	386	HIS	-	cloning artifact	UNP Q6N1P6
A	387	HIS	-	cloning artifact	UNP Q6N1P6
B	21	MSE	MET	modified residue	UNP Q6N1P6
B	27	MSE	MET	modified residue	UNP Q6N1P6
B	60	MSE	MET	modified residue	UNP Q6N1P6
B	94	MSE	MET	modified residue	UNP Q6N1P6
B	95	MSE	MET	modified residue	UNP Q6N1P6
B	317	MSE	MET	modified residue	UNP Q6N1P6
B	343	MSE	MET	modified residue	UNP Q6N1P6
B	346	MSE	MET	modified residue	UNP Q6N1P6
B	380	LEU	-	cloning artifact	UNP Q6N1P6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	381	GLU	-	cloning artifact	UNP Q6N1P6
B	382	HIS	-	cloning artifact	UNP Q6N1P6
B	383	HIS	-	cloning artifact	UNP Q6N1P6
B	384	HIS	-	cloning artifact	UNP Q6N1P6
B	385	HIS	-	cloning artifact	UNP Q6N1P6
B	386	HIS	-	cloning artifact	UNP Q6N1P6
B	387	HIS	-	cloning artifact	UNP Q6N1P6

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	132	Total 132	O 132	0	0
2	B	139	Total 139	O 139	0	0



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	79.80Å 79.80Å 247.35Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	22.19 – 2.10 22.19 – 2.10	Depositor EDS
% Data completeness (in resolution range)	92.4 (22.19-2.10) 95.9 (22.19-2.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	13.90 (at 2.10Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.223 , 0.258 0.230 , 0.266	Depositor DCC
$R_{free}$ test set	2430 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.8	Xtriage
Anisotropy	0.008	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 31.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.472 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5740	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.26% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

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	0.32	0/2795	0.59	0/3787
1	B	0.33	0/2784	0.60	0/3773
All	All	0.32	0/5579	0.59	0/7560

There are no bond length outliers.

There are no bond angle outliers.

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	2740	0	2747	37	0
1	B	2729	0	2734	46	0
2	A	132	0	0	1	0
2	B	139	0	0	2	0
All	All	5740	0	5481	79	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 7.

The worst 5 of 79 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:120:ASN:HD22	1:B:123:LEU:HB2	1.47	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:PRO:HA	1:A:208:ARG:HH11	1.52	0.71
1:B:4:GLN:NE2	1:B:268:HIS:H	1.88	0.71
1:B:160:ASP:HB3	1:B:242:ASP:OD1	1.91	0.69
1:B:313:ALA:O	1:B:317:MSE:HG2	1.95	0.67

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	353/387 (91%)	346 (98%)	5 (1%)	2 (1%)	22	19
1	B	352/387 (91%)	346 (98%)	4 (1%)	2 (1%)	22	19
All	All	705/774 (91%)	692 (98%)	9 (1%)	4 (1%)	22	19

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	197	PRO
1	B	197	PRO
1	A	121	PRO
1	B	121	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	284/301 (94%)	275 (97%)	9 (3%)	34	37
1	B	283/301 (94%)	279 (99%)	4 (1%)	62	70
All	All	567/602 (94%)	554 (98%)	13 (2%)	45	51

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	314	LEU
1	A	335	LEU
1	B	314	LEU
1	B	230	ARG
1	B	242	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	125	GLN
1	B	165	HIS
1	B	268	HIS
1	B	175	HIS
1	B	4	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 ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	349/387 (90%)	-1.18	0 100 100	10, 25, 53, 65	0
1	B	348/387 (89%)	-1.18	0 100 100	11, 25, 53, 63	0
All	All	697/774 (90%)	-1.18	0 100 100	10, 25, 53, 65	0

There are no RSRZ outliers to report.

### 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 monosaccharides 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.