



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 3, 2025 – 04:04 PM EDT

PDB ID : 9EE7 / pdb\_00009ee7  
Title : Folded domains of Xrs2 from S.cerevisiae  
Authors : Vigneswaran, A.; Shi, K.; Evans, R.; Aihara, H.; Latham, M.P.  
Deposited on : 2024-11-18  
Resolution : 2.38 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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

<http://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 : 4-5-2 with Phenix2.0rc1  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.45.1

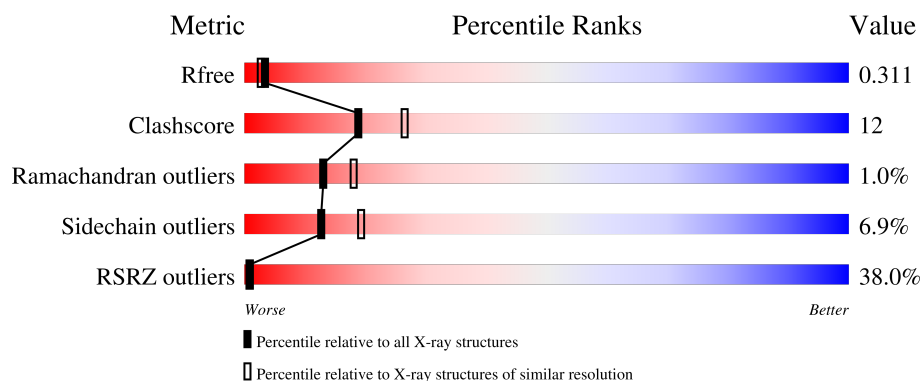
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.38 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	6699 (2.40-2.36)
Clashscore	180529	7414 (2.40-2.36)
Ramachandran outliers	177936	7337 (2.40-2.36)
Sidechain outliers	177891	7338 (2.40-2.36)
RSRZ outliers	164620	6699 (2.40-2.36)

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	325	<div> <div>35%</div> <div>68%</div> <div>22%</div> <div>8%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2182 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 DNA repair protein XRS2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	300	Total	C	N	O	S	0	0	0
			2175	1404	346	411	14			

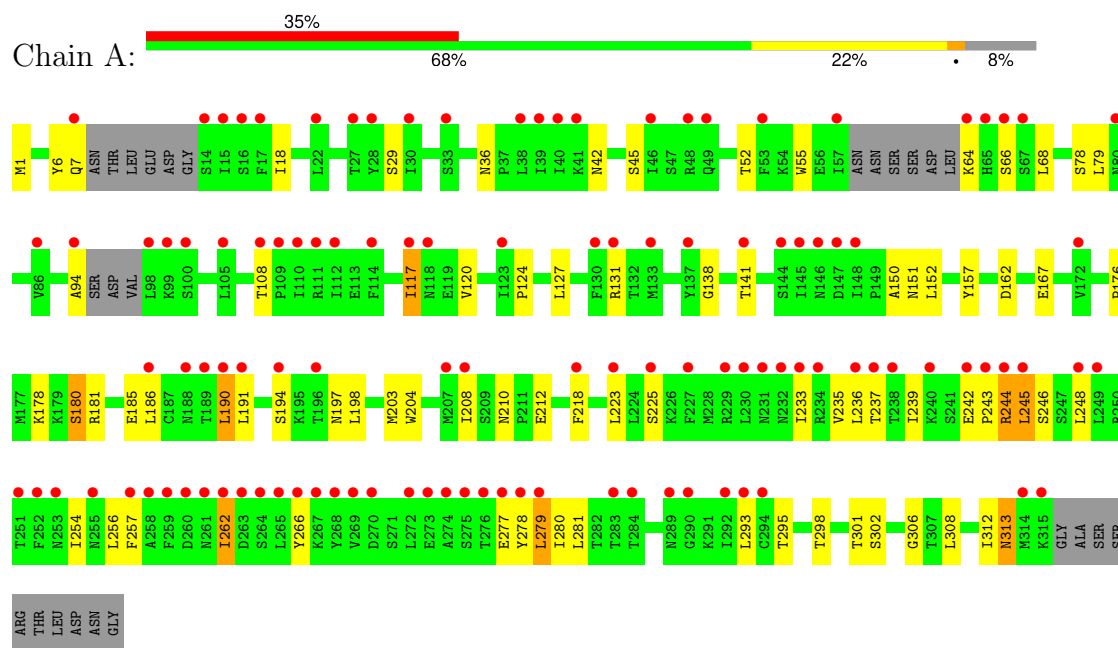
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	7	Total	O	0	0
			7	7		

### 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: DNA repair protein XRS2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	84.84Å 84.84Å 316.72Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	71.58 – 2.38 71.58 – 2.38	Depositor EDS
% Data completeness (in resolution range)	90.2 (71.58-2.38) 90.5 (71.58-2.38)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	0.14	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.33 (at 2.37Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.298 , 0.311 0.298 , 0.311	Depositor DCC
$R_{free}$ test set	1285 reflections (4.54%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	74.1	Xtriage
Anisotropy	0.442	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 67.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	2182	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.41% 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 [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	0.40	0/2217	0.64	0/3037

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 [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	2175	0	1929	48	0
2	A	7	0	0	0	0
All	All	2182	0	1929	48	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 12.

All (48) 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:A:237:THR:HG22	1:A:239:ILE:H	1.50	0.77
1:A:157:TYR:HH	1:A:301:THR:HG1	1.43	0.66
1:A:42:ASN:O	1:A:42:ASN:ND2	2.31	0.64
1:A:236:LEU:HD23	1:A:257:PHE:HB2	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:SER:HB3	1:A:256:LEU:HD12	1.81	0.63
1:A:124:PRO:HD2	1:A:127:LEU:HD12	1.81	0.61
1:A:244:ARG:O	1:A:246:SER:N	2.34	0.60
1:A:237:THR:CG2	1:A:239:ILE:H	2.15	0.59
1:A:243:PRO:O	1:A:245:LEU:N	2.36	0.59
1:A:190:LEU:HD22	1:A:203:MET:HB3	1.84	0.58
1:A:18:ILE:HG23	1:A:198:LEU:HB3	1.85	0.58
1:A:197:ASN:HD21	1:A:203:MET:HE2	1.67	0.58
1:A:278:TYR:CZ	1:A:313:ASN:HB2	2.38	0.58
1:A:181:ARG:NH2	1:A:185:GLU:OE1	2.37	0.58
1:A:237:THR:OG1	1:A:281:LEU:HB2	2.05	0.57
1:A:218:PHE:HB2	1:A:223:LEU:HD12	1.87	0.56
1:A:157:TYR:OH	1:A:301:THR:OG1	2.20	0.56
1:A:233:ILE:HG22	1:A:254:ILE:HD12	1.87	0.55
1:A:1:MET:N	1:A:117:ILE:O	2.41	0.54
1:A:162:ASP:HB3	1:A:295:THR:HG21	1.90	0.52
1:A:218:PHE:HB2	1:A:223:LEU:CD1	2.41	0.49
1:A:233:ILE:HG13	1:A:277:GLU:HG3	1.95	0.49
1:A:204:TRP:NE1	1:A:208:ILE:HG13	2.28	0.48
1:A:131:ARG:HG2	1:A:141:THR:OG1	2.13	0.48
1:A:280:ILE:HG13	1:A:293:LEU:HA	1.94	0.48
1:A:236:LEU:O	1:A:280:ILE:HA	2.14	0.48
1:A:151:ASN:O	1:A:176:PRO:HD2	2.14	0.47
1:A:55:TRP:CZ3	1:A:66:SER:HB3	2.50	0.46
1:A:29:SER:OG	1:A:36:ASN:OD1	2.25	0.46
1:A:278:TYR:CE1	1:A:313:ASN:HB2	2.51	0.45
1:A:55:TRP:HB3	1:A:68:LEU:HD13	1.98	0.44
1:A:181:ARG:HH21	1:A:185:GLU:HG2	1.83	0.44
1:A:152:LEU:HD11	1:A:178:LYS:HD2	1.98	0.44
1:A:302:SER:O	1:A:306:GLY:N	2.50	0.43
1:A:245:LEU:HA	1:A:248:LEU:HD23	1.98	0.43
1:A:6:TYR:HD1	1:A:7:GLN:HB2	1.82	0.43
1:A:235:VAL:HG22	1:A:279:LEU:CD2	2.49	0.43
1:A:308:LEU:O	1:A:312:ILE:HD12	2.19	0.43
1:A:120:VAL:HG13	1:A:150:ALA:HA	2.01	0.43
1:A:127:LEU:HD11	1:A:180:SER:HB3	1.99	0.42
1:A:210:ASN:OD1	1:A:212:GLU:HG2	2.19	0.42
1:A:243:PRO:O	1:A:244:ARG:C	2.62	0.42
1:A:262:ILE:HG13	1:A:266:TYR:CE2	2.55	0.41
1:A:29:SER:HB2	1:A:52:THR:HG22	2.03	0.41
1:A:64:LYS:HA	1:A:94:ALA:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:GLU:H	1:A:167:GLU:CD	2.27	0.41
1:A:1:MET:HA	1:A:138:GLY:HA3	2.02	0.41
1:A:191:LEU:HD23	1:A:191:LEU:HA	1.60	0.40

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	292/325 (90%)	256 (88%)	33 (11%)	3 (1%)	13 18

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	242	GLU
1	A	244	ARG
1	A	245	LEU

### 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	204/307 (66%)	190 (93%)	14 (7%)	13 19

All (14) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	A	45	SER
1	A	78	SER
1	A	79	LEU
1	A	108	THR
1	A	117	ILE
1	A	180	SER
1	A	186	LEU
1	A	190	LEU
1	A	194	SER
1	A	225	SER
1	A	262	ILE
1	A	279	LEU
1	A	298	THR
1	A	313	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	126	HIS
1	A	214	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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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	300/325 (92%)	1.70	114 (38%) <b>1</b> <b>1</b>	58, 81, 110, 120	0

All (114) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	98	LEU	6.2
1	A	14	SER	6.1
1	A	146	ASN	4.6
1	A	15	ILE	4.6
1	A	38	LEU	4.3
1	A	64	LYS	4.0
1	A	65	HIS	4.0
1	A	260	ASP	4.0
1	A	283	THR	4.0
1	A	94	ALA	4.0
1	A	147	ASP	3.9
1	A	148	ILE	3.9
1	A	253	ASN	3.9
1	A	99	LYS	3.8
1	A	289	ASN	3.8
1	A	7	GLN	3.8
1	A	22	LEU	3.7
1	A	17	PHE	3.7
1	A	259	PHE	3.6
1	A	231	ASN	3.6
1	A	227	PHE	3.6
1	A	108	THR	3.6
1	A	284	THR	3.6
1	A	264	SER	3.5
1	A	234	ARG	3.5
1	A	100	SER	3.5
1	A	194	SER	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	263	ASP	3.5
1	A	145	ILE	3.5
1	A	278	TYR	3.5
1	A	292	ILE	3.4
1	A	53	PHE	3.4
1	A	243	PRO	3.4
1	A	30	ILE	3.4
1	A	252	PHE	3.4
1	A	265	LEU	3.4
1	A	57	ILE	3.4
1	A	249	LEU	3.3
1	A	255	ASN	3.3
1	A	191	LEU	3.3
1	A	237	THR	3.2
1	A	232	ASN	3.1
1	A	66	SER	3.1
1	A	261	ASN	3.1
1	A	137	TYR	3.0
1	A	110	ILE	2.9
1	A	186	LEU	2.9
1	A	274	ALA	2.9
1	A	315	LYS	2.9
1	A	40	ILE	2.8
1	A	105	LEU	2.8
1	A	225	SER	2.8
1	A	207	MET	2.8
1	A	276	THR	2.8
1	A	112	ILE	2.7
1	A	270	ASP	2.7
1	A	266	TYR	2.7
1	A	208	ILE	2.7
1	A	67	SER	2.6
1	A	230	LEU	2.6
1	A	275	SER	2.6
1	A	257	PHE	2.6
1	A	28	TYR	2.6
1	A	196	THR	2.6
1	A	269	VAL	2.6
1	A	273	GLU	2.6
1	A	190	LEU	2.5
1	A	272	LEU	2.5
1	A	268	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	238	THR	2.5
1	A	39	ILE	2.5
1	A	117	ILE	2.5
1	A	240	LYS	2.5
1	A	80	ASN	2.5
1	A	144	SER	2.4
1	A	123	ILE	2.4
1	A	277	GLU	2.4
1	A	41	LYS	2.4
1	A	109	PRO	2.4
1	A	233	ILE	2.4
1	A	267	LYS	2.4
1	A	111	ARG	2.4
1	A	293	LEU	2.4
1	A	46	ILE	2.3
1	A	229	ARG	2.3
1	A	118	ASN	2.3
1	A	236	LEU	2.3
1	A	172	VAL	2.3
1	A	133	MET	2.3
1	A	242	GLU	2.3
1	A	251	THR	2.3
1	A	262	ILE	2.2
1	A	131	ARG	2.2
1	A	27	THR	2.2
1	A	189	THR	2.2
1	A	86	VAL	2.2
1	A	294	CYS	2.2
1	A	16	SER	2.2
1	A	258	ALA	2.2
1	A	141	THR	2.2
1	A	248	LEU	2.2
1	A	48	ARG	2.1
1	A	244	ARG	2.1
1	A	49	GLN	2.1
1	A	188	ASN	2.1
1	A	279	LEU	2.1
1	A	114	PHE	2.1
1	A	314	MET	2.1
1	A	223	LEU	2.1
1	A	130	PHE	2.0
1	A	218	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	290	GLY	2.0
1	A	33	SER	2.0
1	A	245	LEU	2.0

## 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.