



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:07 AM UTC

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

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

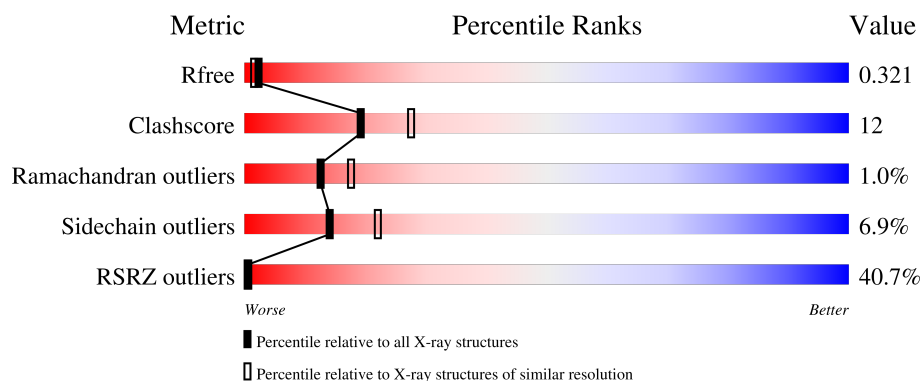
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	7164 (2.40-2.36)
Clashscore	190562	7722 (2.40-2.36)
Ramachandran outliers	187476	7626 (2.40-2.36)
Sidechain outliers	187428	7627 (2.40-2.36)
RSRZ outliers	180081	7170 (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 ≥ 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	

2 Entry composition [i](#)

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			

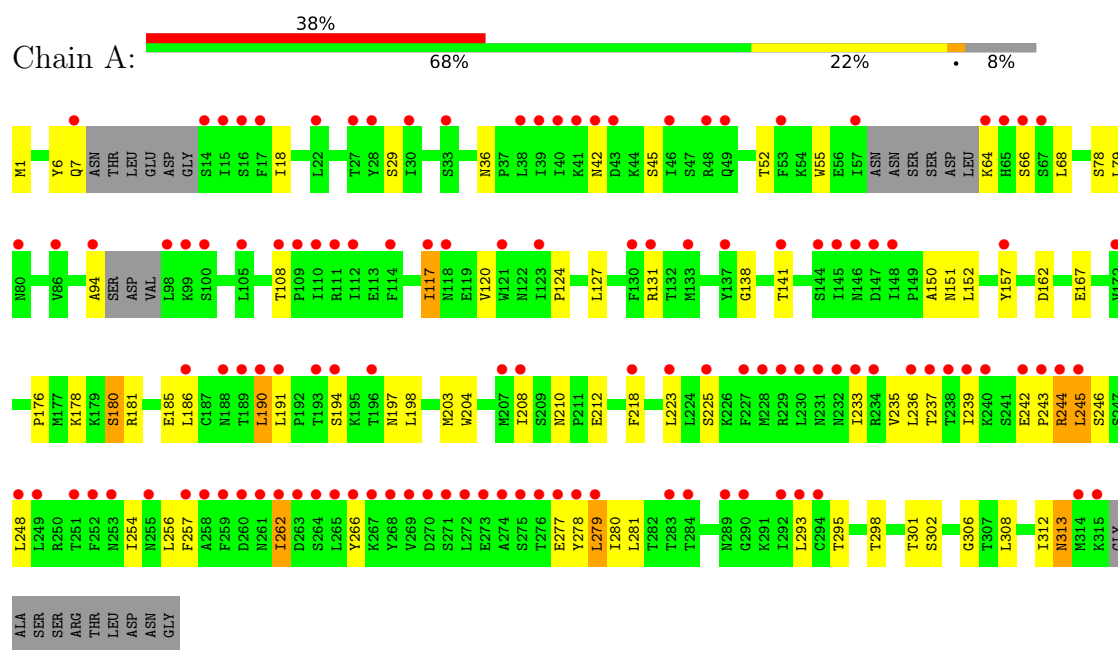
- Molecule 2 is water.

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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	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 0.307 , 0.321	Depositor DCC
R_{free} test set	1285 reflections (4.54%)	wwPDB-VP
Wilson B-factor (Å ²)	74.1	Xtriage
Anisotropy	0.442	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 67.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	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 ²)	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.*

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	0.40	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%)	12 17

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%)	14 22

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, 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	300/325 (92%)	1.79	122 (40%) 0 0	58, 81, 110, 120	0

All (122) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	98	LEU	6.4
1	A	14	SER	6.1
1	A	146	ASN	4.7
1	A	15	ILE	4.7
1	A	38	LEU	4.4
1	A	283	THR	4.1
1	A	65	HIS	4.1
1	A	94	ALA	4.1
1	A	260	ASP	4.1
1	A	148	ILE	4.0
1	A	64	LYS	4.0
1	A	147	ASP	4.0
1	A	253	ASN	3.9
1	A	289	ASN	3.9
1	A	22	LEU	3.8
1	A	7	GLN	3.8
1	A	17	PHE	3.8
1	A	99	LYS	3.8
1	A	259	PHE	3.8
1	A	227	PHE	3.7
1	A	108	THR	3.7
1	A	231	ASN	3.7
1	A	284	THR	3.7
1	A	278	TYR	3.6
1	A	264	SER	3.6
1	A	145	ILE	3.6
1	A	53	PHE	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	100	SER	3.5
1	A	194	SER	3.5
1	A	292	ILE	3.5
1	A	252	PHE	3.5
1	A	243	PRO	3.5
1	A	30	ILE	3.5
1	A	265	LEU	3.5
1	A	263	ASP	3.5
1	A	234	ARG	3.5
1	A	57	ILE	3.5
1	A	249	LEU	3.5
1	A	191	LEU	3.4
1	A	255	ASN	3.4
1	A	237	THR	3.3
1	A	137	TYR	3.2
1	A	232	ASN	3.2
1	A	66	SER	3.1
1	A	261	ASN	3.1
1	A	110	ILE	3.0
1	A	186	LEU	3.0
1	A	274	ALA	3.0
1	A	40	ILE	2.9
1	A	105	LEU	2.9
1	A	315	LYS	2.9
1	A	112	ILE	2.9
1	A	207	MET	2.9
1	A	276	THR	2.9
1	A	225	SER	2.8
1	A	266	TYR	2.8
1	A	208	ILE	2.8
1	A	270	ASP	2.8
1	A	230	LEU	2.7
1	A	28	TYR	2.7
1	A	257	PHE	2.7
1	A	67	SER	2.7
1	A	269	VAL	2.7
1	A	196	THR	2.7
1	A	275	SER	2.7
1	A	190	LEU	2.7
1	A	268	TYR	2.6
1	A	272	LEU	2.6
1	A	273	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	238	THR	2.6
1	A	39	ILE	2.6
1	A	117	ILE	2.6
1	A	80	ASN	2.5
1	A	123	ILE	2.5
1	A	144	SER	2.5
1	A	109	PRO	2.5
1	A	233	ILE	2.5
1	A	240	LYS	2.5
1	A	293	LEU	2.5
1	A	277	GLU	2.4
1	A	41	LYS	2.4
1	A	46	ILE	2.4
1	A	172	VAL	2.4
1	A	236	LEU	2.4
1	A	111	ARG	2.4
1	A	267	LYS	2.4
1	A	118	ASN	2.4
1	A	251	THR	2.4
1	A	133	MET	2.4
1	A	229	ARG	2.4
1	A	86	VAL	2.3
1	A	262	ILE	2.3
1	A	258	ALA	2.3
1	A	27	THR	2.3
1	A	189	THR	2.3
1	A	242	GLU	2.3
1	A	294	CYS	2.3
1	A	141	THR	2.3
1	A	16	SER	2.3
1	A	248	LEU	2.3
1	A	131	ARG	2.3
1	A	279	LEU	2.2
1	A	114	PHE	2.2
1	A	49	GLN	2.2
1	A	48	ARG	2.2
1	A	188	ASN	2.2
1	A	244	ARG	2.2
1	A	223	LEU	2.2
1	A	130	PHE	2.2
1	A	218	PHE	2.2
1	A	314	MET	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	121	TRP	2.1
1	A	290	GLY	2.1
1	A	157	TYR	2.1
1	A	245	LEU	2.1
1	A	33	SER	2.1
1	A	193	THR	2.1
1	A	228	MET	2.1
1	A	271	SER	2.0
1	A	42	ASN	2.0
1	A	43	ASP	2.0
1	A	239	ILE	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.