



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 27, 2026 – 05:13 PM EDT

PDB ID : 3UWX / pdb_00003uwx
Title : Crystal structure of UvrA-UvrB complex
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Deposited on : 2011-12-03
Resolution : 4.40 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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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

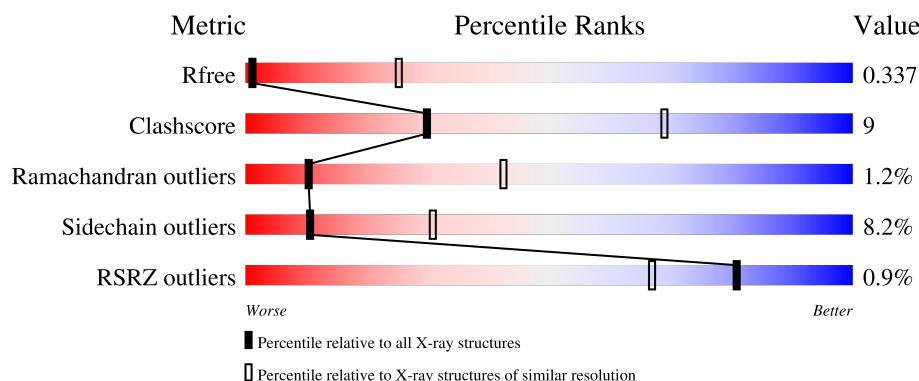
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.40 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	1088 (4.90-3.90)
Clashscore	190562	1135 (4.90-3.90)
Ramachandran outliers	187476	1026 (4.90-3.90)
Sidechain outliers	187428	1010 (4.90-3.90)
RSRZ outliers	180081	1084 (4.90-3.90)

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	972	
2	B	683	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12193 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 Excinuclease ABC, A subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	945	Total	C	N	O	S	0	0	0
			7381	4646	1305	1402	28			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP E8SW61
A	-18	GLY	-	expression tag	UNP E8SW61
A	-17	SER	-	expression tag	UNP E8SW61
A	-16	SER	-	expression tag	UNP E8SW61
A	-15	HIS	-	expression tag	UNP E8SW61
A	-14	HIS	-	expression tag	UNP E8SW61
A	-13	HIS	-	expression tag	UNP E8SW61
A	-12	HIS	-	expression tag	UNP E8SW61
A	-11	HIS	-	expression tag	UNP E8SW61
A	-10	HIS	-	expression tag	UNP E8SW61
A	-9	SER	-	expression tag	UNP E8SW61
A	-8	SER	-	expression tag	UNP E8SW61
A	-7	GLY	-	expression tag	UNP E8SW61
A	-6	LEU	-	expression tag	UNP E8SW61
A	-5	VAL	-	expression tag	UNP E8SW61
A	-4	PRO	-	expression tag	UNP E8SW61
A	-3	ARG	-	expression tag	UNP E8SW61
A	-2	GLY	-	expression tag	UNP E8SW61
A	-1	SER	-	expression tag	UNP E8SW61
A	0	HIS	-	expression tag	UNP E8SW61

- Molecule 2 is a protein called UvrABC system protein B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	595	Total	C	N	O	S	0	0	0
			4809	3031	856	910	12			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-24	MET	-	expression tag	UNP E8SW62
B	-23	GLY	-	expression tag	UNP E8SW62
B	-22	SER	-	expression tag	UNP E8SW62
B	-21	SER	-	expression tag	UNP E8SW62
B	-20	HIS	-	expression tag	UNP E8SW62
B	-19	HIS	-	expression tag	UNP E8SW62
B	-18	HIS	-	expression tag	UNP E8SW62
B	-17	HIS	-	expression tag	UNP E8SW62
B	-16	HIS	-	expression tag	UNP E8SW62
B	-15	HIS	-	expression tag	UNP E8SW62
B	-14	SER	-	expression tag	UNP E8SW62
B	-13	SER	-	expression tag	UNP E8SW62
B	-12	GLY	-	expression tag	UNP E8SW62
B	-11	LEU	-	expression tag	UNP E8SW62
B	-10	VAL	-	expression tag	UNP E8SW62
B	-9	PRO	-	expression tag	UNP E8SW62
B	-8	ARG	-	expression tag	UNP E8SW62
B	-7	GLY	-	expression tag	UNP E8SW62
B	-6	SER	-	expression tag	UNP E8SW62
B	-5	HIS	-	expression tag	UNP E8SW62
B	-3	GLY	-	expression tag	UNP E8SW62
B	-2	PRO	-	expression tag	UNP E8SW62
B	-1	LYS	-	expression tag	UNP E8SW62
B	0	LYS	-	expression tag	UNP E8SW62
B	1	VAL	MET	SEE REMARK 999	UNP E8SW62
B	74	HIS	TYR	SEE REMARK 999	UNP E8SW62

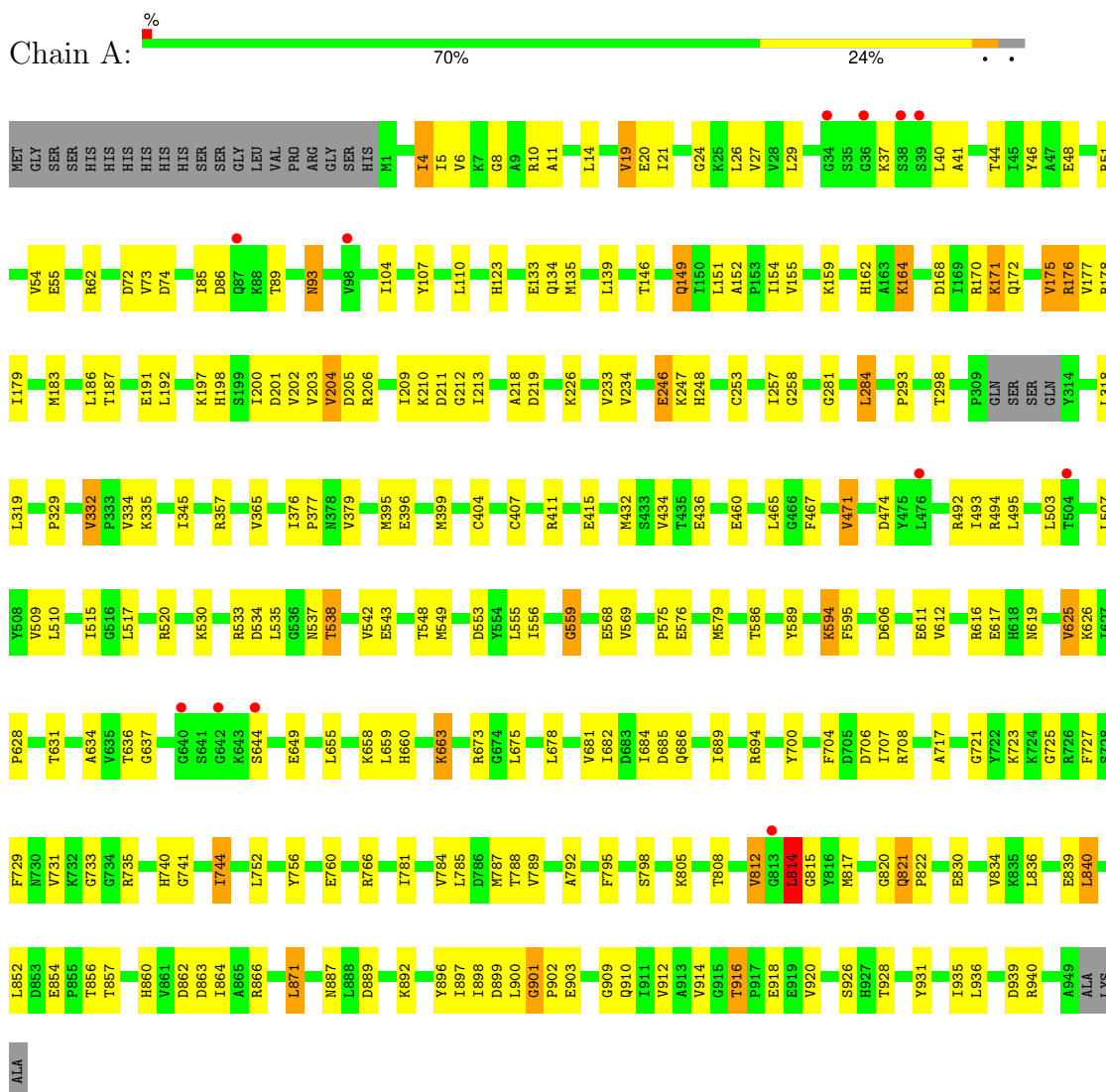
- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	Zn	0	0
			3	3		

3 Residue-property plots

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: Excinuclease ABC, A subunit



- Molecule 2: UvrABC system protein B



GLU	E478	L334	P204	E99	MET
GLU	I479	I335	A205	A100	GLY
THR	K480	I336	S206	R207	SER
GLU	T481		R207	Y101	SER
MET		V342	D208	D106	HIS
TYR	R484	T343	E209		HIS
GLU		L344	H210	E110	HIS
ALA	R489		C211	K111	HIS
LYS		I347	I212	D112	HIS
PRO	L493	Y351	R213	A113	HIS
ALA	G494		V214	K114	SER
ALA	K495		E215	I115	SER
ALA	Y496	K358	F216		GLY
MET	D497				LEU
THR	V498	R367	E220	E118	VAL
THR	L499	L372	I224	I119	PRO
GLN				K121	ARG
GLU	R506	R375	V227	L122	GLY
ARG	E507				SER
ARG		F382	L230	S125	HIS
GLU	V517	K385	L235	L130	MET
GLU	A518	I386			GLY
LEU	I519		E239	R133	SER
ILE	L520	Y391	H240	R134	HIS
ARG		I392	V241	D135	MET
GLU		T395	F244	V139	GLY
LEU	Y552	P396	R252		ARG
ILE	L520	G397		V142	SER
LYS	K558		A259	S143	GLY
LEU		S404	I263	E153	LYS
ALA	E561	P405	E264	E156	LYS
ALA		Q410	R270		V1
LYS	Q565	I411		E166	E12
LYS	E566		Q288	I167	
ALA	T567	T415	R291	I179	Q19
LEU	K568	D419	R298	Q180	
ASP		V424		M184	A40
PHE	R571	Q430	E307	D185	
GLU		I431	R316	I186	T43
ARG		L434	P317	D187	I49
ALA	Y577		S320	T192	P59
ALA		I438	T321	F193	T60
GLN	K580	R444	L326	V195	L61
LEU	H581	L449	D327	R196	V62
ARG		K456	P330	G197	N66
ASP	V588		D331	D198	K67
ILE			D332	V199	A70
ILE	E591		F333	I202	G71
PHE	I592			F203	Q72
GLU	R593				L73
LEU	D594				H74
LYS	V595				K78
LYS					V86
ALA	ILE				E87
ARG	ARG				Y88
ALA	ALA				
GLU	THR				
GLY	ALA				
	TYR				
	ALA				
	ALA				
	ALA				

4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α , β , γ	216.82Å 216.82Å 116.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.06 – 4.40 38.06 – 4.40	Depositor EDS
% Data completeness (in resolution range)	96.7 (38.06-4.40) 85.4 (38.06-4.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 4.44Å)	Xtriage
Refinement program	PHENIX 1.7.2 _869	Depositor
R, R_{free}	0.288 , 0.349 0.275 , 0.337	Depositor DCC
R_{free} test set	900 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	189.5	Xtriage
Anisotropy	0.632	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 348.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	12193	wwPDB-VP
Average B, all atoms (Å ²)	347.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.81% 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: ZN

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	0.31	0/7507	0.79	2/10143 (0.0%)
2	B	0.33	0/4892	0.81	4/6612 (0.1%)
All	All	0.32	0/12399	0.80	6/16755 (0.0%)

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	397	GLY	CA-C-N	6.53	125.76	118.97
2	B	397	GLY	C-N-CA	6.53	125.76	118.97
2	B	244	PHE	CA-C-N	5.79	125.79	119.89
2	B	244	PHE	C-N-CA	5.79	125.79	119.89
1	A	821	GLN	CA-C-N	5.34	125.34	119.90

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	7381	0	7458	147	0
2	B	4809	0	4839	68	0
3	A	3	0	0	0	0
All	All	12193	0	12297	209	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 9.

The worst 5 of 209 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:176:ARG:HB3	1:A:203:VAL:HB	1.61	0.80
1:A:168:ASP:HA	1:A:171:LYS:HB3	1.69	0.75
1:A:432:MET:HE2	1:A:436:GLU:HB3	1.68	0.75
2:B:74:HIS:CE1	2:B:88:TYR:HA	2.22	0.75
1:A:634:ALA:HB3	1:A:897:ILE:HG22	1.70	0.71

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	941/972 (97%)	855 (91%)	72 (8%)	14 (2%)	8	38
2	B	593/683 (87%)	557 (94%)	32 (5%)	4 (1%)	18	55
All	All	1534/1655 (93%)	1412 (92%)	104 (7%)	18 (1%)	10	42

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	901	GLY
1	A	212	GLY
1	A	559	GLY
1	A	617	GLU
1	A	798	SER

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	796/818 (97%)	748 (94%)	48 (6%)	17	39
2	B	523/592 (88%)	463 (88%)	60 (12%)	5	20
All	All	1319/1410 (94%)	1211 (92%)	108 (8%)	10	31

5 of 108 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	114	LYS
2	B	208	ASP
2	B	507	GLU
2	B	118	GLU
2	B	179	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	104	GLN
2	B	116	ASN
2	B	565	GLN
2	B	288	GLN
1	A	302	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](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

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	945/972 (97%)	-0.24	12 (1%) 75 60	250, 336, 486, 771	0
2	B	595/683 (87%)	-0.32	2 (0%) 90 80	252, 325, 437, 576	0
All	All	1540/1655 (93%)	-0.27	14 (0%) 81 67	250, 332, 468, 771	0

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	644	SER	4.1
1	A	476	LEU	3.6
1	A	36	GLY	3.3
1	A	34	GLY	2.9
2	B	434	LEU	2.9

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
3	ZN	A	1006	1/1	0.95	0.08	550,550,550,550	0
3	ZN	A	1004	1/1	0.97	0.04	550,550,550,550	0
3	ZN	A	1005	1/1	0.98	0.06	550,550,550,550	0

6.5 Other polymers [i](#)

There are no such residues in this entry.