



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 8DPE / pdb_00008dpe
Title : Crystal structure of ATP-dependent RNA helicase DDX42
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Deposited on : 2022-07-15
Resolution : 1.53 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

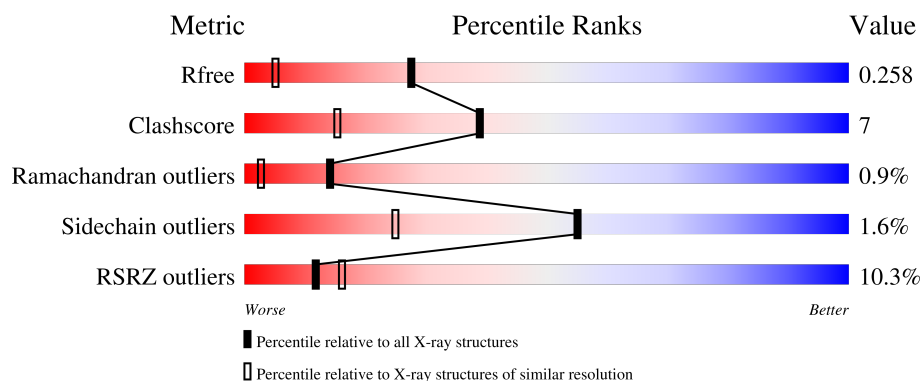
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.53 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	1003 (1.54-1.54)
Clashscore	190562	1025 (1.54-1.54)
Ramachandran outliers	187476	1007 (1.54-1.54)
Sidechain outliers	187428	1007 (1.54-1.54)
RSRZ outliers	180081	1002 (1.54-1.54)

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	444	10% 84% 12% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3802 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 ATP-dependent RNA helicase DDX42.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	436	Total	C	N	O	S	0	0	0
			3449	2175	627	633	14			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	203	MET	-	expression tag	UNP Q86XP3
A	204	GLY	-	expression tag	UNP Q86XP3
A	205	HIS	-	expression tag	UNP Q86XP3
A	206	HIS	-	expression tag	UNP Q86XP3
A	207	HIS	-	expression tag	UNP Q86XP3
A	208	HIS	-	expression tag	UNP Q86XP3
A	209	HIS	-	expression tag	UNP Q86XP3
A	210	HIS	-	expression tag	UNP Q86XP3

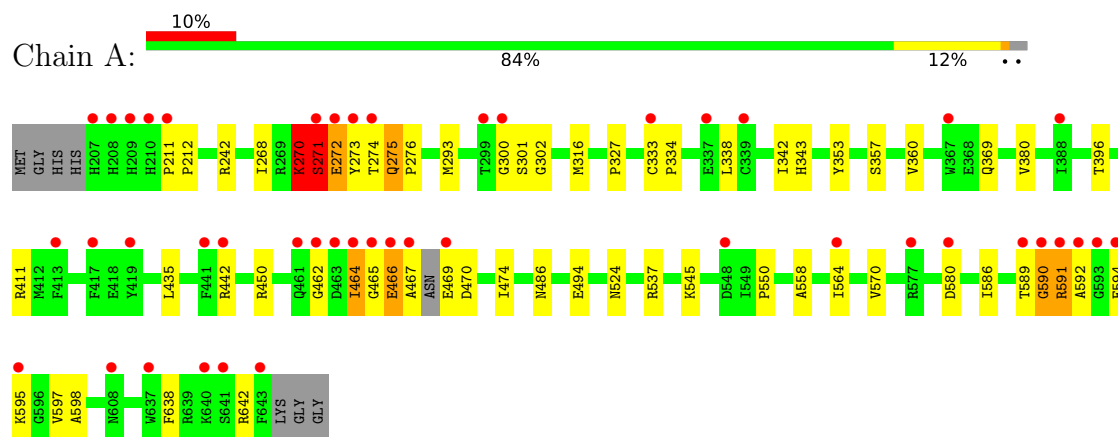
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	353	Total	O	0	0
			353	353		

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: ATP-dependent RNA helicase DDX42



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	42.92Å 73.27Å 134.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.15 – 1.53 38.15 – 1.53	Depositor EDS
% Data completeness (in resolution range)	98.3 (38.15-1.53) 98.3 (38.15-1.53)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.99 (at 1.53Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.212 , 0.255 0.215 , 0.258	Depositor DCC
R_{free} test set	3220 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	20.1	Xtriage
Anisotropy	0.268	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 32.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3802	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.38% 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

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	0.56	1/3521 (0.0%)	0.85	12/4757 (0.3%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	276	PRO	C-O	-7.00	1.15	1.23

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	591	ARG	N-CA-C	-6.83	103.09	113.89
1	A	271	SER	CA-C-N	6.50	133.40	121.70
1	A	271	SER	C-N-CA	6.50	133.40	121.70
1	A	592	ALA	N-CA-C	-6.25	104.52	111.71
1	A	271	SER	N-CA-C	-6.03	97.95	110.80
1	A	464	ILE	CB-CA-C	-5.96	104.28	111.85
1	A	270	LYS	N-CA-C	-5.90	104.80	112.23
1	A	275	GLN	CA-C-N	-5.75	114.04	119.85
1	A	275	GLN	C-N-CA	-5.75	114.04	119.85
1	A	275	GLN	N-CA-CB	5.60	116.98	111.10
1	A	464	ILE	N-CA-C	5.36	117.27	112.17
1	A	462	GLY	N-CA-C	5.16	118.88	112.64

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	590	GLY	Peptide

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	3449	0	3452	47	0
2	A	353	0	0	4	2
All	All	3802	0	3452	47	2

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.

All (47) 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:465:GLY:O	1:A:466:GLU:HB2	1.34	1.15
1:A:469:GLU:HB3	1:A:591:ARG:HD3	1.53	0.90
1:A:465:GLY:O	1:A:466:GLU:CB	2.19	0.89
1:A:268:ILE:O	1:A:271:SER:HB3	1.75	0.87
1:A:268:ILE:O	1:A:271:SER:CB	2.28	0.82
1:A:300:GLY:O	1:A:302:GLY:N	2.12	0.80
1:A:271:SER:HA	1:A:272:GLU:HB3	1.65	0.79
1:A:537:ARG:NH1	2:A:704:HOH:O	2.16	0.78
1:A:469:GLU:HB3	1:A:591:ARG:CD	2.14	0.78
1:A:494:GLU:OE1	2:A:701:HOH:O	2.12	0.68
1:A:268:ILE:O	1:A:271:SER:OG	2.11	0.67
1:A:486:ASN:OD1	2:A:702:HOH:O	2.13	0.65
1:A:586:ILE:O	1:A:589:THR:HG23	1.95	0.65
1:A:270:LYS:C	1:A:271:SER:O	2.34	0.65
1:A:396:THR:O	2:A:703:HOH:O	2.15	0.65
1:A:271:SER:CA	1:A:272:GLU:HB3	2.29	0.62
1:A:242:ARG:HH22	1:A:465:GLY:HA3	1.65	0.60
1:A:464:ILE:O	1:A:464:ILE:HG22	2.01	0.60
1:A:300:GLY:C	1:A:302:GLY:H	2.06	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:ILE:C	1:A:271:SER:HB3	2.26	0.59
1:A:537:ARG:NH2	1:A:558:ALA:O	2.33	0.57
1:A:474:ILE:HD12	1:A:597:VAL:HG11	1.88	0.55
1:A:293:MET:HB3	1:A:435:LEU:HD22	1.90	0.54
1:A:589:THR:HG21	1:A:598:ALA:HB2	1.90	0.54
1:A:638:PHE:O	1:A:642:ARG:HB2	2.09	0.53
1:A:450:ARG:NH2	1:A:580:ASP:OD2	2.41	0.53
1:A:360:VAL:HG12	1:A:369:GLN:HB3	1.92	0.51
1:A:545:LYS:HE2	1:A:564:ILE:HD11	1.93	0.49
1:A:316:MET:SD	1:A:353:TYR:HB3	2.54	0.47
1:A:271:SER:OG	1:A:273:TYR:N	2.47	0.47
1:A:591:ARG:NH1	1:A:594:GLU:HG3	2.30	0.47
1:A:524:ASN:O	1:A:550:PRO:HD2	2.14	0.47
1:A:333:CYS:SG	1:A:342:ILE:HD12	2.55	0.46
1:A:466:GLU:HG2	1:A:467:ALA:H	1.80	0.46
1:A:590:GLY:O	1:A:594:GLU:HA	2.16	0.45
1:A:272:GLU:HG3	1:A:272:GLU:O	2.16	0.45
1:A:467:ALA:CA	1:A:469:GLU:N	2.80	0.45
1:A:467:ALA:C	1:A:469:GLU:N	2.77	0.43
1:A:334:PRO:HD2	1:A:338:LEU:HD23	2.01	0.42
1:A:470:ASP:O	1:A:591:ARG:NE	2.52	0.42
1:A:343:HIS:HE1	1:A:357:SER:O	2.03	0.42
1:A:467:ALA:HA	1:A:469:GLU:N	2.35	0.42
1:A:469:GLU:HB3	1:A:591:ARG:HD2	1.99	0.42
1:A:211:PRO:HA	1:A:212:PRO:HD3	1.88	0.41
1:A:466:GLU:HB3	1:A:467:ALA:H	1.41	0.41
1:A:570:VAL:CG2	1:A:589:THR:HG22	2.51	0.41
1:A:327:PRO:HB3	1:A:380:VAL:HG23	2.03	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:988:HOH:O	2:A:1031:HOH:O[3_546]	2.17	0.03
2:A:859:HOH:O	2:A:995:HOH:O[4_456]	2.18	0.02

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	432/444 (97%)	420 (97%)	8 (2%)	4 (1%)	14 3

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	301	SER
1	A	466	GLU
1	A	595	LYS
1	A	272	GLU

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	372/377 (99%)	366 (98%)	6 (2%)	55 25

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	270	LYS
1	A	271	SER
1	A	274	THR
1	A	275	GLN
1	A	411	ARG
1	A	442	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	207	HIS
1	A	209	HIS
1	A	219	ASN
1	A	266	HIS
1	A	343	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](#)

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	436/444 (98%)	0.82	45 (10%) 12 16	12, 24, 42, 66	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	441	PHE	9.0
1	A	592	ALA	6.9
1	A	643	PHE	6.0
1	A	467	ALA	5.4
1	A	590	GLY	5.3
1	A	464	ILE	5.2
1	A	591	ARG	5.1
1	A	593	GLY	5.0
1	A	466	GLU	4.0
1	A	274	THR	3.9
1	A	564	ILE	3.9
1	A	271	SER	3.6
1	A	272	GLU	3.6
1	A	465	GLY	3.5
1	A	333	CYS	3.4
1	A	300	GLY	3.3
1	A	207	HIS	3.2
1	A	209	HIS	3.2
1	A	589	THR	3.2
1	A	273	TYR	3.2
1	A	641	SER	3.1
1	A	367	TRP	3.1
1	A	208	HIS	3.1
1	A	299	THR	3.0
1	A	339	CYS	3.0
1	A	419	TYR	2.9
1	A	469	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	210	HIS	2.8
1	A	640	LYS	2.6
1	A	594	GLU	2.6
1	A	595	LYS	2.5
1	A	608	ASN	2.5
1	A	637	TRP	2.5
1	A	580	ASP	2.4
1	A	442	ARG	2.4
1	A	337	GLU	2.4
1	A	461	GLN	2.4
1	A	211	PRO	2.4
1	A	417	PHE	2.3
1	A	462	GLY	2.2
1	A	388	ILE	2.1
1	A	548	ASP	2.1
1	A	577	ARG	2.0
1	A	463	ASP	2.0
1	A	413	PHE	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.