



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 21, 2024 – 10:43 PM EDT

PDB ID : 2QFD  
Title : Crystal structure of the regulatory domain of human RIG-I with bound Hg  
Authors : Cui, S.; Lammens, A.; Lammens, K.; Hopfner, K.P.  
Deposited on : 2007-06-27  
Resolution : 2.70 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

<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	:	4.02b-467
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)
Validation Pipeline (wwPDB-VP)	:	2.39

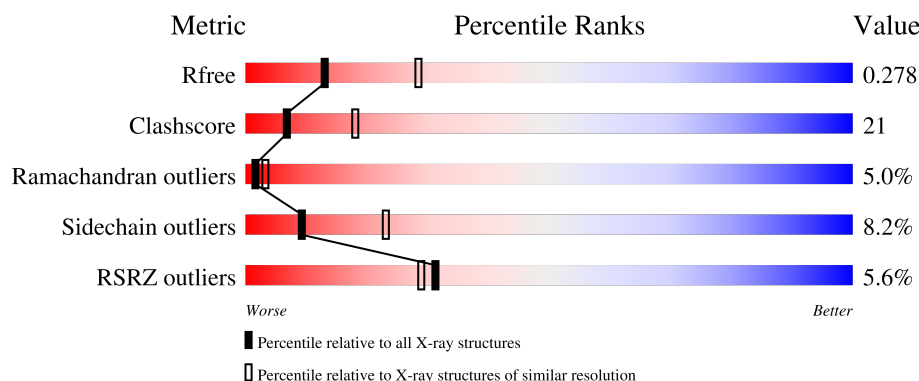
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	3333 (2.70-2.70)
Clashscore	180529	3684 (2.70-2.70)
Ramachandran outliers	177936	3633 (2.70-2.70)
Sidechain outliers	177891	3633 (2.70-2.70)
RSRZ outliers	164620	3333 (2.70-2.70)

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	145	<div> <div>0%</div> <div> <div>63%</div> <div>17%</div> <div>•</div> <div>17%</div> </div> </div>
1	B	145	<div> <div>2%</div> <div> <div>59%</div> <div>21%</div> <div>•</div> <div>17%</div> </div> </div>
1	C	145	<div> <div>3%</div> <div> <div>48%</div> <div>30%</div> <div>5%</div> <div>17%</div> </div> </div>
1	D	145	<div> <div>0%</div> <div> <div>50%</div> <div>28%</div> <div>•</div> <div>17%</div> </div> </div>
1	E	145	<div> <div>6%</div> <div> <div>43%</div> <div>33%</div> <div>7%</div> <div>17%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	145	<div><div></div><div>2%</div><div>41%</div><div>35%</div><div>7%</div><div>17%</div></div>
1	G	145	<div><div></div><div>6%</div><div>56%</div><div>23%</div><div>• •</div><div>17%</div></div>
1	H	145	<div><div></div><div>6%</div><div>48%</div><div>29%</div><div>7%</div><div>17%</div></div>
1	I	145	<div><div></div><div>4%</div><div>43%</div><div>35%</div><div>• •</div><div>17%</div></div>
1	J	145	<div><div></div><div>15%</div><div>49%</div><div>28%</div><div>6%</div><div>•</div><div>17%</div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10092 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 Probable ATP-dependent RNA helicase DDX58.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	121	Total	C	N	O	S	36	0	0
			998	648	169	173	8			
1	B	121	Total	C	N	O	S	73	0	0
			998	648	169	173	8			
1	C	121	Total	C	N	O	S	85	0	0
			998	648	169	173	8			
1	D	121	Total	C	N	O	S	130	0	0
			998	648	169	173	8			
1	E	121	Total	C	N	O	S	109	0	0
			998	648	169	173	8			
1	F	121	Total	C	N	O	S	86	0	0
			998	648	169	173	8			
1	G	121	Total	C	N	O	S	123	0	0
			998	648	169	173	8			
1	H	121	Total	C	N	O	S	98	0	0
			998	648	169	173	8			
1	I	121	Total	C	N	O	S	86	0	0
			998	648	169	173	8			
1	J	121	Total	C	N	O	S	176	0	0
			998	648	169	173	8			

There are 210 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	781	MET	-	expression tag	UNP O95786
A	782	GLY	-	expression tag	UNP O95786
A	783	SER	-	expression tag	UNP O95786
A	784	SER	-	expression tag	UNP O95786
A	785	HIS	-	expression tag	UNP O95786
A	786	HIS	-	expression tag	UNP O95786
A	787	HIS	-	expression tag	UNP O95786
A	788	HIS	-	expression tag	UNP O95786
A	789	HIS	-	expression tag	UNP O95786

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Chain	Residue	Modelled	Actual	Comment	Reference
A	790	HIS	-	expression tag	UNP O95786
A	791	SER	-	expression tag	UNP O95786
A	792	SER	-	expression tag	UNP O95786
A	793	GLY	-	expression tag	UNP O95786
A	794	LEU	-	expression tag	UNP O95786
A	795	VAL	-	expression tag	UNP O95786
A	796	PRO	-	expression tag	UNP O95786
A	797	ARG	-	expression tag	UNP O95786
A	798	GLY	-	expression tag	UNP O95786
A	799	SER	-	expression tag	UNP O95786
A	800	HIS	-	expression tag	UNP O95786
A	801	MET	-	expression tag	UNP O95786
B	781	MET	-	expression tag	UNP O95786
B	782	GLY	-	expression tag	UNP O95786
B	783	SER	-	expression tag	UNP O95786
B	784	SER	-	expression tag	UNP O95786
B	785	HIS	-	expression tag	UNP O95786
B	786	HIS	-	expression tag	UNP O95786
B	787	HIS	-	expression tag	UNP O95786
B	788	HIS	-	expression tag	UNP O95786
B	789	HIS	-	expression tag	UNP O95786
B	790	HIS	-	expression tag	UNP O95786
B	791	SER	-	expression tag	UNP O95786
B	792	SER	-	expression tag	UNP O95786
B	793	GLY	-	expression tag	UNP O95786
B	794	LEU	-	expression tag	UNP O95786
B	795	VAL	-	expression tag	UNP O95786
B	796	PRO	-	expression tag	UNP O95786
B	797	ARG	-	expression tag	UNP O95786
B	798	GLY	-	expression tag	UNP O95786
B	799	SER	-	expression tag	UNP O95786
B	800	HIS	-	expression tag	UNP O95786
B	801	MET	-	expression tag	UNP O95786
C	781	MET	-	expression tag	UNP O95786
C	782	GLY	-	expression tag	UNP O95786
C	783	SER	-	expression tag	UNP O95786
C	784	SER	-	expression tag	UNP O95786
C	785	HIS	-	expression tag	UNP O95786
C	786	HIS	-	expression tag	UNP O95786
C	787	HIS	-	expression tag	UNP O95786
C	788	HIS	-	expression tag	UNP O95786
C	789	HIS	-	expression tag	UNP O95786

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Chain	Residue	Modelled	Actual	Comment	Reference
C	790	HIS	-	expression tag	UNP O95786
C	791	SER	-	expression tag	UNP O95786
C	792	SER	-	expression tag	UNP O95786
C	793	GLY	-	expression tag	UNP O95786
C	794	LEU	-	expression tag	UNP O95786
C	795	VAL	-	expression tag	UNP O95786
C	796	PRO	-	expression tag	UNP O95786
C	797	ARG	-	expression tag	UNP O95786
C	798	GLY	-	expression tag	UNP O95786
C	799	SER	-	expression tag	UNP O95786
C	800	HIS	-	expression tag	UNP O95786
C	801	MET	-	expression tag	UNP O95786
D	781	MET	-	expression tag	UNP O95786
D	782	GLY	-	expression tag	UNP O95786
D	783	SER	-	expression tag	UNP O95786
D	784	SER	-	expression tag	UNP O95786
D	785	HIS	-	expression tag	UNP O95786
D	786	HIS	-	expression tag	UNP O95786
D	787	HIS	-	expression tag	UNP O95786
D	788	HIS	-	expression tag	UNP O95786
D	789	HIS	-	expression tag	UNP O95786
D	790	HIS	-	expression tag	UNP O95786
D	791	SER	-	expression tag	UNP O95786
D	792	SER	-	expression tag	UNP O95786
D	793	GLY	-	expression tag	UNP O95786
D	794	LEU	-	expression tag	UNP O95786
D	795	VAL	-	expression tag	UNP O95786
D	796	PRO	-	expression tag	UNP O95786
D	797	ARG	-	expression tag	UNP O95786
D	798	GLY	-	expression tag	UNP O95786
D	799	SER	-	expression tag	UNP O95786
D	800	HIS	-	expression tag	UNP O95786
D	801	MET	-	expression tag	UNP O95786
E	781	MET	-	expression tag	UNP O95786
E	782	GLY	-	expression tag	UNP O95786
E	783	SER	-	expression tag	UNP O95786
E	784	SER	-	expression tag	UNP O95786
E	785	HIS	-	expression tag	UNP O95786
E	786	HIS	-	expression tag	UNP O95786
E	787	HIS	-	expression tag	UNP O95786
E	788	HIS	-	expression tag	UNP O95786
E	789	HIS	-	expression tag	UNP O95786

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Chain	Residue	Modelled	Actual	Comment	Reference
E	790	HIS	-	expression tag	UNP O95786
E	791	SER	-	expression tag	UNP O95786
E	792	SER	-	expression tag	UNP O95786
E	793	GLY	-	expression tag	UNP O95786
E	794	LEU	-	expression tag	UNP O95786
E	795	VAL	-	expression tag	UNP O95786
E	796	PRO	-	expression tag	UNP O95786
E	797	ARG	-	expression tag	UNP O95786
E	798	GLY	-	expression tag	UNP O95786
E	799	SER	-	expression tag	UNP O95786
E	800	HIS	-	expression tag	UNP O95786
E	801	MET	-	expression tag	UNP O95786
F	781	MET	-	expression tag	UNP O95786
F	782	GLY	-	expression tag	UNP O95786
F	783	SER	-	expression tag	UNP O95786
F	784	SER	-	expression tag	UNP O95786
F	785	HIS	-	expression tag	UNP O95786
F	786	HIS	-	expression tag	UNP O95786
F	787	HIS	-	expression tag	UNP O95786
F	788	HIS	-	expression tag	UNP O95786
F	789	HIS	-	expression tag	UNP O95786
F	790	HIS	-	expression tag	UNP O95786
F	791	SER	-	expression tag	UNP O95786
F	792	SER	-	expression tag	UNP O95786
F	793	GLY	-	expression tag	UNP O95786
F	794	LEU	-	expression tag	UNP O95786
F	795	VAL	-	expression tag	UNP O95786
F	796	PRO	-	expression tag	UNP O95786
F	797	ARG	-	expression tag	UNP O95786
F	798	GLY	-	expression tag	UNP O95786
F	799	SER	-	expression tag	UNP O95786
F	800	HIS	-	expression tag	UNP O95786
F	801	MET	-	expression tag	UNP O95786
G	781	MET	-	expression tag	UNP O95786
G	782	GLY	-	expression tag	UNP O95786
G	783	SER	-	expression tag	UNP O95786
G	784	SER	-	expression tag	UNP O95786
G	785	HIS	-	expression tag	UNP O95786
G	786	HIS	-	expression tag	UNP O95786
G	787	HIS	-	expression tag	UNP O95786
G	788	HIS	-	expression tag	UNP O95786
G	789	HIS	-	expression tag	UNP O95786

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Chain	Residue	Modelled	Actual	Comment	Reference
G	790	HIS	-	expression tag	UNP O95786
G	791	SER	-	expression tag	UNP O95786
G	792	SER	-	expression tag	UNP O95786
G	793	GLY	-	expression tag	UNP O95786
G	794	LEU	-	expression tag	UNP O95786
G	795	VAL	-	expression tag	UNP O95786
G	796	PRO	-	expression tag	UNP O95786
G	797	ARG	-	expression tag	UNP O95786
G	798	GLY	-	expression tag	UNP O95786
G	799	SER	-	expression tag	UNP O95786
G	800	HIS	-	expression tag	UNP O95786
G	801	MET	-	expression tag	UNP O95786
H	781	MET	-	expression tag	UNP O95786
H	782	GLY	-	expression tag	UNP O95786
H	783	SER	-	expression tag	UNP O95786
H	784	SER	-	expression tag	UNP O95786
H	785	HIS	-	expression tag	UNP O95786
H	786	HIS	-	expression tag	UNP O95786
H	787	HIS	-	expression tag	UNP O95786
H	788	HIS	-	expression tag	UNP O95786
H	789	HIS	-	expression tag	UNP O95786
H	790	HIS	-	expression tag	UNP O95786
H	791	SER	-	expression tag	UNP O95786
H	792	SER	-	expression tag	UNP O95786
H	793	GLY	-	expression tag	UNP O95786
H	794	LEU	-	expression tag	UNP O95786
H	795	VAL	-	expression tag	UNP O95786
H	796	PRO	-	expression tag	UNP O95786
H	797	ARG	-	expression tag	UNP O95786
H	798	GLY	-	expression tag	UNP O95786
H	799	SER	-	expression tag	UNP O95786
H	800	HIS	-	expression tag	UNP O95786
H	801	MET	-	expression tag	UNP O95786
I	781	MET	-	expression tag	UNP O95786
I	782	GLY	-	expression tag	UNP O95786
I	783	SER	-	expression tag	UNP O95786
I	784	SER	-	expression tag	UNP O95786
I	785	HIS	-	expression tag	UNP O95786
I	786	HIS	-	expression tag	UNP O95786
I	787	HIS	-	expression tag	UNP O95786
I	788	HIS	-	expression tag	UNP O95786
I	789	HIS	-	expression tag	UNP O95786

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Chain	Residue	Modelled	Actual	Comment	Reference
I	790	HIS	-	expression tag	UNP O95786
I	791	SER	-	expression tag	UNP O95786
I	792	SER	-	expression tag	UNP O95786
I	793	GLY	-	expression tag	UNP O95786
I	794	LEU	-	expression tag	UNP O95786
I	795	VAL	-	expression tag	UNP O95786
I	796	PRO	-	expression tag	UNP O95786
I	797	ARG	-	expression tag	UNP O95786
I	798	GLY	-	expression tag	UNP O95786
I	799	SER	-	expression tag	UNP O95786
I	800	HIS	-	expression tag	UNP O95786
I	801	MET	-	expression tag	UNP O95786
J	781	MET	-	expression tag	UNP O95786
J	782	GLY	-	expression tag	UNP O95786
J	783	SER	-	expression tag	UNP O95786
J	784	SER	-	expression tag	UNP O95786
J	785	HIS	-	expression tag	UNP O95786
J	786	HIS	-	expression tag	UNP O95786
J	787	HIS	-	expression tag	UNP O95786
J	788	HIS	-	expression tag	UNP O95786
J	789	HIS	-	expression tag	UNP O95786
J	790	HIS	-	expression tag	UNP O95786
J	791	SER	-	expression tag	UNP O95786
J	792	SER	-	expression tag	UNP O95786
J	793	GLY	-	expression tag	UNP O95786
J	794	LEU	-	expression tag	UNP O95786
J	795	VAL	-	expression tag	UNP O95786
J	796	PRO	-	expression tag	UNP O95786
J	797	ARG	-	expression tag	UNP O95786
J	798	GLY	-	expression tag	UNP O95786
J	799	SER	-	expression tag	UNP O95786
J	800	HIS	-	expression tag	UNP O95786
J	801	MET	-	expression tag	UNP O95786

- Molecule 2 is MERCURY (II) ION (three-letter code: HG) (formula: Hg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Hg 1 1	0	0
2	B	1	Total Hg 1 1	0	0
2	C	1	Total Hg 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total Hg 1 1	0	0
2	E	1	Total Hg 1 1	0	0
2	F	1	Total Hg 1 1	0	0
2	G	1	Total Hg 1 1	0	0
2	H	1	Total Hg 1 1	0	0
2	I	1	Total Hg 1 1	0	0
2	J	1	Total Hg 1 1	0	0

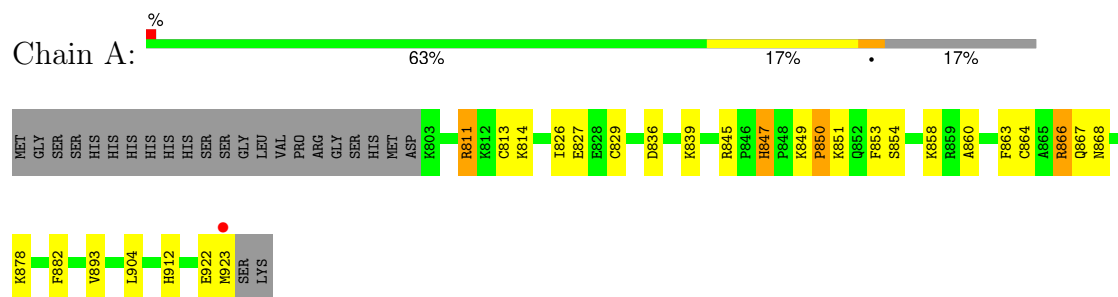
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	27	Total O 27 27	0	0
3	B	25	Total O 25 25	0	0
3	C	12	Total O 12 12	0	0
3	D	15	Total O 15 15	0	0
3	E	8	Total O 8 8	0	0
3	F	4	Total O 4 4	0	0
3	G	8	Total O 8 8	0	0
3	H	3	Total O 3 3	0	0

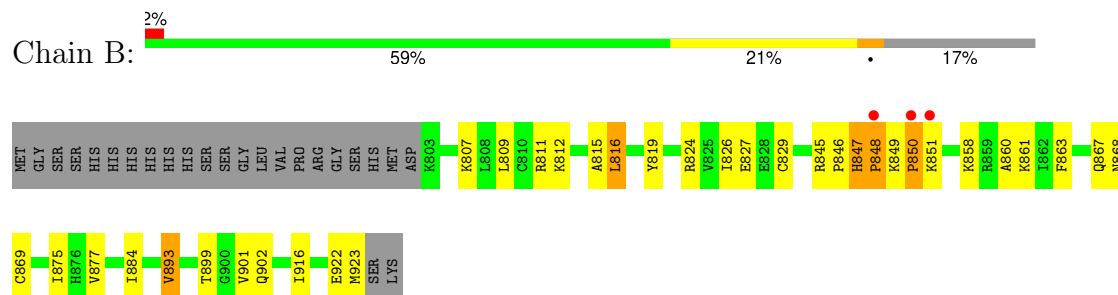
### 3 Residue-property plots [i](#)

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.

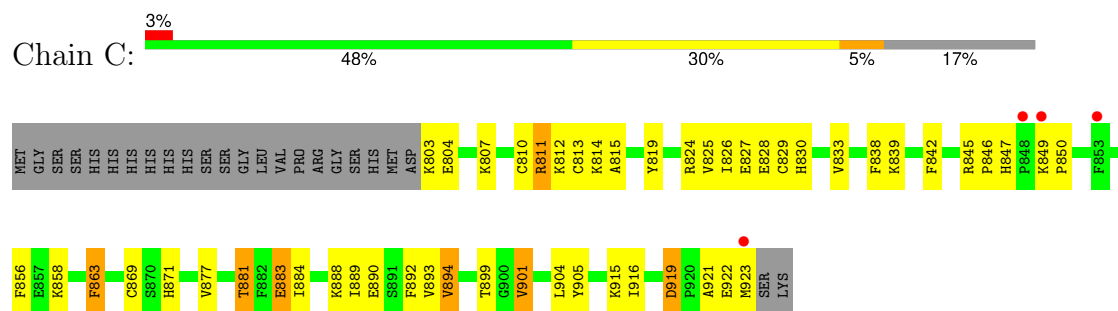
- Molecule 1: Probable ATP-dependent RNA helicase DDX58



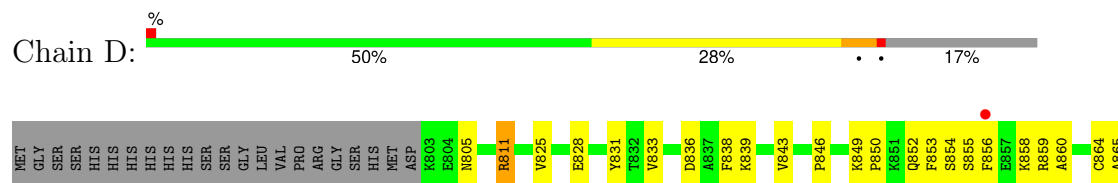
- Molecule 1: Probable ATP-dependent RNA helicase DDX58



- Molecule 1: Probable ATP-dependent RNA helicase DDX58

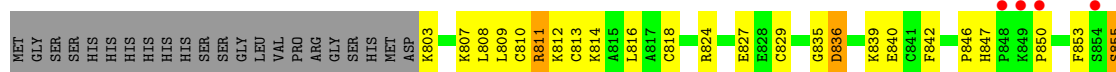
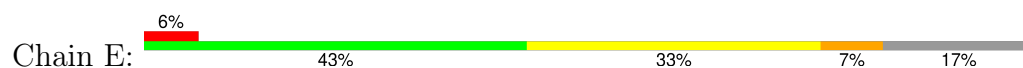


- Molecule 1: Probable ATP-dependent RNA helicase DDX58

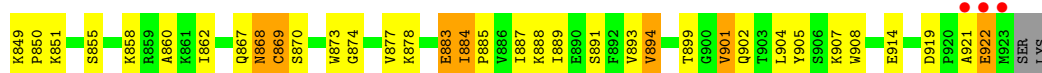




- Molecule 1: Probable ATP-dependent RNA helicase DDX58



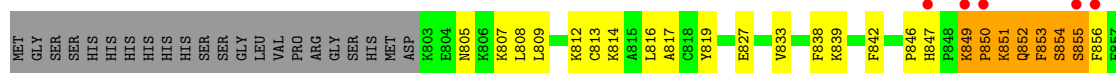
- Molecule 1: Probable ATP-dependent RNA helicase DDX58



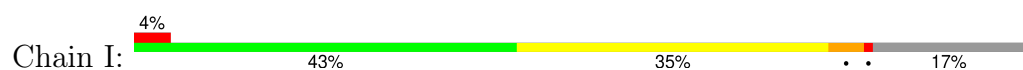
- Molecule 1: Probable ATP-dependent RNA helicase DDX58

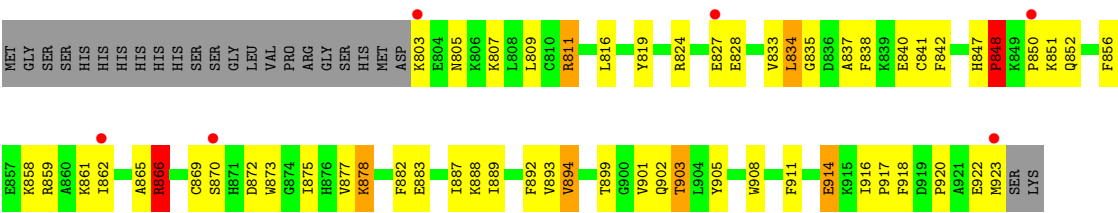


- Molecule 1: Probable ATP-dependent RNA helicase DDX58

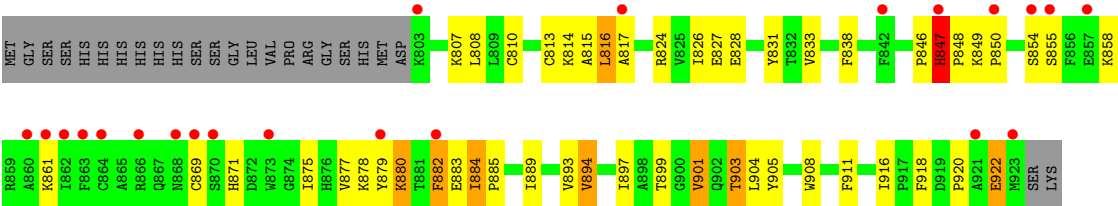


- Molecule 1: Probable ATP-dependent RNA helicase DDX58





● Molecule 1: Probable ATP-dependent RNA helicase DDX58



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	97.15Å 76.54Å 137.90Å 90.00° 93.07° 90.00°	Depositor
Resolution (Å)	20.00 – 2.70 20.00 – 2.71	Depositor EDS
% Data completeness (in resolution range)	97.6 (20.00-2.70) 97.8 (20.00-2.71)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.49 (at 2.69Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.241 , 0.276 0.241 , 0.278	Depositor DCC
$R_{free}$ test set	5535 reflections (10.18%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	55.7	Xtriage
Anisotropy	0.227	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 50.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	10092	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: HG

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	0.45	0/1026	0.70	0/1380
1	B	0.46	0/1026	0.71	0/1380
1	C	0.42	0/1026	0.70	0/1380
1	D	0.43	0/1026	0.64	0/1380
1	E	0.41	0/1026	0.68	0/1380
1	F	0.39	0/1026	0.64	0/1380
1	G	0.38	0/1026	0.67	1/1380 (0.1%)
1	H	0.40	0/1026	0.69	1/1380 (0.1%)
1	I	0.37	0/1026	0.60	0/1380
1	J	0.37	0/1026	0.66	1/1380 (0.1%)
All	All	0.41	0/10260	0.67	3/13800 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	847	HIS	C-N-CD	-7.77	103.50	120.60
1	H	852	GLN	N-CA-C	6.82	129.40	111.00
1	G	922	GLU	N-CA-C	-6.26	94.10	111.00

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	998	0	993	24	0
1	B	998	0	993	23	0
1	C	998	0	993	45	0
1	D	998	0	994	36	0
1	E	998	0	996	41	0
1	F	998	0	993	49	0
1	G	998	0	994	28	0
1	H	998	0	995	46	0
1	I	998	0	993	49	0
1	J	998	0	993	34	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
3	A	27	0	0	1	0
3	B	25	0	0	1	0
3	C	12	0	0	1	0
3	D	15	0	0	1	0
3	E	8	0	0	0	0
3	F	4	0	0	1	0
3	G	8	0	0	2	0
3	H	3	0	0	0	0
All	All	10092	0	9937	370	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 21.

The worst 5 of 370 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:H:897:ILE:HD12	1:H:897:ILE:H	1.20	1.05
1:D:858:LYS:HA	1:D:877:VAL:HG12	1.39	1.03
1:D:897:ILE:HD13	1:D:897:ILE:H	1.23	1.00
1:D:897:ILE:H	1:D:897:ILE:CD1	1.81	0.92
1:D:894:VAL:HG13	1:D:903:THR:HG23	1.51	0.91



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	119/145 (82%)	110 (92%)	8 (7%)	1 (1%)	16	38
1	B	119/145 (82%)	110 (92%)	4 (3%)	5 (4%)	2	5
1	C	119/145 (82%)	100 (84%)	16 (13%)	3 (2%)	4	12
1	D	119/145 (82%)	99 (83%)	12 (10%)	8 (7%)	1	1
1	E	119/145 (82%)	95 (80%)	17 (14%)	7 (6%)	1	2
1	F	119/145 (82%)	104 (87%)	11 (9%)	4 (3%)	3	7
1	G	119/145 (82%)	102 (86%)	10 (8%)	7 (6%)	1	2
1	H	119/145 (82%)	100 (84%)	10 (8%)	9 (8%)	1	1
1	I	119/145 (82%)	93 (78%)	21 (18%)	5 (4%)	2	5
1	J	119/145 (82%)	91 (76%)	18 (15%)	10 (8%)	0	1
All	All	1190/1450 (82%)	1004 (84%)	127 (11%)	59 (5%)	1	3

5 of 59 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	850	PRO
1	B	847	HIS
1	B	850	PRO
1	C	850	PRO
1	D	849	LYS

### 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	110/131 (84%)	105 (96%)	5 (4%)	23	50
1	B	110/131 (84%)	107 (97%)	3 (3%)	40	69
1	C	110/131 (84%)	103 (94%)	7 (6%)	14	34
1	D	110/131 (84%)	101 (92%)	9 (8%)	9	23
1	E	110/131 (84%)	96 (87%)	14 (13%)	3	9
1	F	110/131 (84%)	98 (89%)	12 (11%)	5	13
1	G	110/131 (84%)	101 (92%)	9 (8%)	9	23
1	H	110/131 (84%)	100 (91%)	10 (9%)	7	19
1	I	110/131 (84%)	98 (89%)	12 (11%)	5	13
1	J	110/131 (84%)	101 (92%)	9 (8%)	9	23
All	All	1100/1310 (84%)	1010 (92%)	90 (8%)	9	23

5 of 90 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	922	GLU
1	I	811	ARG
1	H	850	PRO
1	H	882	PHE
1	I	866	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	876	HIS
1	I	876	HIS
1	F	805	ASN
1	J	830	HIS
1	H	867	GLN

### 5.3.3 RNA ⓘ

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 10 ligands modelled in this entry, 10 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 ⓘ

### 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	121/145 (83%)	-0.57	1 (0%) 82 82	13, 33, 60, 76	14 (11%)
1	B	119/145 (82%)	-0.34	3 (2%) 58 57	9, 31, 54, 77	20 (16%)
1	C	119/145 (82%)	-0.10	4 (3%) 48 46	10, 41, 67, 85	24 (20%)
1	D	112/145 (77%)	-0.13	2 (1%) 67 67	9, 41, 67, 98	18 (16%)
1	E	118/145 (81%)	0.33	9 (7%) 21 19	14, 48, 79, 94	24 (20%)
1	F	120/145 (82%)	0.05	3 (2%) 58 57	12, 44, 62, 94	27 (22%)
1	G	118/145 (81%)	0.01	8 (6%) 25 23	14, 45, 69, 95	29 (24%)
1	H	118/145 (81%)	0.13	8 (6%) 25 23	25, 50, 87, 100	25 (21%)
1	I	120/145 (82%)	0.44	6 (5%) 35 33	12, 61, 91, 96	30 (25%)
1	J	116/145 (80%)	0.98	22 (18%) 4 4	16, 65, 96, 100	36 (31%)
All	All	1181/1450 (81%)	0.08	66 (5%) 31 29	9, 45, 84, 100	247 (20%)

The worst 5 of 66 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	851	LYS	15.4
1	J	868	ASN	8.5
1	J	847	HIS	7.6
1	G	853	PHE	6.9
1	D	923	MET	5.8

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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](#)

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, 95<sup>th</sup> 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
2	HG	I	1009	1/1	0.98	0.14	51,51,51,51	1
2	HG	J	1010	1/1	0.98	0.21	48,48,48,48	1
2	HG	C	1003	1/1	0.99	0.15	37,37,37,37	1
2	HG	D	1004	1/1	0.99	0.11	49,49,49,49	1
2	HG	E	1005	1/1	0.99	0.10	59,59,59,59	1
2	HG	F	1006	1/1	0.99	0.10	54,54,54,54	1
2	HG	H	1008	1/1	0.99	0.12	51,51,51,51	1
2	HG	A	1001	1/1	0.99	0.12	45,45,45,45	1
2	HG	B	1002	1/1	0.99	0.10	44,44,44,44	1
2	HG	G	1007	1/1	1.00	0.07	51,51,51,51	1

### 6.5 Other polymers [i](#)

There are no such residues in this entry.