



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 11:47 AM GMT

PDB ID : 3PUF  
Title : Crystal structure of human RNase H2 complex  
Authors : Figiel, M.; Chon, H.; Cerritelli, S.M.; Cybulska, M.; Crouch, R.J.; Nowotny, M.  
Deposited on : 2010-12-04  
Resolution : 3.10 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

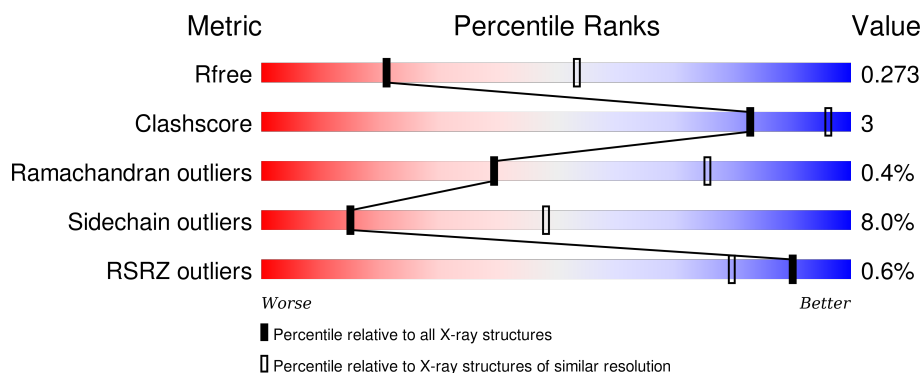
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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))
$R_{free}$	91344	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	302	<div> <div>73%</div> <div>16%</div> <div>11%</div> </div>
1	D	302	<div> <div>73%</div> <div>17%</div> <div>• 9%</div> </div>
1	G	302	<div> <div>75%</div> <div>12%</div> <div>• 12%</div> </div>
1	J	302	<div> <div>77%</div> <div>11%</div> <div>• 11%</div> </div>
1	M	302	<div> <div>82%</div> <div>8%</div> <div>10%</div> </div>

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Mol	Chain	Length	Quality of chain
1	P	302	<p>2% 74% 11% 14%</p>
2	B	224	<p>% 67% 14% 17%</p>
2	E	224	<p>% 69% 11% 19%</p>
2	H	224	<p>82% 8% 10%</p>
2	K	224	<p>72% 9% 19%</p>
2	N	224	<p>74% 9% 17%</p>
2	Q	224	<p>2% 73% 5% 21%</p>
3	C	167	<p>% 65% 10% 24%</p>
3	F	167	<p>63% 11% 23%</p>
3	I	167	<p>73% 11% 16%</p>
3	L	167	<p>61% 8% 31%</p>
3	O	167	<p>64% 5% 31%</p>
3	R	167	<p>% 63% 5% 31%</p>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 25820 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 Ribonuclease H2 subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	270	Total	C	N	O	S	0	0	0
			2031	1300	340	380	11			
1	D	274	Total	C	N	O	S	0	0	0
			2040	1299	348	384	9			
1	G	266	Total	C	N	O	S	0	0	0
			1999	1274	334	382	9			
1	J	270	Total	C	N	O	S	0	0	0
			1965	1251	330	374	10			
1	M	272	Total	C	N	O	S	0	0	0
			1995	1273	333	381	8			
1	P	259	Total	C	N	O	S	0	0	0
			1895	1211	318	357	9			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	EXPRESSION TAG	UNP O75792
A	-1	PRO	-	EXPRESSION TAG	UNP O75792
A	0	HIS	-	EXPRESSION TAG	UNP O75792
D	-2	GLY	-	EXPRESSION TAG	UNP O75792
D	-1	PRO	-	EXPRESSION TAG	UNP O75792
D	0	HIS	-	EXPRESSION TAG	UNP O75792
G	-2	GLY	-	EXPRESSION TAG	UNP O75792
G	-1	PRO	-	EXPRESSION TAG	UNP O75792
G	0	HIS	-	EXPRESSION TAG	UNP O75792
J	-2	GLY	-	EXPRESSION TAG	UNP O75792
J	-1	PRO	-	EXPRESSION TAG	UNP O75792
J	0	HIS	-	EXPRESSION TAG	UNP O75792
M	-2	GLY	-	EXPRESSION TAG	UNP O75792
M	-1	PRO	-	EXPRESSION TAG	UNP O75792
M	0	HIS	-	EXPRESSION TAG	UNP O75792
P	-2	GLY	-	EXPRESSION TAG	UNP O75792
P	-1	PRO	-	EXPRESSION TAG	UNP O75792

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Chain	Residue	Modelled	Actual	Comment	Reference
P	0	HIS	-	EXPRESSION TAG	UNP O75792

- Molecule 2 is a protein called Ribonuclease H2 subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	185	Total	C	N	O	S	0	0	0
			1459	961	233	261	4			
2	E	181	Total	C	N	O	S	0	0	0
			1355	883	228	240	4			
2	H	202	Total	C	N	O	S	0	0	0
			1546	1010	249	281	6			
2	K	182	Total	C	N	O	S	0	0	0
			1357	891	222	240	4			
2	N	186	Total	C	N	O	S	0	0	0
			1387	906	227	250	4			
2	Q	176	Total	C	N	O	S	0	0	0
			1299	852	211	233	3			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	10	GLY	-	EXPRESSION TAG	UNP Q5TBB1
B	11	SER	-	EXPRESSION TAG	UNP Q5TBB1
B	12	HIS	-	EXPRESSION TAG	UNP Q5TBB1
B	13	MET	-	EXPRESSION TAG	UNP Q5TBB1
E	10	GLY	-	EXPRESSION TAG	UNP Q5TBB1
E	11	SER	-	EXPRESSION TAG	UNP Q5TBB1
E	12	HIS	-	EXPRESSION TAG	UNP Q5TBB1
E	13	MET	-	EXPRESSION TAG	UNP Q5TBB1
H	10	GLY	-	EXPRESSION TAG	UNP Q5TBB1
H	11	SER	-	EXPRESSION TAG	UNP Q5TBB1
H	12	HIS	-	EXPRESSION TAG	UNP Q5TBB1
H	13	MET	-	EXPRESSION TAG	UNP Q5TBB1
K	10	GLY	-	EXPRESSION TAG	UNP Q5TBB1
K	11	SER	-	EXPRESSION TAG	UNP Q5TBB1
K	12	HIS	-	EXPRESSION TAG	UNP Q5TBB1
K	13	MET	-	EXPRESSION TAG	UNP Q5TBB1
N	10	GLY	-	EXPRESSION TAG	UNP Q5TBB1
N	11	SER	-	EXPRESSION TAG	UNP Q5TBB1
N	12	HIS	-	EXPRESSION TAG	UNP Q5TBB1
N	13	MET	-	EXPRESSION TAG	UNP Q5TBB1
Q	10	GLY	-	EXPRESSION TAG	UNP Q5TBB1

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	11	SER	-	EXPRESSION TAG	UNP Q5TBB1
Q	12	HIS	-	EXPRESSION TAG	UNP Q5TBB1
Q	13	MET	-	EXPRESSION TAG	UNP Q5TBB1

- Molecule 3 is a protein called Ribonuclease H2 subunit C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	127	Total	C	N	O	S	0	0	0
			933	601	166	163	3			
3	F	128	Total	C	N	O	S	0	0	0
			952	609	176	164	3			
3	I	140	Total	C	N	O	S	0	0	0
			1048	669	193	183	3			
3	L	116	Total	C	N	O	S	0	0	0
			840	543	148	146	3			
3	O	116	Total	C	N	O	S	0	0	0
			828	537	145	143	3			
3	R	115	Total	C	N	O	S	0	0	0
			800	519	145	133	3			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	GLY	-	EXPRESSION TAG	UNP Q8TDP1
C	-1	SER	-	EXPRESSION TAG	UNP Q8TDP1
C	0	HIS	-	EXPRESSION TAG	UNP Q8TDP1
F	-2	GLY	-	EXPRESSION TAG	UNP Q8TDP1
F	-1	SER	-	EXPRESSION TAG	UNP Q8TDP1
F	0	HIS	-	EXPRESSION TAG	UNP Q8TDP1
I	-2	GLY	-	EXPRESSION TAG	UNP Q8TDP1
I	-1	SER	-	EXPRESSION TAG	UNP Q8TDP1
I	0	HIS	-	EXPRESSION TAG	UNP Q8TDP1
L	-2	GLY	-	EXPRESSION TAG	UNP Q8TDP1
L	-1	SER	-	EXPRESSION TAG	UNP Q8TDP1
L	0	HIS	-	EXPRESSION TAG	UNP Q8TDP1
O	-2	GLY	-	EXPRESSION TAG	UNP Q8TDP1
O	-1	SER	-	EXPRESSION TAG	UNP Q8TDP1
O	0	HIS	-	EXPRESSION TAG	UNP Q8TDP1
R	-2	GLY	-	EXPRESSION TAG	UNP Q8TDP1
R	-1	SER	-	EXPRESSION TAG	UNP Q8TDP1
R	0	HIS	-	EXPRESSION TAG	UNP Q8TDP1

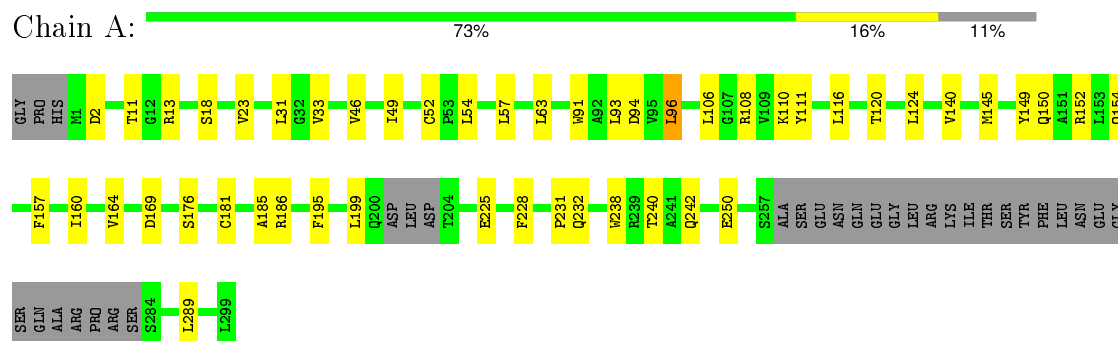
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	11	Total 11	O 11	0	0
4	B	5	Total 5	O 5	0	0
4	C	6	Total 6	O 6	0	0
4	D	4	Total 4	O 4	0	0
4	E	3	Total 3	O 3	0	0
4	F	7	Total 7	O 7	0	0
4	G	7	Total 7	O 7	0	0
4	H	8	Total 8	O 8	0	0
4	I	9	Total 9	O 9	0	0
4	J	11	Total 11	O 11	0	0
4	K	4	Total 4	O 4	0	0
4	L	3	Total 3	O 3	0	0
4	M	1	Total 1	O 1	0	0
4	N	2	Total 2	O 2	0	0
4	O	3	Total 3	O 3	0	0
4	P	4	Total 4	O 4	0	0
4	Q	2	Total 2	O 2	0	0
4	R	1	Total 1	O 1	0	0

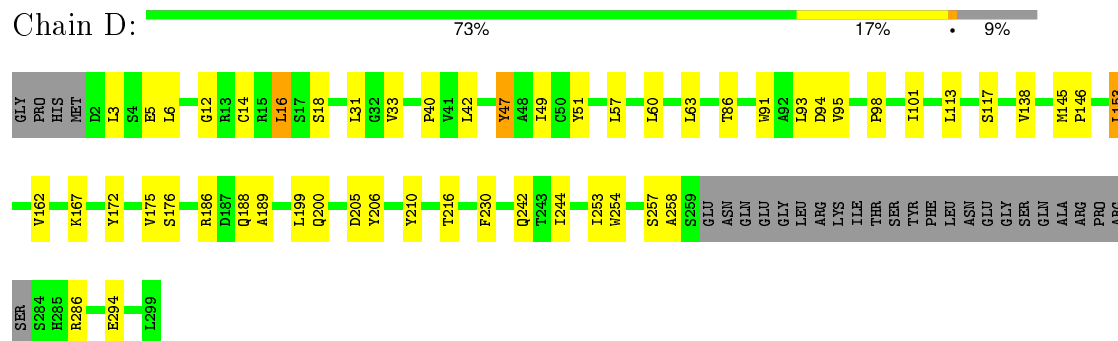
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

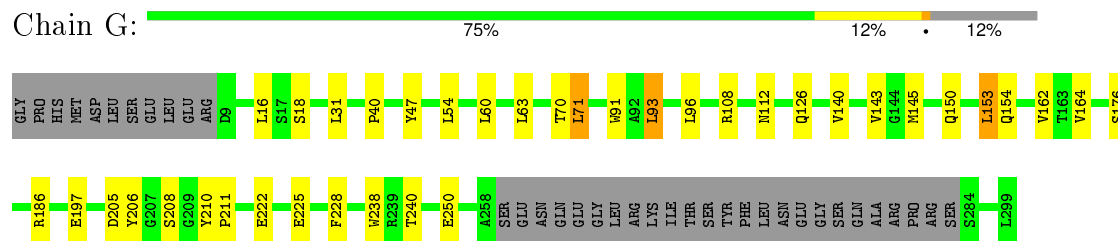
#### • Molecule 1: Ribonuclease H2 subunit A



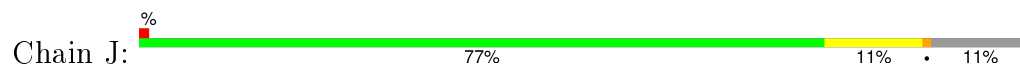
#### • Molecule 1: Ribonuclease H2 subunit A



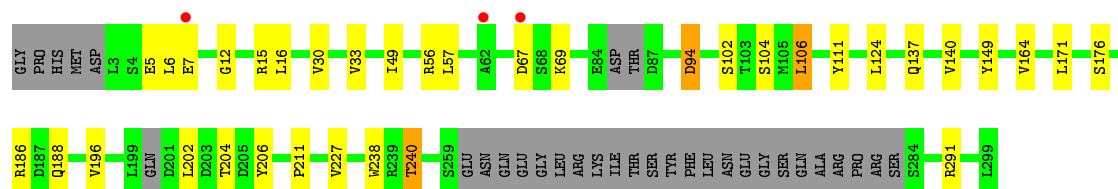
#### • Molecule 1: Ribonuclease H2 subunit A



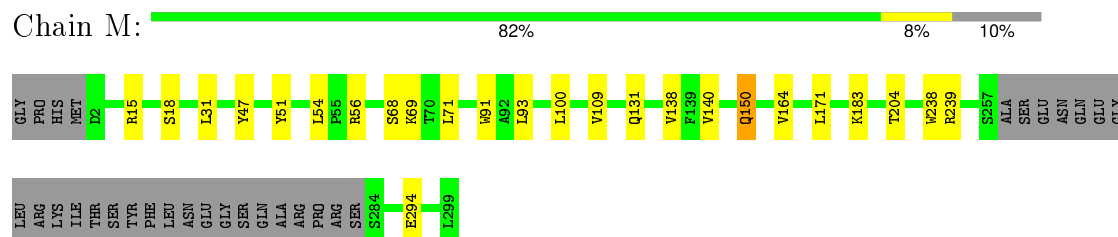
#### • Molecule 1: Ribonuclease H2 subunit A



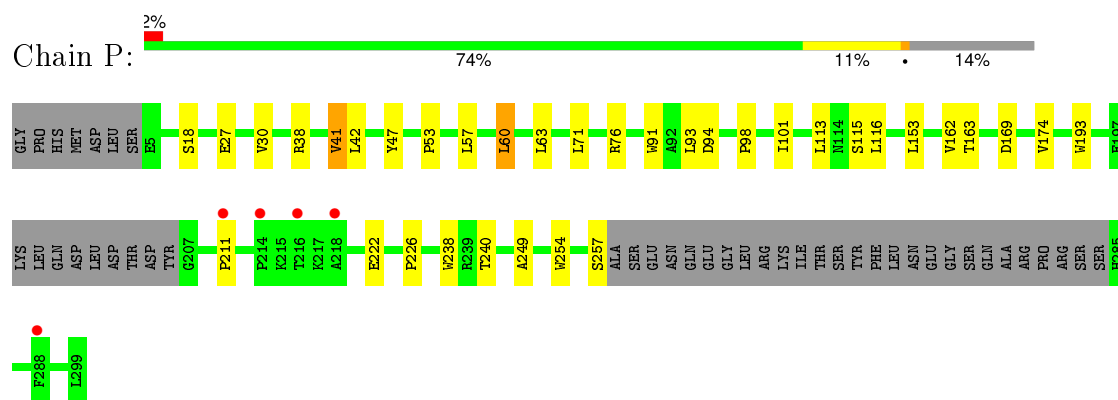




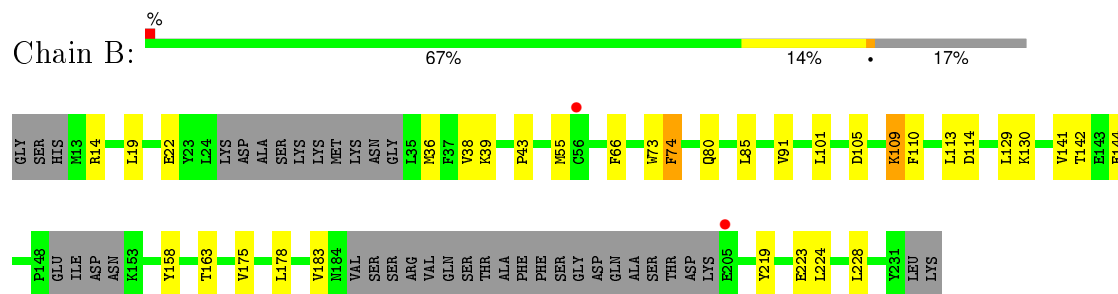
• Molecule 1: Ribonuclease H2 subunit A



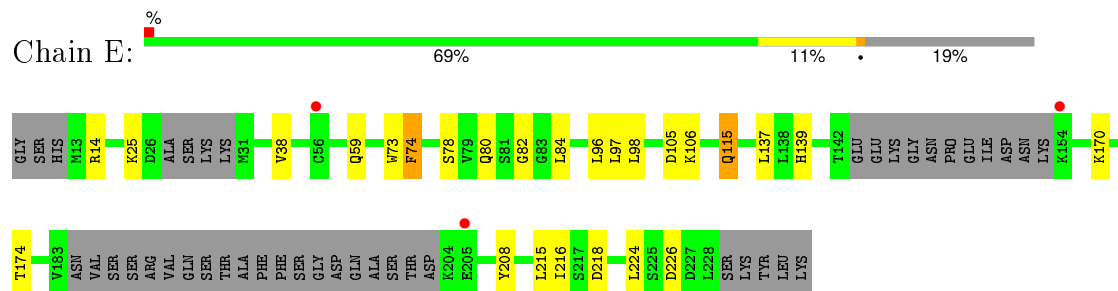
• Molecule 1: Ribonuclease H2 subunit A




• Molecule 2: Ribonuclease H2 subunit B

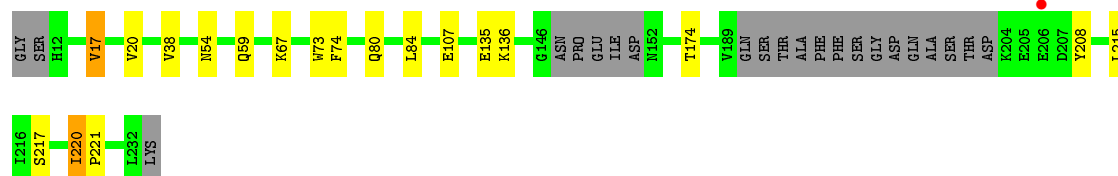


• Molecule 2: Ribonuclease H2 subunit B



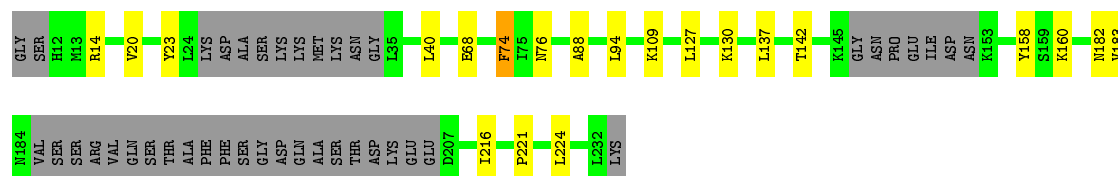
- Molecule 2: Ribonuclease H2 subunit B

Chain H: 



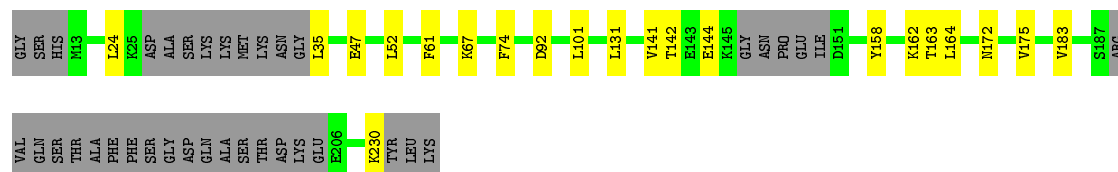
- Molecule 2: Ribonuclease H2 subunit B

Chain K: 




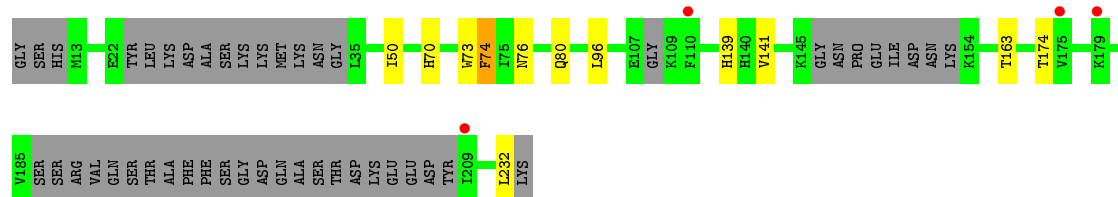
- Molecule 2: Ribonuclease H2 subunit B

Chain N: 



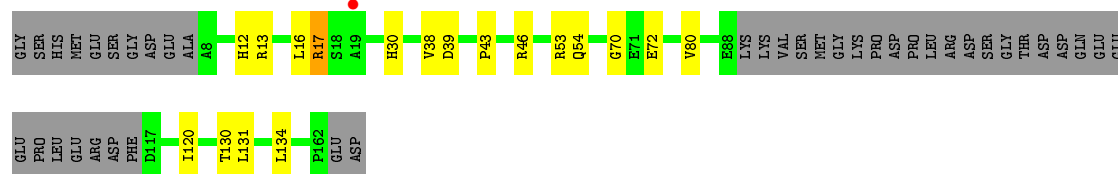
- Molecule 2: Ribonuclease H2 subunit B

Chain Q: 



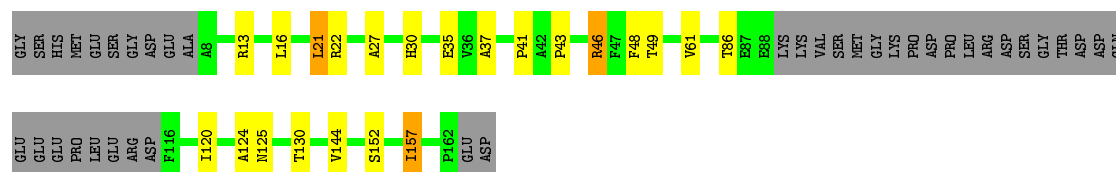
- Molecule 3: Ribonuclease H2 subunit C

Chain C: 



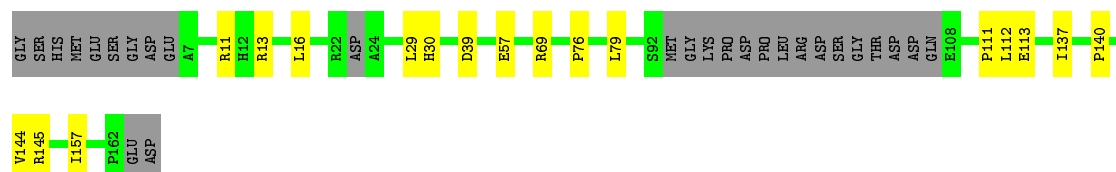
- Molecule 3: Ribonuclease H2 subunit C

Chain F: 



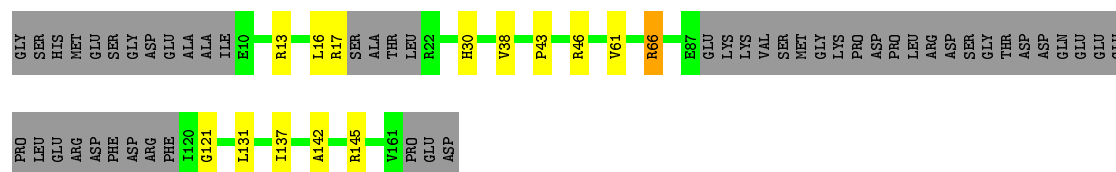
• Molecule 3: Ribonuclease H2 subunit C

Chain I: 



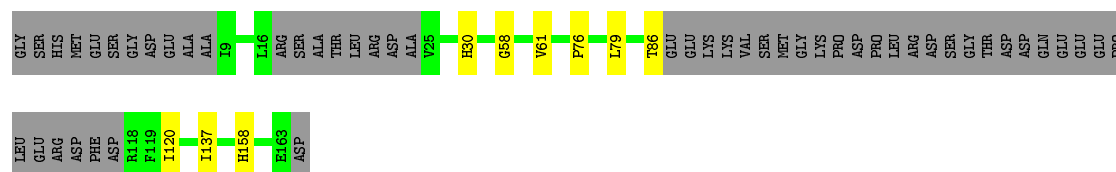
• Molecule 3: Ribonuclease H2 subunit C

Chain L: 



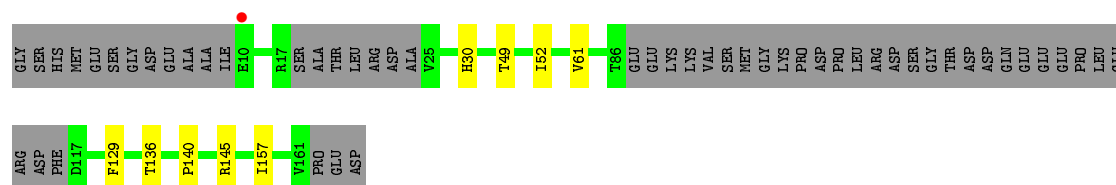
• Molecule 3: Ribonuclease H2 subunit C

Chain O: 



• Molecule 3: Ribonuclease H2 subunit C

Chain R: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.07Å 108.37Å 114.26Å 105.90° 103.71° 111.42°	Depositor
Resolution (Å)	44.10 – 3.10 44.10 – 3.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (44.10-3.10) 82.7 (44.10-3.10)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.97 (at 3.12Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, $R_{free}$	0.203 , 0.255 0.216 , 0.273	Depositor DCC
$R_{free}$ test set	3207 reflections (5.35%)	DCC
Wilson B-factor (Å <sup>2</sup> )	63.1	Xtriage
Anisotropy	0.189	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 60.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 63136 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	25820	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.99% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0/2075	0.64	0/2830
1	D	0.41	0/2084	0.63	0/2851
1	G	0.41	0/2044	0.64	0/2797
1	J	0.40	0/2008	0.60	0/2748
1	M	0.40	0/2039	0.63	0/2795
1	P	0.39	0/1937	0.60	0/2656
2	B	0.38	0/1494	0.64	0/2028
2	E	0.39	0/1385	0.61	0/1887
2	H	0.39	0/1581	0.62	0/2148
2	K	0.39	0/1391	0.62	0/1899
2	N	0.39	0/1421	0.63	0/1938
2	Q	0.37	0/1329	0.57	0/1815
3	C	0.40	0/958	0.61	0/1312
3	F	0.40	0/977	0.64	0/1335
3	I	0.40	0/1074	0.66	0/1465
3	L	0.41	0/862	0.68	0/1181
3	O	0.39	0/850	0.62	0/1166
3	R	0.41	0/821	0.60	0/1127
All	All	0.40	0/26330	0.62	0/35978

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	2031	0	1951	17	0
1	D	2040	0	1932	21	0
1	G	1999	0	1886	10	0
1	J	1965	0	1800	14	0
1	M	1995	0	1850	5	0
1	P	1895	0	1766	11	0
2	B	1459	0	1402	15	0
2	E	1355	0	1248	8	0
2	H	1546	0	1448	8	0
2	K	1357	0	1212	6	0
2	N	1387	0	1235	9	0
2	Q	1299	0	1160	4	0
3	C	933	0	921	12	0
3	F	952	0	945	14	0
3	I	1048	0	1032	9	0
3	L	840	0	821	7	0
3	O	828	0	804	6	0
3	R	800	0	764	4	0
4	A	11	0	0	0	0
4	B	5	0	0	0	0
4	C	6	0	0	0	0
4	D	4	0	0	0	0
4	E	3	0	0	0	0
4	F	7	0	0	0	0
4	G	7	0	0	0	0
4	H	8	0	0	0	0
4	I	9	0	0	0	0
4	J	11	0	0	0	0
4	K	4	0	0	0	0
4	L	3	0	0	0	0
4	M	1	0	0	0	0
4	N	2	0	0	0	0
4	O	3	0	0	0	0
4	P	4	0	0	0	0
4	Q	2	0	0	0	0
4	R	1	0	0	0	0
All	All	25820	0	24177	153	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 3.

The worst 5 of 153 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)
2:E:174:THR:HG22	3:F:157:ILE:HB	1.60	0.84
3:I:111:PRO:HA	3:I:112:LEU:HB3	1.64	0.78
3:I:111:PRO:HA	3:I:112:LEU:CB	2.22	0.69
1:D:153:LEU:HB3	1:D:162:VAL:HG11	1.75	0.69
1:M:150:GLN:HG2	1:M:164:VAL:HG12	1.74	0.68

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	264/302 (87%)	255 (97%)	9 (3%)	0	100	100
1	D	270/302 (89%)	255 (94%)	13 (5%)	2 (1%)	26	65
1	G	262/302 (87%)	252 (96%)	9 (3%)	1 (0%)	39	75
1	J	262/302 (87%)	250 (95%)	10 (4%)	2 (1%)	24	63
1	M	268/302 (89%)	255 (95%)	13 (5%)	0	100	100
1	P	253/302 (84%)	244 (96%)	9 (4%)	0	100	100
2	B	177/224 (79%)	165 (93%)	10 (6%)	2 (1%)	17	55
2	E	173/224 (77%)	160 (92%)	12 (7%)	1 (1%)	30	68
2	H	196/224 (88%)	185 (94%)	11 (6%)	0	100	100
2	K	174/224 (78%)	163 (94%)	7 (4%)	4 (2%)	8	35
2	N	178/224 (80%)	166 (93%)	11 (6%)	1 (1%)	30	68
2	Q	166/224 (74%)	161 (97%)	4 (2%)	1 (1%)	30	68
3	C	123/167 (74%)	119 (97%)	4 (3%)	0	100	100
3	F	124/167 (74%)	119 (96%)	4 (3%)	1 (1%)	24	63
3	I	134/167 (80%)	129 (96%)	5 (4%)	0	100	100
3	L	110/167 (66%)	103 (94%)	7 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	O	110/167 (66%)	106 (96%)	4 (4%)	0	100	100
3	R	109/167 (65%)	102 (94%)	7 (6%)	0	100	100
All	All	3353/4158 (81%)	3189 (95%)	149 (4%)	15 (0%)	39	75

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	110	PHE
2	E	82	GLY
3	F	37	ALA
2	B	183	VAL
1	D	12	GLY

### 5.3.2 Protein sidechains ⓘ

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	207/259 (80%)	186 (90%)	21 (10%)	9	33
1	D	205/259 (79%)	186 (91%)	19 (9%)	11	39
1	G	203/259 (78%)	182 (90%)	21 (10%)	9	32
1	J	190/259 (73%)	174 (92%)	16 (8%)	14	46
1	M	196/259 (76%)	179 (91%)	17 (9%)	13	44
1	P	187/259 (72%)	171 (91%)	16 (9%)	13	45
2	B	151/204 (74%)	139 (92%)	12 (8%)	15	49
2	E	130/204 (64%)	112 (86%)	18 (14%)	4	19
2	H	154/204 (76%)	142 (92%)	12 (8%)	16	49
2	K	126/204 (62%)	118 (94%)	8 (6%)	22	58
2	N	130/204 (64%)	123 (95%)	7 (5%)	27	64
2	Q	122/204 (60%)	116 (95%)	6 (5%)	31	68
3	C	92/134 (69%)	88 (96%)	4 (4%)	35	72
3	F	94/134 (70%)	85 (90%)	9 (10%)	10	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	I	104/134 (78%)	98 (94%)	6 (6%)	25	61
3	L	81/134 (60%)	76 (94%)	5 (6%)	23	59
3	O	79/134 (59%)	78 (99%)	1 (1%)	76	91
3	R	71/134 (53%)	68 (96%)	3 (4%)	36	73
All	All	2522/3582 (70%)	2321 (92%)	201 (8%)	15	48

5 of 201 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	126	GLN
2	H	136	LYS
1	P	116	LEU
1	G	150	GLN
1	G	238	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	242	GLN
2	K	77	GLN
3	O	160	GLN
1	G	114	ASN
1	P	154	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates 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	270/302 (89%)	-0.52	0 100 100	21, 48, 77, 104	0
1	D	274/302 (90%)	-0.42	0 100 100	34, 59, 88, 106	0
1	G	266/302 (88%)	-0.53	0 100 100	24, 45, 77, 90	0
1	J	270/302 (89%)	-0.26	3 (1%) 82 66	33, 74, 106, 121	0
1	M	272/302 (90%)	-0.37	0 100 100	40, 68, 95, 109	0
1	P	259/302 (85%)	-0.29	5 (1%) 70 48	46, 76, 101, 109	0
2	B	185/224 (82%)	-0.45	2 (1%) 82 66	38, 59, 80, 95	0
2	E	181/224 (80%)	-0.35	3 (1%) 73 52	33, 77, 105, 117	0
2	H	202/224 (90%)	-0.50	1 (0%) 91 83	31, 60, 85, 107	0
2	K	182/224 (81%)	-0.46	0 100 100	44, 73, 96, 127	0
2	N	186/224 (83%)	-0.31	0 100 100	44, 79, 109, 137	0
2	Q	176/224 (78%)	-0.35	4 (2%) 64 40	55, 81, 99, 118	0
3	C	127/167 (76%)	-0.48	1 (0%) 87 75	28, 56, 89, 104	0
3	F	128/167 (76%)	-0.59	0 100 100	34, 52, 78, 95	0
3	I	140/167 (83%)	-0.63	0 100 100	26, 44, 75, 95	0
3	L	116/167 (69%)	-0.44	0 100 100	32, 63, 100, 119	0
3	O	116/167 (69%)	-0.47	0 100 100	39, 66, 85, 102	0
3	R	115/167 (68%)	-0.42	1 (0%) 85 72	54, 75, 90, 110	0
All	All	3465/4158 (83%)	-0.42	20 (0%) 90 80	21, 64, 96, 137	0

The worst 5 of 20 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	7	GLU	5.6
2	B	56	CYS	3.4
2	E	56	CYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	P	216	THR	3.0
2	E	205	GLU	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 carbohydrates 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.