



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:08 AM UTC

PDB ID : 3P5J / pdb_00003p5j
Title : The structure of the human RNase H2 complex defines key interaction interfaces relevant to enzyme function and human disease
Authors : Bubeck, D.; Graham, S.C.; Jones, E.Y.
Deposited on : 2010-10-08
Resolution : 2.90 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

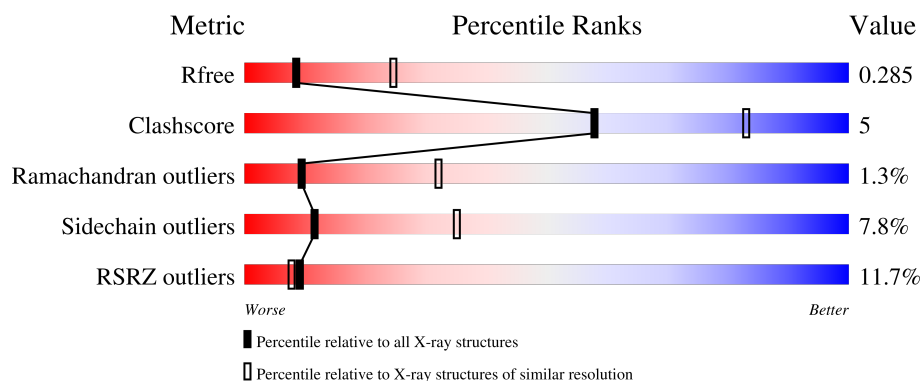
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	301	5% 64% 22% • 13%
2	B	332	14% 45% 6% • 48%
3	C	166	2% 60% 7% •• 30%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4016 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	262	Total	C	N	O	S	0	0	0
			1995	1275	343	368	9			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	171	Total	C	N	O	S	0	0	0
			1179	761	207	208	3			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-23	MET	-	expression tag	UNP Q80ZV0
B	-22	GLY	-	expression tag	UNP Q80ZV0
B	-21	SER	-	expression tag	UNP Q80ZV0
B	-20	SER	-	expression tag	UNP Q80ZV0
B	-19	HIS	-	expression tag	UNP Q80ZV0
B	-18	HIS	-	expression tag	UNP Q80ZV0
B	-17	HIS	-	expression tag	UNP Q80ZV0
B	-16	HIS	-	expression tag	UNP Q80ZV0
B	-15	HIS	-	expression tag	UNP Q80ZV0
B	-14	HIS	-	expression tag	UNP Q80ZV0
B	-13	SER	-	expression tag	UNP Q80ZV0
B	-12	GLN	-	expression tag	UNP Q80ZV0
B	-11	ASP	-	expression tag	UNP Q80ZV0
B	-10	PRO	-	expression tag	UNP Q80ZV0
B	-9	ASN	-	expression tag	UNP Q80ZV0
B	-8	SER	-	expression tag	UNP Q80ZV0
B	-7	LEU	-	expression tag	UNP Q80ZV0
B	-6	GLU	-	expression tag	UNP Q80ZV0
B	-5	VAL	-	expression tag	UNP Q80ZV0
B	-4	LEU	-	expression tag	UNP Q80ZV0

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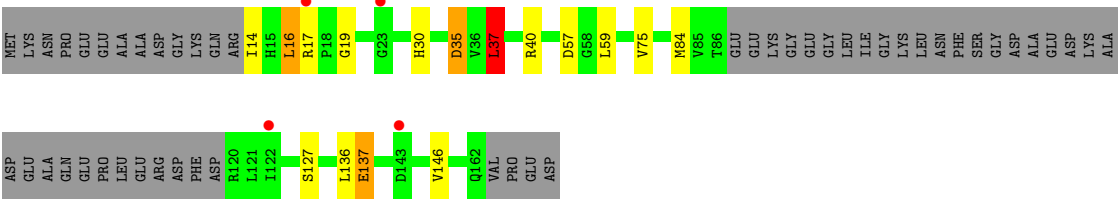
Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	PHE	-	expression tag	UNP Q80ZV0
B	-2	GLN	-	expression tag	UNP Q80ZV0
B	-1	GLY	-	expression tag	UNP Q80ZV0
B	0	PRO	-	expression tag	UNP Q80ZV0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	116	Total	C	N	O	S	0	0	0
			842	542	156	142	2			

- Molecule 1: Ribonuclease H2 subunit A





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	279.29Å 40.42Å 67.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.61 – 2.90 24.61 – 2.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (24.61-2.90) 99.1 (24.61-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.92 (at 2.89Å)	Xtriage
Refinement program	BUSTER 2.9.2	Depositor
R, R_{free}	0.210 , 0.272 0.223 , 0.285	Depositor DCC
R_{free} test set	925 reflections (5.20%)	wwPDB-VP
Wilson B-factor (Å ²)	49.9	Xtriage
Anisotropy	0.011	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 70.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	4016	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.20% 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	1.01	1/2041 (0.0%)	1.49	27/2779 (1.0%)
2	B	0.84	0/1208	1.46	8/1652 (0.5%)
3	C	0.93	0/867	1.40	7/1183 (0.6%)
All	All	0.95	1/4116 (0.0%)	1.46	42/5614 (0.7%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	231	PHE	CA-C	5.26	1.58	1.52

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	39	GLY	N-CA-C	7.33	127.30	112.34
3	C	40	ARG	N-CA-CB	-7.11	104.59	111.27
3	C	40	ARG	CB-CA-C	-6.73	100.81	110.03
1	A	118	SER	CA-C-N	6.59	129.12	120.28
1	A	118	SER	C-N-CA	6.59	129.12	120.28
2	B	225	LEU	N-CA-C	-6.46	105.22	113.23
1	A	297	SER	CA-C-N	6.21	129.42	120.79
1	A	297	SER	C-N-CA	6.21	129.42	120.79
3	C	75	VAL	N-CA-C	-6.17	103.28	109.02
2	B	221	LEU	N-CA-C	-6.15	104.48	112.23
1	A	41	VAL	N-CA-C	-6.04	104.17	113.16
1	A	200	LEU	N-CA-C	-5.99	104.44	110.97
2	B	224	ASP	N-CA-C	-5.96	105.50	112.89
1	A	231	PHE	CA-CB-CG	5.95	119.75	113.80
3	C	37	LEU	N-CA-C	5.91	120.03	112.34
2	B	54	ASP	CA-CB-CG	5.89	118.49	112.60
3	C	35	ASP	CA-CB-CG	5.87	118.47	112.60
1	A	103	SER	CA-C-N	5.84	128.11	120.28
1	A	103	SER	C-N-CA	5.84	128.11	120.28
1	A	76	ARG	CA-C-N	5.83	128.09	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	76	ARG	C-N-CA	5.83	128.09	120.28
1	A	231	PHE	N-CA-C	5.77	116.77	110.13
1	A	202	ASP	CA-CB-CG	5.76	118.36	112.60
1	A	214	ASP	CA-CB-CG	5.69	118.29	112.60
3	C	16	LEU	N-CA-C	5.52	117.03	107.93
1	A	120	ASP	CA-C-N	5.44	127.58	120.28
1	A	120	ASP	C-N-CA	5.44	127.58	120.28
1	A	285	HIS	CA-C-N	5.42	129.76	120.71
1	A	285	HIS	C-N-CA	5.42	129.76	120.71
2	B	127	LEU	CA-C-N	5.42	127.48	120.44
2	B	127	LEU	C-N-CA	5.42	127.48	120.44
1	A	251	GLU	CB-CG-CD	5.41	121.79	112.60
1	A	249	GLU	N-CA-C	5.33	120.79	113.97
2	B	222	SER	N-CA-C	-5.27	106.69	113.23
1	A	255	TRP	CA-C-N	5.17	127.21	120.28
1	A	255	TRP	C-N-CA	5.17	127.21	120.28
1	A	297	SER	N-CA-C	-5.13	106.18	112.90
3	C	40	ARG	N-CA-C	5.11	112.73	108.13
1	A	109	ARG	N-CA-C	-5.10	105.90	111.82
1	A	151	GLN	CA-C-N	5.04	127.30	120.65
1	A	151	GLN	C-N-CA	5.04	127.30	120.65
2	B	74	PHE	N-CA-C	-5.01	99.64	108.20

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	1995	0	1923	27	0
2	B	1179	0	944	7	0
3	C	842	0	822	4	0
All	All	4016	0	3689	35	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 5.

All (35) 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:33:VAL:HG22	1:A:49:ILE:HG22	1.74	0.69
1:A:42:LEU:HD12	1:A:210:GLY:HA2	1.75	0.67
1:A:86:ASP:HB2	1:A:89:PHE:CE2	2.38	0.59
1:A:118:SER:O	1:A:121:THR:HB	2.06	0.56
1:A:147:PRO:HB3	1:A:165:VAL:HG12	1.88	0.56
1:A:32:GLY:O	1:A:49:ILE:HA	2.07	0.54
1:A:42:LEU:HD11	1:A:217:THR:HG23	1.90	0.53
2:B:74:PHE:HB2	3:C:30:HIS:HB2	1.90	0.52
1:A:20:VAL:HG21	1:A:132:GLN:HB3	1.91	0.52
1:A:42:LEU:HB3	1:A:234:PHE:CE1	2.45	0.52
1:A:21:PRO:HG2	1:A:24:CYS:SG	2.51	0.51
1:A:201:GLN:HG3	1:A:203:LEU:HG	1.93	0.51
1:A:97:LEU:HD11	1:A:121:THR:HG21	1.93	0.50
1:A:32:GLY:HA3	1:A:175:VAL:HG12	1.93	0.49
2:B:54:ASP:HB3	2:B:59:GLN:H	1.79	0.48
1:A:18:SER:HB3	1:A:92:TRP:CE2	2.48	0.48
1:A:252:ASP:HB2	3:C:37:LEU:HD12	1.97	0.47
1:A:32:GLY:N	1:A:175:VAL:HG12	2.30	0.47
3:C:17:ARG:HH11	3:C:19:GLY:HA3	1.80	0.46
1:A:47:TYR:HB3	1:A:125:LEU:HD12	1.98	0.46
1:A:284:PRO:HG2	1:A:286:ARG:HB2	1.96	0.46
1:A:86:ASP:HB2	1:A:89:PHE:HE2	1.79	0.45
2:B:14:GLN:H	2:B:80:GLN:NE2	2.15	0.45
1:A:32:GLY:CA	1:A:175:VAL:HG12	2.48	0.43
1:A:46:VAL:HG11	1:A:186:ALA:HB3	2.00	0.43
1:A:244:ALA:O	1:A:248:LYS:HG3	2.19	0.43
1:A:157:HIS:C	1:A:159:PRO:HD3	2.44	0.42
2:B:98:LEU:HD22	2:B:217:ILE:HD11	2.02	0.42
2:B:70:HIS:HA	3:C:35:ASP:HB2	2.01	0.41
1:A:157:HIS:O	1:A:159:PRO:HD3	2.20	0.41
2:B:66:PHE:HB3	2:B:85:LEU:HB3	2.02	0.41
1:A:180:SER:O	1:A:184:LYS:HG3	2.21	0.41
1:A:22:ALA:HA	1:A:25:LEU:HD12	2.01	0.41
1:A:43:GLY:C	1:A:99:PRO:HG3	2.46	0.41
2:B:167:LYS:O	2:B:171:THR:HG23	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	256/301 (85%)	239 (93%)	14 (6%)	3 (1%)	10	34
2	B	161/332 (48%)	144 (89%)	15 (9%)	2 (1%)	10	34
3	C	112/166 (68%)	102 (91%)	8 (7%)	2 (2%)	6	25
All	All	529/799 (66%)	485 (92%)	37 (7%)	7 (1%)	9	32

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	137	GLU
1	A	148	GLU
2	B	130	ARG
1	A	146	MET
2	B	102	LEU
3	C	37	LEU
1	A	234	PHE

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	205/257 (80%)	191 (93%)	14 (7%)	14	42
2	B	88/292 (30%)	82 (93%)	6 (7%)	14	42
3	C	80/127 (63%)	71 (89%)	9 (11%)	5	19
All	All	373/676 (55%)	344 (92%)	29 (8%)	11	35

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ARG
1	A	14	CYS
1	A	27	GLU
1	A	41	VAL
1	A	52	CYS
1	A	54	LEU
1	A	65	VAL
1	A	110	VAL
1	A	166	LYS
1	A	168	LYS
1	A	173	PHE
1	A	188	ASP
1	A	285	HIS
1	A	291	ARG
2	B	19	LEU
2	B	65	VAL
2	B	98	LEU
2	B	125	CYS
2	B	136	LYS
2	B	217	ILE
3	C	14	ILE
3	C	16	LEU
3	C	57	ASP
3	C	59	LEU
3	C	84	MET
3	C	127	SER
3	C	136	LEU
3	C	137	GLU
3	C	146	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	115	ASN
1	A	132	GLN
1	A	233	GLN
2	B	42	ASN
2	B	80	GLN
2	B	86	HIS
2	B	210	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	262/301 (87%)	0.10	14 (5%) 32 25	19, 37, 95, 152	0
2	B	171/332 (51%)	1.34	46 (26%) 1 1	26, 110, 150, 173	0
3	C	116/166 (69%)	0.16	4 (3%) 48 39	18, 50, 91, 126	0
All	All	549/799 (68%)	0.50	64 (11%) 9 8	18, 50, 125, 173	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	143	GLU	5.9
2	B	45	SER	4.8
1	A	74	ASN	4.3
3	C	143	ASP	4.0
2	B	207	ARG	3.9
2	B	128	LEU	3.9
2	B	34	SER	3.7
2	B	96	LEU	3.7
2	B	123	PRO	3.6
2	B	231	LEU	3.6
2	B	97	LEU	3.4
2	B	206	VAL	3.4
2	B	56	CYS	3.3
1	A	66	ALA	3.3
1	A	60	LEU	3.3
2	B	228	PHE	3.3
1	A	89	PHE	3.3
1	A	10	ASN	3.2
2	B	213	ILE	3.2
2	B	47	GLU	3.1
2	B	106	LYS	3.1
3	C	23	GLY	3.0
1	A	258	SER	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	37	PHE	2.9
2	B	99	HIS	2.9
2	B	181	ASN	2.8
2	B	100	TYR	2.8
1	A	299	LEU	2.8
2	B	127	LEU	2.8
2	B	221	LEU	2.8
2	B	216	TYR	2.7
1	A	284	PRO	2.7
2	B	153	TYR	2.6
2	B	155	TYR	2.6
2	B	152	TYR	2.6
2	B	220	GLU	2.6
1	A	285	HIS	2.5
2	B	94	LEU	2.5
2	B	222	SER	2.5
2	B	178	ASN	2.5
2	B	43	PRO	2.4
1	A	65	VAL	2.4
2	B	157	SER	2.4
2	B	203	GLU	2.3
1	A	11	THR	2.3
3	C	122	ILE	2.3
2	B	60	LEU	2.3
2	B	212	LEU	2.3
2	B	142	THR	2.3
2	B	217	ILE	2.3
2	B	226	SER	2.3
3	C	17	ARG	2.3
1	A	175	VAL	2.3
2	B	151	LYS	2.2
2	B	158	GLU	2.2
1	A	286	ARG	2.2
2	B	205	TYR	2.2
2	B	204	ASP	2.1
2	B	104	ALA	2.1
1	A	297	SER	2.1
2	B	161	LEU	2.0
2	B	179	ASN	2.0
2	B	165	GLU	2.0
2	B	98	LEU	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.