



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 05:47 AM UTC

PDB ID : 6HTU / pdb_00006htu
Title : Structure of hStau1 dsRBD3-4 in complex with ARF1 RNA
Authors : Emmerich, C.; Lazzaretti, D.; Bandholz-Cajamarca, L.; Bono, F.
Deposited on : 2018-10-04
Resolution : 2.89 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

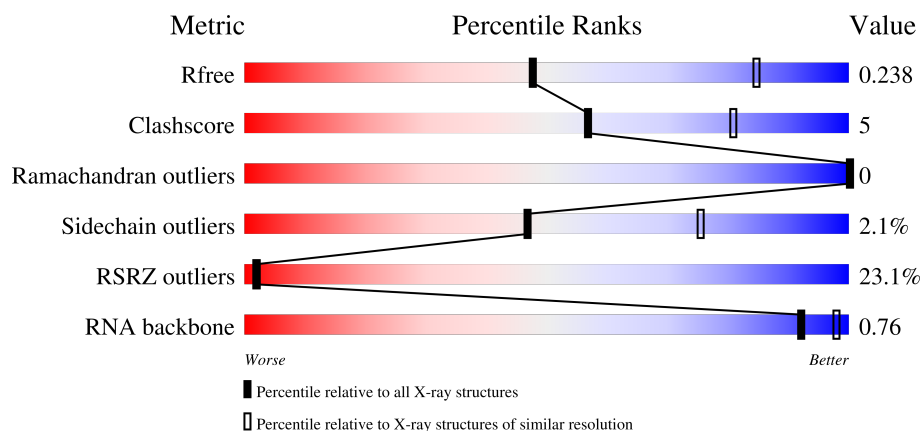
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.89 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	3557 (2.90-2.86)
Clashscore	190562	3801 (2.90-2.86)
Ramachandran outliers	187476	3699 (2.90-2.86)
Sidechain outliers	187428	3702 (2.90-2.86)
RSRZ outliers	180081	3558 (2.90-2.86)
RNA backbone	3983	1174 (3.10-2.66)

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	D	19	95% 5%
2	F	19	79% 21%
3	A	182	4% 36% 6% 58%
3	B	182	6% 35% 7% 58%

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Mol	Chain	Length	Quality of chain
3	C	182	22% 31% 47%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4226 atoms, of which 1906 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 RNA chain called RNA (19-MER).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	D	19	Total	C	H	N	O	P	0	0	0
			611	181	208	74	130	18			

- Molecule 2 is a RNA chain called RNA (19-MER).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	F	19	Total	C	H	N	O	P	0	0	0
			606	180	205	69	134	18			

- Molecule 3 is a protein called Double-stranded RNA-binding protein Staufen homolog 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	A	76	Total	C	H	N	O	S	0	0	0
			1119	354	567	95	101	2			
3	B	76	Total	C	H	N	O	S	0	0	0
			1121	355	565	94	105	2			
3	C	65	Total	C	H	N	O	S	0	0	0
			766	251	361	76	76	2			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	179	GLY	-	expression tag	UNP O95793
A	180	HIS	-	expression tag	UNP O95793
A	181	MET	-	expression tag	UNP O95793
A	359	ARG	ALA	conflict	UNP O95793
B	179	GLY	-	expression tag	UNP O95793
B	180	HIS	-	expression tag	UNP O95793
B	181	MET	-	expression tag	UNP O95793
B	359	ARG	ALA	conflict	UNP O95793
C	179	GLY	-	expression tag	UNP O95793
C	180	HIS	-	expression tag	UNP O95793

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Chain	Residue	Modelled	Actual	Comment	Reference
C	181	MET	-	expression tag	UNP O95793
C	359	ARG	ALA	conflict	UNP O95793

- Molecule 4 is water.

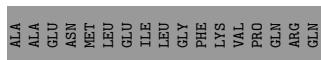
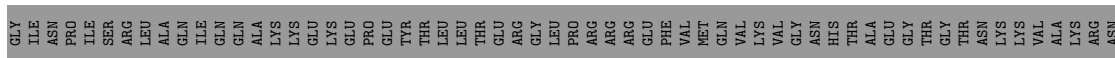
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O 1 1	0	0
4	B	2	Total O 2 2	0	0

- Molecule 1: RNA (19-MER)

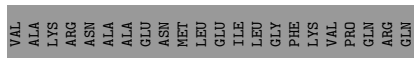
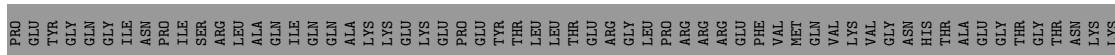


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- A diagram showing a sequence of nodes: G194, A199, G200, U201, U202, U205, and C212. Nodes G194, G200, and C212 are green, while A199, U201, U202, and U205 are yellow. They are connected by horizontal lines, with vertical lines indicating connections to a common vertical line on the left.

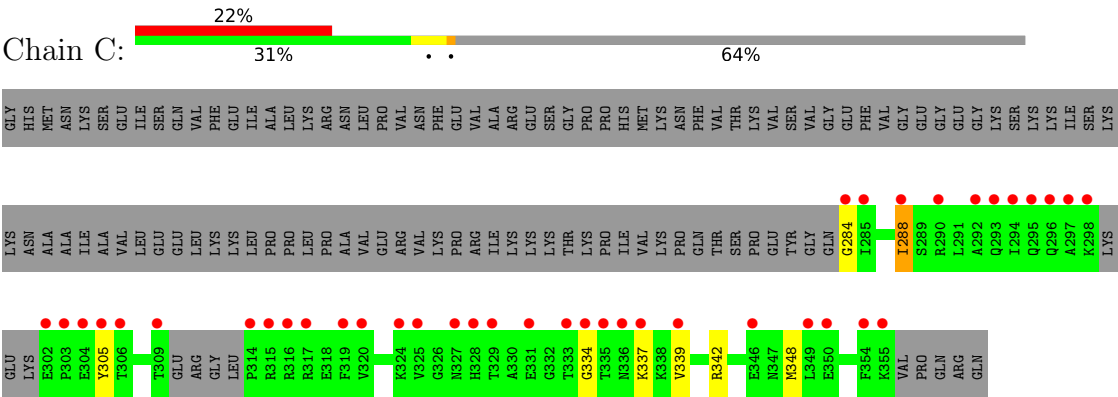
- GLY
 H180
 M181
 E185
 I186
 V189
 L194
 N197
 N201
 V204
 A205
 R206
 V217
 V220
 E224
 K239
 I243
 A244
 V245
 L255
 PRO
 ALA
 VAL
 GLU
 ARG
 VAL
 LYS
 PRO
 ARG
 ILE
 LYS
 LYS
 LYS
 THR
 LYS
 PRO
 ILE
 VAL
 LYS
 PRO
 PRO
 GLN
 THR
 SER
 PRO
 PRO
 GLU
 TYR
 GLY
 GLN



- [illegible]



● Molecule 3: Double-stranded RNA-binding protein Staufen homolog 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	105.89Å 105.89Å 169.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.35 – 2.89 47.35 – 2.89	Depositor EDS
% Data completeness (in resolution range)	99.1 (47.35-2.89) 99.4 (47.35-2.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.13 (at 2.91Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.217 , 0.240 0.220 , 0.238	Depositor DCC
R_{free} test set	1109 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	90.2	Xtriage
Anisotropy	0.206	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 60.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4226	wwPDB-VP
Average B, all atoms (Å ²)	109.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.53% 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	D	0.14	0/450	0.30	0/700
2	F	0.11	0/447	0.28	0/695
3	A	0.17	0/561	0.32	0/757
3	B	0.49	1/565 (0.2%)	0.45	1/763 (0.1%)
3	C	0.18	0/408	0.35	0/553
All	All	0.27	1/2431 (0.0%)	0.35	1/3468 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	212	HIS	CA-C	6.00	1.60	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	210	PRO	O-C-N	5.06	123.53	121.15

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	D	403	208	208	1	0
2	F	401	205	205	3	0
3	A	552	567	552	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	556	565	549	6	0
3	C	405	361	315	6	0
4	A	1	0	0	0	0
4	B	2	0	0	0	0
All	All	2320	1906	1829	19	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 (19) 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)
3:B:220:VAL:HG13	3:B:245:VAL:HG21	1.85	0.59
3:B:186:ILE:HD12	3:B:186:ILE:H	1.72	0.54
3:A:186:ILE:HD12	3:A:186:ILE:H	1.75	0.51
3:C:334:GLY:HA3	3:C:339:VAL:HG23	1.93	0.49
3:A:205:ALA:HB3	3:A:217:VAL:HG23	1.94	0.49
3:B:196:ARG:HH12	3:B:252:LEU:HB3	1.77	0.48
3:A:186:ILE:HD11	3:A:239:LYS:HA	1.95	0.48
3:A:185:GLU:HG2	3:A:243:ILE:HG12	1.96	0.47
3:B:218:THR:HG23	3:B:237:SER:OG	2.15	0.46
2:F:201:U:H2'	2:F:202:U:C6	2.53	0.44
3:A:201:ASN:OD1	3:C:342:ARG:NH2	2.44	0.43
3:C:288:ILE:HD11	3:C:305:TYR:CE2	2.53	0.43
3:A:197:ASN:HA	3:C:284:GLY:HA3	2.01	0.43
3:B:225:PHE:CZ	3:B:252:LEU:HD11	2.55	0.42
3:A:204:VAL:HG23	3:A:204:VAL:O	2.20	0.42
1:D:81:C:OP1	3:C:337:LYS:HB2	2.20	0.41
2:F:205:U:O2'	3:B:183:LYS:HE2	2.20	0.41
3:A:220:VAL:HG13	3:A:245:VAL:HG21	2.02	0.41
2:F:199:A:H5'	3:C:288:ILE:CG2	2.51	0.41

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	
3	A	74/182 (41%)	69 (93%)	5 (7%)	0	100	100
3	B	74/182 (41%)	72 (97%)	2 (3%)	0	100	100
3	C	59/182 (32%)	58 (98%)	1 (2%)	0	100	100
All	All	207/546 (38%)	199 (96%)	8 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	
3	A	57/157 (36%)	57 (100%)	0	100	100
3	B	58/157 (37%)	57 (98%)	1 (2%)	53	80
3	C	25/157 (16%)	23 (92%)	2 (8%)	11	31
All	All	140/471 (30%)	137 (98%)	3 (2%)	47	75

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	B	207	GLU
3	C	288	ILE
3	C	348	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
3	B	215	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	D	18/19 (94%)	0	0
2	F	18/19 (94%)	0	0
All	All	36/38 (94%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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	D	19/19 (100%)	-0.87	0 100 100	64, 74, 91, 91	0
2	F	19/19 (100%)	-0.83	0 100 100	71, 78, 83, 87	0
3	A	76/182 (41%)	0.73	8 (10%) 11 10	66, 98, 176, 203	0
3	B	76/182 (41%)	1.08	11 (14%) 6 5	69, 100, 152, 198	0
3	C	65/182 (35%)	2.80	40 (61%) 0 0	115, 165, 220, 244	0
All	All	255/584 (43%)	1.13	59 (23%) 2 2	64, 104, 199, 244	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	309	THR	8.9
3	B	212	HIS	7.5
3	C	302	GLU	7.2
3	C	298	LYS	6.1
3	A	255	LEU	6.0
3	B	180	HIS	6.0
3	C	315	ARG	5.5
3	C	314	PRO	5.4
3	C	296	GLN	5.4
3	C	355	LYS	5.2
3	A	206	ARG	5.1
3	B	255	LEU	4.8
3	C	303	PRO	4.7
3	C	327	ASN	4.6
3	A	180	HIS	4.4
3	C	297	ALA	4.4
3	C	285	ILE	4.3
3	C	336	ASN	4.1
3	C	319	PHE	4.1
3	C	316	ARG	4.0

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Mol	Chain	Res	Type	RSRZ
3	C	292	ALA	4.0
3	B	211	PRO	4.0
3	B	206	ARG	4.0
3	C	339	VAL	3.9
3	C	350	GLU	3.8
3	C	335	THR	3.7
3	C	295	GLN	3.6
3	C	293	GLN	3.6
3	A	181	MET	3.6
3	C	328	HIS	3.5
3	B	213	MET	3.4
3	C	317	ARG	3.4
3	C	329	THR	3.2
3	C	305	TYR	3.1
3	C	337	LYS	3.1
3	C	320	VAL	3.0
3	C	290	ARG	3.0
3	C	294	ILE	2.9
3	C	331	GLU	2.9
3	C	325	VAL	2.8
3	C	349	LEU	2.7
3	C	324	LYS	2.6
3	A	224	GLU	2.6
3	C	346	GLU	2.5
3	C	354	PHE	2.4
3	C	288	ILE	2.4
3	C	333	THR	2.4
3	B	217	VAL	2.3
3	C	306	THR	2.3
3	C	284	GLY	2.3
3	C	304	GLU	2.1
3	B	202	PHE	2.1
3	C	334	GLY	2.1
3	B	192	ILE	2.1
3	B	193	ALA	2.1
3	B	181	MET	2.0
3	A	205	ALA	2.0
3	A	189	VAL	2.0
3	A	194	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.