



wwPDB X-ray Structure Validation Summary Report ⓘ

May 23, 2020 – 07:50 pm BST

PDB ID : 4EBA
Title : Crystal structure of the Rna14-Rna15 complex
Authors : Paulson, A.R.; Tong, L.
Deposited on : 2012-03-23
Resolution : 3.30 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

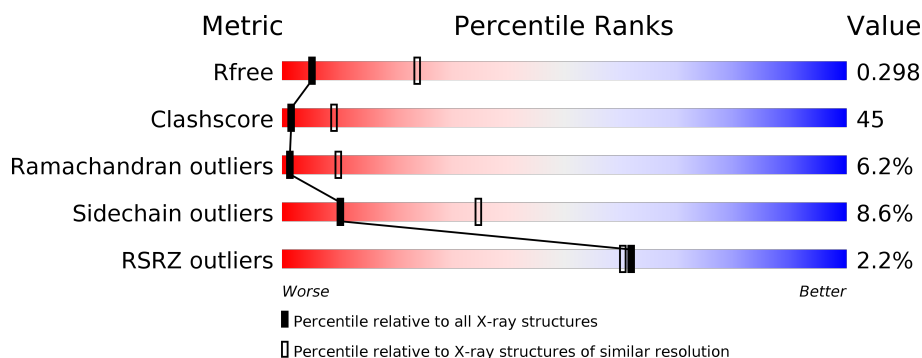
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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}	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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 ≥ 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	645	
1	B	645	
1	C	645	
1	D	645	
1	E	645	
1	F	645	

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Mol	Chain	Length	Quality of chain
2	G	174	<div><div></div><div>16%24%7%53%</div></div>
2	H	174	<div><div>2%</div><div></div><div>11%28%6%53%</div></div>
2	I	174	<div><div>%</div><div></div><div>13%27%6%53%</div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 30268 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 mRNA 3'-end-processing protein Rna14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	585	Total	C	N	O	S	0	0	0
			4874	3149	803	897	25			
1	B	558	Total	C	N	O	S	0	0	0
			4646	2990	772	859	25			
1	C	585	Total	C	N	O	S	0	0	0
			4874	3149	803	897	25			
1	D	551	Total	C	N	O	S	0	0	0
			4589	2957	759	848	25			
1	E	578	Total	C	N	O	S	0	0	0
			4823	3118	795	885	25			
1	F	553	Total	C	N	O	S	0	0	0
			4608	2967	764	852	25			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	17	MET	-	EXPRESSION TAG	UNP Q6CII8
B	17	MET	-	EXPRESSION TAG	UNP Q6CII8
C	17	MET	-	EXPRESSION TAG	UNP Q6CII8
D	17	MET	-	EXPRESSION TAG	UNP Q6CII8
E	17	MET	-	EXPRESSION TAG	UNP Q6CII8
F	17	MET	-	EXPRESSION TAG	UNP Q6CII8

- Molecule 2 is a protein called Rna15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	81	Total	C	N	O	S	0	0	0
			618	395	98	119	6			
2	I	81	Total	C	N	O	S	0	0	0
			618	395	98	119	6			
2	H	81	Total	C	N	O	S	0	0	0
			618	395	98	119	6			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	85	MET	-	EXPRESSION TAG	UNP Q6CKN2
G	86	GLY	-	EXPRESSION TAG	UNP Q6CKN2
G	87	SER	-	EXPRESSION TAG	UNP Q6CKN2
G	88	SER	-	EXPRESSION TAG	UNP Q6CKN2
G	89	HIS	-	EXPRESSION TAG	UNP Q6CKN2
G	90	HIS	-	EXPRESSION TAG	UNP Q6CKN2
G	91	HIS	-	EXPRESSION TAG	UNP Q6CKN2
G	92	HIS	-	EXPRESSION TAG	UNP Q6CKN2
G	93	HIS	-	EXPRESSION TAG	UNP Q6CKN2
G	94	HIS	-	EXPRESSION TAG	UNP Q6CKN2
G	95	SER	-	EXPRESSION TAG	UNP Q6CKN2
G	96	SER	-	EXPRESSION TAG	UNP Q6CKN2
G	97	GLY	-	EXPRESSION TAG	UNP Q6CKN2
G	98	LEU	-	EXPRESSION TAG	UNP Q6CKN2
G	99	VAL	-	EXPRESSION TAG	UNP Q6CKN2
G	100	PRO	-	EXPRESSION TAG	UNP Q6CKN2
G	101	ARG	-	EXPRESSION TAG	UNP Q6CKN2
G	102	GLY	-	EXPRESSION TAG	UNP Q6CKN2
G	103	SER	-	EXPRESSION TAG	UNP Q6CKN2
G	104	HIS	-	EXPRESSION TAG	UNP Q6CKN2
I	85	MET	-	EXPRESSION TAG	UNP Q6CKN2
I	86	GLY	-	EXPRESSION TAG	UNP Q6CKN2
I	87	SER	-	EXPRESSION TAG	UNP Q6CKN2
I	88	SER	-	EXPRESSION TAG	UNP Q6CKN2
I	89	HIS	-	EXPRESSION TAG	UNP Q6CKN2
I	90	HIS	-	EXPRESSION TAG	UNP Q6CKN2
I	91	HIS	-	EXPRESSION TAG	UNP Q6CKN2
I	92	HIS	-	EXPRESSION TAG	UNP Q6CKN2
I	93	HIS	-	EXPRESSION TAG	UNP Q6CKN2
I	94	HIS	-	EXPRESSION TAG	UNP Q6CKN2
I	95	SER	-	EXPRESSION TAG	UNP Q6CKN2
I	96	SER	-	EXPRESSION TAG	UNP Q6CKN2
I	97	GLY	-	EXPRESSION TAG	UNP Q6CKN2
I	98	LEU	-	EXPRESSION TAG	UNP Q6CKN2
I	99	VAL	-	EXPRESSION TAG	UNP Q6CKN2
I	100	PRO	-	EXPRESSION TAG	UNP Q6CKN2
I	101	ARG	-	EXPRESSION TAG	UNP Q6CKN2
I	102	GLY	-	EXPRESSION TAG	UNP Q6CKN2
I	103	SER	-	EXPRESSION TAG	UNP Q6CKN2
I	104	HIS	-	EXPRESSION TAG	UNP Q6CKN2
H	85	MET	-	EXPRESSION TAG	UNP Q6CKN2
H	86	GLY	-	EXPRESSION TAG	UNP Q6CKN2

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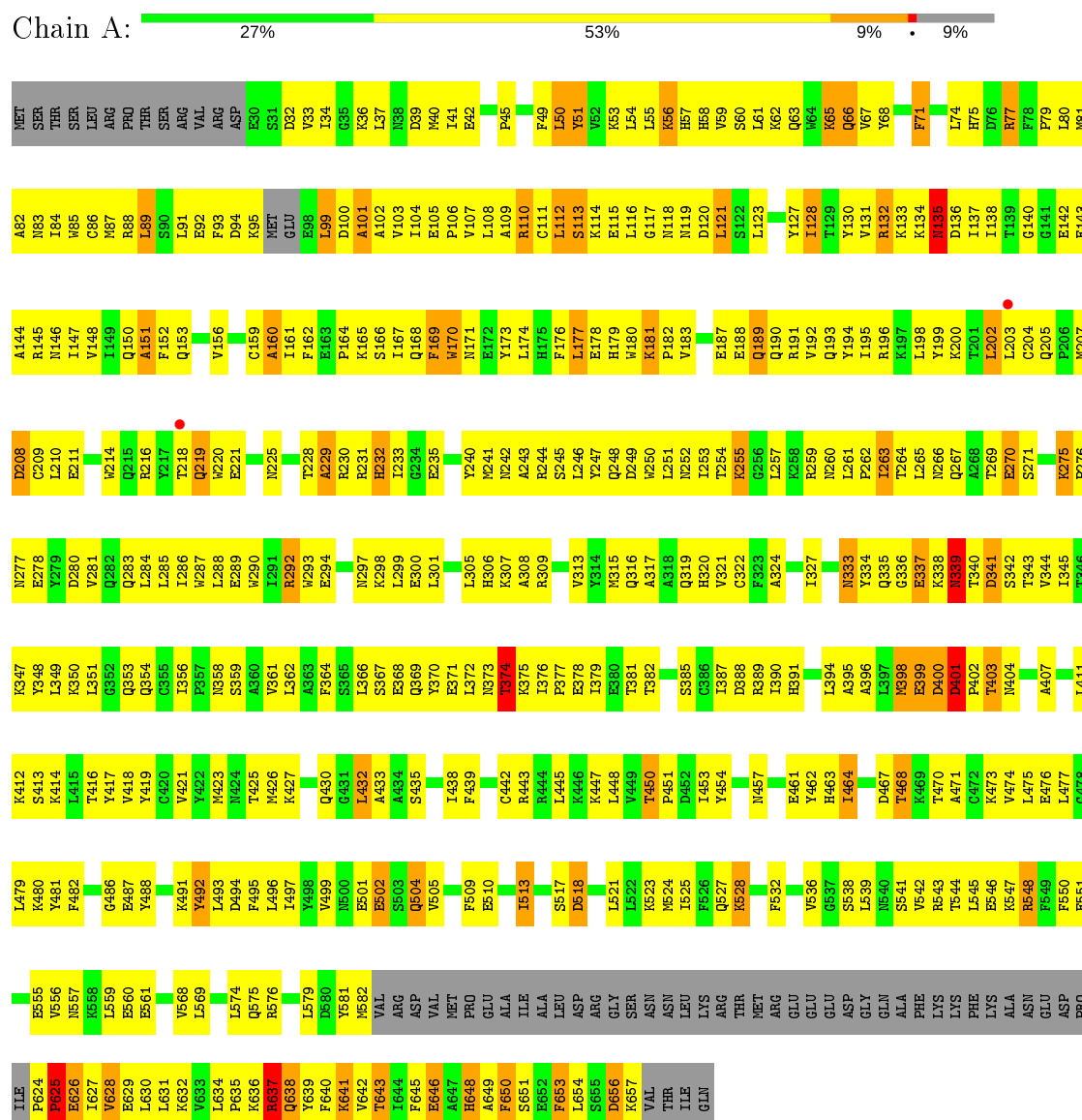
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Chain	Residue	Modelled	Actual	Comment	Reference
H	87	SER	-	EXPRESSION TAG	UNP Q6CKN2
H	88	SER	-	EXPRESSION TAG	UNP Q6CKN2
H	89	HIS	-	EXPRESSION TAG	UNP Q6CKN2
H	90	HIS	-	EXPRESSION TAG	UNP Q6CKN2
H	91	HIS	-	EXPRESSION TAG	UNP Q6CKN2
H	92	HIS	-	EXPRESSION TAG	UNP Q6CKN2
H	93	HIS	-	EXPRESSION TAG	UNP Q6CKN2
H	94	HIS	-	EXPRESSION TAG	UNP Q6CKN2
H	95	SER	-	EXPRESSION TAG	UNP Q6CKN2
H	96	SER	-	EXPRESSION TAG	UNP Q6CKN2
H	97	GLY	-	EXPRESSION TAG	UNP Q6CKN2
H	98	LEU	-	EXPRESSION TAG	UNP Q6CKN2
H	99	VAL	-	EXPRESSION TAG	UNP Q6CKN2
H	100	PRO	-	EXPRESSION TAG	UNP Q6CKN2
H	101	ARG	-	EXPRESSION TAG	UNP Q6CKN2
H	102	GLY	-	EXPRESSION TAG	UNP Q6CKN2
H	103	SER	-	EXPRESSION TAG	UNP Q6CKN2
H	104	HIS	-	EXPRESSION TAG	UNP Q6CKN2

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 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: mRNA 3'-end-processing protein RNA14



• Molecule 1: mRNA 3'-end-processing protein RNA14

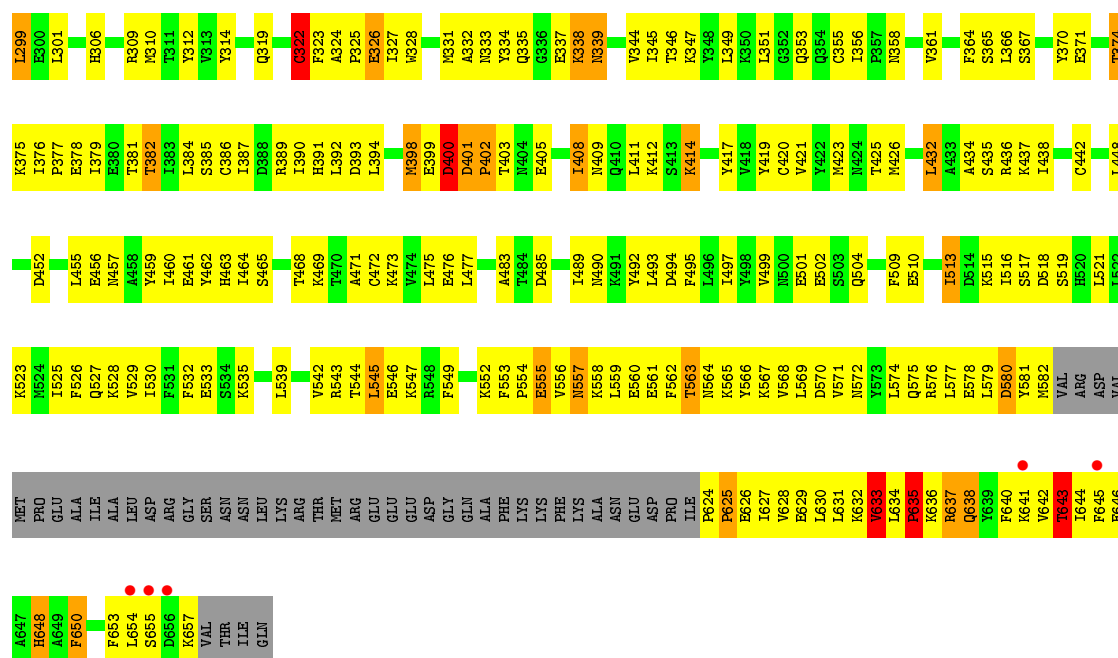


PRO	F562	D494	T425	L349	V281	M146	M81	MET
GLU	T563	F495	M426	K350	Q282	I147	A82	THR
ILE	N564	L496	K427	L351	Q283	V148	N83	SER
VAL	K565	I497	R428	G352	Q215	I149	I84	THR
GLU		V498	I429	Q353	L285	Q150	W85	LEU
LEU	V568	V499		Q354	L286	A151	C86	ARG
L569		M500	A434	C355	W287	F152	M87	
L575		E501	S435	L356	L288	R88	R88	P23
VAL	M572	E502	L534	P357	W220	V155	L89	S25
LEU		S503	I438	N358	W290		S90	R26
PRO	Q575	Q504	F439	S359	T291	C159	L91	V27
LYS	R576	V505	G440		R292	A160	E92	R28
ARG	L577	K441	F364			I161	F93	D29
GLN	E578	S507	C442	S365	D296	F162	D94	E30
TYR	L579	L508	R443	L366	N297		K95	S31
PHE	D580	F509	R444	E367	K298	R230	GLU	
LYS	Y581		L445	E368	L299	R231	MET	
VAL	M582	I513	K446	Q369		H232	E98	V33
THR	VAL	I516	K447	Y370	S302	I167	L99	I34
ILE	ARG	I516	L448	E371	D303	Q168	G35	
GLU	ASP	V449	T450	F370	L304	F169	L100	K36
PHE	GLU	L521	G450		L305	W170	A101	L37
ALA	VAL	L522	V451	P377	R306	N171	A02	N38
HIS	MET	K523	P451	E378	K307	E172	V103	D59
ALA	PRO	M524	D452	I379	A308	Y173	I104	M40
GLU	ALA	I525	I453		R309	F176	E105	I41
PHE	ALA	F526	E456		G310	L177	P106	E42
SER	ILE	F526	N457	T382	T311	H178	V107	E43
GLU	ALA	K528				H179	L108	Q44
PHE	LEU	V529	Y462	R389		W180		
LEU	ASP	V529	H463	I390	Y314	E187	C111	I48
SER	ARG	I530	H463	H391	Q315	K181	L112	F49
GLY	ASP	F531	L464	L392	R316	P182	S113	
LYS	VAL	F532	S465	D393	A317	V183	K114	Y51
ASN	ASN	ASN	K466	L394	A318	M184	E115	V52
ASN	ASN	K535	D467	L395	Q319	K185	L116	V53
LEU	LEU	V536	T468	A396	H320	F186	G117	L54
LYS	LYS	G537	K469	L397	R321	E187	M118	L55
ARG	ARG	S538	T470	M398	C322	Q188	D120	K56
THR	THR	L539	A471	C399	F323	Q189	N119	H57
MET	MET		C472	D400	A324	Q190	L121	H58
ARG	ARG	V542	K473	D401	P325	R191	S122	V59
GLU	GLU	R543	V474	F402		V192	L123	S60
GLU	GLU	T544	L475	T403	M331	Q193	L61	
GLU	GLU	L545	E476	L404	A332	Y194	I128	K62
ASP	E546	K547	L477		N333	I195	T129	Q63
GLY	GLY	K547	G478	I408	Y334	R196	K65	W64
GLN	GLN	R548	L479		Q335	K197	V130	K65
ALA	ALA	F549	K480	L411	G336	L198	V131	Q66
PHE	PHE	F550	Y481	K412	G336	Y199	R132	
LYS	LYS	K551	F482	S413	K338	K200	K134	Y68
LYS	LYS	F552		K414	N339	T201	C134	E69
PHE	PHE	F553	D485	L415	T340	L202	N135	T70
LYS	LYS	P554	G486	T416	D341	L203	D136	F71
ALA	ALA	E555	E487	Y419	S342	C204	I137	
ASN	ASN	V556	Y488	C420	T274	Q205	I138	L74
GLU	GLU	N557	L489	E489	V344	T206	T139	
ASP	ASP	K558	N490	Y421	T345	M207	G140	F77
PRO	PRO	L559	K491	Y422	T346	D208		F78
ILE	ILE	E560	Y492	M423	K347	Y279	A144	P79
PRO	PRO	E561	N493	M423	T348	E282	R145	L50

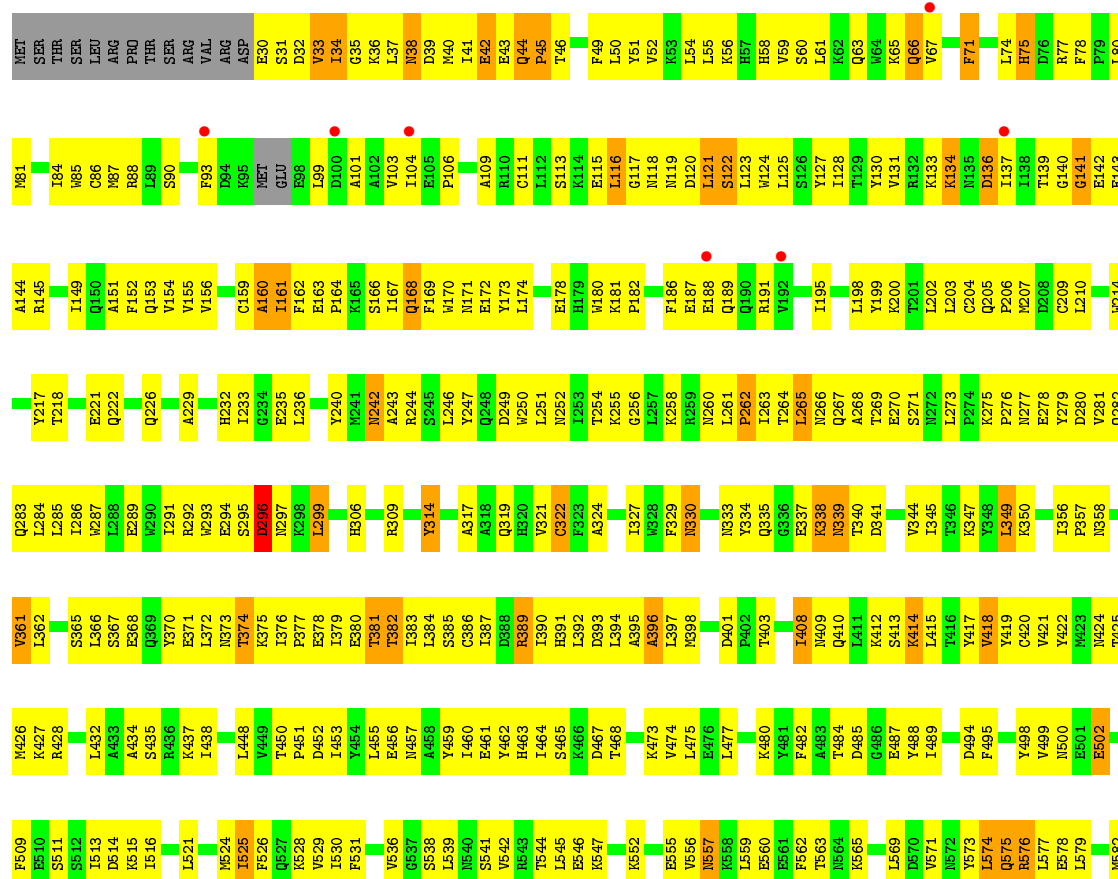
• Molecule 1: mRNA 3'-end-processing protein RNA14



MET	SER	THR	SER	THR	LEU	ARG	PRO	THR	SER	THR	VAL	ARG	ASP	E30	S31	D32	V33	I34	G35	K36	L37	N38	D39	I40	E41	E42	E43	Q44	P45	D46	T47	L48	F49	L50	K53	L54	L55	B58	V59	S60	L61	K62	Q63	Q66	T70	F71	L74	H75	F78	P79	L80	P81	I84
M85	M88	R88	D157	E92	K95	MET	GLU	E98	A101	A102	V103	I104	E105	P106	V107	L108	A109	R110	C111	L112	S113	K114	E115	L116	G117	N118	L121	S122	L123	M124	L125	S126	Y127	I128	Y131	K134	N135	D136	I137	I138	T139	G140	G141	E142	E143	A144	R145	H146	I147	Q150	A151	F152	Q153
V154	V155	V156	D157	K158	C159	A160	I161	E163	P164	K165	S166	I167	Q168	F169	W170	Y173	L174	H175	F176	L177	E178	H179	W180	K181	P182	F186	E187	E188	R191	V192	Q193	R196	K197	L198	Y199	K200	L201	L202	L203	C204	Q205	P206	M207	D208	C209	L210	E211	Y217	T218	Q226	L227	T228	
R231	H232	I233	G234	E235	L236	S237	Y240	M241	M242	A243	R244	S245	L246	Y247	Q248	D249	W250	L251	N252	I253	G256	L257	P262	L263	T264	L265	N266	Q267	A268	T269	E270	S271	N272	L273	P274	K275	P276	N277	E278	Y279	D280	V281	Q282	Q283	L284	L285	L286	W287	W290	S295	D296	N297	K298



• Molecule 1: mRNA 3'-end-processing protein RNA14

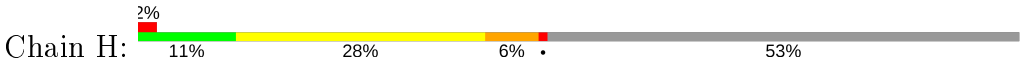






GLU	LYS	VAL	ASP	LEU	LEU	ARG	GLN	GLN	GLN	LEU	GLN	ASP	SER	ASP	ASP	ILE	ARG	ALA	GLY	MET	LEU	PRO	GLN	ASP	GLU	LYS	LYS	MET	ALA	VAL	TRP	GLU	LEU	LYS	GLN	ARG	ALA	MET	LYS	GLY	GLU	PHE	GLY	HIS	LEU
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● Molecule 2: Rna15



MET	GLY	SER	SER	Q151	H152	HIS	HIS	HIS	HIS	HIS	SER	SER	GLY	LEU	VAL	PRO	ARG	GLY	SER	SER	HIS	MET	VAL	GLU	ASP	LYS	VAL	LYS	PHE	P112	W113	L114	P115	V116	G117	V118	D119	V120	H121	I122	T125	T126	M129	C130	I131	E134	L135	G136	K137	L138	Q139	K140	D141	Q142	Q143	H144	A145	L146	L147
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K148	V149	I150	Q151	H152	F153	C154	K155	D156	ASP	LYS	E159	T160	F161	V162	A163	E166	E167	A168	P169	Q170	L171	S172	V173	A174	I175	A176	E177	L178	L179	L180	V184	C185	S186	V187	D188	Q189	L190	T191	Q192	L193	A194	MET	ALA	SER	LYS	GLN	ARG	PRO	GLU	GLU	GLN	THR	ASP	ASN	THR	VAL	GLU
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ASP	GLY	LEU	ASP	GLU	GLU	LYS	VAL	ASP	LEU	LEU	ARG	GLN	VAL	LEU	GLN	LEU	GLN	ASP	SER	ASP	ASP	ILE	ALA	MET	LEU	PRO	GLN	ASP	GLU	LYS	MET	ALA	VAL	TRP	GLU	LEU	LYS	GLN	ARG	ALA	MET	LYS	GLY	GLU	PHE	GLY	HIS	LEU
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4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	162.04Å 162.04Å 177.54Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.79 – 3.30 47.79 – 3.30	Depositor EDS
% Data completeness (in resolution range)	86.4 (47.79-3.30) 86.3 (47.79-3.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 3.33Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.226 , 0.298 0.226 , 0.298	Depositor DCC
R_{free} test set	3646 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	84.8	Xtriage
Anisotropy	0.158	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 76.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.018 for -h,-k,l 0.038 for h,-h-k,-l 0.025 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	30268	wwPDB-VP
Average B, all atoms (Å ²)	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.09% 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 [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	0.46	0/4982	0.64	0/6732
1	B	0.44	0/4747	0.67	1/6416 (0.0%)
1	C	0.40	0/4982	0.60	0/6732
1	D	0.40	0/4689	0.59	0/6338
1	E	0.46	0/4931	0.66	1/6664 (0.0%)
1	F	0.42	0/4708	0.61	0/6363
2	G	0.39	0/626	0.71	0/849
2	H	0.37	0/626	0.67	0/849
2	I	0.38	0/626	0.63	0/849
All	All	0.43	0/30917	0.63	2/41792 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	31	SER	N-CA-C	-5.59	95.91	111.00
1	E	112	LEU	CA-CB-CG	5.05	126.91	115.30

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	4874	0	4885	509	0
1	B	4646	0	4650	399	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	4874	0	4885	391	0
1	D	4589	0	4591	385	0
1	E	4823	0	4834	511	0
1	F	4608	0	4608	398	0
2	G	618	0	632	81	0
2	H	618	0	632	93	0
2	I	618	0	632	92	0
All	All	30268	0	30349	2735	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 45.

The worst 5 of 2735 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:D:563:THR:HG22	1:D:574:LEU:HD12	1.23	1.17
1:C:557:ASN:HD22	1:C:560:GLU:HB2	1.11	1.16
1:D:468:THR:HG21	1:D:499:VAL:HG11	1.31	1.07
1:A:345:ILE:HD12	1:A:345:ILE:H	1.19	1.03
1:A:225:ASN:HB2	1:A:229:ALA:HB2	1.37	1.02

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	579/645 (90%)	433 (75%)	110 (19%)	36 (6%)	1	10
1	B	554/645 (86%)	414 (75%)	108 (20%)	32 (6%)	1	11
1	C	579/645 (90%)	435 (75%)	110 (19%)	34 (6%)	1	10
1	D	547/645 (85%)	398 (73%)	117 (21%)	32 (6%)	1	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	572/645 (89%)	429 (75%)	106 (18%)	37 (6%)	1	9
1	F	549/645 (85%)	422 (77%)	95 (17%)	32 (6%)	1	11
2	G	77/174 (44%)	57 (74%)	12 (16%)	8 (10%)	0	3
2	H	77/174 (44%)	56 (73%)	12 (16%)	9 (12%)	0	2
2	I	77/174 (44%)	58 (75%)	14 (18%)	5 (6%)	1	9
All	All	3611/4392 (82%)	2702 (75%)	684 (19%)	225 (6%)	1	10

5 of 225 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	62	LYS
1	A	110	ARG
1	A	135	ASN
1	A	255	LYS
1	A	337	GLU

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	544/598 (91%)	483 (89%)	61 (11%)	6	23
1	B	519/598 (87%)	472 (91%)	47 (9%)	9	31
1	C	544/598 (91%)	506 (93%)	38 (7%)	15	43
1	D	512/598 (86%)	476 (93%)	36 (7%)	15	43
1	E	538/598 (90%)	487 (90%)	51 (10%)	8	29
1	F	514/598 (86%)	479 (93%)	35 (7%)	16	44
2	G	71/154 (46%)	62 (87%)	9 (13%)	4	19
2	H	71/154 (46%)	65 (92%)	6 (8%)	10	35
2	I	71/154 (46%)	64 (90%)	7 (10%)	8	28
All	All	3384/4050 (84%)	3094 (91%)	290 (9%)	10	35

5 of 290 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	419	TYR
1	D	314	TYR
2	G	120	VAL
1	C	545	LEU
1	D	42	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 144 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	575	GLN
1	D	354	GLN
2	I	170	GLN
1	D	58	HIS
1	D	219	GLN

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 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 ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	585/645 (90%)	-0.29	2 (0%) 94 94	39, 76, 136, 149	0
1	B	558/645 (86%)	-0.29	0 100 100	36, 73, 136, 148	0
1	C	585/645 (90%)	-0.10	13 (2%) 62 60	60, 106, 149, 151	0
1	D	551/645 (85%)	-0.13	7 (1%) 77 77	58, 104, 149, 151	0
1	E	578/645 (89%)	0.20	43 (7%) 14 14	57, 106, 150, 151	0
1	F	553/645 (85%)	-0.08	8 (1%) 75 75	55, 104, 148, 151	0
2	G	81/174 (46%)	-0.30	0 100 100	63, 102, 138, 151	0
2	H	81/174 (46%)	0.06	4 (4%) 29 27	90, 128, 148, 151	0
2	I	81/174 (46%)	-0.03	2 (2%) 57 54	96, 125, 147, 151	0
All	All	3653/4392 (83%)	-0.11	79 (2%) 62 60	36, 99, 148, 151	0

The worst 5 of 79 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	125	LEU	4.9
1	E	214	TRP	4.3
1	E	215	GLN	4.3
1	E	218	THR	4.1
1	C	655	SER	4.0

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 carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.