



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:31 PM BST

PDB ID : 5FLX
EMDB ID: : EMD-3221
Title : Mammalian 40S HCV-IRES complex
Authors : Yamamoto, H.; Collier, M.; Loerke, J.; Ismer, J.; Schmidt, A.; Hilal, T.;
Sprink, T.; Yamamoto, K.; Mielke, T.; Burger, J.; Shaikh, T.R.; Dabrowski,
M.; Hildebrand, P.W.; Scheerer, P.; Spahn, C.M.T.
Deposited on : 2015-10-28
Resolution : 3.90 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could
stem from errors in the original structure(s) used in the fitting.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

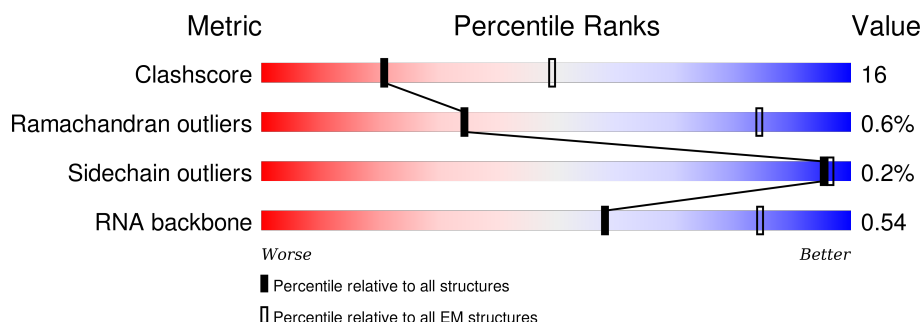
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 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)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	1	1869	<div> <div>39%</div> <div>45%</div> <div>8%</div> <div>9%</div> </div>
2	A	295	<div> <div>49%</div> <div>23%</div> <div>27%</div> </div>
3	B	264	<div> <div>53%</div> <div>27%</div> <div>20%</div> </div>
4	C	293	<div> <div>50%</div> <div>26%</div> <div>24%</div> </div>
5	D	243	<div> <div>72%</div> <div>17%</div> <div>•</div> <div>9%</div> </div>
6	E	263	<div> <div>64%</div> <div>33%</div> <div>•</div> </div>
7	F	204	<div> <div>61%</div> <div>31%</div> <div>•</div> <div>7%</div> </div>
8	G	249	<div> <div>71%</div> <div>22%</div> <div>7%</div> </div>

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Mol	Chain	Length	Quality of chain
9	H	194	
10	I	208	
11	J	194	
12	K	165	
13	L	158	
14	M	132	
15	N	151	
16	O	151	
17	P	145	
18	Q	146	
19	R	135	
20	S	152	
21	T	145	
22	U	119	
23	V	83	
24	W	130	
25	X	143	
26	Y	133	
27	Z	125	
28	a	115	
29	b	84	
30	c	69	
31	d	56	
32	e	59	
33	f	156	

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Mol	Chain	Length	Quality of chain
34	g	317	<div><div></div><div>99%</div><div>.</div></div>
35	z	504	<div><div><div></div><div>42%</div></div><div><div></div><div>10%</div><div>.</div></div><div><div></div><div>48%</div></div></div>

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 80592 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 18S RRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	1708	Total	C	N	O	P	0	0
			36456	16274	6546	11928	1708		

- Molecule 2 is a protein called 40S RIBOSOMAL PROTEIN SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	215	Total	C	N	O	S	0	0
			1704	1083	298	315	8		

- Molecule 3 is a protein called 40S RIBOSOMAL PROTEIN S3A.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	212	Total	C	N	O	S	0	0
			1722	1093	308	307	14		

- Molecule 4 is a protein called 40S RIBOSOMAL PROTEIN S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	222	Total	C	N	O	S	0	0
			1724	1114	296	304	10		

- Molecule 5 is a protein called 40S RIBOSOMAL PROTEIN S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	220	Total	C	N	O	S	0	0
			1709	1090	308	304	7		

- Molecule 6 is a protein called 40S RIBOSOMAL PROTEIN S4, Y ISOFORM 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	257	Total	C	N	O	S	0	0
			2031	1298	381	344	8		

- Molecule 7 is a protein called 40S RIBOSOMAL PROTEIN S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	190	Total	C	N	O	S	0	0
			1502	939	285	271	7		

- Molecule 8 is a protein called 40S RIBOSOMAL PROTEIN S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	232	Total	C	N	O	S	0	0
			1884	1176	379	322	7		

- Molecule 9 is a protein called 40S RIBOSOMAL PROTEIN S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	H	183	Total	C	N	O	S	0	0
			1479	941	272	265	1		

- Molecule 10 is a protein called 40S RIBOSOMAL PROTEIN S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	I	207	Total	C	N	O	S	0	0
			1696	1064	334	293	5		

- Molecule 11 is a protein called 40S RIBOSOMAL PROTEIN S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	J	179	Total	C	N	O	S	0	0
			1495	953	299	241	2		

- Molecule 12 is a protein called 40S RIBOSOMAL PROTEIN S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	K	98	Total	C	N	O	S	0	0
			827	539	148	134	6		

- Molecule 13 is a protein called 40S RIBOSOMAL PROTEIN S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	L	153	Total	C	N	O	S	0	0
			1258	804	235	213	6		

- Molecule 14 is a protein called 40S RIBOSOMAL PROTEIN S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	M	120	Total	C	N	O	S	0	0
			931	584	164	174	9		

- Molecule 15 is a protein called 40S RIBOSOMAL PROTEIN S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	N	149	Total	C	N	O	S	0	0
			1202	770	228	203	1		

- Molecule 16 is a protein called 40S RIBOSOMAL PROTEIN S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	O	136	Total	C	N	O	S	0	0
			1016	621	199	190	6		

- Molecule 17 is a protein called 40S RIBOSOMAL PROTEIN S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	P	120	Total	C	N	O	S	0	0
			999	636	188	168	7		

- Molecule 18 is a protein called 40S RIBOSOMAL PROTEIN S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Q	139	Total	C	N	O	S	0	0
			1109	704	210	192	3		

- Molecule 19 is a protein called 40S RIBOSOMAL PROTEIN S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	R	121	Total	C	N	O	S	0	0
			985	618	183	181	3		

- Molecule 20 is a protein called 40S RIBOSOMAL PROTEIN S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	S	139	Total	C	N	O	S	0	0
			1154	725	233	195	1		

- Molecule 21 is a protein called 40S RIBOSOMAL PROTEIN S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	T	143	Total	C	N	O	S	0	0
			1112	697	214	198	3		

- Molecule 22 is a protein called 40S RIBOSOMAL PROTEIN S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	U	97	Total	C	N	O	S	0	0
			769	483	144	138	4		

- Molecule 23 is a protein called 40S RIBOSOMAL PROTEIN S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	V	81	Total	C	N	O	S	0	0
			617	380	114	118	5		

- Molecule 24 is a protein called 40S RIBOSOMAL PROTEIN S15A.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	W	129	Total	C	N	O	S	0	0
			1034	659	193	176	6		

- Molecule 25 is a protein called 40S RIBOSOMAL PROTEIN S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	X	139	Total	C	N	O	S	0	0
			1080	682	214	181	3		

- Molecule 26 is a protein called 40S RIBOSOMAL PROTEIN S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Y	125	Total	C	N	O	S	0	0
			1015	642	199	169	5		

- Molecule 27 is a protein called 40S RIBOSOMAL PROTEIN S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Z	73	Total	C	N	O	S	0	0
			585	374	108	102	1		

- Molecule 28 is a protein called 40S RIBOSOMAL PROTEIN S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	a	97	Total	C	N	O	S	0	0
			774	481	160	128	5		

- Molecule 29 is a protein called 40S RIBOSOMAL PROTEIN S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	b	80	Total	C	N	O	S	0	0
			625	391	116	111	7		

- Molecule 30 is a protein called 40S RIBOSOMAL PROTEIN S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	c	61	Total	C	N	O	S	0	0
			480	291	96	91	2		

- Molecule 31 is a protein called 40S RIBOSOMAL PROTEIN S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	d	51	Total	C	N	O	S	0	0
			427	269	87	66	5		

- Molecule 32 is a protein called 40S RIBOSOMAL PROTEIN S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	e	55	Total	C	N	O	S	0	0
			437	272	96	68	1		

- Molecule 33 is a protein called UBIQUITIN-40S RIBOSOMAL PROTEIN S27A.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	f	73	Total	C	N	O	S	0	0
			601	379	115	100	7		

- Molecule 34 is a protein called GUANINE NUCLEOTIDE-BINDING PROTEIN SUBUNIT BETA-2-LIKE 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	g	314	Total	C	N	O	S	0	0
			2440	1537	425	466	12		

- Molecule 35 is a RNA chain called HCV-IRES.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	z	264	Total	C	N	O	P	0	0
			5637	2512	1009	1852	264		

- Molecule 36 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
36	X	1	Total	Mg	0
			1	1	
36	1	72	Total	Mg	0
			72	72	
36	D	1	Total	Mg	0
			1	1	

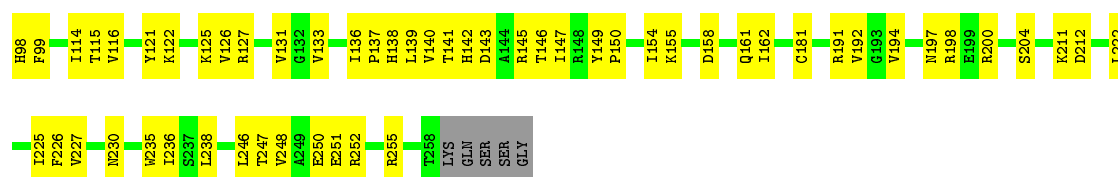
- Molecule 37 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
37	a	1	Total	Zn	0
			1	1	
37	d	1	Total	Zn	0
			1	1	

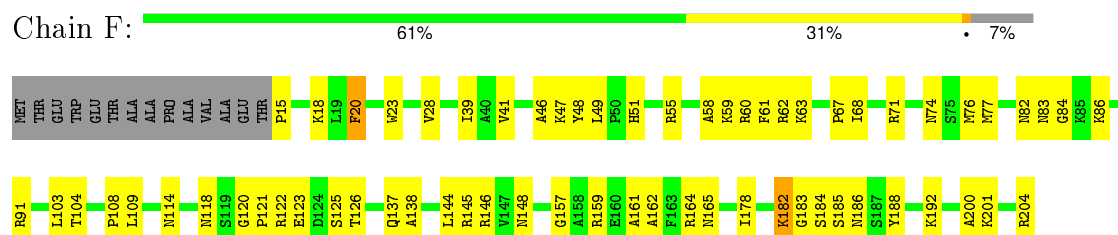
• Molecule 2: 40S RIBOSOMAL PROTEIN SA

Category	Percentage
Very bad	49%
Bad	23%
Good	27%

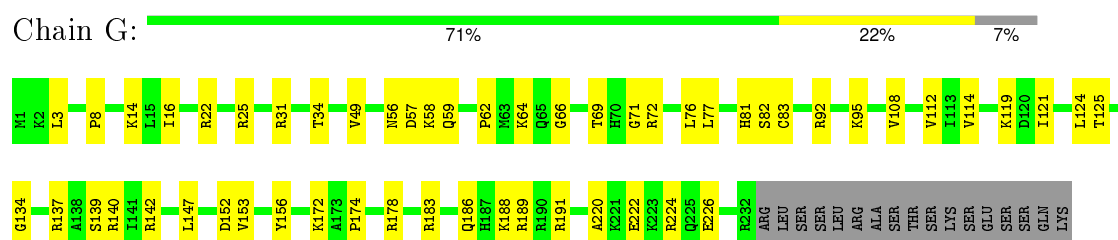


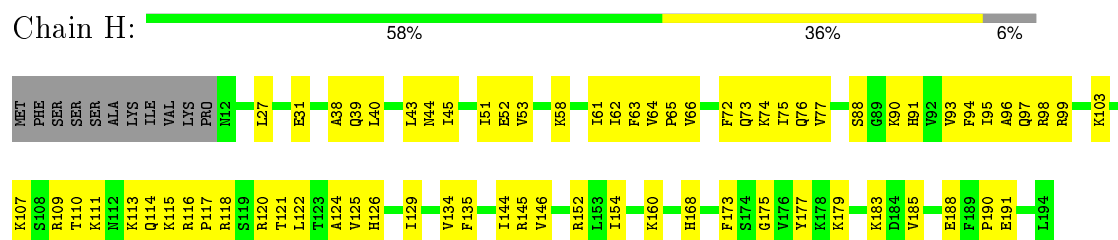
• Molecule 7: 40S RIBOSOMAL PROTEIN S5



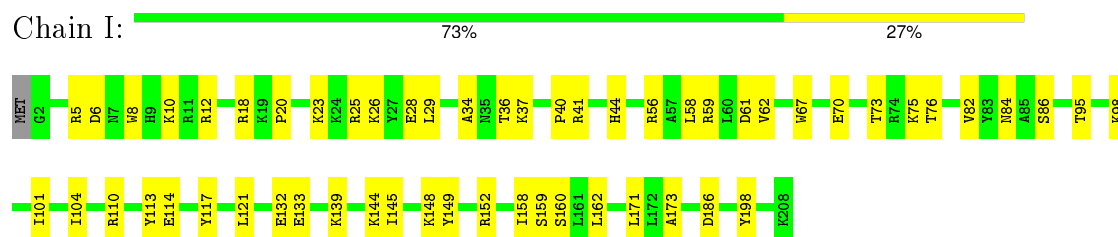
• Molecule 8: 40S RIBOSOMAL PROTEIN S6



• Molecule 9: 40S RIBOSOMAL PROTEIN S7



• Molecule 10: 40S RIBOSOMAL PROTEIN S8

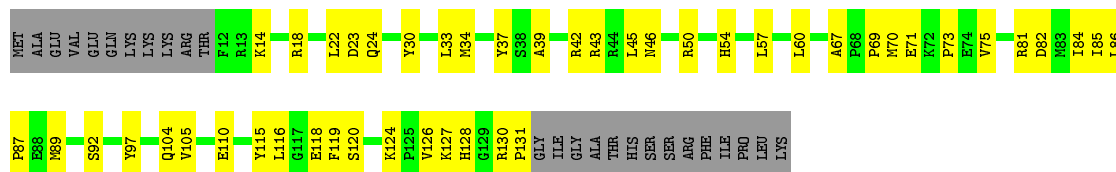


• Molecule 11: 40S RIBOSOMAL PROTEIN S9

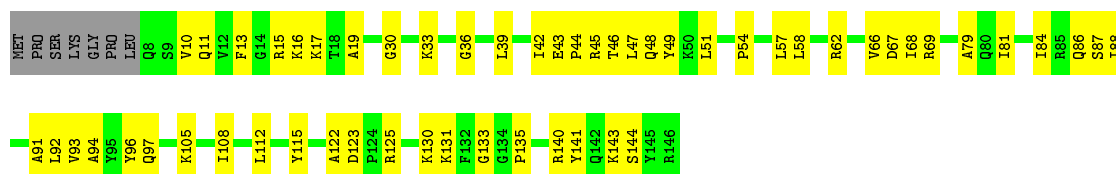




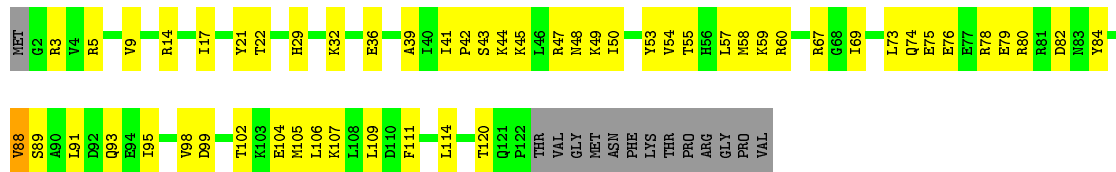
• Molecule 17: 40S RIBOSOMAL PROTEIN S15



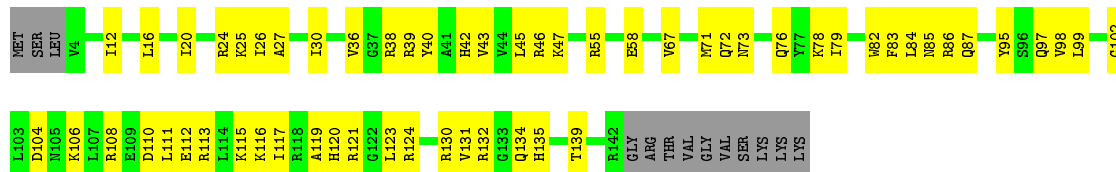
• Molecule 18: 40S RIBOSOMAL PROTEIN S16



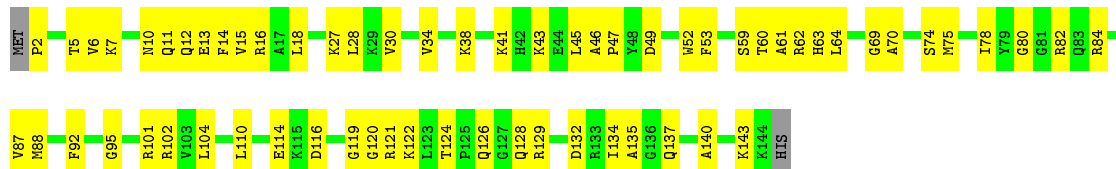
• Molecule 19: 40S RIBOSOMAL PROTEIN S17



• Molecule 20: 40S RIBOSOMAL PROTEIN S18




• Molecule 21: 40S RIBOSOMAL PROTEIN S19



Chain a:  75% 8% 16%




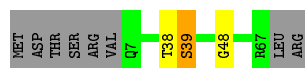
- Molecule 29: 40S RIBOSOMAL PROTEIN S27

Chain b:  90% 5%




- Molecule 30: 40S RIBOSOMAL PROTEIN S28

Chain c:  84% 12%




- Molecule 31: 40S RIBOSOMAL PROTEIN S29

Chain d:  91% 9%



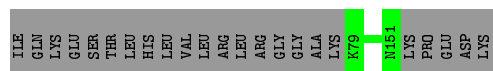
- Molecule 32: 40S RIBOSOMAL PROTEIN S30

Chain e:  92% 7%



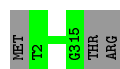
- Molecule 33: UBIQUITIN-40S RIBOSOMAL PROTEIN S27A

Chain f:  47% 53%

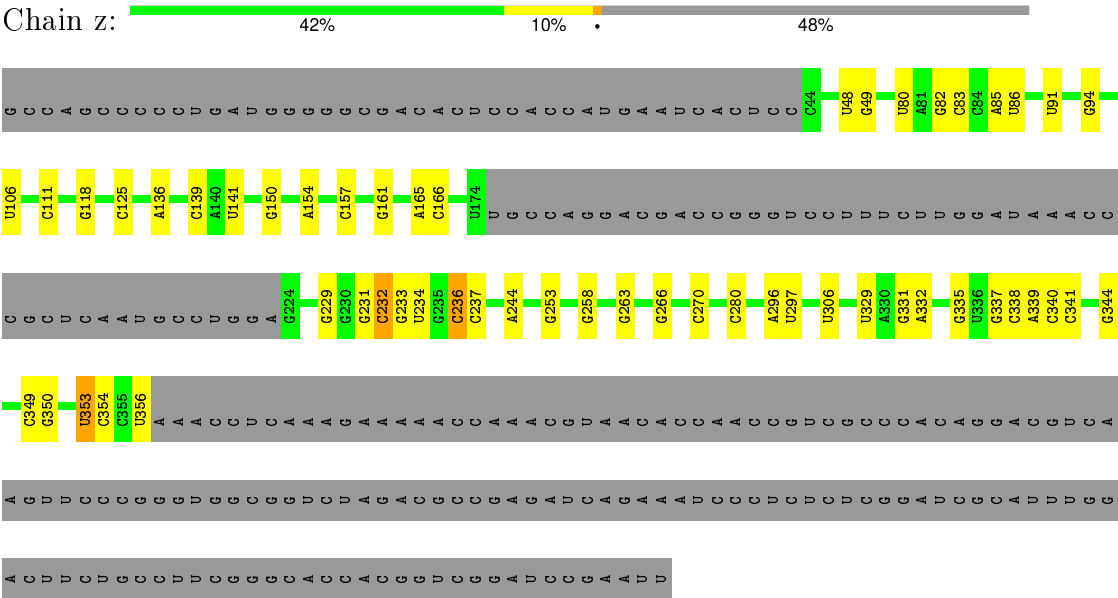


- Molecule 34: GUANINE NUCLEOTIDE-BINDING PROTEIN SUBUNIT BETA-2-LIKE 1

Chain g:  99%



- Molecule 35: HCV-IRES



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	CTFFIND3, Not provided	Depositor
Microscope	OTHER	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	4500	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON II (4K X 4K)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	1	0.19	1/40766 (0.0%)	0.78	23/63532 (0.0%)
10	I	0.24	0/1725	0.44	0/2298
11	J	0.23	0/1520	0.40	0/2030
12	K	0.25	0/851	0.48	0/1147
13	L	0.24	0/1281	0.49	0/1710
14	M	0.24	0/941	0.42	0/1264
15	N	0.23	0/1226	0.44	0/1649
16	O	0.25	0/1029	0.50	0/1380
17	P	0.24	0/1019	0.49	0/1361
18	Q	0.24	0/1126	0.49	0/1506
19	R	0.25	0/997	0.48	0/1338
2	A	0.25	0/1741	0.46	0/2366
20	S	0.24	0/1172	0.44	0/1570
21	T	0.25	0/1131	0.44	0/1515
22	U	0.22	0/778	0.43	0/1045
23	V	0.24	0/623	0.41	0/833
24	W	0.24	0/1051	0.44	0/1406
25	X	0.24	0/1097	0.44	0/1464
26	Y	0.24	0/1032	0.43	0/1371
27	Z	0.24	0/591	0.49	0/794
28	a	0.71	4/786 (0.5%)	1.26	6/1053 (0.6%)
29	b	0.25	0/637	0.54	0/854
3	B	0.23	0/1749	0.48	0/2340
30	c	1.01	1/482 (0.2%)	1.07	5/645 (0.8%)
31	d	0.27	0/437	0.50	0/580
32	e	0.65	3/443 (0.7%)	0.83	2/583 (0.3%)
33	f	0.24	0/613	0.48	0/811
34	g	0.24	0/2497	0.44	0/3399
35	z	0.34	4/6299 (0.1%)	0.92	24/9818 (0.2%)
4	C	0.25	0/1761	0.43	0/2379
5	D	0.25	0/1736	0.44	0/2338
6	E	0.24	0/2072	0.45	0/2793

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
7	F	0.24	0/1524	0.45	0/2048
8	G	0.24	0/1907	0.43	0/2538
9	H	0.28	0/1501	0.49	0/2009
All	All	0.25	13/86141 (0.0%)	0.69	60/125767 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
13	L	0	1
16	O	0	1
17	P	0	1
18	Q	0	1
28	a	2	1
30	c	1	0
5	D	0	1
6	E	0	1
7	F	0	1
All	All	3	8

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	c	39	SER	CA-CB	-20.82	1.21	1.52
35	z	353	U	N1-C2	-12.82	1.27	1.38
28	a	48	ALA	CA-CB	-11.41	1.28	1.52
1	1	1	U	OP3-P	-10.53	1.48	1.61
28	a	44	ILE	CA-CB	-9.59	1.32	1.54

The worst 5 of 60 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	a	48	ALA	CB-CA-C	29.24	153.96	110.10
30	c	39	SER	CB-CA-C	18.56	145.36	110.10
35	z	234	U	O5'-P-OP1	-16.34	90.99	105.70
35	z	353	U	N3-C4-O4	-16.19	108.06	119.40
35	z	234	U	P-O5'-C5'	15.32	145.42	120.90

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
28	a	44	ILE	CA
28	a	48	ALA	CA
30	c	39	SER	CA

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	D	76	ARG	Peptide
6	E	92	ILE	Peptide
7	F	20	PHE	Peptide
13	L	15	THR	Peptide
16	O	141	ARG	Peptide

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	1	36456	0	18413	792	0
2	A	1704	0	1704	68	0
3	B	1722	0	1793	60	0
4	C	1724	0	1808	59	0
5	D	1709	0	1803	34	0
6	E	2031	0	2138	74	0
7	F	1502	0	1556	53	0
8	G	1884	0	2044	38	0
9	H	1479	0	1564	98	0
10	I	1696	0	1785	50	0
11	J	1495	0	1615	50	0
12	K	827	0	854	40	0
13	L	1258	0	1334	36	0
14	M	931	0	961	33	0
15	N	1202	0	1289	37	0
16	O	1016	0	1039	60	0
17	P	999	0	1046	35	0
18	Q	1109	0	1174	50	0
19	R	985	0	1035	45	0
20	S	1154	0	1210	49	0
21	T	1112	0	1146	52	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	U	769	0	837	13	0
23	V	617	0	622	14	0
24	W	1034	0	1080	31	0
25	X	1080	0	1147	37	0
26	Y	1015	0	1086	28	0
27	Z	585	0	640	45	0
28	a	774	0	819	0	0
29	b	625	0	646	0	0
30	c	480	0	502	0	0
31	d	427	0	428	0	0
32	e	437	0	483	0	0
33	f	601	0	622	0	0
34	g	2440	0	2396	0	0
35	z	5637	0	2849	0	0
36	1	72	0	0	0	0
36	D	1	0	0	0	0
36	X	1	0	0	0	0
37	a	1	0	0	0	0
37	d	1	0	0	0	0
All	All	80592	0	61468	1693	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 16.

The worst 5 of 1693 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)
9:H:52:GLU:HG3	9:H:58:LYS:CG	1.15	1.63
9:H:62:ILE:HD11	9:H:94:PHE:CE1	1.43	1.54
9:H:62:ILE:CD1	9:H:94:PHE:HE1	1.23	1.45
9:H:52:GLU:CG	9:H:58:LYS:CG	2.11	1.26
9:H:52:GLU:HG3	9:H:58:LYS:CD	1.69	1.22

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 PDB entries followed by that with respect to all EM entries.

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	
2	A	213/295 (72%)	202 (95%)	11 (5%)	0	100	100
3	B	210/264 (80%)	182 (87%)	26 (12%)	2 (1%)	19	64
4	C	220/293 (75%)	209 (95%)	9 (4%)	2 (1%)	21	65
5	D	218/243 (90%)	206 (94%)	11 (5%)	1 (0%)	34	76
6	E	255/263 (97%)	244 (96%)	11 (4%)	0	100	100
7	F	188/204 (92%)	165 (88%)	22 (12%)	1 (0%)	34	76
8	G	230/249 (92%)	221 (96%)	9 (4%)	0	100	100
9	H	181/194 (93%)	165 (91%)	16 (9%)	0	100	100
10	I	205/208 (99%)	186 (91%)	19 (9%)	0	100	100
11	J	177/194 (91%)	163 (92%)	13 (7%)	1 (1%)	30	73
12	K	96/165 (58%)	90 (94%)	4 (4%)	2 (2%)	9	51
13	L	151/158 (96%)	142 (94%)	8 (5%)	1 (1%)	26	70
14	M	118/132 (89%)	111 (94%)	7 (6%)	0	100	100
15	N	147/151 (97%)	131 (89%)	16 (11%)	0	100	100
16	O	134/151 (89%)	119 (89%)	13 (10%)	2 (2%)	13	57
17	P	118/145 (81%)	107 (91%)	10 (8%)	1 (1%)	24	68
18	Q	137/146 (94%)	132 (96%)	5 (4%)	0	100	100
19	R	119/135 (88%)	108 (91%)	9 (8%)	2 (2%)	11	55
20	S	137/152 (90%)	125 (91%)	12 (9%)	0	100	100
21	T	141/145 (97%)	135 (96%)	6 (4%)	0	100	100
22	U	95/119 (80%)	94 (99%)	1 (1%)	0	100	100
23	V	79/83 (95%)	77 (98%)	1 (1%)	1 (1%)	15	59
24	W	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
25	X	137/143 (96%)	128 (93%)	9 (7%)	0	100	100
26	Y	123/133 (92%)	118 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	Z	71/125 (57%)	64 (90%)	7 (10%)	0	100	100
28	a	95/115 (83%)	78 (82%)	10 (10%)	7 (7%)	1	21
29	b	78/84 (93%)	67 (86%)	7 (9%)	4 (5%)	2	31
30	c	59/69 (86%)	48 (81%)	10 (17%)	1 (2%)	11	55
31	d	49/56 (88%)	43 (88%)	6 (12%)	0	100	100
32	e	53/59 (90%)	49 (92%)	4 (8%)	0	100	100
33	f	71/156 (46%)	66 (93%)	5 (7%)	0	100	100
34	g	312/317 (98%)	298 (96%)	14 (4%)	0	100	100
All	All	4744/5476 (87%)	4395 (93%)	321 (7%)	28 (1%)	34	73

5 of 28 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	O	62	VAL
23	V	42	VAL
28	a	92	ARG
28	a	94	ASP
29	b	74	THR

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 PDB entries followed by that with respect to all EM entries.

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	
2	A	180/243 (74%)	180 (100%)	0	100	100
3	B	193/231 (84%)	192 (100%)	1 (0%)	92	96
4	C	188/225 (84%)	188 (100%)	0	100	100
5	D	183/202 (91%)	183 (100%)	0	100	100
6	E	220/225 (98%)	220 (100%)	0	100	100
7	F	160/170 (94%)	159 (99%)	1 (1%)	90	95
8	G	202/218 (93%)	202 (100%)	0	100	100
9	H	164/174 (94%)	164 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	I	179/180 (99%)	179 (100%)	0	100	100
11	J	160/168 (95%)	160 (100%)	0	100	100
12	K	89/136 (65%)	89 (100%)	0	100	100
13	L	138/142 (97%)	138 (100%)	0	100	100
14	M	102/108 (94%)	102 (100%)	0	100	100
15	N	130/131 (99%)	130 (100%)	0	100	100
16	O	106/119 (89%)	105 (99%)	1 (1%)	84	92
17	P	109/130 (84%)	109 (100%)	0	100	100
18	Q	115/121 (95%)	115 (100%)	0	100	100
19	R	110/122 (90%)	110 (100%)	0	100	100
20	S	121/132 (92%)	121 (100%)	0	100	100
21	T	113/115 (98%)	113 (100%)	0	100	100
22	U	90/107 (84%)	90 (100%)	0	100	100
23	V	65/67 (97%)	65 (100%)	0	100	100
24	W	112/113 (99%)	112 (100%)	0	100	100
25	X	111/115 (96%)	111 (100%)	0	100	100
26	Y	107/115 (93%)	107 (100%)	0	100	100
27	Z	65/103 (63%)	64 (98%)	1 (2%)	72	89
28	a	84/98 (86%)	81 (96%)	3 (4%)	42	76
29	b	72/76 (95%)	71 (99%)	1 (1%)	74	89
30	c	54/62 (87%)	53 (98%)	1 (2%)	65	86
31	d	45/49 (92%)	45 (100%)	0	100	100
32	e	44/48 (92%)	44 (100%)	0	100	100
33	f	66/140 (47%)	66 (100%)	0	100	100
34	g	272/275 (99%)	272 (100%)	0	100	100
All	All	4149/4660 (89%)	4140 (100%)	9 (0%)	95	97

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
28	a	15	ARG
30	c	39	SER
28	a	89	ARG

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Mol	Chain	Res	Type
16	O	150	ARG
28	a	46	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 62 such sidechains are listed below:

Mol	Chain	Res	Type
12	K	42	ASN
17	P	35	GLN
34	g	20	GLN
15	N	62	GLN
17	P	103	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	1700/1869 (90%)	286 (16%)	9 (0%)
35	z	262/504 (51%)	52 (19%)	0
All	All	1962/2373 (82%)	338 (17%)	9 (0%)

5 of 338 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	4	C
1	1	33	G
1	1	41	G
1	1	42	A
1	1	49	C

5 of 9 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	797	C
1	1	1756	C
1	1	1211	G
1	1	369	C
1	1	869	A

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 ⓘ

Of 76 ligands modelled in this entry, 76 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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.