Full wwPDB X-ray Structure Validation Report (i)

Oct 4, 2023 – 06:26 PM EDT

PDB ID	:	6U8K
Title	:	Crystal structure of hepatitis C virus IRES junction IIIabc in complex with Fab HCV3
Authors	:	Koirala, D.; Lewicka, A.; Koldobskaya, Y.; Huang, H.; Piccirilli, J.A.
Deposited on	:	2019-09-05
Resolution	:	2.75 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 (i) 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 (1)) were used in the production of this report:

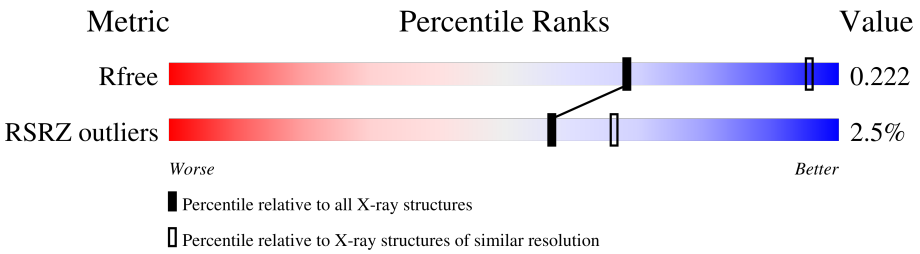
MolProbity	:	FAILED
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1235 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 14455 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 RNA chain called JIIIabc RNA (68-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	A	68	1460	650	270	472	68	0	0	0
1	B	68	1460	650	270	472	68	0	0	0
1	C	68	1460	650	270	472	68	0	0	0

- Molecule 2 is a protein called Heavy chain of Fab HCV3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	D	222	1661	1046	283	327	5	0	0	0
2	F	222	1661	1046	283	327	5	0	0	0
2	H	222	1661	1046	283	327	5	0	0	0

- Molecule 3 is a protein called Light chain of Fab HCV3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	E	215	1644	1025	275	338	6	0	0	0
3	G	215	1644	1025	275	338	6	0	0	0
3	L	215	1644	1025	275	338	6	0	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	20	20	20	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	B	18	18	18	0	0
			Total	O		
4	C	5	5	5	0	0
			Total	O		
4	D	19	19	19	0	0
			Total	O		
4	E	16	16	16	0	0
			Total	O		
4	F	14	14	14	0	0
			Total	O		
4	G	12	12	12	0	0
			Total	O		
4	H	26	26	26	0	0
			Total	O		
4	L	30	30	30	0	0

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3 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α, β, γ	173.29Å 173.29Å 140.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	173.29 – 2.75 173.29 – 2.75	Depositor EDS
% Data completeness (in resolution range)	98.5 (173.29-2.75) 94.3 (173.29-2.75)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.95 (at 2.73Å)	Xtriage
Refinement program	PHENIX (1.14_3260)	Depositor
R, R_{free}	0.186 , 0.222 0.187 , 0.222	Depositor DCC
R_{free} test set	2006 reflections (1.89%)	wwPDB-VP
Wilson B-factor (Å^2)	59.3	Xtriage
Anisotropy	0.163	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 64.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	0.177 for h,-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	14455	wwPDB-VP
Average B, all atoms (Å^2)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.93% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

4 Model quality (i)

4.1 Standard geometry (i)

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4.2 Too-close contacts (i)

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4.3 Torsion angles (i)

4.3.1 Protein backbone (i)

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4.3.2 Protein sidechains (i)

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4.3.3 RNA (i)

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains (i)

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

4.5 Carbohydrates (i)

There are no monosaccharides in this entry.

4.6 Ligand geometry (i)

There are no ligands in this entry.

4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

5 Fit of model and data (i)

5.1 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	68/68 (100%)	-0.11	0	100	100	62, 83, 130, 156	0
1	B	68/68 (100%)	-0.20	0	100	100	57, 83, 112, 136	0
1	C	68/68 (100%)	-0.18	0	100	100	70, 108, 198, 232	0
2	D	222/232 (95%)	0.69	8 (3%)	42	51	40, 59, 100, 175	0
2	F	222/232 (95%)	0.75	8 (3%)	42	51	42, 66, 107, 178	0
2	H	222/232 (95%)	0.68	6 (2%)	54	63	41, 58, 90, 150	0
3	E	215/215 (100%)	0.55	3 (1%)	75	82	37, 62, 99, 173	0
3	G	215/215 (100%)	0.61	9 (4%)	36	43	47, 77, 110, 147	0
3	L	215/215 (100%)	0.58	4 (1%)	66	75	41, 59, 91, 161	0
All	All	1515/1545 (98%)	0.54	38 (2%)	57	66	37, 65, 119, 232	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	142	THR	10.4
2	F	143	SER	6.5
2	D	142	THR	5.4
2	F	107	TYR	4.5
3	G	215	CYS	4.3
2	D	107	TYR	4.0
2	H	143	SER	3.9
2	H	138	SER	3.8
2	H	139	SER	3.7
3	G	30	VAL	3.7
2	F	144	GLY	3.6
3	G	20	VAL	3.5
2	D	139	SER	3.2
3	G	16	VAL	3.0
3	G	101	GLN	2.9

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Mol	Chain	Res	Type	RSRZ
2	D	144	GLY	2.8
3	L	155	LEU	2.6
2	D	140	LYS	2.5
3	G	3	ILE	2.5
2	F	139	SER	2.5
2	H	142	THR	2.4
2	F	145	GLY	2.4
3	E	214	GLU	2.3
3	G	76	ILE	2.3
2	H	151	CYS	2.2
2	D	143	SER	2.2
2	F	186	LEU	2.2
3	L	215	CYS	2.2
2	D	51	VAL	2.1
2	F	21	LEU	2.1
3	G	22	ILE	2.1
3	G	105	VAL	2.1
3	L	214	GLU	2.1
3	L	150	LYS	2.1
2	D	26	ALA	2.1
2	H	6	GLN	2.0
3	E	146	LYS	2.0
3	E	134	VAL	2.0

5.2 Non-standard residues in protein, DNA, RNA chains (i)

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

5.3 Carbohydrates (i)

There are no monosaccharides in this entry.

5.4 Ligands (i)

There are no ligands in this entry.

5.5 Other polymers (i)

There are no such residues in this entry.