



wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2020 – 02:01 am BST

PDB ID : 5JZE
Title : Erve virus viral OTU domain protease in complex with mouse ISG15
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Deposited on : 2016-05-16
Resolution : 2.47 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
Mogul : 1.8.5 (274361), CSD as541be (2020)
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

i

X-RAY DIFFRACTION

A.



R_{free}	130704	5857 (2.50-2.46)
Clashscore	141614	6594 (2.50-2.46)
Ramachandran outliers	138981	6469 (2.50-2.46)
Sidechain outliers	138945	6471 (2.50-2.46)
RSRZ outliers	127900	5738 (2.50-2.46)

that have poor fit to the electron density. The numeric value is given above the bar.

1	B	76	<div><div></div><div></div></div> 95%5%
1	D	76	<div><div></div><div></div></div> 82%18%
2	A	159	<div><div></div><div></div><div></div></div> 89%9%•
2	C	159	<div><div></div><div></div><div></div></div> 87%12%••

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4142 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.

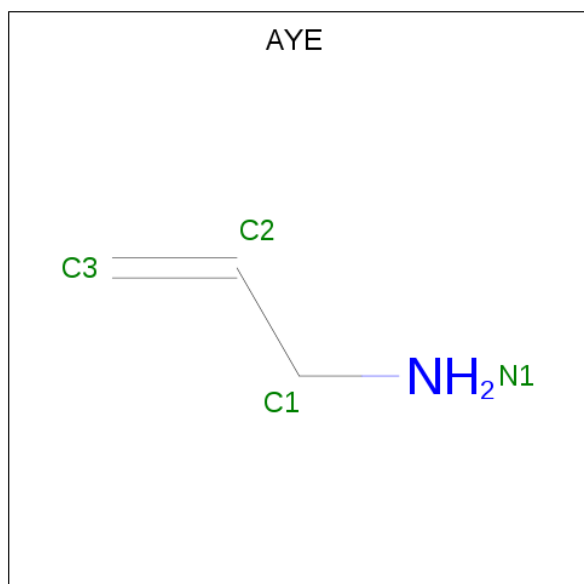
- Molecule 1 is a protein called Ubiquitin-like protein ISG15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	76	Total	C	N	O	S	0	1	0
			637	404	115	116	2			
1	D	76	Total	C	N	O	S	0	0	0
			631	400	114	115	2			

- Molecule 2 is a protein called RNA-dependent RNA polymerase.

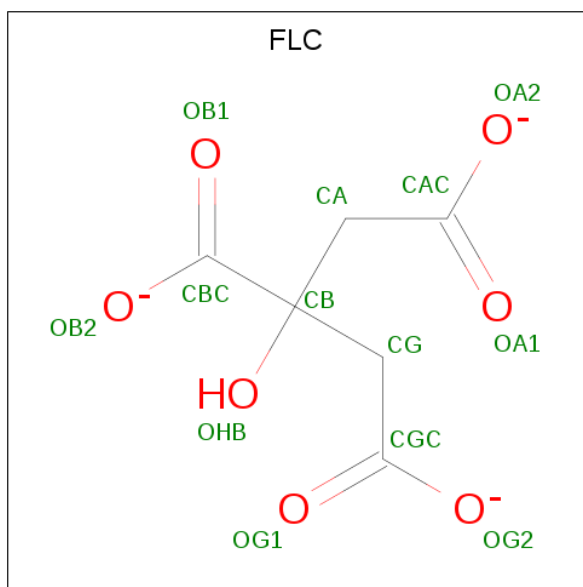
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	159	Total	C	N	O	S	0	1	0
			1281	816	219	242	4			
2	C	158	Total	C	N	O	S	0	2	0
			1280	815	219	242	4			

- Molecule 3 is prop-2-en-1-amine (three-letter code: AYE) (formula: C₃H₇N).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	N	0	0
			4	3	1		
3	D	1	Total	C	N	0	0
			4	3	1		

- Molecule 4 is CITRATE ANION (three-letter code: FLC) (formula: $C_6H_5O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			13	6	7		
4	A	1	Total	C	O	0	0
			13	6	7		
4	D	1	Total	C	O	0	0
			13	6	7		
4	C	1	Total	C	O	0	0
			13	6	7		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	48	Total	O	0	0
			48	48		
5	A	81	Total	O	0	0
			81	81		
5	D	40	Total	O	0	0
			40	40		
5	C	84	Total	O	0	0
			84	84		

3 Residue-property plots [i](#)


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: Ubiquitin-like protein ISG15

Chain B:  95% 5%



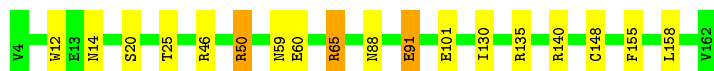
- Molecule 1: Ubiquitin-like protein ISG15

Chain D:  82% 18%




- Molecule 2: RNA-dependent RNA polymerase

Chain A:  89% 9% .



- Molecule 2: RNA-dependent RNA polymerase

Chain C:  87% 12% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	65.99 Å 65.99 Å 121.99 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	65.99 – 2.47 44.79 – 2.47	Depositor EDS
% Data completeness (in resolution range)	100.0 (65.99-2.47) 100.0 (44.79-2.47)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.71 (at 2.48 Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.174 , 0.226 0.180 , 0.232	Depositor DCC
R_{free} test set	986 reflections (5.27%)	wwPDB-VP
Wilson B-factor (Å ²)	23.8	Xtriage
Anisotropy	0.227	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 1.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.478 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4142	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.07% 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](#)

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

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	B	0.66	0/652	0.88	0/875
1	D	0.75	0/643	0.88	0/863
2	A	0.71	0/1308	0.91	6/1773 (0.3%)
2	C	0.70	0/1310	0.91	3/1775 (0.2%)
All	All	0.71	0/3913	0.90	9/5286 (0.2%)

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	C	65	ARG	NE-CZ-NH2	-10.03	115.28	120.30
2	A	65	ARG	NE-CZ-NH2	-8.12	116.24	120.30
2	A	50	ARG	NE-CZ-NH2	-7.80	116.40	120.30
2	C	65	ARG	NE-CZ-NH1	6.95	123.78	120.30
2	A	50	ARG	NE-CZ-NH1	6.59	123.59	120.30

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	B	637	0	647	4	0
1	D	631	0	639	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1281	0	1246	10	0
2	C	1280	0	1245	13	0
3	B	4	0	4	0	0
3	D	4	0	4	1	0
4	A	13	0	5	1	0
4	B	13	0	5	2	0
4	C	13	0	5	1	0
4	D	13	0	5	0	0
5	A	81	0	0	2	0
5	B	48	0	0	1	0
5	C	84	0	0	1	0
5	D	40	0	0	1	0
All	All	4142	0	3805	37	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.

The worst 5 of 37 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:96:VAL:HG13	1:D:135:LEU:HD13	1.70	0.74
2:A:140[A]:ARG:HG3	5:A:342:HOH:O	1.93	0.68
1:B:90:HIS:HB2	4:B:202:FLC:HA1	1.75	0.67
1:D:129:MET:CE	1:D:146:VAL:HG13	2.30	0.60
2:C:46:ARG:HB3	2:C:58:SER:HB2	1.87	0.56

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	B	75/76 (99%)	75 (100%)	0	0	100	100
1	D	74/76 (97%)	72 (97%)	2 (3%)	0	100	100
2	A	158/159 (99%)	152 (96%)	6 (4%)	0	100	100
2	C	158/159 (99%)	155 (98%)	3 (2%)	0	100	100
All	All	465/470 (99%)	454 (98%)	11 (2%)	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	
1	B	72/71 (101%)	71 (99%)	1 (1%)	67	84
1	D	71/71 (100%)	69 (97%)	2 (3%)	43	67
2	A	137/136 (101%)	134 (98%)	3 (2%)	52	75
2	C	137/136 (101%)	135 (98%)	2 (2%)	65	83
All	All	417/414 (101%)	409 (98%)	8 (2%)	57	78

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	158	LEU
2	C	161	ARG
1	D	133	GLU
2	A	91	GLU
1	D	103	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

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](#)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	FLC	B	202	-	3,12,12	0.85	0	3,17,17	0.97	0
3	AYE	D	201	1,2	3,3,3	0.28	0	1,2,2	2.01	1 (100%)
4	FLC	C	201	-	3,12,12	1.24	0	3,17,17	2.08	2 (66%)
3	AYE	B	201	1,2	3,3,3	0.25	0	1,2,2	1.67	0
4	FLC	D	202	-	3,12,12	0.61	0	3,17,17	1.80	1 (33%)
4	FLC	A	201	-	3,12,12	0.91	0	3,17,17	2.26	2 (66%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FLC	B	202	-	-	3/6/16/16	-
3	AYE	D	201	1,2	-	0/1/1/1	-
4	FLC	C	201	-	-	3/6/16/16	-
3	AYE	B	201	1,2	-	0/1/1/1	-
4	FLC	D	202	-	-	3/6/16/16	-
4	FLC	A	201	-	-	3/6/16/16	-

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	C	201	FLC	CB-CG-CGC	-2.82	110.47	114.98
4	A	201	FLC	CB-CG-CGC	-2.81	110.49	114.98
4	A	201	FLC	CB-CA-CAC	-2.32	111.26	114.98
4	C	201	FLC	CB-CA-CAC	-2.25	111.39	114.98
4	D	202	FLC	CG-CB-CA	2.21	115.23	109.33

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	202	FLC	CAC-CA-CB-CBC
4	B	202	FLC	CAC-CA-CB-CG
4	B	202	FLC	CAC-CA-CB-OHB
4	D	202	FLC	CA-CB-CG-CGC
4	D	202	FLC	CBC-CB-CG-CGC

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	202	FLC	2	0
3	D	201	AYE	1	0
4	C	201	FLC	1	0
4	A	201	FLC	1	0

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 [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	B	76/76 (100%)	-1.09	0 100 100	15, 23, 34, 65	0
1	D	76/76 (100%)	-1.04	0 100 100	15, 23, 35, 60	0
2	A	159/159 (100%)	-1.00	0 100 100	13, 21, 43, 65	0
2	C	158/159 (99%)	-1.01	0 100 100	14, 21, 40, 63	0
All	All	469/470 (99%)	-1.03	0 100 100	13, 22, 39, 65	0

There are no RSRZ outliers to report.

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 [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	FLC	A	201	13/13	0.86	0.15	55,64,75,77	0
4	FLC	D	202	13/13	0.90	0.15	40,53,57,59	0
4	FLC	B	202	13/13	0.92	0.15	50,57,60,60	0
4	FLC	C	201	13/13	0.92	0.12	53,57,66,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	AYE	B	201	4/4	0.97	0.10	16,16,17,17	0
3	AYE	D	201	4/4	0.98	0.09	15,16,16,16	0

6.5 Other polymers [i](#)

There are no such residues in this entry.