



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 30, 2017 – 12:13 PM EST

PDB ID : 1I9W
Title : CRYSTAL STRUCTURE OF THE FUSION GLYCOPROTEIN E1 FROM
SEMLIKI FOREST VIRUS
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Wengler, G.; Rey, F.A.
Deposited on : 2001-03-21
Resolution : 3.00 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

<http://wwpdb.org/validation/2016/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	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

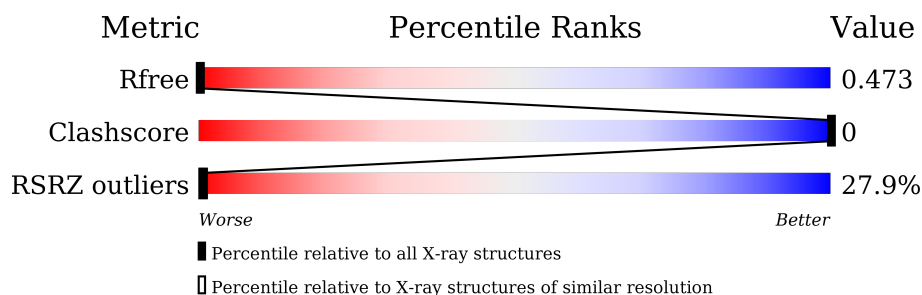
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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. 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	390	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 369 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.

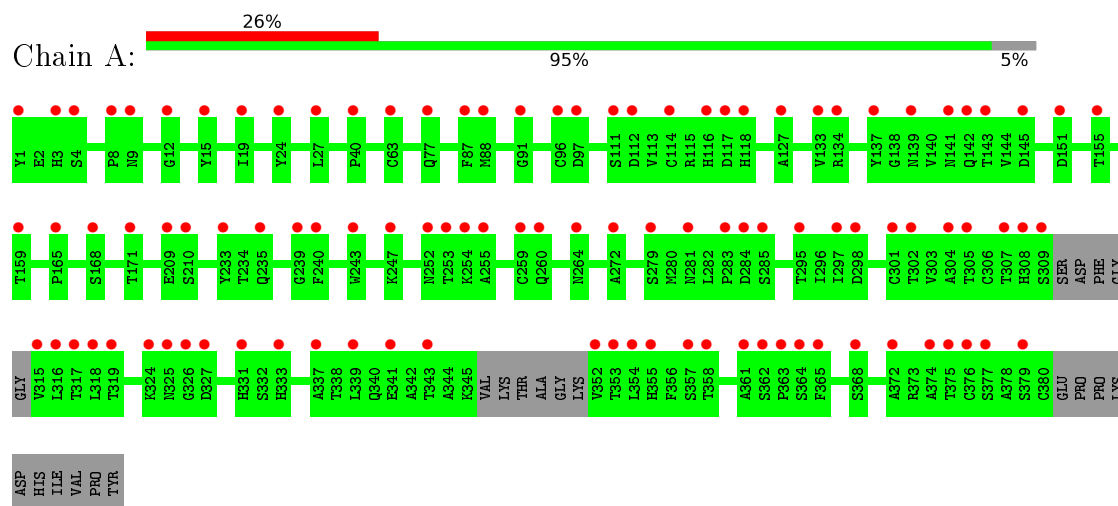
- Molecule 1 is a protein called FUSION PROTEIN E1.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
1	A	369	Total 369	C 369	0	0	369

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 errors 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: FUSION PROTEIN E1



4 Data and refinement statistics

Property	Value	Source
Space group	P 64 2 2	Depositor
Cell constants a, b, c, α , β , γ	79.46 Å 79.46 Å 334.76 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	15.00 – 3.00 39.27 – 2.69	Depositor EDS
% Data completeness (in resolution range)	86.5 (15.00-3.00) 83.7 (39.27-2.69)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.00 (at 2.69 Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.275 , 0.344 0.467 , 0.473	Depositor DCC
R_{free} test set	1161 reflections (10.11%)	DCC
Wilson B-factor (Å ²)	69.5	Xtriage
Anisotropy	0.761	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 207.9	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	0.63	EDS
Total number of atoms	369	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.21% 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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

There are no bond length outliers.

There are no bond angle outliers.

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	A	369	0	0	0	0
All	All	369	0	0	0	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 0.

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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 [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	A	369/390 (94%)	2.18	103 (27%) 1 0	15, 63, 99, 99	0

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	319	THR	34.1
1	A	304	ALA	22.1
1	A	353	THR	20.5
1	A	209	GLU	20.1
1	A	97	ASP	18.4
1	A	139	ASN	17.1
1	A	376	CYS	15.9
1	A	352	VAL	15.6
1	A	264	ASN	15.6
1	A	243	TRP	14.2
1	A	87	PHE	13.9
1	A	302	THR	13.4
1	A	357	SER	13.4
1	A	337	ALA	11.7
1	A	252	ASN	11.2
1	A	284	ASP	11.2
1	A	355	HIS	11.1
1	A	114	CYS	10.5
1	A	15	TYR	10.3
1	A	116	HIS	10.2
1	A	295	THR	10.0
1	A	333	HIS	9.9
1	A	24	TYR	9.7
1	A	364	SER	9.7
1	A	331	HIS	9.6
1	A	372	ALA	9.3
1	A	233	TYR	9.1

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Mol	Chain	Res	Type	RSRZ
1	A	324	LYS	8.9
1	A	317	THR	8.4
1	A	318	LEU	8.3
1	A	343	THR	8.3
1	A	305	THR	8.3
1	A	283	PRO	8.2
1	A	316	LEU	8.2
1	A	168	SER	8.1
1	A	117	ASP	8.1
1	A	77	GLN	8.1
1	A	4	SER	8.0
1	A	374	ALA	7.0
1	A	111	SER	7.0
1	A	365	PHE	6.8
1	A	272	ALA	6.8
1	A	326	GLY	6.8
1	A	363	PRO	6.8
1	A	255	ALA	6.7
1	A	141	ASN	6.6
1	A	379	SER	6.6
1	A	361	ALA	6.4
1	A	247	LYS	6.3
1	A	253	THR	6.2
1	A	308	HIS	5.7
1	A	155	THR	5.7
1	A	260	GLN	5.7
1	A	327	ASP	5.5
1	A	301	CYS	5.4
1	A	91	GLY	5.3
1	A	375	THR	5.3
1	A	325	ASN	5.3
1	A	354	LEU	4.9
1	A	88	MET	4.8
1	A	143	THR	4.6
1	A	307	THR	4.4
1	A	112	ASP	4.2
1	A	281	ASN	4.2
1	A	8	PRO	4.1
1	A	368	SER	4.0
1	A	235	GLN	3.9
1	A	151	ASP	3.9
1	A	171	THR	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	165	PRO	3.4
1	A	341	GLU	3.4
1	A	254	LYS	3.3
1	A	12	GLY	3.3
1	A	239	GLY	3.3
1	A	309	SER	3.2
1	A	315	VAL	3.2
1	A	279	SER	3.2
1	A	134	ARG	3.0
1	A	259	CYS	2.9
1	A	297	ILE	2.9
1	A	285	SER	2.9
1	A	27	LEU	2.8
1	A	298	ASP	2.8
1	A	358	THR	2.7
1	A	159	THR	2.7
1	A	137	TYR	2.6
1	A	40	PRO	2.6
1	A	3	HIS	2.5
1	A	210	SER	2.5
1	A	377	SER	2.4
1	A	1	TYR	2.4
1	A	118	HIS	2.4
1	A	142	GLN	2.3
1	A	362	SER	2.3
1	A	96	CYS	2.3
1	A	145	ASP	2.2
1	A	339	LEU	2.2
1	A	9	ASN	2.2
1	A	133	VAL	2.2
1	A	127	ALA	2.1
1	A	19	ILE	2.1
1	A	240	PHE	2.0
1	A	63	CYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.