



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 04:31 AM UTC

PDB ID : 8FUQ / pdb_00008fuq
Title : Crystal structure of rabies virus (strain CVS-11) P3 dimerization domain
Authors : Donnelly, C.M.; Cross, E.M.; Forwood, J.K.
Deposited on : 2023-01-18
Resolution : 1.80 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

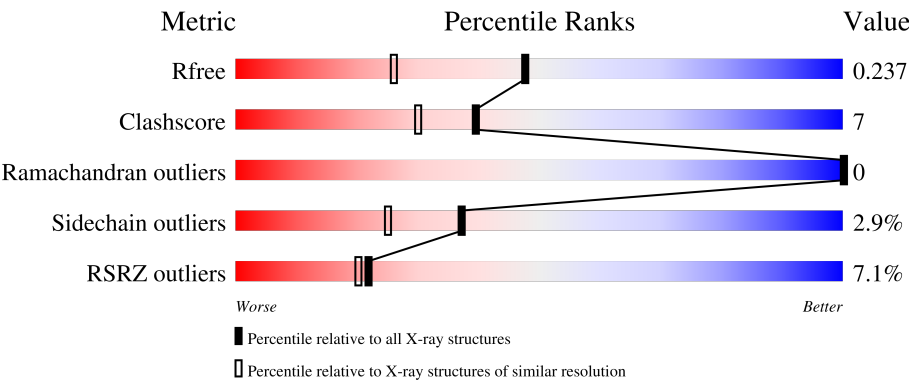
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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 of 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	119	3% 36% 7% 57%
1	B	119	3% 31% 11% 57%
1	C	119	% 38% . 58%
1	D	119	3% 32% 7% 61%
1	E	119	5% 32% 8% 59%

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Mol	Chain	Length	Quality of chain
1	F	119	 3% 34% 5% 61%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 4970 atoms, of which 2370 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 Phosphoprotein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	51	Total	C	H	N	O	S	0	1	0
			821	272	398	70	80	1			
1	B	51	Total	C	H	N	O	S	0	1	0
			831	271	410	72	77	1			
1	C	50	Total	C	H	N	O	S	0	0	0
			794	261	388	66	78	1			
1	D	47	Total	C	H	N	O	S	0	1	0
			778	252	389	65	71	1			
1	E	49	Total	C	H	N	O	S	0	0	0
			795	259	394	67	74	1			
1	F	47	Total	C	H	N	O	S	0	2	0
			782	256	391	62	72	1			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	53	SER	-	expression tag	UNP P15198
B	53	SER	-	expression tag	UNP P15198
C	53	SER	-	expression tag	UNP P15198
D	53	SER	-	expression tag	UNP P15198
E	53	SER	-	expression tag	UNP P15198
F	53	SER	-	expression tag	UNP P15198

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	30	Total	O	0	0
			30	30		
2	B	46	Total	O	0	0
			46	46		
2	C	30	Total	O	0	0
			30	30		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	29	Total 29	O 29	0	0
2	E	12	Total 12	O 12	0	0
2	F	22	Total 22	O 22	0	0

- Molecule 1: Phosphoprotein



GLU	ASP	LYS	SER	THR	GLN	THR	THR	GLY	ARG	GLU	LEU	SER	LYS	LYS	GLU	THR	THR	SER	SER	ALA	PHE	SER	GLN	ARG	GLU	SER	GLN	PRO	SER	LYS	ALA
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● Molecule 1: Phosphoprotein



SER	LYS	ARG	GLU	ASP	LEU	HIS	LEU	ASP	ASP	GLN	THR	THR	GLY	LYS	SER	GLY	SER	ASN	LEU	GLY	LYS	GLU	GLY	THR	VAL	ARG	VAL	GLY	GLY	GLY	LYS	TYR	ARG	GLU	SER	GLN	ASP	PHE	GLN	GLN	MET	ASP	GLU	GLU	GLU	GLU	D88	L91	Y96	V105	M108	F114	L115	S119	E124	I125	V126	P134	M135	P136	PRO	ARG	ARG
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SER	SER	GLU	GLU	LYS	ASP	THR	THR	GLN	THR	THR	GLY	LYS	SER	ARG	GLU	ASN	LEU	GLY	LYS	GLU	GLY	THR	THR	THR	ALA	SER	PHE	GLY	GLY	GLY	GLY	LYS	GLN	ARG	GLU	GLU	SER	GLN	ASP	PRO	SER	LYS	ALA
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● Molecule 1: Phosphoprotein



SER	LYS	ARG	LEU	HIS	LEU	ASP	ASP	GLU	LYS	SER	SER	ASN	LEU	GLY	LYS	GLU	GLY	THR	VAL	ARG	VAL	GLY	GLY	GLY	LYS	TYR	ARG	GLU	SER	GLN	ASP	PHE	GLN	GLN	MET	ASP	GLU	GLY	GLU	GLU	D88	L91	V102	V105	R109	S110	L115	G120	V126	P134	ASN	PRO	PRO	ARG	ARG	SER	SER
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GLU	ASP	LYS	SER	THR	GLN	THR	THR	GLY	ARG	GLU	LEU	SER	LYS	LYS	GLU	THR	THR	SER	SER	ALA	PHE	SER	GLN	ARG	GLU	SER	GLN	PRO	SER	LYS	ALA
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4 Data and refinement statistics

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	67.05Å 44.10Å 111.79Å 90.00° 100.44° 90.00°	Depositor
Resolution (Å)	52.51 – 1.80 52.51 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (52.51-1.80) 99.9 (52.51-1.80)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.10 (at 1.80Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.208 , 0.237 0.207 , 0.237	Depositor DCC
R_{free} test set	1499 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	24.2	Xtriage
Anisotropy	0.109	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.44 , 49.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4970	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.99% 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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.96	0/436	1.15	0/594
1	B	1.08	1/434 (0.2%)	1.30	0/592
1	C	0.99	0/414	1.13	0/562
1	D	0.94	0/400	1.19	0/542
1	E	0.92	0/410	1.22	1/558 (0.2%)
1	F	0.98	1/402 (0.2%)	1.16	1/547 (0.2%)
All	All	0.98	2/2496 (0.1%)	1.19	2/3395 (0.1%)

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
1	A	0	2
1	B	0	1
1	C	0	1
1	D	0	2
1	F	0	1
All	All	0	7

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	126	VAL	C-N	-8.50	1.22	1.33
1	B	114	PHE	C-O	-6.21	1.17	1.24

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	114	PHE	CA-C-O	-5.34	115.21	120.82
1	F	126	VAL	CA-C-O	-5.06	115.69	120.95

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	109	ARG	Sidechain
1	A	113	ARG	Sidechain
1	B	113	ARG	Sidechain
1	C	109	ARG	Sidechain
1	D	109	ARG	Sidechain
1	D	113	ARG	Sidechain
1	F	109	ARG	Sidechain

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	423	398	416	9	0
1	B	421	410	411	12	0
1	C	406	388	393	4	0
1	D	389	389	389	7	0
1	E	401	394	394	10	0
1	F	391	391	384	6	0
2	A	30	0	0	0	0
2	B	46	0	0	0	1
2	C	30	0	0	0	0
2	D	29	0	0	0	1
2	E	12	0	0	0	0
2	F	22	0	0	0	0
All	All	2600	2370	2387	32	1

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 7.

All (32) 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:E:115:LEU:HD23	1:F:105:VAL:CG1	2.22	0.69
1:A:136:PRO:HG3	1:B:133:PHE:CD2	2.29	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:115:LEU:HD23	1:F:105:VAL:HG13	1.76	0.66
1:A:104:ILE:HG22	1:A:108:MET:HE2	1.84	0.59
1:B:122:VAL:O	1:B:126:VAL:HG23	2.06	0.55
1:B:98:ASP:HB3	1:D:102:VAL:HG13	1.92	0.52
1:C:135:ASN:ND2	1:D:135:ASN:C	2.68	0.52
1:A:108:MET:HE1	1:B:114:PHE:CB	2.40	0.51
1:A:136:PRO:HG3	1:B:133:PHE:CE2	2.45	0.50
1:E:105:VAL:HG21	1:F:115:LEU:HG	1.93	0.50
1:E:115:LEU:HD23	1:F:105:VAL:HG11	1.96	0.46
1:D:118:TRP:O	1:D:122:VAL:HG23	2.16	0.45
1:A:112:GLU:HB2	1:A:117:ILE:HD11	1.98	0.45
1:A:136:PRO:HG2	1:B:89:PRO:HB2	2.00	0.44
1:C:108:MET:HE1	1:D:108:MET:HE1	2.00	0.44
1:E:96:TYR:OH	1:E:124:GLU:HG3	2.18	0.44
1:E:125:ILE:O	1:E:126:VAL:C	2.57	0.44
1:D:104:ILE:HD11	1:D:121:THR:HG21	1.98	0.44
1:A:108:MET:HE1	1:B:114:PHE:HB2	2.01	0.43
1:B:88:ASP:HB3	1:B:89:PRO:HD3	2.01	0.43
1:B:118:TRP:CE2	1:B:122:VAL:CG2	3.02	0.42
1:E:135:ASN:CB	1:E:136:PRO:HD2	2.49	0.42
1:B:102:VAL:O	1:B:105:VAL:HG12	2.19	0.42
1:C:108:MET:SD	1:D:108:MET:HE1	2.60	0.42
1:E:115:LEU:HD22	1:E:115:LEU:HA	1.82	0.42
1:F:91:LEU:HD12	1:F:91:LEU:O	2.19	0.42
1:E:105:VAL:HA	1:E:108:MET:HE2	2.02	0.41
1:A:136:PRO:HB2	1:B:89:PRO:HB3	2.03	0.40
1:A:118:TRP:CD1	1:B:101:GLY:HA3	2.56	0.40
1:C:108:MET:HE1	1:D:108:MET:CE	2.51	0.40
1:E:91:LEU:HD12	1:E:91:LEU:HA	1.81	0.40
1:F:102:VAL:HA	1:F:105:VAL:HG22	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:216:HOH:O	2:D:218:HOH:O[4_545]	2.19	0.01

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 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	50/119 (42%)	50 (100%)	0	0	100	100
1	B	50/119 (42%)	50 (100%)	0	0	100	100
1	C	48/119 (40%)	47 (98%)	1 (2%)	0	100	100
1	D	46/119 (39%)	46 (100%)	0	0	100	100
1	E	47/119 (40%)	47 (100%)	0	0	100	100
1	F	47/119 (40%)	47 (100%)	0	0	100	100
All	All	288/714 (40%)	287 (100%)	1 (0%)	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	A	50/110 (46%)	50 (100%)	0	100	100
1	B	48/110 (44%)	46 (96%)	2 (4%)	26	14
1	C	46/110 (42%)	42 (91%)	4 (9%)	9	3
1	D	45/110 (41%)	44 (98%)	1 (2%)	45	34
1	E	46/110 (42%)	45 (98%)	1 (2%)	45	34
1	F	44/110 (40%)	44 (100%)	0	100	100
All	All	279/660 (42%)	271 (97%)	8 (3%)	37	25

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	90	ASN
1	B	112	GLU
1	C	109	ARG
1	C	112	GLU
1	C	116	LYS
1	C	135	ASN
1	D	113	ARG
1	E	115	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	120	GLN
1	B	103	GLN
1	B	107	GLN
1	B	120	GLN
1	C	132	ASN
1	D	107	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	51/119 (42%)	0.35	4 (7%) 19 17	17, 31, 53, 87	1 (1%)
1	B	51/119 (42%)	0.42	4 (7%) 19 17	14, 27, 51, 69	1 (1%)
1	C	50/119 (42%)	0.15	1 (2%) 65 65	17, 28, 50, 56	0
1	D	47/119 (39%)	0.16	3 (6%) 25 24	12, 27, 51, 68	1 (2%)
1	E	49/119 (41%)	1.00	6 (12%) 8 7	24, 39, 59, 104	0
1	F	47/119 (39%)	0.64	3 (6%) 25 24	13, 38, 58, 60	2 (4%)
All	All	295/714 (41%)	0.45	21 (7%) 22 20	12, 32, 58, 104	5 (1%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	136	PRO	4.6
1	A	137	PRO	4.5
1	C	135	ASN	4.3
1	D	135	ASN	3.8
1	E	134	PRO	3.5
1	E	91	LEU	3.4
1	E	135	ASN	3.3
1	B	87	GLU	3.2
1	D	89	PRO	3.1
1	E	119	SER	2.9
1	A	87	GLU	2.7
1	B	88	ASP	2.5
1	B	115	LEU	2.4
1	A	136	PRO	2.3
1	E	115	LEU	2.3
1	F	115	LEU	2.3
1	F	120	GLN	2.2
1	D	134	PRO	2.2
1	F	110	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	119	SER	2.1
1	A	99	ASN	2.0

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 oligosaccharides 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.