



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:36 AM UTC

PDB ID : 8PU3 / pdb_00008pu3
Title : Complex of the toxin/antitoxin FaRel2/ATfaRel2
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Deposited on : 2023-07-16
Resolution : 2.17 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

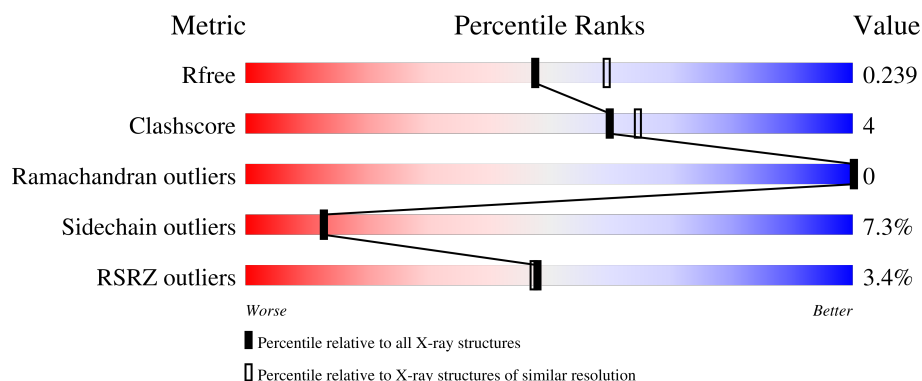
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

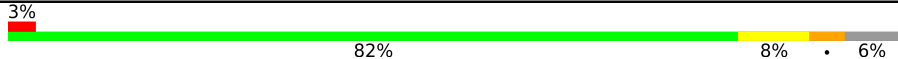
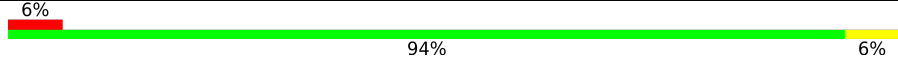
The reported resolution of this entry is 2.17 Å.

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	8975 (2.20-2.16)
Clashscore	190562	9786 (2.20-2.16)
Ramachandran outliers	187476	9664 (2.20-2.16)
Sidechain outliers	187428	9664 (2.20-2.16)
RSRZ outliers	180081	8979 (2.20-2.16)

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	79	 3% 82% 8% 6%
1	B	79	 6% 94% 6%
2	C	206	 2% 85% 11% 2%
2	D	206	 3% 80% 15% 2%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4830 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 ATfaRel2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	74	Total	C	N	O	S	0	0	0
			585	378	97	107	3			
1	B	79	Total	C	N	O	S	0	0	0
			618	401	102	112	3			

- Molecule 2 is a protein called FaRel2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	203	Total	C	N	O	S	0	0	0
			1704	1093	281	323	7			
2	D	203	Total	C	N	O	S	0	0	0
			1702	1093	281	321	7			

- Molecule 3 is water.

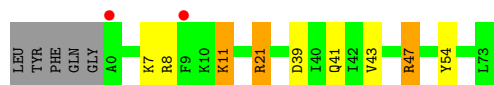
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	23	Total	O	0	0
			23	23		
3	B	22	Total	O	0	0
			22	22		
3	C	99	Total	O	0	0
			99	99		
3	D	77	Total	O	0	0
			77	77		

3 Residue-property plots [i](#)

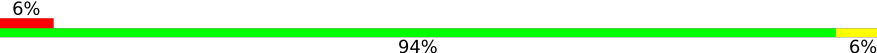
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

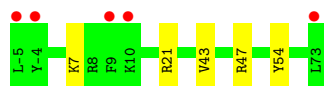
• Molecule 1: ATfaRel2

Chain A: 



• Molecule 1: ATfaRel2

Chain B: 



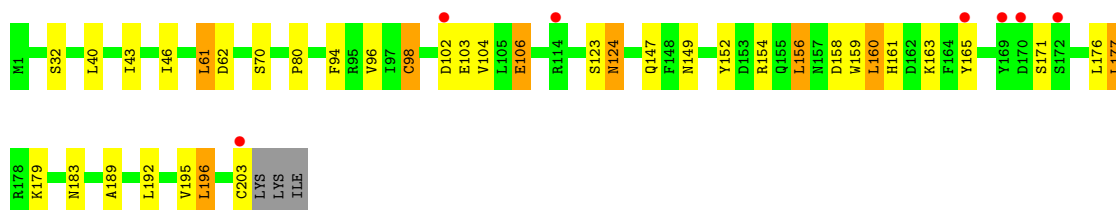
• Molecule 2: FaRel2

Chain C: 



• Molecule 2: FaRel2

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	51.96Å 106.23Å 135.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	67.55 – 2.17 67.55 – 2.17	Depositor EDS
% Data completeness (in resolution range)	62.6 (67.55-2.17) 62.6 (67.55-2.17)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 2.16Å)	Xtriage
Refinement program	BUSTER 1.19.2_4158, PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.184 , 0.239 0.191 , 0.239	Depositor DCC
R_{free} test set	1213 reflections (3.01%)	wwPDB-VP
Wilson B-factor (Å ²)	42.3	Xtriage
Anisotropy	0.089	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 49.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4830	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.03% 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	0.62	0/595	0.95	0/795
1	B	0.63	0/630	0.93	0/844
2	C	0.73	0/1742	1.10	0/2345
2	D	0.78	0/1740	1.16	7/2342 (0.3%)
All	All	0.72	0/4707	1.08	7/6326 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	171	SER	CA-C-N	5.78	128.30	120.38
2	D	171	SER	C-N-CA	5.78	128.30	120.38
2	D	104	VAL	N-CA-C	5.74	115.93	110.42
2	D	106	GLU	CB-CG-CD	5.72	122.32	112.60
2	D	124	ASN	CA-CB-CG	5.44	118.04	112.60
2	D	103	GLU	CA-C-N	5.35	127.30	120.56
2	D	103	GLU	C-N-CA	5.35	127.30	120.56

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	585	0	596	8	0
1	B	618	0	615	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1704	0	1644	15	0
2	D	1702	0	1644	20	0
3	A	23	0	0	2	0
3	B	22	0	0	0	0
3	C	99	0	0	0	0
3	D	77	0	0	1	0
All	All	4830	0	4499	39	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 4.

All (39) 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)
2:D:98:CYS:SG	3:D:325:HOH:O	2.42	0.74
2:C:32:SER:HB3	2:C:80:PRO:HB2	1.77	0.66
2:D:32:SER:HB3	2:D:80:PRO:HB2	1.78	0.65
2:C:155:GLN:HE21	2:D:152:TYR:H	1.47	0.61
2:D:61:LEU:HD22	2:D:94:PHE:HB3	1.83	0.60
2:D:163:LYS:HB2	2:D:192:LEU:HD12	1.83	0.59
2:D:147:GLN:NE2	2:D:154:ARG:HH21	2.01	0.57
2:C:61:LEU:HD22	2:C:94:PHE:HB3	1.86	0.57
1:A:8:ARG:HB3	1:A:11:LYS:HZ2	1.69	0.56
1:A:8:ARG:HB3	1:A:11:LYS:NZ	2.21	0.56
2:D:159:TRP:CD1	2:D:189:ALA:HB2	2.42	0.55
2:D:156:LEU:HD13	2:D:160:LEU:HD22	1.89	0.54
2:D:161:HIS:HA	2:D:165:TYR:CD2	2.42	0.54
2:C:147:GLN:HE21	2:C:149:ASN:HD21	1.55	0.53
2:C:156:LEU:HD13	2:C:160:LEU:HD22	1.91	0.53
2:D:147:GLN:HE22	2:D:154:ARG:NH2	2.07	0.52
2:D:149:ASN:HD22	2:D:154:ARG:HE	1.60	0.49
2:C:12:GLU:H	2:C:12:GLU:CD	2.22	0.48
2:D:147:GLN:HE22	2:D:154:ARG:HH21	1.59	0.48
2:C:163:LYS:NZ	2:C:164:PHE:CE1	2.78	0.47
2:C:113:ILE:HG23	2:C:133:VAL:HG13	1.96	0.46
2:D:43:ILE:HA	2:D:46:ILE:HD12	1.98	0.46
2:D:154:ARG:NH1	2:D:158:ASP:OD1	2.42	0.46
2:C:96:VAL:HG22	2:C:148:PHE:CD2	2.52	0.45
2:C:155:GLN:NE2	2:D:152:TYR:H	2.12	0.45
1:A:7:LYS:HD2	1:A:54:TYR:HD1	1.82	0.45
1:B:7:LYS:HD2	1:B:54:TYR:HD1	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:149:ASN:HD21	2:D:154:ARG:HH21	1.65	0.45
1:A:39:ASP:HB2	3:A:114:HOH:O	2.17	0.44
2:D:177:LEU:HD21	2:D:196:LEU:HG	1.98	0.44
1:A:41:GLN:NE2	3:A:101:HOH:O	2.51	0.44
2:C:43:ILE:HA	2:C:46:ILE:HD12	1.99	0.44
2:C:170:ASP:HB3	2:C:173:CYS:HB3	2.00	0.43
2:C:155:GLN:HG2	2:D:152:TYR:HB2	2.01	0.42
2:D:160:LEU:HB3	2:D:165:TYR:CZ	2.54	0.42
1:A:47:ARG:HH22	2:D:62:ASP:CG	2.27	0.42
1:A:8:ARG:HD2	1:A:11:LYS:HZ2	1.85	0.42
1:A:21:ARG:HD2	2:C:53:LEU:O	2.20	0.41
2:C:25:MET:HE2	2:C:25:MET:HB2	1.89	0.40

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 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	72/79 (91%)	71 (99%)	1 (1%)	0	100	100
1	B	77/79 (98%)	76 (99%)	1 (1%)	0	100	100
2	C	201/206 (98%)	196 (98%)	5 (2%)	0	100	100
2	D	201/206 (98%)	197 (98%)	4 (2%)	0	100	100
All	All	551/570 (97%)	540 (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	A	59/65 (91%)	55 (93%)	4 (7%)	14	15
1	B	60/65 (92%)	57 (95%)	3 (5%)	22	25
2	C	186/194 (96%)	175 (94%)	11 (6%)	18	19
2	D	185/194 (95%)	167 (90%)	18 (10%)	8	7
All	All	490/518 (95%)	454 (93%)	36 (7%)	13	13

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LYS
1	A	21	ARG
1	A	43	VAL
1	A	47	ARG
1	B	21	ARG
1	B	43	VAL
1	B	47	ARG
2	C	40	LEU
2	C	55	ILE
2	C	61	LEU
2	C	70	SER
2	C	96	VAL
2	C	156	LEU
2	C	160	LEU
2	C	163	LYS
2	C	172	SER
2	C	183	ASN
2	C	196	LEU
2	D	40	LEU
2	D	61	LEU
2	D	70	SER
2	D	96	VAL
2	D	98	CYS
2	D	102	ASP
2	D	106	GLU
2	D	123	SER
2	D	124	ASN
2	D	156	LEU

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Mol	Chain	Res	Type
2	D	160	LEU
2	D	176	LEU
2	D	177	LEU
2	D	179	LYS
2	D	183	ASN
2	D	195	VAL
2	D	196	LEU
2	D	203	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	GLN
2	C	149	ASN
2	C	155	GLN
2	D	35	ASN
2	D	139	ASN
2	D	147	GLN
2	D	149	ASN

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 oligosaccharides 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	74/79 (93%)	0.06	2 (2%) 56 55	30, 51, 67, 76	0
1	B	79/79 (100%)	0.18	5 (6%) 26 25	32, 51, 77, 87	0
2	C	203/206 (98%)	0.05	5 (2%) 58 57	28, 45, 69, 103	0
2	D	203/206 (98%)	0.18	7 (3%) 48 47	30, 45, 71, 91	1 (0%)
All	All	559/570 (98%)	0.12	19 (3%) 48 47	28, 46, 71, 103	1 (0%)

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	165	TYR	7.4
1	A	0	ALA	3.0
1	B	-5	LEU	3.0
2	D	169	TYR	3.0
1	B	-4	TYR	2.8
2	D	172	SER	2.8
2	D	114	ARG	2.7
1	B	73	LEU	2.7
2	C	203	CYS	2.7
2	C	202	HIS	2.5
2	D	203	CYS	2.4
2	D	102	ASP	2.3
1	B	9	PHE	2.3
2	C	198	ASP	2.3
1	A	9	PHE	2.2
2	D	170	ASP	2.2
2	C	164	PHE	2.1
1	B	10	LYS	2.1
2	C	1	MET	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.