



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 29, 2026 – 03:59 PM UTC

PDB ID : 6XAY / pdb_00006xay
Title : Structure of a fragment of human fibronectin containing the 10th, 11th and 12th type III domains
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Deposited on : 2020-06-05
Resolution : 2.48 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 : **FAILED**
Mogul : 2022.3.0, CSD as543be (2022)
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

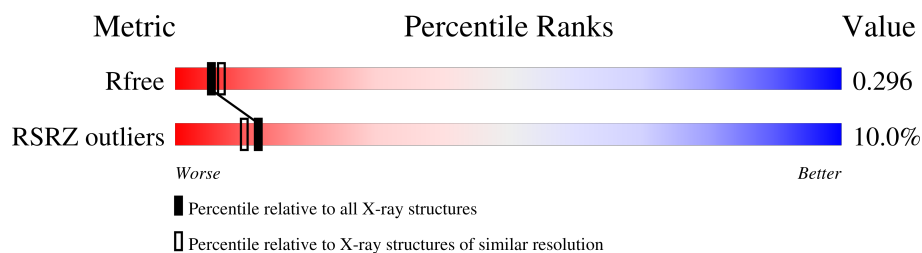
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.48 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	7589 (2.50-2.46)
RSRZ outliers	180081	7593 (2.50-2.46)

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

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8315 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.

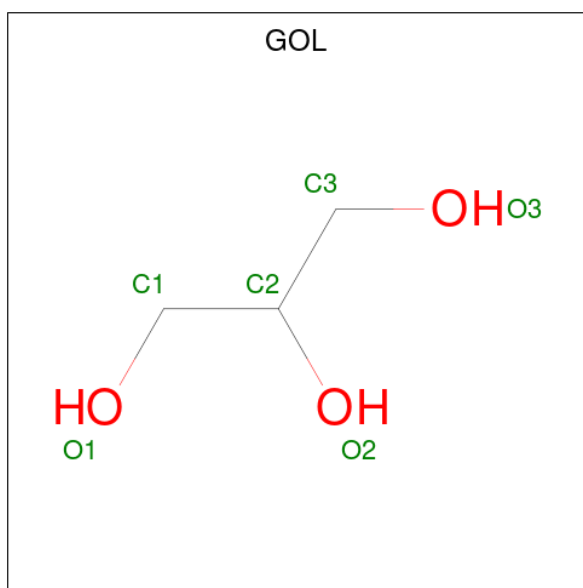
- Molecule 1 is a protein called Fibronectin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	272	Total	C	N	O	S	0	0	0
			2042	1286	336	416	4			
1	B	269	Total	C	N	O	S	0	0	0
			2022	1274	332	412	4			
1	C	271	Total	C	N	O	S	0	0	0
			2036	1283	335	414	4			
1	D	272	Total	C	N	O	S	0	0	0
			2042	1286	336	416	4			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1443	GLY	-	expression tag	UNP P02751
A	1444	SER	-	expression tag	UNP P02751
A	1445	HIS	-	expression tag	UNP P02751
A	1446	MET	-	expression tag	UNP P02751
A	1643	GLY	VAL	engineered mutation	UNP P02751
B	1443	GLY	-	expression tag	UNP P02751
B	1444	SER	-	expression tag	UNP P02751
B	1445	HIS	-	expression tag	UNP P02751
B	1446	MET	-	expression tag	UNP P02751
B	1643	GLY	VAL	engineered mutation	UNP P02751
C	1443	GLY	-	expression tag	UNP P02751
C	1444	SER	-	expression tag	UNP P02751
C	1445	HIS	-	expression tag	UNP P02751
C	1446	MET	-	expression tag	UNP P02751
C	1643	GLY	VAL	engineered mutation	UNP P02751
D	1443	GLY	-	expression tag	UNP P02751
D	1444	SER	-	expression tag	UNP P02751
D	1445	HIS	-	expression tag	UNP P02751
D	1446	MET	-	expression tag	UNP P02751
D	1643	GLY	VAL	engineered mutation	UNP P02751

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	44	Total	O	0	0
			44	44		
3	B	20	Total	O	0	0
			20	20		
3	C	27	Total	O	0	0
			27	27		
3	D	46	Total	O	0	0
			46	46		

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3 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	125.08Å 440.37Å 60.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.40 – 2.48 37.40 – 2.48	Depositor EDS
% Data completeness (in resolution range)	92.1 (37.40-2.48) 92.2 (37.40-2.48)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.84 (at 2.48Å)	Xtriage
Refinement program	PHENIX 1.16	Depositor
R, R_{free}	0.246 , 0.296 0.246 , 0.296	Depositor DCC
R_{free} test set	2000 reflections (3.33%)	wwPDB-VP
Wilson B-factor (Å ²)	41.8	Xtriage
Anisotropy	0.624	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 59.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8315	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 39.23 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.2757e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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.

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 oligosaccharides in this entry.

4.6 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	$\# Z > 2$
2	GOL	B	1803	-	5,5,5	0.97	0	5,5,5	1.13	1 (20%)
2	GOL	B	1802	-	5,5,5	1.00	0	5,5,5	1.03	0
2	GOL	B	1801	-	5,5,5	0.90	0	5,5,5	1.12	1 (20%)
2	GOL	D	1801	-	5,5,5	0.85	0	5,5,5	1.12	0
2	GOL	A	1801	-	5,5,5	0.99	0	5,5,5	1.16	0
2	GOL	A	1802	-	5,5,5	1.05	1 (20%)	5,5,5	1.11	0

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
2	GOL	B	1803	-	-	2/4/4/4	-
2	GOL	B	1802	-	-	0/4/4/4	-
2	GOL	B	1801	-	-	0/4/4/4	-
2	GOL	D	1801	-	-	0/4/4/4	-
2	GOL	A	1801	-	-	2/4/4/4	-
2	GOL	A	1802	-	-	0/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1802	GOL	O2-C2	-2.06	1.37	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1803	GOL	C3-C2-C1	-2.01	104.43	111.80
2	B	1801	GOL	C3-C2-C1	-2.00	104.46	111.80

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1803	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
2	B	1803	GOL	O2-C2-C3-O3
2	A	1801	GOL	O1-C1-C2-C3
2	A	1801	GOL	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

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	272/280 (97%)	0.24	12 (4%) 39 35	38, 55, 102, 145	0
1	B	269/280 (96%)	0.87	31 (11%) 9 8	48, 81, 113, 156	0
1	C	271/280 (96%)	1.04	54 (19%) 3 2	28, 91, 139, 185	0
1	D	272/280 (97%)	0.17	11 (4%) 42 38	29, 53, 102, 146	0
All	All	1084/1120 (96%)	0.58	108 (9%) 12 10	28, 67, 122, 185	0

All (108) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1674	PRO	5.7
1	C	1522	THR	5.1
1	A	1581	GLY	4.7
1	C	1560	VAL	4.5
1	C	1470	ALA	4.2
1	C	1528	PRO	4.1
1	C	1529	ALA	4.1
1	A	1722	GLU	4.1
1	D	1582	PRO	4.0
1	B	1582	PRO	3.7
1	A	1529	ALA	3.7
1	C	1538	TYR	3.7
1	B	1628	ALA	3.7
1	C	1473	VAL	3.6
1	D	1672	THR	3.6
1	C	1511	GLY	3.5
1	B	1722	GLU	3.5
1	C	1516	ILE	3.5
1	A	1673	GLY	3.5
1	B	1523	GLY	3.5
1	C	1481	THR	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	1618	SER	3.4
1	C	1521	VAL	3.3
1	C	1457	VAL	3.3
1	C	1597	MET	3.3
1	A	1582	PRO	3.2
1	C	1456	VAL	3.2
1	C	1582	PRO	3.2
1	C	1520	ALA	3.1
1	A	1675	MET	3.1
1	C	1590	ALA	3.0
1	C	1480	ILE	3.0
1	C	1598	THR	3.0
1	C	1496	VAL	2.9
1	C	1490	PRO	2.9
1	C	1535	SER	2.9
1	B	1708	THR	2.9
1	C	1519	TYR	2.9
1	A	1708	THR	2.8
1	C	1491	VAL	2.8
1	B	1548	MET	2.8
1	C	1568	PRO	2.8
1	C	1581	GLY	2.7
1	B	1529	ALA	2.7
1	B	1519	TYR	2.7
1	C	1483	GLY	2.6
1	B	1610	VAL	2.6
1	C	1505	ILE	2.6
1	C	1558	ILE	2.6
1	C	1474	THR	2.6
1	B	1550	VAL	2.5
1	B	1507	GLY	2.5
1	D	1581	GLY	2.5
1	B	1473	VAL	2.5
1	D	1656	ASN	2.5
1	C	1587	THR	2.5
1	C	1464	LEU	2.4
1	A	1448	SER	2.4
1	C	1628	ALA	2.4
1	B	1674	PRO	2.4
1	B	1583	GLY	2.4
1	C	1514	TYR	2.4
1	C	1722	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	1547	GLN	2.3
1	C	1492	GLN	2.3
1	B	1515	THR	2.3
1	B	1665	ARG	2.3
1	C	1619	GLY	2.3
1	C	1673	GLY	2.3
1	C	1600	GLU	2.3
1	C	1458	ALA	2.3
1	B	1524	ARG	2.3
1	C	1510	PRO	2.3
1	B	1656	ASN	2.2
1	C	1477	TYR	2.3
1	B	1648	LEU	2.2
1	D	1451	PRO	2.2
1	D	1473	VAL	2.2
1	D	1472	ALA	2.2
1	C	1564	PRO	2.2
1	C	1460	THR	2.2
1	B	1453	ASP	2.2
1	B	1670	GLU	2.2
1	C	1562	TRP	2.2
1	A	1473	VAL	2.2
1	B	1487	GLY	2.2
1	B	1528	PRO	2.2
1	C	1530	SER	2.1
1	C	1617	PRO	2.1
1	D	1528	PRO	2.1
1	D	1470	ALA	2.1
1	B	1691	GLY	2.1
1	C	1589	THR	2.1
1	B	1678	ILE	2.1
1	C	1671	LYS	2.1
1	B	1491	VAL	2.0
1	B	1581	GLY	2.0
1	A	1672	THR	2.0
1	C	1579	LYS	2.0
1	D	1448	SER	2.0
1	B	1457	VAL	2.0
1	C	1459	ALA	2.0
1	D	1523	GLY	2.0
1	B	1522	THR	2.0
1	C	1495	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	1540	THR	2.0
1	C	1674	PRO	2.0
1	B	1506	SER	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 oligosaccharides in this entry.

5.4 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($\text{\AA}^2$)	Q<0.9
2	GOL	B	1803	6/6	0.82	0.25	83,102,126,131	0
2	GOL	B	1802	6/6	0.84	0.23	85,95,124,142	0
2	GOL	A	1801	6/6	0.85	0.24	44,60,76,84	0
2	GOL	B	1801	6/6	0.89	0.16	65,69,84,91	6
2	GOL	A	1802	6/6	0.92	0.14	43,50,62,69	6
2	GOL	D	1801	6/6	0.95	0.21	43,43,69,84	0

5.5 Other polymers [i](#)

There are no such residues in this entry.