



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 07:33 PM GMT

PDB ID : 1FZC
Title : CRYSTAL STRUCTURE OF FRAGMENT DOUBLE-D FROM HUMAN FIBRIN WITH TWO DIFFERENT BOUND LIGANDS
Authors : Everse, S.J.; Spraggon, G.; Veerapandian, L.; Riley, M.; Doolittle, R.F.
Deposited on : 1998-05-19
Resolution : 2.30 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
<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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

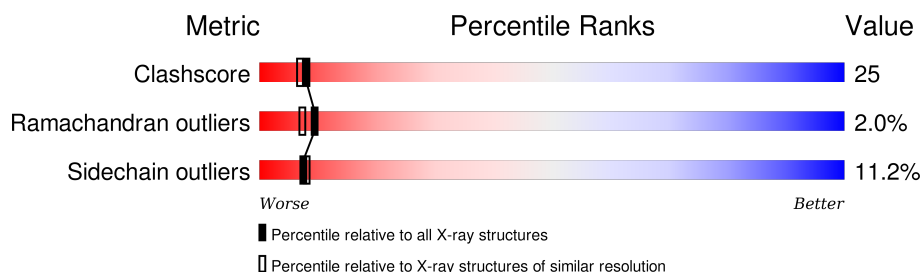
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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))
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)




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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	87	
1	D	87	
2	B	328	
2	E	328	
3	C	319	
3	F	319	
4	G	4	

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Mol	Chain	Length	Quality of chain
4	H	4	 75%25%
5	I	4	 75%25%
5	J	4	 75%25%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 11594 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 FIBRIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	74	Total	C	N	O	S	0	0	0
			608	377	115	113	3			
1	D	74	Total	C	N	O	S	0	0	0
			608	377	115	113	3			

- Molecule 2 is a protein called FIBRIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	308	Total	C	N	O	S	0	0	0
			2473	1544	434	473	22			
2	E	308	Total	C	N	O	S	0	0	0
			2473	1544	434	473	22			

- Molecule 3 is a protein called FIBRIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	301	Total	C	N	O	S	0	0	0
			2404	1523	405	465	11			
3	F	301	Total	C	N	O	S	0	0	0
			2404	1523	405	465	11			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	88	LYS	ILE	CONFLICT	UNP P02679
F	88	LYS	ILE	CONFLICT	UNP P02679

- Molecule 4 is a protein called FIBRIN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	4	Total	C	N	O	0	0	0
			29	18	7	4			

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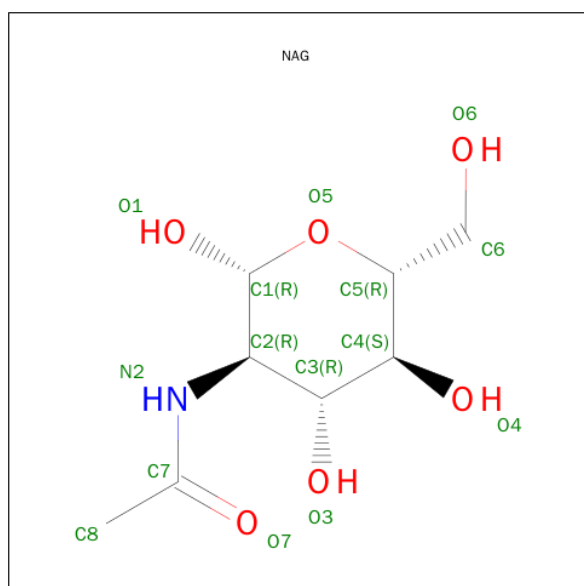
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	H	4	Total	C	N	O	0	0	0
			29	18	7	4			

- Molecule 5 is a protein called FIBRIN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	I	4	Total	C	N	O	0	0	0
			32	19	9	4			
5	J	4	Total	C	N	O	0	0	0
			32	19	9	4			

- Molecule 6 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	N	O	0	0
			14	8	1	5		
6	I	1	Total	C	N	O	0	0
			14	8	1	5		
6	E	1	Total	C	N	O	0	0
			14	8	1	5		
6	J	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 7 is SUGAR (ALPHA-D-MANNOSE) (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			11	6	5		

- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total	Ca	0	0
			1	1		
8	C	1	Total	Ca	0	0
			1	1		
8	F	1	Total	Ca	0	0
			1	1		
8	E	1	Total	Ca	0	0
			1	1		

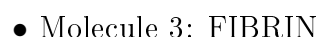
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	15	Total	O	0	0
			15	15		
9	B	124	Total	O	0	0
			124	124		
9	C	71	Total	O	0	0
			71	71		
9	D	16	Total	O	0	0
			16	16		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	E	119	Total 119	O 119	0	0
9	F	82	Total 82	O 82	0	0
9	G	1	Total 1	O 1	0	0
9	H	1	Total 1	O 1	0	0
9	I	1	Total 1	O 1	0	0
9	J	1	Total 1	O 1	0	0



● Molecule 4: FIBRIN

Chain H:  75% 25%

G1	P2	R3	P4
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● Molecule 5: FIBRIN

Chain I:  75% 25%

G1	H2	R3	P4
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● Molecule 5: FIBRIN

Chain J:  75% 25%

G1	P4
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4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	83.44Å 95.60Å 113.64Å 90.00° 90.19° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30	Depositor
% Data completeness (in resolution range)	94.5 (20.00-2.30)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.220 , 0.290	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11594	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, NAG, MAN

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	0.60	0/609	1.86	13/811 (1.6%)
1	D	0.58	0/609	1.62	11/811 (1.4%)
2	B	0.98	3/2535 (0.1%)	1.94	82/3425 (2.4%)
2	E	0.92	3/2535 (0.1%)	1.94	81/3425 (2.4%)
3	C	0.73	1/2469 (0.0%)	1.68	50/3339 (1.5%)
3	F	0.75	1/2469 (0.0%)	1.61	30/3339 (0.9%)
4	G	0.75	0/30	4.32	4/40 (10.0%)
4	H	0.97	0/30	2.53	2/40 (5.0%)
5	I	0.75	0/33	1.89	1/43 (2.3%)
5	J	0.91	0/33	1.42	0/43
All	All	0.83	8/11352 (0.1%)	1.81	274/15316 (1.8%)

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
3	C	0	1

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	295	GLY	N-CA	12.22	1.64	1.46
2	B	434	GLY	N-CA	11.47	1.63	1.46
2	E	295	GLY	N-CA	11.01	1.62	1.46
2	E	258	GLY	N-CA	10.33	1.61	1.46
2	B	258	GLY	N-CA	7.23	1.56	1.46

The worst 5 of 274 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	3	ARG	NE-CZ-NH2	-23.44	108.58	120.30
1	A	167	ARG	NE-CZ-NH1	18.52	129.56	120.30
2	E	255	ARG	NE-CZ-NH2	15.11	127.86	120.30
2	E	264	ARG	NE-CZ-NH2	-14.71	112.94	120.30
3	C	375	ARG	NE-CZ-NH1	14.15	127.38	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	274	TYR	Mainchain

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	608	0	647	31	0
1	D	608	0	649	58	0
2	B	2473	0	2336	119	0
2	E	2473	0	2335	181	0
3	C	2404	0	2249	109	0
3	F	2404	0	2249	135	0
4	G	29	0	32	1	0
4	H	29	0	32	0	0
5	I	32	0	32	0	0
5	J	32	0	32	1	0
6	B	14	0	13	0	0
6	E	14	0	13	2	0
6	I	14	0	13	2	0
6	J	14	0	13	2	0
7	B	11	0	10	2	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0
8	E	1	0	0	0	0
8	F	1	0	0	0	0
9	A	15	0	0	6	0
9	B	124	0	0	18	0
9	C	71	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	D	16	0	0	3	0
9	E	119	0	0	6	0
9	F	82	0	0	11	0
9	G	1	0	0	1	0
9	H	1	0	0	0	0
9	I	1	0	0	0	0
9	J	1	0	0	0	0
All	All	11594	0	10655	536	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 25.

The worst 5 of 536 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)
3:C:277:THR:HG21	3:F:303:PHE:CD2	1.37	1.59
3:C:277:THR:CG2	3:F:303:PHE:CE2	1.83	1.42
1:A:135:LEU:HD12	9:A:207:HOH:O	1.27	1.34
2:E:423:THR:H	2:E:426:MET:CE	1.40	1.34
2:E:423:THR:N	2:E:426:MET:CE	1.91	1.33

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	A	72/87 (83%)	67 (93%)	3 (4%)	2 (3%)	6 4
1	D	72/87 (83%)	64 (89%)	6 (8%)	2 (3%)	6 4
2	B	306/328 (93%)	286 (94%)	15 (5%)	5 (2%)	12 11
2	E	306/328 (93%)	281 (92%)	21 (7%)	4 (1%)	15 15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	299/319 (94%)	275 (92%)	17 (6%)	7 (2%)	8	6
3	F	299/319 (94%)	276 (92%)	16 (5%)	7 (2%)	8	6
4	G	2/4 (50%)	2 (100%)	0	0	100	100
4	H	2/4 (50%)	2 (100%)	0	0	100	100
5	I	2/4 (50%)	2 (100%)	0	0	100	100
5	J	2/4 (50%)	2 (100%)	0	0	100	100
All	All	1362/1484 (92%)	1257 (92%)	78 (6%)	27 (2%)	9	7

5 of 27 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	240	SER
3	C	392	LEU
2	E	156	THR
3	F	101	LEU
3	F	240	SER

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	69/82 (84%)	59 (86%)	10 (14%)	4	3
1	D	69/82 (84%)	62 (90%)	7 (10%)	9	11
2	B	266/286 (93%)	235 (88%)	31 (12%)	7	7
2	E	266/286 (93%)	235 (88%)	31 (12%)	7	7
3	C	252/267 (94%)	220 (87%)	32 (13%)	5	5
3	F	252/267 (94%)	231 (92%)	21 (8%)	14	17
4	G	3/3 (100%)	2 (67%)	1 (33%)	0	0
4	H	3/3 (100%)	3 (100%)	0	100	100
5	I	3/3 (100%)	3 (100%)	0	100	100
5	J	3/3 (100%)	3 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1186/1282 (92%)	1053 (89%)	133 (11%)	7 8

5 of 133 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	303	PHE
1	D	125	LYS
3	F	317	ASN
3	C	317	ASN
3	C	376	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 57 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	319	ASN
2	E	189	GLN
3	F	319	ASN
3	C	325	ASN
3	C	390	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 for Mogul analysis.

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
6	NAG	B	470	2,6	14,14,15	1.23	1 (7%)	15,19,21	1.35	3 (20%)
7	MAN	B	472	-	11,11,12	1.12	1 (9%)	14,15,17	2.62	4 (28%)
6	NAG	E	470	2	14,14,15	1.22	1 (7%)	15,19,21	1.49	2 (13%)
6	NAG	I	471	6	14,14,15	1.28	1 (7%)	15,19,21	1.16	1 (6%)
6	NAG	J	471	-	14,14,15	1.23	1 (7%)	15,19,21	1.38	1 (6%)

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
6	NAG	B	470	2,6	-	0/6/23/26	0/1/1/1
7	MAN	B	472	-	-	0/2/19/22	0/1/1/1
6	NAG	E	470	2	-	0/6/23/26	0/1/1/1
6	NAG	I	471	6	-	0/6/23/26	0/1/1/1
6	NAG	J	471	-	-	0/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	470	NAG	O7-C7	-4.00	1.13	1.23
6	E	470	NAG	O7-C7	-3.80	1.14	1.23
6	I	471	NAG	O7-C7	-3.62	1.14	1.23
6	J	471	NAG	O7-C7	-3.52	1.15	1.23
7	B	472	MAN	O5-C1	-3.18	1.38	1.43

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	472	MAN	O3-C3-C2	-2.53	105.43	110.00
6	E	470	NAG	O3-C3-C2	-2.33	104.50	109.11
6	B	470	NAG	C6-C5-C4	-2.28	107.40	113.02
6	I	471	NAG	C1-O5-C5	2.31	115.17	112.25
6	B	470	NAG	C1-O5-C5	2.35	115.22	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	472	MAN	2	0
6	E	470	NAG	2	0
6	I	471	NAG	2	0
6	J	471	NAG	2	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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.