



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 26, 2016 – 10:54 PM EDT

PDB ID : 5KF4
Title : Crystal structure of FN3 domain (Residues P368-P466) of Human collagen XX
Authors : Xie, Y.; Cheng, Z.; Zhao, J.
Deposited on : 2016-06-12
Resolution : 2.50 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-20027790
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-20027790

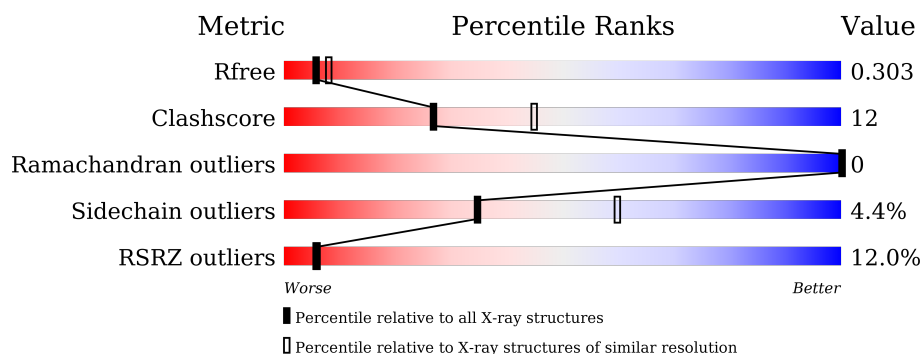
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	100	<div> <div>15%</div> <div>59%</div> <div>39%</div> <div>..</div> </div>
1	B	100	<div> <div>%</div> <div>84%</div> <div>15%</div> <div>.</div> </div>
1	C	100	<div> <div>13%</div> <div>67%</div> <div>28%</div> <div>..</div> </div>
1	D	100	<div> <div>18%</div> <div>67%</div> <div>30%</div> <div>.</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2985 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 Collagen alpha-1(XX) chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	99	Total	C	N	O	0	0	0
			738	471	129	138			
1	B	99	Total	C	N	O	0	0	0
			738	471	129	138			
1	C	96	Total	C	N	O	0	0	0
			718	458	126	134			
1	D	97	Total	C	N	O	0	0	0
			723	461	127	135			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	367	GLY	-	expression tag	UNP Q9P218
B	367	GLY	-	expression tag	UNP Q9P218
C	367	GLY	-	expression tag	UNP Q9P218
D	367	GLY	-	expression tag	UNP Q9P218

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	23	Total	O	0	0
			23	23		
2	B	18	Total	O	0	0
			18	18		
2	C	16	Total	O	0	0
			16	16		
2	D	11	Total	O	0	0
			11	11		

- Molecule 1: Collagen alpha-1(XX) chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	56.48Å 78.60Å 81.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.86 – 2.50 46.51 – 2.50	Depositor EDS
% Data completeness (in resolution range)	92.2 (45.86-2.50) 98.1 (46.51-2.50)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	11.90 (at 2.51Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.258 , 0.284 0.276 , 0.303	Depositor DCC
R_{free} test set	637 reflections (4.95%)	DCC
Wilson B-factor (Å ²)	27.0	Xtriage
Anisotropy	1.232	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 43.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.002 for -h,l,k	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	2985	wwPDB-VP
Average B, all atoms (Å ²)	32.0	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 34.47 % 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 6.7868e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

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	0.27	0/758	0.55	0/1041
1	B	0.25	0/758	0.52	0/1041
1	C	0.27	0/736	0.54	0/1011
1	D	0.27	0/741	0.59	0/1018
All	All	0.26	0/2993	0.55	0/4111

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 [i](#)

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	738	0	752	32	0
1	B	738	0	752	8	0
1	C	718	0	732	18	0
1	D	723	0	737	15	0
2	A	23	0	0	14	0
2	B	18	0	0	2	0
2	C	16	0	0	2	0
2	D	11	0	0	2	0
All	All	2985	0	2973	71	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 12.

All (71) 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:D:443:LEU:HD21	1:D:459:ARG:HD2	1.48	0.93
1:A:397:TRP:O	2:A:501:HOH:O	1.99	0.81
1:A:374:LEU:HG	2:A:507:HOH:O	1.85	0.76
1:D:410:VAL:HG22	1:D:421:GLU:HG2	1.68	0.75
1:B:451:GLU:OE2	2:B:501:HOH:O	2.03	0.75
1:A:459:ARG:NH1	2:A:506:HOH:O	2.20	0.75
1:B:439:ARG:HG2	1:B:466:PRO:HA	1.70	0.74
1:B:443:LEU:HD21	1:B:459:ARG:HD2	1.70	0.73
1:A:402:ARG:O	2:A:502:HOH:O	2.07	0.72
1:C:410:VAL:HG22	1:C:421:GLU:HG2	1.73	0.70
1:A:404:PRO:HG2	1:A:426:GLY:HA2	1.74	0.69
1:A:382:SER:HB2	1:C:458:LEU:HD12	1.75	0.69
1:B:410:VAL:HG22	1:B:421:GLU:HG2	1.75	0.67
1:A:453:GLY:O	2:A:503:HOH:O	2.14	0.66
1:C:409:ILE:HD13	1:C:431:THR:HG21	1.79	0.65
1:A:410:VAL:HG22	1:A:421:GLU:HG2	1.78	0.65
1:D:395:LEU:HD11	1:D:444:VAL:HG11	1.79	0.65
1:A:408:LEU:HB3	1:A:447:PHE:HB2	1.78	0.64
1:B:408:LEU:HB3	1:B:447:PHE:HB2	1.77	0.64
1:A:454:VAL:N	2:A:507:HOH:O	2.30	0.63
1:C:395:LEU:HD11	1:C:444:VAL:HG11	1.81	0.62
1:A:439:ARG:HG2	1:A:466:PRO:HA	1.82	0.62
1:D:412:ARG:HH21	1:D:419:PRO:HG3	1.66	0.61
1:C:401:PRO:HB3	1:D:401:PRO:HB3	1.82	0.60
1:C:441:GLU:HA	1:C:463:THR:HA	1.84	0.59
1:A:404:PRO:O	1:A:426:GLY:HA3	2.02	0.59
1:C:388:VAL:HG13	1:C:393:ILE:HG22	1.87	0.57
1:A:428:ALA:O	2:A:504:HOH:O	2.18	0.56
1:D:370:ALA:C	2:D:503:HOH:O	2.42	0.56
1:C:393:ILE:HD11	1:C:433:LEU:HD12	1.88	0.56
1:A:404:PRO:HB3	1:A:450:TYR:CE1	2.41	0.56
1:A:399:PRO:HD3	2:A:501:HOH:O	2.07	0.55
1:D:446:VAL:O	1:D:457:GLY:HA3	2.07	0.55
1:D:371:ALA:N	2:D:503:HOH:O	2.40	0.53
1:C:386:SER:N	2:C:501:HOH:O	2.40	0.52
1:A:375:ASP:HA	1:A:456:GLU:HB2	1.91	0.52
1:D:408:LEU:HB3	1:D:447:PHE:HB2	1.91	0.52
1:A:446:VAL:O	1:A:457:GLY:HA3	2.10	0.51
1:C:380:PRO:HG2	1:C:458:LEU:HD22	1.92	0.51
1:D:441:GLU:HA	1:D:463:THR:HA	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:446:VAL:O	1:B:457:GLY:HA3	2.12	0.50
1:A:415:ARG:NH1	2:A:511:HOH:O	2.46	0.49
1:A:406:LYS:HD3	1:A:425:GLU:HA	1.95	0.48
1:C:369:ALA:N	2:C:503:HOH:O	2.46	0.48
1:D:388:VAL:HG13	1:D:393:ILE:HG22	1.96	0.47
1:A:406:LYS:HB2	1:A:449:ILE:HB	1.96	0.46
1:D:393:ILE:O	1:D:432:GLU:HG3	2.15	0.46
1:A:402:ARG:NH2	2:A:512:HOH:O	2.48	0.46
1:A:383:LEU:N	2:A:508:HOH:O	2.35	0.46
1:A:379:ALA:O	2:A:505:HOH:O	2.20	0.46
1:C:411:TRP:HZ3	1:C:422:VAL:HG12	1.80	0.46
1:A:412:ARG:NH2	1:A:417:GLY:O	2.50	0.45
1:A:425:GLU:OE1	1:A:425:GLU:N	2.51	0.44
1:D:393:ILE:HD13	1:D:462:VAL:HG11	1.99	0.43
1:C:408:LEU:HB2	1:C:449:ILE:HD11	2.00	0.43
1:A:375:ASP:OD1	1:A:376:THR:HG23	2.18	0.43
1:A:407:TYR:HB2	1:A:424:VAL:HG23	2.00	0.43
1:A:453:GLY:HA3	2:A:507:HOH:O	2.19	0.43
1:C:436:LEU:HD23	1:C:442:TYR:CD1	2.54	0.43
1:A:371:ALA:HA	1:A:372:PRO:HD3	1.88	0.43
1:C:371:ALA:HA	1:C:372:PRO:HD3	1.90	0.42
1:B:388:VAL:HG13	1:B:393:ILE:HG22	2.02	0.41
1:D:384:VAL:HB	1:D:396:SER:HB3	2.02	0.41
1:B:439:ARG:NH2	2:B:503:HOH:O	2.39	0.41
1:C:411:TRP:CZ3	1:C:422:VAL:HG12	2.56	0.41
1:A:394:ARG:NH2	1:A:430:SER:OG	2.54	0.41
1:A:402:ARG:HB3	2:A:502:HOH:O	2.21	0.41
1:D:448:PRO:HB2	1:D:450:TYR:CE1	2.56	0.41
1:C:384:VAL:HB	1:C:396:SER:OG	2.21	0.41
1:C:408:LEU:HB3	1:C:447:PHE:HB2	2.03	0.41
1:A:408:LEU:N	1:A:447:PHE:O	2.40	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	97/100 (97%)	94 (97%)	3 (3%)	0	100	100
1	B	97/100 (97%)	94 (97%)	3 (3%)	0	100	100
1	C	94/100 (94%)	91 (97%)	3 (3%)	0	100	100
1	D	95/100 (95%)	91 (96%)	4 (4%)	0	100	100
All	All	383/400 (96%)	370 (97%)	13 (3%)	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	80/80 (100%)	76 (95%)	4 (5%)	30	53
1	B	80/80 (100%)	78 (98%)	2 (2%)	55	82
1	C	78/80 (98%)	75 (96%)	3 (4%)	40	67
1	D	78/80 (98%)	73 (94%)	5 (6%)	22	39
All	All	316/320 (99%)	302 (96%)	14 (4%)	35	60

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	377	LEU
1	A	390	SER
1	A	394	ARG
1	A	431	THR
1	B	395	LEU
1	B	405	LEU
1	C	406	LYS
1	C	420	ARG
1	C	458	LEU
1	D	390	SER

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Mol	Chain	Res	Type
1	D	424	VAL
1	D	430	SER
1	D	433	LEU
1	D	438	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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	99/100 (99%)	0.94	15 (15%) 3 3	13, 34, 70, 95	0
1	B	99/100 (99%)	0.04	1 (1%) 84 86	9, 18, 47, 58	0
1	C	96/100 (96%)	0.69	13 (13%) 4 4	8, 30, 74, 132	0
1	D	97/100 (97%)	1.05	18 (18%) 2 2	14, 35, 65, 129	0
All	All	391/400 (97%)	0.68	47 (12%) 6 6	8, 29, 69, 132	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	415	ARG	6.3
1	A	368	PRO	5.2
1	C	440	THR	4.8
1	A	374	LEU	4.7
1	A	375	ASP	4.4
1	D	426	GLY	4.1
1	C	415	ARG	3.9
1	D	412	ARG	3.7
1	D	442	TYR	3.6
1	C	442	TYR	3.6
1	C	438	SER	3.5
1	A	427	PRO	3.5
1	C	417	GLY	3.4
1	D	369	ALA	3.1
1	A	450	TYR	3.1
1	C	441	GLU	3.1
1	D	392	SER	3.1
1	A	401	PRO	3.0
1	B	369	ALA	2.9
1	A	451	GLU	2.9
1	C	439	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	369	ALA	2.7
1	A	453	GLY	2.6
1	D	388	VAL	2.6
1	C	414	SER	2.6
1	D	371	ALA	2.6
1	D	423	VAL	2.6
1	D	443	LEU	2.5
1	D	464	THR	2.5
1	A	377	LEU	2.4
1	D	403	HIS	2.3
1	C	392	SER	2.3
1	A	428	ALA	2.3
1	A	399	PRO	2.2
1	A	403	HIS	2.2
1	C	437	ALA	2.2
1	C	382	SER	2.2
1	C	464	THR	2.2
1	D	431	THR	2.2
1	A	404	PRO	2.2
1	D	414	SER	2.2
1	D	410	VAL	2.2
1	A	425	GLU	2.1
1	D	424	VAL	2.1
1	D	425	GLU	2.1
1	D	440	THR	2.1
1	C	436	LEU	2.1

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 ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.