



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:22 PM GMT

PDB ID : 1TDQ
Title : Structural basis for the interactions between tenascins and the C-type lectin domains from lecticans: evidence for a cross-linking role for tenascins
Authors : Lundell, A.; Olin, A.I.; Moergelin, M.; al-Karadaghi, S.; Aspberg, A.; Logan, D.T.
Deposited on : 2004-05-24
Resolution : 2.60 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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
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) : trunk26865

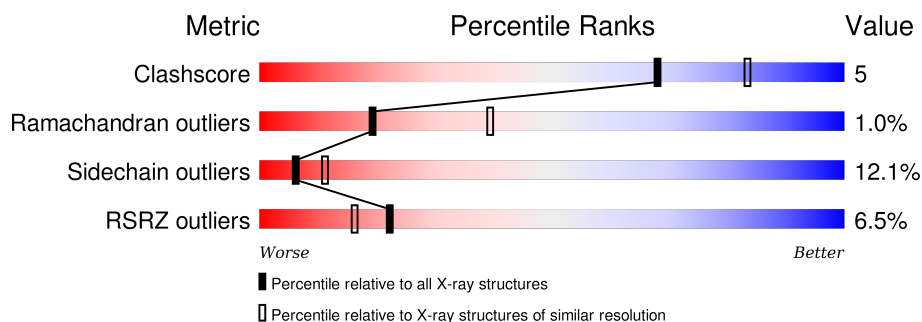
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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	283	<div> <div>9%</div> <div>78%</div> <div>17%</div> <div>• •</div> </div>
2	B	130	<div> <div>%</div> <div>71%</div> <div>19%</div> <div>7%</div> <div>•</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3181 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 Tenascin-R.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	271	Total	C	N	O	S	0	0	0
			2068	1293	347	425	3			

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	GLY	-	CLONING ARTIFACT	UNP Q05546
A	-9	SER	-	CLONING ARTIFACT	UNP Q05546
A	-8	PRO	-	CLONING ARTIFACT	UNP Q05546
A	-7	GLY	-	CLONING ARTIFACT	UNP Q05546
A	-6	ILE	-	CLONING ARTIFACT	UNP Q05546
A	-5	SER	-	CLONING ARTIFACT	UNP Q05546
A	-4	GLY	-	CLONING ARTIFACT	UNP Q05546
A	-3	GLY	-	CLONING ARTIFACT	UNP Q05546
A	-2	GLY	-	CLONING ARTIFACT	UNP Q05546
A	-1	GLY	-	CLONING ARTIFACT	UNP Q05546
A	0	GLY	-	CLONING ARTIFACT	UNP Q05546
A	1	ILE	-	CLONING ARTIFACT	UNP Q05546
A	2	PRO	-	CLONING ARTIFACT	UNP Q05546

- Molecule 2 is a protein called AggreCAN core protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	126	Total	C	N	O	S	0	0	0
			1072	669	192	204	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	ARG	-	CLONING ARTIFACT	UNP P07897

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	3	Total 3	Ca 3	0	0

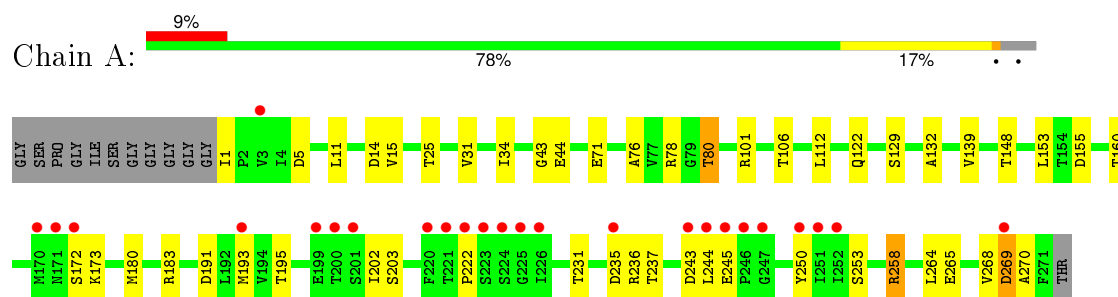
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	10	Total 10	O 10	0	0
4	B	28	Total 28	O 28	0	0

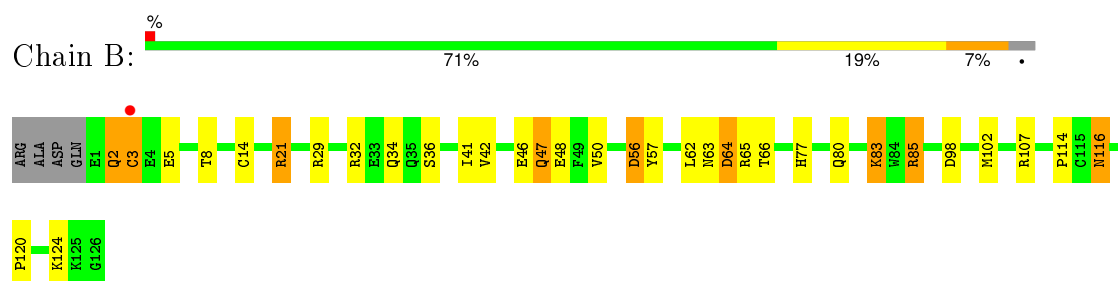
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ($\text{RSRZ} > 2$). 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: Tenascin-R



• Molecule 2: Aggregran core protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	112.52Å 86.42Å 57.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.00 – 2.60 36.48 – 2.57	Depositor EDS
% Data completeness (in resolution range)	99.1 (39.00-2.60) 97.0 (36.48-2.57)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.69 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.209 , 0.234 0.212 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	52.4	Xtriage
Anisotropy	0.259	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 45.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 17947 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3181	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 5.69% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.51	0/2108	0.79	6/2877 (0.2%)
2	B	0.65	1/1107 (0.1%)	0.87	3/1499 (0.2%)
All	All	0.56	1/3215 (0.0%)	0.82	9/4376 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	5	GLU	CD-OE2	7.80	1.34	1.25

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	56	ASP	CB-CG-OD2	8.14	125.62	118.30
2	B	64	ASP	CB-CG-OD2	6.36	124.02	118.30
2	B	21	ARG	NE-CZ-NH2	-6.34	117.13	120.30
1	A	269	ASP	CB-CG-OD2	5.82	123.53	118.30
1	A	235	ASP	CB-CG-OD2	5.68	123.42	118.30
1	A	243	ASP	CB-CG-OD2	5.33	123.10	118.30
1	A	5	ASP	CB-CG-OD2	5.27	123.04	118.30
1	A	191	ASP	CB-CG-OD2	5.16	122.94	118.30
1	A	14	ASP	CB-CG-OD2	5.03	122.83	118.30

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	2068	0	2042	12	1
2	B	1072	0	955	19	0
3	B	3	0	0	0	0
4	A	10	0	0	1	0
4	B	28	0	0	0	0
All	All	3181	0	2997	29	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 5.

All (29) 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:B:2:GLN:O	2:B:3:CYS:HB2	1.95	0.67
2:B:116:ASN:H	2:B:116:ASN:HD22	1.43	0.66
2:B:42:VAL:HG13	2:B:80:GLN:HE21	1.65	0.62
1:A:258:ARG:HD2	4:A:282:HOH:O	2.03	0.58
1:A:31:VAL:HG11	1:A:76:ALA:HB1	1.87	0.57
1:A:193:MET:HA	1:A:268:VAL:HG21	1.88	0.55
2:B:50:VAL:HG12	2:B:102:MET:HE1	1.86	0.55
1:A:183:ARG:NH2	2:B:56:ASP:OD1	2.39	0.54
1:A:132:ALA:O	2:B:85:ARG:HD3	2.12	0.50
2:B:83:LYS:NZ	2:B:107:ARG:NH1	2.61	0.48
1:A:112:LEU:HD11	1:A:153:LEU:HD11	1.95	0.48
2:B:46:GLU:OE2	2:B:124:LYS:NZ	2.41	0.48
2:B:41:ILE:HG21	2:B:47:GLN:HG2	1.96	0.47
2:B:114:PRO:HB3	2:B:116:ASN:HD21	1.80	0.46
1:A:15:VAL:HG23	1:A:15:VAL:O	2.15	0.46
2:B:3:CYS:HG	2:B:14:CYS:HG	1.63	0.45
2:B:116:ASN:ND2	2:B:116:ASN:H	2.13	0.45
1:A:31:VAL:CG1	1:A:76:ALA:HB1	2.46	0.44
2:B:83:LYS:HE3	2:B:107:ARG:CZ	2.48	0.43
2:B:64:ASP:OD1	2:B:98:ASP:HA	2.18	0.43
1:A:244:LEU:HD22	1:A:250:TYR:CZ	2.54	0.43
2:B:50:VAL:HG12	2:B:102:MET:CE	2.48	0.42
2:B:57:TYR:O	2:B:120:PRO:HD2	2.20	0.42
2:B:114:PRO:HB3	2:B:116:ASN:ND2	2.35	0.41
1:A:80:THR:OG1	1:A:80:THR:O	2.38	0.41
2:B:42:VAL:HG13	2:B:80:GLN:NE2	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:ILE:HD13	1:A:270:ALA:CB	2.51	0.41
1:A:202:ILE:HD13	1:A:270:ALA:HB3	2.02	0.41
2:B:63:ASN:HD22	2:B:65:ARG:H	1.69	0.41

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)
1:A:106:THR:OG1	1:A:155:ASP:OD2[2_555]	2.17	0.03

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	269/283 (95%)	253 (94%)	13 (5%)	3 (1%)	17	36
2	B	124/130 (95%)	118 (95%)	5 (4%)	1 (1%)	24	46
All	All	393/413 (95%)	371 (94%)	18 (5%)	4 (1%)	19	39

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	43	GLY
2	B	3	CYS
1	A	44	GLU
1	A	222	PRO

5.3.2 Protein sidechains [i](#)

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	233/239 (98%)	206 (88%)	27 (12%)	7	12
2	B	115/118 (98%)	100 (87%)	15 (13%)	5	9
All	All	348/357 (98%)	306 (88%)	42 (12%)	6	11

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	ILE
1	A	11	LEU
1	A	25	THR
1	A	34	ILE
1	A	71	GLU
1	A	78	ARG
1	A	80	THR
1	A	101	ARG
1	A	122	GLN
1	A	129	SER
1	A	139	VAL
1	A	148	THR
1	A	160	THR
1	A	172	SER
1	A	173	LYS
1	A	180	MET
1	A	195	THR
1	A	203	SER
1	A	231	THR
1	A	236	ARG
1	A	237	THR
1	A	245	GLU
1	A	253	SER
1	A	258	ARG
1	A	264	LEU
1	A	265	GLU
1	A	269	ASP
2	B	2	GLN
2	B	8	THR
2	B	21	ARG
2	B	29	ARG
2	B	32	ARG
2	B	34	GLN

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Mol	Chain	Res	Type
2	B	36	SER
2	B	47	GLN
2	B	48	GLU
2	B	62	LEU
2	B	66	THR
2	B	77	HIS
2	B	83	LYS
2	B	85	ARG
2	B	116	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	116	ASN
2	B	63	ASN
2	B	80	GLN
2	B	105	HIS
2	B	116	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	271/283 (95%)	0.40	25 (9%) 11 7	21, 42, 59, 79	0
2	B	126/130 (96%)	-0.15	1 (0%) 87 85	8, 17, 30, 52	0
All	All	397/413 (96%)	0.22	26 (6%) 22 16	8, 36, 57, 79	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	3	VAL	7.2
1	A	225	GLY	5.6
1	A	269	ASP	5.3
1	A	224	SER	4.9
1	A	251	ILE	4.8
1	A	226	ILE	4.3
1	A	199	GLU	3.1
1	A	222	PRO	3.1
1	A	243	ASP	3.1
1	A	221	THR	3.0
1	A	250	TYR	3.0
1	A	245	GLU	2.9
1	A	220	PHE	2.9
1	A	223	SER	2.9
1	A	246	PRO	2.8
2	B	3	CYS	2.8
1	A	172	SER	2.7
1	A	170	MET	2.7
1	A	193	MET	2.7
1	A	244	LEU	2.5
1	A	252	ILE	2.5
1	A	171	ASN	2.2
1	A	201	SER	2.2
1	A	235	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	200	THR	2.0
1	A	247	GLY	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 carbohydrates in this entry.

6.4 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
3	CA	B	127	1/1	0.99	0.15	-0.41	10,10,10,10	0
3	CA	B	128	1/1	0.95	0.13	-0.52	17,17,17,17	0
3	CA	B	129	1/1	0.98	0.07	-2.72	18,18,18,18	0

6.5 Other polymers [i](#)

There are no such residues in this entry.