



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:44 AM UTC

PDB ID : 8FXS / pdb_00008fxs
Title : Crystal structure of human pro-TGF-beta2 in complex with Nb9
Authors : Le, V.Q.; Springer, T.A.
Deposited on : 2023-01-25
Resolution : 3.15 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
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

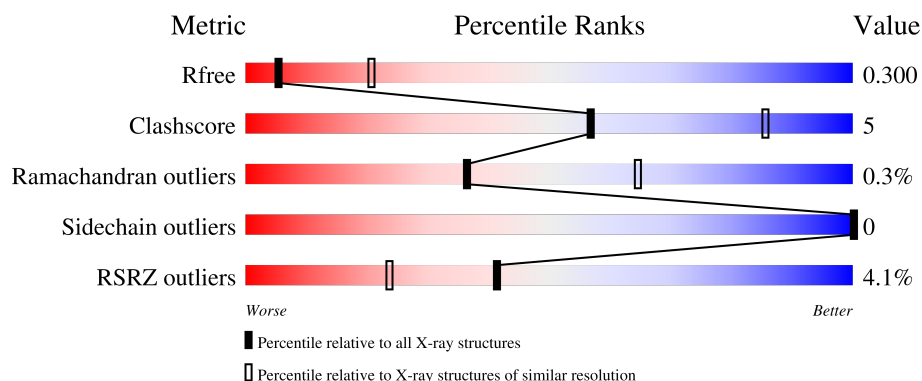
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 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	2361 (3.20-3.12)
Clashscore	190562	2486 (3.20-3.12)
Ramachandran outliers	187476	2405 (3.20-3.12)
Sidechain outliers	187428	2404 (3.20-3.12)
RSRZ outliers	180081	2361 (3.20-3.12)

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	393	
1	B	393	
2	D	124	
2	E	124	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13221 atoms, of which 6511 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 Transforming growth factor beta-2 proprotein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	307	Total	C	H	N	O	S	0	0	0
			4960	1606	2455	423	458	18			
1	B	301	Total	C	H	N	O	S	0	0	0
			4889	1577	2432	420	443	17			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	18	GLY	-	expression tag	UNP P61812
A	19	PRO	-	expression tag	UNP P61812
A	20	SER	-	expression tag	UNP P61812
A	24	SER	CYS	engineered mutation	UNP P61812
A	140	ARG	ASN	engineered mutation	UNP P61812
A	298	GLY	ARG	engineered mutation	UNP P61812
A	?	-	ARG	deletion	UNP P61812
A	?	-	LYS	deletion	UNP P61812
A	?	-	LYS	deletion	UNP P61812
A	?	-	ARG	deletion	UNP P61812
B	18	GLY	-	expression tag	UNP P61812
B	19	PRO	-	expression tag	UNP P61812
B	20	SER	-	expression tag	UNP P61812
B	24	SER	CYS	engineered mutation	UNP P61812
B	140	ARG	ASN	engineered mutation	UNP P61812
B	298	GLY	ARG	engineered mutation	UNP P61812
B	?	-	ARG	deletion	UNP P61812
B	?	-	LYS	deletion	UNP P61812
B	?	-	LYS	deletion	UNP P61812
B	?	-	ARG	deletion	UNP P61812

- Molecule 2 is a protein called Nanobody clone 9.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	D	110	Total	C	H	N	O	S	0	0	0
			1638	537	783	148	166	4			
2	E	111	Total	C	H	N	O	S	0	0	0
			1676	540	815	149	168	4			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
3	B	1	Total	C	H	N	O	0	0
			27	8	13	1	5		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	O	0	0
			2	2		
4	B	1	Total	O	0	0
			1	1		
4	E	1	Total	O	0	0
			1	1		

● Molecule 2: Nanobody clone 9



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	69.68Å 89.55Å 89.74Å 90.00° 95.00° 90.00°	Depositor
Resolution (Å)	48.27 – 3.15 48.27 – 3.15	Depositor EDS
% Data completeness (in resolution range)	98.3 (48.27-3.15) 98.3 (48.27-3.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.249 , 0.301 0.248 , 0.300	Depositor DCC
R_{free} test set	1911 reflections (9.96%)	wwPDB-VP
Wilson B-factor (Å ²)	85.0	Xtriage
Anisotropy	0.205	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 63.4	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	0.89	EDS
Total number of atoms	13221	wwPDB-VP
Average B, all atoms (Å ²)	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.56% 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

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

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	0.11	0/2563	0.29	0/3459
1	B	0.10	0/2513	0.28	0/3387
2	D	0.10	0/871	0.30	0/1175
2	E	0.08	0/878	0.27	0/1186
All	All	0.10	0/6825	0.28	0/9207

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

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	2505	2455	2467	21	1
1	B	2457	2432	2440	25	1
2	D	855	783	808	13	0
2	E	861	815	814	12	1
3	A	14	13	13	0	1
3	B	14	13	13	0	0
4	A	2	0	0	1	0
4	B	1	0	0	0	0
4	E	1	0	0	0	0
All	All	6710	6511	6555	61	2

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 (61) 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:A:81:LYS:NZ	4:A:601:HOH:O	2.18	0.75
2:E:9:GLY:HA2	2:E:18:LEU:HD21	1.69	0.73
2:E:62:SER:O	2:E:66:ARG:NH2	2.25	0.69
2:E:48:VAL:HG13	2:E:63:VAL:HG11	1.78	0.66
1:B:305:CYS:SG	1:B:315:LEU:N	2.72	0.63
2:E:82:MET:HE2	2:E:85:LEU:HD21	1.80	0.62
1:A:106:ILE:HD11	1:A:137:MET:HG3	1.82	0.61
1:B:301:ASP:OD1	1:B:302:ALA:N	2.35	0.60
1:A:397:GLU:OE1	1:B:290:ARG:NH1	2.33	0.58
1:B:159:ALA:HB3	1:B:193:ARG:HG2	1.87	0.57
1:A:30:ASP:OD1	1:A:31:GLN:N	2.37	0.56
1:A:225:HIS:O	1:A:226:CYS:O	2.24	0.55
2:D:2:VAL:HG12	2:D:3:GLN:H	1.71	0.55
1:A:171:ILE:HD11	1:A:221:LYS:HB2	1.88	0.54
2:D:23:ALA:HA	2:D:77:THR:HG22	1.90	0.54
2:D:90:THR:HG23	2:D:115:THR:HA	1.89	0.54
2:D:85:LEU:HD23	2:D:116:VAL:HG22	1.90	0.54
1:A:67:VAL:HG13	1:B:396:ILE:HD11	1.90	0.53
1:A:179:SER:HB3	1:A:180:PRO:CD	2.39	0.53
1:A:228:CYS:HA	1:B:226:CYS:HB2	1.92	0.52
1:B:300:LEU:HD13	1:B:313:CYS:O	2.09	0.52
2:D:99:ASN:OD1	2:D:100:ARG:N	2.44	0.51
1:B:387:LEU:HD13	1:B:396:ILE:HG13	1.93	0.50
1:B:346:CYS:HB2	1:B:374:PRO:HB2	1.93	0.50
2:E:2:VAL:HG12	2:E:3:GLN:H	1.77	0.50
1:B:168:LEU:HD11	1:B:220:PHE:HB3	1.93	0.49
1:B:320:ILE:O	1:B:320:ILE:HG23	2.12	0.49
1:A:167:GLU:OE1	1:A:169:TYR:OH	2.19	0.49
2:E:12:VAL:HG11	2:E:85:LEU:HD13	1.93	0.49
1:A:74:THR:OG1	1:A:103:VAL:HG11	2.12	0.49
2:D:2:VAL:HG12	2:D:3:GLN:N	2.29	0.47
1:A:377:VAL:HG21	1:B:377:VAL:HG21	1.97	0.47
2:E:90:THR:HG22	2:E:116:VAL:H	1.80	0.47
1:A:349:LEU:C	1:A:349:LEU:HD12	2.40	0.47
2:D:81:GLN:NE2	2:D:83:ASN:OD1	2.43	0.47
1:B:49:LYS:HD2	1:B:290:ARG:HA	1.97	0.46
1:A:389:TYR:CG	1:B:58:PRO:HG3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:286:LEU:HD23	1:B:291:LEU:HD21	1.99	0.44
1:A:48:LEU:CD2	1:B:397:GLU:OE1	2.66	0.44
2:E:2:VAL:HG12	2:E:3:GLN:N	2.33	0.43
1:A:102:GLU:HA	1:B:397:GLU:HG2	2.01	0.43
1:A:54:PRO:HD2	1:B:330:TRP:CD2	2.54	0.42
1:A:178:THR:O	1:A:179:SER:OG	2.30	0.42
1:A:179:SER:HB3	1:A:180:PRO:HD2	2.01	0.42
1:B:114:SER:O	2:E:45:ARG:NH1	2.53	0.42
1:B:77:LEU:HD11	1:B:148:GLU:OE1	2.20	0.42
1:B:320:ILE:HD11	1:B:326:LEU:HG	2.02	0.42
1:B:321:ASP:HB3	1:B:324:ARG:HB3	2.02	0.42
2:D:48:VAL:HG22	2:D:63:VAL:HG21	2.02	0.42
1:A:159:ALA:HB3	1:A:193:ARG:HG2	2.02	0.41
2:E:34:MET:HG2	2:E:97:ALA:HA	2.02	0.41
2:D:4:LEU:HD22	2:D:22:CYS:SG	2.60	0.41
2:D:100:ARG:HH11	2:D:100:ARG:HG3	1.85	0.41
2:E:38:ARG:HG3	2:E:91:ALA:HB3	2.01	0.41
1:B:381:LEU:HD23	1:B:404:VAL:HA	2.02	0.41
2:D:52:GLY:O	2:D:53:TYR:C	2.62	0.41
2:D:72:ASP:O	2:D:76:ASN:N	2.52	0.41
1:B:390:ILE:O	1:B:390:ILE:HG13	2.22	0.40
1:A:380:ASP:C	1:A:381:LEU:HD12	2.45	0.40
1:B:118:ILE:HB	2:E:103:TRP:HE3	1.86	0.40
2:D:48:VAL:CG2	2:D:63:VAL:HG21	2.52	0.40

All (2) 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:308:ASN:OD1	2:E:43:LYS:NZ[2_455]	2.06	0.14
1:B:212:HIS:NE2	3:A:501:NAG:O4[2_545]	2.11	0.09

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	287/393 (73%)	273 (95%)	12 (4%)	2 (1%)	18	49
1	B	282/393 (72%)	264 (94%)	18 (6%)	0	100	100
2	D	102/124 (82%)	92 (90%)	10 (10%)	0	100	100
2	E	105/124 (85%)	96 (91%)	9 (9%)	0	100	100
All	All	776/1034 (75%)	725 (93%)	49 (6%)	2 (0%)	36	64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	226	CYS
1	A	227	PRO

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	280/357 (78%)	280 (100%)	0	100	100
1	B	274/357 (77%)	274 (100%)	0	100	100
2	D	87/99 (88%)	87 (100%)	0	100	100
2	E	88/99 (89%)	88 (100%)	0	100	100
All	All	729/912 (80%)	729 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	GLN
1	A	143	ASN
1	A	225	HIS
1	A	398	GLN

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Mol	Chain	Res	Type
1	B	31	GLN
1	B	225	HIS
1	B	308	ASN
1	B	379	GLN
2	D	73	ASN
2	E	99	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 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	$\# Z > 2$
3	NAG	A	501	1	14,14,15	0.15	0	17,19,21	0.82	1 (5%)
3	NAG	B	501	1	14,14,15	0.23	0	17,19,21	0.86	1 (5%)

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
3	NAG	A	501	1	-	4/6/23/26	0/1/1/1
3	NAG	B	501	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	501	NAG	C1-O5-C5	3.09	116.33	112.19
3	A	501	NAG	C1-O5-C5	2.77	115.90	112.19

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	NAG	O5-C5-C6-O6
3	B	501	NAG	O5-C5-C6-O6
3	A	501	NAG	C4-C5-C6-O6
3	B	501	NAG	C4-C5-C6-O6
3	A	501	NAG	C1-C2-N2-C7
3	A	501	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	NAG	0	1

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	307/393 (78%)	0.36	9 (2%)	53	34	56, 87, 144, 164	0
1	B	301/393 (76%)	0.41	11 (3%)	45	26	54, 89, 147, 199	0
2	D	110/124 (88%)	0.73	9 (8%)	17	10	72, 115, 137, 163	0
2	E	111/124 (89%)	0.62	5 (4%)	38	22	72, 112, 137, 163	0
All	All	829/1034 (80%)	0.46	34 (4%)	41	24	54, 97, 145, 199	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	55	SER	4.6
1	A	372	ALA	3.8
2	D	24	ALA	3.5
1	B	371	SER	3.4
1	A	32	PHE	3.3
1	A	309	VAL	3.1
1	A	116	ASN	2.9
1	B	32	PHE	2.9
1	B	309	VAL	2.8
2	E	55	SER	2.8
2	D	102	GLY	2.8
2	E	53	TYR	2.8
2	D	101	ASP	2.7
1	B	374	PRO	2.6
1	B	293	SER	2.5
1	A	349	LEU	2.5
2	D	106	TYR	2.4
1	B	305	CYS	2.4
1	B	372	ALA	2.3
1	B	349	LEU	2.3
2	E	102	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	27	THR	2.2
1	B	302	ALA	2.2
2	D	53	TYR	2.2
2	E	65	SER	2.2
1	A	255	GLY	2.2
1	A	300	LEU	2.2
1	A	302	ALA	2.2
2	E	112	THR	2.1
1	B	255	GLY	2.1
1	A	54	PRO	2.1
1	B	254	ASP	2.1
2	D	104	TYR	2.1
2	D	21	SER	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](#)

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
3	NAG	A	501	14/15	0.67	0.15	79,112,136,139	0
3	NAG	B	501	14/15	0.71	0.16	80,104,126,139	0

6.5 Other polymers [i](#)

There are no such residues in this entry.