



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:48 AM UTC

PDB ID : 7ASC / pdb_00007asc
Title : TGFBIP mutant A546T
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Deposited on : 2020-10-27
Resolution : 4.80 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
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

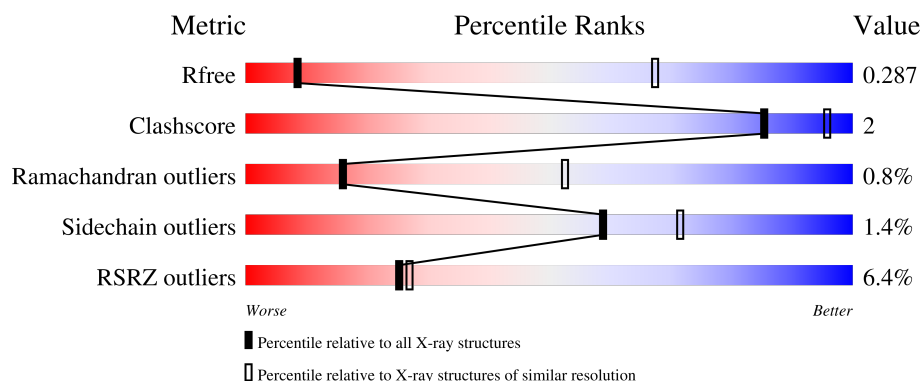
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.80 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	1018 (5.66-3.94)
Clashscore	190562	1001 (5.60-3.98)
Ramachandran outliers	187476	1104 (5.70-3.90)
Sidechain outliers	187428	1085 (5.70-3.90)
RSRZ outliers	180081	1013 (5.66-3.94)

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	594	6% 91% 8% .
1	B	594	6% 91% 8% ..

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 9022 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 Transforming growth factor-beta-induced protein ig-h3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	588	Total	C	N	O	S	0	0	0
			4511	2837	786	865	23			
1	B	588	Total	C	N	O	S	0	0	0
			4511	2837	786	865	23			

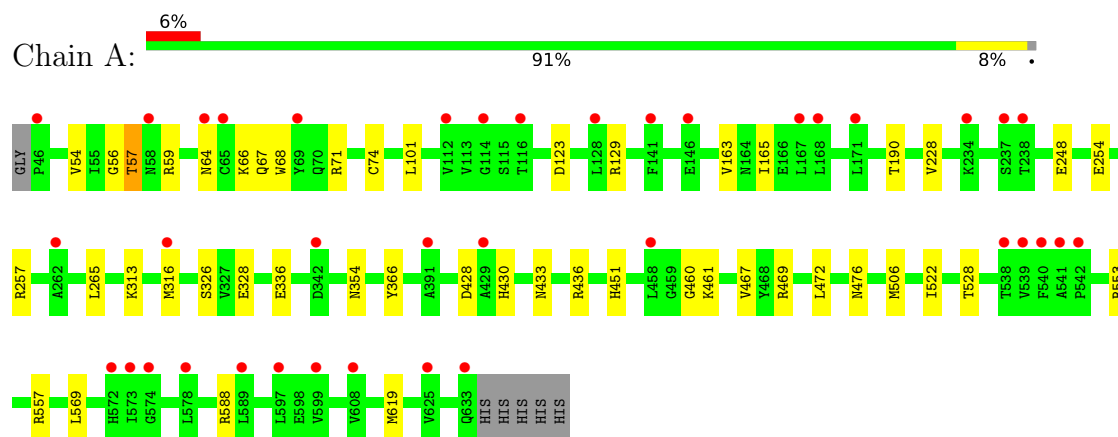
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	546	THR	ALA	engineered mutation	UNP Q15582
A	634	HIS	-	expression tag	UNP Q15582
A	635	HIS	-	expression tag	UNP Q15582
A	636	HIS	-	expression tag	UNP Q15582
A	637	HIS	-	expression tag	UNP Q15582
A	638	HIS	-	expression tag	UNP Q15582
B	546	THR	ALA	engineered mutation	UNP Q15582
B	634	HIS	-	expression tag	UNP Q15582
B	635	HIS	-	expression tag	UNP Q15582
B	636	HIS	-	expression tag	UNP Q15582
B	637	HIS	-	expression tag	UNP Q15582
B	638	HIS	-	expression tag	UNP Q15582

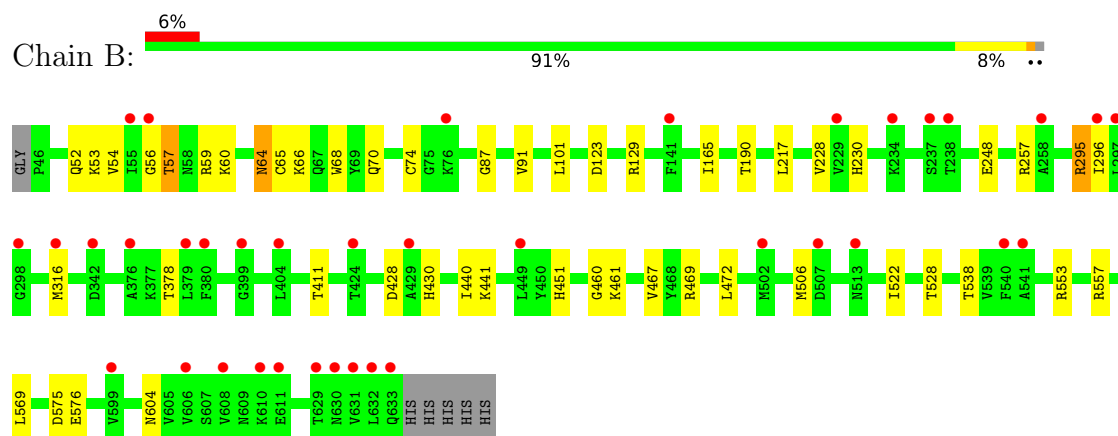
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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 ($RSRZ > 2$). 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: Transforming growth factor-beta-induced protein ig-h3



- Molecule 1: Transforming growth factor-beta-induced protein ig-h3



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	206.76Å 206.76Å 127.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	80.31 – 4.80 80.31 – 4.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (80.31-4.80) 99.9 (80.31-4.80)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.23 (at 4.87Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.250 , 0.259 0.274 , 0.287	Depositor DCC
R_{free} test set	1401 reflections (9.99%)	wwPDB-VP
Wilson B-factor (Å ²)	279.5	Xtriage
Anisotropy	0.008	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 386.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	9022	wwPDB-VP
Average B, all atoms (Å ²)	332.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.50% 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

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	0.34	0/4584	0.89	1/6224 (0.0%)
1	B	0.36	0/4584	0.89	5/6224 (0.1%)
All	All	0.35	0/9168	0.89	6/12448 (0.0%)

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
1	A	0	2
1	B	0	2
All	All	0	4

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	295	ARG	N-CA-C	9.60	121.50	111.14
1	B	296	ILE	N-CA-C	6.33	116.48	110.53
1	A	67	GLN	CA-CB-CG	5.45	125.00	114.10
1	B	441	LYS	CA-C-N	5.43	131.90	121.54
1	B	441	LYS	C-N-CA	5.43	131.90	121.54
1	B	64	ASN	N-CA-C	5.28	122.04	110.80

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	56	GLY	Peptide
1	A	57	THR	Peptide
1	B	56	GLY	Peptide

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Mol	Chain	Res	Type	Group
1	B	57	THR	Peptide

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	4511	0	4571	23	0
1	B	4511	0	4571	23	0
All	All	9022	0	9142	40	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 2.

All (40) 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:469:ARG:HH12	1:B:101:LEU:HB2	1.49	0.75
1:A:248:GLU:HA	1:A:257:ARG:HH11	1.56	0.70
1:A:66:LYS:NZ	1:A:68:TRP:O	2.23	0.69
1:B:248:GLU:HA	1:B:257:ARG:HH11	1.58	0.68
1:A:588:ARG:HH12	1:B:91:VAL:HG22	1.61	0.65
1:A:101:LEU:HB2	1:B:469:ARG:HH12	1.62	0.64
1:A:101:LEU:HB2	1:B:469:ARG:NH1	2.14	0.62
1:B:506:MET:HE2	1:B:528:THR:HG23	1.82	0.61
1:B:66:LYS:NZ	1:B:68:TRP:O	2.31	0.60
1:A:469:ARG:NH1	1:B:101:LEU:HB2	2.17	0.59
1:A:326:SER:OG	1:A:336:GLU:OE2	2.14	0.58
1:B:52:GLN:NE2	1:B:70:GLN:O	2.40	0.54
1:B:248:GLU:HA	1:B:257:ARG:HD3	1.88	0.54
1:B:295:ARG:NH1	1:B:378:THR:HG23	2.23	0.53
1:A:57:THR:HB	1:A:59:ARG:H	1.73	0.53
1:B:451:HIS:NE2	1:B:467:VAL:O	2.43	0.51
1:A:428:ASP:OD2	1:A:430:HIS:HB3	2.11	0.50
1:B:428:ASP:OD2	1:B:430:HIS:HB3	2.12	0.50
1:B:553:ARG:HD2	1:B:557:ARG:HD3	1.93	0.50
1:A:553:ARG:HD2	1:A:557:ARG:HD3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:451:HIS:NE2	1:A:467:VAL:O	2.45	0.48
1:B:53:LYS:HG3	1:B:60:LYS:HG2	1.96	0.48
1:A:506:MET:HE2	1:A:528:THR:HG23	1.97	0.47
1:B:538:THR:OG1	1:B:576:GLU:O	2.33	0.46
1:B:57:THR:HB	1:B:59:ARG:H	1.81	0.46
1:B:522:ILE:HD13	1:B:569:LEU:HD13	1.97	0.46
1:A:254:GLU:HG3	1:A:257:ARG:HH21	1.81	0.46
1:B:316:MET:HE2	1:B:316:MET:HB3	1.85	0.45
1:A:123:ASP:CG	1:A:129:ARG:HH11	2.25	0.45
1:B:217:LEU:HD11	1:B:230:HIS:HB3	1.99	0.45
1:B:123:ASP:CG	1:B:129:ARG:HH11	2.25	0.45
1:A:354:ASN:HB2	1:A:366:TYR:HB2	1.99	0.45
1:B:411:THR:HB	1:B:440:ILE:HB	2.00	0.44
1:A:265:LEU:HD23	1:A:265:LEU:HA	1.90	0.44
1:A:313:LYS:NZ	1:A:328:GLU:HB3	2.34	0.43
1:A:522:ILE:HD13	1:A:569:LEU:HD13	2.01	0.43
1:A:316:MET:HE2	1:A:316:MET:HB3	1.84	0.42
1:A:469:ARG:NH1	1:B:87:GLY:HA2	2.35	0.42
1:A:476:ASN:HB3	1:A:619:MET:HE3	2.01	0.41
1:A:433:ASN:OD1	1:A:436:ARG:NH2	2.55	0.40

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	586/594 (99%)	562 (96%)	20 (3%)	4 (1%)	18	55
1	B	586/594 (99%)	560 (96%)	21 (4%)	5 (1%)	14	49
All	All	1172/1188 (99%)	1122 (96%)	41 (4%)	9 (1%)	16	52

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	64	ASN
1	B	64	ASN
1	A	74	CYS
1	A	165	ILE
1	B	74	CYS
1	B	165	ILE
1	A	460	GLY
1	B	460	GLY
1	B	65	CYS

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	501/506 (99%)	494 (99%)	7 (1%)	59	71
1	B	501/506 (99%)	494 (99%)	7 (1%)	59	71
All	All	1002/1012 (99%)	988 (99%)	14 (1%)	59	71

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

Mol	Chain	Res	Type
1	A	54	VAL
1	A	71	ARG
1	A	163	VAL
1	A	190	THR
1	A	228	VAL
1	A	461	LYS
1	A	472	LEU
1	B	54	VAL
1	B	190	THR
1	B	228	VAL
1	B	461	LYS
1	B	472	LEU
1	B	575	ASP
1	B	604	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	197	ASN
1	A	222	HIS
1	A	223	HIS
1	A	294	ASN
1	A	443	GLN
1	A	453	GLN
1	A	630	ASN
1	B	244	GLN
1	B	294	ASN
1	B	470	ASN
1	B	523	GLN
1	B	604	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 oligosaccharides 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	588/594 (98%)	0.44	38 (6%) 25 26	258, 325, 438, 524	0
1	B	588/594 (98%)	0.33	37 (6%) 26 27	256, 314, 407, 537	0
All	All	1176/1188 (98%)	0.39	75 (6%) 25 27	256, 321, 432, 537	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	541	ALA	6.5
1	A	540	PHE	6.1
1	A	64	ASN	5.1
1	B	316	MET	4.6
1	A	69	TYR	4.5
1	B	540	PHE	4.2
1	B	611	GLU	4.1
1	A	539	VAL	3.9
1	A	141	PHE	3.7
1	A	168	LEU	3.7
1	B	296	ILE	3.6
1	A	429	ALA	3.5
1	B	376	ALA	3.4
1	B	297	LEU	3.3
1	A	342	ASP	3.3
1	A	167	LEU	3.2
1	B	298	GLY	3.2
1	B	630	ASN	3.2
1	A	238	THR	3.1
1	B	541	ALA	3.1
1	A	578	LEU	3.0
1	A	573	ILE	3.0
1	B	238	THR	3.0
1	A	574	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	65	CYS	2.9
1	A	538	THR	2.9
1	A	171	LEU	2.9
1	A	599	VAL	2.8
1	B	55	ILE	2.8
1	A	316	MET	2.8
1	B	342	ASP	2.8
1	A	542	PRO	2.7
1	B	237	SER	2.6
1	B	608	VAL	2.6
1	B	502	MET	2.6
1	B	76	LYS	2.6
1	A	58	ASN	2.6
1	A	625	VAL	2.6
1	B	606	VAL	2.5
1	A	589	LEU	2.5
1	B	229	VAL	2.5
1	B	633	GLN	2.5
1	B	429	ALA	2.5
1	B	424	THR	2.4
1	A	633	GLN	2.3
1	B	629	THR	2.3
1	B	399	GLY	2.3
1	A	112	VAL	2.3
1	A	608	VAL	2.3
1	A	572	HIS	2.3
1	A	46	PRO	2.2
1	A	237	SER	2.2
1	B	404	LEU	2.2
1	A	128	LEU	2.2
1	B	56	GLY	2.2
1	B	379	LEU	2.2
1	B	599	VAL	2.2
1	A	114	GLY	2.1
1	B	507	ASP	2.1
1	A	597	LEU	2.1
1	A	146	GLU	2.1
1	B	380	PHE	2.1
1	B	632	LEU	2.1
1	B	513	ASN	2.1
1	A	116	THR	2.1
1	A	234	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	458	LEU	2.1
1	B	610	LYS	2.1
1	A	262	ALA	2.1
1	A	391	ALA	2.1
1	B	631	VAL	2.1
1	B	234	LYS	2.0
1	B	141	PHE	2.0
1	B	258	ALA	2.0
1	B	449	LEU	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.