WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Sep 3, 2024 – 10:04 AM EDT

PDB ID	:	8GDT
Title	:	Heligmosomoides polygyrus TGF-beta Mimic 6 Domain 3 (TGM6-D3) Bound to Human TGF-beta Type II Receptor Extracellular Domain
Authors	:	White, S.E.; Schwartze, T.A.; Hinck, A.P.
Deposited on	:	2023-03-06
Resolution	:	1.40 Å(reported)

The following versions of software and data (see references (i)) were used in the production of this report:

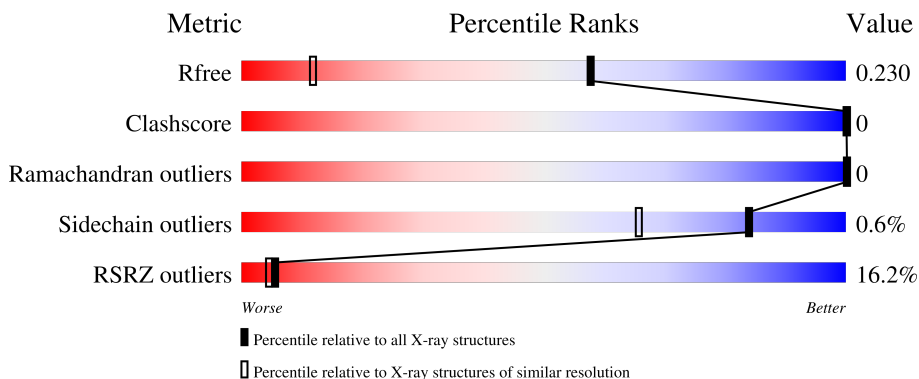|		
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.002 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.38.3

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 1.40 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	Percentile Ranks	Value
Rfree		0.230
Clashscore		0
Ramachandran outliers		0
Sidechain outliers		0.6%
RSRZ outliers		16.2%

Worse   *Better*

▮ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	2247 (1.40-1.40)
Clashscore	180529	2446 (1.40-1.40)
Ramachandran outliers	177936	2398 (1.40-1.40)
Sidechain outliers	177891	2397 (1.40-1.40)
RSRZ outliers	164620	2246 (1.40-1.40)

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 <=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	118	8% / 88% / 11%
2	B	92	22% / 86% / 13%

2 Entry composition ⓘ

There are 7 unique types of molecules in this entry. The entry contains 3113 atoms, of which 1445 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 TGF-beta receptor type-2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	105	Total	C	H	N	O	S	21	4	0
			1657	528	813	136	163	17			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	37	MET	-	initiating methionine	UNP P37173

- Molecule 2 is a protein called Transforming growth factor beta mimic 6.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	80	Total	C	H	N	O	S	23	1	0
			1258	413	598	116	127	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	11	GLY	-	expression tag	UNP A0A2P1IQ80
B	12	SER	-	expression tag	UNP A0A2P1IQ80
B	13	GLY	-	expression tag	UNP A0A2P1IQ80
B	14	THR	-	expression tag	UNP A0A2P1IQ80

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

GOL

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 14	C 3	H 8	O 3	2	0
3	B	1	Total 14	C 3	H 8	O 3	2	0

- Molecule 4 is CACODYLATE ION (three-letter code: CAC) (formula: $C_2H_6AsO_2$).

CAC

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 11	As 1	C 2	H 6	O 2	0	0
4	A	1	Total 11	As 1	C 2	H 6	O 2	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	As	C	H	O	0	0
			11	1	2	6	2		

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Na	0	0
			1	1		

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Cl	0	0
			1	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	83	Total	O	0	0
			83	83		
7	B	52	Total	O	0	0
			52	52		

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.
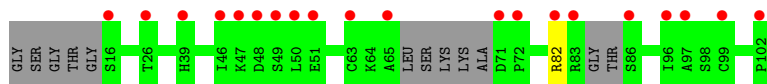
• Molecule 1: TGF-beta receptor type-2

Chain A:
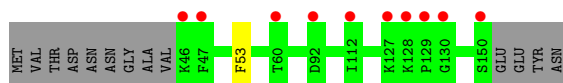
• Molecule 2: Transforming growth factor beta mimic 6

Chain B:

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	56.04Å 128.39Å 29.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.25 – 1.40 42.25 – 1.40	Depositor EDS
% Data completeness (in resolution range)	98.3 (42.25-1.40) 98.3 (42.25-1.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.50 (at 1.40Å)	Xtriage
Refinement program	REFMAC 5.8.0411	Depositor
R, R_{free}	0.218 , 0.230 0.219 , 0.230	Depositor DCC
R_{free} test set	2092 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å^2)	16.9	Xtriage
Anisotropy	0.665	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.44 , 44.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	3113	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.19% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.
[2] Theoretical values of $< \|L\| >$, $< L^2 >$ 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: CL, NA, CAC, GOL

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	0.61	0/873	0.79	0/1175
2	B	0.54	0/685	0.79	0/932
All	All	0.58	0/1558	0.79	0/2107

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
2	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	82	ARG	Sidechain

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	844	813	814	0	0
2	B	660	598	593	0	0
3	A	6	8	8	0	0
3	B	6	8	8	0	0
4	A	15	18	0	0	0
5	B	1	0	0	0	0
6	B	1	0	0	0	0
7	A	83	0	0	0	0
7	B	52	0	0	0	0
All	All	1668	1445	1423	0	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 0.

There are no clashes within the asymmetric unit.

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	107/118 (91%)	104 (97%)	3 (3%)	0	100	100
2	B	75/92 (82%)	73 (97%)	2 (3%)	0	100	100
All	All	182/210 (87%)	177 (97%)	5 (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	105/112 (94%)	104 (99%)	1 (1%)	73	49
2	B	71/77 (92%)	71 (100%)	0	100	100
All	All	176/189 (93%)	175 (99%)	1 (1%)	84	66

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	PHE

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

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 ⓘ

Of 7 ligands modelled in this entry, 2 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	#$|Z| > 2$
4	CAC	A	203	-	2,4,4	0.60	0	2,6,6	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$\|Z\|$ > 2	Counts	RMSZ	#$\|Z\|$ > 2
4	CAC	A	202	-	2,4,4	0.47	0	2,6,6	0.39	0
3	GOL	A	201	-	5,5,5	0.12	0	5,5,5	0.22	0
3	GOL	B	201	-	5,5,5	0.08	0	5,5,5	0.26	0
4	CAC	A	204	-	2,4,4	0.67	0	2,6,6	1.51	0

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	GOL	B	201	-	-	0/4/4/4	-
3	GOL	A	201	-	-	1/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	201	GOL	O2-C2-C3-O3

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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(Å²)	Q<0.9
1	A	105/118 (88%)	0.50	10 (9%)	15	13	10, 19, 40, 125	4 (3%)
2	B	80/92 (86%)	1.71	20 (25%)	2	2	15, 29, 66, 99	1 (1%)
All	All	185/210 (88%)	1.02	30 (16%)	5	4	10, 23, 56, 125	5 (2%)

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	46	LYS	10.2
2	B	83	ARG	7.3
1	A	47	PHE	7.2
2	B	86	SER	6.1
2	B	47	LYS	5.0
2	B	50	LEU	4.9
2	B	82	ARG	4.8
2	B	49	SER	4.8
1	A	129	PRO	4.8
2	B	71	ASP	4.5
2	B	51	GLU	4.3
2	B	65	ALA	4.3
1	A	150	SER	4.1
2	B	102	PRO	4.0
1	A	128	LYS	3.9
2	B	46	ILE	3.8
1	A	92	ASP	3.4
2	B	96	ILE	3.3
2	B	16	SER	3.2
1	A	130	GLY	2.8
2	B	97	ALA	2.8
2	B	63	CYS	2.7
2	B	72	PRO	2.6
1	A	60	THR	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	99	CYS	2.3
1	A	112	ILE	2.2
2	B	39	HIS	2.2
2	B	26	THR	2.1
1	A	127	LYS	2.1
2	B	48	ASP	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 monosaccharides in this entry.

6.4 Ligands ⓘ

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(Å^2)	Q<0.9
4	CAC	A	203	5/5	0.59	0.40	15,36,43,55	11
4	CAC	A	204	5/5	0.72	0.27	21,24,34,55	11
3	GOL	A	201	6/6	0.79	0.14	20,20,20,20	2
3	GOL	B	201	6/6	0.83	0.13	20,20,20,20	2
6	CL	B	203	1/1	0.91	0.25	30,30,30,30	0
5	NA	B	202	1/1	0.96	0.09	30,30,30,30	0
4	CAC	A	202	5/5	0.97	0.13	23,27,30,32	11

6.5 Other polymers ⓘ

There are no such residues in this entry.