WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 10, 2023 – 01:01 AM EDT

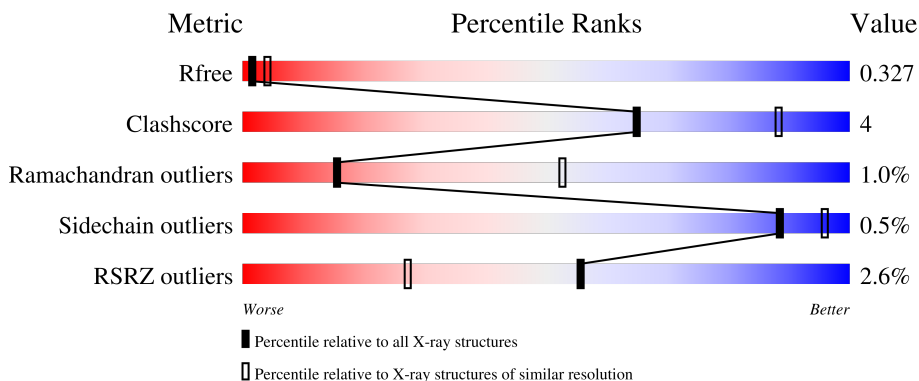|		
PDB ID	:	7MRZ
Title	:	Structure of GDF11 bound to fused ActRIIB-ECD and Alk4-ECD with Anti-ActRIIB Fab fragment
Authors	:	Goebel, E.J.; Kattamuri, C.; Gipson, G.R.; Thompson, T.B.
Deposited on	:	2021-05-10
Resolution	:	3.00 Å(reported)

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 3.00 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		0.327
Clashscore		4
Ramachandran outliers		1.0%
Sidechain outliers		0.5%
RSRZ outliers		2.6%

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}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	109	91% — 7% ··
2	C	254	61% — 6% · — 33%
3	X	222	90% — 10%
4	Y	221	94% — 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	SO4	X	301	-	-	X	-

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 10892 atoms, of which 5305 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 Growth/differentiation factor 11.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	108	Total	C	H	N	O	S	0	7	0
			1661	541	802	147	157	14			

- Molecule 2 is a protein called Activin receptor type-2B,Activin receptor type-1B.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	171	Total	C	H	N	O	S	0	0	0
			2582	835	1222	233	270	22			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1007	GLY	-	linker	UNP Q13705
C	1008	GLY	-	linker	UNP Q13705
C	1009	GLY	-	linker	UNP Q13705
C	1010	THR	-	linker	UNP Q13705
C	1011	HIS	-	linker	UNP Q13705
C	1012	THR	-	linker	UNP Q13705
C	1013	CYS	-	linker	UNP Q13705
C	1014	PRO	-	linker	UNP Q13705
C	1015	PRO	-	linker	UNP Q13705
C	1016	CYS	-	linker	UNP Q13705
C	1017	PRO	-	linker	UNP Q13705
C	1018	ALA	-	linker	UNP Q13705
C	1019	PRO	-	linker	UNP Q13705
C	1020	GLU	-	linker	UNP Q13705
C	1021	LEU	-	linker	UNP Q13705
C	1022	LEU	-	linker	UNP Q13705
C	1023	GLY	-	linker	UNP Q13705
C	1067	ALA	ARG	conflict	UNP P36896
C	1127	THR	-	expression tag	UNP P36896
C	1128	GLY	-	expression tag	UNP P36896

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1129	GLY	-	expression tag	UNP P36896
C	1130	GLY	-	expression tag	UNP P36896
C	1131	THR	-	expression tag	UNP P36896
C	1132	HIS	-	expression tag	UNP P36896
C	1133	THR	-	expression tag	UNP P36896
C	1134	CYS	-	expression tag	UNP P36896
C	1135	PRO	-	expression tag	UNP P36896
C	1136	PRO	-	expression tag	UNP P36896
C	1137	CYS	-	expression tag	UNP P36896
C	1138	PRO	-	expression tag	UNP P36896
C	1139	ALA	-	expression tag	UNP P36896
C	1140	PRO	-	expression tag	UNP P36896
C	1141	GLU	-	expression tag	UNP P36896
C	1142	LEU	-	expression tag	UNP P36896
C	1143	LEU	-	expression tag	UNP P36896
C	1144	GLY	-	expression tag	UNP P36896

- Molecule 3 is a protein called Fab Heavy Chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
3	X	222	3265	1036	1618	272	333	6	0	0	0

- Molecule 4 is a protein called Fab Light Chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
4	Y	221	3352	1065	1650	286	345	6	0	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

NAG

O6
OH

O1
HO

O5
O

C6

C1(R) C5(R)

C2(R) C4(S)
C3(R)

N2
HN

OH
O4

C7
OH
O3

C8
O
O7
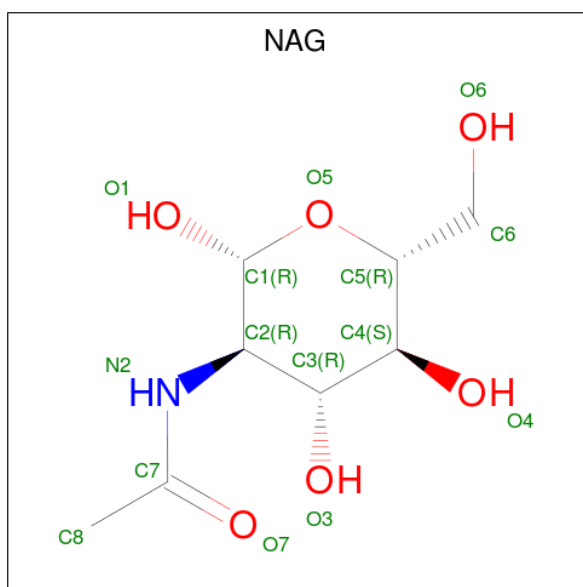
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
5	C	1	27	8	13	1	5	0	0

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

SO4

O1
O

O3 O⁻ — S — O⁻ O4
S

O
O2
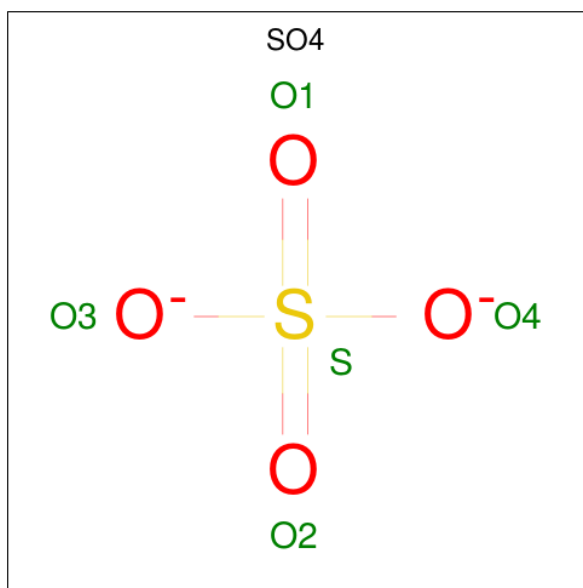
| Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
6	X	1	5	4	1	0	0

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.
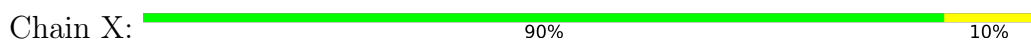
- Molecule 1: Growth/differentiation factor 11
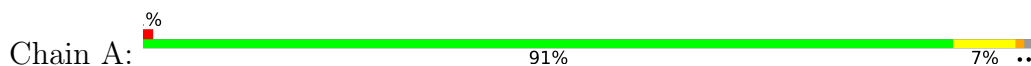
Chain A:

- Molecule 2: Activin receptor type-2B,Activin receptor type-1B
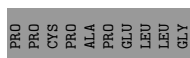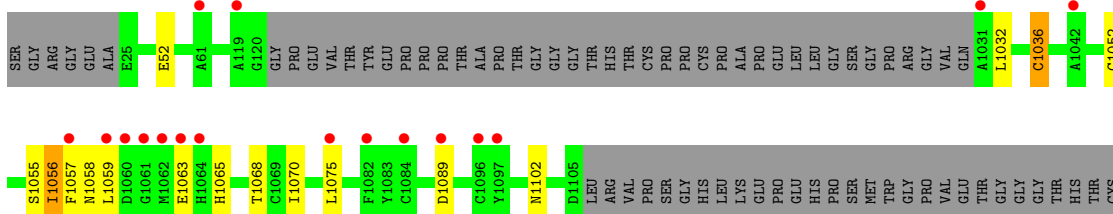
Chain C:

- Molecule 3: Fab Heavy Chain

Chain X:

- Molecule 4: Fab Light Chain

Chain Y:

4   Data and refinement statistics   (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α, β, γ	68.26Å 68.26Å 990.38Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.06 – 3.00 48.06 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.7 (48.06-3.00) 98.7 (48.06-3.00)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.34 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.288 , 0.327 0.288 , 0.327	Depositor DCC
R_{free} test set	1411 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å^2)	89.2	Xtriage
Anisotropy	0.081	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 60.6	EDS
L-test for twinning[2]	$< |L| > = 0.35$, $< L^2 > = 0.17$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	10892	wwPDB-VP
Average B, all atoms (Å^2)	108.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.17% 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: NAG, SO4

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	0/884	0.46	0/1194
2	C	0.27	0/1389	0.48	0/1881
3	X	0.26	0/1687	0.48	0/2302
4	Y	0.25	0/1739	0.45	0/2362
All	All	0.26	0/5699	0.47	0/7739

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	859	802	795	5	0
2	C	1360	1222	1223	13	0
3	X	1647	1618	1623	16	0
4	Y	1702	1650	1650	9	0
5	C	14	13	13	3	0
6	X	5	0	0	3	0
All	All	5587	5305	5304	45	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 4.

The worst 5 of 45 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)
4:Y:354:LEU:O	4:Y:412:LYS:NZ	2.05	0.90
2:C:1055:SER:O	2:C:1056:ILE:HG23	1.72	0.89
5:C:301:NAG:H3	5:C:301:NAG:H83	1.66	0.77
3:X:12:VAL:HG21	3:X:18:LEU:HD13	1.78	0.66
2:C:1056:ILE:HG21	2:C:1065:HIS:CA	2.25	0.66

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	106/109 (97%)	94 (89%)	10 (9%)	2 (2%)	8	36
2	C	167/254 (66%)	145 (87%)	21 (13%)	1 (1%)	25	64
3	X	220/222 (99%)	195 (89%)	22 (10%)	3 (1%)	11	43
4	Y	219/221 (99%)	205 (94%)	13 (6%)	1 (0%)	29	68
All	All	712/806 (88%)	639 (90%)	66 (9%)	7 (1%)	15	53

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	310[A]	GLU
3	X	33	SER
1	A	364	PRO
2	C	1056	ILE
3	X	86	SER

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	95/96 (99%)	94 (99%)	1 (1%)	73	90
2	C	152/216 (70%)	150 (99%)	2 (1%)	69	89
3	X	192/192 (100%)	192 (100%)	0	100	100
4	Y	193/193 (100%)	193 (100%)	0	100	100
All	All	632/697 (91%)	629 (100%)	3 (0%)	88	96

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	311	SER
2	C	1036	CYS
2	C	1089	ASP

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 monosaccharides 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	$\#|Z| > 2$
5	NAG	C	301	2	14,14,15	0.27	0	17,19,21	1.05	1 (5%)
6	SO4	X	301	-	4,4,4	0.15	0	6,6,6	0.13	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
5	NAG	C	301	2	-	5/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	301	NAG	C2-N2-C7	2.95	127.11	122.90

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	301	NAG	O5-C5-C6-O6
5	C	301	NAG	C8-C7-N2-C2
5	C	301	NAG	O7-C7-N2-C2
5	C	301	NAG	C4-C5-C6-O6
5	C	301	NAG	C3-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	301	NAG	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	X	301	SO4	3	0

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	108/109 (99%)	0.09	1 (0%)	84	63	86, 118, 156, 188	1 (0%)
2	C	171/254 (67%)	0.51	17 (9%)	7	2	80, 116, 211, 249	38 (22%)
3	X	222/222 (100%)	-0.06	1 (0%)	91	75	52, 83, 126, 255	0
4	Y	221/221 (100%)	-0.05	0	100	100	53, 77, 116, 179	0
All	All	722/806 (89%)	0.10	19 (2%)	56	27	52, 93, 162, 255	39 (5%)

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	1060	ASP	6.2
2	C	1059	LEU	5.7
2	C	1064	HIS	5.7
3	X	222	CYS	5.3
2	C	1061	GLY	4.5

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
5	NAG	C	301	14/15	0.77	0.17	101,122,147,151	0
6	SO4	X	301	5/5	0.84	0.20	115,122,135,137	0

6.5   Other polymers ⓘ

There are no such residues in this entry.

W O R L D W I D E
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