

Full wwPDB X-ray Structure Validation Report (i)

Oct 5, 2023 – 04:54 AM EDT

PDB ID	:	6UMX
Title	:	Structural basis for specific inhibition of extracellular activation of pro/latent
		myostatin by SRK-015
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Deposited on	:	2019-10-10
Resolution	:	2.79 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 (i) 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 (1)) were used in the production of this report:

MolProbity	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\hbox{-}RAY\,DIFFRACTION$

The reported resolution of this entry is 2.79 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 10849 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.

Mol	Chain	Residues		Atoms				ZeroOcc	AltConf	Trace
1	Δ	270	Total	С	Ν	0	\mathbf{S}	0	0	0
	219	2175	1390	364	404	17	0	0	0	
1	D	072	Total	С	Ν	0	S	0	0	0
	213	2101	1336	355	393	17	0	0		

• Molecule 1 is a protein called Growth/differentiation factor 8.

Chain	Residue	Modelled	Actual	Comment	Reference
А	11	HIS	-	expression tag	UNP 014793
A	12	HIS	-	expression tag	UNP 014793
А	13	HIS	-	expression tag	UNP 014793
А	14	HIS	-	expression tag	UNP 014793
А	15	HIS	-	expression tag	UNP 014793
А	16	HIS	-	expression tag	UNP 014793
A	17	GLU	-	expression tag	UNP 014793
А	18	ASN	-	expression tag	UNP 014793
A	19	LEU	-	expression tag	UNP 014793
А	20	TYR	-	expression tag	UNP 014793
А	21	PHE	-	expression tag	UNP 014793
А	22	GLN	-	expression tag	UNP 014793
А	23	SER	-	expression tag	UNP 014793
А	99	ALA	ASP	engineered mutation	UNP 014793
А	263	ALA	ARG	engineered mutation	UNP 014793
A	266	ALA	ARG	engineered mutation	UNP 014793
В	11	HIS	-	expression tag	UNP 014793
В	12	HIS	-	expression tag	UNP 014793
В	13	HIS	-	expression tag	UNP 014793
В	14	HIS	-	expression tag	UNP 014793
В	15	HIS	-	expression tag	UNP 014793
В	16	HIS	-	expression tag	UNP 014793
В	17	GLU	-	expression tag	UNP 014793
В	18	ASN	-	expression tag	UNP 014793
B	19	LEU	-	expression tag	UNP 014793

There are 32 discrepancies between the modelled and reference sequences:

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Chain	Residue	Modelled	Actual	Comment	Reference
В	20	TYR	-	expression tag	UNP 014793
В	21	PHE	-	expression tag	UNP 014793
В	22	GLN	-	expression tag	UNP 014793
В	23	SER	-	expression tag	UNP 014793
В	99	ALA	ASP	engineered mutation	UNP 014793
В	263	ALA	ARG	engineered mutation	UNP 014793
В	266	ALA	ARG	engineered mutation	UNP 014793

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• Molecule 2 is a protein called GL29H4-16 Fab Light Chain, GL29H4-16 Fab Light Chain.

Mol	Chain	Residues		Atoms				ZeroOcc	AltConf	Trace
2	L	214	Total	С	Ν	0	S	0	0	0
		1583	985	266	327	5	Ŭ	U U		
0	1	210	Total	С	Ν	0	\mathbf{S}	0	0	0
		210	1555	969	261	321	4	0	0	

• Molecule 3 is a protein called GL29H4-16 Fab Heavy Chain, GL29H4-16 Fab Heavy Chain.

Mol	Chain	Residues		Atoms				ZeroOcc	AltConf	Trace
2	Ц	226	Total	С	Ν	0	S	0	0	0
3 11	220	1718	1090	293	328	7	0	0	0	
2	h	225	Total	С	Ν	0	S	0	0	0
	223	1709	1084	291	327	7		U	0	

• Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	h	1	Total 6	$\begin{array}{c} \mathrm{C} \\ \mathrm{3} \end{array}$	O 3	0	0

• Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	Н	1	Total O 1 1	0	0
5	1	1	Total O 1 1	0	0

MolProbity and EDS failed to run properly - this section is therefore empty.



3 Data and refinement statistics (i)

Property	Value	Source	
Space group	P 21 21 21	Depositor	
Cell constants	59.62Å 110.01Å 293.27Å	Depositor	
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor	
Resolution (Å)	40.43 - 2.79	Depositor	
% Data completeness	99.8(40.43-2.79)	Depositor	
(in resolution range)	55.0 (40.45-2.15)	Depositor	
R _{merge}	(Not available)	Depositor	
R_{sym}	(Not available)	Depositor	
$< I/\sigma(I) > 1$	2.10 (at 2.81\AA)	Xtriage	
Refinement program	REFMAC 5.8.0189	Depositor	
R, R_{free}	0.217 , 0.264	Depositor	
Wilson B-factor $(Å^2)$	81.1	Xtriage	
Anisotropy	0.325	Xtriage	
L-test for twinning ²	$ < L >=0.49, < L^2>=0.32$	Xtriage	
Estimated twinning fraction	No twinning to report.	Xtriage	
Total number of atoms	10849	wwPDB-VP	
Average B, all atoms $(Å^2)$	97.0	wwPDB-VP	

EDS failed to run properly - this section is therefore incomplete.

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.96% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

4 Model quality (i)

4.1 Standard geometry (i)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts (i)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles (i)

4.3.1 Protein backbone (i)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains (i)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA (i)

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

4.5 Carbohydrates (i)

There are no monosaccharides in this entry.

4.6 Ligand geometry (i)

1 ligand is 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	Dec	Tiple	B	ond leng	gths	Bond angles		
NIOI	Type	Unam	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
4	GOL	h	301	-	5,5,5	0.89	0	$5,\!5,\!5$	0.98	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
4	GOL	h	301	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	h	301	GOL	O1-C1-C2-O2
4	h	301	GOL	O1-C1-C2-C3
4	h	301	GOL	C1-C2-C3-O3
4	h	301	GOL	O2-C2-C3-O3

There are no ring outliers.

No monomer is involved in short contacts.

4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



5 Fit of model and data (i)

5.1 Protein, DNA and RNA chains (i)

EDS failed to run properly - this section is therefore empty.

5.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS failed to run properly - this section is therefore empty.

5.3 Carbohydrates (i)

EDS failed to run properly - this section is therefore empty.

5.4 Ligands (i)

EDS failed to run properly - this section is therefore empty.

5.5 Other polymers (i)

EDS failed to run properly - this section is therefore empty.

