



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:01 PM UTC

PDB ID : 6F2O / pdb_00006f2o
Title : Crystal structure of mouse SALM5 adhesion protein extracellular LRR-Ig domain fragment
Authors : Karki, S.; Paudel, P.; Sele, C.; Kajander, T.
Deposited on : 2017-11-25
Resolution : 3.00 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

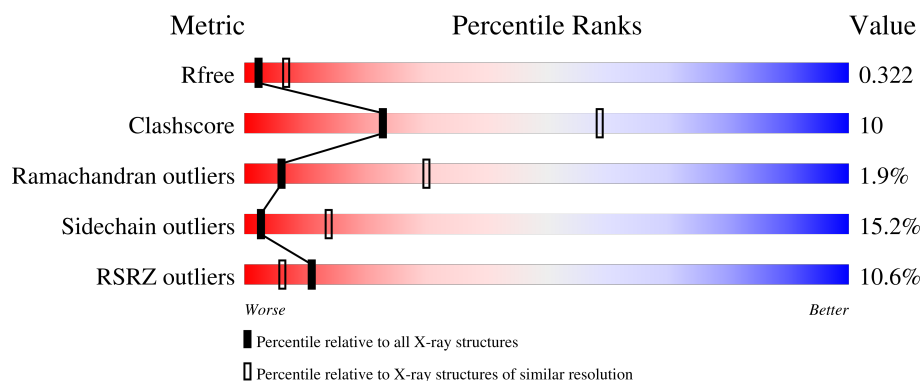
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (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 $\leq 5\%$. 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	388	9% 57% 24% • 15%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2457 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 Leucine-rich repeat and fibronectin type-III domain-containing protein 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	330	Total	C	N	O	S	0	0	0
			2457	1551	424	467	15			

There are 29 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	MET	-	initiating methionine	UNP Q8BXA0
A	-3	PRO	-	expression tag	UNP Q8BXA0
A	-2	LEU	-	expression tag	UNP Q8BXA0
A	-1	LEU	-	expression tag	UNP Q8BXA0
A	0	LEU	-	expression tag	UNP Q8BXA0
A	1	LEU	-	expression tag	UNP Q8BXA0
A	2	LEU	-	expression tag	UNP Q8BXA0
A	3	PRO	-	expression tag	UNP Q8BXA0
A	4	LEU	-	expression tag	UNP Q8BXA0
A	5	LEU	-	expression tag	UNP Q8BXA0
A	6	TRP	-	expression tag	UNP Q8BXA0
A	7	ALA	-	expression tag	UNP Q8BXA0
A	8	GLY	-	expression tag	UNP Q8BXA0
A	9	ALA	-	expression tag	UNP Q8BXA0
A	10	LEU	-	expression tag	UNP Q8BXA0
A	11	ALA	-	expression tag	UNP Q8BXA0
A	12	MET	-	expression tag	UNP Q8BXA0
A	13	ASP	-	expression tag	UNP Q8BXA0
A	14	LYS	-	expression tag	UNP Q8BXA0
A	15	LEU	-	expression tag	UNP Q8BXA0
A	16	GLU	-	expression tag	UNP Q8BXA0
A	17	PHE	-	expression tag	UNP Q8BXA0
A	377	GLY	-	expression tag	UNP Q8BXA0
A	378	SER	-	expression tag	UNP Q8BXA0
A	379	GLU	-	expression tag	UNP Q8BXA0
A	380	VAL	-	expression tag	UNP Q8BXA0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	381	LEU	-	expression tag	UNP Q8BXA0
A	382	PHE	-	expression tag	UNP Q8BXA0
A	383	GLN	-	expression tag	UNP Q8BXA0

- Molecule 1: Leucine-rich repeat and fibronectin type-III domain-containing protein 5



4 Data and refinement statistics

Property	Value	Source
Space group	F 41 3 2	Depositor
Cell constants a, b, c, α , β , γ	254.01 Å 254.01 Å 254.01 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.94 – 3.00 29.94 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.1 (29.94-3.00) 98.9 (29.94-3.00)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.95 (at 3.00 Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.252 , 0.282 0.271 , 0.322	Depositor DCC
R_{free} test set	721 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	131.8	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 100.6	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	0.92	EDS
Total number of atoms	2457	wwPDB-VP
Average B, all atoms (Å ²)	142.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.09% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.92	3/2505 (0.1%)	1.42	20/3427 (0.6%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	74	MET	SD-CE	-10.15	1.54	1.79
1	A	264	ALA	CA-C	8.61	1.64	1.52
1	A	118	MET	SD-CE	-5.12	1.66	1.79

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	48	ASN	CA-CB-CG	7.08	119.68	112.60
1	A	133	ASN	CA-C-N	-6.34	112.56	122.08
1	A	133	ASN	C-N-CA	-6.34	112.56	122.08
1	A	288	LEU	CD1-CG-CD2	-5.87	97.88	110.80
1	A	184	ASP	CA-CB-CG	5.83	118.43	112.60
1	A	41	GLY	CA-C-N	5.69	128.79	120.71
1	A	41	GLY	C-N-CA	5.69	128.79	120.71
1	A	68	ARG	CA-C-N	5.29	129.14	120.63
1	A	68	ARG	C-N-CA	5.29	129.14	120.63
1	A	107	ASN	CA-CB-CG	5.22	117.82	112.60
1	A	189	GLY	CA-C-N	5.22	131.50	121.54
1	A	189	GLY	C-N-CA	5.22	131.50	121.54
1	A	115	THR	CA-C-N	5.15	127.18	120.28
1	A	115	THR	C-N-CA	5.15	127.18	120.28
1	A	160	GLU	N-CA-C	-5.14	107.56	113.88
1	A	179	ASP	CA-CB-CG	5.13	117.73	112.60
1	A	246	CYS	CA-C-N	5.05	129.22	120.58
1	A	246	CYS	C-N-CA	5.05	129.22	120.58
1	A	163	PRO	CA-C-N	5.01	127.00	120.28
1	A	163	PRO	C-N-CA	5.01	127.00	120.28

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	2457	0	2333	50	0
All	All	2457	0	2333	50	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 10.

All (50) 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:30:SER:HB3	1:A:31:PRO:CD	1.90	1.01
1:A:30:SER:HB3	1:A:31:PRO:HD3	1.40	1.01
1:A:299:LEU:HD11	1:A:302:GLN:CB	1.92	1.00
1:A:26:CYS:HB2	1:A:34:ALA:O	1.76	0.85
1:A:30:SER:CB	1:A:31:PRO:CD	2.62	0.78
1:A:299:LEU:CD1	1:A:302:GLN:CB	2.67	0.72
1:A:286:PRO:O	1:A:288:LEU:HD12	1.96	0.66
1:A:203:THR:HG22	1:A:238:GLY:H	1.62	0.65
1:A:286:PRO:O	1:A:288:LEU:CD1	2.47	0.63
1:A:274:PHE:O	1:A:275:TRP:HD1	1.82	0.62
1:A:287:PRO:HB3	1:A:316:PRO:HB3	1.82	0.60
1:A:56:LEU:HB2	1:A:77:LEU:HD11	1.83	0.60
1:A:51:ARG:HD3	1:A:74:MET:HE2	1.88	0.56
1:A:77:LEU:HD21	1:A:80:LEU:HG	1.88	0.56
1:A:203:THR:CG2	1:A:238:GLY:H	2.22	0.52
1:A:349:VAL:HA	1:A:352:THR:HG23	1.92	0.52
1:A:278:PRO:HB2	1:A:283:LEU:HD23	1.91	0.52
1:A:349:VAL:HA	1:A:352:THR:CG2	2.41	0.51
1:A:348:THR:HG22	1:A:350:LYS:H	1.75	0.51
1:A:203:THR:HG22	1:A:238:GLY:N	2.25	0.50
1:A:30:SER:CB	1:A:31:PRO:HD2	2.42	0.50
1:A:131:ASN:HA	1:A:155:SER:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:PRO:HG3	1:A:360:SER:HA	1.96	0.47
1:A:74:MET:HB3	1:A:77:LEU:HB2	1.96	0.47
1:A:238:GLY:HA2	1:A:261:GLU:HG3	1.97	0.47
1:A:300:GLU:OE1	1:A:349:VAL:HG13	2.14	0.47
1:A:244:CYS:H	1:A:265:SER:HB2	1.79	0.46
1:A:25:VAL:HG13	1:A:36:LEU:HB2	1.98	0.46
1:A:133:ASN:O	1:A:157:ASN:ND2	2.45	0.46
1:A:61:ASN:C	1:A:85:ASN:OD1	2.60	0.45
1:A:293:THR:HB	1:A:370:VAL:HG21	1.98	0.45
1:A:40:LYS:HB3	1:A:42:LEU:HD13	1.99	0.45
1:A:132:ASN:H	1:A:156:TYR:HB2	1.81	0.45
1:A:114:ILE:HD11	1:A:130:LEU:HD13	1.99	0.44
1:A:286:PRO:O	1:A:288:LEU:HD11	2.18	0.43
1:A:299:LEU:C	1:A:299:LEU:HD12	2.44	0.43
1:A:17:PHE:HD1	1:A:17:PHE:O	2.01	0.43
1:A:205:ASN:O	1:A:240:ASN:OD1	2.37	0.43
1:A:21:PRO:HD2	1:A:24:CYS:HB2	2.01	0.42
1:A:39:LYS:HA	1:A:60:ASP:O	2.19	0.42
1:A:278:PRO:HD2	1:A:282:PHE:HB2	2.01	0.42
1:A:107:ASN:HA	1:A:131:ASN:O	2.20	0.42
1:A:46:PRO:HA	1:A:47:PRO:HD3	1.93	0.41
1:A:80:LEU:HB2	1:A:101:LEU:HD11	2.02	0.41
1:A:26:CYS:HB3	1:A:35:THR:HA	2.00	0.41
1:A:74:MET:HB2	1:A:98:LEU:CD2	2.50	0.41
1:A:157:ASN:O	1:A:181:ASN:HA	2.21	0.40
1:A:179:ASP:HA	1:A:203:THR:O	2.21	0.40
1:A:133:ASN:H	1:A:157:ASN:ND2	2.20	0.40
1:A:274:PHE:O	1:A:275:TRP:CD1	2.69	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	322/388 (83%)	285 (88%)	31 (10%)	6 (2%)	6	30

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	30	SER
1	A	266	PRO
1	A	298	VAL
1	A	346	ILE
1	A	69	LYS
1	A	269	LEU

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	263/347 (76%)	223 (85%)	40 (15%)	3	14

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	20	CYS
1	A	25	VAL
1	A	27	GLN
1	A	28	ILE
1	A	33	LEU
1	A	36	LEU
1	A	40	LYS
1	A	42	LEU
1	A	48	ASN
1	A	56	LEU
1	A	64	THR
1	A	74	MET
1	A	80	LEU
1	A	102	ARG

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Mol	Chain	Res	Type
1	A	112	THR
1	A	122	LEU
1	A	137	LEU
1	A	139	SER
1	A	158	ASN
1	A	161	THR
1	A	183	ILE
1	A	190	THR
1	A	207	LEU
1	A	209	LYS
1	A	210	LEU
1	A	236	SER
1	A	242	LEU
1	A	247	GLU
1	A	249	LEU
1	A	254	LEU
1	A	255	SER
1	A	268	LEU
1	A	277	ILE
1	A	283	LEU
1	A	306	LEU
1	A	321	ILE
1	A	342	LEU
1	A	344	ILE
1	A	369	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	73	ASN
1	A	116	ASN
1	A	157	ASN
1	A	319	HIS

5.3.3 RNA ⓘ

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	330/388 (85%)	0.55	35 (10%) 11 6	92, 134, 234, 249	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	215	LEU	5.1
1	A	365	GLU	4.4
1	A	327	LEU	3.6
1	A	273	TYR	3.1
1	A	304	ALA	3.1
1	A	143	PHE	3.1
1	A	283	LEU	3.1
1	A	305	THR	3.1
1	A	238	GLY	3.0
1	A	151	GLU	3.0
1	A	30	SER	3.0
1	A	328	ILE	2.9
1	A	335	LEU	2.9
1	A	235	LEU	2.9
1	A	336	VAL	2.8
1	A	306	LEU	2.7
1	A	290	THR	2.7
1	A	234	ALA	2.6
1	A	344	ILE	2.6
1	A	343	ASP	2.6
1	A	351	ASP	2.3
1	A	367	THR	2.3
1	A	46	PRO	2.3
1	A	318	ILE	2.3
1	A	269	LEU	2.3
1	A	264	ALA	2.3
1	A	320	TRP	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	48	ASN	2.3
1	A	342	LEU	2.2
1	A	275	TRP	2.2
1	A	17	PHE	2.2
1	A	55	GLU	2.1
1	A	190	THR	2.1
1	A	147	PHE	2.1
1	A	34	ALA	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.