



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 07:41 PM UTC

PDB ID : 1DLP / pdb_00001dlp
Title : STRUCTURAL CHARACTERIZATION OF THE NATIVE FETUIN-BINDING PROTEIN SCILLA CAMPANULATA AGGLUTININ (SCAFET): A NOVEL TWO-DOMAIN LECTIN
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Deposited on : 1999-12-11
Resolution : 3.30 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

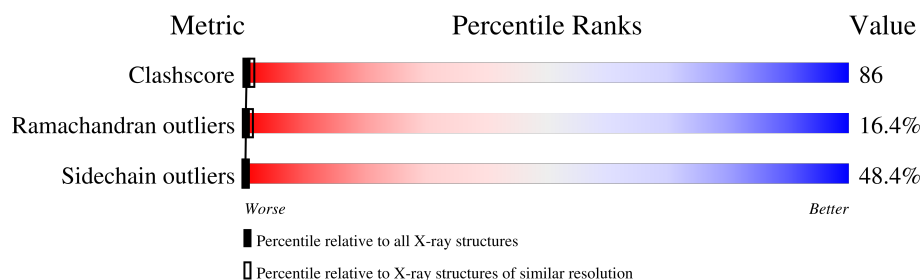
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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))
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	236	11% 35% 53% .
1	B	236	11% 31% 51% 6%
1	C	236	17% 30% 52% .
1	D	236	9% 35% 50% 6%
1	E	236	. 11% 42% 44% .
1	F	236	12% 37% 42% 8%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10431 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 LECTIN SCAFET PRECURSOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	233	Total	C	N	O	S	18	0	0
			1778	1102	322	347	7			
1	B	221	Total	C	N	O	S	21	0	0
			1694	1053	305	329	7			
1	C	234	Total	C	N	O	S	25	0	0
			1772	1097	323	345	7			
1	D	223	Total	C	N	O	S	28	0	0
			1702	1057	307	331	7			
1	E	231	Total	C	N	O	S	17	0	0
			1759	1093	318	341	7			
1	F	216	Total	C	N	O	S	40	0	0
			1659	1034	298	320	7			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	19	Total	O	0	0
			19	19		
2	B	15	Total	O	0	0
			15	15		
2	C	6	Total	O	0	0
			6	6		
2	D	8	Total	O	0	0
			8	8		
2	E	8	Total	O	0	0
			8	8		
2	F	11	Total	O	0	0
			11	11		

Note EDS was not executed.

[illegible]

Chain B: 11% 31% 51% 6%

M1	M2	M3	M4	M5	M6	M7	M8	M9	M10	M11	M12	M13	M14	M15	M16	M17	M18	M19	M20	M21	M22	M23	M24	M25	M26	M27	M28	M29	M30	M31	M32	M33	M34	M35	M36	M37	M38	M39	M40	M41	M42	M43	M44	M45	M46	M47	M48	M49	M50	M51	M52	M53	M54	M55	M56	M57	M58	M59	M60				
ALA	ASN	NI23	G183	G184	G185	G186	G187	G188	G189	G190	G191	G192	GLY	ASN	ASP	NI36	H137	H138	Q139	T140	H141	H142	H143	T144	Q145	S146	L147	Q148	N208	L149	S150	H151	H152	H153	L154	S155	M156	E157	T158	D159	C160	L161	L162	L163	M164	F165	L166	H167	D168	D169	R170	G171	H172	H173	S174	GLY	L175	S176	GLY	VAL	L178	VAL	C180

Chain C:

Index	Value	Category
N1	0.05	Red
N2	0.05	Red
N3	0.05	Red
N4	0.05	Red
N5	0.05	Red
N6	0.05	Red
N7	0.05	Red
N8	0.05	Red
N9	0.05	Red
N10	0.05	Red
N11	0.05	Red
N12	0.05	Red
N13	0.05	Red
N14	0.05	Red
N15	0.05	Red
N16	0.05	Red
N17	0.05	Red
N18	0.05	Red
N19	0.05	Red
N20	0.05	Red
N21	0.05	Red
N22	0.05	Red
N23	0.05	Red
N24	0.05	Red
N25	0.05	Red
N26	0.05	Red
N27	0.05	Red
N28	0.05	Red
N29	0.05	Red
N30	0.05	Red
N31	0.05	Red
N32	0.05	Red
N33	0.05	Red
N34	0.05	Red
N35	0.05	Red
N36	0.05	Red
N37	0.05	Red
N38	0.05	Red
N39	0.05	Red
N40	0.05	Red
N41	0.05	Red
N42	0.05	Red
N43	0.05	Red
N44	0.05	Red
N45	0.05	Red
N46	0.05	Red
N47	0.05	Red
N48	0.05	Red
N49	0.05	Red
N50	0.05	Red
N51	0.05	Red
N52	0.05	Red
N53	0.05	Red
N54	0.05	Red
N55	0.05	Red
N56	0.05	Red
N57	0.05	Red
N58	0.05	Red
N59	0.05	Red
N60	0.05	Red

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	277.94Å 164.10Å 53.60Å 90.00° 95.38° 90.00°	Depositor
Resolution (Å)	20.00 – 3.30	Depositor
% Data completeness (in resolution range)	95.3 (20.00-3.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.189 , 0.293	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10431	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

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	3.27	209/1812 (11.5%)	8.06	1086/2470 (44.0%)
1	B	3.25	188/1726 (10.9%)	8.17	1068/2351 (45.4%)
1	C	3.04	138/1805 (7.6%)	7.69	1054/2459 (42.9%)
1	D	3.82	191/1735 (11.0%)	8.75	1128/2365 (47.7%)
1	E	2.75	130/1793 (7.3%)	7.27	988/2444 (40.4%)
1	F	2.80	114/1691 (6.7%)	8.06	992/2303 (43.1%)
All	All	3.17	970/10562 (9.2%)	8.01	6316/14392 (43.9%)

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	2	60
1	B	2	73
1	C	0	66
1	D	0	51
1	E	0	39
1	F	2	53
All	All	6	342

The worst 5 of 970 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	1	ASN	CG-ND2	59.49	2.58	1.33
1	D	78	ARG	CG-CD	38.85	2.69	1.52
1	C	168	ASP	CG-OD1	36.39	1.94	1.25
1	D	167	ARG	CD-NE	-35.41	0.96	1.46
1	F	224	ASN	CA-CB	-30.70	1.01	1.53

The worst 5 of 6316 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	109	ASP	CA-CB-CG	62.65	175.25	112.60
1	D	1	ASN	OD1-CG-ND2	-62.32	60.28	122.60
1	D	104	GLY	CA-C-N	59.86	178.98	120.31
1	D	104	GLY	C-N-CA	59.86	178.98	120.31
1	E	1	ASN	CA-CB-CG	55.29	167.89	112.60

5 of 6 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	9	HIS	CA
1	A	87	ILE	CA
1	B	60	ALA	CA
1	B	168	ASP	CA
1	F	60	ALA	CA

5 of 342 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	13	HIS	Mainchain
1	A	19	ALA	Mainchain
1	A	2	ASN	Peptide
1	A	25	LEU	Mainchain
1	A	5	PHE	Mainchain

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	1778	0	1709	286	0
1	B	1694	0	1618	274	0
1	C	1772	0	1706	283	0
1	D	1702	0	1624	324	0
1	E	1759	0	1700	321	0
1	F	1659	0	1591	311	0
2	A	19	0	0	1	0
2	B	15	0	0	0	0
2	C	6	0	0	0	0
2	D	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	8	0	0	0	0
2	F	11	0	0	0	0
All	All	10431	0	9948	1721	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 86.

The worst 5 of 1721 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:D:77:ILE:CD1	1:D:77:ILE:CG1	1.80	1.57
1:E:131:THR:CA	1:E:131:THR:C	1.75	1.53
1:E:136:ASN:CA	1:E:136:ASN:CB	1.88	1.49
1:A:131:THR:OG1	1:A:131:THR:CB	1.64	1.46
1:D:64:SER:OG	1:D:64:SER:CB	1.67	1.43

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	229/236 (97%)	158 (69%)	41 (18%)	30 (13%)	0	1
1	B	213/236 (90%)	132 (62%)	42 (20%)	39 (18%)	0	0
1	C	230/236 (98%)	150 (65%)	42 (18%)	38 (16%)	0	1
1	D	217/236 (92%)	148 (68%)	30 (14%)	39 (18%)	0	0
1	E	227/236 (96%)	150 (66%)	39 (17%)	38 (17%)	0	1
1	F	208/236 (88%)	138 (66%)	37 (18%)	33 (16%)	0	1
All	All	1324/1416 (94%)	876 (66%)	231 (17%)	217 (16%)	0	1

5 of 217 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	10	GLU
1	A	11	GLY
1	A	14	PRO
1	A	19	ALA
1	A	20	ALA

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	197/198 (100%)	94 (48%)	103 (52%)	0	0
1	B	187/198 (94%)	88 (47%)	99 (53%)	0	0
1	C	195/198 (98%)	101 (52%)	94 (48%)	0	0
1	D	187/198 (94%)	96 (51%)	91 (49%)	0	0
1	E	194/198 (98%)	109 (56%)	85 (44%)	0	0
1	F	183/198 (92%)	102 (56%)	81 (44%)	0	0
All	All	1143/1188 (96%)	590 (52%)	553 (48%)	0	0

5 of 553 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	217	PHE
1	F	12	SER
1	E	216	VAL
1	F	150	SER
1	B	220	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 73 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	199	GLN
1	F	175	ASN

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Mol	Chain	Res	Type
1	E	208	ASN
1	F	63	GLN
1	B	188	GLN

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	3
1	A	1
1	C	1
1	E	1

The worst 5 of 6 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	25:LEU	C	26:SER	N	1.19

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	8:SER	C	9:HIS	N	1.19
1	C	229:GLY	C	230:GLY	N	1.19
1	E	85:GLY	C	86:SER	N	1.19
1	B	30:PHE	C	31:THR	N	1.16

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.