



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 13, 2024 – 04:06 PM EDT

PDB ID : 8UCY
Title : Sterile Alpha Motif (SAM) domain from Tric1, Arabidopsis thaliana
Authors : Olasz, B.; Vrieling, A.; Evans, G.L.
Deposited on : 2023-09-27
Resolution : 1.48 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 : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.36.2
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

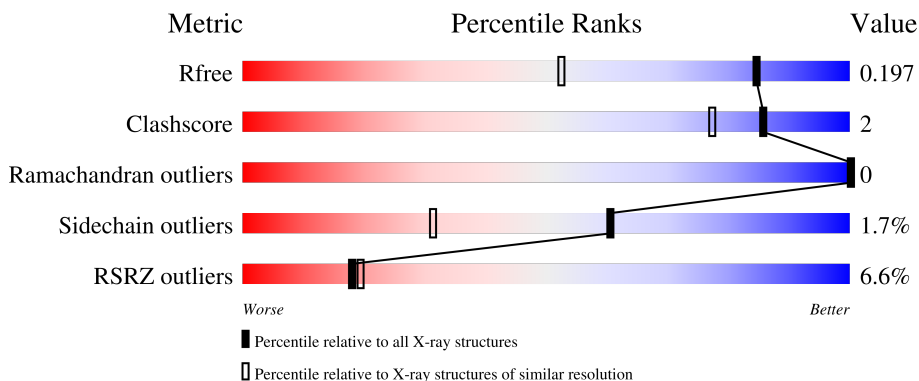
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.48 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}	130704	4690 (1.50-1.46)
Clashscore	141614	4955 (1.50-1.46)
Ramachandran outliers	138981	4846 (1.50-1.46)
Sidechain outliers	138945	4844 (1.50-1.46)
RSRZ outliers	127900	4614 (1.50-1.46)

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	90	
1	B	90	
1	C	90	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3429 atoms, of which 1652 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 Chloroplastic import inner membrane translocase subunit HP30-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	A	65	1079	343	547	90	97	2	0	3	0
1	B	66	1087	342	555	93	95	2	0	1	0
1	C	67	1082	342	550	91	97	2	0	2	0

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	172	MET	-	initiating methionine	UNP Q9SCK3
A	173	GLY	-	expression tag	UNP Q9SCK3
A	174	SER	-	expression tag	UNP Q9SCK3
A	175	SER	-	expression tag	UNP Q9SCK3
A	176	HIS	-	expression tag	UNP Q9SCK3
A	177	HIS	-	expression tag	UNP Q9SCK3
A	178	HIS	-	expression tag	UNP Q9SCK3
A	179	HIS	-	expression tag	UNP Q9SCK3
A	180	HIS	-	expression tag	UNP Q9SCK3
A	181	HIS	-	expression tag	UNP Q9SCK3
A	182	SER	-	expression tag	UNP Q9SCK3
A	183	SER	-	expression tag	UNP Q9SCK3
A	184	GLY	-	expression tag	UNP Q9SCK3
A	185	LEU	-	expression tag	UNP Q9SCK3
A	186	VAL	-	expression tag	UNP Q9SCK3
A	187	PRO	-	expression tag	UNP Q9SCK3
A	188	ARG	-	expression tag	UNP Q9SCK3
A	189	GLY	-	expression tag	UNP Q9SCK3
B	172	MET	-	initiating methionine	UNP Q9SCK3
B	173	GLY	-	expression tag	UNP Q9SCK3
B	174	SER	-	expression tag	UNP Q9SCK3
B	175	SER	-	expression tag	UNP Q9SCK3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	176	HIS	-	expression tag	UNP Q9SCK3
B	177	HIS	-	expression tag	UNP Q9SCK3
B	178	HIS	-	expression tag	UNP Q9SCK3
B	179	HIS	-	expression tag	UNP Q9SCK3
B	180	HIS	-	expression tag	UNP Q9SCK3
B	181	HIS	-	expression tag	UNP Q9SCK3
B	182	SER	-	expression tag	UNP Q9SCK3
B	183	SER	-	expression tag	UNP Q9SCK3
B	184	GLY	-	expression tag	UNP Q9SCK3
B	185	LEU	-	expression tag	UNP Q9SCK3
B	186	VAL	-	expression tag	UNP Q9SCK3
B	187	PRO	-	expression tag	UNP Q9SCK3
B	188	ARG	-	expression tag	UNP Q9SCK3
B	189	GLY	-	expression tag	UNP Q9SCK3
C	172	MET	-	initiating methionine	UNP Q9SCK3
C	173	GLY	-	expression tag	UNP Q9SCK3
C	174	SER	-	expression tag	UNP Q9SCK3
C	175	SER	-	expression tag	UNP Q9SCK3
C	176	HIS	-	expression tag	UNP Q9SCK3
C	177	HIS	-	expression tag	UNP Q9SCK3
C	178	HIS	-	expression tag	UNP Q9SCK3
C	179	HIS	-	expression tag	UNP Q9SCK3
C	180	HIS	-	expression tag	UNP Q9SCK3
C	181	HIS	-	expression tag	UNP Q9SCK3
C	182	SER	-	expression tag	UNP Q9SCK3
C	183	SER	-	expression tag	UNP Q9SCK3
C	184	GLY	-	expression tag	UNP Q9SCK3
C	185	LEU	-	expression tag	UNP Q9SCK3
C	186	VAL	-	expression tag	UNP Q9SCK3
C	187	PRO	-	expression tag	UNP Q9SCK3
C	188	ARG	-	expression tag	UNP Q9SCK3
C	189	GLY	-	expression tag	UNP Q9SCK3

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

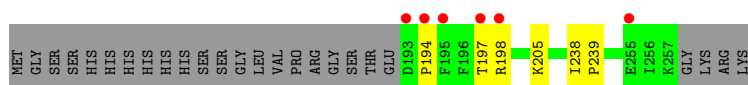
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	58	Total 58	O 58	0	0
3	B	65	Total 65	O 65	0	0
3	C	57	Total 57	O 57	0	0

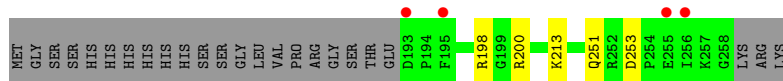
3 Residue-property plots [i](#)

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.

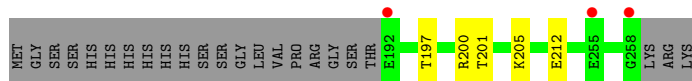
- Molecule 1: Chloroplastic import inner membrane translocase subunit HP30-1



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- Molecule 1: Chloroplastic import inner membrane translocase subunit HP30-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	28.64Å 92.12Å 93.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.17 – 1.48 29.17 – 1.48	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.17-1.48) 100.0 (29.17-1.48)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.56 (at 1.48Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.179 , 0.198 0.178 , 0.197	Depositor DCC
R_{free} test set	2116 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	19.2	Xtrriage
Anisotropy	0.316	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.44 , 49.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.012 for -h,l,k	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	3429	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.62% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL

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	0.56	0/554	0.75	0/748
1	B	0.57	0/543	0.73	0/733
1	C	0.50	0/551	0.71	0/745
All	All	0.54	0/1648	0.73	0/2226

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	0	1
1	B	0	2
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	198	ARG	Sidechain
1	B	198[A]	ARG	Sidechain
1	B	200	ARG	Sidechain

5.2 Too-close contacts [i](#)

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	532	547	534	3	0
1	B	532	555	554	0	0
1	C	532	550	542	4	0
2	B	1	0	0	0	0
3	A	58	0	0	0	0
3	B	65	0	0	0	0
3	C	57	0	0	0	0
All	All	1777	1652	1630	7	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 2.

The worst 5 of 7 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:C:200:ARG:HG2	1:C:212:GLU:HG2	1.91	0.53
1:C:197:THR:HA	1:C:200:ARG:NH2	2.29	0.48
1:A:194:PRO:HA	1:A:197:THR:HG23	1.96	0.48
1:C:201:THR:O	1:C:205:LYS:HG3	2.14	0.47
1:A:238:ILE:HA	1:A:239:PRO:HD3	1.91	0.42

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	66/90 (73%)	66 (100%)	0	0	100	100
1	B	65/90 (72%)	65 (100%)	0	0	100	100
1	C	67/90 (74%)	66 (98%)	1 (2%)	0	100	100
All	All	198/270 (73%)	197 (100%)	1 (0%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	60/80 (75%)	60 (100%)	0	100	100
1	B	59/80 (74%)	56 (95%)	3 (5%)	24	3
1	C	60/80 (75%)	60 (100%)	0	100	100
All	All	179/240 (75%)	176 (98%)	3 (2%)	60	31

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

Mol	Chain	Res	Type
1	B	213	LYS
1	B	251	GLN
1	B	253	ASP

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

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	65/90 (72%)	0.53	6 (9%) 9 9	16, 23, 60, 66	0
1	B	66/90 (73%)	0.24	4 (6%) 21 22	14, 22, 49, 75	0
1	C	67/90 (74%)	0.21	3 (4%) 33 36	16, 23, 50, 73	0
All	All	198/270 (73%)	0.33	13 (6%) 18 19	14, 23, 62, 75	0

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	195	PHE	7.0
1	A	194	PRO	6.8
1	B	193	ASP	6.3
1	A	193	ASP	5.0
1	C	192	GLU	3.9

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 monosaccharides in this entry.

6.4 Ligands [i](#)

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(\AA^2)	Q<0.9
2	CL	B	301	1/1	0.89	0.08	50,50,50,50	0

6.5 Other polymers [i](#)

There are no such residues in this entry.