



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 14, 2023 – 01:37 PM EDT

PDB ID : 8DN6
Title : The crystal structure of the Arabidopsis thaliana Toc75 POTRA domains in complex with fab tc2
Authors : Srinivasan, K.; Noinaj, N.
Deposited on : 2022-07-10
Resolution : 3.00 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
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

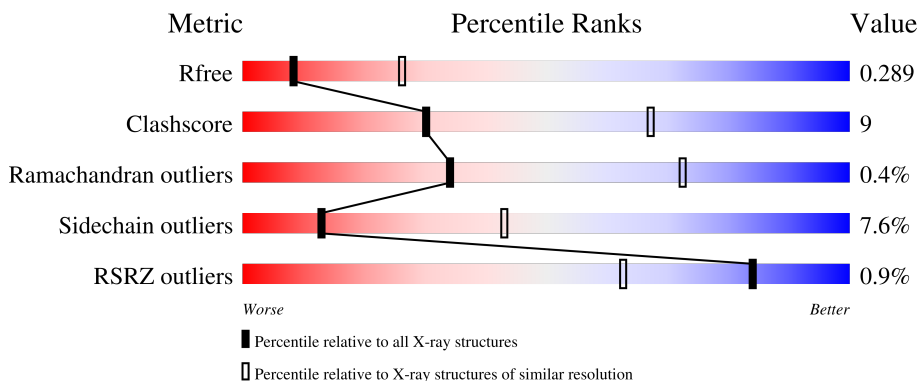
1 Overall quality at a glance i

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}	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 $\leq 5\%$. 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	313	 45% 16% 2% 37%
1	B	313	 48% 15% 2% 37%
2	C	239	 2% 71% 21% 7%
2	E	239	 2% 72% 18% 8%
3	D	215	 76% 22%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	F	215	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into two segments: a green segment on the left representing 79% and a yellow segment on the right representing 21%. A small red square is located at the beginning of the bar, followed by a percentage sign (%).</p>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 9639 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 Protein TOC75-3, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	198	1566	982	283	292	9	0	0	0
1	B	198	1565	982	281	294	8	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	137	GLY	-	expression tag	UNP Q9STE8
A	138	ALA	-	expression tag	UNP Q9STE8
A	139	MET	-	expression tag	UNP Q9STE8
A	140	GLY	-	expression tag	UNP Q9STE8
B	137	GLY	-	expression tag	UNP Q9STE8
B	138	ALA	-	expression tag	UNP Q9STE8
B	139	MET	-	expression tag	UNP Q9STE8
B	140	GLY	-	expression tag	UNP Q9STE8

- Molecule 2 is a protein called fabtc2_HC.

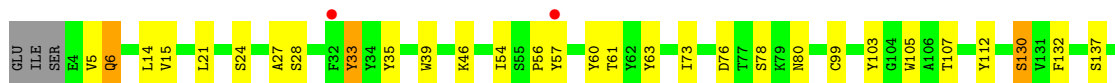
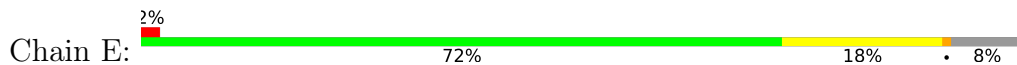
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	222	1631	1038	267	321	5	0	0	0
2	E	220	1635	1043	263	324	5	0	1	0

- Molecule 3 is a protein called fabtc2_LC.

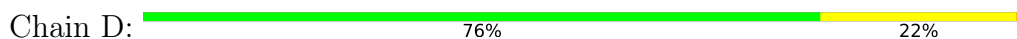
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	D	214	1619	1011	271	331	6	0	0	0
3	F	215	1623	1013	271	333	6	0	1	0



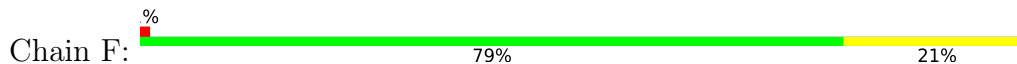
• Molecule 2: fabtc2_HC



• Molecule 3: fabtc2_LC



• Molecule 3: fabtc2_LC



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	276.09Å 51.48Å 172.08Å 90.00° 123.06° 90.00°	Depositor
Resolution (Å)	49.30 – 3.00 49.30 – 2.98	Depositor EDS
% Data completeness (in resolution range)	98.9 (49.30-3.00) 98.9 (49.30-2.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 3.01Å)	Xtrriage
Refinement program	PHENIX 1.20_4459	Depositor
R, R_{free}	0.240 , 0.293 0.238 , 0.289	Depositor DCC
R_{free} test set	1990 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å ²)	59.8	Xtrriage
Anisotropy	0.672	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 69.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	9639	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.27% 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	0.33	0/1587	0.65	0/2140
1	B	0.31	0/1587	0.61	1/2143 (0.0%)
2	C	0.29	0/1677	0.59	0/2299
2	E	0.28	0/1684	0.59	0/2306
3	D	0.29	0/1655	0.60	0/2254
3	F	0.27	0/1662	0.57	0/2266
All	All	0.29	0/9852	0.60	1/13408 (0.0%)

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
2	C	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	261	LEU	CA-CB-CG	6.09	129.31	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	5	VAL	Peptide

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	1566	0	1576	37	0
1	B	1565	0	1558	33	0
2	C	1631	0	1537	34	0
2	E	1635	0	1550	28	0
3	D	1619	0	1530	32	0
3	F	1623	0	1532	22	0
All	All	9639	0	9283	175	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 9.

The worst 5 of 175 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)
3:D:19:ARG:HD3	3:D:77:SER:HA	1.26	1.11
3:D:19:ARG:CD	3:D:77:SER:HA	2.02	0.89
2:E:27:ALA:HB3	2:E:80:ASN:HB3	1.65	0.79
1:A:269:GLU:O	1:A:282:TYR:OH	2.02	0.77
2:C:50:TRP:HE1	2:C:53:SER:HG	1.35	0.72

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	196/313 (63%)	182 (93%)	10 (5%)	4 (2%)	7 34

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	196/313 (63%)	186 (95%)	10 (5%)	0	100	100
2	C	220/239 (92%)	205 (93%)	14 (6%)	1 (0%)	29	68
2	E	219/239 (92%)	202 (92%)	17 (8%)	0	100	100
3	D	212/215 (99%)	203 (96%)	9 (4%)	0	100	100
3	F	214/215 (100%)	205 (96%)	9 (4%)	0	100	100
All	All	1257/1534 (82%)	1183 (94%)	69 (6%)	5 (0%)	34	72

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	264	GLN
1	A	267	PRO
1	A	268	ILE
1	A	269	GLU
2	C	57	TYR

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	170/276 (62%)	159 (94%)	11 (6%)	17	50
1	B	169/276 (61%)	153 (90%)	16 (10%)	8	32
2	C	174/200 (87%)	161 (92%)	13 (8%)	13	43
2	E	176/200 (88%)	163 (93%)	13 (7%)	13	44
3	D	182/190 (96%)	167 (92%)	15 (8%)	11	39
3	F	183/190 (96%)	171 (93%)	12 (7%)	16	49
All	All	1054/1332 (79%)	974 (92%)	80 (8%)	13	43

5 of 80 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	14	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	F	23	THR
2	E	33	TYR
2	E	179	VAL
3	F	130	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
3	F	91	GLN
3	F	138	ASN

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](#)

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 [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	198/313 (63%)	-0.18	1 (0%) 91 75	36, 66, 127, 176	0
1	B	198/313 (63%)	-0.18	0 100 100	24, 63, 115, 142	0
2	C	222/239 (92%)	0.02	4 (1%) 68 40	48, 82, 133, 197	0
2	E	220/239 (92%)	-0.06	4 (1%) 68 40	46, 75, 126, 204	0
3	D	214/215 (99%)	-0.21	0 100 100	49, 71, 118, 141	0
3	F	215/215 (100%)	-0.22	2 (0%) 84 63	43, 69, 120, 137	0
All	All	1267/1534 (82%)	-0.14	11 (0%) 84 63	24, 72, 125, 204	0

The worst 5 of 11 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	141	THR	7.0
2	E	57	TYR	5.5
1	A	252	ASP	3.6
2	E	141	THR	2.9
2	C	78	SER	2.9

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.