



wwPDB X-ray Structure Validation Summary Report ⓘ

May 21, 2020 – 05:19 pm BST

PDB ID : 5O3U
Title : Structural characterization of the fast and promiscuous macrocyclase from plant - PCY1-S562A bound to Presegetalin F1
Authors : Ludewig, H.; Czekster, C.M.; Bent, A.F.; Naismith, J.H.
Deposited on : 2017-05-25
Resolution : 1.86 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 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 : 2.11
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) : 2.11

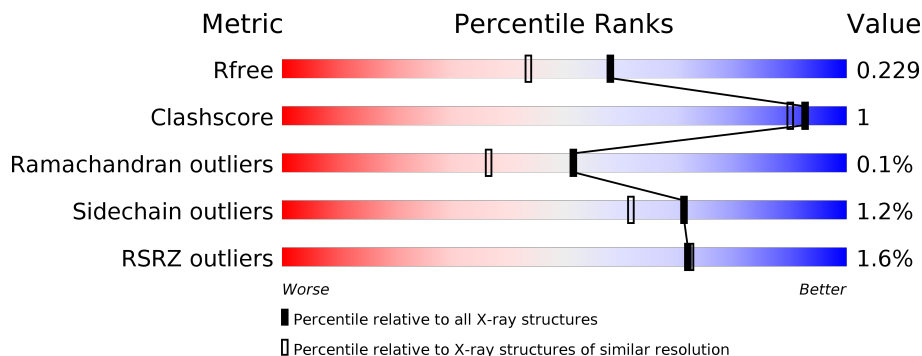
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.86 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.



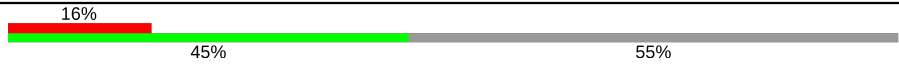

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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 on 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	724	
1	B	724	
1	C	724	
1	D	724	
2	L	38	
2	M	38	

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Mol	Chain	Length	Quality of chain
2	N	38	 16% 45% 55%
2	O	38	 8% 45% 53%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 24284 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 Peptide cyclase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	711	Total 5729	C 3663	N 970	O 1066	S 30	0	6	0
1	B	703	Total 5670	C 3629	N 959	O 1054	S 28	0	5	0
1	C	706	Total 5714	C 3659	N 969	O 1059	S 27	0	4	0
1	D	710	Total 5722	C 3659	N 972	O 1065	S 26	0	4	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	562	ALA	SER	engineered mutation	UNP R4P353
B	562	ALA	SER	engineered mutation	UNP R4P353
C	562	ALA	SER	engineered mutation	UNP R4P353
D	562	ALA	SER	engineered mutation	UNP R4P353

- Molecule 2 is a protein called Putative presegetalin F1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	L	18	Total 131	C 82	N 21	O 28	0	0	0
2	M	18	Total 132	C 82	N 21	O 29	0	0	0
2	N	17	Total 124	C 78	N 20	O 26	0	0	0
2	O	18	Total 132	C 82	N 21	O 29	0	0	0

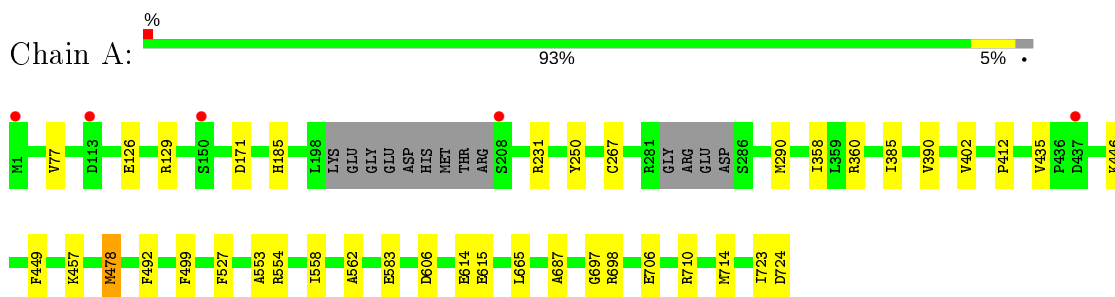
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	271	Total 271	O 271	0	0
3	B	243	Total 243	O 243	0	0
3	C	226	Total 226	O 226	0	0
3	D	179	Total 179	O 179	0	0
3	L	2	Total 2	O 2	0	0
3	M	3	Total 3	O 3	0	0
3	N	3	Total 3	O 3	0	0
3	O	3	Total 3	O 3	0	0

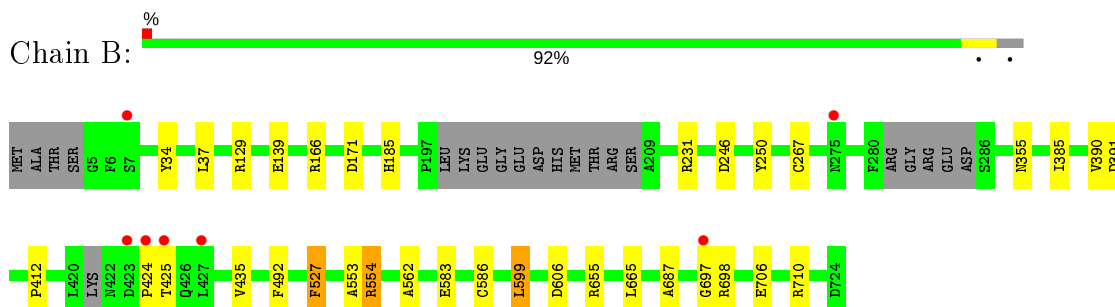
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

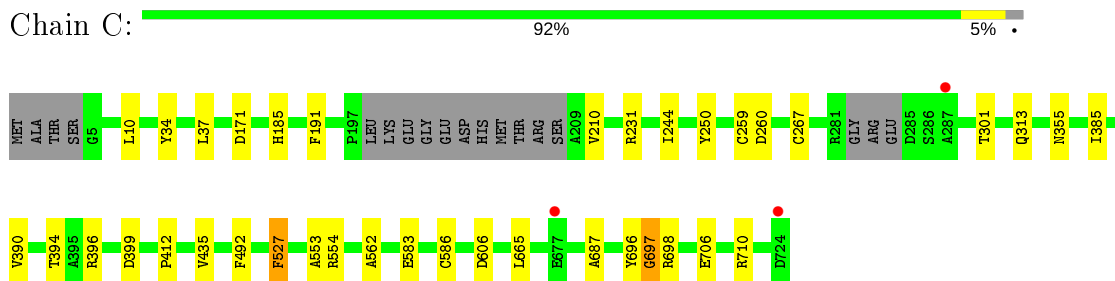
- Molecule 1: Peptide cyclase 1



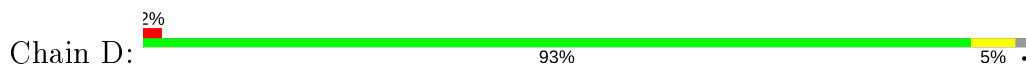
- Molecule 1: Peptide cyclase 1

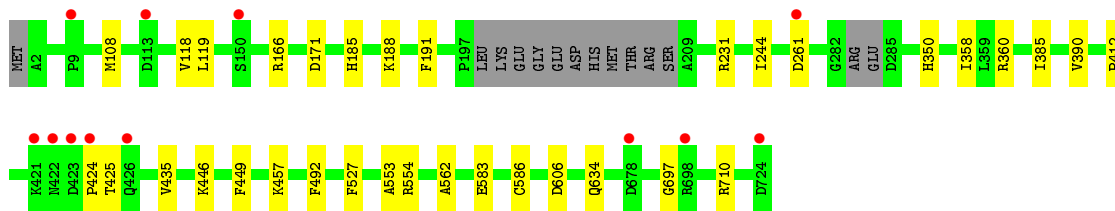


- Molecule 1: Peptide cyclase 1

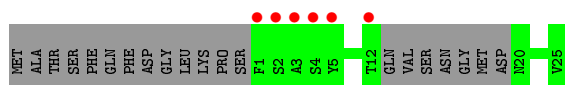


- Molecule 1: Peptide cyclase 1

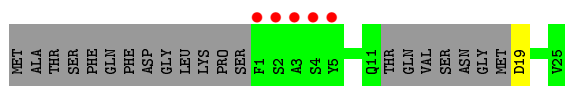




- Molecule 2: Putative presegetalin F1



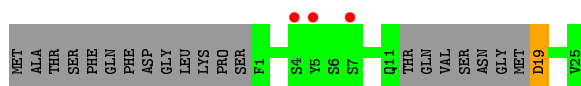
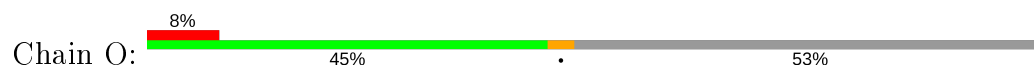
- Molecule 2: Putative presegetalin F1



- Molecule 2: Putative presegetalin F1



- Molecule 2: Putative presegetalin F1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	64.86Å 85.82Å 137.87Å 87.64° 78.32° 89.52°	Depositor
Resolution (Å)	73.72 – 1.86 73.72 – 1.86	Depositor EDS
% Data completeness (in resolution range)	95.8 (73.72-1.86) 95.8 (73.72-1.86)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 1.86Å)	Xtrriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.193 , 0.223 0.201 , 0.229	Depositor DCC
R_{free} test set	11725 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	22.4	Xtrriage
Anisotropy	0.341	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 37.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.049 for h,-k,h-l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	24284	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.89% 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	0.57	0/5894	0.74	7/7980 (0.1%)
1	B	0.57	0/5830	0.74	4/7897 (0.1%)
1	C	0.58	1/5874 (0.0%)	0.76	3/7956 (0.0%)
1	D	0.56	0/5880	0.74	4/7964 (0.1%)
2	L	0.60	0/133	0.60	0/178
2	M	0.62	0/134	0.62	0/179
2	N	0.59	0/126	0.55	0/168
2	O	0.62	0/134	0.56	0/179
All	All	0.57	1/24005 (0.0%)	0.74	18/32501 (0.1%)

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	C	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	697	GLY	C-O	-7.18	1.12	1.23

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	399	ASP	CB-CG-OD2	-7.29	111.74	118.30
1	D	231	ARG	NE-CZ-NH1	6.89	123.75	120.30
1	D	231	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	A	231	ARG	NE-CZ-NH1	5.83	123.22	120.30
1	B	231	ARG	NE-CZ-NH1	5.69	123.14	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	696	TYR	Peptide
1	C	697	GLY	Peptide

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	5729	0	5590	21	0
1	B	5670	0	5505	15	0
1	C	5714	0	5556	17	0
1	D	5722	0	5563	15	0
2	L	131	0	127	0	0
2	M	132	0	124	0	0
2	N	124	0	120	0	0
2	O	132	0	124	1	0
3	A	271	0	0	0	0
3	B	243	0	0	1	0
3	C	226	0	0	2	0
3	D	179	0	0	0	0
3	L	2	0	0	0	0
3	M	3	0	0	0	0
3	N	3	0	0	0	0
3	O	3	0	0	0	0
All	All	24284	0	22709	68	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 1.

The worst 5 of 68 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:478[A]:MET:HG3	1:A:558:ILE:HG22	1.61	0.83
1:A:499:PHE:CE1	1:A:714:MET:CE	2.63	0.82
1:A:478[A]:MET:CG	1:A:558:ILE:HG22	2.13	0.79
1:A:553:ALA:O	1:A:554:ARG:HB3	1.87	0.74
1:A:499:PHE:CE1	1:A:714:MET:HE1	2.25	0.71

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	711/724 (98%)	690 (97%)	20 (3%)	1 (0%)	51	36
1	B	700/724 (97%)	679 (97%)	20 (3%)	1 (0%)	51	36
1	C	705/724 (97%)	685 (97%)	20 (3%)	0	100	100
1	D	708/724 (98%)	687 (97%)	20 (3%)	1 (0%)	51	36
2	L	14/38 (37%)	12 (86%)	2 (14%)	0	100	100
2	M	14/38 (37%)	13 (93%)	1 (7%)	0	100	100
2	N	13/38 (34%)	12 (92%)	1 (8%)	0	100	100
2	O	14/38 (37%)	13 (93%)	1 (7%)	0	100	100
All	All	2879/3048 (94%)	2791 (97%)	85 (3%)	3 (0%)	51	36

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	697	GLY
1	A	697	GLY
1	B	697	GLY

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	623/628 (99%)	617 (99%)	6 (1%)	76	69
1	B	614/628 (98%)	607 (99%)	7 (1%)	73	65
1	C	618/628 (98%)	610 (99%)	8 (1%)	69	58
1	D	619/628 (99%)	613 (99%)	6 (1%)	76	69
2	L	15/32 (47%)	15 (100%)	0	100	100
2	M	15/32 (47%)	14 (93%)	1 (7%)	16	4
2	N	14/32 (44%)	14 (100%)	0	100	100
2	O	15/32 (47%)	14 (93%)	1 (7%)	16	4
All	All	2533/2640 (96%)	2504 (99%)	29 (1%)	71	65

5 of 29 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	171	ASP
1	C	260	ASP
1	D	634	GLN
1	C	185	HIS
1	C	394	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	422	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 carbohydrates 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	711/724 (98%)	-0.28	5 (0%) 87 88	11, 22, 47, 76	0
1	B	703/724 (97%)	-0.21	7 (0%) 82 82	12, 23, 49, 101	0
1	C	706/724 (97%)	-0.23	3 (0%) 92 92	13, 23, 47, 67	0
1	D	710/724 (98%)	-0.12	12 (1%) 70 70	13, 28, 53, 97	0
2	L	18/38 (47%)	1.20	6 (33%) 0 0	17, 31, 65, 65	0
2	M	18/38 (47%)	1.36	5 (27%) 0 0	17, 33, 67, 77	0
2	N	17/38 (44%)	1.36	6 (35%) 0 0	19, 32, 68, 86	0
2	O	18/38 (47%)	0.80	3 (16%) 1 1	21, 40, 59, 64	0
All	All	2901/3048 (95%)	-0.18	47 (1%) 72 72	11, 24, 51, 101	0

The worst 5 of 47 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	N	4	SER	6.6
2	M	4	SER	6.2
1	A	150	SER	5.3
2	L	4	SER	4.6
2	M	2	SER	4.6

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 carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.