



wwPDB NMR Structure Validation Summary Report ⓘ

Mar 8, 2026 – 03:29 PM UTC

PDB ID : 5MYE / pdb_00005mye
BMRB ID : 34093
Title : Solution structure of C20S variant of Dehydroascorbate reductase 3A from Populus trichocarpa in complex with dehydroascorbic acid.
Authors : Roret, T.; Tsan, P.
Deposited on : 2017-01-26

This is a wwPDB NMR 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/NMRValidationReportHelp>

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
Mogul : 2022.3.0, CSD as543be (2022)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

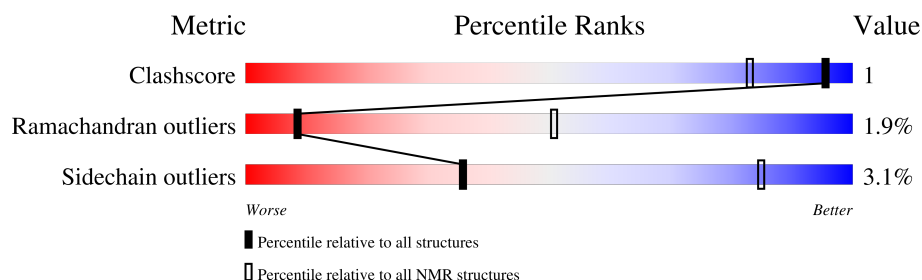
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 13%.

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)	NMR archive (#Entries)
Clashscore	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	218	 88% 9% .

2 Ensemble composition and analysis

This entry contains 20 models. Model 12 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *target function*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:1-A:212 (212)	0.42	12

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 5 clusters. No single-model clusters were found.

Cluster number	Models
1	8, 9, 10, 11, 12
2	13, 14, 15, 16, 17
3	2, 18, 19, 20
4	5, 6, 7
5	1, 3, 4

3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 3379 atoms, of which 1706 are hydrogens and 0 are deuteriums.

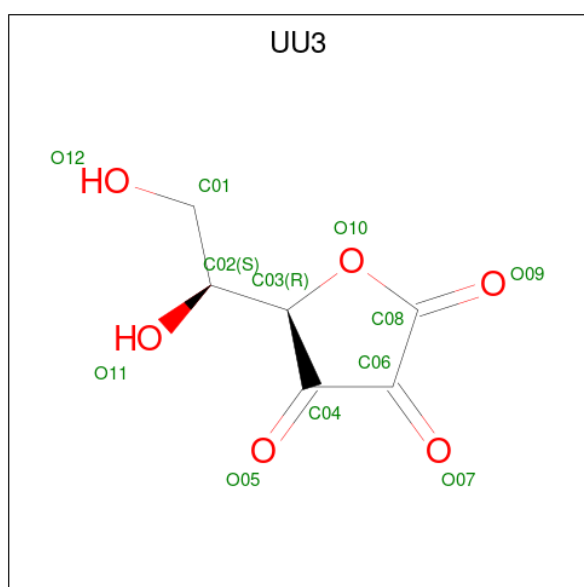
- Molecule 1 is a protein called Dehydroascorbate reductase family protein.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	212	3361	1085	1700	272	301	3	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	SER	CYS	engineered mutation	UNP B9HM36
A	40	HIS	TYR	conflict	UNP B9HM36
A	171	PRO	THR	conflict	UNP B9HM36
A	213	HIS	-	expression tag	UNP B9HM36
A	214	HIS	-	expression tag	UNP B9HM36
A	215	HIS	-	expression tag	UNP B9HM36
A	216	HIS	-	expression tag	UNP B9HM36
A	217	HIS	-	expression tag	UNP B9HM36
A	218	HIS	-	expression tag	UNP B9HM36

- Molecule 2 is (5R)-5-[(1S)-1,2-bis(oxidanyl)ethyl]oxolane-2,3,4-trione (CCD ID: UU3) (formula: C₆H₆O₆).



Mol	Chain	Residues	Atoms			
			Total	C	H	O
2	A	1	18	6	6	6

5 Refinement protocol and experimental data overview

The models were refined using the following method: *molecular dynamics*.

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
YASARA	refinement	
UCSF Chimera	refinement	
PELE web server	structure calculation	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	2
Total number of shifts	748
Number of shifts mapped to atoms	748
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	13%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: UU3

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 (average) 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	0.84±0.01	0±0/1706 (0.0± 0.0%)	1.42±0.02	4±2/2319 (0.2± 0.1%)
All	All	0.84	1/34120 (0.0%)	1.42	74/46380 (0.2%)

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	Planarity
1	A	0.0±0.0	10.2±1.9
All	All	0	203

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	87	PRO	CA-C	5.08	1.54	1.51	11	1

5 of 26 unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	114	ASP	CA-CB-CG	7.42	120.02	112.60	1	1
1	A	190	GLU	CA-C-N	6.97	129.50	120.44	14	9
1	A	190	GLU	C-N-CA	6.97	129.50	120.44	14	9
1	A	20	SER	O-C-N	-6.30	115.62	121.36	9	5
1	A	174	ASP	CA-CB-CG	6.28	118.88	112.60	16	6

There are no chirality outliers.

5 of 32 unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	49	GLN	Mainchain	19
1	A	31	GLU	Sidechain	17
1	A	74	ASP	Sidechain,Mainchain	15
1	A	198	ALA	Peptide,Mainchain	13
1	A	190	GLU	Sidechain	11

6.2 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 each 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 averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1661	1700	1700	3±1
All	All	33460	34120	34000	69

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.

5 of 16 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:8:LYS:N	1:A:23:CYS:SG	0.76	2.59	10	18
1:A:20:SER:HB2	1:A:23:CYS:SG	0.53	2.43	3	1
1:A:190:GLU:H	1:A:190:GLU:CD	0.51	2.13	1	6
1:A:8:LYS:HB3	1:A:23:CYS:SG	0.50	2.45	2	9
1:A:20:SER:CB	1:A:23:CYS:SG	0.49	3.00	3	1

6.3 Torsion angles [i](#)

6.3.1 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 PDB entries followed by that with respect to all NMR entries. 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	210/218 (96%)	189±3 (90±2%)	17±4 (8±2%)	4±1 (2±1%)	8	51
All	All	4200/4360 (96%)	3786 (90%)	335 (8%)	79 (2%)	8	51

5 of 10 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	112	SER	19
1	A	19	ASP	16
1	A	71	ALA	16
1	A	2	ALA	8
1	A	72	ASP	7

6.3.2 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 PDB entries followed by that with respect to all NMR entries. 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	183/189 (97%)	177±1 (97±1%)	6±1 (3±1%)	36	85
All	All	3660/3780 (97%)	3547 (97%)	113 (3%)	36	85

5 of 28 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	7	VAL	20
1	A	177	THR	20
1	A	191	SER	10
1	A	174	ASP	9
1	A	76	ILE	8

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
2	UU3	A	301	-	10,12,12	3.27±0.04	1±0 (10±0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	UU3	A	301	-	11,17,17	3.57±0.28	4±1 (36±6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	UU3	A	301	-	-	0±0,6,22,22	0±0,1,1,1

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	A	301	UU3	O07-C06	10.39	1.46	1.23	1	20

5 of 7 unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	A	301	UU3	O07-C06-C08	11.03	111.13	122.17	7	20
2	A	301	UU3	C08-C06-C04	5.11	101.45	107.45	4	20
2	A	301	UU3	O09-C08-C06	5.01	122.59	129.74	13	20
2	A	301	UU3	O10-C08-O09	2.72	124.85	121.27	13	13
2	A	301	UU3	C03-O10-C08	2.54	112.06	109.27	20	5

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation [i](#)

The completeness of assignment taking into account all chemical shift lists is 13% for the well-defined parts and 13% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *PtDHAR3A.txt*

7.1.1 Bookkeeping [i](#)

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	374
Number of shifts mapped to atoms	374
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	0	—	None (insufficient data)
$^{13}\text{C}_\beta$	0	—	None (insufficient data)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	187	0.96 ± 0.28	Should be applied

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 13%, i.e. 374 atoms were assigned a chemical shift out of a possible 2917. 0 out of 42 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	374/1036 (36%)	187/418 (45%)	0/424 (0%)	187/194 (96%)
Sidechain	0/1657 (0%)	0/1085 (0%)	0/530 (0%)	0/42 (0%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	0/224 (0%)	0/114 (0%)	0/99 (0%)	0/11 (0%)
Overall	374/2917 (13%)	187/1617 (12%)	0/1053 (0%)	187/247 (76%)

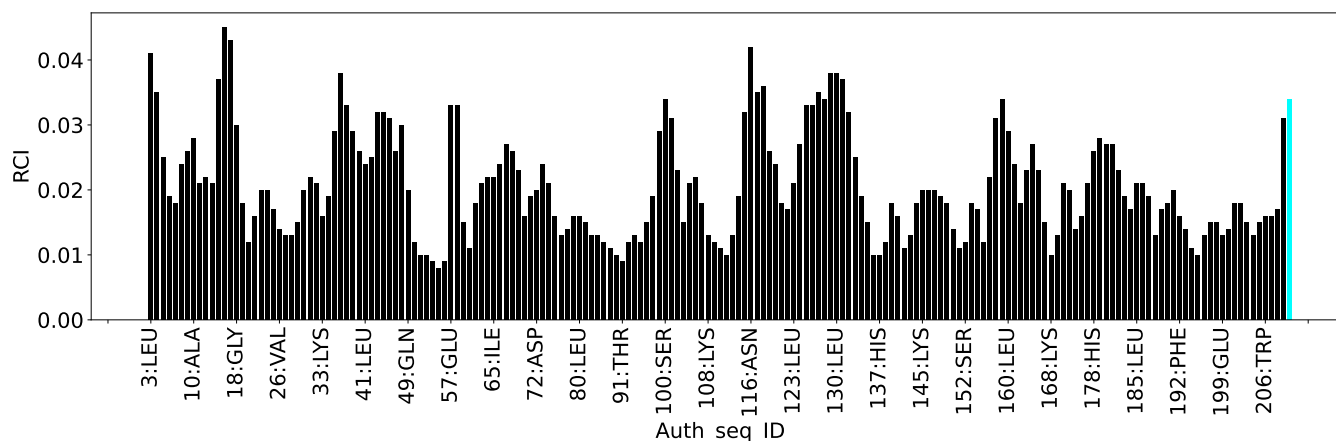
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots [i](#)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:



7.2 Chemical shift list 2

File name: working_cs.cif

Chemical shift list name: *PtDHAR3A_-DHA_O37gAFw.txt*

7.2.1 Bookkeeping [i](#)

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	374
Number of shifts mapped to atoms	374
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.2.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	0	—	None (insufficient data)
$^{13}\text{C}_\beta$	0	—	None (insufficient data)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	187	0.93 ± 0.29	Should be applied

7.2.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 13%, i.e. 374 atoms were assigned a chemical shift out of a possible 2917. 0 out of 42 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	374/1036 (36%)	187/418 (45%)	0/424 (0%)	187/194 (96%)
Sidechain	0/1657 (0%)	0/1085 (0%)	0/530 (0%)	0/42 (0%)
Aromatic	0/224 (0%)	0/114 (0%)	0/99 (0%)	0/11 (0%)
Overall	374/2917 (13%)	187/1617 (12%)	0/1053 (0%)	187/247 (76%)

7.2.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

7.2.5 Random Coil Index (RCI) plots [i](#)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble

composition. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:

