

wwPDB X-ray Structure Validation Summary Report (i)

Feb 17, 2024 – 10:12 PM EST

PDB ID : 4DDM

Title : Pantothenate synthetase in complex with 2,1,3-benzothiadiazole-5-carboxylic

acid

Authors : Silvestre, H.L. Deposited on : 2012-01-18

Resolution : 1.83 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 (i) 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 (1)) were used in the production of this report:

Mol Probity : 4.02b-467

Mogul: 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13 EDS : 2.36

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

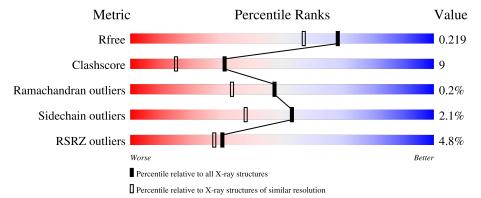
Validation Pipeline (wwPDB-VP) : 2.36

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 1.83 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	Similar resolution
Metric	$(\# ext{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
R_{free}	130704	4003 (1.86-1.82)
Clashscore	141614	4233 (1.86-1.82)
Ramachandran outliers	138981	4185 (1.86-1.82)
Sidechain outliers	138945	4186 (1.86-1.82)
RSRZ outliers	127900	3957 (1.86-1.82)

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 <=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	301	82%	13% • •
1	В	301	78%	13% • 9%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:



Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	EOH	A	403	-	-	X	-
3	EOH	В	403	-	-	X	-
4	0HO	A	406	-	-	X	-



2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 4805 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.

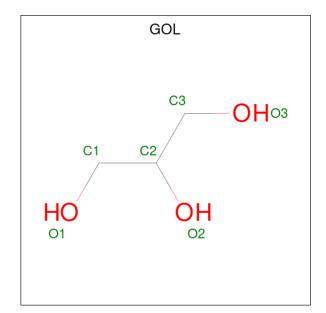
• Molecule 1 is a protein called Pantothenate synthetase.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	А	289	Total	С	N	О	S	0	7	0
1	11	203	2167	1369	389	403	6		•	
1	D	275	Total	С	N	Ο	\mathbf{S}	0	0	0
1	Б	210	2095	1325	381	383	6		0	U

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ALA	THR	engineered mutation	UNP P0A5R0
A	77	GLY	GLU	engineered mutation	UNP P0A5R0
В	2	ALA	THR	engineered mutation	UNP P0A5R0
В	77	GLY	GLU	engineered mutation	UNP P0A5R0

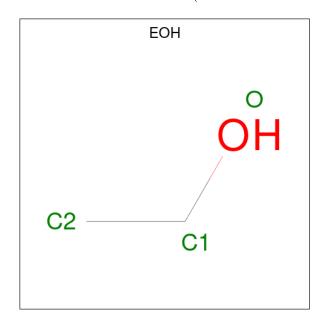
• Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0

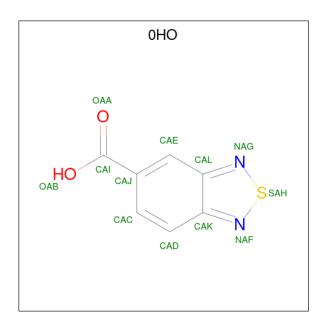
• Molecule 3 is ETHANOL (three-letter code: EOH) (formula: C₂H₆O).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 3 2 1	0	0
3	A	1	Total C O 3 2 1	0	0
3	В	1	Total C O 3 2 1	0	0

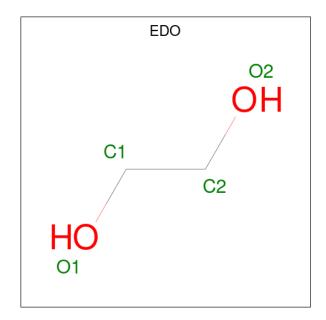
 \bullet Molecule 4 is 2,1,3-benzothia diazole-5-carboxylic acid (three-letter code: 0HO) (formula: $\rm C_7H_4N_2O_2S).$





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf			
4	Λ	1	Total	С	N	О	S	0	0	
4	4 A	1	12	7	2	2	1	0		
1	D	1	Total	С	N	О	S	0	0	
4	Б	1	12	7	2	2	1		U	

 \bullet Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $\mathrm{C_2H_6O_2}).$



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	В	1	Total C O 4 2 2	0	0

• Molecule 6 is water.



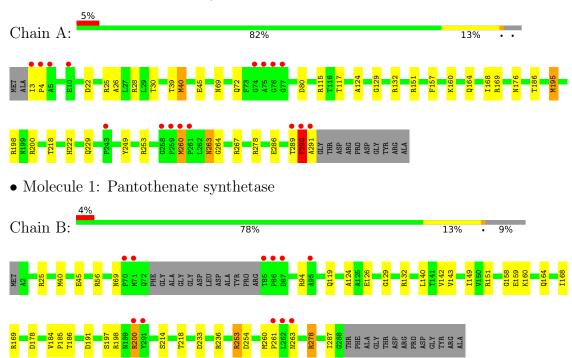
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	249	Total O 249 249	0	0
6	В	239	Total O 239 239	0	0



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: Pantothenate synthetase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	48.45Å 71.04Å 81.97Å	Donositor
a, b, c, α , β , γ	90.00° 99.49° 90.00°	Depositor
Resolution (Å)	35.52 - 1.83	Depositor
Resolution (A)	35.52 - 1.83	EDS
% Data completeness	99.9 (35.52-1.83)	Depositor
(in resolution range)	99.9 (35.52-1.83)	EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) > 1$	2.34 (at 1.83Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
D D.	0.164 , 0.221	Depositor
R, R_{free}	0.163 , 0.219	DCC
R_{free} test set	2446 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	22.4	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.38, 58.3	EDS
L-test for twinning ²	$ < L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4805	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.56% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of <|L|>, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 0HO, EDO, GOL, EOH

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	Bo	nd lengths	Bond angles		
MIOI	Chain	RMSZ = # Z > 5		RMSZ	# Z > 5	
1	A	1.09	$1/2206 \ (0.0\%)$	1.01	8/3014 (0.3%)	
1	В	1.14	0/2135	0.97	5/2914 (0.2%)	
All	All	1.11	1/4341 (0.0%)	0.99	$13/5928 \ (0.2\%)$	

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\text{\AA})$	$\operatorname{Ideal}(ext{\AA})$
1	A	249	TYR	CD1-CE1	5.38	1.47	1.39

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\operatorname{Ideal}(^{o})$
1	A	40	MET	CG-SD-CE	-13.40	78.76	100.20
1	A	278	ARG	NE-CZ-NH1	-9.08	115.76	120.30
1	A	28	ARG	NE-CZ-NH2	-7.92	116.34	120.30
1	В	278	ARG	NE-CZ-NH1	-7.13	116.73	120.30
1	A	169	ARG	NE-CZ-NH2	-6.89	116.86	120.30

There are no chirality outliers.

There are no planarity outliers.

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	2167	0	2200	32	0
1	В	2095	0	2159	46	0
2	A	18	0	24	2	0
3	A	6	0	12	4	0
3	В	3	0	6	18	0
4	A	12	0	3	6	0
4	В	12	0	3	3	0
5	В	4	0	6	1	0
6	A	249	0	0	9	2
6	В	239	0	0	9	1
All	All	4805	0	4413	80	2

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 80 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	Clash overlap (Å)
1:A:164:GLN:HE22	4:A:406:0HO:H3	1.17	1.05
1:B:158:GLY:HA3	3:B:403:EOH:H11	1.45	0.95
1:A:263:ASN:CG	1:A:264:GLY:H	1.71	0.94
1:B:164:GLN:HE22	4:B:401:0HO:H3	1.37	0.90
1:A:229[B]:GLN:NE2	6:A:530:HOH:O	2.04	0.89

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$egin{aligned} ext{Clash} \ ext{overlap } (ext{Å}) \end{aligned}$
6:A:571:HOH:O	6:B:724:HOH:O[2_656]	1.86	0.34
6:A:615:HOH:O	6:A:649:HOH:O[2_645]	2.13	0.07

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	Perce	ntiles
1	A	$292/301 \ (97\%)$	284 (97%)	7 (2%)	1 (0%)	41	27
1	В	280/301 (93%)	276 (99%)	4 (1%)	0	100	100
All	All	572/602 (95%)	560 (98%)	11 (2%)	1 (0%)	47	33

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	290	PHE

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	$220/223 \ (99\%)$	214 (97%)	6 (3%)	44 28		
1	В	214/223 (96%)	211 (99%)	3 (1%)	67 55		
All	All	434/446 (97%)	425 (98%)	9 (2%)	53 38		

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	В	200	ARG
1	В	263	ASN
1	A	263	ASN
1	A	289	THR
1	A	290	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	148	GLN
1	A	164	GLN
1	A	222	HIS
1	В	164	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

9 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or 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 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| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Во	ond leng	ths	Bond angles		
MIOI	Type	Chain	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	A	401	-	5,5,5	0.77	0	5,5,5	0.77	0
2	GOL	A	405	-	5,5,5	0.29	0	5,5,5	0.87	0
3	EOH	В	403	-	2,2,2	0.42	0	1,1,1	0.33	0
4	0HO	A	406	-	13,13,13	2.69	4 (30%)	11,18,18	1.96	4 (36%)
4	0HO	В	401	-	13,13,13	2.31	4 (30%)	11,18,18	2.06	4 (36%)
3	EOH	A	403	-	2,2,2	0.43	0	1,1,1	0.41	0
3	EOH	A	404	-	2,2,2	0.49	0	1,1,1	0.44	0
2	GOL	A	402	-	5,5,5	0.25	0	5,5,5	1.22	0
5	EDO	В	402	-	3,3,3	0.30	0	2,2,2	0.91	0

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.

\mathbf{Mol}	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	A	401	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	A	405	-	-	4/4/4/4	-
4	0HO	A	406	-	-	0/4/4/4	0/2/2/2
4	0HO	В	401	-	-	0/4/4/4	0/2/2/2
2	GOL	A	402	-	-	2/4/4/4	-
5	EDO	В	402	-	-	1/1/1/1	-

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	Observed(A)	$Ideal(\AA)$
4	A	406	0HO	CAE-CAL	-6.01	1.32	1.41
4	A	406	0HO	CAD-CAK	-5.02	1.33	1.41
4	В	401	0HO	CAD-CAK	-4.78	1.33	1.41
4	В	401	0HO	CAE-CAL	-4.62	1.34	1.41
4	A	406	0HO	CAJ-CAI	-4.39	1.40	1.49

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	${f Atoms}$	\mathbf{Z}	$\mathbf{Observed}(^{o})$	$\operatorname{Ideal}(^{o})$
4	В	401	0HO	CAD-CAC-CAJ	-4.06	116.21	120.79
4	A	406	0HO	CAD-CAC-CAJ	-3.87	116.42	120.79
4	A	406	0HO	NAF-SAH-NAG	-3.36	96.55	101.49
4	В	401	0HO	OAB-CAI-CAJ	2.61	121.62	114.85
4	В	401	OHO	CAC-CAD-CAK	2.47	123.94	120.84

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	405	GOL	O1-C1-C2-C3
2	A	401	GOL	O1-C1-C2-C3
2	A	402	GOL	C1-C2-C3-O3
2	A	405	GOL	C1-C2-C3-O3
2	A	402	GOL	O2-C2-C3-O3

There are no ring outliers.

6 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	405	GOL	2	0
3	В	403	EOH	18	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	406	0HO	6	0
4	В	401	0HO	3	0
3	A	403	EOH	4	0
5	В	402	EDO	1	0

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, 95^{th} 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 $>$	$\#\mathrm{RSRZ}{>}2$	$OWAB(Å^2)$	Q<0.9
1	A	289/301 (96%)	-0.08	16 (5%) 25 22	10, 22, 46, 58	4 (1%)
1	В	275/301 (91%)	-0.14	11 (4%) 38 35	11, 21, 41, 60	1 (0%)
All	All	564/602 (93%)	-0.11	27 (4%) 30 28	10, 21, 45, 60	5 (0%)

The worst 5 of 27 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	85	THR	5.8
1	A	3	ILE	4.9
1	A	290	PHE	4.4
1	A	76	GLY	4.3
1	A	243	PRO	4.1

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, 95^{th} 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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
2	GOL	A	402	6/6	0.79	0.17	33,42,46,49	0
2	GOL	A	405	6/6	0.82	0.20	43,53,54,57	0
3	EOH	A	403	3/3	0.82	0.16	30,30,35,35	0
3	ЕОН	A	404	3/3	0.85	0.19	31,31,32,32	0
4	0HO	A	406	12/12	0.86	0.15	19,32,37,47	12
3	EOH	В	403	3/3	0.87	0.22	36,36,40,41	0
4	0HO	В	401	12/12	0.90	0.12	18,23,30,41	12
5	EDO	В	402	4/4	0.97	0.14	25,25,27,30	0
2	GOL	A	401	6/6	0.98	0.11	14,16,17,17	0

6.5 Other polymers (i)

There are no such residues in this entry.

