



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 11, 2024 – 10:03 AM EDT

PDB ID : 9CBD
Title : Pikromycin Thioesterase Domain
Authors : McCullough, T.M.; Smith, J.L.
Deposited on : 2024-06-19
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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
Xtrriage (Phenix) : 1.20.1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.002 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.38.3

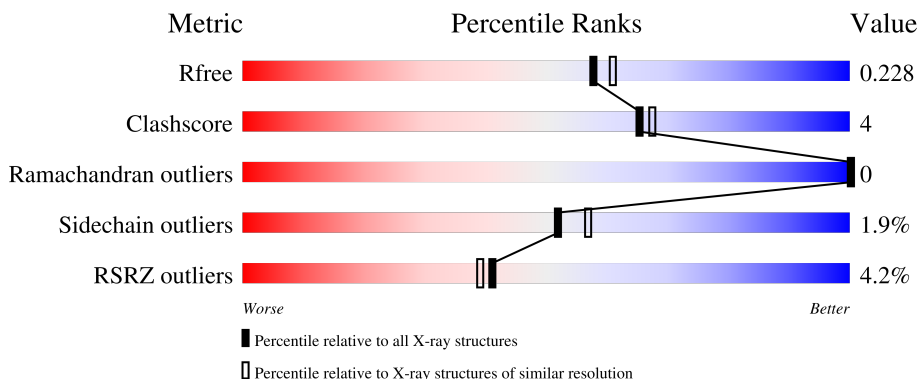
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	164625	9409 (2.00-2.00)
Clashscore	180529	10737 (2.00-2.00)
Ramachandran outliers	177936	10628 (2.00-2.00)
Sidechain outliers	177891	10627 (2.00-2.00)
RSRZ outliers	164620	9409 (2.00-2.00)

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	293	 3% 85% 9% • 5%
1	B	293	 5% 91% • 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4495 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 Narbonolide/10-deoxymethynolide synthase PikA4, module 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	277	2095	1324	374	390	7	0	0	0
1	B	277	2095	1324	374	390	7	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1054	SER	-	expression tag	UNP Q9ZGI2
A	1055	ASN	-	expression tag	UNP Q9ZGI2
A	1056	ALA	-	expression tag	UNP Q9ZGI2
B	1054	SER	-	expression tag	UNP Q9ZGI2
B	1055	ASN	-	expression tag	UNP Q9ZGI2
B	1056	ALA	-	expression tag	UNP Q9ZGI2

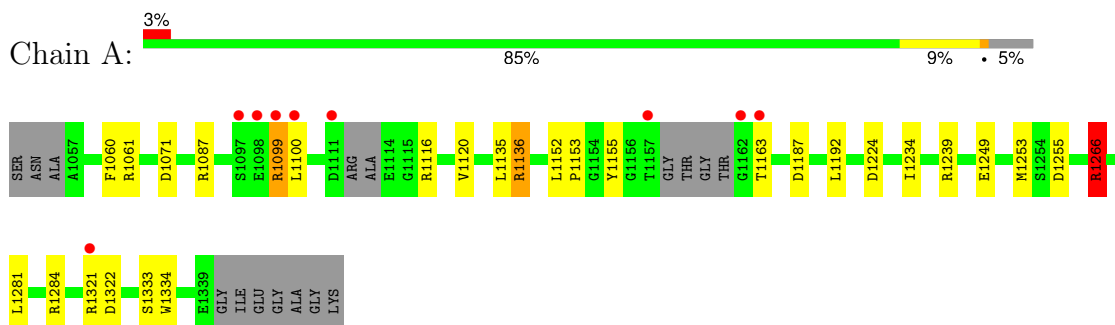
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	176	176	176	0	0
2	B	129	129	129	0	0

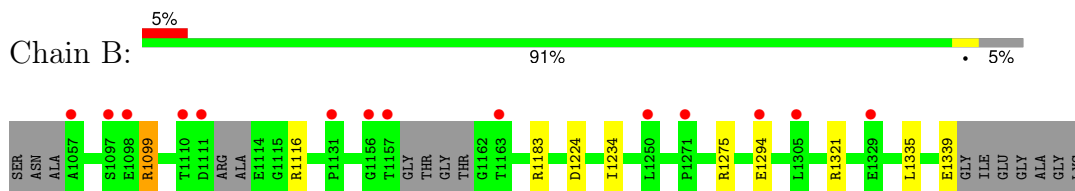
3 Residue-property plots [i](#)

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: Narbonolide/10-deoxymethynolide synthase PikA4, module 6



- Molecule 1: Narbonolide/10-deoxymethynolide synthase PikA4, module 6



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	58.58Å 105.93Å 114.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.04 – 2.00 48.04 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.04-2.00) 99.7 (48.04-2.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.12 (at 2.00Å)	Xtrriage
Refinement program	PHENIX (1.15.2_3472: ???)	Depositor
R, R_{free}	0.198 , 0.228 0.198 , 0.228	Depositor DCC
R_{free} test set	47557 reflections (2.41%)	wwPDB-VP
Wilson B-factor (Å ²)	41.7	Xtrriage
Anisotropy	0.207	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 38.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4495	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.31% 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	0.43	0/2150	0.60	1/2930 (0.0%)
1	B	0.41	0/2150	0.54	0/2930
All	All	0.42	0/4300	0.57	1/5860 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1266	ARG	NE-CZ-NH1	5.04	122.82	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	2095	0	2019	22	0
1	B	2095	0	2019	8	0
2	A	176	0	0	5	0
2	B	129	0	0	5	0
All	All	4495	0	4038	30	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 4.

All (30) 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:1266:ARG:HH11	1:A:1266:ARG:HG3	1.41	0.84
1:A:1087:ARG:HH22	1:A:1163:THR:HB	1.50	0.76
1:B:1116:ARG:NH1	2:B:1402:HOH:O	2.20	0.71
1:B:1294:GLU:CD	1:B:1294:GLU:H	1.95	0.69
1:B:1275:ARG:NH1	2:B:1403:HOH:O	2.29	0.57
1:B:1183:ARG:NH2	2:B:1405:HOH:O	2.37	0.55
1:A:1136:ARG:HD2	1:A:1321:ARG:HA	1.89	0.54
1:A:1099:ARG:NE	1:A:1099:ARG:HA	2.25	0.51
1:A:1100:LEU:HD11	1:A:1153:PRO:HG3	1.92	0.51
1:A:1060:PHE:HB2	1:A:1255:ASP:CG	2.31	0.51
1:B:1099:ARG:NH1	2:B:1410:HOH:O	2.42	0.51
1:A:1321:ARG:HG3	1:A:1322:ASP:H	1.80	0.47
1:A:1061:ARG:NH1	2:A:1412:HOH:O	2.48	0.47
1:A:1071:ASP:HB2	1:A:1239:ARG:NH2	2.30	0.46
1:B:1321:ARG:NH2	2:B:1401:HOH:O	2.19	0.46
1:A:1116:ARG:NH1	2:A:1409:HOH:O	2.42	0.44
1:A:1249:GLU:OE1	2:A:1401:HOH:O	2.21	0.44
1:B:1335:LEU:O	1:B:1339:GLU:HG2	2.17	0.44
1:A:1152:LEU:HD23	1:A:1155:TYR:CE1	2.52	0.44
1:A:1120:VAL:HB	1:A:1192:LEU:HD23	2.01	0.43
1:A:1266:ARG:NH2	2:A:1413:HOH:O	2.50	0.43
1:A:1135:LEU:HD23	1:A:1135:LEU:HA	1.88	0.42
1:A:1060:PHE:HB2	1:A:1255:ASP:OD1	2.20	0.42
1:A:1266:ARG:HH11	1:A:1266:ARG:CG	2.20	0.41
1:A:1087:ARG:HH22	1:A:1163:THR:CB	2.26	0.41
1:A:1249:GLU:OE2	1:A:1253:MET:HG3	2.20	0.41
1:A:1281:LEU:HB2	1:A:1334:TRP:CD2	2.55	0.41
1:A:1234:ILE:HA	1:A:1234:ILE:HD12	1.83	0.40
1:B:1234:ILE:HD12	1:B:1234:ILE:HA	1.86	0.40
1:A:1284:ARG:NH1	2:A:1407:HOH:O	2.39	0.40

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	271/293 (92%)	265 (98%)	6 (2%)	0	100	100
1	B	271/293 (92%)	264 (97%)	7 (3%)	0	100	100
All	All	542/586 (92%)	529 (98%)	13 (2%)	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	207/215 (96%)	201 (97%)	6 (3%)	37	39
1	B	207/215 (96%)	205 (99%)	2 (1%)	73	78
All	All	414/430 (96%)	406 (98%)	8 (2%)	52	57

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1099	ARG
1	A	1136	ARG
1	A	1187	ASP
1	A	1224	ASP
1	A	1266	ARG
1	A	1333	SER
1	B	1099	ARG
1	B	1224	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 oligosaccharides 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

6.1 Protein, DNA and RNA chains

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	277/293 (94%)	0.16	9 (3%) 50 48	26, 38, 64, 88	0
1	B	277/293 (94%)	0.42	14 (5%) 34 32	33, 43, 70, 89	0
All	All	554/586 (94%)	0.29	23 (4%) 41 39	26, 40, 66, 89	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1157	THR	4.2
1	B	1157	THR	3.7
1	A	1163	THR	3.4
1	B	1097	SER	3.1
1	A	1100	LEU	3.0
1	B	1098	GLU	2.8
1	A	1098	GLU	2.7
1	B	1329	GLU	2.7
1	A	1099	ARG	2.6
1	B	1156	GLY	2.5
1	A	1321	ARG	2.4
1	B	1111	ASP	2.4
1	A	1097	SER	2.3
1	B	1294	GLU	2.3
1	B	1057	ALA	2.3
1	B	1271	PRO	2.3
1	A	1162	GLY	2.3
1	B	1110	THR	2.3
1	A	1111	ASP	2.2
1	B	1250	LEU	2.1
1	B	1163	THR	2.1
1	B	1305	LEU	2.0
1	B	1131	PRO	2.0

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.