



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 12, 2024 – 06:41 AM JST

PDB ID : 9K71
Title : Three-dimensional structure of homo-dimer of cystathione beta lyase/PLP from *Bacillus cereus*(BcPatB)
Authors : Liu, Y.; Yang, C.
Deposited on : 2024-10-23
Resolution : 2.28 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
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.003 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

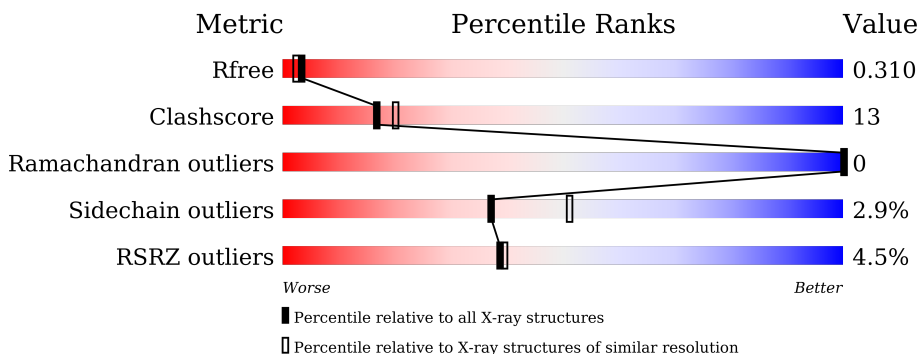
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.28 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	8487 (2.30-2.26)
Clashscore	180529	9437 (2.30-2.26)
Ramachandran outliers	177936	9341 (2.30-2.26)
Sidechain outliers	177891	9342 (2.30-2.26)
RSRZ outliers	164620	8487 (2.30-2.26)

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	383	 2% 71% 27%
1	B	383	 7% 69% 29%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 6343 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 cysteine-S-conjugate beta-lyase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	382	3114	2002	525	570	1	16	0	0	0
1	B	383	3123	2007	526	573	1	16	0	0	0

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	51	LYS	GLU	engineered mutation	UNP Q816F3
A	66	ASP	ASN	engineered mutation	UNP Q816F3
A	131	CYS	TYR	engineered mutation	UNP Q816F3
A	147	LYS	GLN	engineered mutation	UNP Q816F3
A	179	ILE	LEU	engineered mutation	UNP Q816F3
A	180	LYS	GLN	engineered mutation	UNP Q816F3
A	220	GLU	ALA	engineered mutation	UNP Q816F3
A	251	HIS	GLN	engineered mutation	UNP Q816F3
A	255	ALA	SER	engineered mutation	UNP Q816F3
A	286	LYS	GLU	engineered mutation	UNP Q816F3
A	296	LYS	GLN	engineered mutation	UNP Q816F3
A	299	CYS	TRP	engineered mutation	UNP Q816F3
A	302	MET	ILE	engineered mutation	UNP Q816F3
A	304	ASP	THR	engineered mutation	UNP Q816F3
A	308	THR	ALA	engineered mutation	UNP Q816F3
A	326	ALA	ARG	engineered mutation	UNP Q816F3
A	328	ASN	LYS	engineered mutation	UNP Q816F3
A	332	ASP	ASN	engineered mutation	UNP Q816F3
A	336	LYS	ALA	engineered mutation	UNP Q816F3
B	51	LYS	GLU	engineered mutation	UNP Q816F3
B	66	ASP	ASN	engineered mutation	UNP Q816F3
B	131	CYS	TYR	engineered mutation	UNP Q816F3
B	147	LYS	GLN	engineered mutation	UNP Q816F3
B	179	ILE	LEU	engineered mutation	UNP Q816F3
B	180	LYS	GLN	engineered mutation	UNP Q816F3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	220	GLU	ALA	engineered mutation	UNP Q816F3
B	251	HIS	GLN	engineered mutation	UNP Q816F3
B	255	ALA	SER	engineered mutation	UNP Q816F3
B	286	LYS	GLU	engineered mutation	UNP Q816F3
B	296	LYS	GLN	engineered mutation	UNP Q816F3
B	299	CYS	TRP	engineered mutation	UNP Q816F3
B	302	MET	ILE	engineered mutation	UNP Q816F3
B	304	ASP	THR	engineered mutation	UNP Q816F3
B	308	THR	ALA	engineered mutation	UNP Q816F3
B	326	ALA	ARG	engineered mutation	UNP Q816F3
B	328	ASN	LYS	engineered mutation	UNP Q816F3
B	332	ASP	ASN	engineered mutation	UNP Q816F3
B	336	LYS	ALA	engineered mutation	UNP Q816F3

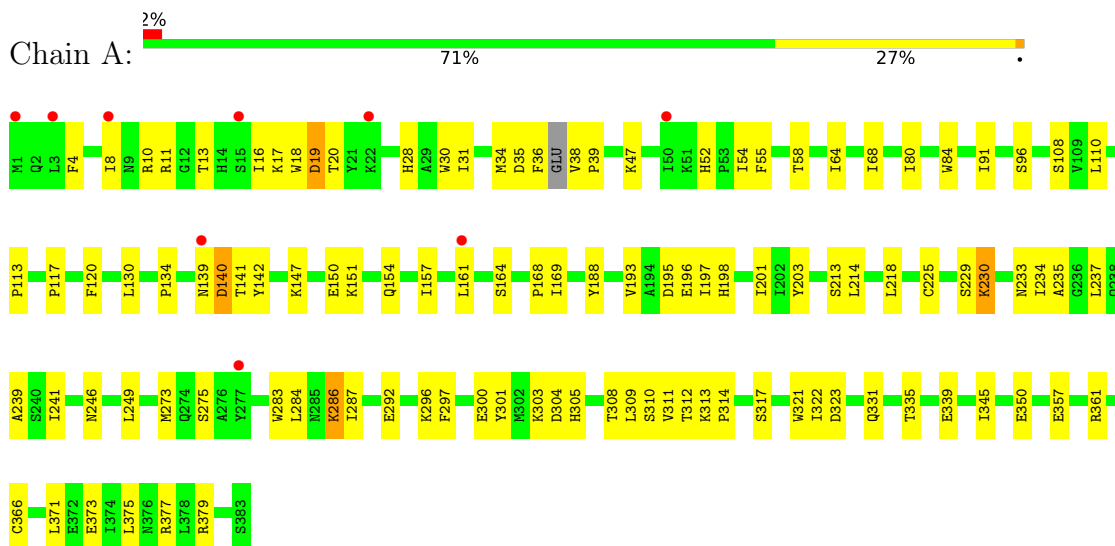
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	46	Total O 46 46	0	0
2	B	60	Total O 60 60	0	0

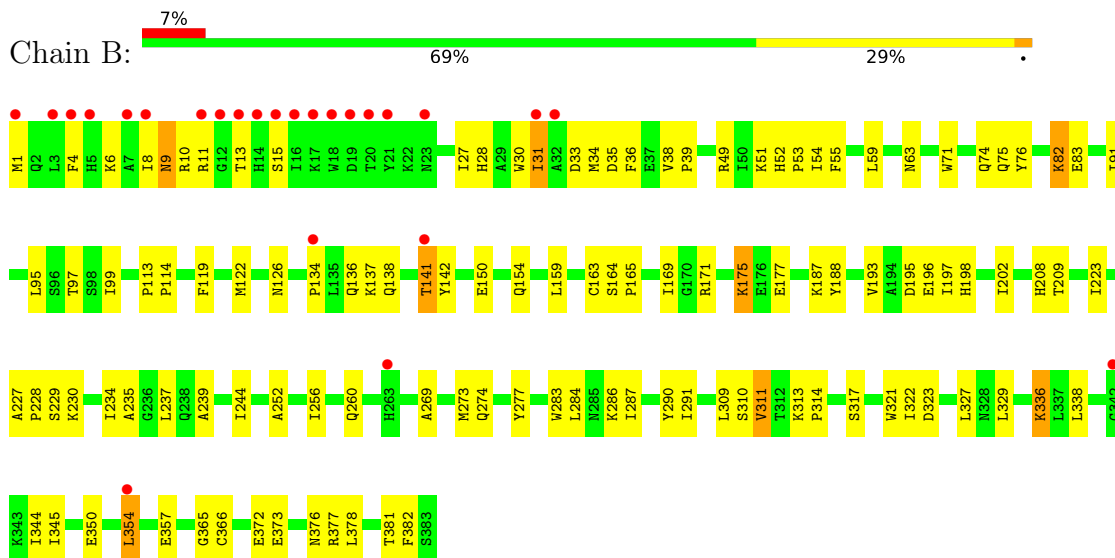
3 Residue-property plots [i](#)

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: cysteine-S-conjugate beta-lyase



- Molecule 1: cysteine-S-conjugate beta-lyase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	53.42Å 84.65Å 163.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.33 – 2.28 42.33 – 2.28	Depositor EDS
% Data completeness (in resolution range)	99.4 (42.33-2.28) 95.3 (42.33-2.28)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.38 (at 2.29Å)	Xtrriage
Refinement program	PHENIX 1.16	Depositor
R, R_{free}	0.229 , 0.310 0.229 , 0.310	Depositor DCC
R_{free} test set	32658 reflections (5.90%)	wwPDB-VP
Wilson B-factor (Å ²)	33.3	Xtrriage
Anisotropy	0.489	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 45.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.19$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6343	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.27% 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](#)

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

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	0.53	0/3167	0.68	0/4296
1	B	0.51	0/3177	0.69	0/4311
All	All	0.52	0/6344	0.69	0/8607

There are no bond length outliers.

There are no bond angle outliers.

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	3114	0	3098	80	0
1	B	3123	0	3105	92	0
2	A	46	0	0	1	0
2	B	60	0	0	1	0
All	All	6343	0	6203	157	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 13.

The worst 5 of 157 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:17:LYS:HD3	1:A:31:ILE:HG22	1.44	1.00
1:A:310:SER:OG	1:A:323:ASP:HB3	1.64	0.95
1:A:312:THR:HG1	1:A:321:TRP:HD1	1.08	0.95
1:A:91:ILE:HG13	1:A:197:ILE:HD12	1.66	0.77
1:A:91:ILE:HB	1:A:230:LLP:H5'1	1.66	0.76

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	377/383 (98%)	361 (96%)	16 (4%)	0	100	100
1	B	380/383 (99%)	363 (96%)	17 (4%)	0	100	100
All	All	757/766 (99%)	724 (96%)	33 (4%)	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	342/343 (100%)	334 (98%)	8 (2%)	45	60
1	B	343/343 (100%)	331 (96%)	12 (4%)	31	43
All	All	685/686 (100%)	665 (97%)	20 (3%)	37	51

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	141	THR
1	B	317	SER
1	B	354	LEU
1	B	336	LYS
1	A	296	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	HIS
1	A	198	HIS
1	B	9	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](#)

2 non-standard protein/DNA/RNA residues 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	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	LLP	B	230	1	23,24,25	1.96	6 (26%)	25,32,34	3.78	6 (24%)
1	LLP	A	230	1	23,24,25	1.73	4 (17%)	25,32,34	3.06	4 (16%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	LLP	B	230	1	-	5/16/17/19	0/1/1/1
1	LLP	A	230	1	-	8/16/17/19	0/1/1/1

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	230	LLP	C4'-NZ	5.07	1.44	1.27
1	A	230	LLP	C4'-NZ	4.87	1.43	1.27
1	B	230	LLP	CE-NZ	4.64	1.56	1.46
1	A	230	LLP	C3-C2	-3.75	1.37	1.40
1	B	230	LLP	C4-C4'	2.90	1.52	1.46

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	230	LLP	CE-NZ-C4'	16.82	170.54	118.90
1	A	230	LLP	CE-NZ-C4'	12.86	158.40	118.90
1	A	230	LLP	OP4-C5'-C5	5.51	119.85	109.35
1	B	230	LLP	C2'-C2-C3	-4.58	115.23	120.89
1	B	230	LLP	C2'-C2-N1	3.60	124.70	117.67

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	230	LLP	C4-C5-C5'-OP4
1	A	230	LLP	C6-C5-C5'-OP4
1	A	230	LLP	C5'-OP4-P-OP3
1	B	230	LLP	C3-C4-C4'-NZ
1	B	230	LLP	C4-C4'-NZ-CE

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	230	LLP	2	0

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 [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	381/383 (99%)	0.21	9 (2%) 59 61	18, 34, 66, 91	0
1	B	382/383 (99%)	0.40	25 (6%) 26 27	19, 39, 75, 103	0
All	All	763/766 (99%)	0.31	34 (4%) 39 39	18, 36, 69, 103	0

The worst 5 of 34 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	15	SER	4.4
1	B	18	TRP	4.3
1	B	23	ASN	4.0
1	B	32	ALA	3.9
1	B	20	THR	3.9

6.2 Non-standard residues in protein, DNA, RNA chains [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, 95th 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	B-factors(Å ²)	Q<0.9
1	LLP	A	230	24/25	0.88	0.11	19,38,63,76	0
1	LLP	B	230	24/25	0.90	0.12	18,42,68,75	0

6.3 Carbohydrates [i](#)

There are no monosaccharides 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.