



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 20, 2025 – 04:52 PM EST

PDB ID : 9BT7
Title : Crystal structure of Chorismate Mutase from Mycobacterium tuberculosis in complex with the cyclic peptide inhibitor D1.3
Authors : Liu, L.; Lovell, S.; Battaile, K.P.; Inglese, J.
Deposited on : 2024-05-14
Resolution : 1.80 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 : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 1.21
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.004 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41.4

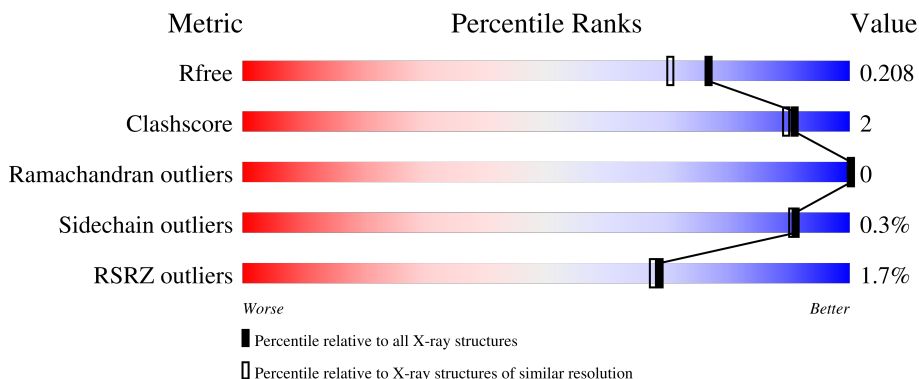
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7108 (1.80-1.80)
Clashscore	180529	8162 (1.80-1.80)
Ramachandran outliers	177936	8077 (1.80-1.80)
Sidechain outliers	177891	8076 (1.80-1.80)
RSRZ outliers	164620	7108 (1.80-1.80)

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	205	<div> <div> <div></div> <div>76%</div> <div></div> <div>21%</div> </div> <div></div> </div>
1	B	205	<div> <div> <div></div> <div>76%</div> <div></div> <div>21%</div> </div> <div></div> </div>
2	C	15	<div> <div>100%</div> </div>
2	D	15	<div> <div>100%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3121 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 Secreted chorismate mutase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	161	Total	C	N	O	S	0	3	0
			1283	795	231	254	3			
1	B	161	Total	C	N	O	S	0	5	0
			1306	808	239	256	3			

There are 78 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	200	GLY	-	expression tag	UNP P9WIB9
A	201	LEU	-	expression tag	UNP P9WIB9
A	202	ASN	-	expression tag	UNP P9WIB9
A	203	ASP	-	expression tag	UNP P9WIB9
A	204	ILE	-	expression tag	UNP P9WIB9
A	205	PHE	-	expression tag	UNP P9WIB9
A	206	GLU	-	expression tag	UNP P9WIB9
A	207	ALA	-	expression tag	UNP P9WIB9
A	208	GLN	-	expression tag	UNP P9WIB9
A	209	LYS	-	expression tag	UNP P9WIB9
A	210	ILE	-	expression tag	UNP P9WIB9
A	211	GLU	-	expression tag	UNP P9WIB9
A	212	TRP	-	expression tag	UNP P9WIB9
A	213	HIS	-	expression tag	UNP P9WIB9
A	214	GLU	-	expression tag	UNP P9WIB9
A	215	SER	-	expression tag	UNP P9WIB9
A	216	SER	-	expression tag	UNP P9WIB9
A	217	GLY	-	expression tag	UNP P9WIB9
A	218	LEU	-	expression tag	UNP P9WIB9
A	219	VAL	-	expression tag	UNP P9WIB9
A	220	PRO	-	expression tag	UNP P9WIB9
A	221	ARG	-	expression tag	UNP P9WIB9
A	222	GLY	-	expression tag	UNP P9WIB9
A	223	SER	-	expression tag	UNP P9WIB9
A	224	ALA	-	expression tag	UNP P9WIB9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	225	ALA	-	expression tag	UNP P9WIB9
A	226	GLY	-	expression tag	UNP P9WIB9
A	227	HIS	-	expression tag	UNP P9WIB9
A	228	HIS	-	expression tag	UNP P9WIB9
A	229	HIS	-	expression tag	UNP P9WIB9
A	230	HIS	-	expression tag	UNP P9WIB9
A	231	HIS	-	expression tag	UNP P9WIB9
A	232	HIS	-	expression tag	UNP P9WIB9
A	233	HIS	-	expression tag	UNP P9WIB9
A	234	HIS	-	expression tag	UNP P9WIB9
A	235	HIS	-	expression tag	UNP P9WIB9
A	236	HIS	-	expression tag	UNP P9WIB9
A	237	GLU	-	expression tag	UNP P9WIB9
A	238	LEU	-	expression tag	UNP P9WIB9
B	200	GLY	-	expression tag	UNP P9WIB9
B	201	LEU	-	expression tag	UNP P9WIB9
B	202	ASN	-	expression tag	UNP P9WIB9
B	203	ASP	-	expression tag	UNP P9WIB9
B	204	ILE	-	expression tag	UNP P9WIB9
B	205	PHE	-	expression tag	UNP P9WIB9
B	206	GLU	-	expression tag	UNP P9WIB9
B	207	ALA	-	expression tag	UNP P9WIB9
B	208	GLN	-	expression tag	UNP P9WIB9
B	209	LYS	-	expression tag	UNP P9WIB9
B	210	ILE	-	expression tag	UNP P9WIB9
B	211	GLU	-	expression tag	UNP P9WIB9
B	212	TRP	-	expression tag	UNP P9WIB9
B	213	HIS	-	expression tag	UNP P9WIB9
B	214	GLU	-	expression tag	UNP P9WIB9
B	215	SER	-	expression tag	UNP P9WIB9
B	216	SER	-	expression tag	UNP P9WIB9
B	217	GLY	-	expression tag	UNP P9WIB9
B	218	LEU	-	expression tag	UNP P9WIB9
B	219	VAL	-	expression tag	UNP P9WIB9
B	220	PRO	-	expression tag	UNP P9WIB9
B	221	ARG	-	expression tag	UNP P9WIB9
B	222	GLY	-	expression tag	UNP P9WIB9
B	223	SER	-	expression tag	UNP P9WIB9
B	224	ALA	-	expression tag	UNP P9WIB9
B	225	ALA	-	expression tag	UNP P9WIB9
B	226	GLY	-	expression tag	UNP P9WIB9
B	227	HIS	-	expression tag	UNP P9WIB9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	228	HIS	-	expression tag	UNP P9WIB9
B	229	HIS	-	expression tag	UNP P9WIB9
B	230	HIS	-	expression tag	UNP P9WIB9
B	231	HIS	-	expression tag	UNP P9WIB9
B	232	HIS	-	expression tag	UNP P9WIB9
B	233	HIS	-	expression tag	UNP P9WIB9
B	234	HIS	-	expression tag	UNP P9WIB9
B	235	HIS	-	expression tag	UNP P9WIB9
B	236	HIS	-	expression tag	UNP P9WIB9
B	237	GLU	-	expression tag	UNP P9WIB9
B	238	LEU	-	expression tag	UNP P9WIB9

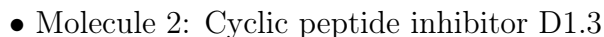
- Molecule 2 is a protein called Cyclic peptide inhibitor D1.3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	15	Total	C	N	O	S	0	0	0
			135	87	25	22	1			
2	D	15	Total	C	N	O	S	0	0	0
			135	87	25	22	1			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	118	Total	O	0	0
			118	118		
3	B	115	Total	O	0	0
			115	115		
3	C	16	Total	O	0	0
			16	16		
3	D	13	Total	O	0	0
			13	13		

- Molecule 1: Secreted chorismate mutase



- Molecule 2: Cyclic peptide inhibitor D1.3



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	70.19Å 71.10Å 71.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.95 – 1.80 49.95 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.95-1.80) 100.0 (49.95-1.80)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 1.79Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.176 , 0.208 0.175 , 0.208	Depositor DCC
R_{free} test set	1786 reflections (5.27%)	wwPDB-VP
Wilson B-factor (Å ²)	19.5	Xtriage
Anisotropy	0.387	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 41.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.007 for -h,l,k 0.006 for -l,-k,-h 0.008 for k,h,-l 0.000 for k,l,h 0.000 for l,h,k	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3121	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.16% 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: ACE, DTY

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	0.37	0/1312	0.56	0/1786
1	B	0.36	0/1336	0.57	0/1818
2	C	0.31	0/124	0.58	0/164
2	D	0.39	0/124	0.60	0/164
All	All	0.36	0/2896	0.57	0/3932

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	1283	0	1240	5	0
1	B	1306	0	1271	4	0
2	C	135	0	117	0	0
2	D	135	0	117	0	0
3	A	118	0	0	1	0
3	B	115	0	0	1	0
3	C	16	0	0	0	0
3	D	13	0	0	0	0
All	All	3121	0	2745	9	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 2.

The worst 5 of 9 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:169:ARG:HE	1:A:173:ARG:HH12	1.45	0.63
1:B:134[A]:ARG:HH11	1:B:134[A]:ARG:HB2	1.73	0.54
1:A:96:ARG:NH1	3:A:302:HOH:O	2.44	0.49
1:A:169:ARG:NE	1:A:173:ARG:HH12	2.12	0.45
1:B:130:LEU:O	1:B:134[A]:ARG:HD3	2.18	0.43

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	162/205 (79%)	160 (99%)	2 (1%)	0	100	100
1	B	164/205 (80%)	163 (99%)	1 (1%)	0	100	100
2	C	12/15 (80%)	11 (92%)	1 (8%)	0	100	100
2	D	12/15 (80%)	11 (92%)	1 (8%)	0	100	100
All	All	350/440 (80%)	345 (99%)	5 (1%)	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	138/171 (81%)	138 (100%)	0	100	100
1	B	141/171 (82%)	139 (99%)	2 (1%)	62	56
2	C	11/11 (100%)	11 (100%)	0	100	100
2	D	11/11 (100%)	11 (100%)	0	100	100
All	All	301/364 (83%)	299 (99%)	2 (1%)	91	79

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	134[A]	ARG
1	B	134[B]	ARG

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

Mol	Chain	Res	Type
1	A	190	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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	$\# Z > 2$
2	DTY	D	1	2	11,12,13	0.45	0	10,15,17	0.13	0
2	DTY	C	1	2	11,12,13	0.45	0	10,15,17	0.14	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.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DTY	D	1	2	-	0/5/6/8	0/1/1/1
2	DTY	C	1	2	-	0/5/6/8	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	161/205 (78%)	-0.31	3 (1%) 66 64	8, 18, 31, 44	3 (1%)
1	B	161/205 (78%)	-0.27	3 (1%) 66 64	8, 18, 31, 45	5 (3%)
2	C	13/15 (86%)	-0.35	0 100 100	16, 18, 26, 38	0
2	D	13/15 (86%)	-0.17	0 100 100	18, 20, 38, 43	0
All	All	348/440 (79%)	-0.29	6 (1%) 69 67	8, 18, 32, 45	8 (2%)

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	196	LEU	3.6
1	A	36	THR	3.1
1	A	196	LEU	3.0
1	B	134[A]	ARG	2.9
1	B	36	THR	2.3

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
2	DTY	C	1	12/13	0.97	0.06	14,15,17,18	0
2	DTY	D	1	12/13	0.97	0.06	14,15,16,16	0

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.