Full wwPDB X-ray Structure Validation Report (i)

Nov 18, 2024 – 03:03 pm GMT

PDB ID	:	8RIN
Title	:	Crystal structure of EccC5 DUF domain of Mycobacterium tuberculosis
Authors	:	Ceballos-Zuniga, F.; Perez-Dorado, I.
Deposited on	:	2023-12-19
Resolution	:	2.05 Å(reported)

The following versions of software and data (see references (i)) were used in the production of this report:

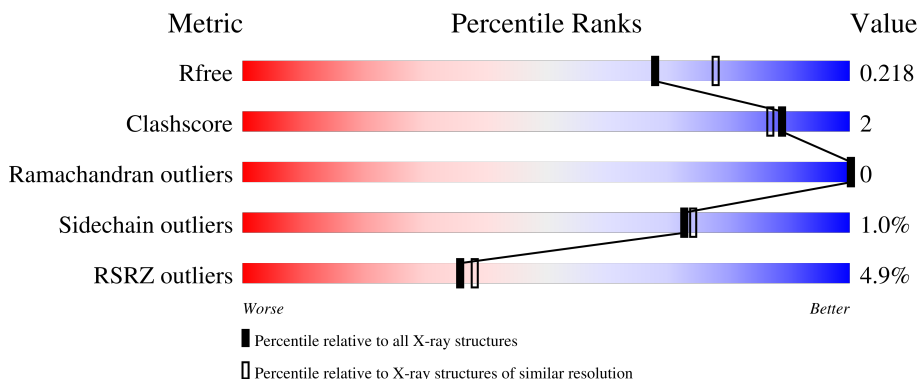|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 2.05 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	Percentile Ranks	Value
Rfree		0.218
Clashscore		2
Ramachandran outliers		0
Sidechain outliers		1.0%
RSRZ outliers		4.9%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	2096 (2.04-2.04)
Clashscore	180529	2229 (2.04-2.04)
Ramachandran outliers	177936	2217 (2.04-2.04)
Sidechain outliers	177891	2217 (2.04-2.04)
RSRZ outliers	164620	2096 (2.04-2.04)

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	292	3% 82% • 14%
1	B	292	5% 84% • 13%

2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 4254 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 ESX-5 secretion system protein EccC5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	251	Total 1971	C 1270	N 337	O 354	S 10	0	3	0
1	B	255	Total 1996	C 1283	N 341	O 361	S 11	0	4	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	97	GLY	-	expression tag	UNP P9WNA5
A	98	PRO	-	expression tag	UNP P9WNA5
A	115	GLY	-	linker	UNP P9WNA5
A	116	SER	-	linker	UNP P9WNA5
A	117	SER	-	linker	UNP P9WNA5
A	118	GLY	-	linker	UNP P9WNA5
A	166A	GLY	-	linker	UNP P9WNA5
A	166B	SER	-	linker	UNP P9WNA5
A	166C	GLY	-	linker	UNP P9WNA5
B	97	GLY	-	expression tag	UNP P9WNA5
B	98	PRO	-	expression tag	UNP P9WNA5
B	115	GLY	-	linker	UNP P9WNA5
B	116	SER	-	linker	UNP P9WNA5
B	117	SER	-	linker	UNP P9WNA5
B	118	GLY	-	linker	UNP P9WNA5
B	166A	GLY	-	linker	UNP P9WNA5
B	166B	SER	-	linker	UNP P9WNA5
B	166C	GLY	-	linker	UNP P9WNA5

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	149	Total 149	O 149	0	0

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| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	138	Total 138	O 138	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: ESX-5 secretion system protein EccC5

Chain A:

• Molecule 1: ESX-5 secretion system protein EccC5

Chain B:
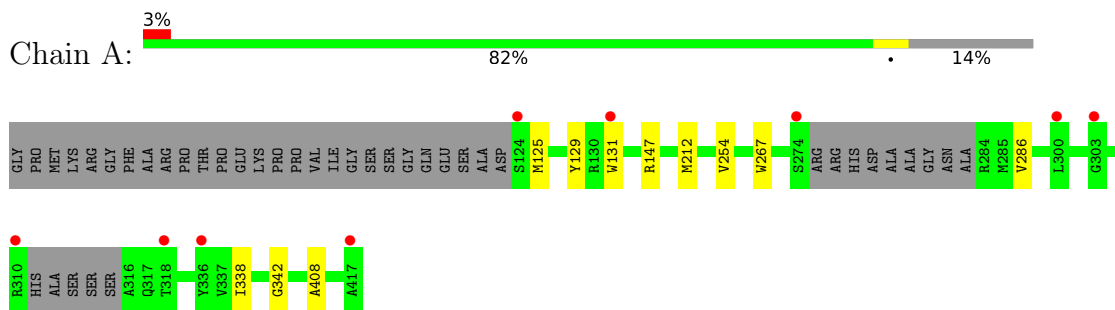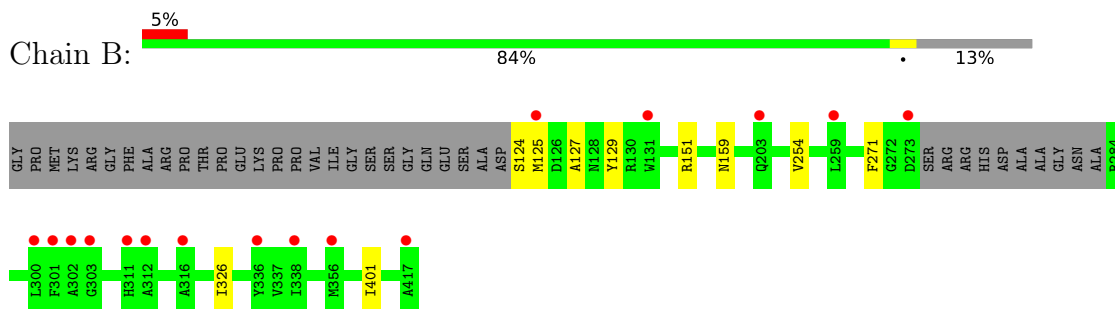
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	48.30Å 52.24Å 57.44Å 88.39° 84.60° 80.17°	Depositor
Resolution (Å)	57.18 – 2.05 57.18 – 2.05	Depositor EDS
% Data completeness (in resolution range)	95.1 (57.18-2.05) 95.1 (57.18-2.05)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.53 (at 2.05Å)	Xtriage
Refinement program	BUSTER 2.10.4, PHENIX 1.20-4459	Depositor
R, R_{free}	0.185 , 0.224 0.180 , 0.218	Depositor DCC
R_{free} test set	1731 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	29.0	Xtriage
Anisotropy	0.454	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 35.2	EDS
L-test for twinning [2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	4254	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.08% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical 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.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	0.41	0/2037	0.55	0/2777
1	B	0.40	0/2065	0.56	0/2813
All	All	0.40	0/4102	0.56	0/5590

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 ⓘ

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	1971	0	1870	6	0
1	B	1996	0	1897	8	0
2	A	149	0	0	0	0
2	B	138	0	0	0	0
All	All	4254	0	3767	14	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.

All (14) 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:131:TRP:HE3	1:A:147:ARG:HD2	1.48	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:TRP:CE3	1:A:147:ARG:HD2	2.30	0.65
1:B:125:MET:CE	1:B:159:ASN:HD21	2.19	0.55
1:B:254:VAL:HG23	1:B:271:PHE:HE2	1.73	0.54
1:B:125:MET:HE1	1:B:159:ASN:HD21	1.80	0.47
1:B:254:VAL:HG23	1:B:271:PHE:CE2	2.52	0.45
1:B:151:ARG:HA	1:B:151:ARG:NE	2.33	0.44
1:A:254:VAL:HG13	1:A:286:VAL:HG13	2.01	0.43
1:B:254:VAL:HG22	1:B:326:ILE:HB	2.00	0.43
1:B:125:MET:HB3	1:B:125:MET:HE3	1.87	0.43
1:A:267:TRP:HB2	1:A:408:ALA:HB1	2.01	0.42
1:B:124:SER:HB3	1:B:127:ALA:HB3	2.03	0.41
1:A:125:MET:HE3	1:A:125:MET:HB3	2.00	0.40
1:A:338:ILE:CD1	1:A:342:GLY:HA2	2.51	0.40

There are no symmetry-related clashes.

5.3   Torsion angles ⓘ

5.3.1   Protein backbone ⓘ

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	248/292 (85%)	246 (99%)	2 (1%)	0	100	100
1	B	255/292 (87%)	248 (97%)	7 (3%)	0	100	100
All	All	503/584 (86%)	494 (98%)	9 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2   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 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	200/241 (83%)	198 (99%)	2 (1%)	73	74
1	B	203/241 (84%)	201 (99%)	2 (1%)	73	74
All	All	403/482 (84%)	399 (99%)	4 (1%)	73	74

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	129	TYR
1	A	212	MET
1	B	129	TYR
1	B	401	ILE

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

Mol	Chain	Res	Type
1	B	159	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	251/292 (85%)	0.00	9 (3%) 46	48	18, 30, 52, 58	3 (1%)
1	B	255/292 (87%)	0.15	16 (6%) 27	28	17, 32, 58, 64	4 (1%)
All	All	506/584 (86%)	0.08	25 (4%) 36	38	17, 31, 54, 64	7 (1%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	131	TRP	4.3
1	A	417	ALA	3.7
1	B	316	ALA	3.5
1	A	303	GLY	3.2
1	B	203	GLN	3.0
1	B	300	LEU	3.0
1	B	125	MET	2.8
1	B	273	ASP	2.8
1	B	417	ALA	2.7
1	B	301	PHE	2.7
1	B	303	GLY	2.6
1	B	336	TYR	2.6
1	B	311	HIS	2.6
1	A	124	SER	2.5
1	A	274	SER	2.4
1	B	131	TRP	2.4
1	A	336	TYR	2.4
1	B	312	ALA	2.3
1	B	302	ALA	2.3
1	A	300	LEU	2.3
1	B	259	LEU	2.2
1	A	318	THR	2.2
1	B	338	ILE	2.2
1	A	310	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	356	MET	2.0

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

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

6.3 Carbohydrates ⓘ

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.