



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 09:07 PM GMT

PDB ID : 1NL3
Title : CRYSTAL STRUCTURE OF THE SECA PROTEIN TRANSLOCATION
ATPASE FROM MYCOBACTERIUM TUBERCULOSIS in APO FORM
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Consortium (TBSGC)
Deposited on : 2003-01-06
Resolution : 2.80 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

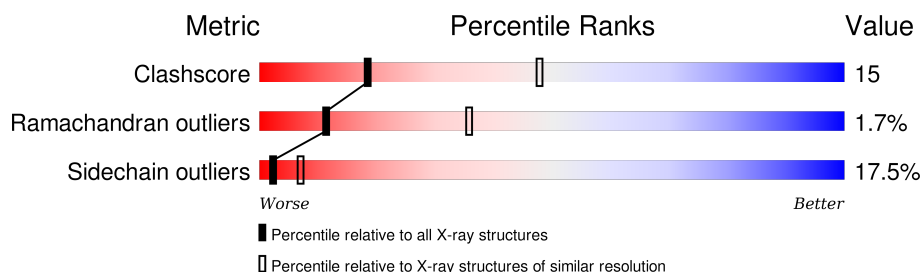
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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))
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	922	 60% 25% 6% • 9%
1	B	922	 56% 27% 7% • 9%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14209 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 PREPROTEIN TRANSLOCASE SECA 1 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	839	Total	C	N	O	S	0	0	0
			6639	4157	1169	1288	25			
1	B	838	Total	C	N	O	S	0	0	0
			6640	4157	1171	1287	25			

There are 62 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-29	MET	-	CLONING ARTIFACT	UNP P0A5Y8
A	-28	LYS	-	CLONING ARTIFACT	UNP P0A5Y8
A	-27	GLU	-	CLONING ARTIFACT	UNP P0A5Y8
A	-26	THR	-	CLONING ARTIFACT	UNP P0A5Y8
A	-25	ALA	-	CLONING ARTIFACT	UNP P0A5Y8
A	-24	ALA	-	CLONING ARTIFACT	UNP P0A5Y8
A	-23	ALA	-	CLONING ARTIFACT	UNP P0A5Y8
A	-22	LYS	-	CLONING ARTIFACT	UNP P0A5Y8
A	-21	PHE	-	CLONING ARTIFACT	UNP P0A5Y8
A	-20	GLU	-	CLONING ARTIFACT	UNP P0A5Y8
A	-19	ARG	-	CLONING ARTIFACT	UNP P0A5Y8
A	-18	GLN	-	CLONING ARTIFACT	UNP P0A5Y8
A	-17	HIS	-	CLONING ARTIFACT	UNP P0A5Y8
A	-16	MET	-	CLONING ARTIFACT	UNP P0A5Y8
A	-15	ASP	-	CLONING ARTIFACT	UNP P0A5Y8
A	-14	SER	-	CLONING ARTIFACT	UNP P0A5Y8
A	-13	PRO	-	CLONING ARTIFACT	UNP P0A5Y8
A	-12	ASP	-	CLONING ARTIFACT	UNP P0A5Y8
A	-11	LEU	-	CLONING ARTIFACT	UNP P0A5Y8
A	-10	GLY	-	CLONING ARTIFACT	UNP P0A5Y8
A	-9	THR	-	CLONING ARTIFACT	UNP P0A5Y8
A	-8	LEU	-	CLONING ARTIFACT	UNP P0A5Y8
A	-7	VAL	-	CLONING ARTIFACT	UNP P0A5Y8
A	-6	PRO	-	CLONING ARTIFACT	UNP P0A5Y8
A	-5	ARG	-	CLONING ARTIFACT	UNP P0A5Y8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	CLONING ARTIFACT	UNP P0A5Y8
A	-3	SER	-	CLONING ARTIFACT	UNP P0A5Y8
A	-2	MET	-	CLONING ARTIFACT	UNP P0A5Y8
A	-1	ALA	-	CLONING ARTIFACT	UNP P0A5Y8
A	0	ASP	-	CLONING ARTIFACT	UNP P0A5Y8
A	1	ILE	-	CLONING ARTIFACT	UNP P0A5Y8
B	-29	MET	-	CLONING ARTIFACT	UNP P0A5Y8
B	-28	LYS	-	CLONING ARTIFACT	UNP P0A5Y8
B	-27	GLU	-	CLONING ARTIFACT	UNP P0A5Y8
B	-26	THR	-	CLONING ARTIFACT	UNP P0A5Y8
B	-25	ALA	-	CLONING ARTIFACT	UNP P0A5Y8
B	-24	ALA	-	CLONING ARTIFACT	UNP P0A5Y8
B	-23	ALA	-	CLONING ARTIFACT	UNP P0A5Y8
B	-22	LYS	-	CLONING ARTIFACT	UNP P0A5Y8
B	-21	PHE	-	CLONING ARTIFACT	UNP P0A5Y8
B	-20	GLU	-	CLONING ARTIFACT	UNP P0A5Y8
B	-19	ARG	-	CLONING ARTIFACT	UNP P0A5Y8
B	-18	GLN	-	CLONING ARTIFACT	UNP P0A5Y8
B	-17	HIS	-	CLONING ARTIFACT	UNP P0A5Y8
B	-16	MET	-	CLONING ARTIFACT	UNP P0A5Y8
B	-15	ASP	-	CLONING ARTIFACT	UNP P0A5Y8
B	-14	SER	-	CLONING ARTIFACT	UNP P0A5Y8
B	-13	PRO	-	CLONING ARTIFACT	UNP P0A5Y8
B	-12	ASP	-	CLONING ARTIFACT	UNP P0A5Y8
B	-11	LEU	-	CLONING ARTIFACT	UNP P0A5Y8
B	-10	GLY	-	CLONING ARTIFACT	UNP P0A5Y8
B	-9	THR	-	CLONING ARTIFACT	UNP P0A5Y8
B	-8	LEU	-	CLONING ARTIFACT	UNP P0A5Y8
B	-7	VAL	-	CLONING ARTIFACT	UNP P0A5Y8
B	-6	PRO	-	CLONING ARTIFACT	UNP P0A5Y8
B	-5	ARG	-	CLONING ARTIFACT	UNP P0A5Y8
B	-4	GLY	-	CLONING ARTIFACT	UNP P0A5Y8
B	-3	SER	-	CLONING ARTIFACT	UNP P0A5Y8
B	-2	MET	-	CLONING ARTIFACT	UNP P0A5Y8
B	-1	ALA	-	CLONING ARTIFACT	UNP P0A5Y8
B	0	ASP	-	CLONING ARTIFACT	UNP P0A5Y8
B	1	ILE	-	CLONING ARTIFACT	UNP P0A5Y8

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	475	Total O 475 475	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	455	Total	O	0	0
			455	455		

Note EDS was not executed.

- Chain A:

60% 25% 6% 9%

Chain A: MET D84 Q86 Q86 A90 M101 K102 T103 K107 T110 C111 V112 L113 P114 A115 Y116 L120 M123 V128 D132 K136 E140 W141 R144 V145 H146 R147 F148 L149 Q152 V155 K156 Y169 D172 F173 G176 R177 N179 M190 A191 S193 Q199 E203 S203 Y204 A205 Y210 D211 D216 R219 L222 L223 L224 S225 G226 P227 A228 S232 N233 R240 L241 A242 P243 D245 E246 K247 V248 R249 E250 D254 L255 R256 K257 R258 T259 V262 E263 E264 K265 E268 F269 G270 E271 D272 L276 D277 E281 A282 Q283 N284 E285 P286 S289 Y290 L291 K296 L300 D304 K305 D306 R310 D311 I316 V317 D318 E319 F320 T321 G322 K323 L324 L325 I326 G327 K328 R329 H335 D336 K347 N350 T357 L358 Q359 Y365 M371 T372 A375 E381 E384 K387 N396 R401 D402 Q404 S405 K410 E413 I417 D421 R426 Y427 L434 I435 G436 T437 T438 T555 E556 R557 H558 R561 S562 L563 D564 S571 Q574 G587 D588 R592 R593 L599 P600 T601 L602 L603 T604 R605 D611 W612 P615 A616 K617 W618 Q632 L633 D634 D645 E646 V647 Q650 R659 R660 R661 I662 N667 L668 K669 A672 L673 D674 M675 E676 R677 D678 R679 I680 V684 T688 G689 E690 A693 R694 D695 W696 R697 L698 D699 W702 T703 L708 Y709 I713 T714 A715 D716 S717 L718 T719 ARG LYS HIS PHE C190 D820 G821 M822 E825 S826 V827 F831 V835 L740 K741 D742 A743 E744 R745 R750 E755 G761 R764 E767 L771 L772 R777 K778 W779 R780 E781 I793 G794 L795 R796 A797 W798 Y799 D800 R801 D802 P803 E806 Q807 Q808 R809 E810 D813 L814 L815

- Chain B: 56% 27% 7% 9%

V835	GLU	D678	E579	R490	E384	Y290	R200	M55	MET
GLU	D678	E579	E586	D493	E384	L291	R200	P64	LYS
ALA	Y683	E586	E586	D493	V391	L295	A205	L78	THR
VAL	D685	E592	E593	D501	V397	E299	V210	D79	ALA
PRO	M763	E592	E593	D501	K410	R303	D216	Q80	ALA
ALA	M764	E593	E593	D501	T411	D304	S212	M81	LYS
PRO	E767	E687	E688	D505	E413	K305	D216	M88	PHE
VAL	M768	E688	E688	D505	E413	V309	R219	M101	GLU
ALA	M769	E688	E688	D505	E413	R310	R219	M101	GLN
PRO	M770	E688	E688	D505	E413	D311	L222	K107	HIS
ALA	M771	E688	E688	D505	E413	D318	L222	T108	MET
GLU	M774	E688	E688	D505	E413	E319	L222	K107	D-15
PRO	M775	E688	E688	D505	E413	F320	L222	T108	S-14
ALA	M776	E688	E688	D505	E413	G226	L222	G111	P-13
ALA	M777	E688	E688	D505	E413	T321	L222	G111	D-12
GLU	M778	E688	E688	D505	E413	G322	L222	G111	R-5
LEU	M779	E688	E688	D505	E413	R323	L222	G111	G-4
ALA	M780	E688	E688	D505	E413	V324	L222	G111	L2
GLU	M784	E688	E688	D505	E413	L325	L222	G111	R3
PHE	M785	E688	E688	D505	E413	I326	L222	G111	K4
ALA	M788	E688	E688	D505	E413	G327	L222	G111	L5
ALA	M791	E688	E688	D505	E413	R328	L222	G111	L6
ALA	M792	E688	E688	D505	E413	R329	L222	G111	R7
ALA	M793	E688	E688	D505	E413	Q336	L222	G111	L8
ALA	M794	E688	E688	D505	E413	K341	L222	G111	R12
GLN	M795	E688	E688	D505	E413	E342	L222	G111	K15
GLN	M796	E688	E688	D505	E413	E345	L222	G111	K18
ARG	M797	E688	E688	D505	E413	I346	L222	G111	A21
SER	M798	E688	E688	D505	E413	K347	L222	G111	V24
ALA	M799	E688	E688	D505	E413	A348	L222	G111	D30
VAL	M800	E688	E688	D505	E413	E349	L222	G111	V31
ASP	M801	E688	E688	D505	E413	N350	L222	G111	T35
GLY	M802	E688	E688	D505	E413	T357	L222	G111	D36
ALA	M803	E688	E688	D505	E413	L358	L222	G111	L39
ALA	M806	E688	E688	D505	E413	Q359	L222	G111	R40
ARG	M807	E688	E688	D505	E413	L364	L222	G111	A41
GLU	M808	E688	E688	D505	E413	Y365	L222	G111	K42
LEU	M809	E688	E688	D505	E413	D366	L222	G111	D44
ARG	M810	E688	E688	D505	E413	K367	L222	G111	D44
ALA	M814	E688	E688	D505	E413	M371	L222	G111	R48
LEU	M820	E688	E688	D505	E413	T372	L222	G111	L50
ARG	M822	E688	E688	D505	E413	A375	L222	G111	A51
LYS	M823	E688	E688	D505	E413	E381	L222	G111	D52
GLY	M824	E688	E688	D505	E413	E381	L222	G111	Q53
VAL	M825	E688	E688	D505	E413	E381	L222	G111	K54
ALA	M826	E688	E688	D505	E413	E381	L222	G111	
SER	M827	E688	E688	D505	E413	E381	L222	G111	
GLU	M828	E688	E688	D505	E413	E381	L222	G111	
SER	M829	E688	E688	D505	E413	E381	L222	G111	
PRO	M831	E688	E688	D505	E413	E381	L222	G111	
ALA	M832	E688	E688	D505	E413	E381	L222	G111	

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 62 2 2	Depositor
Cell constants a, b, c, α , β , γ	206.20 Å 206.20 Å 295.41 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 2.80	Depositor
% Data completeness (in resolution range)	99.4 (8.00-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
Refinement program	REFMAC 5.1.25	Depositor
R, R_{free}	0.193 , 0.259	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	14209	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

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	0.59	0/6743	0.87	26/9116 (0.3%)
1	B	0.59	0/6744	0.88	25/9116 (0.3%)
All	All	0.59	0/13487	0.87	51/18232 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

The worst 5 of 51 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	820	ASP	CB-CG-OD2	7.49	125.04	118.30
1	B	79	ASP	CB-CG-OD2	7.42	124.98	118.30
1	A	248	ASP	CB-CG-OD2	7.18	124.76	118.30
1	A	820	ASP	CB-CG-OD2	6.83	124.45	118.30
1	A	318	ASP	CB-CG-OD2	6.68	124.31	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	320	PHE	Peptide

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	6639	0	6576	197	0
1	B	6640	0	6585	220	0
2	A	475	0	0	57	0
2	B	455	0	0	67	0
All	All	14209	0	13161	409	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 15.

The worst 5 of 409 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:615:GLU:HG3	1:B:323:ARG:HG3	1.37	1.06
1:A:702:TRP:NE1	1:A:714:THR:HA	1.73	1.03
1:A:660:ARG:HG2	2:A:1748:HOH:O	1.60	1.01
1:B:359:GLN:H	1:B:359:GLN:HE21	1.08	1.00
1:A:734:GLU:O	1:A:735:LEU:HB3	1.64	0.94

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	835/922 (91%)	765 (92%)	57 (7%)	13 (2%)	12	38
1	B	834/922 (90%)	758 (91%)	60 (7%)	16 (2%)	10	32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1669/1844 (90%)	1523 (91%)	117 (7%)	29 (2%)	11	36

5 of 29 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	264	GLU
1	A	714	THR
1	A	715	ALA
1	A	716	ASP
1	B	695	ASP

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	696/755 (92%)	577 (83%)	119 (17%)	2	7
1	B	697/755 (92%)	572 (82%)	125 (18%)	2	6
All	All	1393/1510 (92%)	1149 (82%)	244 (18%)	2	7

5 of 244 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	798	MET
1	B	107	LYS
1	B	718	LEU
1	A	809	ARG
1	B	7	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	632	GLN
1	B	118	ASN
1	B	671	GLN

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Mol	Chain	Res	Type
1	A	649	ASN
1	B	53	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 carbohydrates 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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.