



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
Authors : Sharma, V.; Arockiasamy, A.; Ronning, D.R.; Savva, C.G.; Holzenburg, A.;
Braunstein, M.; Jacobs Jr., W.R.; Sacchettini, J.C.; TB Structural Genomics
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)
Xtrriage (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

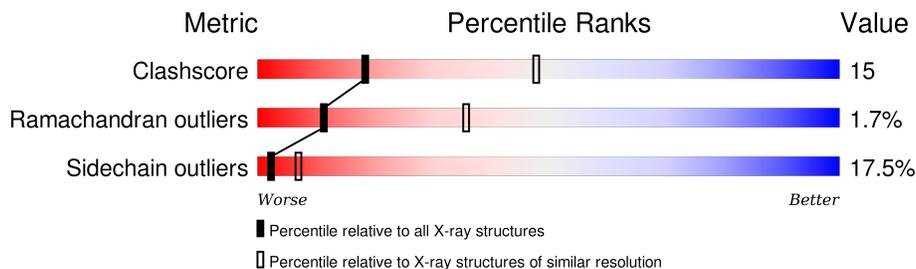
1 Overall quality at a glance

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	
1	B	922	

2 Entry composition [i](#)

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
			Total	C	N	O	S			
1	A	839	6639	4157	1169	1288	25	0	0	0
1	B	838	6640	4157	1171	1287	25	0	0	0

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 455	O 455	0	0

ALA	V835	ALA	D678	ALA	E579	ALA	R490	ALA	Y290	ALA	Y200	ALA	M85	ALA	MET
ALA	G759	ALA	Y683	ALA	L586	ALA	D493	ALA	L291	ALA	R200	ALA	P64	ALA	LYS
ALA	E760	ALA	V684	ALA	L592	ALA	D501	ALA	L295	ALA	A205	ALA	L78	ALA	THR
ALA	M763	ALA	D685	ALA	R593	ALA	D505	ALA	E299	ALA	V210	ALA	D79	ALA	ALA
ALA	R764	ALA	G686	ALA	L603	ALA	Q506	ALA	R303	ALA	D313	ALA	O80	ALA	ALA
ALA	A687	ALA	T688	ALA	L604	ALA	R507	ALA	D304	ALA	S212	ALA	N81	ALA	LYS
ALA	A693	ALA	L602	ALA	L608	ALA	E510	ALA	K305	ALA	D216	ALA	M88	ALA	PHE
ALA	M694	ALA	L603	ALA	P609	ALA	R511	ALA	D309	ALA	R219	ALA	M101	ALA	GLU
ALA	M696	ALA	L604	ALA	D610	ALA	D514	ALA	R310	ALA	R310	ALA	M101	ALA	ARG
ALA	D697	ALA	L605	ALA	E615	ALA	E521	ALA	R323	ALA	L222	ALA	K107	ALA	HIS
ALA	L698	ALA	L705	ALA	A616	ALA	Y522	ALA	R324	ALA	L223	ALA	T108	ALA	MET
ALA	L699	ALA	Y709	ALA	K617	ALA	E523	ALA	V324	ALA	S232	ALA	S-14	ALA	D-15
ALA	D699	ALA	Y709	ALA	M618	ALA	E528	ALA	I325	ALA	I224	ALA	G111	ALA	S-14
ALA	A700	ALA	I713	ALA	V619	ALA	H527	ALA	I326	ALA	S225	ALA	P-13	ALA	P-13
ALA	A701	ALA	T714	ALA	R621	ALA	S528	ALA	G327	ALA	G226	ALA	D-12	ALA	D-12
ALA	A702	ALA	T714	ALA	R622	ALA	E529	ALA	R328	ALA	P227	ALA	V112	ALA	P-13
ALA	L705	ALA	A715	ALA	E616	ALA	E531	ALA	G322	ALA	A228	ALA	Y116	ALA	R-5
ALA	D716	ALA	D716	ALA	K617	ALA	Y522	ALA	R323	ALA	L117	ALA	L117	ALA	G-4
ALA	I717	ALA	D717	ALA	M618	ALA	E523	ALA	V324	ALA	M118	ALA	M118	ALA	L2
ALA	I718	ALA	I718	ALA	V619	ALA	E528	ALA	I326	ALA	T129	ALA	T129	ALA	R3
ALA	I719	ALA	I719	ALA	R621	ALA	H527	ALA	G327	ALA	V130	ALA	V130	ALA	K4
ALA	A791	ALA	A791	ALA	R622	ALA	E529	ALA	R328	ALA	Y133	ALA	Y133	ALA	L5
ALA	G792	ALA	D792	ALA	E616	ALA	E531	ALA	G322	ALA	R240	ALA	R137	ALA	L6
ALA	I793	ALA	D793	ALA	K617	ALA	Y522	ALA	R323	ALA	L241	ALA	K136	ALA	R7
ALA	G794	ALA	D794	ALA	M618	ALA	E523	ALA	V324	ALA	A242	ALA	R137	ALA	L8
ALA	G795	ALA	I795	ALA	V619	ALA	E528	ALA	I326	ALA	P243	ALA	K137	ALA	R12
ALA	L796	ALA	I796	ALA	R621	ALA	E529	ALA	R328	ALA	E246	ALA	M141	ALA	K15
ALA	R796	ALA	I796	ALA	E616	ALA	E531	ALA	G322	ALA	K247	ALA	M142	ALA	K15
ALA	A797	ALA	D797	ALA	K617	ALA	Y522	ALA	R323	ALA	D248	ALA	G143	ALA	K18
ALA	M798	ALA	D798	ALA	M618	ALA	E523	ALA	V324	ALA	V249	ALA	R144	ALA	K18
ALA	A799	ALA	I799	ALA	V619	ALA	E528	ALA	I326	ALA	H250	ALA	H146	ALA	A21
ALA	A800	ALA	I800	ALA	R621	ALA	E529	ALA	R328	ALA	Y251	ALA	R147	ALA	A21
ALA	R801	ALA	I801	ALA	E616	ALA	E531	ALA	G322	ALA	D254	ALA	F148	ALA	V24
ALA	D802	ALA	I802	ALA	K617	ALA	Y522	ALA	R323	ALA	L255	ALA	L151	ALA	D30
ALA	P803	ALA	I803	ALA	M618	ALA	E523	ALA	V324	ALA	K265	ALA	Q152	ALA	V31
ALA	E806	ALA	I806	ALA	V619	ALA	E528	ALA	I326	ALA	R265	ALA	Q152	ALA	D30
ALA	Y807	ALA	I807	ALA	R621	ALA	E529	ALA	R328	ALA	K257	ALA	Y185	ALA	R48
ALA	Q808	ALA	I808	ALA	E616	ALA	E531	ALA	G322	ALA	R258	ALA	Y185	ALA	R49
ALA	R809	ALA	I809	ALA	K617	ALA	Y522	ALA	R323	ALA	T259	ALA	L186	ALA	R49
ALA	E810	ALA	I810	ALA	M618	ALA	E523	ALA	V324	ALA	V260	ALA	D163	ALA	D36
ALA	M814	ALA	I814	ALA	V619	ALA	E528	ALA	I326	ALA	D264	ALA	D163	ALA	D36
ALA	D820	ALA	I820	ALA	R621	ALA	E529	ALA	R328	ALA	L265	ALA	R166	ALA	L39
ALA	G821	ALA	I821	ALA	E616	ALA	E531	ALA	G322	ALA	K265	ALA	R166	ALA	R40
ALA	M822	ALA	I822	ALA	K617	ALA	Y522	ALA	R323	ALA	V270	ALA	M178	ALA	A41
ALA	E824	ALA	I824	ALA	M618	ALA	E523	ALA	V324	ALA	I276	ALA	M179	ALA	K42
ALA	E825	ALA	I825	ALA	V619	ALA	E528	ALA	I326	ALA	D277	ALA	M179	ALA	K42
ALA	S826	ALA	I826	ALA	R621	ALA	E529	ALA	R328	ALA	K278	ALA	D184	ALA	D44
ALA	S827	ALA	I827	ALA	E616	ALA	E531	ALA	G322	ALA	E281	ALA	D184	ALA	D44
ALA	V827	ALA	I827	ALA	K617	ALA	Y522	ALA	R323	ALA	M371	ALA	Y185	ALA	R48
ALA	F831	ALA	I831	ALA	M618	ALA	E523	ALA	V324	ALA	T372	ALA	L186	ALA	R49
ALA	M832	ALA	I832	ALA	V619	ALA	E528	ALA	I326	ALA	A375	ALA	L186	ALA	R49
ALA	E755	ALA	I755	ALA	R621	ALA	E529	ALA	R328	ALA	M284	ALA	A191	ALA	L50
ALA	E756	ALA	I756	ALA	E616	ALA	E531	ALA	G322	ALA	E284	ALA	A191	ALA	L50
ALA	I757	ALA	I757	ALA	K617	ALA	Y522	ALA	R323	ALA	S289	ALA	D195	ALA	D52
ALA	I757	ALA	I757	ALA	M618	ALA	E523	ALA	V324	ALA	E311	ALA	D195	ALA	D52
ALA	I757	ALA	I757	ALA	V619	ALA	E528	ALA	I326	ALA	E311	ALA	D195	ALA	D52
ALA	I757	ALA	I757	ALA	R621	ALA	E529	ALA	R328	ALA	E311	ALA	D195	ALA	D52
ALA	I757	ALA	I757	ALA	E616	ALA	E531	ALA	G322	ALA	E311	ALA	D195	ALA	D52
ALA	I757	ALA	I757	ALA	K617	ALA	Y522	ALA	R323	ALA	E311	ALA	D195	ALA	D52
ALA	I757	ALA	I757	ALA	M618	ALA	E523	ALA	V324	ALA	E311	ALA	D195	ALA	D52
ALA	I757	ALA	I757	ALA	V619	ALA	E528	ALA	I326	ALA	E311	ALA	D195	ALA	D52
ALA	I757	ALA	I757	ALA	R621	ALA	E529	ALA	R328	ALA	E311	ALA	D195	ALA	D52
ALA	I757	ALA	I757	ALA	E616	ALA	E531	ALA	G322	ALA	E311	ALA	D195	ALA	D52
ALA	I757	ALA	I757	ALA	K617	ALA	Y522	ALA	R323	ALA	E311	ALA	D195	ALA	D52
ALA	I757	ALA	I757	ALA	M618	ALA	E523	ALA	V324	ALA	E311	ALA	D195	ALA	D52
ALA	I757	ALA	I757	ALA	V619	ALA	E528	ALA	I326	ALA	E311	ALA	D195	ALA	D52
ALA	I757	ALA	I757	ALA	R621	ALA	E529	ALA	R328	ALA	E311	ALA	D195	ALA	D52
ALA	I757	ALA	I757	ALA	E616	ALA	E531	ALA	G322	ALA	E311	ALA	D195	ALA	D52
ALA	I757	ALA	I757	ALA	K617	ALA	Y522	ALA	R323	ALA	E311	ALA	D195	ALA	D52
ALA	I757	ALA	I757	ALA	M618	ALA	E523	ALA	V324	ALA	E311	ALA	D195	ALA	D52
ALA	I757	ALA	I757	ALA	V619	ALA	E528	ALA	I326	ALA	E311	ALA	D195	ALA	D52
ALA	I757	ALA	I757	ALA	R621	ALA	E529	ALA	R328	ALA	E311	ALA	D195	ALA	D52
ALA	I757	ALA	I757	ALA	E616	ALA	E531	ALA	G322	ALA	E311	ALA	D195	ALA	D52
ALA	I757	ALA	I757	ALA	K617	ALA	Y522	ALA	R323	ALA	E311	ALA	D195	ALA	D52
ALA	I757	ALA	I757	ALA	M618	ALA	E523	ALA	V324	ALA	E311	ALA	D195	ALA	D52
ALA	I757	ALA	I757	ALA	V619	ALA	E528	ALA	I326	ALA	E311	ALA	D195	ALA	D52
ALA	I757	ALA	I757	ALA	R621	ALA	E529	ALA	R328	ALA	E311	ALA	D195	ALA	D52
ALA	I757	ALA	I757	ALA	E616	ALA	E531	ALA	G322	ALA	E311	ALA	D195	ALA	D52
ALA	I757	ALA	I757	ALA	K617	ALA	Y522	ALA	R323	ALA	E311	ALA	D195	ALA	D52
ALA	I757	ALA	I757	ALA	M618	ALA	E523	ALA	V324	ALA	E311	ALA	D195	ALA	D52
ALA	I757	ALA	I757	ALA	V619	ALA	E528	ALA	I326	ALA	E311	ALA	D195	ALA	D52
ALA	I757	ALA	I757	ALA	R621	ALA	E529	ALA	R328	ALA	E311	ALA	D195	ALA	D52
ALA	I757	ALA	I757	ALA	E616	ALA	E531	ALA	G322	ALA	E311	ALA	D195	ALA	D52
ALA	I757	ALA	I757	ALA	K617	ALA	Y522	ALA	R323	ALA	E311	ALA	D195	ALA	D52
ALA	I757	ALA	I757	ALA	M618	ALA	E523	ALA	V324	ALA	E311	ALA	D195	ALA	D52
ALA	I757	ALA	I757	ALA	V619	ALA	E528	ALA	I326	ALA	E311	ALA	D195	ALA	D52
ALA	I757	ALA	I757	ALA	R621	ALA	E529	ALA	R328	ALA	E311	ALA	D195	ALA	D52
ALA	I757	ALA	I757	ALA	E616	ALA	E531	ALA	G322	ALA	E311	ALA	D195	ALA	D52
ALA	I757	ALA	I757	ALA	K617	ALA	Y522	ALA	R323	ALA	E311	ALA	D195	ALA	D52
ALA	I757	ALA	I757	ALA	M618	ALA	E523	ALA	V324	ALA	E311	ALA	D195	ALA	D52
ALA	I757	ALA	I757	ALA	V619	ALA	E528	ALA	I326	ALA	E311	ALA	D195	ALA	D52
ALA	I757	ALA	I757	ALA	R621	ALA	E529	ALA	R328	ALA	E311	ALA	D195	ALA	D52
ALA	I757	ALA	I757	ALA	E616	ALA	E531	ALA	G322	ALA	E311	ALA	D195	ALA	D52
ALA	I757	ALA	I757	ALA	K617	ALA	Y522	ALA	R323	ALA	E311	ALA	D195	ALA	D52
ALA	I757	ALA	I757	ALA	M618	ALA	E523	ALA	V324	ALA	E311	ALA	D195	ALA	D52
ALA	I757	ALA	I757	ALA	V619	ALA	E528	ALA	I326	ALA	E311	ALA	D195	ALA	D52
ALA	I757	ALA	I757	ALA	R621	ALA	E529	ALA	R328	ALA	E311	ALA	D195	ALA	D52
ALA	I757	ALA	I757	ALA	E616	ALA	E531	ALA	G322	ALA	E311	ALA	D195	ALA	D52
ALA	I757	ALA	I757	ALA	K617	ALA	Y522	ALA	R323	ALA	E311	ALA	D195	ALA	D52
ALA	I757	ALA	I757	ALA	M618	ALA	E523	ALA	V324	ALA	E311	ALA	D195	ALA	D52
ALA	I757	ALA	I757	ALA	V619	ALA	E528	ALA	I326	ALA	E311	ALA	D195	ALA	D52
ALA	I757	ALA	I757	ALA	R621	ALA	E529	ALA	R328	ALA	E311	ALA	D195	ALA	D52
ALA	I757	ALA	I757	ALA	E616	ALA	E531	ALA	G322	ALA	E311	ALA	D195	ALA	D52
ALA	I757	ALA	I757	ALA	K617	ALA	Y522	ALA	R323	ALA	E311	ALA	D195	ALA	D52
ALA	I757	ALA	I757	ALA	M618	ALA	E523	ALA	V324	ALA	E311	ALA	D195	ALA	D52
ALA	I757	ALA	I757	ALA	V619										

4 Data and refinement statistics

Xtrriage (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	206.20Å 206.20Å 295.41Å 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.	Xtrriage
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 [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	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 [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	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 [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	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.