



wwPDB X-ray Structure Validation Summary Report ⓘ

May 25, 2020 – 03:53 am BST

PDB ID : 1NL3
Title : CRYSTAL STRUCTURE OF THE SECA PROTEIN TRANSLOCATION
ATPASE FROM MYCOBACTERIUM TUBERCULOSIS in APO FORM
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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

<https://www.wwpdb.org/validation/2017/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
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

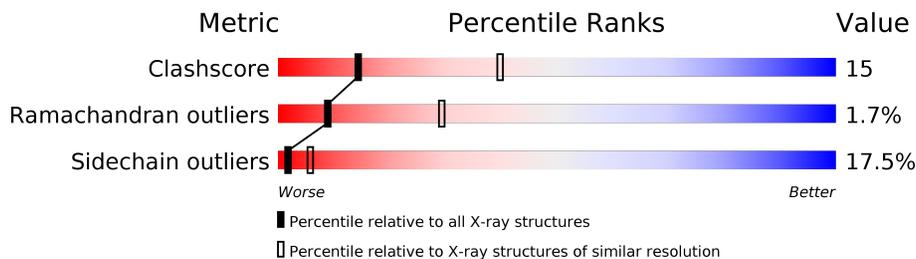
1 Overall quality at a glance

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	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (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 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 $\leq 5\%$

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

V835	MET
GLU	LYS
ALA	GLU
VAL	THR
PRO	ALA
VAL	ALA
VAL	ALA
PRO	ALA
PRO	ALA
ALA	ALA
ALA	ALA
GLU	GLU
PRO	GLU
PRO	GLU
ALA	ARG
ALA	GLN
ALA	HIS
ALA	MET
ALA	D-15
ALA	S-14
ALA	P-13
ALA	D-12
ALA	R-5
ALA	G-4
ALA	L2
ALA	S3
ALA	K4
ALA	L5
ALA	L6
ALA	R7
ALA	L8
ALA	R12
ALA	K15
ALA	K18
ALA	A21
ALA	V24
ALA	D30
ALA	V31
ALA	R31
ALA	T35
ALA	D36
ALA	L39
ALA	R40
ALA	A41
ALA	K42
ALA	T43
ALA	D44
ALA	R48
ALA	R49
ALA	L50
ALA	A51
ALA	D52
ALA	Q53
ALA	K54
ALA	M65
ALA	P64
ALA	L78
ALA	D79
ALA	O80
ALA	N81
ALA	M88
ALA	D16
ALA	M101
ALA	K107
ALA	T108
ALA	G111
ALA	V112
ALA	Y116
ALA	L117
ALA	N118
ALA	T129
ALA	V130
ALA	Y133
ALA	R136
ALA	R137
ALA	W141
ALA	M142
ALA	G143
ALA	R144
ALA	V145
ALA	H146
ALA	R147
ALA	F148
ALA	L151
ALA	Q152
ALA	Y155
ALA	D163
ALA	R166
ALA	M178
ALA	M179
ALA	D184
ALA	Y185
ALA	L186
ALA	A191
ALA	D195
ALA	Q196
ALA	R200
ALA	A205
ALA	V210
ALA	D211
ALA	S212
ALA	D216
ALA	R219
ALA	L222
ALA	I223
ALA	I224
ALA	S225
ALA	G226
ALA	P227
ALA	A228
ALA	D229
ALA	N118
ALA	T129
ALA	V130
ALA	Y133
ALA	R240
ALA	L241
ALA	A242
ALA	P243
ALA	E246
ALA	R247
ALA	D248
ALA	R144
ALA	V249
ALA	H250
ALA	Y251
ALA	D254
ALA	L255
ALA	R256
ALA	K257
ALA	R258
ALA	T259
ALA	V260
ALA	K265
ALA	V270
ALA	I276
ALA	D277
ALA	N278
ALA	L186
ALA	E281
ALA	N284
ALA	S289
ALA	Y290
ALA	L291
ALA	L295
ALA	E299
ALA	R303
ALA	D304
ALA	K305
ALA	V309
ALA	R310
ALA	D311
ALA	D318
ALA	E319
ALA	F320
ALA	T321
ALA	G322
ALA	R323
ALA	V324
ALA	L325
ALA	I326
ALA	G327
ALA	R328
ALA	R329
ALA	Q336
ALA	K341
ALA	E342
ALA	E345
ALA	I346
ALA	K347
ALA	A348
ALA	E349
ALA	R350
ALA	Q351
ALA	T352
ALA	L353
ALA	A354
ALA	T355
ALA	I356
ALA	T357
ALA	L358
ALA	Q359
ALA	L364
ALA	Y365
ALA	D366
ALA	K367
ALA	M371
ALA	T372
ALA	A375
ALA	M486
ALA	E381
ALA	E384
ALA	V391
ALA	M397
ALA	K410
ALA	T411
ALA	E413
ALA	D421
ALA	D422
ALA	V423
ALA	A424
ALA	E425
ALA	R426
ALA	K429
ALA	G430
ALA	V433
ALA	L434
ALA	I435
ALA	G436
ALA	T437
ALA	S439
ALA	V440
ALA	R441
ALA	R442
ALA	S443
ALA	E444
ALA	S447
ALA	R448
ALA	Q449
ALA	F450
ALA	R453
ALA	R454
ALA	I455
ALA	E456
ALA	H457
ALA	L460
ALA	K463
ALA	Y464
ALA	E468
ALA	I472
ALA	R478
ALA	M486
ALA	G489
ALA	R490
ALA	D493
ALA	D501
ALA	D505
ALA	Q506
ALA	R507
ALA	E510
ALA	R511
ALA	D514
ALA	E517
ALA	T518
ALA	P519
ALA	E520
ALA	E521
ALA	Y522
ALA	E523
ALA	H527
ALA	S528
ALA	E529
ALA	L530
ALA	P531
ALA	I532
ALA	V533
ALA	K534
ALA	E535
ALA	E536
ALA	A537
ALA	E444
ALA	S447
ALA	K539
ALA	E540
ALA	E543
ALA	E546
ALA	R651
ALA	R652
ALA	K653
ALA	V654
ALA	L655
ALA	R659
ALA	R660
ALA	R661
ALA	L662
ALA	L663
ALA	K669
ALA	D670
ALA	Q671
ALA	A672
ALA	L673
ALA	D674
ALA	R677
ALA	D678
ALA	Y683
ALA	V684
ALA	D685
ALA	G686
ALA	A687
ALA	T688
ALA	A693
ALA	E694
ALA	D695
ALA	M696
ALA	E697
ALA	L698
ALA	D699
ALA	A700
ALA	L701
ALA	W702
ALA	L705
ALA	Y709
ALA	T713
ALA	T714
ALA	A715
ALA	D716
ALA	S717
ALA	L718
ALA	T719
ALA	ARG
ALA	LYS
ALA	ASP
ALA	HIS
ALA	GLU
ALA	PHE
ALA	GLU
ALA	ARG
ALA	ASP
ALA	ASP
ALA	LEU
ALA	THR
ALA	ARG
ALA	E733
ALA	E734
ALA	L736
ALA	E737
ALA	L740
ALA	R741
ALA	D742
ALA	R750
ALA	L754
ALA	E755
ALA	E756
ALA	R757
ALA	I757
ALA	A758
ALA	G759
ALA	E760
ALA	V763
ALA	R764
ALA	E767
ALA	R768
ALA	M769
ALA	V770
ALA	L771
ALA	V774
ALA	I775
ALA	D776
ALA	R777
ALA	K778
ALA	W779
ALA	R780
ALA	Y784
ALA	E785
ALA	Y788
ALA	E791
ALA	G792
ALA	I793
ALA	G794
ALA	L795
ALA	R796
ALA	A797
ALA	M798
ALA	A799
ALA	Q800
ALA	R801
ALA	D802
ALA	F803
ALA	E806
ALA	Y807
ALA	Q808
ALA	R809
ALA	E810
ALA	M814
ALA	D820
ALA	G821
ALA	M822
ALA	R823
ALA	E824
ALA	E825
ALA	S826
ALA	W827
ALA	F831
ALA	N832
ALA	V835
ALA	P64
ALA	L78
ALA	D79
ALA	O80
ALA	N81
ALA	M88
ALA	D16
ALA	M101
ALA	K107
ALA	T108
ALA	G111
ALA	V112
ALA	Y116
ALA	L117
ALA	N118
ALA	T129
ALA	V130
ALA	Y133
ALA	R136
ALA	R137
ALA	W141
ALA	M142
ALA	G143
ALA	R144
ALA	V145
ALA	H146
ALA	R147
ALA	F148
ALA	L151
ALA	Q152
ALA	Y155
ALA	D163
ALA	R166
ALA	M178
ALA	M179
ALA	D184
ALA	Y185
ALA	L186
ALA	A191
ALA	D195
ALA	Q196
ALA	R200
ALA	A205
ALA	V210
ALA	D211
ALA	S212
ALA	D216
ALA	R219
ALA	L222
ALA	I223
ALA	I224
ALA	S225
ALA	G226
ALA	P227
ALA	A228
ALA	D229
ALA	N118
ALA	T129
ALA	V130
ALA	Y133
ALA	R240
ALA	L241
ALA	A242
ALA	P243
ALA	E246
ALA	R247
ALA	D248
ALA	R144
ALA	V249
ALA	H250
ALA	Y251
ALA	D254
ALA	L255
ALA	R256
ALA	K257
ALA	R258
ALA	T259
ALA	V260
ALA	K265
ALA	V270
ALA	I276
ALA	D277
ALA	N278
ALA	L186
ALA	E281
ALA	N284
ALA	S289
ALA	Y290
ALA	L291
ALA	L295
ALA	E299
ALA	R303
ALA	D304
ALA	K305
ALA	V309
ALA	R310
ALA	D311
ALA	D318
ALA	E319
ALA	F320
ALA	T321
ALA	G322
ALA	R323
ALA	V324
ALA	L325
ALA	I326
ALA	G327
ALA	R328
ALA	R329
ALA	Q336
ALA	K341
ALA	E342
ALA	E345
ALA	I346
ALA	K347
ALA	A348
ALA	E349
ALA	R350
ALA	Q351
ALA	T352
ALA	L353
ALA	A354
ALA	T355
ALA	I356
ALA	T357
ALA	L358
ALA	Q359
ALA	L364
ALA	Y365
ALA	D366
ALA	K367
ALA	M371
ALA	T372
ALA	A375
ALA	M486
ALA	E381
ALA	E384
ALA	V391
ALA	M397
ALA	K410
ALA	T411
ALA	E413
ALA	D421
ALA	D422
ALA	V423
ALA	A424
ALA	E425
ALA	R426
ALA	K429
ALA	G430
ALA	V433
ALA	L434
ALA	I435
ALA	G436
ALA	T437
ALA	S439
ALA	V440
ALA	R441
ALA	R442
ALA	S443
ALA	E444
ALA	S447
ALA	K539
ALA	E540
ALA	E543
ALA	E546
ALA	R651
ALA	R652
ALA	K653
ALA	V654
ALA	L655
ALA	R659
ALA	R660
ALA	R661
ALA	L662
ALA	L663
ALA	K669
ALA	D670
ALA	Q671
ALA	A672
ALA	L673
ALA	D674
ALA	R677
ALA	D678
ALA	Y683
ALA	V684
ALA	D685
ALA	G686
ALA	A687
ALA	T688
ALA	A693
ALA	E694
ALA	D695
ALA	M696
ALA	E697
ALA	L698
ALA	D699
ALA	A700
ALA	L701
ALA	W702
ALA	L705
ALA	Y709
ALA	T713
ALA	T714
ALA	A715
ALA	D716
ALA	S717
ALA	L718
ALA	T719
ALA	ARG
ALA	LYS
ALA	ASP
ALA	HIS
ALA	GLU
ALA	PHE
ALA	GLU
ALA	ARG
ALA	ASP
ALA	ASP
ALA	LEU
ALA	THR
ALA	ARG
ALA	E733
ALA	E734
ALA	L736
ALA	E737
ALA	L740
ALA	R741
ALA	D742
ALA	R750
ALA	L754
ALA	E755
ALA	E756
ALA	R757
ALA	I757
ALA	A758
ALA	G759
ALA	E760
ALA	V763
ALA	R764
ALA	E767
ALA	R768
ALA	M769
ALA	V770
ALA	L771
ALA	V774
ALA	I775
ALA	D776
ALA	R777
ALA	K778
ALA	W779
ALA	R780
ALA	Y784
ALA	E785
ALA	Y788
ALA	E791
ALA	G792
ALA	I793
ALA	G794
ALA	L795
ALA	

4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 6 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%)	9	31
1	B	834/922 (90%)	758 (91%)	60 (7%)	16 (2%)	8	26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1669/1844 (90%)	1523 (91%)	117 (7%)	29 (2%)	9	29

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	6
1	B	697/755 (92%)	572 (82%)	125 (18%)	2	5
All	All	1393/1510 (92%)	1149 (82%)	244 (18%)	2	6

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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.