



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 29, 2020 – 11:01 am BST

PDB ID : 1NKT  
Title : CRYSTAL STRUCTURE OF THE SECA PROTEIN TRANSLOCATION  
ATPASE FROM MYCOBACTERIUM TUBERCULOSIS COMPLEX WITH  
ADPBS  
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 : 2003-01-03  
Resolution : 2.60 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
buster-report : 1.1.7 (2018)  
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

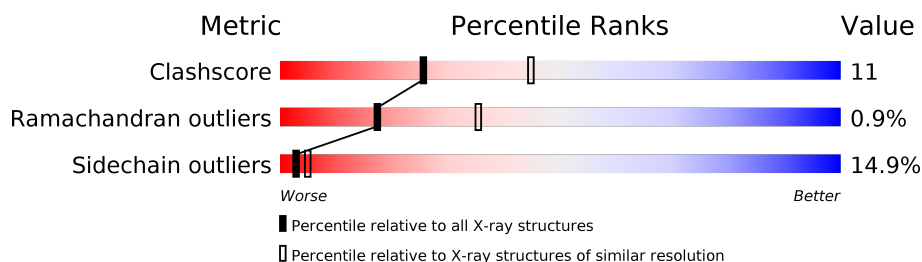
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)

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  $\geq 3$ , 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

There are 4 unique types of molecules in this entry. The entry contains 13862 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	836	Total	C	N	O	S	0	0	0
			6630	4151	1169	1285	25			
1	B	836	Total	C	N	O	S	0	0	0
			6630	4151	1169	1285	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 MAGNESIUM ION (three-letter code: MG) (formula: Mg).

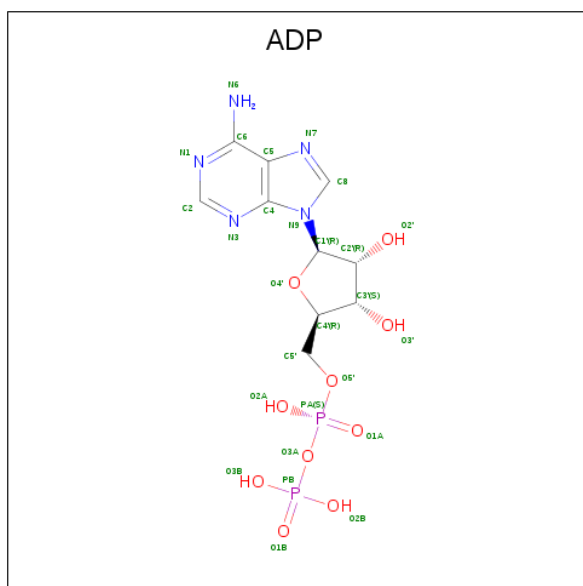
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Mg 1 1	0	0
2	A	1	Total Mg 1 1	0	0

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O P 27 10 5 10 2	0	0
3	B	1	Total C N O P 27 10 5 10 2	0	0

- Molecule 4 is water.

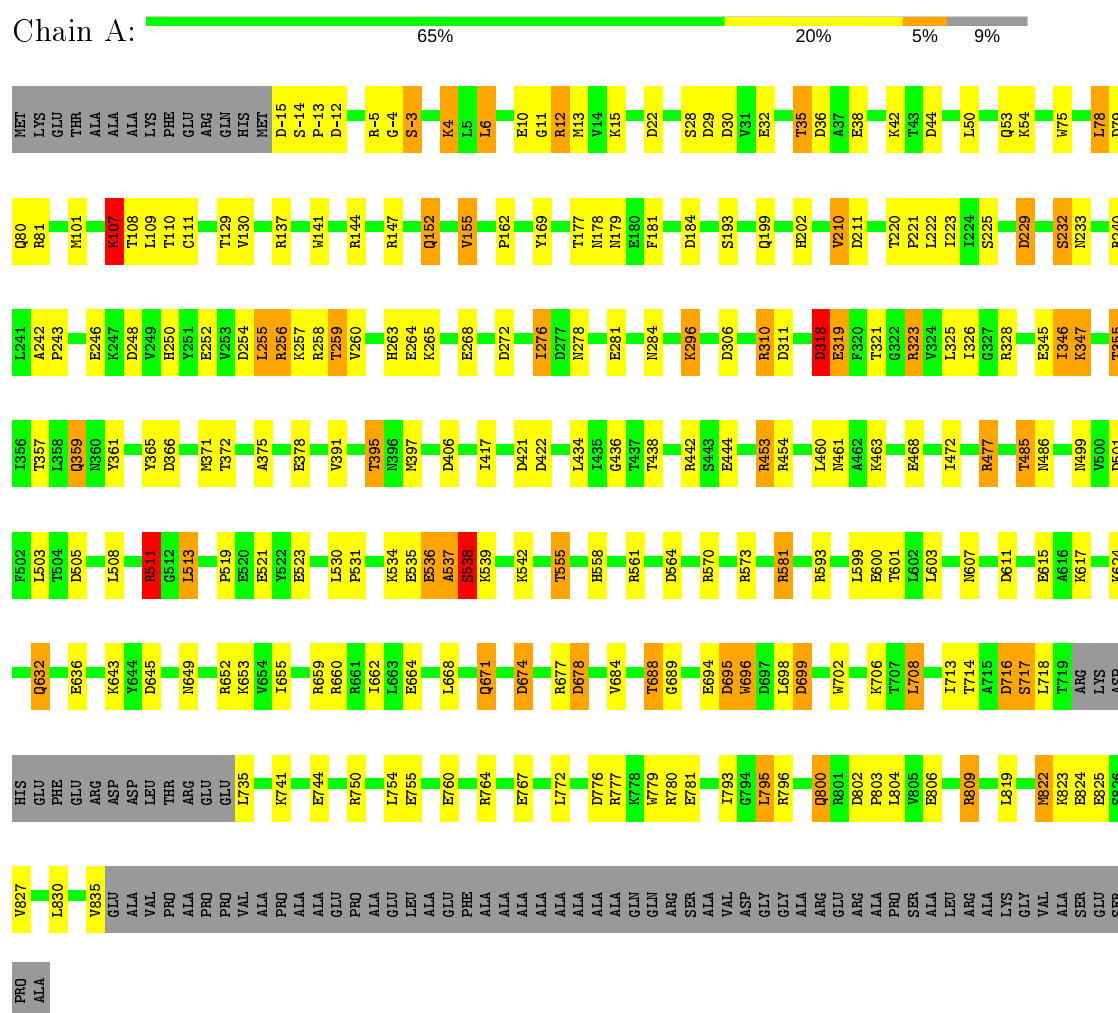
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	246	Total O 246 246	0	0
4	B	300	Total O 300 300	0	0

### 3 Residue-property plots

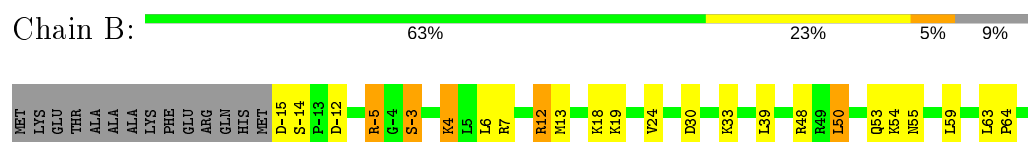
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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. 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.

Note EDS was not executed.

- Molecule 1: Preprotein translocase secA 1 subunit



- Molecule 1: Preprotein translocase secA 1 subunit



VAL	P803	D699	D610	R477	A348	I223	D84
ASP	L804	A700	D611	R478	E349	I224	M101
GLY	V805	L701	V612		N350	S225	
ALA	E806	W702	P613	T485	T355	A228	K107
ARG	Q808	T703	E615	N466	I356	D229	T108
GLU	R809	L708	A616	T482	T357	G230	L109
ARG	E810		K617	D493	L358	N233	T110
ALA		T714	M618		Q359		G111
ALA	D813	A715	K624	D501	D366	R240	V112
SER		D716			K367	A241	L113
LEU	M818	S717	Q632	R507	M371	A242	N118
LEU	L819	L718	Q633	R511	T372	P243	
ARG	D820	ARG					T129
ALA	G821	LYS	R638	E520	A375	E246	V130
LYS	M822	ASP	K639	E523	E381	V249	
GLY	K823	HIS	K643	E529	E394	H250	R137
VAL	E824	GLU		L530	K387	D254	D138
ALA	E825	PHE	E646	I532		K257	G143
SER	S826	ARG	N649	P531	T395	R258	R144
GLU	V827	ASP		E533	K396	T259	V145
SER	L830	ASP	R652	K534	M397	E264	H146
PRQ		LEU	K653	E535	P398	E268	F148
ALA		THR	R659	E536	M399		Q152
	V833	GLU	R660	A537	D406	L276	V153
	T834	ARG	R661	S538	E413	D277	G154
	V835	GLU	E666	K539	E417	E281	V155
ALA		GLU	M667	E540	I417	N284	R165
ALA		VAL	L668	A541			D172
PRQ		VAL	K669	E543	E425	R303	N178
ALA		ALA	D670	T555	K429	D304	N179
ALA		L754	Q671	H558		K305	
ALA		E755	A672	D564	I434	R310	D184
GLU		G759	D674		I435	D311	
ALA			M675	R570	G436		R187
GLU		E767	V676		T437	D318	
LEU			R677	R573	T438	E319	A191
ALA		D776	I680			F320	H192
ALA		R777	T681	R593	E441		
GLU			V684		R442	R323	D195
PHE		R780	D685	A597	S443		
ALA			G686	A598	E444	I326	D208
ALA		E785	A687	L599	K452	G327	E209
ALA		Y788	T688	E600	R453	R328	V210
ALA			G689	T601	R454	R329	
ALA		R796	E690	L602			D216
ALA		A797		L603		E342	
GLN		M798	E694	T604	M461		R219
GLN		A799	D695		A462	E345	T220
ARG		Q800	D696	R605	R463	I346	P221
ARG		R801	M697	L608		K347	
SER		D802	L698	P609	I472		
ALA							

## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 62 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	206.05Å 206.05Å 292.86Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	95.35 – 2.60	Depositor
% Data completeness (in resolution range)	99.0 (95.35-2.60)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
Refinement program	REFMAC 5.1.25	Depositor
R, $R_{free}$	0.213 , 0.265	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13862	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ADP

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	0.66	2/6734 (0.0%)	0.92	27/9102 (0.3%)
1	B	0.68	1/6734 (0.0%)	0.92	29/9102 (0.3%)
All	All	0.67	3/13468 (0.0%)	0.92	56/18204 (0.3%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	511	ARG	C-N	6.67	1.45	1.33
1	B	511	ARG	NE-CZ	6.06	1.41	1.33
1	A	513	LEU	CB-CG	5.59	1.68	1.52

The worst 5 of 56 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	79	ASP	CB-CG-OD2	7.64	125.18	118.30
1	A	318	ASP	CB-CG-OD2	7.41	124.96	118.30
1	B	79	ASP	CB-CG-OD2	7.12	124.71	118.30
1	A	505	ASP	CB-CG-OD2	7.03	124.63	118.30
1	B	84	ASP	CB-CG-OD2	6.83	124.44	118.30

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	6630	0	6581	136	0
1	B	6630	0	6581	151	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	27	0	12	0	0
3	B	27	0	12	1	0
4	A	246	0	0	35	0
4	B	300	0	0	42	0
All	All	13862	0	13186	282	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 11.

The worst 5 of 282 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:11:GLY:HA2	4:A:1387:HOH:O	1.53	1.08
1:A:809:ARG:HB3	1:A:809:ARG:HH11	1.26	1.00
1:A:107:LYS:HD3	4:A:1370:HOH:O	1.62	0.98
1:A:107:LYS:CD	4:A:1370:HOH:O	2.14	0.95
1:A:660:ARG:HG2	4:A:1349:HOH:O	1.66	0.93

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	832/922 (90%)	781 (94%)	41 (5%)	10 (1%)	13 27
1	B	832/922 (90%)	784 (94%)	43 (5%)	5 (1%)	25 47
All	All	1664/1844 (90%)	1565 (94%)	84 (5%)	15 (1%)	17 35

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	319	GLU
1	A	486	ASN
1	A	538	SER
1	A	689	GLY
1	A	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	697/755 (92%)	592 (85%)	105 (15%)	3	4
1	B	697/755 (92%)	594 (85%)	103 (15%)	3	5
All	All	1394/1510 (92%)	1186 (85%)	208 (15%)	3	5

5 of 208 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	744	GLU
1	B	53	GLN
1	B	708	LEU
1	A	754	LEU
1	B	-14	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	649	ASN
1	B	118	ASN
1	B	632	GLN
1	A	671	GLN
1	B	80	GLN

### 5.3.3 RNA ⓘ

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](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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	$\# Z  > 2$
3	ADP	A	900	2	24,29,29	1.34	3 (12%)	29,45,45	1.74	3 (10%)
3	ADP	B	901	2	24,29,29	1.31	3 (12%)	29,45,45	1.69	4 (13%)

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
3	ADP	A	900	2	-	4/12/32/32	0/3/3/3
3	ADP	B	901	2	-	2/12/32/32	0/3/3/3

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	901	ADP	C2-N3	4.26	1.39	1.32
3	A	900	ADP	C2-N3	4.18	1.38	1.32
3	B	901	ADP	C2-N1	2.99	1.39	1.33
3	A	900	ADP	C2-N1	2.65	1.38	1.33
3	B	901	ADP	PB-O3B	2.36	1.63	1.54

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	900	ADP	N3-C2-N1	-6.55	118.44	128.68
3	B	901	ADP	N3-C2-N1	-5.50	120.07	128.68
3	B	901	ADP	O3B-PB-O3A	3.48	116.32	104.64
3	A	900	ADP	O3A-PB-O1B	-3.36	92.56	111.19
3	B	901	ADP	O3A-PB-O1B	-3.26	93.11	111.19

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

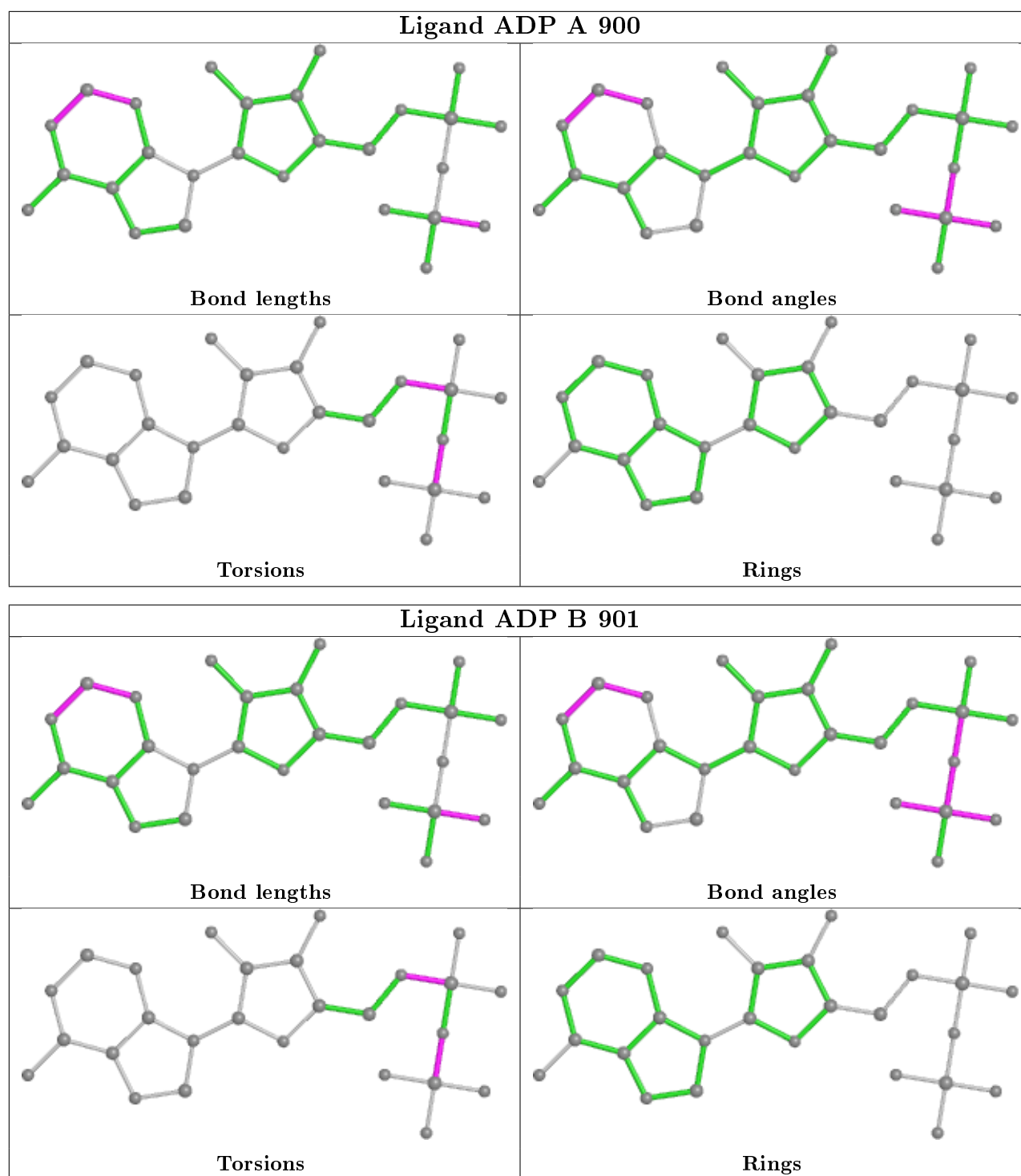
Mol	Chain	Res	Type	Atoms
3	A	900	ADP	PA-O3A-PB-O2B
3	B	901	ADP	PA-O3A-PB-O1B
3	A	900	ADP	PA-O3A-PB-O1B
3	A	900	ADP	PA-O3A-PB-O3B
3	A	900	ADP	C5'-O5'-PA-O1A

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	901	ADP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 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 ⓘ

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.