wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 09:07 PM GMT

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
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

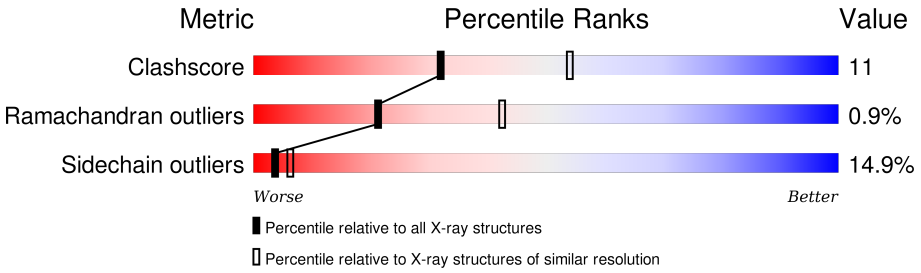
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance (i)

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	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (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 >=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 <=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	65% 20% 5% 9%
1	B	922	63% 23% 5% 9%

2 Entry composition (i)

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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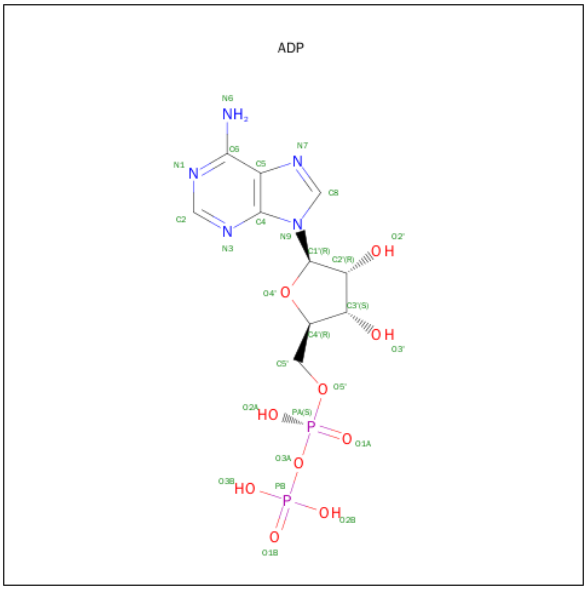
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf

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

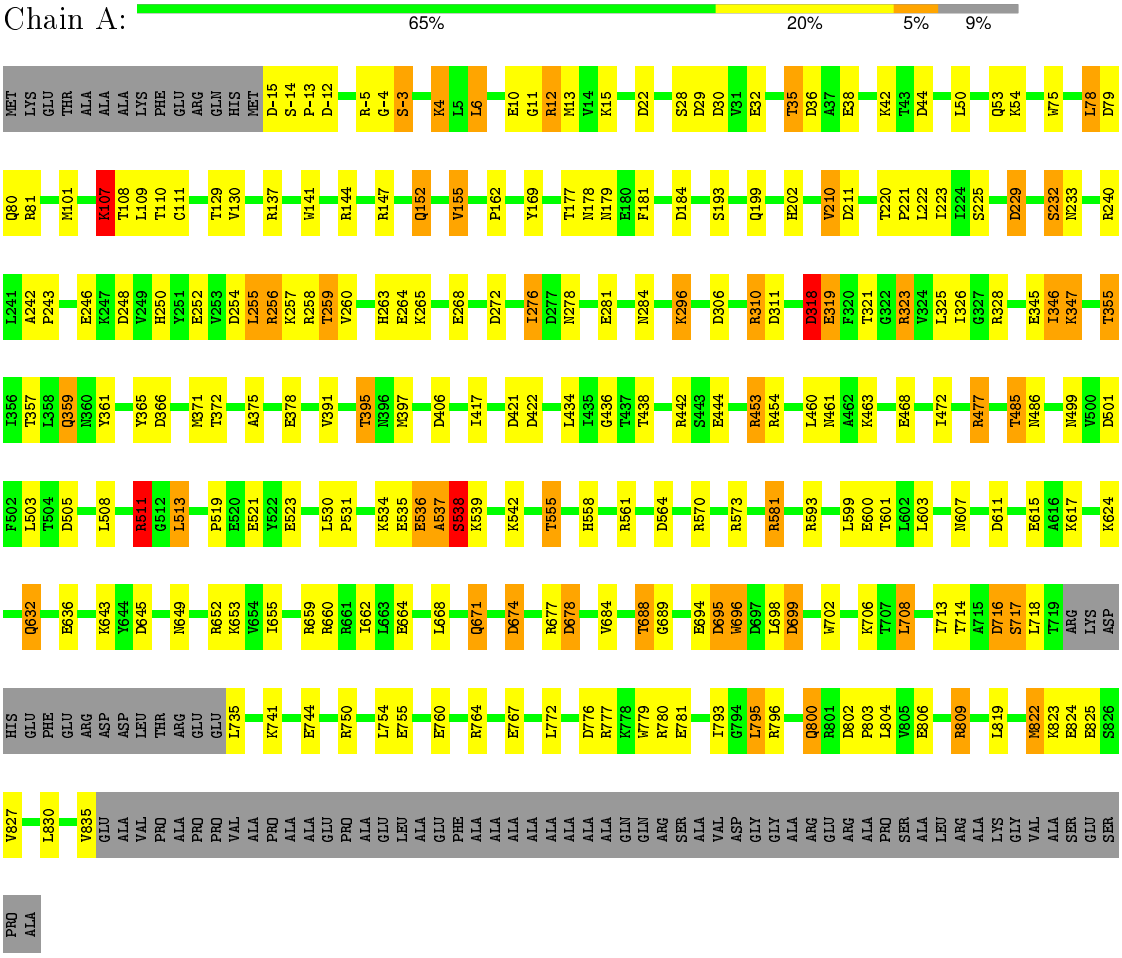
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

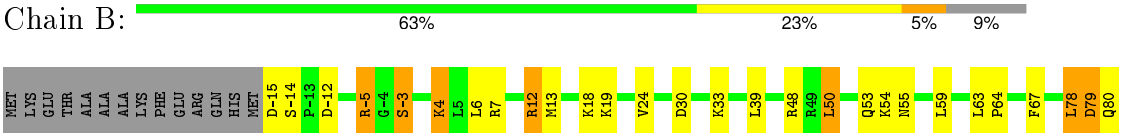
- Molecule 1: Preprotein translocase secA 1 subunit

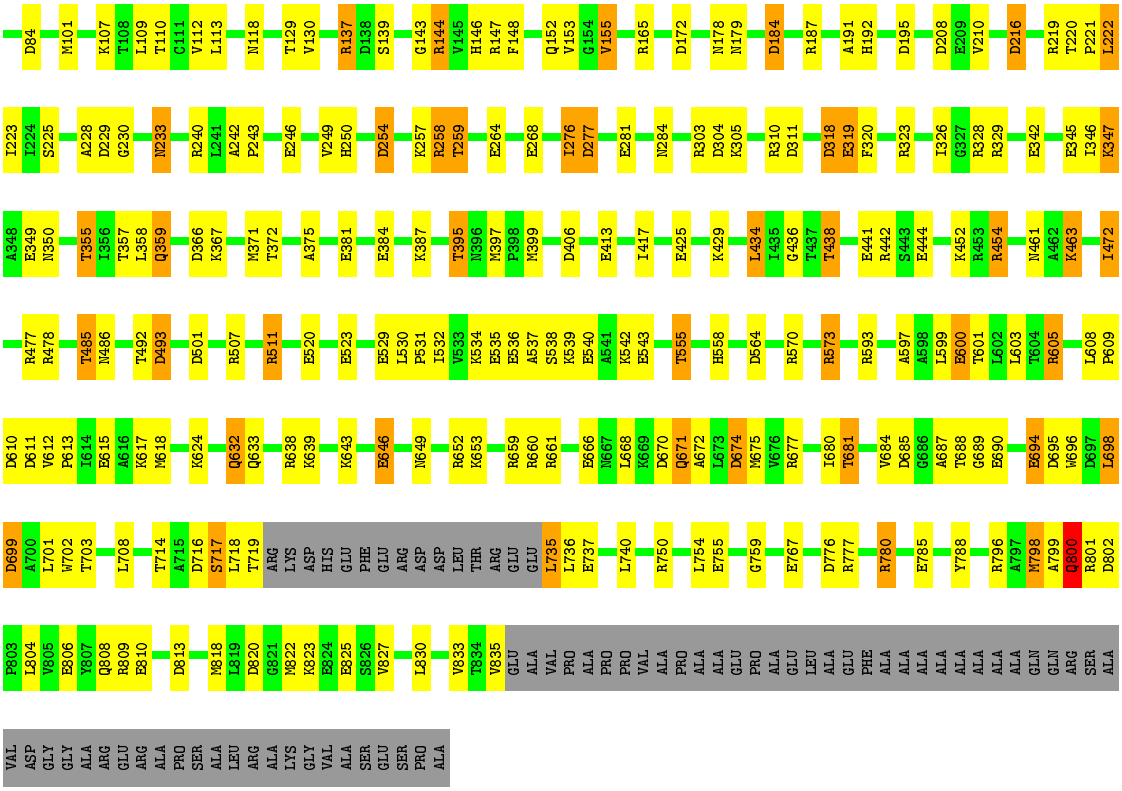
Chain A:



- Molecule 1: Preprotein translocase secA 1 subunit

Chain B:




D84 M101 K107 T108 L109 T110 C111 V112 L113 N118 T129 V130 R137 D138 S139 G143 R144 V145 H146 R147 F148 Q152 V153 G154 V155 R165 D172 N178 N179 D184 R187 A191 H192 D195 D208 E209 V210 D216 R219 T220 P221 L222
I223 I224 S225 A228 D229 G230 N233 R240 I241 A242 P243 E246 V249 H250 D254 K257 R258 T259 E264 E268 I276 D277 E281 N284 R303 D304 K305 R310 D311 D318 E319 F320 R323 I326 G327 R328 R329 E342 E345 I346 K347
A348 E349 N350 T355 I356 T357 L358 Q359 D366 K367 M371 T372 A375 E381 E384 K387 T395 N396 M397 P398 M399 D406 E413 I417 E425 K429 L434 I435 G436 T437 T438 E441 R442 S443 E444 K452 R453 R454 N461 A462 K463 I472
R477 R478 T485 N486 T492 D493 D501 R507 R511 E520 E523 E529 L530 P531 I532 V533 K534 E535 E536 A537 S538 K539 E540 A541 K542 E543 T555 H558 D564 R570 R573 R593 A597 A598 L599 E600 T601 L602 L603 T604 R605 L608 P609
D610 D611 V612 P613 I614 E615 A616 K617 M618 K624 Q632 Q633 R638 K639 K643 E646 M649 R652 K653 R659 R660 R661 E666 W667 L668 K669 D670 Q671 A672 L673 D674 M675 V676 R677 I680 T681 V684 D685 G686 A687 T688 G689 E690 E694 D695 W696 D697 L698
D699 A700 L701 W702 T703 L708 T714 A715 D716 S717 L718 T719 ARG LYS ASP HIS GLU PHE GLU ARG ASP ASP LEU THR ARG GLU GLU L735 L736 E737 L740 R750 L754 E755 G759 E767 D776 R777 R780 E785 Y788 R796 A797 M798 A799 Q800 R801 D802
P803 L804 V805 E806 Y807 Q808 R809 E810 D813 M818 L819 D820 G821 M822 K823 E824 E825 S826 V827 L830 V833 T834 V835 GLU ALA VAL PRO ALA PRO PRO VAL ALA PRO ALA ALA GLU PRO ALA GLU LEU ALA GLU PHE ALA ALA ALA ALA ALA ALA ALA GLN GLN ARG SER ALA
VAL ASP GLY GLY ALA ARG GLU ARG ALA PRO SER ALA LEU ARG ALA LYS GLY VAL ALA SER GLU SER PRO ALA

4 Data and refinement statistics (i)

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	206.05Å 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^2)	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(^{o})	Ideal(^{o})
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:B:101:MET:HE1	1:B:110:THR:HG21	1.47	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%)	16 33
1	B	832/922 (90%)	784 (94%)	43 (5%)	5 (1%)	30 56
All	All	1664/1844 (90%)	1565 (94%)	84 (5%)	15 (1%)	21 42

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 (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	697/755 (92%)	592 (85%)	105 (15%)	3	6
1	B	697/755 (92%)	594 (85%)	103 (15%)	4	6
All	All	1394/1510 (92%)	1186 (85%)	208 (15%)	4	6

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 (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)

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	22,29,29	1.31	3 (13%)	27,45,45	2.90	2 (7%)
3	ADP	B	901	2	22,29,29	1.29	3 (13%)	27,45,45	2.53	3 (11%)

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	-	0/12/32/32	0/3/3/3
3	ADP	B	901	2	-	0/12/32/32	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	A	900	ADP	PB-O3B	2.32	1.63	1.54
3	B	901	ADP	PB-O3B	2.57	1.63	1.54
3	A	900	ADP	C2-N1	2.60	1.38	1.33
3	B	901	ADP	C2-N1	2.93	1.39	1.33
3	A	900	ADP	C2-N3	3.76	1.38	1.32

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	900	ADP	N3-C2-N1	-13.66	118.44	128.89
3	B	901	ADP	N3-C2-N1	-11.52	120.07	128.89
3	B	901	ADP	PA-O3A-PB	-2.40	124.61	132.67
3	A	900	ADP	O2A-PA-O3A	2.39	115.93	105.09
3	B	901	ADP	O3B-PB-O3A	2.47	116.32	105.09

There are no chirality outliers.

There are no torsion outliers.

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

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.