



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2018 – 11:05 pm GMT

PDB ID : 2FSG  
Title : Complex SecA:ATP from Escherichia coli  
Authors : Papanikolau, Y.; Petratos, K.; Economou, A.  
Deposited on : 2006-01-23  
Resolution : 2.20 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 : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk30967  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30967

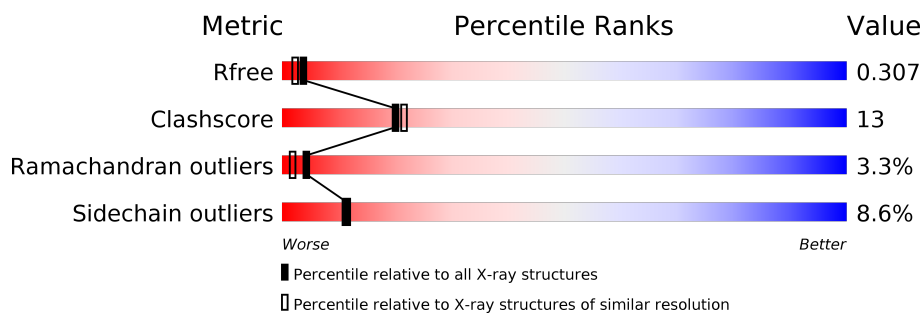
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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))
$R_{free}$	111664	4343 (2.20-2.20)
Clashscore	122126	5027 (2.20-2.20)
Ramachandran outliers	120053	4952 (2.20-2.20)
Sidechain outliers	120020	4953 (2.20-2.20)

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. 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	853	
1	B	853	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11809 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 subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	679	Total	C	N	O	S	Se	0	0	0
			5401	3392	953	1030	1	25			
1	B	743	Total	C	N	O	S	Se	0	0	0
			5915	3712	1045	1128	1	29			

There are 64 discrepancies between the modelled and reference sequences:

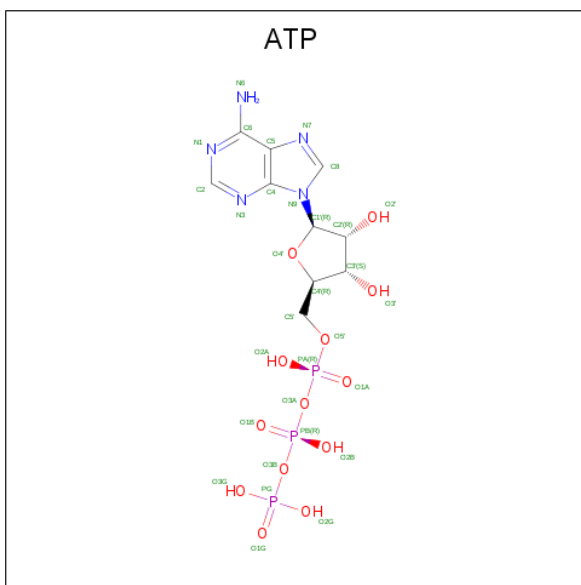
Chain	Residue	Modelled	Actual	Comment	Reference
A	21	MSE	MET	MODIFIED RESIDUE	UNP P10408
A	31	MSE	MET	MODIFIED RESIDUE	UNP P10408
A	35	MSE	MET	MODIFIED RESIDUE	UNP P10408
A	81	MSE	MET	MODIFIED RESIDUE	UNP P10408
A	92	MSE	MET	MODIFIED RESIDUE	UNP P10408
A	102	MSE	MET	MODIFIED RESIDUE	UNP P10408
A	161	MSE	MET	MODIFIED RESIDUE	UNP P10408
A	191	MSE	MET	MODIFIED RESIDUE	UNP P10408
A	235	MSE	MET	MODIFIED RESIDUE	UNP P10408
A	292	MSE	MET	MODIFIED RESIDUE	UNP P10408
A	305	MSE	MET	MODIFIED RESIDUE	UNP P10408
A	307	MSE	MET	MODIFIED RESIDUE	UNP P10408
A	344	MSE	MET	MODIFIED RESIDUE	UNP P10408
A	390	MSE	MET	MODIFIED RESIDUE	UNP P10408
A	418	MSE	MET	MODIFIED RESIDUE	UNP P10408
A	429	MSE	MET	MODIFIED RESIDUE	UNP P10408
A	506	MSE	MET	MODIFIED RESIDUE	UNP P10408
A	590	MSE	MET	MODIFIED RESIDUE	UNP P10408
A	595	MSE	MET	MODIFIED RESIDUE	UNP P10408
A	606	MSE	MET	MODIFIED RESIDUE	UNP P10408
A	607	MSE	MET	MODIFIED RESIDUE	UNP P10408
A	612	MSE	MET	MODIFIED RESIDUE	UNP P10408
A	700	MSE	MET	MODIFIED RESIDUE	UNP P10408
A	758	MSE	MET	MODIFIED RESIDUE	UNP P10408
A	759	MSE	MET	MODIFIED RESIDUE	UNP P10408

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Chain	Residue	Modelled	Actual	Comment	Reference
A	767	MSE	MET	MODIFIED RESIDUE	UNP P10408
A	782	MSE	MET	MODIFIED RESIDUE	UNP P10408
A	810	MSE	MET	MODIFIED RESIDUE	UNP P10408
A	814	MSE	MET	MODIFIED RESIDUE	UNP P10408
A	833	MSE	MET	MODIFIED RESIDUE	UNP P10408
A	846	MSE	MET	MODIFIED RESIDUE	UNP P10408
A	854	MSE	MET	MODIFIED RESIDUE	UNP P10408
B	21	MSE	MET	MODIFIED RESIDUE	UNP P10408
B	31	MSE	MET	MODIFIED RESIDUE	UNP P10408
B	35	MSE	MET	MODIFIED RESIDUE	UNP P10408
B	81	MSE	MET	MODIFIED RESIDUE	UNP P10408
B	92	MSE	MET	MODIFIED RESIDUE	UNP P10408
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B	846	MSE	MET	MODIFIED RESIDUE	UNP P10408
B	854	MSE	MET	MODIFIED RESIDUE	UNP P10408

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 31	C 10	N 5	O 13	P 3	0	0
2	B	1	Total 31	C 10	N 5	O 13	P 3	0	0

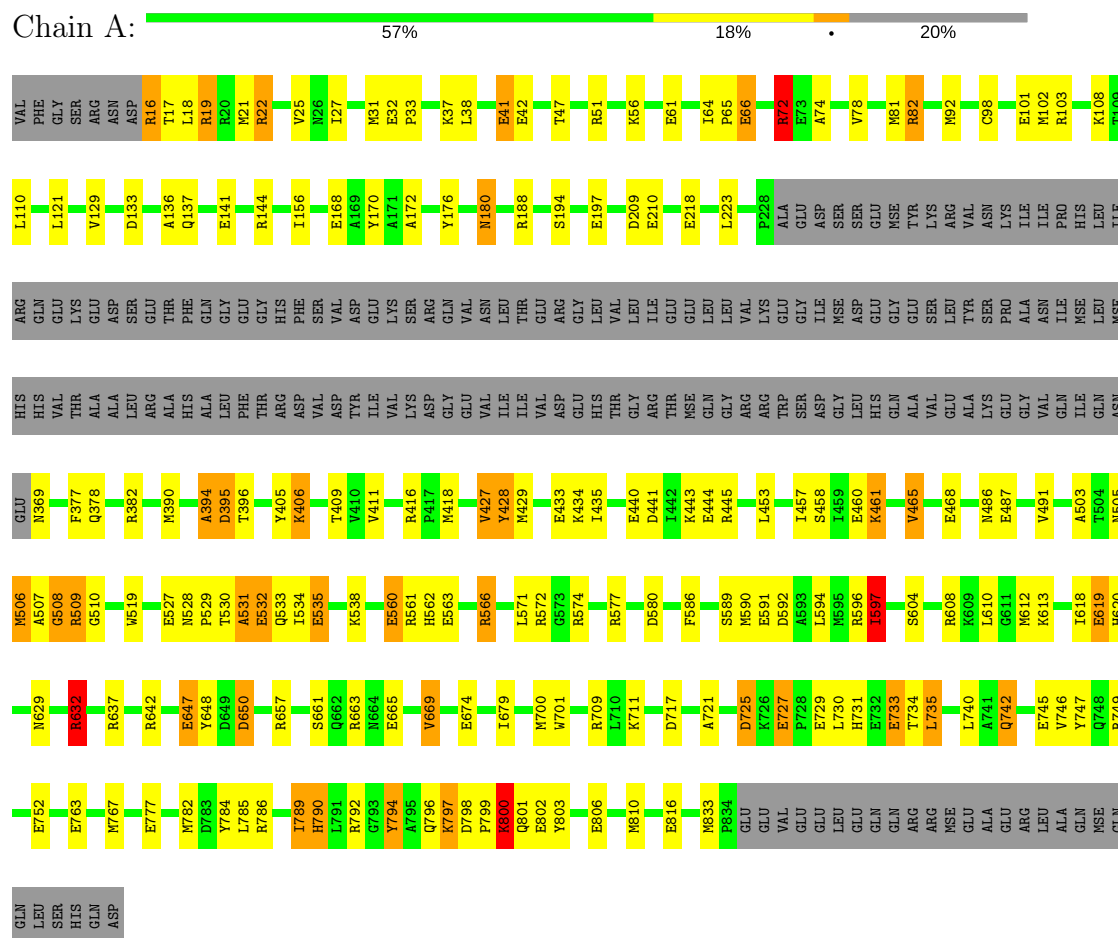
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	198	Total O 198 198	0	0
3	B	233	Total O 233 233	0	0

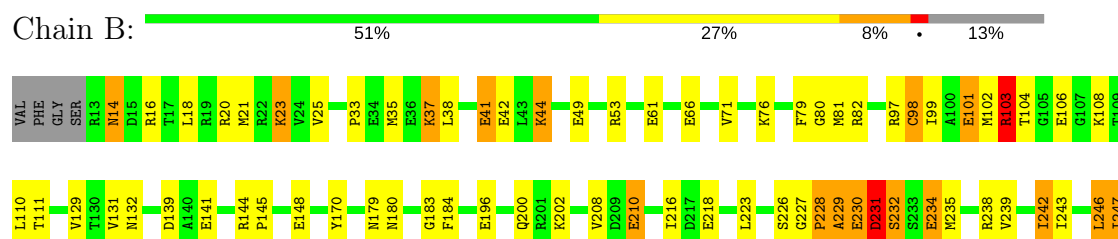
### 3 Residue-property plots

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.

#### • Molecule 1: Preprotein translocase secA subunit



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M810	E727	E647		K461	Q378				R248
E816	F728	Y648	S564	S462	R382	S564	E648	E463	GLN
I823	E729	V651	I567	E463	E385	I567	E468	E463	GLU
L826	H731	D654	B572	E468	A388	B572	A481	A388	LYS
	E732	Q655	S575	A481	M390	S575	P483	M390	ASP
V829	E733	R656	R577	P483	T391	R577	E487	T391	GLU
Q830	L734	R657	B585	E487	T393	B585	V491	T393	GLN
R736	T735	Y660	F586	V491	D396	F586	A492	D396	GLY
E737	L736		L588	A492	T396	L588	Q493	T396	GLY
R738	R737		S589	Q493	F399	S589	Y496	F399	PHE
R832	E738	E665	M590	Y496	F401	M590	P497	F401	LYS
M833	Q742	L666	L594	P497	I404	L594	V500	I404	ASP
P834	S743	V669	M595	V500	Y405	M595	T504	Y405	GLY
GLU	I744	D670	M596	T504	K406	D670	M505	K406	ILE
GLU	E745	S671	S600	M505	L407	S600	M506	L407	ARG
GLU	R749	E672	D601	M506	D403	D601	A507	D403	GLN
GLN	K750	E674	V603	A507	T409	V603	G508	T409	VAL
GLU	V754	I679	S604	G508	V410	S604	R509	V410	ASN
GLN		R680	G605	R509	T511	R680	G510	T511	LEU
ARG	E757	E681	M606	G510	R416	E681	D512	R416	GLY
ARG	M758	D682	R608	D512	P417	D682	S518	P417	ARG
MSE	R759	V683	R609	S518	M413	V683	M519	M413	GLY
GLU	R760	A690	L610	M519	D425	A690	Q520	D425	THR
ALA	E763	Y691	M612	Q520	L426	Y691	A521	L426	MSE
ARG	K764	F692	G613	A521	V427	F692	E522	V427	GLN
LEU	L779	P693	P614	E522	M423	P693	V523	M423	LEU
ALA	A780		A617	V523	E433	A780	M528	E433	ASP
GLN	A781	S696	I618	M528	E434	A781	P529	E434	GLY
MSE	M781	L697	E619	P529	I435	M781	T530	I435	LEU
GLN	M782	E698	V623	T530	Q436	E698	A531	Q436	HIS
GLN	L785	F699	T624	A531	I437	F699	E532	I437	GLN
LEU	R786	M700	K625	E532	I438	M700	R536	I438	ALA
SER	Q787	W701	A626	R536	E440	Q787	I537	E440	VAL
HIS	G788	I703	A628	I537	E444	G788	K538	E444	GLU
GLN	I789	L706	N629	K538	E445	I789	A539	E445	LYS
ASP	H790	Q707	R632	A539	T446	H790	D540	T446	GLY
	L791	E708	E635	D540	Q450	L791	Q542	Q450	VAL
	R792	K711	B637	Q542	V454	R792	R544	V454	ILE
	G793	N712	T641	R544	I457	G793	H545	I457	Q366
	Y794	L716	D644	H545	S458	Y794	G553	S458	N367
	Q796	D717		G553	I459	Q796	T559	I459	E368
	K797	L718		T559	E460	K797		E460	N369
	D798	P719		E460		D798			S374
	P799	I720				P799			
	K800	A721				K800			
	Q801	E722				Q801			
	E802	K723				E802			
	Y803	L724				Y803			
	K804	K726				K804			
	R805					R805			
	E806					E806			
	S807					S807			

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	75.38Å 89.48Å 163.35Å 90.00° 100.73° 90.00°	Depositor
Resolution (Å)	19.61 – 2.20 19.84 – 2.20	Depositor EDS
% Data completeness (in resolution range)	96.9 (19.61-2.20) 96.9 (19.84-2.20)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.79 (at 2.19Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.208 , 0.270 0.262 , 0.307	Depositor DCC
$R_{free}$ test set	5245 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.3	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 40.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.018 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	11809	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.12% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality

### 5.1 Standard geometry

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

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	1.52	46/5466 (0.8%)	1.22	27/7334 (0.4%)
1	B	1.59	70/5983 (1.2%)	1.22	36/8023 (0.4%)
All	All	1.55	116/11449 (1.0%)	1.22	63/15357 (0.4%)

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	3
1	B	0	7
All	All	0	10

The worst 5 of 116 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	210	GLU	CG-CD	11.27	1.68	1.51
1	B	23	LYS	CE-NZ	11.05	1.76	1.49
1	B	385	GLU	CD-OE1	9.99	1.36	1.25
1	B	66	GLU	CD-OE2	9.65	1.36	1.25
1	B	665	GLU	CG-CD	9.55	1.66	1.51

The worst 5 of 63 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	572	ARG	NE-CZ-NH1	12.70	126.65	120.30
1	B	23	LYS	CD-CE-NZ	10.37	135.56	111.70
1	A	72	ARG	NE-CZ-NH2	9.47	125.03	120.30
1	B	97	ARG	NE-CZ-NH1	9.17	124.88	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	572	ARG	NE-CZ-NH1	9.06	124.83	120.30

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	394	ALA	Peptide
1	A	796	GLN	Peptide
1	A	800	LYS	Peptide
1	B	228	PRO	Peptide
1	B	246	LEU	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	5401	0	5406	119	0
1	B	5915	0	5921	188	0
2	A	31	0	12	0	0
2	B	31	0	12	2	0
3	A	198	0	0	15	0
3	B	233	0	0	17	0
All	All	11809	0	11351	306	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 13.

The worst 5 of 306 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:B:44:LYS:CE	1:B:44:LYS:NZ	1.67	1.55
1:B:406:LYS:NZ	1:B:406:LYS:CE	1.69	1.52
1:B:759:MSE:SE	1:B:759:MSE:CE	2.14	1.45
1:B:23:LYS:NZ	1:B:23:LYS:CE	1.76	1.45
1:A:429:MSE:SE	1:A:429:MSE:CE	2.14	1.45

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	675/853 (79%)	635 (94%)	31 (5%)	9 (1%)	13	10
1	B	737/853 (86%)	651 (88%)	49 (7%)	37 (5%)	2	1
All	All	1412/1706 (83%)	1286 (91%)	80 (6%)	46 (3%)	4	2

5 of 46 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	394	ALA
1	A	395	ASP
1	A	508	GLY
1	A	509	ARG
1	A	531	ALA

#### 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	575/696 (83%)	538 (94%)	37 (6%)	19	22
1	B	632/696 (91%)	565 (89%)	67 (11%)	7	7
All	All	1207/1392 (87%)	1103 (91%)	104 (9%)	11	11

5 of 104 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	247	ILE
1	B	409	THR
1	B	779	LEU
1	B	248	ARG
1	B	292	MSE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	180	ASN
1	B	520	GLN
1	B	748	GLN
1	B	486	ASN
1	B	528	ASN

### 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](#)

2 ligands are modelled in this entry.

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
2	ATP	A	900	-	27,33,33	1.39	4 (14%)	27,52,52	2.38	8 (29%)
2	ATP	B	901	-	27,33,33	2.15	9 (33%)	27,52,52	2.45	11 (40%)

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
2	ATP	A	900	-	-	0/18/38/38	0/3/3/3
2	ATP	B	901	-	-	0/18/38/38	0/3/3/3

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	901	ATP	C8-N9	-3.82	1.32	1.36
2	A	900	ATP	PB-O2B	-2.03	1.45	1.55
2	B	901	ATP	C5-N7	-2.02	1.32	1.39
2	B	901	ATP	C2-N3	2.08	1.35	1.32
2	A	900	ATP	C2-N3	2.58	1.36	1.32

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	900	ATP	N3-C2-N1	-8.46	121.62	128.86
2	B	901	ATP	N3-C2-N1	-6.06	123.68	128.86
2	B	901	ATP	O3'-C3'-C2'	-3.61	100.27	111.83
2	A	900	ATP	PB-O3B-PG	-3.41	121.17	132.63
2	B	901	ATP	O4'-C4'-C3'	-3.10	99.03	105.15

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	901	ATP	2	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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.