



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 02:08 AM 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
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)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

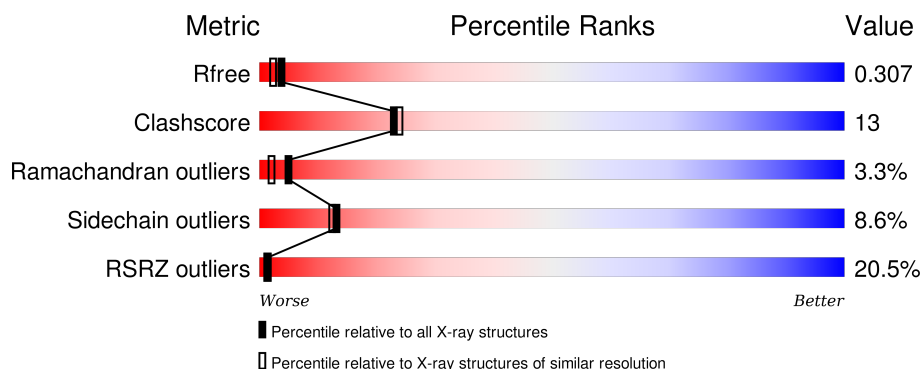
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (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 ≥ 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.

Mol	Chain	Length	Quality of chain
1	A	853	<div> <div>9%</div> <div>57%</div> <div>18%</div> <div>•</div> <div>20%</div> </div>
1	B	853	<div> <div>24%</div> <div>51%</div> <div>27%</div> <div>8%</div> <div>•</div> <div>13%</div> </div>

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
B	102	MSE	MET	MODIFIED RESIDUE	UNP P10408
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B	833	MSE	MET	MODIFIED RESIDUE	UNP P10408
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: C₁₀H₁₆N₅O₁₃P₃).



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

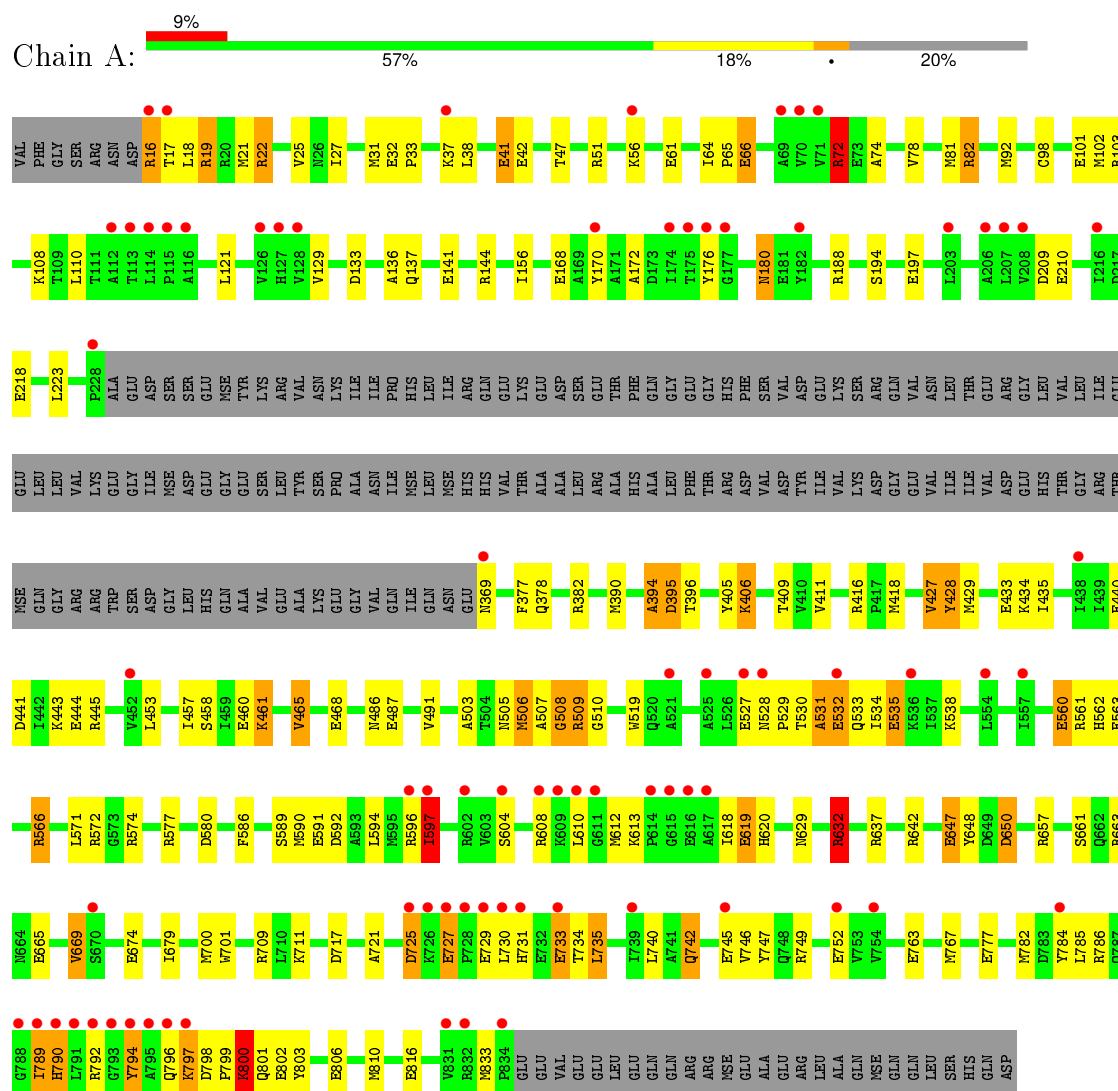
- Molecule 3 is water.

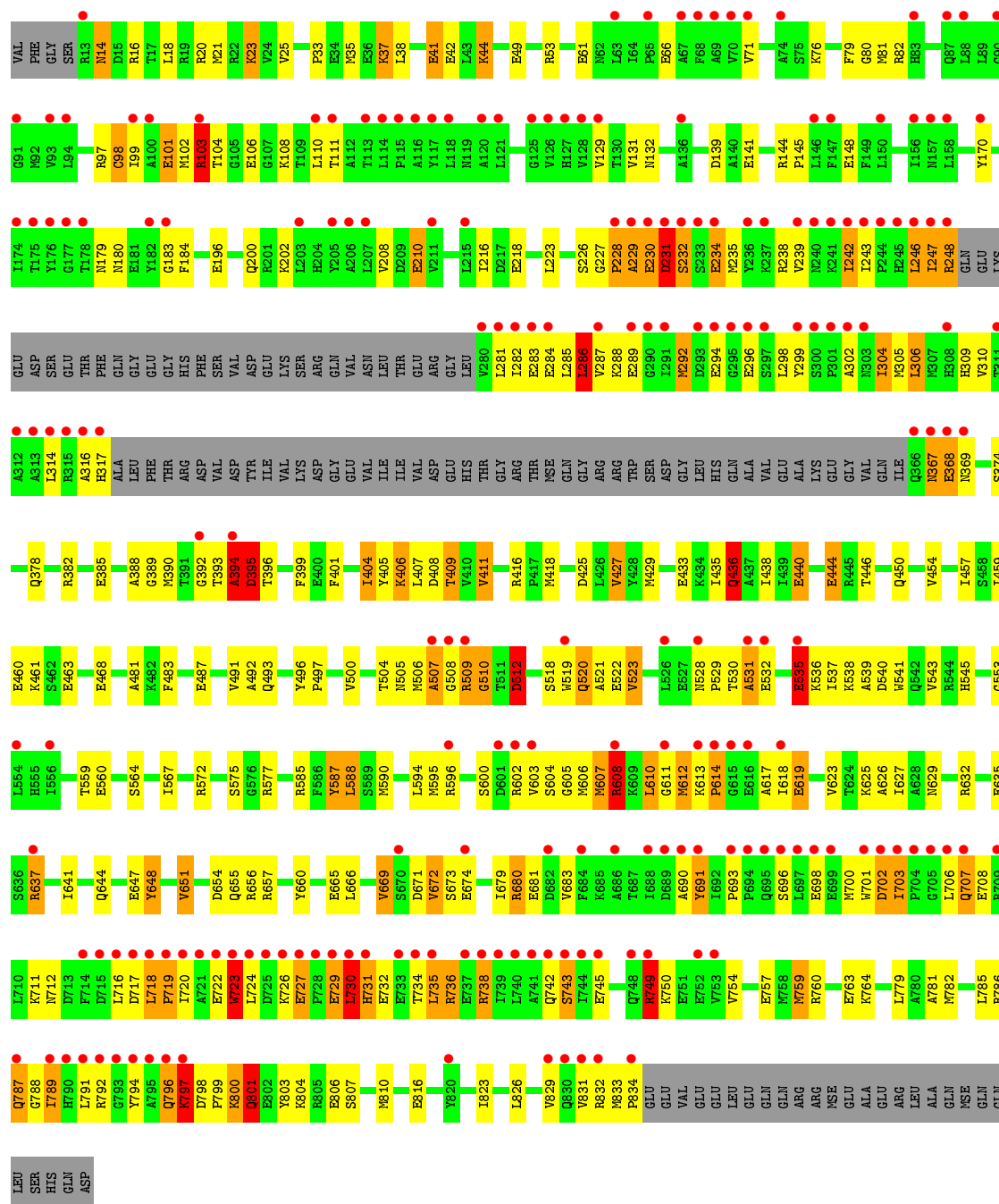
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	198	Total	O	0	0
			198	198		
3	B	233	Total	O	0	0
			233	233		

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.

• Molecule 1: Preprotein translocase secA subunit





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 2.19Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.208 , 0.270 0.261 , 0.307	Depositor DCC
R_{free} test set	5246 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	34.3	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 40.9	EDS
Estimated twinning fraction	0.018 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 104944 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	11809	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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%)	15	11
1	B	737/853 (86%)	651 (88%)	49 (7%)	37 (5%)	3	1
All	All	1412/1706 (83%)	1286 (91%)	80 (6%)	46 (3%)	5	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%)	22	24
1	B	632/696 (91%)	565 (89%)	67 (11%)	8	7
All	All	1207/1392 (87%)	1103 (91%)	104 (9%)	13	12

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	-	24,33,33	1.26	3 (12%)	31,52,52	2.55	10 (32%)
2	ATP	B	901	-	24,33,33	2.03	7 (29%)	31,52,52	2.55	13 (41%)

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 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	900	ATP	PB-O2B	-2.26	1.45	1.54
2	B	901	ATP	PA-O2A	-2.03	1.46	1.54
2	B	901	ATP	C5-N7	-2.02	1.32	1.39
2	A	900	ATP	C2-N3	2.35	1.36	1.32
2	B	901	ATP	C5'-C4'	2.69	1.60	1.51

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	900	ATP	N3-C2-N1	-9.50	121.62	128.89
2	B	901	ATP	N3-C2-N1	-6.81	123.68	128.89
2	A	900	ATP	O3A-PA-O5'	-5.15	89.28	102.94
2	B	901	ATP	O3A-PA-O5'	-3.76	92.96	102.94
2	B	901	ATP	O3'-C3'-C2'	-3.56	100.27	111.83

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	654/853 (76%)	0.70	77 (11%) 6 6	5, 19, 43, 63	0
1	B	714/853 (83%)	1.40	204 (28%) 1 1	3, 21, 46, 64	0
All	All	1368/1706 (80%)	1.06	281 (20%) 1 1	3, 20, 44, 64	0

The worst 5 of 281 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	791	LEU	12.0
1	B	287	VAL	10.8
1	A	793	GLY	10.8
1	A	794	TYR	10.0
1	B	794	TYR	9.8

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	ATP	A	900	31/31	0.91	0.20	0.82	11,24,29,30	0
2	ATP	B	901	31/31	0.87	0.16	-1.11	9,19,24,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.