wwPDB X-ray Structure Validation Summary Report (i)

Aug 23, 2023 – 06:49 AM EDT

PDB ID	:	3BXZ
Title	:	Crystal structure of the isolated DEAD motor domains from Escherichia coli SecA
Authors	:	Nithianantham, S.; Namjoshi, S.; Shilton, B.H.
Deposited on	:	2008-01-15
Resolution	:	3.00 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

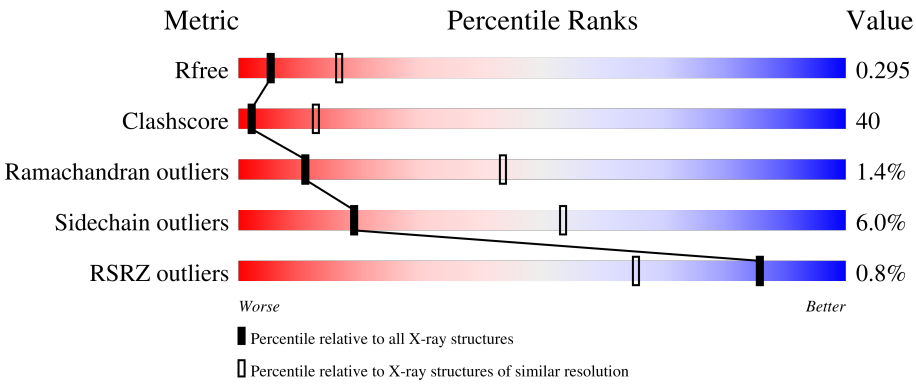
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

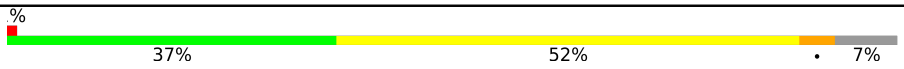
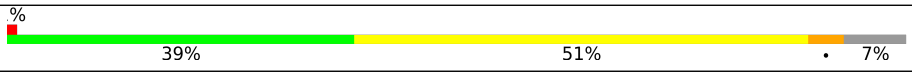
The reported resolution of this entry is 3.00 Å.

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}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 of 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 <=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	471	
1	B	471	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SPD	A	905	-	-	-	X
3	SPD	B	906	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7106 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 subunit secA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	438	3420	2143	608	655	14	0	0	0
1	B	440	3439	2154	613	657	15	0	0	0

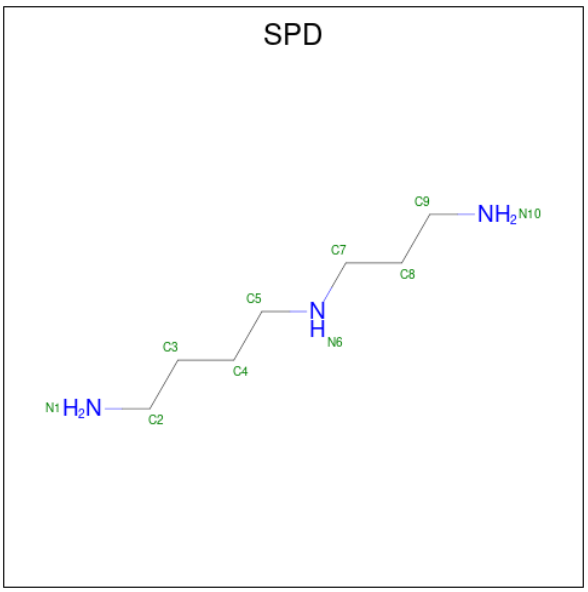
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	expression tag	UNP P10408
A	0	HIS	-	expression tag	UNP P10408
A	1	HIS	-	expression tag	UNP P10408
A	2	HIS	-	expression tag	UNP P10408
A	3	HIS	-	expression tag	UNP P10408
A	4	HIS	-	expression tag	UNP P10408
A	5	HIS	-	expression tag	UNP P10408
A	368	ALA	GLU	engineered mutation	UNP P10408
B	-1	MET	-	expression tag	UNP P10408
B	0	HIS	-	expression tag	UNP P10408
B	1	HIS	-	expression tag	UNP P10408
B	2	HIS	-	expression tag	UNP P10408
B	3	HIS	-	expression tag	UNP P10408
B	4	HIS	-	expression tag	UNP P10408
B	5	HIS	-	expression tag	UNP P10408
B	368	ALA	GLU	engineered mutation	UNP P10408

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

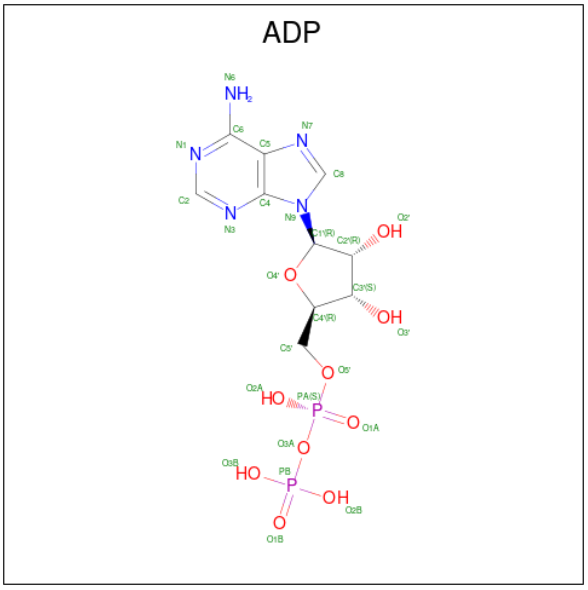
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
2	A	1	1	1	0	0
2	B	1	1	1	0	0

- Molecule 3 is SPERMIDINE (three-letter code: SPD) (formula: $C_7H_{19}N_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	N		
3	A	1	10	7	3	0	0
			Total	C	N		
3	B	1	10	7	3	0	0

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 5 is water.

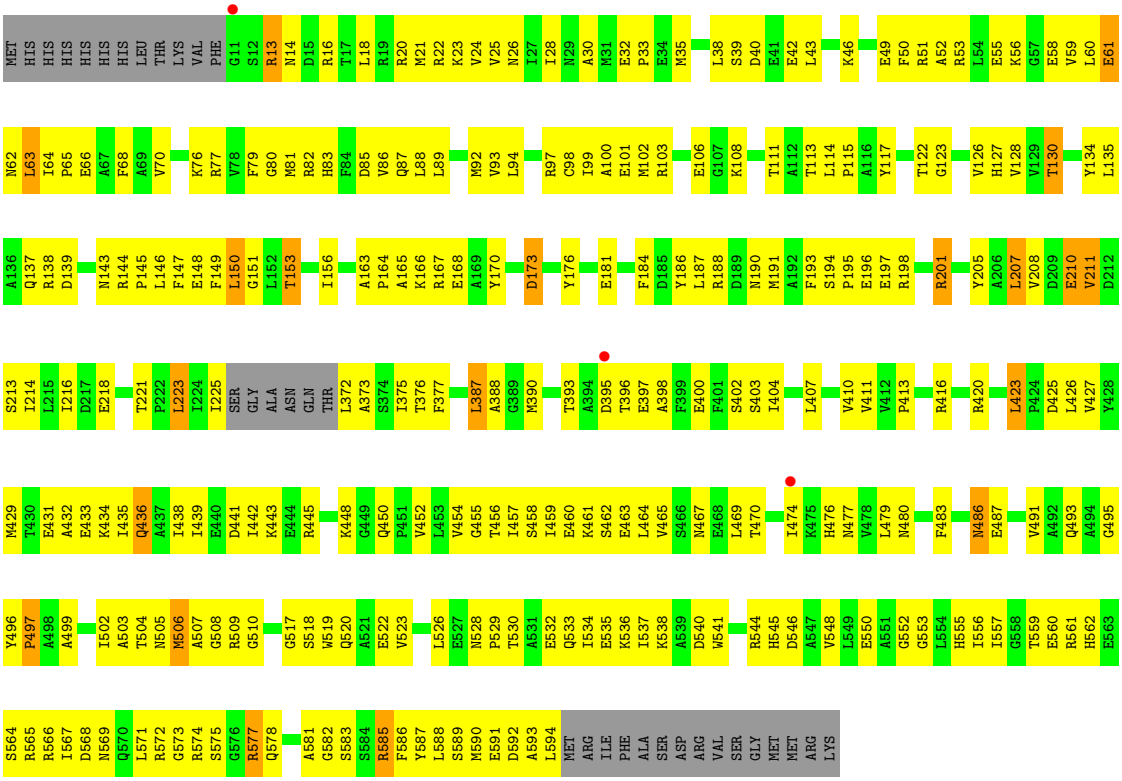
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	89	89	89	0	0
			Total	O		
5	B	82	82	82	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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 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.

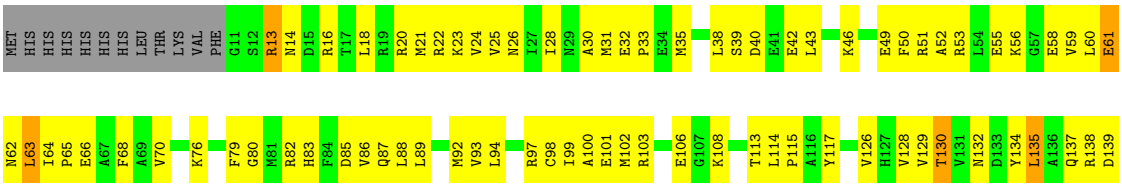
• Molecule 1: Preprotein translocase subunit secA

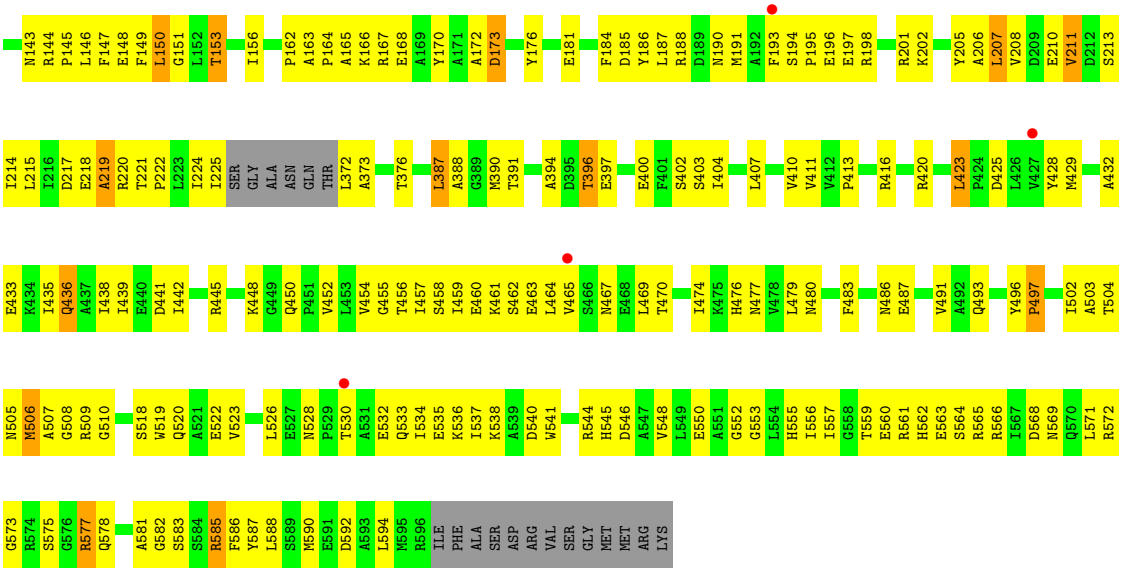
Chain A:



• Molecule 1: Preprotein translocase subunit secA

Chain B:




G573 R574 S575 G576 R577 Q578 A581 G582 S583 S584 R585 F586 Y587 L588 S589 M590 E591 D592 A593 L594 M595 R596 ILE PHE ALA SER ASP ARG VAL SER GLY MET MET ARG LYS
N505 M506 A507 G508 R509 G510 S518 W519 Q520 A521 E522 V523 L526 E527 N528 P529 T530 A531 E532 Q533 I534 E535 K536 I537 K538 A539 D540 W541 R544 H545 D546 A547 V548 L549 E550 A551 G552 G553 L554 H555 I556 I557 G558 T559 E560 R561 H562 E563 S564 R565 R566 I567 D568 N569 Q570 L571 R572
E433 K434 I435 Q436 A437 I438 I439 E440 D441 I442 R445 K448 G449 Q450 P451 V452 L453 V454 G455 T456 I457 S458 I459 E460 K461 S462 E463 L464 V465 S466 N467 E468 L469 T470 I474 K475 H476 N477 V478 L479 N480 F483 N486 E487 V491 A492 Q493 Y496 P497 I502 A503 T504
I214 L215 I216 D217 E218 A219 R220 T221 P222 L223 I224 I225 SER GLY ALA ASN GLN THR L372 A373 T376 L387 A388 G389 M390 T391 A394 D395 T396 E397 E400 F401 S402 S403 I404 L407 V410 V411 V412 P413 R416 R420 L423 P424 D425 L426 V427 Y428 M429 A432
N143 R144 P145 L146 F147 E148 F149 L150 G151 L152 T153 I156 P162 A163 P164 A165 K166 R167 E168 A169 Y170 A171 A172 D173 Y176 E181 F184 D185 Y186 L187 R188 D189 N190 M191 A192 F193 S194 P195 E196 E197 R198 R201 K202 Y205 A206 L207 V208 D209 E210 V211 D212 S213

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	177.82Å 71.36Å 119.54Å 90.00° 128.82° 90.00°	Depositor
Resolution (Å)	46.58 – 3.00 46.57 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.4 (46.58-3.00) 84.1 (46.57-3.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.54 (at 3.01Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.245 , 0.305 0.238 , 0.295	Depositor DCC
R_{free} test set	2317 reflections (9.86%)	wwPDB-VP
Wilson B-factor (Å^2)	83.2	Xtriage
Anisotropy	0.140	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 63.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	7106	wwPDB-VP
Average B, all atoms (Å^2)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.73% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.40	0/3472	0.63	1/4689 (0.0%)
1	B	0.39	0/3491	0.63	0/4713
All	All	0.39	0/6963	0.63	1/9402 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	486	ASN	CB-CA-C	-5.01	100.38	110.40

There are no chirality outliers.

There are no planarity outliers.

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	3420	0	3431	283	0
1	B	3439	0	3453	275	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	10	0	19	4	0
3	B	10	0	19	0	0
4	A	27	0	12	1	0
4	B	27	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	89	0	0	19	0
5	B	82	0	0	22	0
All	All	7106	0	6946	550	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 40.

The worst 5 of 550 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:506:MET:HE2	1:A:506:MET:H	1.12	1.13
1:B:506:MET:HE2	1:B:506:MET:H	1.12	1.06
1:A:221:THR:HG22	1:A:376:THR:HG22	1.05	1.03
1:B:556:ILE:HD13	1:B:571:LEU:HG	1.45	0.98
1:A:504:THR:HG22	1:A:505:ASN:H	1.28	0.98

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	434/471 (92%)	380 (88%)	49 (11%)	5 (1%)	13 48
1	B	436/471 (93%)	382 (88%)	47 (11%)	7 (2%)	9 40
All	All	870/942 (92%)	762 (88%)	96 (11%)	12 (1%)	11 43

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	396	THR
1	A	396	THR

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Mol	Chain	Res	Type
1	B	219	ALA
1	A	150	LEU
1	B	221	THR

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	359/388 (92%)	338 (94%)	21 (6%)	20	55
1	B	361/388 (93%)	339 (94%)	22 (6%)	18	53
All	All	720/776 (93%)	677 (94%)	43 (6%)	19	53

5 of 43 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	162	PRO
1	B	387	LEU
1	B	173	ASP
1	B	210	GLU
1	B	436	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	486	ASN
1	B	533	GLN
1	B	562	HIS
1	B	528	ASN
1	A	562	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
4	ADP	A	901	2	24,29,29	1.83	7 (29%)	29,45,45	1.78	6 (20%)
4	ADP	B	902	-	24,29,29	1.72	7 (29%)	29,45,45	1.75	5 (17%)
3	SPD	A	905	-	9,9,9	0.72	0	8,8,8	0.57	0
3	SPD	B	906	-	9,9,9	0.72	0	8,8,8	0.50	0

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
4	ADP	A	901	2	-	3/12/32/32	0/3/3/3
4	ADP	B	902	-	-	5/12/32/32	0/3/3/3
3	SPD	A	905	-	-	1/7/7/7	-
3	SPD	B	906	-	-	2/7/7/7	-

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	901	ADP	O4'-C1'	4.48	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	902	ADP	O4'-C1'	4.24	1.47	1.41
4	B	902	ADP	C4-N3	3.13	1.40	1.35
4	A	901	ADP	C2-N3	3.02	1.37	1.32
4	A	901	ADP	C2-N1	2.82	1.39	1.33

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	901	ADP	N3-C2-N1	-6.81	118.03	128.68
4	B	902	ADP	N3-C2-N1	-6.05	119.22	128.68
4	B	902	ADP	C4-C5-N7	-3.61	105.63	109.40
4	B	902	ADP	C2'-C3'-C4'	3.42	109.28	102.64
4	A	901	ADP	C2'-C3'-C4'	3.09	108.64	102.64

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	902	ADP	O4'-C4'-C5'-O5'
4	A	901	ADP	C3'-C4'-C5'-O5'
4	B	902	ADP	C3'-C4'-C5'-O5'
4	A	901	ADP	O4'-C4'-C5'-O5'
3	B	906	SPD	C7-C8-C9-N10

There are no ring outliers.

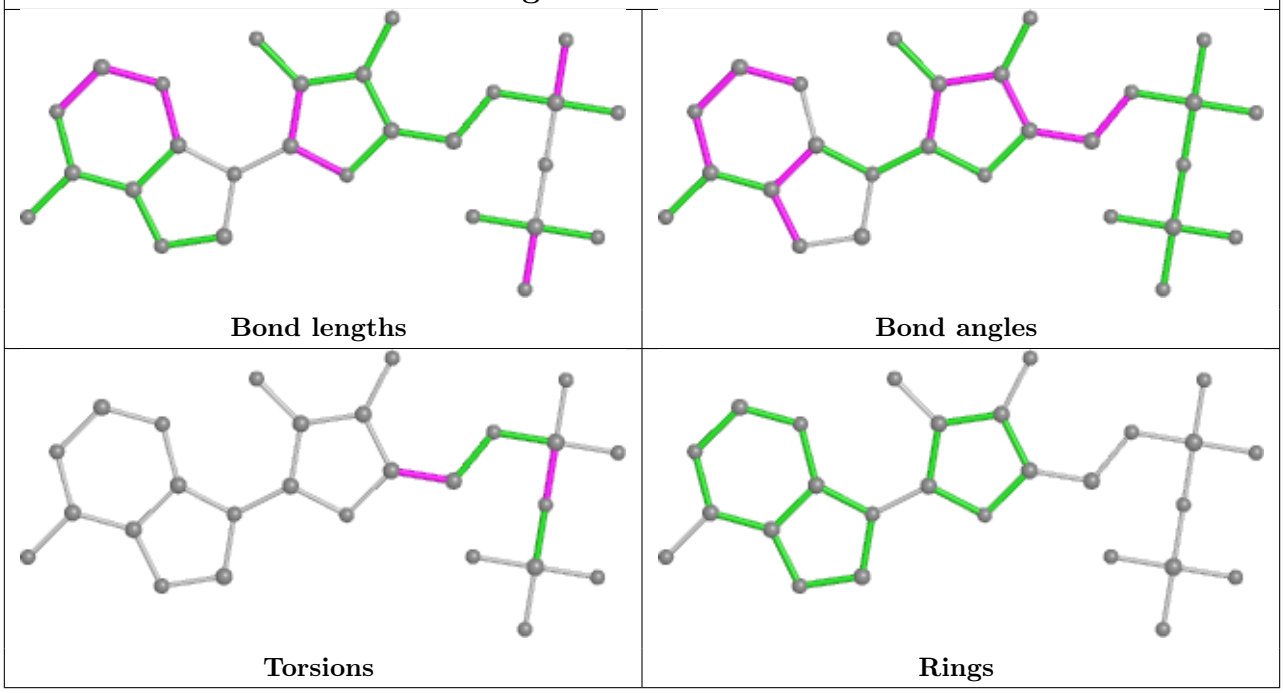
3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	901	ADP	1	0
4	B	902	ADP	1	0
3	A	905	SPD	4	0

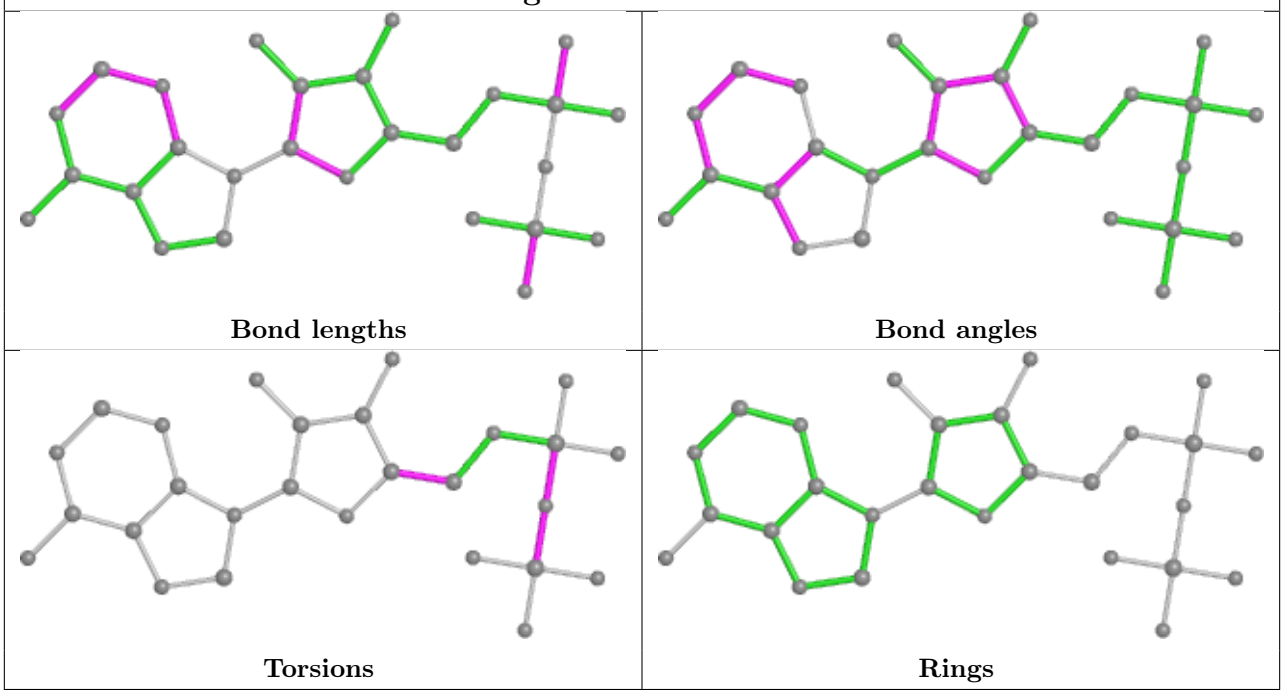
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

Ligand ADP A 901



Ligand ADP B 902



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	438/471 (92%)	0.02	3 (0%)	87	69	46, 78, 128, 152	0
1	B	440/471 (93%)	0.02	4 (0%)	84	63	48, 78, 129, 152	0
All	All	878/942 (93%)	0.02	7 (0%)	86	65	46, 78, 129, 152	0

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	530	THR	3.3
1	B	465	VAL	3.2
1	A	474	ILE	2.7
1	A	11	GLY	2.1
1	B	427	VAL	2.1

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 monosaccharides in this entry.

6.4 Ligands (i)

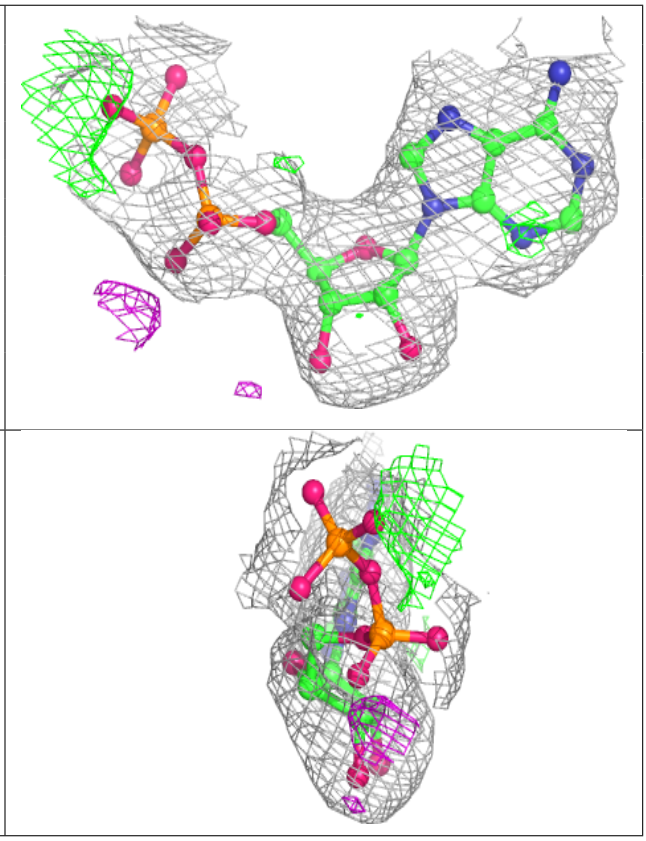
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SPD	B	906	10/10	0.67	0.46	74,80,82,82	0
3	SPD	A	905	10/10	0.69	0.50	76,78,80,81	0
4	ADP	B	902	27/27	0.93	0.22	64,70,71,72	0
4	ADP	A	901	27/27	0.96	0.21	57,63,68,72	0
2	MG	A	903	1/1	0.97	0.23	23,23,23,23	0
2	MG	B	904	1/1	0.98	0.36	41,41,41,41	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

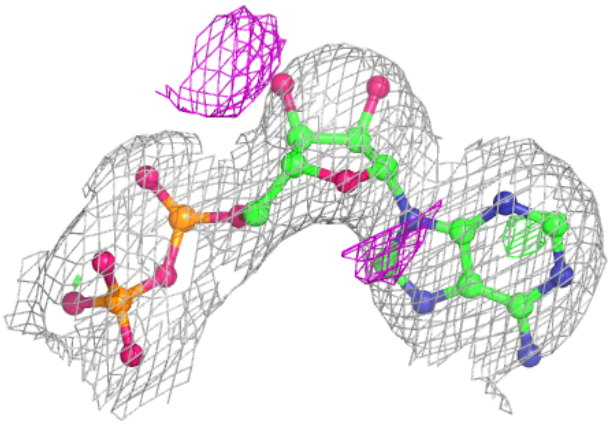
Electron density around ADP B 902:

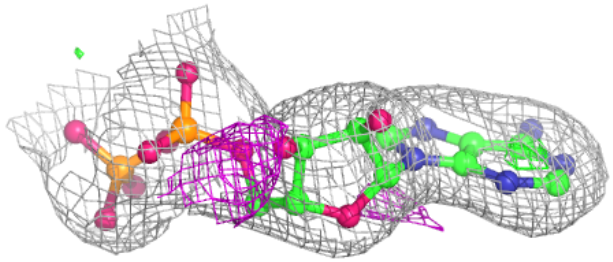
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

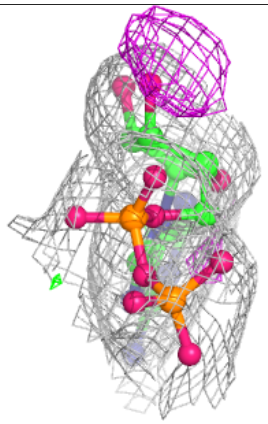


Electron density around ADP A 901:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







6.5 Other polymers (i)

There are no such residues in this entry.