



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 07:36 PM UTC

PDB ID : 3BXZ / pdb_00003bxz
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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

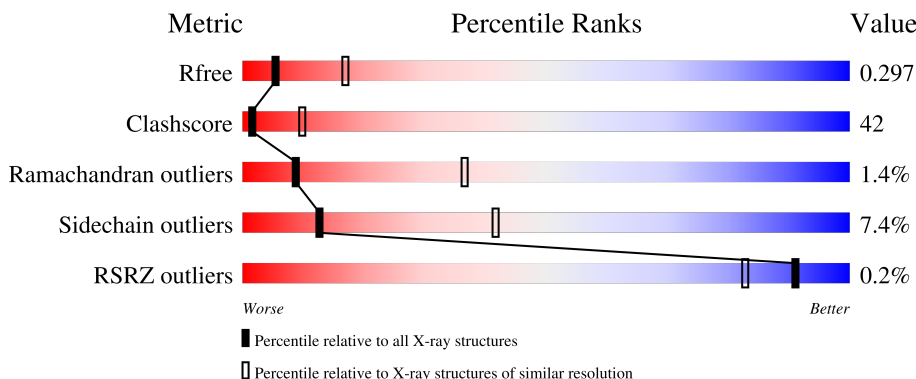
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (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 $\leq 5\%$. 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	471	35% 52% 6% 7%
1	B	471	36% 51% 7% 7%

2 Entry composition

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
1	A	438	Total	C	N	O	S	0	0	0
			3420	2143	608	655	14			
1	B	440	Total	C	N	O	S	0	0	0
			3439	2154	613	657	15			

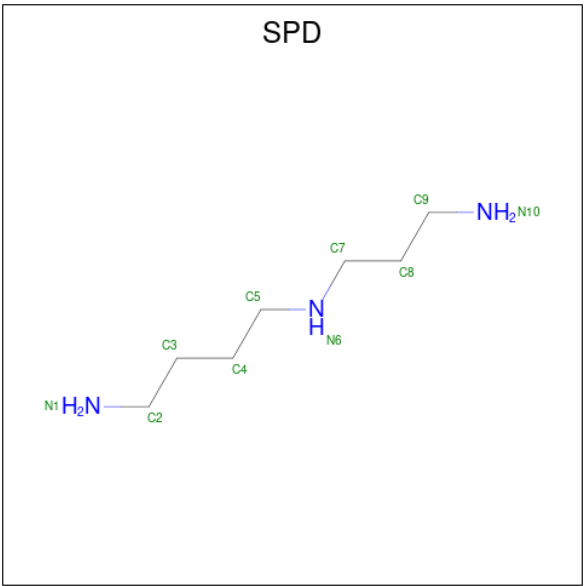
There are 16 discrepancies between the modelled and reference sequences:

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 (CCD ID: MG) (formula: Mg).

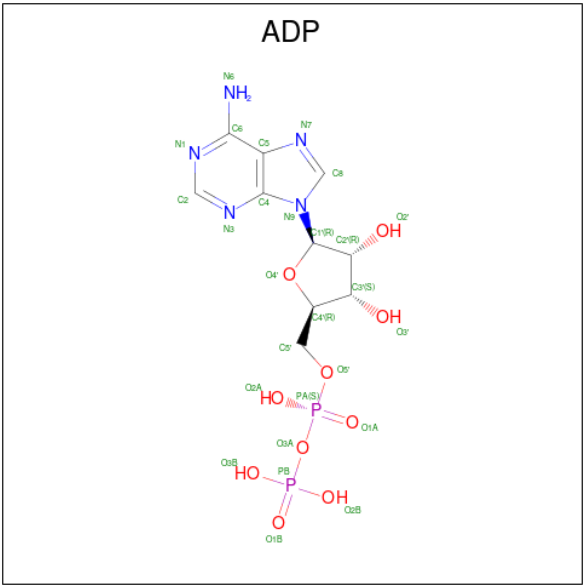
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		

- Molecule 3 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$).



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

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



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

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

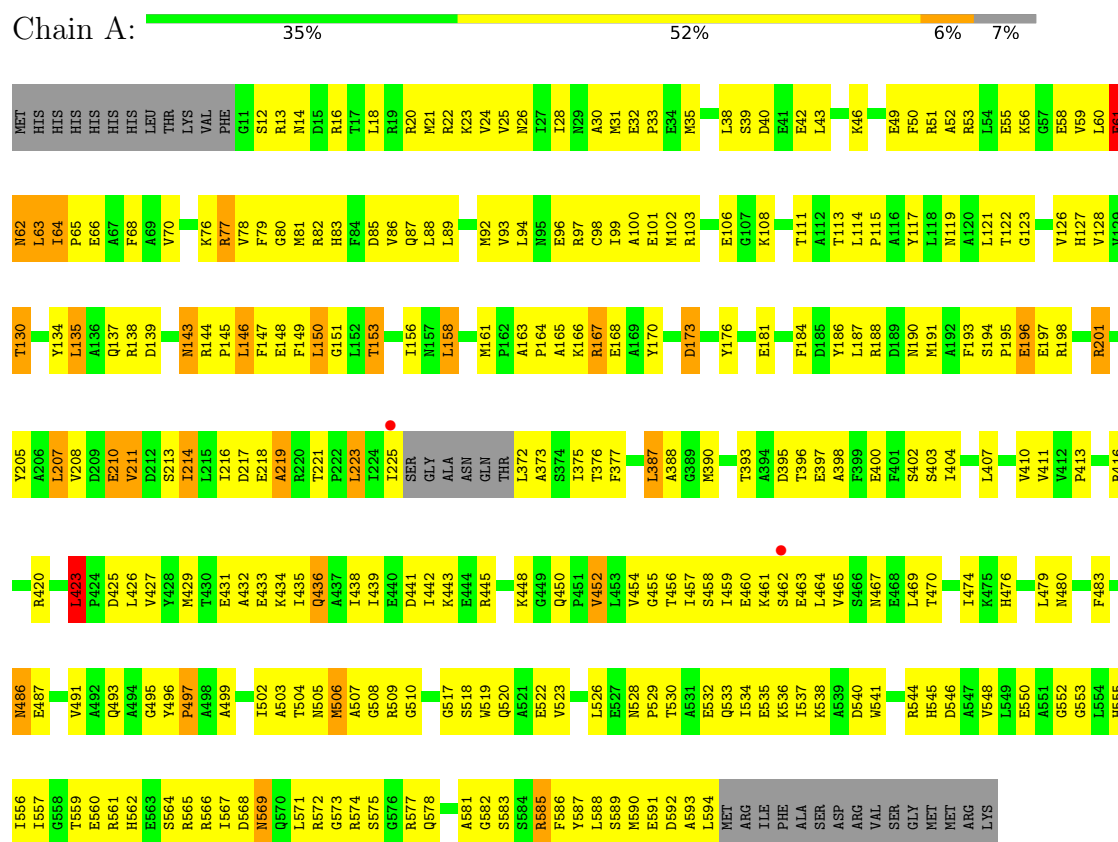
- Molecule 5 is water.

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

3 Residue-property plots

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



• Molecule 1: Preprotein translocase subunit secA



H562	D138	V491	R420	Y205	D139
E563	Y134	A492	R429	A206	D143
S564	L135	A493	L423	L207	R144
R565	A136	A494	L425	V208	P145
R566	P424	G495	Y428	D209	L146
I567	R138	Y496	M429	E210	F147
D568	D139	P497	A432	V211	E148
N569			A433	D212	F149
Q570		I502	E434	I214	L150
Q571		A503	I435	L215	G151
L571		T504	K434	I216	L152
R572		N505	I436	D217	T153
G573		M506	A437	E218	I156
R574		A507	Q436	A219	N157
S575		G508	I439	R220	L158
G576		R509	E440	T221	
R577		G510	D441	P222	
Q578			I442	L223	
		S518	R445	I224	
A581		W519		I225	
Q582		Q520		SER	
S583		A521		GLY	
S584		E522		ALA	
R585		V523		ASN	
F586				GLN	
Y587				THR	
L588		L526		L387	
S589		E527		A388	
N590		N528		G389	
E591		P529		M390	
D592		E591		T391	
D593		T530		A394	
A593		T530		D395	
L594		A531		T396	
L595		E532		Y380	
N596		Q533		L387	
R596		I534		A388	
ILE		E535		G389	
PHE		K536		M390	
ALA		I537		T391	
ALA		K537		A394	
SER		K538		D395	
ASP		A539		T396	
ARG		D540		E397	
ARG		W541		E400	
VAL				F401	
SER		R544		S402	
GLY		H545		S403	
MET		D546		I404	
MET		A547		L407	
ARG		V548		V410	
LYS		L549		V411	
		E550		V412	
		A551		P413	
		G552		R416	
		G553			
		L554			
		H555			
		I556			
		I557			
		G558			
		T559			
		E560			
		R561			

4 Data and refinement statistics

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 46.58 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.4 (46.58-3.00) 99.4 (46.58-3.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.54 (at 3.01Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.245 , 0.305 0.243 , 0.297	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 , 75.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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: MG, SPD, 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	0.51	0/3472	0.99	14/4689 (0.3%)
1	B	0.48	0/3491	0.99	13/4713 (0.3%)
All	All	0.49	0/6963	0.99	27/9402 (0.3%)

There are no bond length outliers.

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	569	ASN	N-CA-C	-9.59	102.16	114.04
1	A	569	ASN	N-CA-C	-9.03	102.85	114.04
1	B	143	ASN	N-CA-C	-8.96	101.02	114.64
1	A	143	ASN	N-CA-C	-8.91	101.09	114.64
1	A	219	ALA	N-CA-C	-8.48	102.48	113.17

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	3420	0	3431	300	0
1	B	3439	0	3453	295	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
5	A	89	0	0	19	0
5	B	82	0	0	22	0
All	All	7106	0	6946	587	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 42.

The worst 5 of 587 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: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
1:A:506:MET:HE2	1:A:506:MET:H	1.30	0.95
1:A:556:ILE:HD13	1:A:571:LEU:HG	1.45	0.94

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%)	10	40
1	B	436/471 (93%)	382 (88%)	47 (11%)	7 (2%)	7	34
All	All	870/942 (92%)	762 (88%)	96 (11%)	12 (1%)	9	36

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	396	THR
1	A	396	THR
1	B	219	ALA
1	A	150	LEU
1	B	221	THR

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	359/388 (92%)	333 (93%)	26 (7%)	13	43
1	B	361/388 (93%)	334 (92%)	27 (8%)	12	41
All	All	720/776 (93%)	667 (93%)	53 (7%)	13	42

5 of 53 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	62	ASN
1	B	146	LEU
1	B	452	VAL
1	B	63	LEU
1	B	86	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	143	ASN
1	B	436	GLN
1	B	415	ASN
1	B	486	ASN
1	A	486	ASN

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 oligosaccharides 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	B	902	-	28,29,29	1.82	10 (35%)	43,45,45	2.10	12 (27%)
3	SPD	A	905	-	9,9,9	0.72	0	8,8,8	0.56	0
4	ADP	A	901	2	28,29,29	1.99	10 (35%)	43,45,45	2.15	11 (25%)
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	B	902	-	-	6/16/32/32	0/3/3/3
3	SPD	A	905	-	-	1/7/7/7	-
4	ADP	A	901	2	-	3/16/32/32	0/3/3/3
3	SPD	B	906	-	-	2/7/7/7	-

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	901	ADP	PA-O3A	-4.58	1.54	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	902	ADP	PA-O3A	-3.95	1.55	1.59
4	A	901	ADP	C5-C4	3.45	1.45	1.39
4	B	902	ADP	C5-C4	3.33	1.45	1.39
4	A	901	ADP	C5-N7	-3.25	1.33	1.39

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	901	ADP	N3-C2-N1	-6.97	118.03	128.58
4	B	902	ADP	N3-C2-N1	-6.19	119.22	128.58
4	A	901	ADP	C5-C4-N3	-5.46	119.19	126.72
4	B	902	ADP	C5-C4-N3	-5.20	119.56	126.72
4	B	902	ADP	C4-C5-N7	-4.33	105.63	110.58

There are no chirality outliers.

5 of 12 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

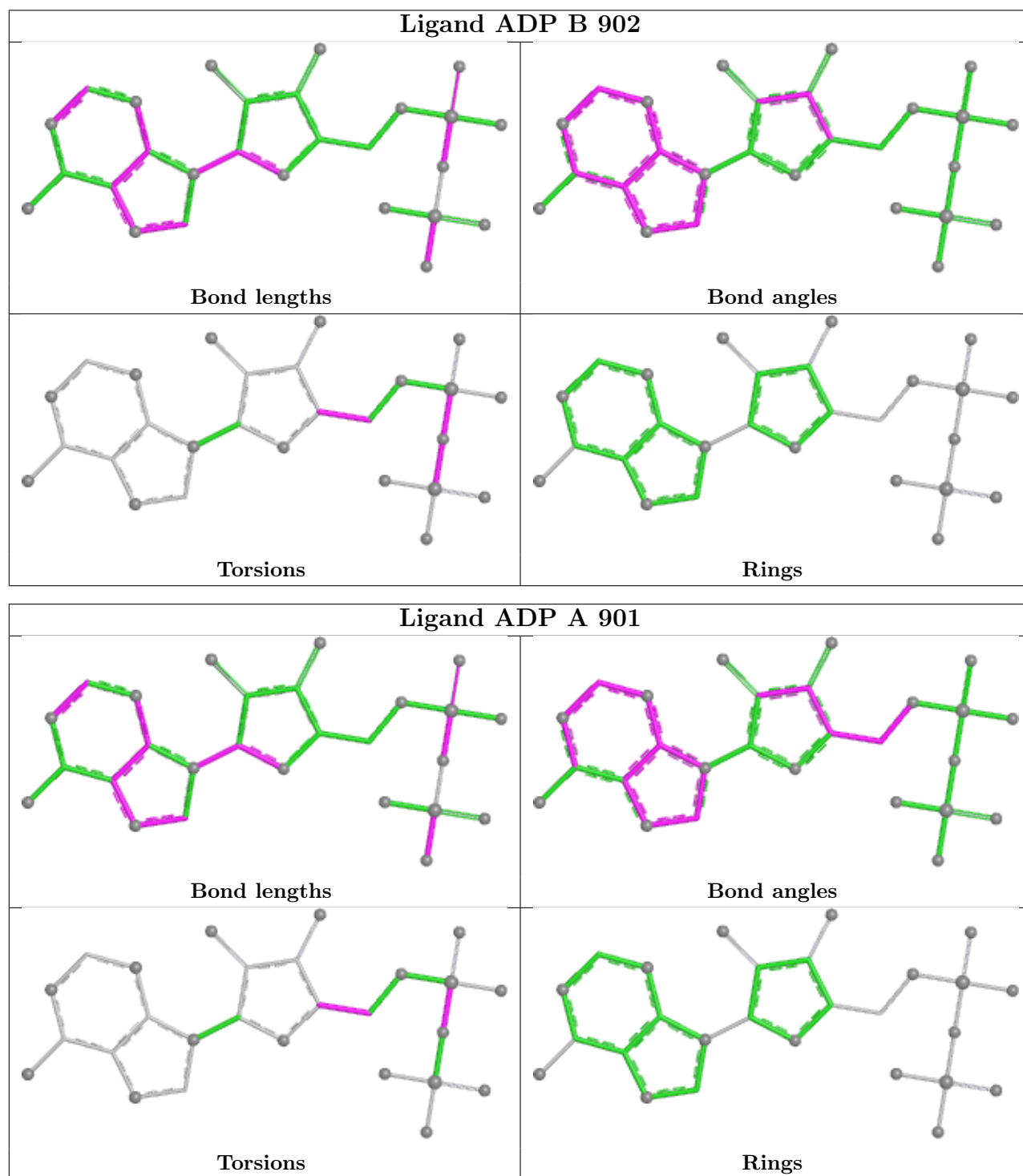
There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	902	ADP	1	0
3	A	905	SPD	4	0
4	A	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 [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%)	0.03	2 (0%) 87 72	46, 78, 128, 152	0
1	B	440/471 (93%)	0.02	0 100 100	48, 78, 129, 152	0
All	All	878/942 (93%)	0.02	2 (0%) 91 83	46, 78, 129, 152	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	462	SER	2.3
1	A	225	ILE	2.0

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 oligosaccharides 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.

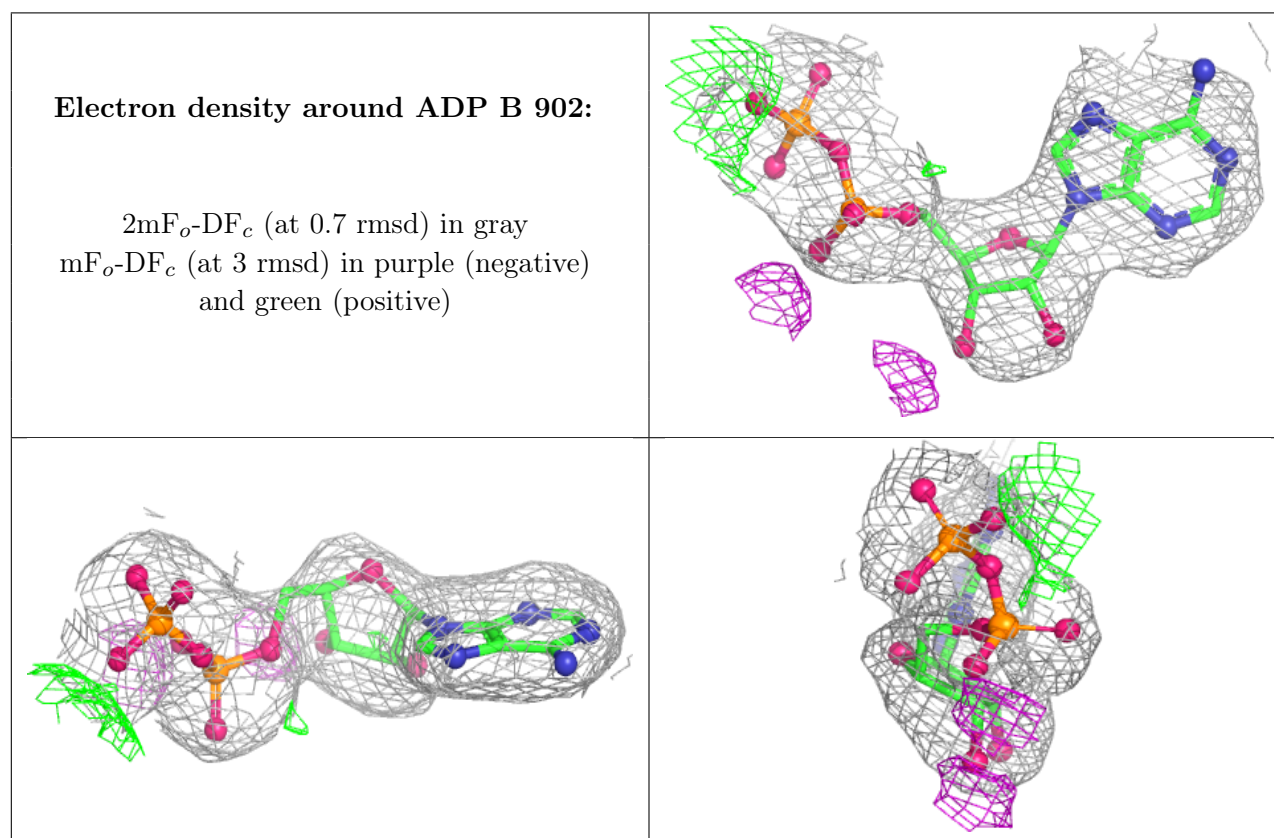
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SPD	A	905	10/10	0.69	0.09	76,78,80,81	0
3	SPD	B	906	10/10	0.78	0.09	74,80,82,82	0
2	MG	B	904	1/1	0.90	0.25	41,41,41,41	0

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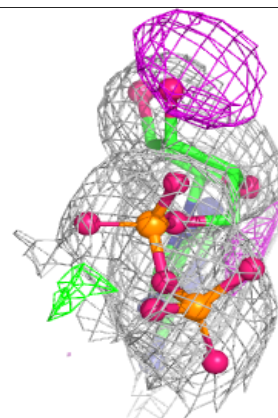
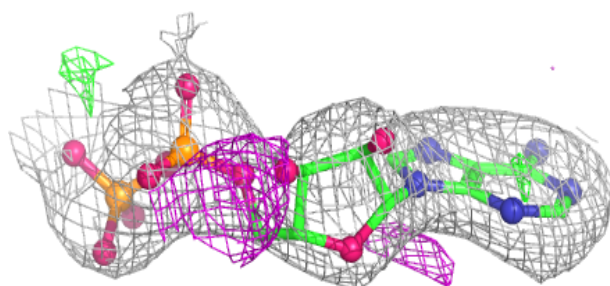
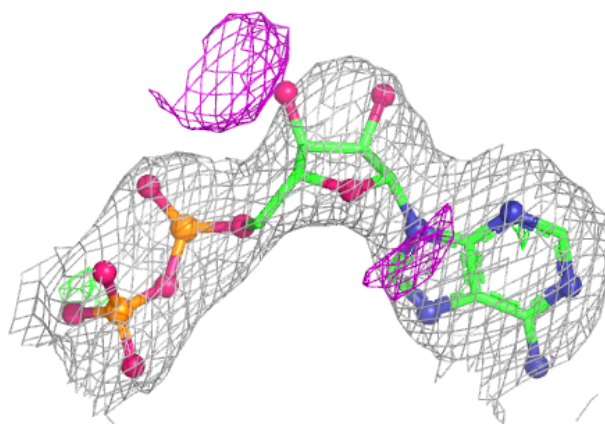
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	ADP	B	902	27/27	0.91	0.11	64,70,71,72	0
4	ADP	A	901	27/27	0.94	0.10	57,63,68,72	0
2	MG	A	903	1/1	0.98	0.10	23,23,23,23	0

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 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.