



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 11, 2021 – 05:19 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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	:	2.23.2
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)	:	2.23.2

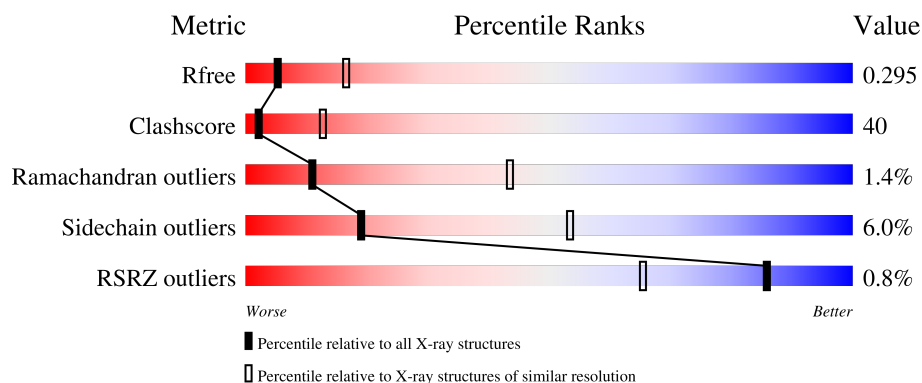
1 Overall quality at a glance

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}	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 $\leq 5\%$. 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	<div> <div></div> <div>37%</div> <div>52%</div> <div>7%</div> </div>
1	B	471	<div> <div></div> <div>39%</div> <div>51%</div> <div>7%</div> </div>

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

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			

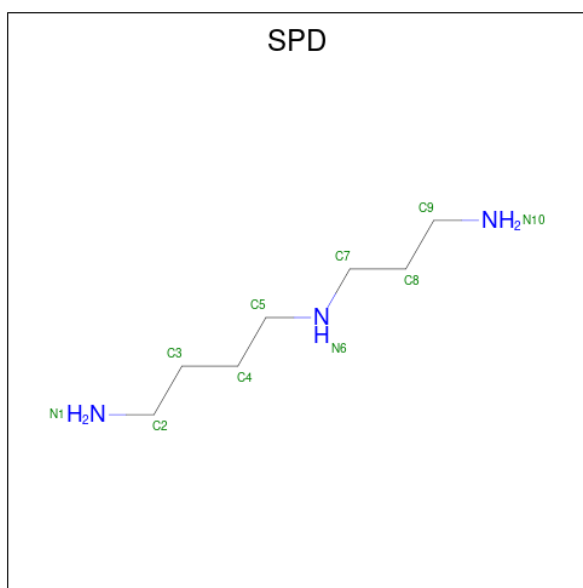
There are 16 discrepancies between the modelled and reference sequences:

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 (three-letter code: MG) (formula: Mg).

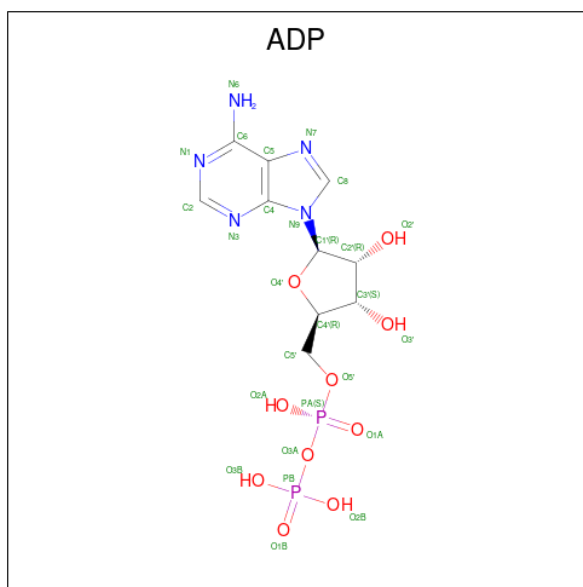
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		

- Molecule 3 is SPERMIDINE (three-letter code: 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 (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

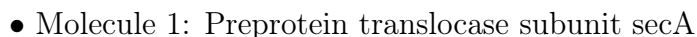


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- 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		

- Molecule 1: Preprotein translocase subunit secA



G573	R574	S575	G576	R577	Q578	G581	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	ARG	LYS																								
N505	M506	A507	G508	R509	G510		S518	W519	Q520	A521	E522	V523	G526	E527	S528	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	R560	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	Q455	T456	I457	S458	T459	E460	K461	S462	E463	L464	V465	S466	M467	E468	L469	T470	I474	K475	H476	N477	V478	L479	M480	F483	N486	E487	V491	A492	Q493	Y496	P497	T502	A503	T504				
K143	L215	D216	D217	E218	A219		R220	T221	P222	L223	I224	T225		SER	GLY	ALA	ASN	GLN	THR	L372	A373	T376	L387	A388	G389	K390	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						
M143	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	M190	M191	F193	S194	P195	E196	E197	R198	R201	K202	Y205	A206	L207	V208	D209	E210	V211	D212	S213					
G573	R574	S575	G576	R577	Q578	G581	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	ARG	LYS																							

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 46.57 – 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
$\langle I/\sigma(I) \rangle$ 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	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	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.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ADP, 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(°)	Ideal(°)
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 ⓘ

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 ⓘ

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%)
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
4	ADP	B	902	-	24,29,29	1.72	7 (29%)	29,45,45	1.75	5 (17%)

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

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(°)	Ideal(°)
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

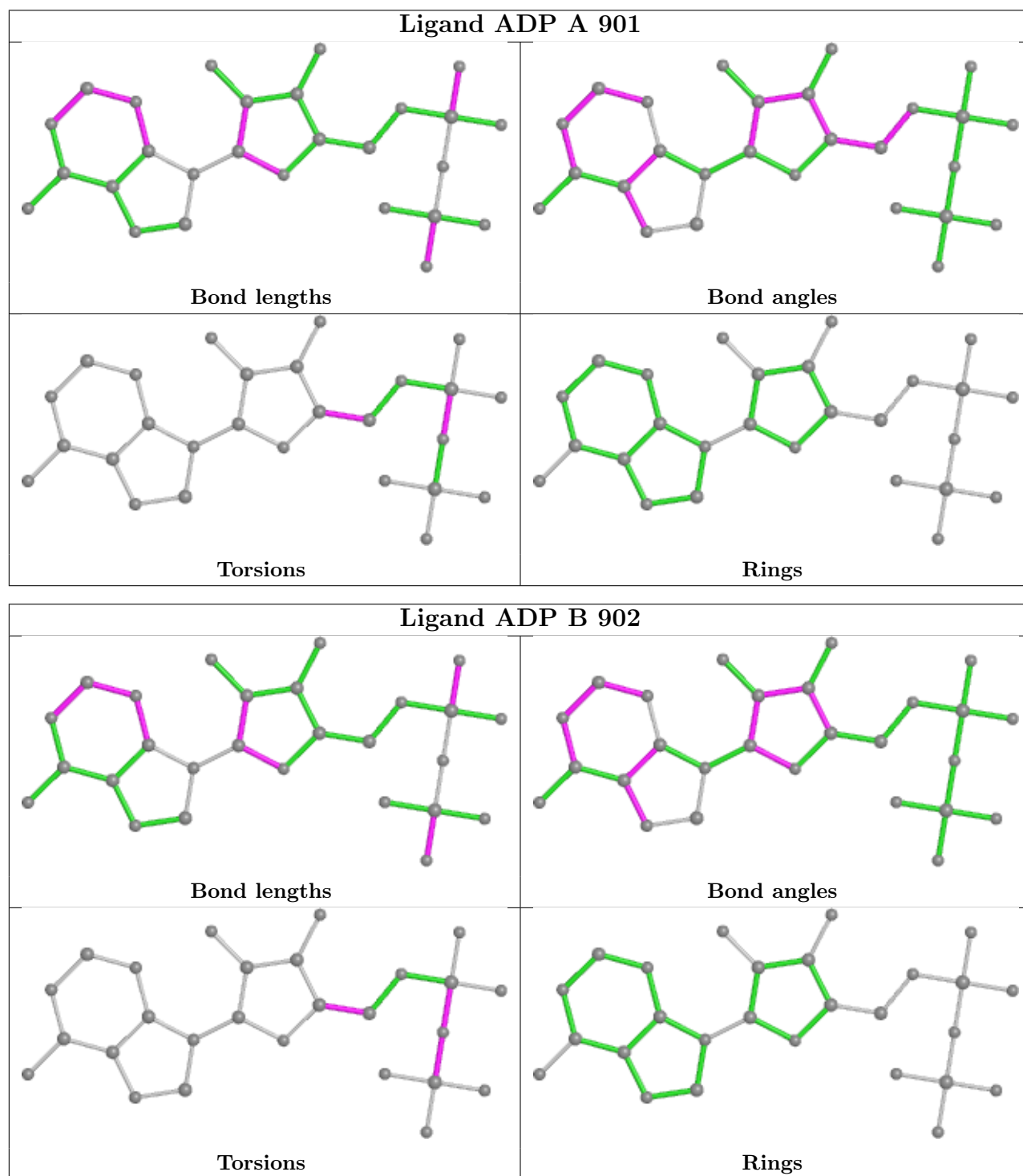
There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	901	ADP	1	0
3	A	905	SPD	4	0
4	B	902	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%)	0.02	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](#)

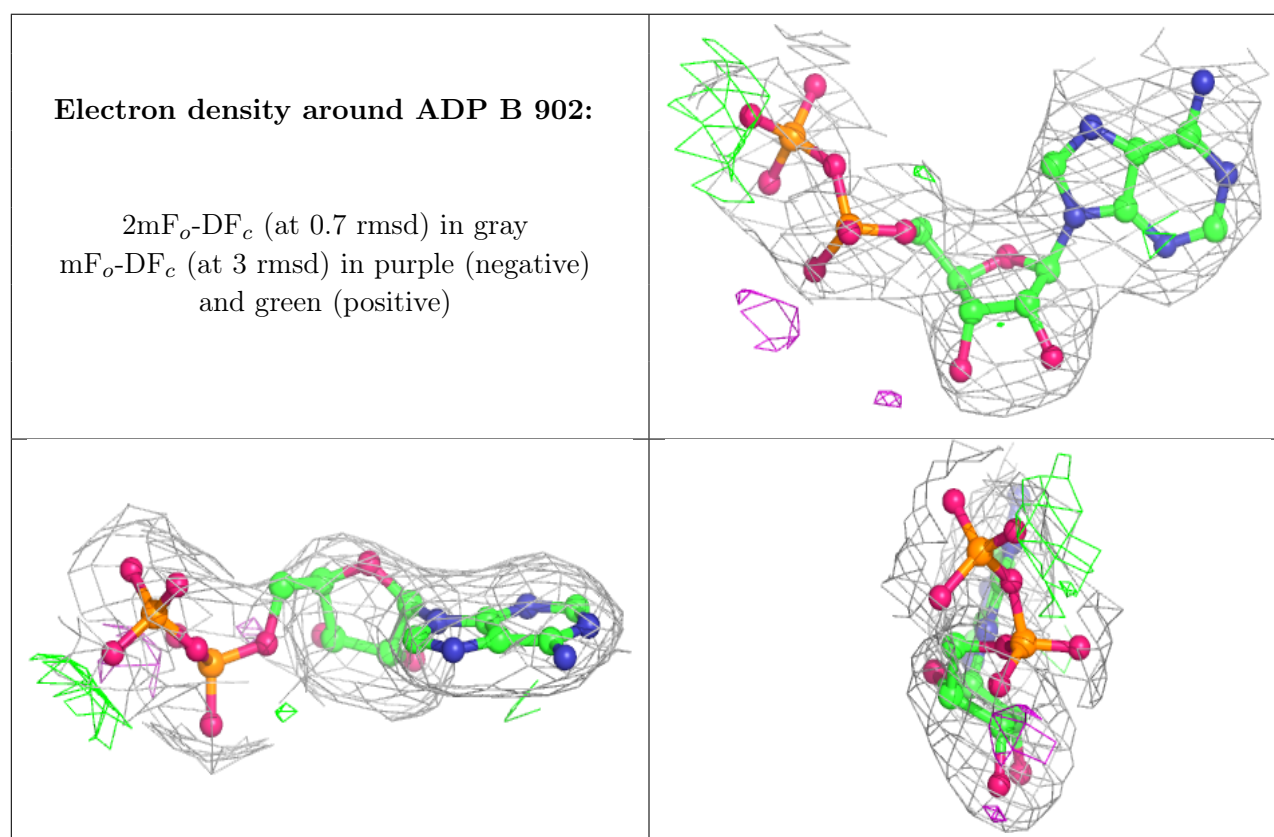
There are no monosaccharides in this entry.

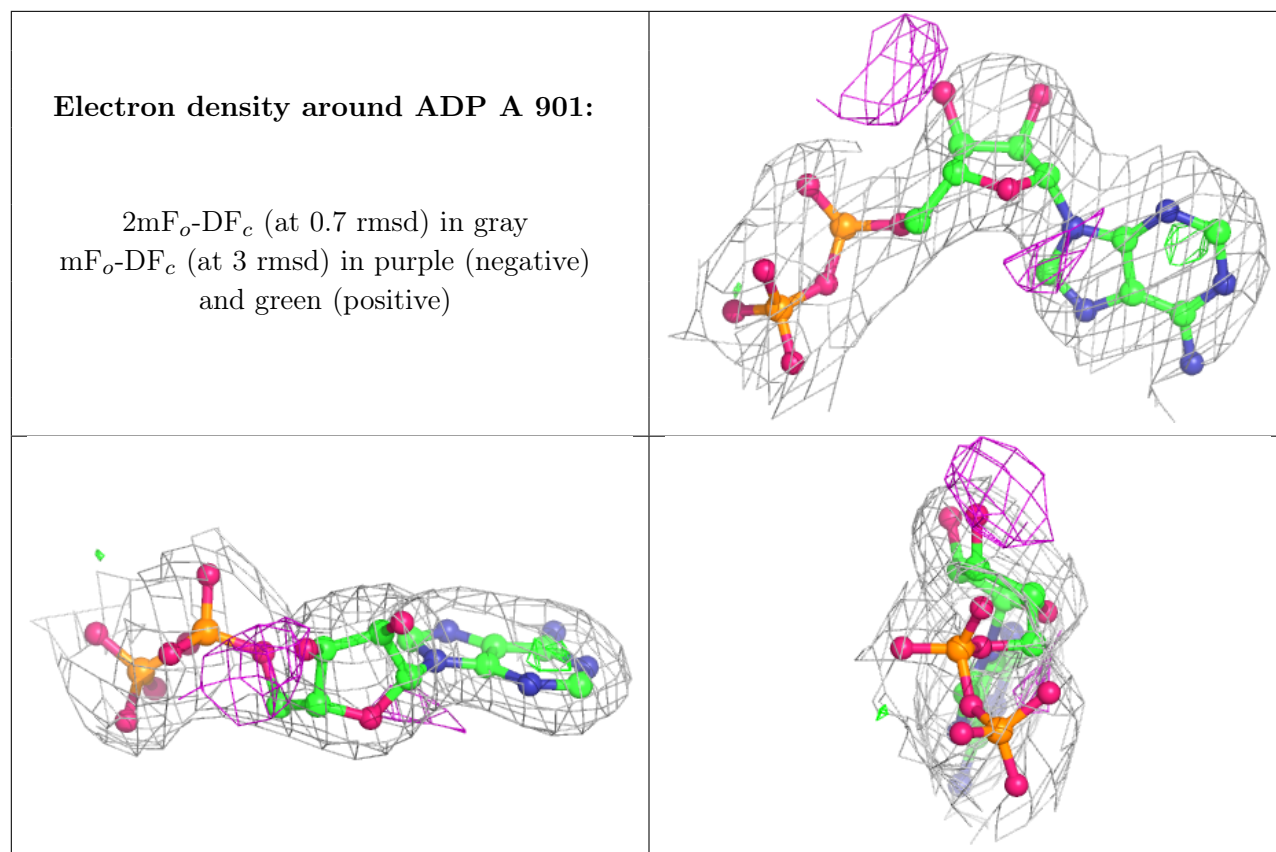
6.4 Ligands [i](#)

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(\AA^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.





6.5 Other polymers [i](#)

There are no such residues in this entry.