wwPDB X-ray Structure Validation Summary Report (i)

Aug 8, 2023 – 11:13 AM EDT

PDB ID	:	1NG9
Title	:	E.coli MutS R697A: an ATPase-asymmetry mutant
Authors	:	Lamers, M.H.; Winterwerp, H.H.K.; Sixma, T.K.
Deposited on	:	2002-12-17
Resolution	:	2.60 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:

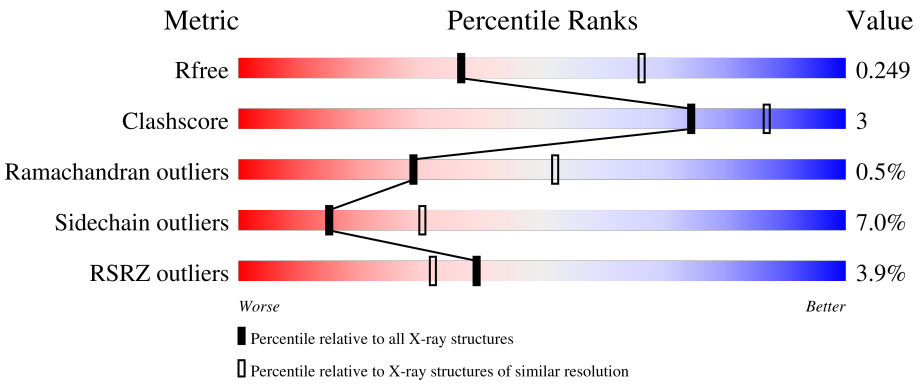
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	E	30	13% 43% 13% • 40%
2	F	30	3% 43% 10% • 43%
3	A	800	4% 85% 13% • •
3	B	800	4% 82% 12% • •

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 13420 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 DNA chain called 5'-D(*AP*GP*CP*TP*GP*CP*CP*AP*GP*GP*CP*AP*CP*CP*AP*GP*TP*GP*TP*CP*AP*GP*CP*GP*TP*CP*CP*TP*AP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	E	18	367	174	72	104	17	0	0	0

- Molecule 2 is a DNA chain called 5'-D(*AP*TP*AP*GP*GP*AP*CP*GP*CP*TP*GP*AP*CP*AP*CP*TP*GP*GP*TP*GP*CP*TP*TP*GP*GP*CP*AP*GP*CP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	F	17	347	166	62	103	16	0	0	0

- Molecule 3 is a protein called DNA mismatch repair protein MutS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	A	794	6241	3925	1109	1177	30	0	0	0
3	B	766	6045	3808	1072	1136	29	0	0	0

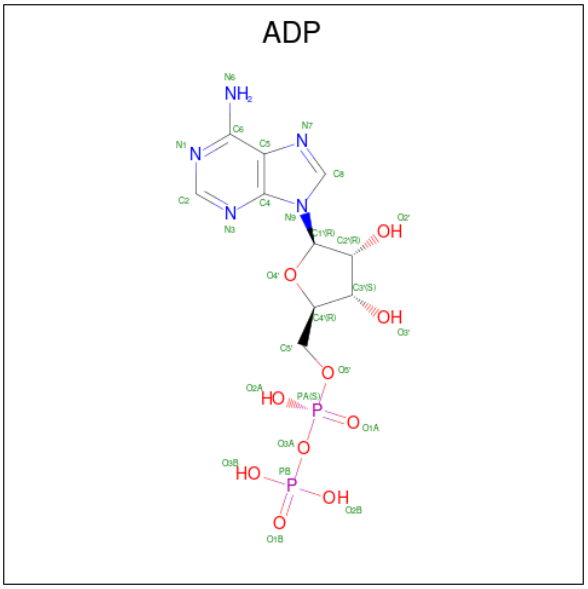
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	697	ALA	ARG	engineered mutation	UNP P23909
B	697	ALA	ARG	engineered mutation	UNP P23909

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 5 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		
5	A	1	27	10	5	10	2	0	0
5	B	1	27	10	5	10	2	0	0

- Molecule 6 is water.

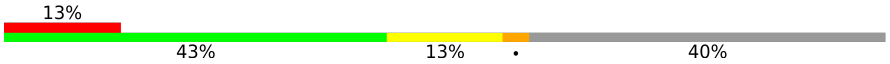
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	E	3	3	3	0	0
6	F	4	4	4	0	0
6	A	165	165	165	0	0
6	B	192	192	192	0	0

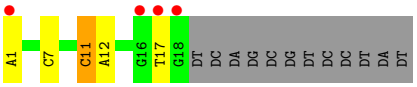
3 Residue-property plots (i)

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: 5'-D(*AP*GP*CP*TP*GP*CP*CP*AP*GP*GP*CP*AP*CP*CP*AP*GP*TP*GP*TP*CP*AP*GP*CP*GP*TP*CP*CP*TP*AP*T)-3'

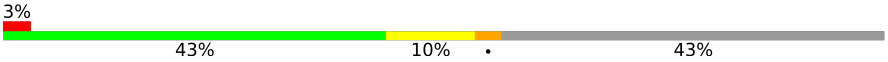
Chain E:

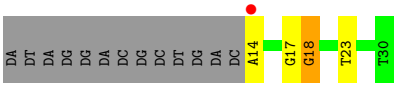




• Molecule 2: 5'-D(*AP*TP*AP*GP*GP*AP*CP*GP*CP*TP*GP*AP*CP*AP*CP*TP*GP*GP*TP*GP*CP*TP*TP*GP*GP*CP*AP*GP*CP*T)-3'

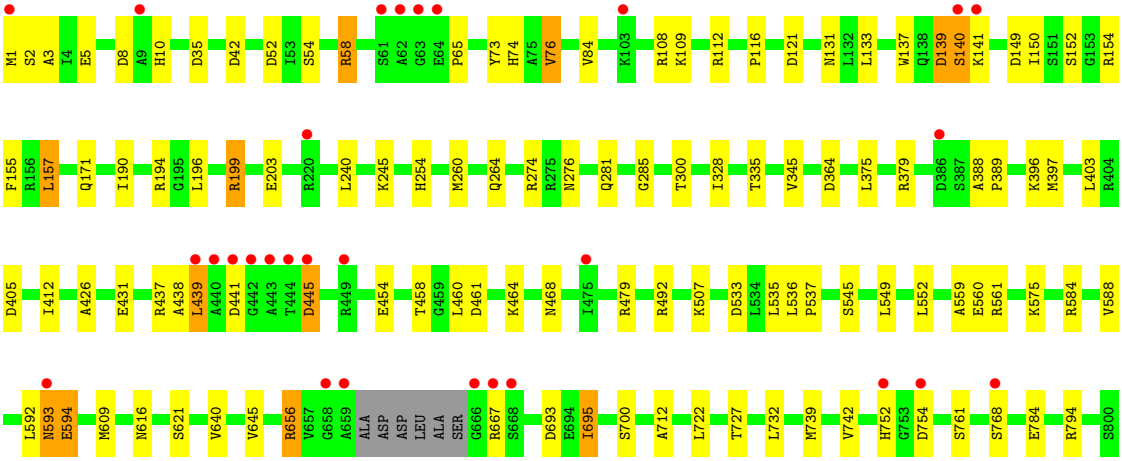
Chain F:





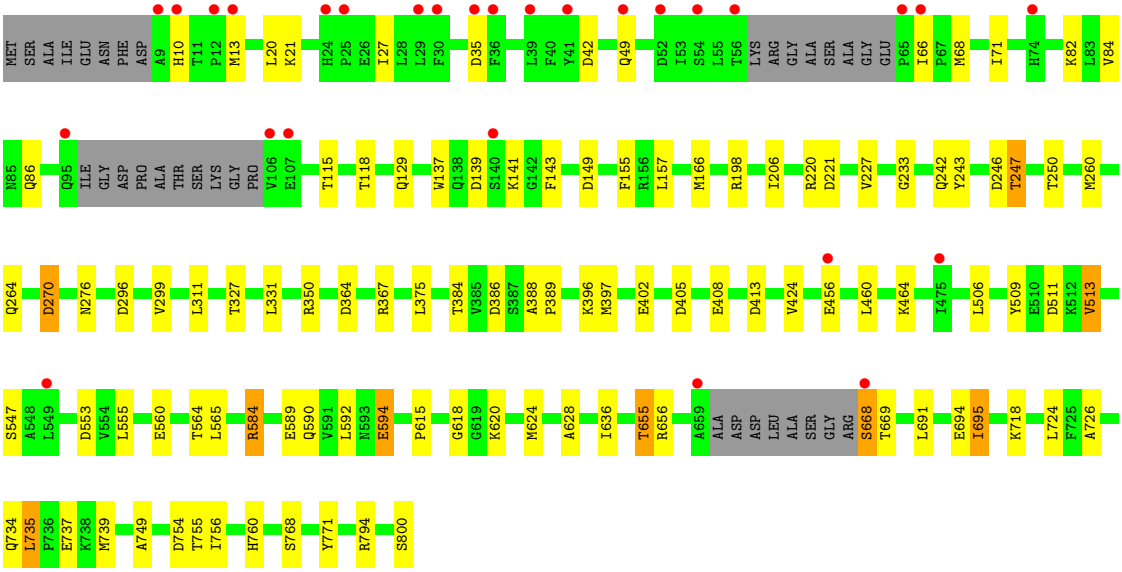
• Molecule 3: DNA mismatch repair protein MutS

Chain A:



• Molecule 3: DNA mismatch repair protein MutS

Chain B:


MET SER ALA ILE GLU ASN PHE ASP A9 H10 T11 P12 M13 L20 K21 H24 P25 E26 I27 L28 L29 F30 D35 F36 L39 F40 Y41 D42 Q49 D52 I53 S54 L55 T56 LYS ARG GLY ALA SER ALA GLY GLU P65 I66 P67 M68 I71 H74 K82 L83 V84
N85 Q86 Q95 ILE GLY ASP PRO ALA THR SER LYS GLY PRO V106 E107 T115 T118 Q129 W137 Q138 D139 S140 K141 G142 F143 D149 F155 R156 L157 M166 R198 I206 R220 D221 V227 G233 Q242 Y243 D246 T247 T250 M260
Q264 D270 N276 D296 V299 L311 T327 L331 R350 D364 R367 L375 T384 V385 D386 S387 A388 P389 K396 M397 E402 D405 E408 D413 V424 E456 L460 K464 I475 L506 Y509 E510 D511 K512 V513
S547 A548 L549 D553 V554 L555 E560 T564 L565 R584 E589 Q590 Y591 L592 N593 E594 P615 G618 G619 K620 M624 A628 I636 T655 R656 A659 ALA ASP ASP LEU ALA SER GLY ARG S668 T669 L691 E694 I695 K718 L724 F725 A726
Q734 L735 P736 E737 K738 M739 A749 D754 T755 I756 H760 S768 Y771 R794 S800

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	89.90Å 92.40Å 261.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.60 20.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.2 (20.00-2.60) 98.2 (20.00-2.60)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	2.09 (at 2.59Å)	Xtriage
Refinement program	REFMAC 5.1.19	Depositor
R, R_{free}	0.215 , 0.249 0.212 , 0.249	Depositor DCC
R_{free} test set	1283 reflections (1.93%)	wwPDB-VP
Wilson B-factor (Å^2)	39.1	Xtriage
Anisotropy	0.790	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 39.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.024 for k,h,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	13420	wwPDB-VP
Average B, all atoms (Å^2)	11.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% 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: MG, 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	E	0.75	0/412	1.40	4/634 (0.6%)
2	F	0.71	0/388	1.50	4/598 (0.7%)
3	A	0.40	0/6347	0.73	12/8591 (0.1%)
3	B	0.42	0/6146	0.71	13/8318 (0.2%)
All	All	0.44	0/13293	0.79	33/18141 (0.2%)

There are no bond length outliers.

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	14	DA	O4'-C1'-N9	9.82	114.87	108.00
2	F	23	DT	O4'-C1'-N1	-7.59	102.69	108.00
1	E	1	DA	O4'-C1'-N9	7.51	113.26	108.00
2	F	18	DG	O4'-C4'-C3'	-7.22	101.61	104.50
3	B	270	ASP	CB-CG-OD2	6.55	124.20	118.30

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	E	367	0	202	1	0
2	F	347	0	194	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	6241	0	6288	43	0
3	B	6045	0	6095	38	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	27	0	12	0	0
5	B	27	0	12	1	0
6	A	165	0	0	9	0
6	B	192	0	0	5	0
6	E	3	0	0	1	0
6	F	4	0	0	0	0
All	All	13420	0	12803	82	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 3.

The worst 5 of 82 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)
6:E:358:HOH:O	3:A:58:ARG:HD3	1.85	0.76
3:B:327:THR:HG21	3:B:555:LEU:HD13	1.71	0.73
3:A:74:HIS:ND1	6:A:2120:HOH:O	2.20	0.72
3:A:74:HIS:CE1	6:A:2120:HOH:O	2.47	0.68
3:A:133:LEU:HG	3:A:240:LEU:HD11	1.78	0.64

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
3	A	790/800 (99%)	765 (97%)	18 (2%)	7 (1%)	17 35
3	B	758/800 (95%)	733 (97%)	25 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1548/1600 (97%)	1498 (97%)	43 (3%)	7 (0%)	29 52

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	2	SER
3	A	594	GLU
3	A	439	LEU
3	A	3	ALA
3	A	140	SER

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
3	A	659/663 (99%)	615 (93%)	44 (7%)	16 33
3	B	640/663 (96%)	593 (93%)	47 (7%)	14 28
All	All	1299/1326 (98%)	1208 (93%)	91 (7%)	15 30

5 of 91 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	B	155	PHE
3	B	460	LEU
3	B	206	ILE
3	B	350	ARG
3	B	547	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
3	B	214	ASN
3	B	590	GLN
3	B	276	ASN

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Mol	Chain	Res	Type
3	B	760	HIS
3	B	344	GLN

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 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	$\#\|Z\| > 2$
5	ADP	A	2001	4	24,29,29	1.26	2 (8%)	29,45,45	1.69	4 (13%)
5	ADP	B	2002	4	24,29,29	1.18	2 (8%)	29,45,45	1.44	3 (10%)

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
5	ADP	A	2001	4	-	2/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ADP	B	2002	4	-	5/12/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	2001	ADP	C2-N3	4.18	1.38	1.32
5	B	2002	ADP	C2-N3	4.06	1.38	1.32
5	A	2001	ADP	C2-N1	2.93	1.39	1.33
5	B	2002	ADP	C2-N1	2.39	1.38	1.33

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	2001	ADP	N3-C2-N1	-6.10	119.14	128.68
5	B	2002	ADP	N3-C2-N1	-5.43	120.19	128.68
5	A	2001	ADP	O3B-PB-O3A	3.56	116.56	104.64
5	A	2001	ADP	PA-O3A-PB	-3.13	122.07	132.83
5	A	2001	ADP	C3'-C2'-C1'	2.84	105.25	100.98

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	2001	ADP	PA-O3A-PB-O2B
5	B	2002	ADP	C5'-O5'-PA-O1A
5	B	2002	ADP	C5'-O5'-PA-O2A
5	B	2002	ADP	C5'-O5'-PA-O3A
5	B	2002	ADP	C4'-C5'-O5'-PA

There are no ring outliers.

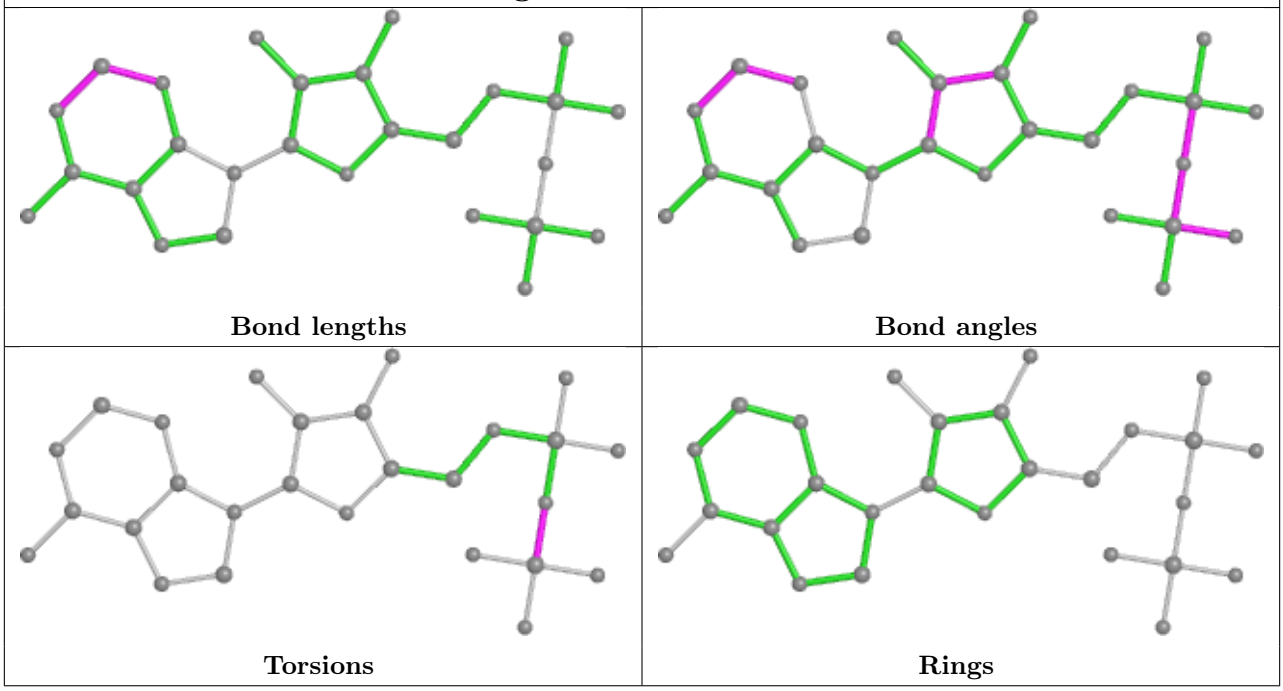
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	2002	ADP	1	0

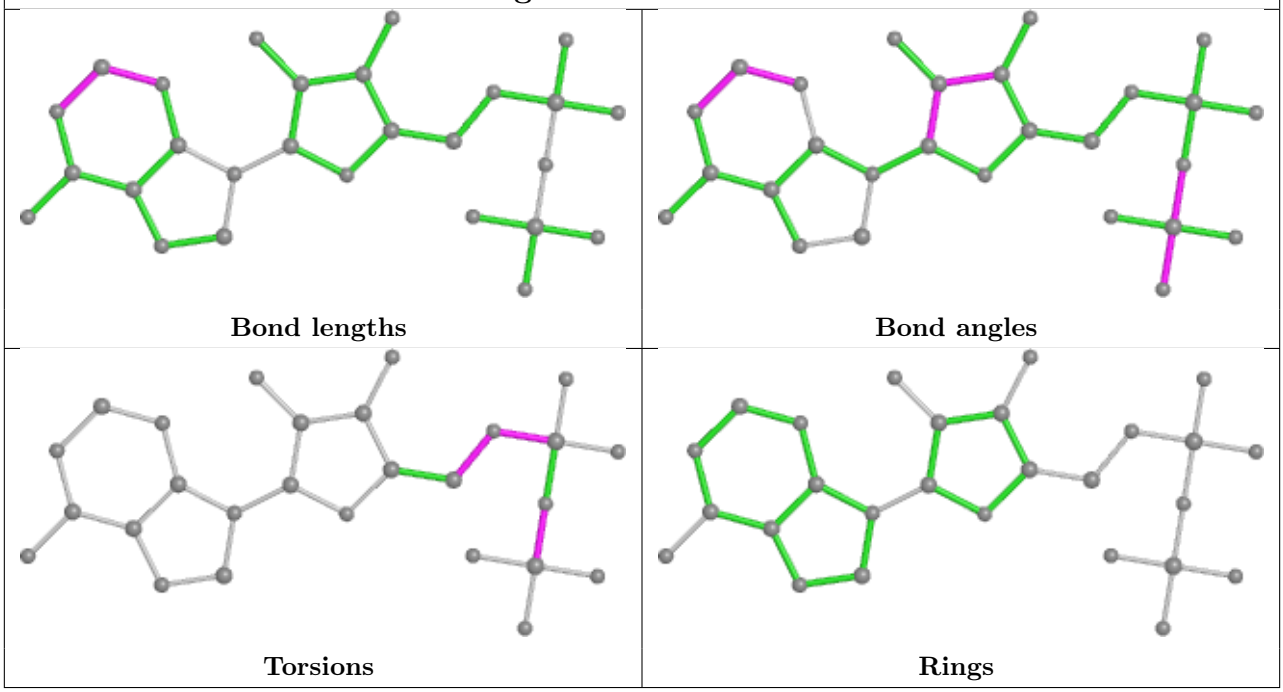
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 2001



Ligand ADP B 2002



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	E	18/30 (60%)	0.84	4 (22%)	0	0	4, 10, 16, 19	0
2	F	17/30 (56%)	0.33	1 (5%)	22	17	5, 10, 15, 18	0
3	A	794/800 (99%)	-0.02	29 (3%)	41	34	4, 10, 14, 20	0
3	B	766/800 (95%)	0.03	28 (3%)	41	34	4, 10, 14, 23	0
All	All	1595/1660 (96%)	0.02	62 (3%)	39	32	4, 10, 14, 23	0

The worst 5 of 62 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	B	106	VAL	6.4
3	B	12	PRO	6.3
1	E	18	DG	6.2
3	B	659	ALA	6.2
3	A	667	ARG	5.1

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)

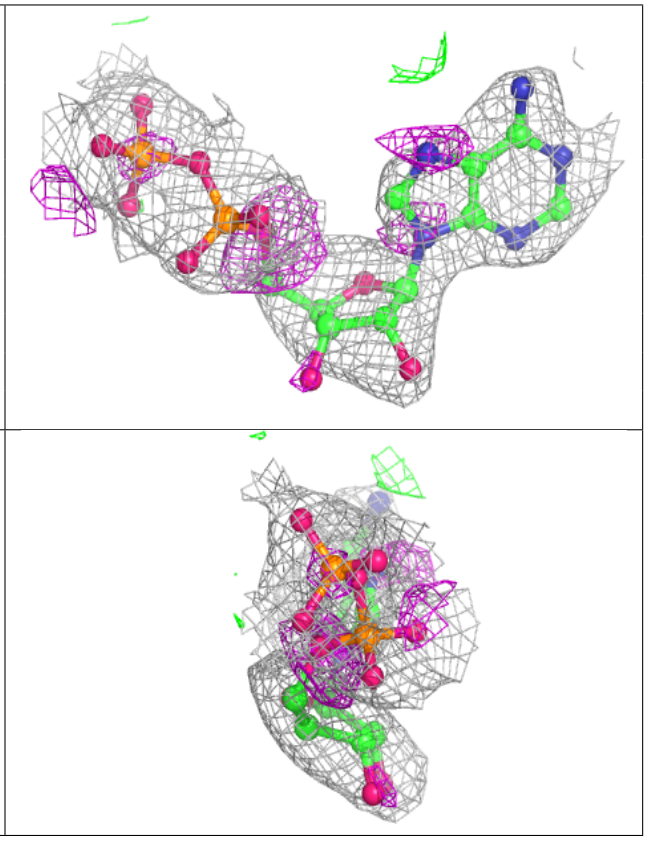
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MG	A	1001	1/1	0.89	0.05	41,41,41,41	0
4	MG	B	1002	1/1	0.90	0.45	54,54,54,54	0
5	ADP	B	2002	27/27	0.90	0.20	64,71,73,76	0
5	ADP	A	2001	27/27	0.96	0.14	50,56,58,58	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.

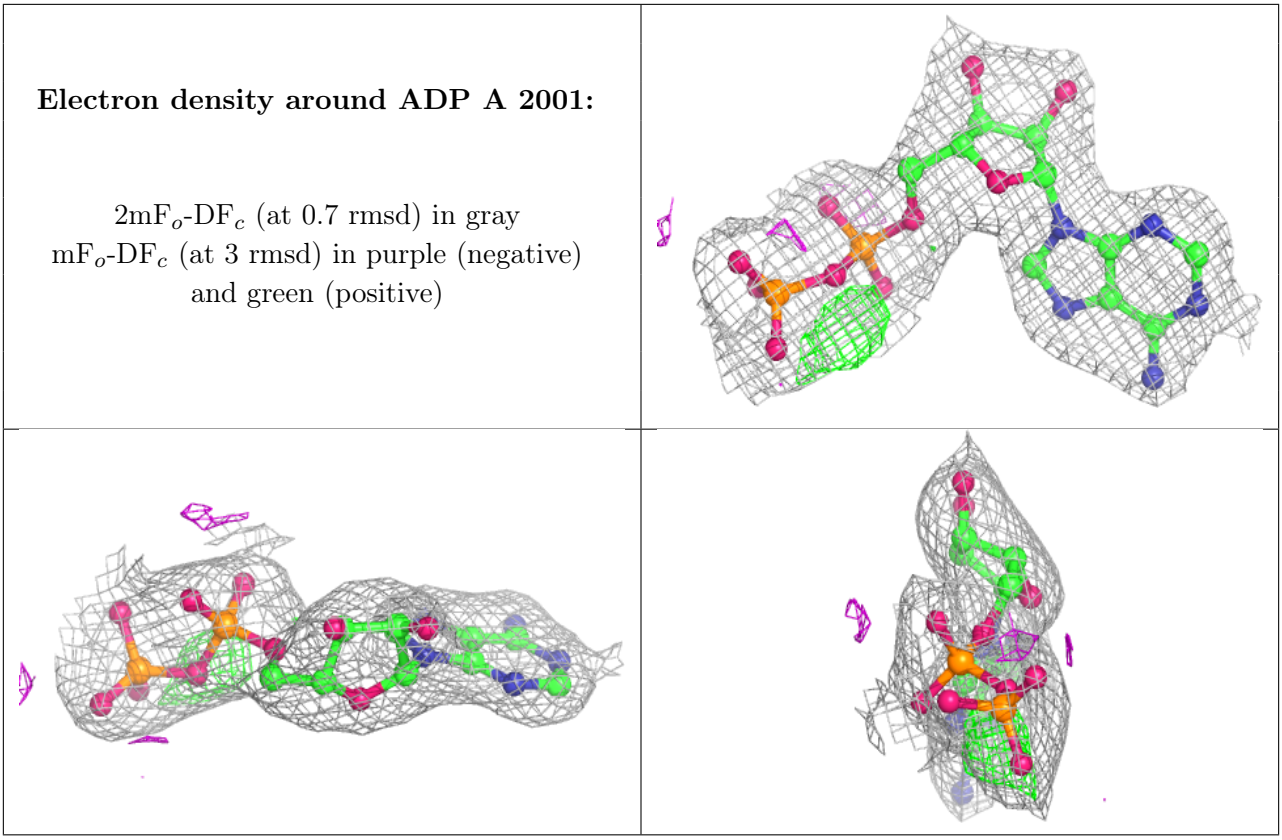
Electron density around ADP B 2002:

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 2001:

$2mF_o$-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.