Full wwPDB X-ray Structure Validation Report ⓘ

Jan 5, 2024 – 01:09 am GMT

PDB ID	:	5JC7
Title	:	Crystal structure of chicken MDA5 with 5'p 24-mer dsRNA and ADP-Mg2+ at 2.75 A resolution.
Authors	:	Cusack, S.; Uchikawa, E.
Deposited on	:	2016-04-14
Resolution	:	2.75 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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:

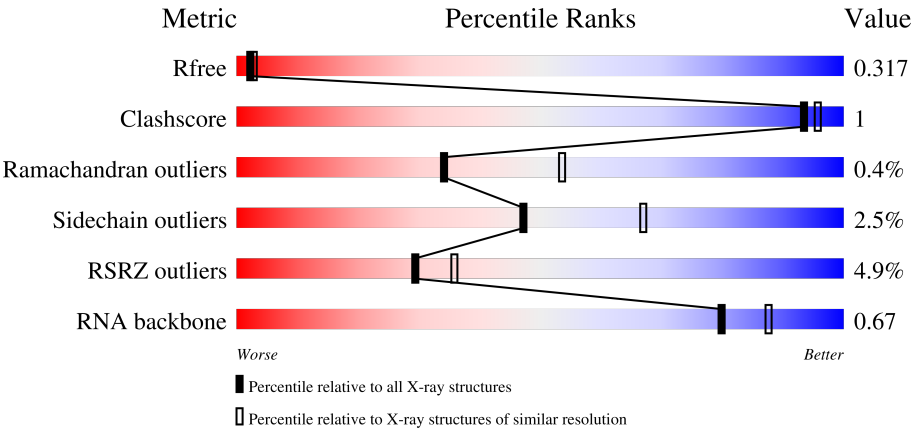
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.75 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)
RNA backbone	3102	1060 (3.02-2.50)

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	701	6% 85% 6% 9%
1	B	701	3% 85% 7% 8%
2	X	25	88% 8% .
3	Y	24	92% 8%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 11616 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 Melanoma differentiation associated protein-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	641	Total	C	N	O	S	0	0	0
			5244	3314	939	959	32			
1	B	647	Total	C	N	O	S	0	0	0
			5293	3347	945	969	32			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	294	GLY	-	expression tag	UNP D9N195
A	295	ALA	-	expression tag	UNP D9N195
A	296	MET	-	expression tag	UNP D9N195
A	297	GLY	-	expression tag	UNP D9N195
A	436	GLN	GLU	engineered mutation	UNP D9N195
B	294	GLY	-	expression tag	UNP D9N195
B	295	ALA	-	expression tag	UNP D9N195
B	296	MET	-	expression tag	UNP D9N195
B	297	GLY	-	expression tag	UNP D9N195
B	436	GLN	GLU	engineered mutation	UNP D9N195

- Molecule 2 is a RNA chain called RNA (5'-R(P*GP*GP*AP*CP*GP*UP*CP*AP*UP*GP *CP*GP*CP*AP*UP*GP*AP*CP*GP*UP*CP*CP*CP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	X	24	Total	C	N	O	P	0	0	0
			509	227	90	168	24			

- Molecule 3 is a RNA chain called RNA (5'-R(P*GP*GP*GP*AP*CP*GP*UP*CP*AP*UP *GP*CP*GP*CP*AP*UP*GP*AP*CP*GP*UP*CP*CP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	Y	24	Total	C	N	O	P	0	0	0
			512	228	92	168	24			

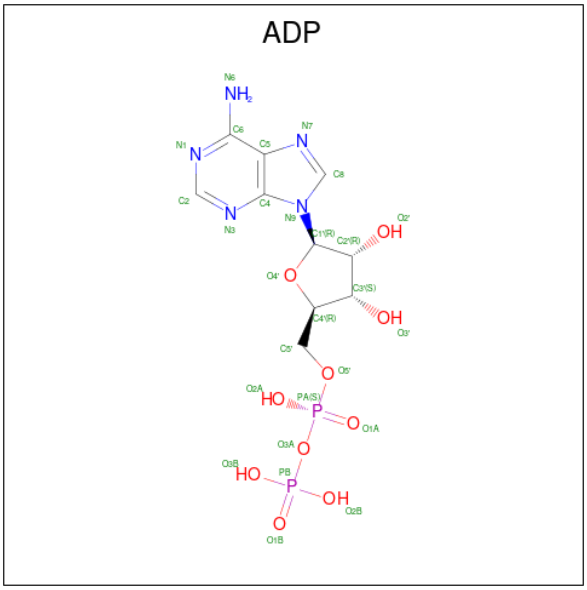
- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



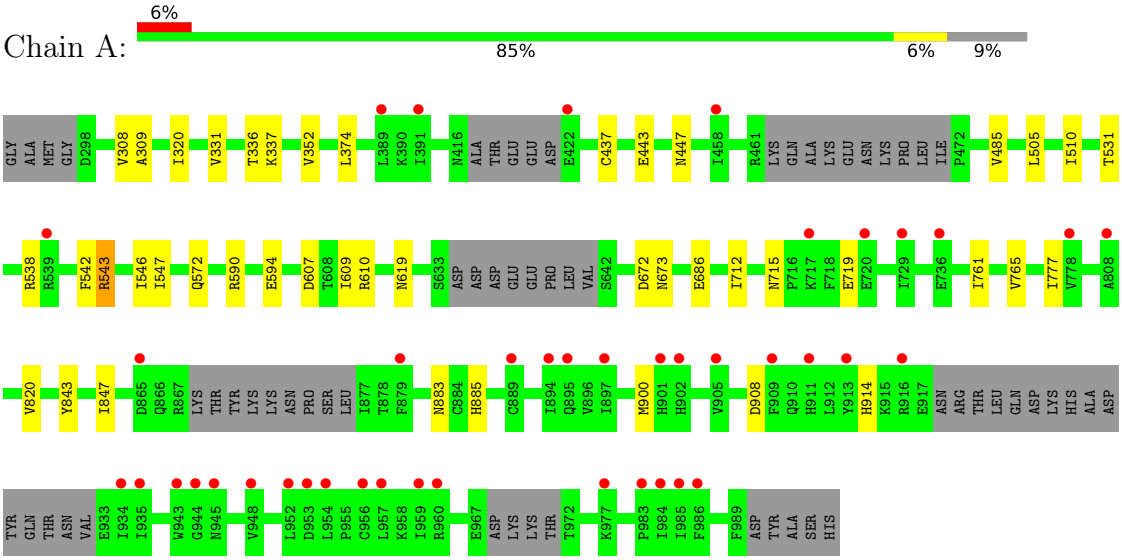
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C N O P 27 10 5 10 2	0	0
6	B	1	Total C N O P 27 10 5 10 2	0	0

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.

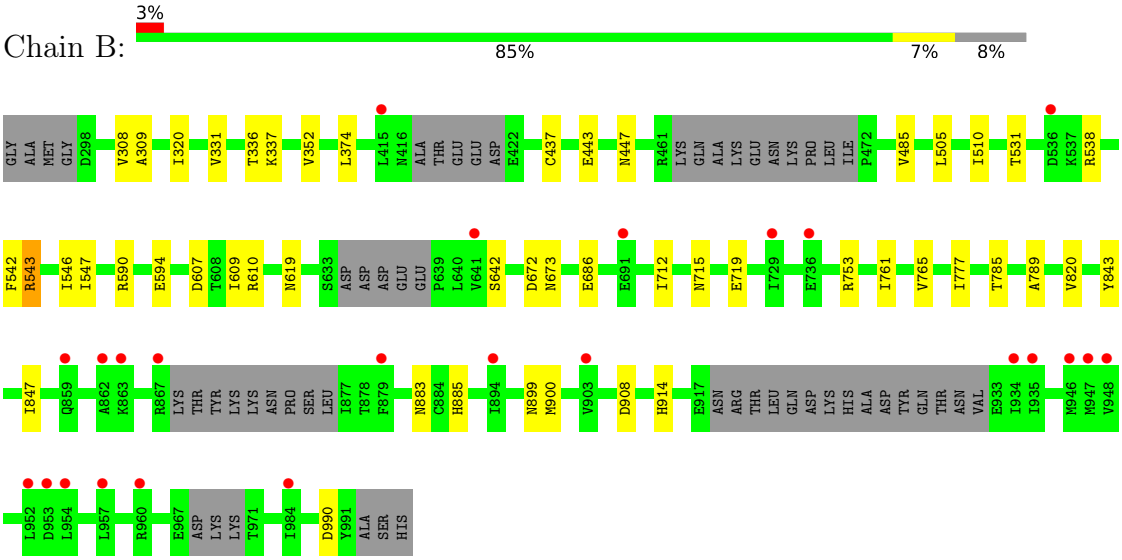
• Molecule 1: Melanoma differentiation associated protein-5

Chain A:



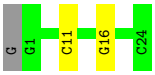
• Molecule 1: Melanoma differentiation associated protein-5

Chain B:



• Molecule 2: RNA (5'-R(P*GP*GP*AP*CP*GP*UP*CP*AP*UP*GP*CP*GP*CP*AP*UP*GP*AP*CP*GP*UP*CP*CP*CP*C)-3')

Chain X:



• Molecule 3: RNA (5'-R(P*GP*GP*GP*AP*CP*GP*UP*CP*AP*UP*GP*CP*GP*CP*AP*UP*GP*AP*CP*GP*UP*CP*CP*C)-3')

Chain Y:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	99.75Å 133.40Å 138.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.75 48.03 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.1 (50.00-2.75) 99.1 (48.03-2.75)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.13 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.8.0131	Depositor
R, R_{free}	0.291 , 0.322 0.291 , 0.317	Depositor DCC
R_{free} test set	2433 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	42.8	Xtriage
Anisotropy	1.103	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 11.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	11616	wwPDB-VP
Average B, all atoms (Å^2)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 44.67 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.4751e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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

5.1 Standard geometry

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

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	0.41	0/5330	0.63	0/7146
1	B	0.41	0/5381	0.63	0/7217
2	X	0.32	0/567	0.71	0/881
3	Y	0.32	0/571	0.72	0/888
All	All	0.40	0/11849	0.64	0/16132

There are no bond length outliers.

There are no bond angle outliers.

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	5244	0	5333	16	0
1	B	5293	0	5381	16	0
2	X	509	0	261	2	0
3	Y	512	0	261	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	27	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	27	0	12	0	0
All	All	11616	0	11260	33	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 1.

All (33) 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:590:ARG:NH1	1:A:883:ASN:OD1	2.29	0.66
1:A:336:THR:HG22	1:A:352:VAL:HG11	1.78	0.65
1:B:336:THR:HG22	1:B:352:VAL:HG11	1.78	0.65
1:B:590:ARG:NH1	1:B:883:ASN:OD1	2.29	0.64
1:B:590:ARG:NH2	1:B:594:GLU:OE1	2.33	0.61
1:A:437:CYS:HB2	1:A:505:LEU:HD11	1.83	0.61
1:B:437:CYS:HB2	1:B:505:LEU:HD11	1.83	0.61
1:A:590:ARG:NH2	1:A:594:GLU:OE1	2.34	0.58
1:B:785:THR:HG23	1:B:789:ALA:HB3	1.89	0.53
1:B:308:VAL:HG11	1:B:320:ILE:HG23	1.91	0.53
1:A:572:GLN:NE2	2:X:11:C:O4'	2.42	0.52
1:A:308:VAL:HG11	1:A:320:ILE:HG23	1.90	0.52
1:B:686:GLU:HG2	1:B:777:ILE:HB	1.94	0.50
1:A:686:GLU:HG2	1:A:777:ILE:HB	1.94	0.49
1:A:609:ILE:HG22	1:A:610:ARG:N	2.28	0.48
1:B:609:ILE:HG22	1:B:610:ARG:N	2.29	0.47
1:A:843:TYR:CE1	1:A:847:ILE:HG13	2.51	0.46
1:A:542:PHE:CE2	1:A:546:ILE:HD11	2.51	0.46
1:B:542:PHE:CE2	1:B:546:ILE:HD11	2.51	0.46
1:A:712:ILE:HD12	1:A:761:ILE:HD11	1.99	0.45
1:A:607:ASP:O	1:A:673:ASN:ND2	2.49	0.45
1:B:607:ASP:O	1:B:673:ASN:ND2	2.49	0.45
1:B:843:TYR:CE1	1:B:847:ILE:HG13	2.51	0.45
1:B:712:ILE:HD12	1:B:761:ILE:HD11	1.98	0.45
1:B:337:LYS:HB2	1:B:374:LEU:HD21	2.01	0.43
1:B:538:ARG:NH1	1:B:672:ASP:O	2.52	0.43
1:A:337:LYS:HB2	1:A:374:LEU:HD21	2.01	0.42
1:A:538:ARG:NH1	1:A:672:ASP:O	2.52	0.42
1:B:543:ARG:HD3	1:B:547:ILE:HD11	2.01	0.41
1:A:309:ALA:HB2	1:A:331:VAL:HG13	2.03	0.41
1:A:543:ARG:HD3	1:A:547:ILE:HD11	2.01	0.41
1:B:309:ALA:HB2	1:B:331:VAL:HG13	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:16:G:C2	3:Y:10:A:C2	3.10	0.40

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	627/701 (89%)	588 (94%)	37 (6%)	2 (0%)	41	60
1	B	633/701 (90%)	593 (94%)	37 (6%)	3 (0%)	29	47
All	All	1260/1402 (90%)	1181 (94%)	74 (6%)	5 (0%)	34	53

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	642	SER
1	A	900	MET
1	B	900	MET
1	A	765	VAL
1	B	765	VAL

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	577/630 (92%)	564 (98%)	13 (2%)	50	69
1	B	583/630 (92%)	567 (97%)	16 (3%)	44	65
All	All	1160/1260 (92%)	1131 (98%)	29 (2%)	47	67

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	443	GLU
1	A	447	ASN
1	A	485	VAL
1	A	510	ILE
1	A	531	THR
1	A	543	ARG
1	A	619	ASN
1	A	715	ASN
1	A	719	GLU
1	A	820	VAL
1	A	885	HIS
1	A	908	ASP
1	A	914	HIS
1	B	443	GLU
1	B	447	ASN
1	B	485	VAL
1	B	510	ILE
1	B	531	THR
1	B	543	ARG
1	B	619	ASN
1	B	715	ASN
1	B	719	GLU
1	B	753	ARG
1	B	820	VAL
1	B	885	HIS
1	B	899	ASN
1	B	908	ASP
1	B	914	HIS
1	B	990	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	416	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	X	23/25 (92%)	0	0
3	Y	23/24 (95%)	1 (4%)	0
All	All	46/49 (93%)	1 (2%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	Y	25	C

There are no RNA pucker outliers to report.

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, 4 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	$\#\|Z\| > 2$
6	ADP	B	1003	5	24,29,29	1.14	3 (12%)	29,45,45	1.36	4 (13%)
6	ADP	A	1003	5	24,29,29	1.15	3 (12%)	29,45,45	1.63	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
6	ADP	B	1003	5	-	2/12/32/32	0/3/3/3
6	ADP	A	1003	5	-	3/12/32/32	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1003	ADP	C5-C4	2.94	1.48	1.40
6	B	1003	ADP	C5-C4	2.77	1.48	1.40
6	B	1003	ADP	C2-N3	2.41	1.36	1.32
6	A	1003	ADP	C2-N3	2.40	1.36	1.32
6	A	1003	ADP	O4'-C1'	2.12	1.44	1.41
6	B	1003	ADP	O4'-C1'	2.02	1.43	1.41

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	1003	ADP	C3'-C2'-C1'	3.97	106.96	100.98
6	A	1003	ADP	N3-C2-N1	-3.70	122.89	128.68
6	B	1003	ADP	N3-C2-N1	-3.64	122.99	128.68
6	A	1003	ADP	PA-O3A-PB	-3.46	120.94	132.83
6	B	1003	ADP	C4-C5-N7	-2.99	106.29	109.40
6	B	1003	ADP	PA-O3A-PB	-2.63	123.81	132.83
6	A	1003	ADP	C4-C5-N7	-2.55	106.74	109.40
6	A	1003	ADP	C2-N1-C6	2.21	122.53	118.75
6	B	1003	ADP	O3B-PB-O2B	2.03	115.40	107.64

There are no chirality outliers.

All (5) torsion outliers are listed below:

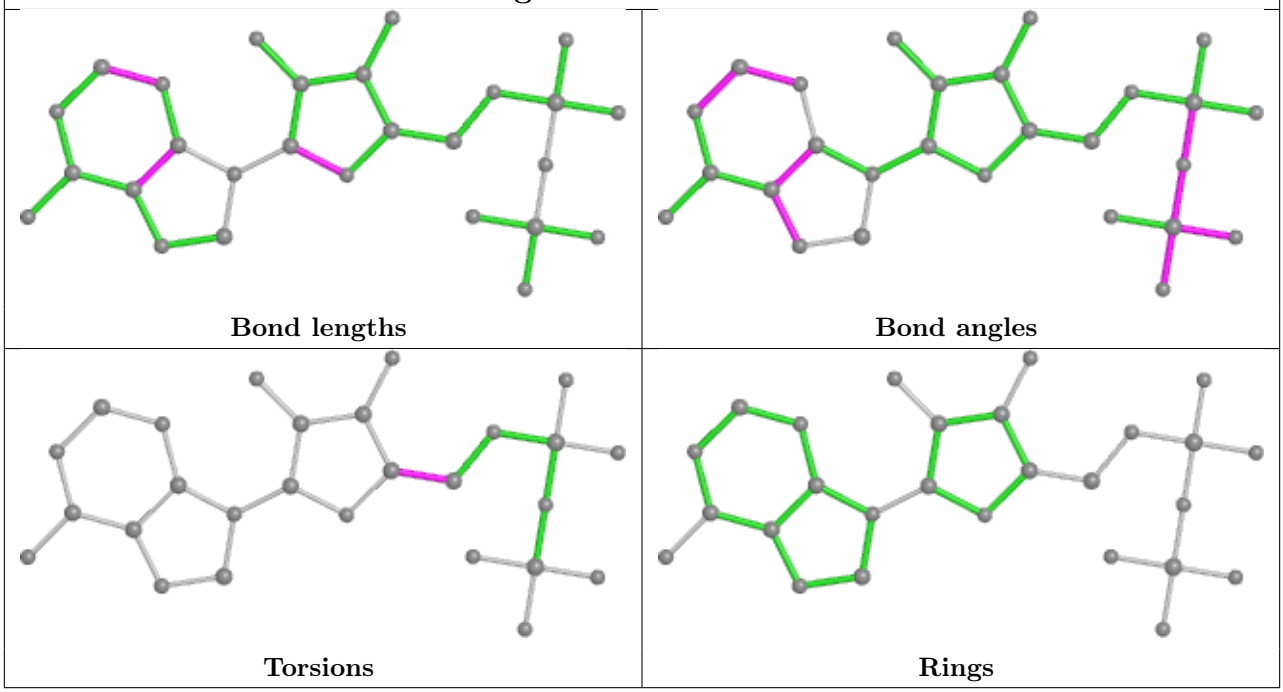
Mol	Chain	Res	Type	Atoms
6	A	1003	ADP	C5'-O5'-PA-O1A
6	B	1003	ADP	C3'-C4'-C5'-O5'
6	B	1003	ADP	O4'-C4'-C5'-O5'
6	A	1003	ADP	C5'-O5'-PA-O3A
6	A	1003	ADP	C5'-O5'-PA-O2A

There are no ring outliers.

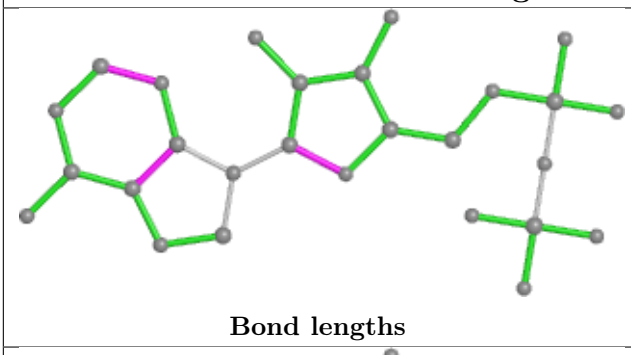
No monomer is involved in short contacts.

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.

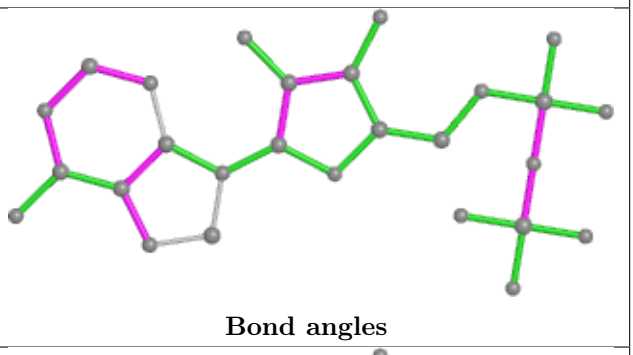
Ligand ADP B 1003



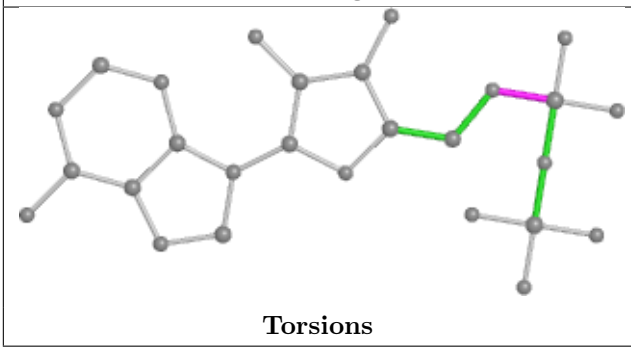
Ligand ADP A 1003



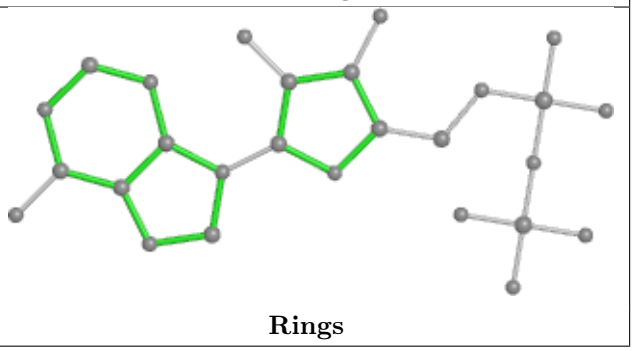
Bond lengths



Bond angles



Torsions



Rings

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

6.1 Protein, DNA and RNA chains

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, 95^{th} 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	641/701 (91%)	0.44	42 (6%) 18 21	36, 67, 113, 148	0
1	B	647/701 (92%)	0.38	24 (3%) 41 49	38, 65, 104, 147	0
2	X	24/25 (96%)	-0.32	0 100 100	40, 52, 77, 86	0
3	Y	24/24 (100%)	-0.22	0 100 100	41, 54, 73, 95	0
All	All	1336/1451 (92%)	0.39	66 (4%) 29 36	36, 66, 109, 148	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	934	ILE	5.8
1	A	957	LEU	5.0
1	A	879	PHE	5.0
1	A	954	LEU	4.9
1	A	894	ILE	4.5
1	A	901	HIS	4.5
1	B	867	ARG	4.3
1	A	895	GLN	4.3
1	A	945	ASN	4.1
1	A	960	ARG	4.1
1	A	985	ILE	4.0
1	A	986	PHE	3.9
1	B	957	LEU	3.7
1	B	947	MET	3.5
1	B	862	ALA	3.4
1	B	879	PHE	3.4
1	A	944	GLY	3.3
1	A	911	HIS	3.2
1	A	948	VAL	3.1
1	B	948	VAL	3.1
1	A	983	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	736	GLU	3.0
1	B	863	LYS	2.9
1	B	894	ILE	2.9
1	B	960	ARG	2.9
1	A	897	ILE	2.8
1	A	391	ILE	2.8
1	B	903	VAL	2.7
1	B	641	VAL	2.6
1	B	946	MET	2.6
1	A	458	ILE	2.6
1	B	953	ASP	2.6
1	A	909	PHE	2.6
1	B	934	ILE	2.6
1	A	956	CYS	2.5
1	A	422	GLU	2.4
1	B	984	ILE	2.4
1	A	913	TYR	2.4
1	A	889	CYS	2.4
1	B	536	ASP	2.4
1	A	808	ALA	2.4
1	A	984	ILE	2.4
1	A	539	ARG	2.3
1	B	415	LEU	2.3
1	A	952	LEU	2.3
1	B	954	LEU	2.3
1	A	905	VAL	2.3
1	A	720	GLU	2.2
1	A	977	LYS	2.2
1	A	943	TRP	2.2
1	B	736	GLU	2.2
1	A	916	ARG	2.2
1	A	729	ILE	2.2
1	B	729	ILE	2.2
1	B	691	GLU	2.2
1	B	952	LEU	2.2
1	A	935	ILE	2.1
1	A	959	ILE	2.1
1	A	778	VAL	2.1
1	A	865	ASP	2.1
1	A	902	HIS	2.1
1	A	953	ASP	2.1
1	B	935	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	717	LYS	2.0
1	B	859	GLN	2.0
1	A	389	LEU	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 monosaccharides in this entry.

6.4 Ligands (i)

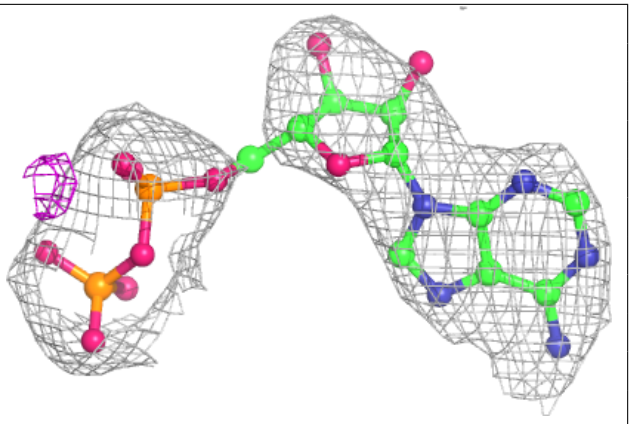
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

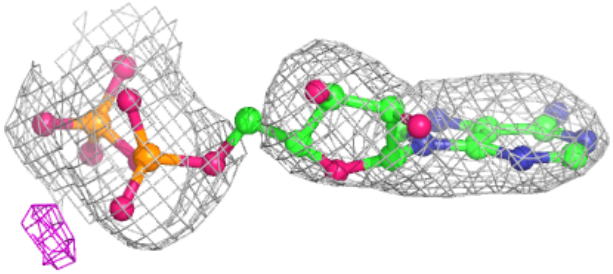
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	ADP	A	1003	27/27	0.91	0.18	68,75,82,82	0
6	ADP	B	1003	27/27	0.91	0.14	71,74,79,82	0
5	MG	B	1002	1/1	0.96	0.07	33,33,33,33	0
4	ZN	B	1001	1/1	0.96	0.10	62,62,62,62	0
5	MG	A	1002	1/1	0.96	0.17	36,36,36,36	0
4	ZN	A	1001	1/1	0.98	0.12	67,67,67,67	0

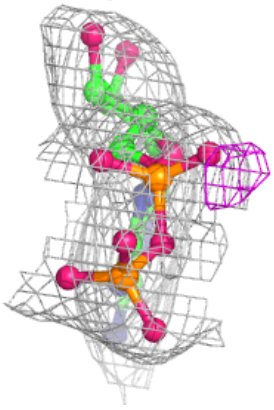
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP A 1003:

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

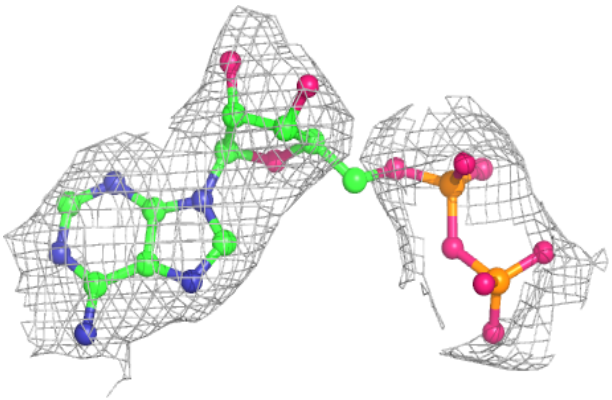


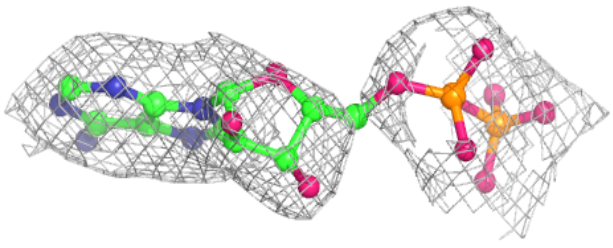


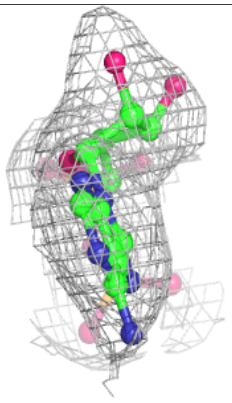


Electron density around ADP B 1003:

$2mF_o$-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.