



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:00 PM UTC

PDB ID : 5JC3 / pdb_00005jc3
Title : Crystal structure of chicken MDA5 with 5'p 10-mer dsRNA and ADP-Mg2+
at 2.6 Å resolution (monoclinic form, twinned).
Authors : Cusack, S.; Uchikawa, E.
Deposited on : 2016-04-14
Resolution : 2.60 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	:	4-5-2 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

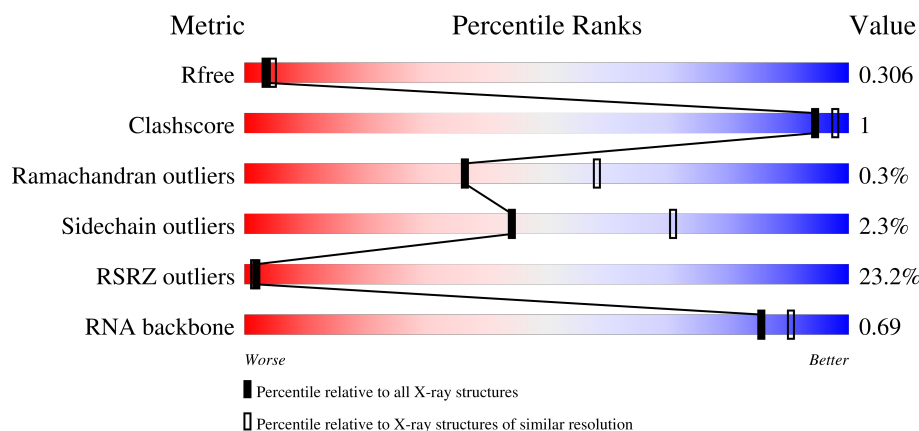
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)
RNA backbone	3983	1014 (2.84-2.36)

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	701	24% 91% 5%
1	B	701	21% 90% 6%
2	C	10	90% 10%
2	D	10	70% 30%

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Mol	Chain	Length	Quality of chain
2	X	10	 90%10%
2	Y	10	 90%10%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11759 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	668	Total	C	N	O	S	0	0	0
			5450	3437	973	1008	32			
1	B	661	Total	C	N	O	S	0	0	0
			5397	3403	964	998	32			

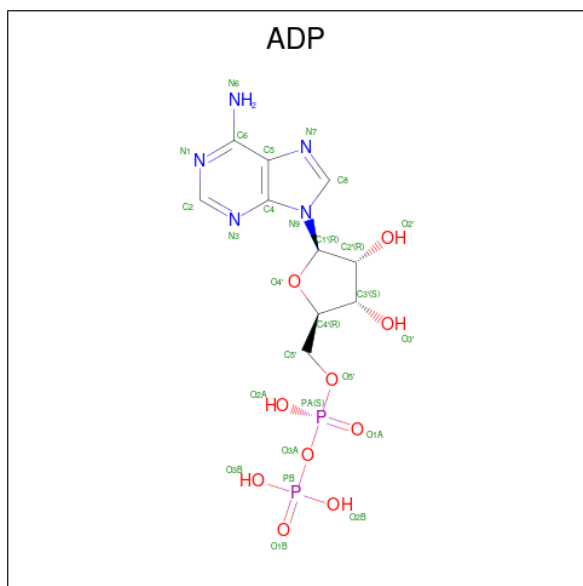
There are 10 discrepancies between the modelled and reference sequences:

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	conflict	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	conflict	UNP D9N195

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	X	10	Total	C	N	O	P	0	0	0
			214	95	38	71	10			
2	Y	10	Total	C	N	O	P	0	0	0
			213	95	38	70	10			
2	C	10	Total	C	N	O	P	0	0	0
			214	95	38	71	10			
2	D	10	Total	C	N	O	P	0	0	0
			213	95	38	70	10			

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

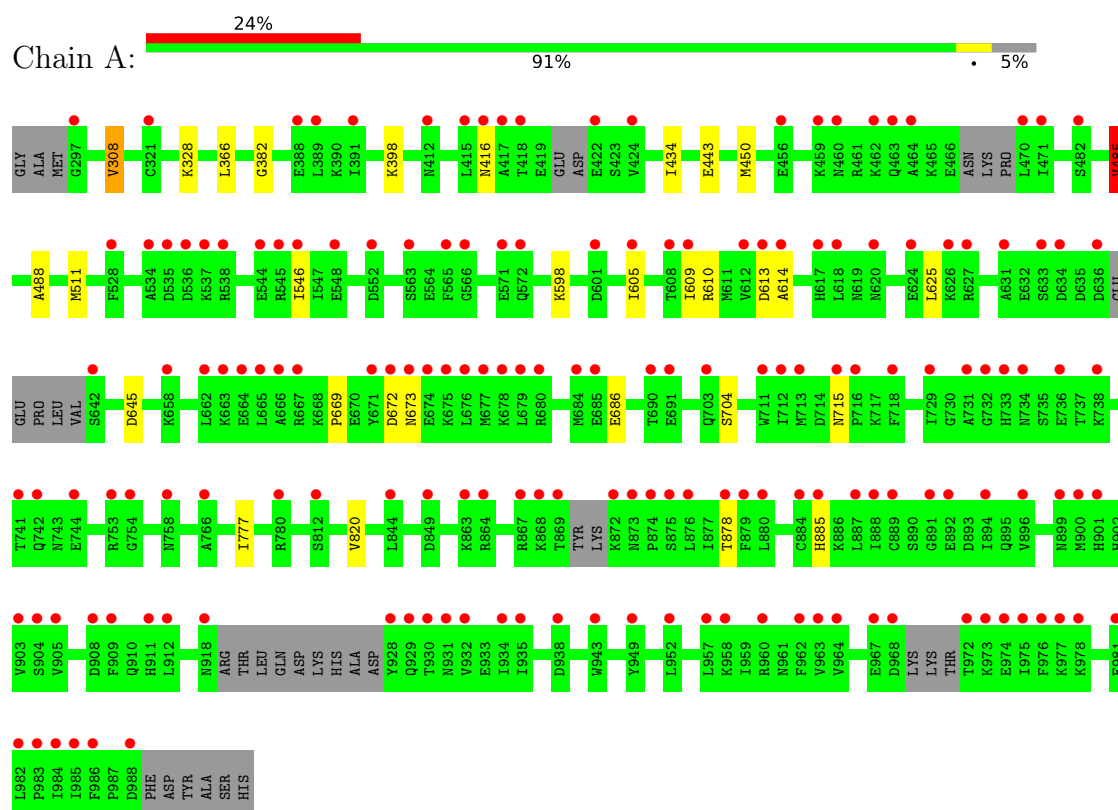
- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

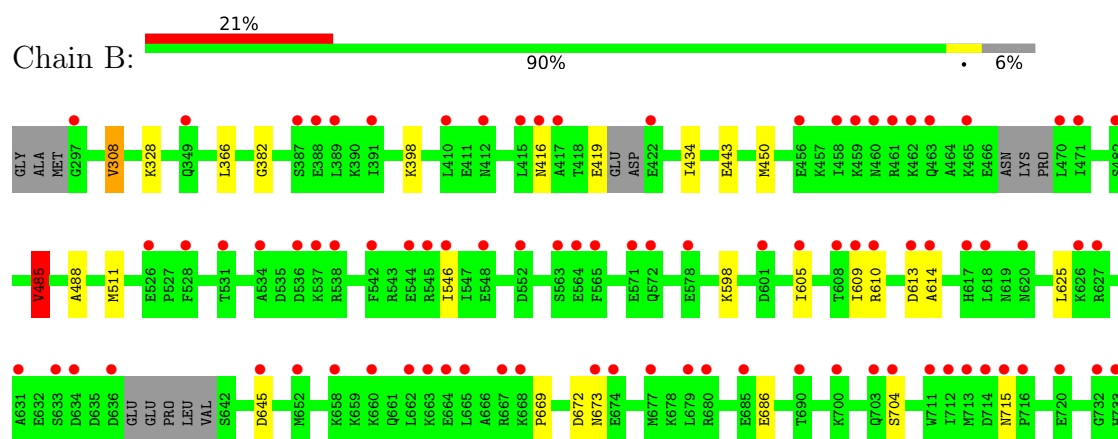
3 Residue-property plots

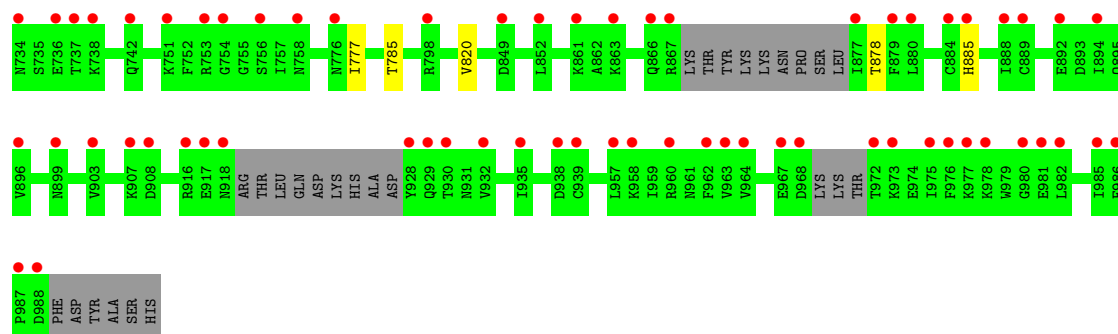
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Melanoma differentiation associated protein-5



- Molecule 1: Melanoma differentiation associated protein-5





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

Chain X:



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

Chain Y:



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

Chain C:



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

Chain D:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	70.16Å 138.70Å 100.43Å 90.00° 109.47° 90.00°	Depositor
Resolution (Å)	50.00 – 2.60 50.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.4 (50.00-2.60) 99.4 (50.00-2.60)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0131	Depositor
R, R_{free}	0.271 , 0.290 0.284 , 0.306	Depositor DCC
R_{free} test set	2811 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	47.1	Xtriage
Anisotropy	0.572	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 19.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	11759	wwPDB-VP
Average B, all atoms (Å ²)	58.0	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 41.20 % 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 2.4451e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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, ZN, 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	0.55	0/5537	0.80	1/7427 (0.0%)
1	B	0.55	1/5483 (0.0%)	0.80	1/7355 (0.0%)
2	C	0.38	0/238	0.69	0/367
2	D	0.35	0/237	0.73	0/367
2	X	0.37	0/238	0.71	0/367
2	Y	0.35	0/237	0.71	0/367
All	All	0.53	1/11970 (0.0%)	0.79	2/16250 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	785	THR	CA-C	5.16	1.55	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	485	VAL	CB-CA-C	5.03	116.05	110.62
1	B	485	VAL	CB-CA-C	5.01	116.03	110.62

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	5450	0	5531	13	0
1	B	5397	0	5470	13	0
2	C	214	0	109	1	0
2	D	213	0	109	2	0
2	X	214	0	109	1	0
2	Y	213	0	109	1	0
3	A	27	0	12	0	0
3	B	27	0	12	0	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
All	All	11759	0	11461	29	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 (29) 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:686:GLU:HG2	1:A:777:ILE:HB	1.86	0.57
1:B:686:GLU:HG2	1:B:777:ILE:HB	1.85	0.57
1:B:434:ILE:HD11	1:B:450:MET:HE3	1.93	0.51
1:B:605:ILE:HD11	1:B:614:ALA:HA	1.93	0.51
1:A:605:ILE:HD11	1:A:614:ALA:HA	1.93	0.50
1:A:434:ILE:HD11	1:A:450:MET:HE3	1.93	0.49
1:B:605:ILE:HD11	1:B:614:ALA:N	2.30	0.47
1:A:609:ILE:CD1	1:A:704:SER:HA	2.45	0.47
1:B:609:ILE:CD1	1:B:704:SER:HA	2.45	0.46
1:A:609:ILE:HD12	1:A:704:SER:HA	1.97	0.46
1:B:609:ILE:HD12	1:B:704:SER:HA	1.97	0.46
1:A:605:ILE:HD11	1:A:614:ALA:N	2.30	0.46
1:B:669:PRO:HA	1:B:672:ASP:HB2	1.96	0.46
1:A:609:ILE:HG22	1:A:610:ARG:N	2.31	0.46
1:A:669:PRO:HA	1:A:672:ASP:HB2	1.96	0.46
1:B:609:ILE:HG22	1:B:610:ARG:N	2.31	0.45
2:D:8:A:H2'	2:D:9:C:C6	2.52	0.45
1:B:485:VAL:HG13	1:B:488:ALA:HB3	2.00	0.44
1:B:308:VAL:HG12	1:B:511:MET:HB3	2.00	0.44
1:A:485:VAL:HG13	1:A:488:ALA:HB3	2.00	0.44
1:B:605:ILE:HD11	1:B:613:ASP:C	2.43	0.43
1:A:308:VAL:HG12	1:A:511:MET:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:605:ILE:HD11	1:A:613:ASP:C	2.43	0.43
2:C:8:A:C2	2:D:4:A:C2	3.07	0.42
1:A:366:LEU:HD11	1:A:382:GLY:HA3	2.01	0.42
1:B:366:LEU:HD11	1:B:382:GLY:HA3	2.00	0.42
1:A:605:ILE:HD11	1:A:614:ALA:CA	2.49	0.42
1:B:605:ILE:HD11	1:B:614:ALA:CA	2.49	0.41
2:X:4:A:C2	2:Y:8:A:C2	3.09	0.41

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	654/701 (93%)	629 (96%)	23 (4%)	2 (0%)	36 58
1	B	647/701 (92%)	623 (96%)	22 (3%)	2 (0%)	36 58
All	All	1301/1402 (93%)	1252 (96%)	45 (4%)	4 (0%)	36 58

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	416	ASN
1	A	673	ASN
1	B	416	ASN
1	B	673	ASN

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	600/630 (95%)	587 (98%)	13 (2%)	45	72
1	B	594/630 (94%)	580 (98%)	14 (2%)	43	70
All	All	1194/1260 (95%)	1167 (98%)	27 (2%)	44	71

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	308	VAL
1	A	328	LYS
1	A	398	LYS
1	A	443	GLU
1	A	485	VAL
1	A	546	ILE
1	A	598	LYS
1	A	625	LEU
1	A	645	ASP
1	A	715	ASN
1	A	820	VAL
1	A	878	THR
1	A	885	HIS
1	B	308	VAL
1	B	328	LYS
1	B	398	LYS
1	B	419	GLU
1	B	443	GLU
1	B	485	VAL
1	B	546	ILE
1	B	598	LYS
1	B	625	LEU
1	B	645	ASP
1	B	715	ASN
1	B	820	VAL
1	B	878	THR
1	B	885	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	448	ASN

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Mol	Chain	Res	Type
1	A	491	ASN
1	A	497	HIS
1	A	522	ASN
1	A	551	GLN
1	A	554	GLN
1	A	558	GLN
1	A	945	ASN
1	B	491	ASN
1	B	497	HIS
1	B	522	ASN
1	B	551	GLN
1	B	554	GLN
1	B	558	GLN
1	B	945	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	C	9/10 (90%)	0	0
2	D	9/10 (90%)	0	0
2	X	9/10 (90%)	0	0
2	Y	9/10 (90%)	0	0
All	All	36/40 (90%)	0	0

There are no RNA backbone outliers to report.

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 oligosaccharides 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
3	ADP	A	1001	4	28,29,29	1.58	5 (17%)	43,45,45	1.87	12 (27%)
3	ADP	B	1001	4	28,29,29	1.53	5 (17%)	43,45,45	1.95	12 (27%)

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
3	ADP	A	1001	4	-	2/16/32/32	0/3/3/3
3	ADP	B	1001	4	-	2/16/32/32	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1001	ADP	C5-C4	5.07	1.48	1.39
3	B	1001	ADP	C5-C4	4.97	1.47	1.39
3	A	1001	ADP	C5-C6	2.97	1.49	1.41
3	B	1001	ADP	C5-C6	2.91	1.49	1.41
3	A	1001	ADP	PA-O3A	2.87	1.62	1.59
3	B	1001	ADP	PA-O3A	2.47	1.62	1.59
3	A	1001	ADP	C8-N7	2.39	1.36	1.31
3	B	1001	ADP	C8-N7	2.33	1.36	1.31
3	A	1001	ADP	C5-N7	-2.33	1.34	1.39
3	B	1001	ADP	C5-N7	-2.31	1.34	1.39

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1001	ADP	C5-C4-N3	-5.85	118.66	126.72
3	A	1001	ADP	C5-C4-N3	-5.73	118.83	126.72
3	B	1001	ADP	N3-C4-N9	4.68	135.12	127.17
3	A	1001	ADP	N3-C4-N9	4.57	134.94	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1001	ADP	C2-N3-C4	3.93	121.43	111.83
3	A	1001	ADP	C2-N3-C4	3.86	121.26	111.83
3	B	1001	ADP	N3-C2-N1	-3.82	122.80	128.58
3	A	1001	ADP	N3-C2-N1	-3.77	122.88	128.58
3	B	1001	ADP	C4-C5-N7	-3.69	106.36	110.58
3	A	1001	ADP	C4-C5-N7	-3.57	106.50	110.58
3	B	1001	ADP	C4-N9-C8	2.79	108.67	105.74
3	A	1001	ADP	C4-N9-C8	2.69	108.56	105.74
3	A	1001	ADP	C5-N7-C8	2.66	107.63	103.45
3	B	1001	ADP	C5-N7-C8	2.63	107.59	103.45
3	B	1001	ADP	C3'-C2'-C1'	2.57	106.32	101.46
3	B	1001	ADP	C6-C5-N7	2.30	136.52	132.09
3	B	1001	ADP	O4'-C1'-N9	2.29	112.48	108.09
3	A	1001	ADP	C6-C5-N7	2.27	136.47	132.09
3	A	1001	ADP	C3'-C2'-C1'	2.25	105.72	101.46
3	A	1001	ADP	C2-N1-C6	2.14	122.24	118.73
3	B	1001	ADP	C2'-C1'-N9	-2.13	108.02	113.30
3	B	1001	ADP	C2-N1-C6	2.13	122.22	118.73
3	A	1001	ADP	O4'-C1'-N9	2.01	111.95	108.09
3	A	1001	ADP	N9-C8-N7	-2.01	111.08	113.94

There are no chirality outliers.

All (4) torsion outliers are listed below:

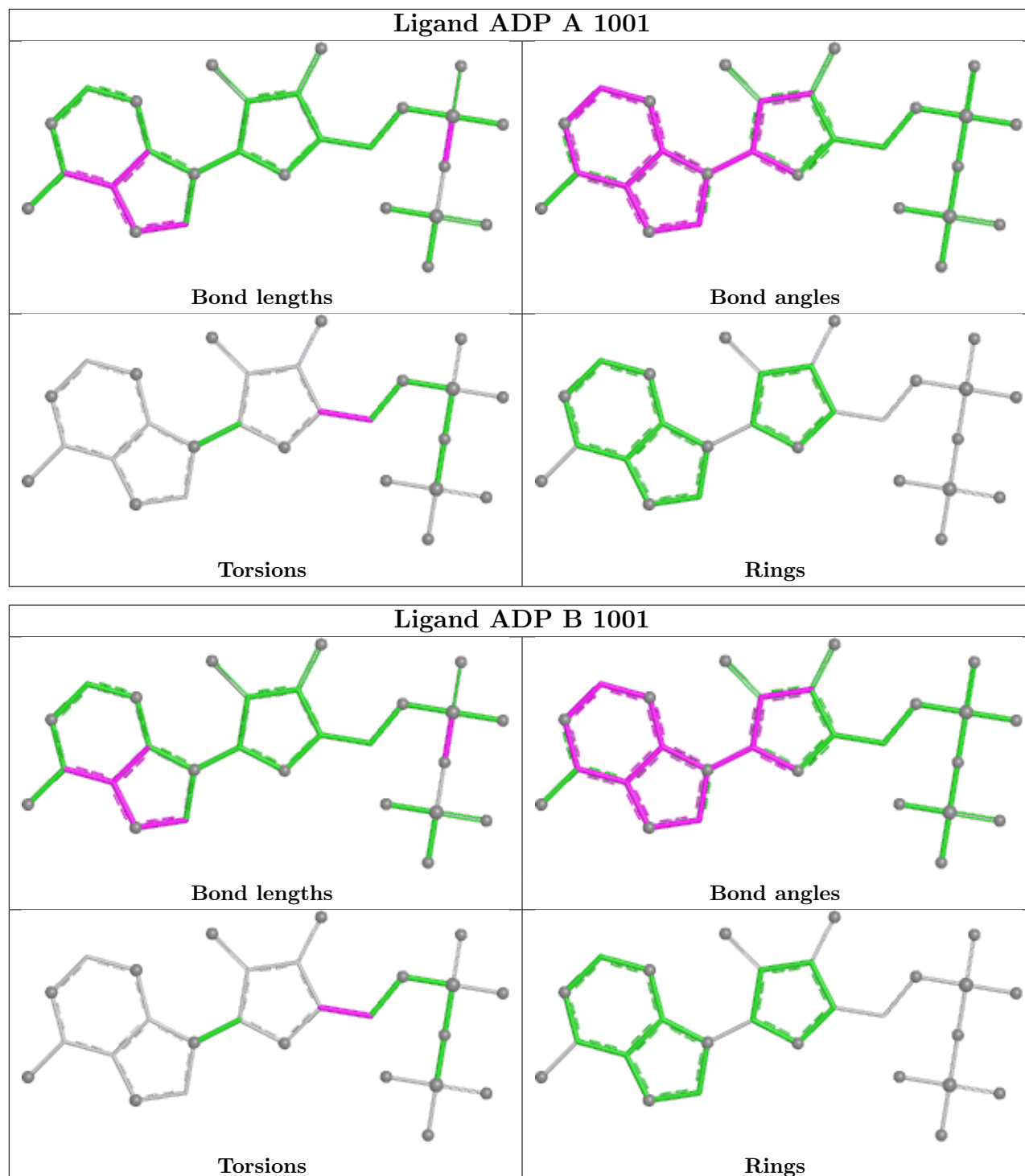
Mol	Chain	Res	Type	Atoms
3	A	1001	ADP	C3'-C4'-C5'-O5'
3	B	1001	ADP	O4'-C4'-C5'-O5'
3	A	1001	ADP	O4'-C4'-C5'-O5'
3	B	1001	ADP	C3'-C4'-C5'-O5'

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 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 ⓘ

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, 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	668/701 (95%)	1.26	167 (25%) 2 1	32, 54, 98, 114	0
1	B	661/701 (94%)	1.23	150 (22%) 2 1	34, 53, 98, 110	0
2	C	10/10 (100%)	0.30	0 100 100	36, 42, 57, 61	0
2	D	10/10 (100%)	0.46	0 100 100	35, 38, 57, 73	0
2	X	10/10 (100%)	0.26	0 100 100	35, 40, 56, 58	0
2	Y	10/10 (100%)	0.31	0 100 100	35, 37, 55, 68	0
All	All	1369/1442 (94%)	1.22	317 (23%) 2 1	32, 53, 98, 114	0

All (317) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	536	ASP	6.4
1	B	677	MET	6.1
1	A	536	ASP	5.7
1	A	605	ILE	5.3
1	A	297	GLY	5.3
1	A	888	ILE	5.3
1	A	869	THR	5.2
1	B	297	GLY	4.9
1	A	928	TYR	4.8
1	A	985	ILE	4.7
1	B	928	TYR	4.7
1	B	885	HIS	4.6
1	A	872	LYS	4.6
1	B	972	THR	4.4
1	B	977	LYS	4.4
1	B	463	GLN	4.3
1	A	470	LEU	4.3
1	B	471	ILE	4.3
1	B	674	GLU	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	867	ARG	4.2
1	B	417	ALA	4.1
1	B	391	ILE	4.1
1	B	470	LEU	4.1
1	B	605	ILE	4.1
1	A	463	GLN	4.0
1	A	534	ALA	4.0
1	A	482	SER	3.9
1	B	888	ILE	3.9
1	A	973	LYS	3.9
1	A	601	ASP	3.9
1	A	674	GLU	3.9
1	A	412	ASN	3.9
1	A	417	ALA	3.9
1	B	734	ASN	3.8
1	A	885	HIS	3.8
1	A	899	ASN	3.8
1	A	391	ILE	3.8
1	B	935	ILE	3.8
1	A	673	ASN	3.7
1	A	677	MET	3.7
1	B	733	HIS	3.6
1	B	462	LYS	3.6
1	B	534	ALA	3.6
1	A	642	SER	3.6
1	B	563	SER	3.6
1	A	459	LYS	3.6
1	B	986	PHE	3.6
1	B	456	GLU	3.6
1	B	667	ARG	3.6
1	A	734	ASN	3.5
1	B	918	ASN	3.4
1	A	608	THR	3.4
1	A	983	PRO	3.4
1	A	733	HIS	3.4
1	A	876	LEU	3.3
1	A	880	LEU	3.3
1	B	601	ASP	3.3
1	A	967	GLU	3.3
1	B	982	LEU	3.2
1	A	535	ASP	3.2
1	B	459	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	972	THR	3.2
1	A	894	ILE	3.2
1	A	905	VAL	3.2
1	A	986	PHE	3.2
1	B	962	PHE	3.2
1	B	973	LYS	3.2
1	A	911	HIS	3.2
1	A	667	ARG	3.1
1	A	321	CYS	3.1
1	B	879	PHE	3.1
1	A	538	ARG	3.1
1	B	460	ASN	3.1
1	B	664	GLU	3.1
1	B	884	CYS	3.1
1	A	680	ARG	3.1
1	B	908	ASP	3.1
1	A	964	VAL	3.1
1	A	736	GLU	3.0
1	A	634	ASP	3.0
1	A	929	GLN	3.0
1	A	863	LYS	3.0
1	B	387	SER	3.0
1	A	691	GLU	3.0
1	A	874	PRO	3.0
1	B	626	LYS	3.0
1	A	984	ILE	3.0
1	B	620	ASN	3.0
1	B	880	LEU	2.9
1	A	958	LYS	2.9
1	A	703	GLN	2.9
1	A	613	ASP	2.9
1	A	631	ALA	2.9
1	A	962	PHE	2.9
1	A	388	GLU	2.9
1	A	671	TYR	2.9
1	B	690	THR	2.9
1	A	571	GLU	2.9
1	B	716	PRO	2.9
1	A	934	ILE	2.9
1	A	889	CYS	2.9
1	B	988	ASP	2.9
1	A	887	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	879	PHE	2.9
1	A	713	MET	2.8
1	A	875	SER	2.8
1	A	868	LYS	2.8
1	A	471	ILE	2.8
1	A	729	ILE	2.8
1	A	738	LYS	2.8
1	A	662	LEU	2.8
1	A	930	THR	2.8
1	A	544	GLU	2.8
1	A	609	ILE	2.8
1	B	975	ILE	2.8
1	A	679	LEU	2.8
1	B	613	ASP	2.8
1	A	685	GLU	2.8
1	A	462	LYS	2.7
1	A	935	ILE	2.7
1	A	664	GLU	2.7
1	A	988	ASP	2.7
1	B	552	ASP	2.7
1	B	634	ASP	2.7
1	B	929	GLN	2.7
1	A	456	GLU	2.7
1	A	552	ASP	2.7
1	A	864	ARG	2.7
1	B	422	GLU	2.7
1	B	680	ARG	2.7
1	A	732	GLY	2.7
1	B	548	GLU	2.7
1	B	618	LEU	2.7
1	A	627	ARG	2.7
1	A	903	VAL	2.7
1	B	738	LYS	2.7
1	B	636	ASP	2.7
1	A	572	GLN	2.6
1	A	949	TYR	2.6
1	B	546	ILE	2.6
1	B	679	LEU	2.6
1	B	685	GLU	2.6
1	B	758	ASN	2.6
1	A	741	THR	2.6
1	A	938	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	618	LEU	2.6
1	A	982	LEU	2.6
1	A	891	GLY	2.6
1	B	899	ASN	2.6
1	B	964	VAL	2.6
1	B	608	THR	2.6
1	A	742	GLN	2.6
1	B	703	GLN	2.6
1	A	712	ILE	2.6
1	B	461	ARG	2.6
1	B	939	CYS	2.6
1	B	987	PRO	2.6
1	B	617	HIS	2.6
1	A	892	GLU	2.6
1	B	544	GLU	2.6
1	A	424	VAL	2.6
1	A	563	SER	2.5
1	A	878	THR	2.5
1	A	636	ASP	2.5
1	B	713	MET	2.5
1	A	626	LYS	2.5
1	A	977	LYS	2.5
1	B	963	VAL	2.5
1	B	930	THR	2.5
1	A	665	LEU	2.5
1	B	465	LYS	2.5
1	A	566	GLY	2.5
1	B	903	VAL	2.5
1	B	412	ASN	2.5
1	B	700	LYS	2.5
1	B	968	ASP	2.5
1	A	901	HIS	2.5
1	B	736	GLU	2.5
1	A	711	TRP	2.5
1	B	415	LEU	2.5
1	A	900	MET	2.5
1	A	614	ALA	2.5
1	B	565	PHE	2.5
1	B	660	LYS	2.4
1	B	545	ARG	2.4
1	B	633	SER	2.4
1	A	675	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	666	ALA	2.4
1	B	528	PHE	2.4
1	A	389	LEU	2.4
1	A	460	ASN	2.4
1	A	715	ASN	2.4
1	B	416	ASN	2.4
1	A	849	ASP	2.4
1	A	678	LYS	2.4
1	B	863	LYS	2.4
1	A	676	LEU	2.4
1	A	912	LEU	2.4
1	B	877	ILE	2.4
1	A	918	ASN	2.4
1	A	931	ASN	2.4
1	B	673	ASN	2.4
1	B	776	ASN	2.4
1	A	943	TRP	2.4
1	A	974	GLU	2.4
1	A	896	VAL	2.4
1	A	565	PHE	2.4
1	A	867	ARG	2.4
1	B	960	ARG	2.4
1	B	410	LEU	2.4
1	B	665	LEU	2.4
1	B	985	ILE	2.4
1	B	756	SER	2.4
1	B	981	GLU	2.4
1	B	645	ASP	2.4
1	A	658	LYS	2.4
1	B	668	LYS	2.4
1	A	976	PHE	2.4
1	A	633	SER	2.3
1	A	684	MET	2.3
1	A	968	ASP	2.3
1	B	663	LYS	2.3
1	A	546	ILE	2.3
1	B	737	THR	2.3
1	B	715	ASN	2.3
1	A	422	GLU	2.3
1	B	388	GLU	2.3
1	A	908	ASP	2.3
1	B	889	CYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	896	VAL	2.3
1	B	627	ARG	2.3
1	B	572	GLN	2.3
1	A	718	PHE	2.3
1	A	909	PHE	2.3
1	B	542	PHE	2.3
1	B	712	ILE	2.3
1	A	672	ASP	2.3
1	A	963	VAL	2.3
1	B	662	LEU	2.3
1	B	957	LEU	2.3
1	B	958	LYS	2.2
1	B	967	GLU	2.2
1	A	812	SER	2.2
1	B	482	SER	2.2
1	B	980	GLY	2.2
1	A	932	VAL	2.2
1	A	617	HIS	2.2
1	B	526	GLU	2.2
1	A	716	PRO	2.2
1	B	537	LYS	2.2
1	B	711	TRP	2.2
1	A	548	GLU	2.2
1	A	744	GLU	2.2
1	A	884	CYS	2.2
1	A	620	ASN	2.2
1	B	742	GLN	2.2
1	B	978	LYS	2.2
1	A	528	PHE	2.2
1	B	720	GLU	2.2
1	A	978	LYS	2.2
1	B	658	LYS	2.2
1	B	976	PHE	2.2
1	A	731	ALA	2.1
1	A	766	ALA	2.1
1	B	571	GLU	2.1
1	B	610	ARG	2.1
1	B	916	ARG	2.1
1	B	866	GLN	2.1
1	A	415	LEU	2.1
1	A	957	LEU	2.1
1	A	754	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	612	VAL	2.1
1	B	564	GLU	2.1
1	B	798	ARG	2.1
1	B	751	LYS	2.1
1	A	873	ASN	2.1
1	B	852	LEU	2.1
1	B	609	ILE	2.1
1	B	849	ASP	2.1
1	B	704	SER	2.1
1	B	614	ALA	2.1
1	A	624	GLU	2.1
1	B	578	GLU	2.1
1	B	538	ARG	2.1
1	A	418	THR	2.1
1	A	904	SER	2.1
1	A	960	ARG	2.1
1	A	537	LYS	2.1
1	A	844	LEU	2.1
1	A	416	ASN	2.1
1	A	545	ARG	2.0
1	A	780	ARG	2.0
1	A	981	GLU	2.0
1	B	753	ARG	2.0
1	B	631	ALA	2.0
1	B	892	GLU	2.0
1	B	917	GLU	2.0
1	B	861	LYS	2.0
1	B	531	THR	2.0
1	B	349	GLN	2.0
1	B	389	LEU	2.0
1	A	758	ASN	2.0
1	A	975	ILE	2.0
1	B	458	ILE	2.0
1	B	754	GLY	2.0
1	B	894	ILE	2.0
1	A	464	ALA	2.0
1	B	714	ASP	2.0
1	B	938	ASP	2.0
1	A	663	LYS	2.0
1	B	907	LYS	2.0
1	A	690	THR	2.0
1	B	652	MET	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	952	LEU	2.0
1	B	732	GLY	2.0
1	A	753	ARG	2.0
1	B	932	VAL	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](#)

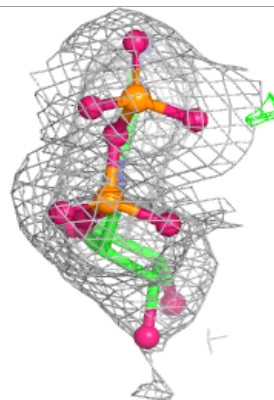
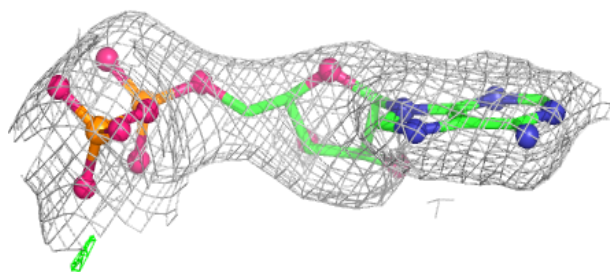
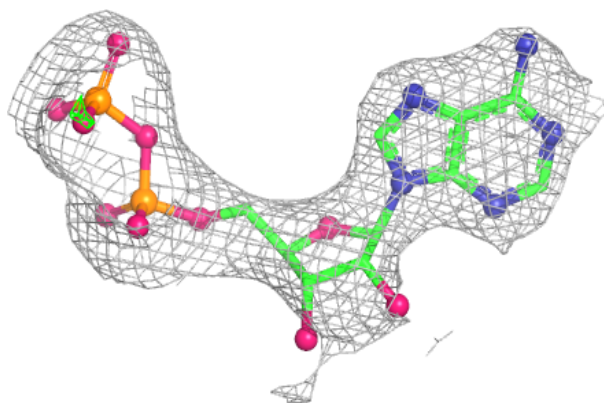
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	ADP	A	1001	27/27	0.90	0.10	55,60,66,69	0
3	ADP	B	1001	27/27	0.92	0.09	53,56,63,63	0
4	MG	B	1002	1/1	0.93	0.17	37,37,37,37	0
4	MG	A	1002	1/1	0.95	0.14	36,36,36,36	0
5	ZN	A	1003	1/1	0.98	0.04	54,54,54,54	0
5	ZN	B	1003	1/1	0.99	0.03	56,56,56,56	0

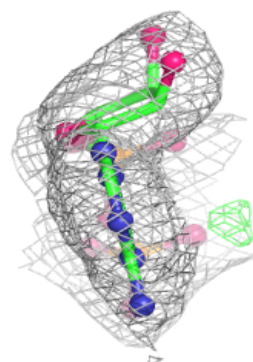
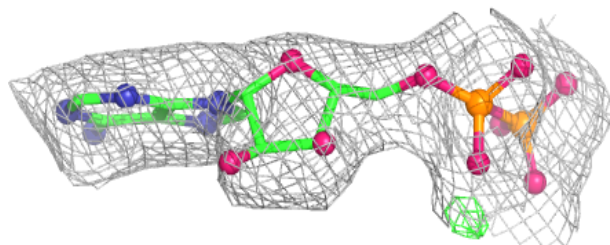
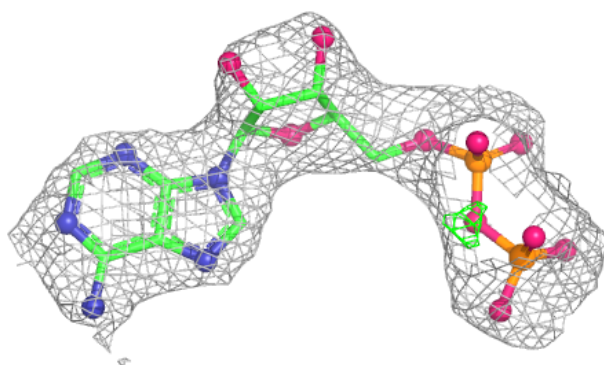
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP A 1001:

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

**Electron density around ADP B 1001:**

$2mF_o-DF_c$ (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.