



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 13, 2024 – 07:08 AM EST

PDB ID : 4KH5
Title : Toxoplasma gondii NTPDase1 C258S/C268S in complex with Mg and AMPNP
Authors : Krug, U.; Totzauer, R.; Strater, N.
Deposited on : 2013-04-30
Resolution : 3.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 1.20.1
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.003 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

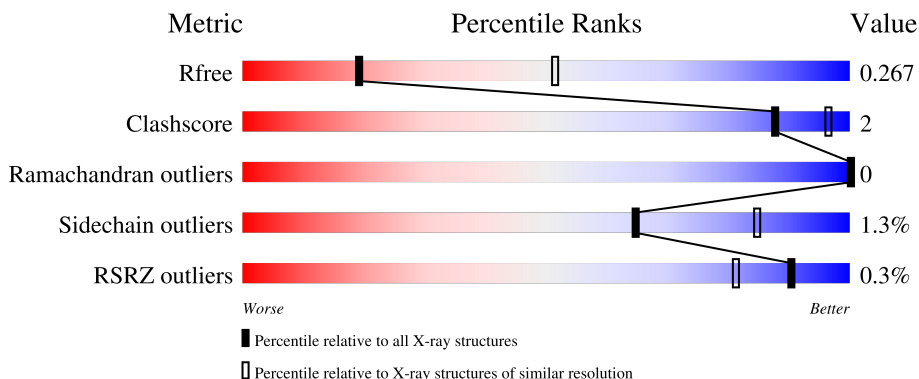
1 Overall quality at a glance

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}	164625	2511 (3.00-3.00)
Clashscore	180529	2866 (3.00-3.00)
Ramachandran outliers	177936	2778 (3.00-3.00)
Sidechain outliers	177891	2781 (3.00-3.00)
RSRZ outliers	164620	2523 (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	612	 90% 7% •
1	B	612	 91% 6% •

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
2	AU1	A	700	-	X	-	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9294 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.

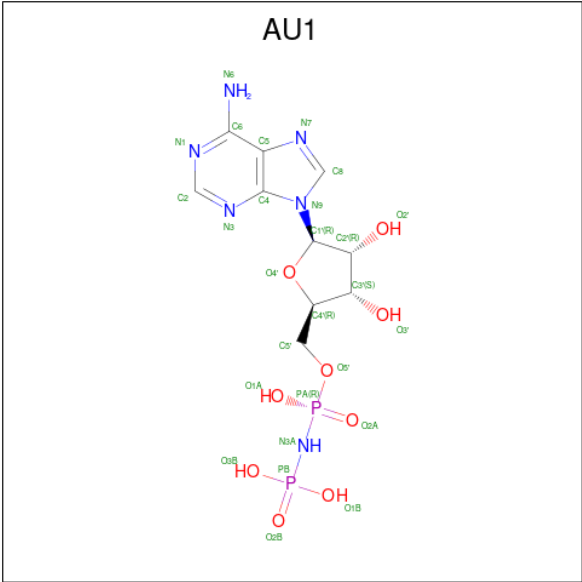
- Molecule 1 is a protein called Nucleoside-triphosphatase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	591	Total	C	N	O	S	0	0	0
			4612	2897	809	881	25			
1	B	591	Total	C	N	O	S	0	0	0
			4617	2901	813	878	25			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	25	MET	-	initiating methionine	UNP Q27895
A	258	SER	CYS	engineered mutation	UNP Q27895
A	268	SER	CYS	engineered mutation	UNP Q27895
A	629	GLU	-	expression tag	UNP Q27895
A	630	GLU	-	expression tag	UNP Q27895
A	631	HIS	-	expression tag	UNP Q27895
A	632	HIS	-	expression tag	UNP Q27895
A	633	HIS	-	expression tag	UNP Q27895
A	634	HIS	-	expression tag	UNP Q27895
A	635	HIS	-	expression tag	UNP Q27895
A	636	HIS	-	expression tag	UNP Q27895
B	25	MET	-	initiating methionine	UNP Q27895
B	258	SER	CYS	engineered mutation	UNP Q27895
B	268	SER	CYS	engineered mutation	UNP Q27895
B	629	GLU	-	expression tag	UNP Q27895
B	630	GLU	-	expression tag	UNP Q27895
B	631	HIS	-	expression tag	UNP Q27895
B	632	HIS	-	expression tag	UNP Q27895
B	633	HIS	-	expression tag	UNP Q27895
B	634	HIS	-	expression tag	UNP Q27895
B	635	HIS	-	expression tag	UNP Q27895
B	636	HIS	-	expression tag	UNP Q27895

- Molecule 2 is 5'-O-[(R)-hydroxy(phosphonoamino)phosphoryl]adenosine (three-letter code: AU1) (formula: C₁₀H₁₆N₆O₉P₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	N	O	P	0	0
			9	1	6	2		
2	B	1	Total	C	N	O	P	27
			54	20	12	18	4	

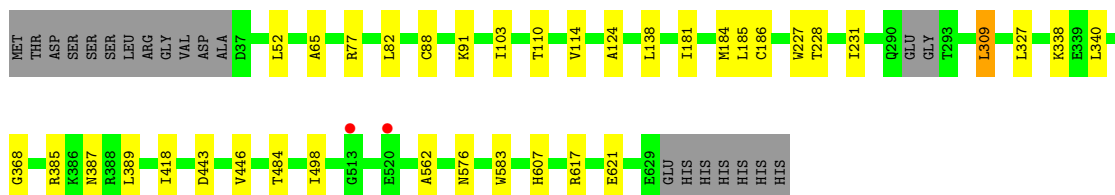
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 1: Nucleoside-triphosphatase 2

A367	G368	V369	R366	K367	R368	L418	V446	V454	V474	L498	D535	L541	PRO	ASN	ALA	ARG	G546	A562	W583	L595	L606	V609	R617	E621	E629	GLU	HIS	HIS	HIS	HIS	HIS	HIS			
Met	THR	ASP	SER	SER	LEU	ARG	GLY	VAL	D35	S73	R77	L82	C88	K91	I103	T110	V114	A124	L138	M184	L185	V191	Y198	R199	W227	T228	G252	R257	T293	L309	F324	L327	A330	K338	S365

Chain B: 91% 6% .



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	73.54Å 150.25Å 240.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.93 – 3.00 38.93 – 3.00	Depositor EDS
% Data completeness (in resolution range)	92.5 (38.93-3.00) 92.4 (38.93-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.14 (at 3.01Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.208 , 0.243 0.227 , 0.267	Depositor DCC
R_{free} test set	524 reflections (2.08%)	wwPDB-VP
Wilson B-factor (Å ²)	37.4	Xtriage
Anisotropy	0.616	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 30.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	9294	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.10% 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, AU1

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	0.37	0/4702	0.58	0/6364
1	B	0.37	0/4708	0.57	0/6373
All	All	0.37	0/9410	0.58	0/12737

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 [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	4612	0	4556	19	0
1	B	4617	0	4569	16	0
2	A	9	0	3	1	0
2	B	54	0	32	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
All	All	9294	0	9160	35	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 2.

The worst 5 of 35 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:B:82:LEU:HG	1:B:103:ILE:HD11	1.56	0.85
1:A:82:LEU:HG	1:A:103:ILE:HD11	1.56	0.85
1:A:252:GLY:HA3	1:A:257:ARG:HE	1.64	0.62
1:A:185:LEU:HB3	1:A:228:THR:HG23	1.80	0.62
1:B:185:LEU:HB3	1:B:228:THR:HG23	1.81	0.61

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	587/612 (96%)	575 (98%)	12 (2%)	0	100	100
1	B	587/612 (96%)	575 (98%)	12 (2%)	0	100	100
All	All	1174/1224 (96%)	1150 (98%)	24 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	509/528 (96%)	503 (99%)	6 (1%)	67	86
1	B	510/528 (97%)	503 (99%)	7 (1%)	62	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1019/1056 (96%)	1006 (99%)	13 (1%)	65 85

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	77	ARG
1	B	110	THR
1	B	443	ASP
1	B	327	LEU
1	B	340	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	412	GLN
1	B	412	GLN
1	B	548	GLN
1	B	607	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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
2	AU1	B	700[A]	3	25,29,29	1.99	7 (28%)	26,45,45	1.73	6 (23%)
2	AU1	A	700	3	8,8,29	3.28	5 (62%)	8,13,45	2.50	4 (50%)
2	AU1	B	700[B]	3	25,29,29	2.00	8 (32%)	26,45,45	1.79	7 (26%)

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
2	AU1	B	700[A]	3	-	5/9/32/32	0/3/3/3
2	AU1	A	700	3	-	2/2/6/32	-
2	AU1	B	700[B]	3	-	6/9/32/32	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	700	AU1	PB-N3A	4.83	1.76	1.63
2	A	700	AU1	PA-N3A	4.79	1.75	1.63
2	B	700[A]	AU1	PA-N3A	4.72	1.75	1.63
2	B	700[A]	AU1	PB-N3A	4.71	1.75	1.63
2	B	700[B]	AU1	PA-N3A	4.70	1.75	1.63

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	700	AU1	O2B-PB-N3A	-4.61	104.98	111.77
2	A	700	AU1	O2A-PA-N3A	-4.33	105.39	111.77
2	B	700[B]	AU1	N3-C2-N1	-4.17	123.01	128.67
2	B	700[A]	AU1	N3-C2-N1	-4.10	123.11	128.67
2	B	700[B]	AU1	O2B-PB-N3A	-3.95	105.96	111.77

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

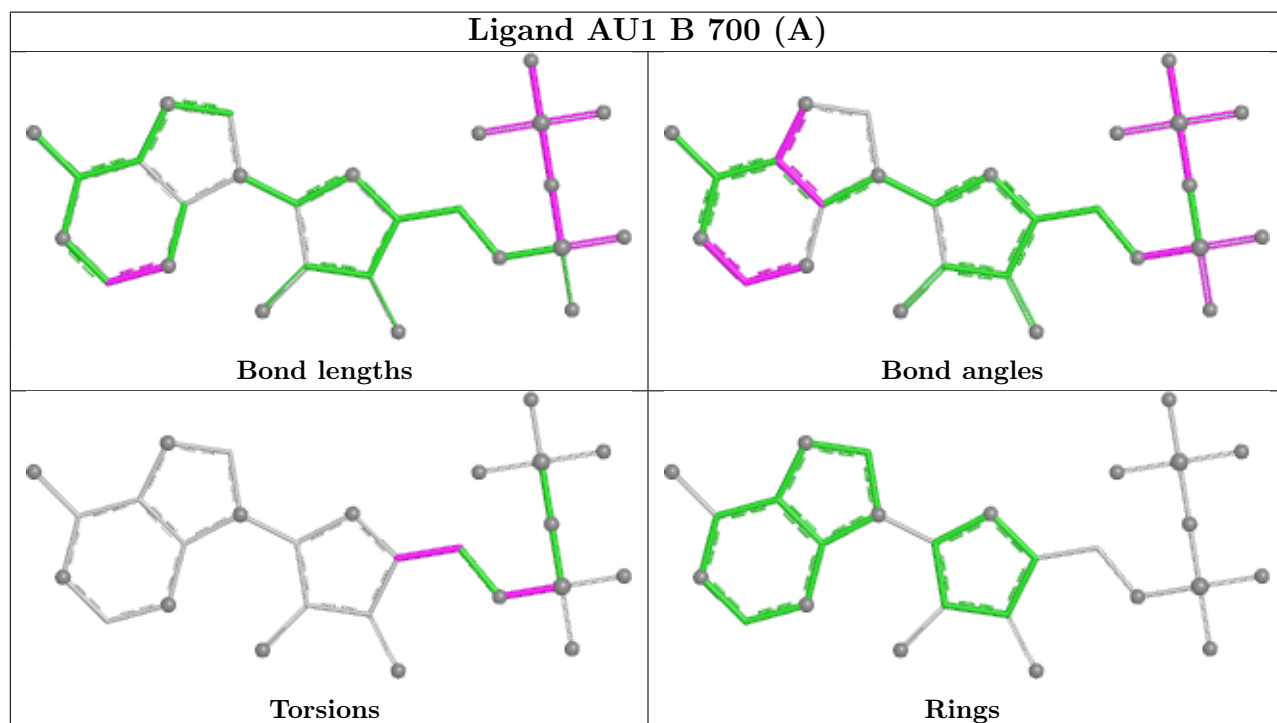
Mol	Chain	Res	Type	Atoms
2	A	700	AU1	PB-N3A-PA-O2A
2	A	700	AU1	PA-N3A-PB-O2B
2	B	700[B]	AU1	C5'-O5'-PA-O1A
2	B	700[B]	AU1	PA-N3A-PB-O2B
2	B	700[B]	AU1	C3'-C4'-C5'-O5'

There are no ring outliers.

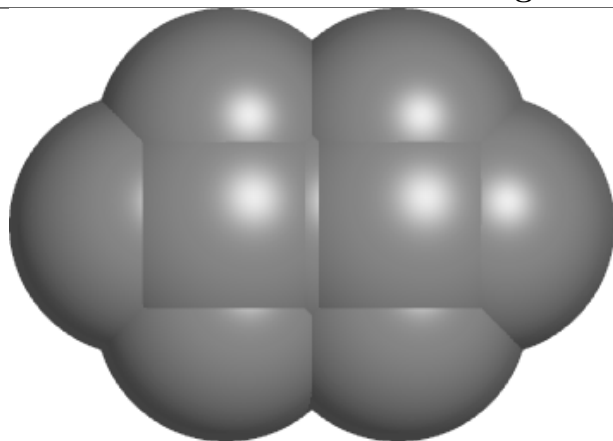
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	700	AU1	1	0

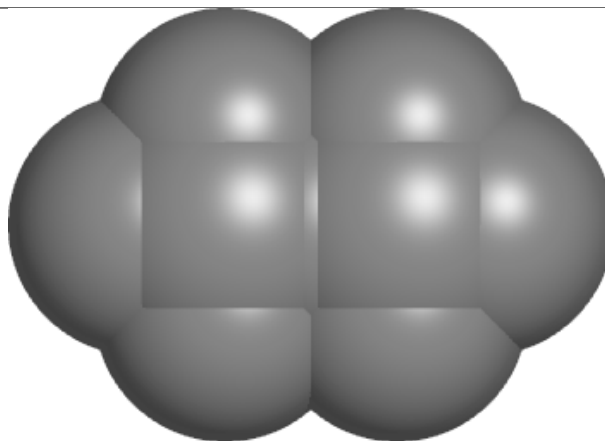
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



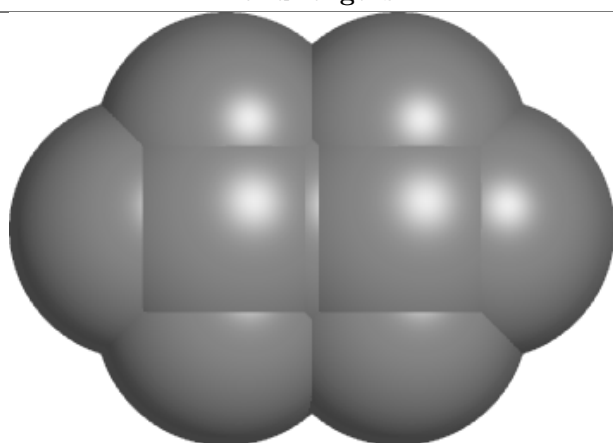
Ligand AU1 A 700



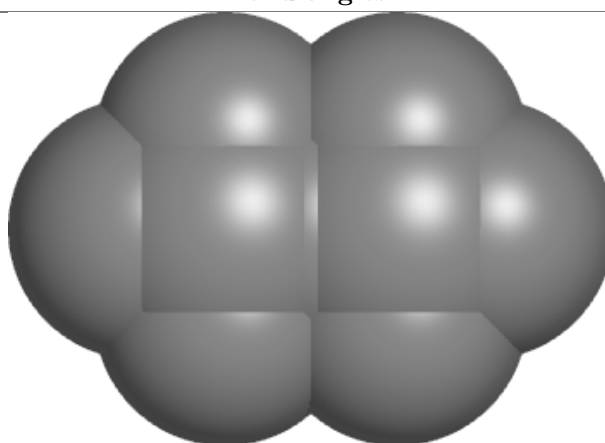
Bond lengths



Bond angles

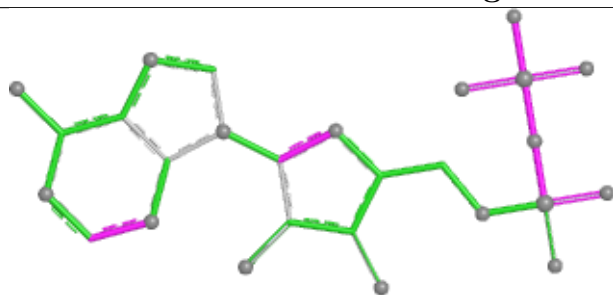


Torsions

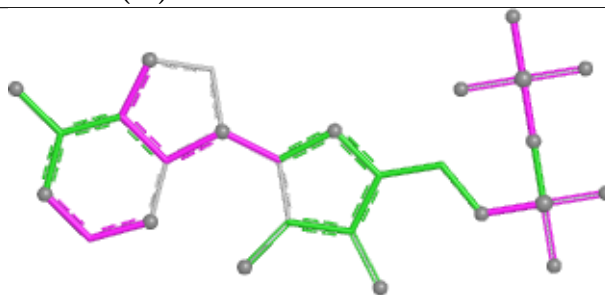


Rings

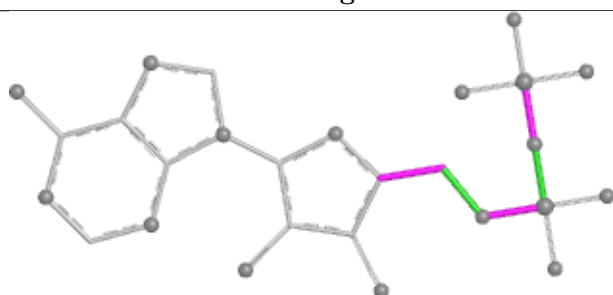
Ligand AU1 B 700 (B)



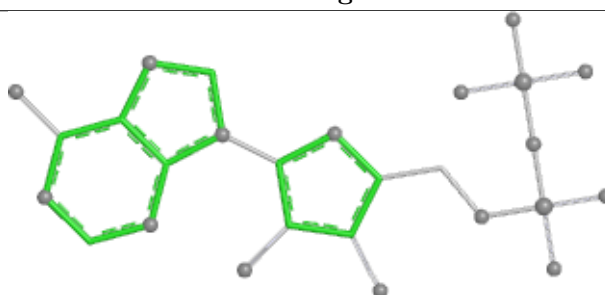
Bond lengths



Bond angles



Torsions



Rings

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	A	591/612 (96%)	-0.10	2 (0%) 90 81	13, 30, 51, 79	0
1	B	591/612 (96%)	-0.01	2 (0%) 90 81	17, 36, 69, 106	0
All	All	1182/1224 (96%)	-0.05	4 (0%) 90 81	13, 33, 62, 106	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	293	THR	2.5
1	B	513	GLY	2.5
1	A	629	GLU	2.1
1	B	520	GLU	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(Å ²)	Q<0.9
2	AU1	B	700[A]	27/27	0.87	0.16	46,50,51,52	27

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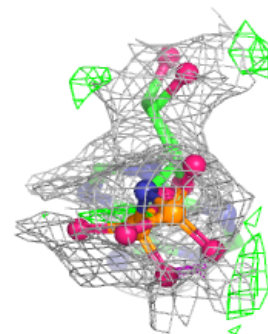
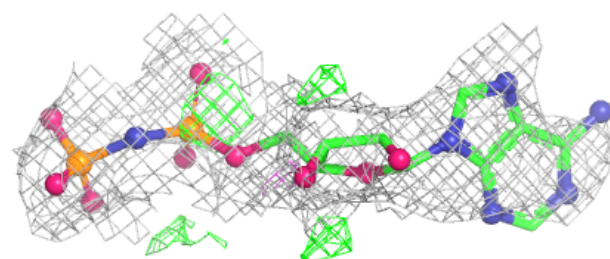
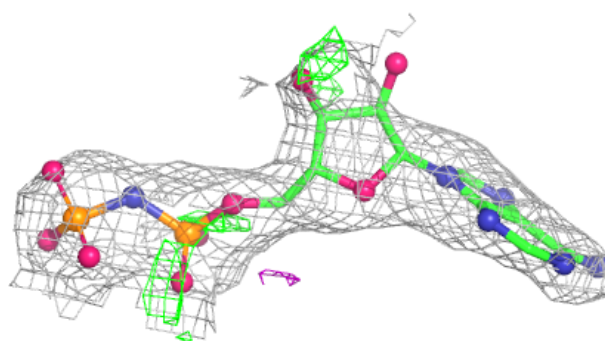
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	AU1	B	700[B]	27/27	0.87	0.16	59,59,59,59	27
2	AU1	A	700	9/27	0.88	0.13	53,53,54,55	9
3	MG	B	701	1/1	0.95	0.12	10,10,10,10	0
3	MG	A	701	1/1	0.97	0.11	9,9,9,9	0

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.

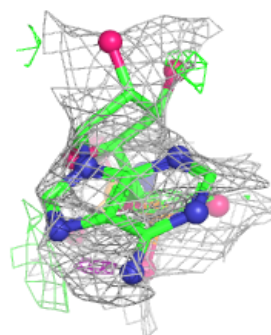
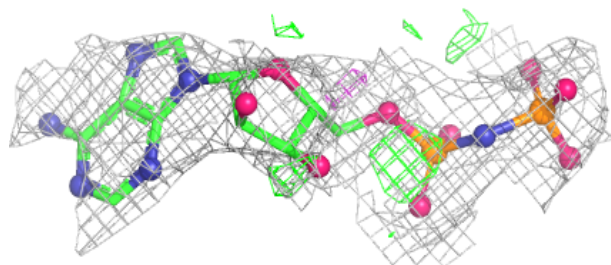
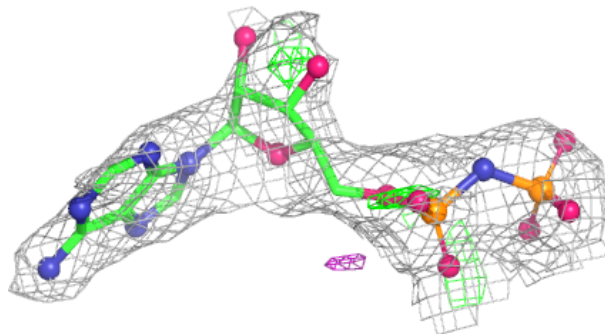
Electron density around AU1 B 700 (A):

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

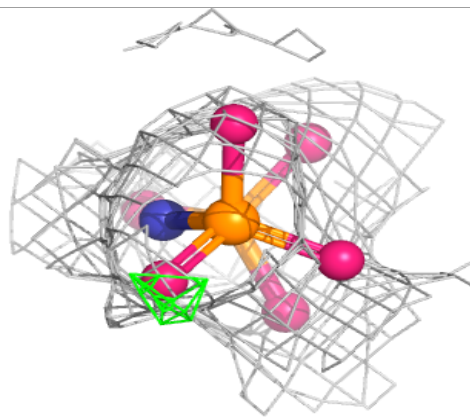
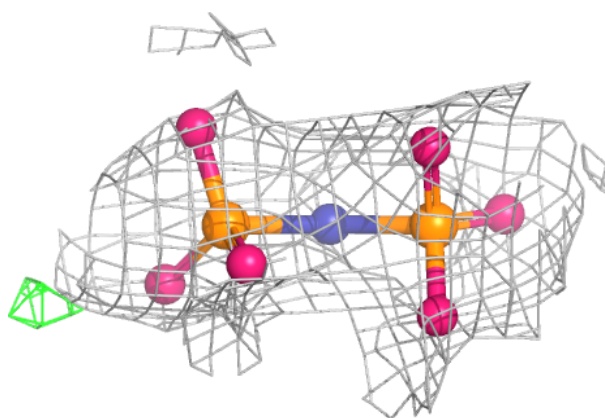


Electron density around AU1 B 700 (B):

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

**Electron density around AU1 A 700:**

$2mF_o-DF_c$ (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.