



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 6, 2021 – 06:12 am BST

PDB ID : 7OMU
Title : Thermosipho africanus DarTG in complex with ADP-ribose
Authors : Ariza, A.
Deposited on : 2021-05-24
Resolution : 2.96 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.2
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0267
CCP4 : 7.1.010 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

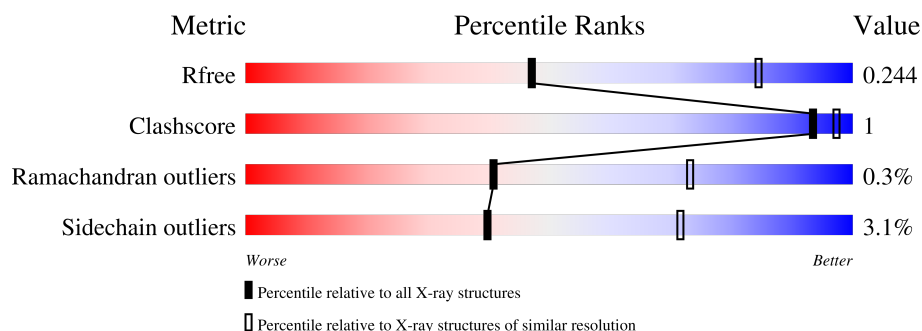
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.96 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	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	AAA	406	
1	BBB	406	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6194 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 Macro domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	376	Total	C	N	O	S	0	0	0
			3061	1979	521	546	15			
1	BBB	376	Total	C	N	O	S	0	0	0
			3061	1979	521	546	15			

There are 38 discrepancies between the modelled and reference sequences:

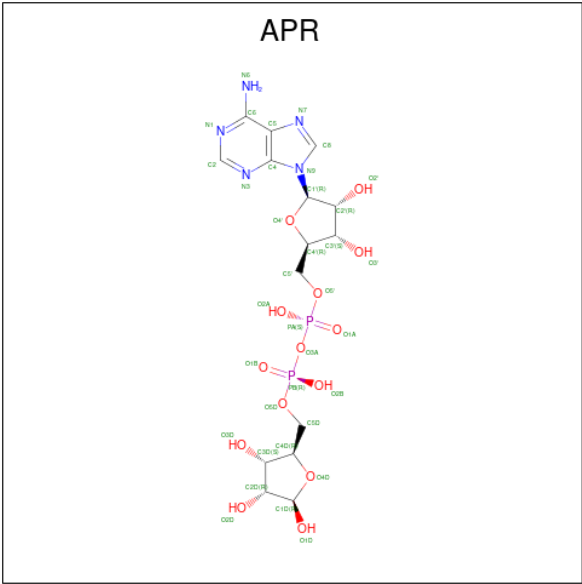
Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-17	GLY	-	expression tag	UNP K2PFJ6
AAA	-16	HIS	-	expression tag	UNP K2PFJ6
AAA	-15	SER	-	expression tag	UNP K2PFJ6
AAA	-14	GLY	-	expression tag	UNP K2PFJ6
AAA	-13	LYS	-	expression tag	UNP K2PFJ6
AAA	-12	PRO	-	expression tag	UNP K2PFJ6
AAA	-11	ILE	-	expression tag	UNP K2PFJ6
AAA	-10	PRO	-	expression tag	UNP K2PFJ6
AAA	-9	ASN	-	expression tag	UNP K2PFJ6
AAA	-8	PRO	-	expression tag	UNP K2PFJ6
AAA	-7	LEU	-	expression tag	UNP K2PFJ6
AAA	-6	LEU	-	expression tag	UNP K2PFJ6
AAA	-5	GLY	-	expression tag	UNP K2PFJ6
AAA	-4	LEU	-	expression tag	UNP K2PFJ6
AAA	-3	ASP	-	expression tag	UNP K2PFJ6
AAA	-2	SER	-	expression tag	UNP K2PFJ6
AAA	-1	THR	-	expression tag	UNP K2PFJ6
AAA	0	HIS	-	expression tag	UNP K2PFJ6
AAA	152	ALA	GLU	engineered mutation	UNP K2PFJ6
BBB	-17	GLY	-	expression tag	UNP K2PFJ6
BBB	-16	HIS	-	expression tag	UNP K2PFJ6
BBB	-15	SER	-	expression tag	UNP K2PFJ6
BBB	-14	GLY	-	expression tag	UNP K2PFJ6
BBB	-13	LYS	-	expression tag	UNP K2PFJ6
BBB	-12	PRO	-	expression tag	UNP K2PFJ6

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Chain	Residue	Modelled	Actual	Comment	Reference
BBB	-11	ILE	-	expression tag	UNP K2PFJ6
BBB	-10	PRO	-	expression tag	UNP K2PFJ6
BBB	-9	ASN	-	expression tag	UNP K2PFJ6
BBB	-8	PRO	-	expression tag	UNP K2PFJ6
BBB	-7	LEU	-	expression tag	UNP K2PFJ6
BBB	-6	LEU	-	expression tag	UNP K2PFJ6
BBB	-5	GLY	-	expression tag	UNP K2PFJ6
BBB	-4	LEU	-	expression tag	UNP K2PFJ6
BBB	-3	ASP	-	expression tag	UNP K2PFJ6
BBB	-2	SER	-	expression tag	UNP K2PFJ6
BBB	-1	THR	-	expression tag	UNP K2PFJ6
BBB	0	HIS	-	expression tag	UNP K2PFJ6
BBB	152	ALA	GLU	engineered mutation	UNP K2PFJ6

- Molecule 2 is ADENOSINE-5-DIPHOSPHORIBOSE (three-letter code: APR) (formula: C₁₅H₂₃N₅O₁₄P₂).

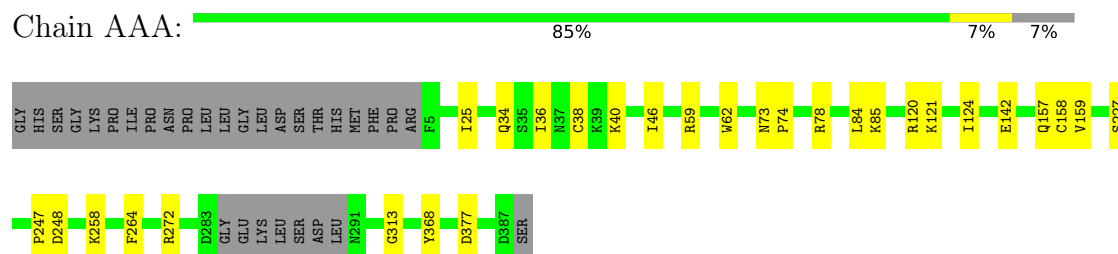


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	AAA	1	Total	C	N	O	P	0	0
			36	15	5	14	2		
2	BBB	1	Total	C	N	O	P	0	0
			36	15	5	14	2		

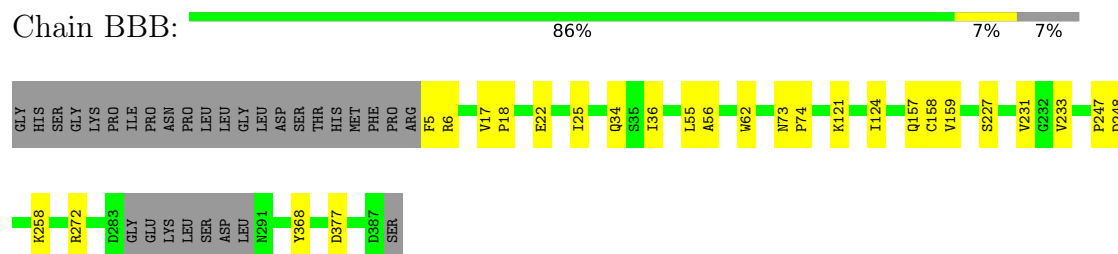
3 Residue-property plots [i](#)

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. 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. 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: Macro domain-containing protein



- Molecule 1: Macro domain-containing protein



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, α , β , γ	187.46Å 187.46Å 187.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	76.65 – 2.96 76.53 – 2.96	Depositor EDS
% Data completeness (in resolution range)	99.5 (76.65-2.96) 99.5 (76.53-2.96)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 2.96Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.211 , 0.248 0.211 , 0.244	Depositor DCC
R_{free} test set	1144 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	93.8	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.018 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6194	wwPDB-VP
Average B, all atoms (Å ²)	110.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.96% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: APR

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	AAA	0.63	0/3128	0.72	0/4225
1	BBB	0.63	0/3128	0.73	0/4225
All	All	0.63	0/6256	0.72	0/8450

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	AAA	3061	0	3147	10	0
1	BBB	3061	0	3147	9	0
2	AAA	36	0	21	1	0
2	BBB	36	0	21	1	0
All	All	6194	0	6336	18	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 (18) 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:AAA:121:LYS:O	1:AAA:124:ILE:HG22	2.08	0.53
1:BBB:55:LEU:HG	1:BBB:56:ALA:N	2.27	0.49
1:BBB:121:LYS:O	1:BBB:124:ILE:HG22	2.12	0.49
1:AAA:248:ASP:OD1	1:AAA:272:ARG:NH1	2.47	0.47
1:AAA:264:PHE:CZ	1:AAA:313:GLY:HA3	2.48	0.47
1:AAA:247:PRO:HB2	1:BBB:247:PRO:HB2	1.97	0.47
1:BBB:248:ASP:OD1	1:BBB:272:ARG:NH1	2.48	0.46
1:AAA:25:ILE:HB	1:AAA:159:VAL:HB	1.97	0.46
1:BBB:25:ILE:HB	1:BBB:159:VAL:HB	1.98	0.46
1:BBB:73:ASN:HB2	1:BBB:74:PRO:HD2	1.99	0.44
1:AAA:73:ASN:HB2	1:AAA:74:PRO:HD2	1.99	0.44
1:AAA:46:ILE:HD11	1:AAA:78:ARG:HD3	2.00	0.42
1:AAA:34:GLN:HB3	1:AAA:36:ILE:HG12	2.02	0.42
1:BBB:17:VAL:HB	1:BBB:18:PRO:HD3	2.02	0.42
1:BBB:368:TYR:HB3	2:BBB:501:APR:H2	2.02	0.41
1:BBB:34:GLN:HB3	1:BBB:36:ILE:HG12	2.03	0.41
1:AAA:368:TYR:HB3	2:AAA:501:APR:H2	2.02	0.41
1:AAA:84:LEU:HD12	1:AAA:84:LEU:HA	1.95	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	AAA	372/406 (92%)	346 (93%)	25 (7%)	1 (0%)	41	73
1	BBB	372/406 (92%)	352 (95%)	19 (5%)	1 (0%)	41	73
All	All	744/812 (92%)	698 (94%)	44 (6%)	2 (0%)	41	73

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	BBB	157	GLN

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Mol	Chain	Res	Type
1	AAA	157	GLN

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AAA	341/367 (93%)	330 (97%)	11 (3%)	39	71
1	BBB	341/367 (93%)	331 (97%)	10 (3%)	42	73
All	All	682/734 (93%)	661 (97%)	21 (3%)	40	71

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	38	CYS
1	AAA	40	LYS
1	AAA	59	ARG
1	AAA	62	TRP
1	AAA	85	LYS
1	AAA	120	ARG
1	AAA	142	GLU
1	AAA	158	CYS
1	AAA	227	SER
1	AAA	258	LYS
1	AAA	377	ASP
1	BBB	5	PHE
1	BBB	6	ARG
1	BBB	22	GLU
1	BBB	62	TRP
1	BBB	158	CYS
1	BBB	227	SER
1	BBB	231	VAL
1	BBB	233	VAL
1	BBB	258	LYS
1	BBB	377	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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](#)

2 ligands are modelled in this entry.

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	APR	AAA	501	-	34,39,39	0.60	0	40,60,60	0.81	1 (2%)
2	APR	BBB	501	-	34,39,39	0.59	0	40,60,60	0.79	1 (2%)

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	APR	AAA	501	-	-	5/18/54/54	0/4/4/4
2	APR	BBB	501	-	-	1/18/54/54	0/4/4/4

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AAA	501	APR	C5-C6-N6	2.37	123.95	120.35
2	BBB	501	APR	C5-C6-N6	2.25	123.77	120.35

There are no chirality outliers.

All (6) torsion outliers are listed below:

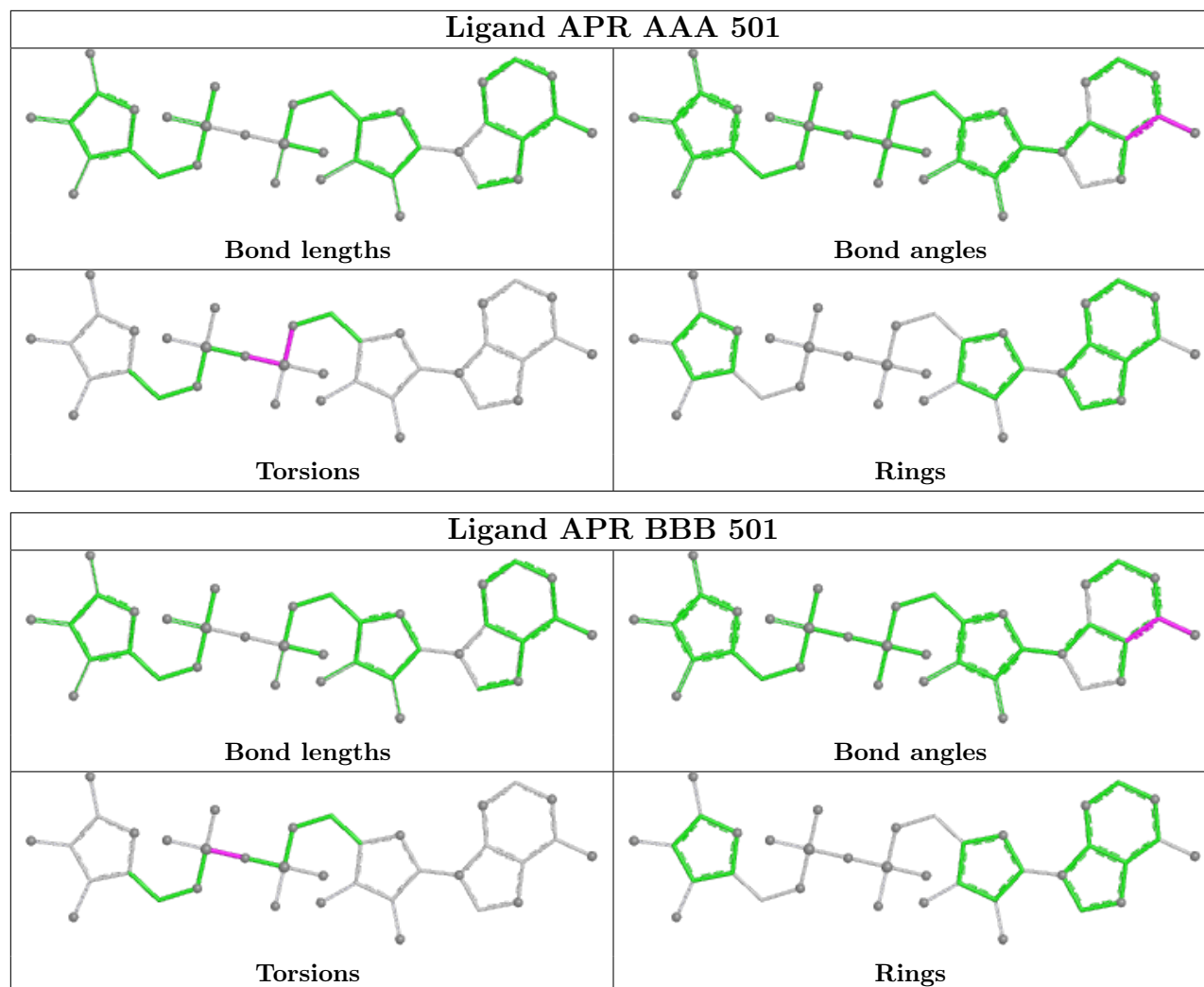
Mol	Chain	Res	Type	Atoms
2	AAA	501	APR	C5'-O5'-PA-O3A
2	BBB	501	APR	PA-O3A-PB-O5D
2	AAA	501	APR	C5'-O5'-PA-O1A
2	AAA	501	APR	C5'-O5'-PA-O2A
2	AAA	501	APR	PB-O3A-PA-O2A
2	AAA	501	APR	PB-O3A-PA-O1A

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	AAA	501	APR	1	0
2	BBB	501	APR	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [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](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

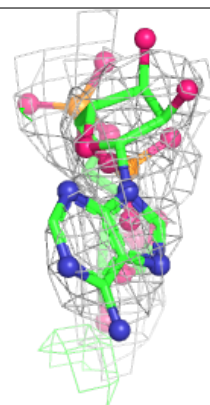
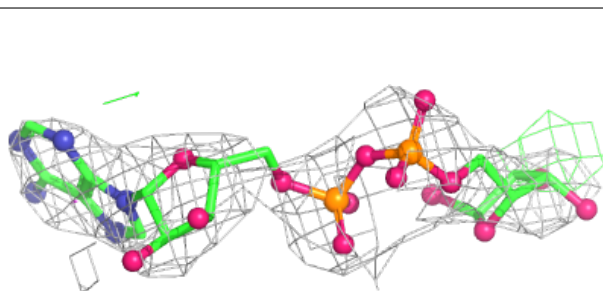
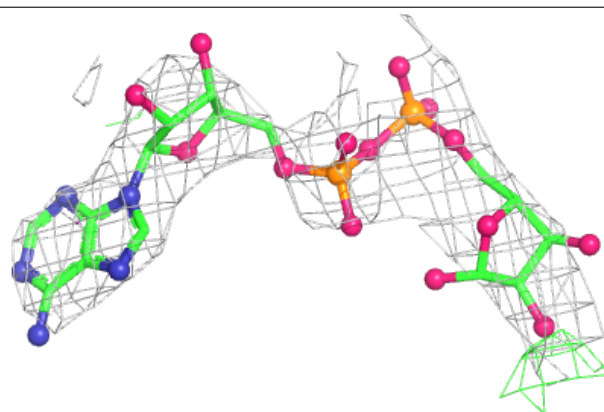
6.4 Ligands [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

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.

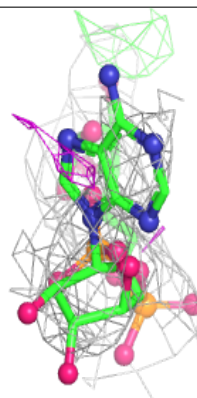
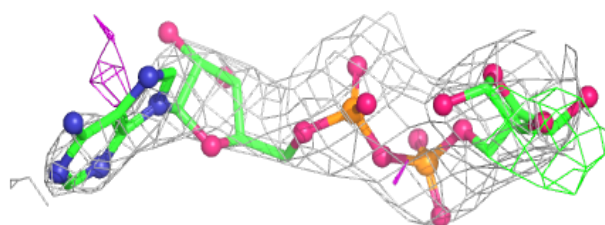
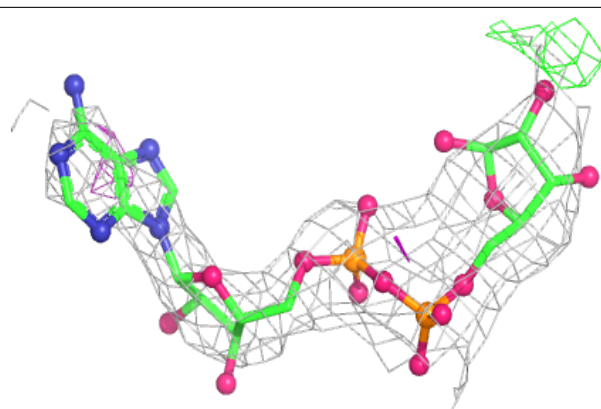
Electron density around APR AAA 501:

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 APR BBB 501:

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



6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.