



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 16, 2023 – 10:37 PM EDT

PDB ID : 2AA3
Title : Crystal structure of Plasmodium vivax lactate dehydrogenase complex with APADH
Authors : Chaikuad, A.; Fairweather, V.; Conners, R.; Joseph-Horne, T.; Turgut-Balik, D.; Brady, R.L.
Deposited on : 2005-07-13
Resolution : 2.05 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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

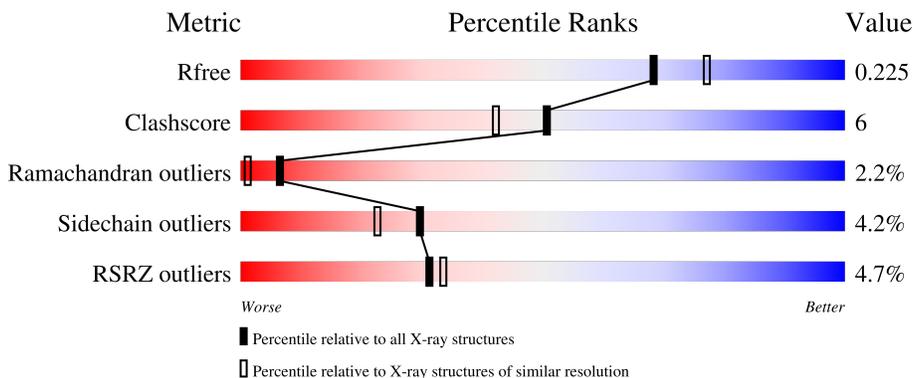
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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	321	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 87%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">87% 8% . .</p>
1	B	321	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 83%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 12%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">83% 12% . .</p>
1	C	321	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 89%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">89% 6% . . .</p>
1	D	321	<div style="display: flex; align-items: center;"> <div style="width: 7%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 80%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 14%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">80% 14% . .</p>

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
3	AP0	A	1401	X	-	-	-
3	AP0	B	1407	X	-	-	-
3	AP0	C	1405	X	-	-	-
3	AP0	D	1403	X	-	-	-

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 10302 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 L-lactate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	316	2408	1540	403	451	14	106	1	0
1	B	315	2398	1534	400	450	14	34	1	0
1	C	318	2433	1557	409	453	14	118	2	0
1	D	315	2398	1534	400	450	14	125	1	0

There are 24 discrepancies between the modelled and reference sequences:

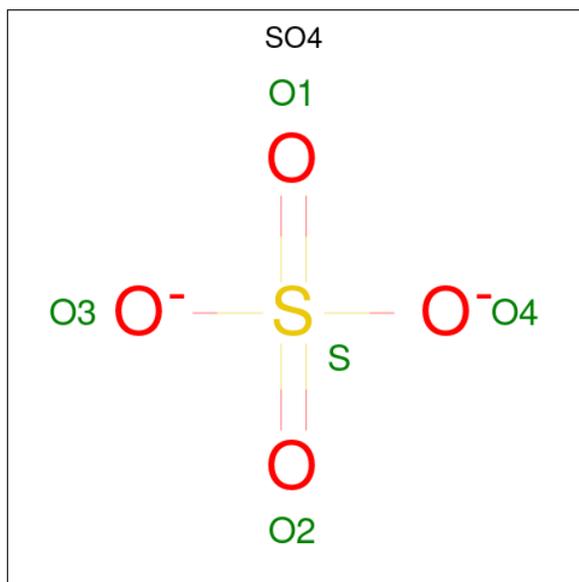
Chain	Residue	Modelled	Actual	Comment	Reference
A	330	HIS	-	expression tag	GB 66967948
A	331	HIS	-	expression tag	GB 66967948
A	332	HIS	-	expression tag	GB 66967948
A	333	HIS	-	expression tag	GB 66967948
A	334	HIS	-	expression tag	GB 66967948
A	335	HIS	-	expression tag	GB 66967948
B	330	HIS	-	expression tag	GB 66967948
B	331	HIS	-	expression tag	GB 66967948
B	332	HIS	-	expression tag	GB 66967948
B	333	HIS	-	expression tag	GB 66967948
B	334	HIS	-	expression tag	GB 66967948
B	335	HIS	-	expression tag	GB 66967948
C	330	HIS	-	expression tag	GB 66967948
C	331	HIS	-	expression tag	GB 66967948
C	332	HIS	-	expression tag	GB 66967948
C	333	HIS	-	expression tag	GB 66967948
C	334	HIS	-	expression tag	GB 66967948
C	335	HIS	-	expression tag	GB 66967948
D	330	HIS	-	expression tag	GB 66967948
D	331	HIS	-	expression tag	GB 66967948
D	332	HIS	-	expression tag	GB 66967948

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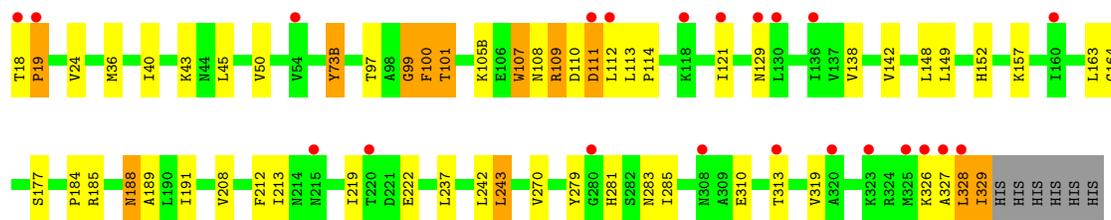
Chain	Residue	Modelled	Actual	Comment	Reference
D	333	HIS	-	expression tag	GB 66967948
D	334	HIS	-	expression tag	GB 66967948
D	335	HIS	-	expression tag	GB 66967948

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is ACETYL PYRIDINE ADENINE DINUCLEOTIDE, REDUCED (three-letter code: AP0) (formula: C₂₂H₃₀N₆O₁₄P₂).



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	81.48Å 128.45Å 130.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	91.67 – 2.05 29.14 – 2.05	Depositor EDS
% Data completeness (in resolution range)	98.3 (91.67-2.05) 98.4 (29.14-2.05)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.46 (at 2.04Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.191 , 0.226 0.191 , 0.225	Depositor DCC
R_{free} test set	4276 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	23.0	Xtrriage
Anisotropy	0.229	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 52.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.008 for -h,l,k	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10302	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% 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: AP0, SO4

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	1.06	4/2448 (0.2%)	0.85	4/3315 (0.1%)
1	B	1.00	4/2437 (0.2%)	0.92	10/3300 (0.3%)
1	C	0.99	3/2478 (0.1%)	0.88	12/3356 (0.4%)
1	D	0.86	3/2437 (0.1%)	0.77	2/3300 (0.1%)
All	All	0.98	14/9800 (0.1%)	0.86	28/13271 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
1	C	2	1
1	D	1	2
All	All	3	6

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	218	LYS	CE-NZ	15.30	1.87	1.49
1	C	222	GLU	CD-OE1	14.62	1.41	1.25
1	A	128	LYS	CE-NZ	14.36	1.84	1.49
1	C	222	GLU	CD-OE2	12.60	1.39	1.25
1	B	226	GLU	CD-OE1	12.25	1.39	1.25

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	106	GLU	CA-CB-CG	15.37	147.21	113.40
1	C	100	PHE	O-C-N	14.45	145.82	122.70
1	C	100	PHE	CA-C-N	-9.95	95.32	117.20
1	A	218	LYS	CD-CE-NZ	-9.86	89.02	111.70
1	B	107	TRP	CB-CA-C	-9.71	90.97	110.40

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	101	THR	CA,CB
1	D	110	ASP	CA

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	107	TRP	Peptide
1	A	108	ASN	Peptide
1	B	244	ALA	Peptide
1	C	108	ASN	Peptide
1	D	99	GLY	Mainchain

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	2408	0	2505	33	0
1	B	2398	0	2498	29	0
1	C	2433	0	2530	31	0
1	D	2398	0	2497	33	0
2	A	5	0	0	0	0
2	C	5	0	0	1	0
3	A	44	0	26	0	0
3	B	44	0	26	1	0
3	C	44	0	26	0	0
3	D	44	0	26	2	0
4	A	149	0	0	1	0
4	B	121	0	0	1	0
4	C	121	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	88	0	0	0	0
All	All	10302	0	10134	109	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 6.

The worst 5 of 109 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:128:LYS:CE	1:A:128:LYS:NZ	1.84	1.39
1:A:218:LYS:CE	1:A:218:LYS:NZ	1.87	1.37
1:D:18:THR:HA	1:D:19:PRO:O	1.27	1.27
1:A:109:ARG:HB2	1:A:110:ASP:HB3	1.33	1.08
1:D:18:THR:HA	1:D:19:PRO:C	1.66	1.06

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	315/321 (98%)	296 (94%)	11 (4%)	8 (2%)	5 1
1	B	314/321 (98%)	302 (96%)	10 (3%)	2 (1%)	25 15
1	C	318/321 (99%)	294 (92%)	17 (5%)	7 (2%)	6 1
1	D	314/321 (98%)	291 (93%)	12 (4%)	11 (4%)	3 0
All	All	1261/1284 (98%)	1183 (94%)	50 (4%)	28 (2%)	6 1

5 of 28 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	102	LYS

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Mol	Chain	Res	Type
1	A	103(C)	GLY
1	A	108	ASN
1	B	245	SER
1	C	20	LYS

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	269/273 (98%)	260 (97%)	9 (3%)	38	31
1	B	268/273 (98%)	256 (96%)	12 (4%)	27	20
1	C	272/273 (100%)	260 (96%)	12 (4%)	28	21
1	D	268/273 (98%)	252 (94%)	16 (6%)	19	11
All	All	1077/1092 (99%)	1028 (96%)	49 (4%)	30	20

5 of 49 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	111	ASP
1	D	101	THR
1	C	148	LEU
1	C	222	GLU
1	D	107	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	152	HIS
1	C	234	ASN
1	D	234	ASN
1	C	188	ASN
1	D	117	ASN

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](#)

6 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	SO4	C	1002	-	4,4,4	0.19	0	6,6,6	0.32	0
3	AP0	B	1407	-	42,48,48	2.03	8 (19%)	48,73,73	2.08	9 (18%)
2	SO4	A	1001	-	4,4,4	0.21	0	6,6,6	0.54	0
3	AP0	A	1401	-	42,48,48	2.19	7 (16%)	48,73,73	2.68	13 (27%)
3	AP0	D	1403	-	42,48,48	2.24	9 (21%)	48,73,73	2.18	13 (27%)
3	AP0	C	1405	-	42,48,48	2.01	8 (19%)	48,73,73	2.27	13 (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	AP0	D	1403	-	2/2/13/16	3/26/72/72	0/5/5/5
3	AP0	A	1401	-	2/2/13/16	3/26/72/72	0/5/5/5
3	AP0	C	1405	-	2/2/13/16	3/26/72/72	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AP0	B	1407	-	2/2/13/16	3/26/72/72	0/5/5/5

The worst 5 of 32 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1403	AP0	C8N-C7N	-7.75	1.34	1.50
3	B	1407	AP0	C8N-C7N	-7.14	1.36	1.50
3	C	1405	AP0	C8N-C7N	-6.51	1.37	1.50
3	D	1403	AP0	C2D-C1D	-6.13	1.33	1.53
3	A	1401	AP0	C2D-C1D	-5.97	1.34	1.53

The worst 5 of 48 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1401	AP0	C2D-C1D-N1N	7.74	132.71	113.30
3	B	1407	AP0	C2D-C1D-N1N	7.29	131.57	113.30
3	C	1405	AP0	C2D-C1D-N1N	7.26	131.48	113.30
3	A	1401	AP0	O7N-C7N-C3N	-6.82	112.62	119.64
3	A	1401	AP0	C3D-C2D-C1D	6.69	114.13	101.43

5 of 8 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	1401	AP0	C2D
3	A	1401	AP0	C1D
3	B	1407	AP0	C2D
3	B	1407	AP0	C1D
3	C	1405	AP0	C2D

5 of 12 torsion outliers are listed below:

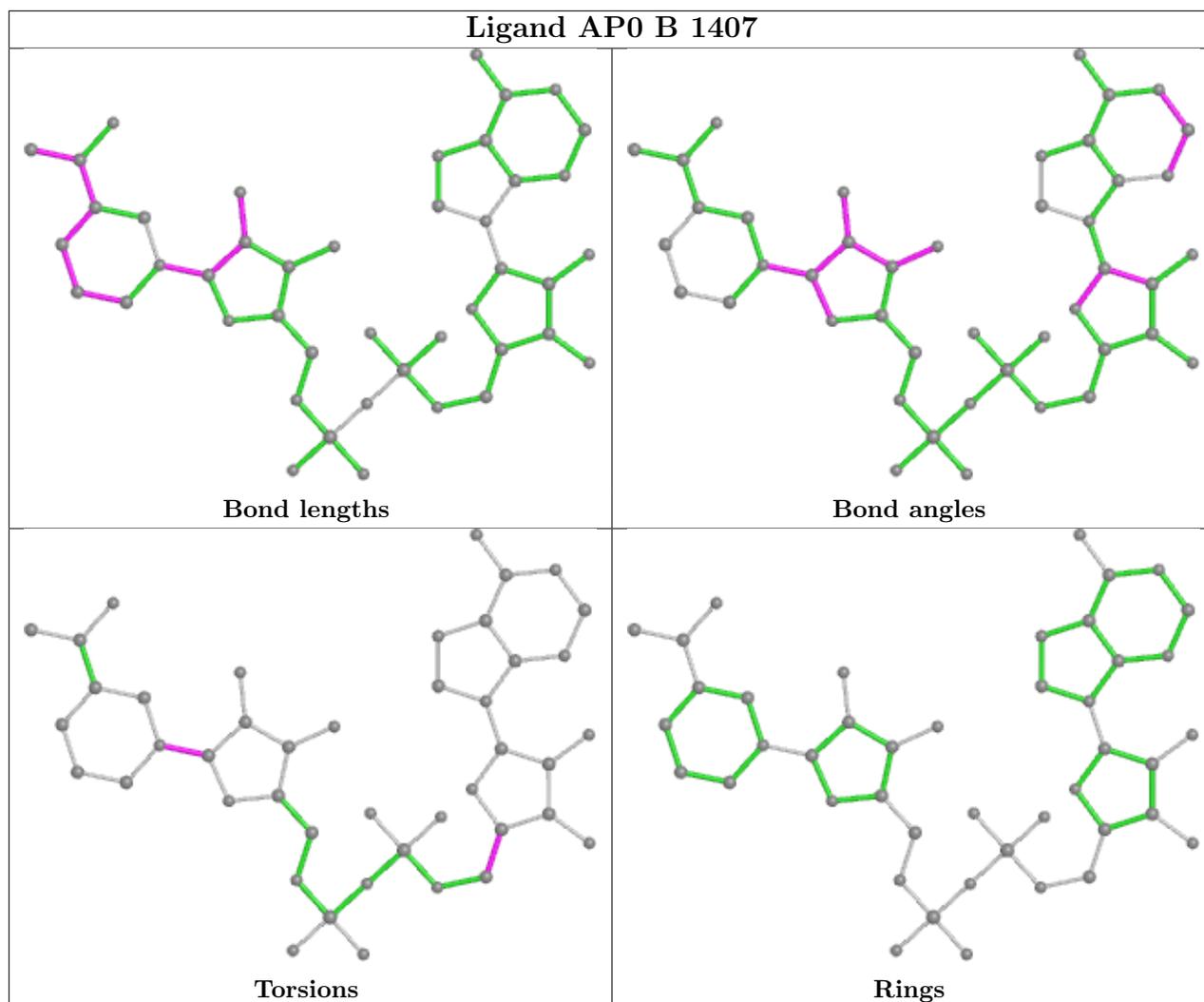
Mol	Chain	Res	Type	Atoms
3	C	1405	AP0	O4D-C1D-N1N-C6N
3	D	1403	AP0	O4D-C1D-N1N-C6N
3	A	1401	AP0	O4D-C1D-N1N-C2N
3	B	1407	AP0	O4D-C1D-N1N-C6N
3	D	1403	AP0	O4D-C1D-N1N-C2N

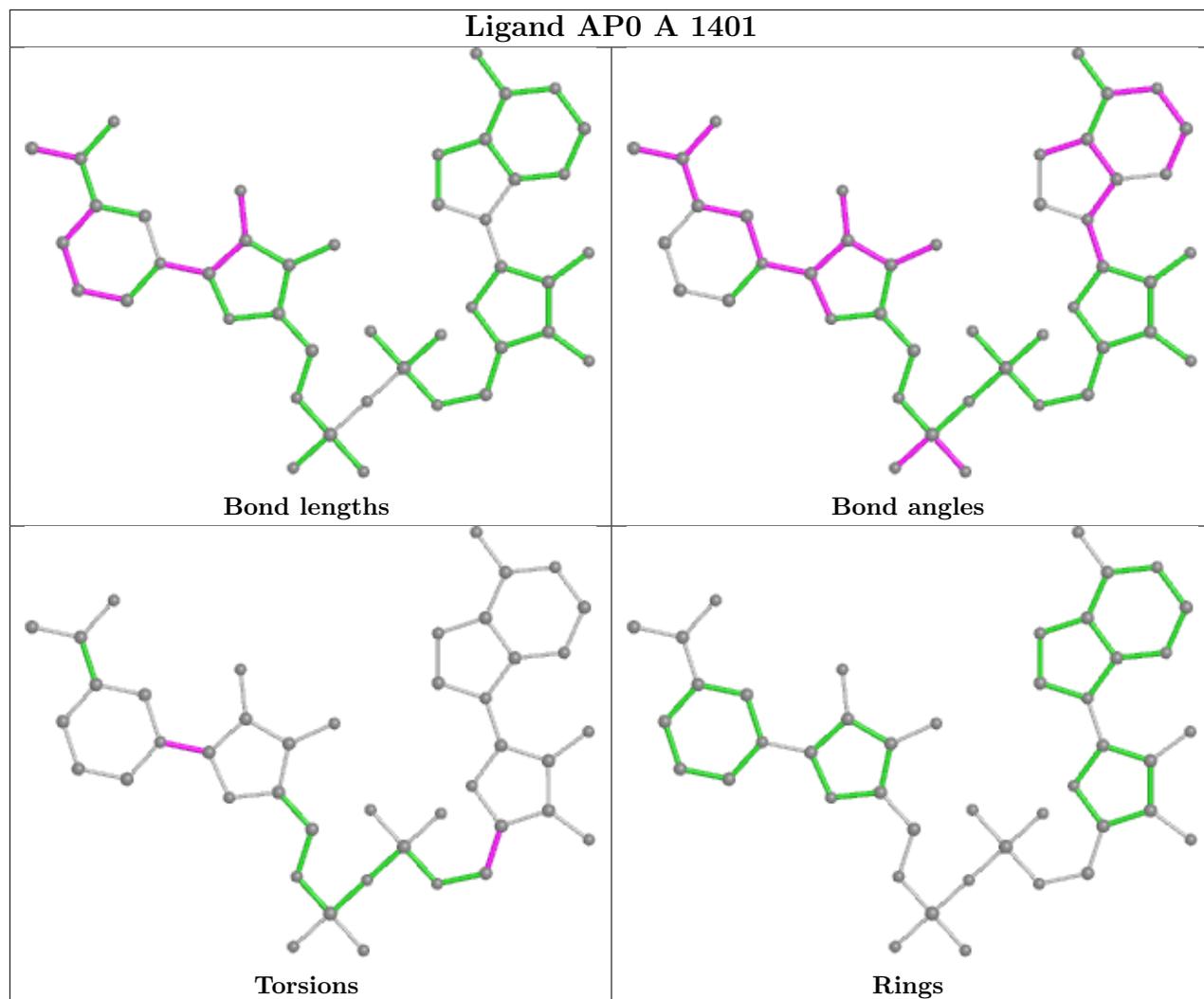
There are no ring outliers.

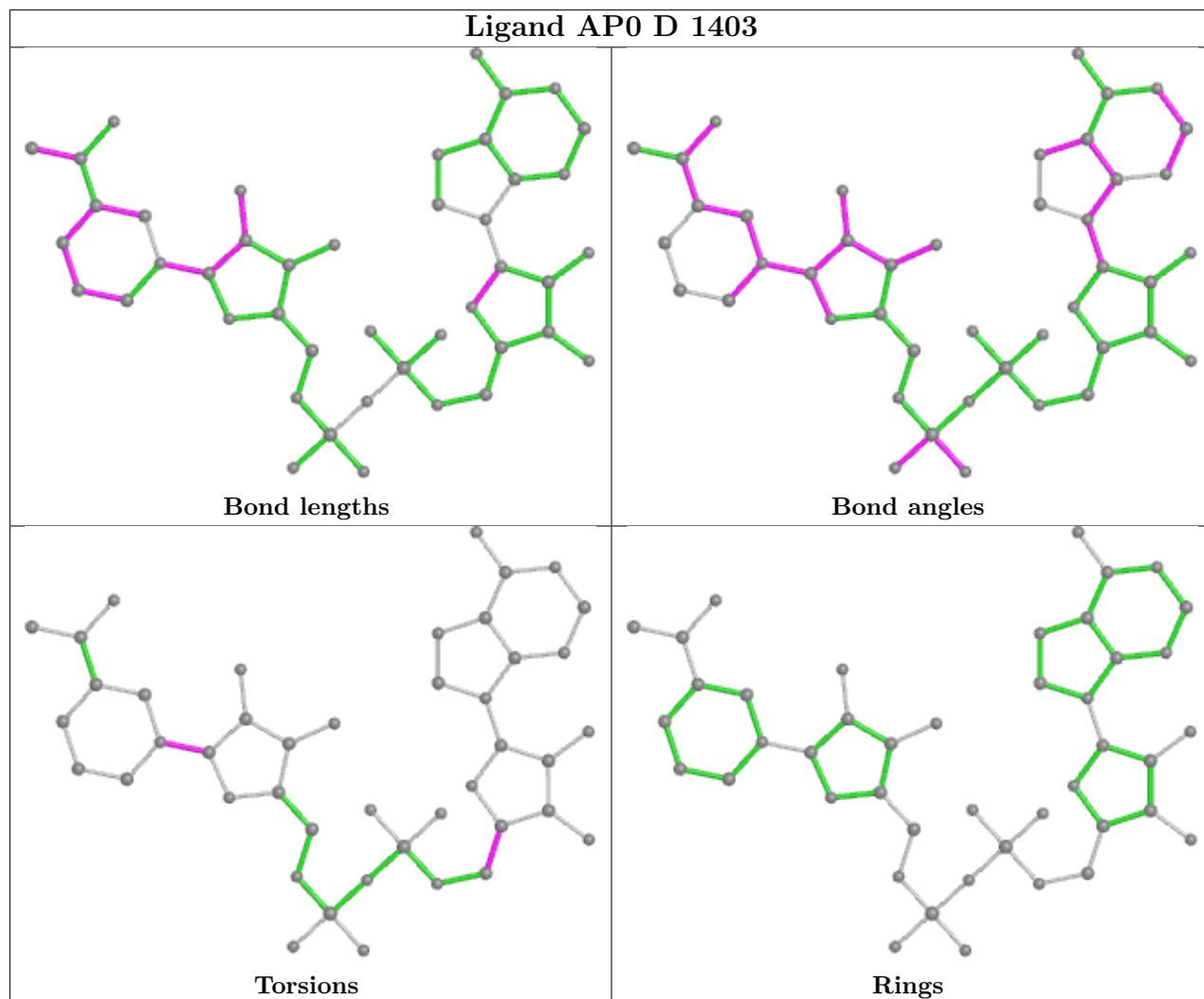
3 monomers are involved in 4 short contacts:

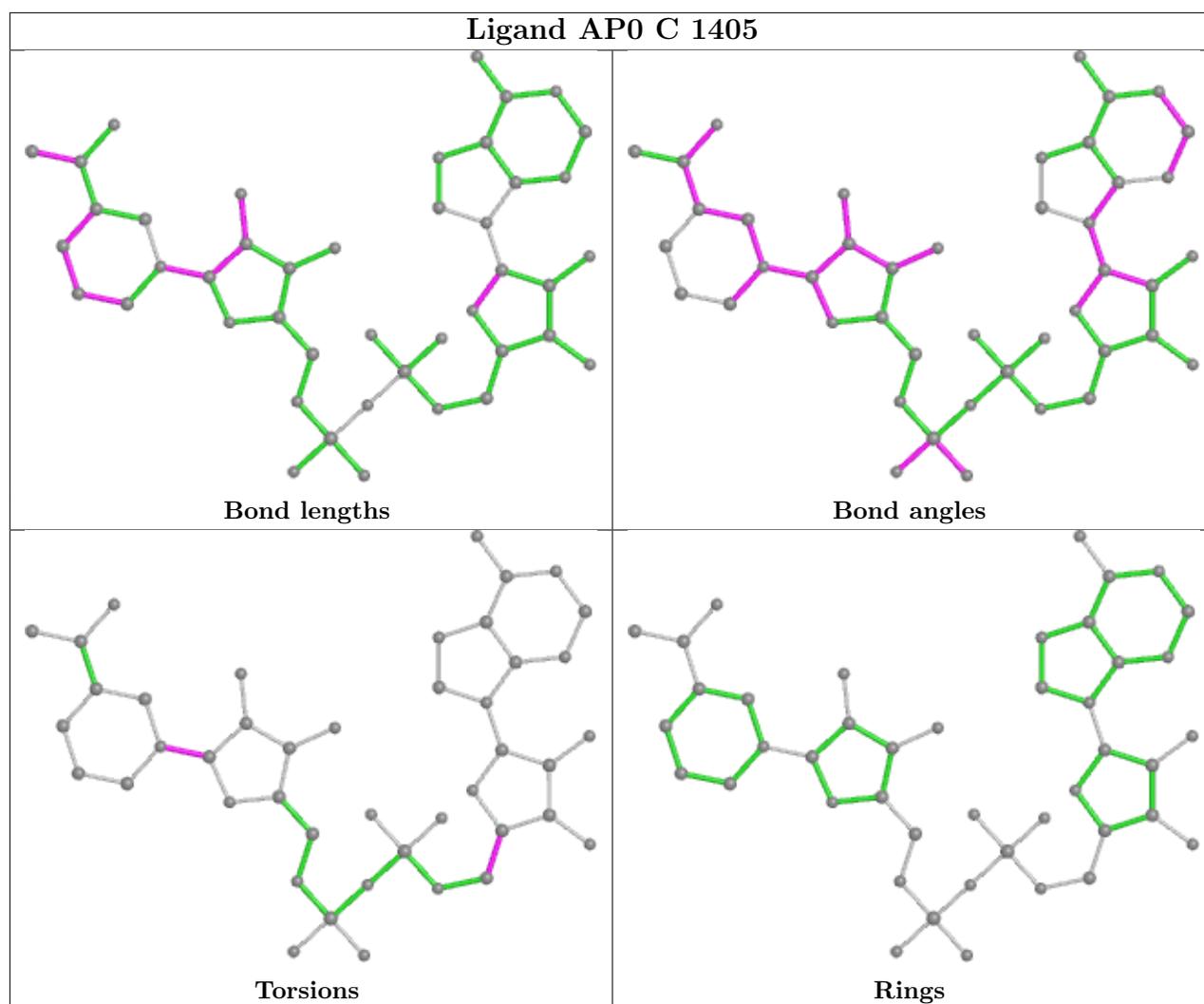
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1002	SO4	1	0
3	B	1407	AP0	1	0
3	D	1403	AP0	2	0

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](#)

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	303/321 (94%)	-0.03	10 (3%) 46 50	9, 17, 29, 43	19 (6%)
1	B	315/321 (98%)	0.09	12 (3%) 40 44	11, 19, 34, 47	32 (10%)
1	C	304/321 (94%)	-0.02	13 (4%) 35 38	9, 20, 30, 42	36 (11%)
1	D	300/321 (93%)	0.35	22 (7%) 15 16	12, 24, 39, 49	40 (13%)
All	All	1222/1284 (95%)	0.10	57 (4%) 31 33	9, 20, 36, 49	127 (10%)

The worst 5 of 57 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	112	LEU	10.0
1	D	18	THR	8.2
1	A	18	THR	7.0
1	C	18	THR	5.9
1	A	330	HIS	4.9

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](#)

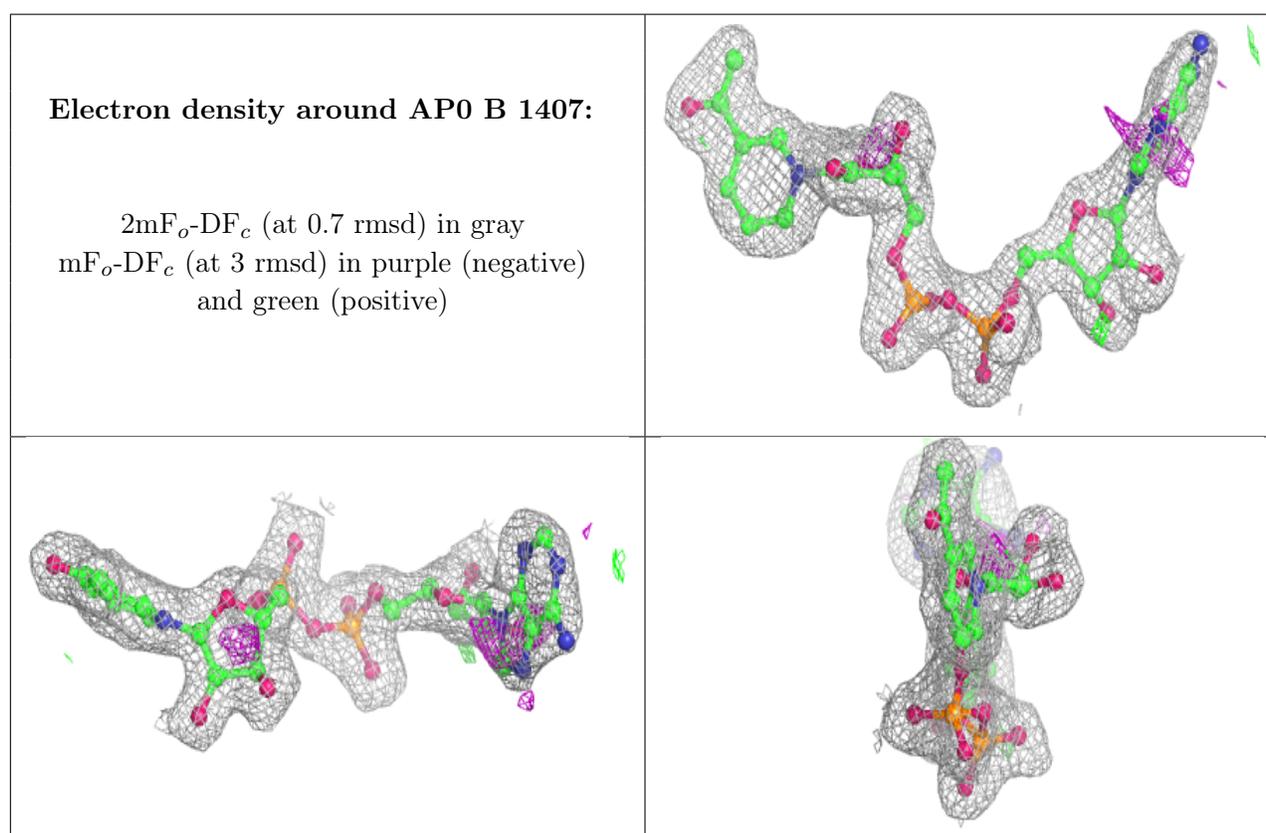
There are no monosaccharides in this entry.

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.

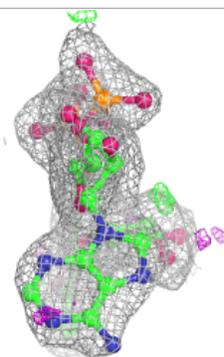
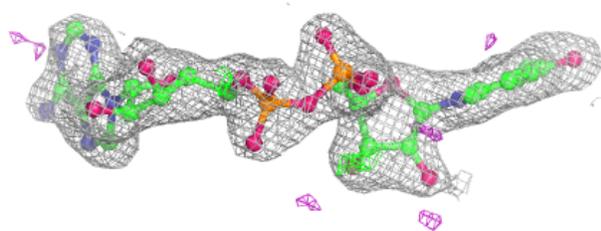
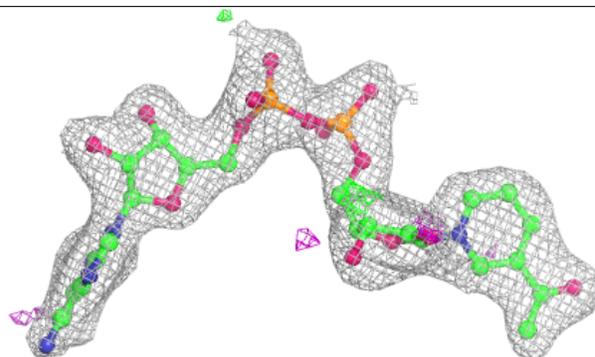
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	$Q < 0.9$
2	SO4	C	1002	5/5	0.86	0.25	35,38,39,40	5
3	AP0	B	1407	44/44	0.93	0.13	17,23,34,36	0
2	SO4	A	1001	5/5	0.94	0.14	29,29,31,32	5
3	AP0	D	1403	44/44	0.94	0.12	24,31,38,39	0
3	AP0	C	1405	44/44	0.95	0.11	14,22,28,33	0
3	AP0	A	1401	44/44	0.96	0.09	14,19,27,28	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.

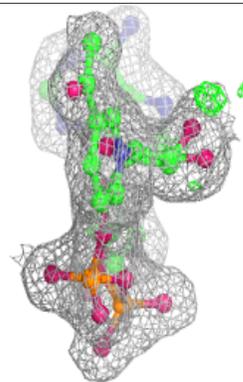
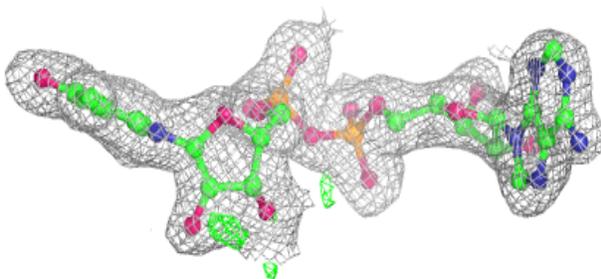
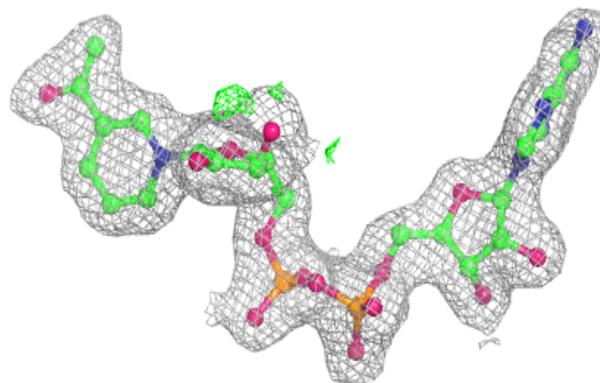


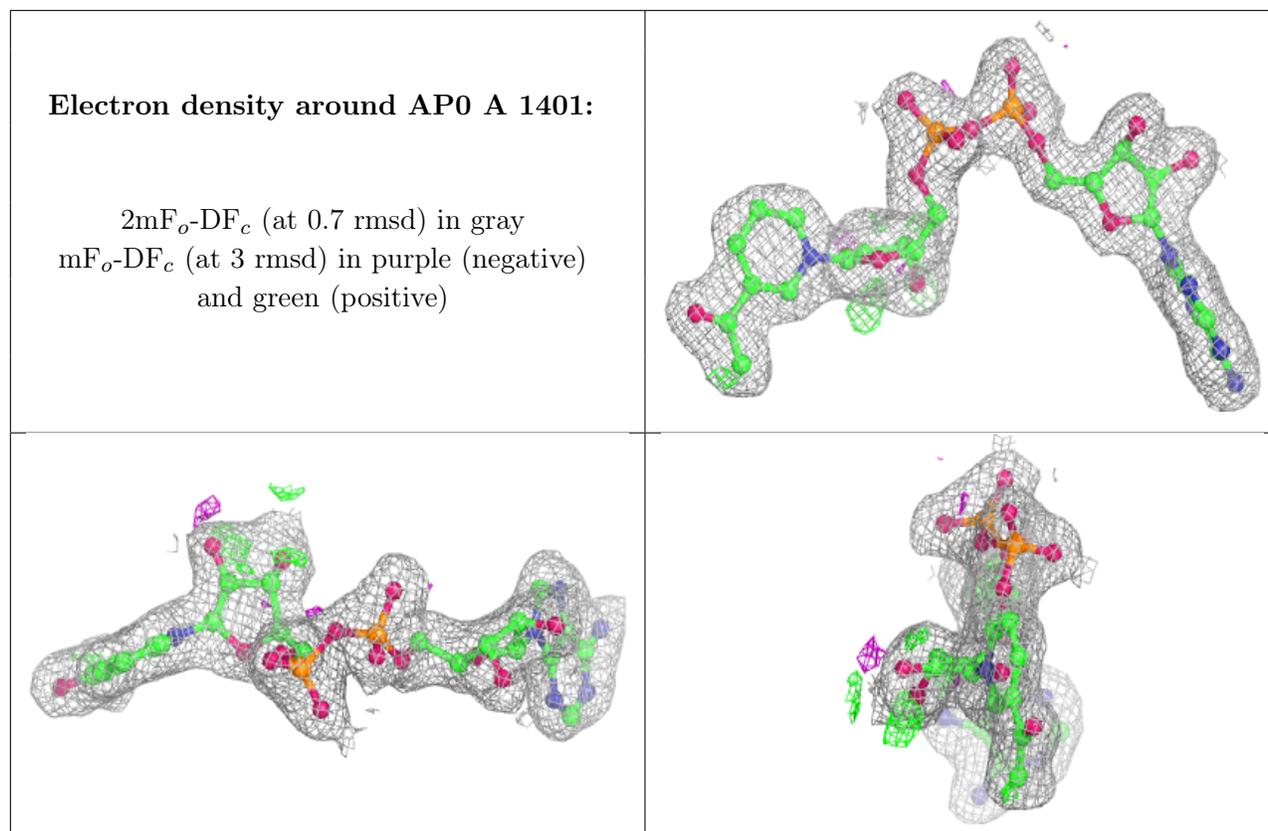
Electron density around AP0 D 1403:

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

**Electron density around AP0 C 1405:**

$2mF_o-DF_c$ (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.