wwPDB X-ray Structure Validation Summary Report (i)

Jun 14, 2020 – 05:20 am BST

PDB ID	:	1M7G
Title	:	Crystal structure of APS kinase from Penicillium Chrysogenum: Ternary structure with ADP and APS
Authors	:	Lansdon, E.B.; Segel, I.H.; Fisher, A.J.
Deposited on	:	2002-07-19
Resolution	:	1.43 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

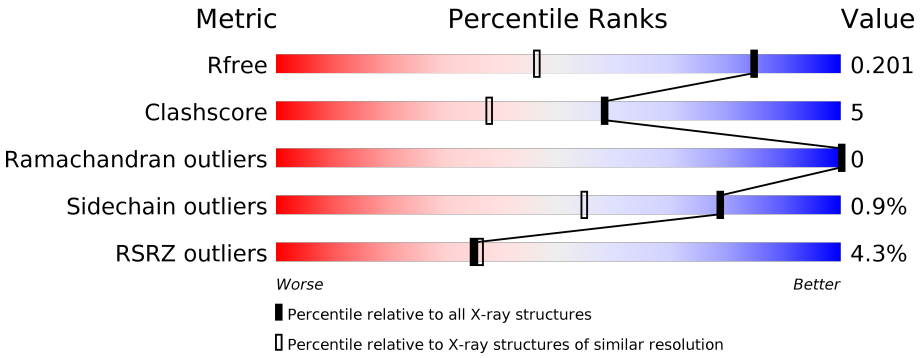
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 1.43 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	2021 (1.46-1.42)
Clashscore	141614	2086 (1.46-1.42)
Ramachandran outliers	138981	2047 (1.46-1.42)
Sidechain outliers	138945	2047 (1.46-1.42)
RSRZ outliers	127900	1993 (1.46-1.42)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	211	5% 90% 9%
1	B	211	% 79% 7% 14%
1	C	211	6% 87% 12%
1	D	211	4% 77% 9% 13%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	GOL	B	2011	-	-	X	-

2 Entry composition (i)

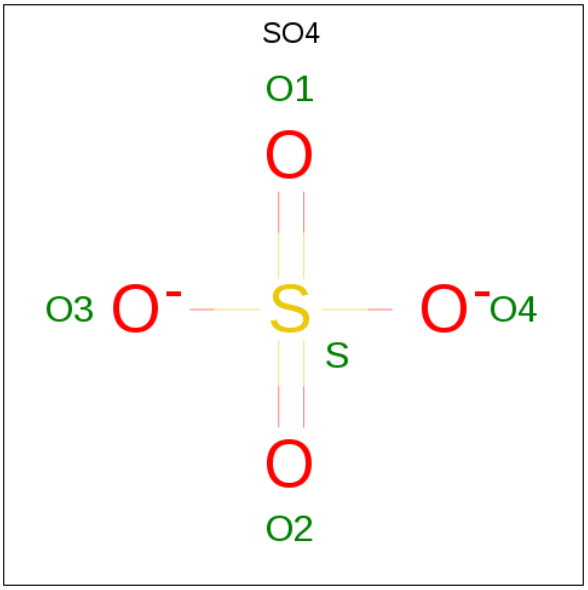
There are 7 unique types of molecules in this entry. The entry contains 7231 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Adenylylsulfate kinase.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	208	Total	C	N	O	0	0	0
			1641	1030	293	318			
1	B	182	Total	C	N	O	0	0	0
			1446	914	256	276			
1	C	209	Total	C	N	O	0	0	0
			1646	1033	294	319			
1	D	183	Total	C	N	O	0	0	0
			1444	913	255	276			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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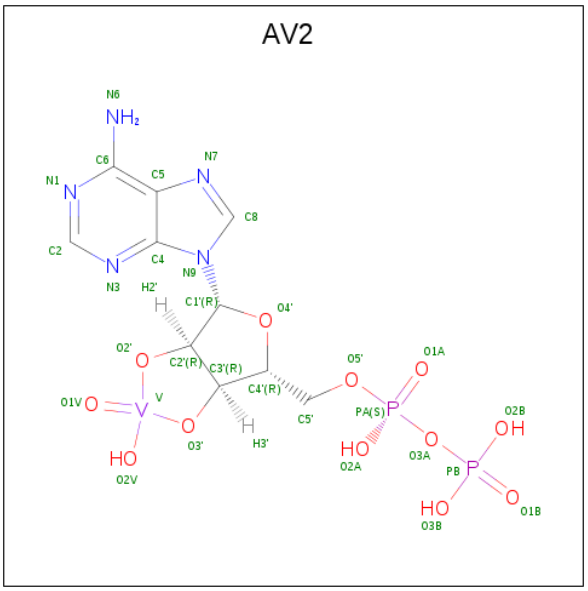
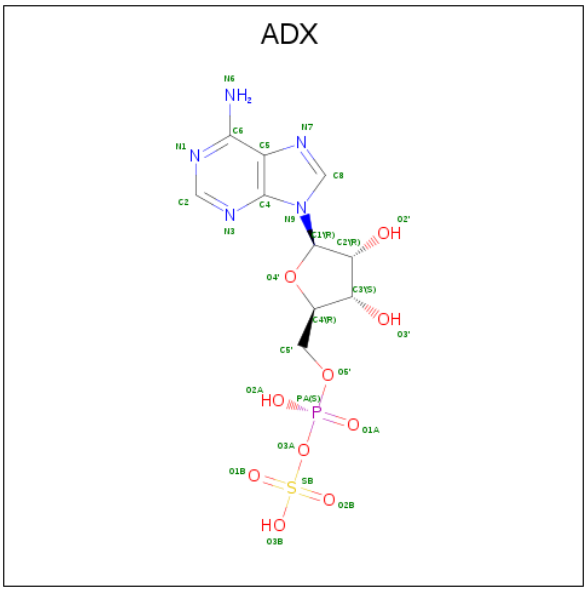
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE-2',3'-VANADATE (three-letter code: AV2) (formula: $C_{10}H_{14}N_5O_{12}P_2V$).



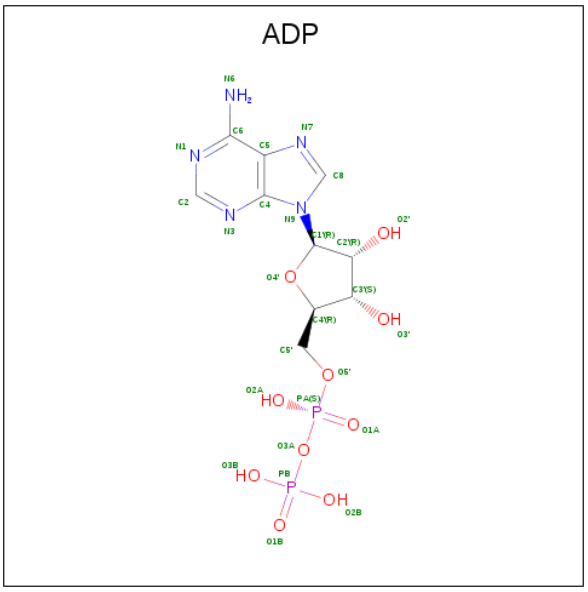
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O P V 30 10 5 12 2 1	0	0
3	C	1	Total C N O P V 30 10 5 12 2 1	0	0

- Molecule 4 is ADENOSINE-5'-PHOSPHOSULFATE (three-letter code: ADX) (formula: $C_{10}H_{14}N_5O_{10}PS$).



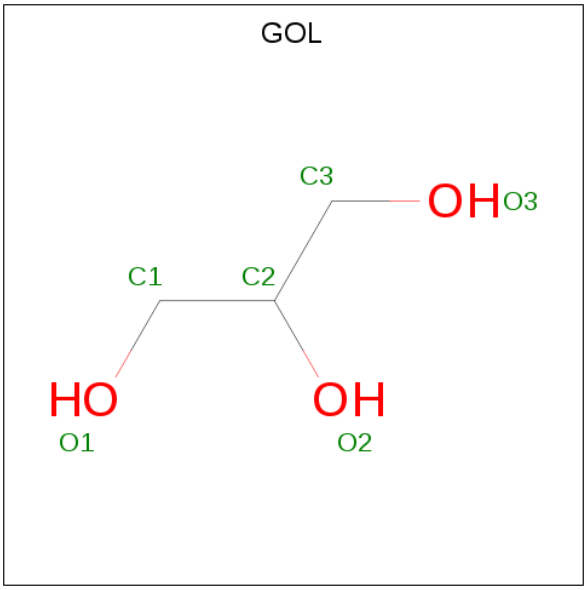
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	S	0	0
			27	10	5	10	1	1		
4	B	1	Total	C	N	O	P	S	0	0
			27	10	5	10	1	1		
4	C	1	Total	C	N	O	P	S	0	0
			27	10	5	10	1	1		
4	D	1	Total	C	N	O	P	S	0	0
			27	10	5	10	1	1		

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



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

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	O		0	0
			6	3	3			
6	C	1	Total	C	O		0	0
			6	3	3			

- Molecule 7 is water.

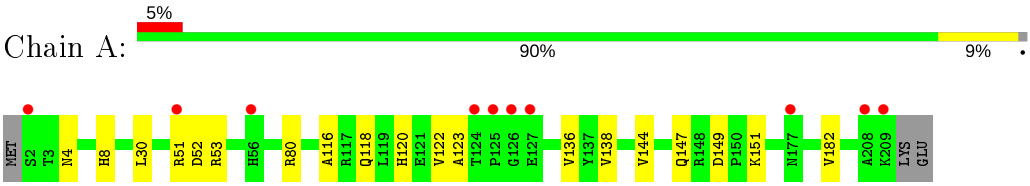
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	230	Total	O	0	0
			230	230		
7	B	189	Total	O	0	0
			189	189		
7	C	188	Total	O	0	0
			188	188		
7	D	183	Total	O	0	0
			183	183		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

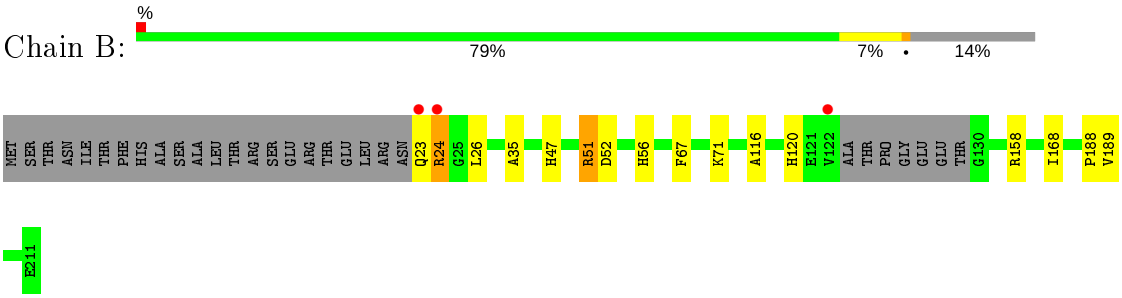
- Molecule 1: Adenylylsulfate kinase

Chain A:



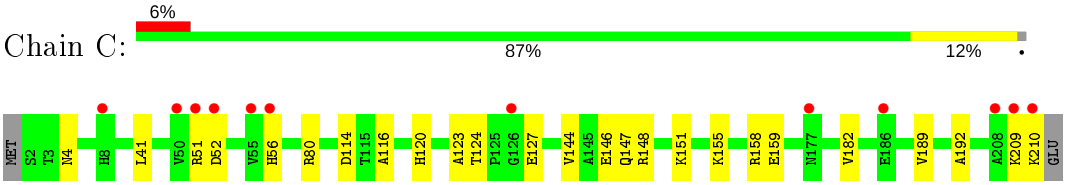
- Molecule 1: Adenylylsulfate kinase

Chain B:



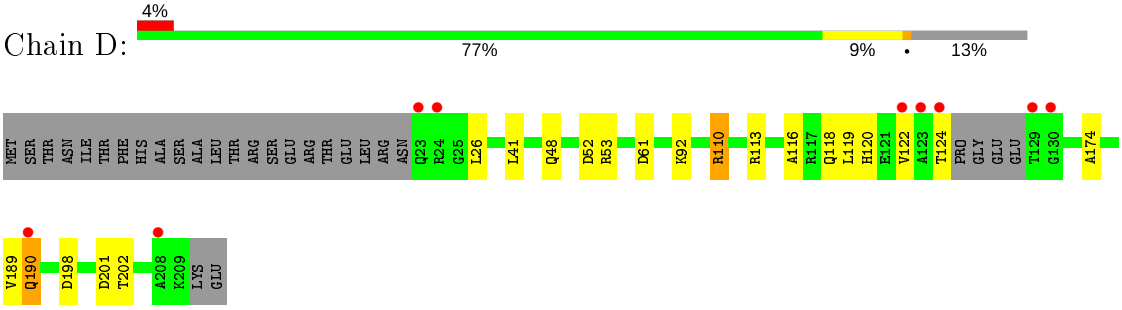
- Molecule 1: Adenylylsulfate kinase

Chain C:



- Molecule 1: Adenylylsulfate kinase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	81.52Å 84.32Å 137.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.61 – 1.43 29.61 – 1.43	Depositor EDS
% Data completeness (in resolution range)	99.1 (29.61-1.43) 99.3 (29.61-1.43)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	4.69 (at 1.43Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.180 , 0.205 0.176 , 0.201	Depositor DCC
R_{free} test set	8730 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	13.4	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 46.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.010 for k,h,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	7231	wwPDB-VP
Average B, all atoms (Å^2)	18.0	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 47.00 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.0560e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AV2, GOL, ADX, ADP, 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	0.68	0/1672	0.92	5/2267 (0.2%)
1	B	0.66	0/1473	0.82	0/1990
1	C	0.64	0/1677	0.87	3/2274 (0.1%)
1	D	0.66	0/1471	0.87	2/1993 (0.1%)
All	All	0.66	0/6293	0.87	10/8524 (0.1%)

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	53	ARG	NE-CZ-NH2	-7.82	116.39	120.30
1	C	80	ARG	NE-CZ-NH2	-7.71	116.44	120.30
1	A	80	ARG	NE-CZ-NH2	-7.54	116.53	120.30
1	C	80	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	A	80	ARG	NE-CZ-NH1	6.60	123.60	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1641	0	1621	14	0
1	B	1446	0	1437	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1646	0	1623	18	0
1	D	1444	0	1433	11	0
2	A	15	0	0	0	0
2	B	5	0	0	0	0
2	C	10	0	0	0	0
3	A	30	0	11	0	0
3	C	30	0	11	0	0
4	A	27	0	11	0	0
4	B	27	0	13	0	0
4	C	27	0	12	0	0
4	D	27	0	12	0	0
5	B	27	0	12	1	0
5	D	27	0	12	0	0
6	B	6	0	8	5	0
6	C	6	0	8	0	0
7	A	230	0	0	2	0
7	B	189	0	0	0	0
7	C	188	0	0	3	0
7	D	183	0	0	2	0
All	All	7231	0	6224	61	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 5.

The worst 5 of 61 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:189:VAL:H	6:B:2011:GOL:H12	1.26	0.98
1:A:4:ASN:HD21	1:A:123:ALA:H	1.15	0.91
1:C:4:ASN:HD21	1:C:123:ALA:H	1.19	0.91
1:B:24:ARG:CZ	1:B:24:ARG:HB2	2.04	0.87
1:A:151:LYS:HA	1:A:151:LYS:HE2	1.58	0.85

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	206/211 (98%)	200 (97%)	6 (3%)	0	100	100
1	B	178/211 (84%)	173 (97%)	5 (3%)	0	100	100
1	C	207/211 (98%)	201 (97%)	6 (3%)	0	100	100
1	D	179/211 (85%)	175 (98%)	4 (2%)	0	100	100
All	All	770/844 (91%)	749 (97%)	21 (3%)	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	175/180 (97%)	175 (100%)	0	100	100
1	B	153/180 (85%)	150 (98%)	3 (2%)	55	21
1	C	175/180 (97%)	175 (100%)	0	100	100
1	D	153/180 (85%)	150 (98%)	3 (2%)	55	21
All	All	656/720 (91%)	650 (99%)	6 (1%)	78	54

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	51	ARG
1	D	190	GLN
1	D	26	LEU

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Mol	Chain	Res	Type
1	B	26	LEU
1	D	118	GLN

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

Mol	Chain	Res	Type
1	B	190	GLN
1	C	4	ASN
1	D	190	GLN
1	B	195	GLN
1	C	48	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry

16 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	$\#\|Z\| > 2$
4	ADX	A	1302	-	25,29,29	2.82	7 (28%)	26,45,45	1.80	6 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	SO4	B	2004	-	4,4,4	0.32	0	6,6,6	0.17	0
4	ADX	B	1305	-	25,29,29	2.89	9 (36%)	26,45,45	1.88	7 (26%)
5	ADP	D	1309	-	24,29,29	1.35	4 (16%)	29,45,45	1.72	3 (10%)
2	SO4	A	2003	-	4,4,4	0.30	0	6,6,6	0.21	0
5	ADP	B	1304	-	24,29,29	1.11	1 (4%)	29,45,45	1.81	4 (13%)
6	GOL	B	2011	-	5,5,5	0.29	0	5,5,5	0.57	0
4	ADX	C	1307	-	25,29,29	2.82	8 (32%)	26,45,45	1.91	6 (23%)
2	SO4	C	2006	-	4,4,4	0.31	0	6,6,6	0.20	0
6	GOL	C	2010	-	5,5,5	0.31	0	5,5,5	0.84	0
2	SO4	A	2002	-	4,4,4	0.34	0	6,6,6	0.53	0
4	ADX	D	1310	-	25,29,29	2.39	9 (36%)	26,45,45	1.83	5 (19%)
2	SO4	A	2001	-	4,4,4	0.38	0	6,6,6	0.55	0
2	SO4	C	2005	-	4,4,4	0.27	0	6,6,6	0.24	0
3	AV2	A	1301	3	26,33,33	4.72	6 (23%)	26,53,53	1.66	4 (15%)
3	AV2	C	1306	3	26,33,33	4.88	8 (30%)	26,53,53	1.64	2 (7%)

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
4	ADX	A	1302	-	-	0/6/32/32	0/3/3/3
4	ADX	B	1305	-	-	0/6/32/32	0/3/3/3
5	ADP	D	1309	-	-	2/12/32/32	0/3/3/3
5	ADP	B	1304	-	-	2/12/32/32	0/3/3/3
6	GOL	B	2011	-	-	2/4/4/4	-
4	ADX	C	1307	-	-	0/6/32/32	0/3/3/3
6	GOL	C	2010	-	-	4/4/4/4	-
4	ADX	D	1310	-	-	0/6/32/32	0/3/3/3
3	AV2	A	1301	3	-	1/12/42/42	0/4/4/4
3	AV2	C	1306	3	-	1/12/42/42	0/4/4/4

The worst 5 of 52 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1301	AV2	O3'-V	17.33	2.00	1.71
3	C	1306	AV2	O3'-V	17.11	1.99	1.71
3	C	1306	AV2	O2'-V	15.74	1.97	1.71
3	A	1301	AV2	O2'-V	15.08	1.96	1.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1305	ADX	PA-O3A	9.01	1.66	1.59

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	1304	ADP	N3-C2-N1	-6.82	118.02	128.68
5	D	1309	ADP	N3-C2-N1	-6.54	118.45	128.68
4	D	1310	ADX	C3'-C2'-C1'	6.17	110.26	100.98
4	C	1307	ADX	C3'-C2'-C1'	6.11	110.18	100.98
3	C	1306	AV2	N3-C2-N1	-6.00	119.31	128.68

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	1304	ADP	PA-O3A-PB-O2B
6	B	2011	GOL	O1-C1-C2-O2
6	B	2011	GOL	O1-C1-C2-C3
6	C	2010	GOL	O1-C1-C2-C3
6	C	2010	GOL	O1-C1-C2-O2

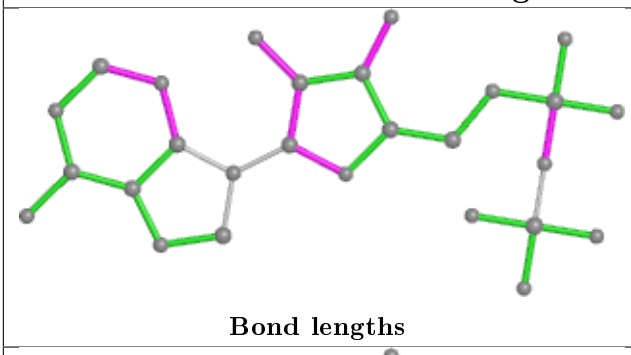
There are no ring outliers.

2 monomers are involved in 6 short contacts:

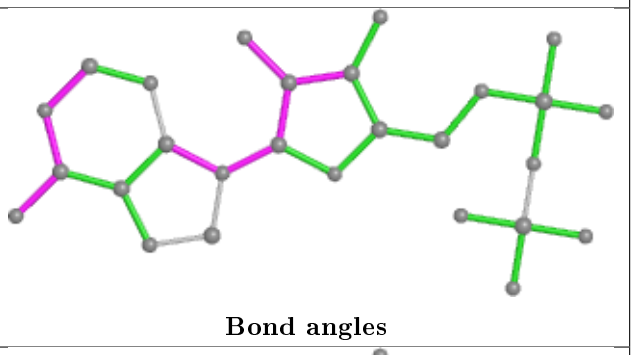
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1304	ADP	1	0
6	B	2011	GOL	5	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

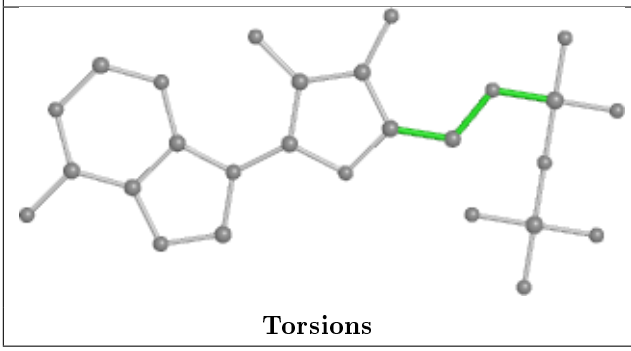
Ligand ADX A 1302



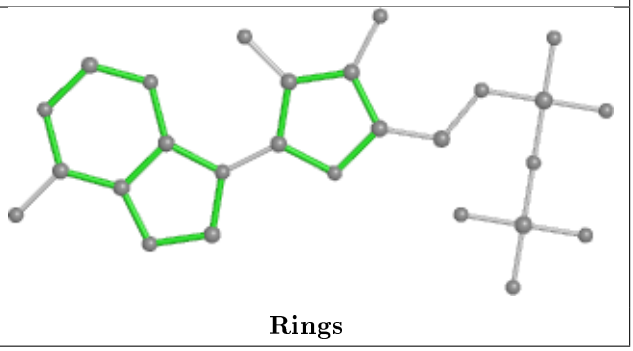
Bond lengths



Bond angles

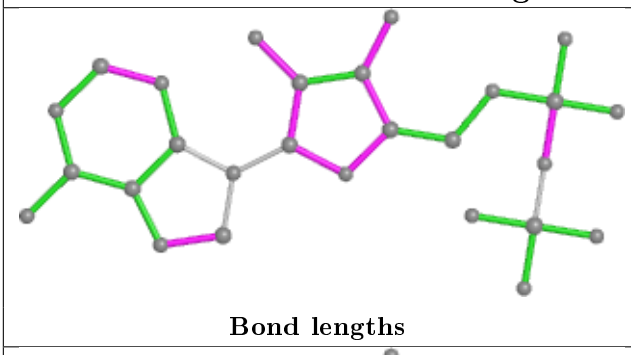


Torsions

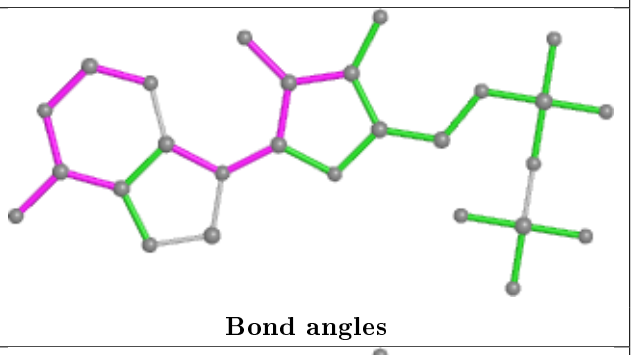


Rings

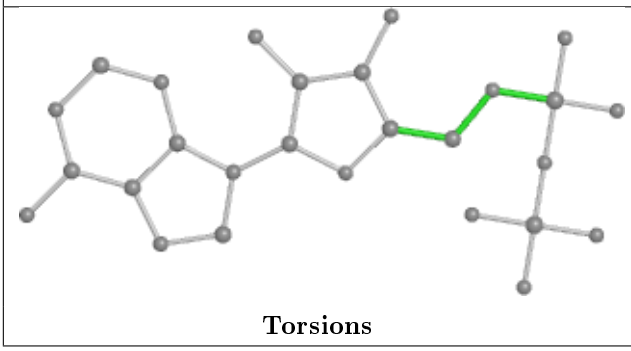
Ligand ADX B 1305



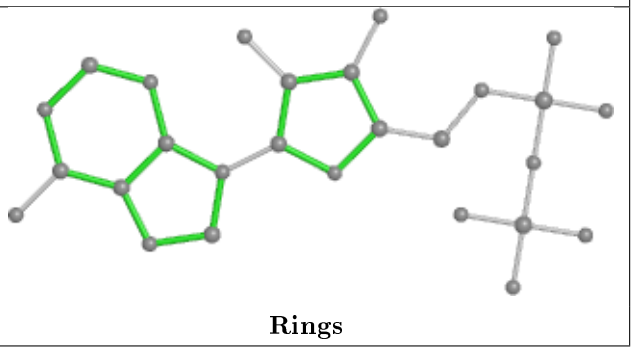
Bond lengths



Bond angles

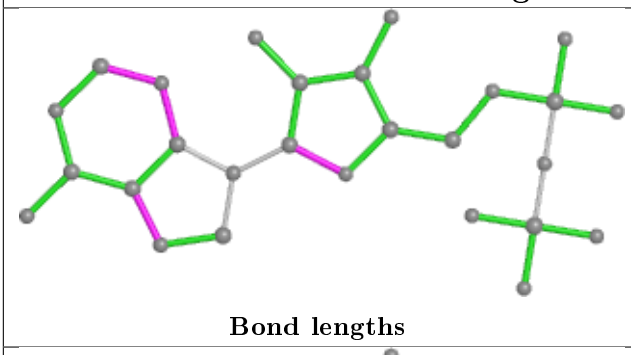


Torsions

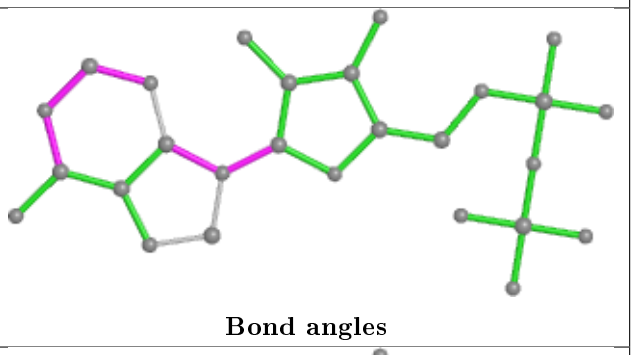


Rings

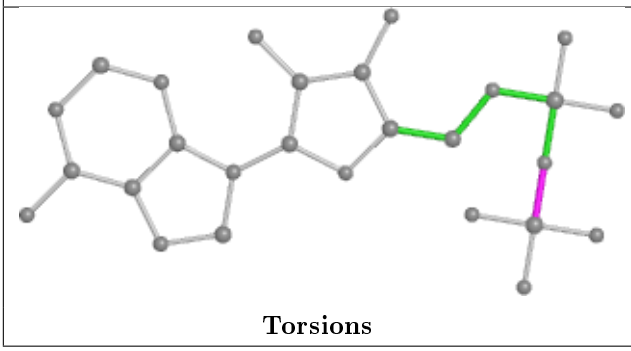
Ligand ADP D 1309



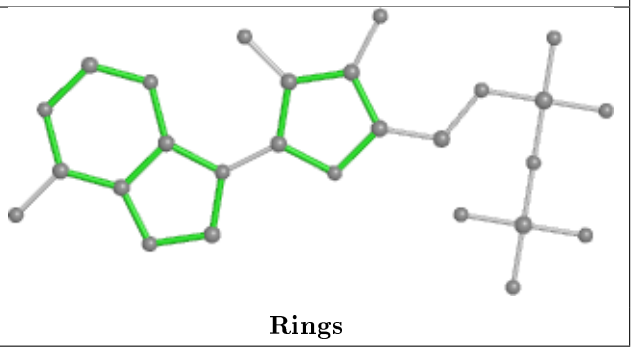
Bond lengths



Bond angles

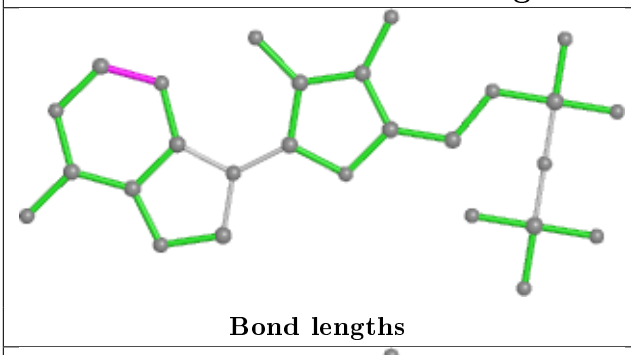


Torsions

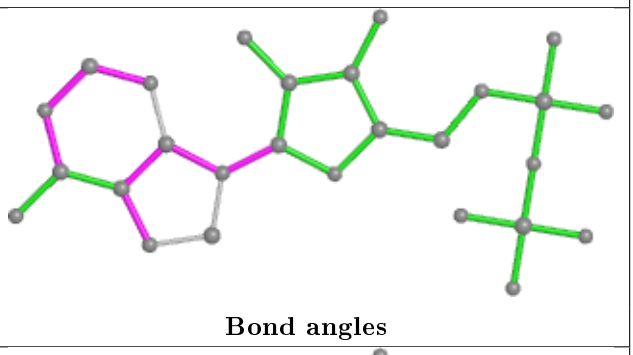


Rings

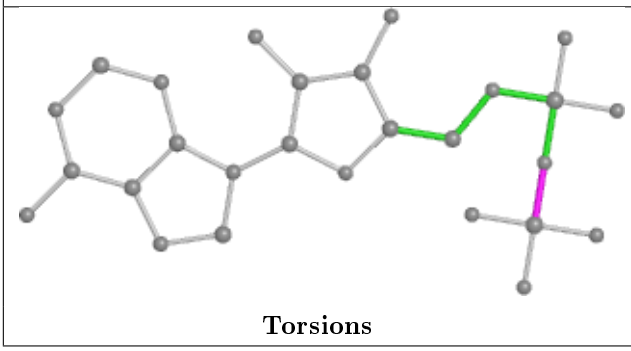
Ligand ADP B 1304



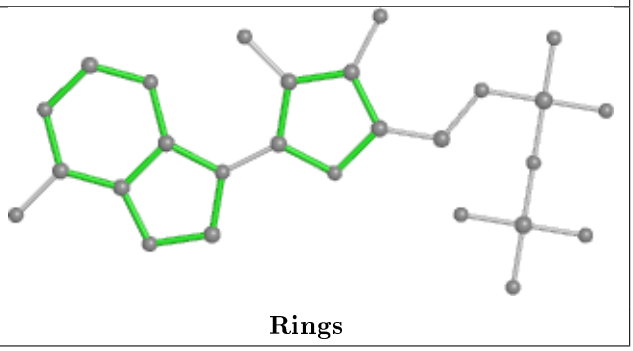
Bond lengths



Bond angles

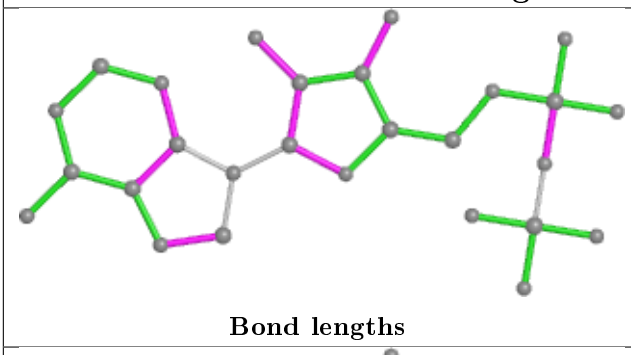


Torsions

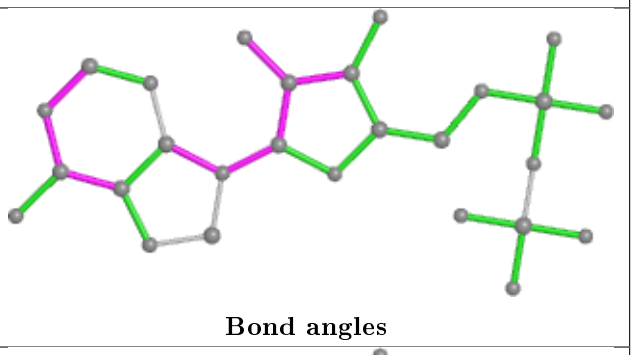


Rings

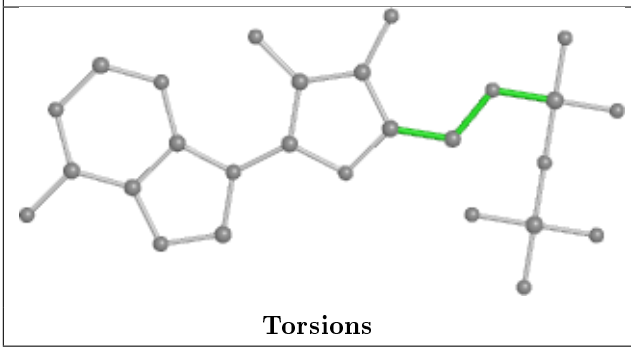
Ligand ADX C 1307



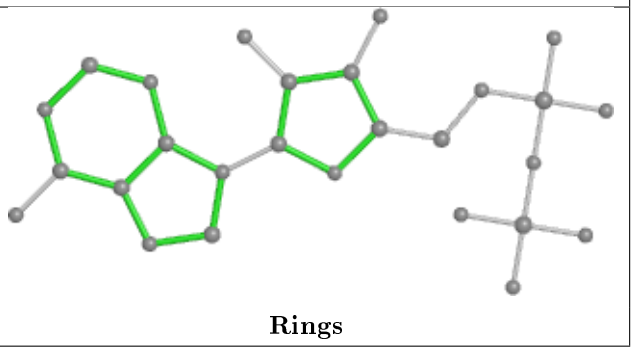
Bond lengths



Bond angles

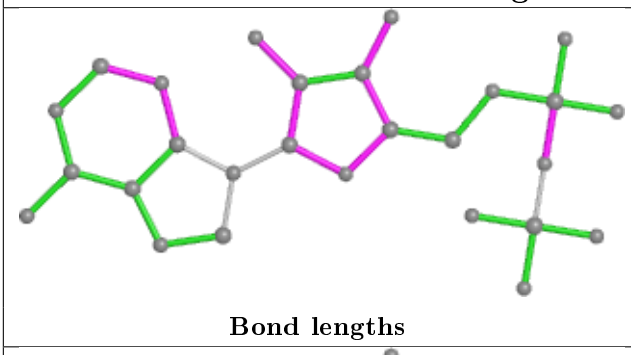


Torsions

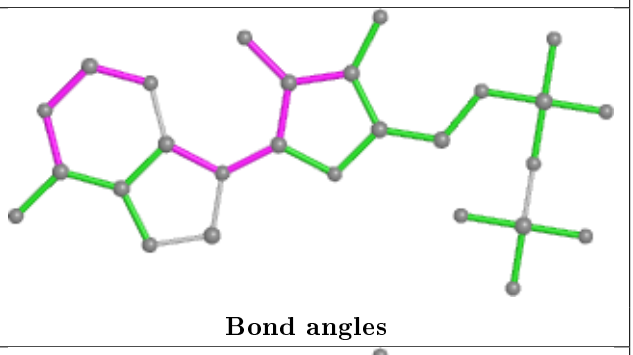


Rings

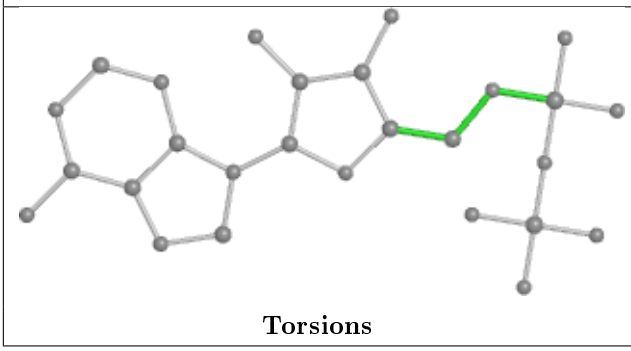
Ligand ADX D 1310



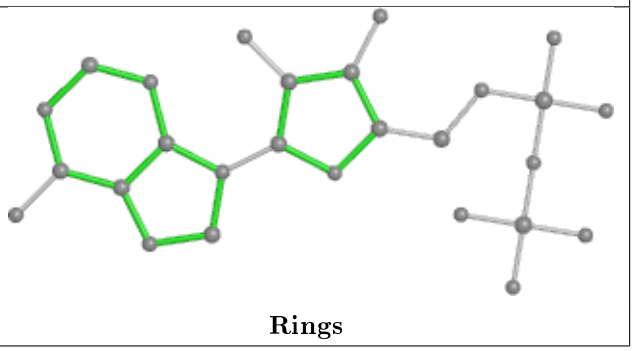
Bond lengths



Bond angles

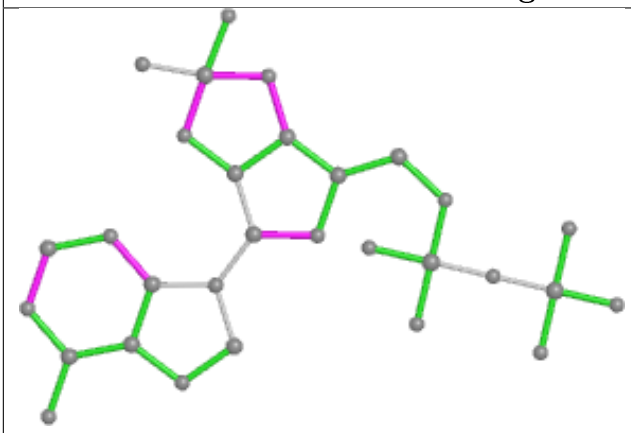


Torsions

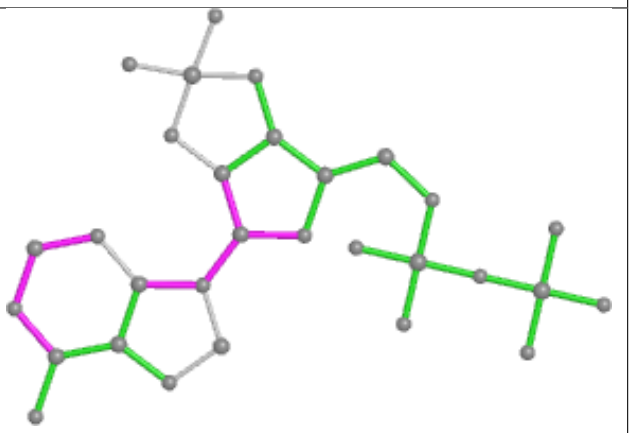


Rings

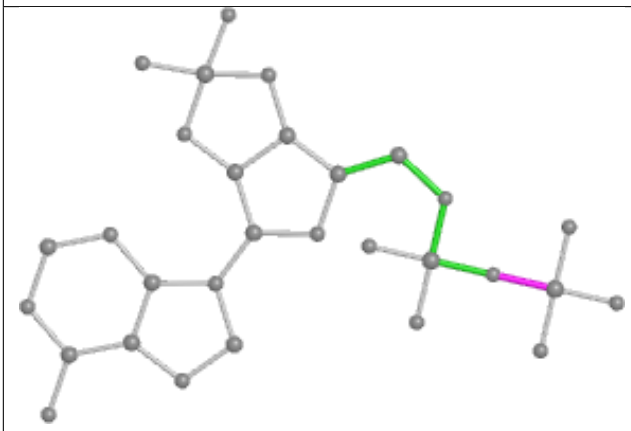
Ligand AV2 A 1301



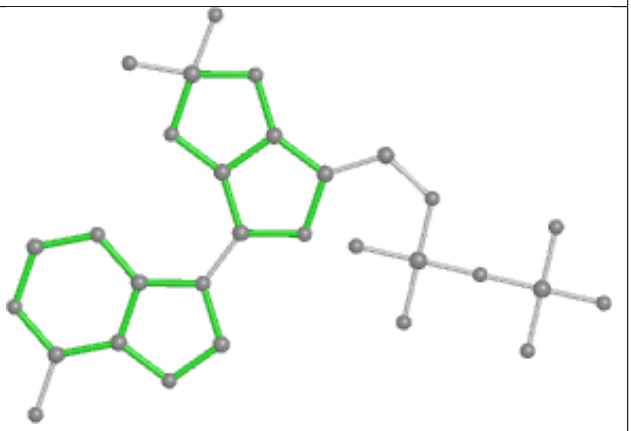
Bond lengths



Bond angles

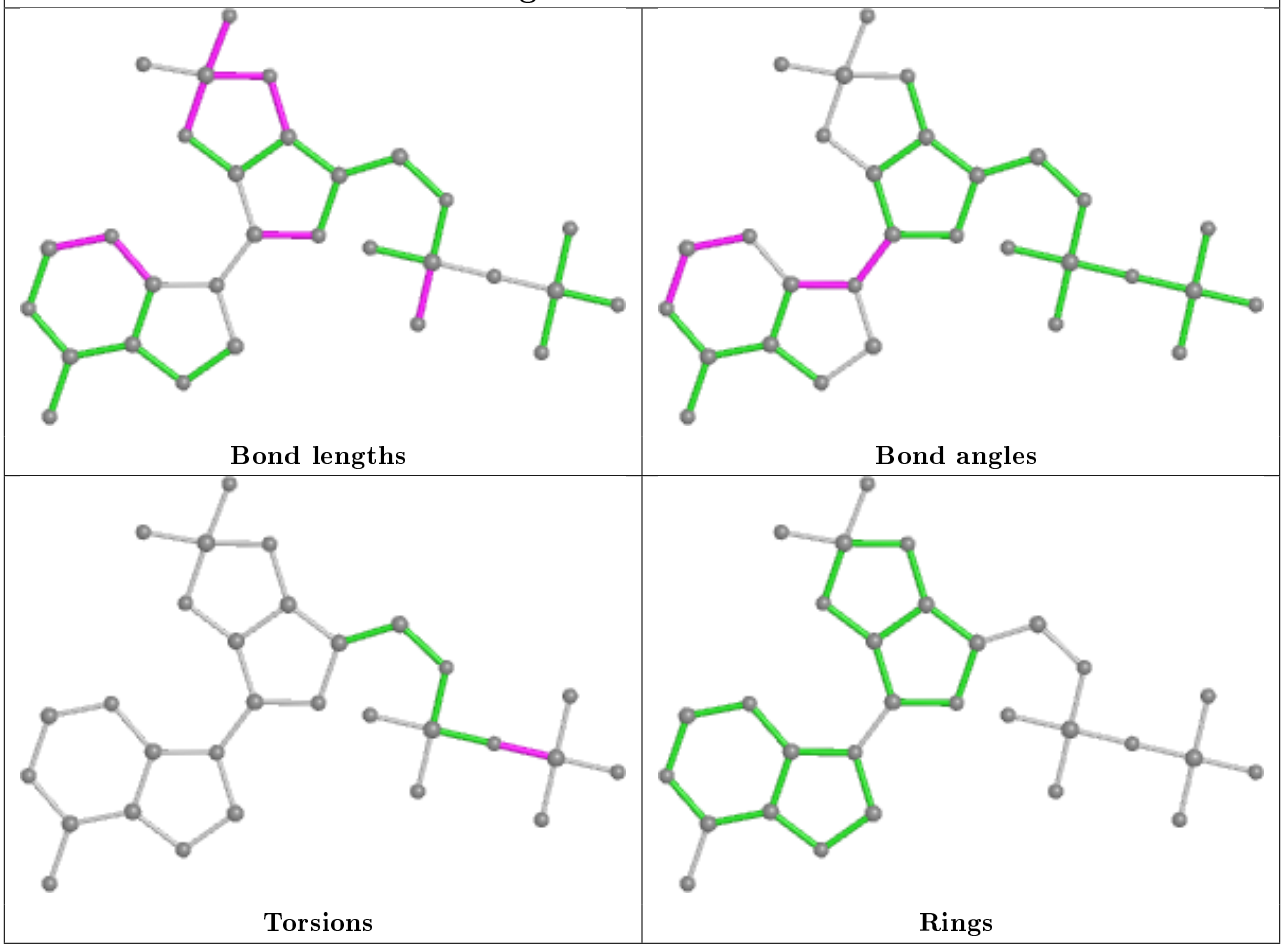


Torsions



Rings

Ligand AV2 C 1306



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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	208/211 (98%)	-0.00	10 (4%)	30	31	8, 14, 34, 49	0
1	B	182/211 (86%)	-0.02	3 (1%)	72	72	10, 15, 31, 53	0
1	C	209/211 (99%)	0.09	12 (5%)	23	23	8, 16, 34, 61	0
1	D	183/211 (86%)	0.09	9 (4%)	29	30	8, 14, 34, 69	0
All	All	782/844 (92%)	0.04	34 (4%)	35	36	8, 15, 34, 69	0

The worst 5 of 34 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	124	THR	10.9
1	D	123	ALA	10.1
1	D	129	THR	6.8
1	C	208	ALA	5.8
1	C	210	LYS	5.6

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

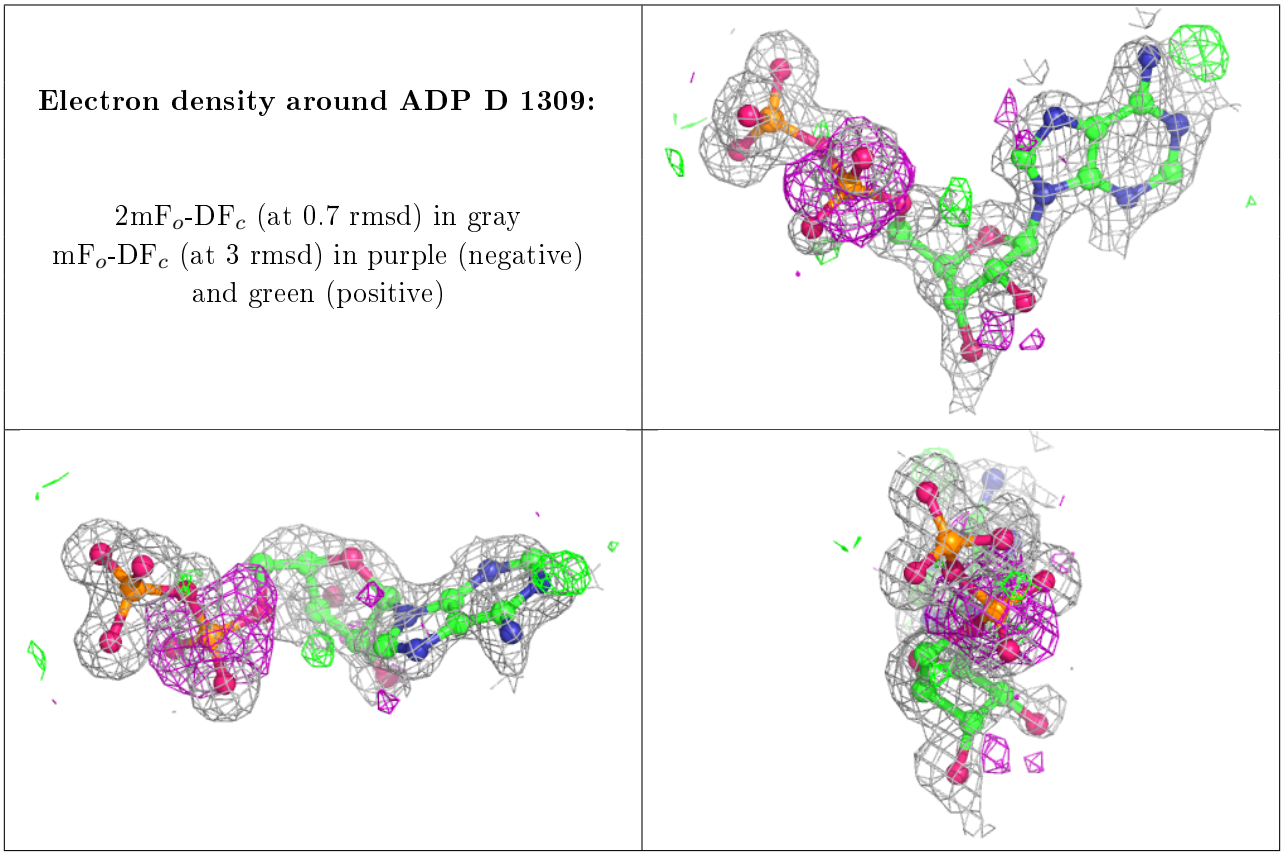
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	GOL	B	2011	6/6	0.66	0.27	47,49,49,50	0
2	SO4	B	2004	5/5	0.69	0.22	63,63,66,66	5
2	SO4	A	2003	5/5	0.83	0.16	55,57,59,59	0
6	GOL	C	2010	6/6	0.83	0.15	23,29,31,34	0
2	SO4	C	2006	5/5	0.87	0.12	49,53,54,54	0
5	ADP	D	1309	27/27	0.95	0.16	11,45,47,50	0
5	ADP	B	1304	27/27	0.96	0.12	12,26,30,32	0
2	SO4	C	2005	5/5	0.96	0.10	38,40,42,42	0
2	SO4	A	2002	5/5	0.98	0.07	24,26,28,31	0
3	AV2	A	1301	30/30	0.98	0.07	9,13,18,18	3
3	AV2	C	1306	30/30	0.98	0.07	10,15,19,21	3
4	ADX	D	1310	27/27	0.99	0.06	8,10,12,15	0
2	SO4	A	2001	5/5	0.99	0.06	18,19,22,26	0
4	ADX	A	1302	27/27	0.99	0.06	9,10,11,14	0
4	ADX	B	1305	27/27	0.99	0.06	10,11,14,15	0
4	ADX	C	1307	27/27	0.99	0.06	8,10,12,15	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.

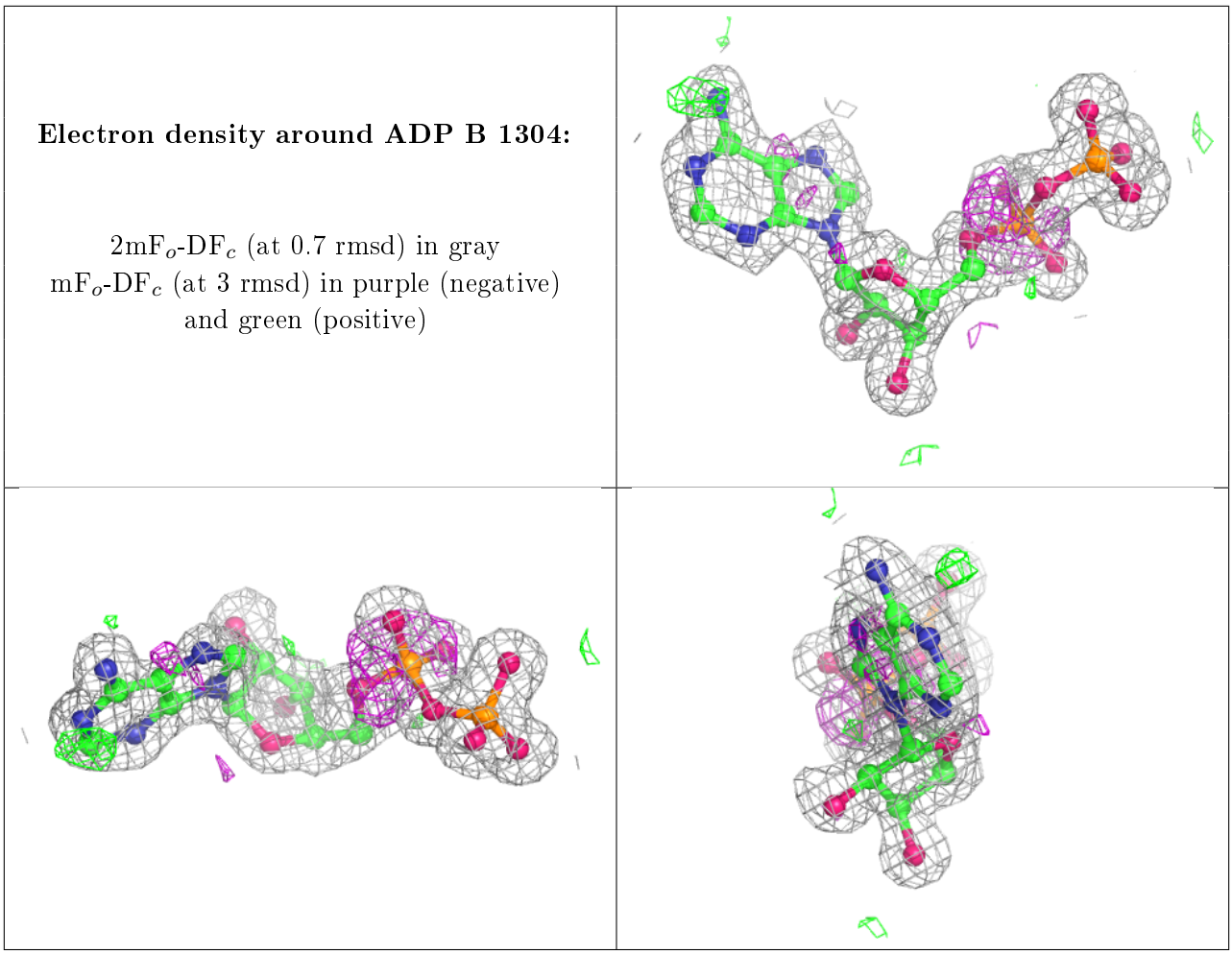
Electron density around ADP D 1309:

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



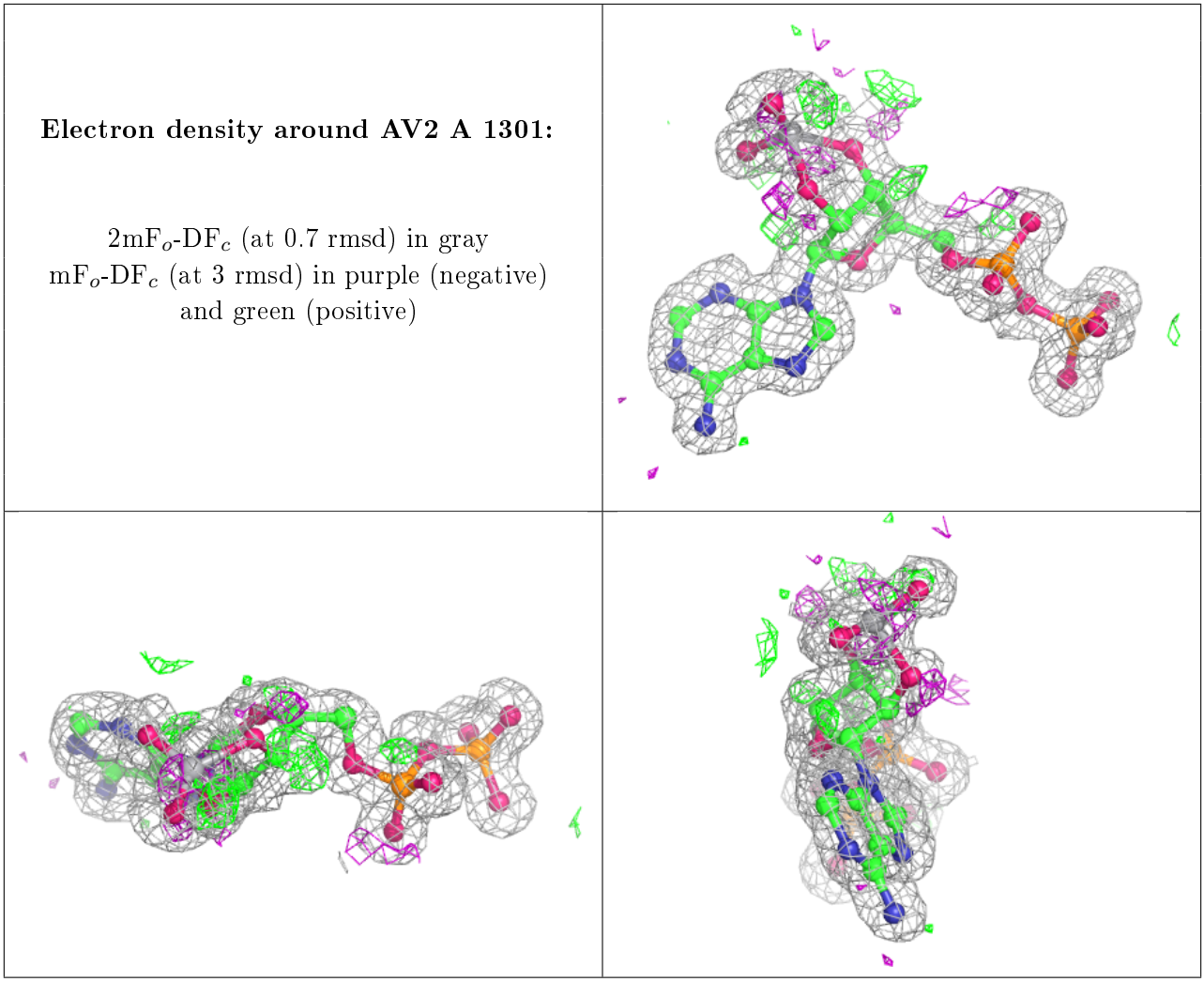
Electron density around ADP B 1304:

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



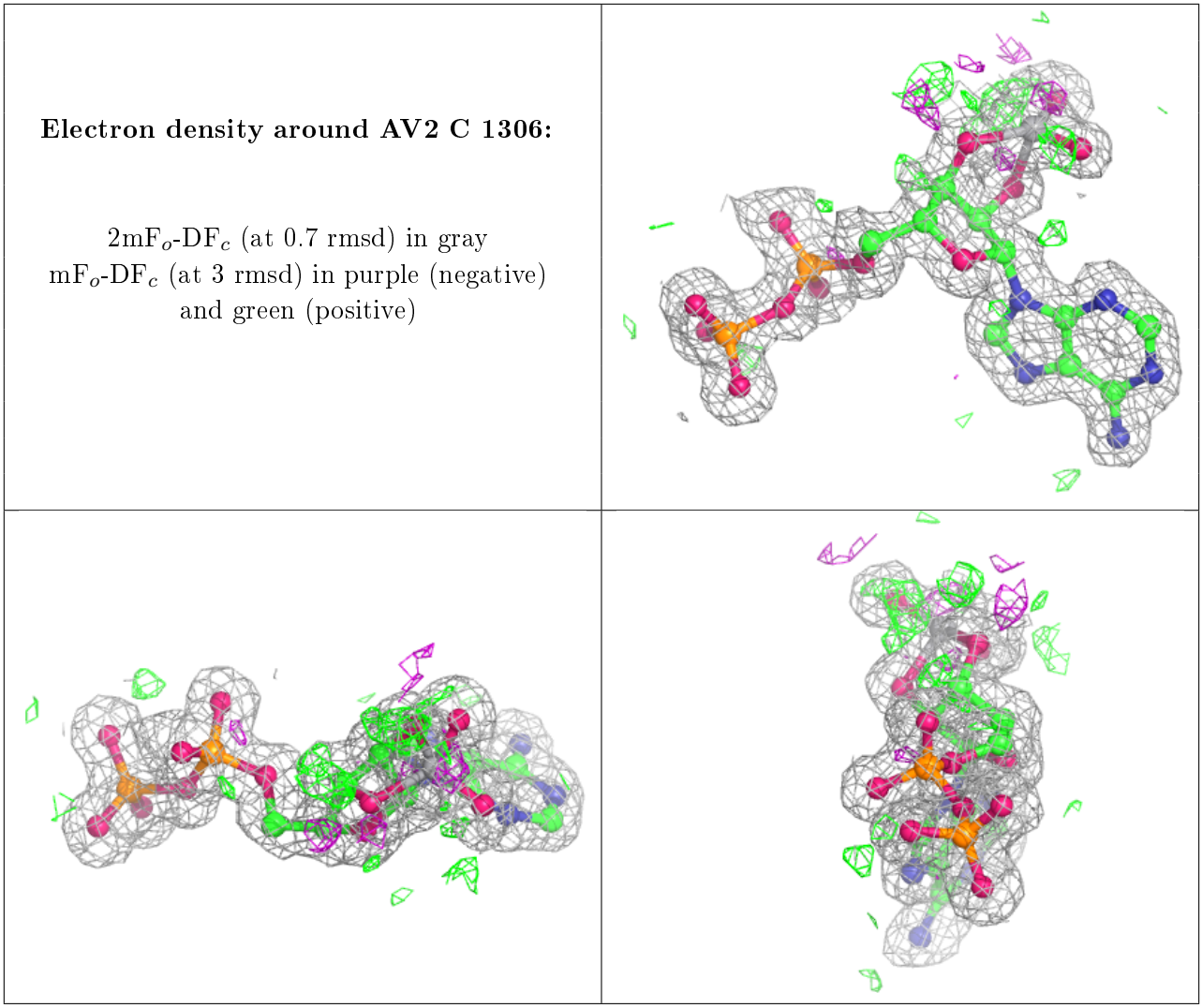
Electron density around AV2 A 1301:

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



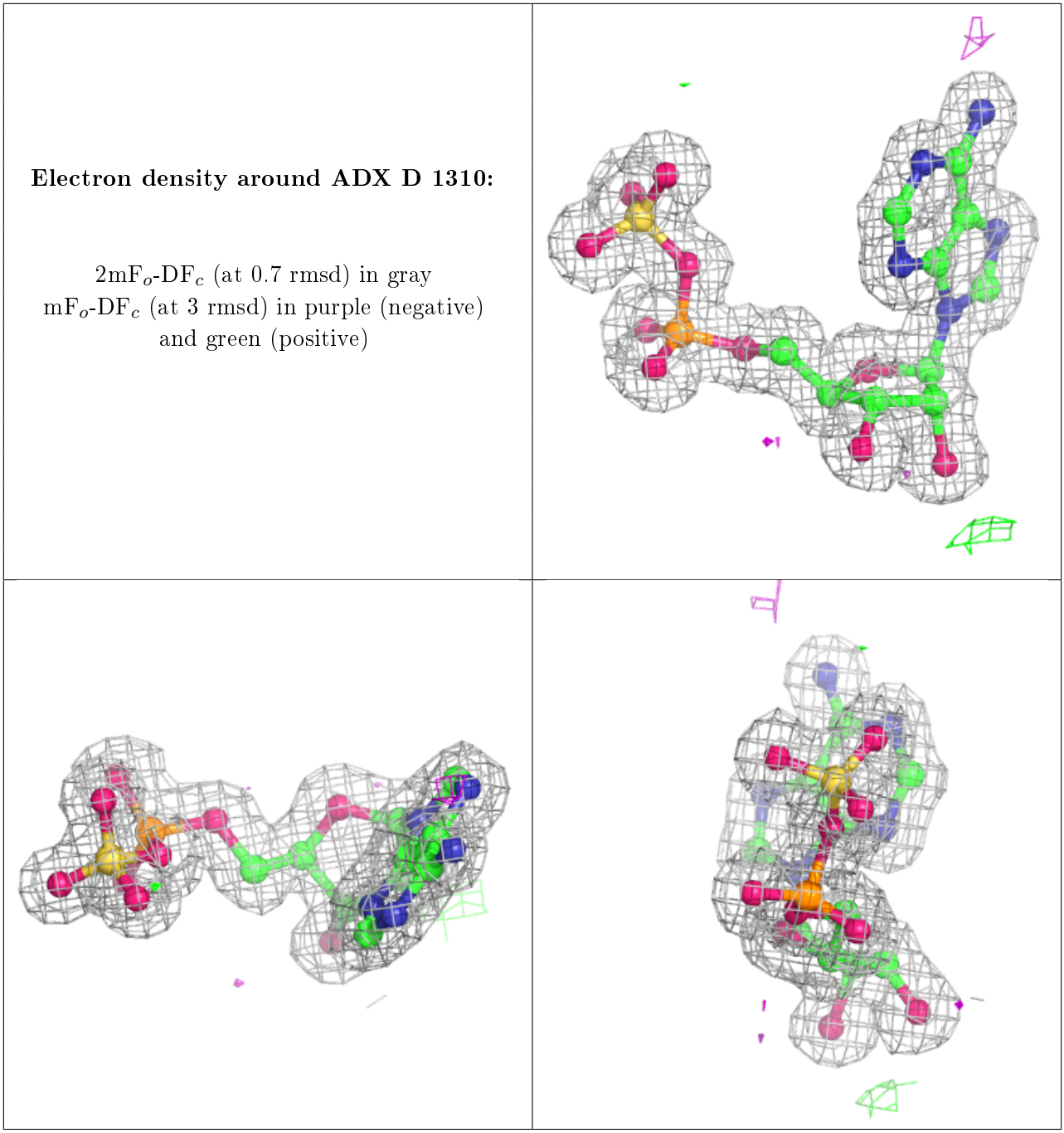
Electron density around AV2 C 1306:

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



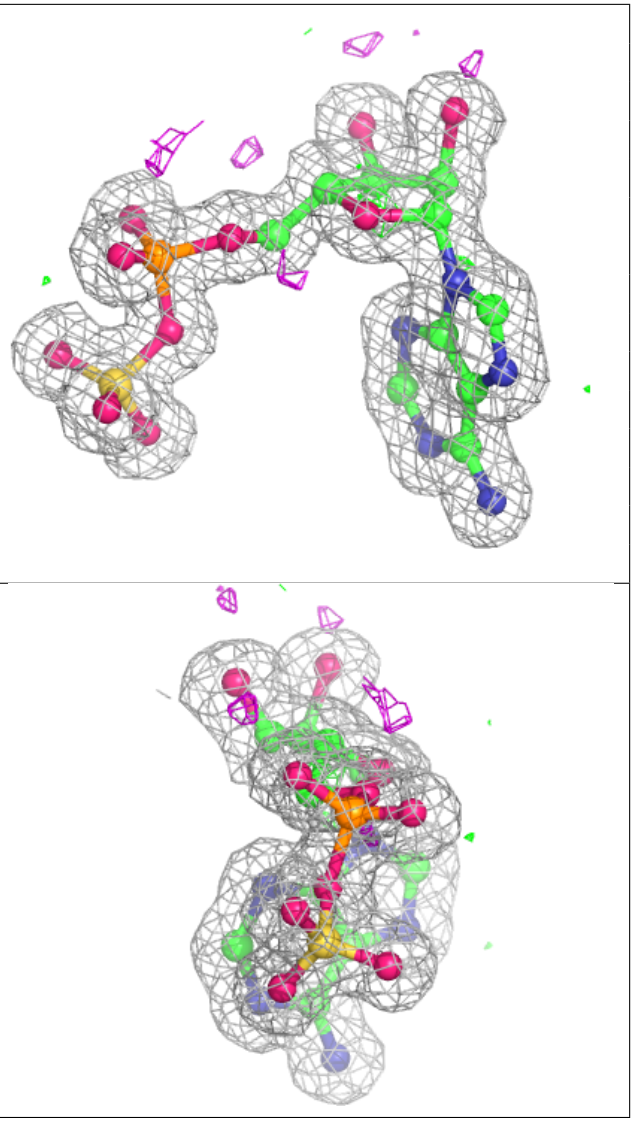
Electron density around ADX D 1310:

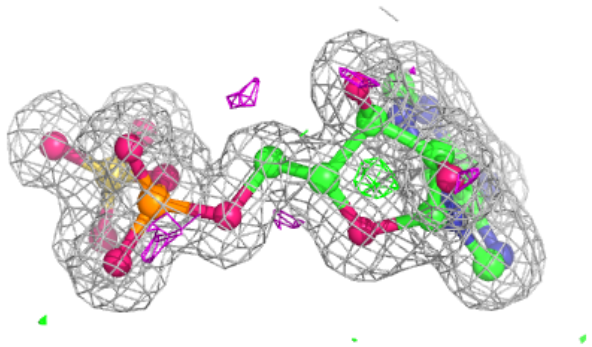
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around ADX A 1302:

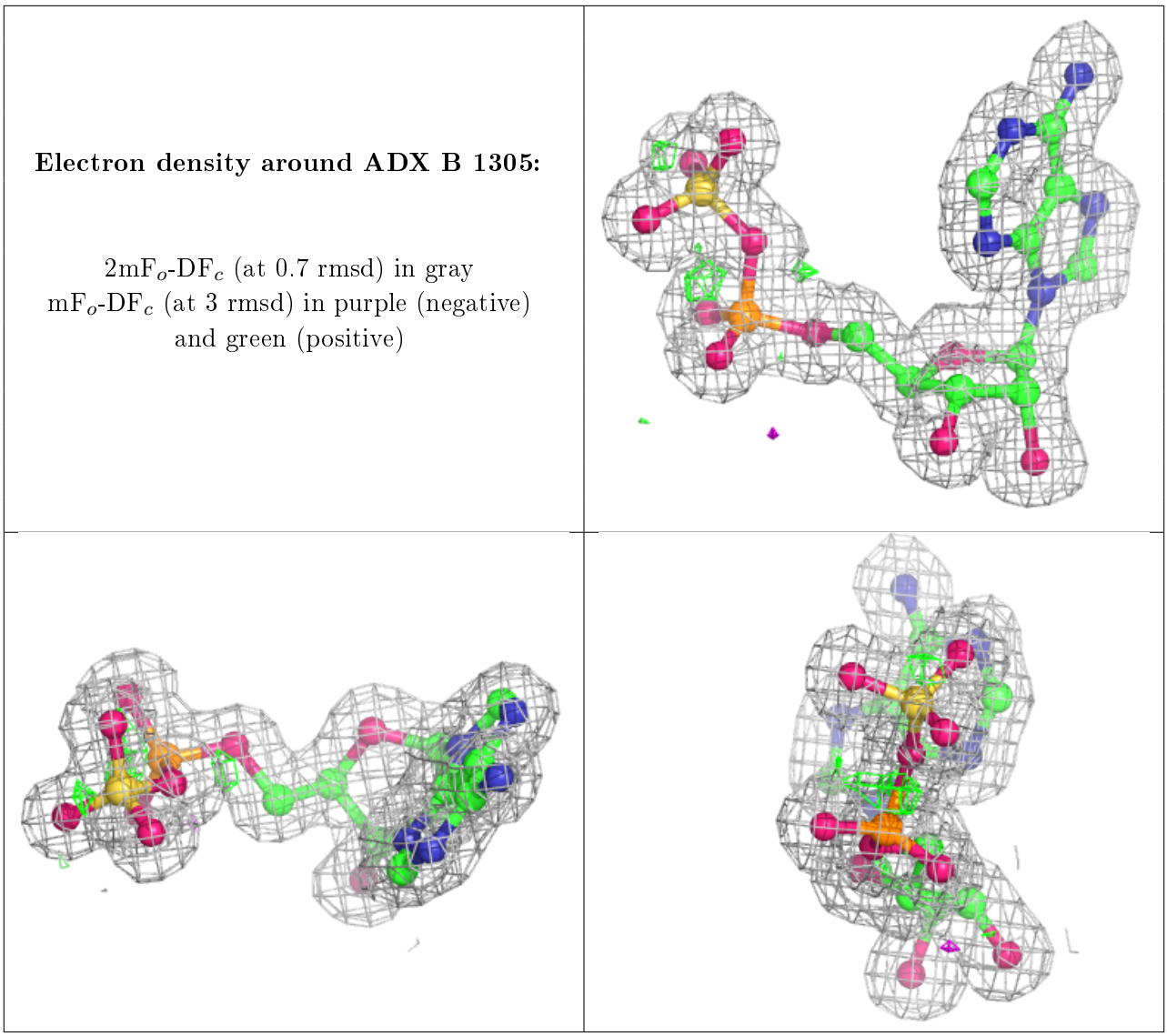
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





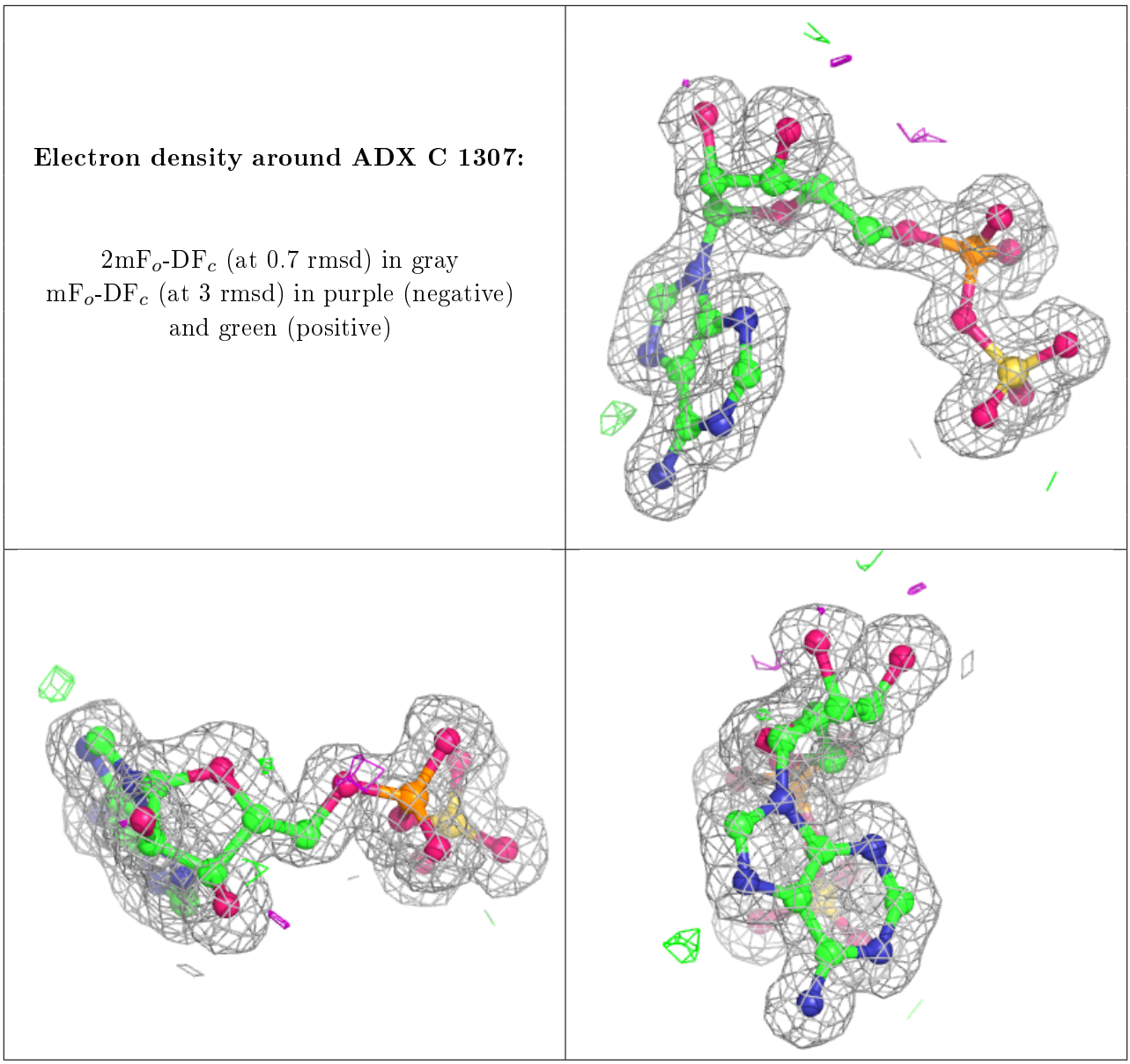
Electron density around ADX B 1305:

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



Electron density around ADX C 1307:

$2mF_o$-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

There are no such residues in this entry.