



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 16, 2020 – 12:21 am BST

PDB ID : 1KEE  
Title : Inactivation of the Amidotransferase Activity of Carbamoyl Phosphate Synthetase by the Antibiotic Acivicin  
Authors : Miles, B.W.; Thoden, J.B.; Holden, H.M.; Raushel, F.M.  
Deposited on : 2001-11-15  
Resolution : 2.10 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](mailto: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	:	2.11
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

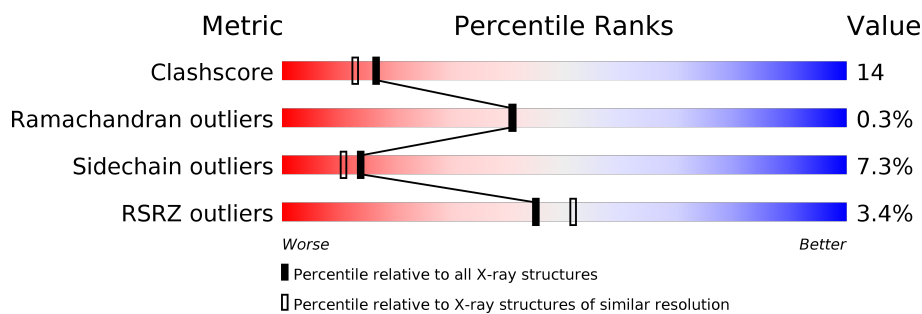
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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))
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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  $\geq 3$ , 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	1073	<div> <div>3%</div> <div>63%</div> <div>29%</div> <div>6%</div> <div>..</div> </div>
1	C	1073	<div> <div>4%</div> <div>63%</div> <div>29%</div> <div>7%</div> <div>..</div> </div>
1	E	1073	<div> <div>4%</div> <div>64%</div> <div>29%</div> <div>5%</div> <div>..</div> </div>
1	G	1073	<div> <div>5%</div> <div>60%</div> <div>30%</div> <div>7%</div> <div>..</div> </div>
2	B	382	<div> <div>%</div> <div>62%</div> <div>32%</div> <div>5%</div> <div>.</div> </div>
2	D	382	<div> <div>61%</div> <div>34%</div> <div>.</div> <div>.</div> </div>
2	F	382	<div> <div>3%</div> <div>61%</div> <div>33%</div> <div>5%</div> <div>.</div> </div>

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
2	H	382	

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	143	B	269	X	-	-	-
2	143	D	269	X	-	-	-
2	143	F	269	X	-	-	-
2	143	H	269	X	-	-	-

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 48896 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 Carbamoyl-phosphate synthetase large chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1058	Total	C	N	O	S	0	5	0
			8181	5136	1425	1575	45			
1	C	1058	Total	C	N	O	S	0	2	0
			8172	5130	1425	1572	45			
1	E	1058	Total	C	N	O	S	0	8	0
			8204	5150	1430	1579	45			
1	G	1058	Total	C	N	O	S	0	0	0
			8160	5123	1422	1570	45			

- Molecule 2 is a protein called Carbamoyl-phosphate synthetase small chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	379	Total	C	N	O	S	0	1	0
			2912	1834	513	555	10			
2	D	379	Total	C	N	O	S	0	1	0
			2907	1831	510	556	10			
2	F	379	Total	C	N	O	S	0	0	0
			2905	1830	510	555	10			
2	H	379	Total	C	N	O	S	0	0	0
			2905	1830	510	555	10			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	269	143	CYS	modified residue	UNP P00907
D	269	143	CYS	modified residue	UNP P00907
F	269	143	CYS	modified residue	UNP P00907
H	269	143	CYS	modified residue	UNP P00907

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	3	Total Mn 3 3	0	0
3	A	3	Total Mn 3 3	0	0
3	C	3	Total Mn 3 3	0	0
3	E	3	Total Mn 3 3	0	0

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	7	Total K 7 7	0	0
4	D	1	Total K 1 1	0	0
4	E	7	Total K 7 7	0	0
4	H	1	Total K 1 1	0	0
4	B	1	Total K 1 1	0	0
4	C	7	Total K 7 7	0	0
4	A	7	Total K 7 7	0	0
4	F	1	Total K 1 1	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

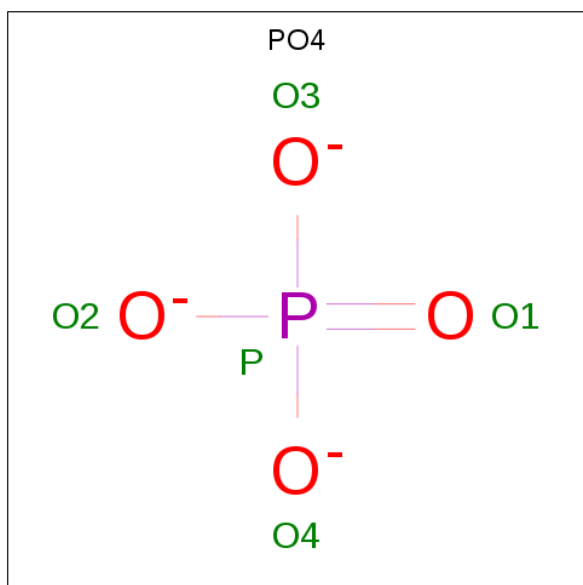
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	G	4	Total Cl 4 4	0	0
5	D	1	Total Cl 1 1	0	0
5	E	4	Total Cl 4 4	0	0
5	H	1	Total Cl 1 1	0	0
5	B	1	Total Cl 1 1	0	0
5	C	5	Total Cl 5 5	0	0

*Continued on next page...*

*Continued from previous page...*

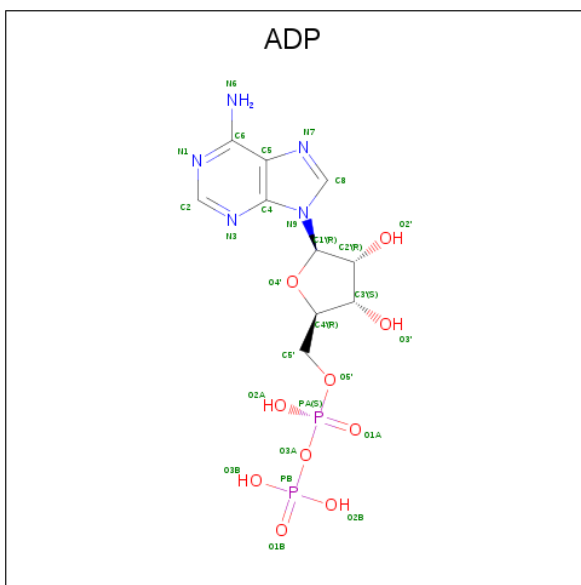
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	5	Total	Cl	0	0
			5	5		
5	F	1	Total	Cl	0	0
			1	1		

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



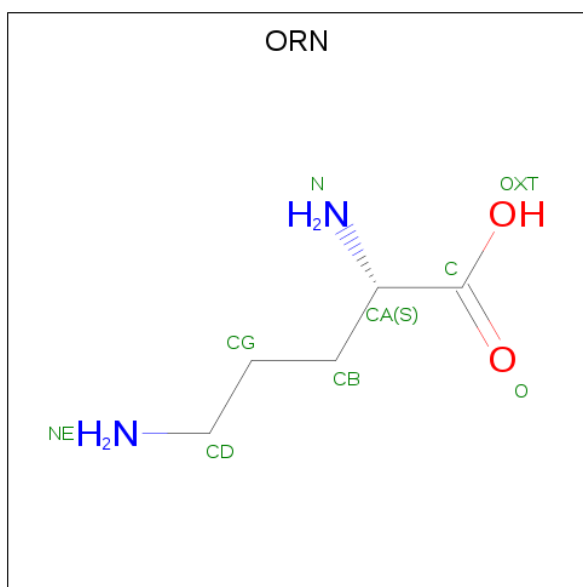
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	P	0	0
			5	4	1		
6	C	1	Total	O	P	0	0
			5	4	1		
6	E	1	Total	O	P	0	0
			5	4	1		
6	G	1	Total	O	P	0	0
			5	4	1		

- Molecule 7 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>).



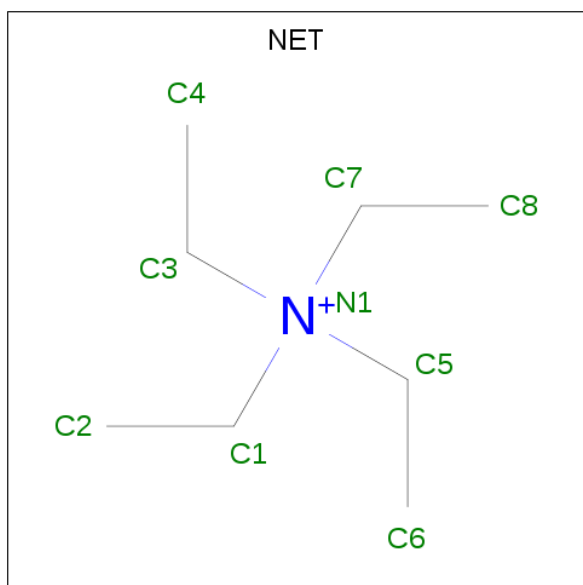
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total 27	C 10	N 5	O 10	P 2	0	0
7	A	1	Total 27	C 10	N 5	O 10	P 2	0	0
7	C	1	Total 27	C 10	N 5	O 10	P 2	0	0
7	C	1	Total 27	C 10	N 5	O 10	P 2	0	0
7	E	1	Total 27	C 10	N 5	O 10	P 2	0	0
7	E	1	Total 27	C 10	N 5	O 10	P 2	0	0
7	G	1	Total 27	C 10	N 5	O 10	P 2	0	0
7	G	1	Total 27	C 10	N 5	O 10	P 2	0	0

- Molecule 8 is L-ornithine (three-letter code: ORN) (formula:  $\text{C}_5\text{H}_{12}\text{N}_2\text{O}_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			9	5	2	2		
8	C	1	Total	C	N	O	0	0
			9	5	2	2		
8	E	1	Total	C	N	O	0	0
			9	5	2	2		
8	G	1	Total	C	N	O	0	0
			9	5	2	2		

- Molecule 9 is TETRAETHYLAMMONIUM ION (three-letter code: NET) (formula: C<sub>8</sub>H<sub>20</sub>N).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C N 9 8 1	0	0
9	C	1	Total C N 9 8 1	0	0
9	E	1	Total C N 9 8 1	0	0
9	G	1	Total C N 9 8 1	0	0

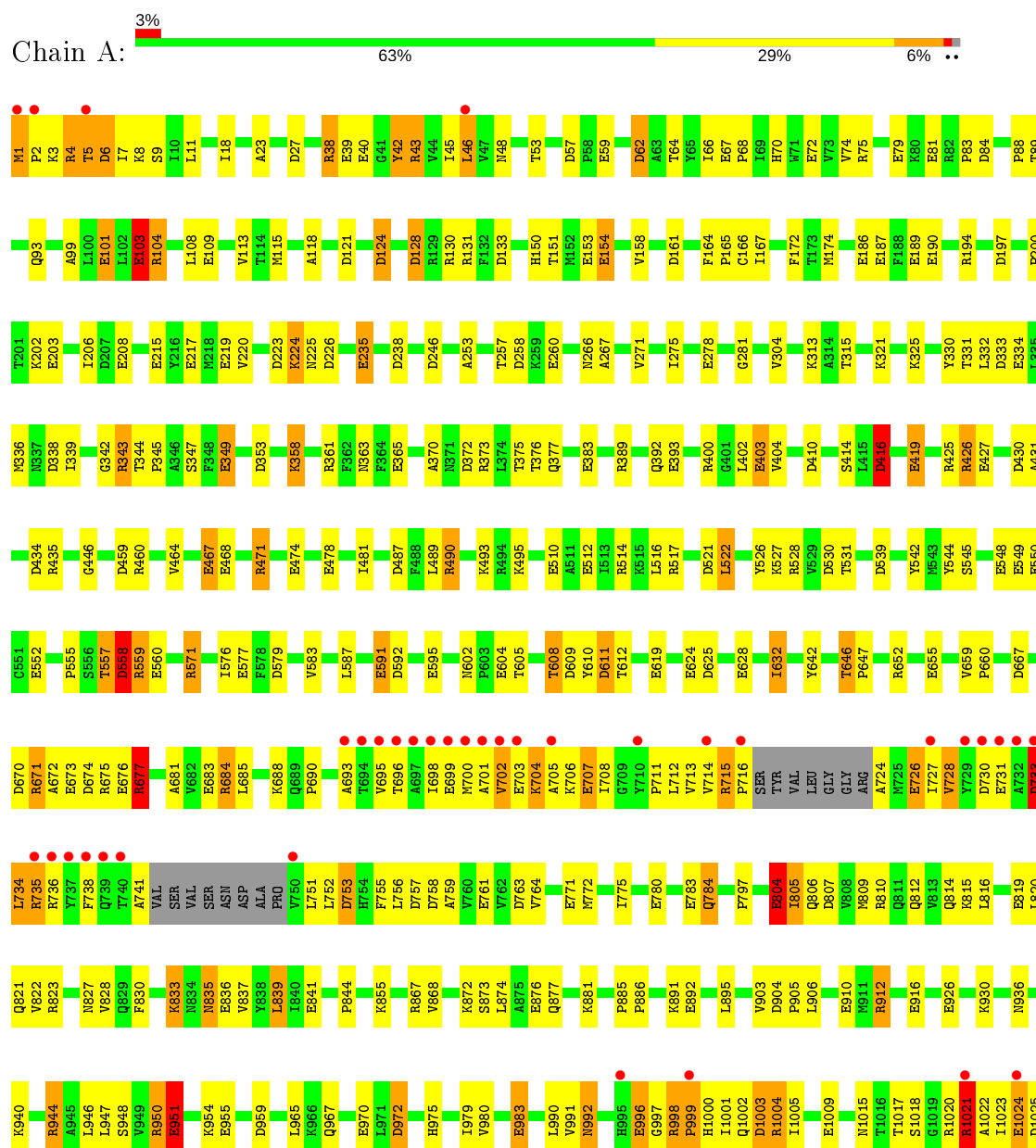
- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	841	Total O 841 841	0	0
10	B	230	Total O 230 230	0	0
10	C	783	Total O 783 783	0	0
10	D	304	Total O 304 304	0	0
10	E	886	Total O 886 886	0	0
10	F	263	Total O 263 263	0	0
10	G	678	Total O 678 678	0	0
10	H	191	Total O 191 191	0	0

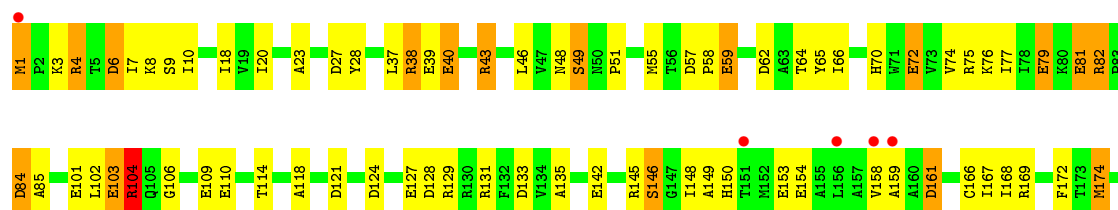
### 3 Residue-property plots [i](#)

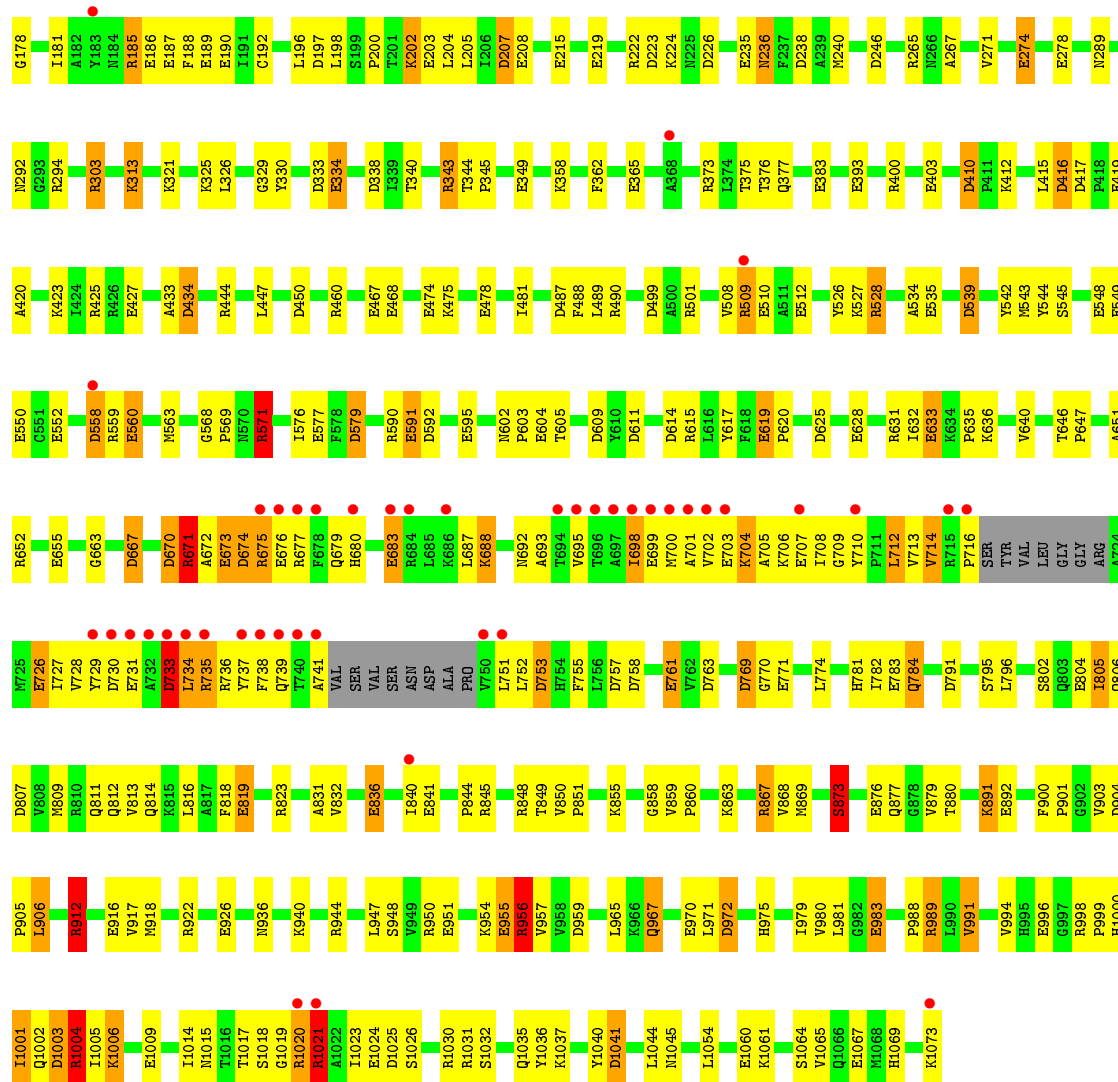
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

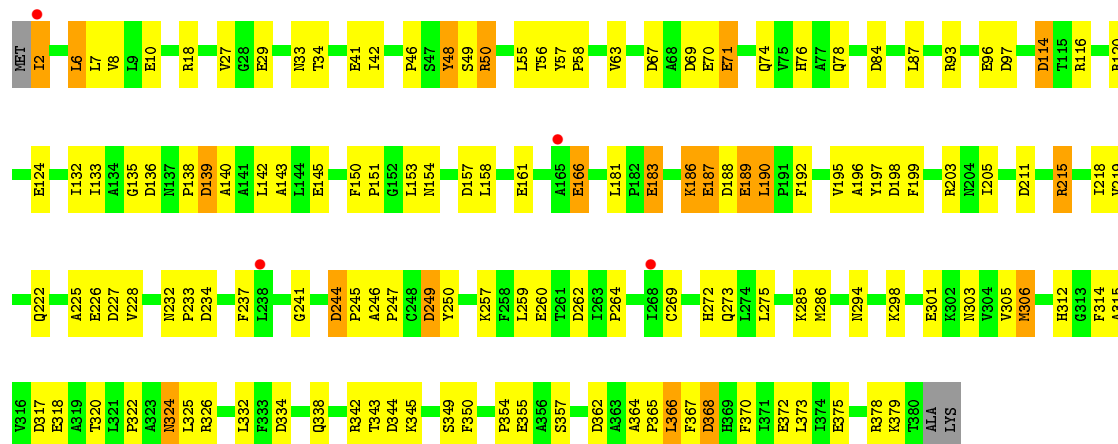




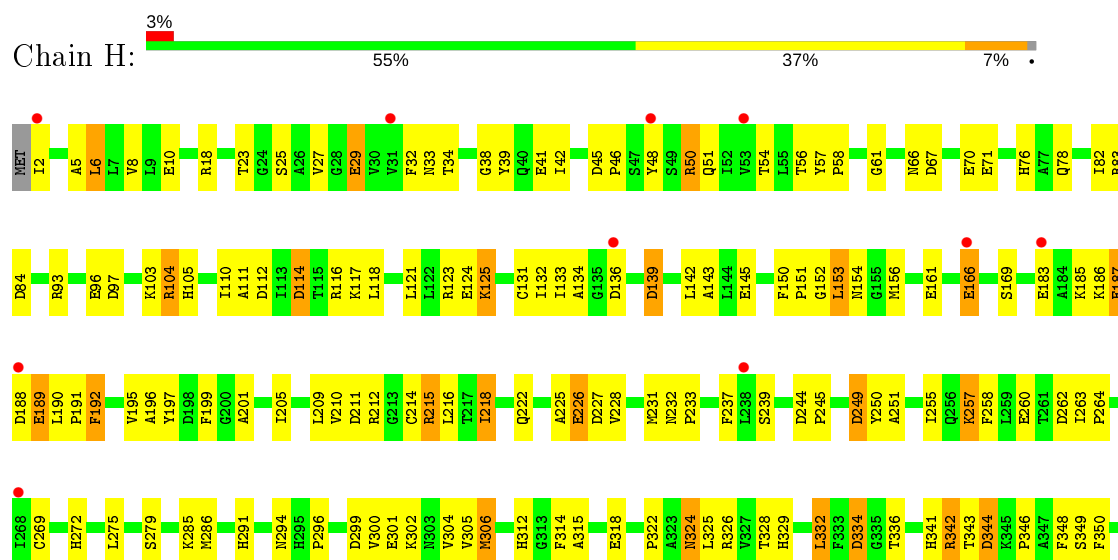




• Molecule 2: Carbamoyl-phosphate synthetase small chain



• Molecule 2: Carbamoyl-phosphate synthetase small chain



P354	E355	A356	S357	P358	D362	A363	A364	P365	L366	F367	D368	H369	F370	I371	E372	E375	T380	ALA	LYS
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	152.40 Å 164.40 Å 333.20 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.10 29.99 – 2.10	Depositor EDS
% Data completeness (in resolution range)	88.9 (30.00-2.10) 88.9 (29.99-2.10)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	0.04	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.07 (at 2.10 Å)	Xtriage
Refinement program	TNT	Depositor
R, $R_{free}$	0.186 , 0.211 0.179 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.4	Xtriage
Anisotropy	0.089	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 108.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	48896	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.83% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: 143, ADP, CL, PO4, MN, ORN, NET, K

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	0.99	76/8327 (0.9%)	1.38	120/11257 (1.1%)
1	C	0.99	79/8306 (1.0%)	1.34	111/11228 (1.0%)
1	E	1.00	77/8362 (0.9%)	1.34	118/11302 (1.0%)
1	G	0.97	74/8286 (0.9%)	1.38	120/11202 (1.1%)
2	B	0.88	20/2961 (0.7%)	1.28	38/4019 (0.9%)
2	D	0.90	19/2956 (0.6%)	1.29	33/4013 (0.8%)
2	F	0.90	18/2950 (0.6%)	1.31	39/4005 (1.0%)
2	H	0.88	20/2950 (0.7%)	1.28	36/4005 (0.9%)
All	All	0.96	383/45098 (0.8%)	1.34	615/61031 (1.0%)

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
2	B	1	0
2	D	1	0
2	F	1	0
2	H	1	0
All	All	4	0

The worst 5 of 383 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	183	GLU	CD-OE2	8.23	1.34	1.25
1	C	110	GLU	CD-OE2	8.18	1.34	1.25
2	D	183	GLU	CD-OE2	8.05	1.34	1.25
1	E	467	GLU	CD-OE2	8.02	1.34	1.25
2	F	355	GLU	CD-OE2	8.01	1.34	1.25

The worst 5 of 615 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	38	ARG	NE-CZ-NH1	11.63	126.11	120.30
1	E	956	ARG	NE-CZ-NH2	-11.36	114.62	120.30
1	A	642	TYR	CB-CG-CD2	-11.19	114.28	121.00
1	E	43	ARG	NE-CZ-NH2	-10.47	115.06	120.30
1	A	1004	ARG	NE-CZ-NH1	10.36	125.48	120.30

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	269	143	CD
2	D	269	143	CD
2	F	269	143	CD
2	H	269	143	CD

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	8181	0	8215	216	0
1	C	8172	0	8206	231	0
1	E	8204	0	8235	208	0
1	G	8160	0	8196	256	0
2	B	2912	0	2874	84	0
2	D	2907	0	2866	90	0
2	F	2905	0	2864	84	0
2	H	2905	0	2864	109	0
3	A	3	0	0	0	0
3	C	3	0	0	0	0
3	E	3	0	0	0	0
3	G	3	0	0	0	0
4	A	7	0	0	0	0
4	B	1	0	0	0	0
4	C	7	0	0	0	0
4	D	1	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	7	0	0	1	0
4	F	1	0	0	0	0
4	G	7	0	0	0	0
4	H	1	0	0	0	0
5	A	5	0	0	1	0
5	B	1	0	0	0	0
5	C	5	0	0	1	0
5	D	1	0	0	0	0
5	E	4	0	0	1	0
5	F	1	0	0	0	0
5	G	4	0	0	1	0
5	H	1	0	0	0	0
6	A	5	0	0	0	0
6	C	5	0	0	1	0
6	E	5	0	0	0	0
6	G	5	0	0	1	0
7	A	54	0	24	0	0
7	C	54	0	24	0	0
7	E	54	0	24	4	0
7	G	54	0	24	4	0
8	A	9	0	11	0	0
8	C	9	0	11	1	0
8	E	9	0	11	1	0
8	G	9	0	11	2	0
9	A	9	0	20	4	0
9	C	9	0	20	0	0
9	E	9	0	20	1	0
9	G	9	0	20	1	0
10	A	841	0	0	23	0
10	B	230	0	0	5	0
10	C	783	0	0	20	0
10	D	304	0	0	8	0
10	E	886	0	0	20	0
10	F	263	0	0	1	0
10	G	678	0	0	13	0
10	H	191	0	0	4	0
All	All	48896	0	44540	1267	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 14.

The worst 5 of 1267 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:E:46:LEU:HD22	1:E:46:LEU:O	1.37	1.20
1:A:46:LEU:O	1:A:46:LEU:HD22	1.42	1.18
1:C:695:VAL:HG11	1:C:701:ALA:HB2	1.27	1.14
2:D:228:VAL:HA	2:D:231:MET:HE2	1.26	1.10
2:H:187:GLU:HG2	2:H:215:ARG:HD2	1.32	1.09

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	1057/1073 (98%)	998 (94%)	56 (5%)	3 (0%)	41	41
1	C	1054/1073 (98%)	1002 (95%)	48 (5%)	4 (0%)	34	32
1	E	1060/1073 (99%)	1012 (96%)	45 (4%)	3 (0%)	41	41
1	G	1052/1073 (98%)	998 (95%)	49 (5%)	5 (0%)	29	26
2	B	377/382 (99%)	363 (96%)	14 (4%)	0	100	100
2	D	377/382 (99%)	363 (96%)	14 (4%)	0	100	100
2	F	376/382 (98%)	364 (97%)	12 (3%)	0	100	100
2	H	376/382 (98%)	362 (96%)	14 (4%)	0	100	100
All	All	5729/5820 (98%)	5462 (95%)	252 (4%)	15 (0%)	41	41

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	996	GLU
1	G	873	SER
1	A	558	ASP
1	A	975	HIS
1	E	675	ARG

### 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	A	870/878 (99%)	808 (93%)	62 (7%)	14	11
1	C	867/878 (99%)	797 (92%)	70 (8%)	11	8
1	E	873/878 (99%)	818 (94%)	55 (6%)	18	15
1	G	865/878 (98%)	793 (92%)	72 (8%)	11	7
2	B	308/309 (100%)	288 (94%)	20 (6%)	17	14
2	D	308/309 (100%)	288 (94%)	20 (6%)	17	14
2	F	307/309 (99%)	281 (92%)	26 (8%)	10	7
2	H	307/309 (99%)	286 (93%)	21 (7%)	16	13
All	All	4705/4748 (99%)	4359 (93%)	346 (7%)	14	10

5 of 346 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	153	LEU
1	E	591	GLU
1	G	1006	LYS
2	D	222	GLN
1	E	68	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 87 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	1071	GLN
1	E	457	ASN
1	G	1055	ASN
2	D	14	GLN
2	D	324	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	143	B	269	2	6,16,17	5.95	2 (33%)	3,21,23	2.51	1 (33%)
2	143	D	269	2	6,16,17	7.65	3 (50%)	3,21,23	1.60	1 (33%)
2	143	F	269	2	6,16,17	9.02	3 (50%)	3,21,23	2.10	1 (33%)
2	143	H	269	2	6,16,17	10.20	3 (50%)	3,21,23	1.65	0

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	143	B	269	2	1/1/5/8	2/5/24/26	0/1/1/1
2	143	D	269	2	1/1/5/8	2/5/24/26	0/1/1/1
2	143	F	269	2	1/1/5/8	3/5/24/26	0/1/1/1
2	143	H	269	2	1/1/5/8	3/5/24/26	0/1/1/1

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	269	143	CD-NX	-20.68	1.17	1.45
2	F	269	143	CD-NX	-19.40	1.19	1.45
2	D	269	143	CD-NX	-16.99	1.22	1.45
2	B	269	143	CD-NX	-13.21	1.27	1.45
2	H	269	143	CD-CE	-12.18	1.33	1.49

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	269	143	CJ-CI-CF	4.13	118.57	112.63

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	269	143	CJ-CI-CF	2.96	116.89	112.63
2	D	269	143	CJ-CI-CF	2.49	116.22	112.63

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	269	143	CD
2	D	269	143	CD
2	F	269	143	CD
2	H	269	143	CD

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	269	143	N-CA-CB-SG
2	B	269	143	OF-CF-CI-CJ
2	D	269	143	N-CA-CB-SG
2	D	269	143	OF-CF-CI-CJ
2	F	269	143	N-CA-CB-SG

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	269	143	2	0
2	D	269	143	3	0
2	F	269	143	2	0
2	H	269	143	2	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 86 ligands modelled in this entry, 66 are monoatomic - leaving 20 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
7	ADP	E	2051	3,4	24,29,29	1.15	4 (16%)	29,45,45	1.06	3 (10%)
8	ORN	E	5055	-	4,8,8	1.29	1 (25%)	3,9,9	0.37	0
7	ADP	A	2007	3,4	24,29,29	1.01	1 (4%)	29,45,45	1.27	3 (10%)
6	PO4	G	2071	3	4,4,4	2.07	1 (25%)	6,6,6	1.05	0
7	ADP	G	2072	3,4	24,29,29	1.20	4 (16%)	29,45,45	1.37	4 (13%)
6	PO4	A	2006	3	4,4,4	1.85	2 (50%)	6,6,6	1.28	1 (16%)
7	ADP	A	2001	3	24,29,29	1.21	2 (8%)	29,45,45	1.26	4 (13%)
9	NET	A	5012	-	8,8,8	0.64	0	10,10,10	0.52	0
7	ADP	C	2023	3	24,29,29	1.26	4 (16%)	29,45,45	1.22	5 (17%)
8	ORN	A	5011	-	4,8,8	0.91	0	3,9,9	0.31	0
9	NET	E	5056	-	8,8,8	0.79	0	10,10,10	0.35	0
8	ORN	C	5033	-	4,8,8	0.82	0	3,9,9	0.63	0
7	ADP	G	2066	3	24,29,29	1.16	3 (12%)	29,45,45	1.28	4 (13%)
6	PO4	C	2028	3	4,4,4	2.28	2 (50%)	6,6,6	0.98	0
9	NET	C	5034	-	8,8,8	0.60	0	10,10,10	0.45	0
9	NET	G	5077	-	8,8,8	0.83	0	10,10,10	0.35	0
6	PO4	E	2050	3	4,4,4	1.99	3 (75%)	6,6,6	1.07	0
8	ORN	G	5076	-	4,8,8	0.29	0	3,9,9	0.73	0
7	ADP	E	2045	3	24,29,29	1.01	2 (8%)	29,45,45	1.25	2 (6%)
7	ADP	C	2029	3,4	24,29,29	1.10	2 (8%)	29,45,45	1.29	4 (13%)

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
7	ADP	E	2051	3,4	-	3/12/32/32	0/3/3/3
8	ORN	E	5055	-	-	3/4/8/8	-
7	ADP	G	2072	3,4	-	3/12/32/32	0/3/3/3
7	ADP	A	2001	3	-	0/12/32/32	0/3/3/3
9	NET	A	5012	-	-	10/12/12/12	-
7	ADP	C	2023	3	-	2/12/32/32	0/3/3/3
8	ORN	A	5011	-	-	4/4/8/8	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NET	E	5056	-	-	3/12/12/12	-
8	ORN	C	5033	-	-	4/4/8/8	-
7	ADP	G	2066	3	-	0/12/32/32	0/3/3/3
9	NET	C	5034	-	-	0/12/12/12	-
9	NET	G	5077	-	-	3/12/12/12	-
7	ADP	A	2007	3,4	-	3/12/32/32	0/3/3/3
8	ORN	G	5076	-	-	4/4/8/8	-
7	ADP	E	2045	3	-	0/12/32/32	0/3/3/3
7	ADP	C	2029	3,4	-	3/12/32/32	0/3/3/3

The worst 5 of 31 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	2029	ADP	O3'-C3'	3.44	1.51	1.43
7	G	2066	ADP	O2'-C2'	2.99	1.50	1.43
7	A	2001	ADP	O3'-C3'	2.96	1.49	1.43
7	C	2023	ADP	O3'-C3'	2.95	1.49	1.43
7	C	2023	ADP	O4'-C1'	-2.94	1.37	1.41

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	2072	ADP	O3B-PB-O3A	3.94	117.86	104.64
7	E	2045	ADP	C5-C6-N6	3.71	125.99	120.35
7	C	2029	ADP	C5-C6-N6	3.35	125.44	120.35
7	G	2066	ADP	O2'-C2'-C3'	3.19	122.15	111.82
7	A	2007	ADP	C5-C6-N6	3.17	125.17	120.35

There are no chirality outliers.

5 of 45 torsion outliers are listed below:

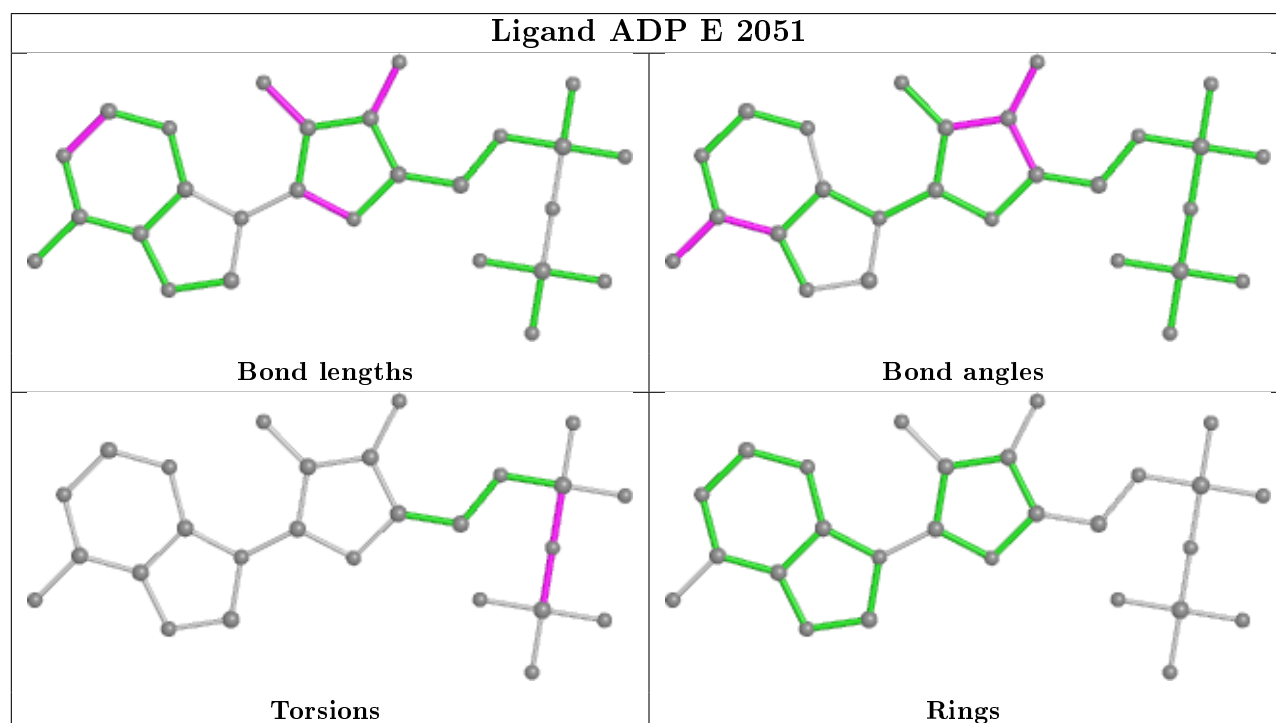
Mol	Chain	Res	Type	Atoms
7	A	2007	ADP	PA-O3A-PB-O3B
7	E	2051	ADP	PA-O3A-PB-O3B
8	C	5033	ORN	N-CA-CB-CG
8	C	5033	ORN	C-CA-CB-CG
8	E	5055	ORN	N-CA-CB-CG

There are no ring outliers.

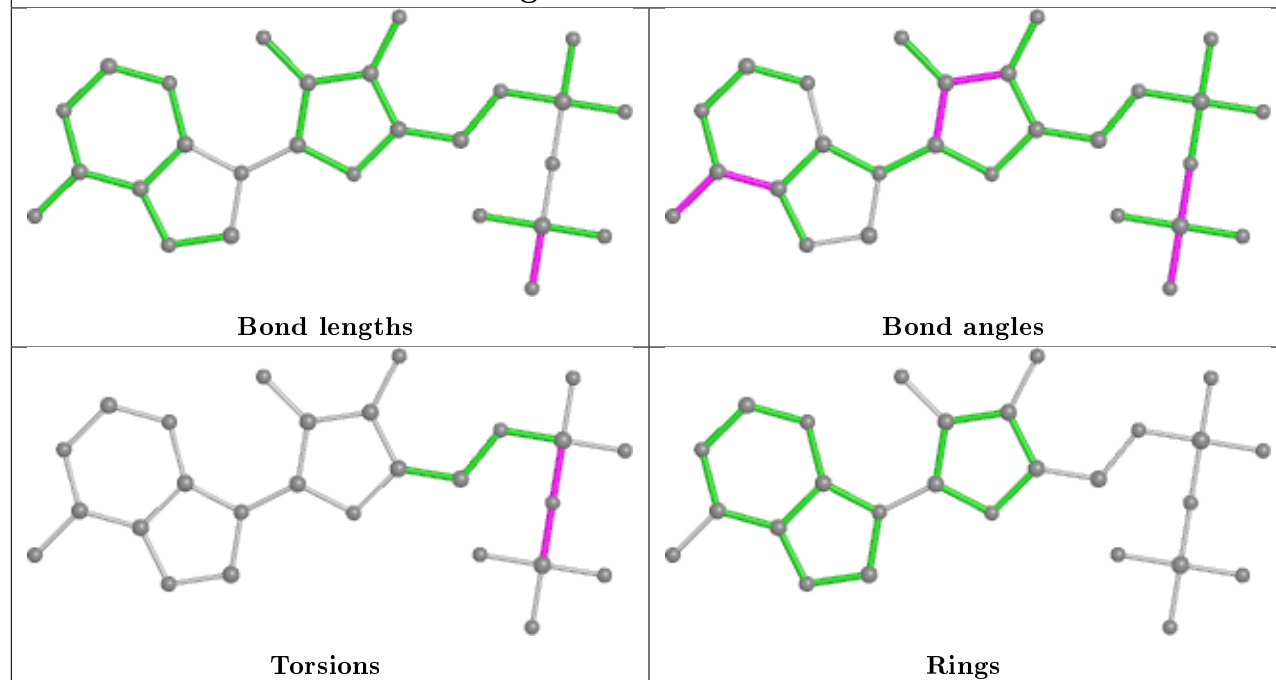
12 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	E	2051	ADP	2	0
8	E	5055	ORN	1	0
6	G	2071	PO4	1	0
7	G	2072	ADP	2	0
9	A	5012	NET	4	0
9	E	5056	NET	1	0
8	C	5033	ORN	1	0
7	G	2066	ADP	2	0
6	C	2028	PO4	1	0
9	G	5077	NET	1	0
8	G	5076	ORN	2	0
7	E	2045	ADP	2	0

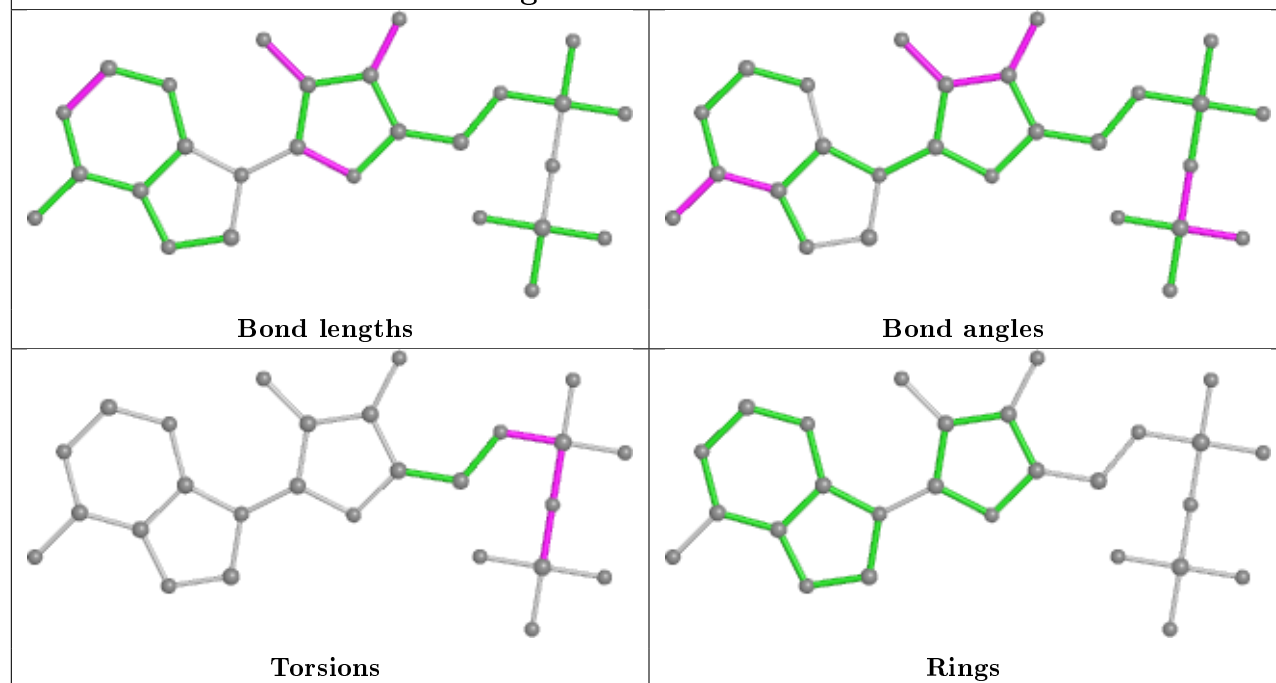
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



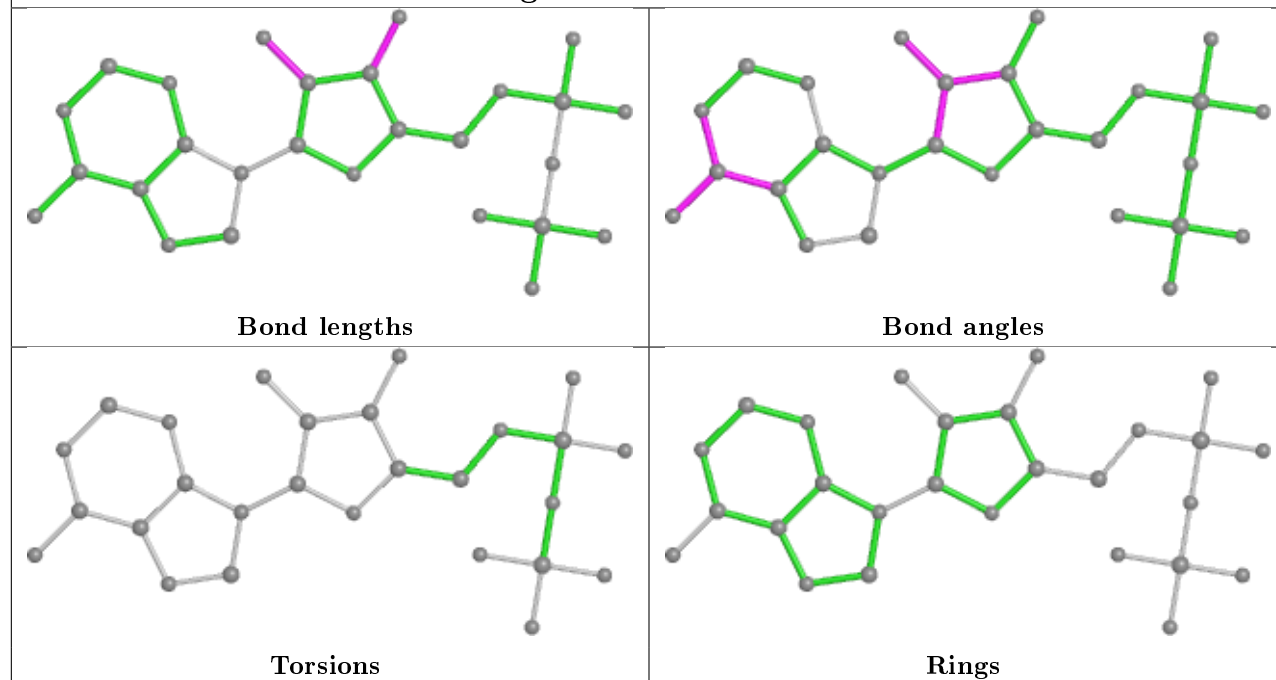
## Ligand ADP A 2007



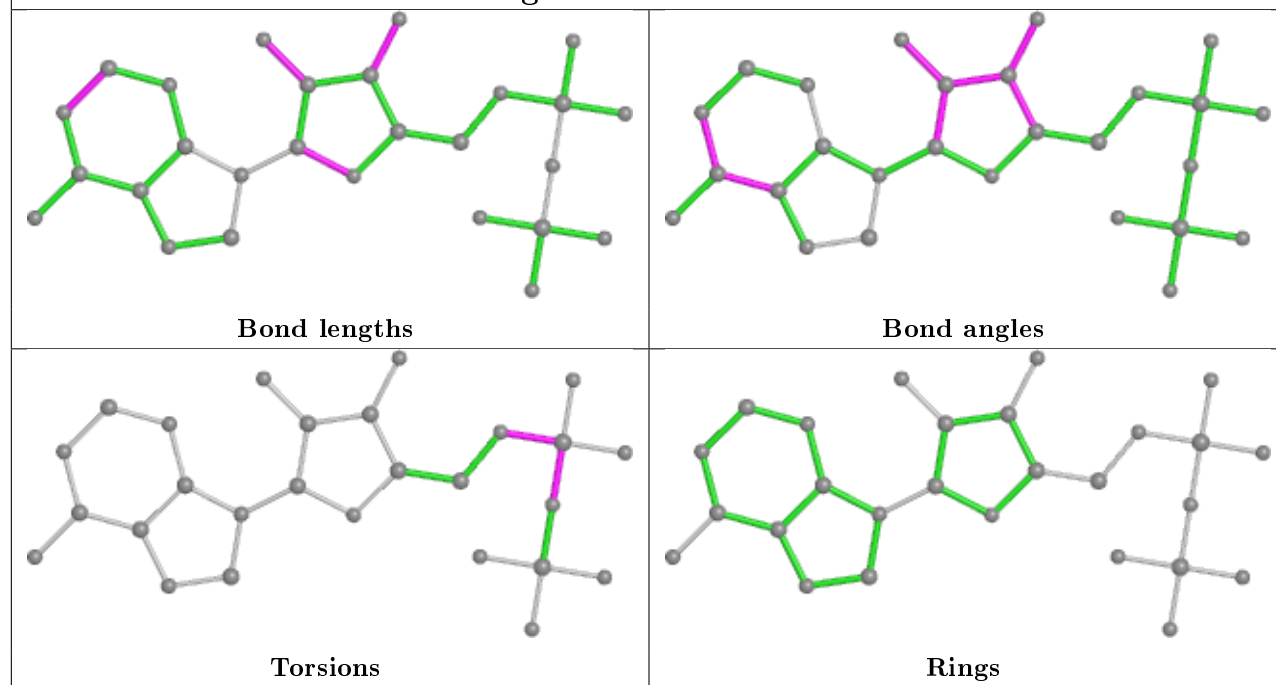
## Ligand ADP G 2072



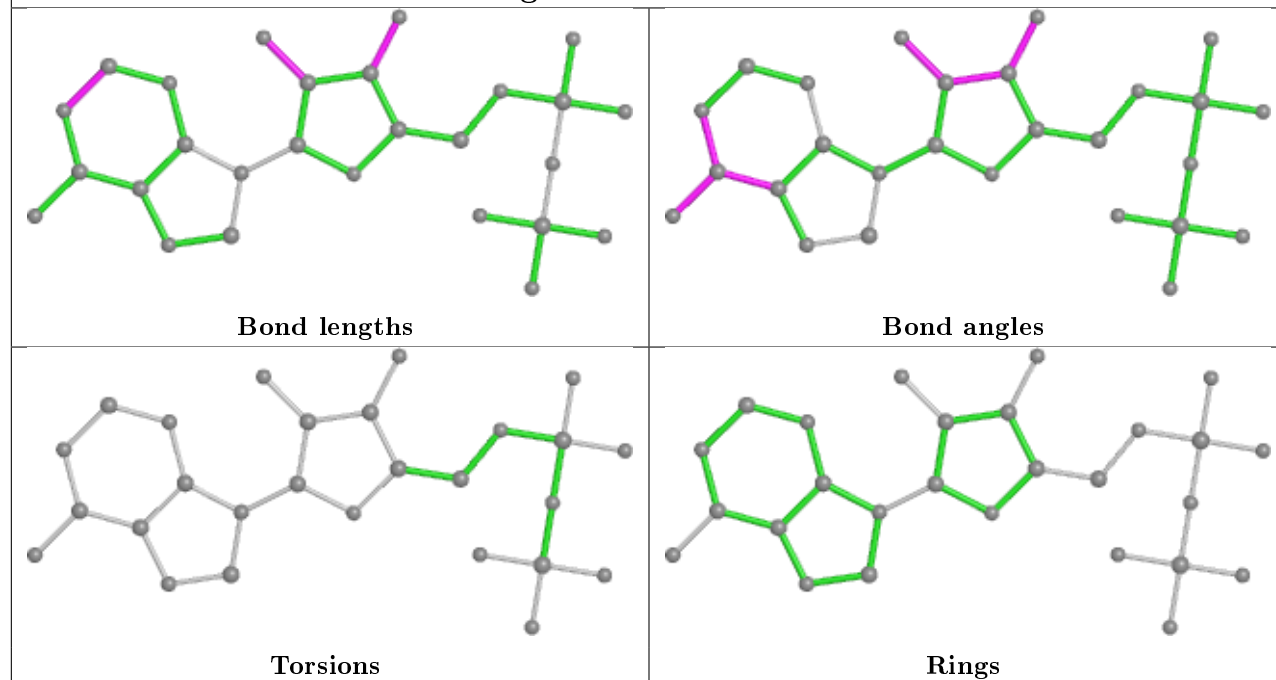
## Ligand ADP A 2001



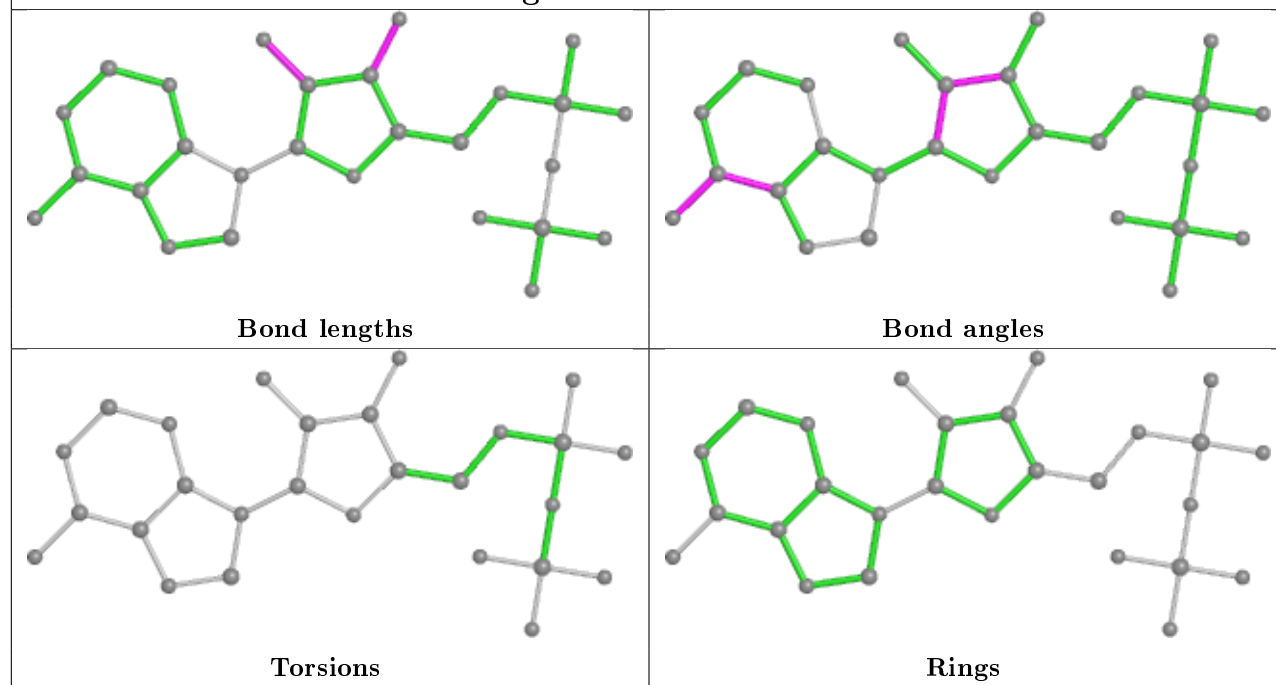
## Ligand ADP C 2023

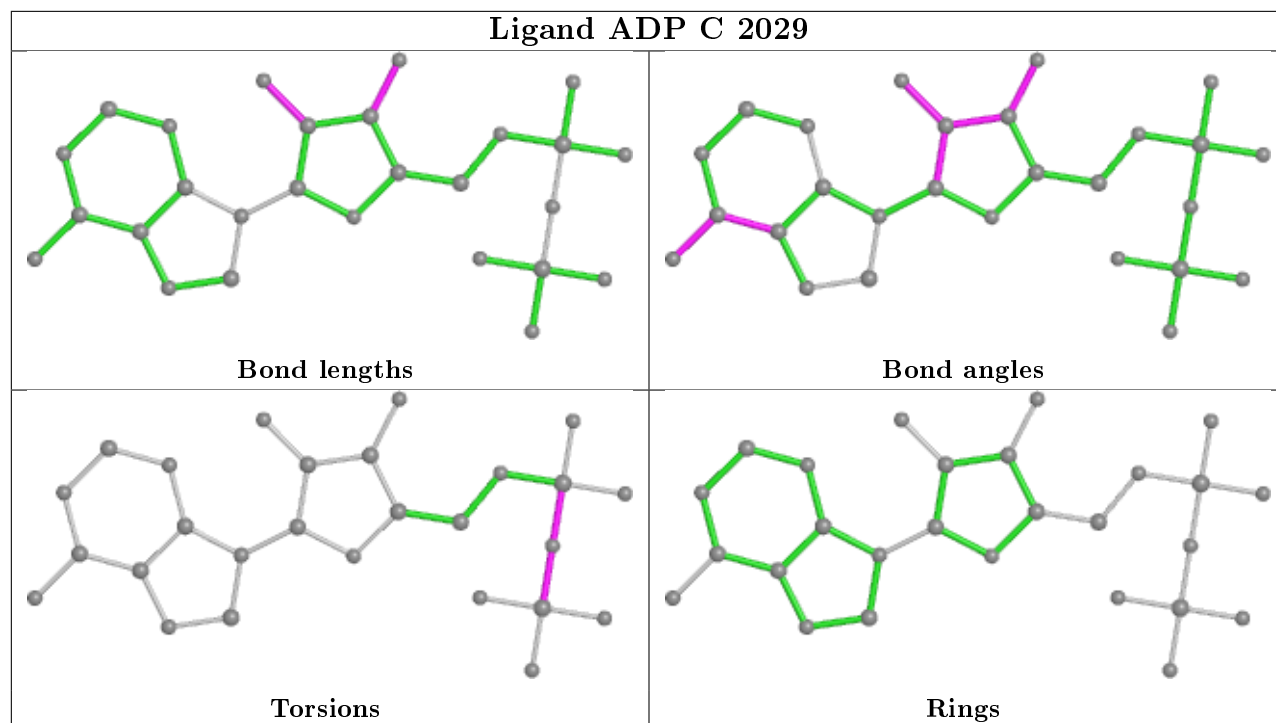


## Ligand ADP G 2066



## Ligand ADP E 2045





## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	1058/1073 (98%)	-0.33	37 (3%) 44 50	15, 32, 80, 100	0
1	C	1058/1073 (98%)	-0.31	42 (3%) 38 44	15, 33, 81, 100	0
1	E	1058/1073 (98%)	-0.32	40 (3%) 40 46	16, 29, 82, 100	0
1	G	1058/1073 (98%)	-0.20	49 (4%) 32 38	16, 37, 87, 100	0
2	B	378/382 (98%)	-0.29	4 (1%) 80 84	19, 41, 75, 100	0
2	D	378/382 (98%)	-0.39	0 100 100	18, 33, 63, 92	0
2	F	378/382 (98%)	-0.28	13 (3%) 45 51	19, 35, 74, 99	0
2	H	378/382 (98%)	-0.12	10 (2%) 56 61	25, 45, 78, 98	0
All	All	5744/5820 (98%)	-0.29	195 (3%) 45 51	15, 34, 80, 100	0

The worst 5 of 195 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	MET	11.4
1	A	738	PHE	10.3
1	A	740	THR	9.9
1	A	739	GLN	8.8
1	C	695	VAL	8.3

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

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	143	H	269	16/17	0.90	0.21	29,71,100,100	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	143	B	269	16/17	0.91	0.18	34,46,87,90	0
2	143	F	269	16/17	0.93	0.20	25,46,100,100	0
2	143	D	269	16/17	0.94	0.20	21,32,100,100	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates 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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
4	K	C	5031	1/1	0.89	0.11	52,52,52,52	0
4	K	A	5013	1/1	0.93	0.10	59,59,59,59	0
5	CL	A	5020	1/1	0.93	0.08	61,61,61,61	0
5	CL	E	5062	1/1	0.94	0.07	59,59,59,59	0
9	NET	E	5056	9/9	0.95	0.15	19,29,41,43	0
8	ORN	G	5076	9/9	0.95	0.16	18,27,35,49	0
4	K	C	5035	1/1	0.95	0.06	48,48,48,48	0
6	PO4	G	2071	5/5	0.96	0.08	20,28,40,56	0
8	ORN	C	5033	9/9	0.96	0.16	12,21,37,46	0
6	PO4	A	2006	5/5	0.96	0.07	22,25,39,50	0
8	ORN	A	5011	9/9	0.96	0.15	21,24,31,40	0
4	K	E	5057	1/1	0.96	0.06	59,59,59,59	0
9	NET	G	5077	9/9	0.96	0.15	23,39,55,64	0
5	CL	G	5084	1/1	0.96	0.11	65,65,65,65	0
4	K	A	5009	1/1	0.97	0.13	38,38,38,38	0
7	ADP	G	2072	27/27	0.97	0.07	24,38,60,83	0
4	K	G	5079	1/1	0.97	0.09	71,71,71,71	0
5	CL	C	5042	1/1	0.97	0.07	55,55,55,55	0
5	CL	C	5040	1/1	0.97	0.04	35,35,35,35	0
4	K	A	5015	1/1	0.97	0.05	54,54,54,54	0
5	CL	G	5083	1/1	0.97	0.05	40,40,40,40	0
5	CL	C	5044	1/1	0.97	0.06	39,39,39,39	0
9	NET	A	5012	9/9	0.97	0.12	20,29,37,45	0
4	K	G	5074	1/1	0.97	0.16	67,67,67,67	0
4	K	E	5058	1/1	0.97	0.09	53,53,53,53	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	K	C	5036	1/1	0.97	0.07	56,56,56,56	0
4	K	C	5037	1/1	0.97	0.08	62,62,62,62	0
5	CL	G	5085	1/1	0.97	0.07	68,68,68,68	0
4	K	G	5080	1/1	0.98	0.07	43,43,43,43	0
7	ADP	C	2029	27/27	0.98	0.07	16,35,60,82	0
7	ADP	E	2051	27/27	0.98	0.07	20,32,49,89	0
5	CL	H	5086	1/1	0.98	0.11	47,47,47,47	0
7	ADP	G	2066	27/27	0.98	0.10	15,21,36,38	0
5	CL	A	5022	1/1	0.98	0.17	74,74,74,74	0
4	K	C	5027	1/1	0.98	0.10	29,29,29,29	0
8	ORN	E	5055	9/9	0.98	0.11	21,23,35,53	0
4	K	E	5059	1/1	0.98	0.04	43,43,43,43	0
6	PO4	E	2050	5/5	0.98	0.07	22,25,48,48	0
5	CL	A	5019	1/1	0.98	0.06	40,40,40,40	0
4	K	E	5053	1/1	0.98	0.09	51,51,51,51	0
4	K	H	5081	1/1	0.98	0.12	57,57,57,57	0
5	CL	E	5063	1/1	0.99	0.05	45,45,45,45	0
3	MN	C	2024	1/1	0.99	0.09	28,28,28,28	0
4	K	A	5010	1/1	0.99	0.08	24,24,24,24	0
4	K	E	5049	1/1	0.99	0.13	30,30,30,30	0
5	CL	G	5082	1/1	0.99	0.08	39,39,39,39	0
4	K	E	2048	1/1	0.99	0.08	24,24,24,24	0
9	NET	C	5034	9/9	0.99	0.12	17,19,27,30	0
4	K	G	5070	1/1	0.99	0.12	36,36,36,36	0
5	CL	B	5021	1/1	0.99	0.06	33,33,33,33	0
7	ADP	C	2023	27/27	0.99	0.12	13,21,23,26	0
5	CL	D	5043	1/1	0.99	0.06	30,30,30,30	0
7	ADP	E	2045	27/27	0.99	0.12	16,27,43,64	0
3	MN	G	2073	1/1	0.99	0.06	42,42,42,42	0
6	PO4	C	2028	5/5	0.99	0.08	13,16,31,35	0
3	MN	G	2067	1/1	0.99	0.06	36,36,36,36	0
7	ADP	A	2007	27/27	0.99	0.07	17,26,37,45	0
4	K	F	5060	1/1	0.99	0.09	42,42,42,42	0
3	MN	A	5008	1/1	0.99	0.06	28,28,28,28	0
4	K	B	5016	1/1	0.99	0.08	45,45,45,45	0
5	CL	E	5064	1/1	0.99	0.05	54,54,54,54	0
4	K	G	5078	1/1	0.99	0.06	54,54,54,54	0
5	CL	A	5018	1/1	0.99	0.04	34,34,34,34	0
7	ADP	A	2001	27/27	0.99	0.10	16,25,33,41	0
4	K	D	5038	1/1	0.99	0.06	37,37,37,37	0
5	CL	F	5065	1/1	0.99	0.08	31,31,31,31	0
4	K	A	5014	1/1	0.99	0.10	52,52,52,52	0

*Continued on next page...*

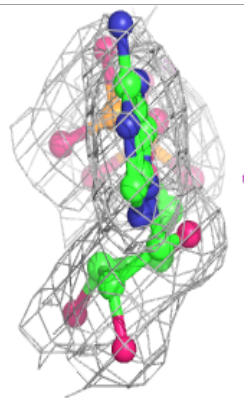
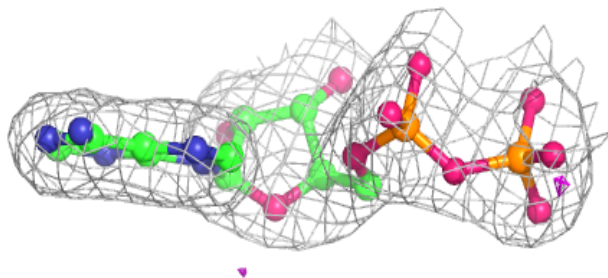
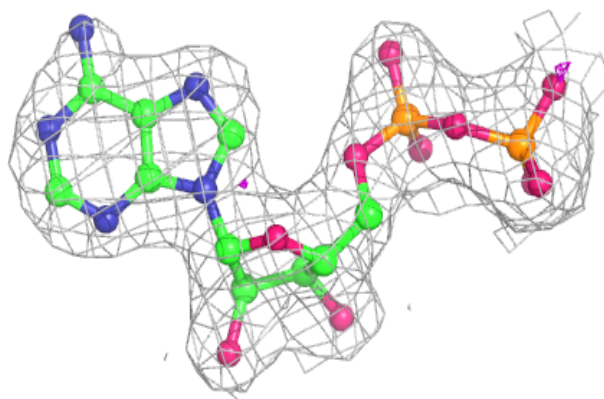
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	MN	A	2003	1/1	1.00	0.08	25,25,25,25	0
5	CL	C	5039	1/1	1.00	0.11	27,27,27,27	0
3	MN	G	2068	1/1	1.00	0.07	25,25,25,25	0
4	K	G	2069	1/1	1.00	0.09	23,23,23,23	0
4	K	A	5004	1/1	1.00	0.10	24,24,24,24	0
4	K	A	5005	1/1	1.00	0.09	27,27,27,27	0
5	CL	A	5017	1/1	1.00	0.07	29,29,29,29	0
3	MN	E	2046	1/1	1.00	0.08	34,34,34,34	0
5	CL	C	5041	1/1	1.00	0.05	36,36,36,36	0
5	CL	E	5061	1/1	1.00	0.12	30,30,30,30	0
4	K	G	5075	1/1	1.00	0.08	29,29,29,29	0
4	K	C	5032	1/1	1.00	0.07	31,31,31,31	0
3	MN	C	2030	1/1	1.00	0.06	38,38,38,38	0
4	K	E	5054	1/1	1.00	0.07	24,24,24,24	0
4	K	C	5026	1/1	1.00	0.12	18,18,18,18	0
3	MN	C	2025	1/1	1.00	0.09	22,22,22,22	0
3	MN	E	2052	1/1	1.00	0.05	34,34,34,34	0
3	MN	E	2047	1/1	1.00	0.08	27,27,27,27	0
3	MN	A	2002	1/1	1.00	0.06	31,31,31,31	0

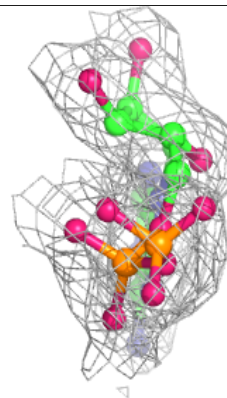
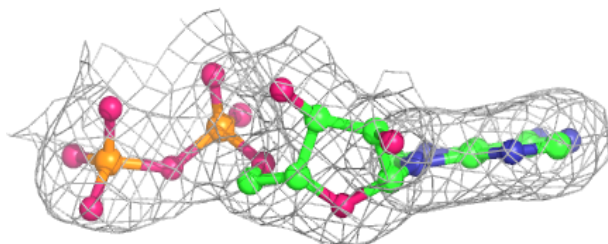
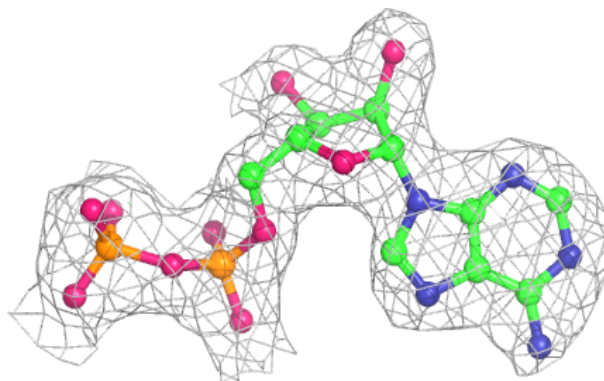
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around ADP G 2072:**

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

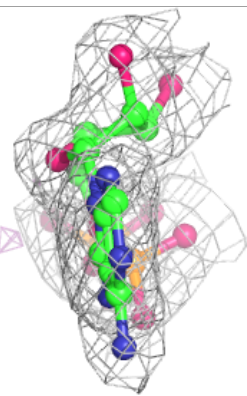
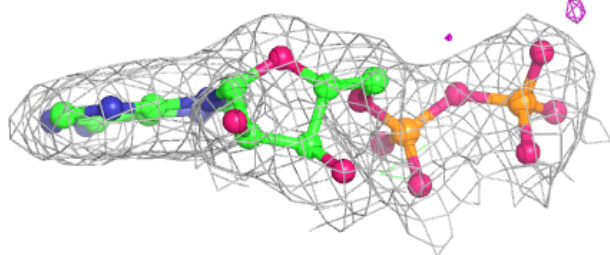
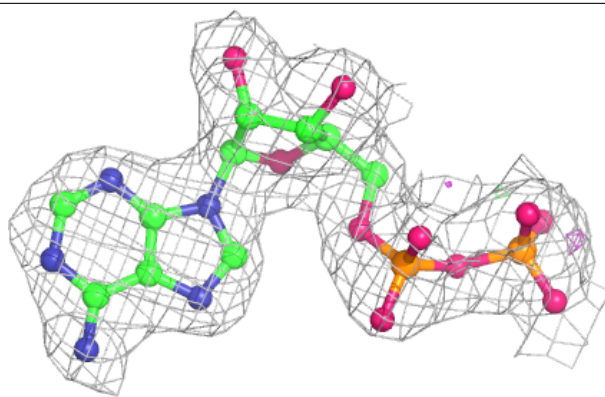
**Electron density around ADP C 2029:**

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

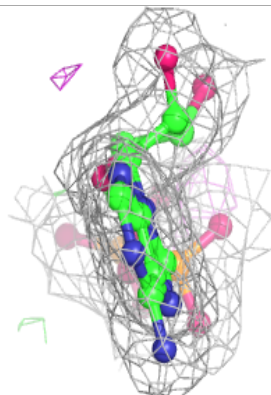
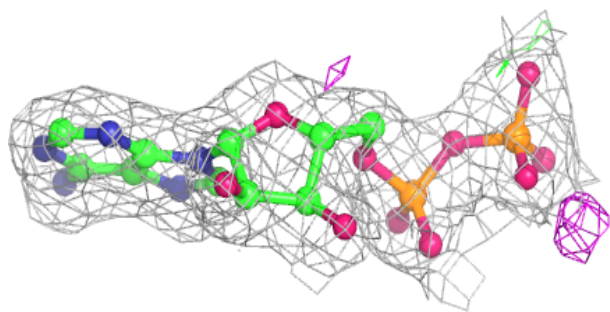
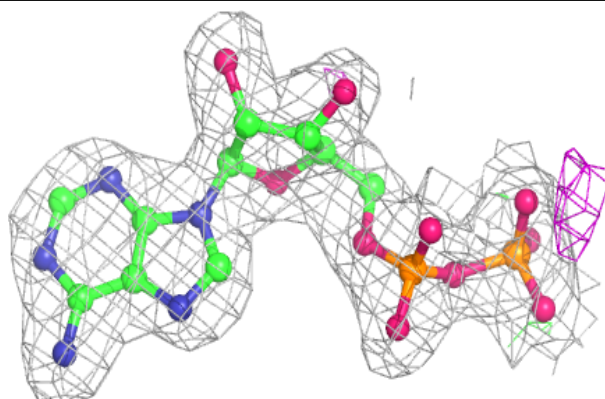


**Electron density around ADP E 2051:**

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

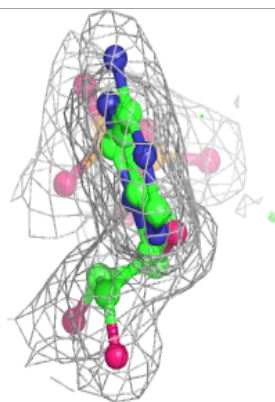
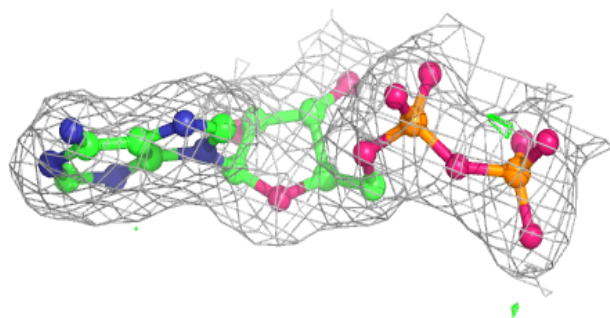
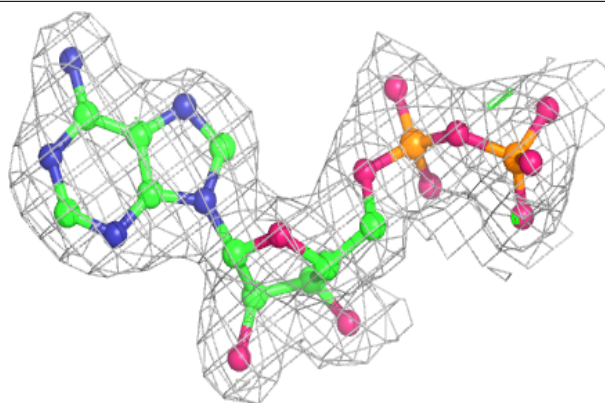
**Electron density around ADP G 2066:**

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

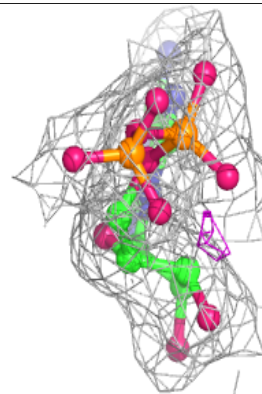
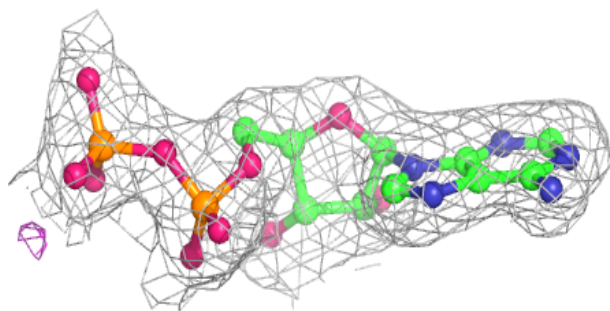
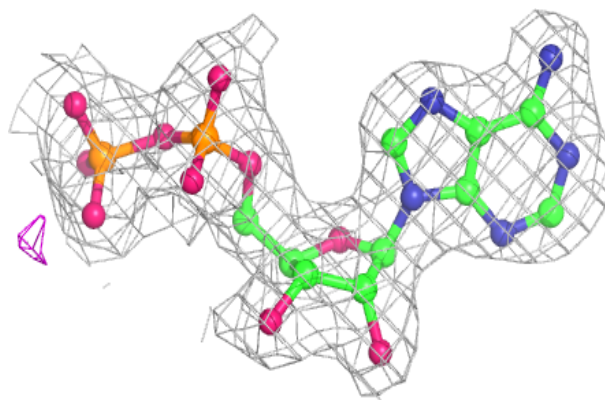


**Electron density around ADP C 2023:**

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

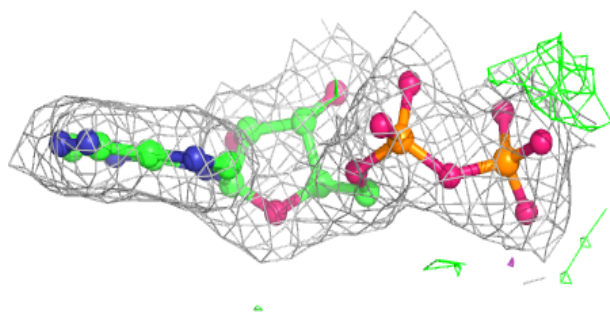
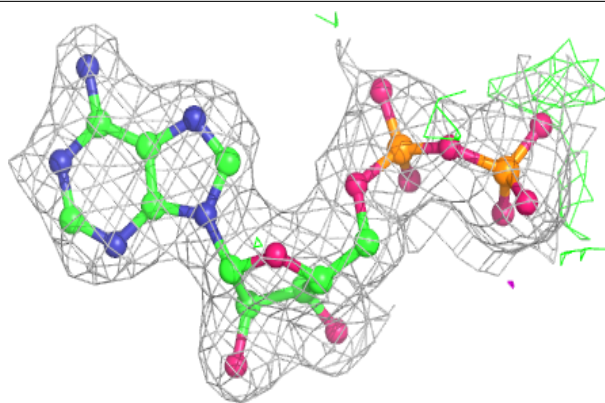
**Electron density around ADP E 2045:**

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

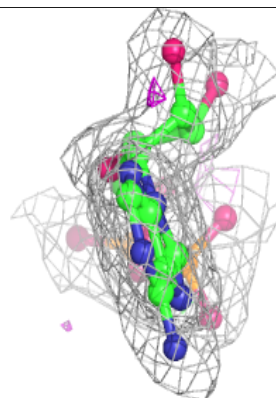
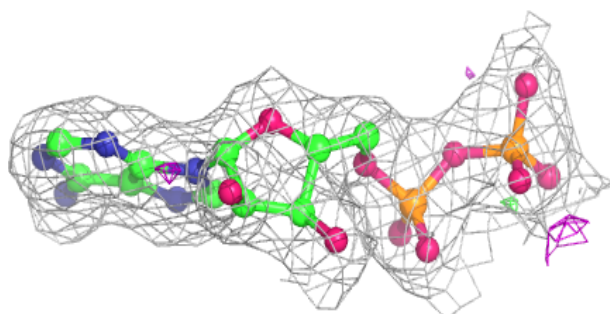
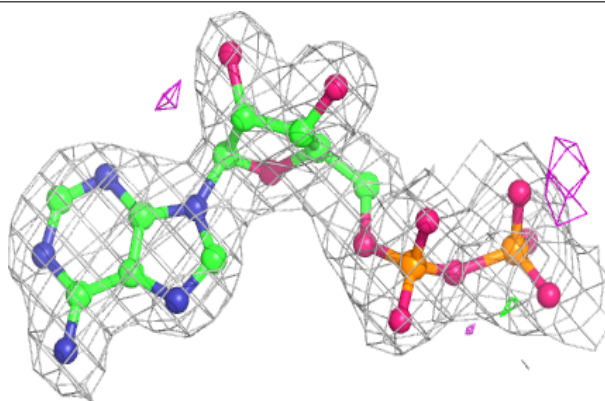


**Electron density around ADP A 2007:**

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

**Electron density around ADP A 2001:**

$2mF_o-DF_c$  (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.