



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 12, 2024 – 02:54 PM EDT

PDB ID : 1CS0  
Title : Crystal structure of carbamoyl phosphate synthetase complexed at CYS269 in the small subunit with the tetrahedral mimic l-glutamate gamma-semialdehyde  
Authors : Thoden, J.B.; Huang, X.; Raushel, F.M.; Holden, H.M.  
Deposited on : 1999-08-16  
Resolution : 2.00 Å(reported)

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

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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>.

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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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

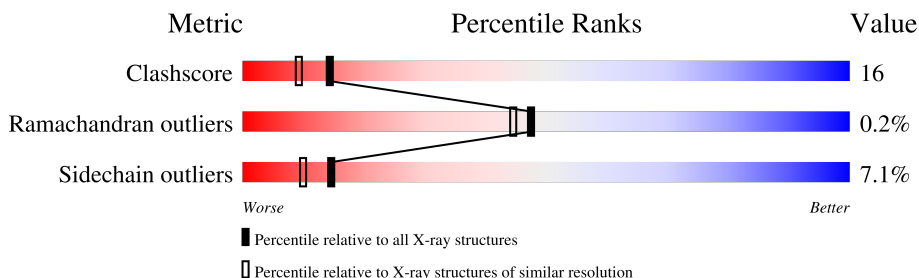
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	1073	60% 31% 6% ..
1	C	1073	60% 31% 6% ..
1	E	1073	65% 27% 6% ..
1	G	1073	61% 30% 7% ..
2	B	382	59% 34% 5% .
2	D	382	59% 34% 7% .
2	F	382	60% 36% ..
2	H	382	53% 38% 8% .

## 2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 48889 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 SUB-UNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1058	Total	C	N	O	S	0	3	0
			8169	5128	1422	1574	45			
1	C	1058	Total	C	N	O	S	0	3	0
			8173	5132	1423	1573	45			
1	E	1058	Total	C	N	O	S	0	6	0
			8186	5140	1424	1576	46			
1	G	1058	Total	C	N	O	S	0	3	0
			8175	5132	1425	1572	46			

- Molecule 2 is a protein called CARBAMOYL PHOSPHATE SYNTHETASE: SMALL SUB-UNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	379	Total	C	N	O	S	0	0	0
			2904	1830	509	555	10			
2	D	379	Total	C	N	O	S	0	1	0
			2909	1833	509	557	10			
2	F	379	Total	C	N	O	S	0	0	0
			2904	1830	509	555	10			
2	H	379	Total	C	N	O	S	0	1	0
			2906	1831	509	556	10			

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

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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	3	Total 3	Mn 3	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	7	Total 7	K 7	0	0
4	B	1	Total 1	K 1	0	0
4	C	7	Total 7	K 7	0	0
4	D	1	Total 1	K 1	0	0
4	E	8	Total 8	K 8	0	0
4	F	1	Total 1	K 1	0	0
4	G	7	Total 7	K 7	0	0
4	H	1	Total 1	K 1	0	0

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

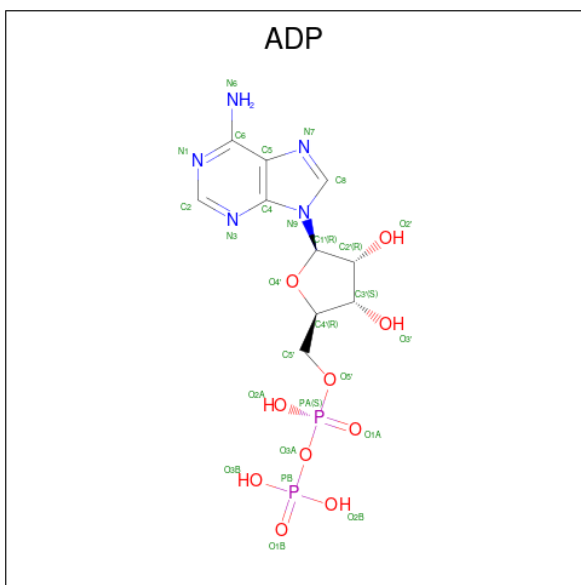
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	6	Total 6	Cl 6	0	0
5	B	2	Total 2	Cl 2	0	0
5	C	5	Total 5	Cl 5	0	0
5	D	2	Total 2	Cl 2	0	0
5	E	5	Total 5	Cl 5	0	0
5	F	2	Total 2	Cl 2	0	0
5	G	5	Total 5	Cl 5	0	0
5	H	2	Total 2	Cl 2	0	0

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula:  $\text{O}_4\text{P}$ ).



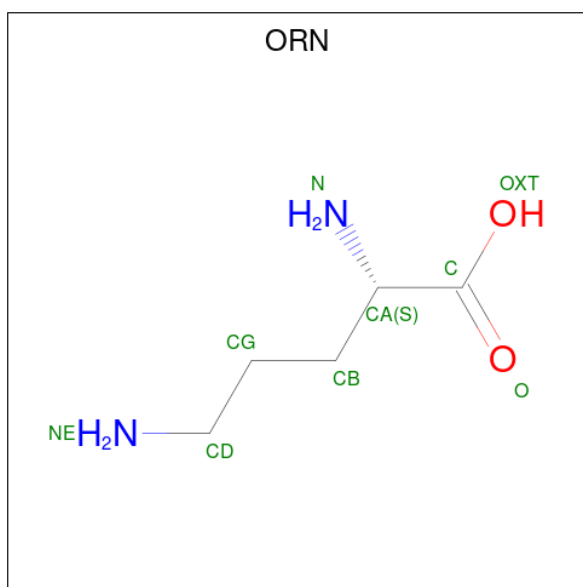
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	P	0	0
			5	4	1		
6	C	1	Total	O	P	0	0
			5	4	1		
6	E	1	Total	O	P	0	0
			5	4	1		
6	E	1	Total	O	P	0	0
			5	4	1		
6	G	1	Total	O	P	0	0
			5	4	1		

- Molecule 7 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$ ).



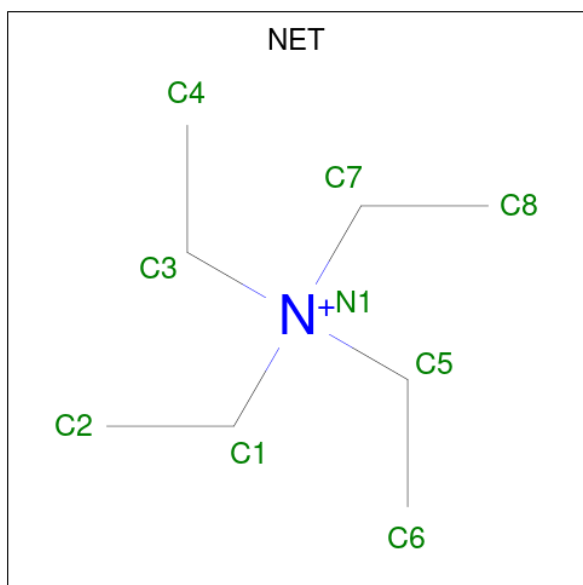
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
7	A	1	Total 27	C 10	N 5	O 10	P 2	0	0
7	A	1	Total 27	C 10	N 5	O 10	P 2	0	0
7	C	1	Total 27	C 10	N 5	O 10	P 2	0	0
7	C	1	Total 27	C 10	N 5	O 10	P 2	0	0
7	E	1	Total 27	C 10	N 5	O 10	P 2	0	0
7	E	1	Total 27	C 10	N 5	O 10	P 2	0	0
7	G	1	Total 27	C 10	N 5	O 10	P 2	0	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	869	Total O 869 869	0	0
10	B	213	Total O 213 213	0	0
10	C	784	Total O 784 784	0	0
10	D	275	Total O 275 275	0	0
10	E	864	Total O 864 864	0	0
10	F	235	Total O 235 235	0	0
10	G	743	Total O 743 743	0	0
10	H	193	Total O 193 193	0	0

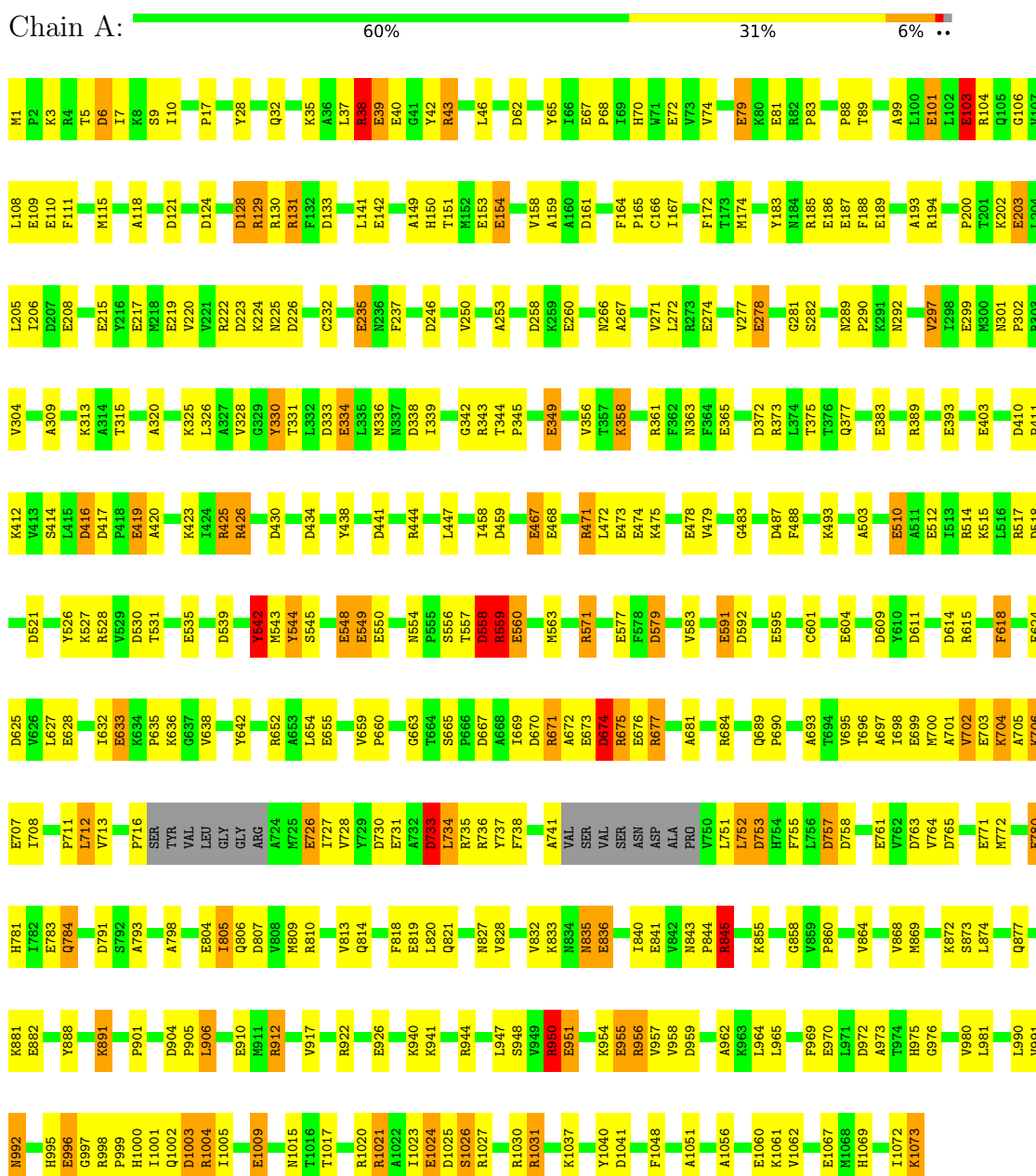


### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

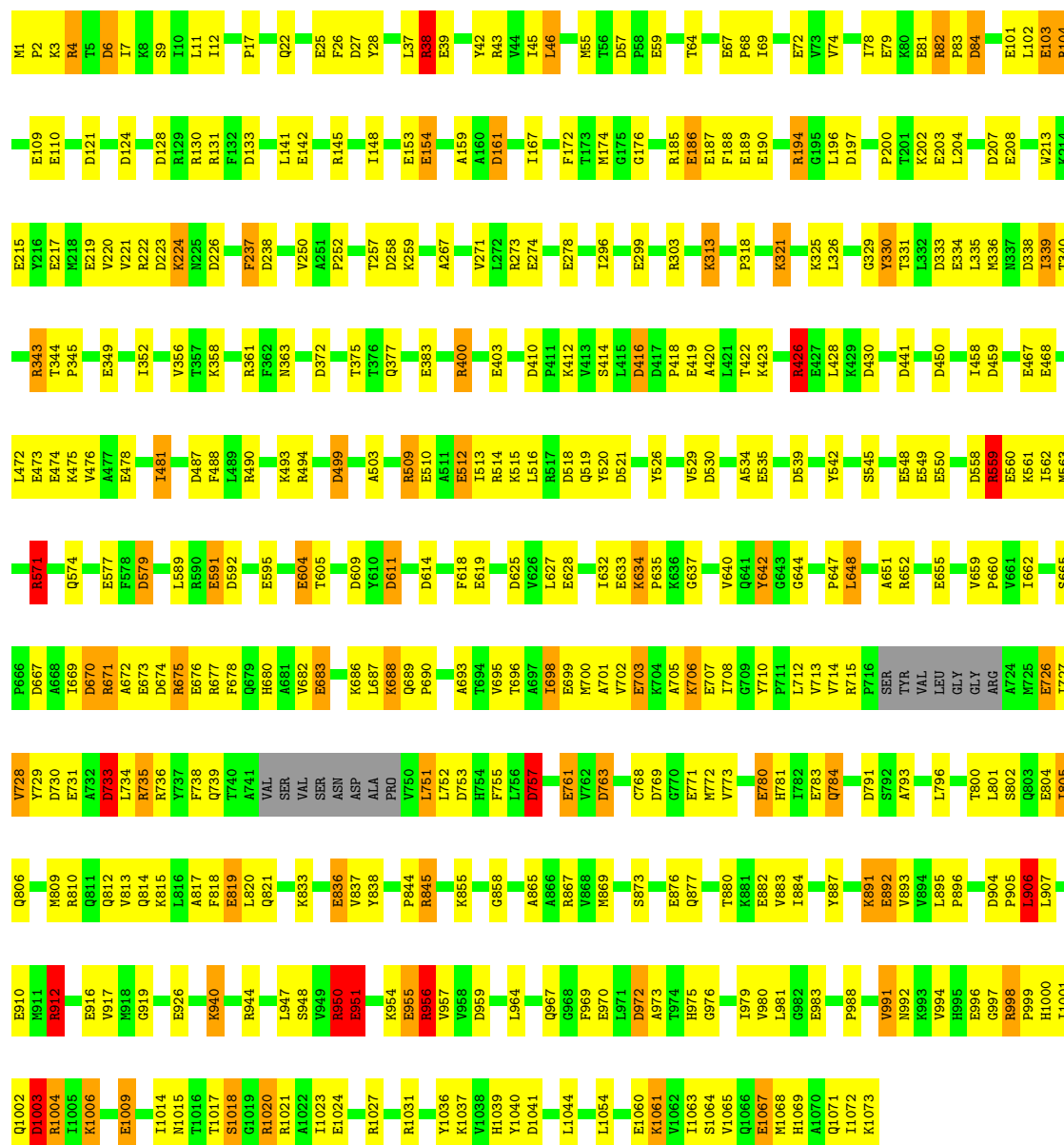
Note EDS was not executed.

#### • Molecule 1: CARBAMOYL PHOSPHATE SYNTHETASE: LARGE SUBUNIT



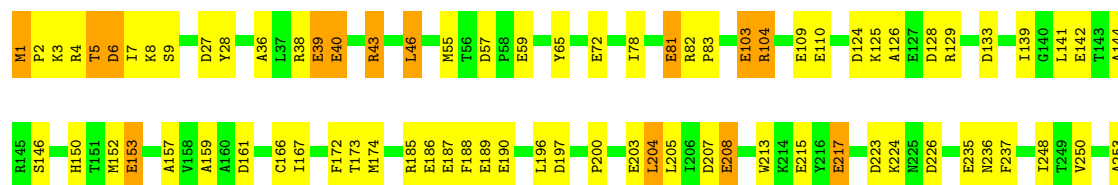
• Molecule 1: CARBAMOYL PHOSPHATE SYNTHETASE: LARGE SUBUNIT

Chain C: 

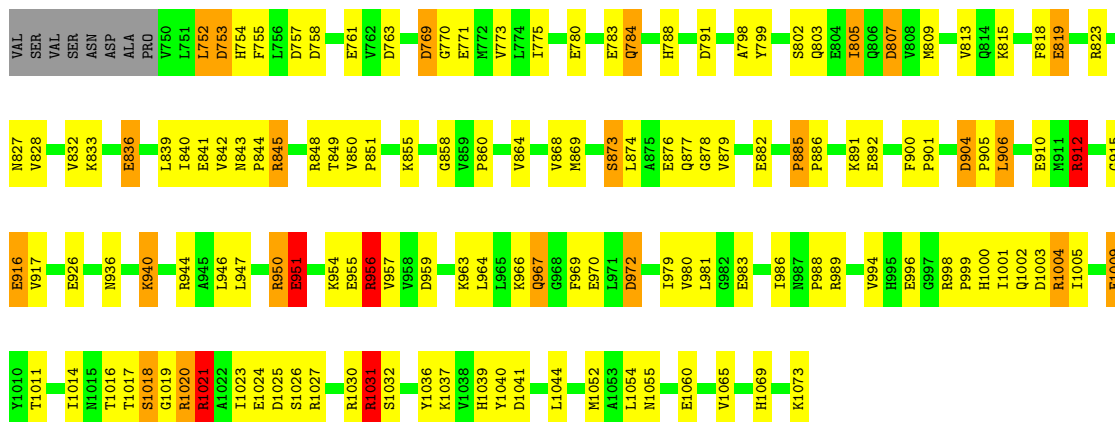


• Molecule 1: CARBAMOYL PHOSPHATE SYNTHETASE: LARGE SUBUNIT

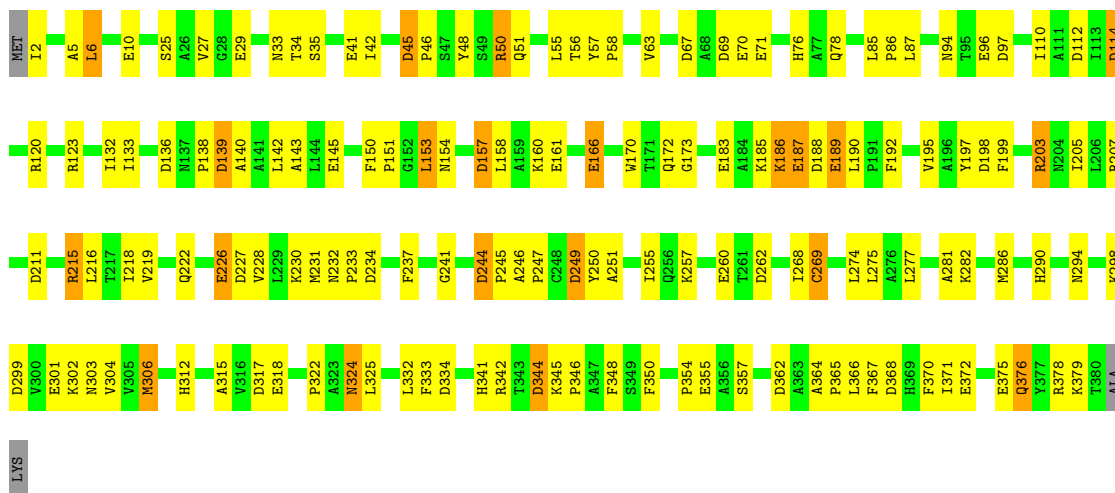
Chain E: 



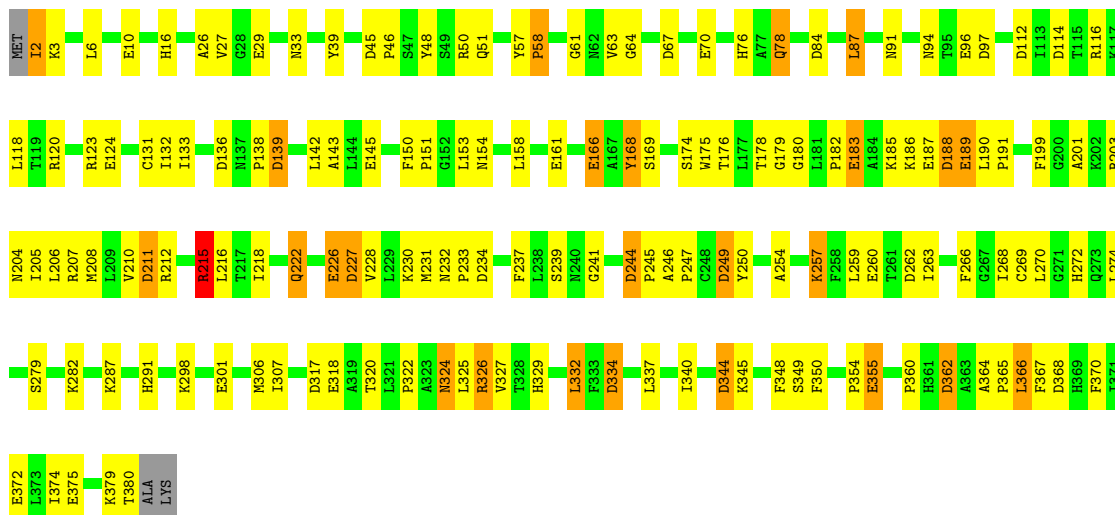




- Molecule 2: CARBAMOYL PHOSPHATE SYNTHETASE: SMALL SUBUNIT

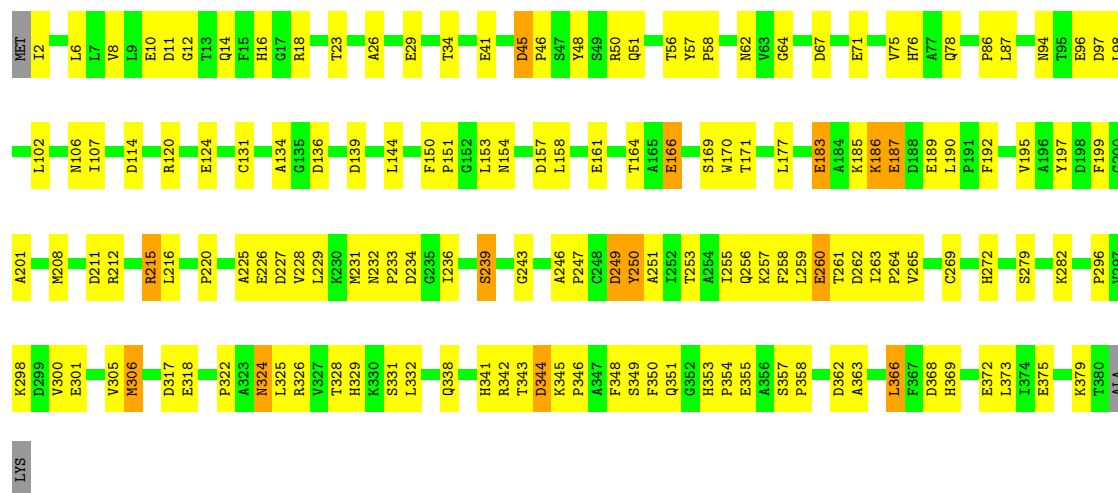


• Molecule 2: CARBAMOYL PHOSPHATE SYNTHETASE: SMALL SUBUNIT



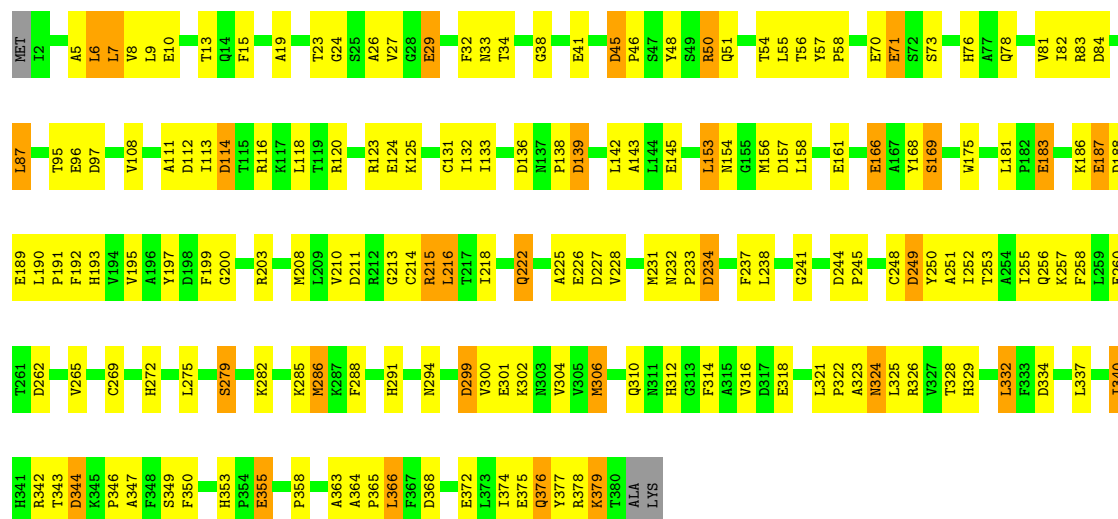
• Molecule 2: CARBAMOYL PHOSPHATE SYNTHETASE: SMALL SUBUNIT

Chain F: 



• Molecule 2: CARBAMOYL PHOSPHATE SYNTHETASE: SMALL SUBUNIT

Chain H: 



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	151.70Å 163.80Å 332.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.00	Depositor
% Data completeness (in resolution range)	98.7 (30.00-2.00)	Depositor
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	TNT	Depositor
R, $R_{free}$	0.186 , 0.242	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	48889	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CL, ADP, PO4, MN, ORN, K, CYG, NET

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	1.05	72/8307 (0.9%)	1.38	129/11230 (1.1%)
1	C	1.04	70/8311 (0.8%)	1.38	130/11236 (1.2%)
1	E	1.05	64/8336 (0.8%)	1.35	129/11267 (1.1%)
1	G	1.04	71/8313 (0.9%)	1.36	109/11237 (1.0%)
2	B	0.92	18/2950 (0.6%)	1.29	32/4005 (0.8%)
2	D	0.98	15/2959 (0.5%)	1.31	40/4017 (1.0%)
2	F	0.96	16/2950 (0.5%)	1.34	31/4005 (0.8%)
2	H	0.93	19/2956 (0.6%)	1.30	36/4013 (0.9%)
All	All	1.02	345/45082 (0.8%)	1.35	636/61010 (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
1	C	1	0

The worst 5 of 345 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	189	GLU	CD-OE2	13.05	1.40	1.25
1	G	39	GLU	CD-OE1	-9.37	1.15	1.25
1	E	403	GLU	CD-OE2	8.00	1.34	1.25
1	E	819	GLU	CD-OE2	7.90	1.34	1.25
1	E	427	GLU	CD-OE2	7.81	1.34	1.25

The worst 5 of 636 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	956	ARG	NE-CZ-NH2	-12.15	114.22	120.30
1	A	677	ARG	NE-CZ-NH1	10.84	125.72	120.30
1	A	677	ARG	NE-CZ-NH2	-10.47	115.07	120.30
1	G	43	ARG	NE-CZ-NH1	10.34	125.47	120.30
1	G	43	ARG	NE-CZ-NH2	-10.24	115.18	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	339	ILE	CA

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8169	0	8201	245	0
1	C	8173	0	8207	259	0
1	E	8186	0	8220	206	0
1	G	8175	0	8210	282	0
2	B	2904	0	2867	95	0
2	D	2909	0	2869	95	0
2	F	2904	0	2867	86	0
2	H	2906	0	2868	129	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
4	E	8	0	0	0	0
4	F	1	0	0	0	0
4	G	7	0	0	0	0
4	H	1	0	0	0	0
5	A	6	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	2	0	0	0	0
5	C	5	0	0	2	0
5	D	2	0	0	0	0
5	E	5	0	0	2	0
5	F	2	0	0	0	0
5	G	5	0	0	3	0
5	H	2	0	0	0	0
6	A	5	0	0	0	0
6	C	5	0	0	0	0
6	E	10	0	0	0	0
6	G	5	0	0	0	0
7	A	54	0	24	0	0
7	C	54	0	24	0	0
7	E	54	0	24	1	0
7	G	54	0	24	3	0
8	A	9	0	11	0	0
8	C	9	0	11	2	0
8	E	9	0	11	3	0
8	G	9	0	11	0	0
9	A	9	0	20	2	0
9	C	9	0	20	0	0
9	E	9	0	20	1	0
9	G	9	0	20	0	0
10	A	869	0	0	26	0
10	B	213	0	0	3	0
10	C	784	0	0	16	0
10	D	275	0	0	6	0
10	E	864	0	0	22	0
10	F	235	0	0	2	0
10	G	743	0	0	25	0
10	H	193	0	0	6	0
All	All	48889	0	44529	1385	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 16.

The worst 5 of 1385 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)
2:B:187:GLU:HG2	2:B:215:ARG:HD2	1.21	1.15
1:G:695:VAL:HG11	1:G:701:ALA:HB2	1.30	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:228:VAL:HA	2:F:231:MET:HE2	1.35	1.06
2:F:187:GLU:HG2	2:F:215:ARG:HD2	1.35	1.05
1:G:1027[B]:ARG:HE	1:G:1031:ARG:HD3	1.17	1.05

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	1055/1073 (98%)	1010 (96%)	43 (4%)	2 (0%)	47	44
1	C	1055/1073 (98%)	999 (95%)	53 (5%)	3 (0%)	41	37
1	E	1058/1073 (99%)	1013 (96%)	42 (4%)	3 (0%)	41	37
1	G	1055/1073 (98%)	1000 (95%)	51 (5%)	4 (0%)	34	30
2	B	376/382 (98%)	357 (95%)	19 (5%)	0	100	100
2	D	377/382 (99%)	364 (97%)	13 (3%)	0	100	100
2	F	376/382 (98%)	361 (96%)	15 (4%)	0	100	100
2	H	377/382 (99%)	367 (97%)	10 (3%)	0	100	100
All	All	5729/5820 (98%)	5471 (96%)	246 (4%)	12 (0%)	47	44

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	954	LYS
1	G	739	GLN
1	A	558	ASP
1	C	739	GLN
1	E	738	PHE

### 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	868/878 (99%)	810 (93%)	58 (7%)	16	11
1	C	868/878 (99%)	798 (92%)	70 (8%)	11	7
1	E	871/878 (99%)	814 (94%)	57 (6%)	17	12
1	G	868/878 (99%)	806 (93%)	62 (7%)	14	10
2	B	307/309 (99%)	284 (92%)	23 (8%)	13	9
2	D	308/309 (100%)	285 (92%)	23 (8%)	13	9
2	F	307/309 (99%)	288 (94%)	19 (6%)	18	13
2	H	308/309 (100%)	283 (92%)	25 (8%)	11	7
All	All	4705/4748 (99%)	4368 (93%)	337 (7%)	14	9

5 of 337 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	2	ILE
1	G	714	VAL
2	F	186	LYS
1	G	236	ASN
1	G	912	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 84 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	1035	GLN
1	G	803	GLN
2	F	78	GLN
1	G	457	ASN
1	G	1000	HIS

### 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	CYG	H	269	2	12,14,15	2.80	5 (41%)	11,17,19	4.24	3 (27%)
2	CYG	B	269	2	12,14,15	2.78	5 (41%)	11,17,19	4.24	3 (27%)
2	CYG	F	269	2	12,14,15	2.79	4 (33%)	11,17,19	4.24	3 (27%)
2	CYG	D	269	2	12,14,15	2.78	4 (33%)	11,17,19	4.23	3 (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
2	CYG	H	269	2	-	5/14/16/18	-
2	CYG	B	269	2	-	5/14/16/18	-
2	CYG	F	269	2	-	5/14/16/18	-
2	CYG	D	269	2	-	5/14/16/18	-

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	269	CYG	OE2-CD1	7.06	1.32	1.21
2	F	269	CYG	OE2-CD1	7.01	1.32	1.21
2	D	269	CYG	OE2-CD1	7.01	1.32	1.21
2	B	269	CYG	OE2-CD1	6.99	1.32	1.21
2	F	269	CYG	O1-C1	4.52	1.35	1.22

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	269	CYG	OE2-CD1-CG1	-10.26	111.88	123.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	269	CYG	OE2-CD1-CG1	-10.25	111.89	123.99
2	F	269	CYG	OE2-CD1-CG1	-10.24	111.89	123.99
2	D	269	CYG	OE2-CD1-CG1	-10.22	111.92	123.99
2	D	269	CYG	OE2-CD1-SG	-8.52	111.55	122.61

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	269	CYG	CA-CB-SG-CD1
2	D	269	CYG	CA-CB-SG-CD1
2	F	269	CYG	CA-CB-SG-CD1
2	H	269	CYG	CA-CB-SG-CD1
2	B	269	CYG	OE2-CD1-SG-CB

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	269	CYG	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 95 ligands modelled in this entry, 74 are monoatomic - leaving 21 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	$\# Z  > 2$
6	PO4	E	5070	-	4,4,4	1.90	2 (50%)	6,6,6	0.97	0
6	PO4	E	5051	3,4	4,4,4	2.62	3 (75%)	6,6,6	0.92	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	PO4	C	5028	3,4	4,4,4	2.24	3 (75%)	6,6,6	1.06	0
9	NET	A	5094	-	8,8,8	0.58	0	10,10,10	0.70	0
7	ADP	E	5046	3	24,29,29	1.14	3 (12%)	29,45,45	1.03	1 (3%)
9	NET	E	5057	-	8,8,8	0.82	0	10,10,10	0.39	0
9	NET	G	5082	-	8,8,8	0.63	0	10,10,10	0.53	0
9	NET	C	5034	-	8,8,8	0.72	0	10,10,10	0.52	0
8	ORN	E	5056	-	7,8,8	0.85	0	8,9,9	1.20	1 (12%)
7	ADP	C	5029	3,4	24,29,29	1.17	3 (12%)	29,45,45	1.31	4 (13%)
8	ORN	A	5010	-	7,8,8	1.08	0	8,9,9	1.61	3 (37%)
7	ADP	E	5052	3,4	24,29,29	1.02	3 (12%)	29,45,45	1.10	3 (10%)
8	ORN	C	5033	-	7,8,8	1.06	1 (14%)	8,9,9	0.95	0
7	ADP	G	5071	3	24,29,29	1.35	4 (16%)	29,45,45	1.54	5 (17%)
7	ADP	C	5023	3	24,29,29	1.26	5 (20%)	29,45,45	1.03	2 (6%)
6	PO4	G	5076	3,4	4,4,4	2.09	2 (50%)	6,6,6	0.93	0
6	PO4	A	5005	3,4	4,4,4	1.98	2 (50%)	6,6,6	1.07	0
7	ADP	A	5000	3	24,29,29	1.26	3 (12%)	29,45,45	1.21	2 (6%)
7	ADP	G	5077	3,4	24,29,29	1.19	4 (16%)	29,45,45	1.38	4 (13%)
8	ORN	G	5081	-	7,8,8	0.77	0	8,9,9	1.41	2 (25%)
7	ADP	A	5006	3,4	24,29,29	1.08	1 (4%)	29,45,45	1.18	5 (17%)

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	5046	3	-	1/12/32/32	0/3/3/3
8	ORN	E	5056	-	-	6/8/8/8	-
9	NET	E	5057	-	-	0/12/12/12	-
7	ADP	C	5029	3,4	-	4/12/32/32	0/3/3/3
7	ADP	A	5000	3	-	1/12/32/32	0/3/3/3
7	ADP	G	5071	3	-	1/12/32/32	0/3/3/3
7	ADP	G	5077	3,4	-	1/12/32/32	0/3/3/3
7	ADP	E	5052	3,4	-	3/12/32/32	0/3/3/3
8	ORN	A	5010	-	-	6/8/8/8	-
8	ORN	G	5081	-	-	6/8/8/8	-
9	NET	C	5034	-	-	0/12/12/12	-
9	NET	G	5082	-	-	0/12/12/12	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	ORN	C	5033	-	-	6/8/8/8	-
7	ADP	A	5006	3,4	-	4/12/32/32	0/3/3/3
7	ADP	C	5023	3	-	1/12/32/32	0/3/3/3
9	NET	A	5094	-	-	8/12/12/12	-

The worst 5 of 39 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	5029	ADP	O3'-C3'	3.82	1.52	1.43
7	G	5071	ADP	O3'-C3'	3.61	1.51	1.43
6	E	5051	PO4	P-O3	-3.59	1.43	1.54
7	A	5000	ADP	O4'-C1'	-3.41	1.36	1.41
7	G	5071	ADP	C2-N1	3.13	1.39	1.33

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	5029	ADP	C5-C6-N6	4.45	127.11	120.35
7	G	5071	ADP	O2'-C2'-C3'	3.93	124.54	111.82
7	G	5077	ADP	O3B-PB-O3A	3.49	116.35	104.64
7	G	5077	ADP	C5-C6-N6	3.26	125.30	120.35
7	G	5071	ADP	O3'-C3'-C2'	3.18	122.10	111.82

There are no chirality outliers.

5 of 48 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	5006	ADP	PA-O3A-PB-O3B
7	C	5029	ADP	PA-O3A-PB-O3B
7	E	5052	ADP	PA-O3A-PB-O3B
8	A	5010	ORN	N-CA-CB-CG
8	A	5010	ORN	C-CA-CB-CG

There are no ring outliers.

7 monomers are involved in 12 short contacts:

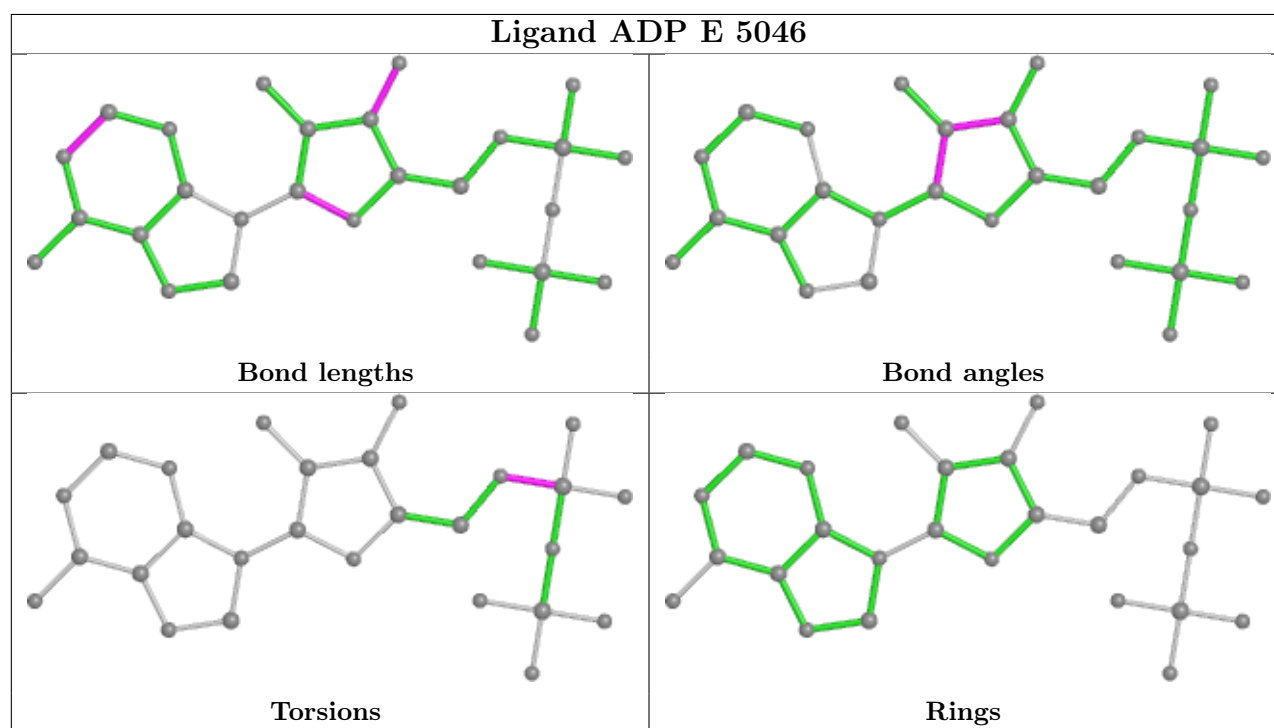
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	5094	NET	2	0
9	E	5057	NET	1	0
8	E	5056	ORN	3	0

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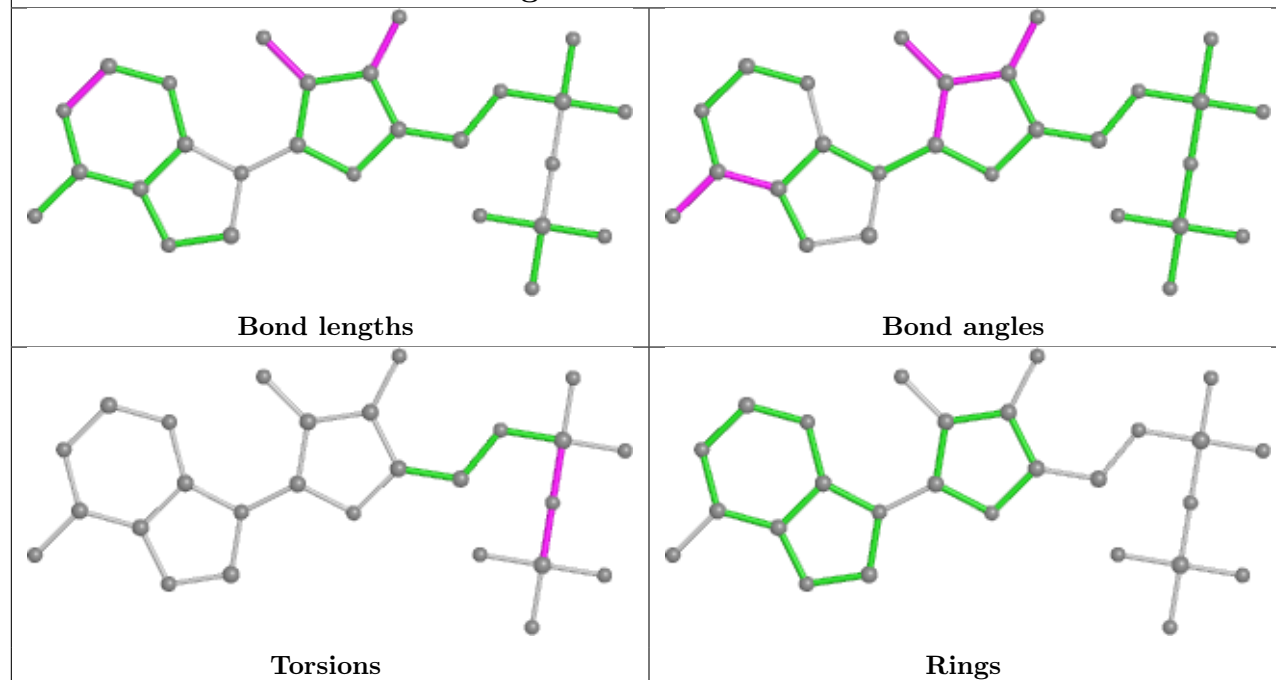
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	E	5052	ADP	1	0
8	C	5033	ORN	2	0
7	G	5071	ADP	1	0
7	G	5077	ADP	2	0

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.

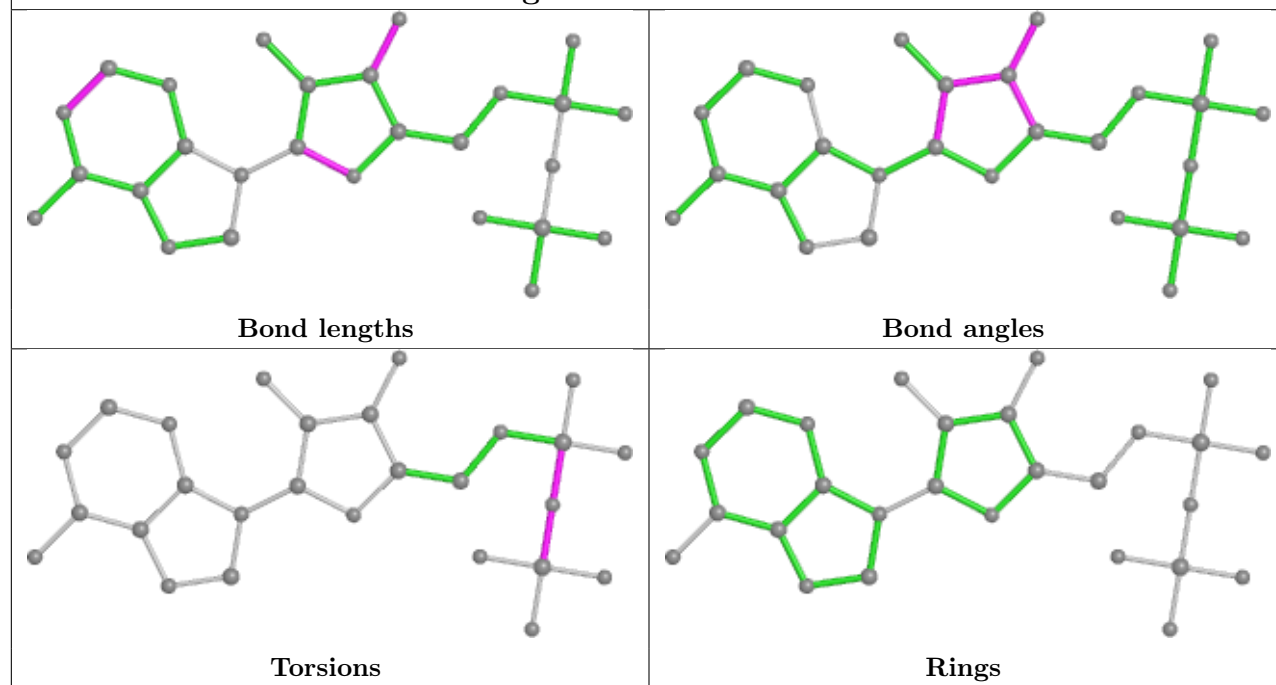




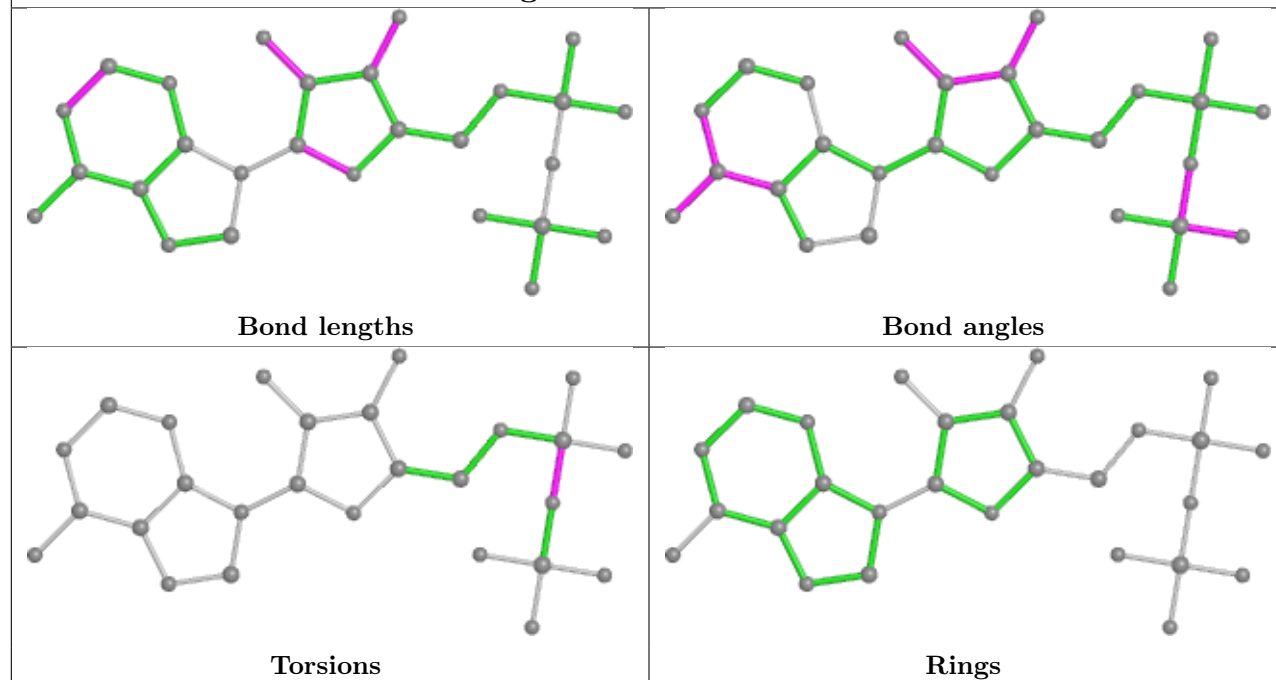
## Ligand ADP C 5029



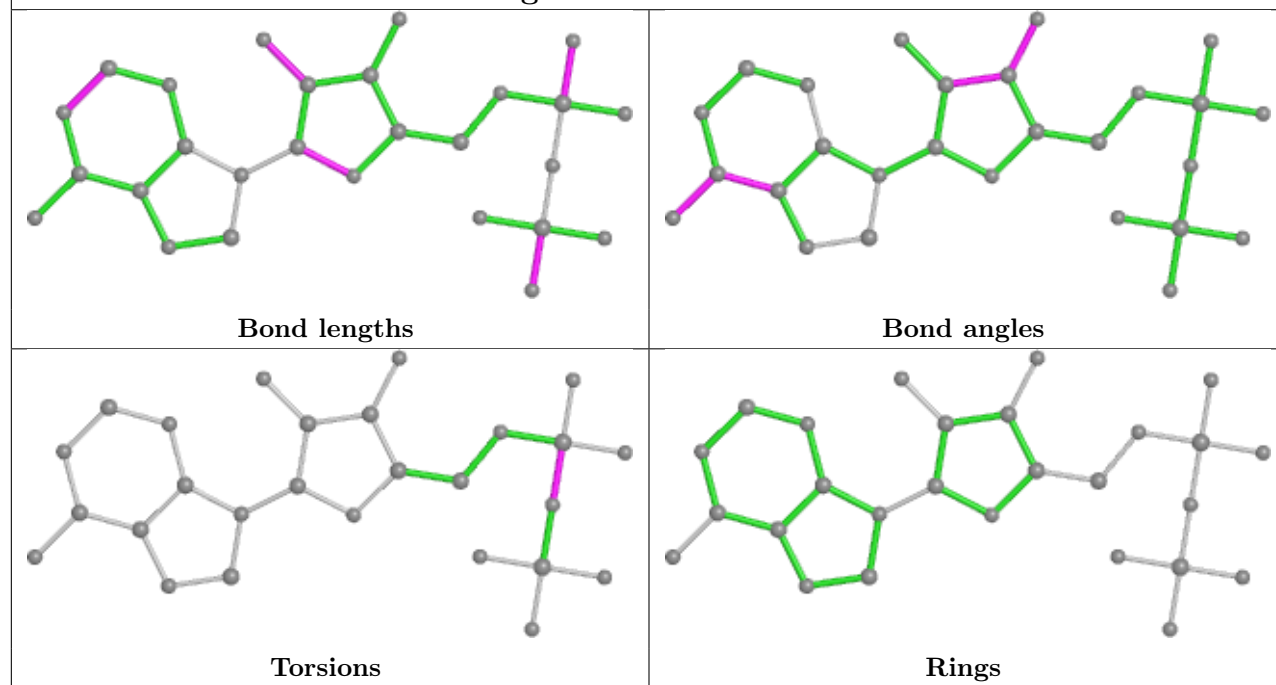
## Ligand ADP E 5052



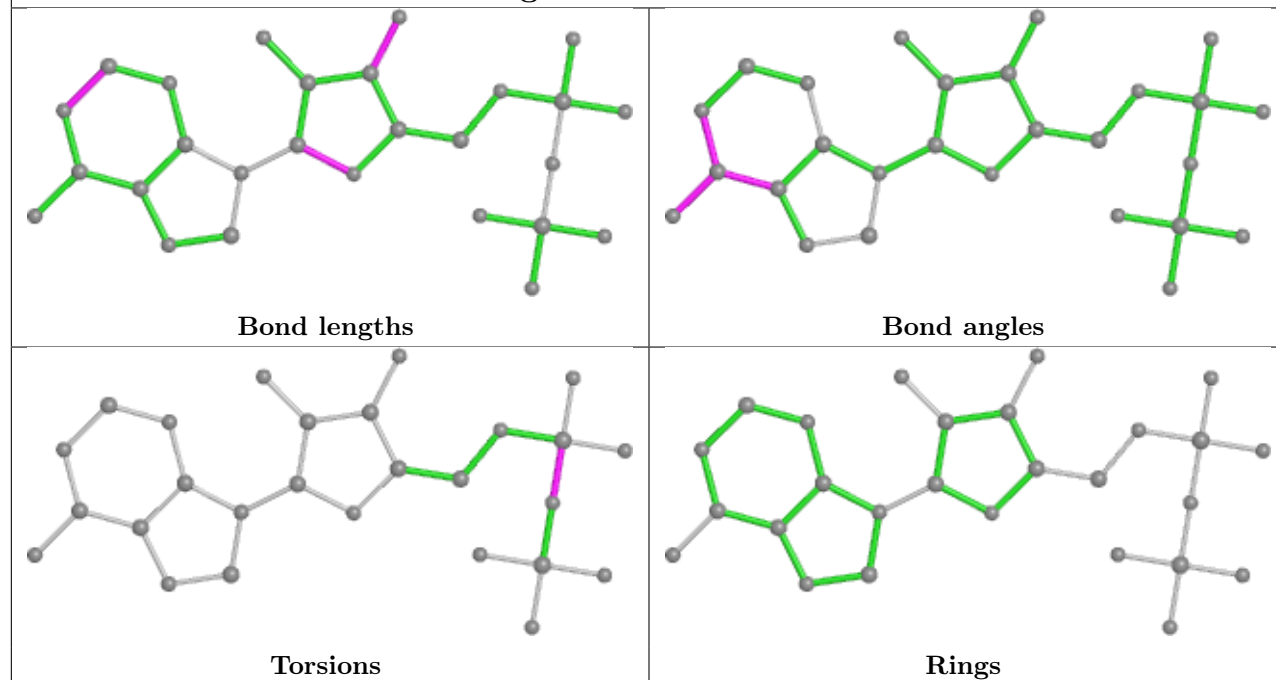
## Ligand ADP G 5071



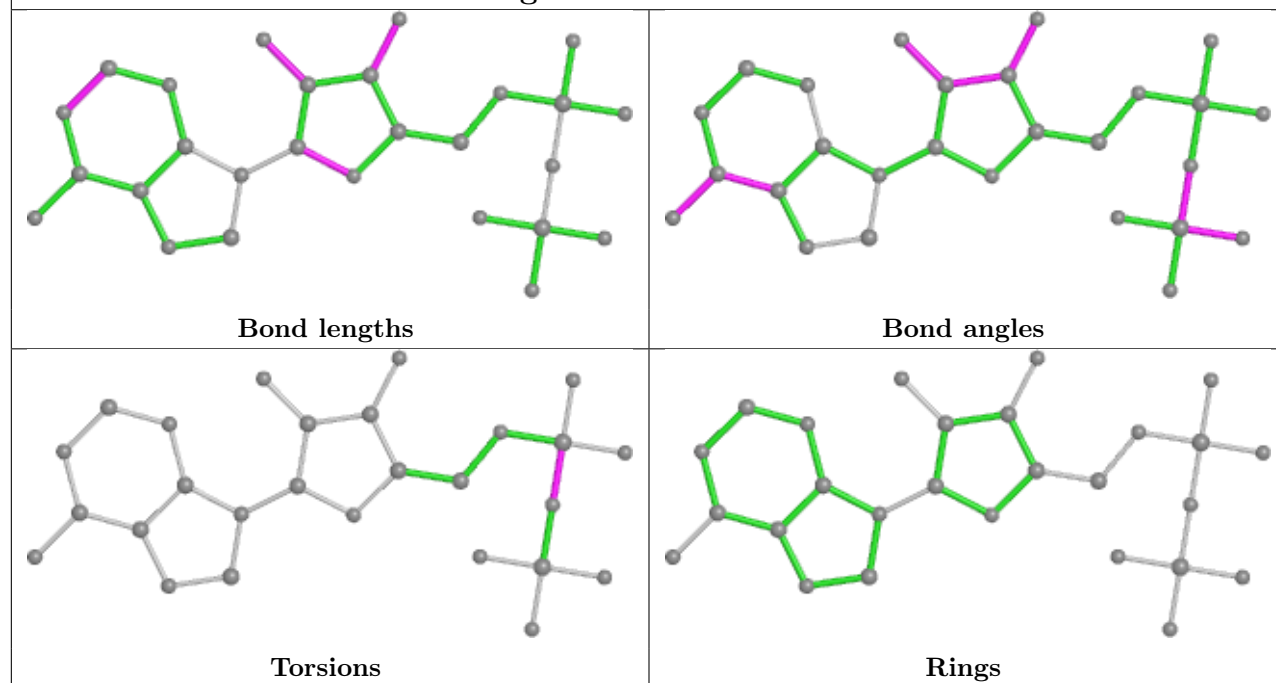
## Ligand ADP C 5023

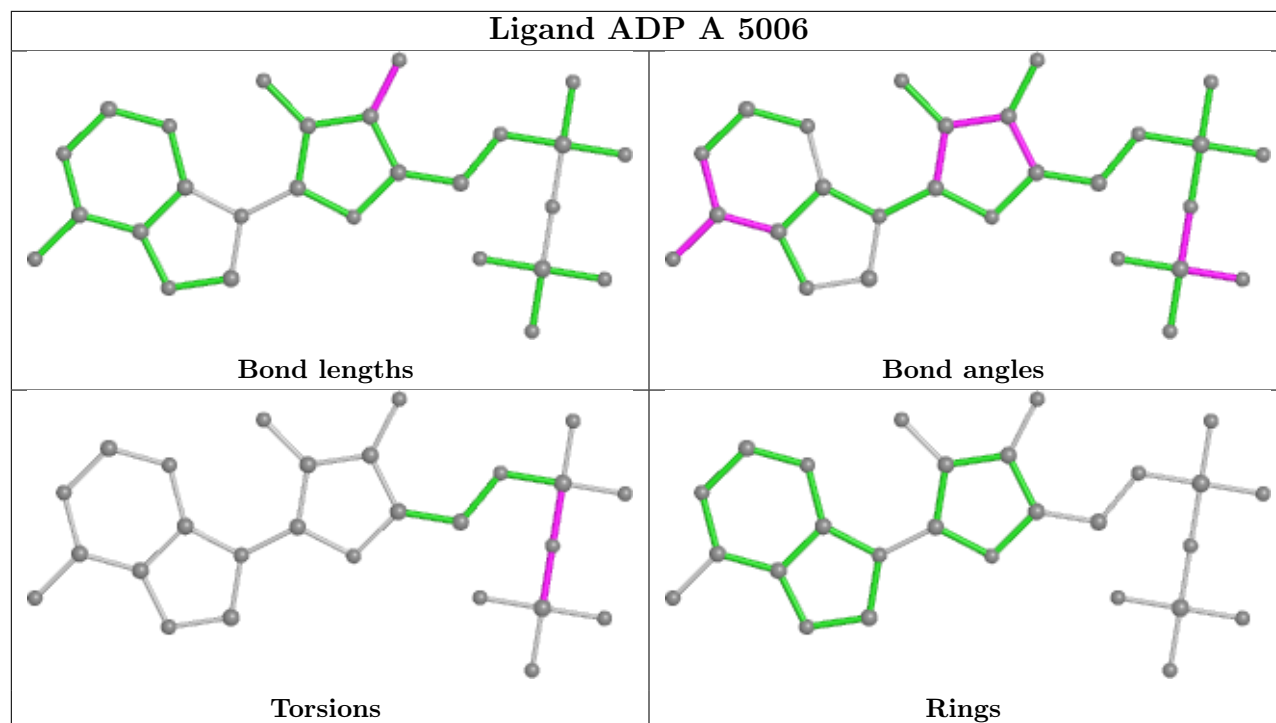


## Ligand ADP A 5000



## Ligand ADP G 5077





## 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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.