



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 27, 2024 – 02:28 PM EST

PDB ID : 1C30  
Title : CRYSTAL STRUCTURE OF CARBAMOYL PHOSPHATE SYNTHETASE:  
SMALL SUBUNIT MUTATION C269S  
Authors : Thoden, J.B.; Huang, X.; Raushel, F.M.; Holden, H.M.  
Deposited on : 1999-07-24  
Resolution : 2.00 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 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)  
Xtrriage (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

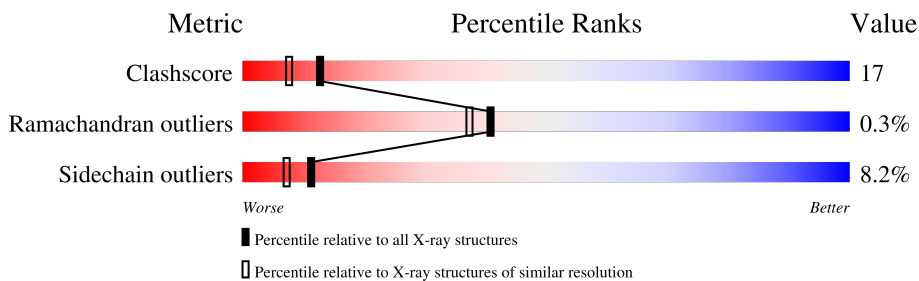
# 1 Overall quality at a glance

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	
1	C	1073	
1	E	1073	
1	G	1073	
2	B	382	
2	D	382	
2	F	382	
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:

<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
6	PO4	C	4025	-	X	-	-

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 48668 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
			Total	C	N	O	S			
1	A	1058	Total 8189	C 5141	N 1429	O 1574	S 45	0	6	0
1	C	1058	Total 8165	C 5126	N 1422	O 1572	S 45	0	1	0
1	E	1058	Total 8188	C 5141	N 1426	O 1575	S 46	0	6	0
1	G	1058	Total 8178	C 5137	N 1424	O 1572	S 45	0	4	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	379	Total 2895	C 1825	N 508	O 553	S 9	0	0	0
2	D	379	Total 2895	C 1825	N 508	O 553	S 9	0	0	0
2	F	379	Total 2895	C 1825	N 508	O 553	S 9	0	0	0
2	H	379	Total 2900	C 1828	N 508	O 555	S 9	0	1	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	269	SER	CYS	engineered mutation	UNP P00907
D	269	SER	CYS	engineered mutation	UNP P00907
F	269	SER	CYS	engineered mutation	UNP P00907
H	269	SER	CYS	engineered mutation	UNP P00907

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

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

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

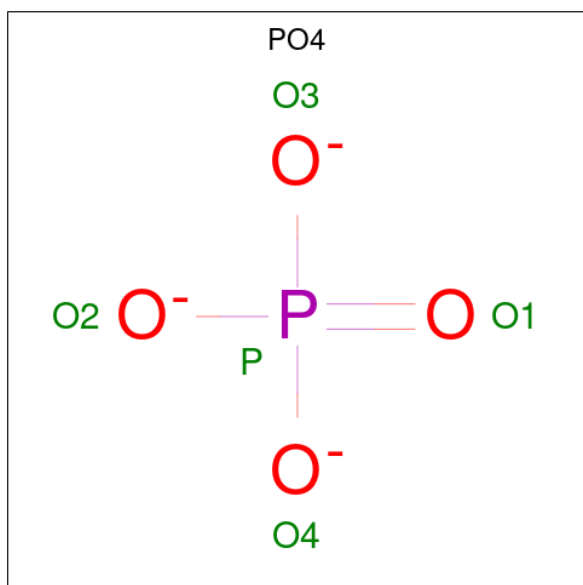
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	3	Total Cl 3 3	0	0
5	B	1	Total Cl 1 1	0	0
5	C	3	Total Cl 3 3	0	0
5	D	1	Total Cl 1 1	0	0
5	E	3	Total Cl 3 3	0	0
5	F	1	Total Cl 1 1	0	0

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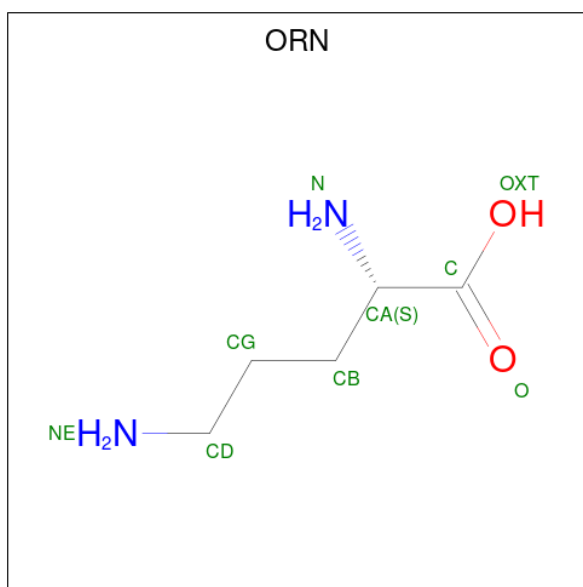
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	G	3	Total Cl 3 3	0	0
5	H	1	Total Cl 1 1	0	0

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



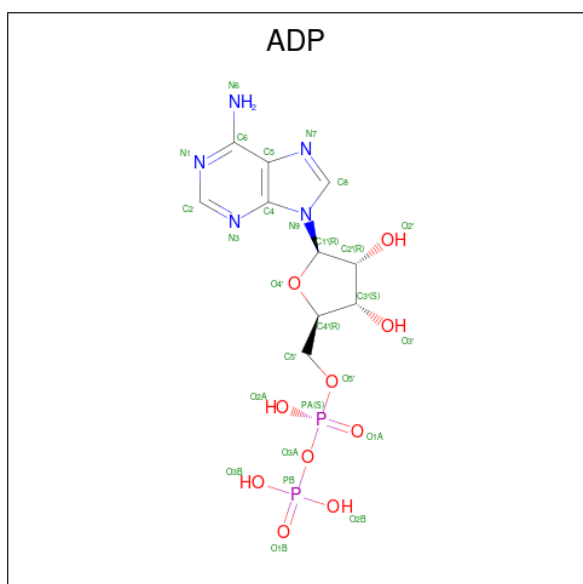
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O P 5 4 1	0	0
6	C	1	Total O P 5 4 1	0	0
6	C	1	Total O P 5 4 1	0	0
6	E	1	Total O P 5 4 1	0	0
6	E	1	Total O P 5 4 1	0	0
6	G	1	Total O P 5 4 1	0	0

- Molecule 7 is L-ornithine (three-letter code: ORN) (formula: C<sub>5</sub>H<sub>12</sub>N<sub>2</sub>O<sub>2</sub>).



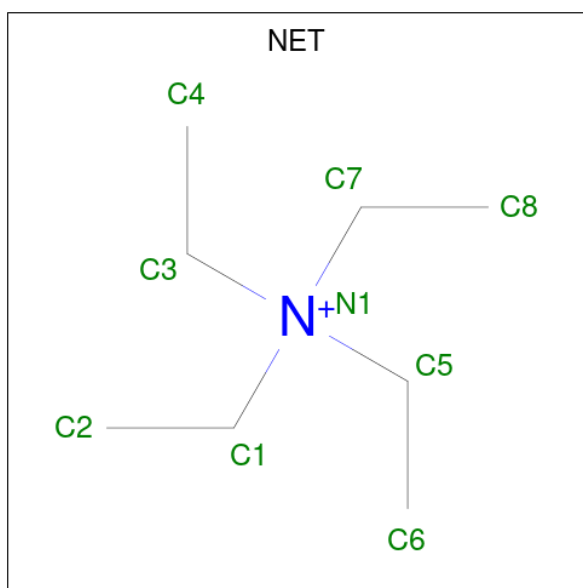
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
7	A	1	9	5	2	2	0	0
7	A	1	8	5	2	1	0	0
7	A	1	8	5	2	1	0	0
7	A	1	9	5	2	2	0	0

- Molecule 8 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
8	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
8	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
8	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
8	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
8	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
8	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
8	G	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
8	G	1	Total	C	N	O	P	0	0
			27	10	5	10	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	0	0
			9	8	1		
9	C	1	Total	C	N	0	0
			9	8	1		
9	E	1	Total	C	N	0	0
			9	8	1		
9	G	1	Total	C	N	0	0
			9	8	1		



- Molecule 10 is water.

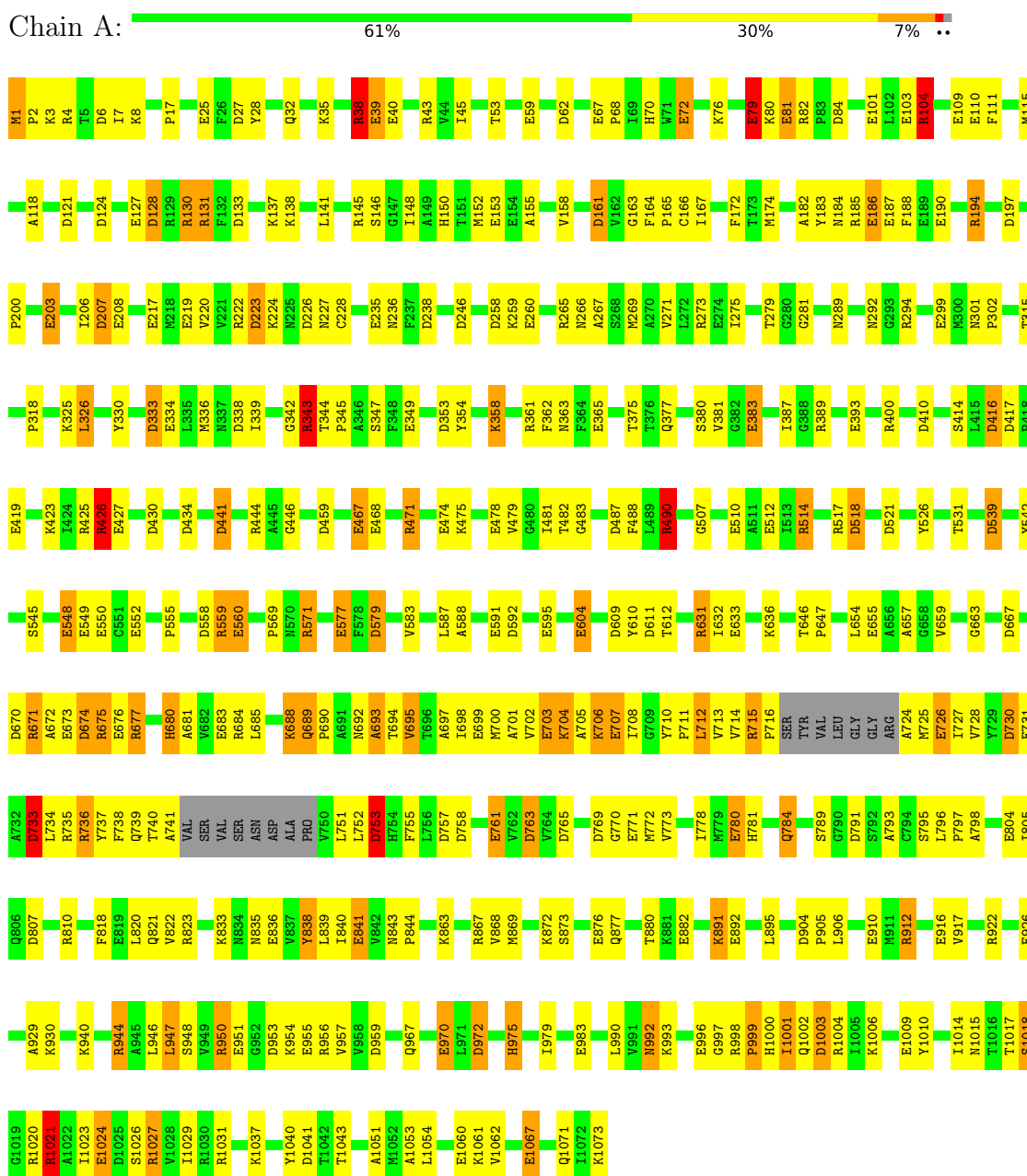
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	830	Total O 830 830	0	0
10	B	230	Total O 230 230	0	0
10	C	683	Total O 683 683	0	0
10	D	238	Total O 238 238	0	0
10	E	884	Total O 884 884	0	0
10	F	272	Total O 272 272	0	0
10	G	666	Total O 666 666	0	0
10	H	184	Total O 184 184	0	0

### 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.

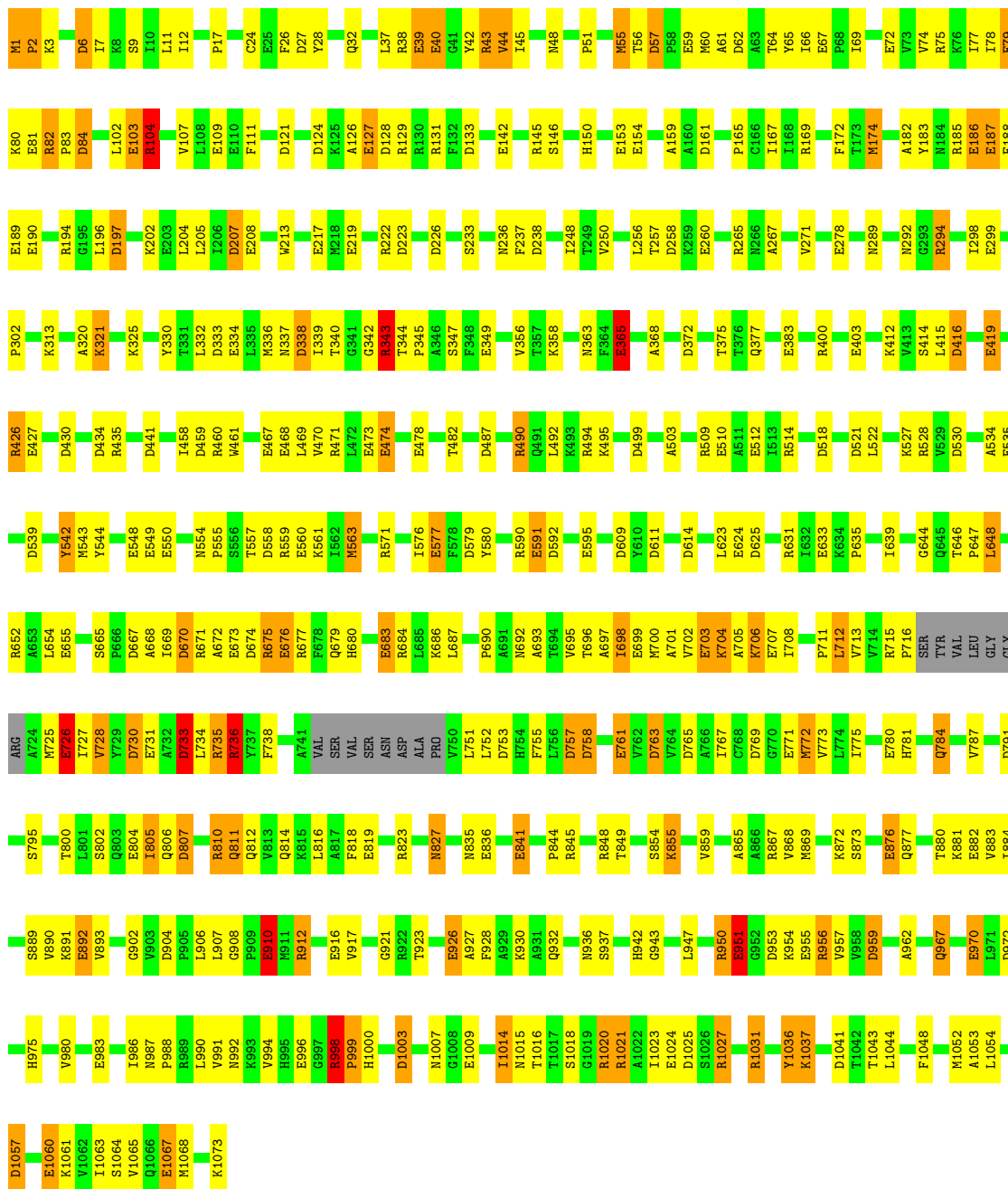
Note EDS was not executed.

- Molecule 1: CARBAMOYL PHOSPHATE SYNTHETASE: LARGE SUBUNIT



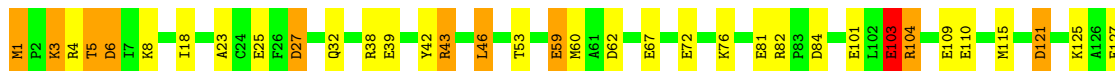
● Molecule 1: CARBAMOYL PHOSPHATE SYNTHETASE: LARGE SUBUNIT

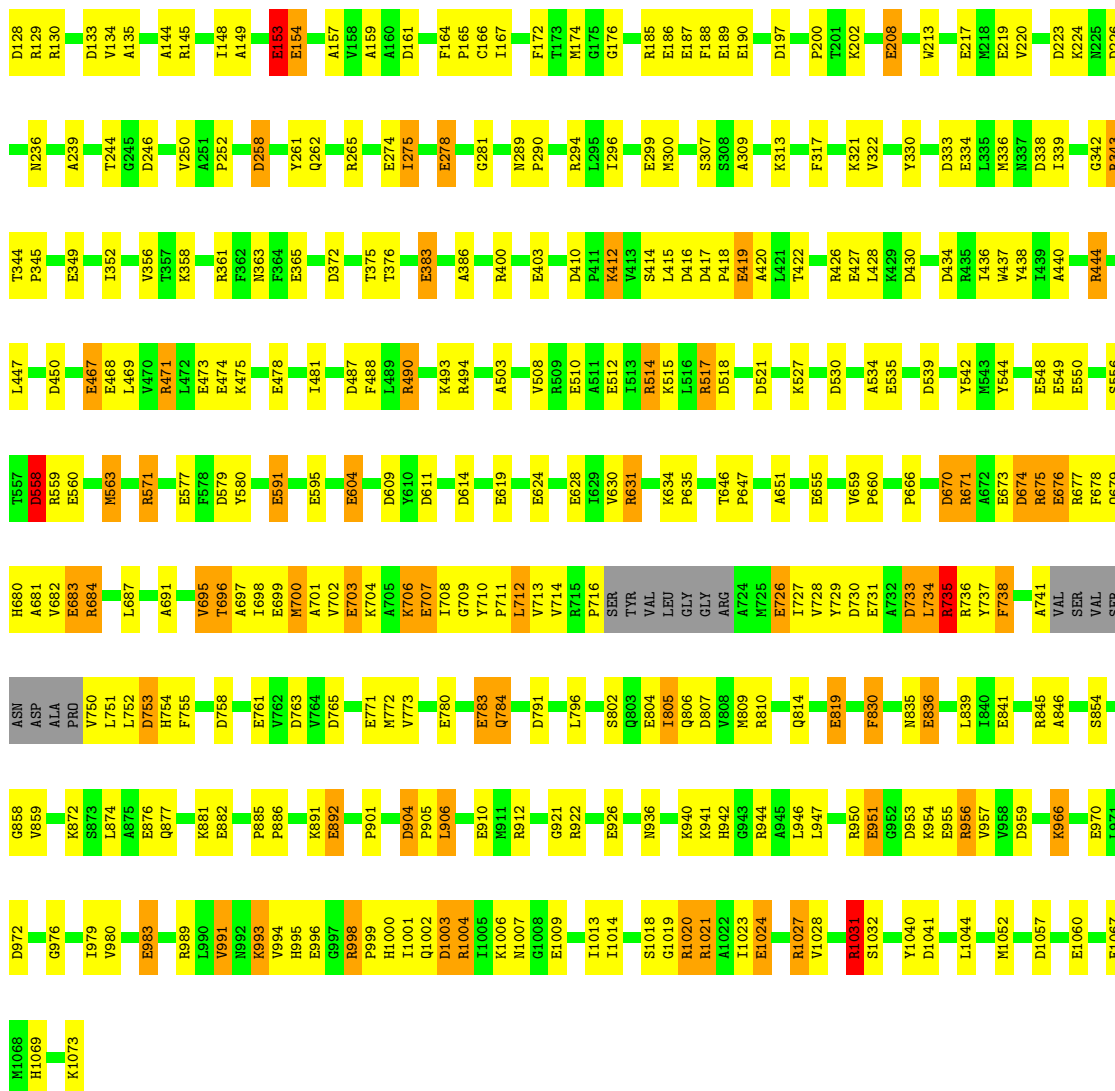
Chain C: 



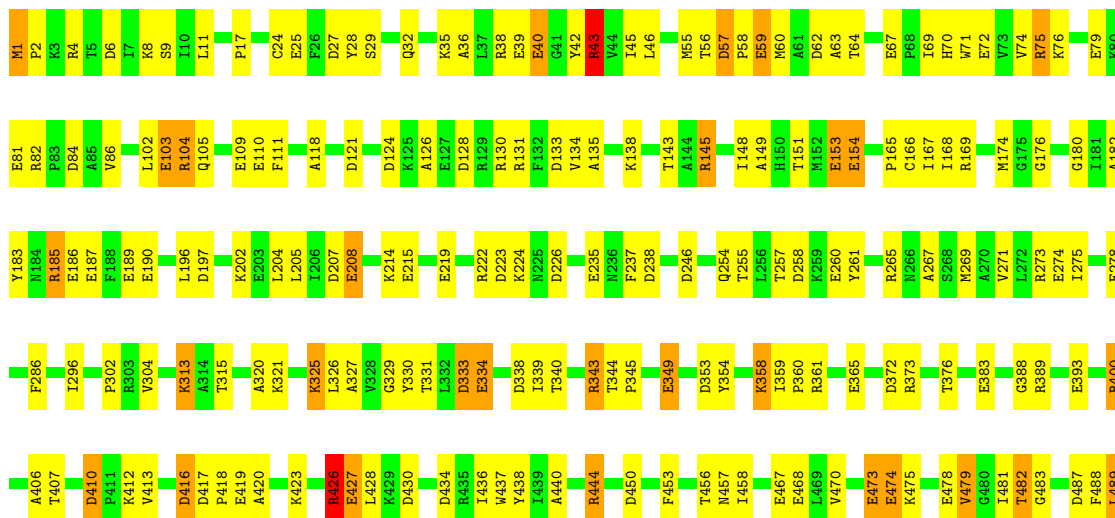
● Molecule 1: CARBAMOYL PHOSPHATE SYNTHETASE: LARGE SUBUNIT

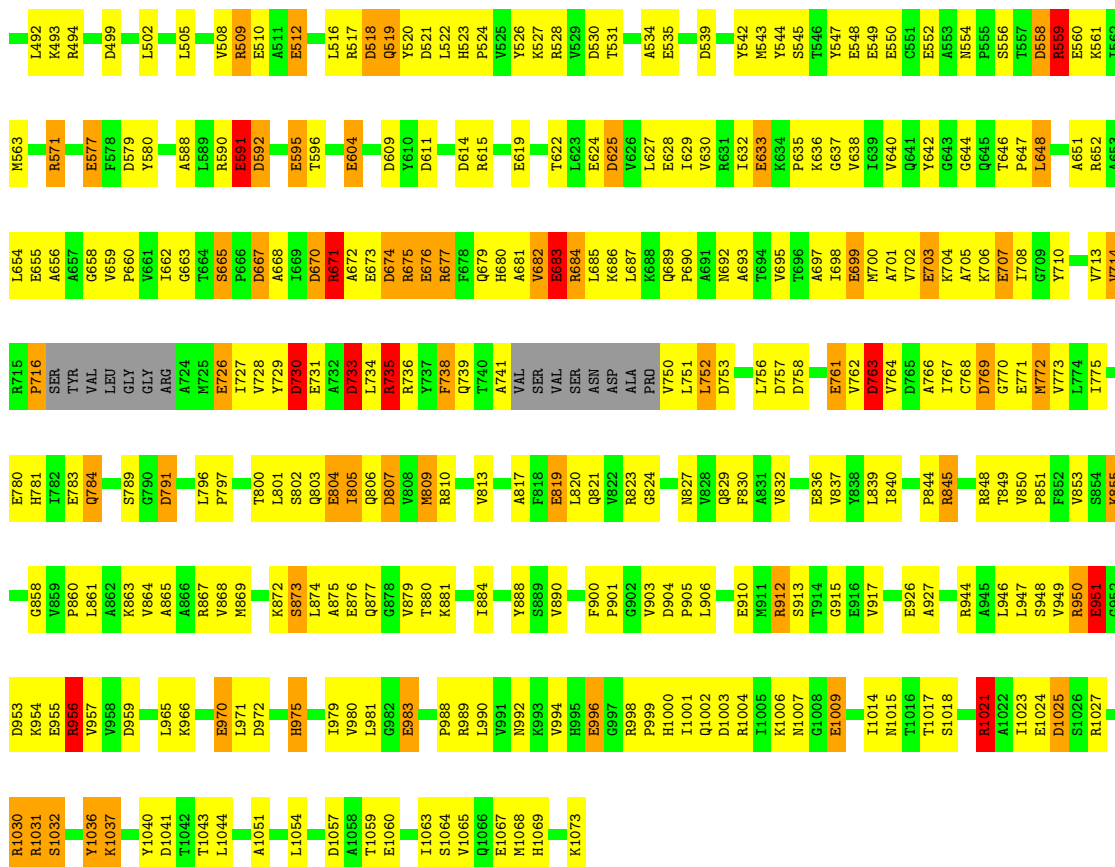
Chain E: 



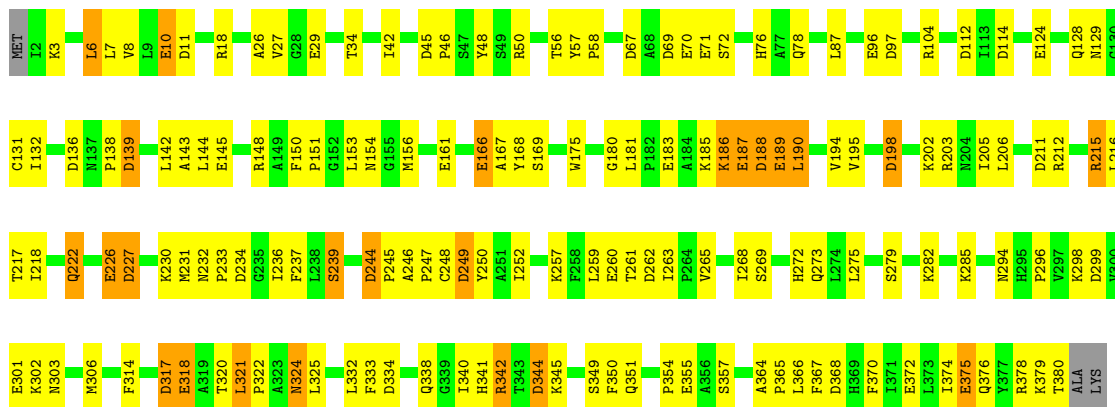


● Molecule 1: CARBAMOYL PHOSPHATE SYNTHETASE: LARGE SUBUNIT

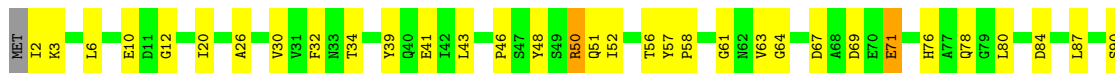


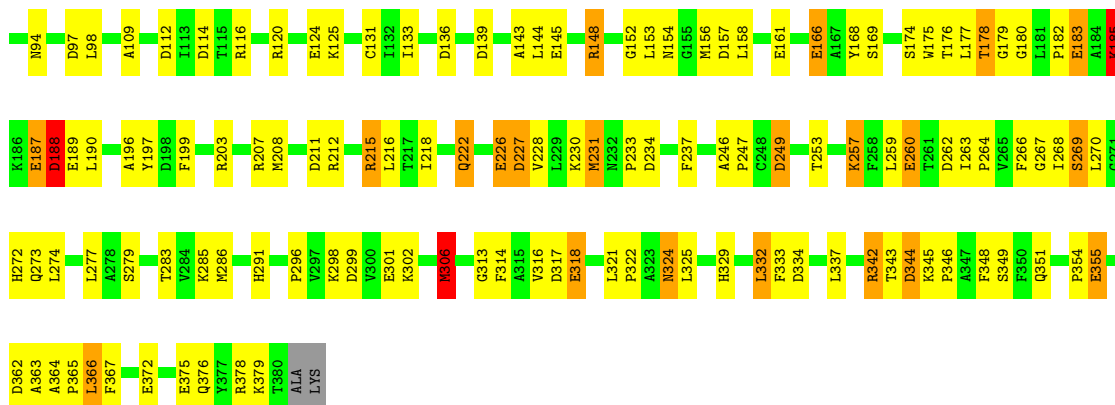


● Molecule 2: CARBAMOYL PHOSPHATE SYNTHETASE: SMALL SUBUNIT

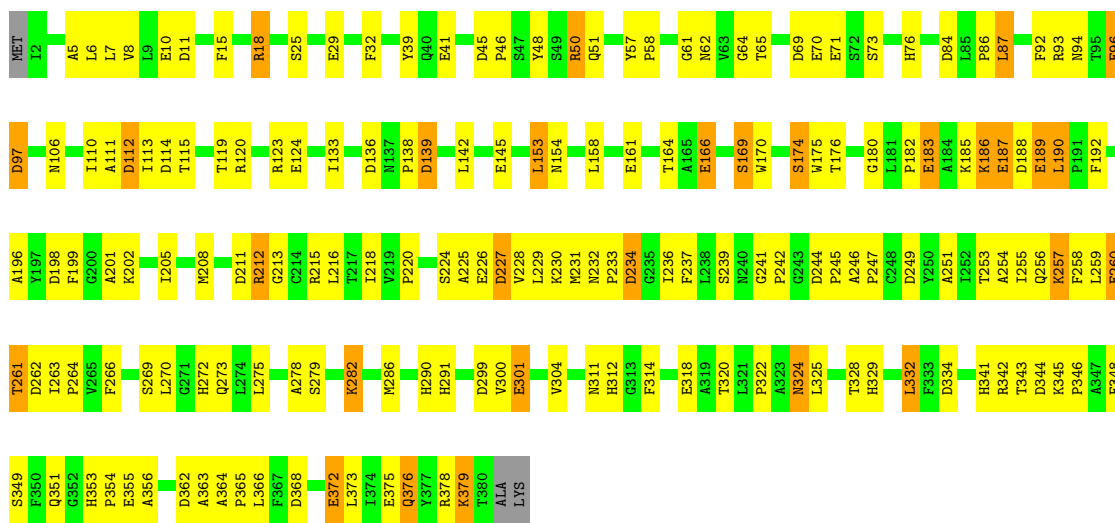


● Molecule 2: CARBAMOYL PHOSPHATE SYNTHETASE: SMALL SUBUNIT

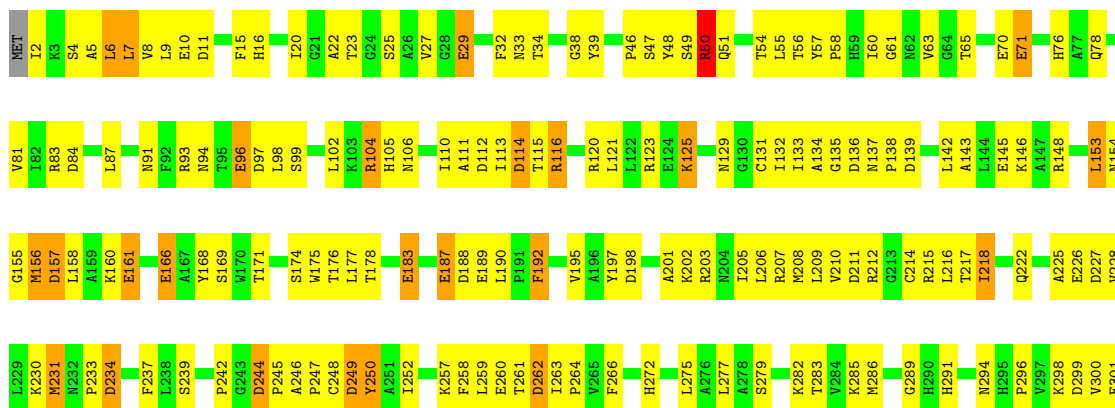


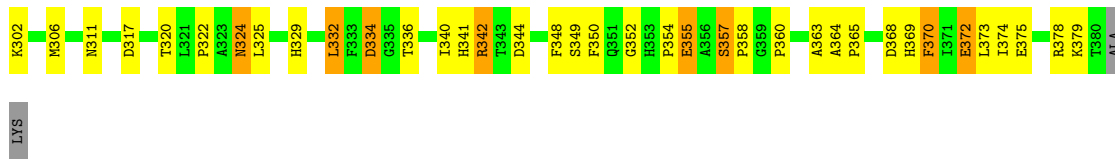


● Molecule 2: CARBAMOYL PHOSPHATE SYNTHETASE: SMALL SUBUNIT



● Molecule 2: CARBAMOYL PHOSPHATE SYNTHETASE: SMALL SUBUNIT





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## 4 Data and refinement statistics

Xtrriage (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, $\alpha$ , $\beta$ , $\gamma$	152.60Å 164.60Å 332.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.00	Depositor
% Data completeness (in resolution range)	97.7 (30.00-2.00)	Depositor
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	TNT 5E	Depositor
R, $R_{free}$	0.189 , 0.246	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	48668	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP



## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, NET, MN, ADP, CL, ORN, 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	1.02	75/8339 (0.9%)	1.40	124/11273 (1.1%)
1	C	1.05	77/8295 (0.9%)	1.45	145/11214 (1.3%)
1	E	1.05	77/8338 (0.9%)	1.40	116/11270 (1.0%)
1	G	1.00	72/8320 (0.9%)	1.44	131/11246 (1.2%)
2	B	0.90	19/2957 (0.6%)	1.29	37/4016 (0.9%)
2	D	0.97	18/2957 (0.6%)	1.36	36/4016 (0.9%)
2	F	0.93	20/2957 (0.7%)	1.35	40/4016 (1.0%)
2	H	0.93	18/2966 (0.6%)	1.36	35/4028 (0.9%)
All	All	1.01	376/45129 (0.8%)	1.40	664/61079 (1.1%)

The worst 5 of 376 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	40	GLU	CD-OE2	10.28	1.36	1.25
1	E	1009[A]	GLU	CD-OE2	9.59	1.36	1.25
1	E	1009[B]	GLU	CD-OE2	9.59	1.36	1.25
1	C	955	GLU	CD-OE2	9.24	1.35	1.25
1	C	951	GLU	CD-OE2	8.93	1.35	1.25

The worst 5 of 664 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	261	TYR	CB-CG-CD2	-14.58	112.25	121.00
1	C	490	ARG	NE-CZ-NH1	11.23	125.91	120.30
1	G	43	ARG	NE-CZ-NH2	-11.22	114.69	120.30
1	E	609	ASP	CB-CG-OD2	-10.78	108.60	118.30
1	E	514	ARG	NE-CZ-NH2	-10.48	115.06	120.30

There are no chirality outliers.

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	8189	0	8227	251	0
1	C	8165	0	8199	238	0
1	E	8188	0	8225	212	0
1	G	8178	0	8221	338	0
2	B	2895	0	2861	107	0
2	D	2895	0	2861	99	0
2	F	2895	0	2861	113	0
2	H	2900	0	2863	144	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	7	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	3	0	0	0	0
5	B	1	0	0	0	0
5	C	3	0	0	0	0
5	D	1	0	0	0	0
5	E	3	0	0	1	0
5	F	1	0	0	0	0
5	G	3	0	0	1	0
5	H	1	0	0	0	0
6	A	5	0	0	0	0
6	C	10	0	0	1	0
6	E	10	0	0	0	0
6	G	5	0	0	0	0
7	A	34	0	44	2	0
8	A	54	0	24	2	0
8	C	54	0	24	0	0
8	E	54	0	24	4	0
8	G	54	0	24	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	A	9	0	20	0	0
9	C	9	0	20	0	0
9	E	9	0	20	0	0
9	G	9	0	20	0	0
10	A	830	0	0	24	0
10	B	230	0	0	5	0
10	C	683	0	0	23	0
10	D	238	0	0	4	0
10	E	884	0	0	21	0
10	F	272	0	0	2	0
10	G	666	0	0	20	0
10	H	184	0	0	3	0
All	All	48668	0	44538	1483	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 17.

The worst 5 of 1483 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:993:LYS:CE	1:E:993:LYS:NZ	1.67	1.55
1:G:695:VAL:HG11	1:G:701:ALA:HB2	1.28	1.12
1:C:998:ARG:HG3	1:C:999:PRO:HA	1.30	1.11
1:C:695:VAL:HG11	1:C:701:ALA:HB2	1.34	1.09
2:H:187:GLU:HG2	2:H:215:ARG:HD2	1.31	1.07

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	1058/1073 (99%)	1012 (96%)	42 (4%)	4 (0%)	34	30
1	C	1053/1073 (98%)	996 (95%)	51 (5%)	6 (1%)	25	19
1	E	1058/1073 (99%)	1014 (96%)	44 (4%)	0	100	100
1	G	1056/1073 (98%)	1000 (95%)	50 (5%)	6 (1%)	25	19
2	B	377/382 (99%)	361 (96%)	16 (4%)	0	100	100
2	D	377/382 (99%)	364 (97%)	13 (3%)	0	100	100
2	F	377/382 (99%)	358 (95%)	18 (5%)	1 (0%)	41	37
2	H	378/382 (99%)	355 (94%)	23 (6%)	0	100	100
All	All	5734/5820 (98%)	5460 (95%)	257 (4%)	17 (0%)	41	37

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	558	ASP
1	A	975	HIS
1	C	698	ILE
1	A	693	ALA
1	C	758	ASP

### 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	871/878 (99%)	808 (93%)	63 (7%)	14	9
1	C	866/878 (99%)	799 (92%)	67 (8%)	13	8
1	E	871/878 (99%)	805 (92%)	66 (8%)	13	8
1	G	869/878 (99%)	791 (91%)	78 (9%)	9	6
2	B	308/310 (99%)	284 (92%)	24 (8%)	12	8
2	D	308/310 (99%)	284 (92%)	24 (8%)	12	8
2	F	308/310 (99%)	279 (91%)	29 (9%)	8	5
2	H	309/310 (100%)	271 (88%)	38 (12%)	4	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	4710/4752 (99%)	4321 (92%)	389 (8%)	11 7

5 of 389 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	950	ARG
1	G	275	ILE
1	E	1018	SER
2	F	190	LEU
1	G	509	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 82 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	1071	GLN
1	G	992	ASN
2	F	154	ASN
1	G	784	GLN
2	H	51	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 82 ligands modelled in this entry, 60 are monoatomic - leaving 22 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	ORN	A	4072	-	7,8,8	0.79	0	8,9,9	1.43	1 (12%)
6	PO4	C	4040	-	4,4,4	1.25	0	6,6,6	0.80	0
8	ADP	C	4026	4,3	24,29,29	1.08	3 (12%)	29,45,45	1.15	3 (10%)
9	NET	E	4052	-	8,8,8	0.67	0	10,10,10	0.62	0
6	PO4	A	4005	4,3	4,4,4	2.30	2 (50%)	6,6,6	1.25	0
9	NET	G	4073	-	8,8,8	0.78	0	10,10,10	0.42	0
8	ADP	E	4047	4,3	24,29,29	1.23	3 (12%)	29,45,45	1.09	3 (10%)
6	PO4	E	4046	4,3	4,4,4	2.02	2 (50%)	6,6,6	1.06	0
6	PO4	G	4067	4,3	4,4,4	2.31	2 (50%)	6,6,6	1.12	0
8	ADP	C	4020	3	24,29,29	1.20	2 (8%)	29,45,45	1.36	3 (10%)
7	ORN	A	4051	-	6,7,8	1.14	1 (16%)	2,7,9	0.41	0
6	PO4	E	4061	-	4,4,4	2.25	3 (75%)	6,6,6	0.91	0
8	ADP	G	4068	4,3	24,29,29	1.14	4 (16%)	29,45,45	1.27	4 (13%)
8	ADP	A	4000	3	24,29,29	1.12	3 (12%)	29,45,45	1.29	3 (10%)
8	ADP	E	4041	3	24,29,29	1.28	3 (12%)	29,45,45	1.42	5 (17%)
6	PO4	C	4025	4,3	4,4,4	2.35	4 (100%)	6,6,6	1.10	0
8	ADP	G	4062	3	24,29,29	1.08	2 (8%)	29,45,45	1.13	3 (10%)
7	ORN	A	4030	-	6,7,8	1.04	1 (16%)	2,7,9	0.93	0
7	ORN	A	4010	-	7,8,8	1.01	1 (14%)	8,9,9	1.52	2 (25%)
9	NET	C	4031	-	8,8,8	0.55	0	10,10,10	0.50	0
8	ADP	A	4006	4,3	24,29,29	1.09	1 (4%)	29,45,45	1.39	4 (13%)
9	NET	A	4011	-	8,8,8	0.67	0	10,10,10	0.56	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
8	ADP	G	4068	4,3	-	3/12/32/32	0/3/3/3
7	ORN	A	4072	-	-	6/8/8/8	-
8	ADP	A	4000	3	-	0/12/32/32	0/3/3/3
8	ADP	E	4041	3	-	1/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	ADP	E	4047	4,3	-	3/12/32/32	0/3/3/3
8	ADP	C	4020	3	-	2/12/32/32	0/3/3/3
8	ADP	G	4062	3	-	0/12/32/32	0/3/3/3
7	ORN	A	4030	-	-	4/5/6/8	-
7	ORN	A	4010	-	-	6/8/8/8	-
9	NET	C	4031	-	-	0/12/12/12	-
8	ADP	C	4026	4,3	-	0/12/32/32	0/3/3/3
7	ORN	A	4051	-	-	3/5/6/8	-
9	NET	E	4052	-	-	3/12/12/12	-
8	ADP	A	4006	4,3	-	3/12/32/32	0/3/3/3
9	NET	G	4073	-	-	0/12/12/12	-
9	NET	A	4011	-	-	0/12/12/12	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	4067	PO4	P-O2	-3.65	1.43	1.54
8	G	4068	ADP	O3'-C3'	3.04	1.50	1.43
8	E	4047	ADP	O2'-C2'	3.02	1.50	1.43
8	E	4041	ADP	O2'-C2'	3.01	1.50	1.43
6	E	4046	PO4	P-O2	-2.91	1.45	1.54

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	4020	ADP	C5-C6-N6	5.01	127.96	120.35
8	A	4000	ADP	C5-C6-N6	4.41	127.06	120.35
8	A	4006	ADP	C5-C6-N6	4.25	126.81	120.35
8	E	4041	ADP	C5-C6-N6	4.24	126.80	120.35
8	G	4068	ADP	C5-C6-N6	3.12	125.09	120.35

There are no chirality outliers.

5 of 34 torsion outliers are listed below:

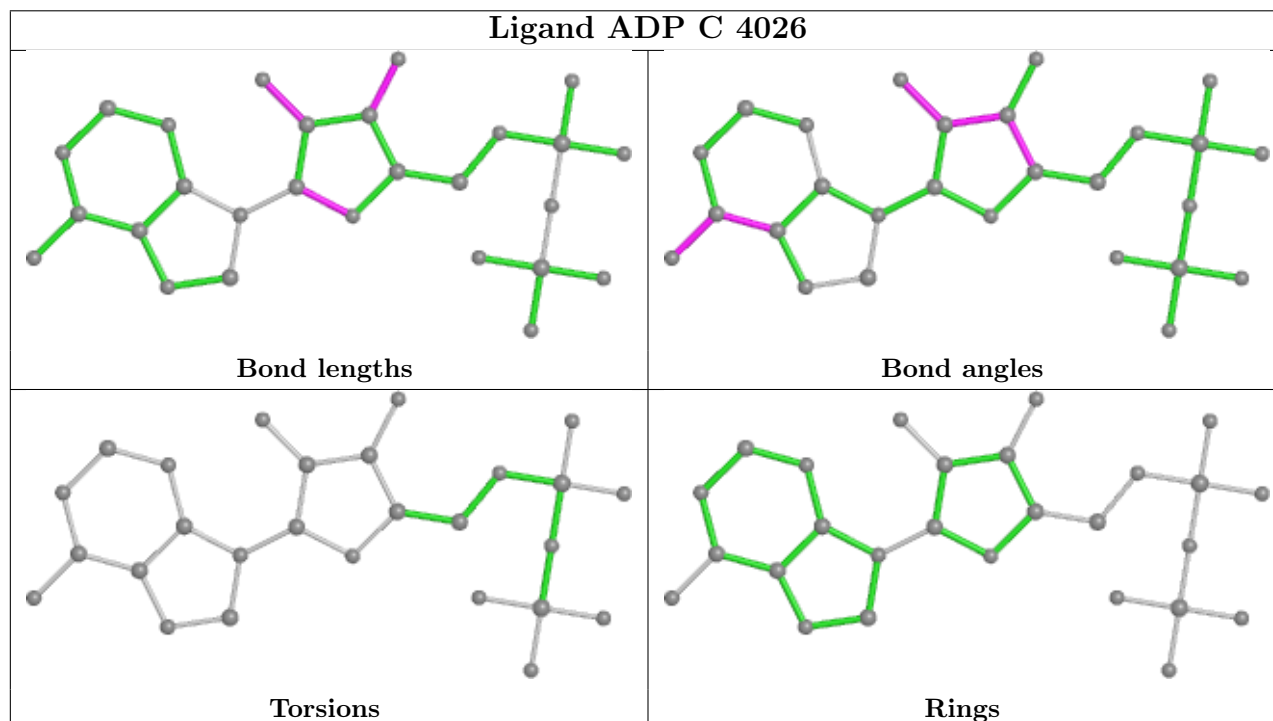
Mol	Chain	Res	Type	Atoms
7	A	4010	ORN	N-CA-CB-CG
7	A	4010	ORN	C-CA-CB-CG
7	A	4030	ORN	N-CA-CB-CG
7	A	4030	ORN	C-CA-CB-CG
7	A	4051	ORN	N-CA-CB-CG

There are no ring outliers.

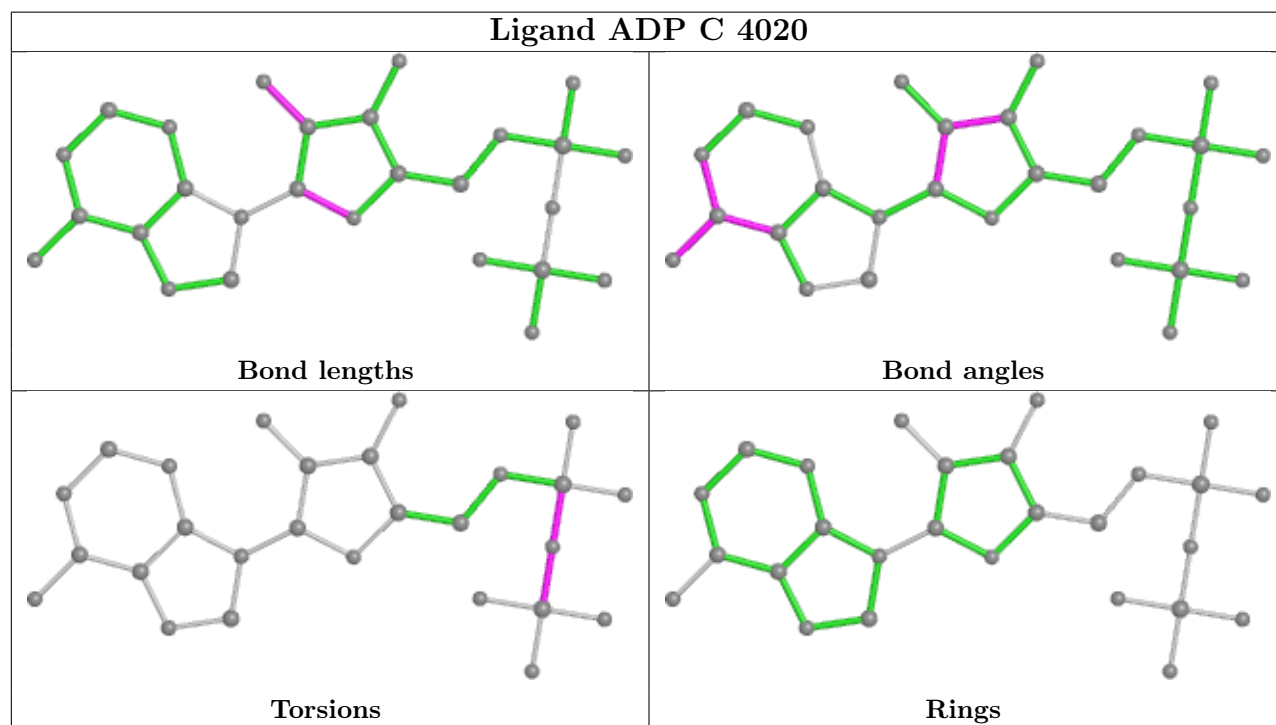
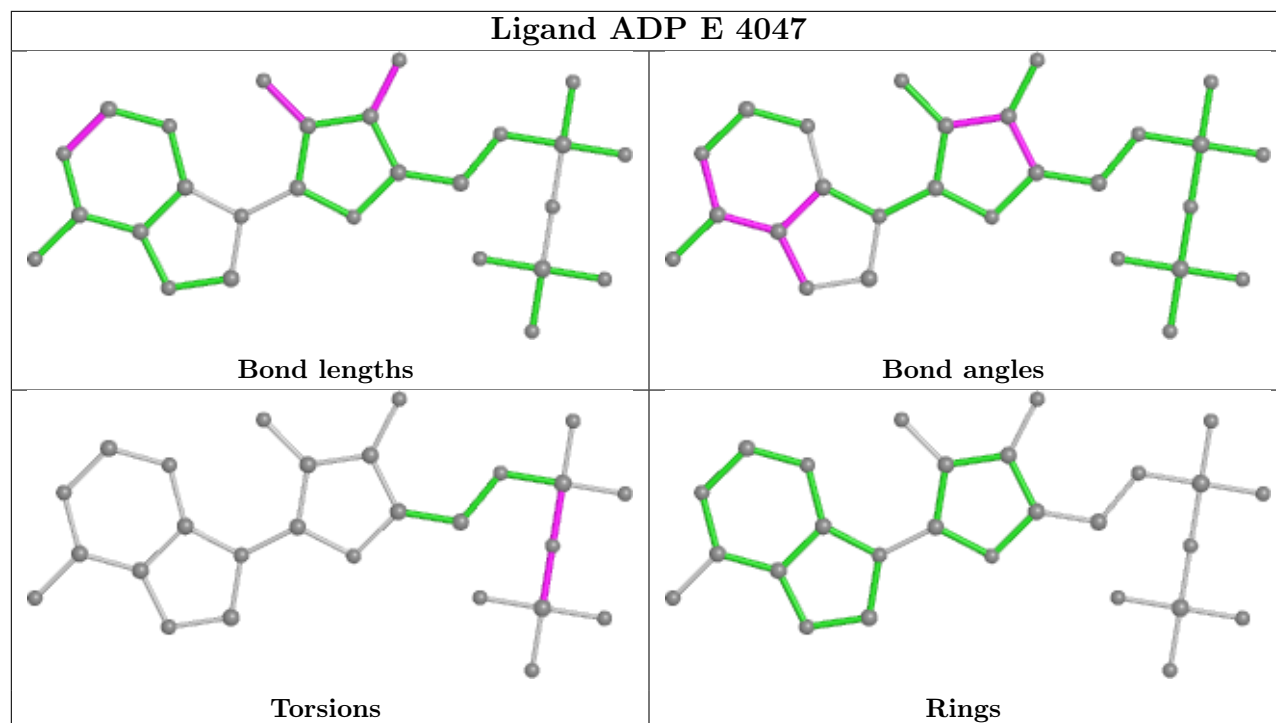
8 monomers are involved in 10 short contacts:

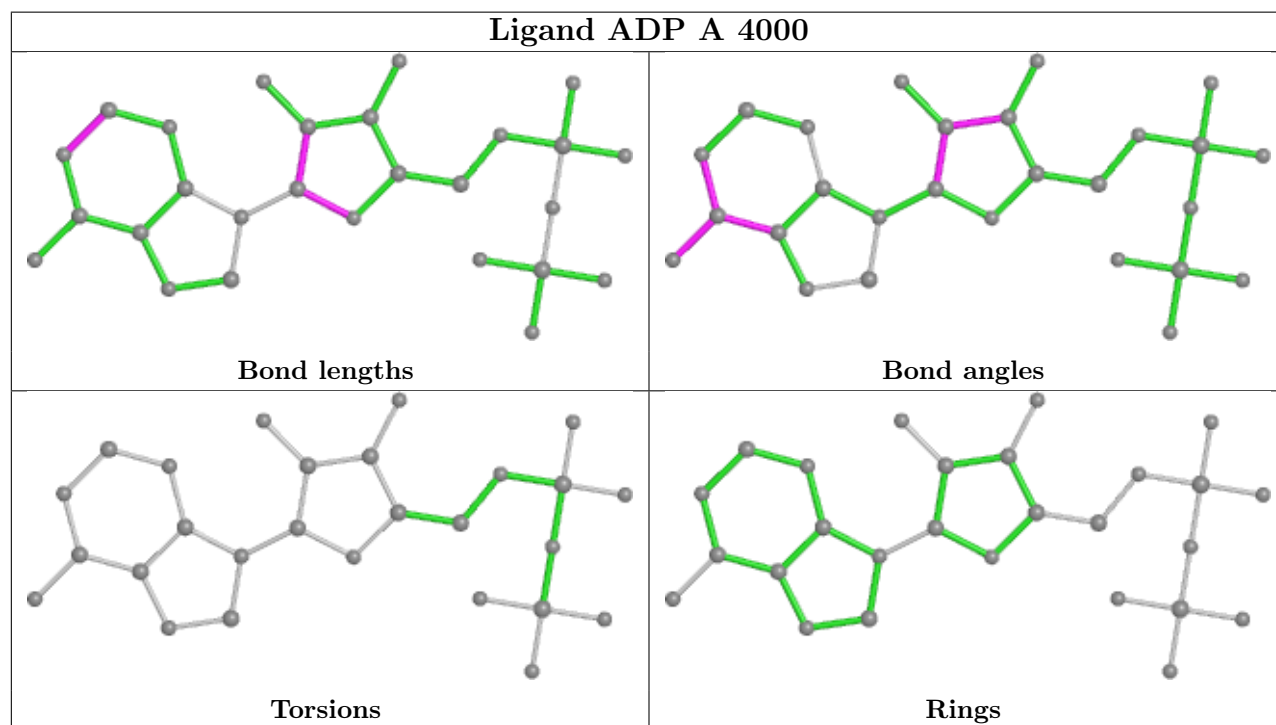
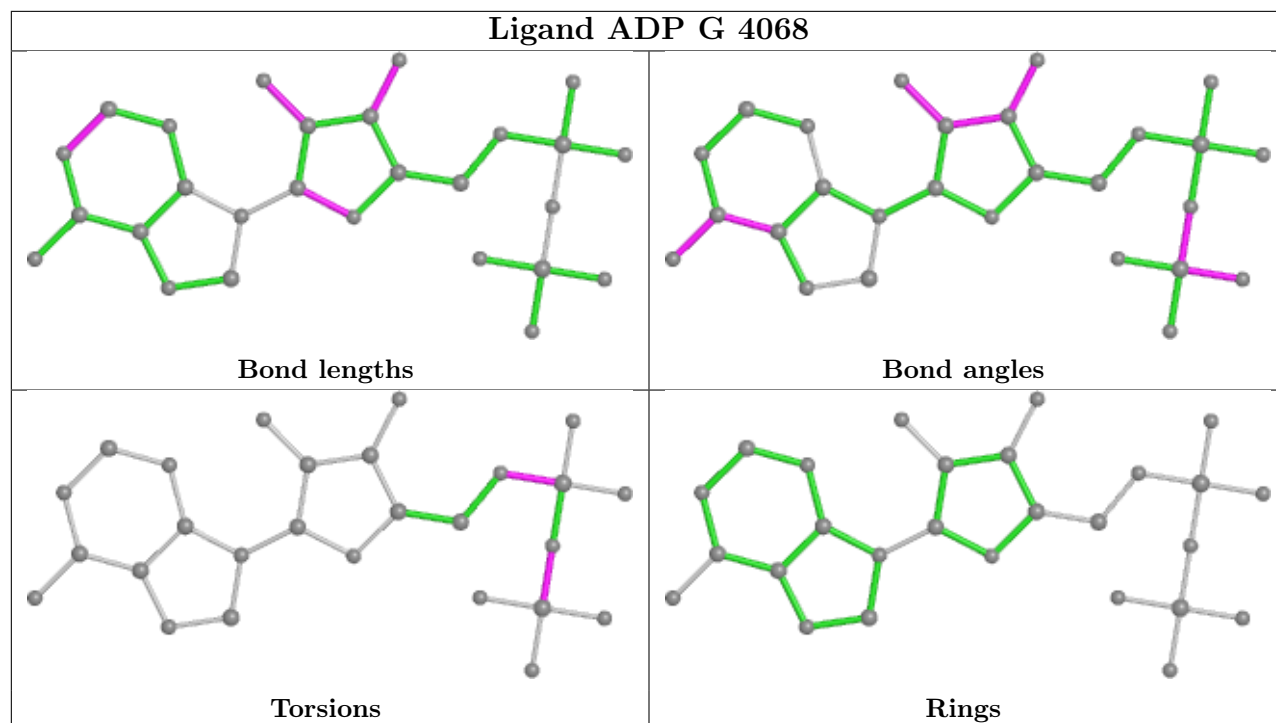
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	E	4047	ADP	2	0
7	A	4051	ORN	1	0
8	A	4000	ADP	1	0
8	E	4041	ADP	2	0
6	C	4025	PO4	1	0
8	G	4062	ADP	1	0
7	A	4030	ORN	1	0
8	A	4006	ADP	1	0

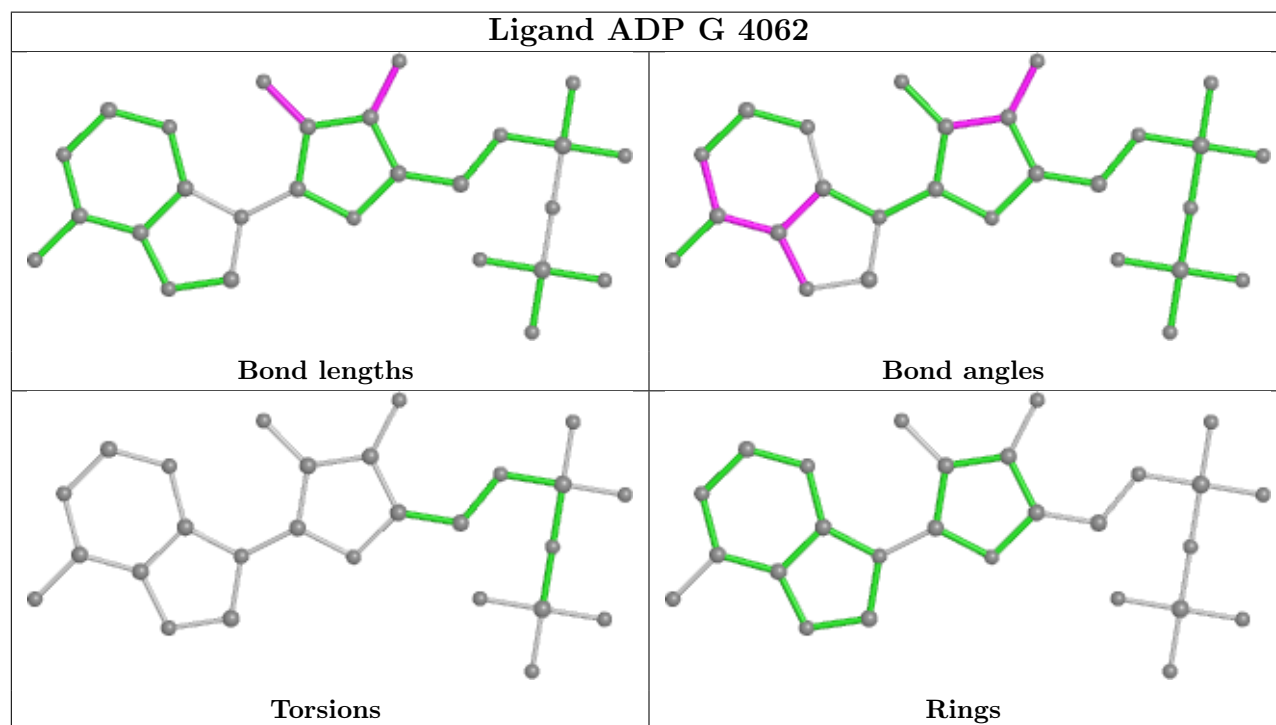
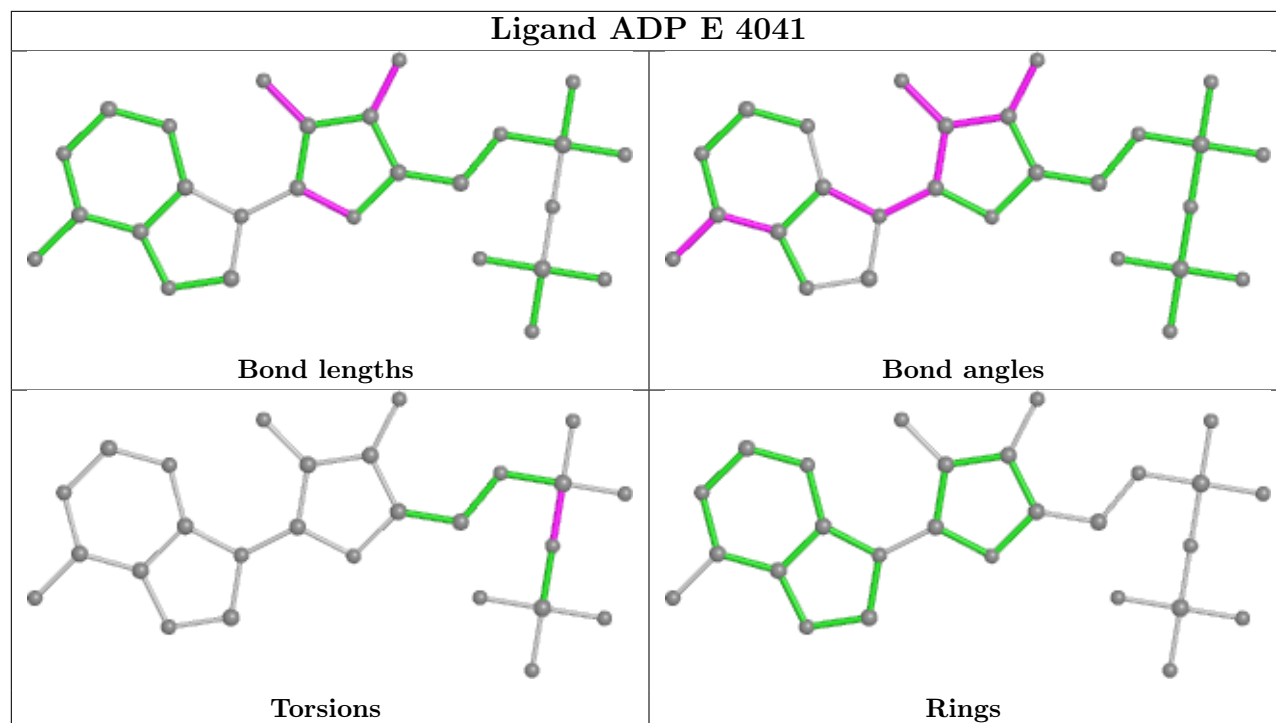
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

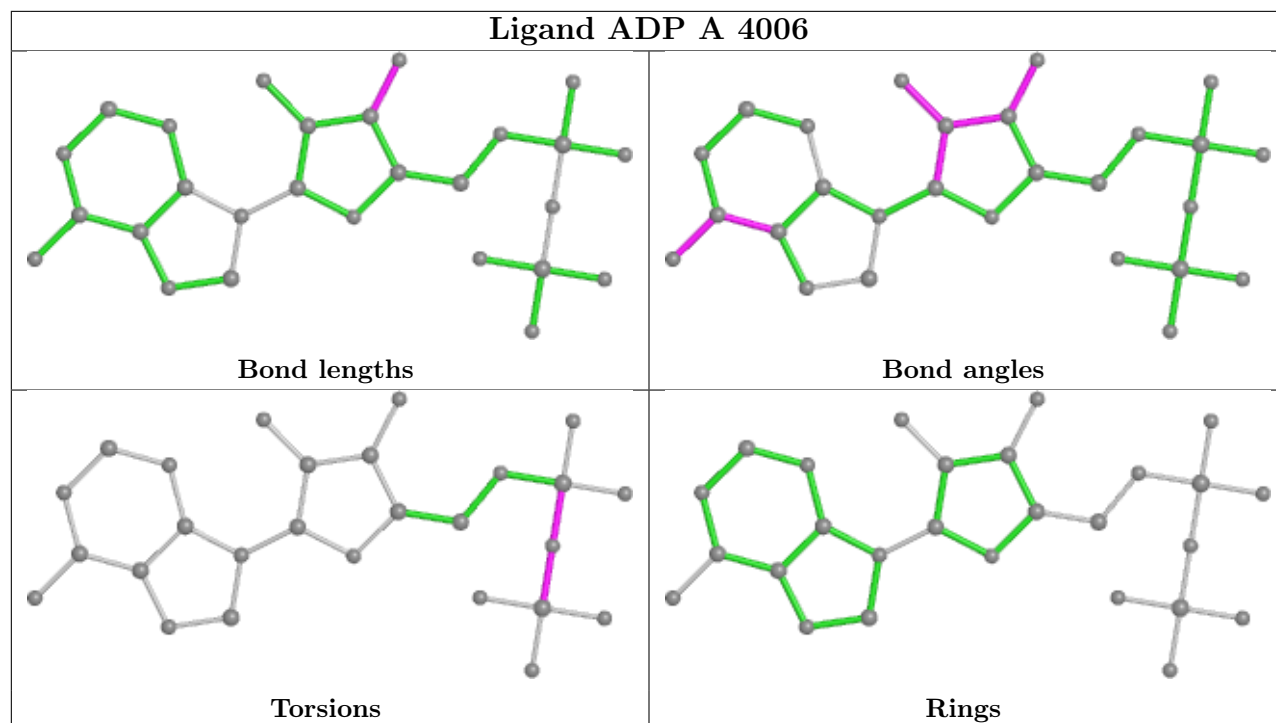












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 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.