



wwPDB X-ray Structure Validation Summary Report ⓘ

May 26, 2020 – 09:46 am BST

PDB ID : 1C3O
Title : CRYSTAL STRUCTURE OF THE CARBAMOYL PHOSPHATE SYNTHETASE: SMALL SUBUNIT MUTANT C269S WITH BOUND GLUTAMINE
Authors : Thoden, J.B.; Huang, X.; Raushel, F.M.; Holden, H.M.
Deposited on : 1999-07-28
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

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) : **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) : 2.11

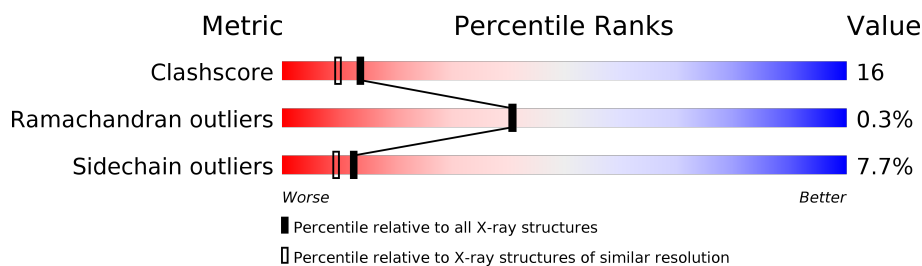
1 Overall quality at a glance

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)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	1073	61% 30% 7% ..
1	C	1073	60% 31% 6% ..
1	E	1073	64% 28% 6% ..
1	G	1073	56% 34% 7% ..
2	B	382	58% 34% 7% .
2	D	382	57% 36% 6% .
2	F	382	55% 36% 7% .
2	H	382	49% 42% 8% .

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
5	CL	G	4083	-	-	X	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 48477 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	6	0
			8195	5146	1433	1570	46			
1	C	1058	Total	C	N	O	S	0	7	0
			8192	5144	1428	1575	45			
1	E	1058	Total	C	N	O	S	0	10	0
			8211	5155	1431	1580	45			
1	G	1058	Total	C	N	O	S	0	4	0
			8180	5135	1425	1574	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
			2895	1825	508	553	9			
2	D	379	Total	C	N	O	S	0	0	0
			2895	1825	508	553	9			
2	F	379	Total	C	N	O	S	0	0	0
			2895	1825	508	553	9			
2	H	379	Total	C	N	O	S	0	0	0
			2895	1825	508	553	9			

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	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).

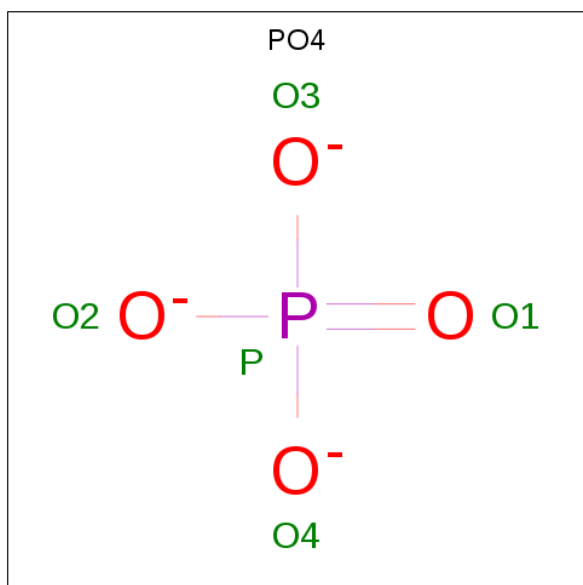
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	G	3	Total Cl 3 3	0	0
5	D	1	Total Cl 1 1	0	0
5	E	3	Total Cl 3 3	0	0
5	H	1	Total Cl 1 1	0	0
5	B	1	Total Cl 1 1	0	0
5	C	3	Total Cl 3 3	0	0

Continued on next page...

Continued from previous page...

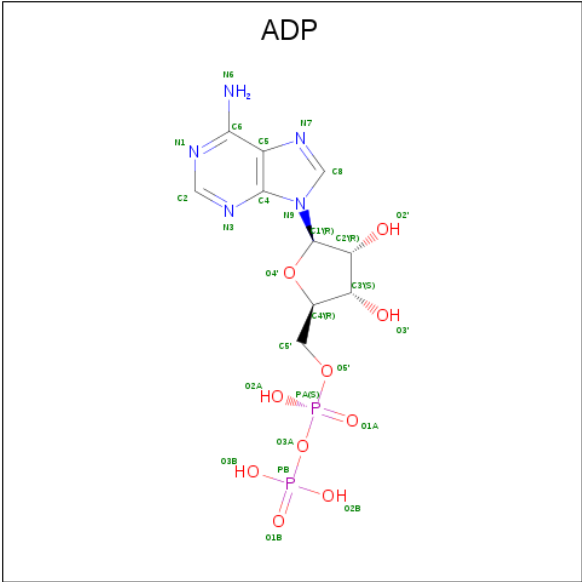
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	3	Total	Cl	0	0
			3	3		
5	F	1	Total	Cl	0	0
			1	1		

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



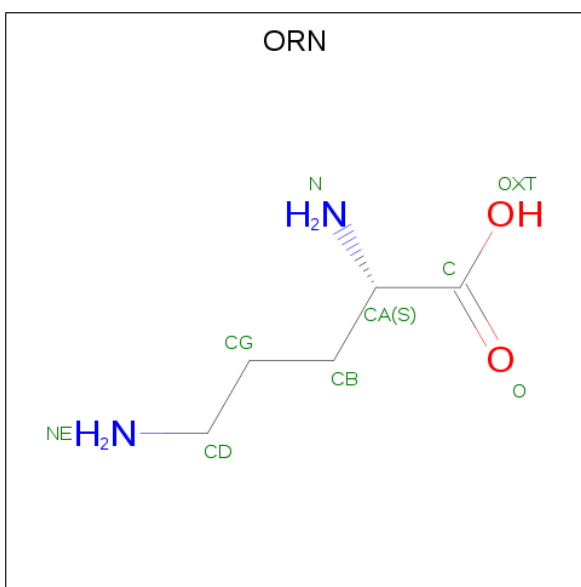
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	P	0	0
			5	4	1		
6	C	1	Total	O	P	0	0
			5	4	1		
6	E	1	Total	O	P	0	0
			5	4	1		
6	E	1	Total	O	P	0	0
			5	4	1		
6	G	1	Total	O	P	0	0
			5	4	1		

- Molecule 7 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



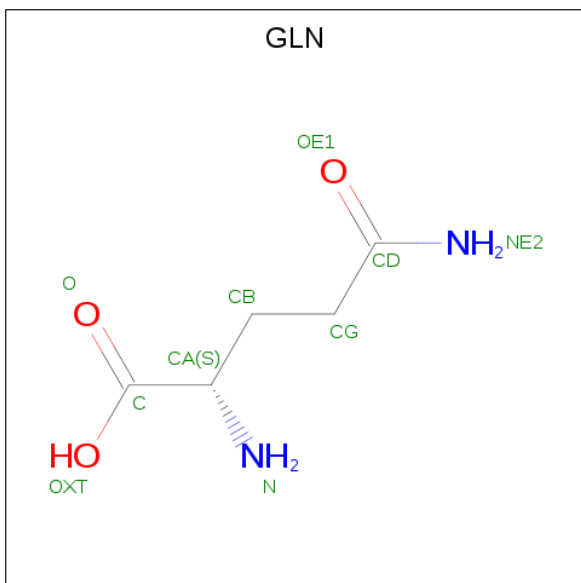
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	G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

- Molecule 8 is L-ornithine (three-letter code: ORN) (formula: C₅H₁₂N₂O₂).



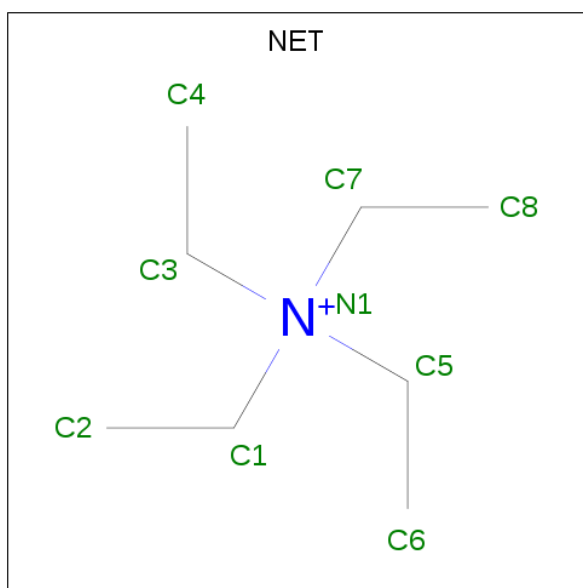
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			9	5	2	2		
8	C	1	Total	C	N	O	0	0
			9	5	2	2		
8	E	1	Total	C	N	O	0	0
			9	5	2	2		
8	G	1	Total	C	N	O	0	0
			9	5	2	2		

- Molecule 9 is GLUTAMINE (three-letter code: GLN) (formula: $C_5H_{10}N_2O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	N	O	0	0
			10	5	2	3		
9	B	1	Total	C	N	O	0	0
			10	5	2	3		
9	C	1	Total	C	N	O	0	0
			10	5	2	3		
9	D	1	Total	C	N	O	0	0
			10	5	2	3		
9	E	1	Total	C	N	O	0	0
			10	5	2	3		
9	F	1	Total	C	N	O	0	0
			10	5	2	3		
9	G	1	Total	C	N	O	0	0
			10	5	2	3		
9	H	1	Total	C	N	O	0	0
			10	5	2	3		

- Molecule 10 is TETRAETHYLAMMONIUM ION (three-letter code: NET) (formula: $C_8H_{20}N$).



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

- Molecule 11 is water.

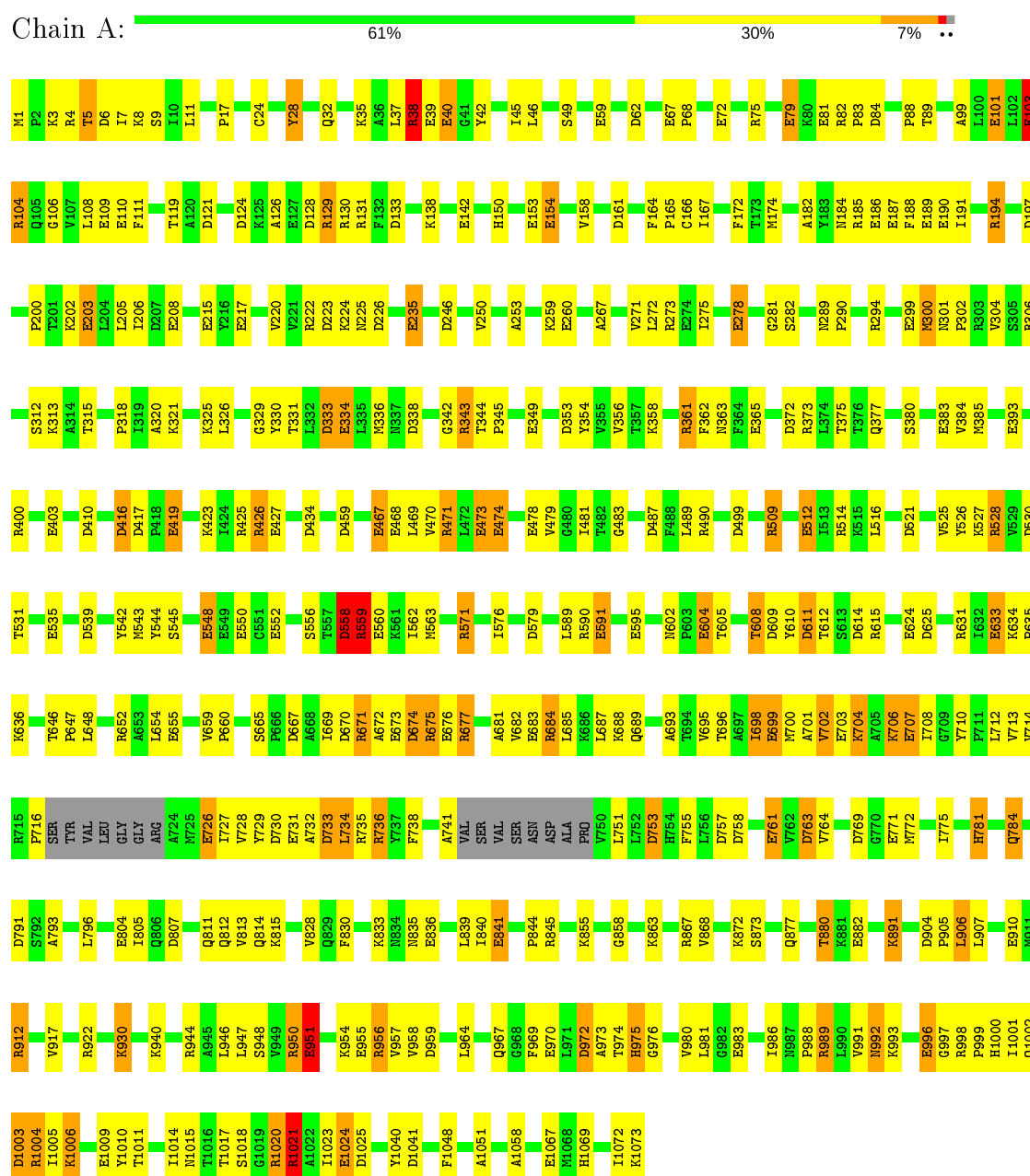
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	699	Total 699	O 699	0	0
11	B	231	Total 231	O 231	0	0
11	C	706	Total 706	O 706	0	0
11	D	250	Total 250	O 250	0	0
11	E	754	Total 754	O 754	0	0
11	F	231	Total 231	O 231	0	0
11	G	622	Total 622	O 622	0	0
11	H	173	Total 173	O 173	0	0

3 Residue-property plots

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. 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.

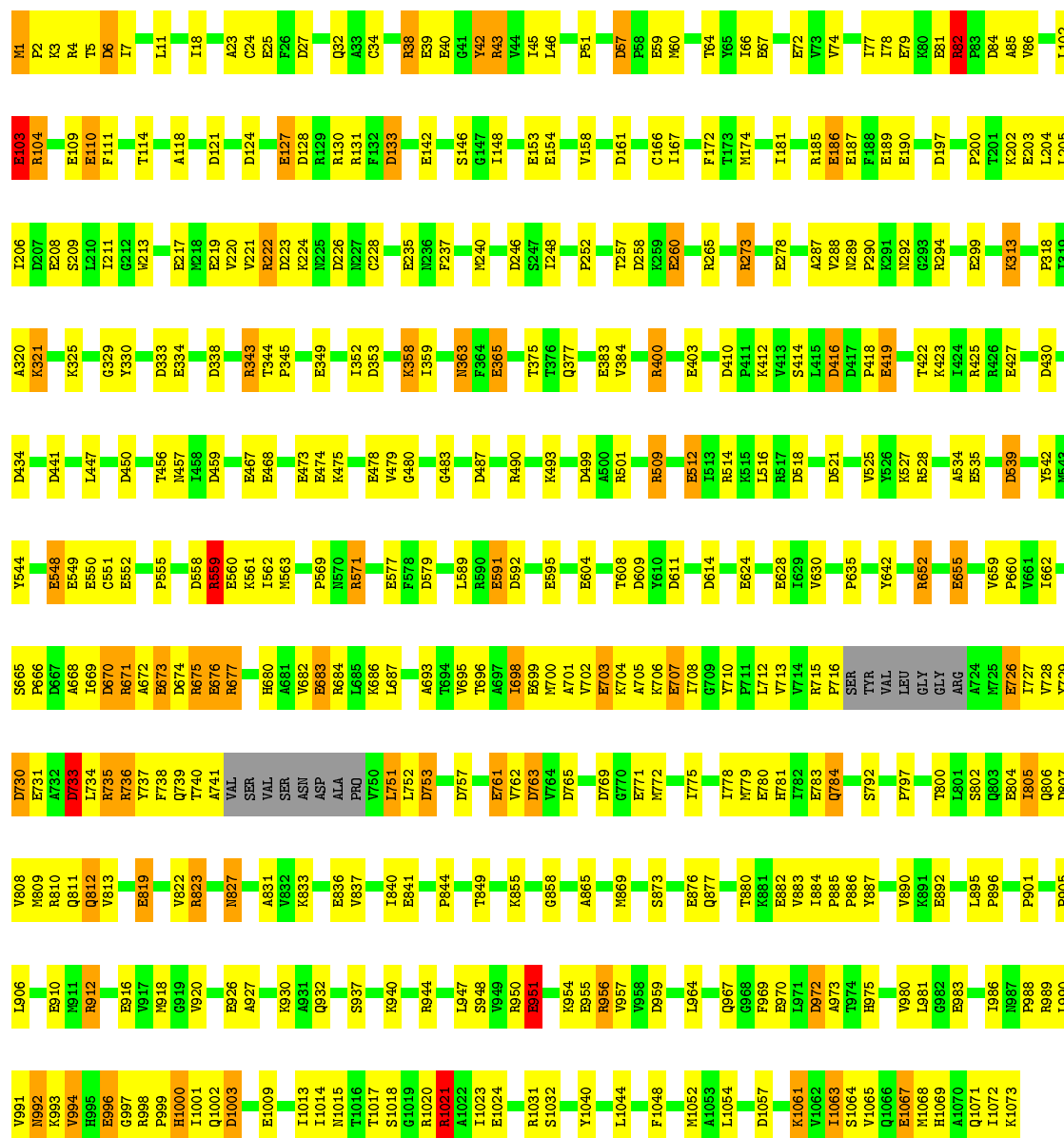
Note EDS was not executed.

• Molecule 1: CARBAMOYL PHOSPHATE SYNTHETASE: LARGE SUBUNIT



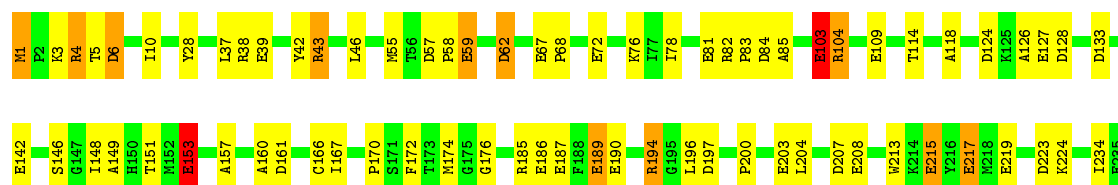
• Molecule 1: CARBAMOYL PHOSPHATE SYNTHETASE: LARGE SUBUNIT

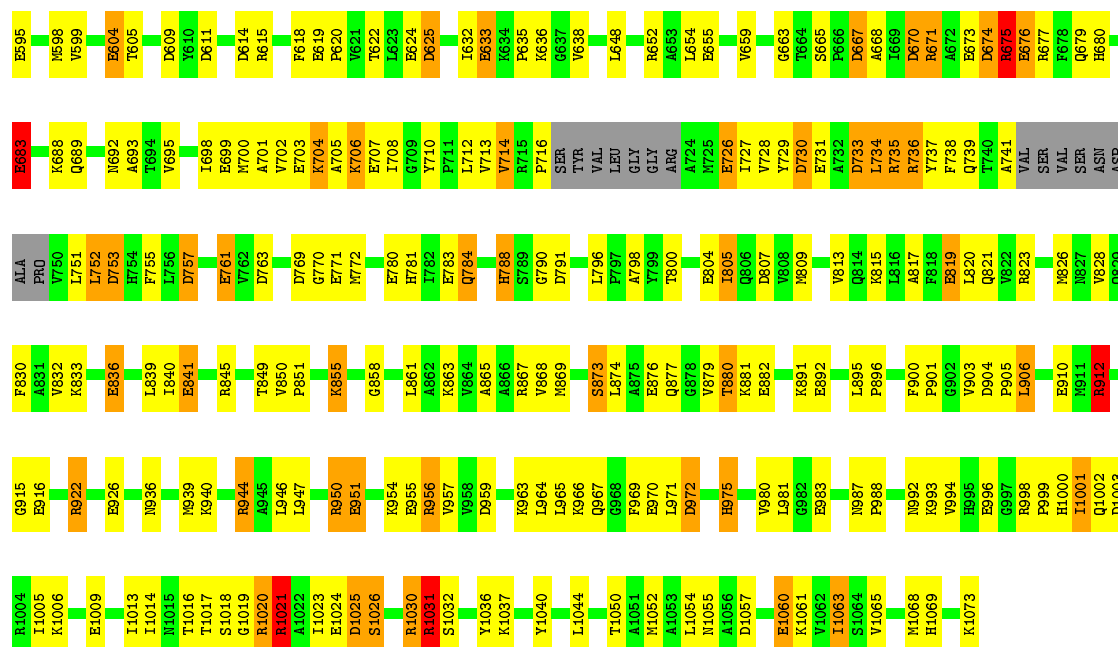
Chain C: 



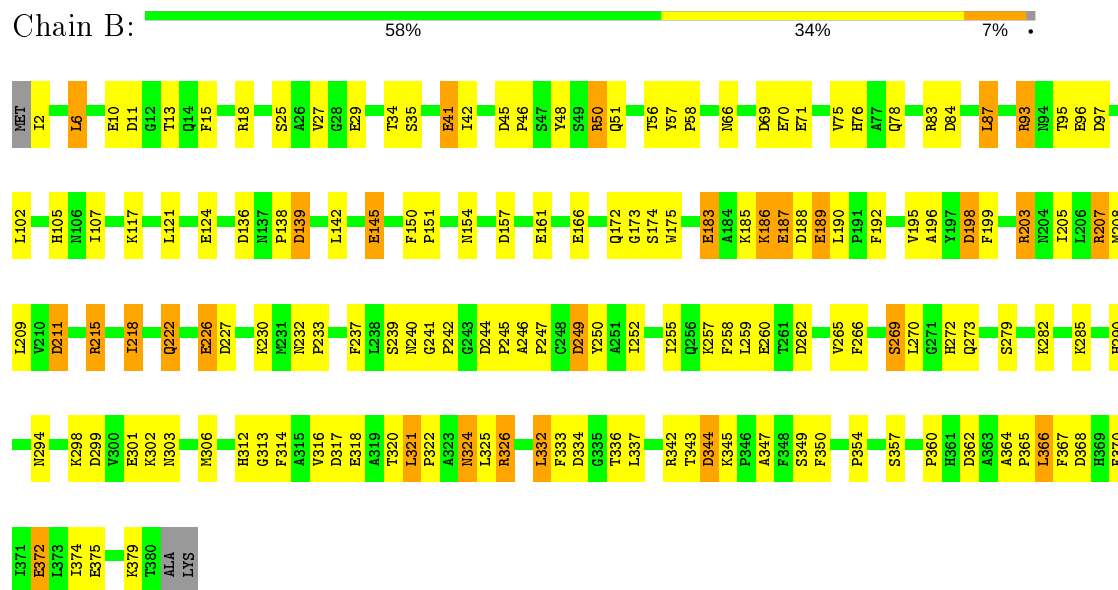
• Molecule 1: CARBAMOYL PHOSPHATE SYNTHETASE: LARGE SUBUNIT

Chain E: 

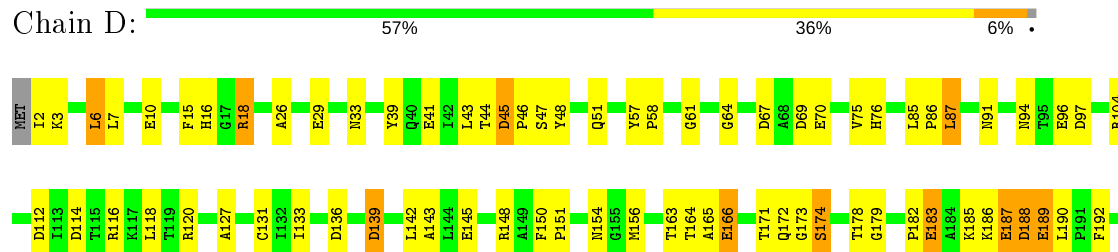


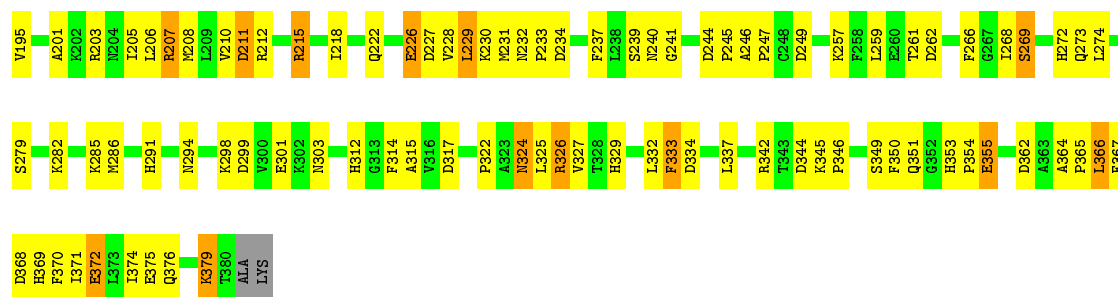


• Molecule 2: CARBAMOYL PHOSPHATE SYNTHETASE: SMALL SUBUNIT



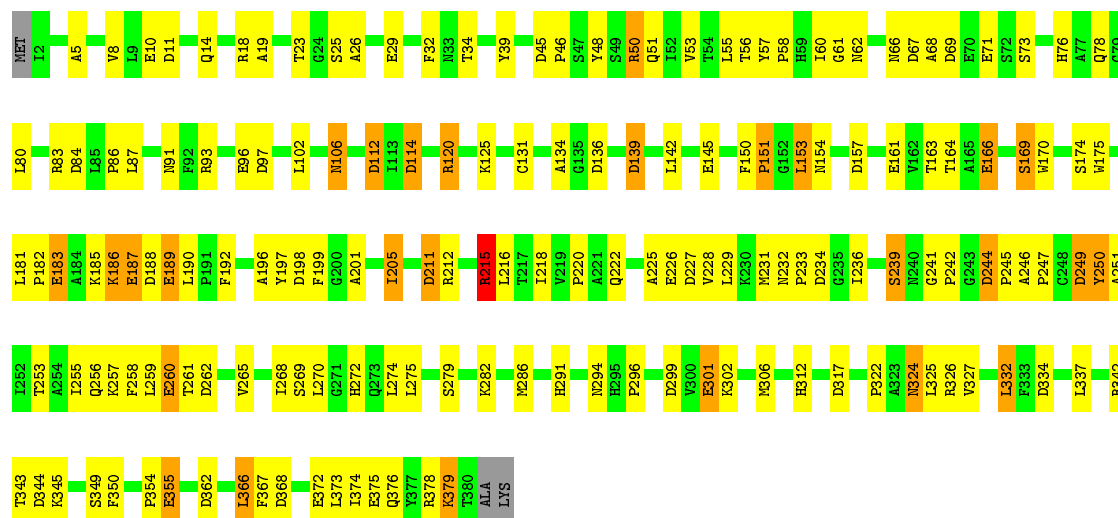
• Molecule 2: CARBAMOYL PHOSPHATE SYNTHETASE: SMALL SUBUNIT





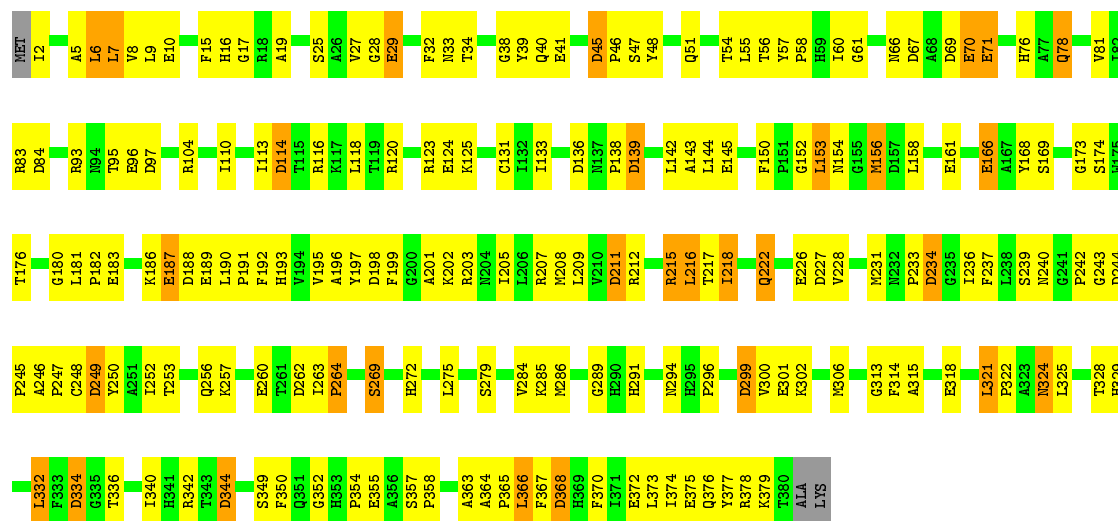
• Molecule 2: CARBAMOYL PHOSPHATE SYNTHETASE: SMALL SUBUNIT

Chain F: 55% 36% 7% .



• Molecule 2: CARBAMOYL PHOSPHATE SYNTHETASE: SMALL SUBUNIT

Chain H: 49% 42% 8% .



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, α , β , γ	152.50 Å 164.40 Å 332.60 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.10	Depositor
% Data completeness (in resolution range)	98.4 (30.00-2.10)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT 5E	Depositor
R, R_{free}	0.188 , 0.258	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	48477	wwPDB-VP
Average B, all atoms (Å ²)	37.0	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: ADP, CL, K, MN, ORN, NET, PO4

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	1.04	72/8345 (0.9%)	1.41	128/11276 (1.1%)
1	C	1.04	77/8346 (0.9%)	1.38	112/11281 (1.0%)
1	E	1.05	68/8377 (0.8%)	1.40	124/11320 (1.1%)
1	G	1.01	79/8322 (0.9%)	1.39	118/11249 (1.0%)
2	B	0.90	18/2957 (0.6%)	1.32	40/4016 (1.0%)
2	D	0.94	15/2957 (0.5%)	1.38	44/4016 (1.1%)
2	F	0.92	15/2957 (0.5%)	1.37	43/4016 (1.1%)
2	H	0.91	18/2957 (0.6%)	1.33	35/4016 (0.9%)
All	All	1.01	362/45218 (0.8%)	1.39	644/61190 (1.1%)

The worst 5 of 362 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	419[A]	GLU	CD-OE2	-10.50	1.14	1.25
1	C	419[B]	GLU	CD-OE2	-10.50	1.14	1.25
1	C	110	GLU	CD-OE1	-10.46	1.14	1.25
1	C	1009	GLU	CD-OE2	9.29	1.35	1.25
1	A	109	GLU	CD-OE2	8.80	1.35	1.25

The worst 5 of 644 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	514	ARG	NE-CZ-NH2	-12.65	113.97	120.30
1	G	75	ARG	NE-CZ-NH2	-12.58	114.01	120.30
1	G	265	ARG	NE-CZ-NH1	12.54	126.57	120.30
2	D	120	ARG	NE-CZ-NH1	12.14	126.37	120.30
1	E	343	ARG	NE-CZ-NH1	11.54	126.07	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8195	0	8247	239	0
1	C	8192	0	8230	247	0
1	E	8211	0	8245	225	0
1	G	8180	0	8214	291	0
2	B	2895	0	2861	91	0
2	D	2895	0	2861	98	0
2	F	2895	0	2861	107	0
2	H	2895	0	2861	134	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	1	0
5	B	1	0	0	0	0
5	C	3	0	0	2	0
5	D	1	0	0	0	0
5	E	3	0	0	0	0
5	F	1	0	0	0	0
5	G	3	0	0	3	0
5	H	1	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	1	0
7	E	54	0	24	4	0
7	G	54	0	24	2	0
8	A	9	0	11	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	C	9	0	11	1	0
8	E	9	0	11	0	0
8	G	9	0	11	0	0
9	A	10	0	7	0	0
9	B	10	0	7	3	0
9	C	10	0	7	0	0
9	D	10	0	7	2	0
9	E	10	0	7	0	0
9	F	10	0	7	3	0
9	G	10	0	7	0	0
9	H	10	0	7	2	0
10	A	9	0	20	0	0
10	C	9	0	20	1	0
10	E	9	0	20	2	0
10	G	9	0	20	0	0
11	A	699	0	0	14	0
11	B	231	0	0	4	0
11	C	706	0	0	19	0
11	D	250	0	0	5	0
11	E	754	0	0	23	0
11	F	231	0	0	4	0
11	G	622	0	0	20	0
11	H	173	0	0	4	0
All	All	48477	0	44656	1411	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 1411 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:808:VAL:HA	1:E:811[B]:GLN:HE21	1.12	1.11
2:H:133:ILE:HD12	2:H:143:ALA:HB2	1.28	1.10
1:A:695:VAL:HG13	1:A:700:MET:HB3	1.36	1.08
1:C:695:VAL:HG11	1:C:701:ALA:HB2	1.38	1.04
2:H:187:GLU:HG2	2:H:215:ARG:HD2	1.35	1.03

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	1004 (95%)	51 (5%)	3 (0%)	41	41
1	C	1059/1073 (99%)	1005 (95%)	50 (5%)	4 (0%)	34	32
1	E	1062/1073 (99%)	1004 (94%)	56 (5%)	2 (0%)	47	49
1	G	1056/1073 (98%)	991 (94%)	59 (6%)	6 (1%)	25	21
2	B	377/382 (99%)	362 (96%)	15 (4%)	0	100	100
2	D	377/382 (99%)	357 (95%)	18 (5%)	2 (0%)	29	26
2	F	377/382 (99%)	358 (95%)	19 (5%)	0	100	100
2	H	377/382 (99%)	353 (94%)	22 (6%)	2 (0%)	29	26
All	All	5743/5820 (99%)	5434 (95%)	290 (5%)	19 (0%)	41	41

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	558	ASP
1	E	954	LYS
1	G	558	ASP
1	G	873	SER
1	A	975	HIS

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	871/878 (99%)	810 (93%)	61 (7%)	15	12

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	872/878 (99%)	805 (92%)	67 (8%)	13	9
1	E	875/878 (100%)	817 (93%)	58 (7%)	16	14
1	G	869/878 (99%)	796 (92%)	73 (8%)	11	7
2	B	308/310 (99%)	277 (90%)	31 (10%)	7	4
2	D	308/310 (99%)	289 (94%)	19 (6%)	18	15
2	F	308/310 (99%)	280 (91%)	28 (9%)	9	6
2	H	308/310 (99%)	283 (92%)	25 (8%)	11	8
All	All	4719/4752 (99%)	4357 (92%)	362 (8%)	13	9

5 of 362 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	154	ASN
1	E	591	GLU
1	G	1061	LYS
2	D	257	LYS
1	E	103	GLU

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

Mol	Chain	Res	Type
2	D	154	ASN
1	E	689	GLN
1	G	1035	GLN
2	D	222	GLN
1	E	105	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 89 ligands modelled in this entry, 60 are monoatomic - leaving 29 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	G	4074	3,4	24,29,29	1.27	3 (12%)	29,45,45	1.37	3 (10%)
6	PO4	A	4006	3,4	4,4,4	2.38	2 (50%)	6,6,6	0.99	0
8	ORN	A	4011	-	4,8,8	0.57	0	3,9,9	0.58	0
6	PO4	G	4073	3,4	4,4,4	1.97	2 (50%)	6,6,6	1.02	0
6	PO4	E	4067	-	4,4,4	1.42	0	6,6,6	0.68	0
6	PO4	E	4050	3,4	4,4,4	2.40	3 (75%)	6,6,6	1.14	0
6	PO4	C	4028	3,4	4,4,4	2.89	3 (75%)	6,6,6	1.13	0
7	ADP	C	4023	3	24,29,29	1.13	1 (4%)	29,45,45	0.96	1 (3%)
8	ORN	G	4078	-	4,8,8	0.29	0	3,9,9	0.44	0
7	ADP	E	4051	3,4	24,29,29	1.05	3 (12%)	29,45,45	0.96	1 (3%)
7	ADP	A	4007	3,4	24,29,29	0.91	0	29,45,45	1.29	2 (6%)
8	ORN	C	4033	-	4,8,8	0.49	0	3,9,9	0.20	0
10	NET	C	4036	-	8,8,8	0.54	0	10,10,10	0.47	0
7	ADP	G	4068	3	24,29,29	1.12	2 (8%)	29,45,45	1.43	6 (20%)
10	NET	G	4081	-	8,8,8	0.66	0	10,10,10	0.46	0
7	ADP	E	4045	3	24,29,29	1.11	2 (8%)	29,45,45	1.20	2 (6%)
7	ADP	A	4000	3	24,29,29	1.20	3 (12%)	29,45,45	1.18	2 (6%)
10	NET	E	4058	-	8,8,8	0.55	0	10,10,10	0.74	0
8	ORN	E	4055	-	4,8,8	0.93	0	3,9,9	0.34	0
10	NET	A	4014	-	8,8,8	0.69	0	10,10,10	0.56	0
7	ADP	C	4029	3,4	24,29,29	1.22	3 (12%)	29,45,45	1.19	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	G	4074	3,4	-	2/12/32/32	0/3/3/3
7	ADP	E	4051	3,4	-	4/12/32/32	0/3/3/3
8	ORN	E	4055	-	-	3/4/8/8	-
8	ORN	A	4011	-	-	3/4/8/8	-
7	ADP	C	4023	3	-	2/12/32/32	0/3/3/3
8	ORN	G	4078	-	-	4/4/8/8	-
7	ADP	A	4007	3,4	-	4/12/32/32	0/3/3/3
8	ORN	C	4033	-	-	4/4/8/8	-
10	NET	C	4036	-	-	3/12/12/12	-
7	ADP	G	4068	3	-	1/12/32/32	0/3/3/3
10	NET	G	4081	-	-	0/12/12/12	-
7	ADP	E	4045	3	-	1/12/32/32	0/3/3/3
7	ADP	A	4000	3	-	1/12/32/32	0/3/3/3
10	NET	E	4058	-	-	3/12/12/12	-
10	NET	A	4014	-	-	0/12/12/12	-
7	ADP	C	4029	3,4	-	3/12/32/32	0/3/3/3

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	4028	PO4	P-O4	-3.77	1.43	1.54
7	G	4074	ADP	O3'-C3'	3.72	1.51	1.43
7	C	4029	ADP	O3'-C3'	3.60	1.51	1.43
6	C	4028	PO4	P-O2	-3.44	1.44	1.54
6	A	4006	PO4	P-O2	-3.12	1.45	1.54

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	4007	ADP	C5-C6-N6	4.26	126.83	120.35
7	G	4068	ADP	O3B-PB-O3A	-3.66	92.38	104.64
7	G	4074	ADP	C5-C6-N6	3.49	125.66	120.35
7	E	4045	ADP	C3'-C2'-C1'	3.00	105.49	100.98
7	G	4074	ADP	O3B-PB-O3A	2.88	114.30	104.64

There are no chirality outliers.

5 of 38 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	C	4033	ORN	N-CA-CB-CG
8	C	4033	ORN	C-CA-CB-CG
8	G	4078	ORN	N-CA-CB-CG
8	G	4078	ORN	C-CA-CB-CG
7	E	4051	ADP	PA-O3A-PB-O3B

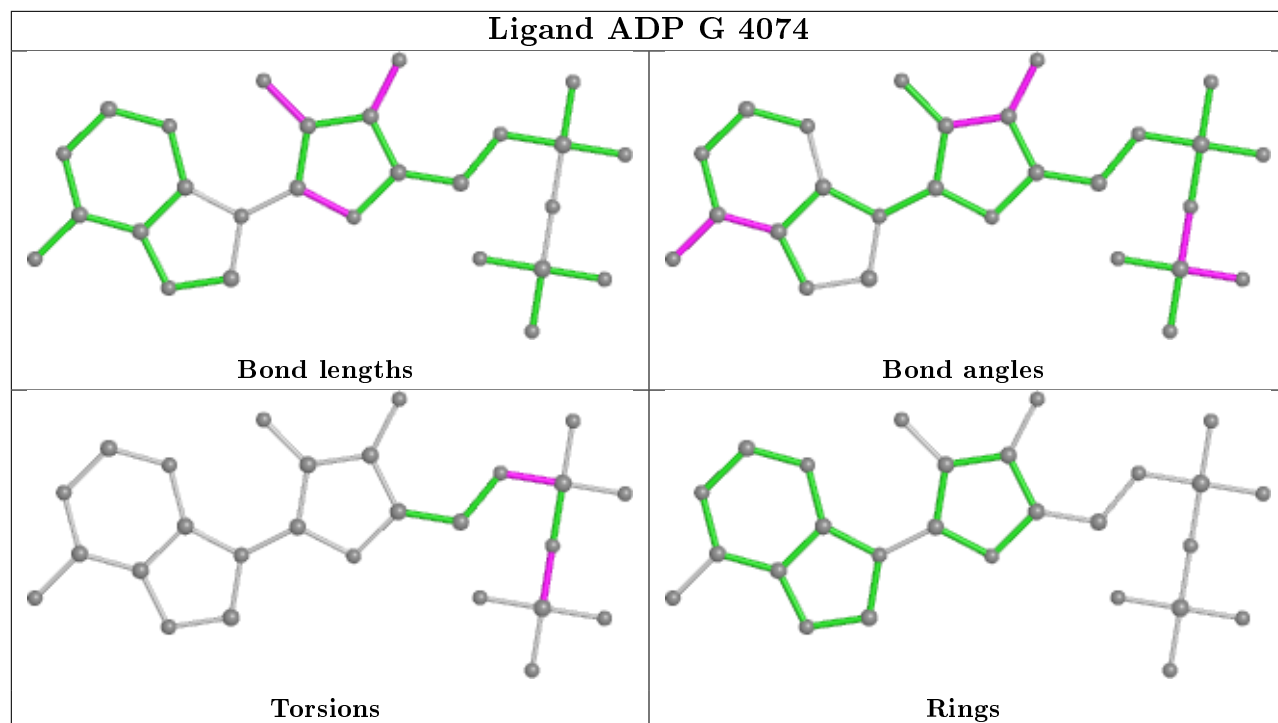
There are no ring outliers.

9 monomers are involved in 12 short contacts:

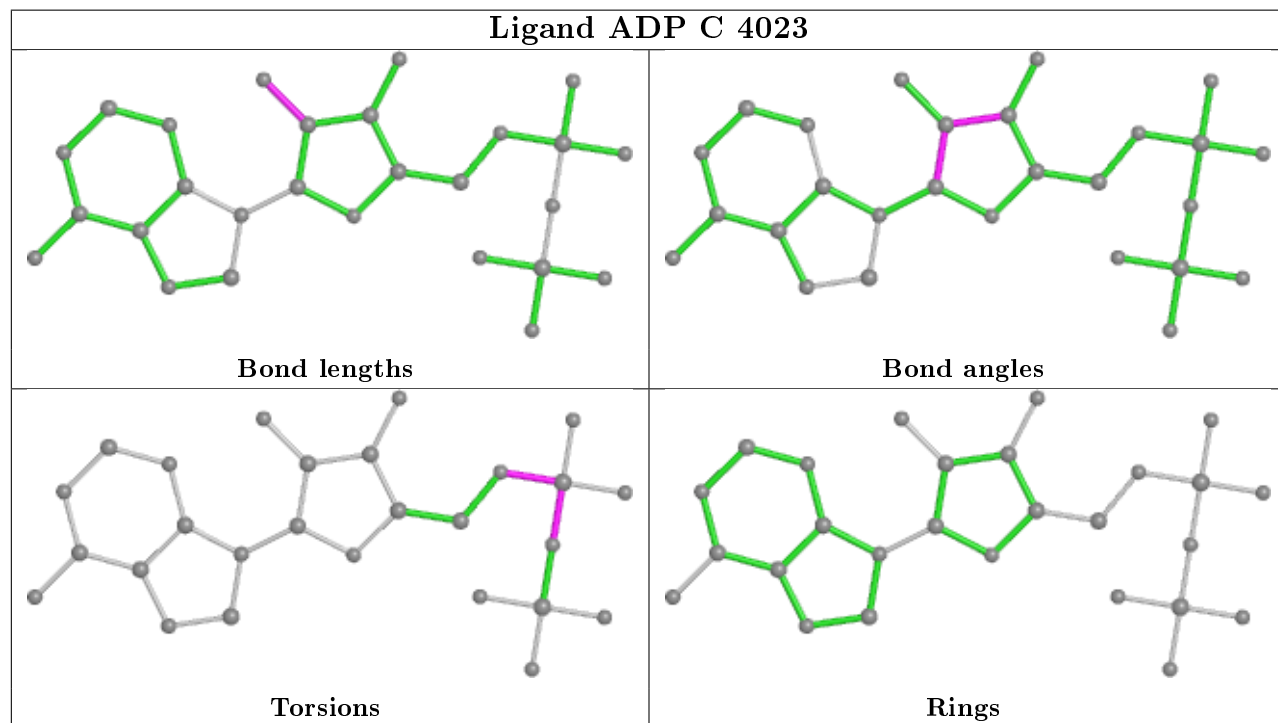
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	G	4074	ADP	1	0
8	A	4011	ORN	1	0
7	E	4051	ADP	2	0
8	C	4033	ORN	1	0
10	C	4036	NET	1	0
7	G	4068	ADP	1	0
7	E	4045	ADP	2	0
10	E	4058	NET	2	0
7	C	4029	ADP	1	0

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.

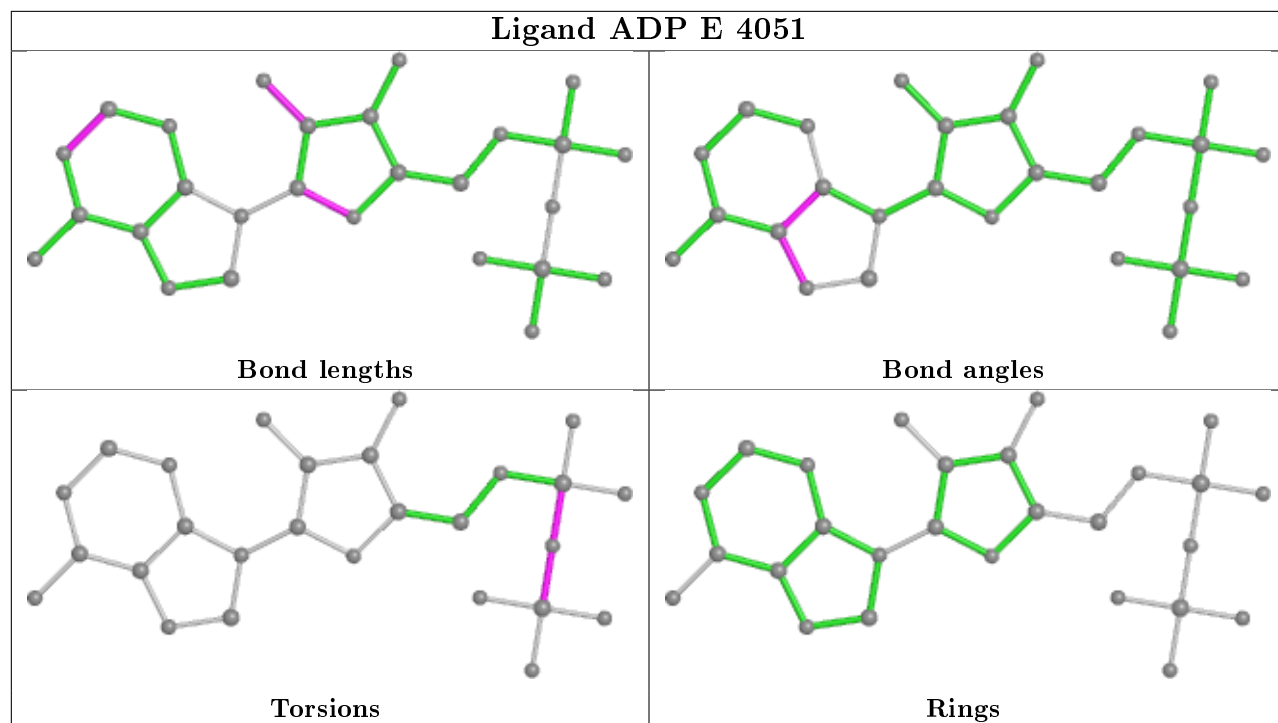
Ligand ADP G 4074



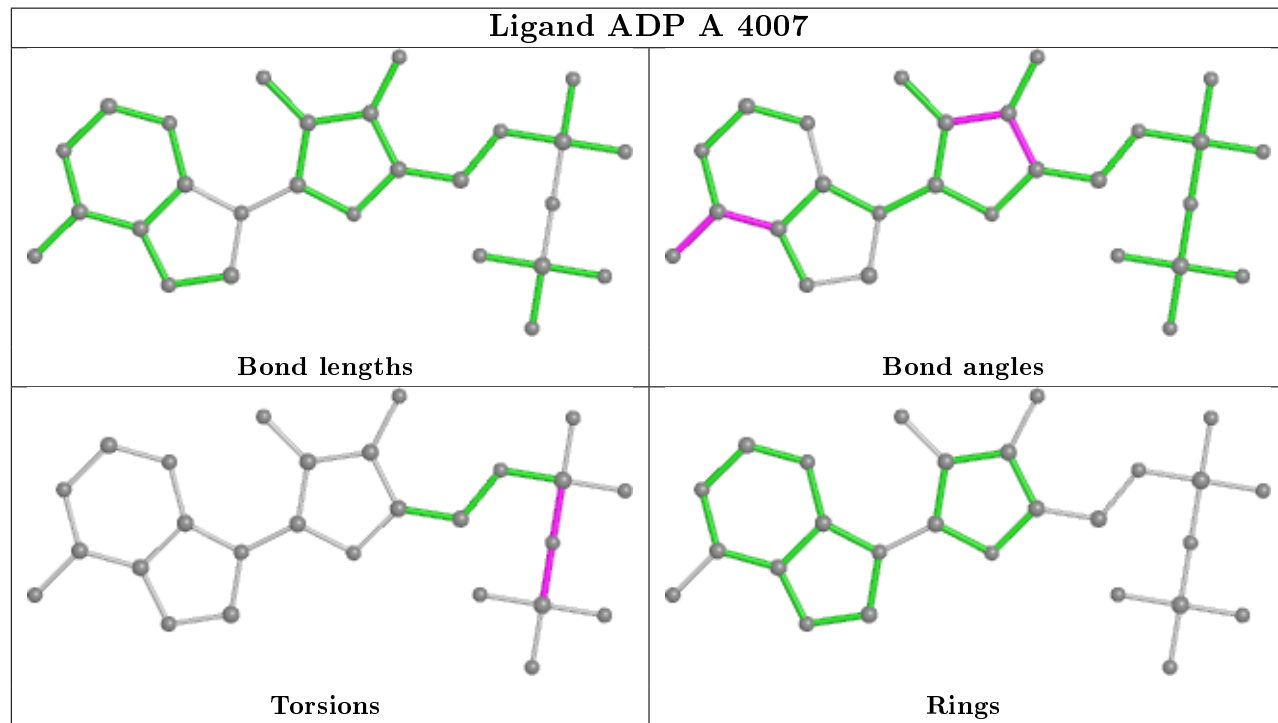
Ligand ADP C 4023



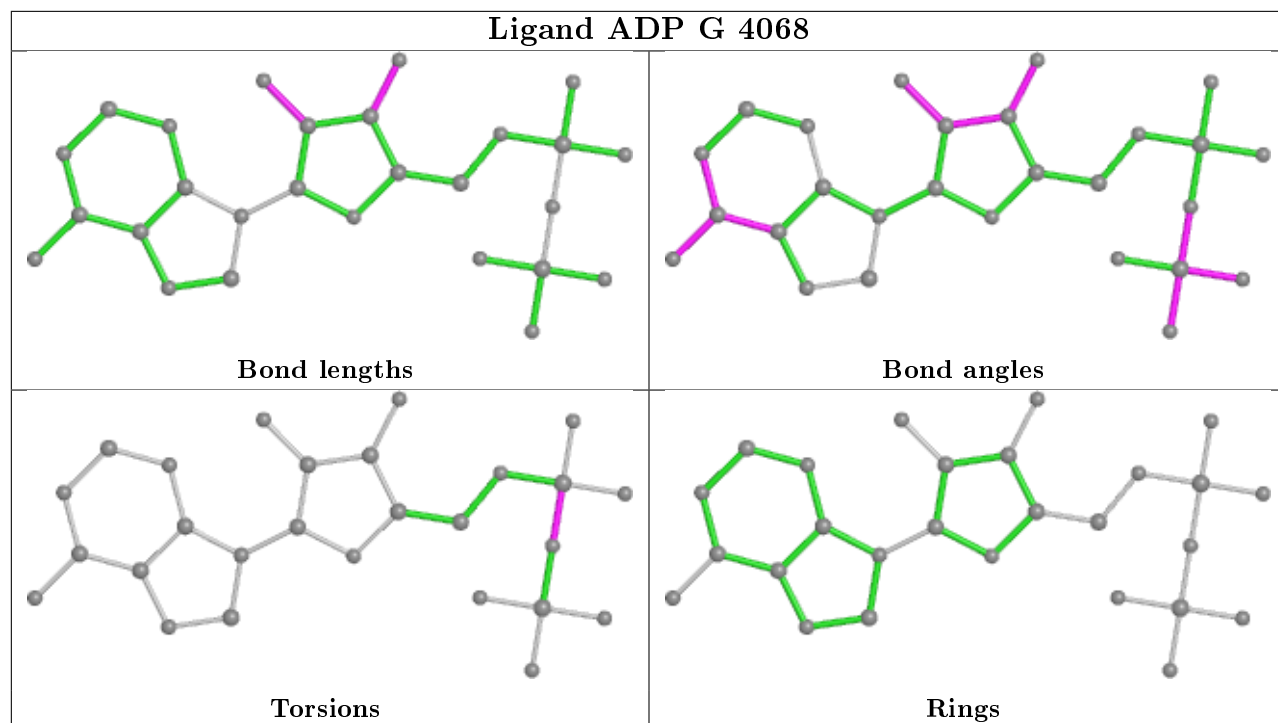
Ligand ADP E 4051



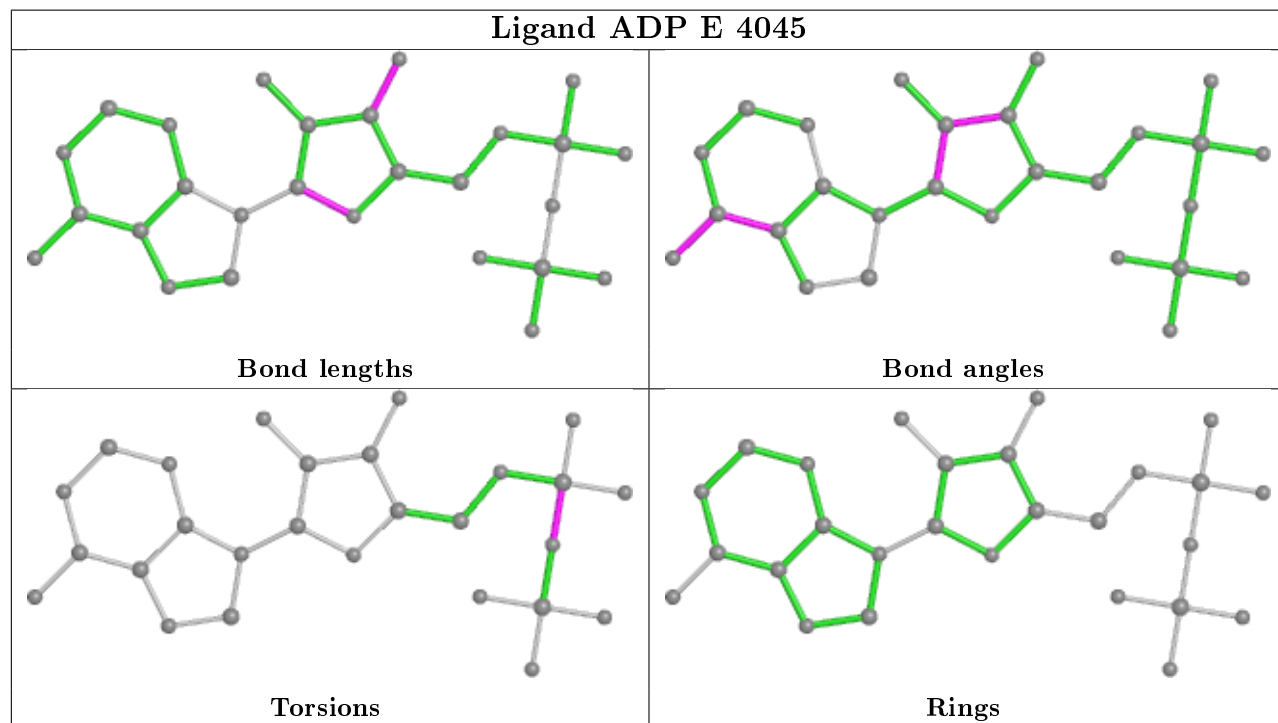
Ligand ADP A 4007

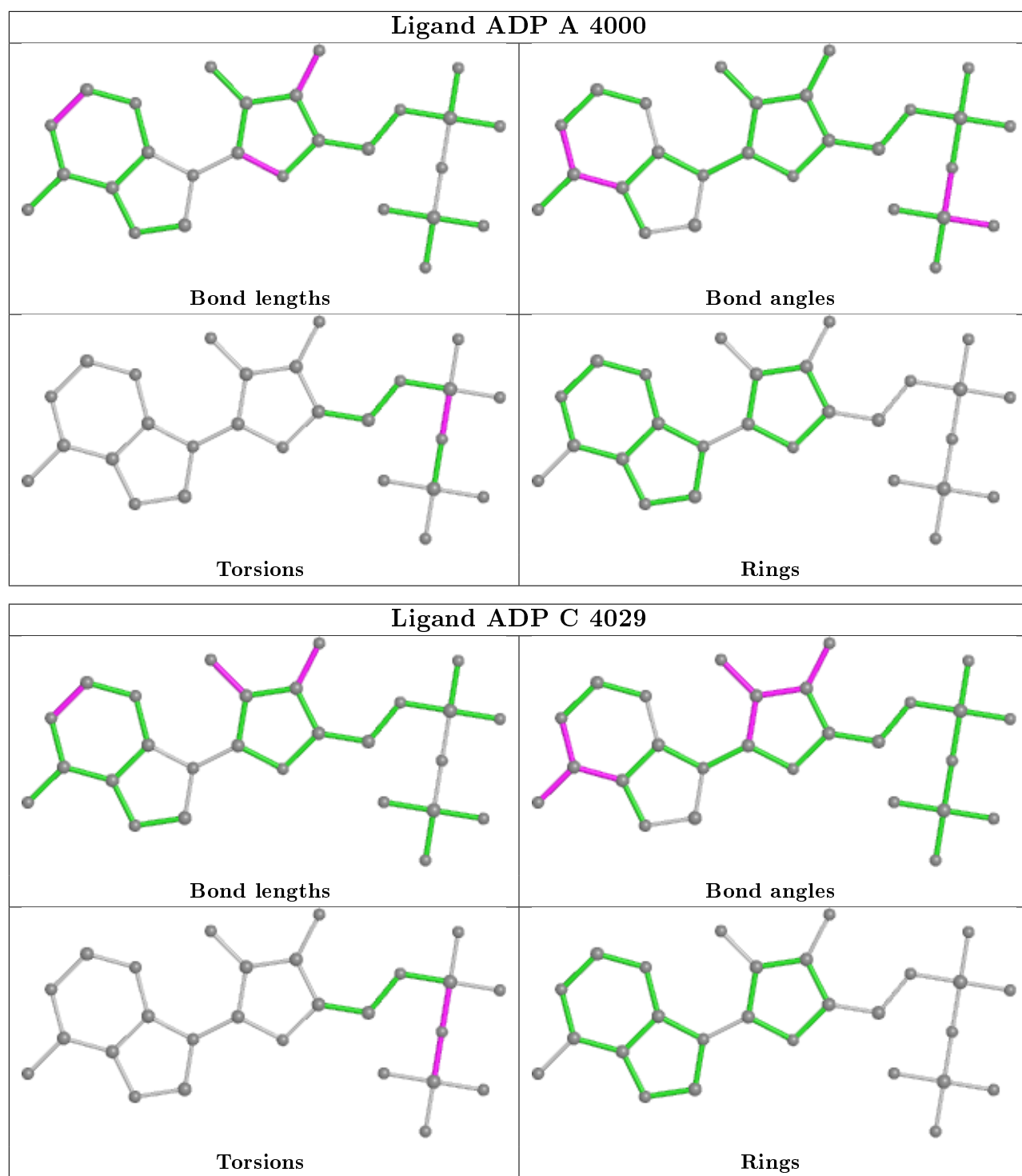


Ligand ADP G 4068



Ligand ADP E 4045





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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.