



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 30, 2024 – 08:04 PM EST

PDB ID : 1JDB
Title : CARBAMOYL PHOSPHATE SYNTHETASE FROM ESCHERICHIA COLI
Authors : Thoden, J.B.; Holden, H.M.; Wesenberg, G.; Raushel, F.M.; Rayment, I.
Deposited on : 1997-03-25
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 types of validation reports are described at

<https://www.wwpdb.org/validation/2017/FAQs#types>.

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

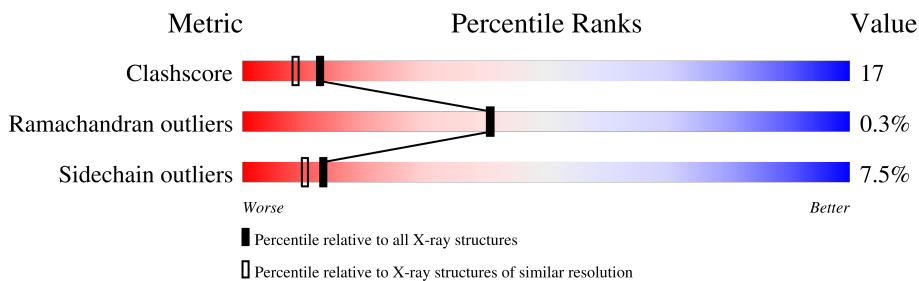
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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 of 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	B	1073	
1	E	1073	
1	H	1073	
1	K	1073	
2	C	382	
2	F	382	
2	I	382	
2	L	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
5	PO4	H	1082	-	-	X	-
5	PO4	K	1082	-	-	X	-
7	GLN	B	1091	-	X	-	-

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 49731 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	B	1057	Total 8195	C 5143	N 1428	O 1579	S 45	0	8	0
1	E	1057	Total 8223	C 5160	N 1440	O 1577	S 46	0	13	0
1	H	1057	Total 8179	C 5136	N 1422	O 1575	S 46	0	6	0
1	K	1060	Total 8201	C 5149	N 1432	O 1575	S 45	0	5	0

- Molecule 2 is a protein called CARBAMOYL PHOSPHATE SYNTHETASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	379	Total 2895	C 1825	N 509	O 551	S 10	0	0	0
2	F	380	Total 2904	C 1830	N 510	O 554	S 10	0	1	0
2	I	379	Total 2895	C 1825	N 509	O 551	S 10	0	0	0
2	L	379	Total 2895	C 1825	N 509	O 551	S 10	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	183	GLN	GLU	conflict	UNP P00907
F	183	GLN	GLU	conflict	UNP P00907
I	183	GLN	GLU	conflict	UNP P00907
L	183	GLN	GLU	conflict	UNP P00907

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	4	Total Mn 4 4	0	0
3	E	4	Total Mn 4 4	0	0
3	H	4	Total Mn 4 4	0	0
3	K	4	Total Mn 4 4	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	6	Total K 6 6	0	0
4	C	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	H	5	Total K 5 5	0	0
4	I	1	Total K 1 1	0	0
4	K	7	Total K 7 7	0	0
4	L	1	Total K 1 1	0	0

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total O P 5 4 1	0	0
5	B	1	Total O P 5 4 1	0	0
5	E	1	Total O P 5 4 1	0	0
5	E	1	Total O P 5 4 1	0	0
5	H	1	Total O P 5 4 1	0	0
5	H	1	Total O P 5 4 1	0	0
5	K	1	Total O P 5 4 1	0	0
5	K	1	Total O P 5 4 1	0	0
5	K	1	Total O P 5 4 1	0	0

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

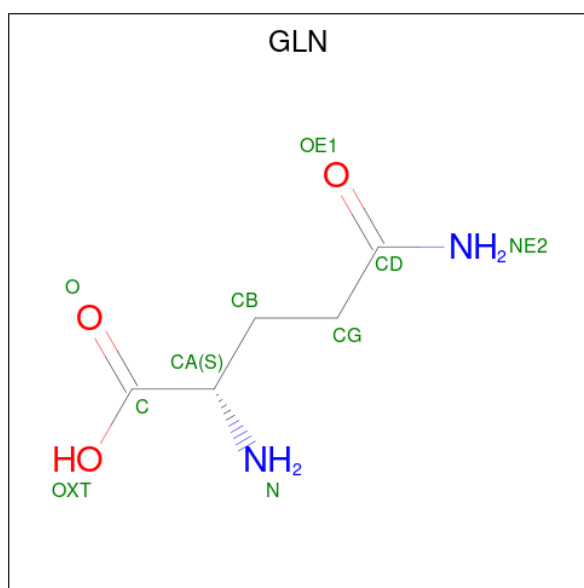
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	6	Total Cl 6 6	0	0
6	C	1	Total Cl 1 1	0	0
6	E	7	Total Cl 7 7	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	1	Total	Cl	0	0
			1	1		
6	H	6	Total	Cl	0	0
			6	6		
6	I	1	Total	Cl	0	0
			1	1		
6	K	6	Total	Cl	0	0
			6	6		
6	L	1	Total	Cl	0	0
			1	1		

- Molecule 7 is GLUTAMINE (three-letter code: GLN) (formula: C₅H₁₀N₂O₃).



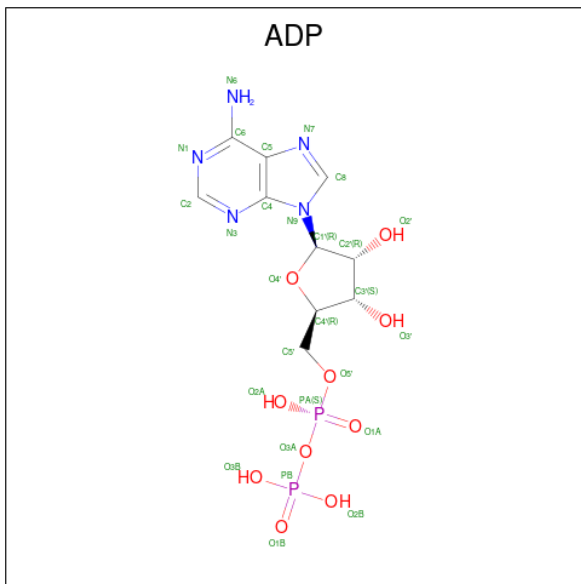
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
7	B	1	Total	C	N	O	0	0
			10	5	2	3		
7	B	1	Total	C	N	O	0	0
			10	5	2	3		
7	E	1	Total	C	N	O	0	0
			10	5	2	3		
7	E	1	Total	C	N	O	0	0
			10	5	2	3		
7	H	1	Total	C	N	O	0	0
			10	5	2	3		
7	H	1	Total	C	N	O	0	0
			10	5	2	3		

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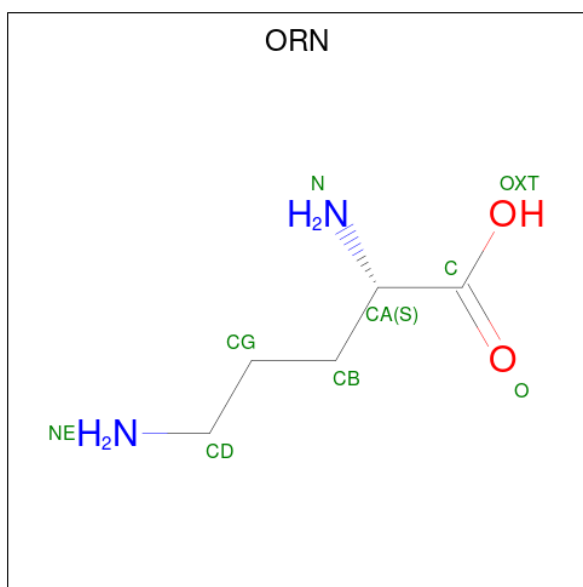
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	K	1	Total	C	N	O	0	0
			10	5	2	3		
7	K	1	Total	C	N	O	0	0
			10	5	2	3		

- Molecule 8 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



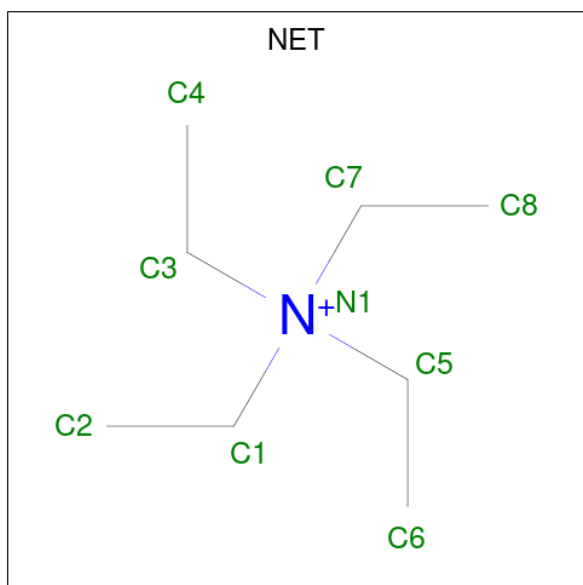
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
8	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
8	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
8	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
8	H	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
8	H	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
8	K	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
8	K	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 9 is L-ornithine (three-letter code: ORN) (formula: $C_5H_{12}N_2O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	B	1	Total	C	N	O	0	0
			9	5	2	2		
9	E	1	Total	C	N	O	0	0
			9	5	2	2		
9	H	1	Total	C	N	O	0	0
			9	5	2	2		
9	K	1	Total	C	N	O	0	0
			9	5	2	2		

- Molecule 10 is TETRAETHYLAMMONIUM ION (three-letter code: NET) (formula: C₈H₂₀N).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	1	Total C N 9 8 1	0	0
10	E	1	Total C N 9 8 1	0	0
10	H	1	Total C N 9 8 1	0	0
10	K	1	Total C N 9 8 1	0	0

- Molecule 11 is water.

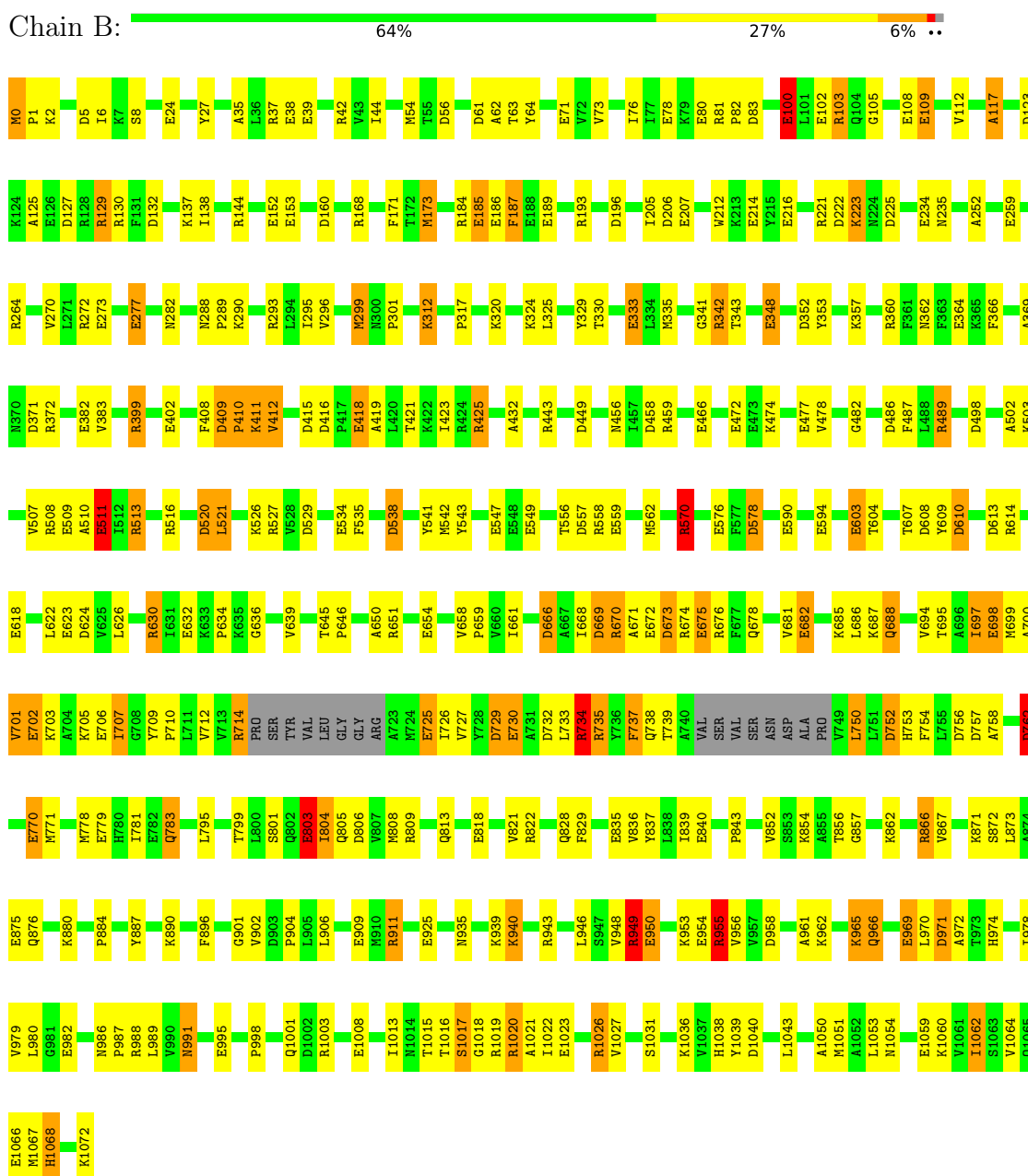
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	B	970	Total O 970 970	0	0
11	C	241	Total O 241 241	0	0
11	E	1022	Total O 1022 1022	0	0
11	F	210	Total O 210 210	0	0
11	H	942	Total O 942 942	0	0
11	I	235	Total O 235 235	0	0
11	K	980	Total O 980 980	0	0
11	L	257	Total O 257 257	0	0

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.

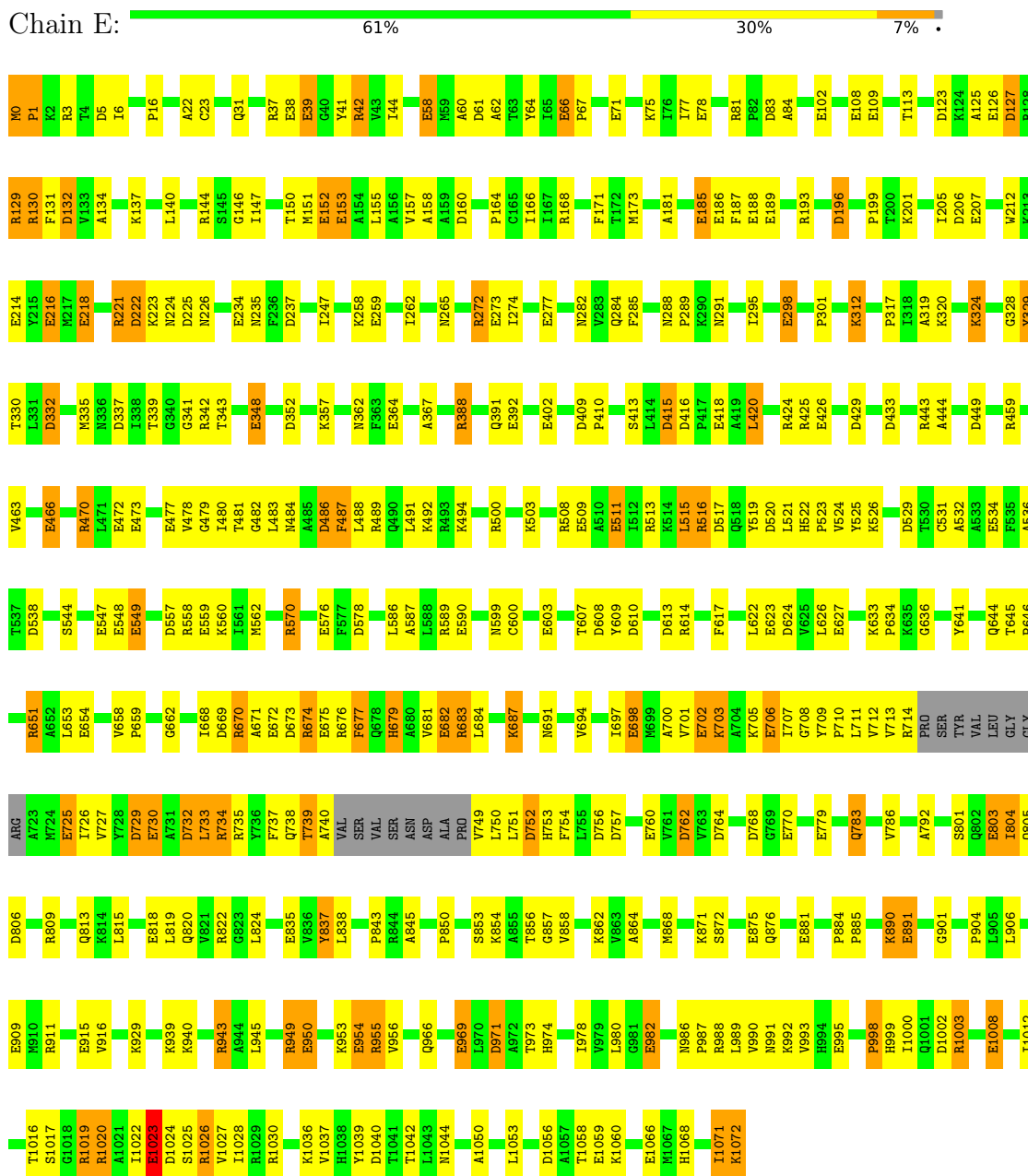
Note EDS was not executed.

- Molecule 1: CARBAMOYL PHOSPHATE SYNTHETASE



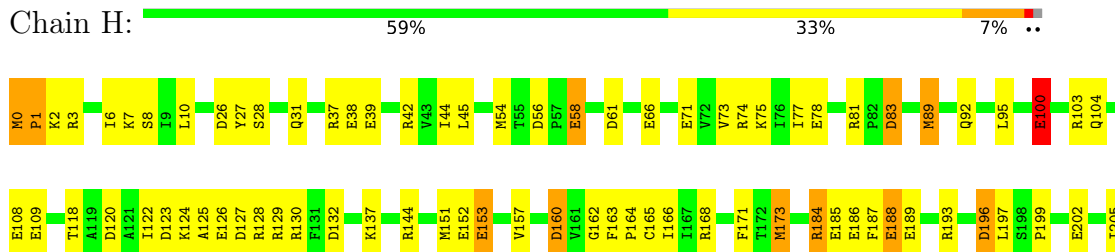
● Molecule 1: CARBAMOYL PHOSPHATE SYNTHETASE

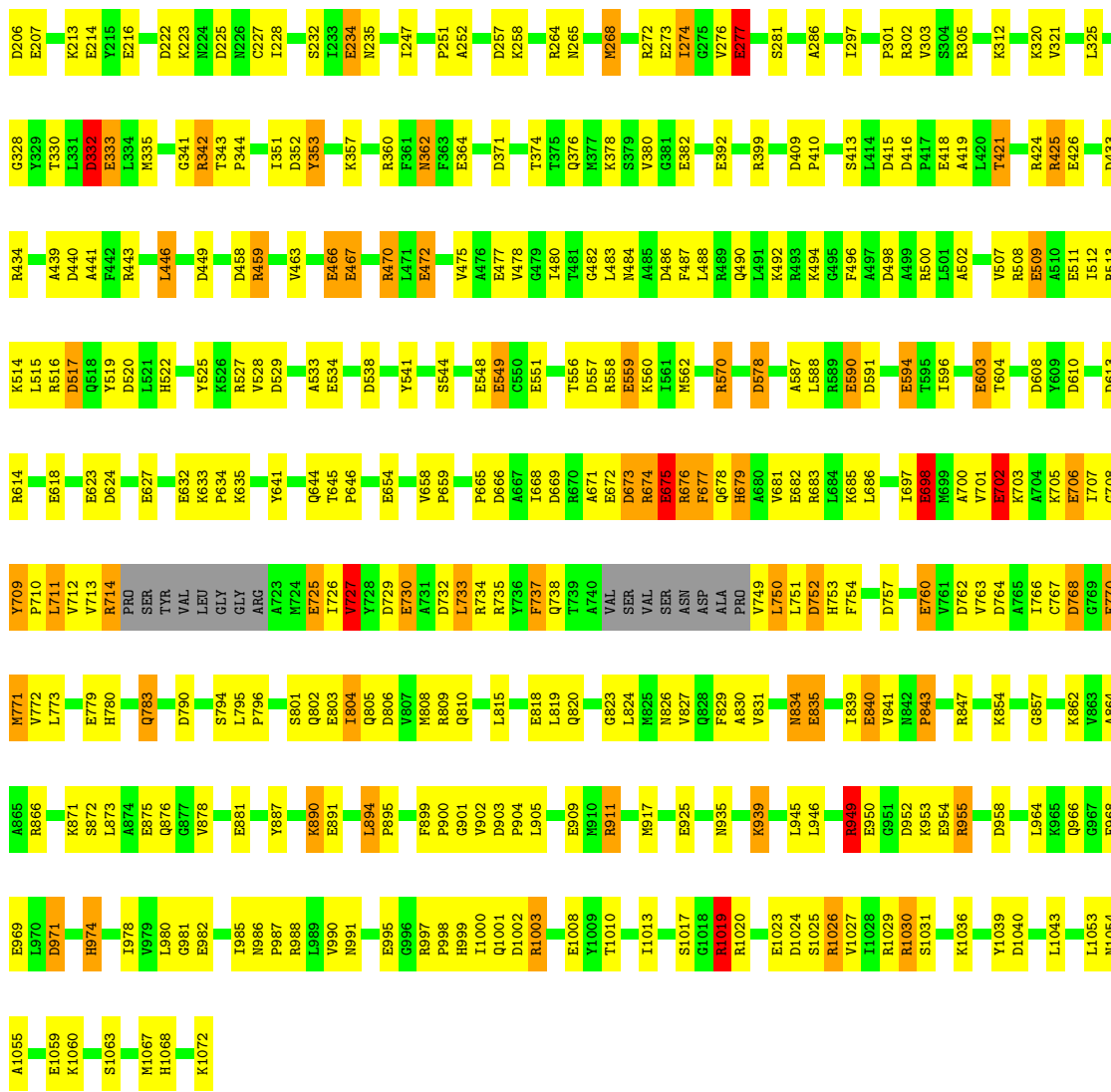
Chain E:



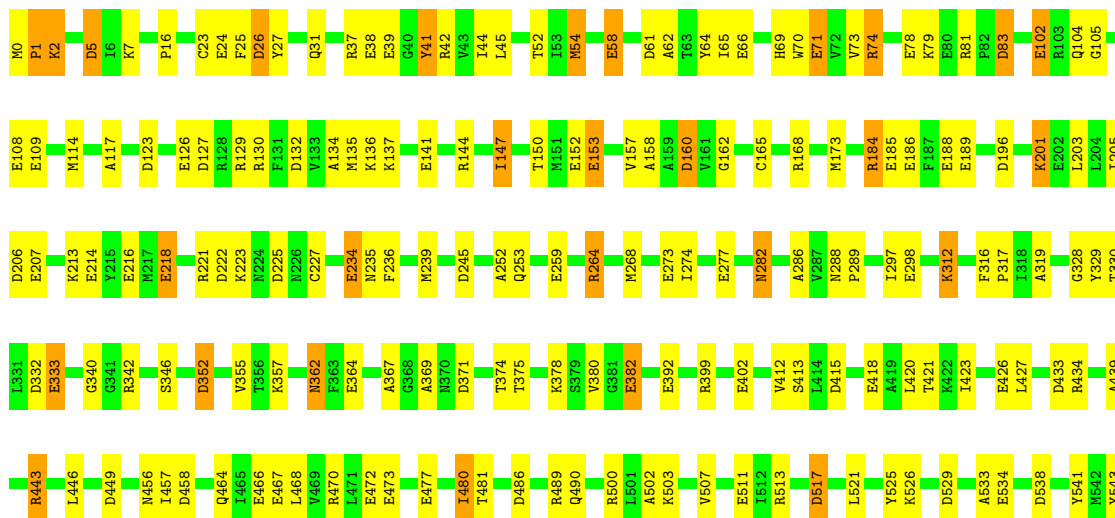
● Molecule 1: CARBAMOYL PHOSPHATE SYNTHETASE

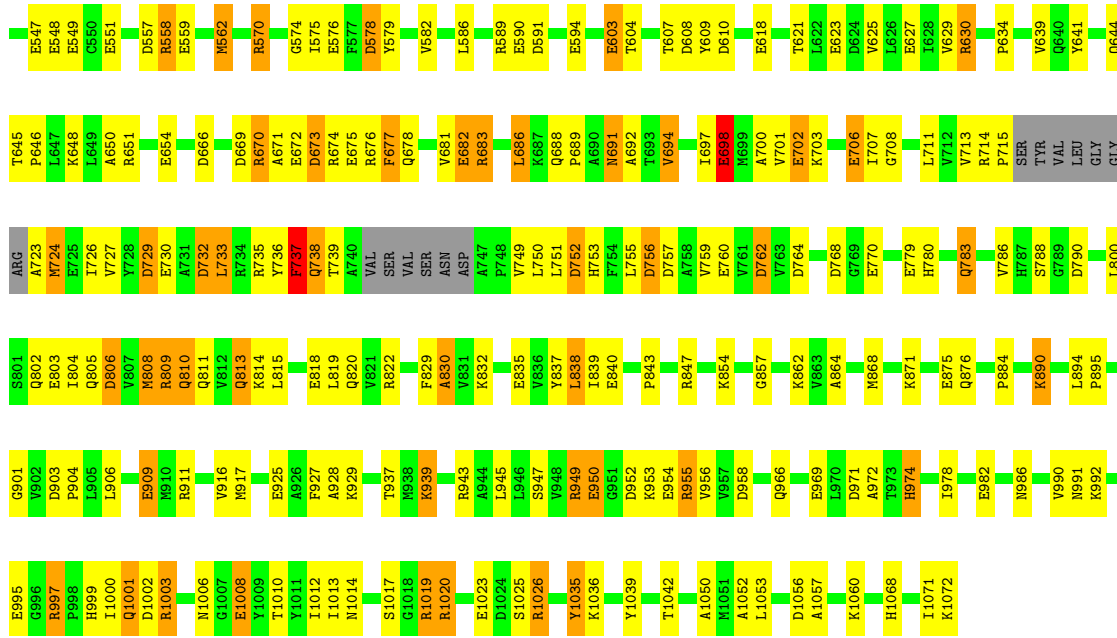
Chain H:



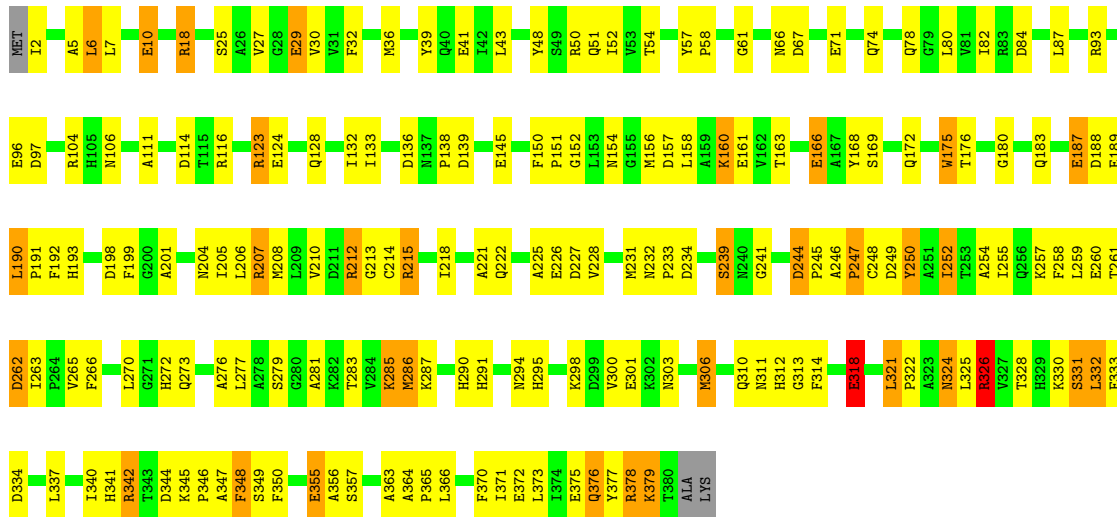


● Molecule 1: CARBAMOYL PHOSPHATE SYNTHETASE

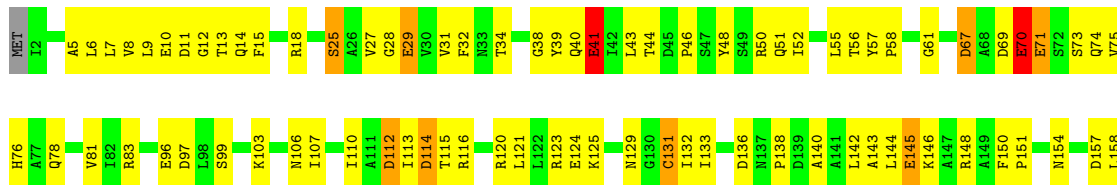




• Molecule 2: CARBAMOYL PHOSPHATE SYNTHETASE

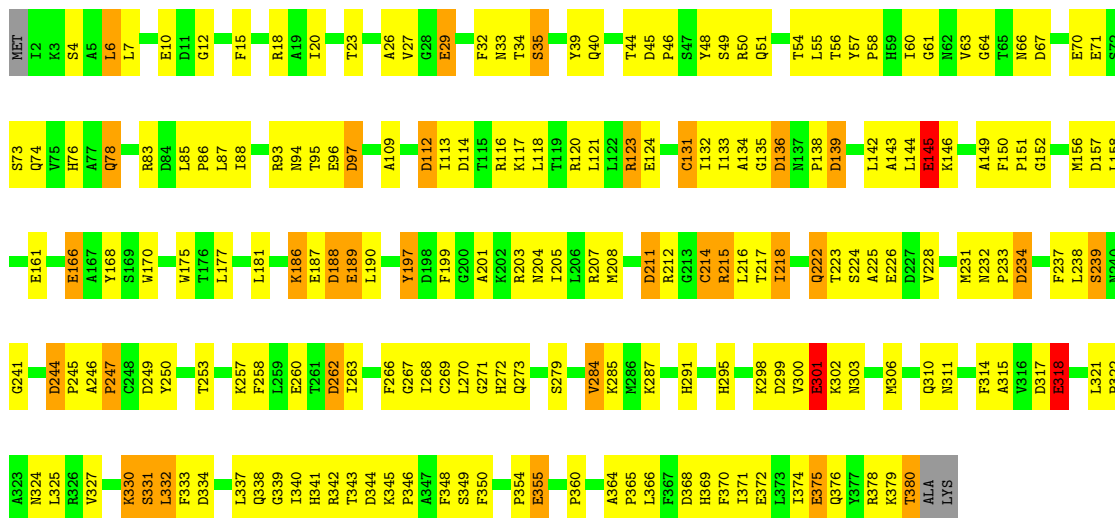


• Molecule 2: CARBAMOYL PHOSPHATE SYNTHETASE

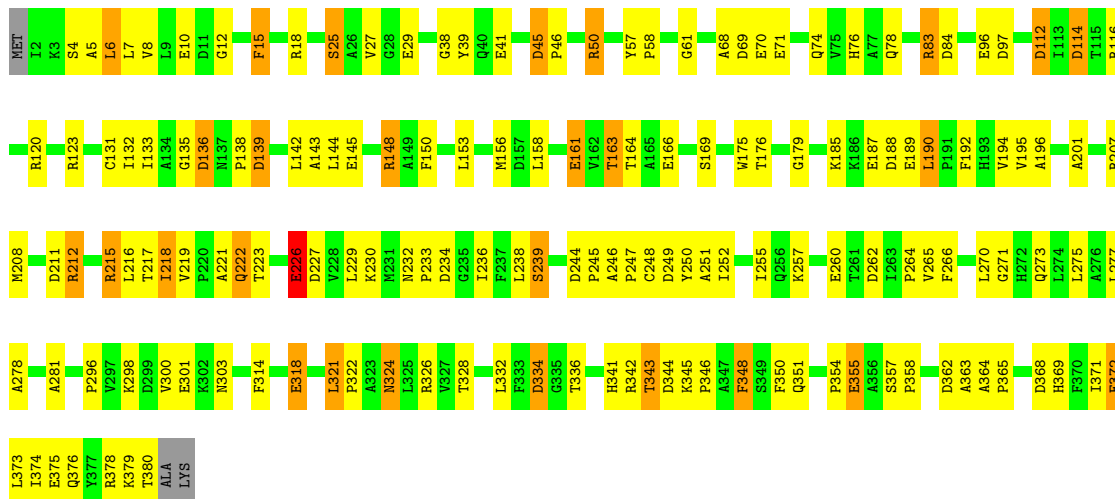




• Molecule 2: CARBAMOYL PHOSPHATE SYNTHETASE



• Molecule 2: CARBAMOYL PHOSPHATE SYNTHETASE



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, α , β , γ	143.80Å 167.70Å 323.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.10	Depositor
% Data completeness (in resolution range)	90.0 (30.00-2.10)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.179 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	49731	wwPDB-VP
Average B, all atoms (Å ²)	33.0	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: CL, NET, PO4, ORN, ADP, MN, 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	B	1.00	65/8353 (0.8%)	1.58	143/11292 (1.3%)
1	E	1.01	73/8401 (0.9%)	1.55	132/11352 (1.2%)
1	H	1.00	72/8329 (0.9%)	1.56	149/11259 (1.3%)
1	K	1.02	73/8349 (0.9%)	1.59	154/11289 (1.4%)
2	C	0.89	18/2957 (0.6%)	1.49	42/4016 (1.0%)
2	F	0.87	16/2970 (0.5%)	1.50	34/4034 (0.8%)
2	I	0.87	16/2957 (0.5%)	1.47	33/4016 (0.8%)
2	L	0.89	16/2957 (0.5%)	1.56	51/4016 (1.3%)
All	All	0.98	349/45273 (0.8%)	1.55	738/61274 (1.2%)

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	E	1	0

The worst 5 of 349 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	216	GLU	CD-OE2	8.36	1.34	1.25
1	E	1008	GLU	CD-OE1	8.23	1.34	1.25
1	B	682	GLU	CD-OE1	8.10	1.34	1.25
1	H	995	GLU	CD-OE2	7.84	1.34	1.25
1	K	995	GLU	CD-OE2	7.74	1.34	1.25

The worst 5 of 738 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	37	ARG	NE-CZ-NH1	16.23	128.42	120.30
1	E	513	ARG	NE-CZ-NH1	15.09	127.84	120.30
1	K	1003[A]	ARG	NE-CZ-NH1	14.27	127.43	120.30
1	K	1003[B]	ARG	NE-CZ-NH1	14.27	127.43	120.30
1	K	943	ARG	NE-CZ-NH1	14.13	127.37	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	E	338	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	B	8195	0	8221	207	0
1	E	8223	0	8265	280	0
1	H	8179	0	8215	257	0
1	K	8201	0	8241	225	0
2	C	2895	0	2863	134	0
2	F	2904	0	2868	154	0
2	I	2895	0	2863	153	0
2	L	2895	0	2863	95	0
3	B	4	0	0	0	0
3	E	4	0	0	0	0
3	H	4	0	0	0	0
3	K	4	0	0	0	0
4	B	6	0	0	0	0
4	C	1	0	0	0	0
4	E	7	0	0	0	0
4	F	1	0	0	0	0
4	H	5	0	0	0	0
4	I	1	0	0	0	0
4	K	7	0	0	0	0
4	L	1	0	0	0	0
5	B	10	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	10	0	0	1	0
5	H	10	0	0	2	0
5	K	15	0	0	2	0
6	B	6	0	0	1	0
6	C	1	0	0	0	0
6	E	7	0	0	1	0
6	F	1	0	0	0	0
6	H	6	0	0	1	0
6	I	1	0	0	1	0
6	K	6	0	0	0	0
6	L	1	0	0	0	0
7	B	20	0	14	0	0
7	E	20	0	14	1	0
7	H	20	0	14	2	0
7	K	20	0	14	1	0
8	B	54	0	24	0	0
8	E	54	0	24	1	0
8	H	54	0	24	0	0
8	K	54	0	24	1	0
9	B	9	0	11	4	0
9	E	9	0	11	3	0
9	H	9	0	11	0	0
9	K	9	0	11	1	0
10	B	9	0	20	1	0
10	E	9	0	20	0	0
10	H	9	0	20	2	0
10	K	9	0	20	0	0
11	B	970	0	0	19	1
11	C	241	0	0	6	0
11	E	1022	0	0	30	1
11	F	210	0	0	6	0
11	H	942	0	0	28	0
11	I	235	0	0	5	0
11	K	980	0	0	21	0
11	L	257	0	0	6	0
All	All	49731	0	44675	1485	1

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 1485 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:0:MET:HB3	1:E:223:LYS:HE3	1.22	1.17
1:H:701:VAL:HG12	1:H:705:LYS:HE3	1.31	1.05
2:I:133:ILE:HG22	2:I:138:PRO:HB3	1.31	1.04
1:B:702:GLU:HA	1:B:705:LYS:HD2	1.38	1.04
1:H:673:ASP:HB3	1:H:676:ARG:HB2	1.37	1.03

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:B:2056:HOH:O	11:E:2344:HOH:O[4_455]	1.95	0.25

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	B	1059/1073 (99%)	1008 (95%)	48 (4%)	3 (0%)	41	41
1	E	1064/1073 (99%)	1008 (95%)	54 (5%)	2 (0%)	47	49
1	H	1057/1073 (98%)	1016 (96%)	38 (4%)	3 (0%)	41	41
1	K	1059/1073 (99%)	1012 (96%)	43 (4%)	4 (0%)	34	32
2	C	377/382 (99%)	356 (94%)	19 (5%)	2 (0%)	29	26
2	F	379/382 (99%)	359 (95%)	19 (5%)	1 (0%)	41	41
2	I	377/382 (99%)	354 (94%)	21 (6%)	2 (0%)	29	26
2	L	377/382 (99%)	362 (96%)	15 (4%)	0	100	100
All	All	5749/5820 (99%)	5475 (95%)	257 (4%)	17 (0%)	41	41

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	1	PRO

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Mol	Chain	Res	Type
2	C	311	ASN
1	H	974	HIS
1	K	737	PHE
1	K	974	HIS

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	B	873/878 (99%)	805 (92%)	68 (8%)	12	9
1	E	878/878 (100%)	828 (94%)	50 (6%)	20	18
1	H	871/878 (99%)	813 (93%)	58 (7%)	16	13
1	K	872/878 (99%)	809 (93%)	63 (7%)	14	11
2	C	308/310 (99%)	277 (90%)	31 (10%)	7	4
2	F	309/310 (100%)	281 (91%)	28 (9%)	9	6
2	I	308/310 (99%)	275 (89%)	33 (11%)	6	3
2	L	308/310 (99%)	284 (92%)	24 (8%)	12	9
All	All	4727/4752 (100%)	4372 (92%)	355 (8%)	13	10

5 of 355 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	1020	ARG
1	K	427	LEU
2	I	35	SER
2	I	318	GLU
1	K	698	GLU

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

Mol	Chain	Res	Type
1	H	1001	GLN

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Mol	Chain	Res	Type
1	K	688	GLN
1	H	1054	ASN
2	I	376	GLN
1	K	941	HIS

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 107 ligands modelled in this entry, 74 are monoatomic - leaving 33 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	$\# Z > 2$
10	NET	K	1098	-	8,8,8	0.58	0	10,10,10	0.89	1 (10%)
5	PO4	B	1078	4,3	4,4,4	1.99	2 (50%)	6,6,6	0.93	0
5	PO4	E	1078	4,3	4,4,4	2.16	2 (50%)	6,6,6	0.82	0
5	PO4	B	1082	-	4,4,4	2.36	2 (50%)	6,6,6	0.84	0
5	PO4	K	1082	-	4,4,4	1.98	1 (25%)	6,6,6	0.65	0
7	GLN	E	1094	-	8,9,9	1.88	3 (37%)	10,11,11	1.16	0
5	PO4	H	1078	4,3	4,4,4	2.19	3 (75%)	6,6,6	0.62	0
9	ORN	H	1094	-	7,8,8	0.94	0	8,9,9	2.12	3 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	ADP	E	1095	3	24,29,29	1.10	2 (8%)	29,45,45	1.16	2 (6%)
9	ORN	K	1097	-	7,8,8	1.00	0	8,9,9	1.87	2 (25%)
8	ADP	K	1096	3	24,29,29	1.18	3 (12%)	29,45,45	1.22	1 (3%)
7	GLN	B	1092	-	8,9,9	1.92	3 (37%)	10,11,11	1.24	1 (10%)
7	GLN	K	1094	-	8,9,9	1.26	1 (12%)	10,11,11	1.16	0
8	ADP	B	1093	3	24,29,29	1.17	3 (12%)	29,45,45	1.15	1 (3%)
9	ORN	E	1097	-	7,8,8	0.88	0	8,9,9	2.77	4 (50%)
8	ADP	H	1093	3	24,29,29	1.22	3 (12%)	29,45,45	1.39	6 (20%)
5	PO4	K	1078	4,3	4,4,4	1.94	2 (50%)	6,6,6	1.30	1 (16%)
8	ADP	E	1096	3	24,29,29	1.27	4 (16%)	29,45,45	1.33	5 (17%)
5	PO4	K	1092	-	4,4,4	0.53	0	6,6,6	1.33	1 (16%)
9	ORN	B	1095	-	7,8,8	1.20	1 (14%)	8,9,9	1.41	0
5	PO4	E	1082	-	4,4,4	2.10	2 (50%)	6,6,6	1.13	0
10	NET	H	1095	-	8,8,8	0.70	0	10,10,10	0.60	0
7	GLN	H	1091	-	8,9,9	1.34	1 (12%)	10,11,11	1.42	3 (30%)
8	ADP	H	1092	3	24,29,29	1.19	2 (8%)	29,45,45	1.42	1 (3%)
5	PO4	H	1082	-	4,4,4	1.95	1 (25%)	6,6,6	0.99	0
10	NET	E	1098	-	8,8,8	0.75	0	10,10,10	0.41	0
10	NET	B	1096	-	8,8,8	0.65	0	10,10,10	0.69	0
7	GLN	K	1093	-	8,9,9	1.30	1 (12%)	10,11,11	1.44	3 (30%)
7	GLN	H	1090	-	8,9,9	1.40	1 (12%)	10,11,11	1.40	2 (20%)
7	GLN	E	1093	-	8,9,9	1.33	1 (12%)	10,11,11	1.71	3 (30%)
8	ADP	K	1095	3	24,29,29	1.06	2 (8%)	29,45,45	1.37	3 (10%)
7	GLN	B	1091	-	8,9,9	1.85	3 (37%)	10,11,11	2.21	5 (50%)
8	ADP	B	1094	3	24,29,29	1.08	1 (4%)	29,45,45	1.28	3 (10%)

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
10	NET	K	1098	-	-	0/12/12/12	-
7	GLN	E	1094	-	-	0/9/9/9	-
8	ADP	E	1095	3	-	1/12/32/32	0/3/3/3
9	ORN	K	1097	-	-	6/8/8/8	-
8	ADP	K	1096	3	-	4/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	GLN	B	1092	-	-	0/9/9/9	-
7	GLN	B	1091	-	-	6/9/9/9	-
7	GLN	K	1094	-	-	0/9/9/9	-
8	ADP	B	1093	3	-	1/12/32/32	0/3/3/3
9	ORN	E	1097	-	-	5/8/8/8	-
8	ADP	H	1093	3	-	1/12/32/32	0/3/3/3
8	ADP	E	1096	3	-	1/12/32/32	0/3/3/3
9	ORN	B	1095	-	-	6/8/8/8	-
10	NET	H	1095	-	-	2/12/12/12	-
7	GLN	H	1091	-	-	1/9/9/9	-
8	ADP	H	1092	3	-	1/12/32/32	0/3/3/3
10	NET	E	1098	-	-	1/12/12/12	-
10	NET	B	1096	-	-	0/12/12/12	-
7	GLN	K	1093	-	-	5/9/9/9	-
7	GLN	H	1090	-	-	7/9/9/9	-
7	GLN	E	1093	-	-	5/9/9/9	-
8	ADP	K	1095	3	-	1/12/32/32	0/3/3/3
9	ORN	H	1094	-	-	6/8/8/8	-
8	ADP	B	1094	3	-	4/12/32/32	0/3/3/3

The worst 5 of 50 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1082	PO4	P-O4	-3.54	1.44	1.54
5	E	1078	PO4	P-O4	-3.47	1.44	1.54
8	E	1096	ADP	O3'-C3'	3.41	1.51	1.43
7	B	1092	GLN	OE1-CD	3.26	1.33	1.24
8	H	1092	ADP	C2'-C1'	-3.18	1.48	1.53

The worst 5 of 51 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	E	1097	ORN	CB-CA-C	-5.48	97.25	110.30
8	H	1092	ADP	C5-C6-N6	5.31	128.42	120.35
8	K	1096	ADP	C5-C6-N6	4.62	127.38	120.35
8	B	1094	ADP	C5-C6-N6	4.38	127.01	120.35
9	H	1094	ORN	CB-CA-C	-4.34	99.97	110.30

There are no chirality outliers.

5 of 64 torsion outliers are listed below:

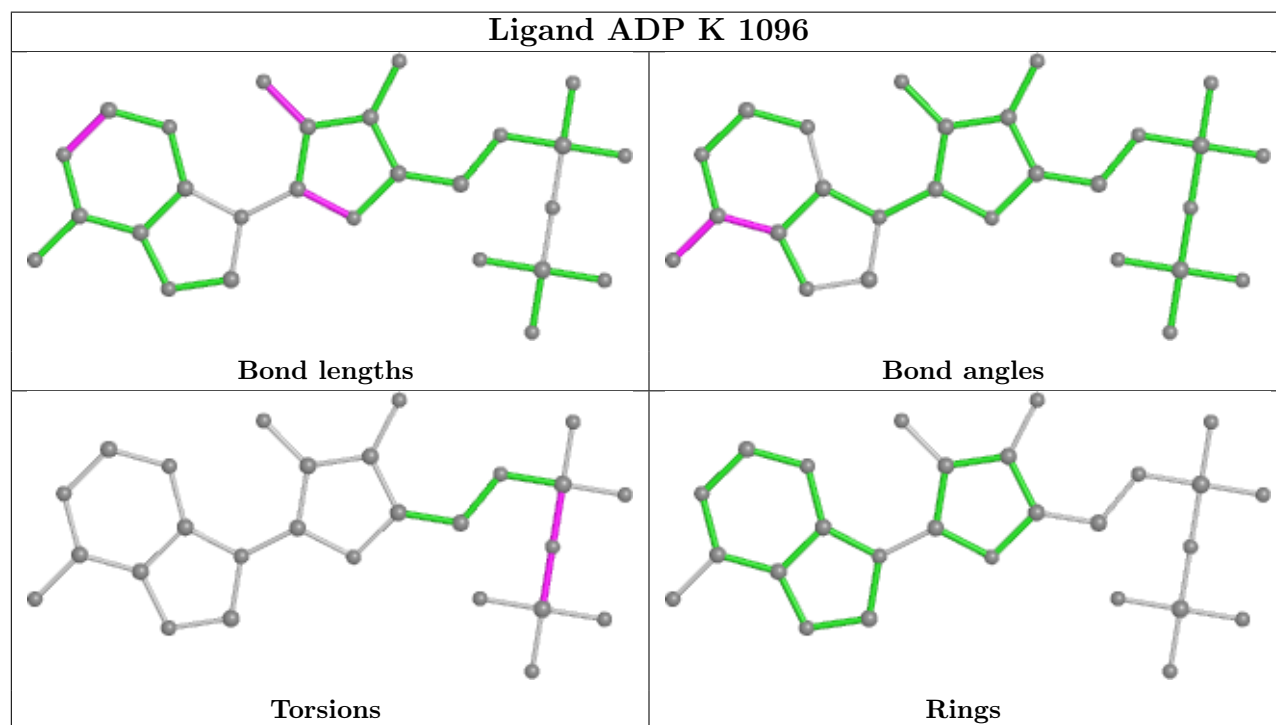
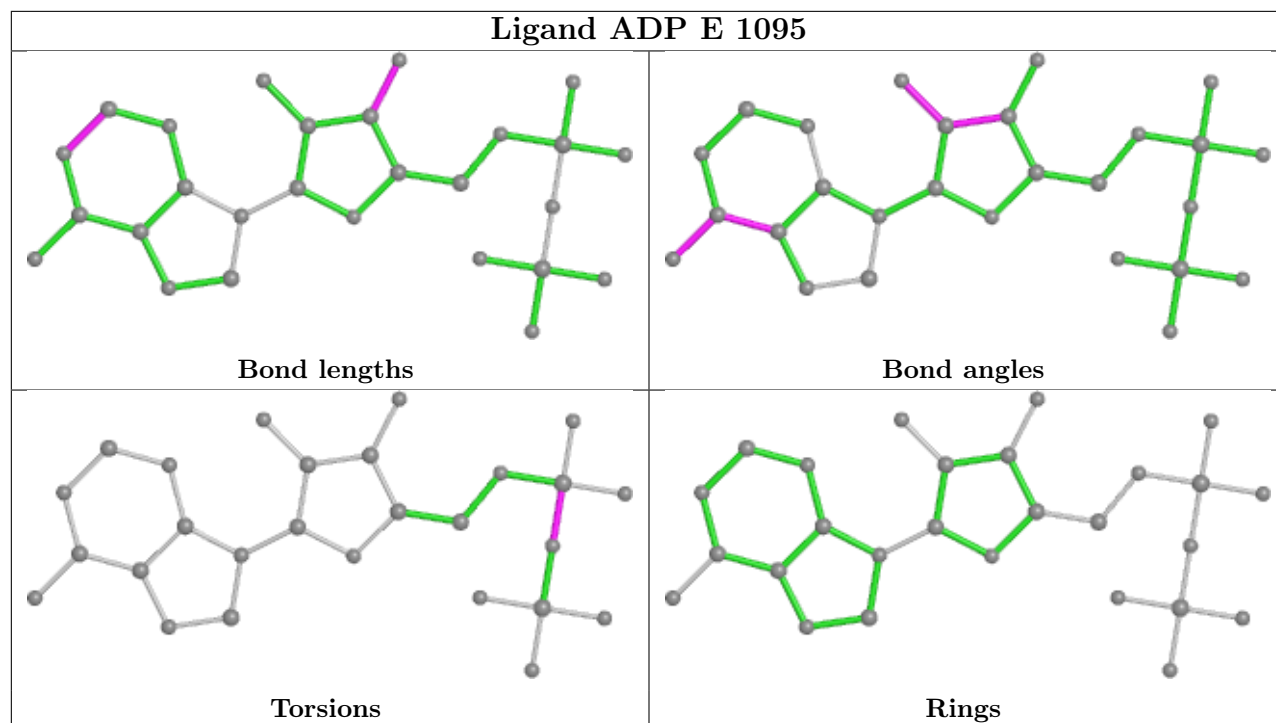
Mol	Chain	Res	Type	Atoms
7	B	1091	GLN	N-CA-CB-CG
7	B	1091	GLN	CA-CB-CG-CD
7	E	1093	GLN	N-CA-CB-CG
7	E	1093	GLN	C-CA-CB-CG
7	H	1090	GLN	N-CA-CB-CG

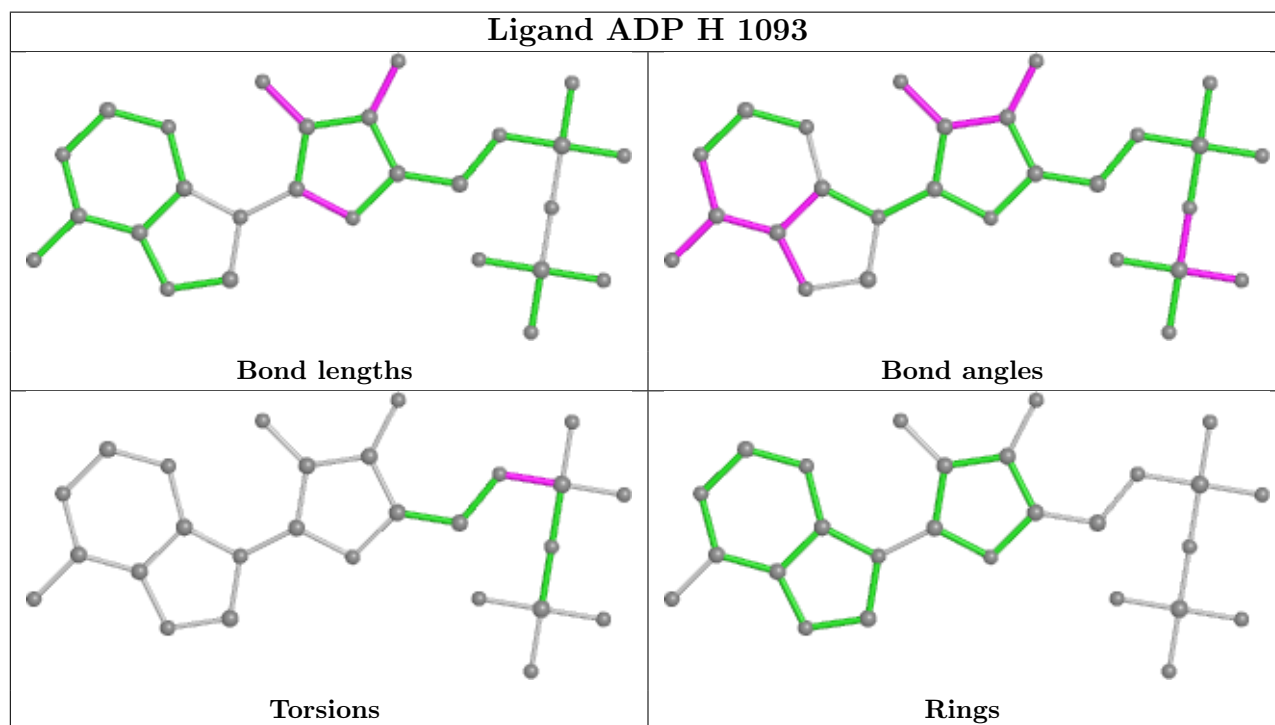
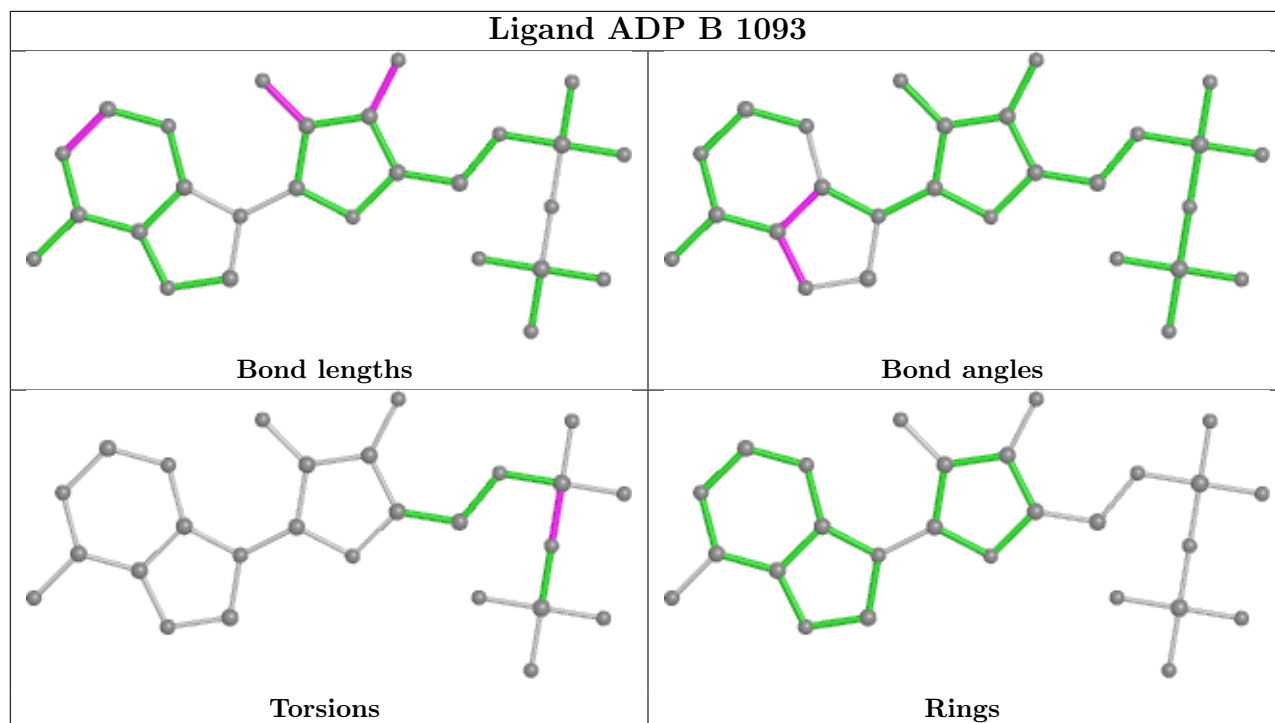
There are no ring outliers.

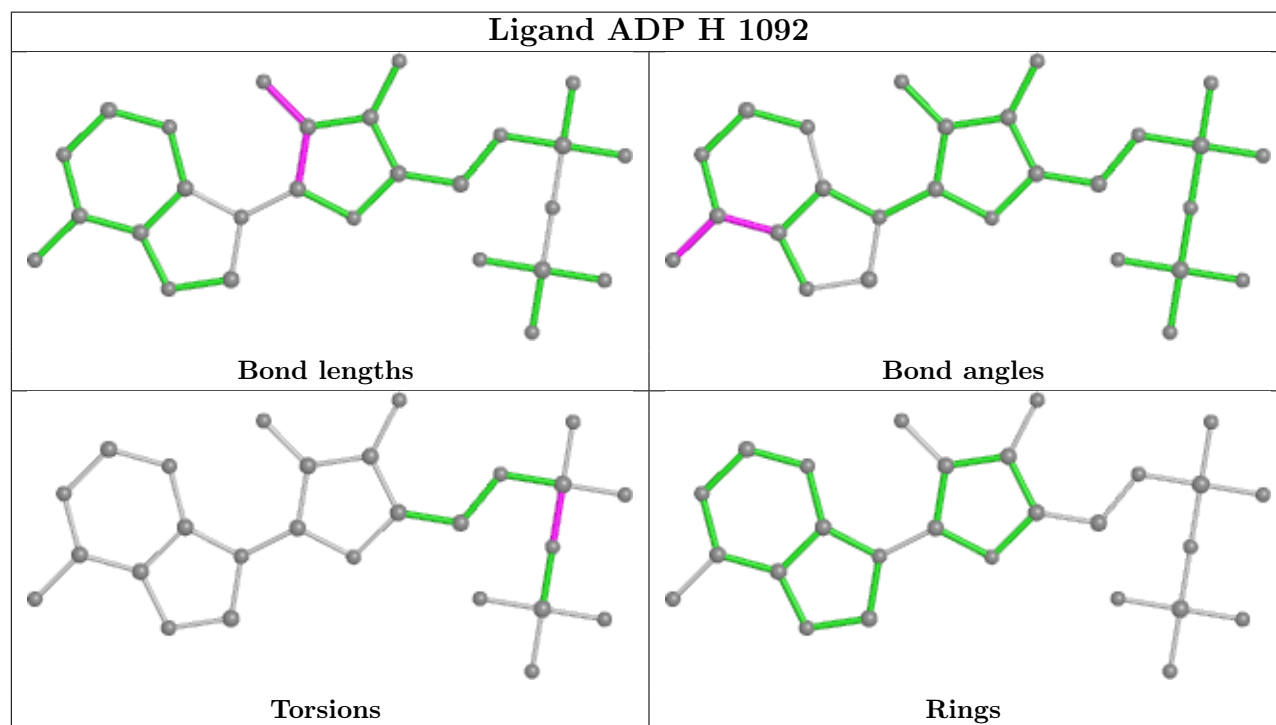
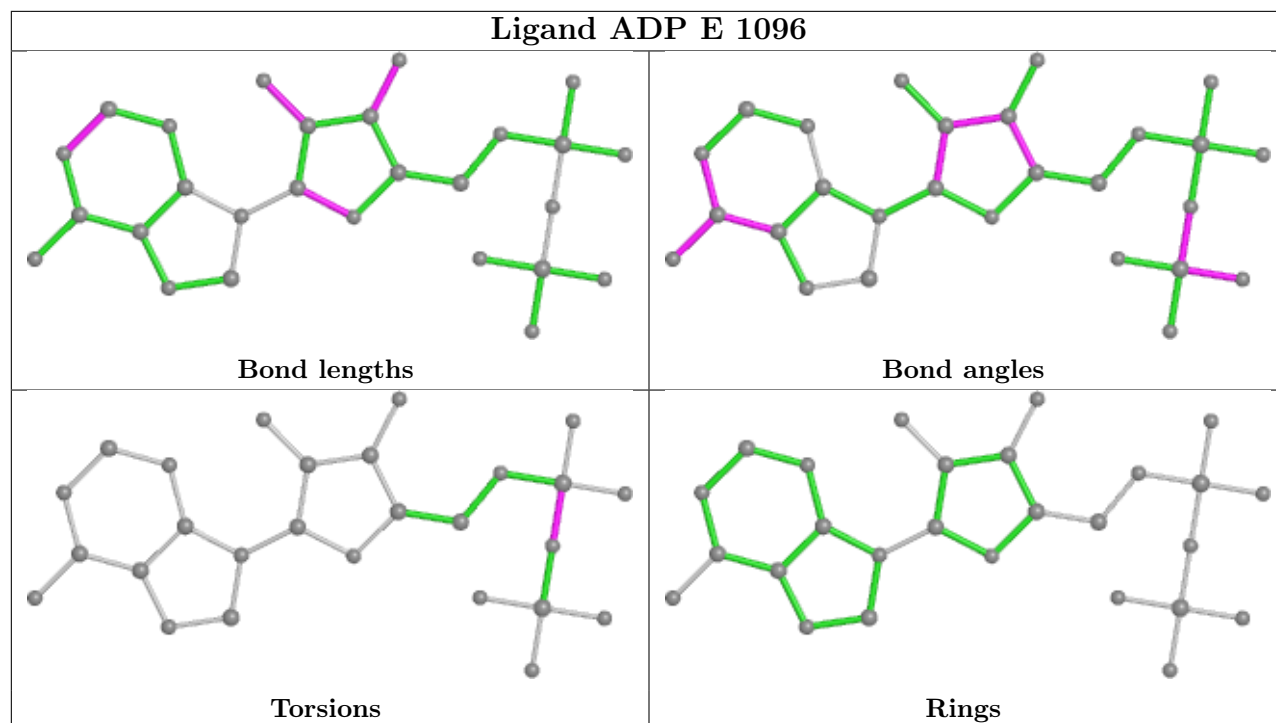
14 monomers are involved in 22 short contacts:

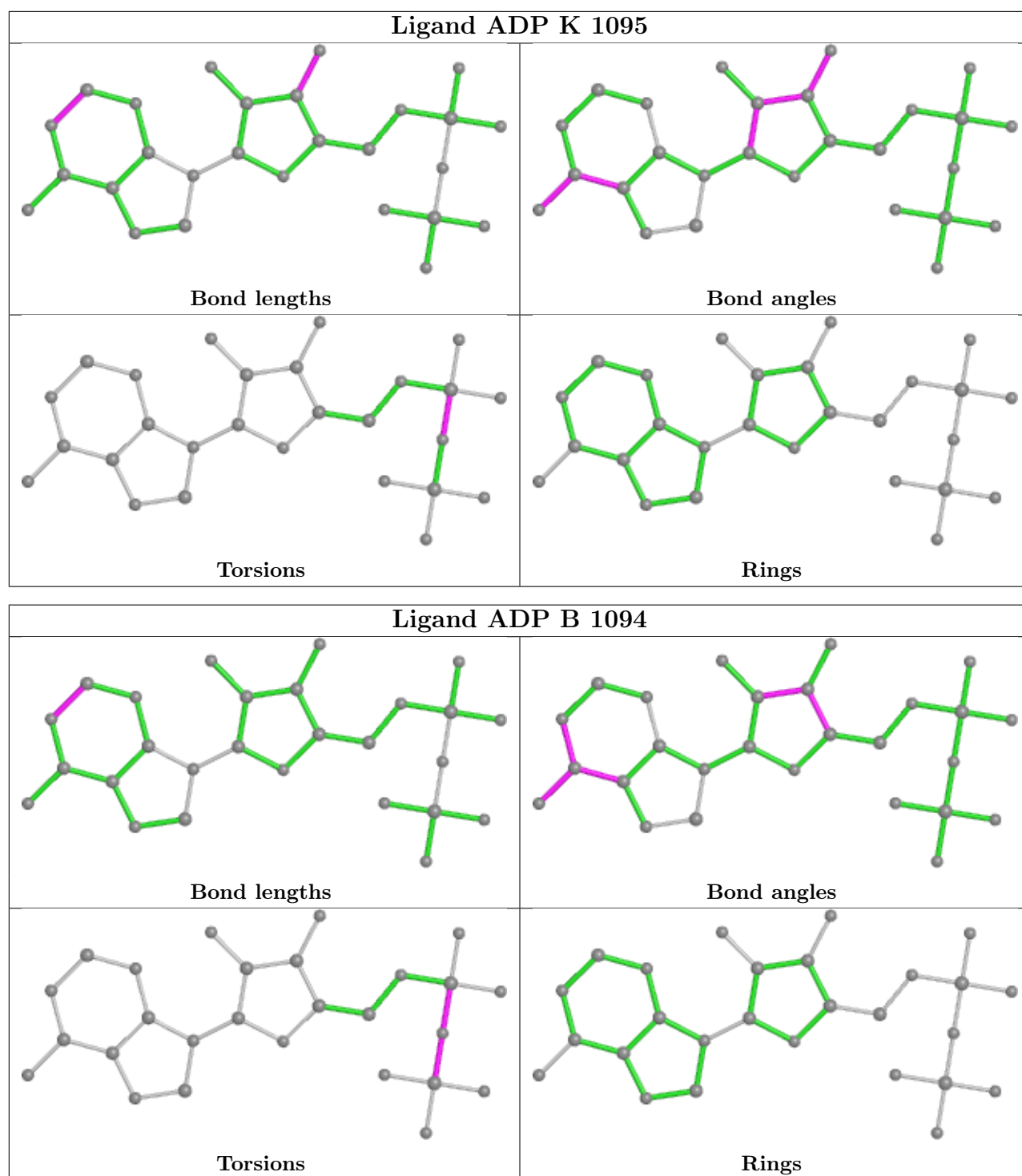
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1078	PO4	1	0
5	K	1082	PO4	2	0
9	K	1097	ORN	1	0
9	E	1097	ORN	3	0
8	E	1096	ADP	1	0
9	B	1095	ORN	4	0
5	E	1082	PO4	1	0
10	H	1095	NET	2	0
5	H	1082	PO4	2	0
10	B	1096	NET	1	0
7	K	1093	GLN	1	0
7	H	1090	GLN	2	0
7	E	1093	GLN	1	0
8	K	1095	ADP	1	0

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

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.