wwPDB X-ray Structure Validation Summary Report (i)

Sep 14, 2023 – 07:56 AM EDT

PDB ID	:	1CE8
Title	:	CARBAMOYL PHOSPHATE SYNTHETASE FROM ESCHERICHIS COLI WITH COMPLEXED WITH THE ALLOSTERIC LIGAND IMP
Authors	:	Thoden, J.B.; Raushel, F.M.; Holden, H.M.
Deposited on	:	1999-03-18
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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

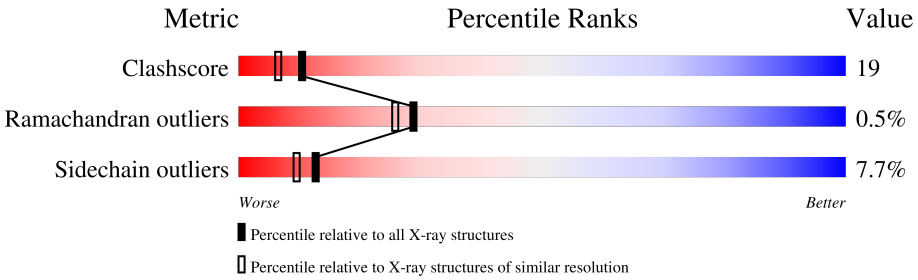
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	1073	59% 31% 8% ••
1	C	1073	61% 31% 7% •
1	E	1073	61% 29% 8% •
1	G	1073	52% 35% 11% ••
2	B	382	49% 40% 9% ••
2	D	382	59% 36% 5% •
2	F	382	51% 40% 8% ••
2	H	382	35% 51% 12% ••

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 48888 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 PROTEIN (CARBAMOYL-PHOSPHATE SYNTHASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1058	Total	C	N	O	S	0	8	0
			8198	5143	1427	1583	45			
1	C	1058	Total	C	N	O	S	0	1	0
			8167	5125	1426	1571	45			
1	E	1058	Total	C	N	O	S	0	12	0
			8232	5165	1444	1578	45			
1	G	1058	Total	C	N	O	S	0	2	0
			8170	5128	1424	1573	45			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	46	ASN	LEU	conflict	UNP P00968
C	46	ASN	LEU	conflict	UNP P00968
E	46	ASN	LEU	conflict	UNP P00968
G	46	ASN	LEU	conflict	UNP P00968

- Molecule 2 is a protein called PROTEIN (CARBAMOYL-PHOSPHATE SYNTHASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	379	Total	C	N	O	S	0	1	0
			2902	1829	512	551	10			
2	D	379	Total	C	N	O	S	0	1	0
			2899	1828	509	551	11			
2	F	379	Total	C	N	O	S	0	1	0
			2900	1828	510	552	10			
2	H	379	Total	C	N	O	S	0	0	0
			2895	1825	509	551	10			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	183	GLN	GLU	conflict	UNP P0A6F1
D	183	GLN	GLU	conflict	UNP P0A6F1
F	183	GLN	GLU	conflict	UNP P0A6F1
H	183	GLN	GLU	conflict	UNP P0A6F1

- 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	6	Total K 6 6	0	0
4	B	1	Total K 1 1	0	0
4	C	6	Total K 6 6	0	0
4	D	1	Total K 1 1	0	0
4	E	6	Total K 6 6	0	0
4	F	1	Total K 1 1	0	0
4	G	6	Total K 6 6	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

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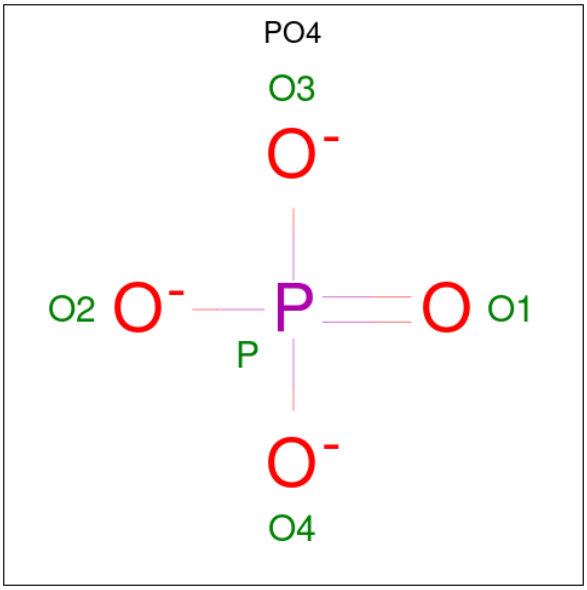
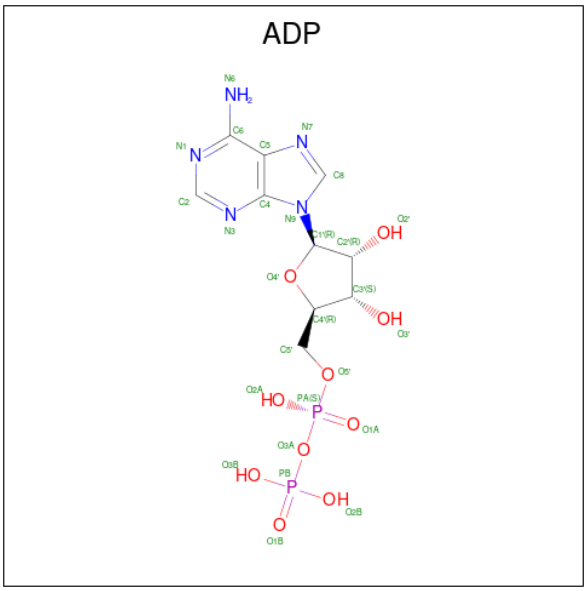
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	3	Total Cl 3 3	0	0
5	E	3	Total Cl 3 3	0	0
5	G	3	Total Cl 3 3	0	0

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



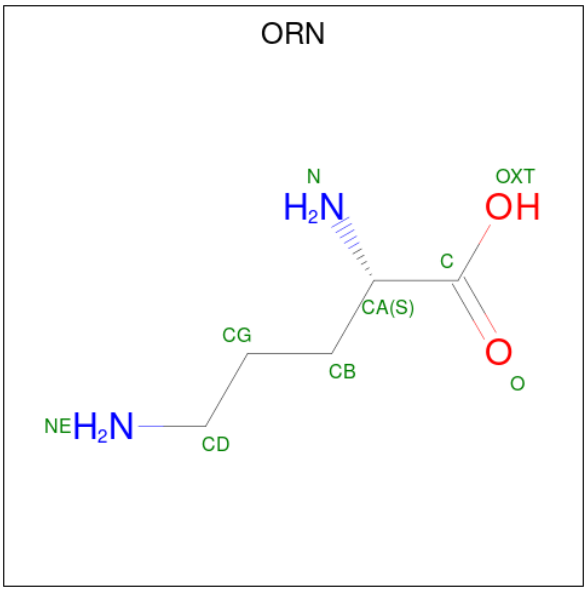
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O P 5 4 1	0	0
6	C	1	Total O P 5 4 1	0	0
6	E	1	Total O P 5 4 1	0	0
6	G	1	Total O P 5 4 1	0	0

- Molecule 7 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



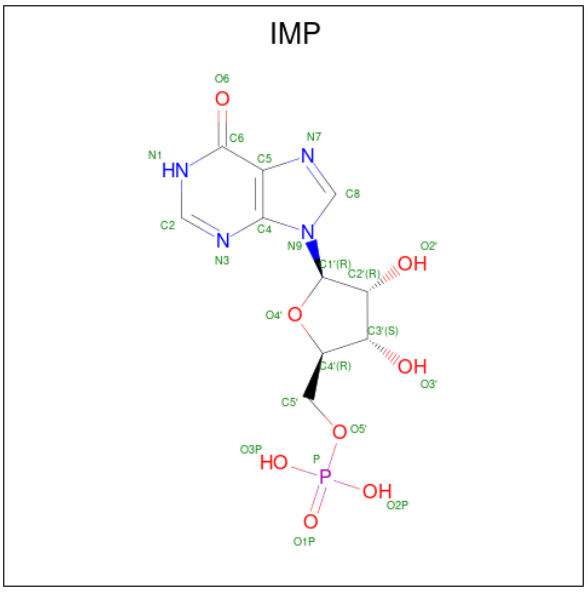
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	G	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: $C_5H_{12}N_2O_2$).



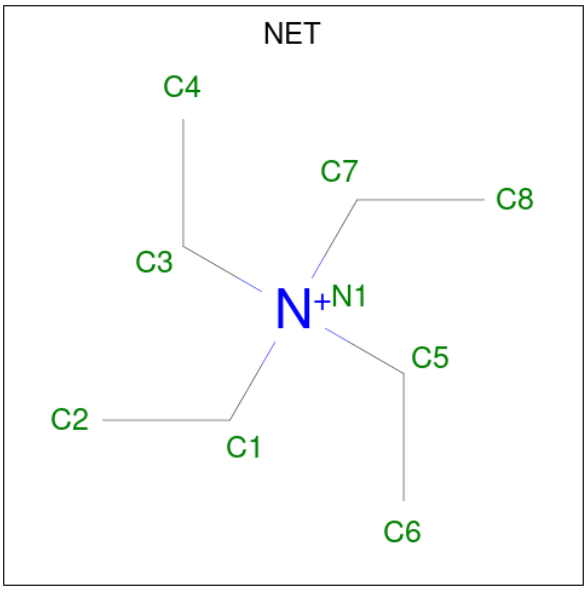
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C N O 9 5 2 2	0	0
8	A	1	Total C N O 9 5 2 2	0	0
8	C	1	Total C N O 9 5 2 2	0	0
8	C	1	Total C N O 9 5 2 2	0	0
8	E	1	Total C N O 9 5 2 2	0	0
8	E	1	Total C N O 9 5 2 2	0	0
8	G	1	Total C N O 9 5 2 2	0	0
8	G	1	Total C N O 9 5 2 2	0	0

- Molecule 9 is INOSINIC ACID (three-letter code: IMP) (formula: $C_{10}H_{13}N_4O_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	A	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
9	C	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
9	E	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
9	G	1	Total	C	N	O	P	0	0
			23	10	4	8	1		

- 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 9 8 1	0	0
10	C	1	Total C N 9 8 1	0	0
10	E	1	Total C N 9 8 1	0	0
10	G	1	Total C N 9 8 1	0	0

- Molecule 11 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	842	Total O 842 842	0	0
11	B	190	Total O 190 190	0	0
11	C	732	Total O 732 732	0	0
11	D	193	Total O 193 193	0	0
11	E	939	Total O 939 939	0	0
11	F	233	Total O 233 233	0	0
11	G	743	Total O 743 743	0	0
11	H	165	Total O 165 165	0	0

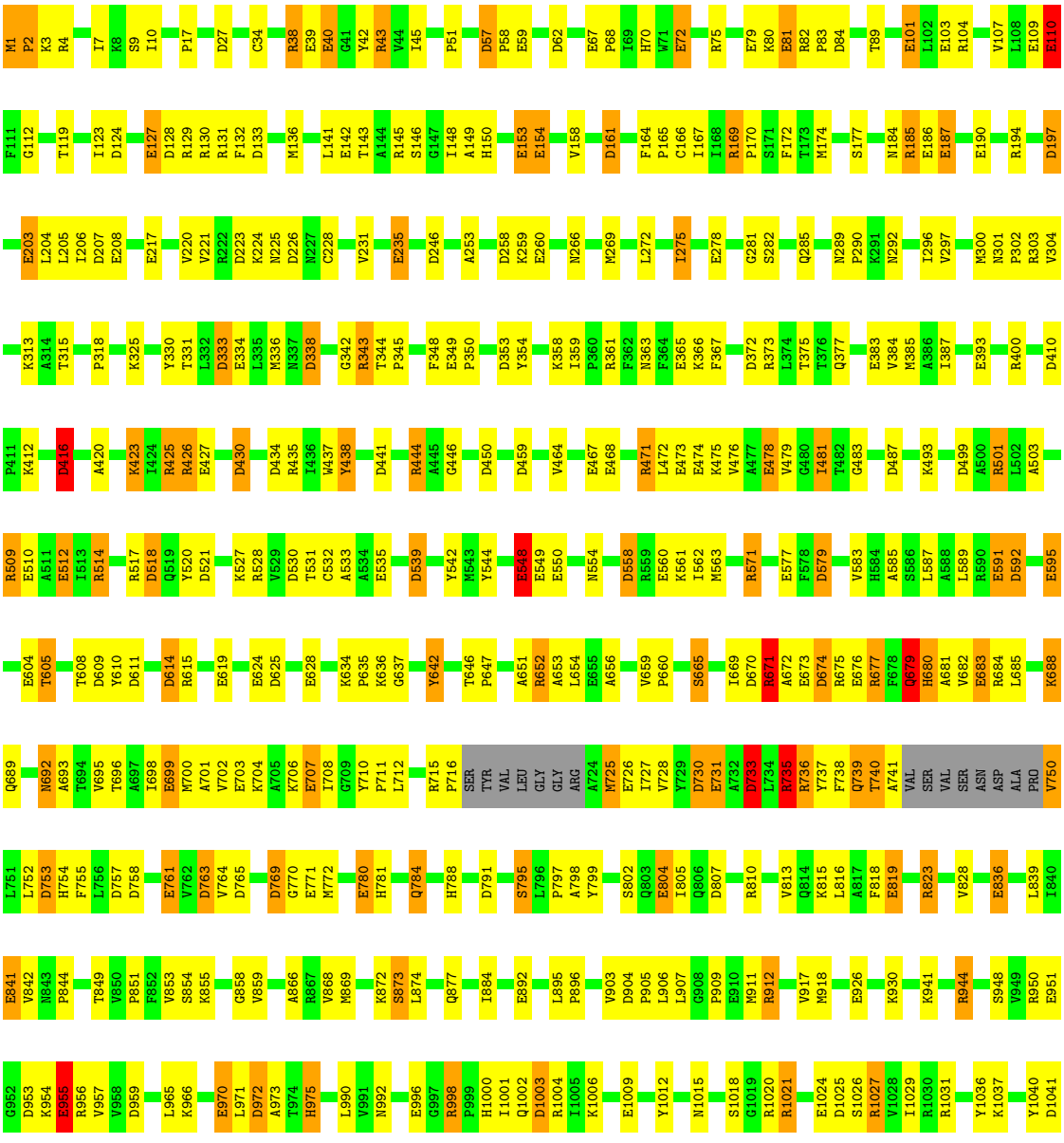
3 Residue-property plots (i)

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.

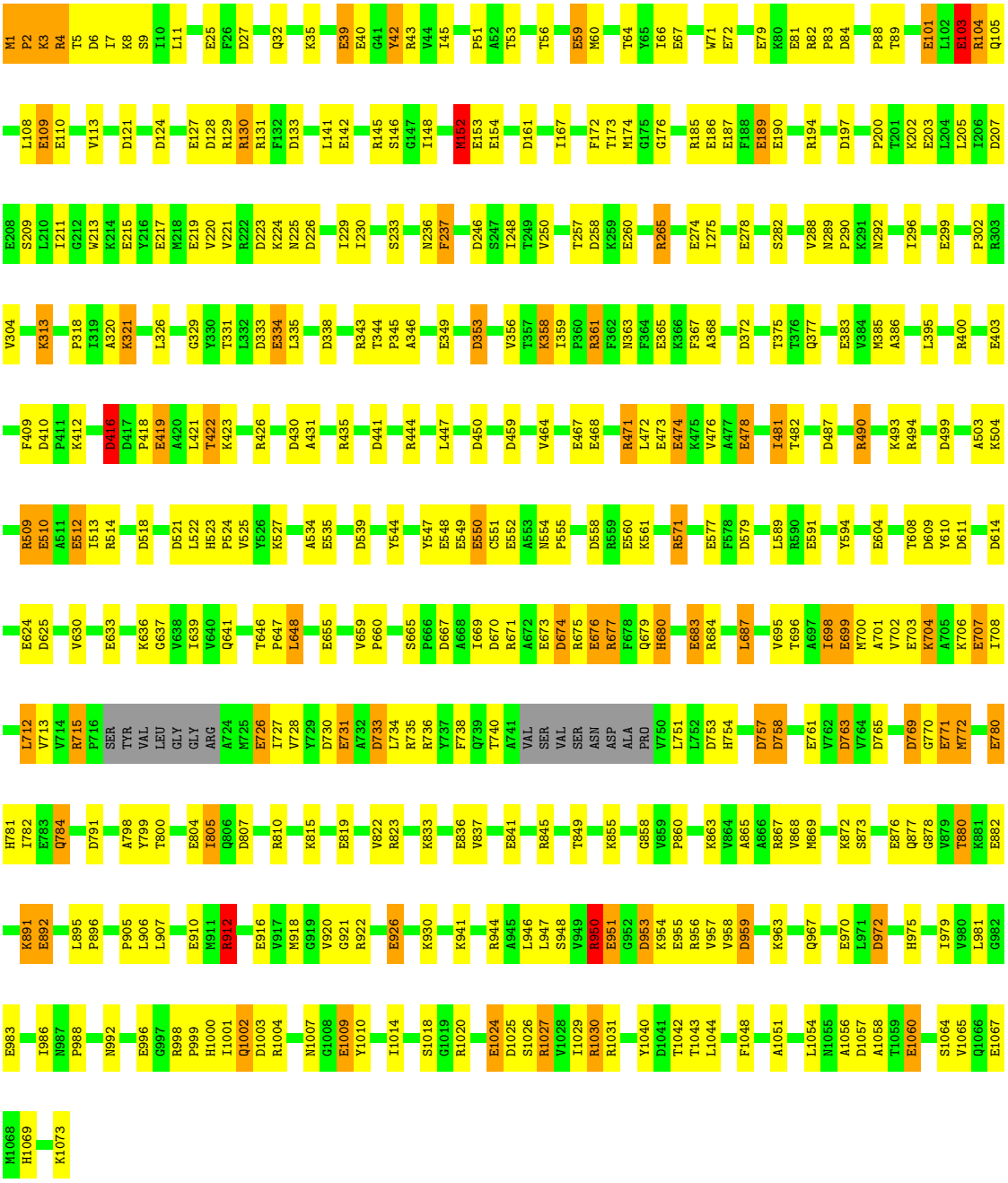
• Molecule 1: PROTEIN (CARBAMOYL-PHOSPHATE SYNTHASE)

Chain A: 59% 31% 8% ••



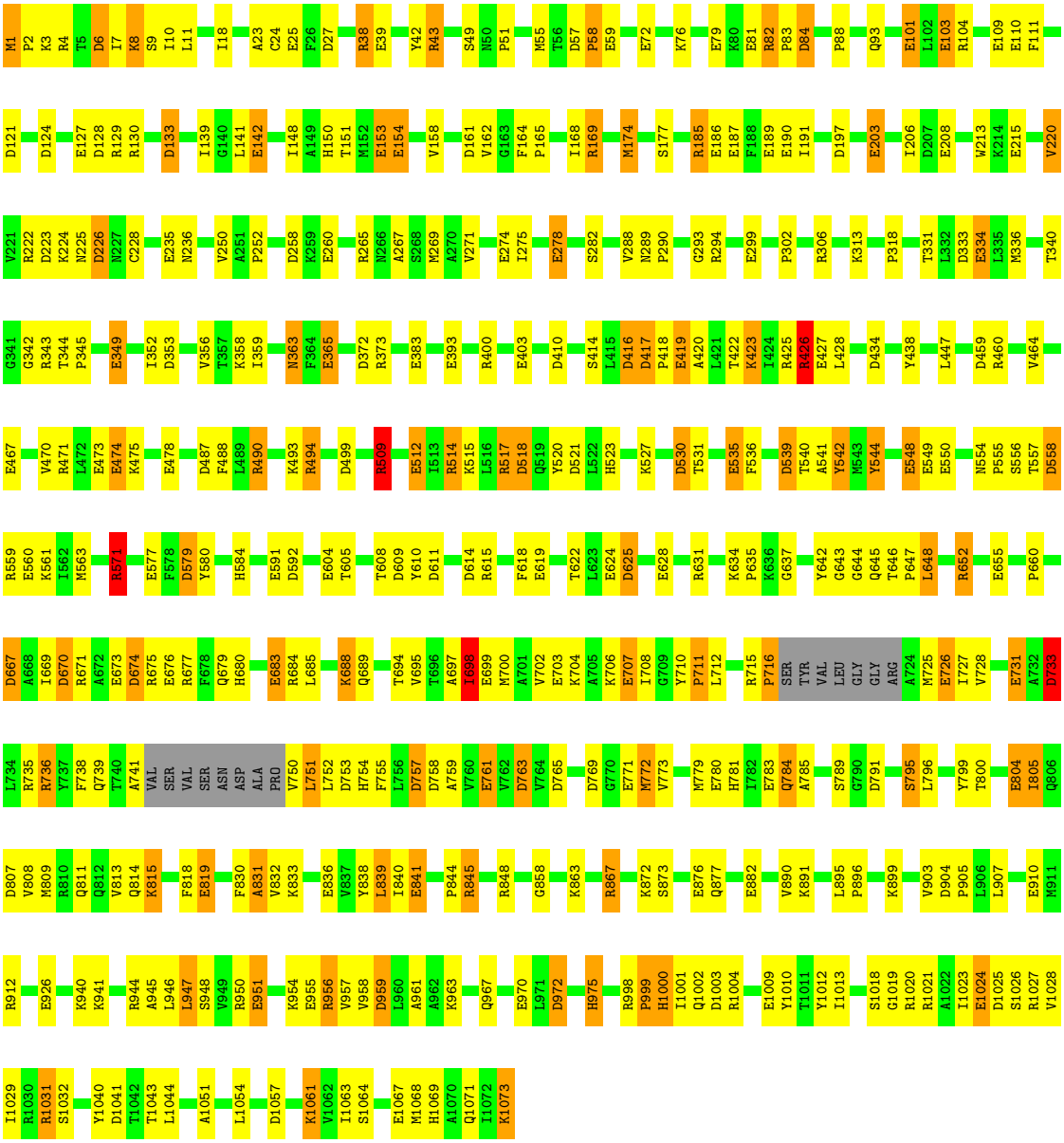
• Molecule 1: PROTEIN (CARBAMOYL-PHOSPHATE SYNTHASE)

Chain C:



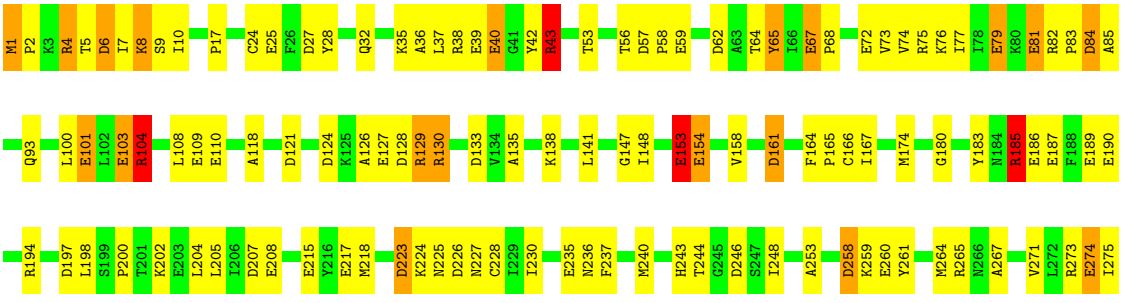
• Molecule 1: PROTEIN (CARBAMOYL-PHOSPHATE SYNTHASE)

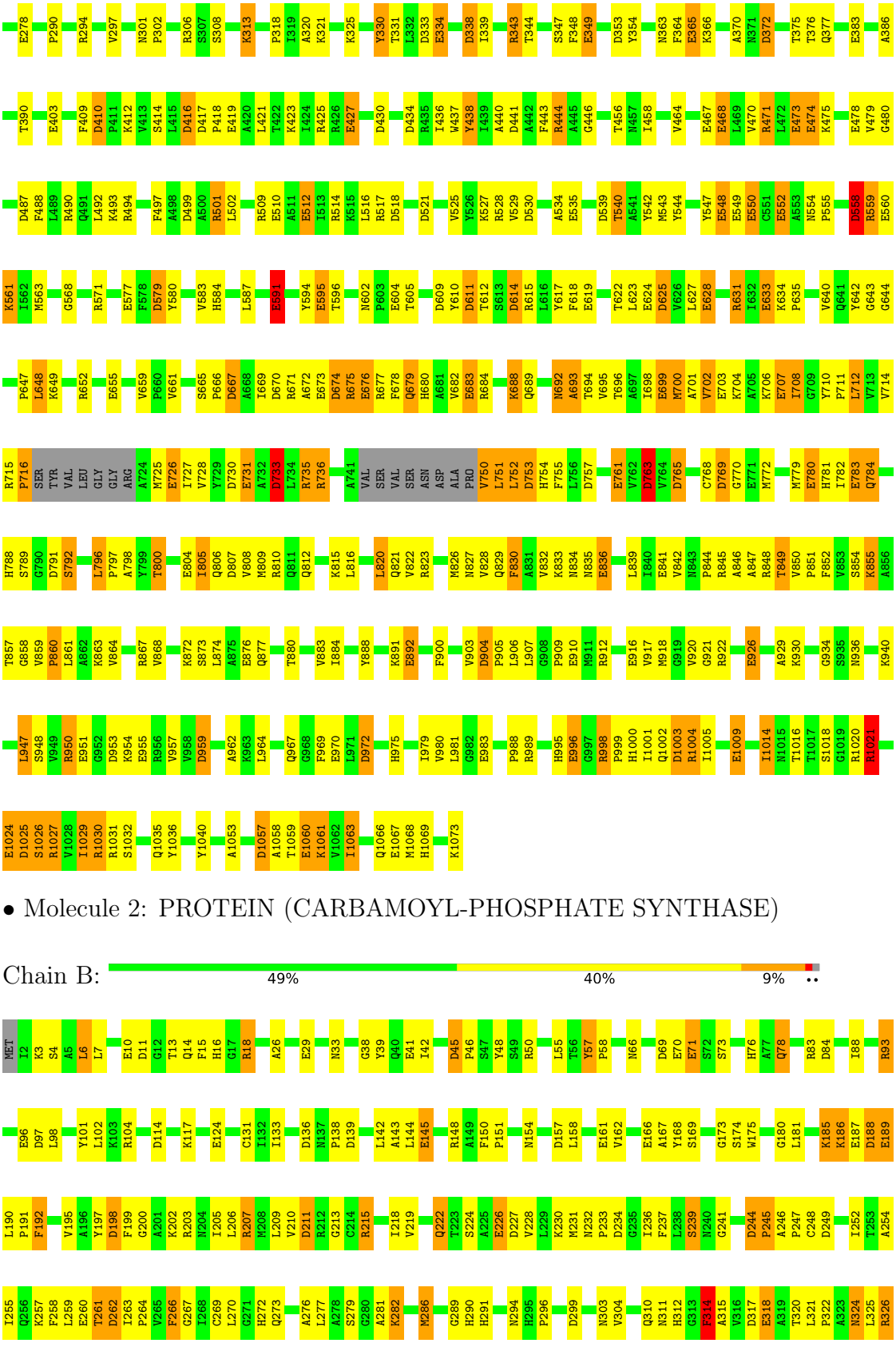
Chain E:



• Molecule 1: PROTEIN (CARBAMOYL-PHOSPHATE SYNTHASE)

Chain G:



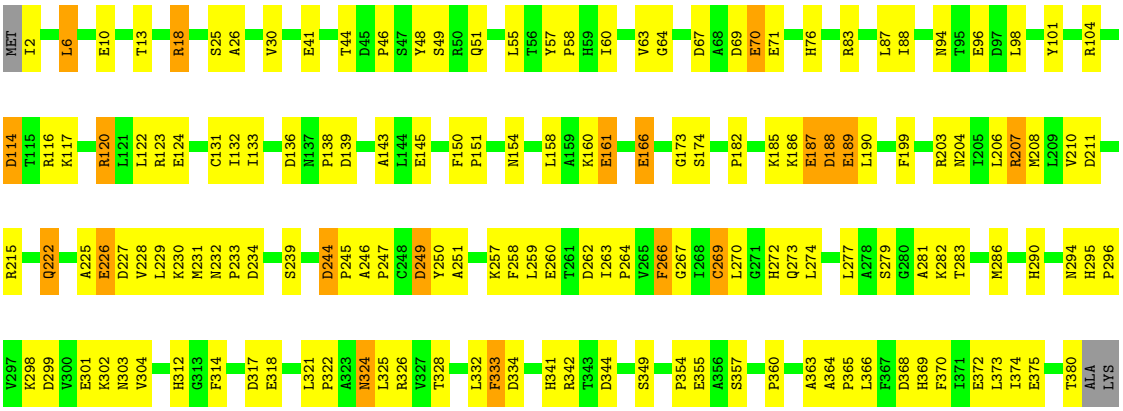


• Molecule 2: PROTEIN (CARBAMOYL-PHOSPHATE SYNTHASE)

Chain B:

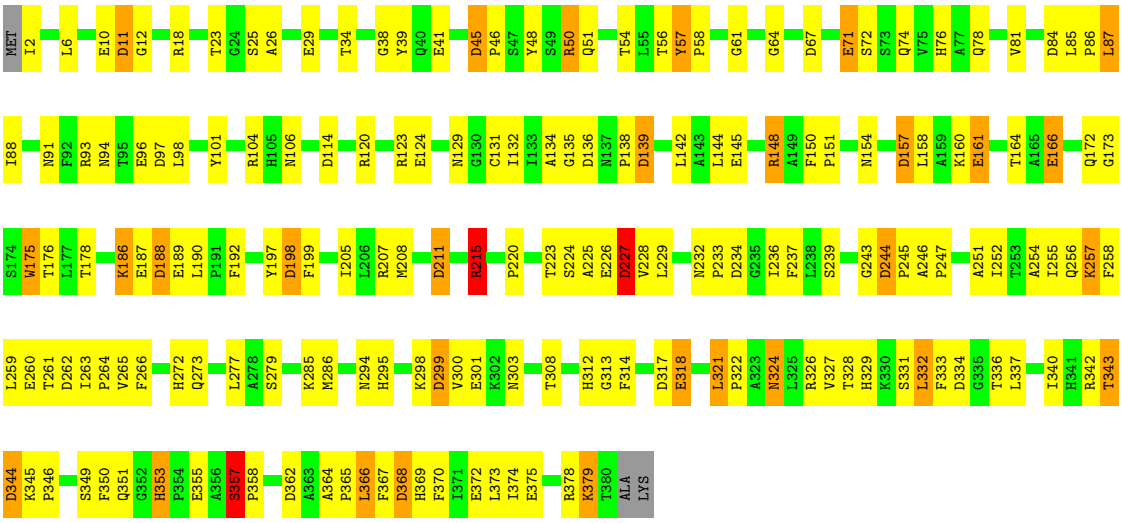
• Molecule 2: PROTEIN (CARBAMOYL-PHOSPHATE SYNTHASE)

Chain D:



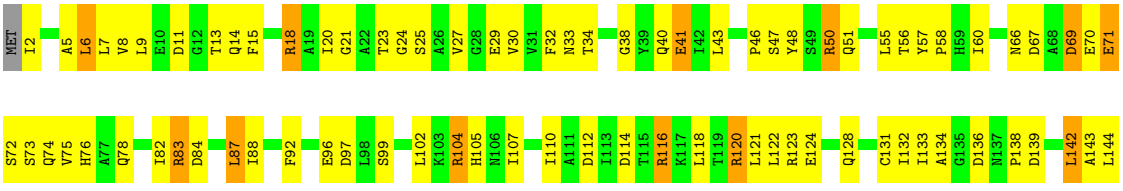
• Molecule 2: PROTEIN (CARBAMOYL-PHOSPHATE SYNTHASE)

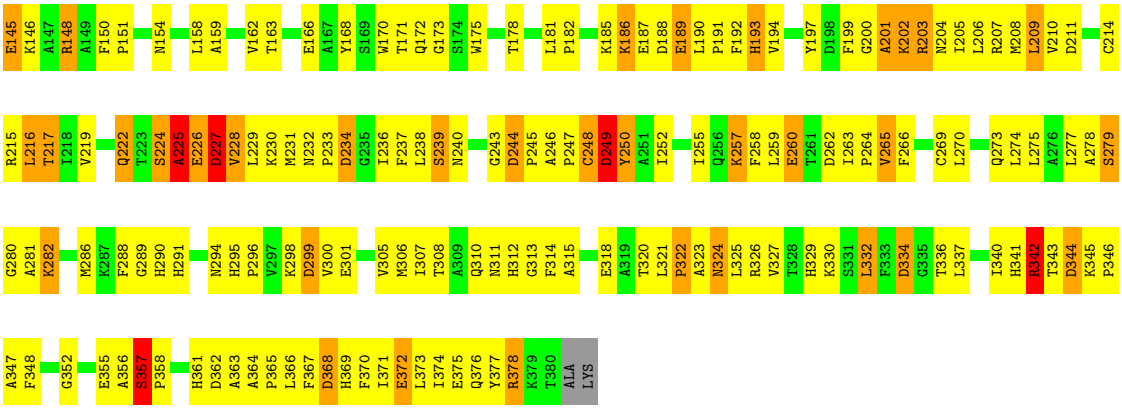
Chain F:



• Molecule 2: PROTEIN (CARBAMOYL-PHOSPHATE SYNTHASE)

Chain H:




E145 K146 A147 R148 A149 F150 P151 N154 L158 A159 V162 T163 E166 A167 Y168 S169 W170 T171 Q172 G173 S174 W175 T178 L181 P182 K185 K186 E187 D188 E189 L190 P191 F192 H193 V194 Y197 D198 F199 G200 A201 K202 R203 N204 I205 L206 R207 M208 L209 V210 D211 C214
R215 L216 T217 I218 V219 Q222 T223 S224 A225 E226 D227 V228 L229 K230 M231 N232 P233 D234 G235 I236 F237 L238 S239 N240 G243 D244 P245 A246 P247 C248 D249 Y250 A251 I252 I255 Q256 K257 F258 L259 E260 T261 D262 I263 P264 V265 F266 C269 L270 Q273 L274 L275 A276 L277 A278 S279
G280 A281 K282 M286 K287 F288 G289 H290 H291 N294 H295 P296 V297 K298 D299 V300 E301 V305 M306 I307 T308 A309 Q310 N311 H312 G313 F314 A315 E318 A319 T320 L321 P322 A323 N324 L325 R326 V327 T328 H329 K330 S331 L332 F333 D334 G335 T336 L337 I340 H341 R342 T343 D344 K345 P346
A347 F348 G352 E355 A356 S357 P358 H361 D362 A363 A364 P365 L366 F367 D368 H369 F370 I371 E372 L373 I374 E375 Q376 Y377 R378 K379 T380 ALA LYS

4 Data and refinement statistics (i)

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	152.10Å 163.90Å 331.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.10	Depositor
% Data completeness (in resolution range)	93.0 (30.00-2.10)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
Refinement program	TNT 5D	Depositor
R, R_{free}	0.193 , 0.250	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	48888	wwPDB-VP
Average B, all atoms (Å^2)	40.0	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: MN, PO4, ADP, K, IMP, CL, ORN, 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	1.03	66/8356 (0.8%)	1.41	138/11295 (1.2%)
1	C	1.04	78/8297 (0.9%)	1.41	118/11216 (1.1%)
1	E	1.04	72/8406 (0.9%)	1.45	135/11358 (1.2%)
1	G	1.04	78/8304 (0.9%)	1.48	144/11225 (1.3%)
2	B	0.92	17/2968 (0.6%)	1.41	55/4030 (1.4%)
2	D	0.94	17/2965 (0.6%)	1.38	42/4026 (1.0%)
2	F	0.95	15/2966 (0.5%)	1.44	49/4028 (1.2%)
2	H	1.00	18/2957 (0.6%)	1.54	55/4016 (1.4%)
All	All	1.02	361/45219 (0.8%)	1.44	736/61194 (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
2	B	0	2
2	H	0	2
All	All	0	4

The worst 5 of 361 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	841	GLU	CD-OE1	-13.34	1.10	1.25
2	H	227	ASP	CG-OD2	9.15	1.46	1.25
2	D	166	GLU	CD-OE2	9.14	1.35	1.25
2	B	372	GLU	CD-OE2	8.34	1.34	1.25
2	H	166	GLU	CD-OE2	8.31	1.34	1.25

The worst 5 of 736 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	227	ASP	CB-CG-OD2	-15.41	104.43	118.30
2	H	249	ASP	CB-CG-OD1	-15.06	104.74	118.30
2	F	120	ARG	NE-CZ-NH1	13.22	126.91	120.30
1	E	642	TYR	CB-CG-CD1	13.16	128.89	121.00
1	E	438	TYR	CB-CG-CD1	13.10	128.86	121.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	314	PHE	Mainchain
2	B	357	SER	Peptide
2	H	250	TYR	Sidechain
2	H	357	SER	Peptide

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	8198	0	8215	275	1
1	C	8167	0	8201	242	0
1	E	8232	0	8274	251	0
1	G	8170	0	8204	343	0
2	B	2902	0	2872	145	0
2	D	2899	0	2868	95	0
2	F	2900	0	2867	118	1
2	H	2895	0	2863	230	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	6	0	0	0	0
4	B	1	0	0	0	0
4	C	6	0	0	0	0
4	D	1	0	0	0	0
4	E	6	0	0	0	0
4	F	1	0	0	0	0
4	G	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	1	0	0	0	0
5	A	3	0	0	0	0
5	C	3	0	0	0	0
5	E	3	0	0	1	0
5	G	3	0	0	2	0
6	A	5	0	0	0	0
6	C	5	0	0	0	0
6	E	5	0	0	0	0
6	G	5	0	0	0	0
7	A	54	0	24	2	0
7	C	54	0	24	1	0
7	E	54	0	24	5	0
7	G	54	0	24	5	0
8	A	18	0	22	4	0
8	C	18	0	22	3	0
8	E	18	0	21	4	0
8	G	18	0	22	4	0
9	A	23	0	11	1	0
9	C	23	0	11	1	0
9	E	23	0	11	2	0
9	G	23	0	11	1	0
10	A	9	0	20	0	0
10	C	9	0	20	0	0
10	E	9	0	20	3	0
10	G	9	0	20	1	0
11	A	842	0	0	26	1
11	B	190	0	0	3	0
11	C	732	0	0	12	0
11	D	193	0	0	3	0
11	E	939	0	0	30	0
11	F	233	0	0	4	1
11	G	743	0	0	19	0
11	H	165	0	0	4	0
All	All	48888	0	44671	1666	2

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 19.

The worst 5 of 1666 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:A:130[B]:ARG:NH2	1:A:130[B]:ARG:CZ	1.70	1.49
2:H:133:ILE:HD12	2:H:143:ALA:HB2	1.26	1.16
2:H:322:PRO:HB2	2:H:324:ASN:HD21	1.06	1.12
1:E:728:VAL:HG13	1:E:733:ASP:HB3	1.13	1.06
1:A:130[B]:ARG:CZ	1:A:130[B]:ARG:NH1	2.18	1.05

All (2) 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)
1:A:130[B]:ARG:NH1	11:F:3079:HOH:O[3_545]	1.65	0.55
2:F:10:GLU:OE1	11:A:5434:HOH:O[3_555]	2.15	0.05

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	1060/1073 (99%)	1010 (95%)	46 (4%)	4 (0%)	34	32
1	C	1053/1073 (98%)	1002 (95%)	48 (5%)	3 (0%)	41	41
1	E	1064/1073 (99%)	1011 (95%)	50 (5%)	3 (0%)	41	41
1	G	1054/1073 (98%)	981 (93%)	67 (6%)	6 (1%)	25	21
2	B	378/382 (99%)	358 (95%)	18 (5%)	2 (0%)	29	26
2	D	378/382 (99%)	362 (96%)	16 (4%)	0	100	100
2	F	378/382 (99%)	360 (95%)	17 (4%)	1 (0%)	41	41
2	H	377/382 (99%)	341 (90%)	27 (7%)	9 (2%)	6	2
All	All	5742/5820 (99%)	5425 (94%)	289 (5%)	28 (0%)	29	26

5 of 28 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	357	SER
1	C	368	ALA
2	F	357	SER
2	H	201	ALA
2	H	248	CYS

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	873/878 (99%)	814 (93%)	59 (7%)	16 13
1	C	866/878 (99%)	813 (94%)	53 (6%)	18 16
1	E	877/878 (100%)	811 (92%)	66 (8%)	13 10
1	G	867/878 (99%)	788 (91%)	79 (9%)	9 6
2	B	309/310 (100%)	281 (91%)	28 (9%)	9 6
2	D	309/310 (100%)	292 (94%)	17 (6%)	21 19
2	F	309/310 (100%)	280 (91%)	29 (9%)	8 5
2	H	308/310 (99%)	272 (88%)	36 (12%)	5 3
All	All	4718/4752 (99%)	4351 (92%)	367 (8%)	13 9

5 of 367 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	154	ASN
1	G	665	SER
2	F	215	ARG
1	G	153	GLU
1	G	751	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 102 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	812	GLN

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Mol	Chain	Res	Type
2	F	154	ASN
2	H	222	GLN
1	E	834	ASN
1	E	1000	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 80 ligands modelled in this entry, 52 are monoatomic - leaving 28 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	C	5027	3,4	24,29,29	1.19	3 (12%)	29,45,45	1.21	3 (10%)
8	ORN	E	5054	-	7,8,8	0.88	0	8,9,9	2.50	4 (50%)
8	ORN	G	5074	-	7,8,8	1.06	1 (14%)	8,9,9	1.02	0
10	NET	C	5033	-	8,8,8	0.61	0	10,10,10	0.51	0
10	NET	G	5073	-	8,8,8	0.69	0	10,10,10	0.49	0
7	ADP	G	5060	3	24,29,29	1.15	2 (8%)	29,45,45	1.35	4 (13%)
9	IMP	C	5032	-	21,25,25	1.84	5 (23%)	24,38,38	1.29	3 (12%)
6	PO4	E	5046	3,4	4,4,4	2.80	3 (75%)	6,6,6	0.63	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	IMP	E	5052	-	21,25,25	1.70	5 (23%)	24,38,38	1.98	4 (16%)
8	ORN	A	5014	-	7,8,8	0.98	1 (14%)	8,9,9	1.06	0
8	ORN	A	5011	-	7,8,8	1.18	1 (14%)	8,9,9	1.31	1 (12%)
7	ADP	E	5047	3,4	24,29,29	1.06	4 (16%)	29,45,45	1.26	4 (13%)
10	NET	E	5053	-	8,8,8	0.82	0	10,10,10	0.37	0
9	IMP	G	5072	-	21,25,25	1.67	5 (23%)	24,38,38	1.52	4 (16%)
7	ADP	A	5007	3,4	24,29,29	1.12	2 (8%)	29,45,45	1.25	3 (10%)
8	ORN	C	5034	-	7,8,8	1.01	1 (14%)	8,9,9	1.09	1 (12%)
7	ADP	A	5000	3	24,29,29	1.15	3 (12%)	29,45,45	1.35	4 (13%)
8	ORN	G	5071	-	7,8,8	0.84	0	8,9,9	1.27	1 (12%)
9	IMP	A	5012	-	21,25,25	1.84	5 (23%)	24,38,38	1.29	3 (12%)
7	ADP	G	5067	3,4	24,29,29	1.21	5 (20%)	29,45,45	1.54	4 (13%)
8	ORN	E	5051	-	7,8,8	0.91	0	8,9,9	1.35	2 (25%)
6	PO4	G	5066	3,4	4,4,4	1.80	2 (50%)	6,6,6	0.98	0
7	ADP	E	5040	3	24,29,29	0.95	1 (4%)	29,45,45	1.33	4 (13%)
10	NET	A	5013	-	8,8,8	0.69	0	10,10,10	0.60	0
6	PO4	C	5026	3,4	4,4,4	2.50	3 (75%)	6,6,6	0.87	0
6	PO4	A	5006	3,4	4,4,4	2.01	2 (50%)	6,6,6	1.28	1 (16%)
7	ADP	C	5020	3	24,29,29	1.28	4 (16%)	29,45,45	1.49	4 (13%)
8	ORN	C	5031	-	7,8,8	0.88	0	8,9,9	1.26	2 (25%)

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	C	5027	3,4	-	4/12/32/32	0/3/3/3
8	ORN	E	5054	-	-	2/8/8/8	-
8	ORN	G	5074	-	-	4/8/8/8	-
10	NET	C	5033	-	-	0/12/12/12	-
10	NET	G	5073	-	-	3/12/12/12	-
7	ADP	G	5060	3	-	1/12/32/32	0/3/3/3
9	IMP	C	5032	-	-	1/6/26/26	0/3/3/3
9	IMP	E	5052	-	-	3/6/26/26	0/3/3/3
8	ORN	A	5014	-	-	6/8/8/8	-
8	ORN	A	5011	-	-	6/8/8/8	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	ADP	E	5047	3,4	-	3/12/32/32	0/3/3/3
10	NET	E	5053	-	-	3/12/12/12	-
9	IMP	G	5072	-	-	1/6/26/26	0/3/3/3
7	ADP	A	5007	3,4	-	3/12/32/32	0/3/3/3
8	ORN	C	5034	-	-	4/8/8/8	-
7	ADP	A	5000	3	-	1/12/32/32	0/3/3/3
8	ORN	G	5071	-	-	6/8/8/8	-
9	IMP	A	5012	-	-	1/6/26/26	0/3/3/3
7	ADP	G	5067	3,4	-	2/12/32/32	0/3/3/3
8	ORN	E	5051	-	-	5/8/8/8	-
7	ADP	E	5040	3	-	1/12/32/32	0/3/3/3
10	NET	A	5013	-	-	0/12/12/12	-
7	ADP	C	5020	3	-	2/12/32/32	0/3/3/3
8	ORN	C	5031	-	-	6/8/8/8	-

The worst 5 of 58 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	5012	IMP	O6-C6	5.66	1.34	1.23
9	C	5032	IMP	O6-C6	5.59	1.34	1.23
9	E	5052	IMP	O6-C6	4.33	1.32	1.23
9	G	5072	IMP	O6-C6	3.96	1.31	1.23
6	E	5046	PO4	P-O2	-3.78	1.43	1.54

The worst 5 of 56 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	E	5052	IMP	O3P-P-O5'	-6.32	89.90	106.73
7	C	5020	ADP	C5-C6-N6	5.69	129.00	120.35
7	A	5000	ADP	C5-C6-N6	4.28	126.86	120.35
8	E	5054	ORN	CB-CA-C	4.22	120.34	110.30
7	G	5067	ADP	O3B-PB-O3A	3.91	117.76	104.64

There are no chirality outliers.

5 of 68 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	5007	ADP	PA-O3A-PB-O3B
7	C	5027	ADP	PA-O3A-PB-O3B

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Mol	Chain	Res	Type	Atoms
7	E	5047	ADP	PA-O3A-PB-O3B
8	A	5011	ORN	N-CA-CB-CG
8	A	5011	ORN	C-CA-CB-CG

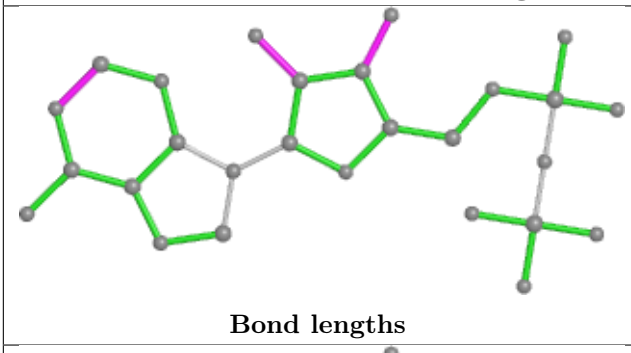
There are no ring outliers.

20 monomers are involved in 37 short contacts:

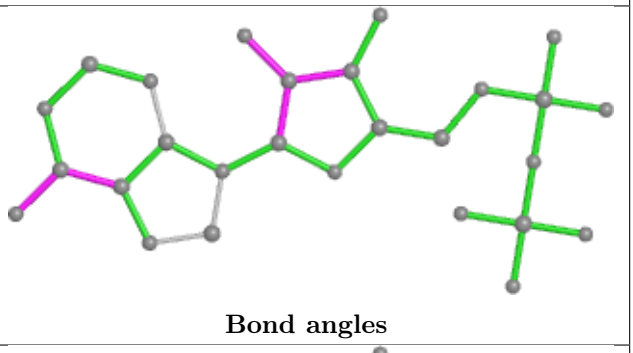
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	5027	ADP	1	0
8	E	5054	ORN	2	0
8	G	5074	ORN	3	0
10	G	5073	NET	1	0
7	G	5060	ADP	2	0
9	C	5032	IMP	1	0
9	E	5052	IMP	2	0
8	A	5014	ORN	3	0
8	A	5011	ORN	1	0
7	E	5047	ADP	4	0
10	E	5053	NET	3	0
9	G	5072	IMP	1	0
7	A	5007	ADP	2	0
8	C	5034	ORN	1	0
8	G	5071	ORN	1	0
9	A	5012	IMP	1	0
7	G	5067	ADP	3	0
8	E	5051	ORN	2	0
7	E	5040	ADP	1	0
8	C	5031	ORN	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 then 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.

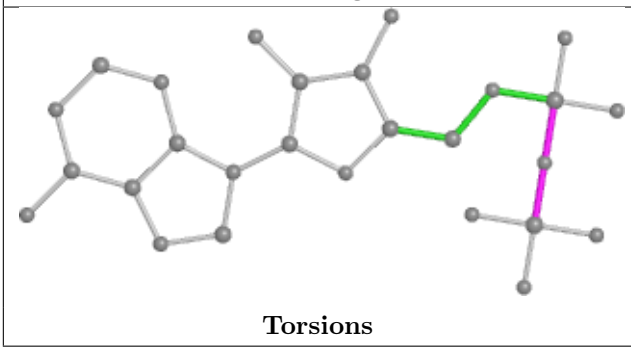
Ligand ADP C 5027



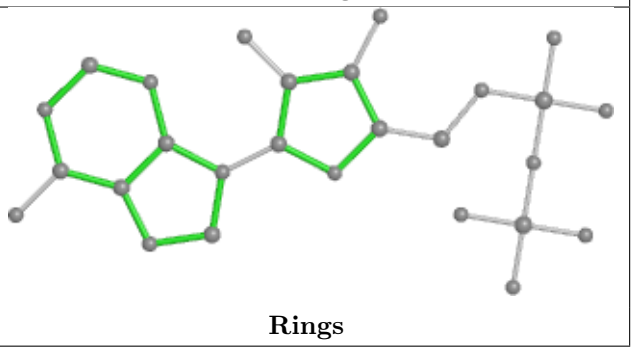
Bond lengths



Bond angles

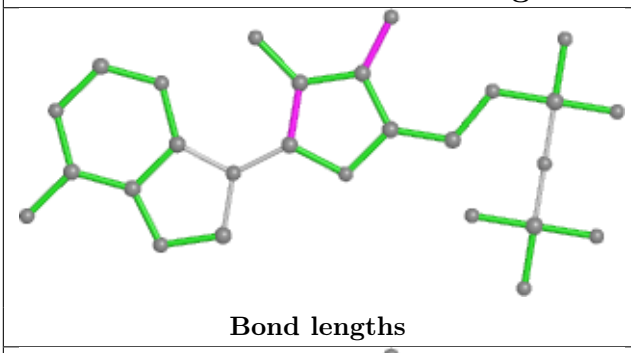


Torsions



Rings

Ligand ADP G 5060



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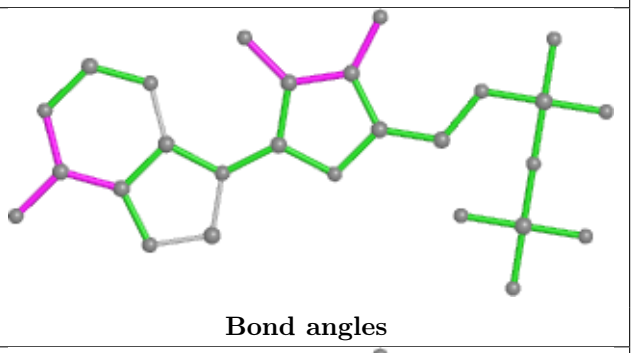

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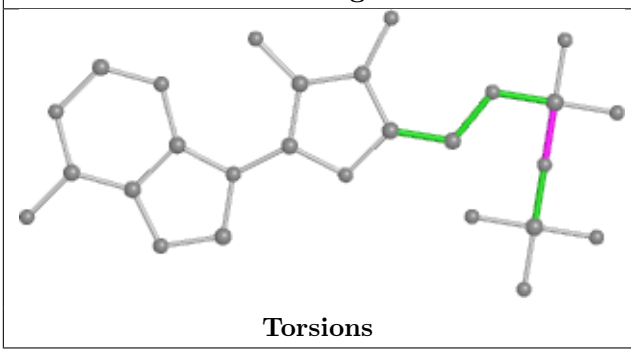

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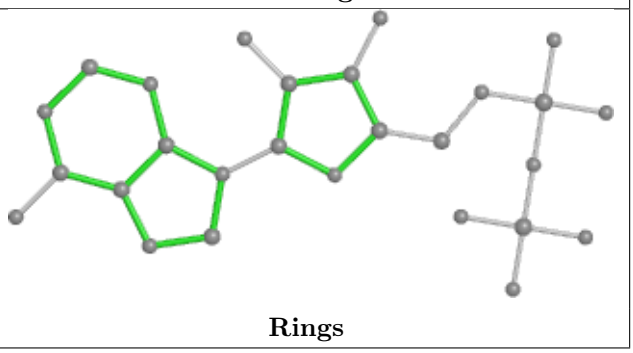
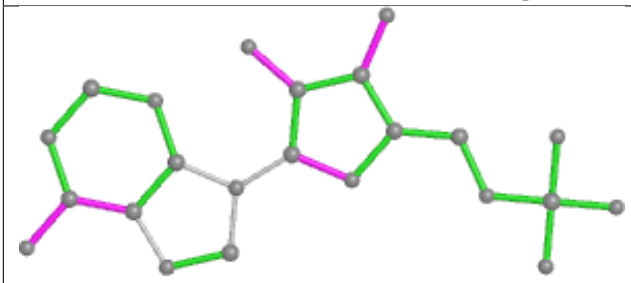
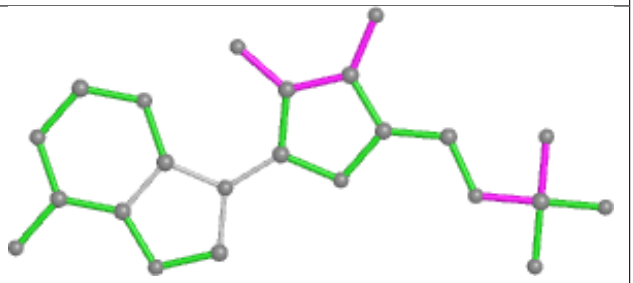


Rings

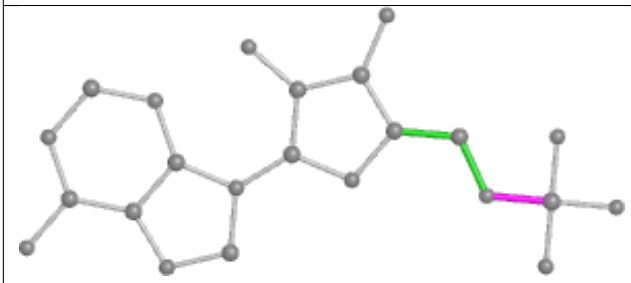
Ligand IMP C 5032



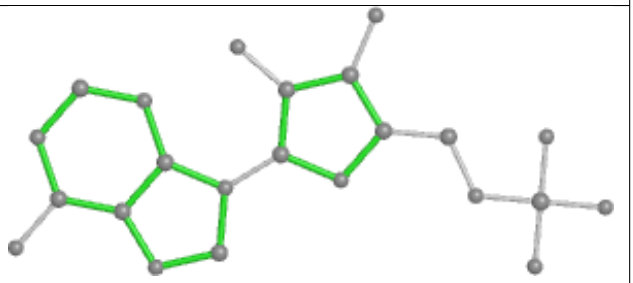
Bond lengths



Bond angles

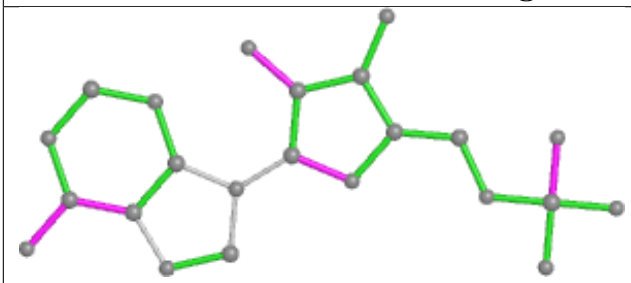


Torsions

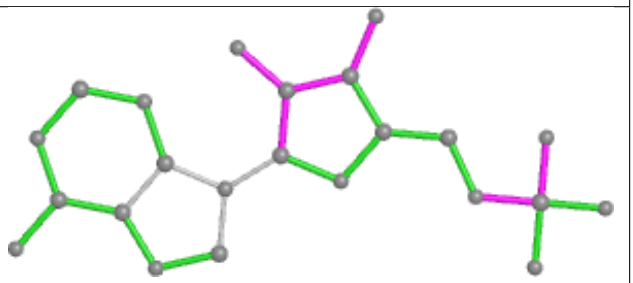


Rings

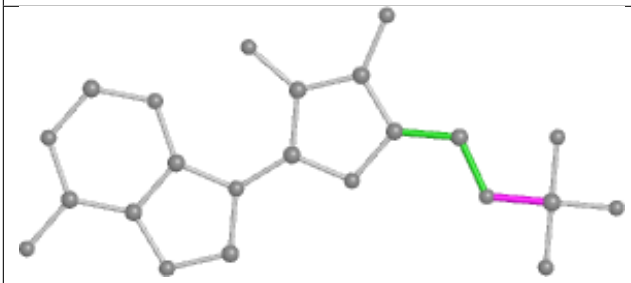
Ligand IMP E 5052



Bond lengths



Bond angles



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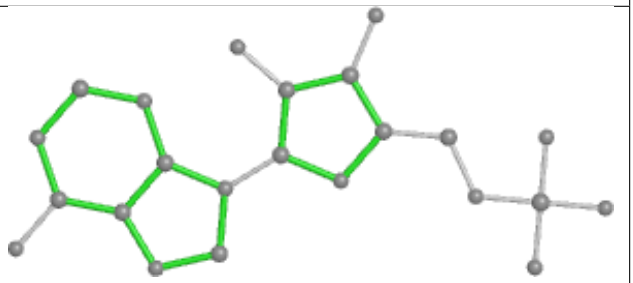
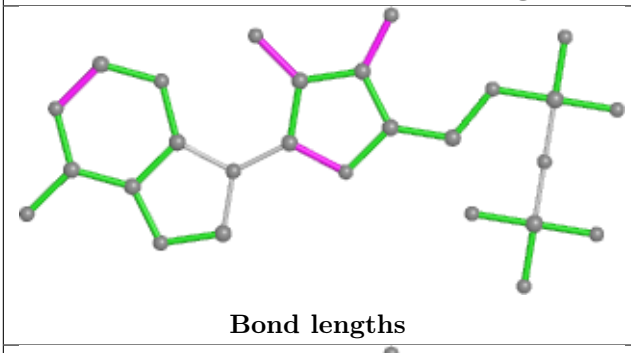
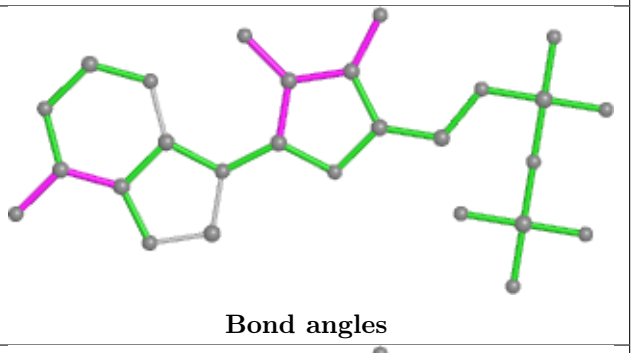


Rings

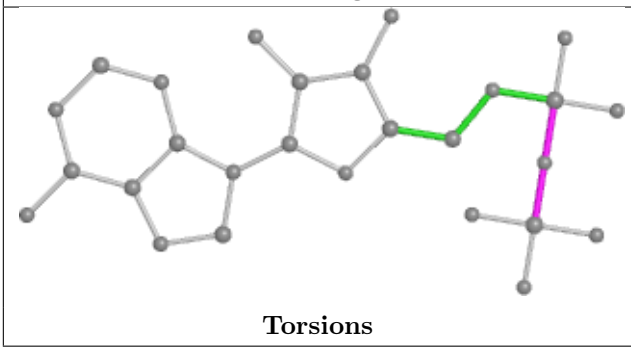
Ligand ADP E 5047



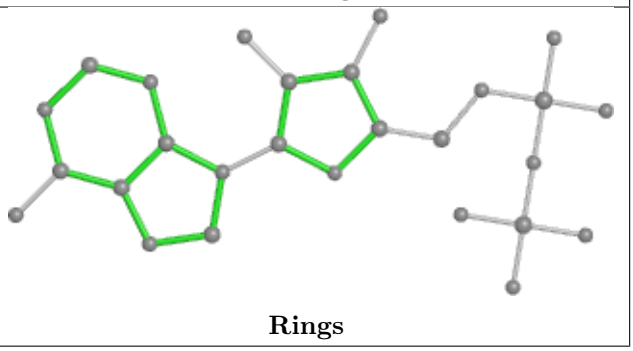
Bond lengths



Bond angles

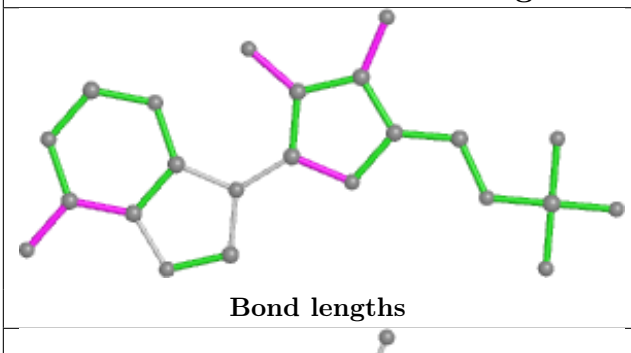


Torsions

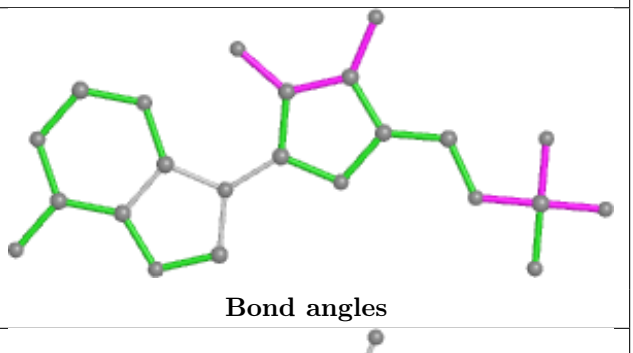


Rings

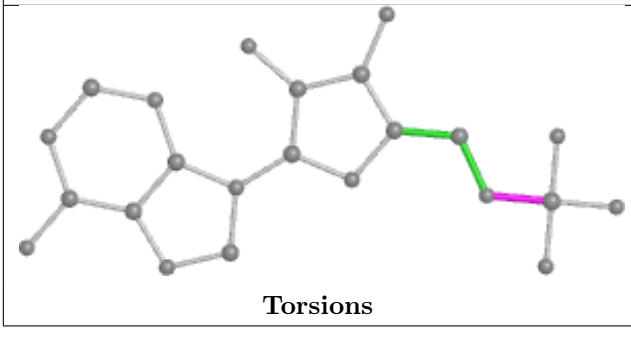
Ligand IMP G 5072



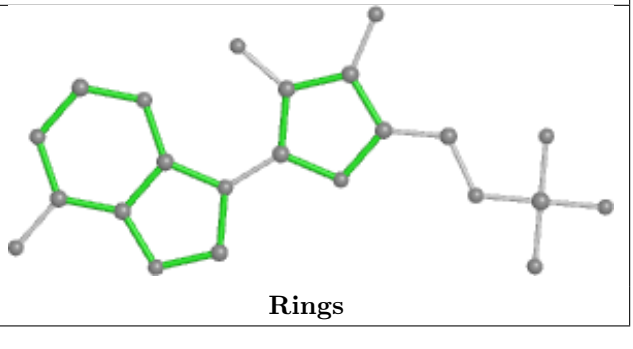
Bond lengths



Bond angles

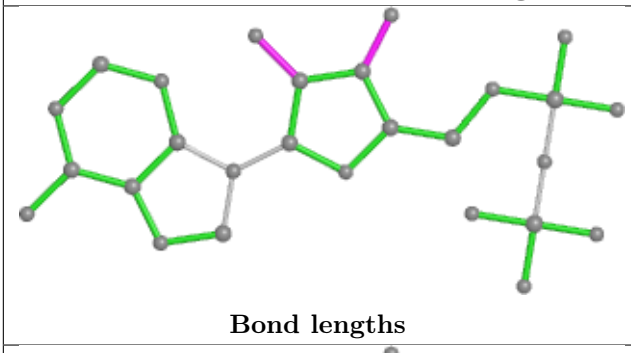


Torsions

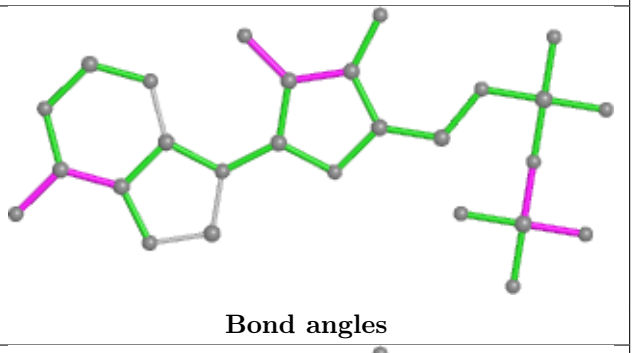


Rings

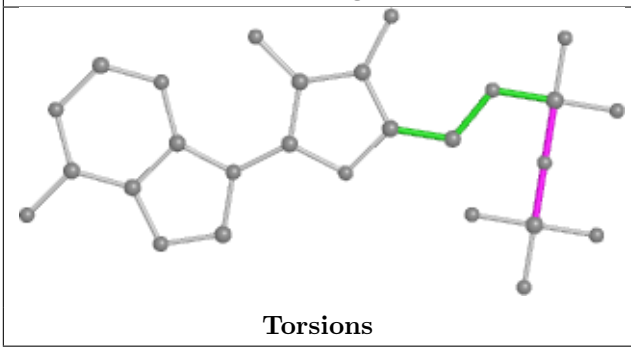
Ligand ADP A 5007



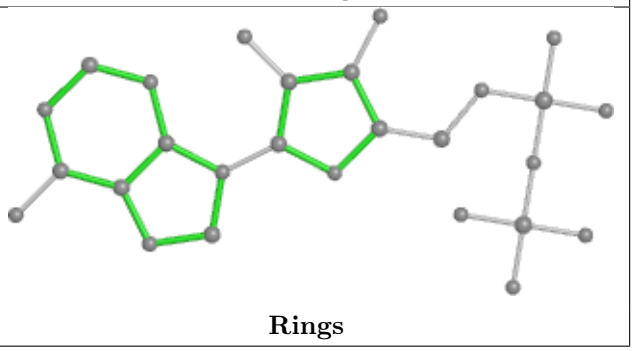
Bond lengths



Bond angles

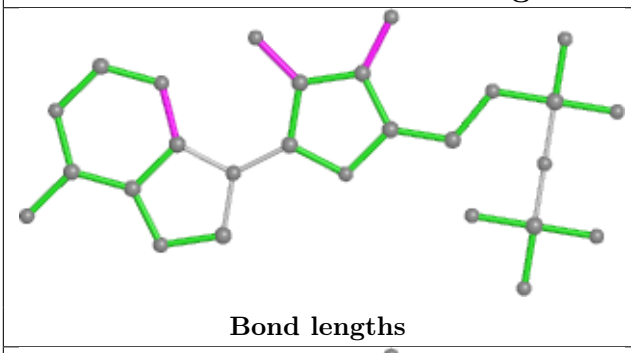


Torsions

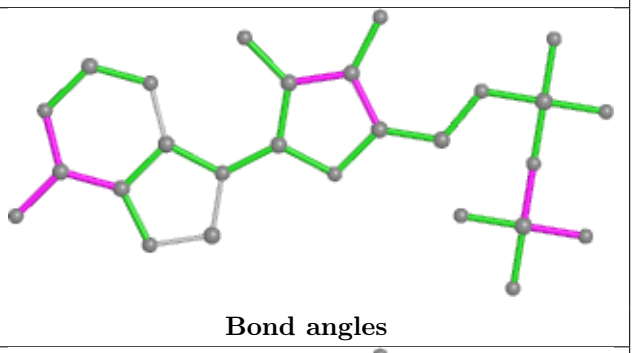


Rings

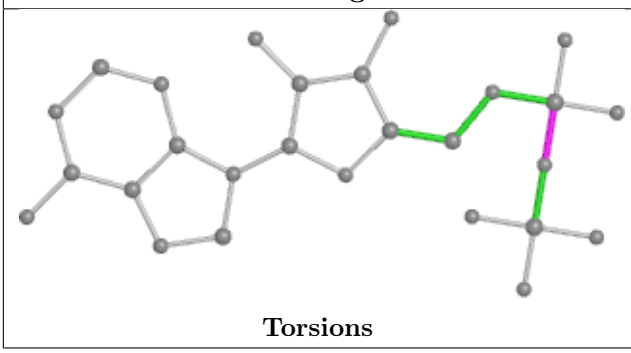
Ligand ADP A 5000



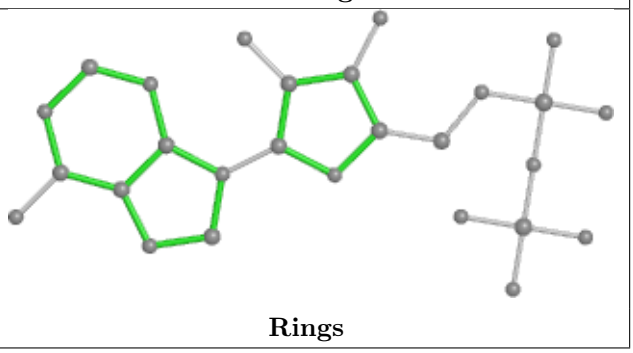
Bond lengths



Bond angles

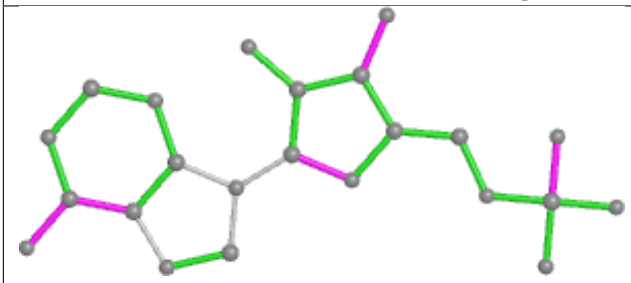


Torsions

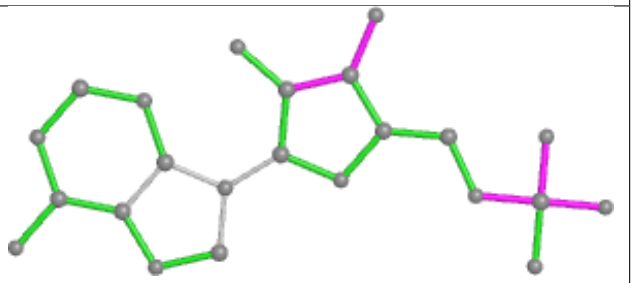


Rings

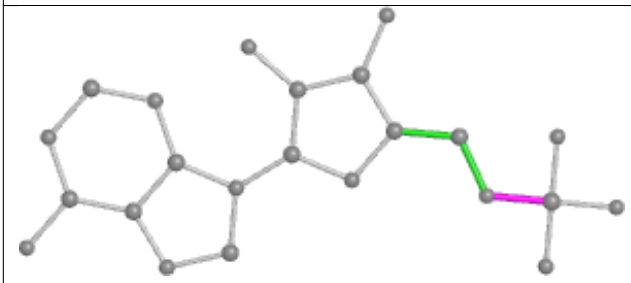
Ligand IMP A 5012



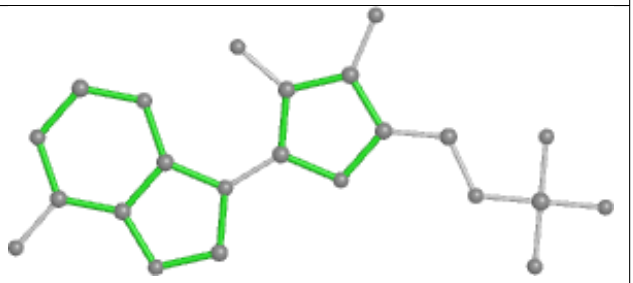
Bond lengths



Bond angles

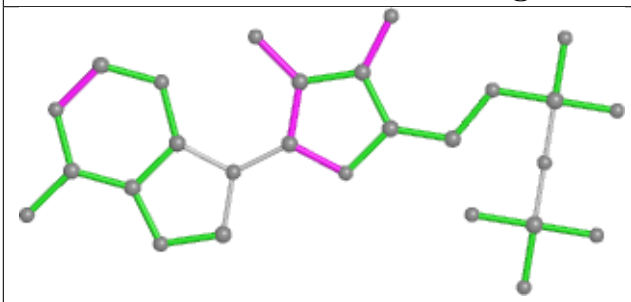


Torsions

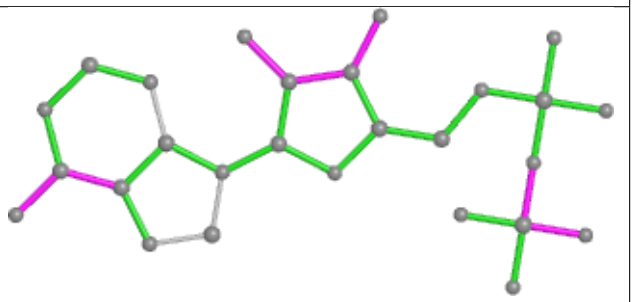


Rings

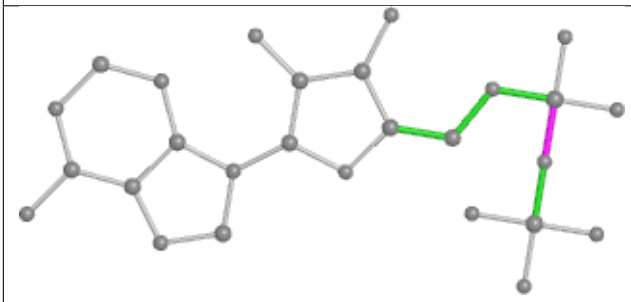
Ligand ADP G 5067



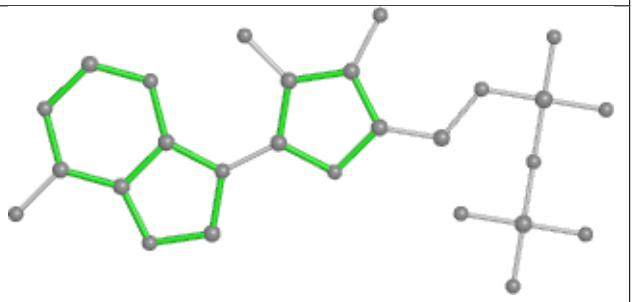
Bond lengths



Bond angles

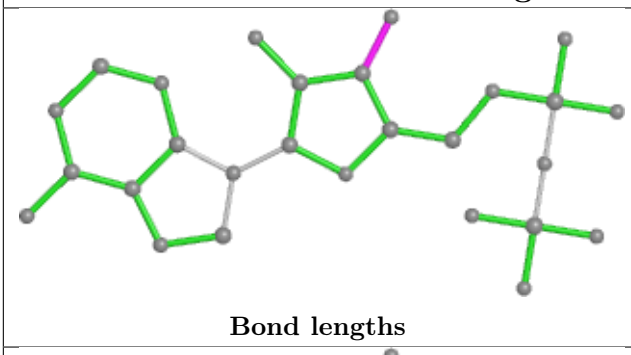


Torsions

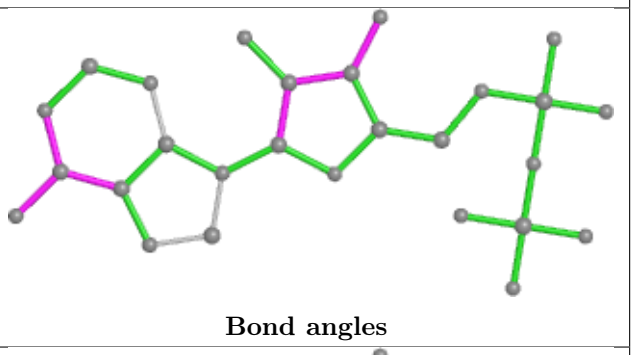


Rings

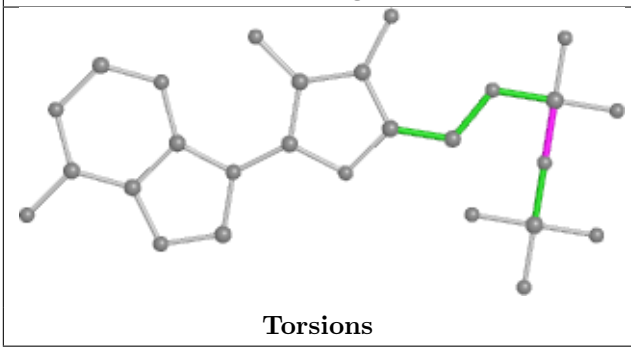
Ligand ADP E 5040



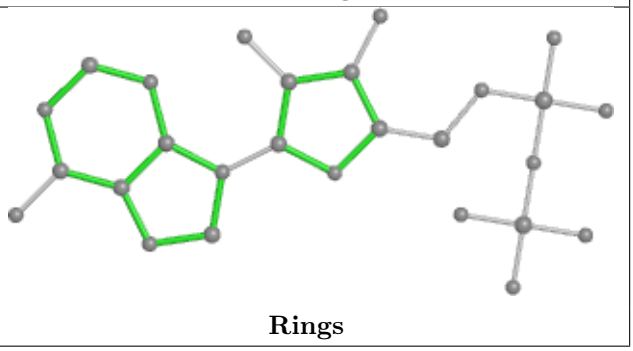
Bond lengths



Bond angles

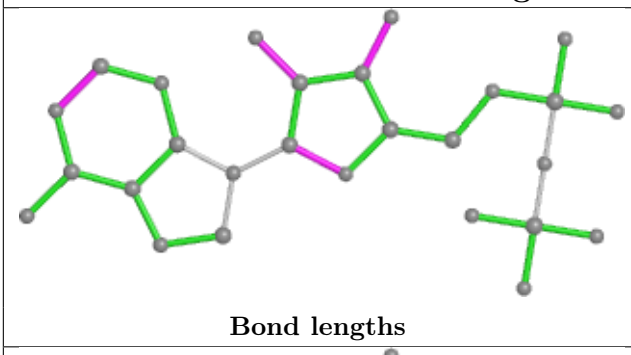


Torsions

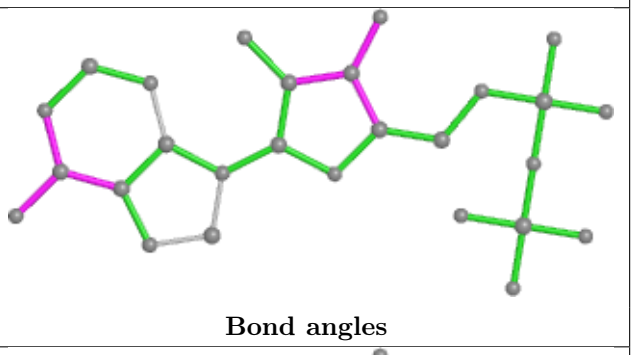


Rings

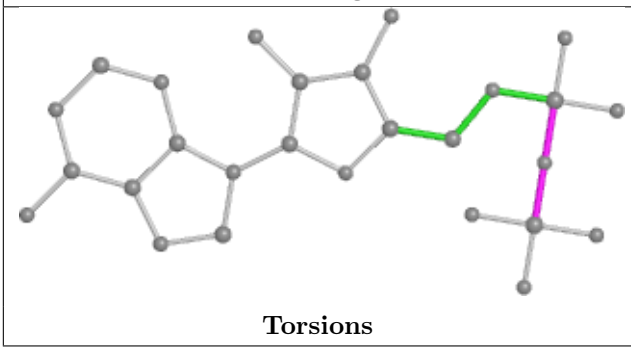
Ligand ADP C 5020



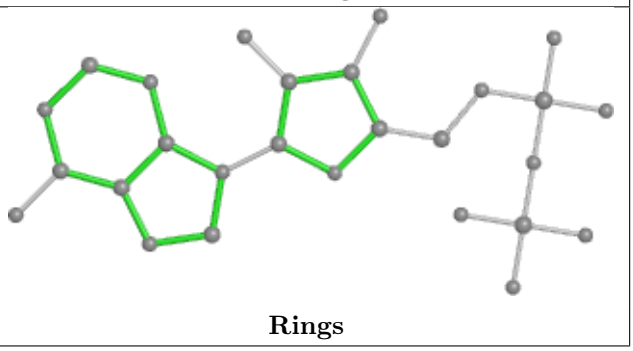
Bond lengths



Bond angles



Torsions



Rings

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.