wwPDB X-ray Structure Validation Summary Report (i)

Jan 27, 2024 – 02:28 PM EST

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

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

We welcome your comments at *validation@mail.wwpdb.org*
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:

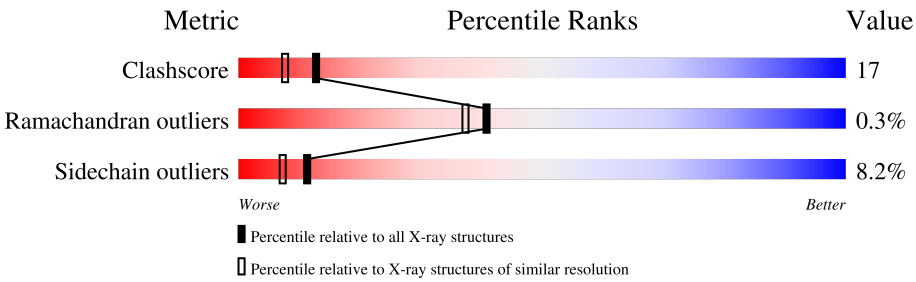
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.00 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=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	61% 30% 7% ••
1	C	1073	59% 31% 7% ••
1	E	1073	64% 28% 7% •
1	G	1073	52% 38% 8% ••
2	B	382	58% 35% 6% •
2	D	382	57% 35% 6% ••
2	F	382	53% 38% 8% •
2	H	382	45% 45% 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
6	PO4	C	4025	-	X	-	-

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 48668 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called CARBAMOYL PHOSPHATE SYNTHETASE: LARGE SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1058	8189	5141	1429	1574	45	0	6	0
1	C	1058	8165	5126	1422	1572	45	0	1	0
1	E	1058	8188	5141	1426	1575	46	0	6	0
1	G	1058	8178	5137	1424	1572	45	0	4	0

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

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

There are 4 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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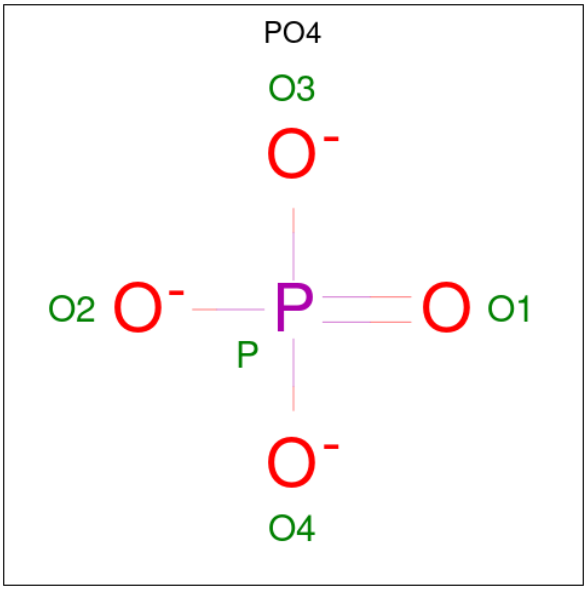
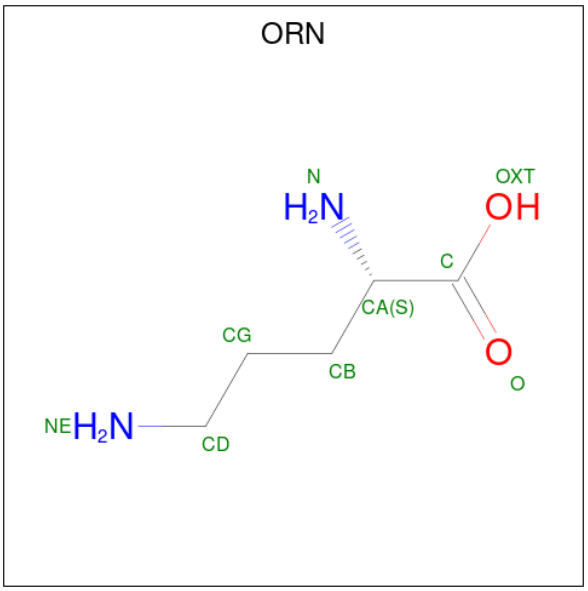
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
5	G	3	3	3	0	0
			Total	Cl		
5	H	1	1	1	0	0

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



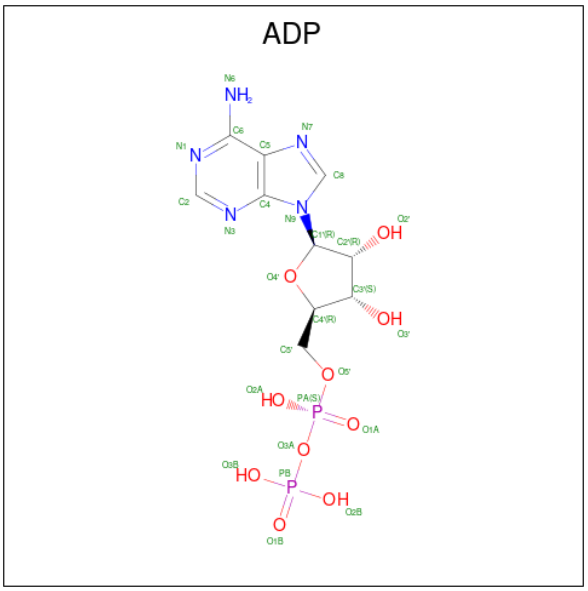
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
6	A	1	5	4	1	0	0
			Total	O	P		
6	C	1	5	4	1	0	0
			Total	O	P		
6	C	1	5	4	1	0	0
			Total	O	P		
6	E	1	5	4	1	0	0
			Total	O	P		
6	E	1	5	4	1	0	0
			Total	O	P		
6	G	1	5	4	1	0	0

- Molecule 7 is L-ornithine (three-letter code: ORN) (formula: $C_5H_{12}N_2O_2$).



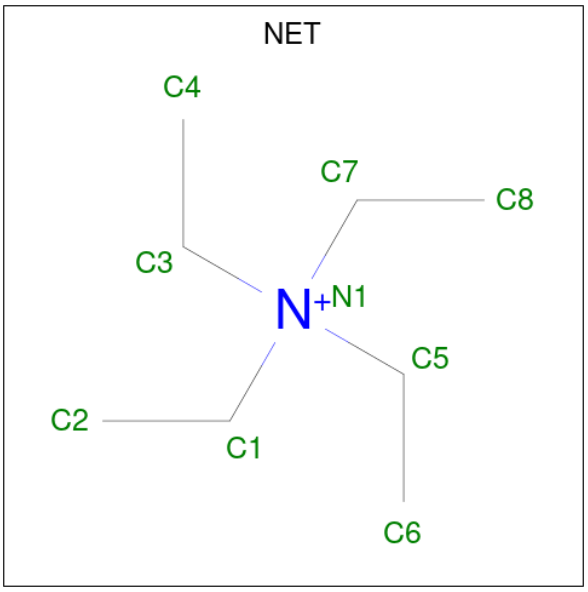
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
7	A	1	9	5	2	2	0	0
			Total	C	N	O		
7	A	1	8	5	2	1	0	0
			Total	C	N	O		
7	A	1	8	5	2	1	0	0
			Total	C	N	O		
7	A	1	9	5	2	2	0	0

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

- Molecule 9 is TETRAETHYLAMMONIUM ION (three-letter code: NET) (formula: $C_8H_{20}N$).



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

- Molecule 10 is water.

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

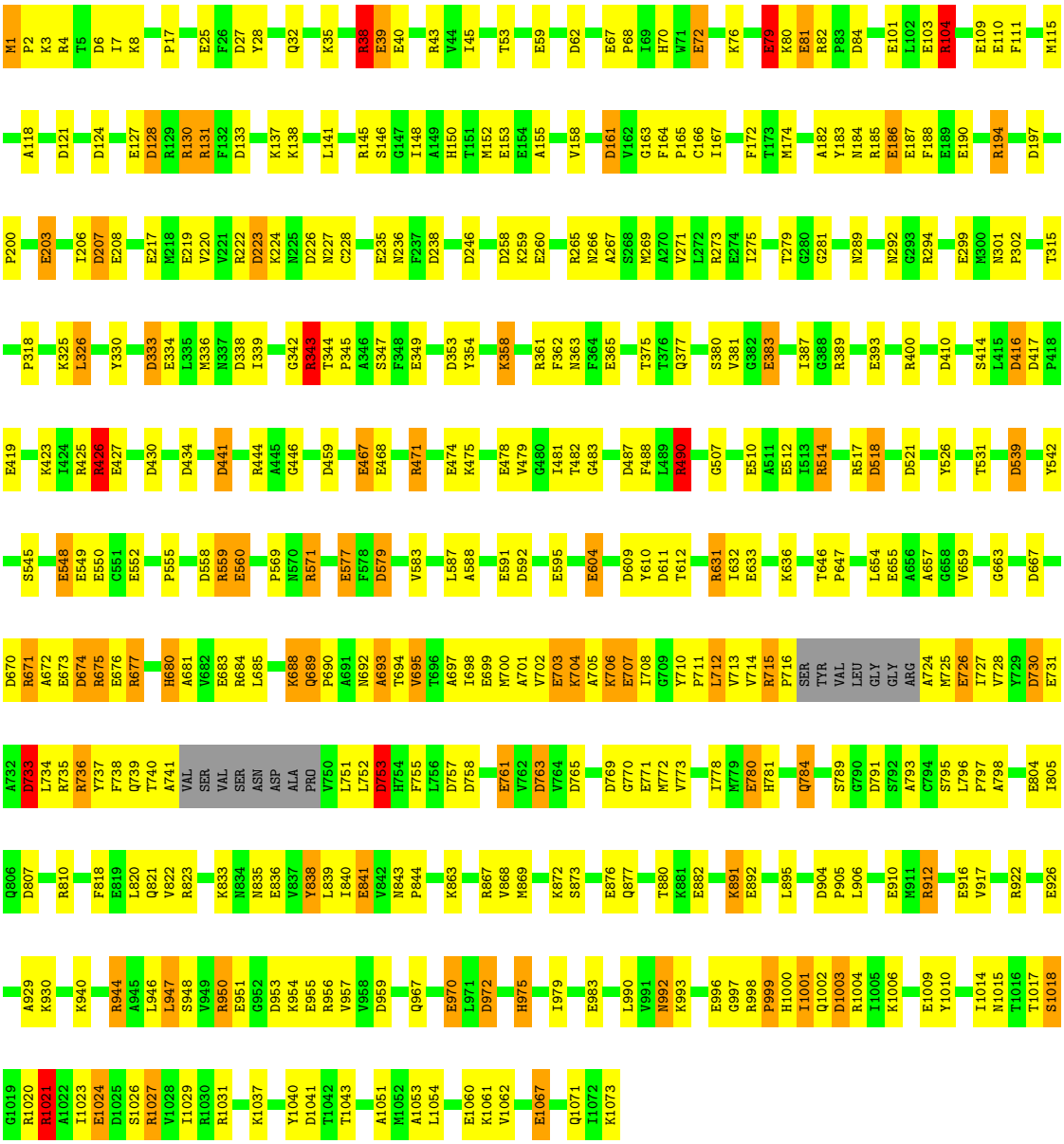
3 Residue-property plots (i)

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: CARBAMOYL PHOSPHATE SYNTHETASE: LARGE SUBUNIT

Chain A: 61% 30% 7% ••



• Molecule 1: CARBAMOYL PHOSPHATE SYNTHETASE: LARGE SUBUNIT

Chain C: 59% 31% 7% ••

M1 P2 K3 D6 I7 K8 S9 I10 L11 I12 P17 C24 E25 F26 D27 Y28 Q32 L37 R38 E39 E40 G41 Y42 R43 V44 I45 N48 P51 M55 T56 D57 P58 E59 M60 A61 D62 A63 T64 Y65 I66 E67 P68 I69 E72 V73 V74 R75 K76 I77 I78 E79

K80 E81 R82 P83 D84 L102 E103 R104 V107 L108 E109 E110 F111 D121 D124 K125 A126 E127 D128 R129 R130 R131 F132 D133 E142 R145 S146 H150 E153 E154 A159 A160 D161 P165 C166 I167 I168 R169 F172 T173 M174 A182 Y183 N184 R185 E186 E187 F188

E189 E190 R194 G195 L196 D197 K202 E203 L204 L205 I206 D207 E208 W213 E217 M218 E219 R222 D223 D226 S233 N236 F237 D238 I248 T249 V250 L256 T257 D258 K259 E260 R265 N266 A267 V271 E278 N289 N292 G293 R294 I298 E299

P302 K313 A320 K321 K325 Y330 T331 L332 D333 E334 L335 M336 N337 D338 I339 T340 G341 G342 R343 T344 P345 A346 S347 F348 E349 V356 T357 K358 N363 F364 E365 A368 D372 T375 T376 Q377 E383 R400 E403 K412 V413 S414 L415 D416 E419

R426 E427 D430 D434 R435 D441 I458 D459 R460 W461 E467 E468 L469 V470 R471 L472 E473 E474 E478 T482 D487 R490 Q491 L492 K493 R494 K495 D499 A503 R509 E510 A511 E512 I513 R514 D518 D521 L522 K527 R528 V529 D530 A534 E535

D539 Y542 M543 Y544 E548 E549 E550 N554 P555 S556 T557 D558 R559 E560 K561 I562 M563 R571 I576 E577 E578 D579 Y580 R590 E591 D592 E595 D609 Y610 D611 D614 L623 E624 D625 R631 I632 E633 K634 P635 I639 G644 Q645 T646 P647 L648

R652 A653 L654 E655 S665 P666 D667 A668 I669 D670 R671 A672 E673 D674 R675 E676 R677 F678 Q679 H680 E683 R684 L685 K686 L687 P690 A691 N692 A693 T694 V695 T696 A697 I698 E699 M700 A701 V702 E703 K704 A705 K706 E707 I708 P711 L712 V713 V714 R715 P716 SER TYR VAL LEU GLY GLY

ARG A724 M725 E726 I727 V728 Y729 D730 E731 A732 D733 L734 R735 R736 Y737 F738 A741 VAL SER VAL SER ASN ASP ALA PRO V750 L751 L752 D753 H754 F755 L756 D757 D758 E761 V762 D763 V764 D765 A766 I767 C768 D769 G770 E771 M772 V773 L774 I775 E780 H781 Q784 V787 D791

S795 T800 L801 S802 Q803 E804 I805 Q806 D807 R810 Q811 Q812 V813 Q814 K815 L816 A817 F818 E819 R823 N827 N835 E836 E841 P844 R845 R848 T849 S854 K855 V859 A865 A866 R867 V868 M869 K872 S873 E876 Q877 T880 K881 E882 V883 I884

S889 V890 K891 E892 V893 G902 V903 D904 P905 L906 L907 G908 P909 E910 M911 R912 E916 V917 G921 R922 T923 E926 A927 F928 A929 K930 A931 Q932 N936 S937 H942 G943 L947 R950 E951 G952 D953 K954 E955 R956 V957 V958 D959 A962 Q967 E970 L971 D972

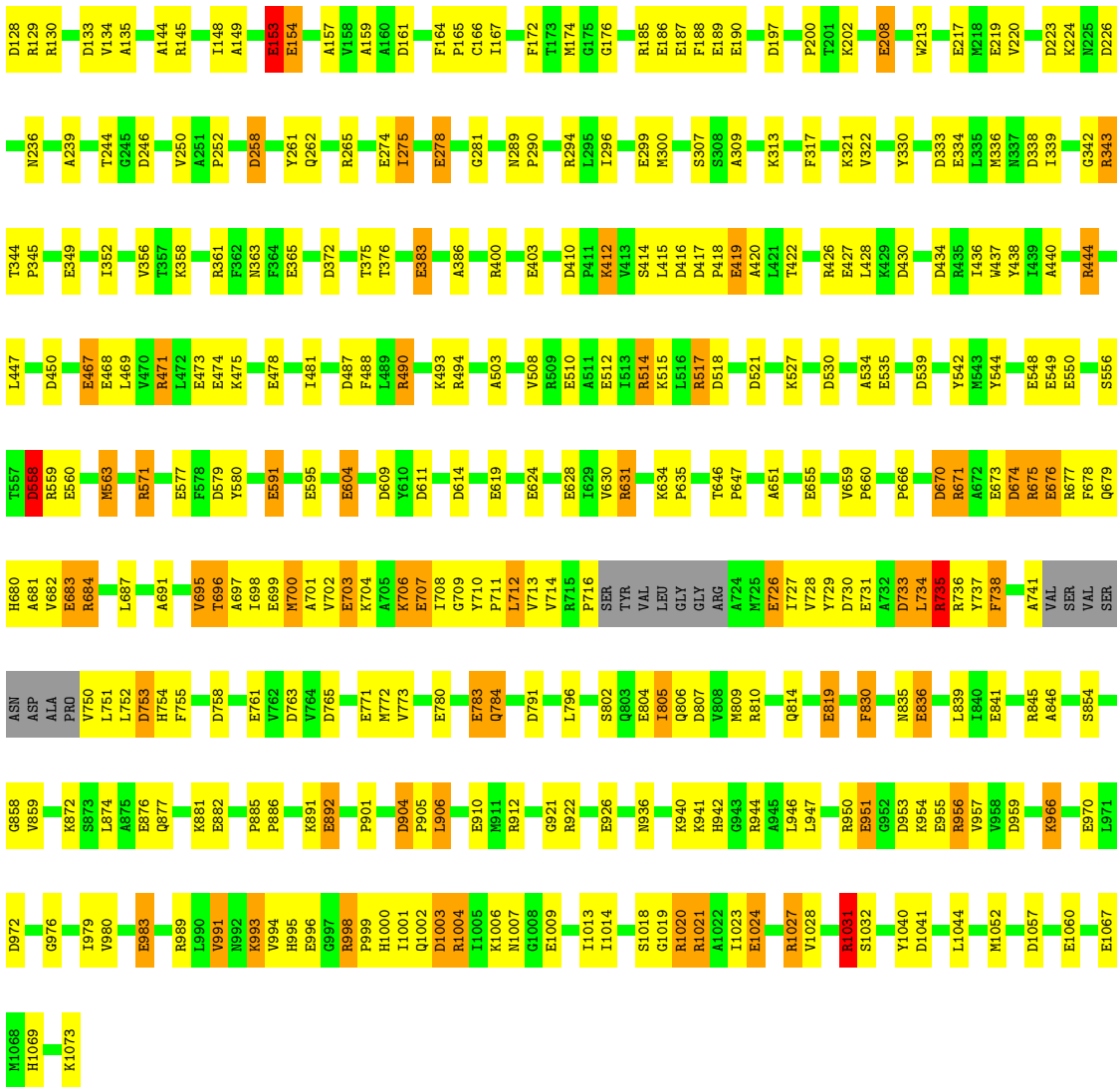
H975 V980 E983 I986 N987 P988 R989 L990 V991 N992 K993 V994 H995 E996 G997 R998 P999 H1000 D1003 N1007 G1008 E1009 I1014 N1015 T1016 T1017 S1018 G1019 R1020 R1021 A1022 I1023 E1024 D1025 S1026 R1027 R1031 Y1036 K1037 D1041 T1042 T1043 L1044 F1048 M1052 A1053 L1054

D1057 E1060 K1061 V1062 I1063 S1064 V1065 Q1066 E1067 M1068 K1073

• Molecule 1: CARBAMOYL PHOSPHATE SYNTHETASE: LARGE SUBUNIT

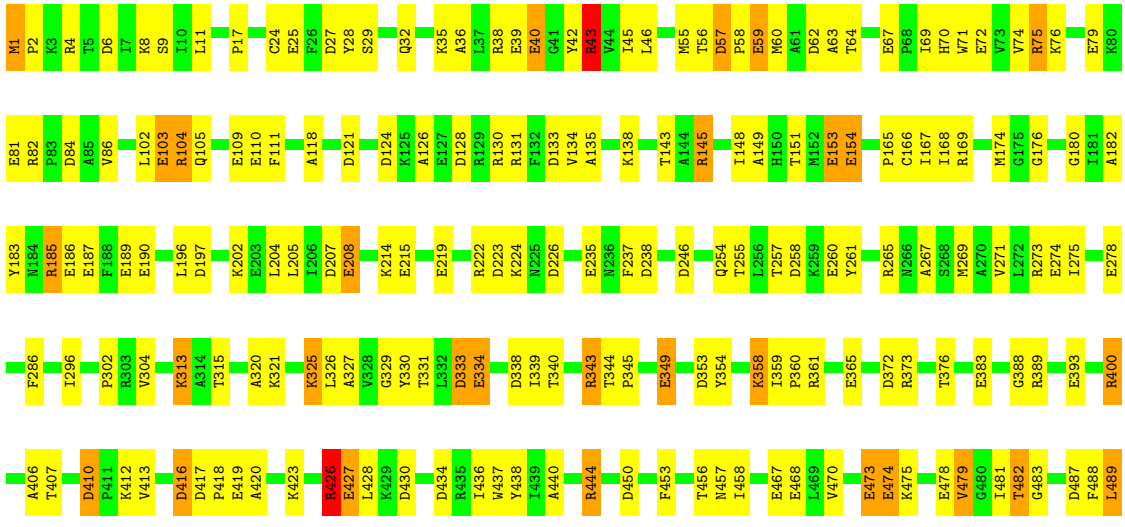
Chain E: 64% 28% 7% •

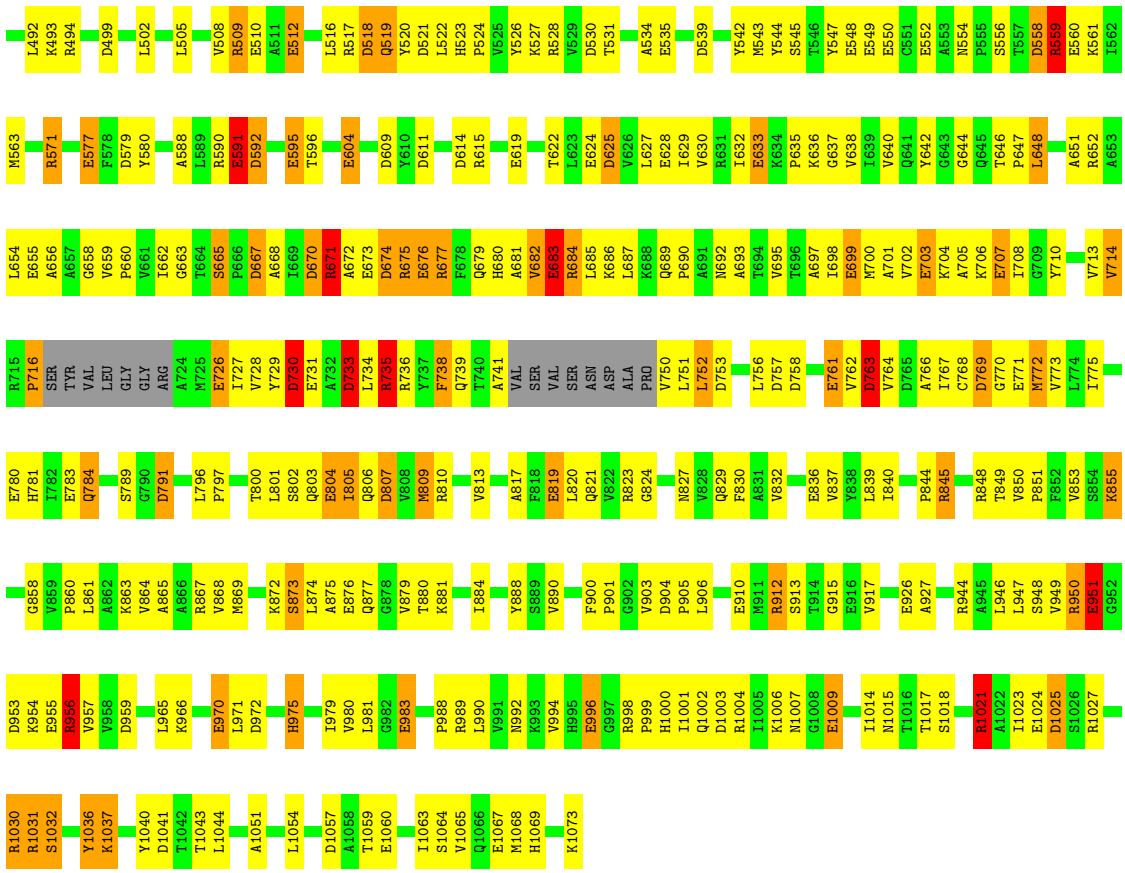
M1 P2 K3 R4 T5 D6 I7 K8 I18 A23 C24 E25 F26 D27 Q32 R38 E39 Y42 R43 L46 T53 E59 M60 A61 D62 E67 E72 K76 E81 R82 P83 D84 E101 L102 E103 R104 E109 E110 M115 D121 K125 A126 E127



- Molecule 1: CARBAMOYL PHOSPHATE SYNTHETASE: LARGE SUBUNIT

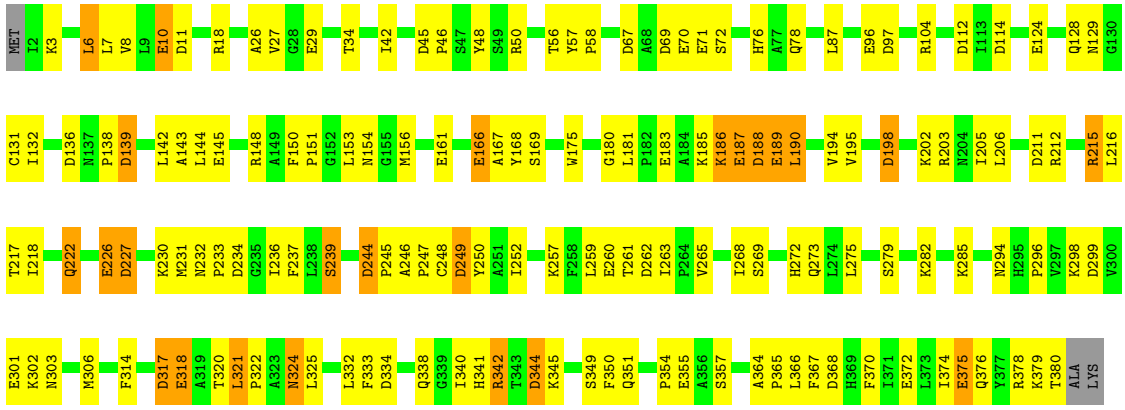
Chain G:





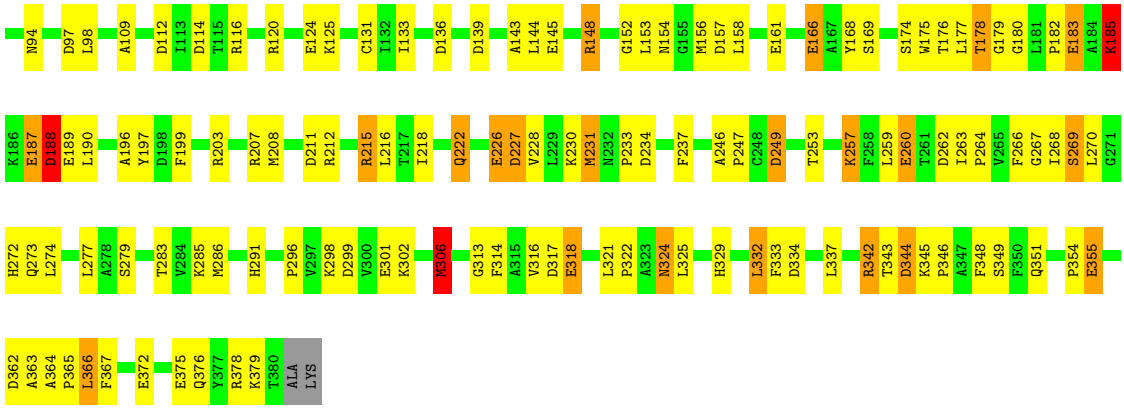
- Molecule 2: CARBAMOYL PHOSPHATE SYNTHETASE: SMALL SUBUNIT

Chain B:



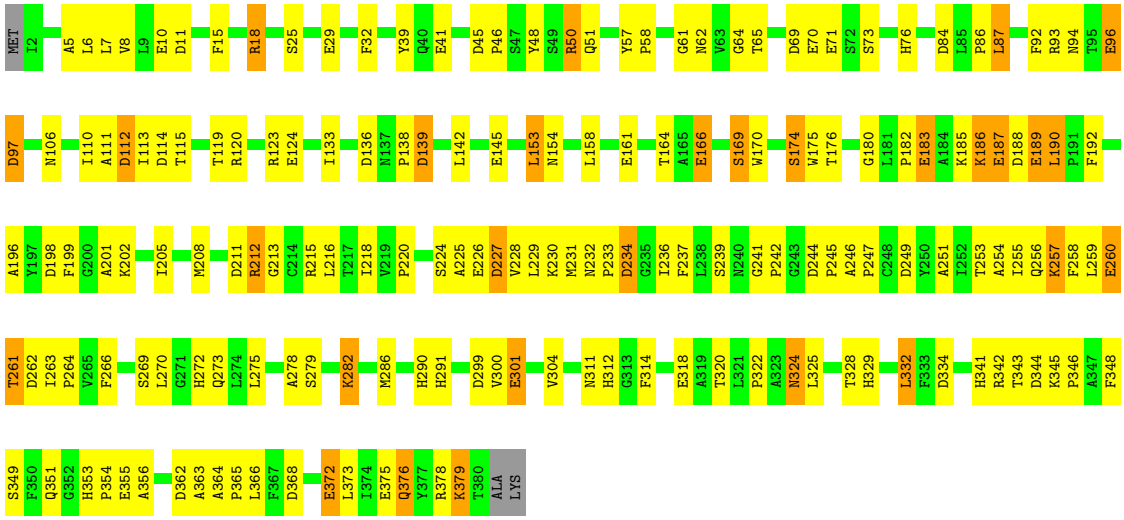
- Molecule 2: CARBAMOYL PHOSPHATE SYNTHETASE: SMALL SUBUNIT

Chain D:



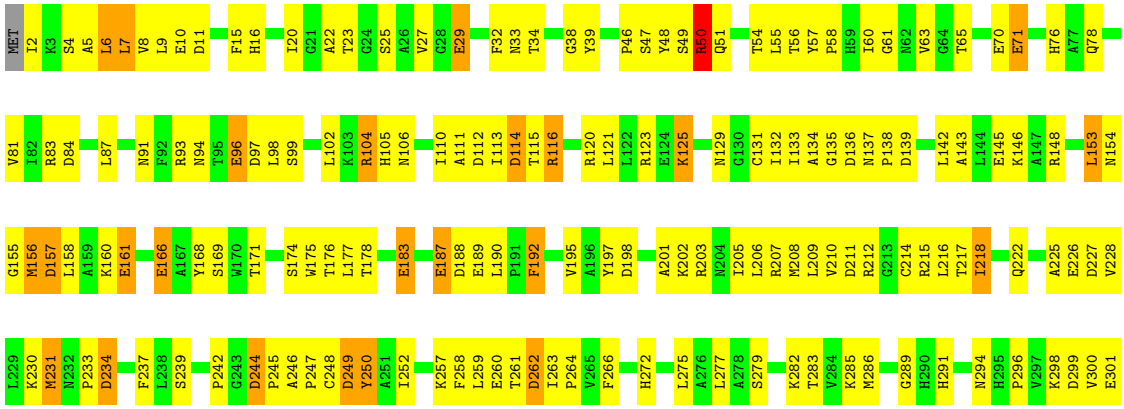
• Molecule 2: CARBAMOYL PHOSPHATE SYNTHETASE: SMALL SUBUNIT

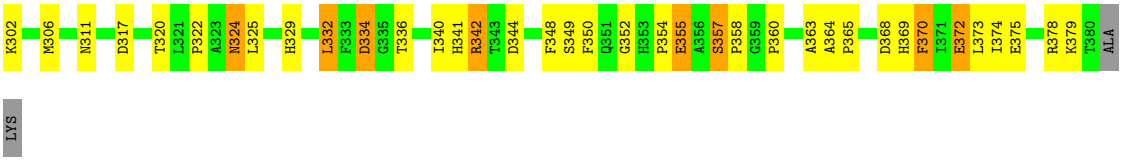
Chain F: 53% 38% 8% •



• Molecule 2: CARBAMOYL PHOSPHATE SYNTHETASE: SMALL SUBUNIT

Chain H: 45% 45% 8% •




K302
M306
N311
D317
T320
L321
P322
A323
N324
L325
H329
L332
F333
D334
G335
T336
I340
H341
R342
T343
D344
F348
S349
F350
Q351
G352
H353
P354
E355
A356
S357
P358
G359
P360
A363
A364
P365
D368
H369
F370
I371
E372
L373
I374
E375
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	152.60Å 164.60Å 332.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.00	Depositor
% Data completeness (in resolution range)	97.7 (30.00-2.00)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT 5E	Depositor
R, R_{free}	0.189 , 0.246	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	48668	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.02	75/8339 (0.9%)	1.40	124/11273 (1.1%)
1	C	1.05	77/8295 (0.9%)	1.45	145/11214 (1.3%)
1	E	1.05	77/8338 (0.9%)	1.40	116/11270 (1.0%)
1	G	1.00	72/8320 (0.9%)	1.44	131/11246 (1.2%)
2	B	0.90	19/2957 (0.6%)	1.29	37/4016 (0.9%)
2	D	0.97	18/2957 (0.6%)	1.36	36/4016 (0.9%)
2	F	0.93	20/2957 (0.7%)	1.35	40/4016 (1.0%)
2	H	0.93	18/2966 (0.6%)	1.36	35/4028 (0.9%)
All	All	1.01	376/45129 (0.8%)	1.40	664/61079 (1.1%)

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

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

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

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

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

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

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

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

The worst 5 of 1483 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:993:LYS:CE	1:E:993:LYS:NZ	1.67	1.55
1:G:695:VAL:HG11	1:G:701:ALA:HB2	1.28	1.12
1:C:998:ARG:HG3	1:C:999:PRO:HA	1.30	1.11
1:C:695:VAL:HG11	1:C:701:ALA:HB2	1.34	1.09
2:H:187:GLU:HG2	2:H:215:ARG:HD2	1.31	1.07

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

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

5 of 17 Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

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

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

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

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

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

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 82 ligands modelled in this entry, 60 are monoatomic - leaving 22 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	ORN	A	4072	-	7,8,8	0.79	0	8,9,9	1.43	1 (12%)
6	PO4	C	4040	-	4,4,4	1.25	0	6,6,6	0.80	0
8	ADP	C	4026	4,3	24,29,29	1.08	3 (12%)	29,45,45	1.15	3 (10%)
9	NET	E	4052	-	8,8,8	0.67	0	10,10,10	0.62	0
6	PO4	A	4005	4,3	4,4,4	2.30	2 (50%)	6,6,6	1.25	0
9	NET	G	4073	-	8,8,8	0.78	0	10,10,10	0.42	0
8	ADP	E	4047	4,3	24,29,29	1.23	3 (12%)	29,45,45	1.09	3 (10%)
6	PO4	E	4046	4,3	4,4,4	2.02	2 (50%)	6,6,6	1.06	0
6	PO4	G	4067	4,3	4,4,4	2.31	2 (50%)	6,6,6	1.12	0
8	ADP	C	4020	3	24,29,29	1.20	2 (8%)	29,45,45	1.36	3 (10%)
7	ORN	A	4051	-	6,7,8	1.14	1 (16%)	2,7,9	0.41	0
6	PO4	E	4061	-	4,4,4	2.25	3 (75%)	6,6,6	0.91	0
8	ADP	G	4068	4,3	24,29,29	1.14	4 (16%)	29,45,45	1.27	4 (13%)
8	ADP	A	4000	3	24,29,29	1.12	3 (12%)	29,45,45	1.29	3 (10%)
8	ADP	E	4041	3	24,29,29	1.28	3 (12%)	29,45,45	1.42	5 (17%)
6	PO4	C	4025	4,3	4,4,4	2.35	4 (100%)	6,6,6	1.10	0
8	ADP	G	4062	3	24,29,29	1.08	2 (8%)	29,45,45	1.13	3 (10%)
7	ORN	A	4030	-	6,7,8	1.04	1 (16%)	2,7,9	0.93	0
7	ORN	A	4010	-	7,8,8	1.01	1 (14%)	8,9,9	1.52	2 (25%)
9	NET	C	4031	-	8,8,8	0.55	0	10,10,10	0.50	0
8	ADP	A	4006	4,3	24,29,29	1.09	1 (4%)	29,45,45	1.39	4 (13%)
9	NET	A	4011	-	8,8,8	0.67	0	10,10,10	0.56	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	ADP	G	4068	4,3	-	3/12/32/32	0/3/3/3
7	ORN	A	4072	-	-	6/8/8/8	-
8	ADP	A	4000	3	-	0/12/32/32	0/3/3/3
8	ADP	E	4041	3	-	1/12/32/32	0/3/3/3

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

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

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

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

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

There are no chirality outliers.

5 of 34 torsion outliers are listed below:

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

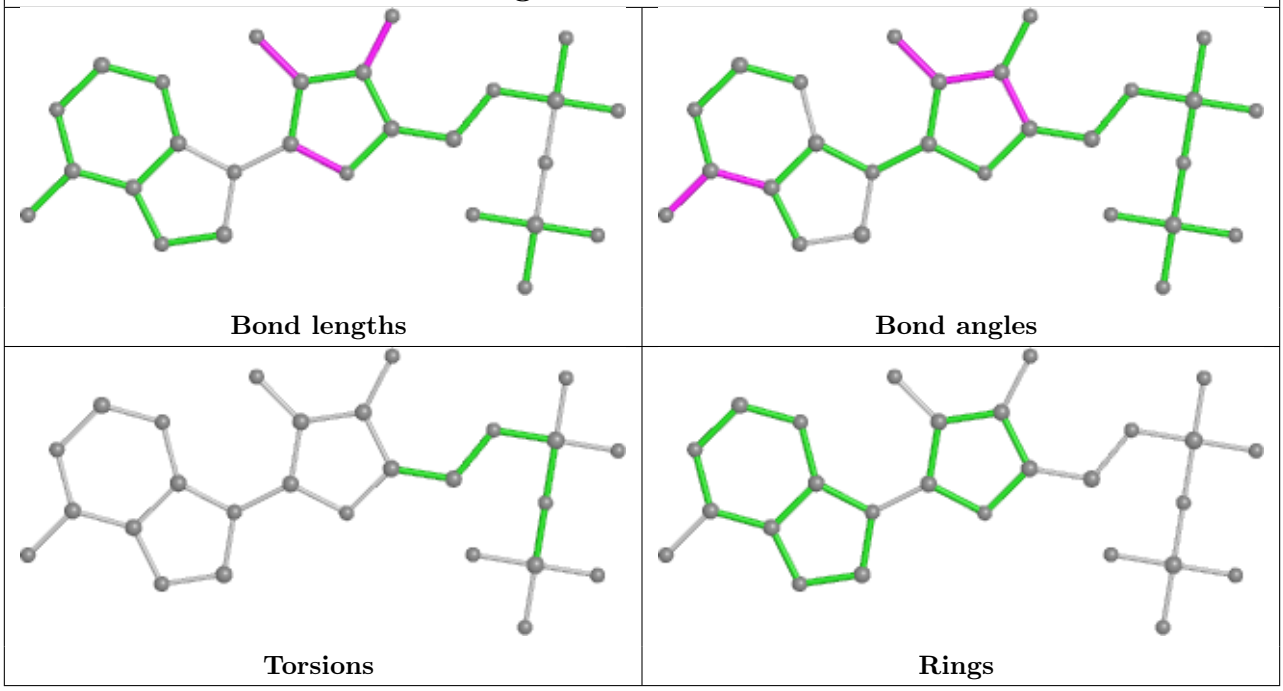
There are no ring outliers.

8 monomers are involved in 10 short contacts:

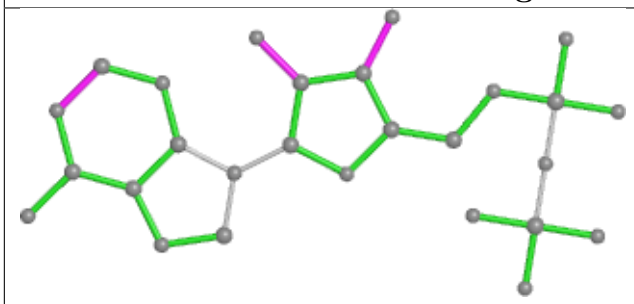
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	E	4047	ADP	2	0
7	A	4051	ORN	1	0
8	A	4000	ADP	1	0
8	E	4041	ADP	2	0
6	C	4025	PO4	1	0
8	G	4062	ADP	1	0
7	A	4030	ORN	1	0
8	A	4006	ADP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

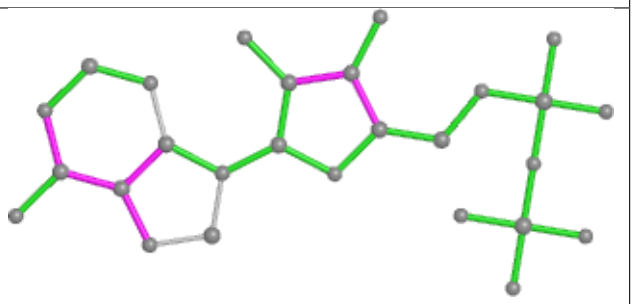
Ligand ADP C 4026



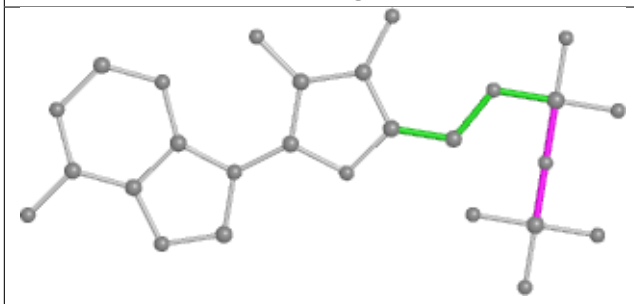
Ligand ADP E 4047



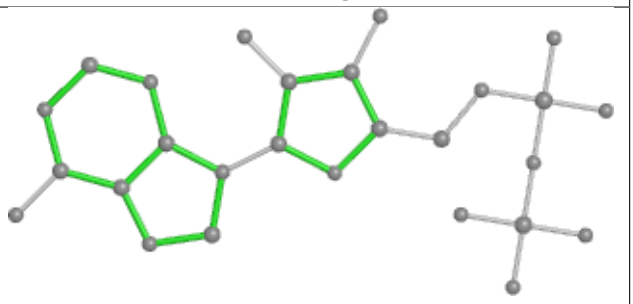
Bond lengths



Bond angles

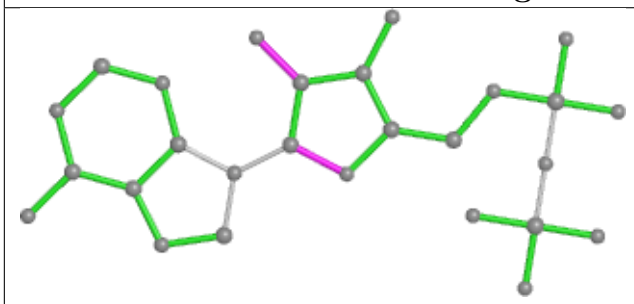


Torsions

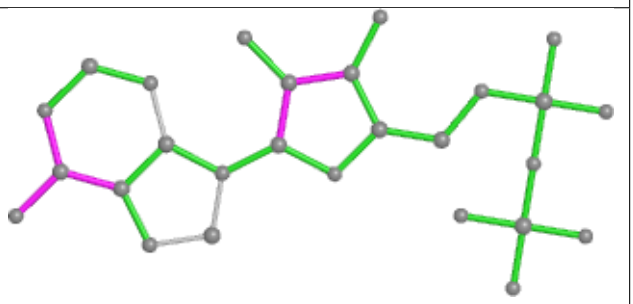


Rings

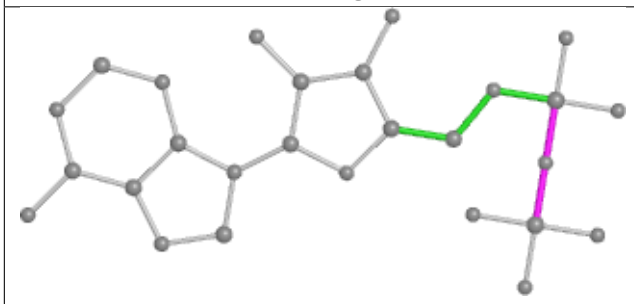
Ligand ADP C 4020



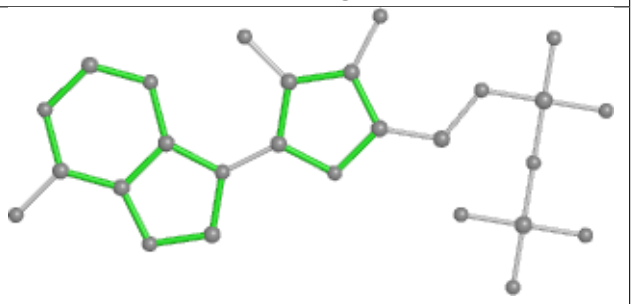
Bond lengths



Bond angles

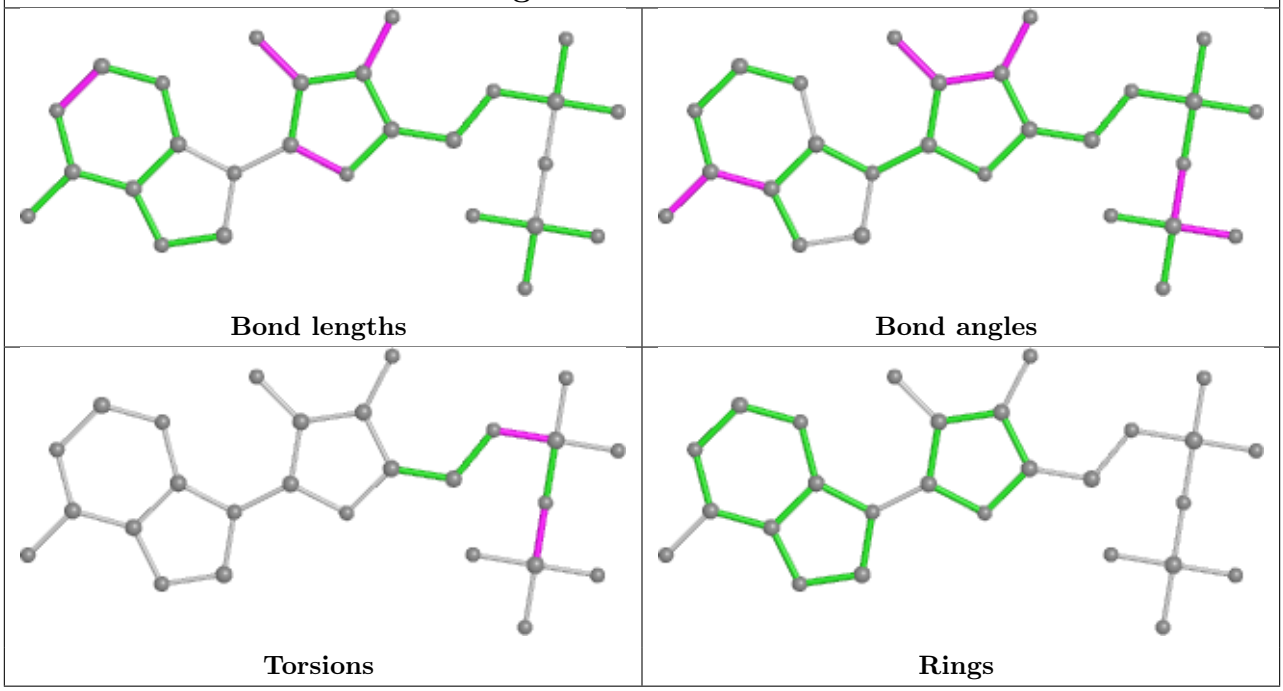


Torsions

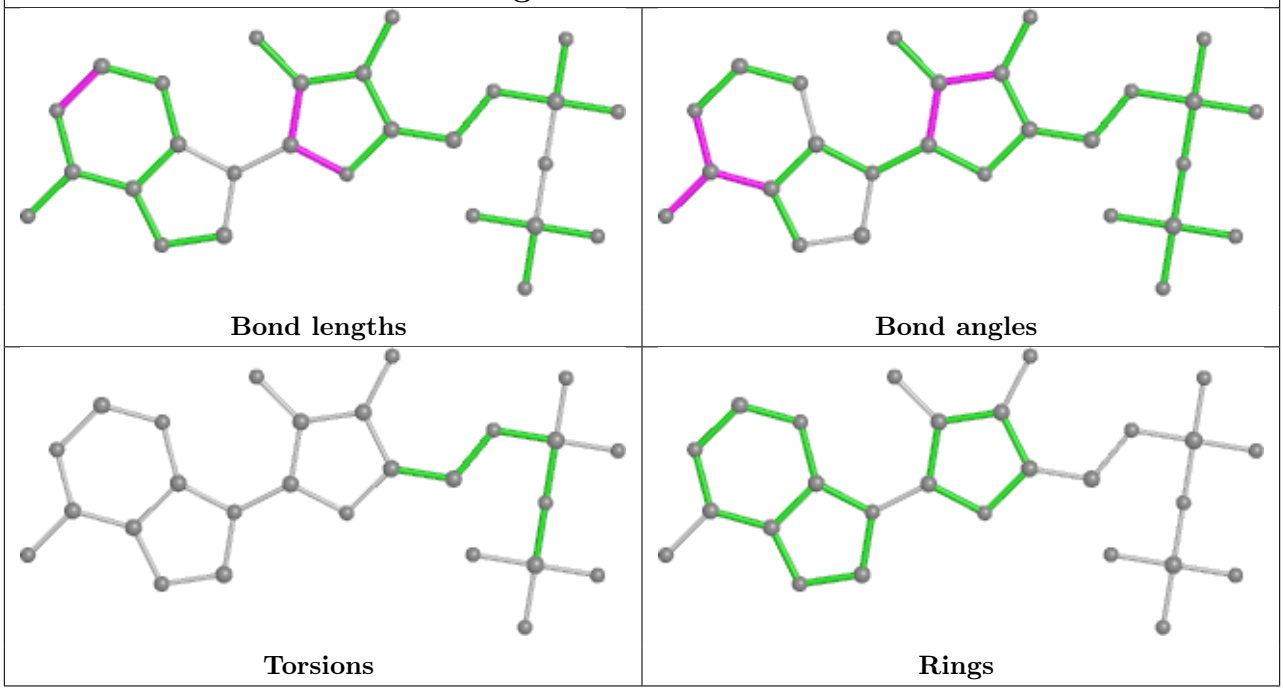


Rings

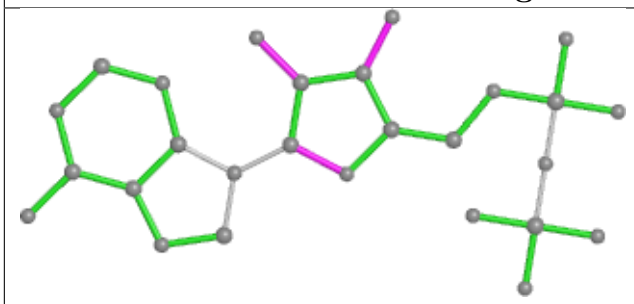
Ligand ADP G 4068



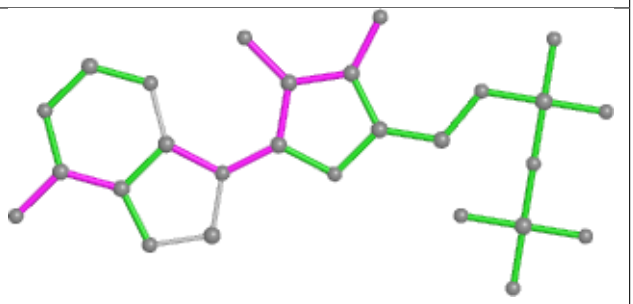
Ligand ADP A 4000



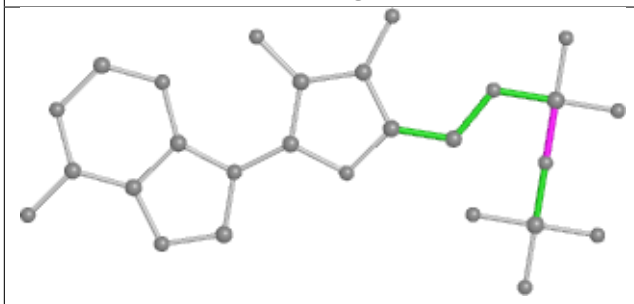
Ligand ADP E 4041



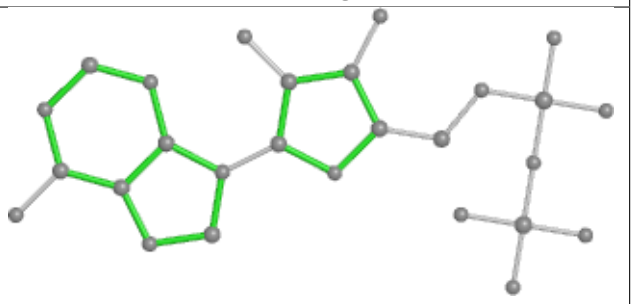
Bond lengths



Bond angles

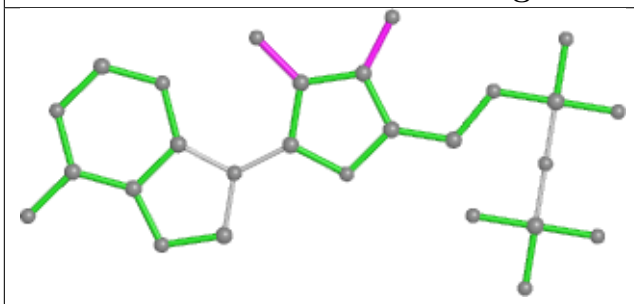


Torsions

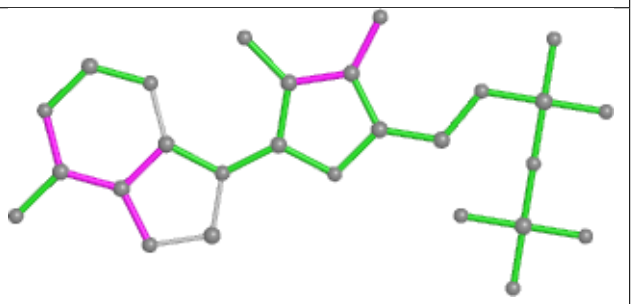


Rings

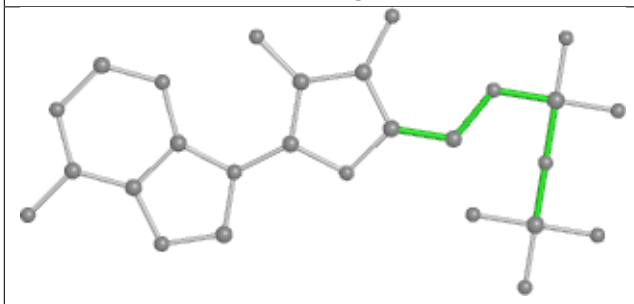
Ligand ADP G 4062



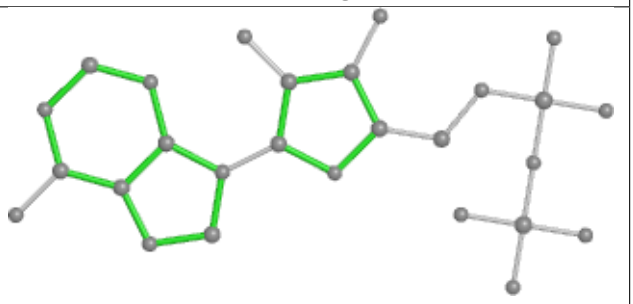
Bond lengths



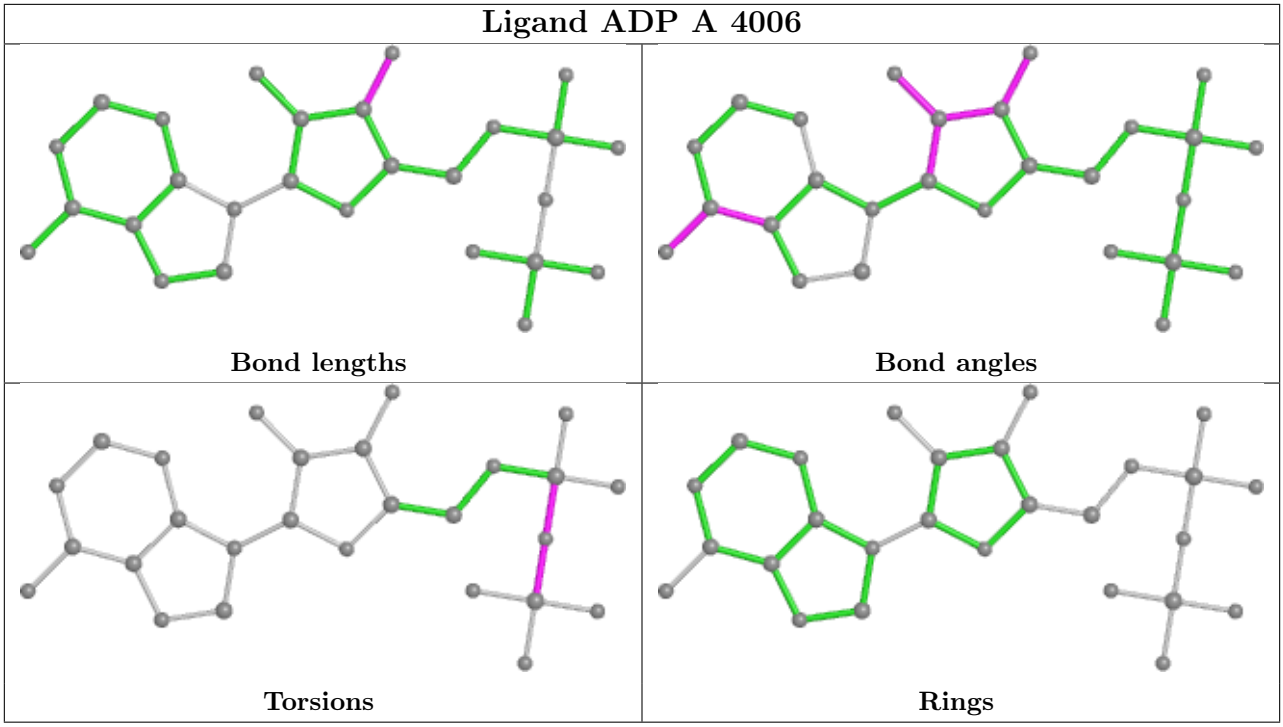
Bond angles



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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.