



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 9, 2024 – 05:44 AM EDT

PDB ID : 1T36
Title : Crystal structure of E. coli carbamoyl phosphate synthetase small subunit mutant C248D complexed with uridine 5'-monophosphate
Authors : Thoden, J.B.; Huang, X.; Raushel, F.M.; Holden, H.M.
Deposited on : 2004-04-24
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

<http://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 : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 1.20.1
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.003 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

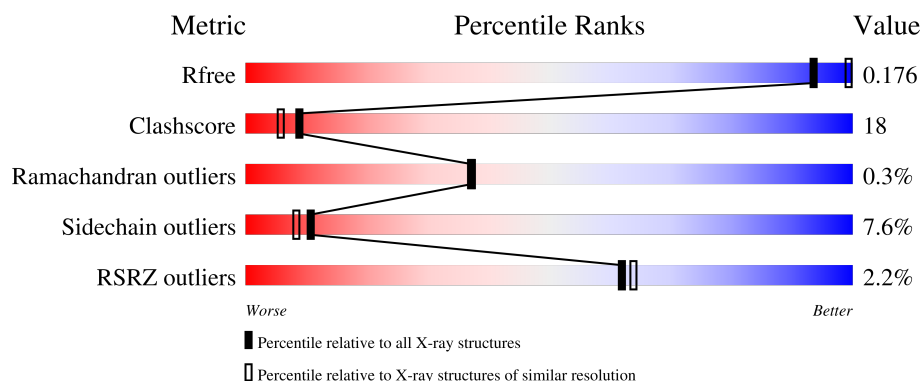
1 Overall quality at a glance

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))
R_{free}	164625	6234 (2.10-2.10)
Clashscore	180529	6893 (2.10-2.10)
Ramachandran outliers	177936	6839 (2.10-2.10)
Sidechain outliers	177891	6840 (2.10-2.10)
RSRZ outliers	164620	6234 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1073	<div> <div>2%</div> <div>62% 30% 7%</div> </div>
1	C	1073	<div> <div>2%</div> <div>58% 32% 7%</div> </div>
1	E	1073	<div> <div>%</div> <div>65% 27% 6%</div> </div>
1	G	1073	<div> <div>%</div> <div>52% 37% 9%</div> </div>
2	B	382	<div> <div>%</div> <div>54% 35% 8%</div> </div>

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Mol	Chain	Length	Quality of chain
2	D	382	
2	F	382	
2	H	382	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	PO4	E	1078	-	X	-	-
5	PO4	G	1078	-	X	-	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 48757 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 synthase large chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1058	Total	C	N	O	S	0	9	0
			8212	5155	1436	1575	46			
1	C	1058	Total	C	N	O	S	0	8	0
			8197	5146	1426	1579	46			
1	E	1058	Total	C	N	O	S	0	5	0
			8182	5137	1425	1575	45			
1	G	1058	Total	C	N	O	S	0	8	0
			8206	5152	1432	1577	45			

- Molecule 2 is a protein called Carbamoyl-phosphate synthase small chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	379	Total	C	N	O	S	0	0	0
			2897	1826	508	554	9			
2	D	379	Total	C	N	O	S	0	1	0
			2904	1830	511	554	9			
2	F	379	Total	C	N	O	S	0	0	0
			2897	1826	508	554	9			
2	H	379	Total	C	N	O	S	0	0	0
			2897	1826	508	554	9			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	248	ASP	CYS	engineered mutation	UNP P00907
D	248	ASP	CYS	engineered mutation	UNP P00907
F	248	ASP	CYS	engineered mutation	UNP P00907
H	248	ASP	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	4	Total K 4 4	0	0
4	B	1	Total K 1 1	0	0
4	C	4	Total K 4 4	0	0
4	D	1	Total K 1 1	0	0
4	E	5	Total K 5 5	0	0
4	F	1	Total K 1 1	0	0
4	G	5	Total K 5 5	0	0
4	H	1	Total K 1 1	0	0

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

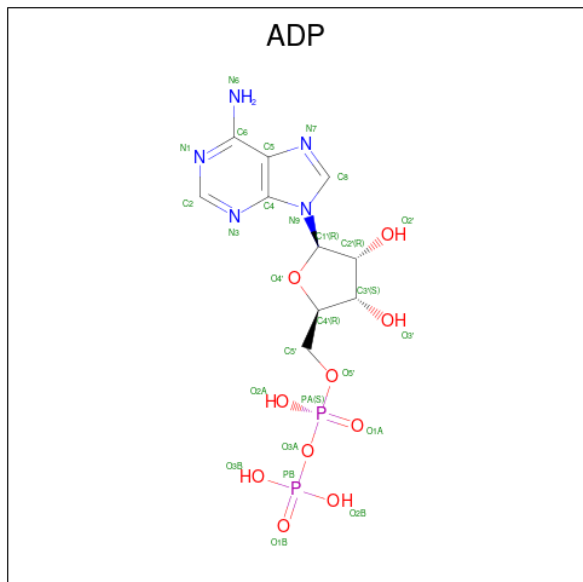


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	P	0	0
			5	4	1		
5	C	1	Total	O	P	0	0
			5	4	1		
5	C	1	Total	O	P	0	0
			5	4	1		
5	E	1	Total	O	P	0	0
			5	4	1		
5	G	1	Total	O	P	0	0
			5	4	1		

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

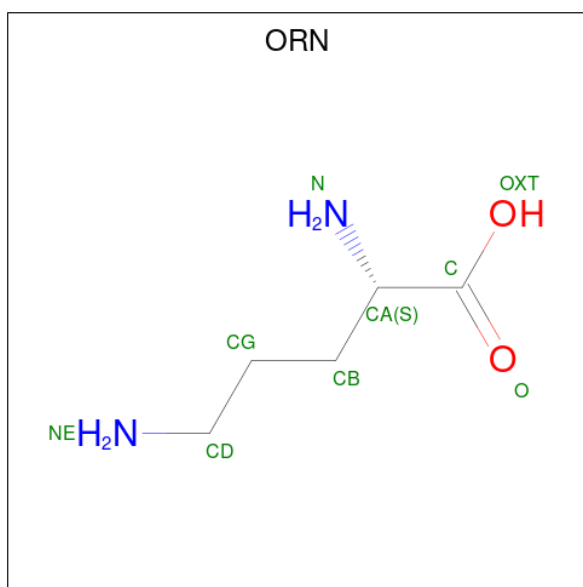
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	5	Total	Cl	0	0
			5	5		
6	C	6	Total	Cl	0	0
			6	6		
6	D	1	Total	Cl	0	0
			1	1		
6	E	6	Total	Cl	0	0
			6	6		
6	F	1	Total	Cl	0	0
			1	1		
6	G	6	Total	Cl	0	0
			6	6		
6	H	2	Total	Cl	0	0
			2	2		

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



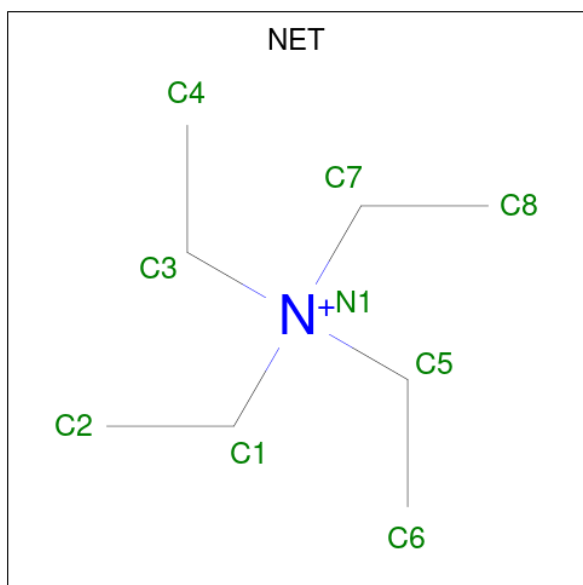
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	G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



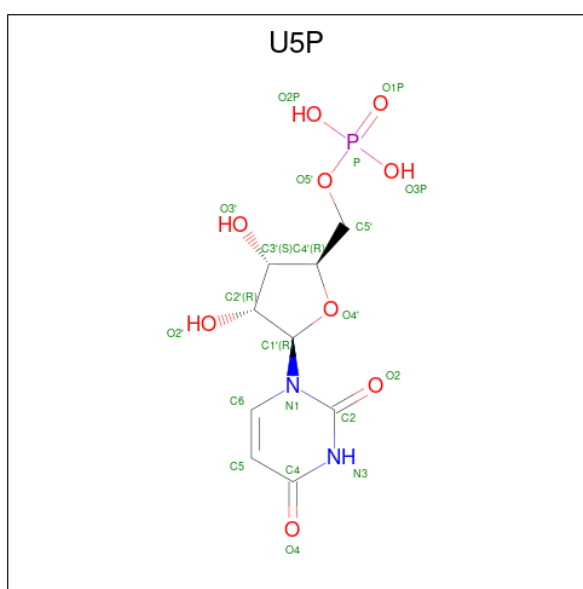
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			9	5	2	2		
8	C	1	Total	C	N	O	0	0
			9	5	2	2		
8	E	1	Total	C	N	O	0	0
			9	5	2	2		
8	G	1	Total	C	N	O	0	0
			9	5	2	2		

- Molecule 9 is TETRAETHYLAMMONIUM ION (three-letter code: NET) (formula: C₈H₂₀N).



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

- Molecule 10 is URIDINE-5'-MONOPHOSPHATE (three-letter code: U5P) (formula: $C_9H_{13}N_2O_9P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total C N O P 21 9 2 9 1	0	0
10	C	1	Total C N O P 21 9 2 9 1	0	0
10	E	1	Total C N O P 21 9 2 9 1	0	0
10	G	1	Total C N O P 21 9 2 9 1	0	0

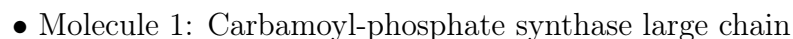
- Molecule 11 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	851	Total O 851 851	0	0

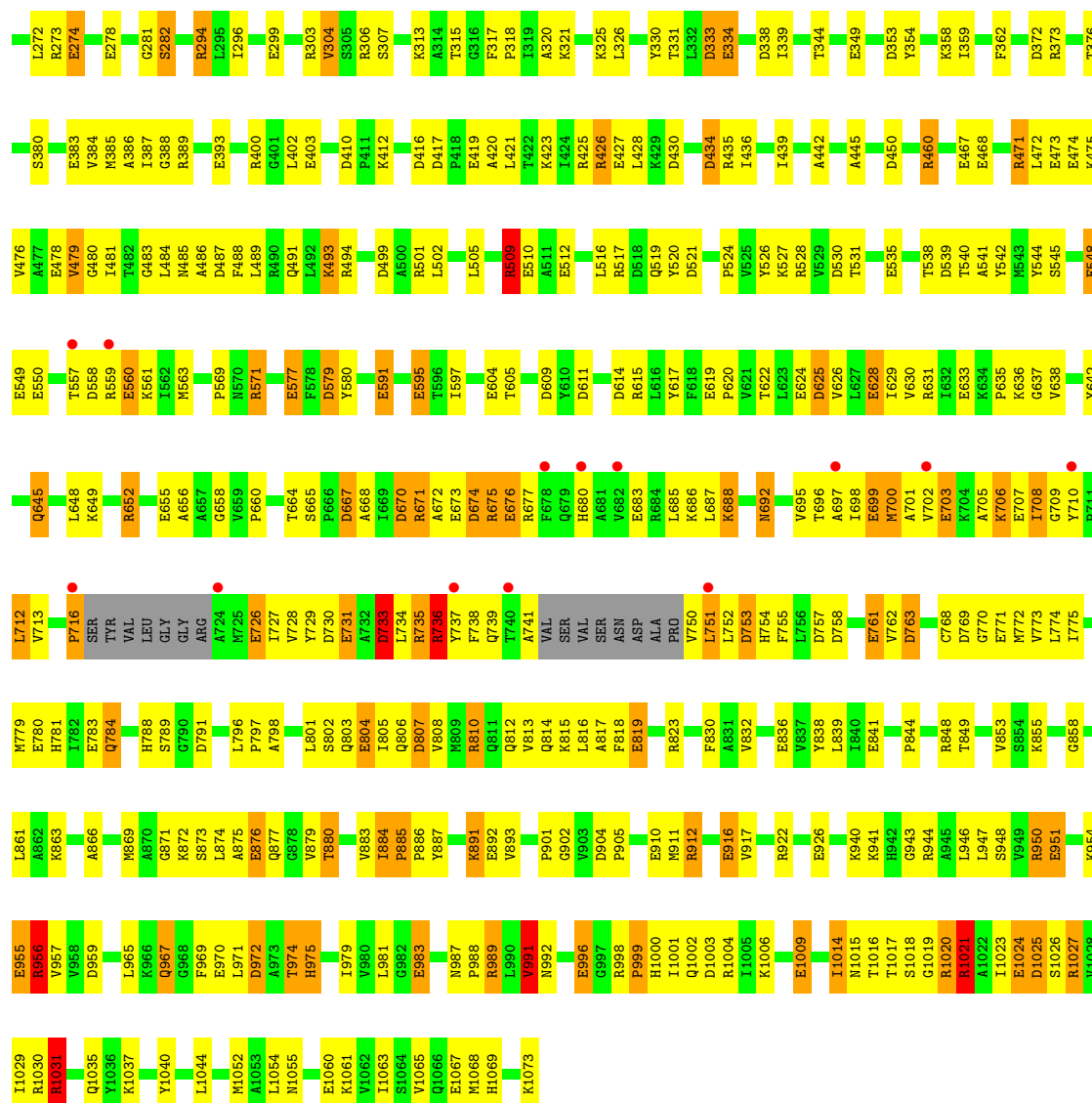
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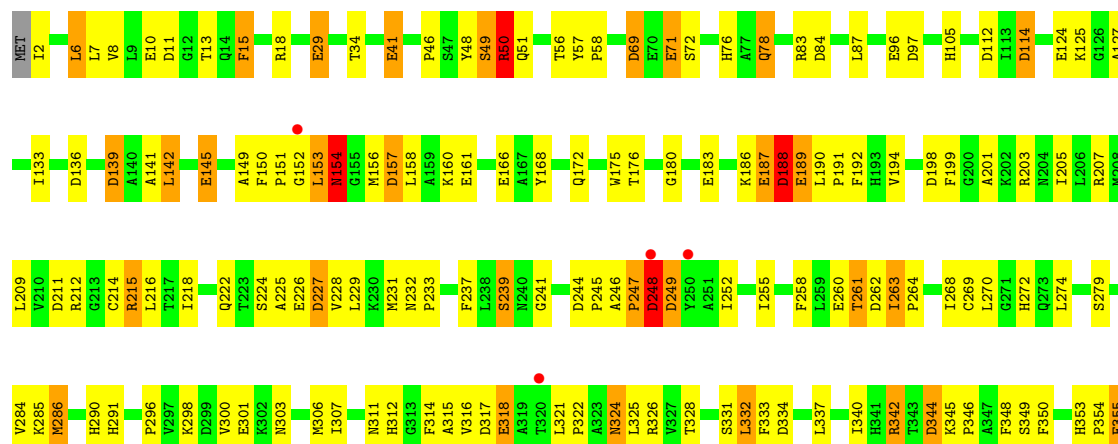
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	B	161	Total 161	O 161	0	0
11	C	819	Total 819	O 819	0	0
11	D	221	Total 221	O 221	0	0
11	E	832	Total 832	O 832	0	0
11	F	200	Total 200	O 200	0	0
11	G	705	Total 705	O 705	0	0
11	H	118	Total 118	O 118	0	0





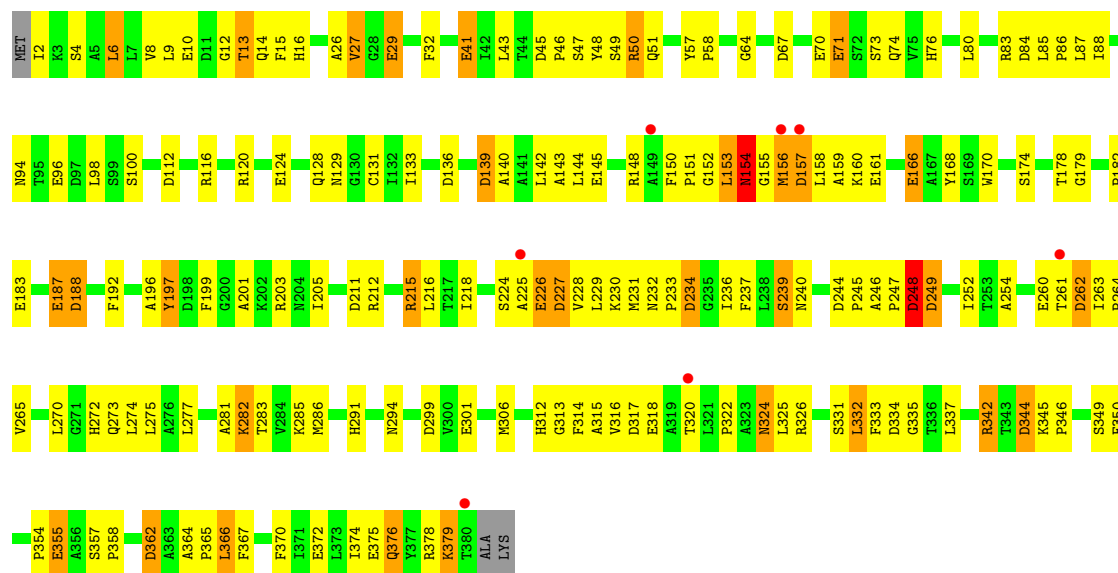


• Molecule 2: Carbamoyl-phosphate synthase small chain

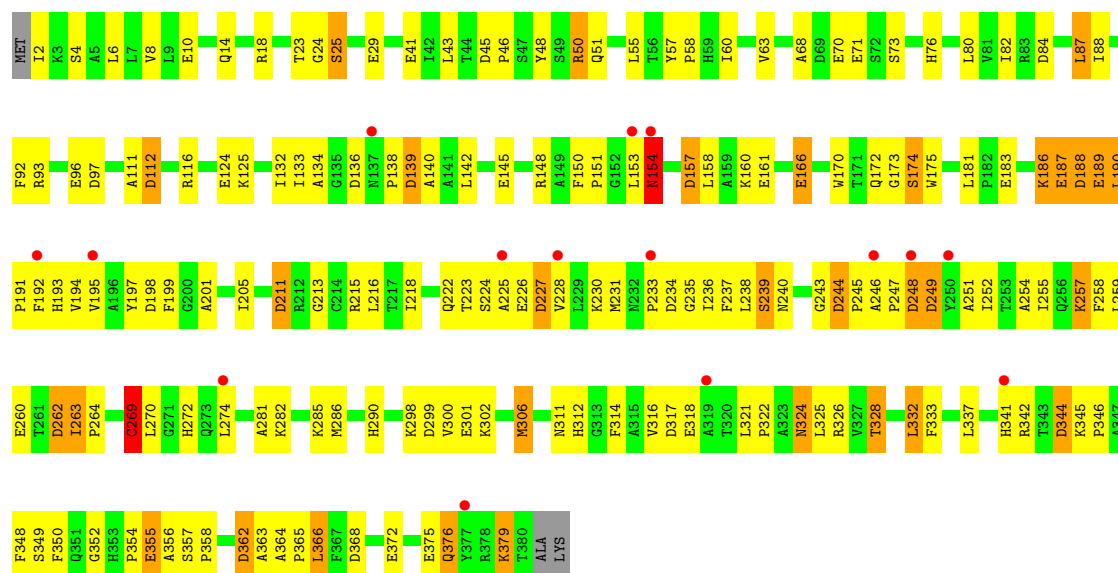




• Molecule 2: Carbamoyl-phosphate synthase small chain



• Molecule 2: Carbamoyl-phosphate synthase small chain



• Molecule 2: Carbamoyl-phosphate synthase small chain





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	152.50Å 164.90Å 333.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.10 30.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	90.0 (30.00-2.10) 88.6 (30.00-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.88 (at 2.10Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.176 , 0.209 0.175 , 0.176	Depositor DCC
R_{free} test set	42730 reflections (9.94%)	wwPDB-VP
Wilson B-factor (Å ²)	28.2	Xtriage
Anisotropy	0.072	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 130.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	48757	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.52% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, K, ADP, MN, ORN, CL, U5P, 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	1.05	68/8374 (0.8%)	1.50	137/11315 (1.2%)
1	C	1.06	81/8355 (1.0%)	1.48	127/11293 (1.1%)
1	E	1.06	74/8328 (0.9%)	1.50	128/11257 (1.1%)
1	G	1.05	74/8368 (0.9%)	1.50	148/11308 (1.3%)
2	B	0.94	19/2959 (0.6%)	1.46	43/4019 (1.1%)
2	D	0.97	17/2970 (0.6%)	1.48	45/4033 (1.1%)
2	F	0.97	19/2959 (0.6%)	1.45	41/4019 (1.0%)
2	H	0.94	20/2959 (0.7%)	1.42	37/4019 (0.9%)
All	All	1.03	372/45272 (0.8%)	1.49	706/61263 (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	1	0
2	D	1	0
2	F	1	0
All	All	3	0

The worst 5 of 372 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	372	GLU	CD-OE2	8.39	1.34	1.25
2	H	166	GLU	CD-OE2	8.34	1.34	1.25
2	D	145	GLU	CD-OE2	8.28	1.34	1.25
1	G	1009[A]	GLU	CD-OE2	8.21	1.34	1.25
1	G	1009[B]	GLU	CD-OE2	8.21	1.34	1.25

The worst 5 of 706 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	514	ARG	NE-CZ-NH2	-15.12	112.74	120.30
1	A	944	ARG	NE-CZ-NH1	14.25	127.42	120.30
1	C	514	ARG	NE-CZ-NH2	-14.00	113.30	120.30
1	A	104	ARG	NE-CZ-NH1	13.43	127.02	120.30
1	A	652	ARG	NE-CZ-NH1	13.13	126.87	120.30

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	154	ASN	CA
2	D	154	ASN	CA
2	F	154	ASN	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	A	8212	0	8255	231	0
1	C	8197	0	8225	253	0
1	E	8182	0	8216	209	0
1	G	8206	0	8247	340	0
2	B	2897	0	2860	147	0
2	D	2904	0	2869	133	0
2	F	2897	0	2860	128	0
2	H	2897	0	2860	213	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	4	0	0	0	0
4	B	1	0	0	0	0
4	C	4	0	0	0	0
4	D	1	0	0	0	0
4	E	5	0	0	0	0
4	F	1	0	0	0	0
4	G	5	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	5	0	0	0	0
5	C	10	0	0	1	0
5	E	5	0	0	0	0
5	G	5	0	0	0	0
6	A	5	0	0	1	0
6	C	6	0	0	0	0
6	D	1	0	0	0	0
6	E	6	0	0	1	0
6	F	1	0	0	0	0
6	G	6	0	0	2	0
6	H	2	0	0	0	0
7	A	54	0	24	2	0
7	C	54	0	24	0	0
7	E	54	0	24	3	0
7	G	54	0	24	0	0
8	A	9	0	11	0	0
8	C	9	0	11	1	0
8	E	9	0	11	2	0
8	G	9	0	11	1	0
9	A	9	0	20	1	0
9	C	9	0	20	1	0
9	E	9	0	20	2	0
9	G	9	0	20	2	0
10	A	21	0	11	1	0
10	C	21	0	11	1	0
10	E	21	0	11	3	0
10	G	21	0	11	1	0
11	A	851	0	0	29	1
11	B	161	0	0	5	0
11	C	819	0	0	23	1
11	D	221	0	0	5	0
11	E	832	0	0	24	0
11	F	200	0	0	2	0
11	G	705	0	0	28	0
11	H	118	0	0	5	0
All	All	48757	0	44656	1643	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 18.

The worst 5 of 1643 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)
2:H:27:VAL:HG22	2:H:131:CYS:HB2	1.13	1.10
2:D:227:ASP:HA	2:D:230:LYS:HD2	1.25	1.07
1:G:784:GLN:NE2	1:G:784:GLN:H	1.53	1.05
2:H:133:ILE:HD12	2:H:143:ALA:HB2	1.41	1.03
1:A:38:ARG:HG3	1:A:38:ARG:HH11	1.25	1.00

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:A:1848:HOH:O	11:C:1912:HOH:O[4_555]	2.14	0.06

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1061/1073 (99%)	1015 (96%)	44 (4%)	2 (0%)	44	45
1	C	1060/1073 (99%)	1005 (95%)	54 (5%)	1 (0%)	48	51
1	E	1057/1073 (98%)	1013 (96%)	42 (4%)	2 (0%)	44	45
1	G	1061/1073 (99%)	996 (94%)	59 (6%)	6 (1%)	22	19
2	B	377/382 (99%)	348 (92%)	26 (7%)	3 (1%)	16	13
2	D	378/382 (99%)	354 (94%)	23 (6%)	1 (0%)	37	37
2	F	377/382 (99%)	355 (94%)	21 (6%)	1 (0%)	37	37
2	H	377/382 (99%)	346 (92%)	27 (7%)	4 (1%)	12	8
All	All	5748/5820 (99%)	5432 (94%)	296 (5%)	20 (0%)	37	37

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	154	ASN

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Mol	Chain	Res	Type
2	D	154	ASN
1	E	738	PHE
1	G	485	ASN
1	G	975	HIS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	874/878 (100%)	811 (93%)	63 (7%)	12	9
1	C	873/878 (99%)	809 (93%)	64 (7%)	11	9
1	E	870/878 (99%)	818 (94%)	52 (6%)	16	14
1	G	874/878 (100%)	800 (92%)	74 (8%)	8	6
2	B	308/310 (99%)	283 (92%)	25 (8%)	9	7
2	D	309/310 (100%)	283 (92%)	26 (8%)	9	6
2	F	308/310 (99%)	276 (90%)	32 (10%)	5	3
2	H	308/310 (99%)	278 (90%)	30 (10%)	6	4
All	All	4724/4752 (99%)	4358 (92%)	366 (8%)	11	8

5 of 366 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	4	SER
1	G	509	ARG
2	F	166	GLU
2	F	376	GLN
1	G	696	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 78 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	266	ASN

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Mol	Chain	Res	Type
1	G	1071	GLN
1	G	679	GLN
1	G	936	ASN
2	H	291	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 86 ligands modelled in this entry, 61 are monoatomic - leaving 25 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	$\# Z > 2$
8	ORN	C	1091	-	7,8,8	1.20	1 (14%)	6,9,9	1.15	1 (16%)
9	NET	C	1092	-	8,8,8	0.52	0	10,10,10	0.79	0
10	U5P	A	1091	-	22,22,22	0.87	1 (4%)	32,33,33	0.84	0
7	ADP	E	1089	3	24,29,29	1.34	3 (12%)	29,45,45	1.17	3 (10%)
7	ADP	A	1088	3	24,29,29	1.26	1 (4%)	29,45,45	1.24	2 (6%)
5	PO4	C	1088	-	4,4,4	2.60	3 (75%)	6,6,6	1.01	0
8	ORN	E	1091	-	7,8,8	1.11	1 (14%)	6,9,9	0.97	0
8	ORN	A	1089	-	7,8,8	0.91	0	6,9,9	1.70	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	PO4	G	1078	3	4,4,4	2.39	3 (75%)	6,6,6	1.24	1 (16%)
9	NET	G	1092	-	8,8,8	0.75	0	10,10,10	0.49	0
10	U5P	E	1093	-	22,22,22	0.99	1 (4%)	32,33,33	1.64	6 (18%)
9	NET	A	1090	-	8,8,8	0.75	0	10,10,10	0.68	0
7	ADP	G	1090	3	24,29,29	1.22	3 (12%)	29,45,45	1.25	5 (17%)
9	NET	E	1092	-	8,8,8	0.41	0	10,10,10	0.78	0
7	ADP	A	1087	3	24,29,29	1.49	3 (12%)	29,45,45	1.02	2 (6%)
10	U5P	C	1093	-	22,22,22	0.85	1 (4%)	32,33,33	0.93	1 (3%)
10	U5P	G	1093	-	22,22,22	0.96	1 (4%)	32,33,33	1.48	3 (9%)
5	PO4	A	1078	3	4,4,4	2.00	1 (25%)	6,6,6	1.43	1 (16%)
5	PO4	C	1078	3	4,4,4	2.37	3 (75%)	6,6,6	1.09	0
7	ADP	C	1089	3	24,29,29	1.87	3 (12%)	29,45,45	1.34	2 (6%)
7	ADP	G	1089	3	24,29,29	1.33	3 (12%)	29,45,45	1.42	5 (17%)
7	ADP	C	1090	3	24,29,29	0.99	1 (4%)	29,45,45	1.18	4 (13%)
7	ADP	E	1090	3	24,29,29	1.26	3 (12%)	29,45,45	1.24	3 (10%)
5	PO4	E	1078	3	4,4,4	2.59	3 (75%)	6,6,6	1.39	1 (16%)
8	ORN	G	1091	-	7,8,8	0.87	0	6,9,9	0.90	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	ORN	C	1091	-	-	6/8/8/8	-
9	NET	C	1092	-	-	0/12/12/12	-
10	U5P	A	1091	-	-	6/10/26/26	0/2/2/2
7	ADP	E	1089	3	-	2/12/32/32	0/3/3/3
7	ADP	A	1088	3	-	4/12/32/32	0/3/3/3
8	ORN	E	1091	-	-	6/8/8/8	-
8	ORN	A	1089	-	-	6/8/8/8	-
9	NET	G	1092	-	-	0/12/12/12	-
10	U5P	E	1093	-	-	6/10/26/26	0/2/2/2
9	NET	A	1090	-	-	3/12/12/12	-
7	ADP	G	1090	3	-	0/12/32/32	0/3/3/3
9	NET	E	1092	-	-	0/12/12/12	-
7	ADP	A	1087	3	-	1/12/32/32	0/3/3/3
10	U5P	C	1093	-	-	5/10/26/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	U5P	G	1093	-	-	6/10/26/26	0/2/2/2
7	ADP	C	1089	3	-	2/12/32/32	0/3/3/3
7	ADP	G	1089	3	-	2/12/32/32	0/3/3/3
7	ADP	C	1090	3	-	4/12/32/32	0/3/3/3
7	ADP	E	1090	3	-	4/12/32/32	0/3/3/3
8	ORN	G	1091	-	-	6/8/8/8	-

The worst 5 of 39 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	1089	ADP	PA-O3A	-6.95	1.52	1.59
7	A	1087	ADP	PA-O3A	-4.43	1.54	1.59
7	A	1088	ADP	PA-O3A	-4.21	1.55	1.59
5	C	1088	PO4	P-O2	-3.58	1.44	1.54
7	E	1089	ADP	PA-O3A	-3.48	1.55	1.59

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	1089	ADP	C5-C6-N6	5.15	128.16	120.31
10	E	1093	U5P	O3P-P-O5'	-5.05	93.51	106.67
10	G	1093	U5P	O3P-P-O5'	-4.42	95.14	106.67
7	A	1088	ADP	C5-C6-N6	4.04	126.47	120.31
7	G	1089	ADP	O4'-C1'-N9	-3.60	103.98	108.75

There are no chirality outliers.

5 of 69 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	1090	ADP	PA-O3A-PB-O3B
7	E	1090	ADP	PA-O3A-PB-O3B
8	A	1089	ORN	N-CA-CB-CG
8	A	1089	ORN	C-CA-CB-CG
8	C	1091	ORN	N-CA-CB-CG

There are no ring outliers.

16 monomers are involved in 22 short contacts:

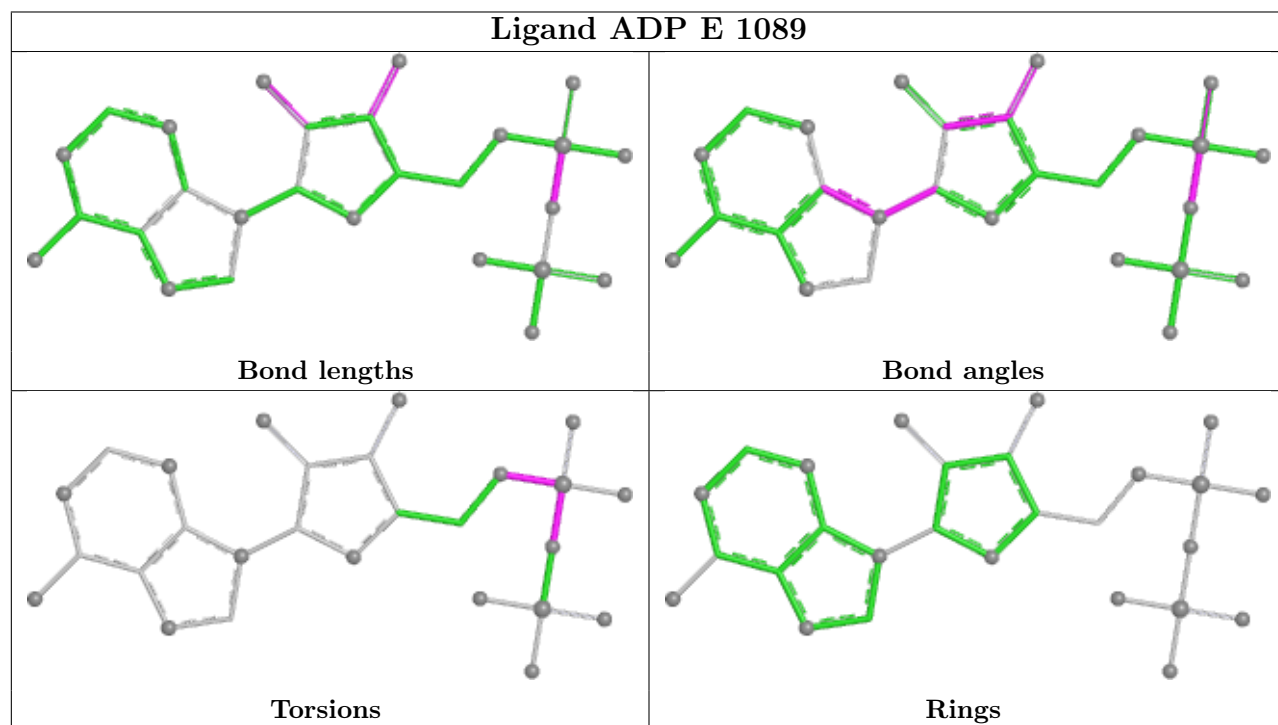
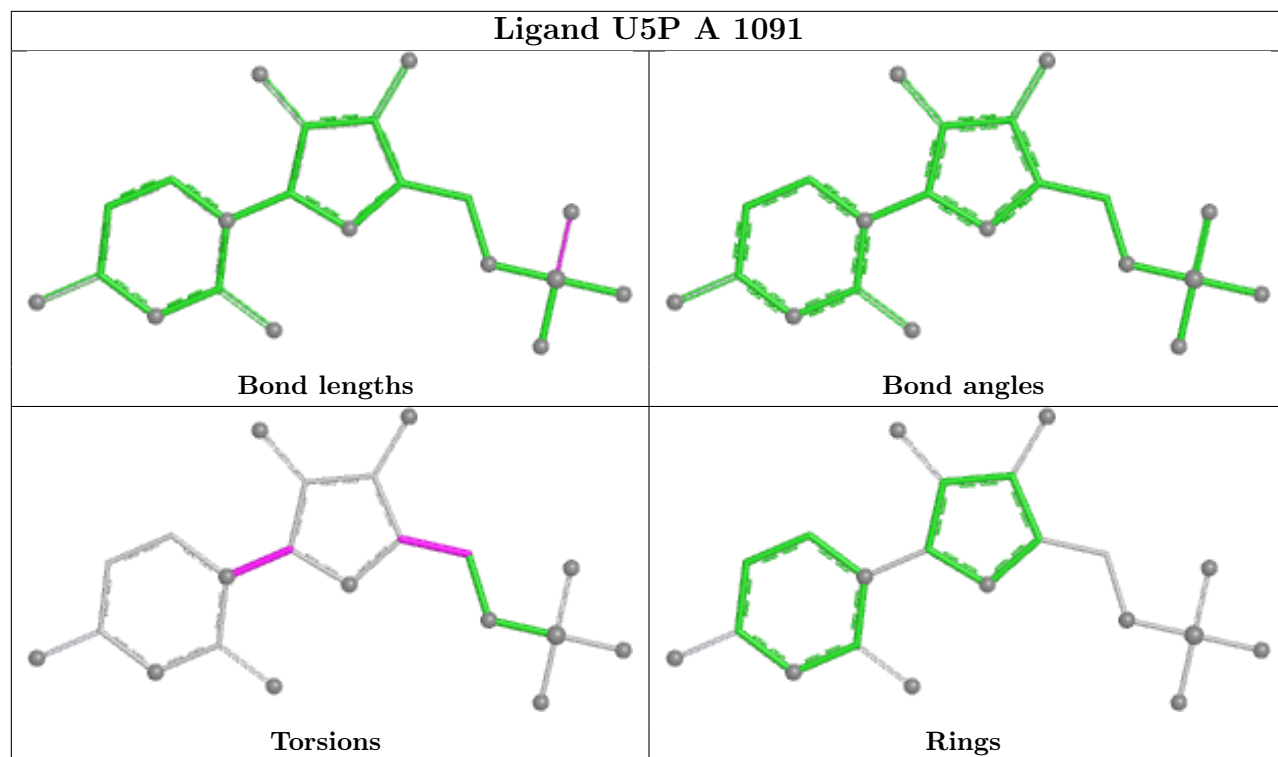
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	1091	ORN	1	0

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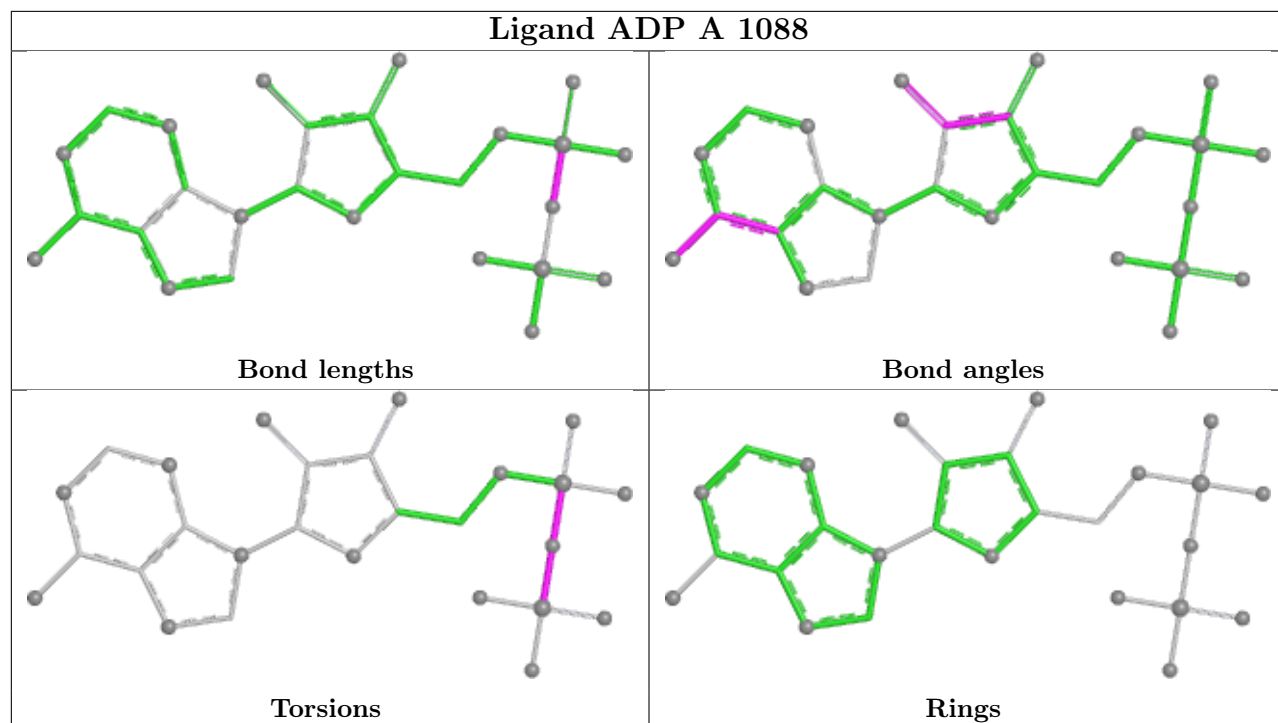
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	C	1092	NET	1	0
10	A	1091	U5P	1	0
7	E	1089	ADP	1	0
7	A	1088	ADP	1	0
8	E	1091	ORN	2	0
9	G	1092	NET	2	0
10	E	1093	U5P	3	0
9	A	1090	NET	1	0
9	E	1092	NET	2	0
7	A	1087	ADP	1	0
10	C	1093	U5P	1	0
10	G	1093	U5P	1	0
5	C	1078	PO4	1	0
7	E	1090	ADP	2	0
8	G	1091	ORN	1	0

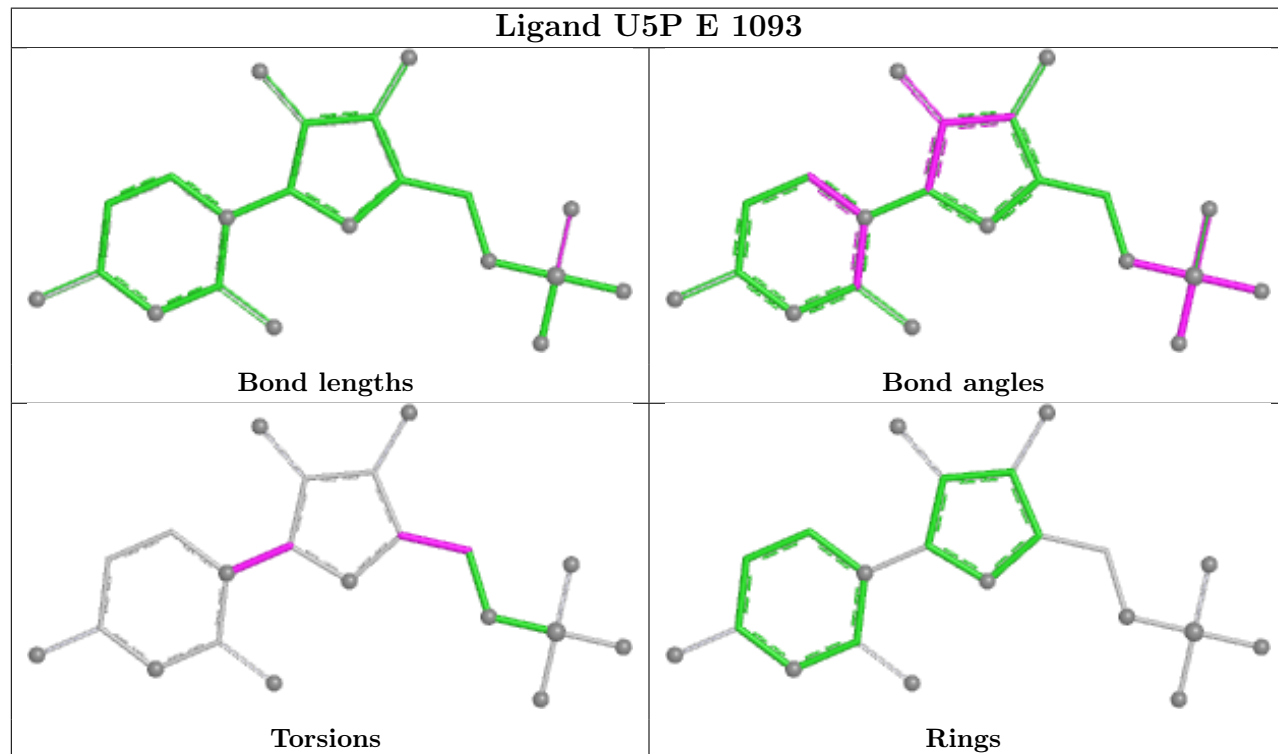
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



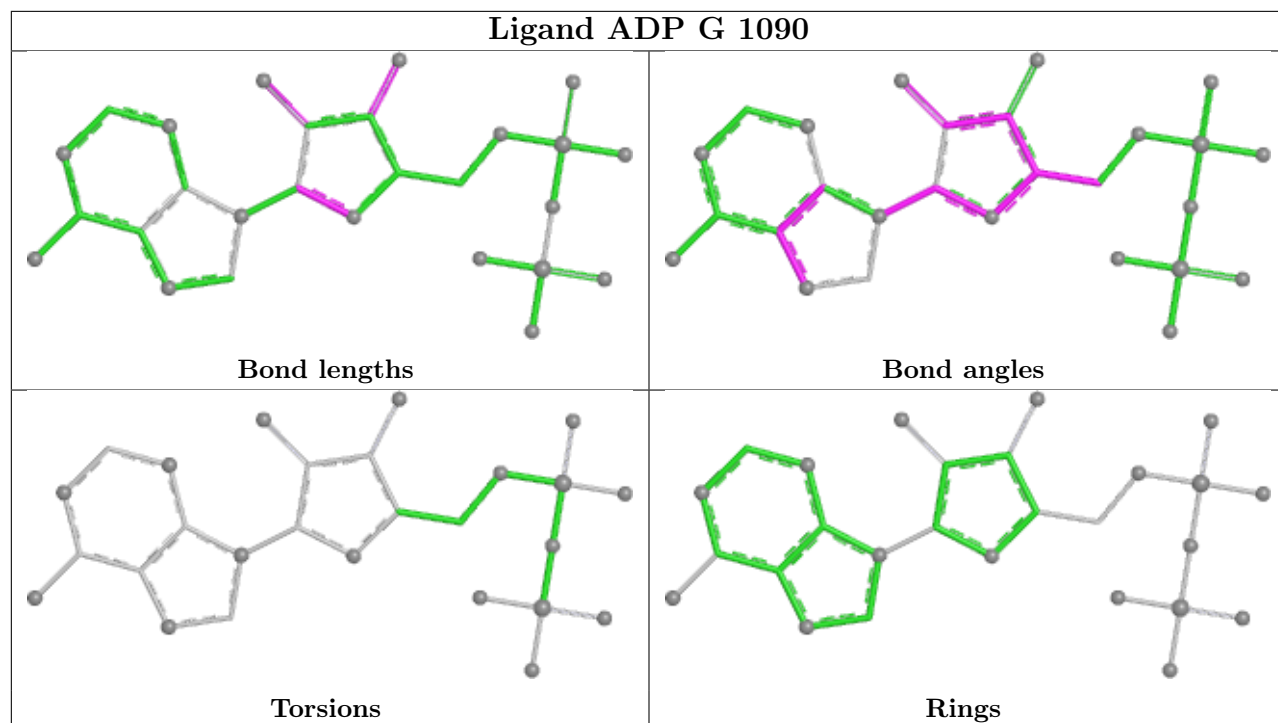
Ligand ADP A 1088



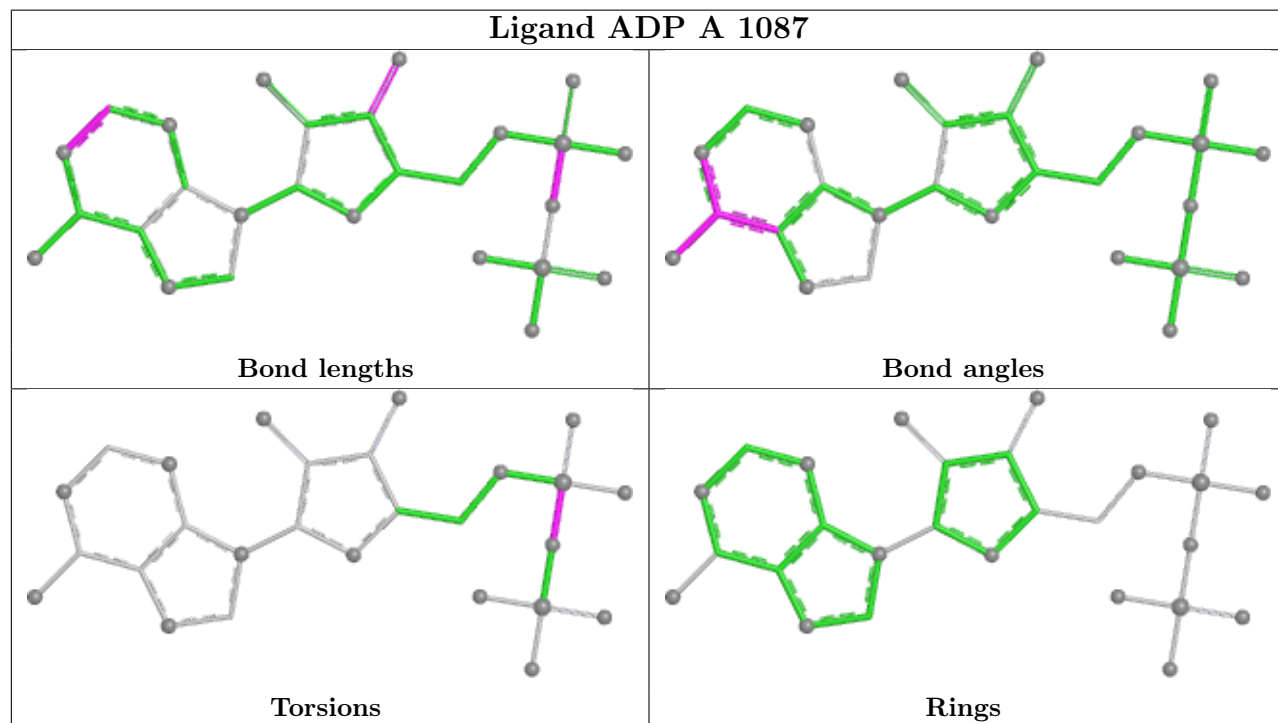
Ligand U5P E 1093



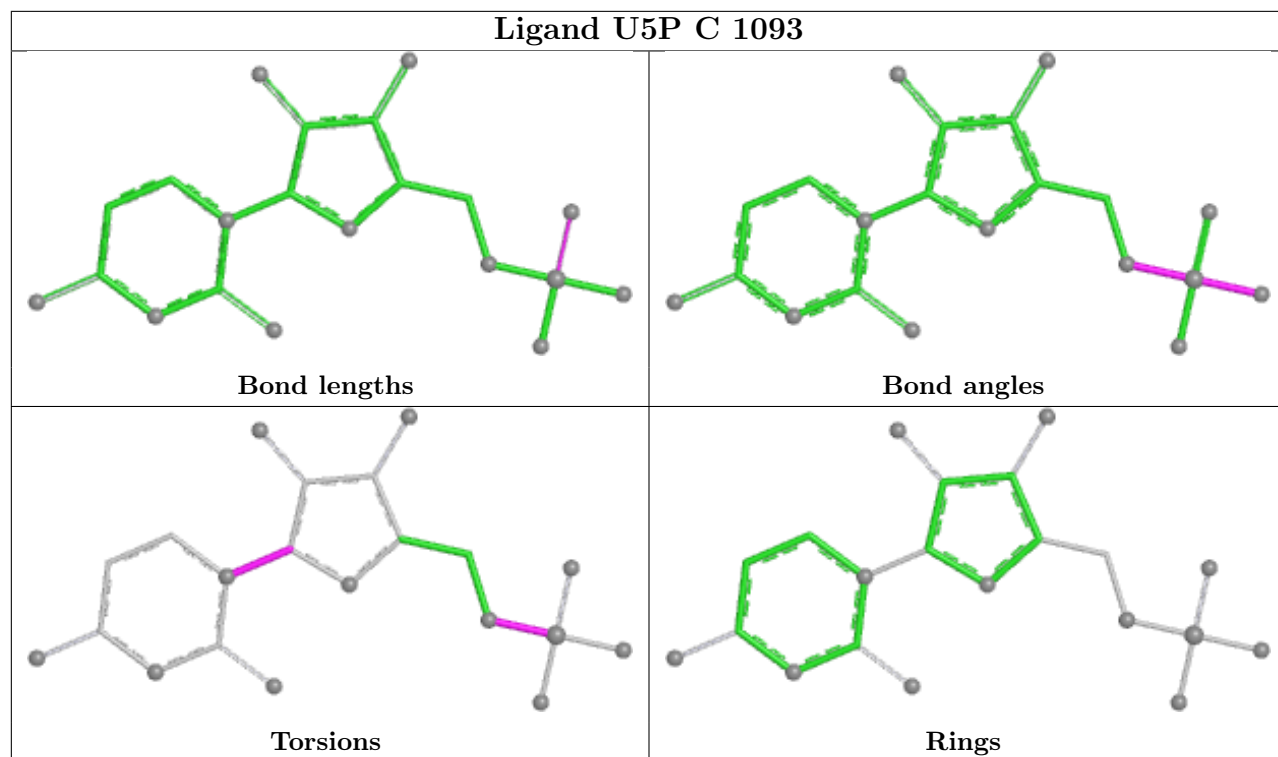
Ligand ADP G 1090



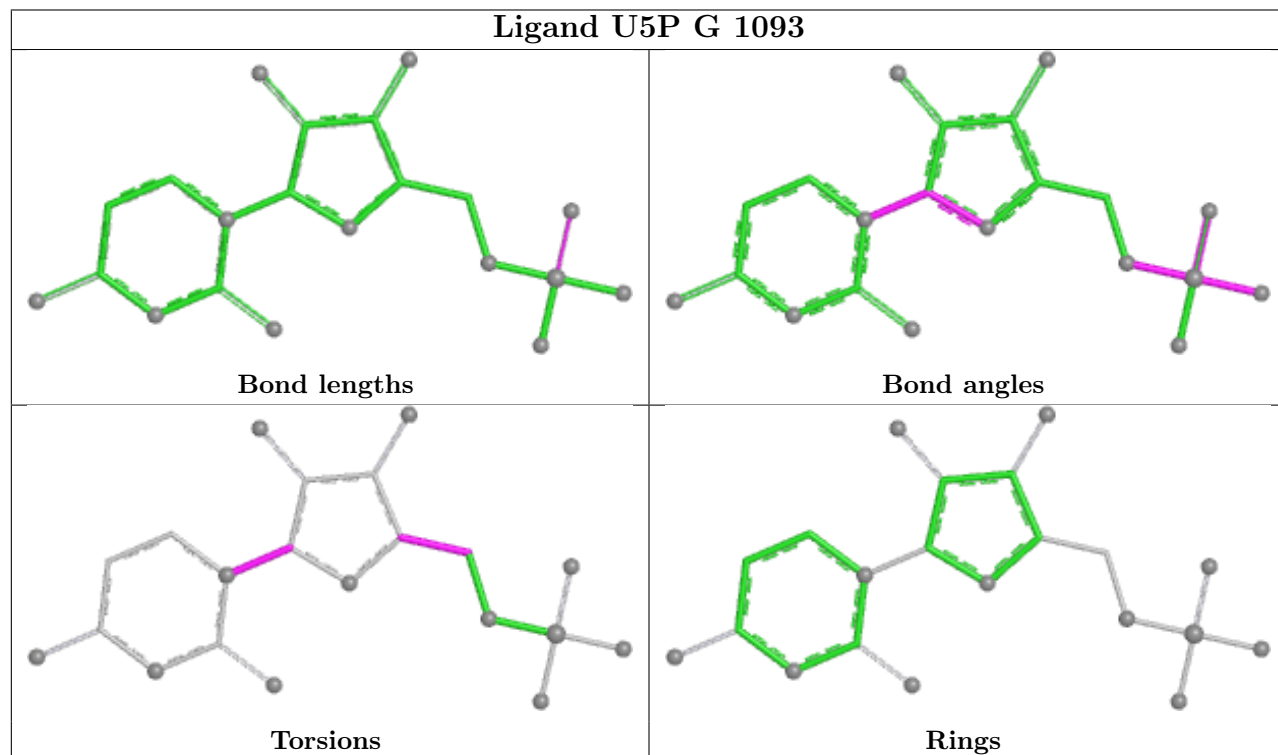
Ligand ADP A 1087



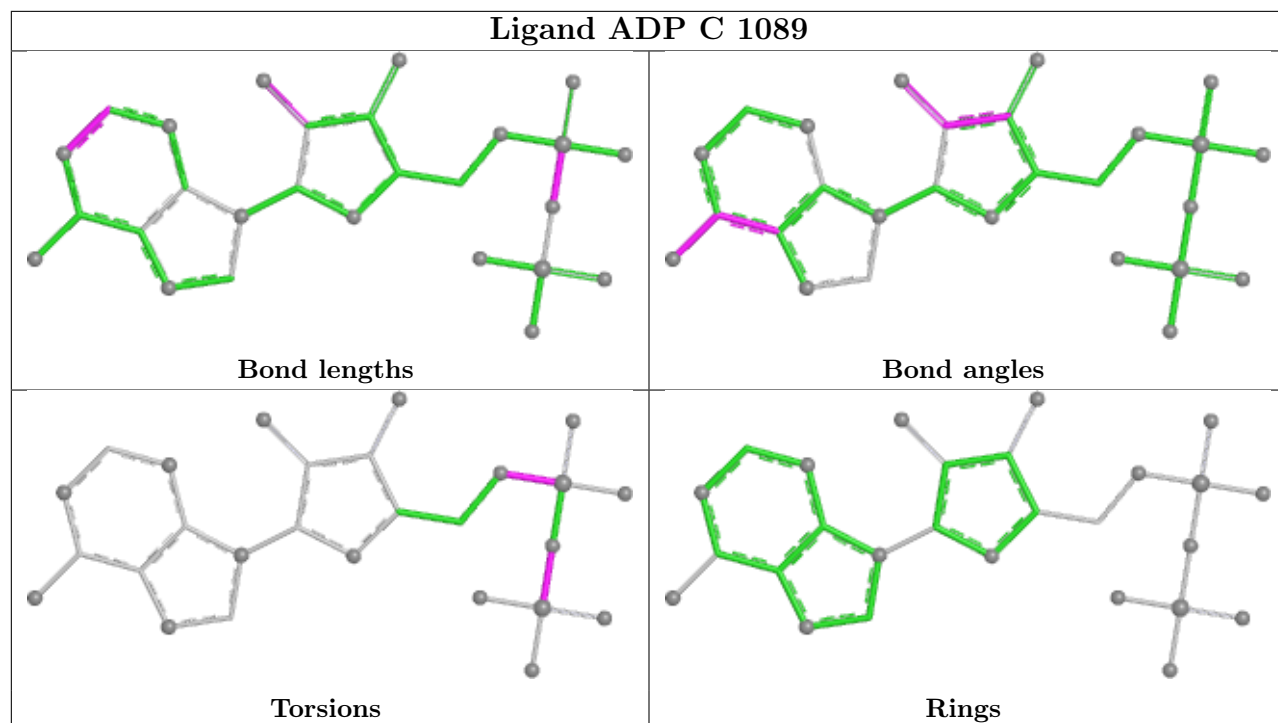
Ligand U5P C 1093



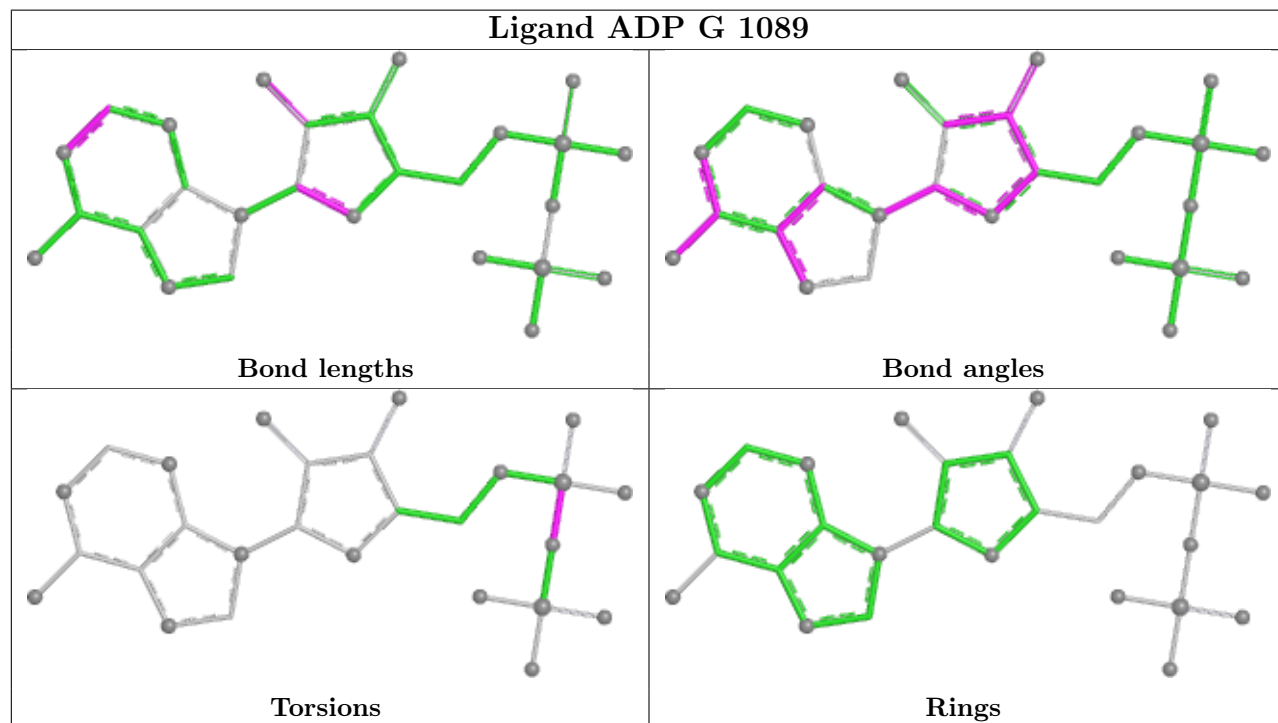
Ligand U5P G 1093

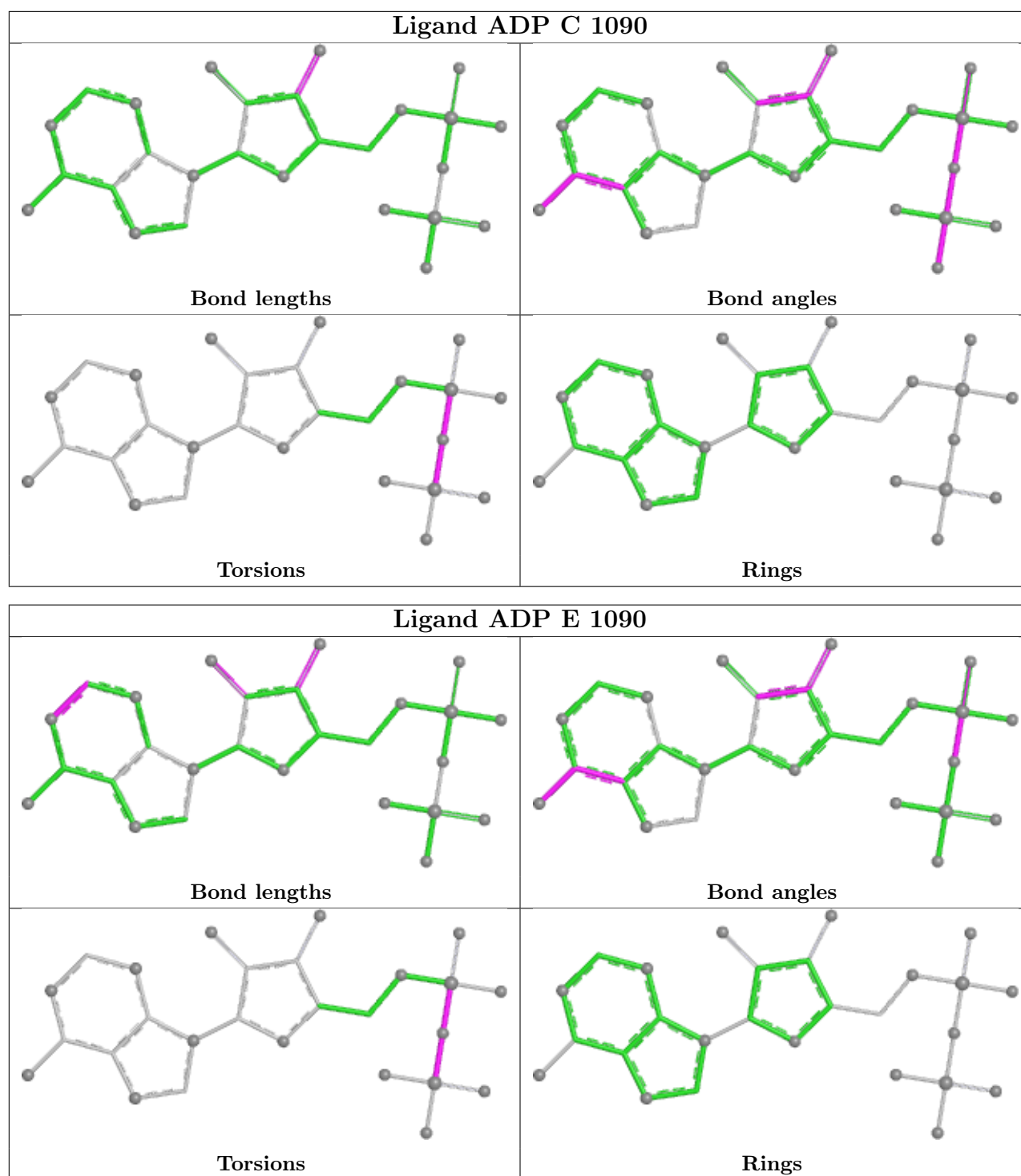


Ligand ADP C 1089



Ligand ADP G 1089





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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1058/1073 (98%)	-0.60	22 (2%) 63 65	17, 33, 73, 100	9 (0%)
1	C	1058/1073 (98%)	-0.51	20 (1%) 66 67	18, 35, 81, 100	8 (0%)
1	E	1058/1073 (98%)	-0.68	11 (1%) 79 80	17, 31, 75, 100	5 (0%)
1	G	1058/1073 (98%)	-0.26	15 (1%) 73 74	20, 41, 84, 100	8 (0%)
2	B	379/382 (99%)	0.01	5 (1%) 74 76	21, 48, 87, 100	0
2	D	379/382 (99%)	-0.13	7 (1%) 67 69	21, 40, 78, 100	1 (0%)
2	F	379/382 (99%)	0.07	15 (3%) 43 45	20, 47, 92, 100	0
2	H	379/382 (99%)	0.61	33 (8%) 17 19	33, 63, 97, 100	0
All	All	5748/5820 (98%)	-0.34	128 (2%) 62 64	17, 38, 84, 100	31 (0%)

The worst 5 of 128 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	2	PRO	5.5
1	E	1	MET	4.4
1	A	751	LEU	4.3
1	C	697	ALA	4.0
2	H	134	ALA	4.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	PO4	C	1088	5/5	0.77	0.12	80,80,80,80	0
6	CL	G	1084	1/1	0.84	0.19	72,72,72,72	0
6	CL	E	1084	1/1	0.86	0.15	74,74,74,74	0
6	CL	A	1083	1/1	0.92	0.10	66,66,66,66	0
6	CL	C	1083	1/1	0.94	0.12	77,77,77,77	0
6	CL	G	1087	1/1	0.94	0.10	81,81,81,81	0
6	CL	H	385	1/1	0.94	0.12	82,82,82,82	0
8	ORN	G	1091	9/9	0.94	0.08	28,33,36,63	0
6	CL	G	1088	1/1	0.95	0.14	67,67,67,67	0
4	K	H	383	1/1	0.95	0.09	64,64,64,64	0
8	ORN	A	1089	9/9	0.95	0.08	24,29,36,37	0
6	CL	E	1087	1/1	0.95	0.08	54,54,54,54	0
10	U5P	G	1093	21/21	0.95	0.10	31,57,80,85	0
8	ORN	C	1091	9/9	0.96	0.07	20,29,35,39	0
8	ORN	E	1091	9/9	0.96	0.06	16,25,37,40	0
6	CL	C	1086	1/1	0.96	0.08	67,67,67,67	0
10	U5P	A	1091	21/21	0.96	0.09	28,58,80,81	0
10	U5P	C	1093	21/21	0.96	0.10	33,51,83,89	0
10	U5P	E	1093	21/21	0.96	0.09	37,54,80,89	0
6	CL	H	384	1/1	0.96	0.09	67,67,67,67	0
6	CL	C	1087	1/1	0.97	0.11	63,63,63,63	0
4	K	G	1083	1/1	0.97	0.06	52,52,52,52	0
9	NET	A	1090	9/9	0.97	0.06	18,23,28,38	0
4	K	E	1081	1/1	0.97	0.06	42,42,42,42	0
7	ADP	G	1090	27/27	0.97	0.07	29,47,80,89	0
6	CL	C	1084	1/1	0.97	0.06	43,43,43,43	0
4	K	E	1083	1/1	0.97	0.08	58,58,58,58	0
4	K	G	1081	1/1	0.98	0.06	46,46,46,46	0
4	K	B	383	1/1	0.98	0.04	45,45,45,45	0
6	CL	G	1086	1/1	0.98	0.07	54,54,54,54	0
6	CL	A	1086	1/1	0.98	0.06	56,56,56,56	0
6	CL	D	384	1/1	0.98	0.04	34,34,34,34	0
4	K	C	1082	1/1	0.98	0.05	44,44,44,44	0
9	NET	C	1092	9/9	0.98	0.05	16,21,23,29	0
9	NET	E	1092	9/9	0.98	0.06	15,23,27,28	0
9	NET	G	1092	9/9	0.98	0.06	18,28,29,37	0
6	CL	E	1085	1/1	0.98	0.05	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	ADP	A	1088	27/27	0.98	0.05	20,33,47,60	0
7	ADP	C	1090	27/27	0.98	0.06	26,42,61,77	0
7	ADP	E	1090	27/27	0.98	0.05	23,35,48,56	0
5	PO4	G	1078	5/5	0.99	0.04	17,24,31,35	0
4	K	E	1077	1/1	0.99	0.03	30,30,30,30	0
6	CL	A	1084	1/1	0.99	0.04	40,40,40,40	0
6	CL	A	1085	1/1	0.99	0.05	39,39,39,39	0
4	K	A	1077	1/1	0.99	0.02	27,27,27,27	0
7	ADP	A	1087	27/27	0.99	0.04	16,22,31,38	0
6	CL	C	1081	1/1	0.99	0.03	29,29,29,29	0
7	ADP	C	1089	27/27	0.99	0.05	16,23,31,44	0
4	K	A	1082	1/1	0.99	0.02	41,41,41,41	0
7	ADP	E	1089	27/27	0.99	0.04	15,26,34,36	0
4	K	F	383	1/1	0.99	0.02	36,36,36,36	0
7	ADP	G	1089	27/27	0.99	0.04	17,27,35,41	0
6	CL	C	1085	1/1	0.99	0.05	39,39,39,39	0
4	K	G	1077	1/1	0.99	0.03	38,38,38,38	0
3	MN	G	1079	1/1	0.99	0.03	47,47,47,47	0
4	K	C	1077	1/1	0.99	0.03	27,27,27,27	0
4	K	C	1080	1/1	0.99	0.03	36,36,36,36	0
5	PO4	A	1078	5/5	0.99	0.03	17,21,24,29	0
6	CL	E	1086	1/1	0.99	0.04	41,41,41,41	0
5	PO4	C	1078	5/5	0.99	0.04	16,22,24,25	0
6	CL	E	1088	1/1	0.99	0.05	44,44,44,44	0
6	CL	F	384	1/1	0.99	0.03	32,32,32,32	0
6	CL	G	1082	1/1	0.99	0.04	29,29,29,29	0
4	K	A	1076	1/1	0.99	0.02	21,21,21,21	0
6	CL	G	1085	1/1	0.99	0.04	46,46,46,46	0
4	K	E	1080	1/1	1.00	0.02	27,27,27,27	0
3	MN	G	1074	1/1	1.00	0.03	31,31,31,31	0
3	MN	G	1075	1/1	1.00	0.03	28,28,28,28	0
3	MN	A	1074	1/1	1.00	0.03	25,25,25,25	0
4	K	G	1076	1/1	1.00	0.02	28,28,28,28	0
3	MN	A	1075	1/1	1.00	0.03	23,23,23,23	0
4	K	G	1080	1/1	1.00	0.03	38,38,38,38	0
6	CL	E	1082	1/1	1.00	0.04	24,24,24,24	0
3	MN	A	1079	1/1	1.00	0.03	37,37,37,37	0
4	K	A	1080	1/1	1.00	0.03	29,29,29,29	0
3	MN	C	1074	1/1	1.00	0.04	27,27,27,27	0
3	MN	C	1075	1/1	1.00	0.03	25,25,25,25	0
4	K	C	1076	1/1	1.00	0.02	22,22,22,22	0
3	MN	C	1079	1/1	1.00	0.03	46,46,46,46	0

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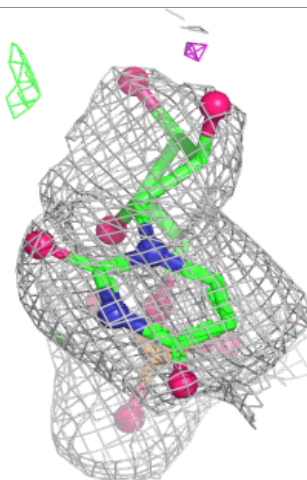
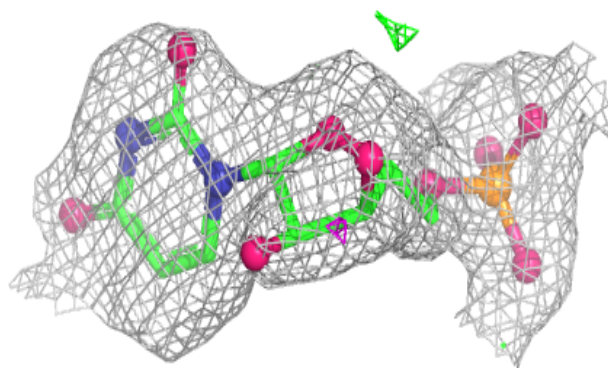
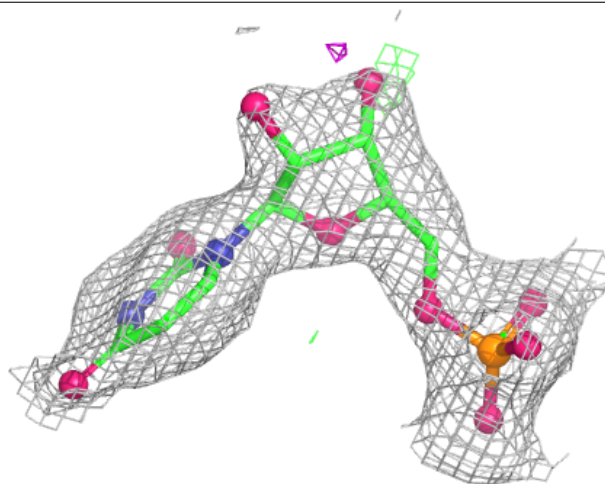
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	PO4	E	1078	5/5	1.00	0.03	19,22,26,27	0
3	MN	E	1074	1/1	1.00	0.03	27,27,27,27	0
6	CL	A	1081	1/1	1.00	0.02	28,28,28,28	0
3	MN	E	1075	1/1	1.00	0.03	27,27,27,27	0
4	K	D	383	1/1	1.00	0.02	34,34,34,34	0
4	K	E	1076	1/1	1.00	0.02	25,25,25,25	0
3	MN	E	1079	1/1	1.00	0.03	41,41,41,41	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

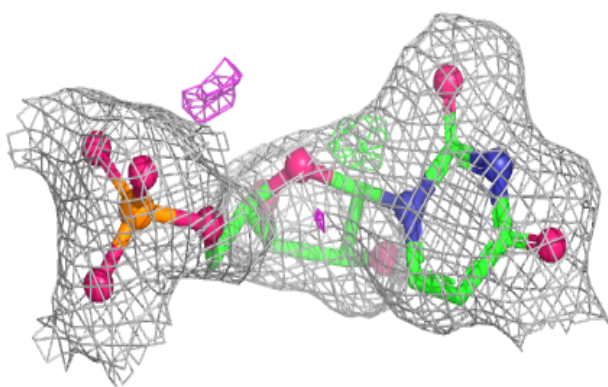
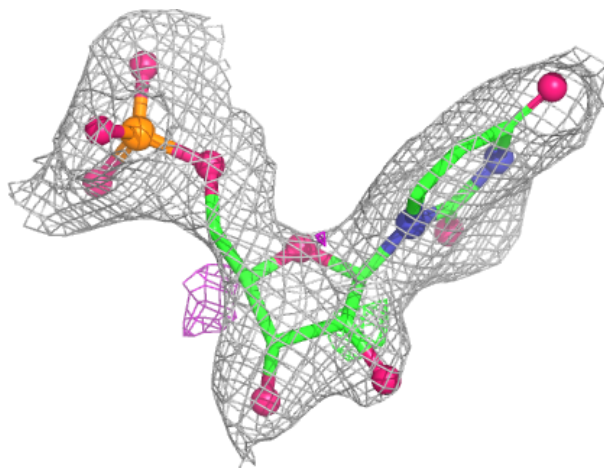
Electron density around U5P G 1093:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



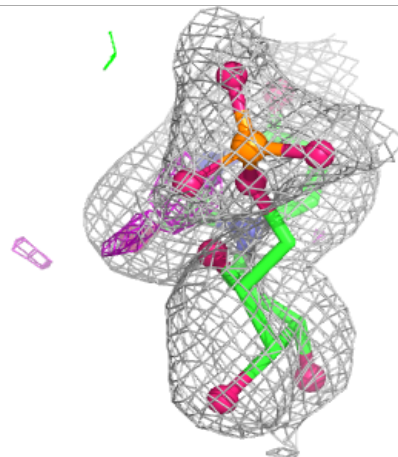
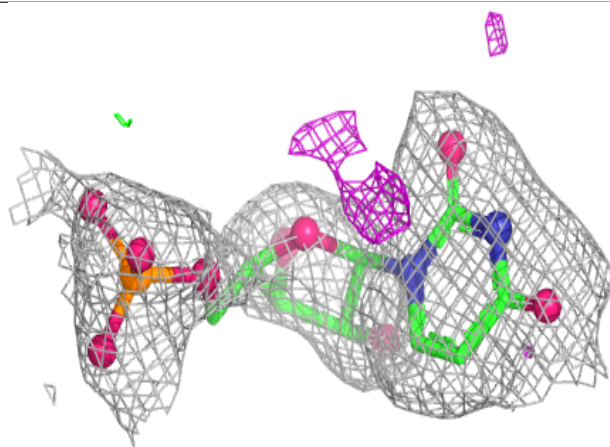
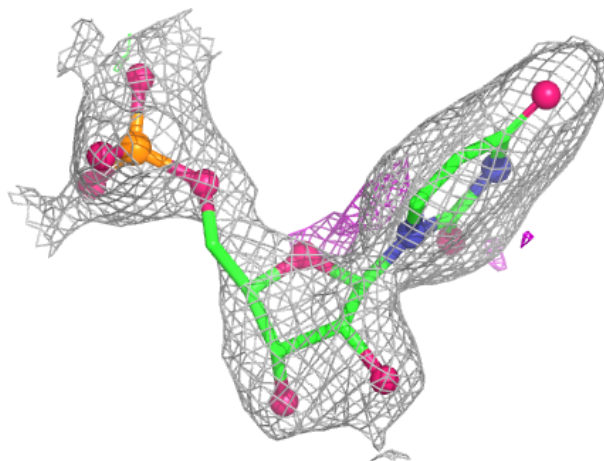
Electron density around U5P A 1091:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



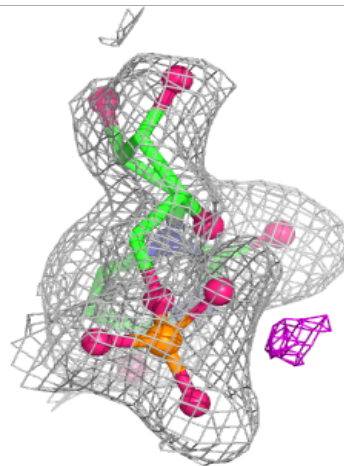
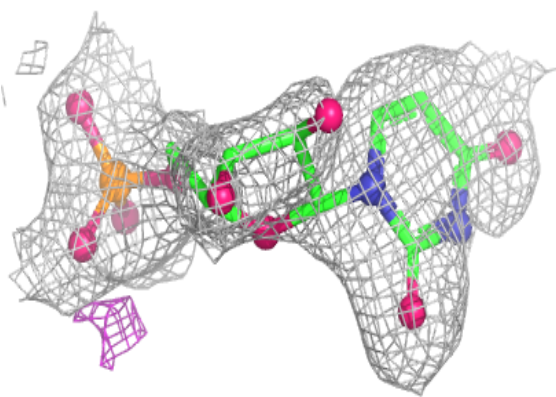
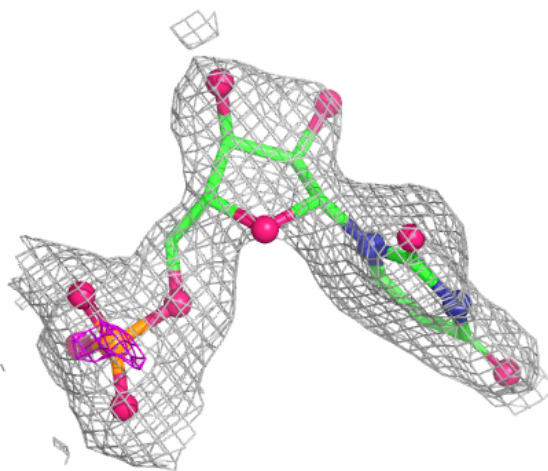
Electron density around U5P C 1093:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



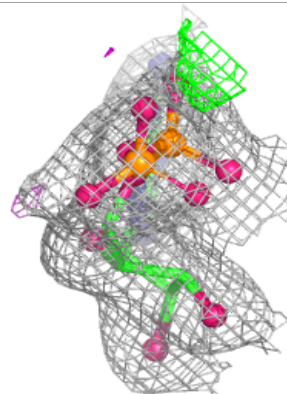
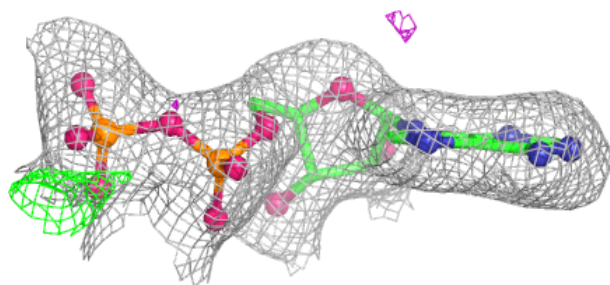
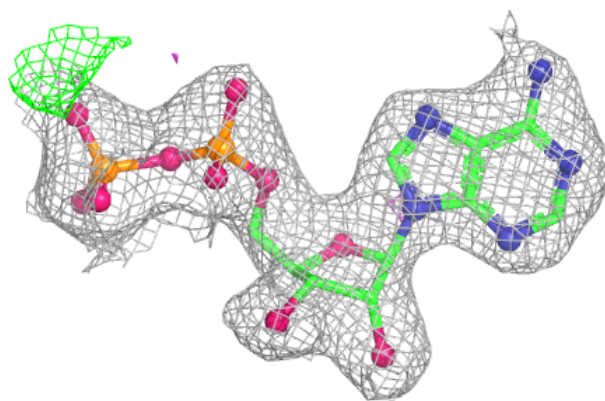
Electron density around U5P E 1093:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

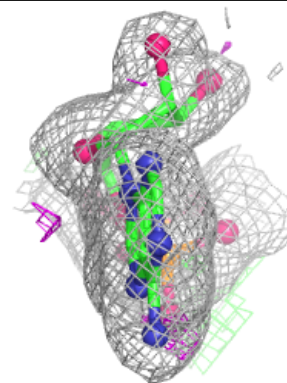
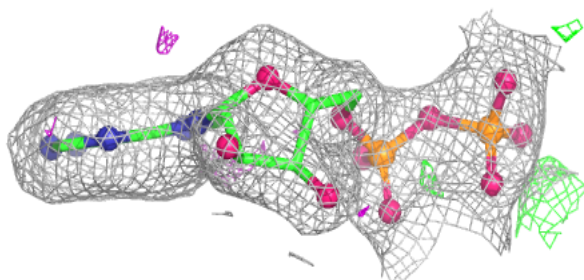
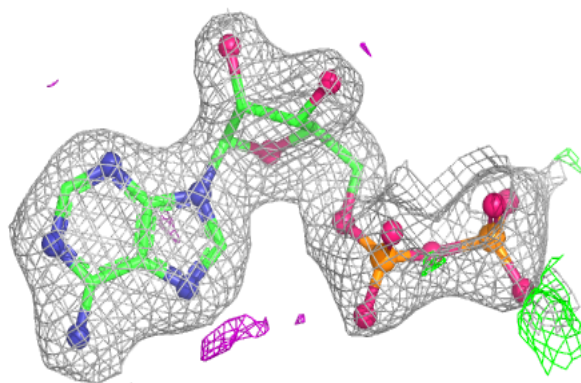


Electron density around ADP G 1090:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

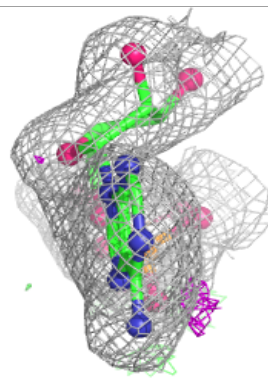
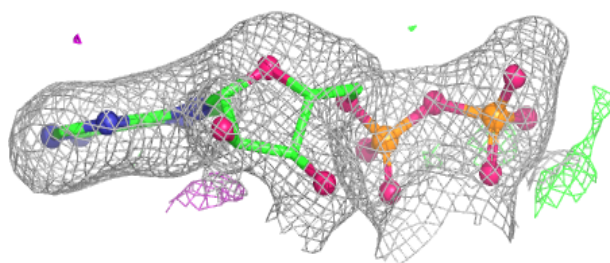
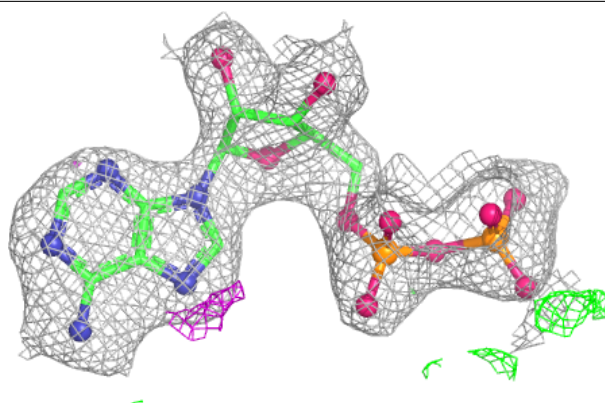
**Electron density around ADP A 1088:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

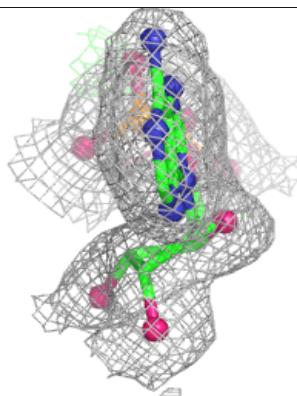
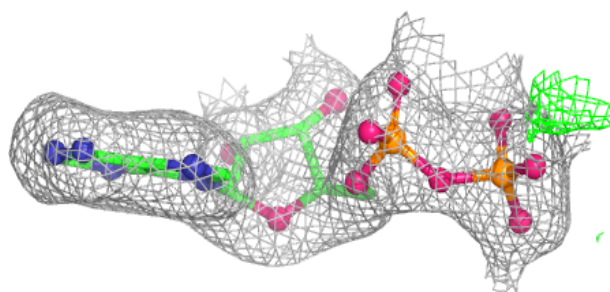
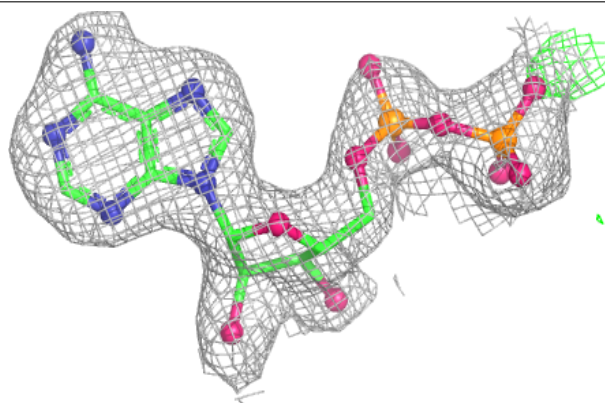


Electron density around ADP C 1090:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

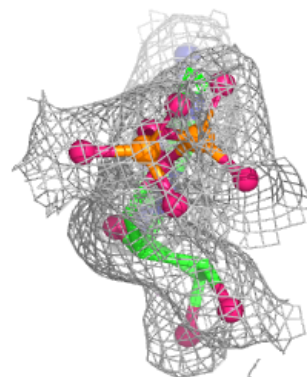
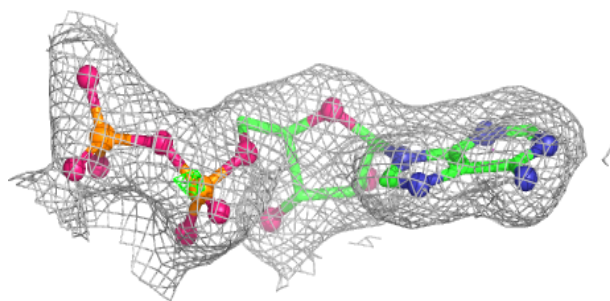
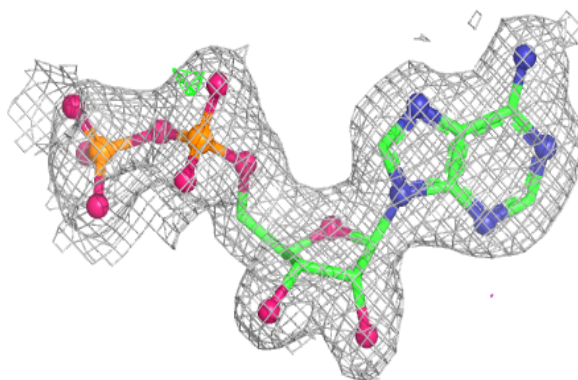
**Electron density around ADP E 1090:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

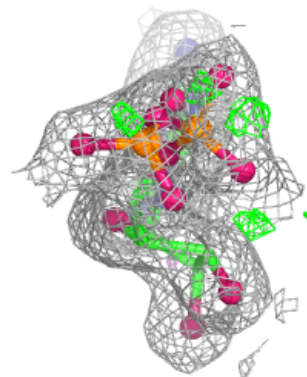
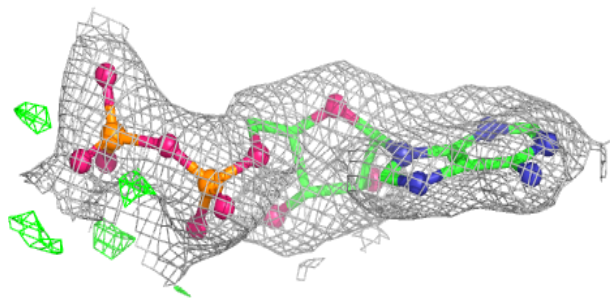
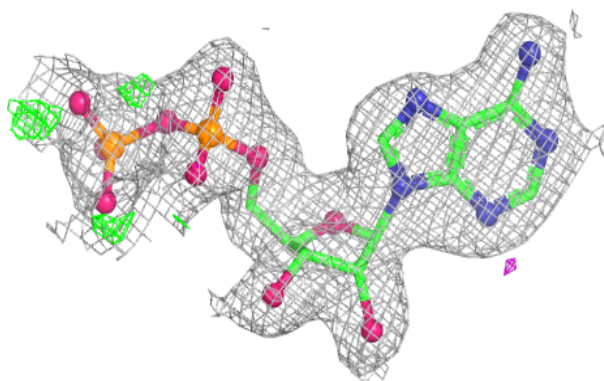


Electron density around ADP A 1087:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

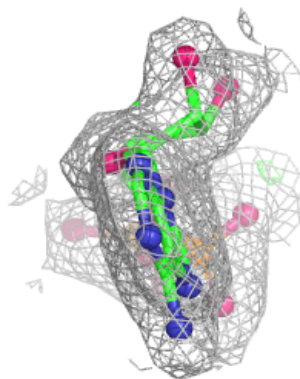
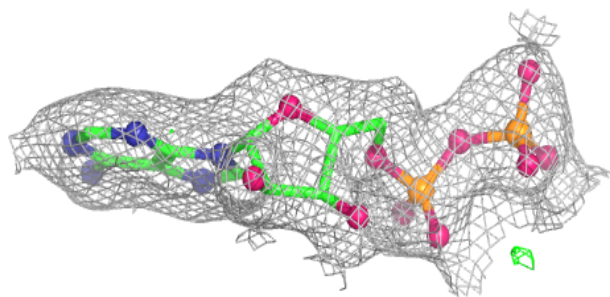
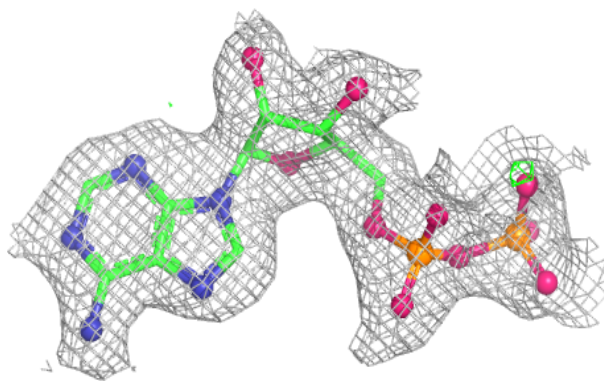
**Electron density around ADP C 1089:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

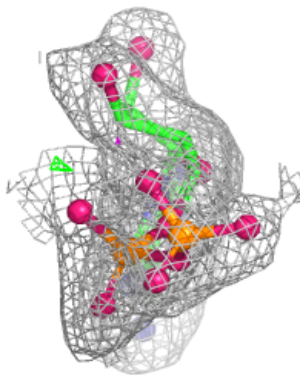
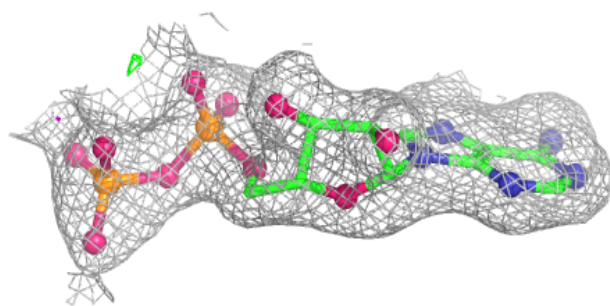
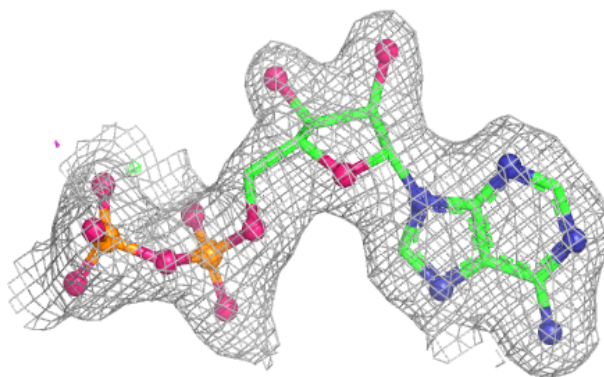


Electron density around ADP E 1089:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around ADP G 1089:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.