



wwPDB X-ray Structure Validation Summary Report

Mar 1, 2014 – 01:12 AM GMT

PDB ID : 1BXR
Title : STRUCTURE OF CARBAMOYL PHOSPHATE SYNTHETASE COM-
PLEXED WITH THE ATP ANALOG AMPPNP
Authors : Thoden, J.B.; Wesenberg, G.; Raushel, F.M.; Holden, H.M.
Deposited on : 1998-10-08
Resolution : 2.10 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

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

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

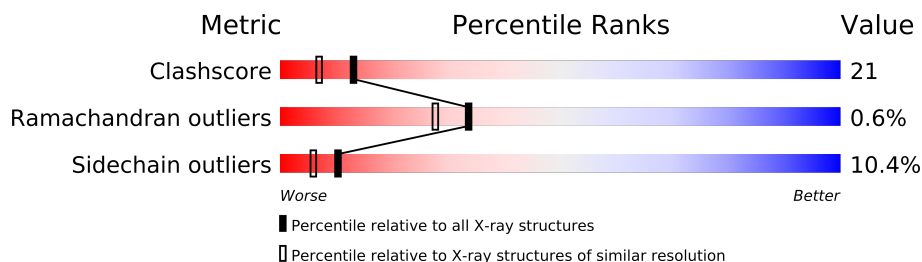
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	21963
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

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	79885	3649 (2.10-2.10)
Ramachandran outliers	78287	3610 (2.10-2.10)
Sidechain outliers	78261	3611 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	1073	
1	C	1073	
1	E	1073	
1	G	1073	
2	B	382	
2	D	382	
2	F	382	
2	H	382	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 48307 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1073	Total	C	N	O	S	0	4	0
			8288	5203	1445	1594	46			
1	C	1073	Total	C	N	O	S	0	0	0
			8268	5190	1441	1592	45			
1	E	1073	Total	C	N	O	S	0	3	0
			8284	5199	1445	1595	45			
1	G	1073	Total	C	N	O	S	0	2	0
			8279	5196	1445	1593	45			

- Molecule 2 is a protein called CARBAMOYL-PHOSPHATE SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	379	Total	C	N	O	S	0	0	0
			2895	1825	509	551	10			
2	D	379	Total	C	N	O	S	0	0	0
			2895	1825	509	551	10			
2	F	379	Total	C	N	O	S	0	0	0
			2895	1825	509	551	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	G	3	Total Mn 3 3	0	0
3	A	3	Total Mn 3 3	0	0
3	C	4	Total Mn 4 4	0	0
3	E	3	Total Mn 3 3	0	0

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

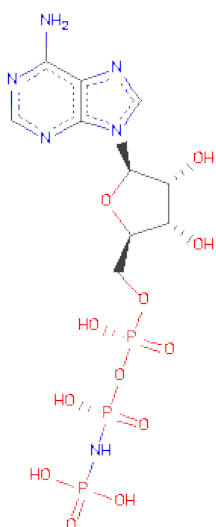
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	4	Total K 4 4	0	0
4	D	1	Total K 1 1	0	0
4	E	5	Total K 5 5	0	0
4	H	1	Total K 1 1	0	0
4	B	1	Total K 1 1	0	0
4	C	4	Total K 4 4	0	0
4	A	3	Total K 3 3	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	G	4	Total Cl 4 4	0	0
5	D	1	Total Cl 1 1	0	0
5	E	2	Total Cl 2 2	0	0
5	B	1	Total Cl 1 1	0	0
5	C	3	Total Cl 3 3	0	0
5	A	3	Total Cl 3 3	0	0

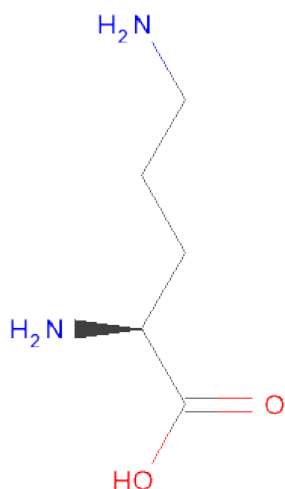
- Molecule 6 is PHOSPHOAMINOPHOSPHONICACID-ADENYLATE ESTER (three-letter

code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



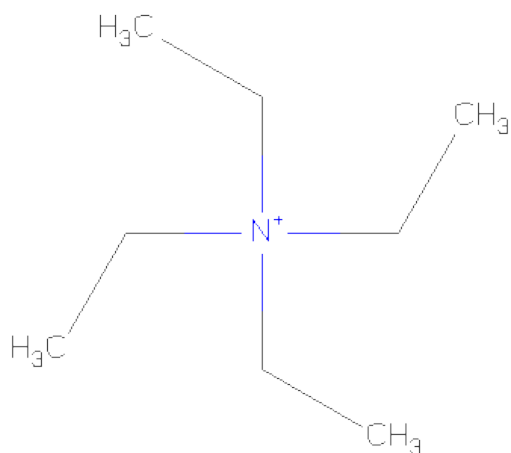
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
6	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
6	C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
6	C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
6	E	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
6	E	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
6	G	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
6	G	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

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



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

- Molecule 8 is TETRAETHYLAMMONIUM ION (three-letter code: NET) (formula: C₈H₂₀N).



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

- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	677	Total O 677 677	0	0
9	B	169	Total O 169 169	0	0
9	C	624	Total O 624 624	0	0
9	D	234	Total O 234 234	0	0
9	E	650	Total O 650 650	0	0
9	F	193	Total O 193 193	0	0
9	G	530	Total O 530 530	0	0
9	H	165	Total O 165 165	0	0

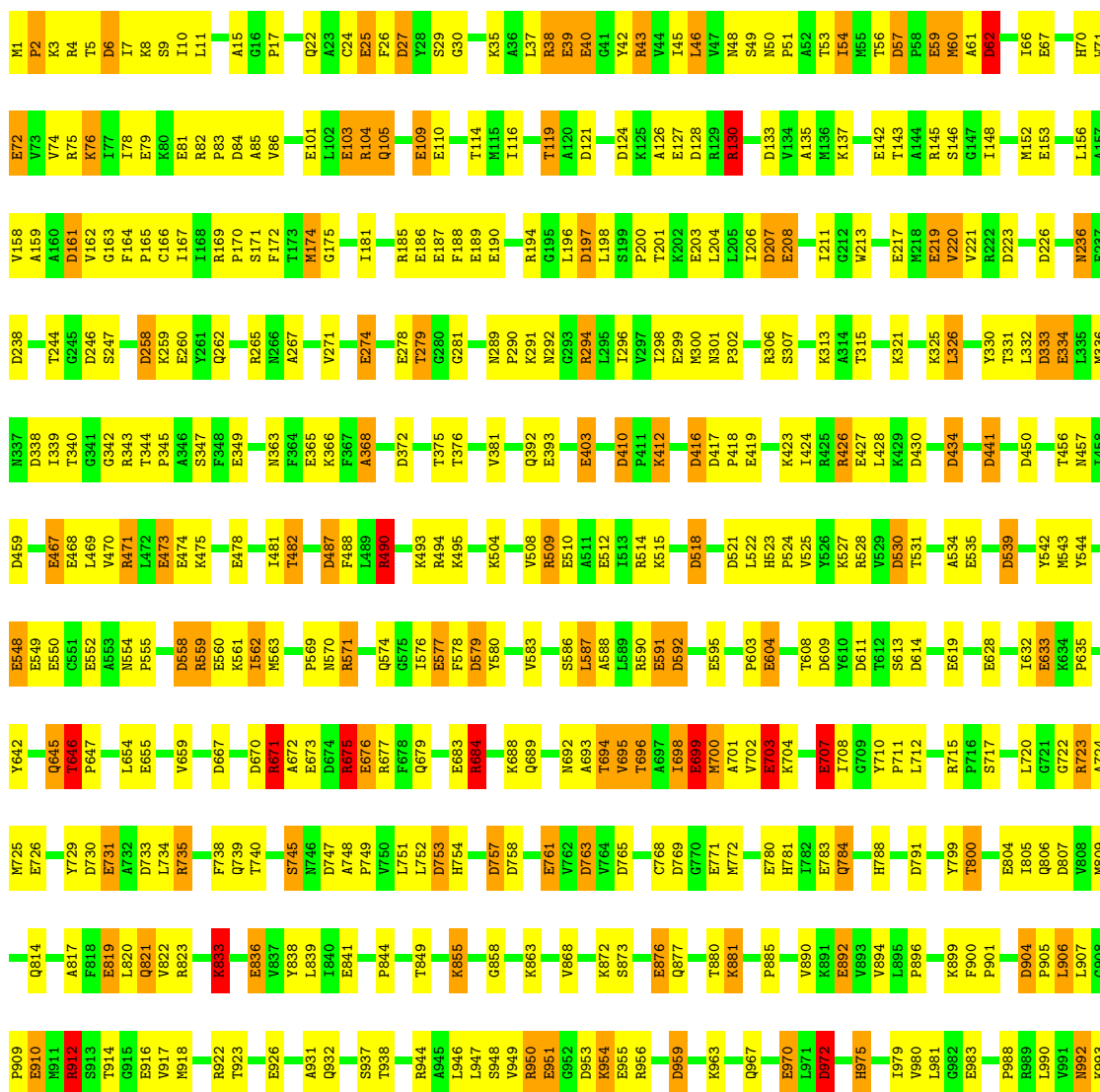
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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 SYNTHASE

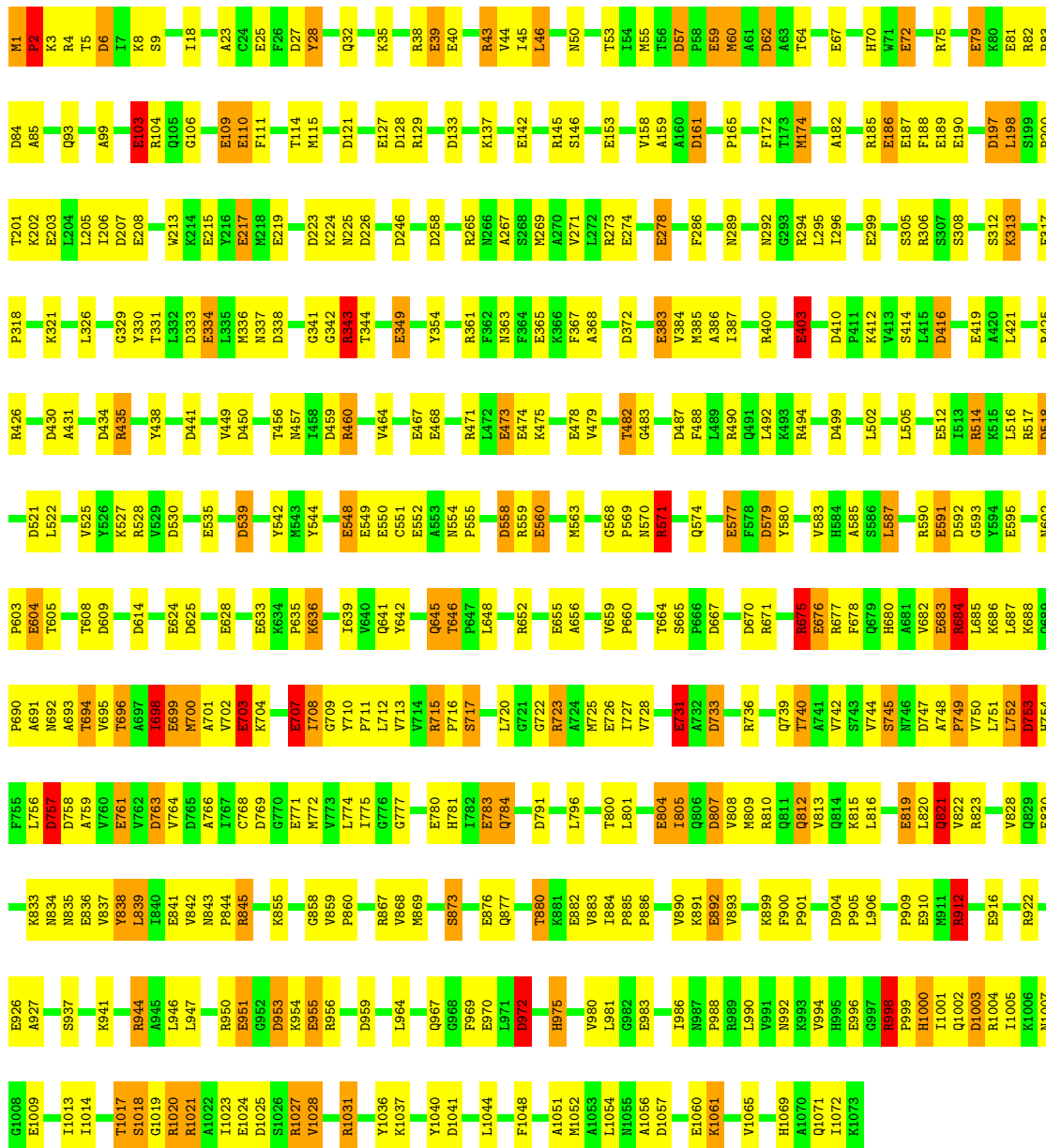
Chain A:





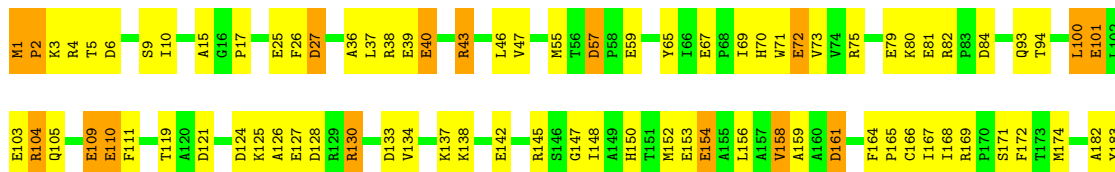
• Molecule 1: CARBAMOYL-PHOSPHATE SYNTHASE

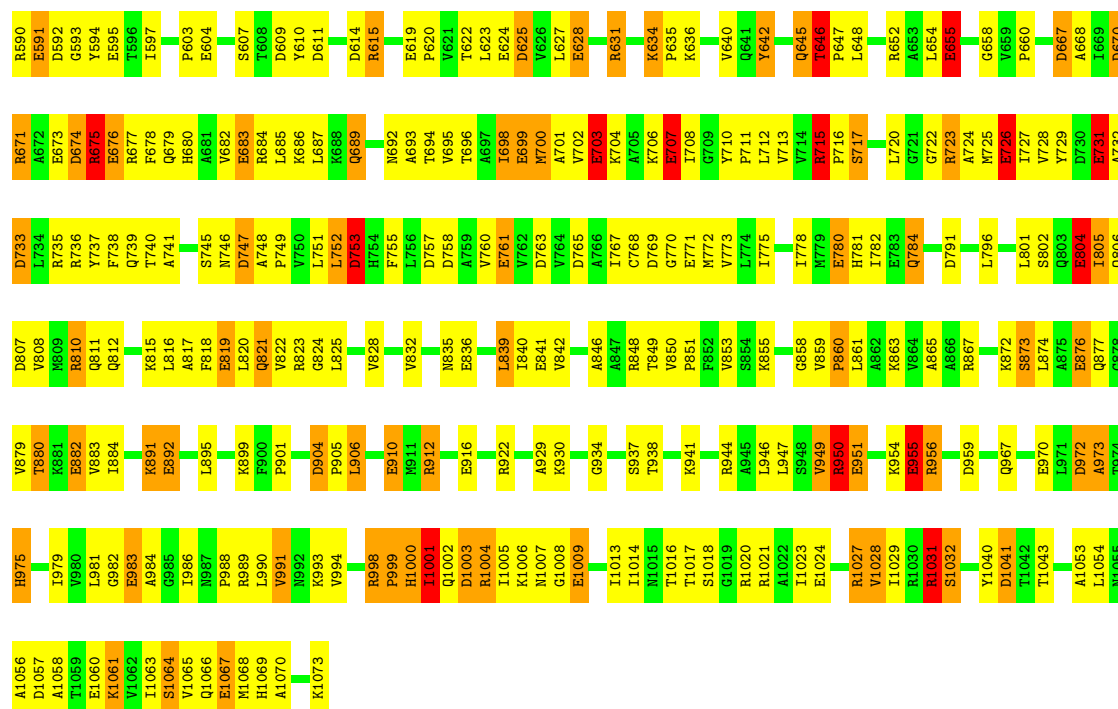
Chain C:



• Molecule 1: CARBAMOYL-PHOSPHATE SYNTHASE

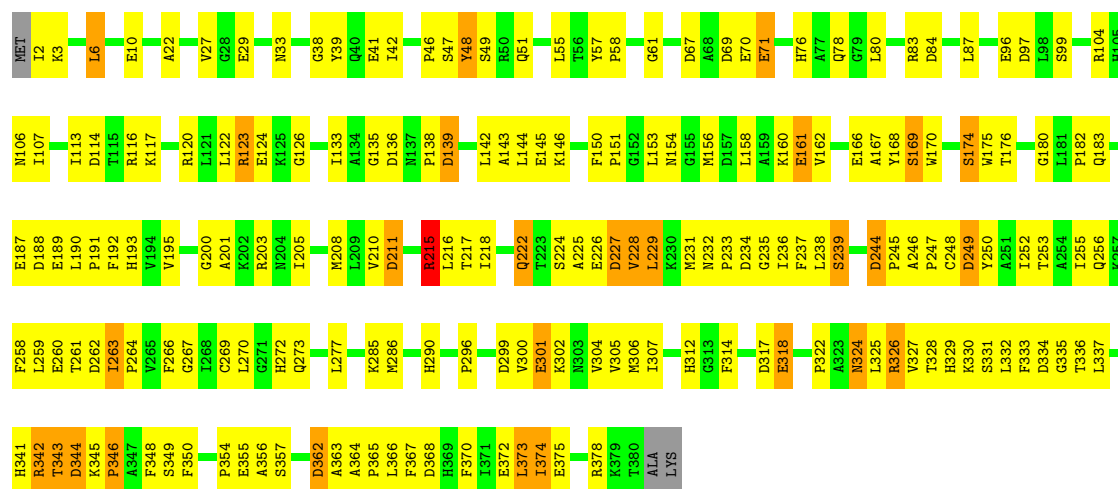
Chain E:





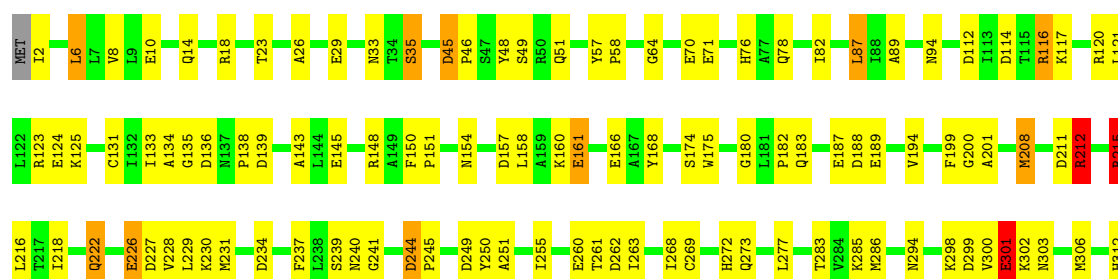
• Molecule 2: CARBAMOYL-PHOSPHATE SYNTHASE

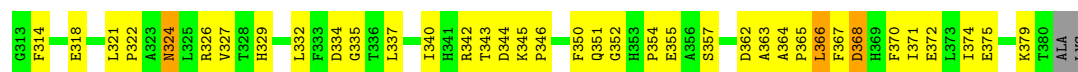
Chain B:



• Molecule 2: CARBAMOYL-PHOSPHATE SYNTHASE

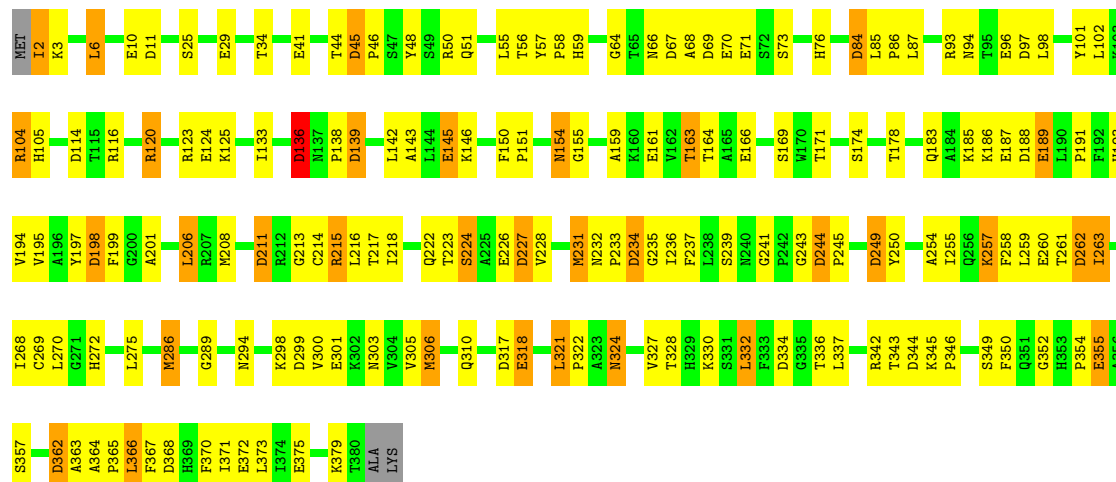
Chain D:





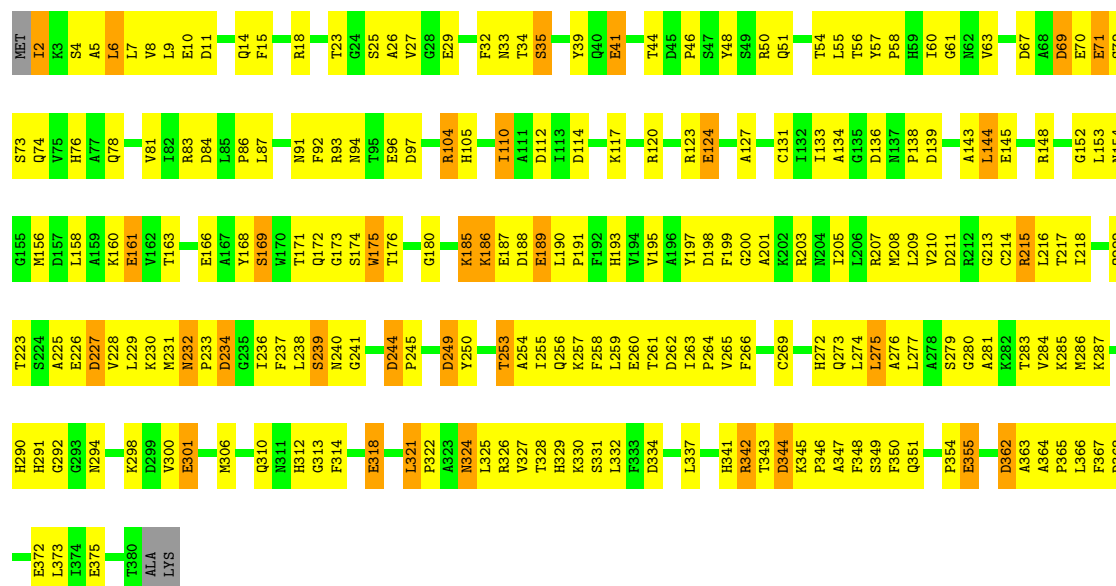
• Molecule 2: CARBAMOYL-PHOSPHATE SYNTHASE

Chain F:



• Molecule 2: CARBAMOYL-PHOSPHATE SYNTHASE

Chain H:



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	151.90Å 164.50Å 332.60Å 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}	(Not available)	Depositor
R_{sym}	0.05	Depositor
Refinement program	TNT V. 5-E	Depositor
R, R_{free}	0.195 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	48307	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, K, MN, ORN, ANP, 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	1.01	83/8435 (1.0%)	1.41	129/11407 (1.1%)
1	C	1.01	81/8399 (1.0%)	1.38	129/11361 (1.1%)
1	E	1.01	82/8427 (1.0%)	1.38	122/11398 (1.1%)
1	G	1.02	82/8418 (1.0%)	1.39	140/11386 (1.2%)
2	B	0.87	19/2957 (0.6%)	1.28	33/4016 (0.8%)
2	D	0.91	16/2957 (0.5%)	1.31	38/4016 (0.9%)
2	F	0.89	19/2957 (0.6%)	1.28	41/4016 (1.0%)
2	H	0.89	19/2957 (0.6%)	1.30	33/4016 (0.8%)
All	All	0.98	401/45507 (0.9%)	1.36	665/61616 (1.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	G	0	1
2	F	1	0
All	All	1	1

The worst 5 of 401 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	39	GLU	CD-OE1	9.89	1.36	1.25
2	H	10	GLU	CD-OE1	9.59	1.36	1.25
1	G	153	GLU	CD-OE1	8.90	1.35	1.25
1	C	110	GLU	CD-OE1	8.43	1.34	1.25
1	G	103	GLU	CD-OE1	8.38	1.34	1.25

The worst 5 of 665 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	912[A]	ARG	NE-CZ-NH2	-15.00	112.80	120.30
1	A	912[B]	ARG	NE-CZ-NH2	-15.00	112.80	120.30
1	A	912[A]	ARG	NE-CZ-NH1	14.54	127.57	120.30
1	A	912[B]	ARG	NE-CZ-NH1	14.54	127.57	120.30
1	C	667	ASP	CB-CG-OD1	-13.42	106.22	118.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	F	50	ARG	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	1008	GLY	Mainchain

5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8288	0	8332	325	0
1	C	8268	0	8308	306	0
1	E	8284	0	8321	276	0
1	G	8279	0	8320	437	0
2	B	2895	0	2863	146	0
2	D	2895	0	2863	85	0
2	F	2895	0	2863	126	0
2	H	2895	0	2863	160	0
3	A	3	0	0	0	0
3	C	4	0	0	0	0
3	E	3	0	0	0	0
3	G	3	0	0	0	0
4	A	3	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	5	0	0	0	0
4	G	4	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	2	0	0	2	0
5	G	4	0	0	0	0
6	A	62	0	26	3	0
6	C	62	0	26	1	0
6	E	62	0	25	3	0
6	G	62	0	26	4	0
7	A	9	0	11	1	0
7	C	9	0	11	1	0
7	E	9	0	11	1	0
7	G	9	0	11	1	0
8	A	9	0	20	6	0
8	C	9	0	20	4	0
8	E	9	0	20	6	0
8	G	9	0	20	4	0
9	A	677	0	0	21	0
9	B	169	0	0	2	0
9	C	624	0	0	20	0
9	D	234	0	0	2	0
9	E	650	0	0	13	0
9	F	193	0	0	7	0
9	G	530	0	0	22	0
9	H	165	0	0	6	0
All	All	48307	0	44960	1851	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 21.

The worst 5 of 1851 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:967:GLN:HG2	1:C:1054:LEU:HD13	1.26	1.16
1:C:574:GLN:NE2	1:C:645:GLN:H	1.44	1.13
1:A:172:PHE:HB3	1:A:200:PRO:HG2	1.32	1.12
2:F:322:PRO:HB2	2:F:324:ASN:HD21	1.12	1.10
1:C:574:GLN:HE22	1:C:645:GLN:N	1.51	1.09

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1075/1073 (100%)	1008 (94%)	63 (6%)	4 (0%)	43	39
1	C	1071/1073 (100%)	1009 (94%)	54 (5%)	8 (1%)	30	23
1	E	1074/1073 (100%)	1020 (95%)	48 (4%)	6 (1%)	33	28
1	G	1073/1073 (100%)	993 (92%)	72 (7%)	8 (1%)	30	23
2	B	377/382 (99%)	350 (93%)	23 (6%)	4 (1%)	21	13
2	D	377/382 (99%)	363 (96%)	14 (4%)	0	100	100
2	F	377/382 (99%)	361 (96%)	14 (4%)	2 (0%)	38	33
2	H	377/382 (99%)	358 (95%)	19 (5%)	0	100	100
All	All	5801/5820 (100%)	5462 (94%)	307 (5%)	32 (1%)	33	28

5 of 32 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	975	HIS
2	F	136	ASP
1	G	975	HIS
2	B	346	PRO
1	C	707	GLU

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	882/878 (100%)	785 (89%)	97 (11%)	9 5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	878/878 (100%)	783 (89%)	95 (11%)	9	5
1	E	881/878 (100%)	800 (91%)	81 (9%)	13	8
1	G	880/878 (100%)	761 (86%)	119 (14%)	6	3
2	B	308/310 (99%)	279 (91%)	29 (9%)	13	8
2	D	308/310 (99%)	290 (94%)	18 (6%)	28	23
2	F	308/310 (99%)	282 (92%)	26 (8%)	16	10
2	H	308/310 (99%)	276 (90%)	32 (10%)	10	6
All	All	4753/4752 (100%)	4256 (90%)	497 (10%)	10	5

5 of 497 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	49	SER
1	E	652	ARG
1	G	1027	ARG
2	D	222	GLN
1	E	236	ASN

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

Mol	Chain	Res	Type
2	D	78	GLN
1	E	689	GLN
2	H	78	GLN
2	D	154	ASN
1	E	105	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 62 ligands modelled in this entry, 46 are monoatomic - leaving 16 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$
6	ANP	A	1083	3	33,33,33	1.84	7 (21%)	51,52,52	1.54	6 (11%)
6	ANP	A	1084	3	33,33,33	1.81	5 (15%)	51,52,52	1.40	6 (11%)
7	ORN	A	1085	-	8,8,8	0.72	0	9,9,9	1.48	2 (22%)
8	NET	A	1086	-	8,8,8	0.70	0	10,10,10	0.44	0
6	ANP	C	1900	3	33,33,33	1.70	7 (21%)	51,52,52	1.50	4 (7%)
6	ANP	C	1910	3	33,33,33	1.75	6 (18%)	51,52,52	1.69	9 (17%)
7	ORN	C	1920	-	8,8,8	0.79	0	9,9,9	1.01	1 (11%)
8	NET	C	1950	-	8,8,8	0.60	0	10,10,10	0.63	0
6	ANP	E	2900	3	33,33,33	1.58	5 (15%)	51,52,52	1.52	5 (9%)
6	ANP	E	2910	3	33,33,33	1.50	4 (12%)	51,52,52	1.56	5 (9%)
7	ORN	E	2920	-	8,8,8	0.77	0	9,9,9	1.02	1 (11%)
8	NET	E	2950	-	8,8,8	0.55	0	10,10,10	0.53	0
6	ANP	G	3900	3	33,33,33	1.47	7 (21%)	51,52,52	1.57	7 (13%)
6	ANP	G	3910	3	33,33,33	1.46	5 (15%)	51,52,52	1.61	6 (11%)
7	ORN	G	3920	-	8,8,8	0.64	0	9,9,9	1.17	2 (22%)
8	NET	G	3950	-	8,8,8	0.62	0	10,10,10	0.51	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
6	ANP	A	1083	3	-	0/18/38/38	0/1/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	ANP	A	1084	3	-	1/18/38/38	0/1/3/3
7	ORN	A	1085	-	-	0/8/8/8	0/0/0/0
8	NET	A	1086	-	-	0/12/12/12	0/0/0/0
6	ANP	C	1900	3	-	2/18/38/38	0/1/3/3
6	ANP	C	1910	3	-	0/18/38/38	0/1/3/3
7	ORN	C	1920	-	-	0/8/8/8	0/0/0/0
8	NET	C	1950	-	-	0/12/12/12	0/0/0/0
6	ANP	E	2900	3	-	1/18/38/38	0/1/3/3
6	ANP	E	2910	3	-	0/18/38/38	0/1/3/3
7	ORN	E	2920	-	-	0/8/8/8	0/0/0/0
8	NET	E	2950	-	-	0/12/12/12	0/0/0/0
6	ANP	G	3900	3	-	1/18/38/38	0/1/3/3
6	ANP	G	3910	3	-	1/18/38/38	0/1/3/3
7	ORN	G	3920	-	-	0/8/8/8	0/0/0/0
8	NET	G	3950	-	-	0/12/12/12	0/0/0/0

The worst 5 of 46 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1083	ANP	PG-O1G	6.51	1.54	1.46
6	C	1900	ANP	PG-N3B	-5.30	1.59	1.64
6	C	1910	ANP	PB-O1B	5.26	1.52	1.46
6	E	2910	ANP	PB-O1B	5.23	1.52	1.46
6	A	1084	ANP	PB-O1B	5.19	1.52	1.46

The worst 5 of 54 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	3910	ANP	N3-C2-N1	-6.95	122.90	128.71
6	E	2910	ANP	N3-C2-N1	-6.66	123.14	128.71
6	C	1900	ANP	N3-C2-N1	-6.50	123.27	128.71
6	E	2900	ANP	N3-C2-N1	-6.48	123.29	128.71
6	A	1083	ANP	N3-C2-N1	-5.88	123.79	128.71

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	G	3900	ANP	O1G-PG-N3B-PB
6	G	3910	ANP	O1G-PG-N3B-PB
6	C	1900	ANP	O1G-PG-N3B-PB

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Mol	Chain	Res	Type	Atoms
6	A	1084	ANP	O1G-PG-N3B-PB
6	E	2900	ANP	O1G-PG-N3B-PB

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.