



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 06:42 PM 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 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

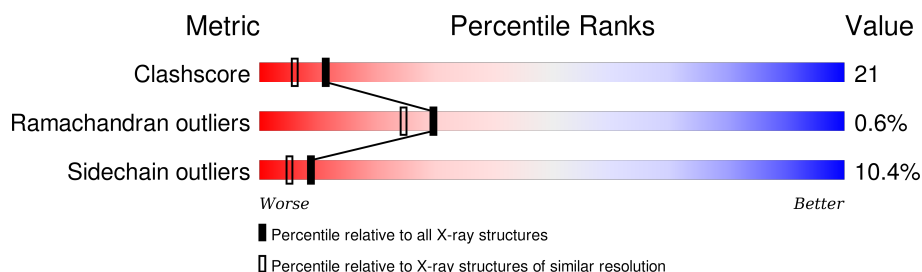
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (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. 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.

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	

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Mol	Chain	Length	Quality of chain
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	CL	E	2980	-	-	X	-
8	NET	A	1086	-	-	X	-
8	NET	E	2950	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 48307 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.

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).

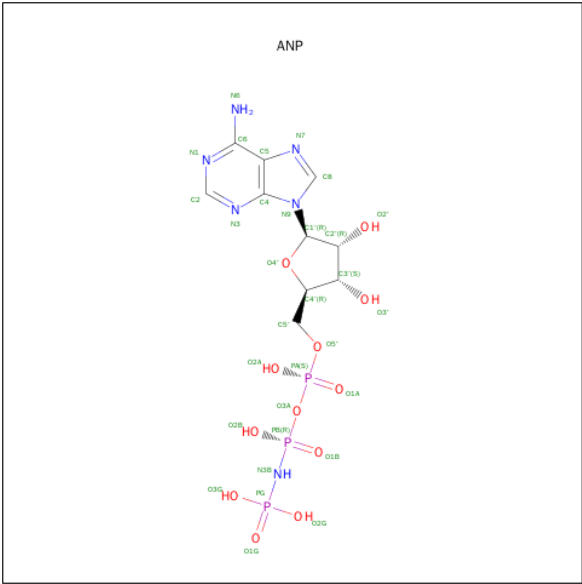
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	4	Total K 4 4	0	0
4	D	1	Total K 1 1	0	0
4	E	5	Total K 5 5	0	0
4	H	1	Total K 1 1	0	0
4	B	1	Total K 1 1	0	0
4	C	4	Total K 4 4	0	0
4	A	3	Total K 3 3	0	0

- 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

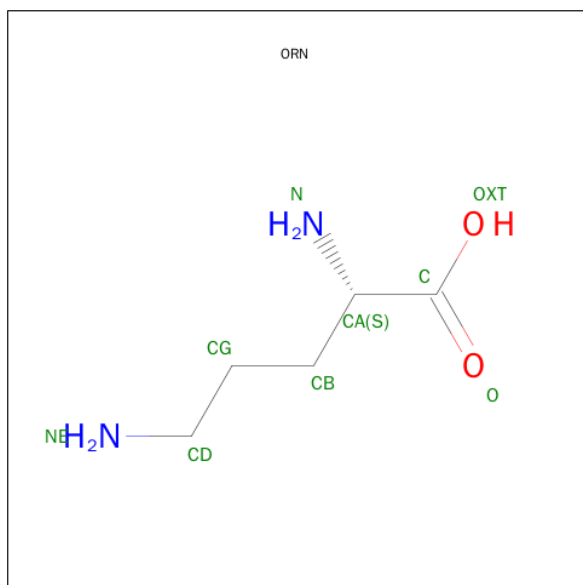
- Molecule 6 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter

code: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



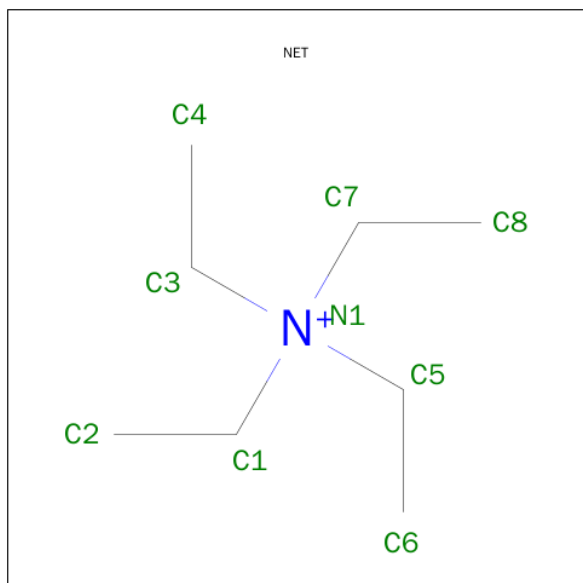
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
6	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
6	C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
6	C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
6	E	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
6	E	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
6	G	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: C₅H₁₂N₂O₂).



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: $C_8H_{20}N$).



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.

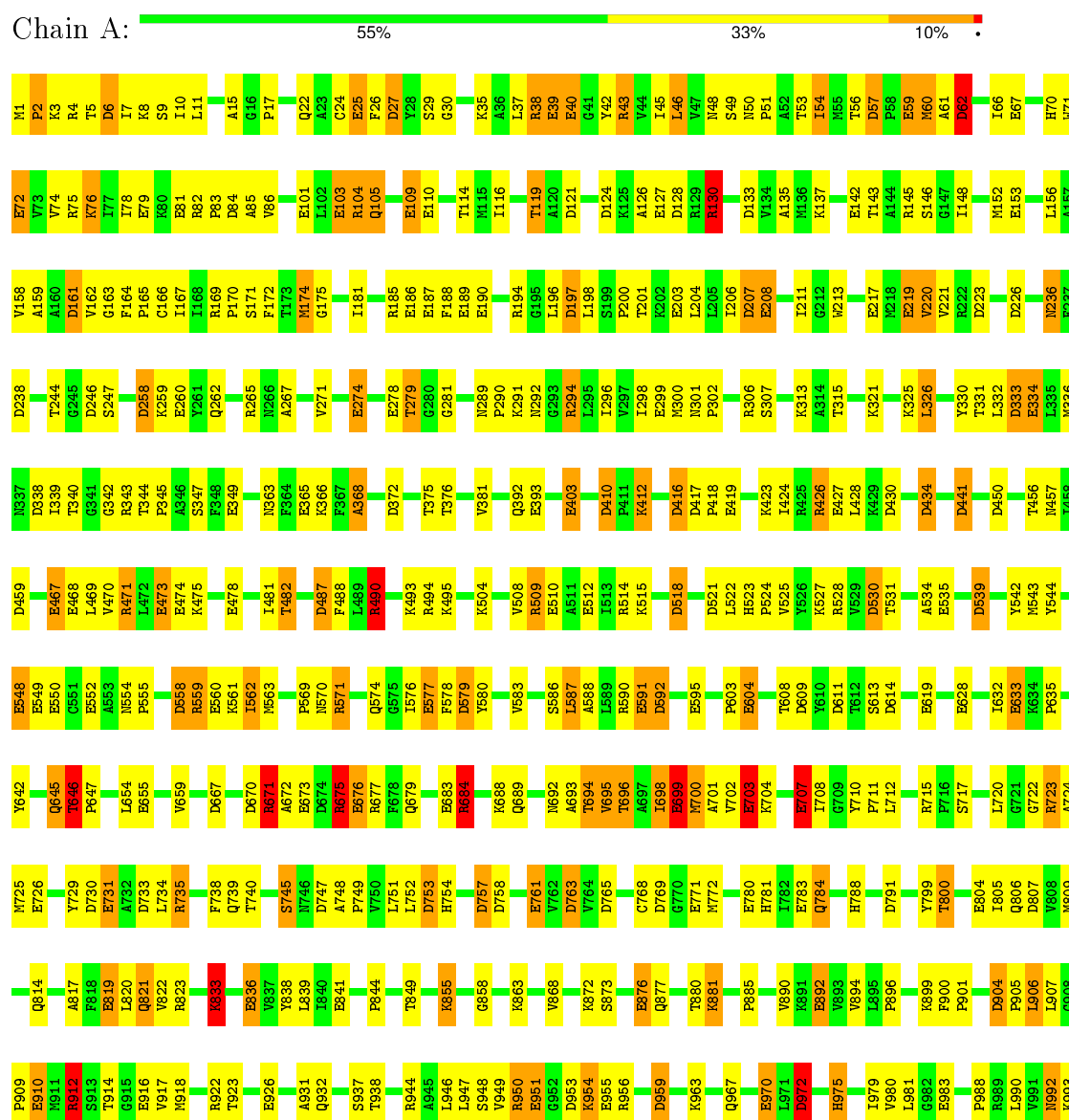
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	677	Total O 677 677	0	0
9	B	169	Total O 169 169	0	0
9	C	624	Total O 624 624	0	0
9	D	234	Total O 234 234	0	0
9	E	650	Total O 650 650	0	0
9	F	193	Total O 193 193	0	0
9	G	530	Total O 530 530	0	0
9	H	165	Total O 165 165	0	0

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.

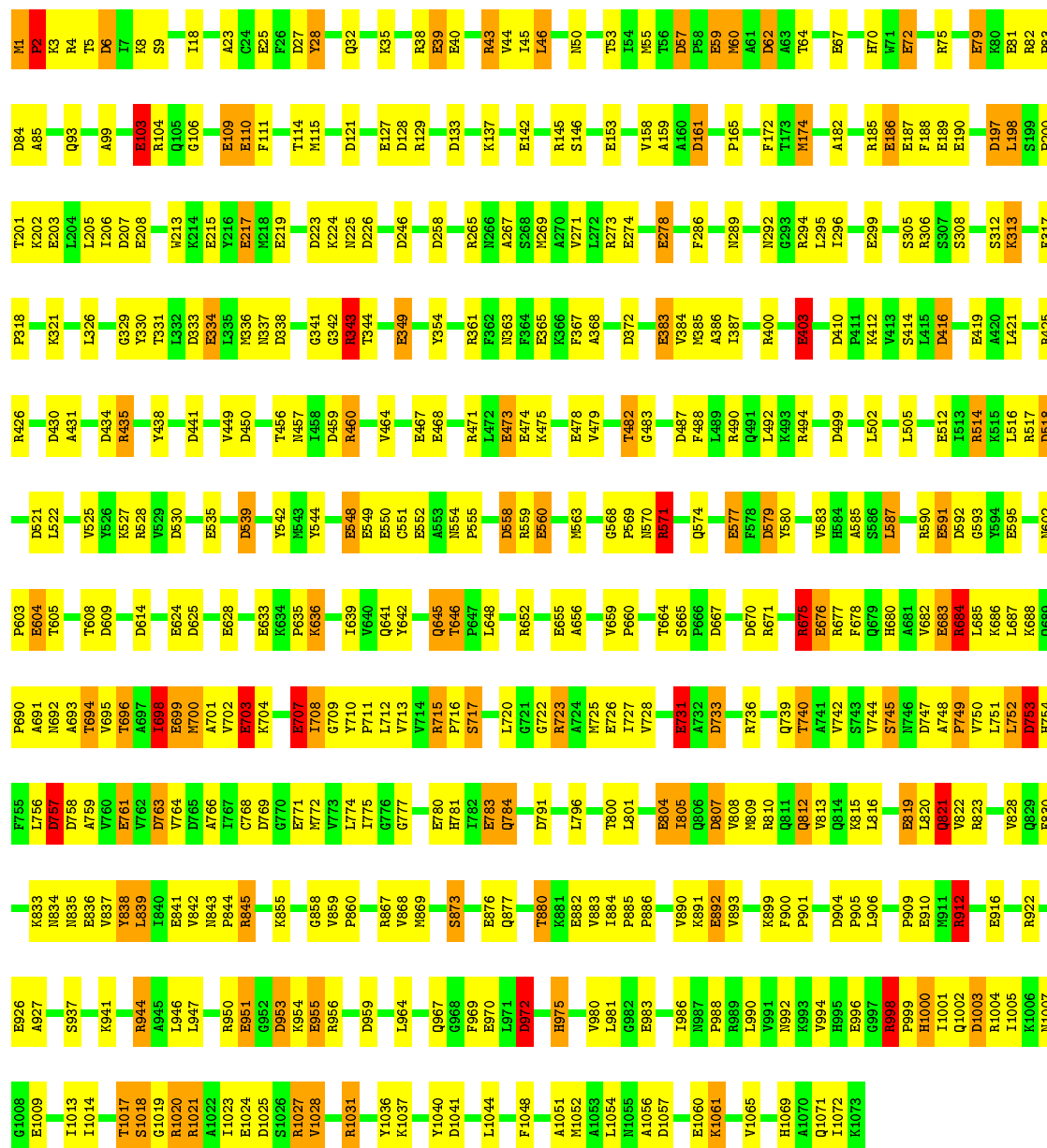
• Molecule 1: CARBAMOYL-PHOSPHATE SYNTHASE





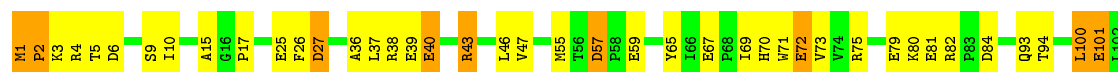
• Molecule 1: CARBAMOYL-PHOSPHATE SYNTHASE

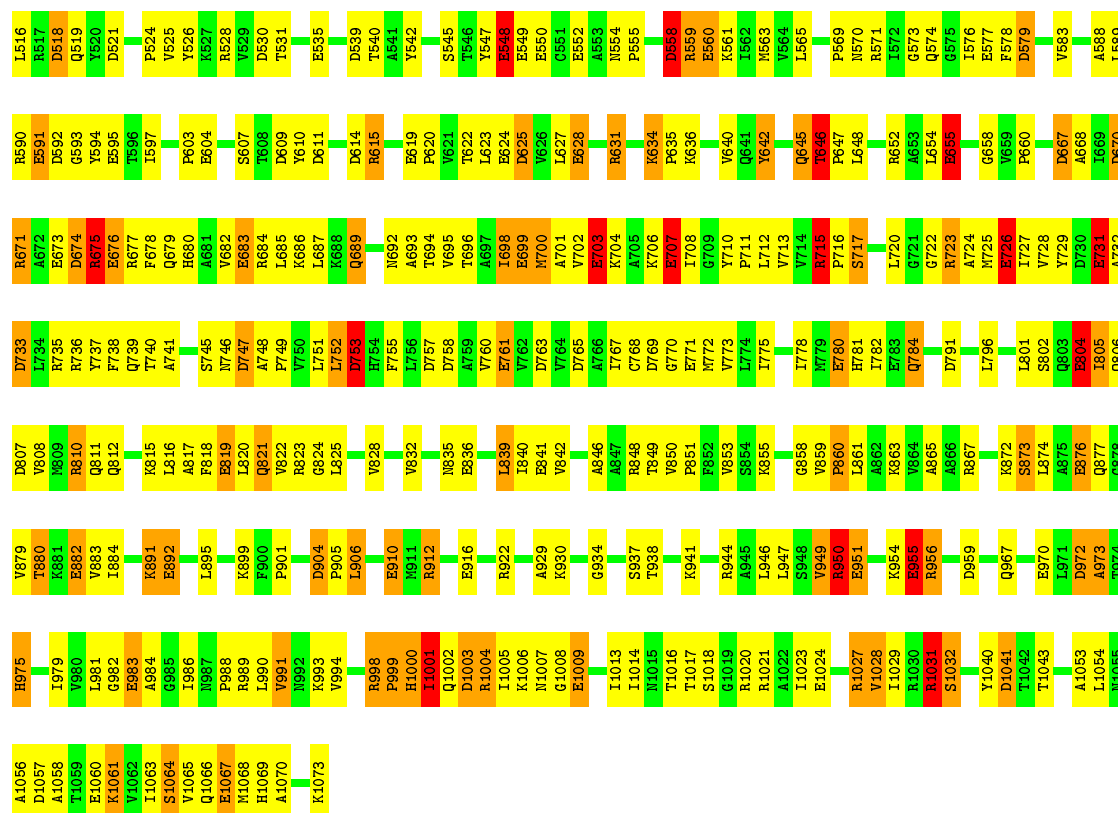
Chain C: 57% 33% 8%



• Molecule 1: CARBAMOYL-PHOSPHATE SYNTHASE

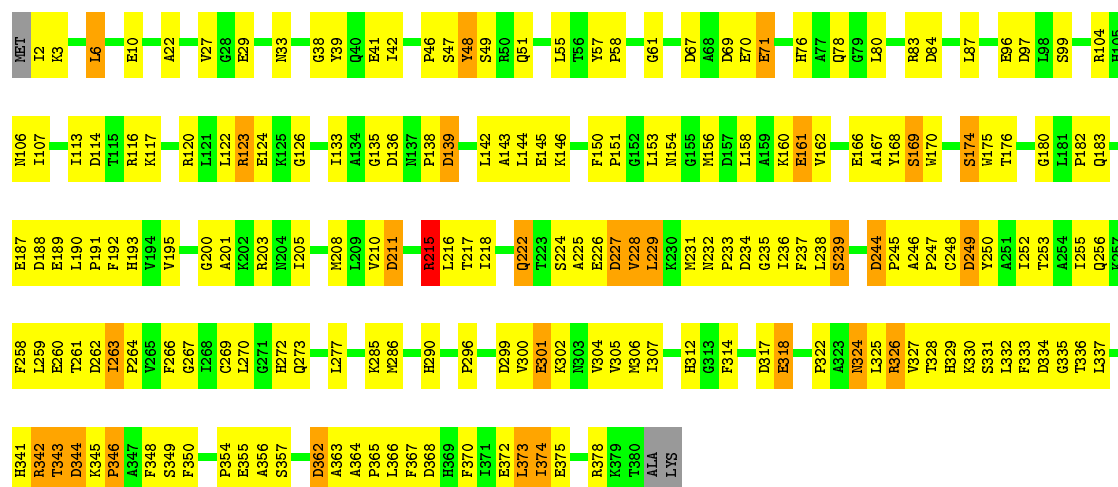
Chain E: 60% 31% 9%





• Molecule 2: CARBAMOYL-PHOSPHATE SYNTHASE

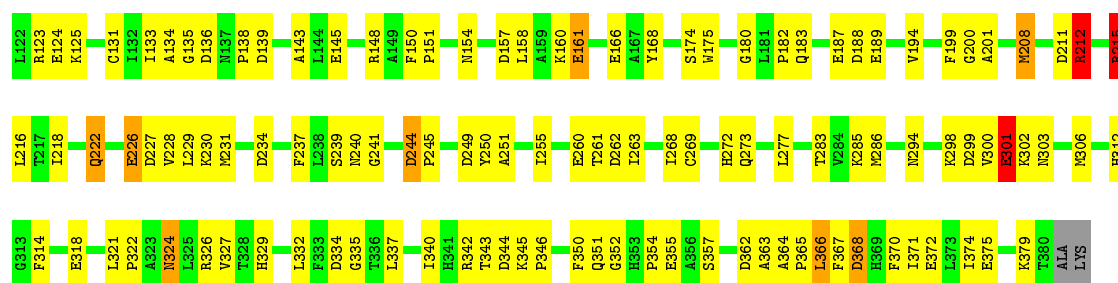
Chain B: 49% 43% 7%



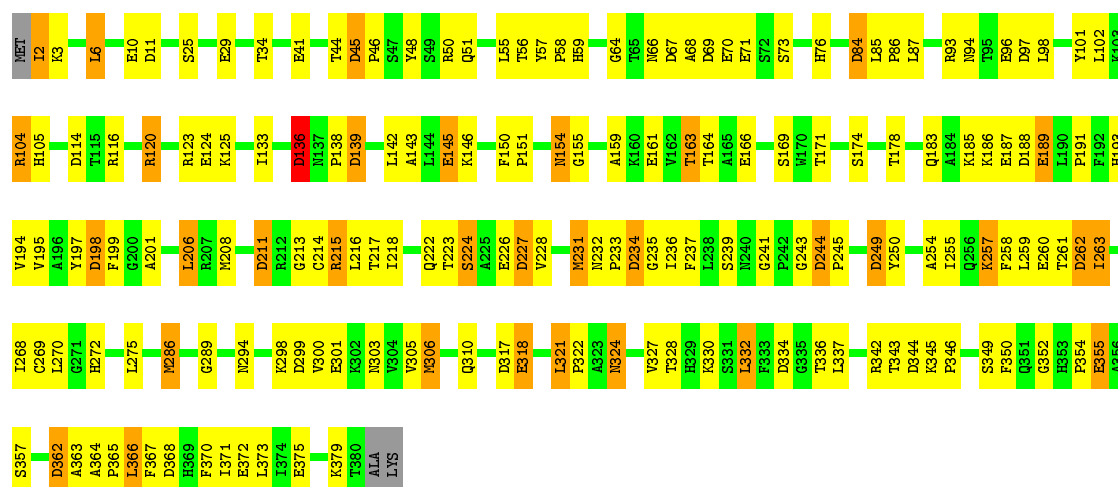
• Molecule 2: CARBAMOYL-PHOSPHATE SYNTHASE

Chain D: 60% 35%

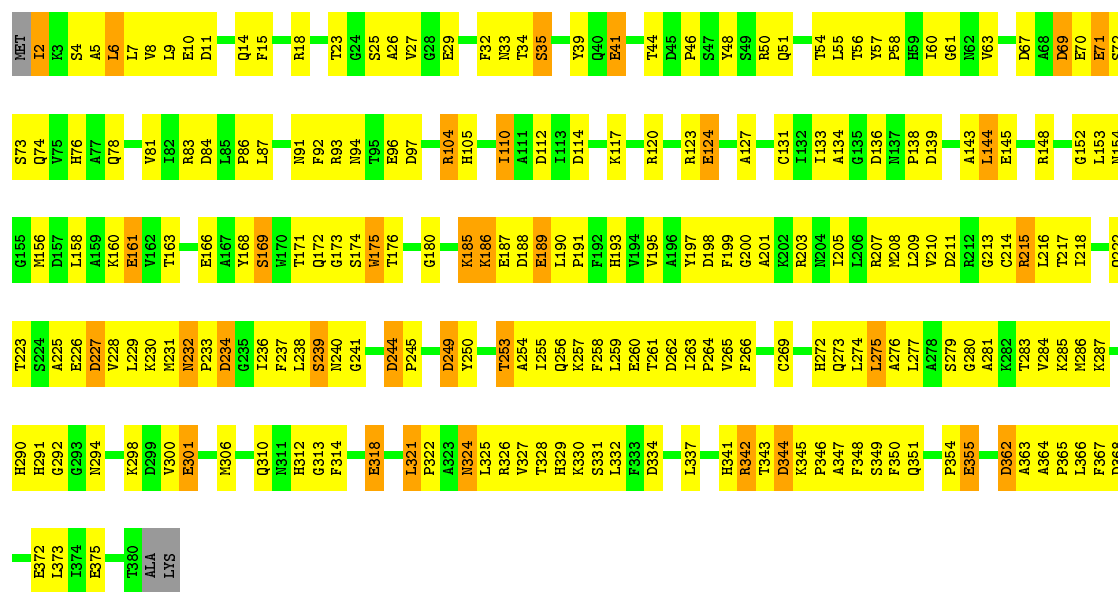




• Molecule 2: CARBAMOYL-PHOSPHATE SYNTHASE



• Molecule 2: CARBAMOYL-PHOSPHATE SYNTHASE



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 Too-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 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	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
4	E	5	0	0	0	0
4	G	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	1	0	0	0	0
5	A	3	0	0	0	0
5	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

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 21.

The worst 5 of 1851 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: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 [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	1075/1073 (100%)	1008 (94%)	63 (6%)	4 (0%)	39	37
1	C	1071/1073 (100%)	1009 (94%)	54 (5%)	8 (1%)	26	21
1	E	1074/1073 (100%)	1020 (95%)	48 (4%)	6 (1%)	30	24
1	G	1073/1073 (100%)	993 (92%)	72 (7%)	8 (1%)	26	21
2	B	377/382 (99%)	350 (93%)	23 (6%)	4 (1%)	17	11
2	D	377/382 (99%)	363 (96%)	14 (4%)	0	100	100
2	F	377/382 (99%)	361 (96%)	14 (4%)	2 (0%)	34	30
2	H	377/382 (99%)	358 (95%)	19 (5%)	0	100	100
All	All	5801/5820 (100%)	5462 (94%)	307 (5%)	32 (1%)	30	24

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 [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	882/878 (100%)	785 (89%)	97 (11%)	8	4
1	C	878/878 (100%)	783 (89%)	95 (11%)	8	4
1	E	881/878 (100%)	800 (91%)	81 (9%)	11	7
1	G	880/878 (100%)	761 (86%)	119 (14%)	5	2
2	B	308/310 (99%)	279 (91%)	29 (9%)	11	7
2	D	308/310 (99%)	290 (94%)	18 (6%)	25	21
2	F	308/310 (99%)	282 (92%)	26 (8%)	14	9
2	H	308/310 (99%)	276 (90%)	32 (10%)	9	5
All	All	4753/4752 (100%)	4256 (90%)	497 (10%)	9	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 molecules 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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	27,33,33	2.01	6 (22%)	30,52,52	1.82	4 (13%)
6	ANP	A	1084	3	27,33,33	1.84	6 (22%)	30,52,52	1.62	3 (10%)
7	ORN	A	1085	-	5,8,8	0.45	0	3,9,9	0.67	0
8	NET	A	1086	-	8,8,8	0.72	0	10,10,10	0.45	0
6	ANP	C	1900	3	27,33,33	1.61	6 (22%)	30,52,52	1.89	5 (16%)
6	ANP	C	1910	3	27,33,33	1.76	5 (18%)	30,52,52	1.75	6 (20%)
7	ORN	C	1920	-	5,8,8	0.49	0	3,9,9	0.16	0
8	NET	C	1950	-	8,8,8	0.63	0	10,10,10	0.64	0
6	ANP	E	2900	3	27,33,33	1.65	7 (25%)	30,52,52	1.84	3 (10%)
6	ANP	E	2910	3	27,33,33	1.75	5 (18%)	30,52,52	1.93	4 (13%)
7	ORN	E	2920	-	5,8,8	0.59	0	3,9,9	0.30	0
8	NET	E	2950	-	8,8,8	0.57	0	10,10,10	0.55	0
6	ANP	G	3900	3	27,33,33	1.55	6 (22%)	30,52,52	1.78	4 (13%)
6	ANP	G	3910	3	27,33,33	1.57	5 (18%)	30,52,52	2.09	7 (23%)
7	ORN	G	3920	-	5,8,8	0.51	0	3,9,9	0.38	0
8	NET	G	3950	-	8,8,8	0.64	0	10,10,10	0.52	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	-	0/12/38/38	0/3/3/3
6	ANP	A	1084	3	-	1/12/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	ORN	A	1085	-	-	0/4/8/8	0/0/0/0
8	NET	A	1086	-	-	0/12/12/12	0/0/0/0
6	ANP	C	1900	3	-	2/12/38/38	0/3/3/3
6	ANP	C	1910	3	-	0/12/38/38	0/3/3/3
7	ORN	C	1920	-	-	0/4/8/8	0/0/0/0
8	NET	C	1950	-	-	0/12/12/12	0/0/0/0
6	ANP	E	2900	3	-	1/12/38/38	0/3/3/3
6	ANP	E	2910	3	-	0/12/38/38	0/3/3/3
7	ORN	E	2920	-	-	0/4/8/8	0/0/0/0
8	NET	E	2950	-	-	0/12/12/12	0/0/0/0
6	ANP	G	3900	3	-	1/12/38/38	0/3/3/3
6	ANP	G	3910	3	-	1/12/38/38	0/3/3/3
7	ORN	G	3920	-	-	0/4/8/8	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	G	3910	ANP	C6-N6	-3.14	1.25	1.34
6	C	1910	ANP	C6-N6	-3.03	1.25	1.34
6	A	1084	ANP	C6-N6	-3.01	1.25	1.34
6	A	1083	ANP	PG-O2G	-2.97	1.48	1.56
6	E	2910	ANP	C6-N6	-2.96	1.25	1.34

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	3910	ANP	N3-C2-N1	-7.83	122.90	128.89
6	E	2910	ANP	N3-C2-N1	-7.51	123.14	128.89
6	C	1900	ANP	N3-C2-N1	-7.34	123.27	128.89
6	E	2900	ANP	N3-C2-N1	-7.31	123.29	128.89
6	A	1083	ANP	N3-C2-N1	-6.66	123.79	128.89

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	1900	ANP	O1B-PB-N3B-PG
6	E	2900	ANP	O1G-PG-N3B-PB
6	A	1084	ANP	O1G-PG-N3B-PB
6	C	1900	ANP	O1G-PG-N3B-PB

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

There are no ring outliers.

13 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1083	ANP	3	0
7	A	1085	ORN	1	0
8	A	1086	NET	6	0
6	C	1910	ANP	1	0
7	C	1920	ORN	1	0
8	C	1950	NET	4	0
6	E	2910	ANP	3	0
7	E	2920	ORN	1	0
8	E	2950	NET	6	0
6	G	3900	ANP	2	0
6	G	3910	ANP	2	0
7	G	3920	ORN	1	0
8	G	3950	NET	4	0

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 will therefore be empty.

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

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

6.3 Carbohydrates [i](#)

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

6.4 Ligands [i](#)

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

6.5 Other polymers [i](#)

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