



wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 03:14 AM GMT

PDB ID : 1A9X
Title : CARBAMOYL PHOSPHATE SYNTHETASE: CAUGHT IN THE ACT OF
GLUTAMINE HYDROLYSIS
Authors : Thoden, J.; Holden, H.
Deposited on : 1998-04-14
Resolution : 1.80 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>

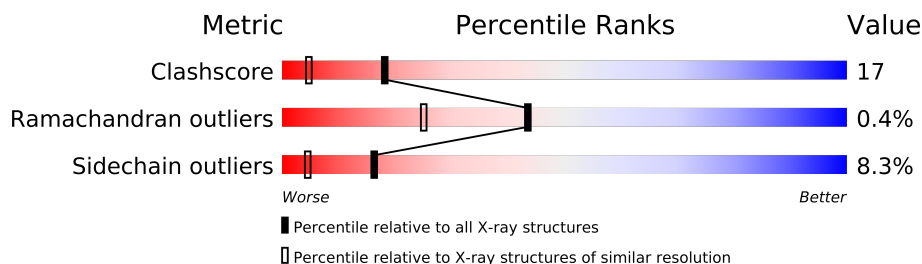
The following versions of software and data (see [references](#)) were used in the production of this report:

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 1.80 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	4461 (1.80-1.80)
Ramachandran outliers	78287	4404 (1.80-1.80)
Sidechain outliers	78261	4403 (1.80-1.80)

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	379	
2	D	379	
2	F	379	
2	H	379	

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 49310 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 SYNTHETASE (LARGE CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1058	Total	C	N	O	S	0	7	0
			8193	5142	1428	1577	46			
1	C	1058	Total	C	N	O	S	0	7	0
			8198	5144	1432	1577	45			
1	E	1058	Total	C	N	O	S	0	2	0
			8169	5126	1423	1575	45			
1	G	1058	Total	C	N	O	S	0	1	0
			8164	5123	1423	1573	45			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	46	ASN	LEU	CONFLICT	UNP P00968
A	716	ALA	PRO	CONFLICT	UNP P00968
C	2046	ASN	LEU	CONFLICT	UNP P00968
C	2716	ALA	PRO	CONFLICT	UNP P00968
E	4046	ASN	LEU	CONFLICT	UNP P00968
E	4716	ALA	PRO	CONFLICT	UNP P00968
G	6046	ASN	LEU	CONFLICT	UNP P00968
G	6716	ALA	PRO	CONFLICT	UNP P00968

- Molecule 2 is a protein called CARBAMOYL PHOSPHATE SYNTHETASE (SMALL CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	379	Total	C	N	O	S	0	1	0
			2904	1829	509	556	10			
2	D	379	Total	C	N	O	S	0	0	0
			2902	1828	509	555	10			
2	F	379	Total	C	N	O	S	0	3	0
			2915	1836	510	558	11			
2	H	379	Total	C	N	O	S	0	0	0
			2902	1828	509	555	10			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1683	GLN	GLU	CONFLICT	UNP P00907
B	1769	CYG	CYS	MODIFIED	UNP P00907
B	1853	ASN	HIS	MUTATION	UNP P00907
D	3683	GLN	GLU	CONFLICT	UNP P00907
D	3769	CYG	CYS	MODIFIED	UNP P00907
D	3853	ASN	HIS	MUTATION	UNP P00907
F	5683	GLN	GLU	CONFLICT	UNP P00907
F	5769	CYG	CYS	MODIFIED	UNP P00907
F	5853	ASN	HIS	MUTATION	UNP P00907
H	7683	GLN	GLU	CONFLICT	UNP P00907
H	7769	CYG	CYS	MODIFIED	UNP P00907
H	7853	ASN	HIS	MUTATION	UNP P00907

- 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	3	Total Mn 3 3	0	0
3	E	3	Total Mn 3 3	0	0

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

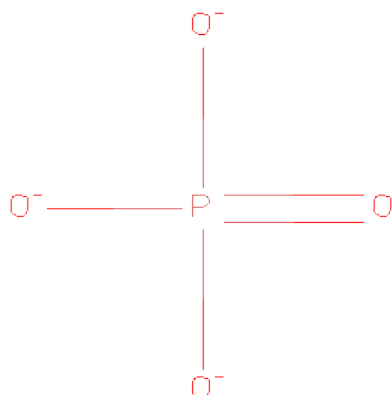
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	7	Total K 7 7	0	0
4	D	1	Total K 1 1	0	0
4	E	7	Total K 7 7	0	0
4	H	1	Total K 1 1	0	0
4	B	1	Total K 1 1	0	0
4	C	7	Total K 7 7	0	0
4	A	7	Total K 7 7	0	0

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

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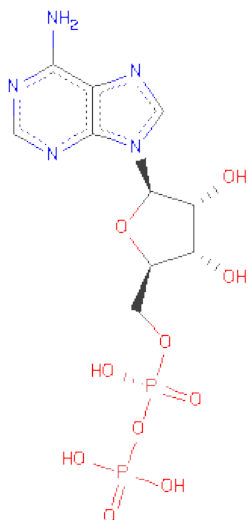
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	E	1	Total	O	P	0	0
			5	4	1		
5	G	1	Total	O	P	0	0
			5	4	1		
5	G	1	Total	O	P	0	0
			5	4	1		
5	G	1	Total	O	P	0	0
			5	4	1		
5	A	1	Total	O	P	0	0
			5	4	1		

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

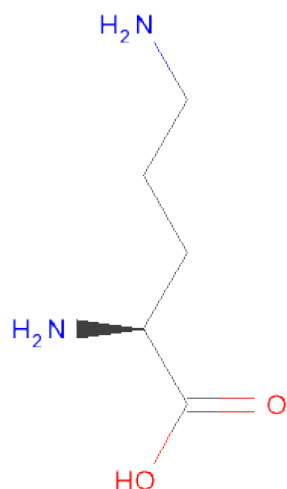
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	G	6	Total	Cl	0	0
			6	6		
6	D	1	Total	Cl	0	0
			1	1		
6	E	6	Total	Cl	0	0
			6	6		
6	H	1	Total	Cl	0	0
			1	1		
6	B	1	Total	Cl	0	0
			1	1		
6	C	6	Total	Cl	0	0
			6	6		
6	A	6	Total	Cl	0	0
			6	6		
6	F	1	Total	Cl	0	0
			1	1		

- Molecule 7 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



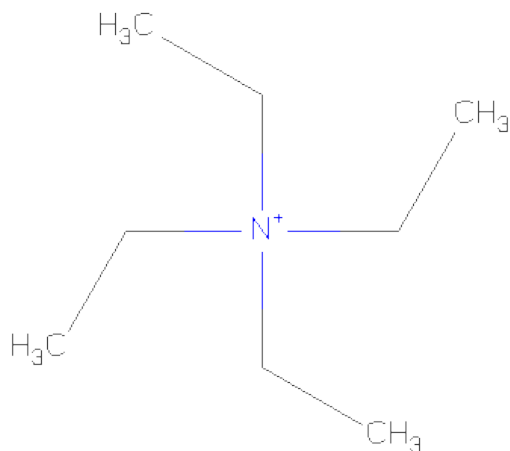
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	G	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	G	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	A	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		

- Molecule 8 is L-ORNITHINE (three-letter code: ORN) (formula: C₅H₁₂N₂O₂).



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

- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	904	Total O 904 904	0	0
10	B	256	Total O 256 256	0	0
10	C	897	Total O 897 897	0	0
10	D	330	Total O 330 330	0	0
10	E	900	Total O 900 900	0	0
10	F	276	Total O 276 276	0	0
10	G	733	Total O 733 733	0	0
10	H	232	Total O 232 232	0	0

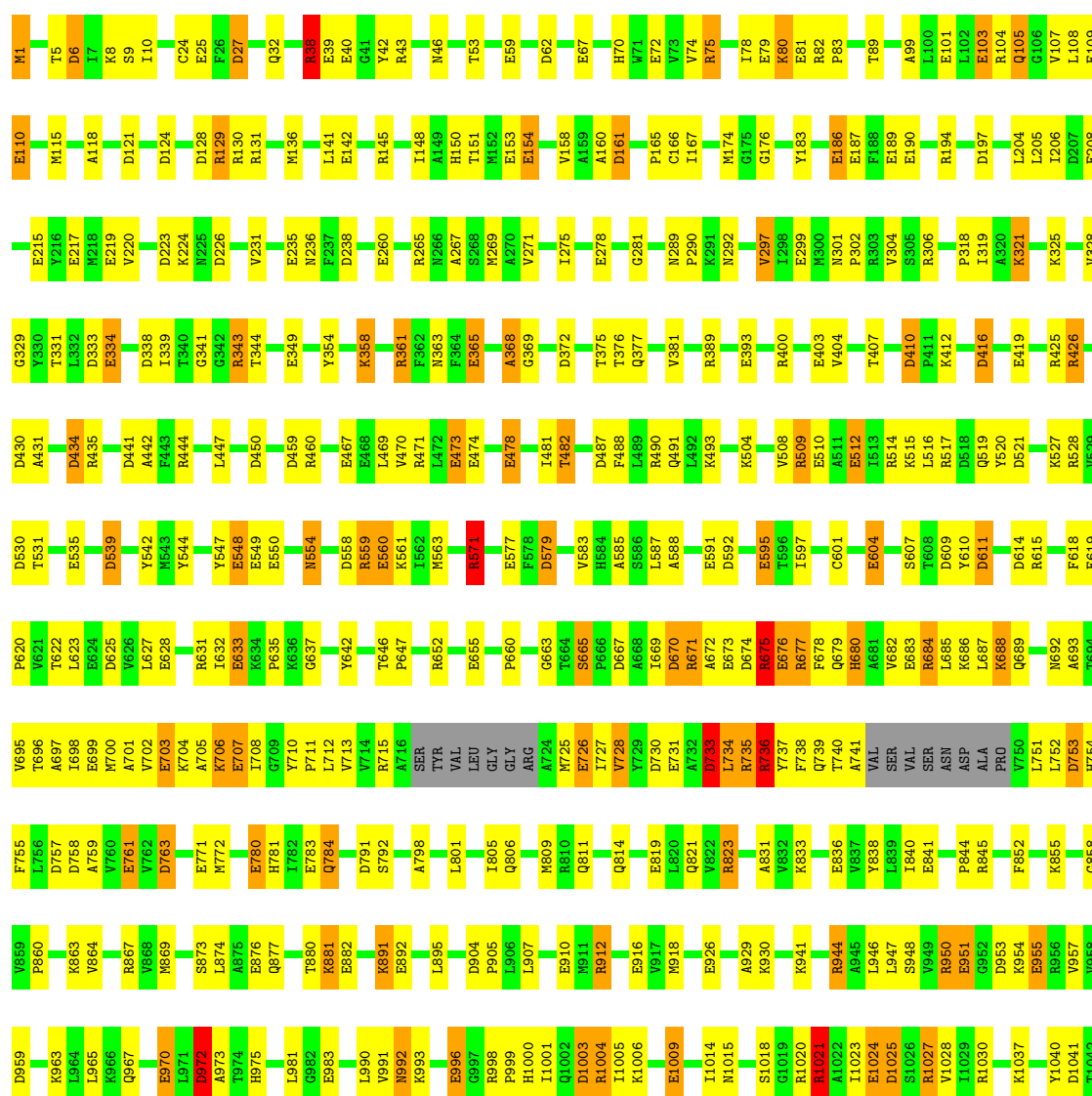
3 Residue-property plots

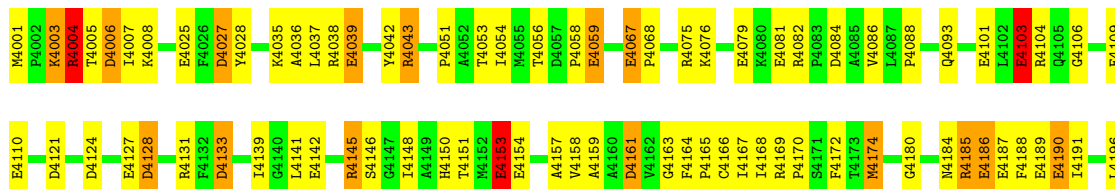
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

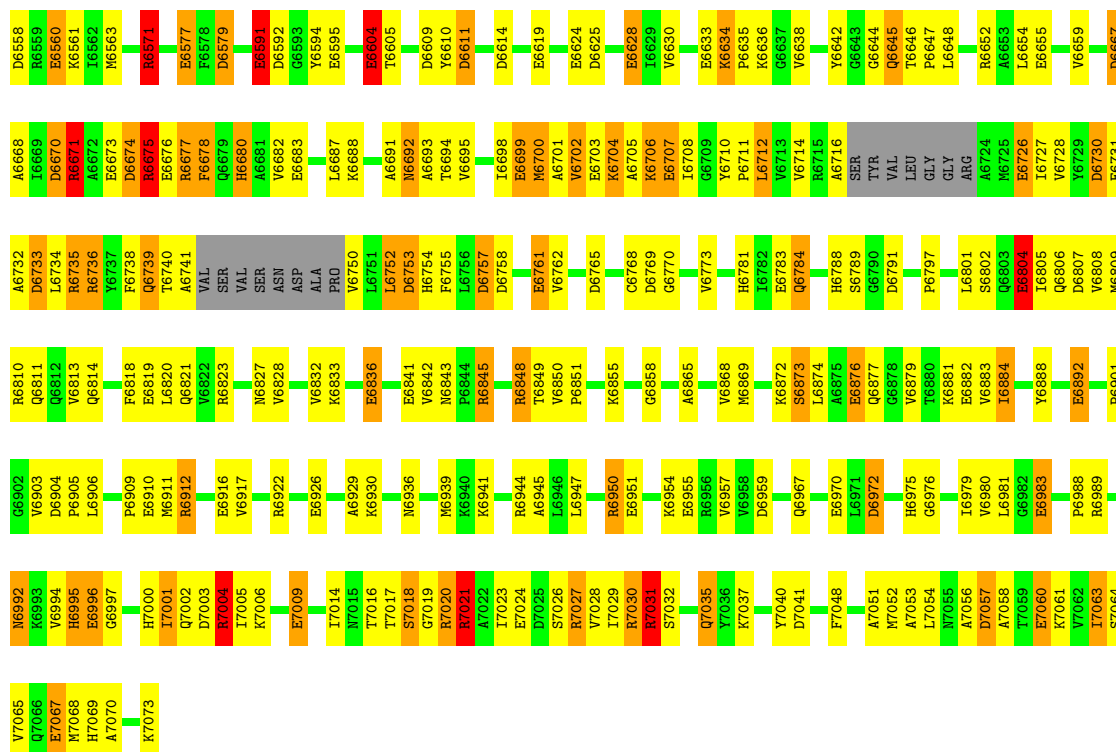
• Molecule 1: CARBAMOYL PHOSPHATE SYNTHETASE (LARGE CHAIN)

Chain A: 



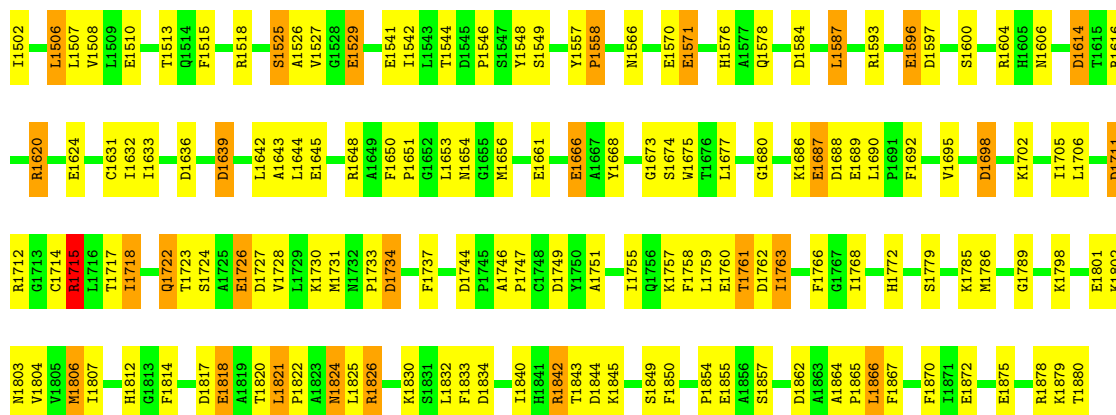






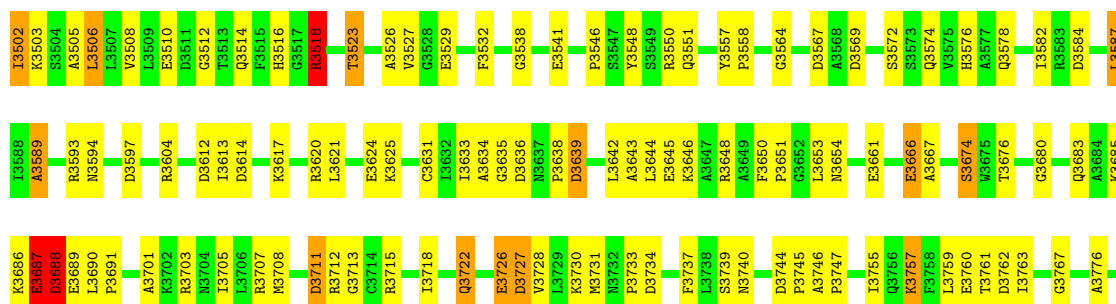
• Molecule 2: CARBAMOYL PHOSPHATE SYNTHETASE (SMALL CHAIN)

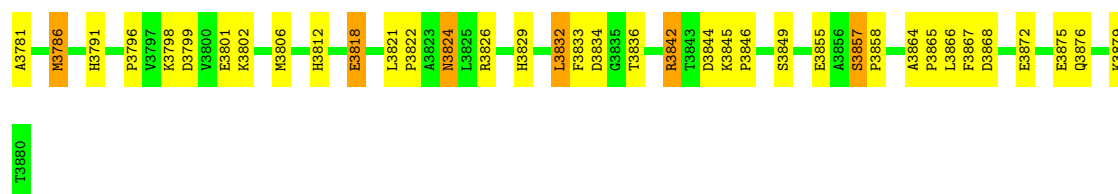
Chain B:



• Molecule 2: CARBAMOYL PHOSPHATE SYNTHETASE (SMALL CHAIN)

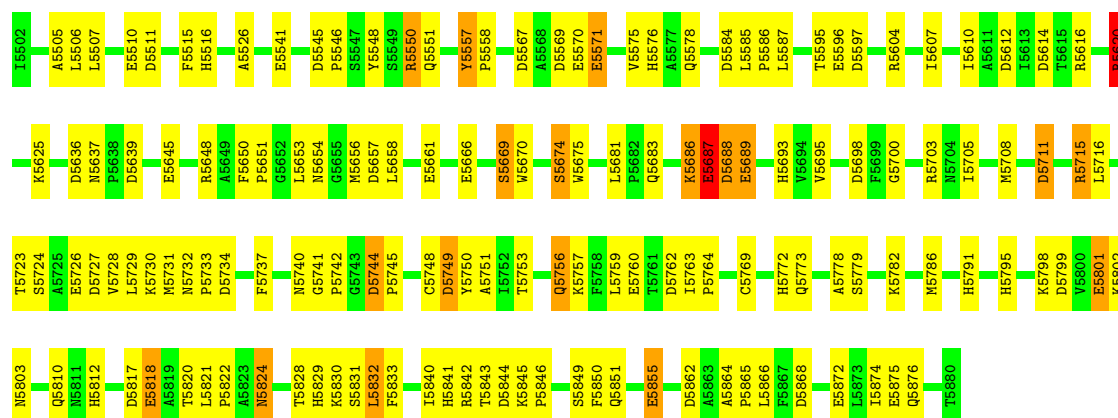
Chain D:





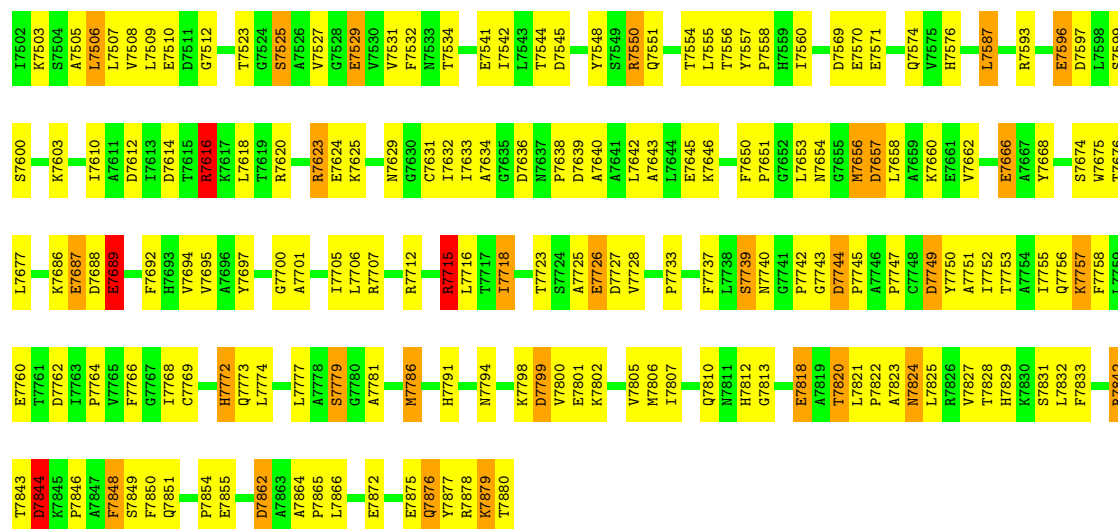
• Molecule 2: CARBAMOYL PHOSPHATE SYNTHETASE (SMALL CHAIN)

Chain F:



• Molecule 2: CARBAMOYL PHOSPHATE SYNTHETASE (SMALL CHAIN)

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	152.10Å 164.40Å 332.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.80	Depositor
% Data completeness (in resolution range)	92.0 (30.00-1.80)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
Refinement program	TNT V. 5-E	Depositor
R, R_{free}	0.191 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	49310	wwPDB-VP
Average B, all atoms (Å ²)	36.0	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: ADP, CL, K, MN, ORN, CYG, NET, PO4

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	1.11	77/8347 (0.9%)	1.53	140/11284 (1.2%)
1	C	1.10	72/8352 (0.9%)	1.48	121/11288 (1.1%)
1	E	1.13	70/8303 (0.8%)	1.55	137/11225 (1.2%)
1	G	1.08	79/8294 (1.0%)	1.49	125/11213 (1.1%)
2	B	0.97	20/2953 (0.7%)	1.39	32/4009 (0.8%)
2	D	1.01	16/2947 (0.5%)	1.42	40/4001 (1.0%)
2	F	0.98	18/2972 (0.6%)	1.42	36/4034 (0.9%)
2	H	0.95	15/2947 (0.5%)	1.45	39/4001 (1.0%)
All	All	1.07	367/45115 (0.8%)	1.49	670/61055 (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	A	1	0

The worst 5 of 367 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	4912	ARG	CZ-NH2	-13.14	1.16	1.33
1	G	6076	LYS	CE-NZ	-11.79	1.19	1.49
1	E	4670	ASP	CG-OD2	-9.89	1.02	1.25
1	E	4655	GLU	CD-OE1	9.63	1.36	1.25
2	D	3872	GLU	CD-OE1	9.12	1.35	1.25

The worst 5 of 670 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	4652	ARG	NE-CZ-NH2	-17.70	111.45	120.30
1	E	4912	ARG	NE-CZ-NH2	-16.36	112.12	120.30
1	C	2043	ARG	NE-CZ-NH1	12.52	126.56	120.30
1	A	671	ARG	NE-CZ-NH2	-12.26	114.17	120.30
1	A	671	ARG	NE-CZ-NH1	12.24	126.42	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	726	GLU	CA

There are no planarity outliers.

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	8193	0	8225	260	0
1	C	8198	0	8230	251	0
1	E	8169	0	8194	264	0
1	G	8164	0	8193	340	0
2	B	2904	0	2868	99	0
2	D	2902	0	2867	88	0
2	F	2915	0	2876	93	0
2	H	2902	0	2868	135	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	1	0	0	0	0
5	A	20	0	0	0	0
5	C	20	0	0	1	0
5	E	15	0	0	0	0
5	G	20	0	0	1	0
6	A	6	0	0	0	0
6	B	1	0	0	0	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	1	0	0	0	0
7	A	54	0	24	2	0
7	C	54	0	24	1	0
7	E	54	0	24	1	0
7	G	54	0	24	4	0
8	A	9	0	11	1	0
8	C	9	0	11	3	0
8	E	9	0	11	1	0
8	G	9	0	11	1	0
9	A	9	0	20	1	0
9	C	9	0	20	0	0
9	E	9	0	20	2	0
9	G	9	0	20	0	0
10	A	904	0	0	32	0
10	B	256	0	0	2	0
10	C	897	0	0	24	0
10	D	330	0	0	8	1
10	E	900	0	0	28	0
10	F	276	0	0	7	0
10	G	733	0	0	27	0
10	H	232	0	0	6	1
All	All	49310	0	44541	1515	1

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 17.

The worst 5 of 1515 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:80:LYS:CE	1:A:80:LYS:NZ	1.68	1.53
1:E:4001:MET:HB3	10:E:6618:HOH:O	1.38	1.21

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:5687:GLU:HG2	2:F:5715:ARG:HD2	1.21	1.13
1:C:2695:VAL:HG21	1:C:2701:ALA:HA	1.30	1.12
1:G:6695:VAL:HG11	1:G:6701:ALA:HB2	1.24	1.12

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	Distance(Å)	Clash(Å)
10:D:4245:HOH:O	10:H:947:HOH:O[3_554]	2.08	0.12

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	1059/1073 (99%)	1010 (95%)	46 (4%)	3 (0%)	50	31
1	C	1059/1073 (99%)	1007 (95%)	49 (5%)	3 (0%)	50	31
1	E	1054/1073 (98%)	1000 (95%)	48 (5%)	6 (1%)	33	15
1	G	1053/1073 (98%)	997 (95%)	50 (5%)	6 (1%)	33	15
2	B	377/379 (100%)	363 (96%)	14 (4%)	0	100	100
2	D	376/379 (99%)	360 (96%)	16 (4%)	0	100	100
2	F	379/379 (100%)	372 (98%)	7 (2%)	0	100	100
2	H	376/379 (99%)	360 (96%)	14 (4%)	2 (0%)	38	19
All	All	5733/5808 (99%)	5469 (95%)	244 (4%)	20 (0%)	43	31

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	368	ALA
1	E	4004	ARG
1	G	6739	GLN
1	A	975	HIS
1	C	2368	ALA

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	872/877 (99%)	814 (93%)	58 (7%)	23	7
1	C	872/877 (99%)	795 (91%)	77 (9%)	14	4
1	E	867/877 (99%)	800 (92%)	67 (8%)	18	5
1	G	866/877 (99%)	786 (91%)	80 (9%)	13	3
2	B	308/307 (100%)	279 (91%)	29 (9%)	13	3
2	D	307/307 (100%)	281 (92%)	26 (8%)	15	4
2	F	310/307 (101%)	284 (92%)	26 (8%)	16	4
2	H	307/307 (100%)	279 (91%)	28 (9%)	14	3
All	All	4709/4736 (99%)	4318 (92%)	391 (8%)	16	4

5 of 391 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	3683	GLN
1	E	4558	ASP
1	G	7063	ILE
2	D	3761	THR
1	E	4174	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 85 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	3071	GLN
1	E	4266	ASN
2	H	7551	GLN
2	D	3514	GLN
2	D	3824	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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$
2	CYG	B	1769	2	14,14,15	6.12	5 (35%)	15,17,19	3.58	5 (33%)
2	CYG	D	3769	2	14,14,15	5.43	5 (35%)	15,17,19	2.81	8 (53%)
2	CYG	F	5769	2	14,14,15	5.21	5 (35%)	15,17,19	2.30	5 (33%)
2	CYG	H	7769	2	14,14,15	5.88	6 (42%)	15,17,19	3.06	6 (40%)

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
2	CYG	B	1769	2	-	0/14/16/18	0/0/0/0
2	CYG	D	3769	2	-	0/14/16/18	0/0/0/0
2	CYG	F	5769	2	-	0/14/16/18	0/0/0/0
2	CYG	H	7769	2	-	0/14/16/18	0/0/0/0

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1769	CYG	O-C	19.24	1.24	1.11
2	H	7769	CYG	O-C	18.27	1.24	1.11
2	D	3769	CYG	O-C	16.45	1.22	1.11
2	F	5769	CYG	O-C	15.70	1.22	1.11
2	B	1769	CYG	OE2-CD1	10.82	1.38	1.21

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	7769	CYG	CB-SG-CD1	-8.84	94.85	100.95
2	B	1769	CYG	OE2-CD1-CG1	-8.25	116.73	123.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	3769	CYG	OE2-CD1-CG1	-7.05	117.78	123.95
2	B	1769	CYG	CB-SG-CD1	7.01	105.78	100.95
2	B	1769	CYG	C1-CA1-N1	6.06	119.40	109.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 103 ligands modelled in this entry, 72 are monoatomic - leaving 31 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	ADP	A	1900	3	29,29,29	1.34	6 (20%)	45,45,45	1.35	5 (11%)
5	PO4	A	1906	3,4	4,4,4	1.02	0	6,6,6	0.35	0
7	ADP	A	1910	3,4	29,29,29	1.21	4 (13%)	45,45,45	1.31	6 (13%)
8	ORN	A	1920	-	8,8,8	0.84	0	9,9,9	1.77	3 (33%)
9	NET	A	1950	-	8,8,8	0.73	0	10,10,10	0.45	0
5	PO4	A	1980	-	4,4,4	1.32	0	6,6,6	0.34	0
5	PO4	A	1981	-	4,4,4	1.49	1 (25%)	6,6,6	0.38	0
5	PO4	A	1982	-	4,4,4	2.14	2 (50%)	6,6,6	0.32	0
7	ADP	C	3900	3	29,29,29	1.34	4 (13%)	45,45,45	1.08	3 (6%)
5	PO4	C	3906	3,4	4,4,4	1.04	0	6,6,6	0.36	0
7	ADP	C	3910	3,4	29,29,29	1.42	5 (17%)	45,45,45	1.43	9 (20%)
8	ORN	C	3920	-	8,8,8	0.91	1 (12%)	9,9,9	0.99	1 (11%)
9	NET	C	3950	-	8,8,8	0.62	0	10,10,10	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	PO4	C	3980	-	4,4,4	1.26	0	6,6,6	0.30	0
5	PO4	C	3981	-	4,4,4	2.61	4 (100%)	6,6,6	0.34	0
5	PO4	C	3982	-	4,4,4	2.18	2 (50%)	6,6,6	0.35	0
7	ADP	E	5900	3	29,29,29	1.53	4 (13%)	45,45,45	1.24	4 (8%)
5	PO4	E	5906	3,4	4,4,4	1.07	0	6,6,6	0.33	0
7	ADP	E	5910	3,4	29,29,29	1.36	5 (17%)	45,45,45	1.12	4 (8%)
8	ORN	E	5920	-	8,8,8	0.86	0	9,9,9	0.86	0
9	NET	E	5950	-	8,8,8	0.71	0	10,10,10	0.48	0
5	PO4	E	5980	-	4,4,4	2.22	2 (50%)	6,6,6	0.35	0
5	PO4	E	5981	-	4,4,4	1.32	0	6,6,6	0.32	0
7	ADP	G	7900	3	29,29,29	1.32	5 (17%)	45,45,45	1.42	6 (13%)
5	PO4	G	7906	3,4	4,4,4	0.91	0	6,6,6	0.31	0
7	ADP	G	7910	3,4	29,29,29	1.37	4 (13%)	45,45,45	1.28	5 (11%)
8	ORN	G	7920	-	8,8,8	1.05	1 (12%)	9,9,9	1.32	1 (11%)
9	NET	G	7950	-	8,8,8	0.61	0	10,10,10	0.46	0
5	PO4	G	7980	-	4,4,4	2.20	1 (25%)	6,6,6	0.34	0
5	PO4	G	7981	-	4,4,4	1.47	0	6,6,6	0.35	0
5	PO4	G	7982	-	4,4,4	2.09	2 (50%)	6,6,6	0.37	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
7	ADP	A	1900	3	-	0/16/32/32	0/1/3/3
5	PO4	A	1906	3,4	-	0/0/0/0	0/0/0/0
7	ADP	A	1910	3,4	-	0/16/32/32	0/1/3/3
8	ORN	A	1920	-	-	0/8/8/8	0/0/0/0
9	NET	A	1950	-	-	0/12/12/12	0/0/0/0
5	PO4	A	1980	-	-	0/0/0/0	0/0/0/0
5	PO4	A	1981	-	-	0/0/0/0	0/0/0/0
5	PO4	A	1982	-	-	0/0/0/0	0/0/0/0
7	ADP	C	3900	3	-	0/16/32/32	0/1/3/3
5	PO4	C	3906	3,4	-	0/0/0/0	0/0/0/0
7	ADP	C	3910	3,4	-	0/16/32/32	0/1/3/3
8	ORN	C	3920	-	-	0/8/8/8	0/0/0/0
9	NET	C	3950	-	-	0/12/12/12	0/0/0/0
5	PO4	C	3980	-	-	0/0/0/0	0/0/0/0
5	PO4	C	3981	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PO4	C	3982	-	-	0/0/0/0	0/0/0/0
7	ADP	E	5900	3	-	0/16/32/32	0/1/3/3
5	PO4	E	5906	3,4	-	0/0/0/0	0/0/0/0
7	ADP	E	5910	3,4	-	0/16/32/32	0/1/3/3
8	ORN	E	5920	-	-	0/8/8/8	0/0/0/0
9	NET	E	5950	-	-	0/12/12/12	0/0/0/0
5	PO4	E	5980	-	-	0/0/0/0	0/0/0/0
5	PO4	E	5981	-	-	0/0/0/0	0/0/0/0
7	ADP	G	7900	3	-	0/16/32/32	0/1/3/3
5	PO4	G	7906	3,4	-	0/0/0/0	0/0/0/0
7	ADP	G	7910	3,4	-	0/16/32/32	0/1/3/3
8	ORN	G	7920	-	-	0/8/8/8	0/0/0/0
9	NET	G	7950	-	-	0/12/12/12	0/0/0/0
5	PO4	G	7980	-	-	0/0/0/0	0/0/0/0
5	PO4	G	7981	-	-	0/0/0/0	0/0/0/0
5	PO4	G	7982	-	-	0/0/0/0	0/0/0/0

The worst 5 of 53 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	E	5900	ADP	O4'-C1'	-4.58	1.34	1.41
7	G	7910	ADP	PA-O3A	-4.24	1.52	1.59
7	C	3900	ADP	PA-O3A	-4.00	1.52	1.59
7	E	5900	ADP	PA-O3A	-3.93	1.52	1.59
7	C	3910	ADP	O3'-C3'	3.62	1.51	1.43

The worst 5 of 47 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1900	ADP	C5-C6-N6	4.60	131.13	120.72
7	G	7900	ADP	C5-C6-N6	4.26	130.35	120.72
7	A	1910	ADP	O4'-C1'-N9	-4.23	104.50	108.44
7	G	7900	ADP	O4'-C1'-N9	-4.02	104.70	108.44
7	E	5900	ADP	O4'-C1'-N9	-3.98	104.73	108.44

There are no chirality outliers.

There are no torsion outliers.

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.