



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 11, 2018 – 04:13 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 X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30967

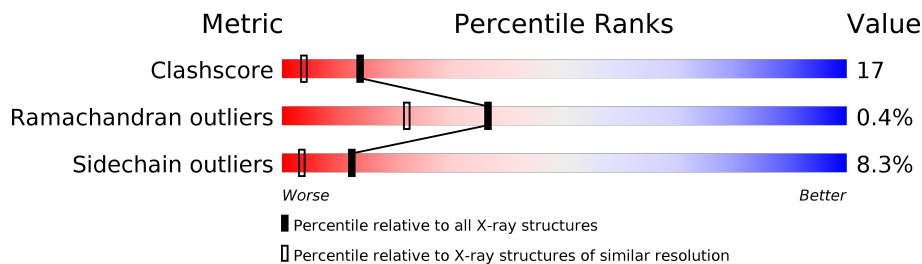
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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	122126	6077 (1.80-1.80)
Ramachandran outliers	120053	6011 (1.80-1.80)
Sidechain outliers	120020	6010 (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  $\geq 3$ , 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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	1073	60% 31% 7% ..
1	C	1073	61% 29% 7% ..
1	E	1073	60% 30% 7% ..
1	G	1073	55% 33% 9% ..
2	B	379	60% 32% 7%
2	D	379	61% 33% 5% .
2	F	379	61% 34% 5% .
2	H	379	53% 38% 8% .

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PO4	C	3981	-	X	-	-

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 49310 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called CARBAMOYL PHOSPHATE SYNTHETASE (LARGE 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

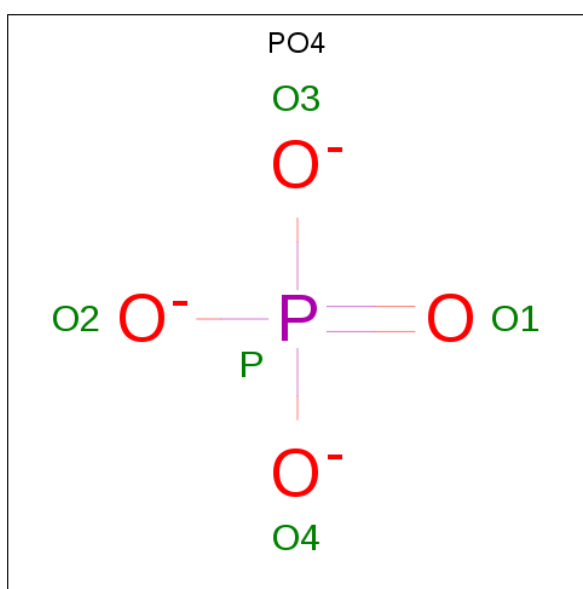
- Molecule 2 is a protein called CARBAMOYL PHOSPHATE SYNTHETASE (SMALL CHAIN).

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	ENGINEERED MUTATION	UNP P00907
D	3683	GLN	GLU	CONFLICT	UNP P00907
D	3769	CYG	CYS	MODIFIED	UNP P00907
D	3853	ASN	HIS	ENGINEERED MUTATION	UNP P00907
F	5683	GLN	GLU	CONFLICT	UNP P00907
F	5769	CYG	CYS	MODIFIED	UNP P00907
F	5853	ASN	HIS	ENGINEERED MUTATION	UNP P00907
H	7683	GLN	GLU	CONFLICT	UNP P00907
H	7769	CYG	CYS	MODIFIED	UNP P00907
H	7853	ASN	HIS	ENGINEERED MUTATION	UNP P00907

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



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

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

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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

- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	7	Total	K	0	0
			7	7		
5	D	1	Total	K	0	0
			1	1		
5	E	7	Total	K	0	0
			7	7		

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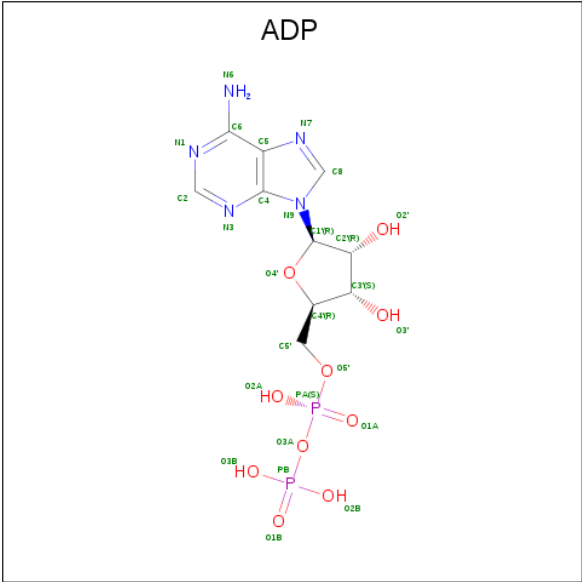
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	1	Total 1	K 1	0	0
5	B	1	Total 1	K 1	0	0
5	C	7	Total 7	K 7	0	0
5	A	7	Total 7	K 7	0	0
5	F	1	Total 1	K 1	0	0

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

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

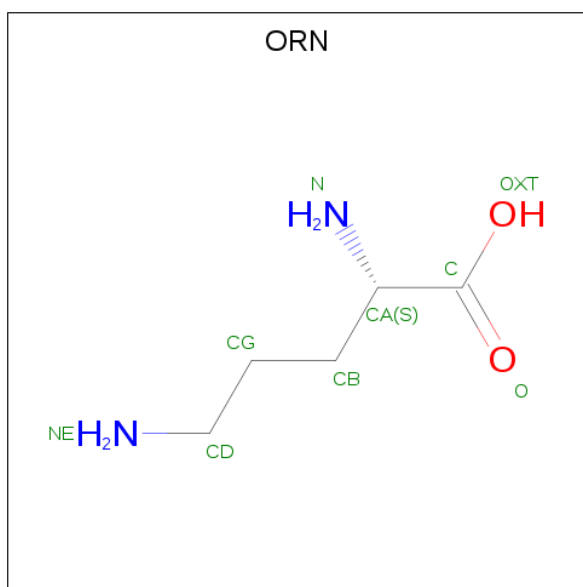
- Molecule 7 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>).



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		

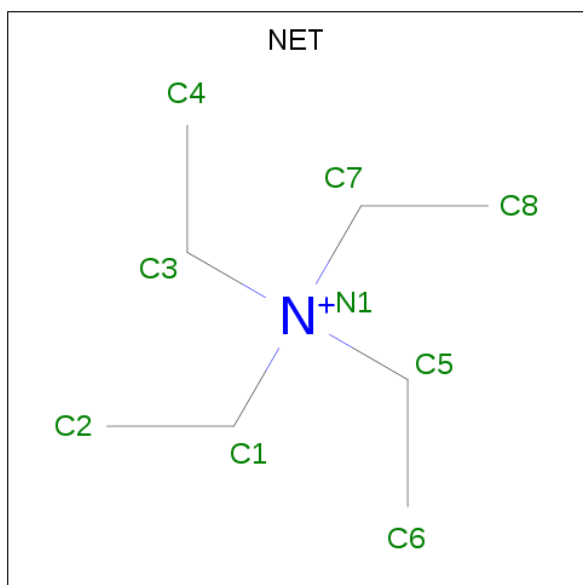
- Molecule 8 is L-ornithine (three-letter code: ORN) (formula: C<sub>5</sub>H<sub>12</sub>N<sub>2</sub>O<sub>2</sub>).





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: C<sub>8</sub>H<sub>20</sub>N).



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 water.

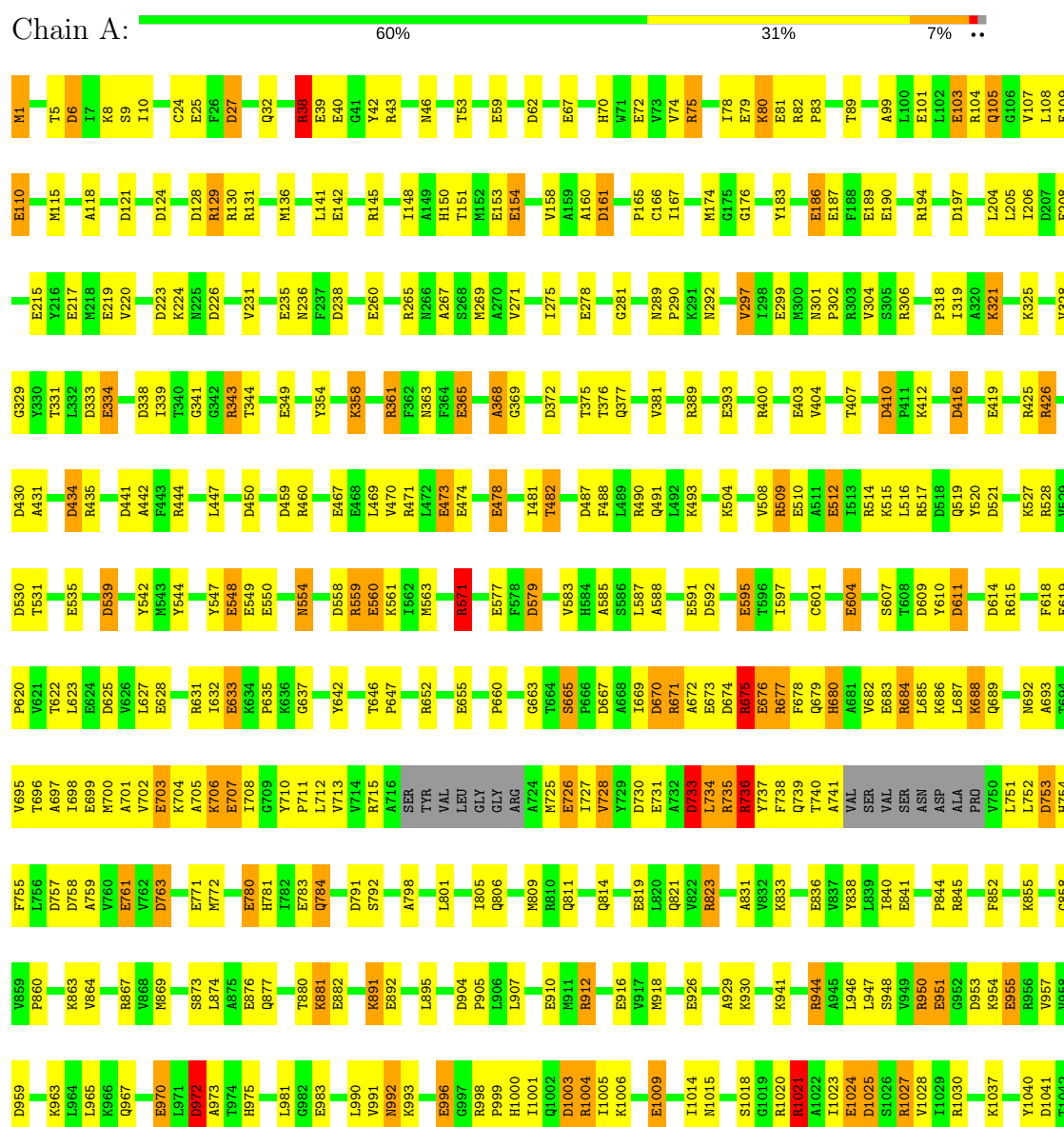
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	904	Total O 904 904	0	0
10	B	256	Total O 256 256	0	0
10	C	897	Total O 897 897	0	0
10	D	330	Total O 330 330	0	0
10	E	900	Total O 900 900	0	0
10	F	276	Total O 276 276	0	0
10	G	733	Total O 733 733	0	0
10	H	232	Total O 232 232	0	0

### 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 the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

#### • Molecule 1: CARBAMOYL PHOSPHATE SYNTHETASE (LARGE CHAIN)

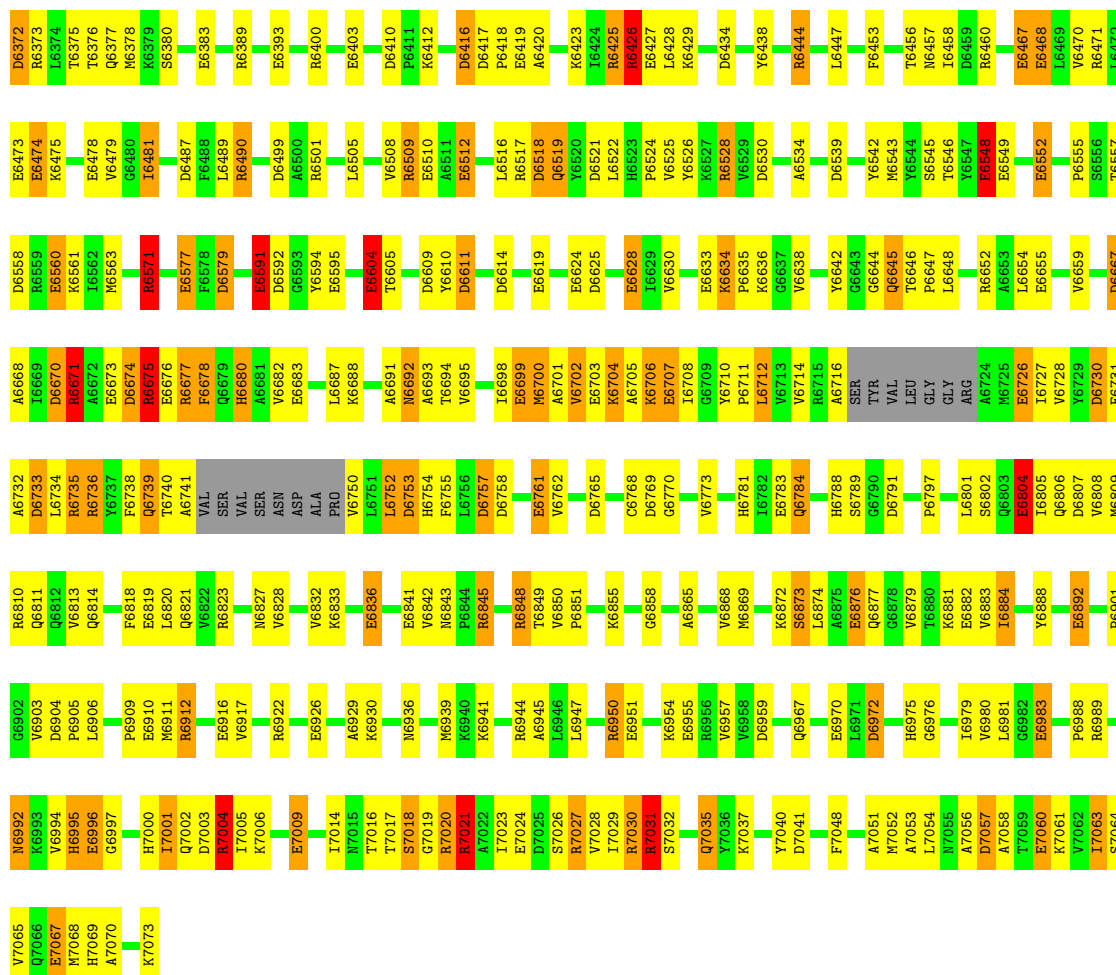






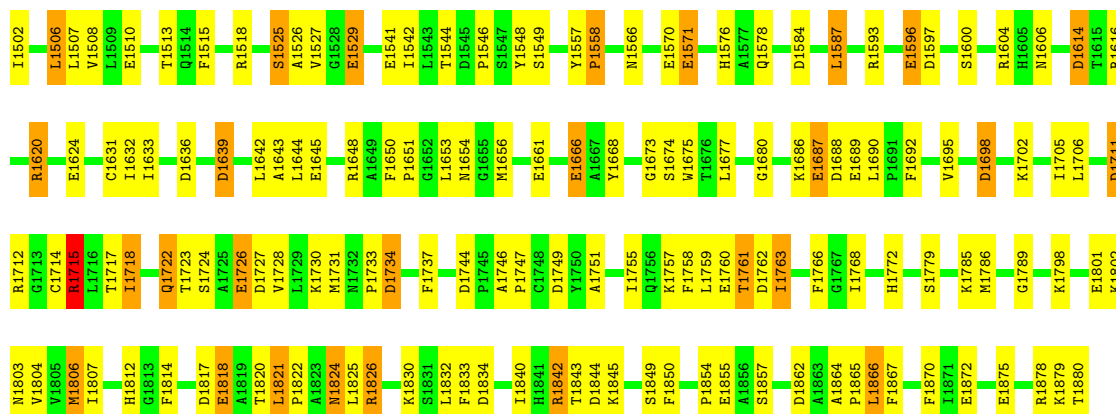
Category	Percentage
Very bad	55%
Bad	33%
Good	9%
Very good	1%





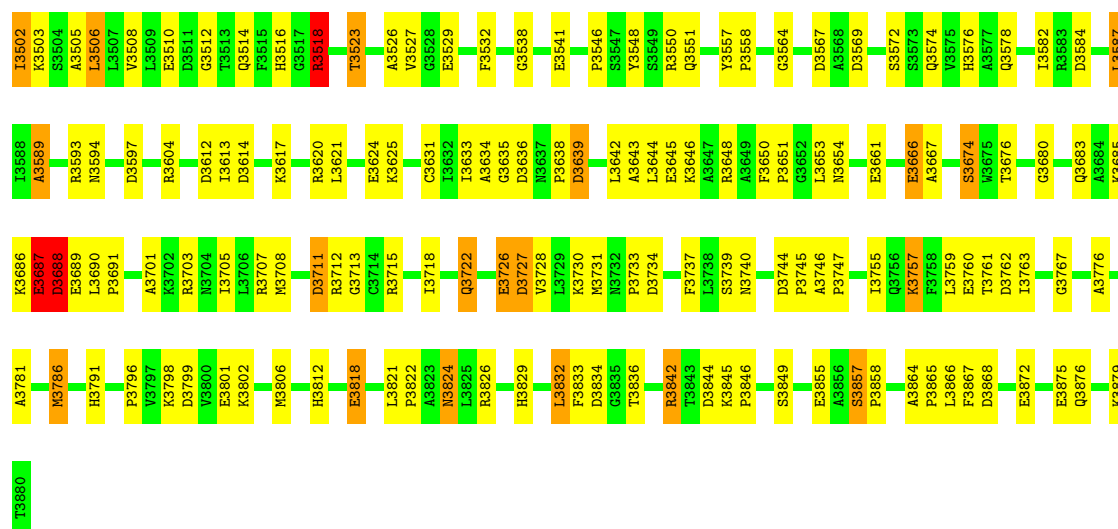
• Molecule 2: CARBAMOYL PHOSPHATE SYNTHETASE (SMALL CHAIN)

Chain B: 60% 32% 7%

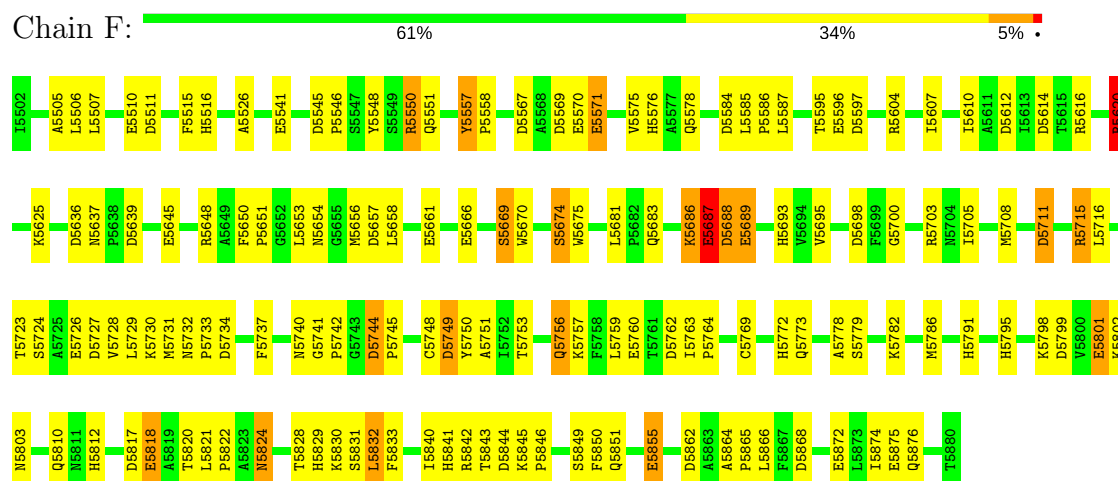


• Molecule 2: CARBAMOYL PHOSPHATE SYNTHETASE (SMALL CHAIN)

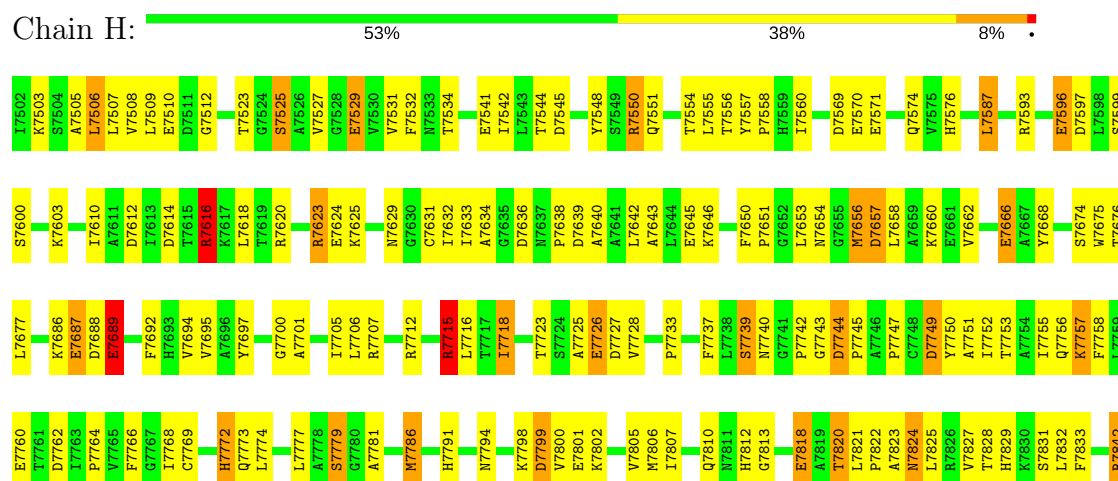
Chain D: 61% 33% 5%



• Molecule 2: CARBAMOYL PHOSPHATE SYNTHETASE (SMALL CHAIN)



• Molecule 2: CARBAMOYL PHOSPHATE SYNTHETASE (SMALL CHAIN)



T7843	D7844	K7845	P7846	A7847	F7848	S7849	F7850	Q7851	P7854	E7855	D7862	A7863	A7864	P7865	L7866	E7872	E7875	Q7876	Y7877	R7878	K7879	T7880
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## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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 5E	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 <sup>2</sup> )	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 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	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	20	0	0	0	0
3	C	20	0	0	1	0
3	E	15	0	0	0	0
3	G	20	0	0	1	0
4	A	3	0	0	0	0
4	C	3	0	0	0	0
4	E	3	0	0	0	0
4	G	3	0	0	0	0
5	A	7	0	0	0	0
5	B	1	0	0	0	0
5	C	7	0	0	0	0
5	D	1	0	0	0	0
5	E	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	1	0	0	0	0
5	G	7	0	0	0	0
5	H	1	0	0	0	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

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

The worst 5 of 1515 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: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	Interatomic distance (Å)	Clash overlap (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	Interatomic distance (Å)	Clash overlap (Å)
10:D:4245:HOH:O	10:H:947:HOH:O[3_554]	2.08	0.12

## 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	1059/1073 (99%)	1010 (95%)	46 (4%)	3 (0%)	43	28
1	C	1059/1073 (99%)	1007 (95%)	49 (5%)	3 (0%)	43	28
1	E	1054/1073 (98%)	1000 (95%)	48 (5%)	6 (1%)	27	13
1	G	1053/1073 (98%)	997 (95%)	50 (5%)	6 (1%)	27	13
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%)	31	16
All	All	5733/5808 (99%)	5469 (95%)	244 (4%)	20 (0%)	36	28

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	368	ALA
1	E	4004	ARG

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Mol	Chain	Res	Type
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%)	18	6
1	C	872/877 (99%)	795 (91%)	77 (9%)	11	3
1	E	867/877 (99%)	800 (92%)	67 (8%)	14	4
1	G	866/877 (99%)	786 (91%)	80 (9%)	10	2
2	B	308/307 (100%)	279 (91%)	29 (9%)	9	2
2	D	307/307 (100%)	281 (92%)	26 (8%)	12	3
2	F	310/307 (101%)	284 (92%)	26 (8%)	12	3
2	H	307/307 (100%)	279 (91%)	28 (9%)	10	2
All	All	4709/4736 (99%)	4318 (92%)	391 (8%)	12	3

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

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Mol	Chain	Res	Type
2	H	7551	GLN
2	D	3514	GLN
2	D	3824	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules 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	9,14,15	3.86	2 (22%)	7,17,19	4.00	5 (71%)
2	CYG	D	3769	2	9,14,15	3.69	2 (22%)	7,17,19	3.32	4 (57%)
2	CYG	F	5769	2	9,14,15	3.47	3 (33%)	7,17,19	2.47	2 (28%)
2	CYG	H	7769	2	9,14,15	3.68	2 (22%)	7,17,19	3.62	3 (42%)

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	-	0/10/16/18	0/0/0/0
2	CYG	D	3769	2	-	0/10/16/18	0/0/0/0
2	CYG	F	5769	2	-	0/10/16/18	0/0/0/0
2	CYG	H	7769	2	-	0/10/16/18	0/0/0/0

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	5769	CYG	CD1-SG	-2.95	1.68	1.76
2	H	7769	CYG	CD1-SG	-2.69	1.69	1.76
2	F	5769	CYG	CA-C	2.12	1.53	1.50
2	B	1769	CYG	CA-C	2.77	1.53	1.50
2	D	3769	CYG	CA-C	3.89	1.55	1.50

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	7769	CYG	CB-SG-CD1	-8.11	94.85	101.21
2	B	1769	CYG	OE2-CD1-CG1	-7.26	116.73	124.14
2	D	3769	CYG	OE2-CD1-CG1	-6.24	117.78	124.14
2	F	5769	CYG	OE2-CD1-SG	-2.97	118.56	122.60
2	H	7769	CYG	OE2-CD1-CG1	-2.58	121.51	124.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	5769	CYG	1	0
2	H	7769	CYG	2	0

## 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	4	25,29,29	1.40	4 (16%)	25,45,45	1.58	4 (16%)
3	PO4	A	1906	5,4	4,4,4	1.52	1 (25%)	6,6,6	0.99	0
7	ADP	A	1910	5,4	25,29,29	1.25	3 (12%)	25,45,45	1.04	2 (8%)
8	ORN	A	1920	-	3,8,8	0.43	0	2,9,9	0.98	0
9	NET	A	1950	-	8,8,8	0.79	0	10,10,10	0.49	0
3	PO4	A	1980	-	4,4,4	2.05	1 (25%)	6,6,6	0.92	0
3	PO4	A	1981	-	4,4,4	2.33	1 (25%)	6,6,6	1.32	1 (16%)
3	PO4	A	1982	-	4,4,4	2.76	3 (75%)	6,6,6	0.64	0
7	ADP	C	3900	4	25,29,29	1.16	3 (12%)	25,45,45	1.16	3 (12%)
3	PO4	C	3906	5,4	4,4,4	1.57	0	6,6,6	1.12	1 (16%)
7	ADP	C	3910	5,4	25,29,29	1.39	3 (12%)	25,45,45	1.42	4 (16%)
8	ORN	C	3920	-	3,8,8	0.50	0	2,9,9	0.58	0
9	NET	C	3950	-	8,8,8	0.67	0	10,10,10	0.62	0
3	PO4	C	3980	-	4,4,4	1.36	0	6,6,6	0.43	0
3	PO4	C	3981	-	4,4,4	3.66	4 (100%)	6,6,6	0.90	0
3	PO4	C	3982	-	4,4,4	2.91	3 (75%)	6,6,6	1.10	0
7	ADP	E	5900	4	25,29,29	1.47	4 (16%)	25,45,45	1.06	2 (8%)
3	PO4	E	5906	5,4	4,4,4	1.60	1 (25%)	6,6,6	0.74	0
7	ADP	E	5910	5,4	25,29,29	1.41	4 (16%)	25,45,45	1.09	3 (12%)
8	ORN	E	5920	-	3,8,8	0.50	0	2,9,9	0.46	0
9	NET	E	5950	-	8,8,8	0.77	0	10,10,10	0.52	0
3	PO4	E	5980	-	4,4,4	3.22	3 (75%)	6,6,6	0.98	0
3	PO4	E	5981	-	4,4,4	1.27	0	6,6,6	0.73	0
7	ADP	G	7900	4	25,29,29	1.32	5 (20%)	25,45,45	1.40	3 (12%)
3	PO4	G	7906	5,4	4,4,4	1.41	1 (25%)	6,6,6	0.59	0
7	ADP	G	7910	5,4	25,29,29	1.21	3 (12%)	25,45,45	1.25	3 (12%)
8	ORN	G	7920	-	3,8,8	0.45	0	2,9,9	0.18	0
9	NET	G	7950	-	8,8,8	0.65	0	10,10,10	0.50	0
3	PO4	G	7980	-	4,4,4	3.01	2 (50%)	6,6,6	0.84	0
3	PO4	G	7981	-	4,4,4	2.70	1 (25%)	6,6,6	0.98	0
3	PO4	G	7982	-	4,4,4	3.30	2 (50%)	6,6,6	1.19	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	4	-	0/12/32/32	0/3/3/3
3	PO4	A	1906	5,4	-	0/0/0/0	0/0/0/0
7	ADP	A	1910	5,4	-	0/12/32/32	0/3/3/3
8	ORN	A	1920	-	-	0/4/8/8	0/0/0/0
9	NET	A	1950	-	-	0/12/12/12	0/0/0/0
3	PO4	A	1980	-	-	0/0/0/0	0/0/0/0
3	PO4	A	1981	-	-	0/0/0/0	0/0/0/0
3	PO4	A	1982	-	-	0/0/0/0	0/0/0/0
7	ADP	C	3900	4	-	0/12/32/32	0/3/3/3
3	PO4	C	3906	5,4	-	0/0/0/0	0/0/0/0
7	ADP	C	3910	5,4	-	0/12/32/32	0/3/3/3
8	ORN	C	3920	-	-	0/4/8/8	0/0/0/0
9	NET	C	3950	-	-	0/12/12/12	0/0/0/0
3	PO4	C	3980	-	-	0/0/0/0	0/0/0/0
3	PO4	C	3981	-	-	0/0/0/0	0/0/0/0
3	PO4	C	3982	-	-	0/0/0/0	0/0/0/0
7	ADP	E	5900	4	-	0/12/32/32	0/3/3/3
3	PO4	E	5906	5,4	-	0/0/0/0	0/0/0/0
7	ADP	E	5910	5,4	-	0/12/32/32	0/3/3/3
8	ORN	E	5920	-	-	0/4/8/8	0/0/0/0
9	NET	E	5950	-	-	0/12/12/12	0/0/0/0
3	PO4	E	5980	-	-	0/0/0/0	0/0/0/0
3	PO4	E	5981	-	-	0/0/0/0	0/0/0/0
7	ADP	G	7900	4	-	0/12/32/32	0/3/3/3
3	PO4	G	7906	5,4	-	0/0/0/0	0/0/0/0
7	ADP	G	7910	5,4	-	0/12/32/32	0/3/3/3
8	ORN	G	7920	-	-	0/4/8/8	0/0/0/0
9	NET	G	7950	-	-	0/12/12/12	0/0/0/0
3	PO4	G	7980	-	-	0/0/0/0	0/0/0/0
3	PO4	G	7981	-	-	0/0/0/0	0/0/0/0
3	PO4	G	7982	-	-	0/0/0/0	0/0/0/0

The worst 5 of 52 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	E	5900	ADP	O4'-C1'	-4.97	1.34	1.41
7	A	1900	ADP	O4'-C1'	-2.74	1.37	1.41
7	E	5910	ADP	O4'-C1'	-2.45	1.37	1.41
7	A	1910	ADP	O4'-C1'	-2.31	1.38	1.41
3	E	5906	PO4	P-O4	-2.30	1.46	1.54

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	3900	ADP	O2B-PB-O1B	-2.19	102.06	110.60
7	C	3900	ADP	C1'-N9-C4	-2.17	122.89	126.64
7	A	1910	ADP	O3B-PB-O2B	-2.09	99.31	107.59
7	A	1900	ADP	C5-C6-N1	-2.01	113.62	119.70
7	E	5900	ADP	C2'-C3'-C4'	-2.00	98.77	102.62

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

13 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1910	ADP	2	0
8	A	1920	ORN	1	0
9	A	1950	NET	1	0
3	C	3906	PO4	1	0
7	C	3910	ADP	1	0
8	C	3920	ORN	3	0
7	E	5900	ADP	1	0
8	E	5920	ORN	1	0
9	E	5950	NET	2	0
7	G	7900	ADP	2	0
3	G	7906	PO4	1	0
7	G	7910	ADP	2	0
8	G	7920	ORN	1	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

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.