wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 06:53 PM GMT

PDB ID	:	1CS0
Title	:	Crystal structure of carbamoyl phosphate synthetase complexed at CYS269 in the small subunit with the tetrahedral mimic l-glutamate gamma-semialdehyde
Authors	:	Thoden, J.B.; Huang, X.; Raushel, F.M.; Holden, H.M.
Deposited on	:	1999-08-16
Resolution	:	2.00 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 (i) symbol.

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

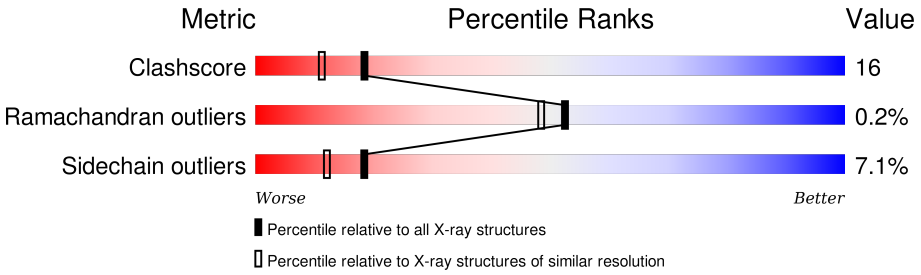
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)

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 <=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	60% 31% 6% ••
1	C	1073	60% 31% 6% ••
1	E	1073	65% 27% 6% ••
1	G	1073	61% 30% 7% ••
2	B	382	59% 35% 5% •
2	D	382	59% 34% 7% •
2	F	382	60% 35% • •

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Mol	Chain	Length	Quality of chain
2	H	382	

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 48889 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 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1058	Total	C	N	O	S	0	3	0
			8169	5128	1422	1574	45			
1	C	1058	Total	C	N	O	S	0	3	0
			8173	5132	1423	1573	45			
1	E	1058	Total	C	N	O	S	0	6	0
			8186	5140	1424	1576	46			
1	G	1058	Total	C	N	O	S	0	3	0
			8175	5132	1425	1572	46			

- Molecule 2 is a protein called CARBAMOYL PHOSPHATE SYNTHETASE: SMALL SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	379	Total	C	N	O	S	0	0	0
			2904	1830	509	555	10			
2	D	379	Total	C	N	O	S	0	1	0
			2909	1833	509	557	10			
2	F	379	Total	C	N	O	S	0	0	0
			2904	1830	509	555	10			
2	H	379	Total	C	N	O	S	0	1	0
			2906	1831	509	556	10			

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	3	Total Mn 3 3	0	0

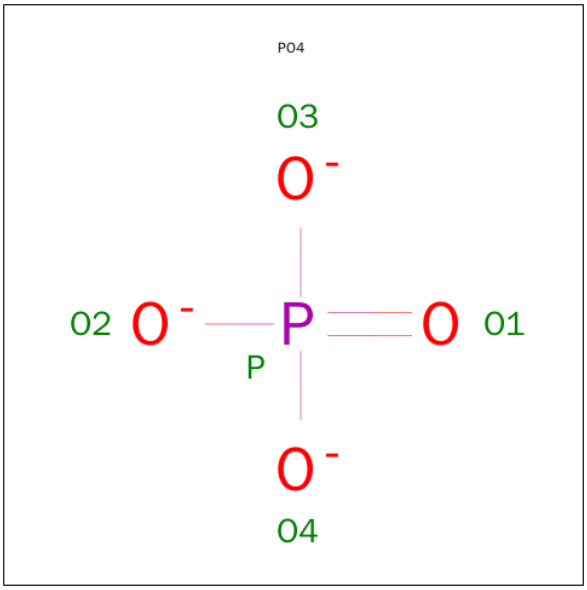
- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

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	8	Total K 8 8	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
4	F	1	Total K 1 1	0	0

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

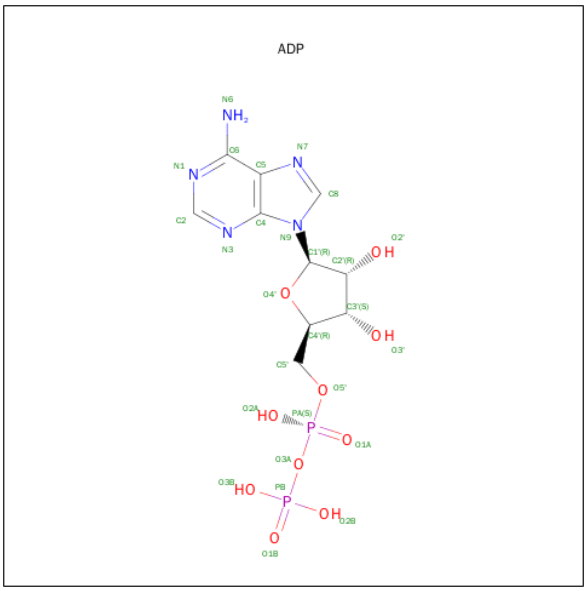
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	G	5	Total Cl 5 5	0	0
5	D	2	Total Cl 2 2	0	0
5	E	5	Total Cl 5 5	0	0
5	H	2	Total Cl 2 2	0	0
5	B	2	Total Cl 2 2	0	0
5	C	5	Total Cl 5 5	0	0
5	A	6	Total Cl 6 6	0	0
5	F	2	Total Cl 2 2	0	0

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



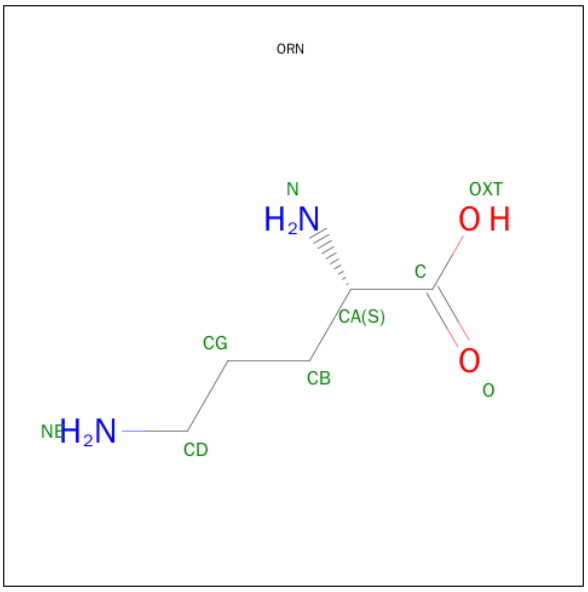
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O P 5 4 1	0	0
6	C	1	Total O P 5 4 1	0	0
6	E	1	Total O P 5 4 1	0	0
6	E	1	Total O P 5 4 1	0	0
6	G	1	Total O P 5 4 1	0	0

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



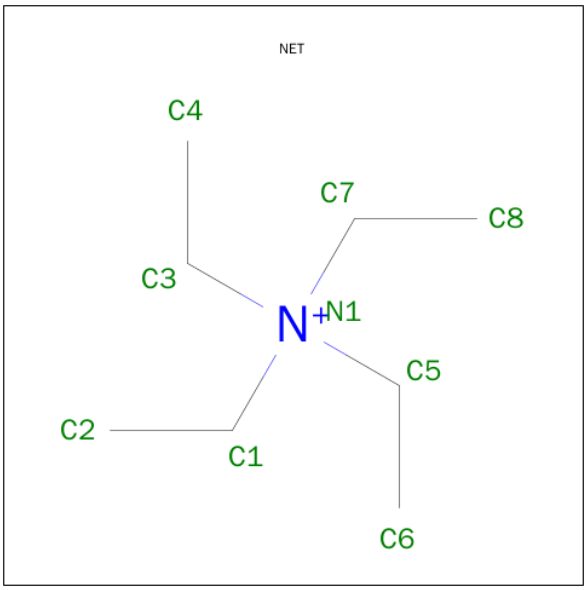
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	G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

- Molecule 8 is L-ORNITHINE (three-letter code: ORN) (formula: $C_5H_{12}N_2O_2$).



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

- Molecule 9 is TETRAETHYLAMMONIUM ION (three-letter code: NET) (formula: $C_8H_{20}N$).



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	869	Total O 869 869	0	0
10	B	213	Total O 213 213	0	0
10	C	784	Total O 784 784	0	0
10	D	275	Total O 275 275	0	0
10	E	864	Total O 864 864	0	0
10	F	235	Total O 235 235	0	0
10	G	743	Total O 743 743	0	0
10	H	193	Total O 193 193	0	0

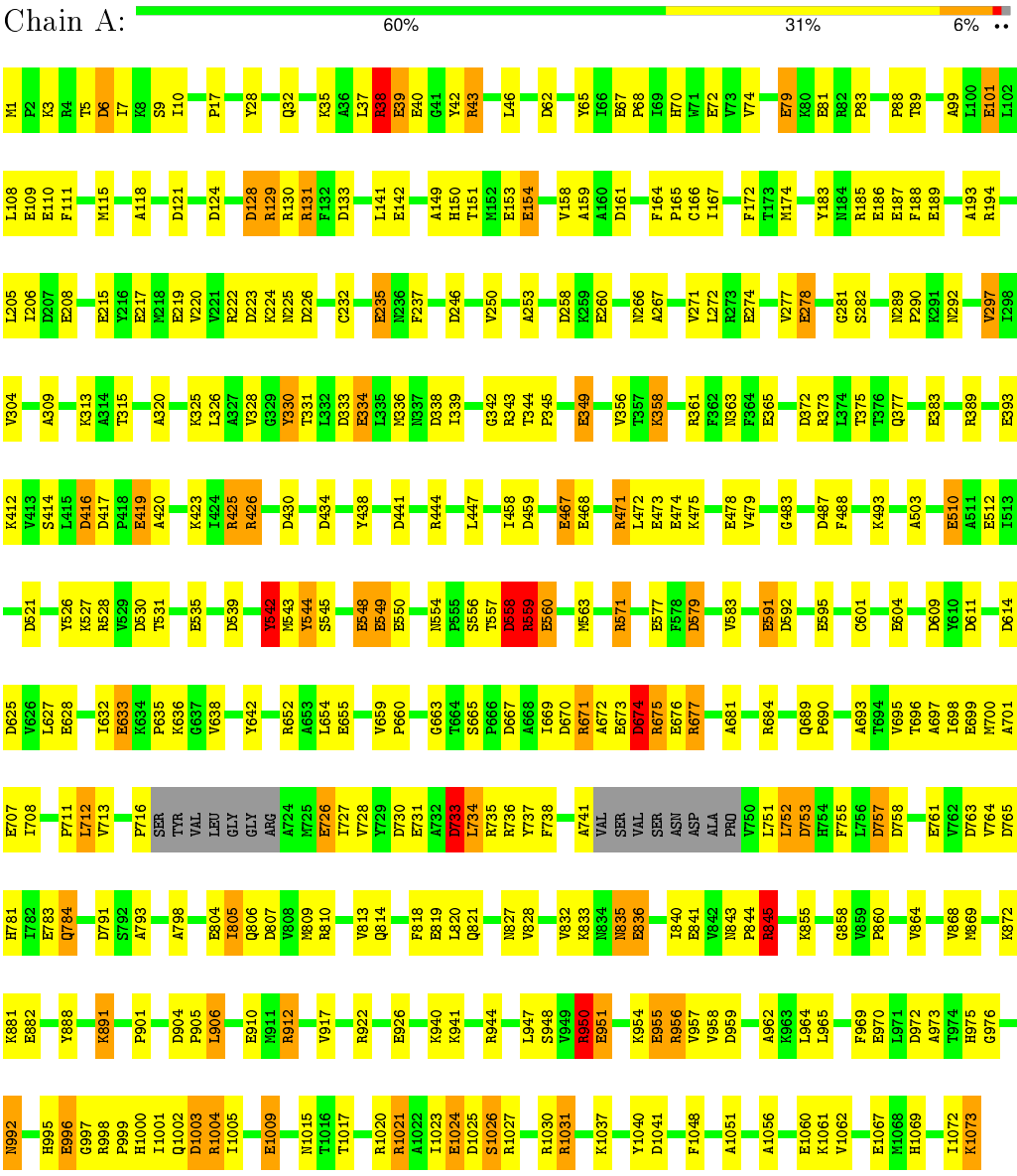
3 Residue-property plots (i)

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.

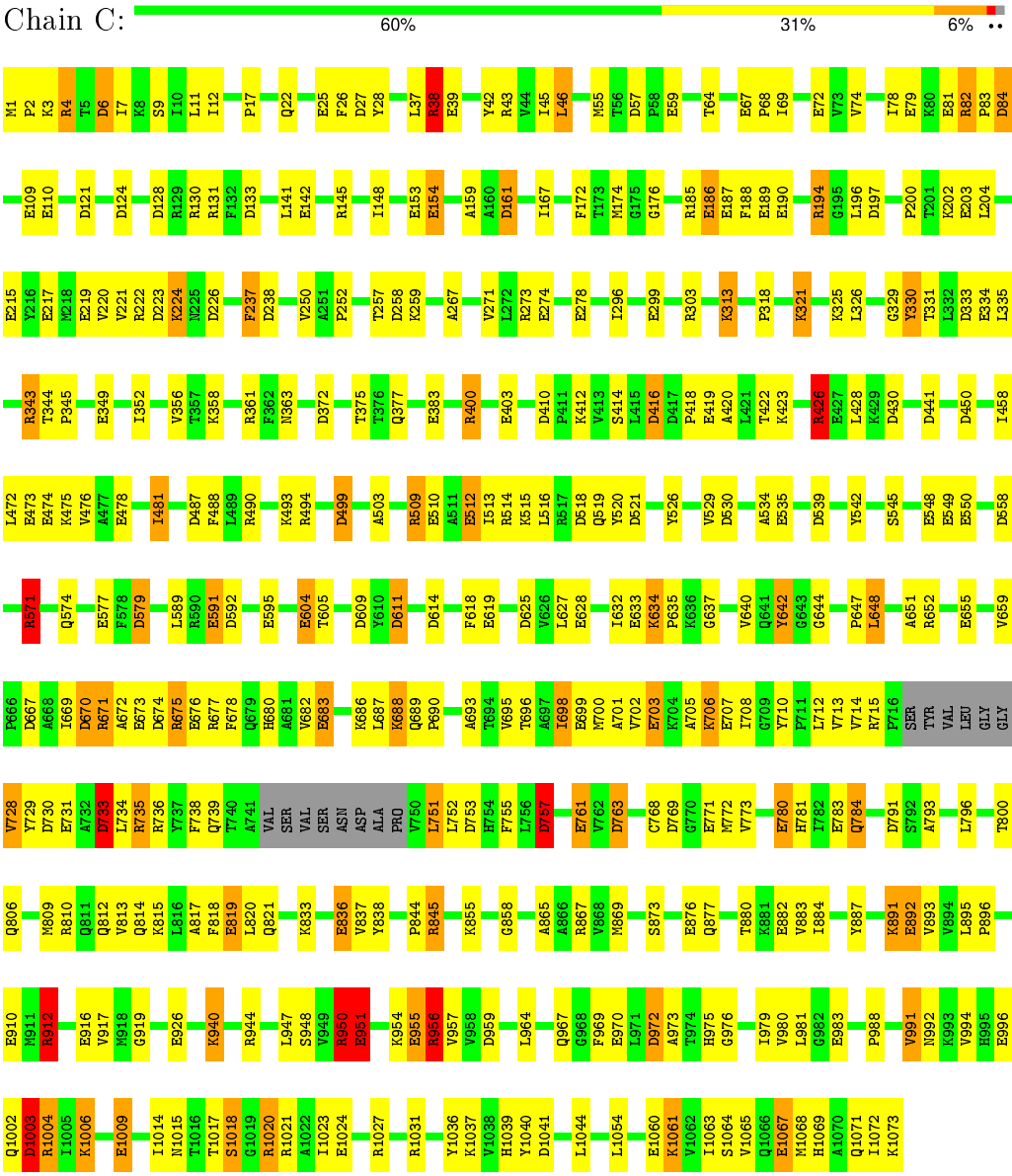
- Molecule 1: CARBAMOYL PHOSPHATE SYNTHETASE: LARGE SUBUNIT

Chain A:



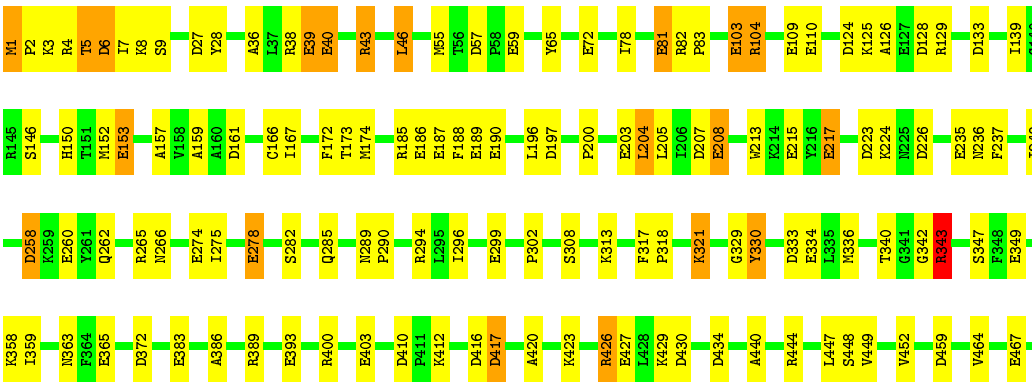
- Molecule 1: CARBAMOYL PHOSPHATE SYNTHETASE: LARGE SUBUNIT

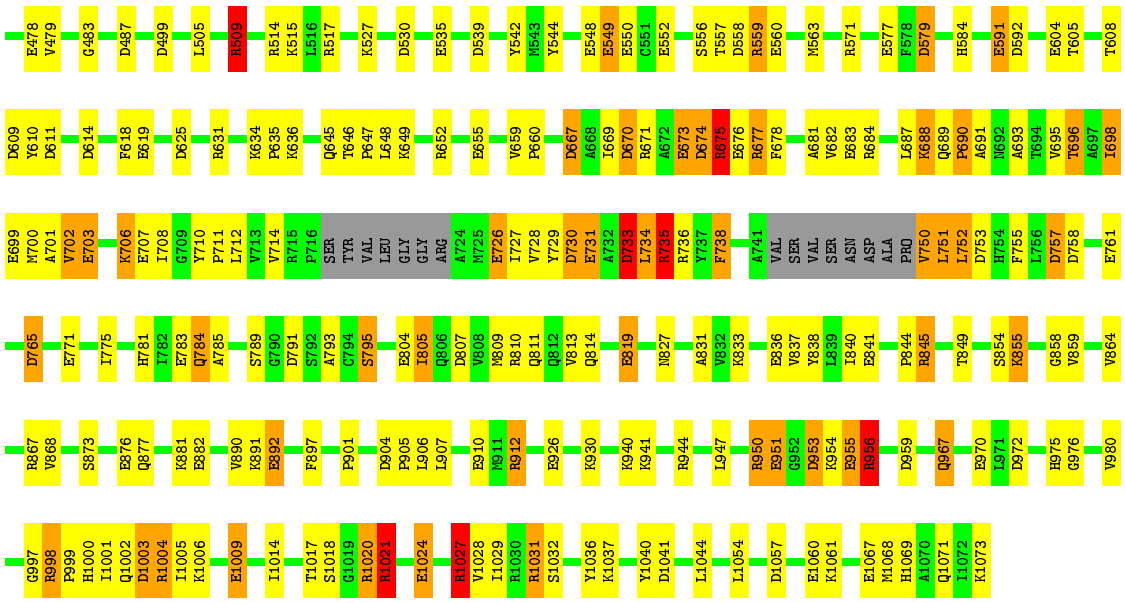
Chain C:



• Molecule 1: CARBAMOYL PHOSPHATE SYNTHETASE: LARGE SUBUNIT

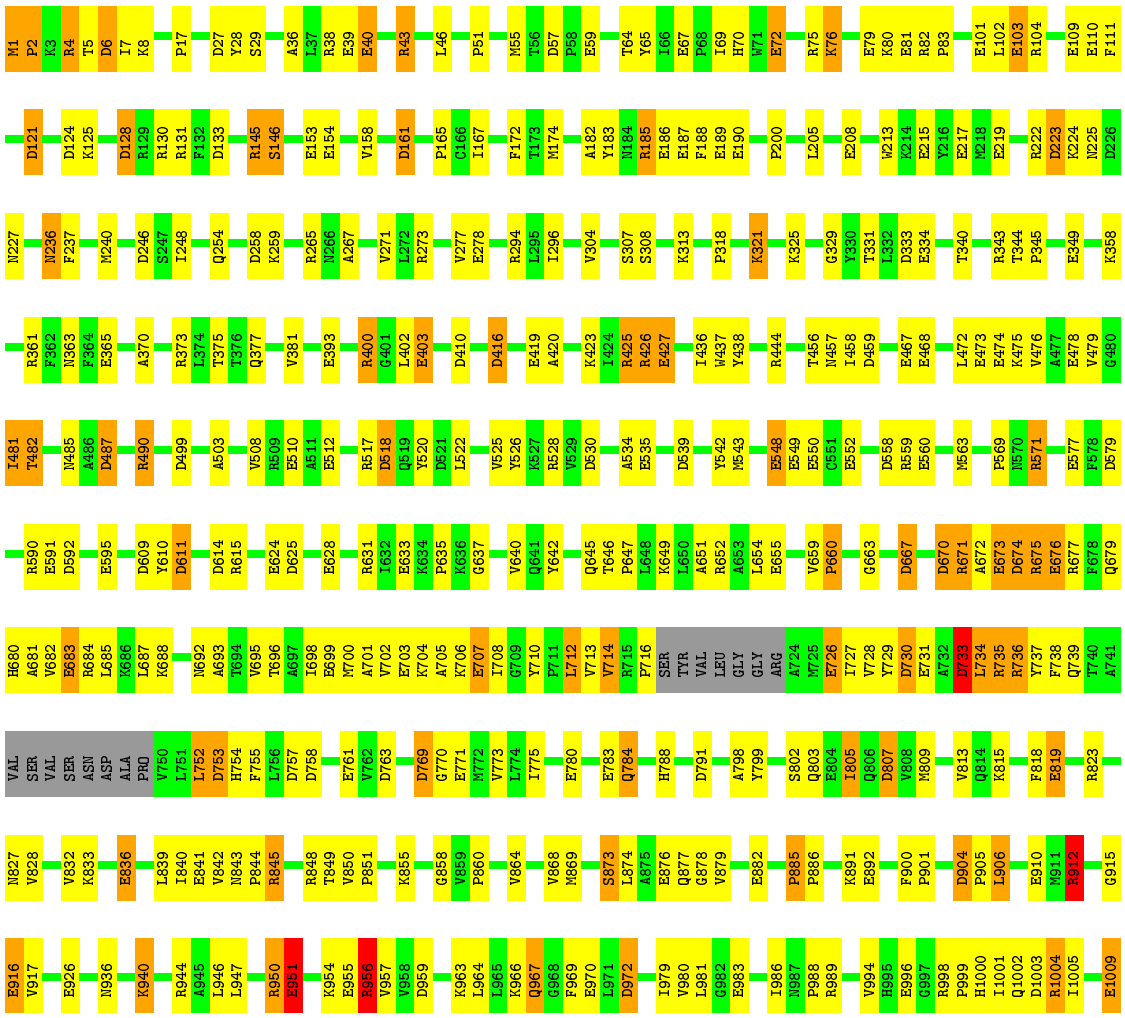
Chain E:





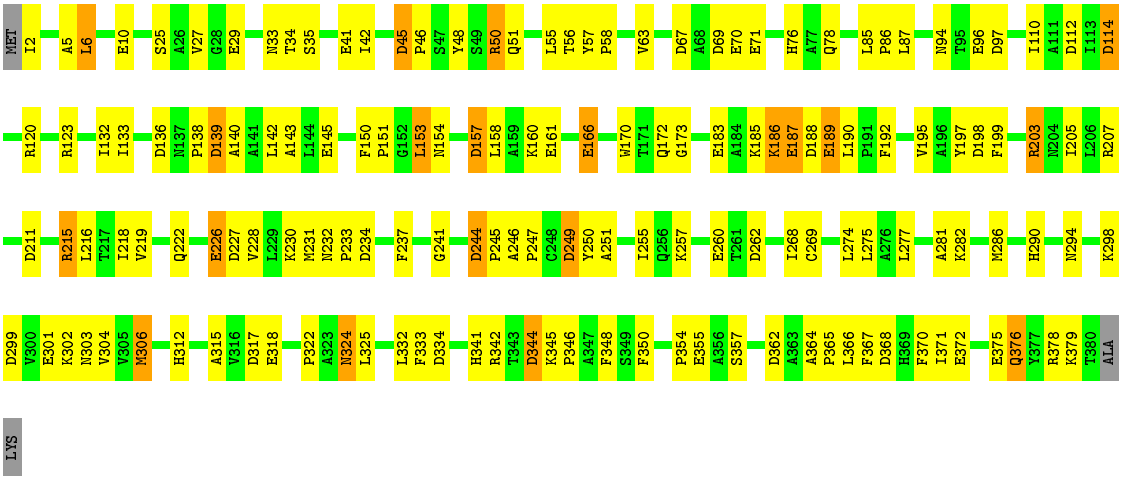
• Molecule 1: CARBAMOYL PHOSPHATE SYNTHETASE: LARGE SUBUNIT

Chain G:



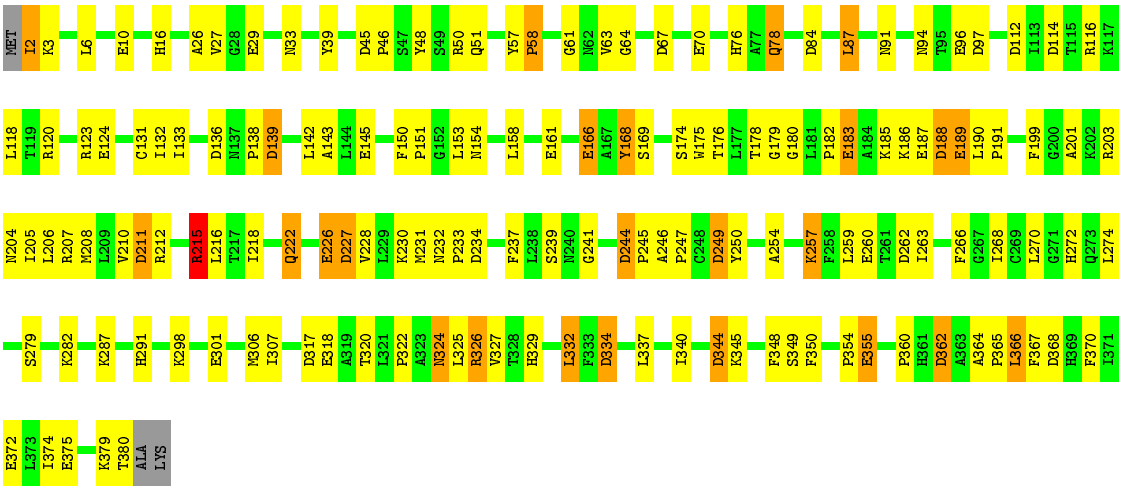
• Molecule 2: CARBAMOYL PHOSPHATE SYNTHETASE: SMALL SUBUNIT

Chain B:



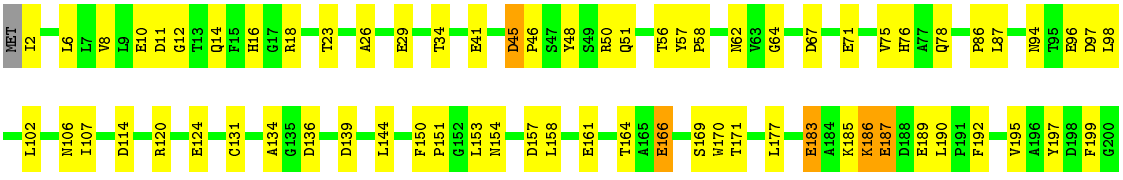
• Molecule 2: CARBAMOYL PHOSPHATE SYNTHETASE: SMALL SUBUNIT

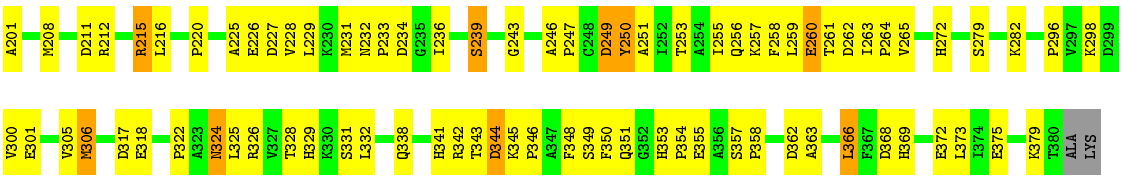
Chain D:



• Molecule 2: CARBAMOYL PHOSPHATE SYNTHETASE: SMALL SUBUNIT

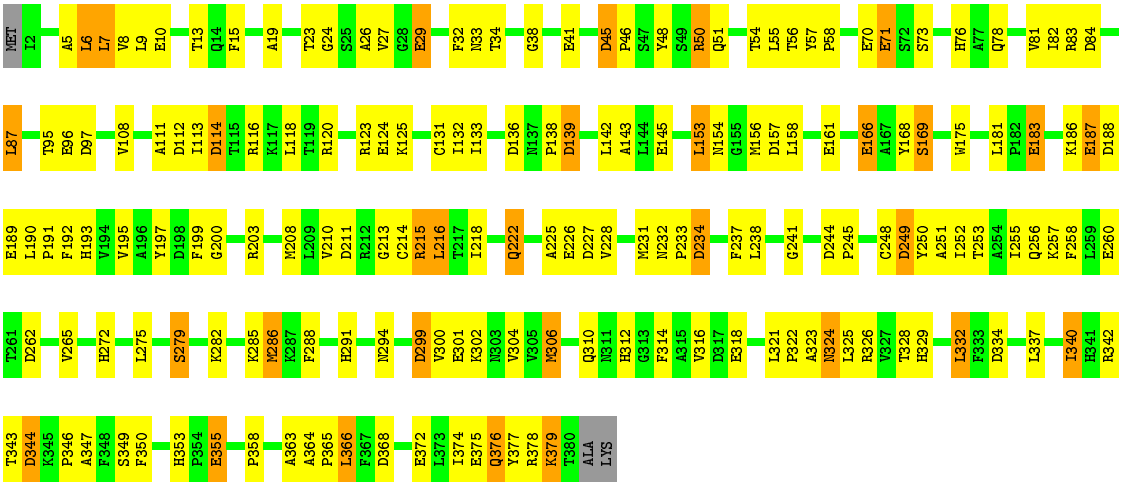
Chain F:





• Molecule 2: CARBAMOYL PHOSPHATE SYNTHETASE: SMALL SUBUNIT

Chain H:



4 Data and refinement statistics (i)

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	151.70Å 163.80Å 332.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.00	Depositor
% Data completeness (in resolution range)	98.7 (30.00-2.00)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.186 , 0.242	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	48889	wwPDB-VP
Average B, all atoms (Å^2)	34.0	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	1.05	72/8307 (0.9%)	1.38	129/11230 (1.1%)
1	C	1.04	70/8311 (0.8%)	1.38	130/11236 (1.2%)
1	E	1.05	64/8336 (0.8%)	1.35	129/11267 (1.1%)
1	G	1.04	71/8313 (0.9%)	1.36	109/11237 (1.0%)
2	B	0.92	18/2950 (0.6%)	1.29	32/4005 (0.8%)
2	D	0.98	15/2959 (0.5%)	1.31	40/4017 (1.0%)
2	F	0.96	16/2950 (0.5%)	1.34	31/4005 (0.8%)
2	H	0.93	19/2956 (0.6%)	1.30	36/4013 (0.9%)
All	All	1.02	345/45082 (0.8%)	1.35	636/61010 (1.0%)

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	C	1	0

The worst 5 of 345 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	189	GLU	CD-OE2	13.05	1.40	1.25
1	G	39	GLU	CD-OE1	-9.37	1.15	1.25
1	E	403	GLU	CD-OE2	8.00	1.34	1.25
1	E	819	GLU	CD-OE2	7.90	1.34	1.25
1	E	427	GLU	CD-OE2	7.81	1.34	1.25

The worst 5 of 636 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	956	ARG	NE-CZ-NH2	-12.15	114.22	120.30
1	A	677	ARG	NE-CZ-NH1	10.84	125.72	120.30
1	A	677	ARG	NE-CZ-NH2	-10.47	115.07	120.30
1	G	43	ARG	NE-CZ-NH1	10.34	125.47	120.30
1	G	43	ARG	NE-CZ-NH2	-10.24	115.18	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	339	ILE	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	8169	0	8201	245	0
1	C	8173	0	8207	259	0
1	E	8186	0	8220	206	0
1	G	8175	0	8210	282	0
2	B	2904	0	2867	95	0
2	D	2909	0	2869	95	0
2	F	2904	0	2867	86	0
2	H	2906	0	2868	129	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	8	0	0	0	0
4	F	1	0	0	0	0
4	G	7	0	0	0	0
4	H	1	0	0	0	0
5	A	6	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	2	0	0	0	0
5	C	5	0	0	2	0
5	D	2	0	0	0	0
5	E	5	0	0	2	0
5	F	2	0	0	0	0
5	G	5	0	0	3	0
5	H	2	0	0	0	0
6	A	5	0	0	0	0
6	C	5	0	0	0	0
6	E	10	0	0	0	0
6	G	5	0	0	0	0
7	A	54	0	24	0	0
7	C	54	0	24	0	0
7	E	54	0	24	1	0
7	G	54	0	24	3	0
8	A	9	0	11	0	0
8	C	9	0	11	2	0
8	E	9	0	11	3	0
8	G	9	0	11	0	0
9	A	9	0	20	2	0
9	C	9	0	20	0	0
9	E	9	0	20	1	0
9	G	9	0	20	0	0
10	A	869	0	0	26	0
10	B	213	0	0	3	0
10	C	784	0	0	16	0
10	D	275	0	0	6	0
10	E	864	0	0	22	0
10	F	235	0	0	2	0
10	G	743	0	0	25	0
10	H	193	0	0	6	0
All	All	48889	0	44529	1385	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 16.

The worst 5 of 1385 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:187:GLU:HG2	2:B:215:ARG:HD2	1.21	1.15
1:G:695:VAL:HG11	1:G:701:ALA:HB2	1.30	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:228:VAL:HA	2:F:231:MET:HE2	1.35	1.06
2:F:187:GLU:HG2	2:F:215:ARG:HD2	1.35	1.05
1:G:1027[B]:ARG:HE	1:G:1031:ARG:HD3	1.17	1.05

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	1055/1073 (98%)	1010 (96%)	43 (4%)	2 (0%)	52	48
1	C	1055/1073 (98%)	999 (95%)	53 (5%)	3 (0%)	46	41
1	E	1058/1073 (99%)	1013 (96%)	42 (4%)	3 (0%)	46	41
1	G	1055/1073 (98%)	1000 (95%)	51 (5%)	4 (0%)	39	33
2	B	376/382 (98%)	357 (95%)	19 (5%)	0	100	100
2	D	377/382 (99%)	364 (97%)	13 (3%)	0	100	100
2	F	376/382 (98%)	361 (96%)	15 (4%)	0	100	100
2	H	377/382 (99%)	367 (97%)	10 (3%)	0	100	100
All	All	5729/5820 (98%)	5471 (96%)	246 (4%)	12 (0%)	52	48

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	954	LYS
1	G	739	GLN
1	A	558	ASP
1	C	739	GLN
1	E	738	PHE

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	868/878 (99%)	810 (93%)	58 (7%)	20 14
1	C	868/878 (99%)	798 (92%)	70 (8%)	15 9
1	E	871/878 (99%)	814 (94%)	57 (6%)	21 15
1	G	868/878 (99%)	806 (93%)	62 (7%)	18 12
2	B	307/309 (99%)	284 (92%)	23 (8%)	17 11
2	D	308/309 (100%)	285 (92%)	23 (8%)	17 11
2	F	307/309 (99%)	288 (94%)	19 (6%)	23 16
2	H	308/309 (100%)	283 (92%)	25 (8%)	15 9
All	All	4705/4748 (99%)	4368 (93%)	337 (7%)	18 12

5 of 337 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	50	ARG
1	E	509	ARG
1	G	1073	LYS
2	D	153	LEU
2	D	372[B]	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 84 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	1071	GLN
1	E	689	GLN
1	G	1055	ASN
2	D	78	GLN
2	D	324	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	269	2	10,14,15	2.73	2 (20%)	6,17,19	9.27	2 (33%)
2	CYG	D	269	2	10,14,15	2.73	2 (20%)	6,17,19	9.25	2 (33%)
2	CYG	F	269	2	10,14,15	2.74	2 (20%)	6,17,19	9.26	2 (33%)
2	CYG	H	269	2	10,14,15	2.76	2 (20%)	6,17,19	9.27	2 (33%)

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	269	2	-	0/10/16/18	0/0/0/0
2	CYG	D	269	2	-	0/10/16/18	0/0/0/0
2	CYG	F	269	2	-	0/10/16/18	0/0/0/0
2	CYG	H	269	2	-	0/10/16/18	0/0/0/0

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	269	CYG	CD1-SG	-4.26	1.67	1.76
2	F	269	CYG	CD1-SG	-4.24	1.67	1.76
2	B	269	CYG	CD1-SG	-4.23	1.67	1.76
2	D	269	CYG	CD1-SG	-4.22	1.67	1.76
2	B	269	CYG	OE2-CD1	7.15	1.32	1.21

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	269	CYG	OE2-CD1-CG1	-17.52	111.88	123.94
2	B	269	CYG	OE2-CD1-CG1	-17.52	111.89	123.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	269	CYG	OE2-CD1-CG1	-17.51	111.89	123.94
2	D	269	CYG	OE2-CD1-CG1	-17.46	111.92	123.94
2	D	269	CYG	OE2-CD1-SG	-14.22	111.55	122.83

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	269	CYG	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 95 ligands modelled in this entry, 74 are monoatomic - leaving 21 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	5000	3	22,29,29	1.31	4 (18%)	27,45,45	1.08	2 (7%)
6	PO4	A	5005	3,4	4,4,4	1.38	0	6,6,6	0.31	0
7	ADP	A	5006	3,4	22,29,29	1.13	2 (9%)	27,45,45	0.84	0
8	ORN	A	5010	-	5,8,8	0.59	0	3,9,9	1.02	0
9	NET	A	5094	-	8,8,8	0.54	0	10,10,10	0.65	0
7	ADP	C	5023	3	22,29,29	1.34	5 (22%)	27,45,45	0.87	1 (3%)
6	PO4	C	5028	3,4	4,4,4	1.60	1 (25%)	6,6,6	0.31	0
7	ADP	C	5029	3,4	22,29,29	1.20	2 (9%)	27,45,45	1.07	3 (11%)
8	ORN	C	5033	-	5,8,8	0.68	0	3,9,9	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	NET	C	5034	-	8,8,8	0.67	0	10,10,10	0.48	0
7	ADP	E	5046	3	22,29,29	1.21	3 (13%)	27,45,45	0.98	0
6	PO4	E	5051	3,4	4,4,4	1.92	2 (50%)	6,6,6	0.30	0
7	ADP	E	5052	3,4	22,29,29	1.06	3 (13%)	27,45,45	1.08	3 (11%)
8	ORN	E	5056	-	5,8,8	0.67	0	3,9,9	0.64	0
9	NET	E	5057	-	8,8,8	0.77	0	10,10,10	0.36	0
6	PO4	E	5070	-	4,4,4	1.34	0	6,6,6	0.31	0
7	ADP	G	5071	3	22,29,29	1.37	4 (18%)	27,45,45	1.41	3 (11%)
6	PO4	G	5076	3,4	4,4,4	1.46	1 (25%)	6,6,6	0.30	0
7	ADP	G	5077	3,4	22,29,29	1.25	4 (18%)	27,45,45	1.15	3 (11%)
8	ORN	G	5081	-	5,8,8	0.47	0	3,9,9	0.30	0
9	NET	G	5082	-	8,8,8	0.60	0	10,10,10	0.49	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	5000	3	-	0/12/32/32	0/3/3/3
6	PO4	A	5005	3,4	-	0/0/0/0	0/0/0/0
7	ADP	A	5006	3,4	-	0/12/32/32	0/3/3/3
8	ORN	A	5010	-	-	0/4/8/8	0/0/0/0
9	NET	A	5094	-	-	0/12/12/12	0/0/0/0
7	ADP	C	5023	3	-	0/12/32/32	0/3/3/3
6	PO4	C	5028	3,4	-	0/0/0/0	0/0/0/0
7	ADP	C	5029	3,4	-	0/12/32/32	0/3/3/3
8	ORN	C	5033	-	-	0/4/8/8	0/0/0/0
9	NET	C	5034	-	-	0/12/12/12	0/0/0/0
7	ADP	E	5046	3	-	0/12/32/32	0/3/3/3
6	PO4	E	5051	3,4	-	0/0/0/0	0/0/0/0
7	ADP	E	5052	3,4	-	0/12/32/32	0/3/3/3
8	ORN	E	5056	-	-	0/4/8/8	0/0/0/0
9	NET	E	5057	-	-	0/12/12/12	0/0/0/0
6	PO4	E	5070	-	-	0/0/0/0	0/0/0/0
7	ADP	G	5071	3	-	0/12/32/32	0/3/3/3
6	PO4	G	5076	3,4	-	0/0/0/0	0/0/0/0
7	ADP	G	5077	3,4	-	0/12/32/32	0/3/3/3
8	ORN	G	5081	-	-	0/4/8/8	0/0/0/0
9	NET	G	5082	-	-	0/12/12/12	0/0/0/0

The worst 5 of 31 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	5000	ADP	O4'-C1'	-3.86	1.36	1.41
7	E	5046	ADP	O4'-C1'	-3.24	1.37	1.41
6	E	5051	PO4	P-O3	-2.67	1.43	1.53
7	C	5023	ADP	O4'-C1'	-2.66	1.37	1.41
7	E	5052	ADP	O4'-C1'	-2.57	1.38	1.41

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	5000	ADP	C1'-N9-C4	-2.49	123.19	126.94
7	E	5052	ADP	C2'-C3'-C4'	-2.26	97.96	102.61
7	G	5071	ADP	O3B-PB-O3A	-2.07	95.68	105.09
7	A	5000	ADP	N6-C6-N1	2.00	123.50	119.20
7	C	5023	ADP	O3'-C3'-C2'	2.07	118.55	111.83

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	5094	NET	2	0
8	C	5033	ORN	2	0
7	E	5052	ADP	1	0
8	E	5056	ORN	3	0
9	E	5057	NET	1	0
7	G	5071	ADP	1	0
7	G	5077	ADP	2	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 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.