wwPDB X-ray Structure Validation Summary Report (i)

Dec 11, 2022 – 02:13 AM EST

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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

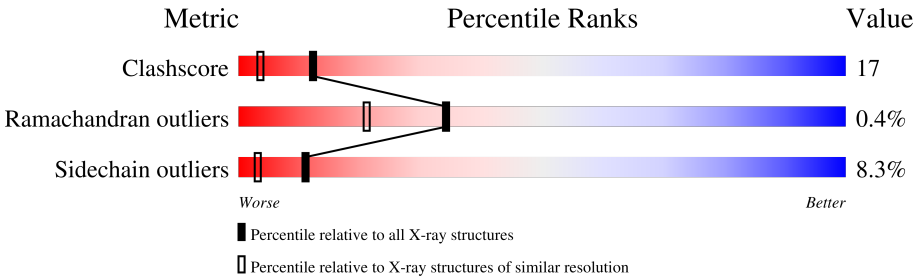
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 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	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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%

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% 34% 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	3906	-	X	-	-
3	PO4	C	3981	-	X	-	-

2 Entry composition (i)

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

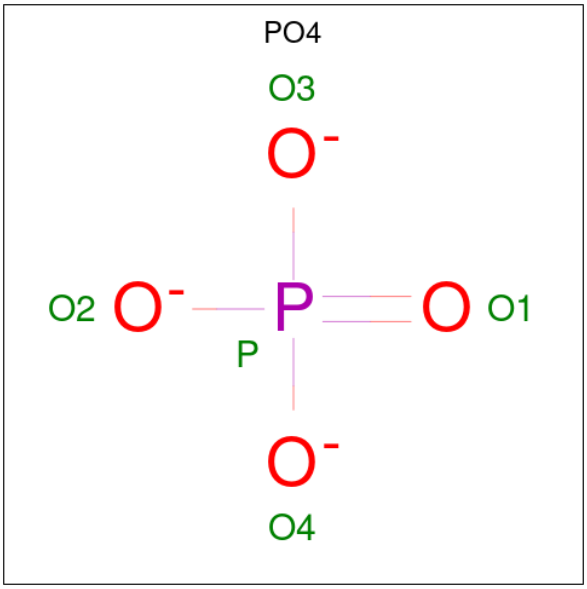
- Molecule 2 is a protein called CARBAMOYL PHOSPHATE SYNTHETASE (SMALL CHAIN).

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 residue	UNP P00907
B	1853	ASN	HIS	engineered mutation	UNP P00907
D	3683	GLN	GLU	conflict	UNP P00907
D	3769	CYG	CYS	modified residue	UNP P00907
D	3853	ASN	HIS	engineered mutation	UNP P00907
F	5683	GLN	GLU	conflict	UNP P00907
F	5769	CYG	CYS	modified residue	UNP P00907
F	5853	ASN	HIS	engineered mutation	UNP P00907
H	7683	GLN	GLU	conflict	UNP P00907
H	7769	CYG	CYS	modified residue	UNP P00907
H	7853	ASN	HIS	engineered mutation	UNP P00907

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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 5 4 1	0	0
3	C	1	Total O P 5 4 1	0	0
3	C	1	Total O P 5 4 1	0	0
3	E	1	Total O P 5 4 1	0	0
3	E	1	Total O P 5 4 1	0	0
3	E	1	Total O P 5 4 1	0	0
3	G	1	Total O P 5 4 1	0	0
3	G	1	Total O P 5 4 1	0	0
3	G	1	Total O P 5 4 1	0	0
3	G	1	Total O P 5 4 1	0	0

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

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

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

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

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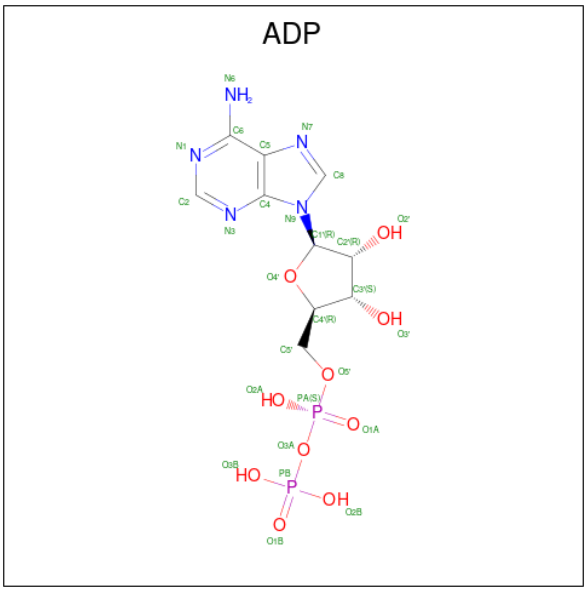
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total K 1 1	0	0
5	E	7	Total K 7 7	0	0
5	F	1	Total K 1 1	0	0
5	G	7	Total K 7 7	0	0
5	H	1	Total K 1 1	0	0

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

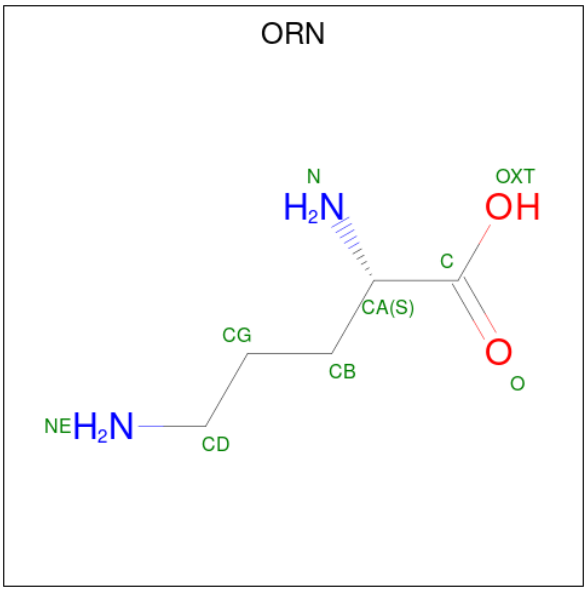
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	6	Total Cl 6 6	0	0
6	B	1	Total Cl 1 1	0	0
6	C	6	Total Cl 6 6	0	0
6	D	1	Total Cl 1 1	0	0
6	E	6	Total Cl 6 6	0	0
6	F	1	Total Cl 1 1	0	0
6	G	6	Total Cl 6 6	0	0
6	H	1	Total Cl 1 1	0	0

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



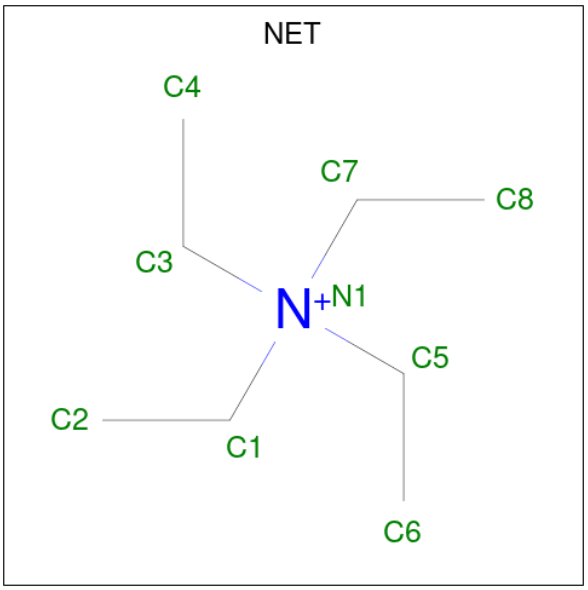
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	G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

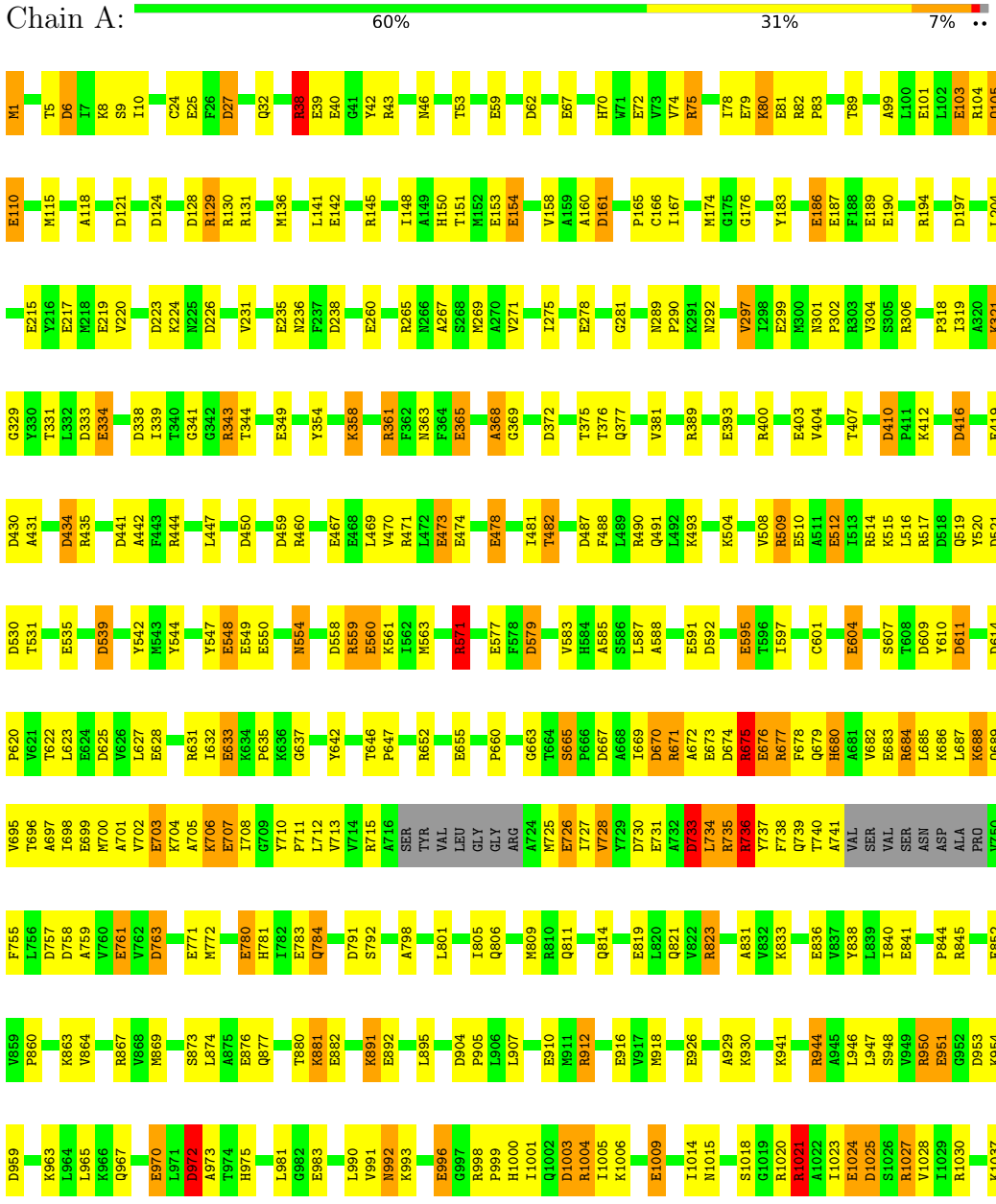
3 Residue-property plots (i)

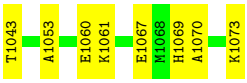
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

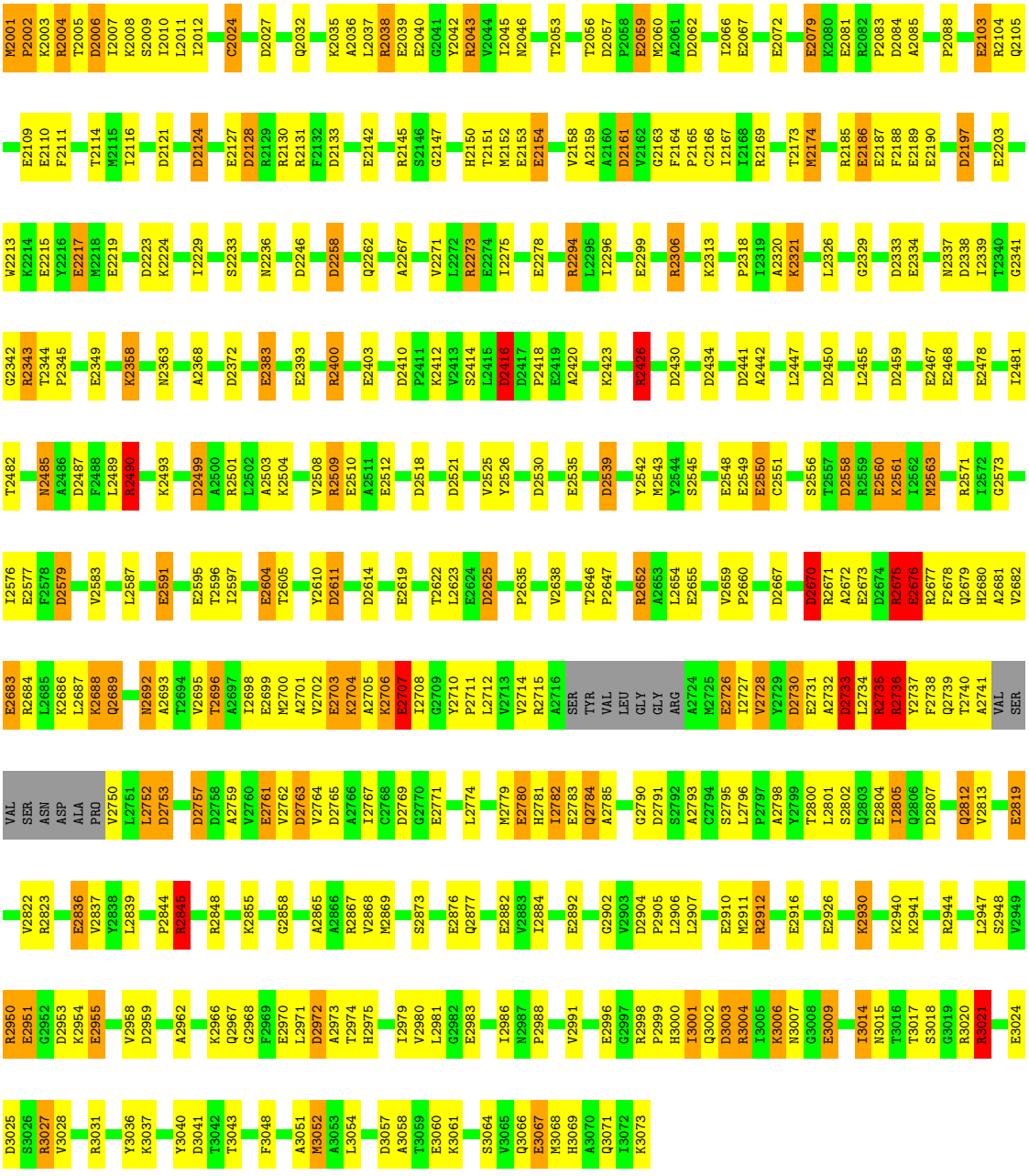
Chain A:





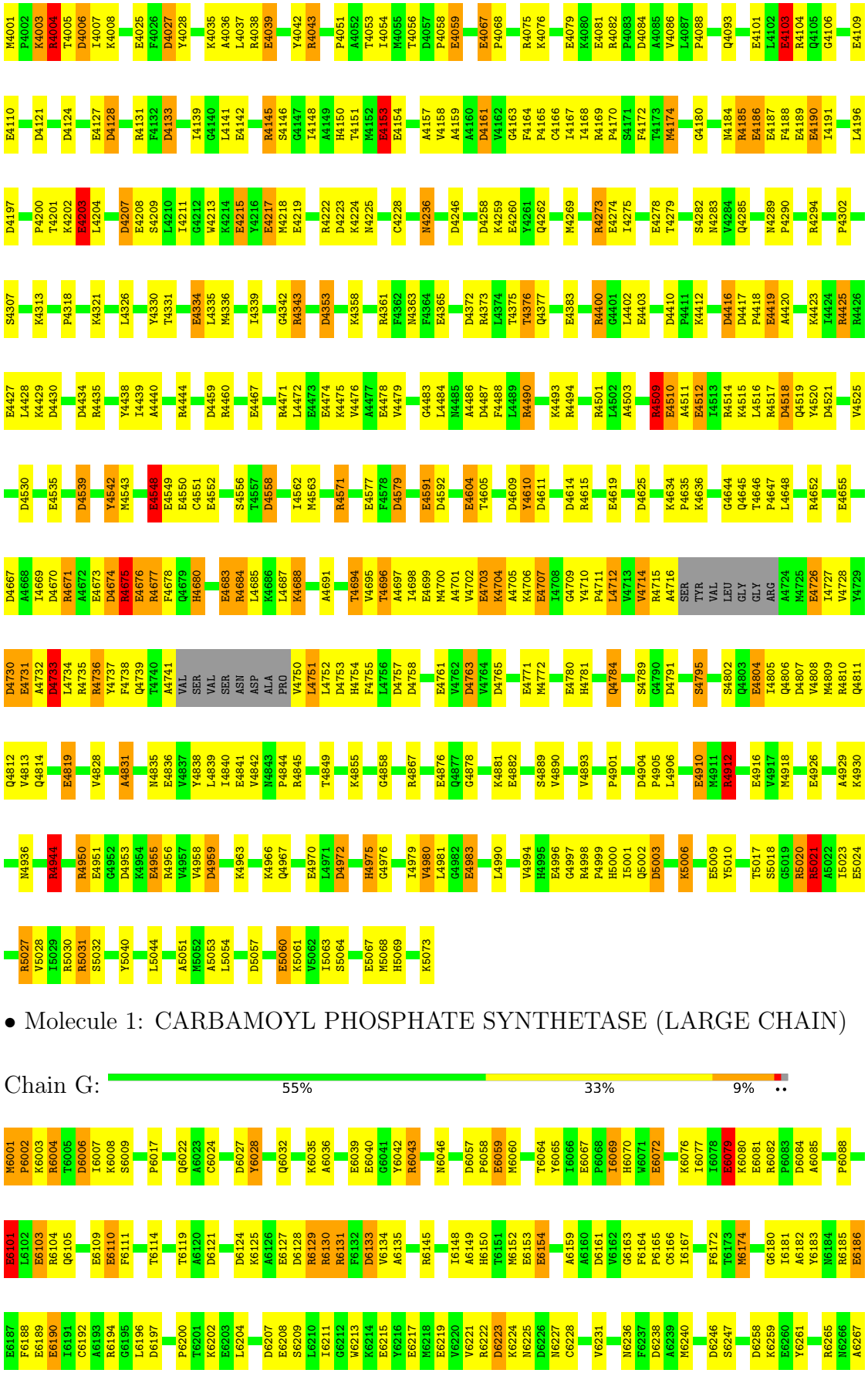
• Molecule 1: CARBAMOYL PHOSPHATE SYNTHETASE (LARGE CHAIN)

Chain C:



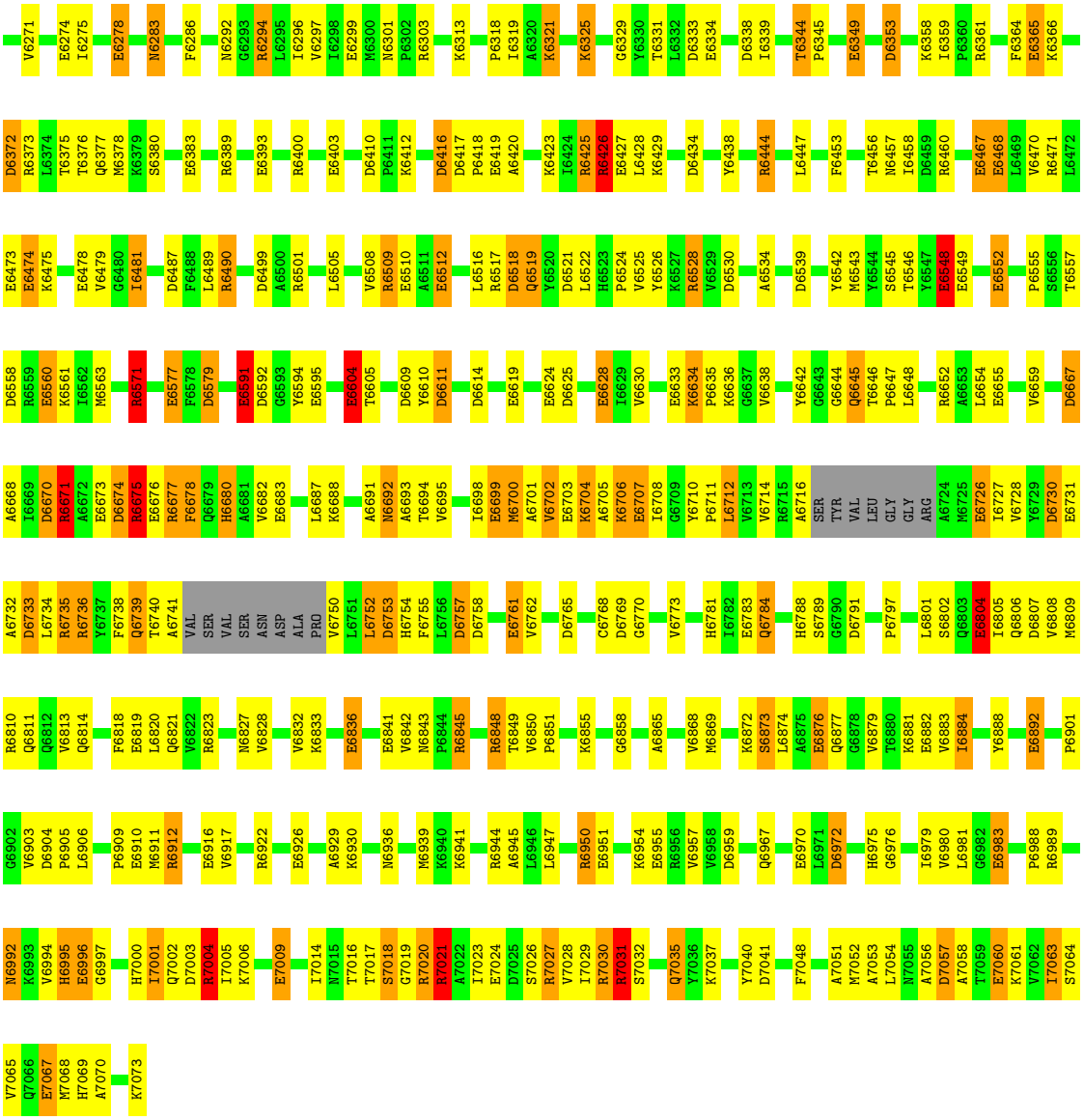
• Molecule 1: CARBAMOYL PHOSPHATE SYNTHETASE (LARGE CHAIN)

Chain E:



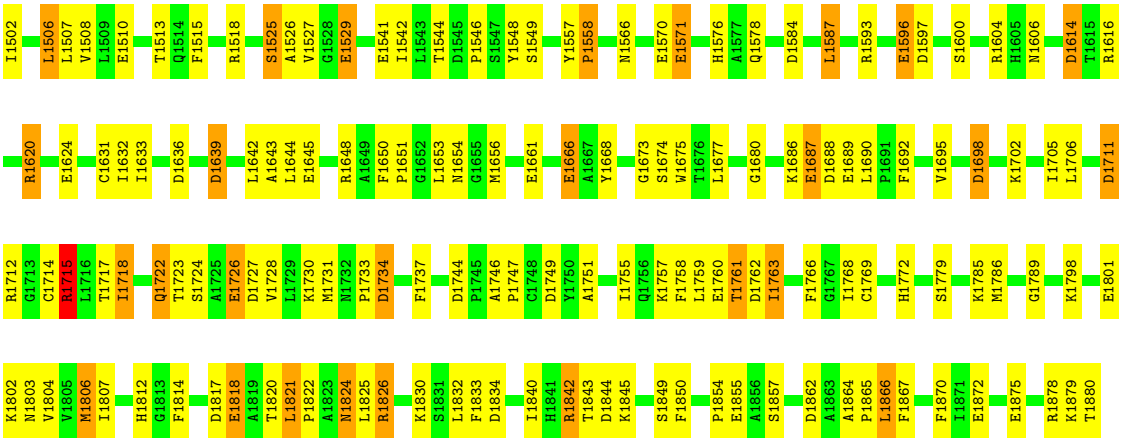
• Molecule 1: CARBAMOYL PHOSPHATE SYNTHETASE (LARGE CHAIN)

Chain G:



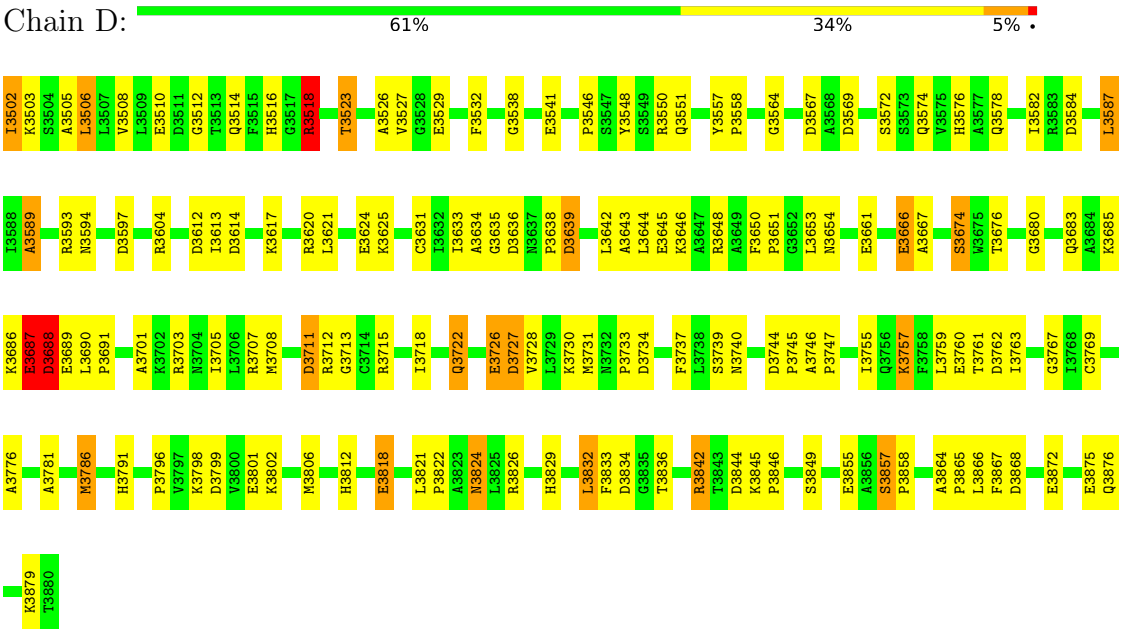
• Molecule 2: CARBAMOYL PHOSPHATE SYNTHETASE (SMALL CHAIN)

Chain B:



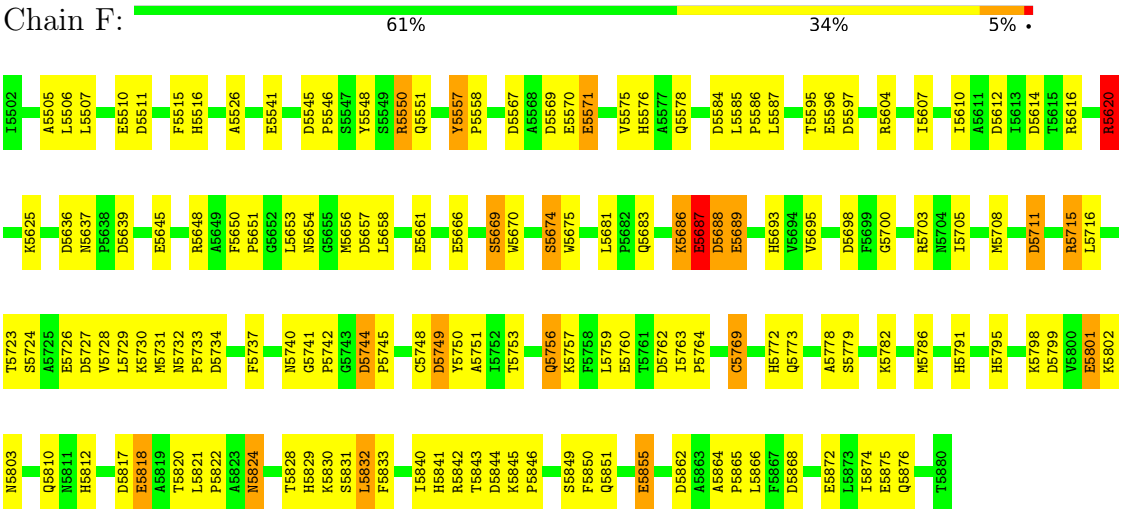
• Molecule 2: CARBAMOYL PHOSPHATE SYNTHETASE (SMALL CHAIN)

Chain D:



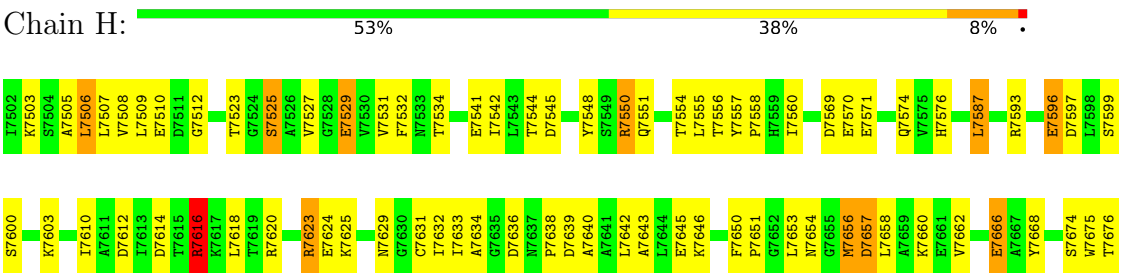
• Molecule 2: CARBAMOYL PHOSPHATE SYNTHETASE (SMALL CHAIN)

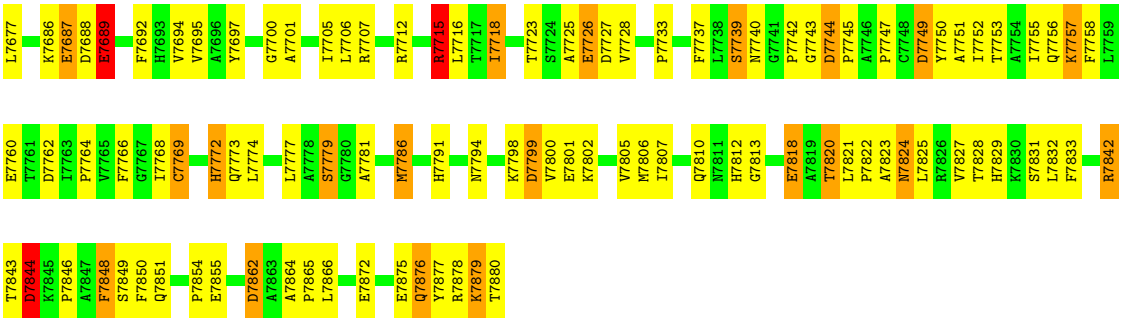
Chain F:



• Molecule 2: CARBAMOYL PHOSPHATE SYNTHETASE (SMALL CHAIN)

Chain H:




L7677 K7686 E7687 D7688 E7689 F7692 H7693 V7694 V7695 A7696 Y7697 G7700 A7701 I7705 L7706 R7707 R7712 R7715 L7716 T7717 I7718 T7723 S7724 A7725 E7726 D7727 V7728 P7733 F7737 L7738 S7739 N7740 G7741 P7742 G7743 D7744 P7745 A7746 P7747 C7748 D7749 Y7750 A7751 I7752 T7753 A7754 I7755 Q7756 K7757 F7758 L7759
E7760 T7761 D7762 I7763 P7764 V7765 F7766 G7767 I7768 C7769 H7772 Q7773 L7774 L7777 A7778 S7779 G7780 A7781 M7786 H7791 N7794 K7798 D7799 V7800 E7801 K7802 V7805 M7806 I7807 Q7810 N7811 H7812 G7813 E7818 A7819 T7820 L7821 P7822 A7823 N7824 L7825 R7826 V7827 T7828 H7829 K7830 S7831 L7832 F7833 R7842
T7843 D7844 K7845 P7846 A7847 F7848 S7849 F7850 Q7851 P7854 E7855 D7862 A7863 A7864 P7865 L7866 E7872 E7875 Q7876 Y7877 R7878 K7879 T7880

4 Data and refinement statistics (i)

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, 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 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^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: PO4, CL, K, NET, ORN, CYG, MN, ADP

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(^{o})	Ideal(^{o})
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%)	41	27
1	C	1059/1073 (99%)	1007 (95%)	49 (5%)	3 (0%)	41	27
1	E	1054/1073 (98%)	1000 (95%)	48 (5%)	6 (1%)	25	12
1	G	1053/1073 (98%)	997 (95%)	50 (5%)	6 (1%)	25	12
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%)	29	15
All	All	5733/5808 (99%)	5469 (95%)	244 (4%)	20 (0%)	34	27

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 (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	872/877 (99%)	814 (93%)	58 (7%)	16 5
1	C	872/877 (99%)	795 (91%)	77 (9%)	10 3
1	E	867/877 (99%)	800 (92%)	67 (8%)	13 4
1	G	866/877 (99%)	786 (91%)	80 (9%)	9 2
2	B	308/307 (100%)	279 (91%)	29 (9%)	8 2
2	D	307/307 (100%)	281 (92%)	26 (8%)	10 3
2	F	310/307 (101%)	284 (92%)	26 (8%)	11 3
2	H	307/307 (100%)	279 (91%)	28 (9%)	9 2
All	All	4709/4736 (99%)	4318 (92%)	391 (8%)	11 3

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

Mol	Chain	Res	Type
1	E	4704	LYS
1	G	6008	LYS
1	E	4784	GLN
2	F	5620	ARG
1	G	6283	ASN

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

Mol	Chain	Res	Type
1	E	5000	HIS
1	G	6803	GLN

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Mol	Chain	Res	Type
1	E	5055	ASN
2	F	5824	ASN
1	G	7007	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	H	7769	2	12,14,15	3.44	4 (33%)	11,17,19	2.01	4 (36%)
2	CYG	F	5769	2	12,14,15	3.17	3 (25%)	11,17,19	1.93	3 (27%)
2	CYG	B	1769	2	12,14,15	3.43	2 (16%)	11,17,19	2.64	5 (45%)
2	CYG	D	3769	2	12,14,15	3.17	2 (16%)	11,17,19	2.30	5 (45%)

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	H	7769	2	-	1/14/16/18	-
2	CYG	F	5769	2	-	0/14/16/18	-
2	CYG	B	1769	2	-	3/14/16/18	-
2	CYG	D	3769	2	-	3/14/16/18	-

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1769	CYG	OE2-CD1	10.57	1.38	1.21
2	H	7769	CYG	OE2-CD1	10.13	1.37	1.21
2	D	3769	CYG	OE2-CD1	9.94	1.37	1.21
2	F	5769	CYG	OE2-CD1	9.29	1.36	1.21
2	H	7769	CYG	O1-C1	4.62	1.36	1.22

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1769	CYG	OE2-CD1-CG1	-6.15	116.73	123.99
2	D	3769	CYG	OE2-CD1-CG1	-5.26	117.78	123.99
2	H	7769	CYG	CB-SG-CD1	-4.29	94.85	100.84
2	F	5769	CYG	CG1-CD1-SG	4.21	118.35	113.46
2	B	1769	CYG	CB-SG-CD1	3.54	105.78	100.84

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1769	CYG	OE2-CD1-SG-CB
2	D	3769	CYG	OE2-CD1-SG-CB
2	B	1769	CYG	CG1-CD1-SG-CB
2	D	3769	CYG	CG1-CD1-SG-CB
2	B	1769	CYG	N-CA-CB-SG

There are no ring outliers.

2 monomers are involved in 3 short contacts:

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	$\#\|Z\| > 2$
3	PO4	C	3980	-	4,4,4	1.40	0	6,6,6	0.50	0
3	PO4	C	3982	-	4,4,4	3.05	3 (75%)	6,6,6	1.27	0
7	ADP	G	7900	4	24,29,29	1.30	4 (16%)	29,45,45	1.69	3 (10%)
8	ORN	C	3920	-	7,8,8	1.09	1 (14%)	8,9,9	1.23	1 (12%)
7	ADP	C	3900	4	24,29,29	1.16	3 (12%)	29,45,45	1.29	3 (10%)
7	ADP	C	3910	5,4	24,29,29	1.29	2 (8%)	29,45,45	1.49	4 (13%)
3	PO4	E	5906	5,4	4,4,4	1.93	1 (25%)	6,6,6	0.85	0
3	PO4	G	7980	-	4,4,4	3.15	2 (50%)	6,6,6	0.96	0
3	PO4	A	1982	-	4,4,4	2.91	3 (75%)	6,6,6	0.73	0
3	PO4	E	5981	-	4,4,4	1.36	0	6,6,6	0.83	0
8	ORN	G	7920	-	7,8,8	1.22	1 (14%)	8,9,9	1.46	1 (12%)
9	NET	E	5950	-	8,8,8	0.79	0	10,10,10	0.53	0
3	PO4	G	7906	5,4	4,4,4	1.69	1 (25%)	6,6,6	0.68	0
8	ORN	A	1920	-	7,8,8	0.95	0	8,9,9	1.61	2 (25%)
3	PO4	E	5980	-	4,4,4	3.34	3 (75%)	6,6,6	1.12	0
3	PO4	C	3981	-	4,4,4	3.84	4 (100%)	6,6,6	1.04	1 (16%)
7	ADP	G	7910	5,4	24,29,29	1.13	2 (8%)	29,45,45	1.32	4 (13%)
8	ORN	E	5920	-	7,8,8	1.14	1 (14%)	8,9,9	0.93	0
7	ADP	E	5910	5,4	24,29,29	1.26	3 (12%)	29,45,45	1.17	4 (13%)
3	PO4	A	1906	5,4	4,4,4	1.84	2 (50%)	6,6,6	1.13	0
7	ADP	E	5900	4	24,29,29	1.46	4 (16%)	29,45,45	1.34	4 (13%)
3	PO4	A	1980	-	4,4,4	2.04	1 (25%)	6,6,6	1.06	0
3	PO4	A	1981	-	4,4,4	2.34	2 (50%)	6,6,6	1.52	1 (16%)
3	PO4	G	7981	-	4,4,4	2.68	1 (25%)	6,6,6	1.12	1 (16%)
3	PO4	G	7982	-	4,4,4	3.36	3 (75%)	6,6,6	1.37	0
3	PO4	C	3906	5,4	4,4,4	1.90	3 (75%)	6,6,6	1.28	1 (16%)
7	ADP	A	1900	4	24,29,29	1.32	4 (16%)	29,45,45	1.81	5 (17%)
9	NET	A	1950	-	8,8,8	0.81	0	10,10,10	0.50	0
9	NET	C	3950	-	8,8,8	0.69	0	10,10,10	0.64	0
9	NET	G	7950	-	8,8,8	0.67	0	10,10,10	0.51	0
7	ADP	A	1910	5,4	24,29,29	1.13	2 (8%)	29,45,45	1.45	4 (13%)

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	E	5900	4	-	2/12/32/32	0/3/3/3
8	ORN	C	3920	-	-	7/8/8/8	-
7	ADP	G	7900	4	-	0/12/32/32	0/3/3/3
8	ORN	G	7920	-	-	6/8/8/8	-
9	NET	E	5950	-	-	9/12/12/12	-
7	ADP	G	7910	5,4	-	0/12/32/32	0/3/3/3
7	ADP	C	3900	4	-	1/12/32/32	0/3/3/3
7	ADP	C	3910	5,4	-	2/12/32/32	0/3/3/3
8	ORN	A	1920	-	-	7/8/8/8	-
9	NET	A	1950	-	-	3/12/12/12	-
9	NET	C	3950	-	-	0/12/12/12	-
9	NET	G	7950	-	-	2/12/12/12	-
7	ADP	A	1910	5,4	-	2/12/32/32	0/3/3/3
8	ORN	E	5920	-	-	5/8/8/8	-
7	ADP	E	5910	5,4	-	0/12/32/32	0/3/3/3
7	ADP	A	1900	4	-	1/12/32/32	0/3/3/3

The worst 5 of 56 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	7982	PO4	P-O1	5.55	1.63	1.50
3	C	3981	PO4	P-O1	5.48	1.63	1.50
3	E	5980	PO4	P-O1	5.03	1.62	1.50
3	G	7981	PO4	P-O1	4.94	1.62	1.50
7	E	5900	ADP	O4'-C1'	-4.86	1.34	1.41

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	1900	ADP	C5-C6-N6	7.09	131.13	120.35
7	G	7900	ADP	C5-C6-N6	6.58	130.35	120.35
7	A	1910	ADP	O3B-PB-O3A	4.21	118.76	104.64
7	C	3900	ADP	C5-C6-N6	4.01	126.44	120.35
7	C	3910	ADP	O3'-C3'-C2'	3.59	123.45	111.82

There are no chirality outliers.

5 of 47 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	1920	ORN	N-CA-CB-CG
8	A	1920	ORN	C-CA-CB-CG
8	C	3920	ORN	N-CA-CB-CG
8	C	3920	ORN	C-CA-CB-CG
8	C	3920	ORN	O-C-CA-N

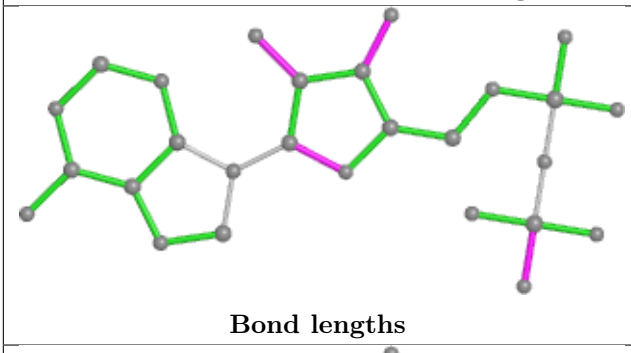
There are no ring outliers.

13 monomers are involved in 19 short contacts:

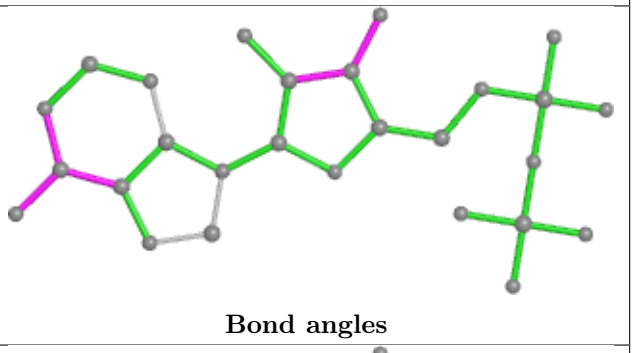
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	G	7900	ADP	2	0
8	C	3920	ORN	3	0
7	C	3910	ADP	1	0
8	G	7920	ORN	1	0
9	E	5950	NET	2	0
3	G	7906	PO4	1	0
8	A	1920	ORN	1	0
7	G	7910	ADP	2	0
8	E	5920	ORN	1	0
7	E	5900	ADP	1	0
3	C	3906	PO4	1	0
9	A	1950	NET	1	0
7	A	1910	ADP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

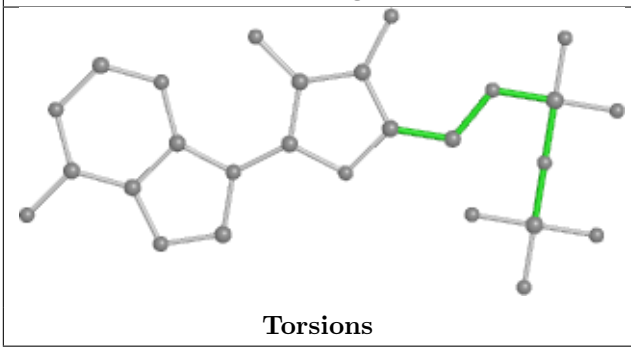
Ligand ADP G 7900



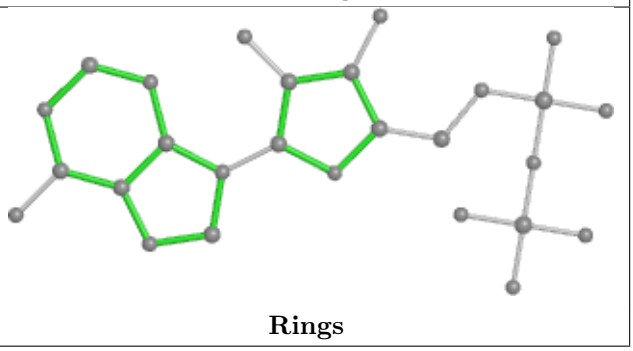
Bond lengths



Bond angles

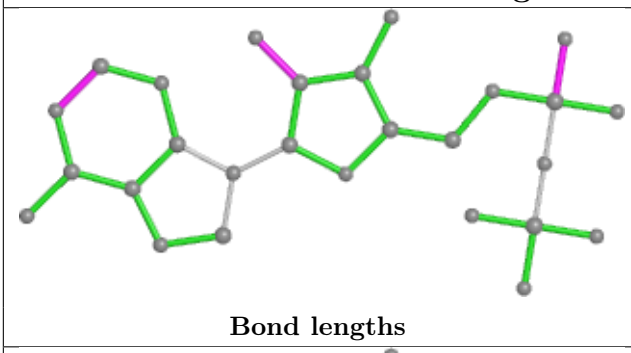


Torsions



Rings

Ligand ADP C 3900



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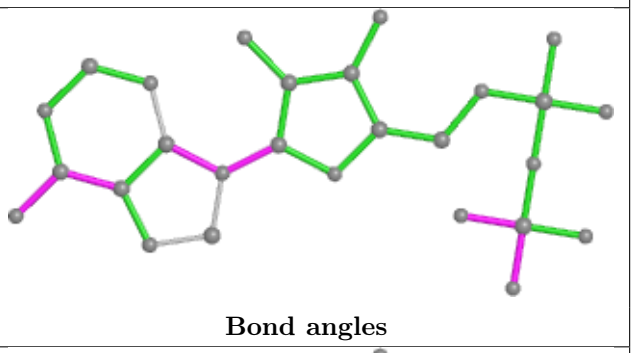
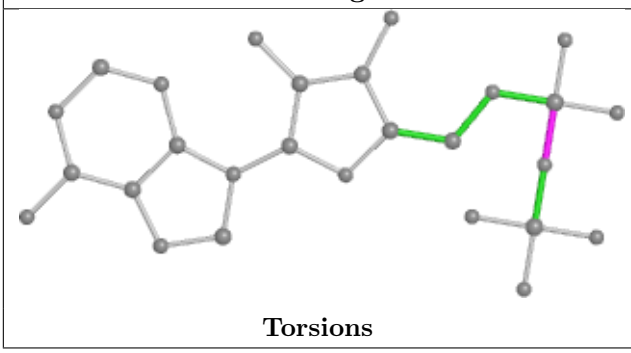


Bond angles



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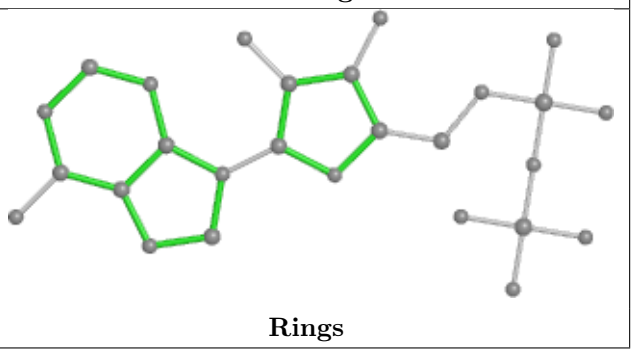
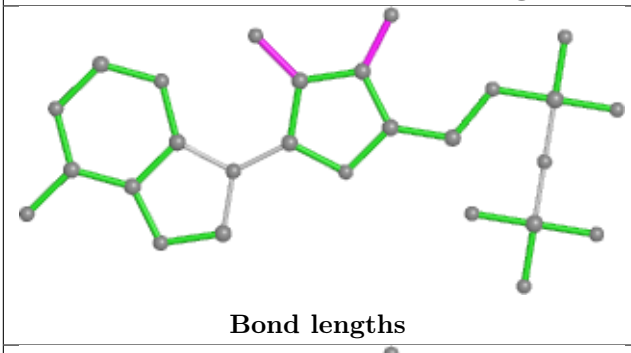
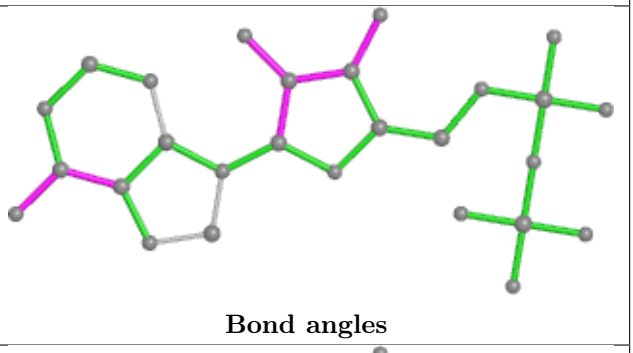


Rings

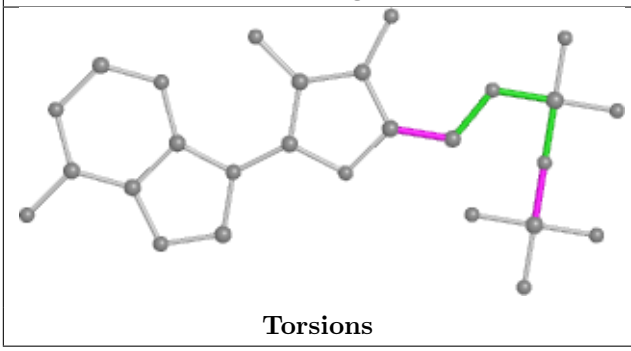
Ligand ADP C 3910



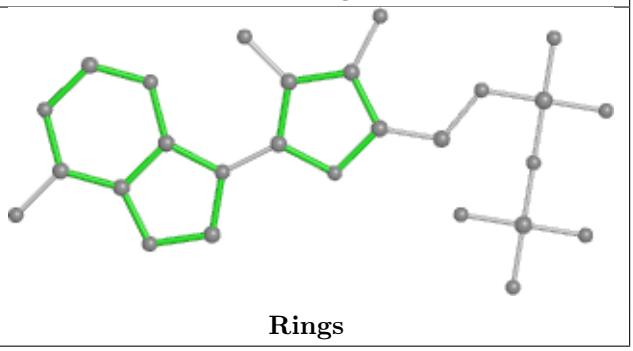
Bond lengths



Bond angles

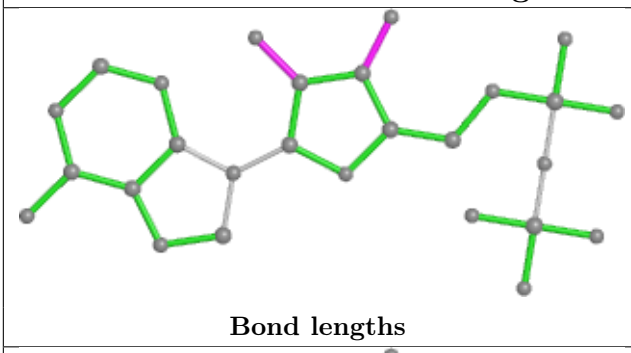


Torsions

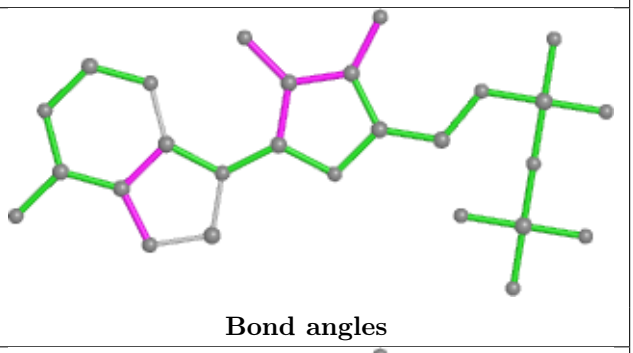


Rings

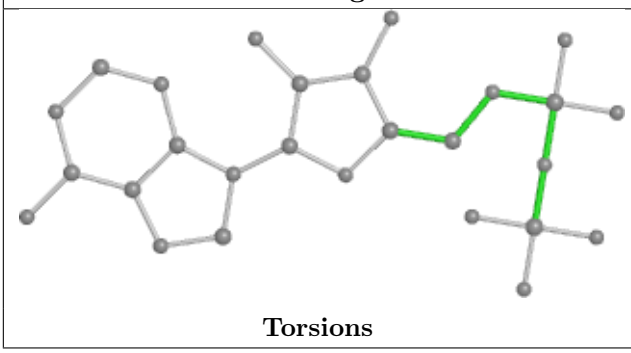
Ligand ADP G 7910



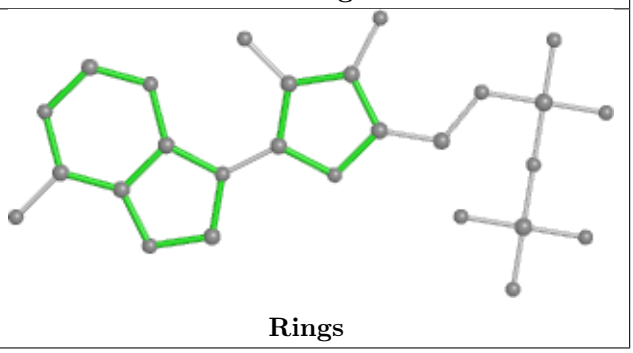
Bond lengths



Bond angles

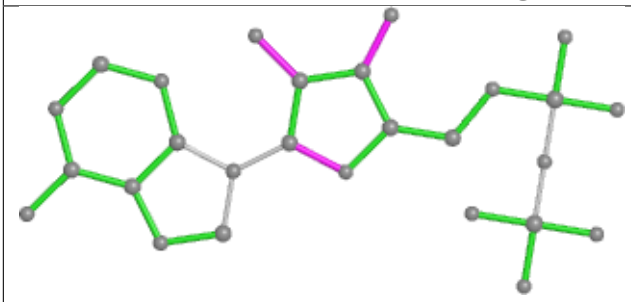


Torsions

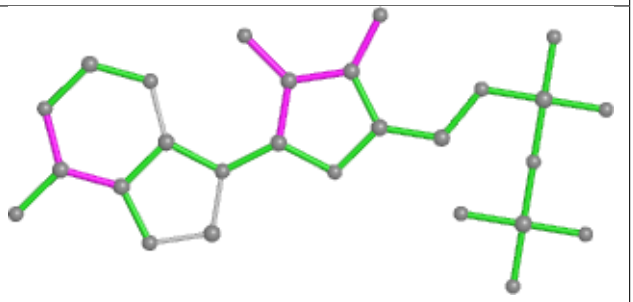


Rings

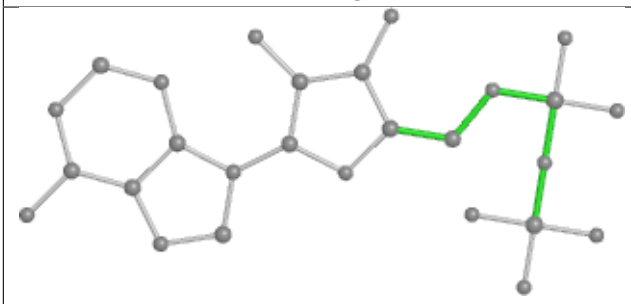
Ligand ADP E 5910



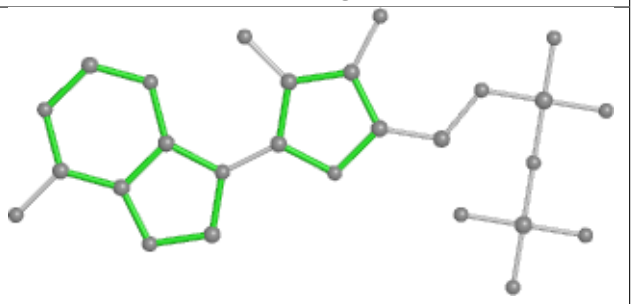
Bond lengths



Bond angles

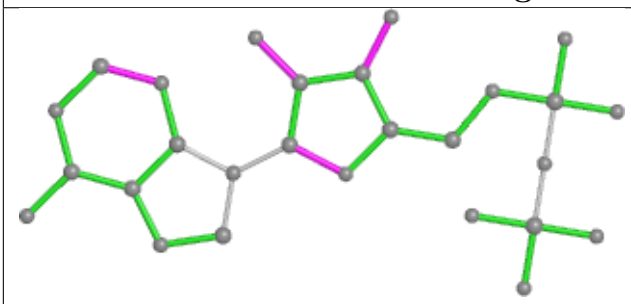


Torsions

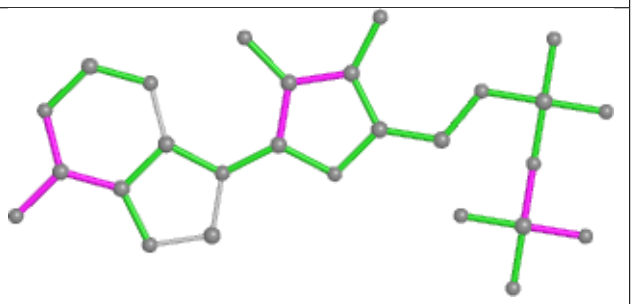


Rings

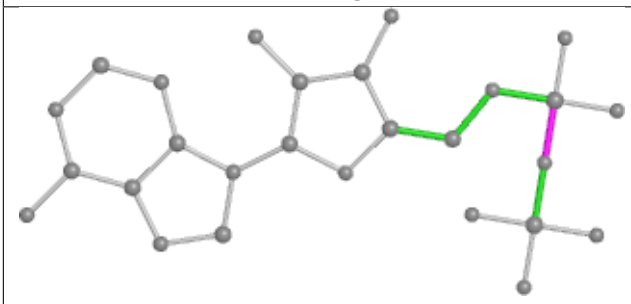
Ligand ADP E 5900



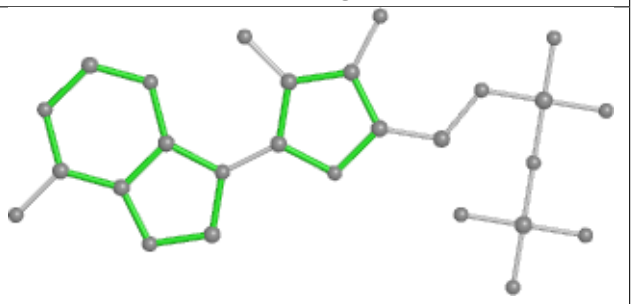
Bond lengths



Bond angles

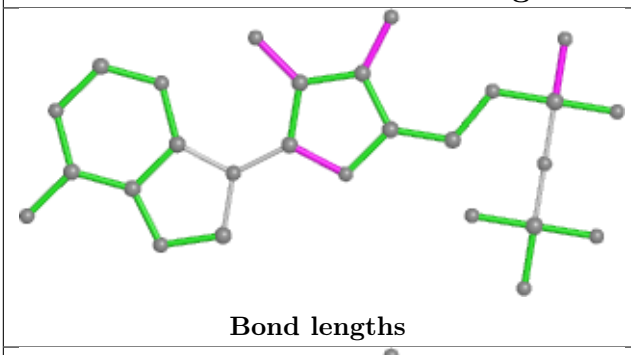


Torsions

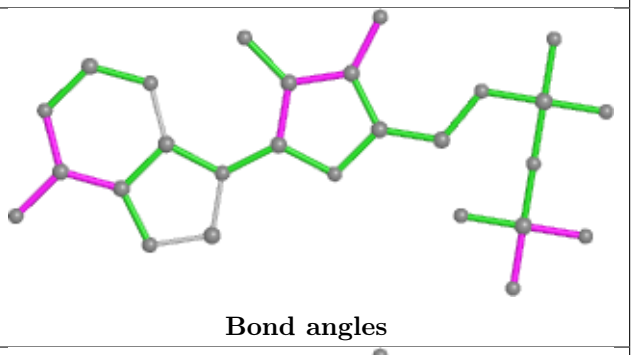


Rings

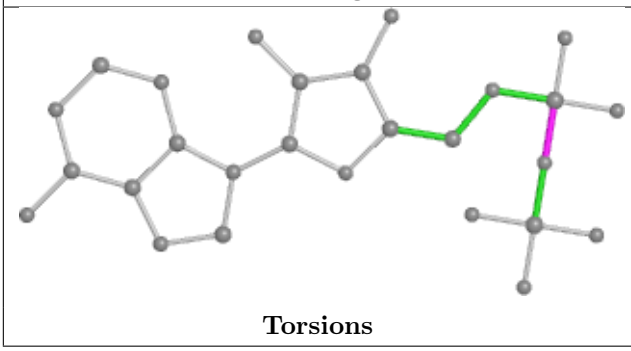
Ligand ADP A 1900



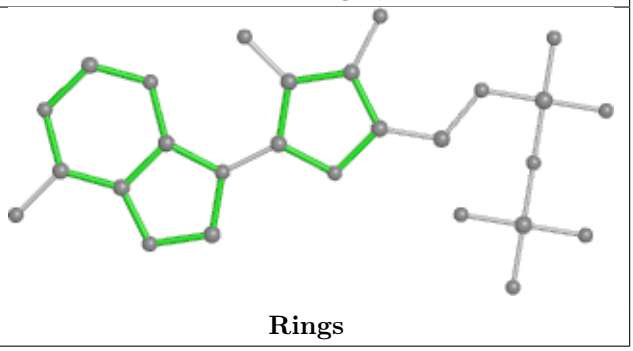
Bond lengths



Bond angles

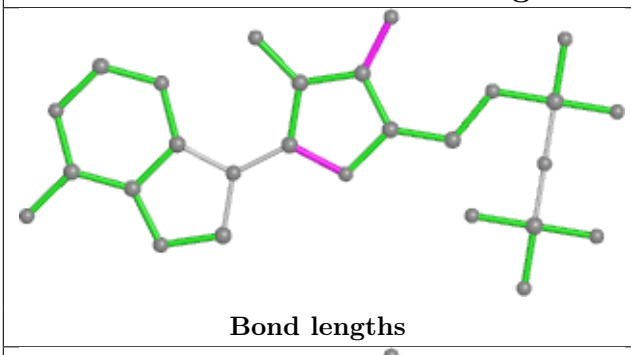


Torsions

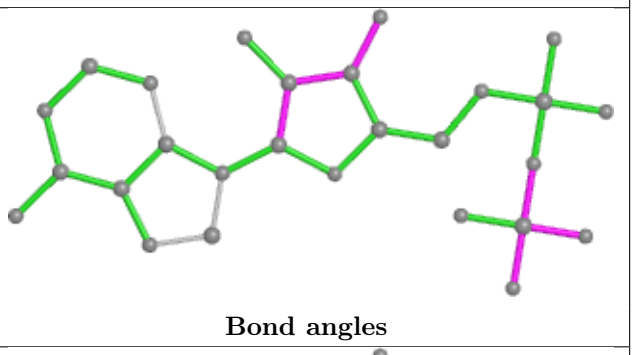


Rings

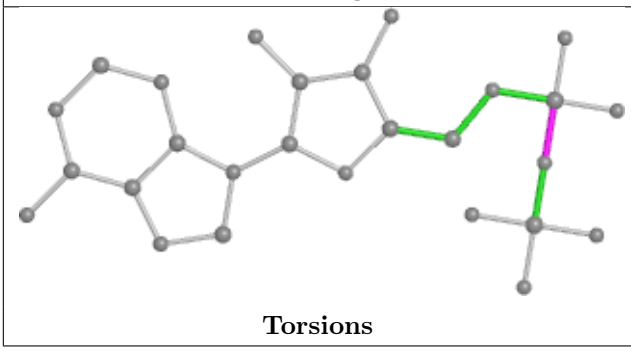
Ligand ADP A 1910



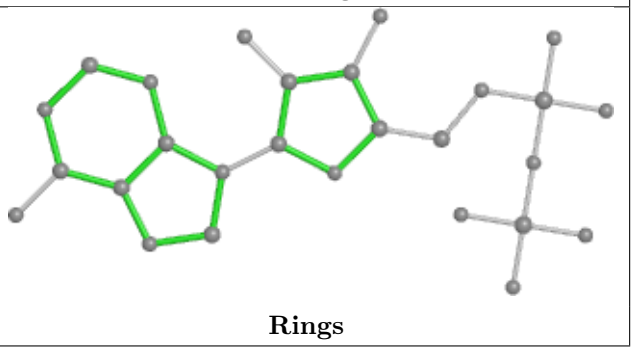
Bond lengths



Bond angles



Torsions



Rings

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.