



wwPDB X-ray Structure Validation Summary Report ⓘ

Jul 31, 2023 – 04:36 AM EDT

PDB ID : 1BXR
Title : STRUCTURE OF CARBAMOYL PHOSPHATE SYNTHETASE COM-
PLEXED WITH THE ATP ANALOG AMPPNP
Authors : Thoden, J.B.; Wesenberg, G.; Raushel, F.M.; Holden, H.M.
Deposited on : 1998-10-08
Resolution : 2.10 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (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) : 2.34

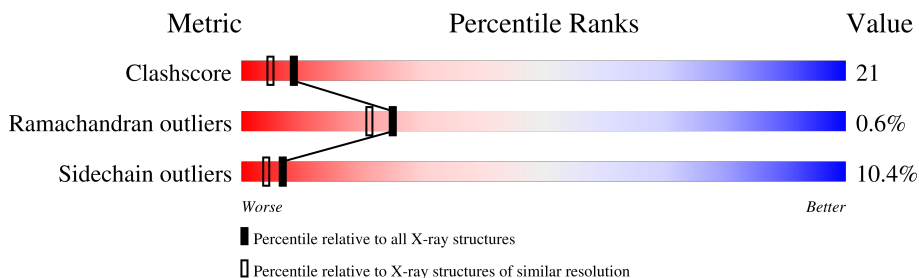
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	1073	55% 33% 10% .
1	C	1073	57% 33% 8% .
1	E	1073	60% 31% 9% .
1	G	1073	48% 39% 11% .
2	B	382	49% 43% 7% .
2	D	382	60% 35% . .
2	F	382	54% 36% 9% .
2	H	382	41% 49% 9% .

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	CL	E	2980	-	-	X	-
8	NET	A	1086	-	-	X	-
8	NET	E	2950	-	X	X	-

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 48307 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called CARBAMOYL-PHOSPHATE SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1073	8288	5203	1445	1594	46	0	4	0
1	C	1073	8268	5190	1441	1592	45	0	0	0
1	E	1073	8284	5199	1445	1595	45	0	3	0
1	G	1073	8279	5196	1445	1593	45	0	2	0

- Molecule 2 is a protein called CARBAMOYL-PHOSPHATE SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	379	2895	1825	509	551	10	0	0	0
2	D	379	2895	1825	509	551	10	0	0	0
2	F	379	2895	1825	509	551	10	0	0	0
2	H	379	2895	1825	509	551	10	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	183	GLN	GLU	conflict	UNP P0A6F1
D	183	GLN	GLU	conflict	UNP P0A6F1
F	183	GLN	GLU	conflict	UNP P0A6F1
H	183	GLN	GLU	conflict	UNP P0A6F1

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

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

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

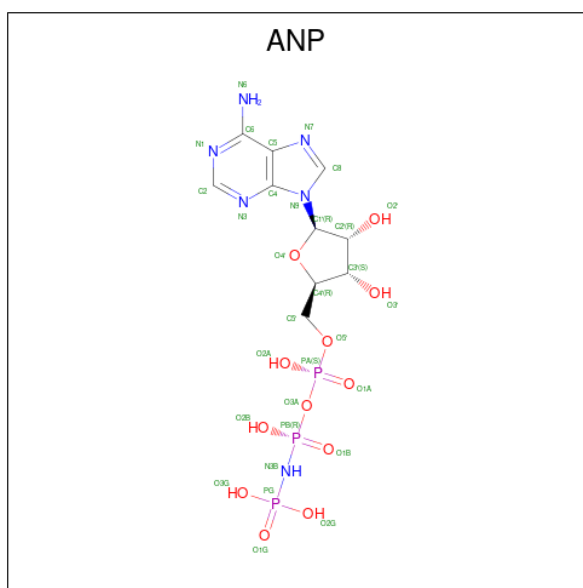
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	3	Total K 3 3	0	0
4	B	1	Total K 1 1	0	0
4	C	4	Total K 4 4	0	0
4	D	1	Total K 1 1	0	0
4	E	5	Total K 5 5	0	0
4	G	4	Total K 4 4	0	0
4	H	1	Total K 1 1	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	3	Total Cl 3 3	0	0
5	B	1	Total Cl 1 1	0	0
5	C	3	Total Cl 3 3	0	0
5	D	1	Total Cl 1 1	0	0
5	E	2	Total Cl 2 2	0	0
5	G	4	Total Cl 4 4	0	0

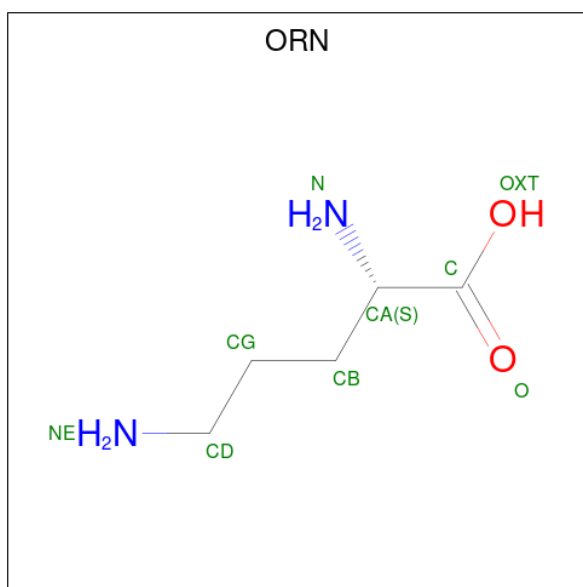
- Molecule 6 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter

code: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



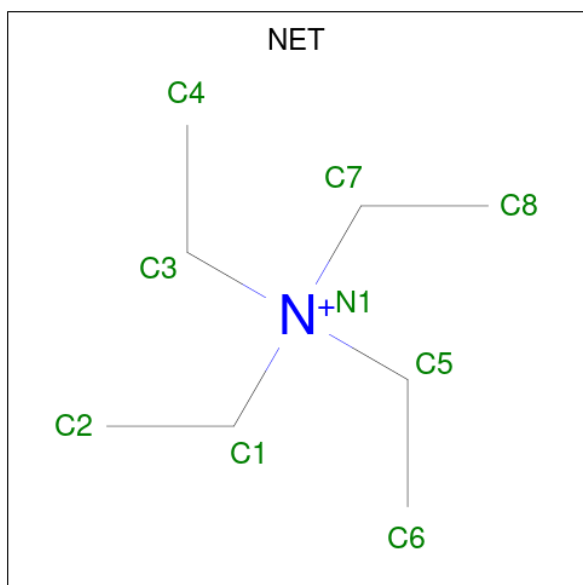
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
6	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
6	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
6	C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
6	C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
6	E	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
6	E	1	Total	C	N	O	P	0	0
		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

- Molecule 7 is L-ornithine (three-letter code: ORN) (formula: C₅H₁₂N₂O₂).



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

- Molecule 8 is TETRAETHYLAMMONIUM ION (three-letter code: NET) (formula: $C_8H_{20}N$).



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

- Molecule 9 is water.

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

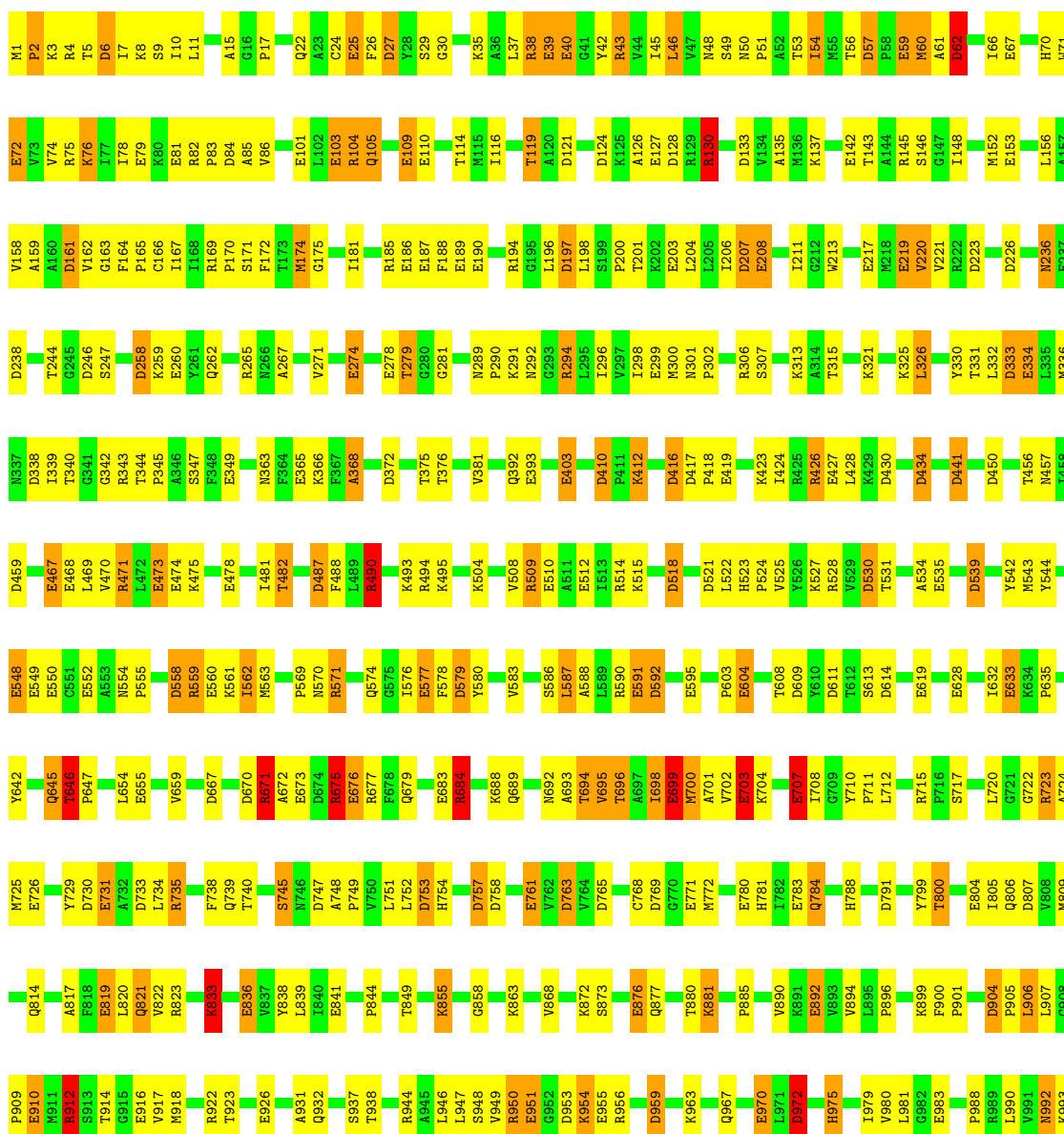
3 Residue-property plots

These plots are drawn for all protein, RNA, 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.

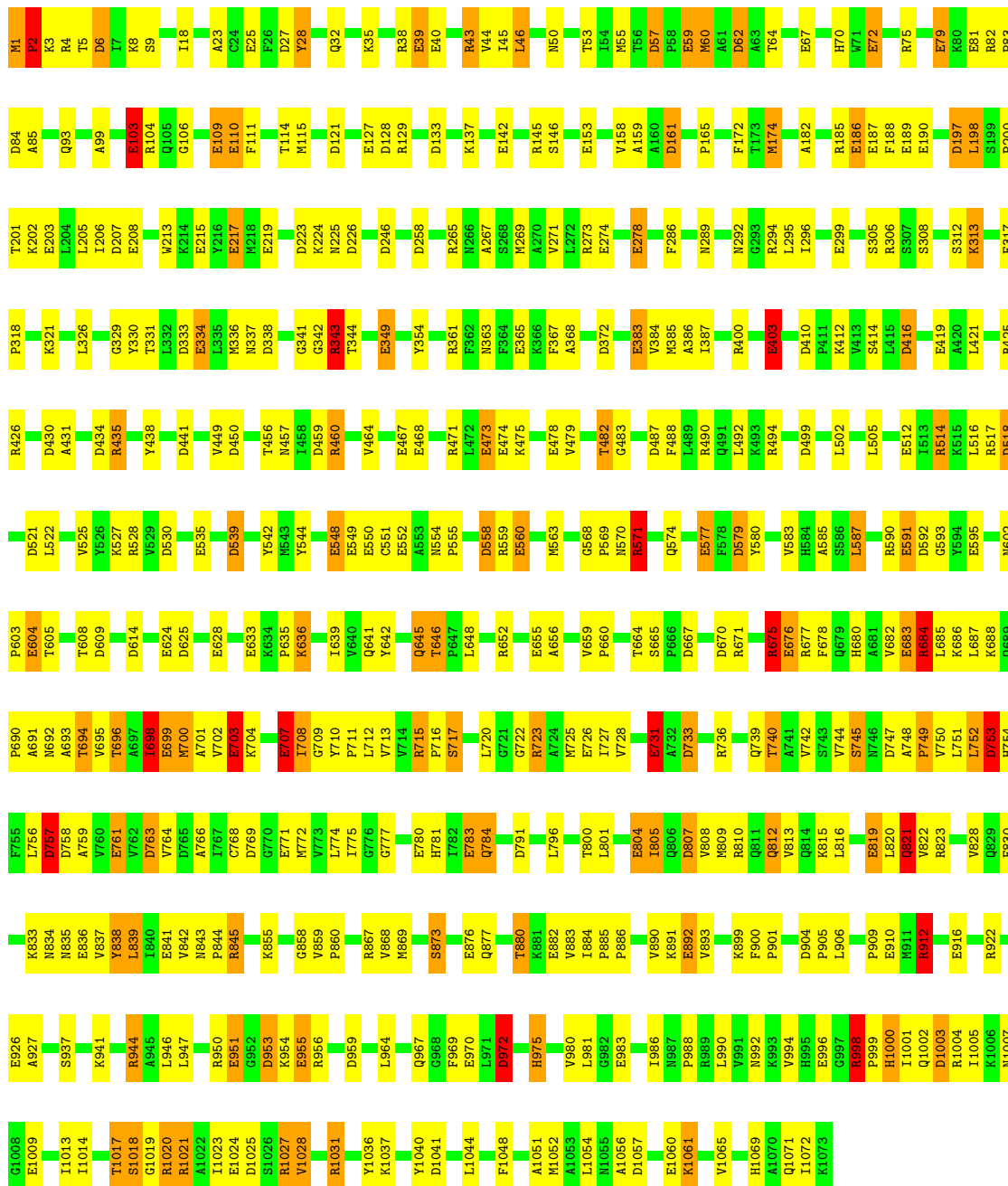
- Molecule 1: CARBAMOYL-PHOSPHATE SYNTHASE

Chain A:  55% 33% 10%



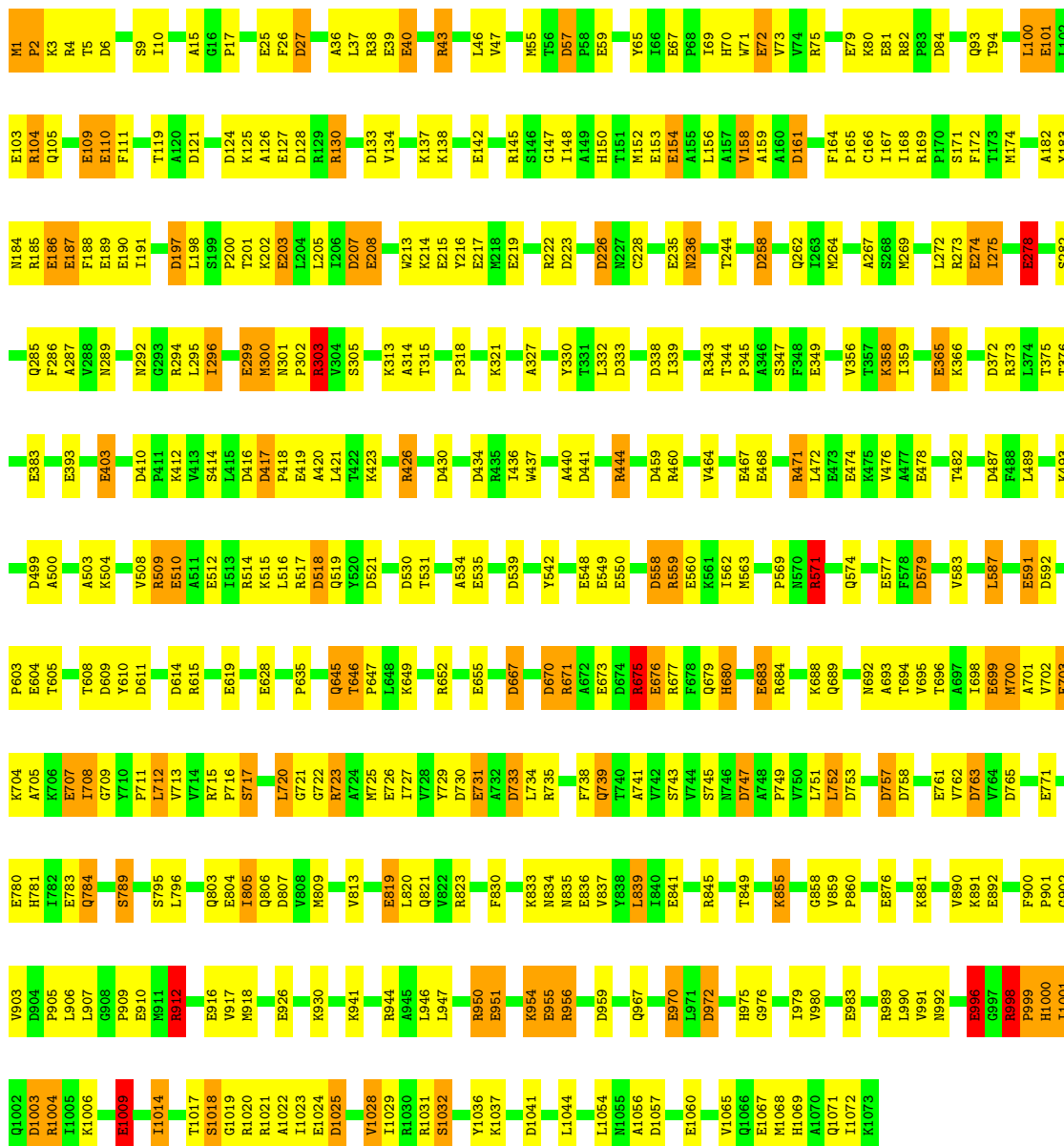


• Molecule 1: CARBAMOYL-PHOSPHATE SYNTHASE

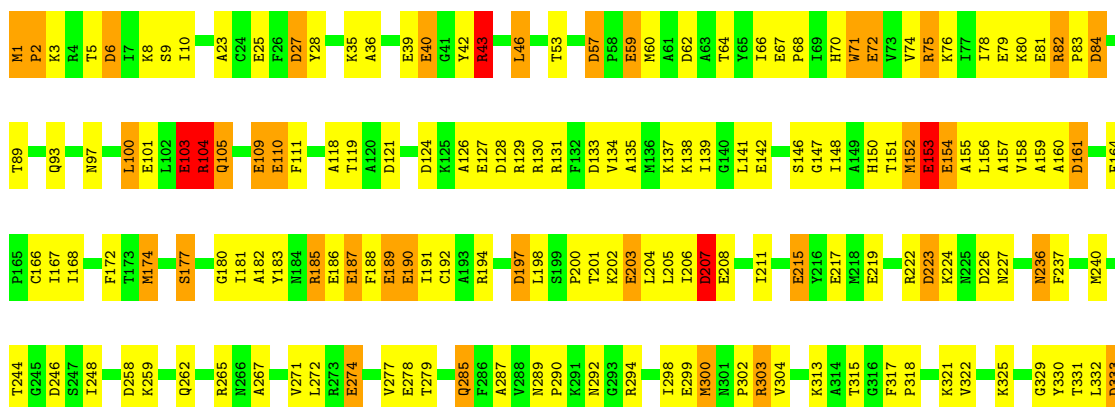


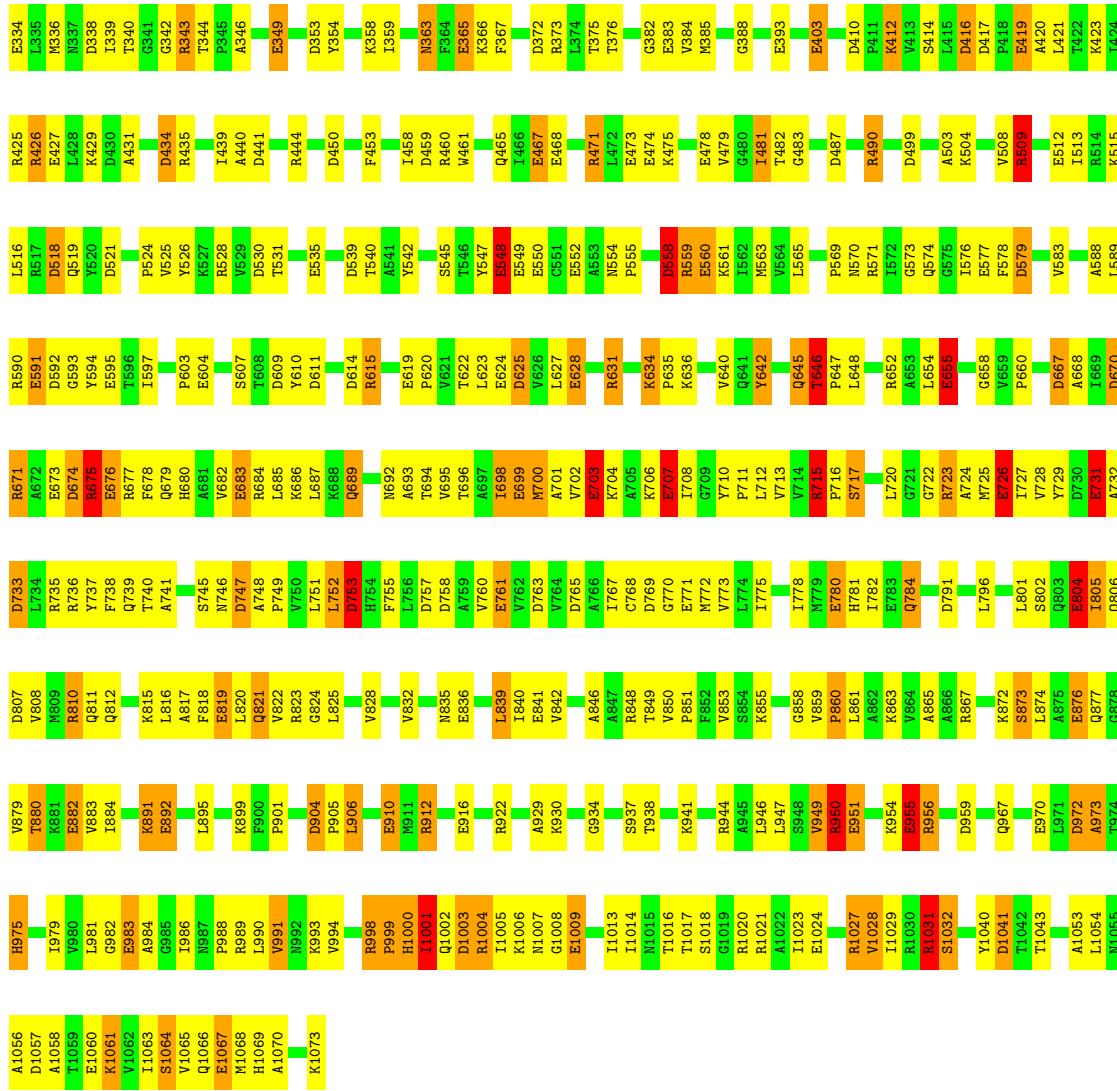
• Molecule 1: CARBAMOYL-PHOSPHATE SYNTHASE



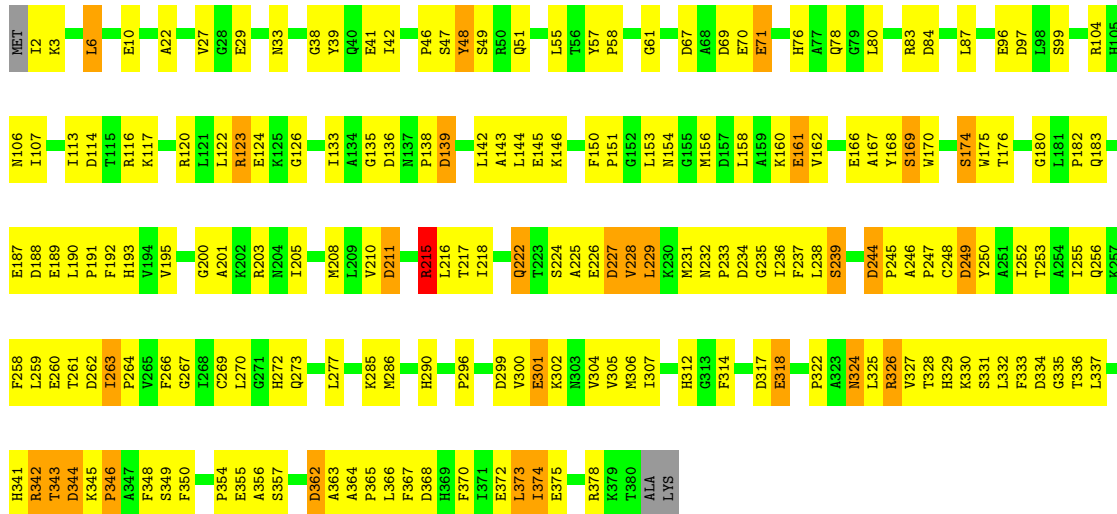


● Molecule 1: CARBAMOYL-PHOSPHATE SYNTHASE



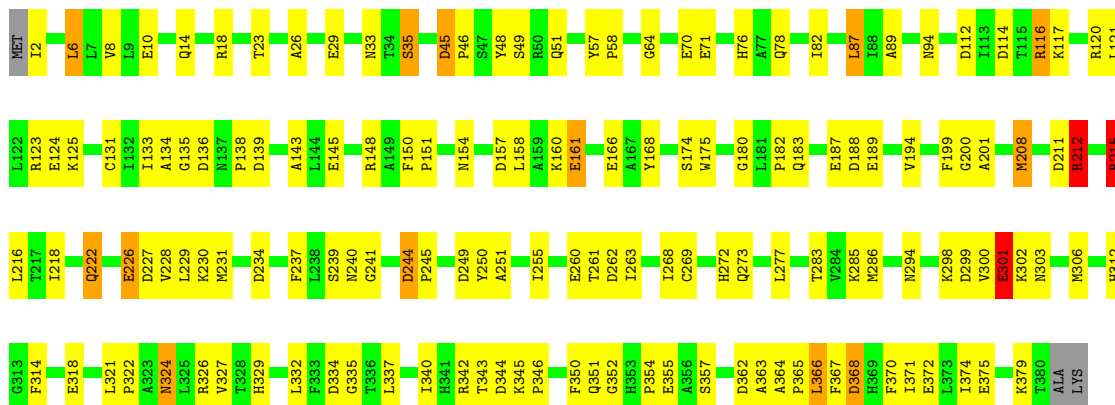


● Molecule 2: CARBAMOYL-PHOSPHATE SYNTHASE



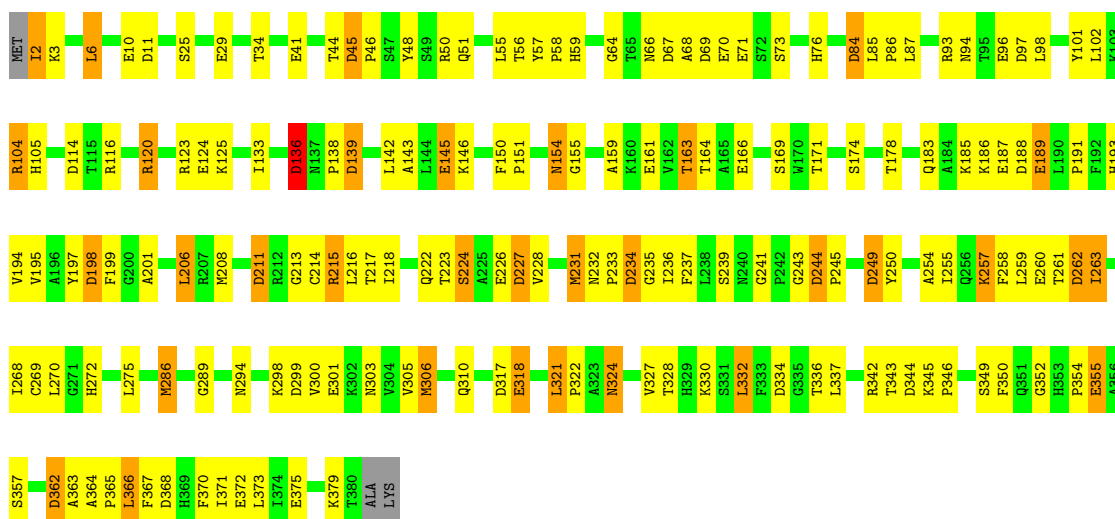
- Molecule 2: CARBAMOYL-PHOSPHATE SYNTHASE

Chain D: 



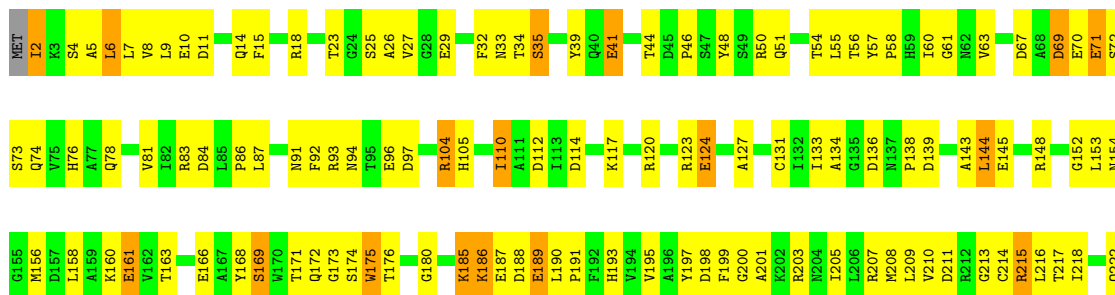
- Molecule 2: CARBAMOYL-PHOSPHATE SYNTHASE

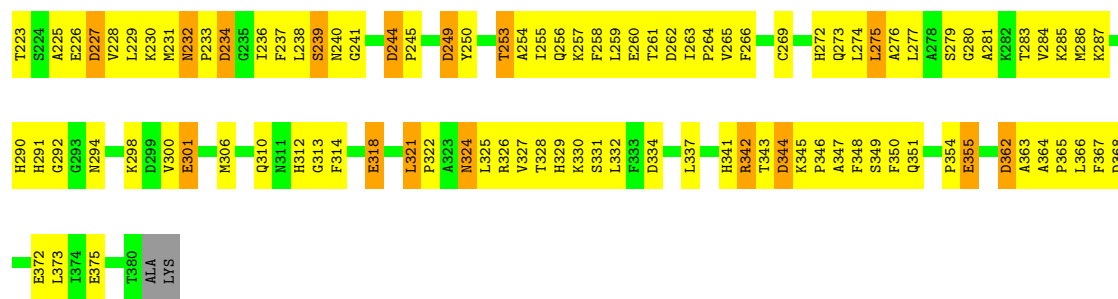
Chain F: 



- Molecule 2: CARBAMOYL-PHOSPHATE SYNTHASE

Chain H: 





4 Data and refinement statistics

Xtrriage (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	151.90Å 164.50Å 332.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.10	Depositor
% Data completeness (in resolution range)	93.0 (30.00-2.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
Refinement program	TNT 5E	Depositor
R, R_{free}	0.195 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	48307	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: CL, NET, ORN, ANP, K, MN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.01	83/8435 (1.0%)	1.41	129/11407 (1.1%)
1	C	1.01	81/8399 (1.0%)	1.38	129/11361 (1.1%)
1	E	1.01	82/8427 (1.0%)	1.38	122/11398 (1.1%)
1	G	1.02	82/8418 (1.0%)	1.39	140/11386 (1.2%)
2	B	0.87	19/2957 (0.6%)	1.28	33/4016 (0.8%)
2	D	0.91	16/2957 (0.5%)	1.31	38/4016 (0.9%)
2	F	0.89	19/2957 (0.6%)	1.28	41/4016 (1.0%)
2	H	0.89	19/2957 (0.6%)	1.30	33/4016 (0.8%)
All	All	0.98	401/45507 (0.9%)	1.36	665/61616 (1.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	G	0	1
2	F	1	0
All	All	1	1

The worst 5 of 401 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	39	GLU	CD-OE1	9.89	1.36	1.25
2	H	10	GLU	CD-OE1	9.59	1.36	1.25
1	G	153	GLU	CD-OE1	8.90	1.35	1.25
1	C	110	GLU	CD-OE1	8.43	1.34	1.25
1	G	103	GLU	CD-OE1	8.38	1.34	1.25

The worst 5 of 665 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	912[A]	ARG	NE-CZ-NH2	-15.00	112.80	120.30
1	A	912[B]	ARG	NE-CZ-NH2	-15.00	112.80	120.30
1	A	912[A]	ARG	NE-CZ-NH1	14.54	127.57	120.30
1	A	912[B]	ARG	NE-CZ-NH1	14.54	127.57	120.30
1	C	667	ASP	CB-CG-OD1	-13.42	106.22	118.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	F	50	ARG	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	1008	GLY	Mainchain

5.2 Too-close contacts [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	8288	0	8332	325	0
1	C	8268	0	8308	306	0
1	E	8284	0	8321	276	0
1	G	8279	0	8320	437	0
2	B	2895	0	2863	146	0
2	D	2895	0	2863	85	0
2	F	2895	0	2863	126	0
2	H	2895	0	2863	160	0
3	A	3	0	0	0	0
3	C	4	0	0	0	0
3	E	3	0	0	0	0
3	G	3	0	0	0	0
4	A	3	0	0	0	0
4	B	1	0	0	0	0
4	C	4	0	0	0	0
4	D	1	0	0	0	0
4	E	5	0	0	0	0
4	G	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	1	0	0	0	0
5	A	3	0	0	0	0
5	B	1	0	0	0	0
5	C	3	0	0	0	0
5	D	1	0	0	0	0
5	E	2	0	0	2	0
5	G	4	0	0	0	0
6	A	62	0	26	3	0
6	C	62	0	26	1	0
6	E	62	0	25	3	0
6	G	62	0	26	4	0
7	A	9	0	11	1	0
7	C	9	0	11	1	0
7	E	9	0	11	1	0
7	G	9	0	11	1	0
8	A	9	0	20	6	0
8	C	9	0	20	4	0
8	E	9	0	20	6	0
8	G	9	0	20	4	0
9	A	677	0	0	21	0
9	B	169	0	0	2	0
9	C	624	0	0	20	0
9	D	234	0	0	2	0
9	E	650	0	0	13	0
9	F	193	0	0	7	0
9	G	530	0	0	22	0
9	H	165	0	0	6	0
All	All	48307	0	44960	1851	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 21.

The worst 5 of 1851 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:967:GLN:HG2	1:C:1054:LEU:HD13	1.26	1.16
1:C:574:GLN:NE2	1:C:645:GLN:H	1.44	1.13
1:A:172:PHE:HB3	1:A:200:PRO:HG2	1.32	1.12
2:F:322:PRO:HB2	2:F:324:ASN:HD21	1.12	1.10
1:C:574:GLN:HE22	1:C:645:GLN:N	1.51	1.09

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1075/1073 (100%)	1008 (94%)	63 (6%)	4 (0%)	34	32
1	C	1071/1073 (100%)	1009 (94%)	54 (5%)	8 (1%)	22	18
1	E	1074/1073 (100%)	1020 (95%)	48 (4%)	6 (1%)	25	21
1	G	1073/1073 (100%)	993 (92%)	72 (7%)	8 (1%)	22	18
2	B	377/382 (99%)	350 (93%)	23 (6%)	4 (1%)	14	9
2	D	377/382 (99%)	363 (96%)	14 (4%)	0	100	100
2	F	377/382 (99%)	361 (96%)	14 (4%)	2 (0%)	29	26
2	H	377/382 (99%)	358 (95%)	19 (5%)	0	100	100
All	All	5801/5820 (100%)	5462 (94%)	307 (5%)	32 (1%)	25	21

5 of 32 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	975	HIS
2	F	136	ASP
1	G	975	HIS
2	B	346	PRO
1	C	707	GLU

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	882/878 (100%)	785 (89%)	97 (11%)	6	3
1	C	878/878 (100%)	783 (89%)	95 (11%)	6	3
1	E	881/878 (100%)	800 (91%)	81 (9%)	9	6
1	G	880/878 (100%)	761 (86%)	119 (14%)	4	2
2	B	308/310 (99%)	279 (91%)	29 (9%)	8	5
2	D	308/310 (99%)	290 (94%)	18 (6%)	20	17
2	F	308/310 (99%)	282 (92%)	26 (8%)	11	7
2	H	308/310 (99%)	276 (90%)	32 (10%)	7	4
All	All	4753/4752 (100%)	4256 (90%)	497 (10%)	7	4

5 of 497 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	222	GLN
1	G	906	LEU
1	E	703	GLU
1	G	849	THR
2	H	104	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 102 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	689	GLN
2	F	105	HIS
2	H	324	ASN
1	E	803	GLN
1	E	1035	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 62 ligands modelled in this entry, 46 are monoatomic - leaving 16 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	ANP	A	1083	3	29,33,33	1.58	6 (20%)	31,52,52	1.83	5 (16%)
7	ORN	A	1085	-	7,8,8	0.81	0	8,9,9	1.64	1 (12%)
6	ANP	E	2910	3	29,33,33	1.39	5 (17%)	31,52,52	1.68	4 (12%)
7	ORN	C	1920	-	7,8,8	0.90	0	8,9,9	1.14	1 (12%)
7	ORN	E	2920	-	7,8,8	0.87	0	8,9,9	1.23	1 (12%)
7	ORN	G	3920	-	7,8,8	0.74	0	8,9,9	1.35	2 (25%)
8	NET	C	1950	-	8,8,8	0.67	0	10,10,10	0.69	0
8	NET	E	2950	-	8,8,8	0.61	0	10,10,10	0.59	0
6	ANP	G	3910	3	29,33,33	1.34	7 (24%)	31,52,52	1.81	7 (22%)
6	ANP	G	3900	3	29,33,33	1.28	6 (20%)	31,52,52	1.86	5 (16%)
8	NET	A	1086	-	8,8,8	0.77	0	10,10,10	0.49	0
6	ANP	A	1084	3	29,33,33	1.49	6 (20%)	31,52,52	1.75	6 (19%)
6	ANP	E	2900	3	29,33,33	1.34	5 (17%)	31,52,52	1.73	5 (16%)
6	ANP	C	1910	3	29,33,33	1.42	5 (17%)	31,52,52	1.76	7 (22%)
8	NET	G	3950	-	8,8,8	0.69	0	10,10,10	0.56	0
6	ANP	C	1900	3	29,33,33	1.35	6 (20%)	31,52,52	1.74	4 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	ANP	A	1083	3	-	3/14/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	ORN	A	1085	-	-	4/8/8/8	-
6	ANP	E	2910	3	-	6/14/38/38	0/3/3/3
7	ORN	C	1920	-	-	6/8/8/8	-
7	ORN	E	2920	-	-	7/8/8/8	-
7	ORN	G	3920	-	-	5/8/8/8	-
8	NET	C	1950	-	-	3/12/12/12	-
8	NET	E	2950	-	-	12/12/12/12	-
6	ANP	G	3910	3	-	4/14/38/38	0/3/3/3
6	ANP	G	3900	3	-	2/14/38/38	0/3/3/3
8	NET	A	1086	-	-	6/12/12/12	-
6	ANP	A	1084	3	-	3/14/38/38	0/3/3/3
6	ANP	E	2900	3	-	3/14/38/38	0/3/3/3
6	ANP	C	1910	3	-	3/14/38/38	0/3/3/3
8	NET	G	3950	-	-	6/12/12/12	-
6	ANP	C	1900	3	-	2/14/38/38	0/3/3/3

The worst 5 of 46 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1083	ANP	PG-O1G	5.08	1.54	1.46
6	C	1910	ANP	PB-O1B	4.11	1.52	1.46
6	E	2910	ANP	PB-O1B	4.08	1.52	1.46
6	A	1084	ANP	PB-O1B	4.05	1.52	1.46
6	A	1084	ANP	PG-O1G	3.58	1.51	1.46

The worst 5 of 48 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	3900	ANP	C5-C6-N6	5.59	128.84	120.35
6	A	1084	ANP	C5-C6-N6	5.12	128.13	120.35
6	C	1900	ANP	C5-C6-N6	4.61	127.35	120.35
6	G	3910	ANP	C2-N1-C6	4.53	126.51	118.75
6	G	3900	ANP	C2-N1-C6	4.53	126.50	118.75

There are no chirality outliers.

5 of 75 torsion outliers are listed below:

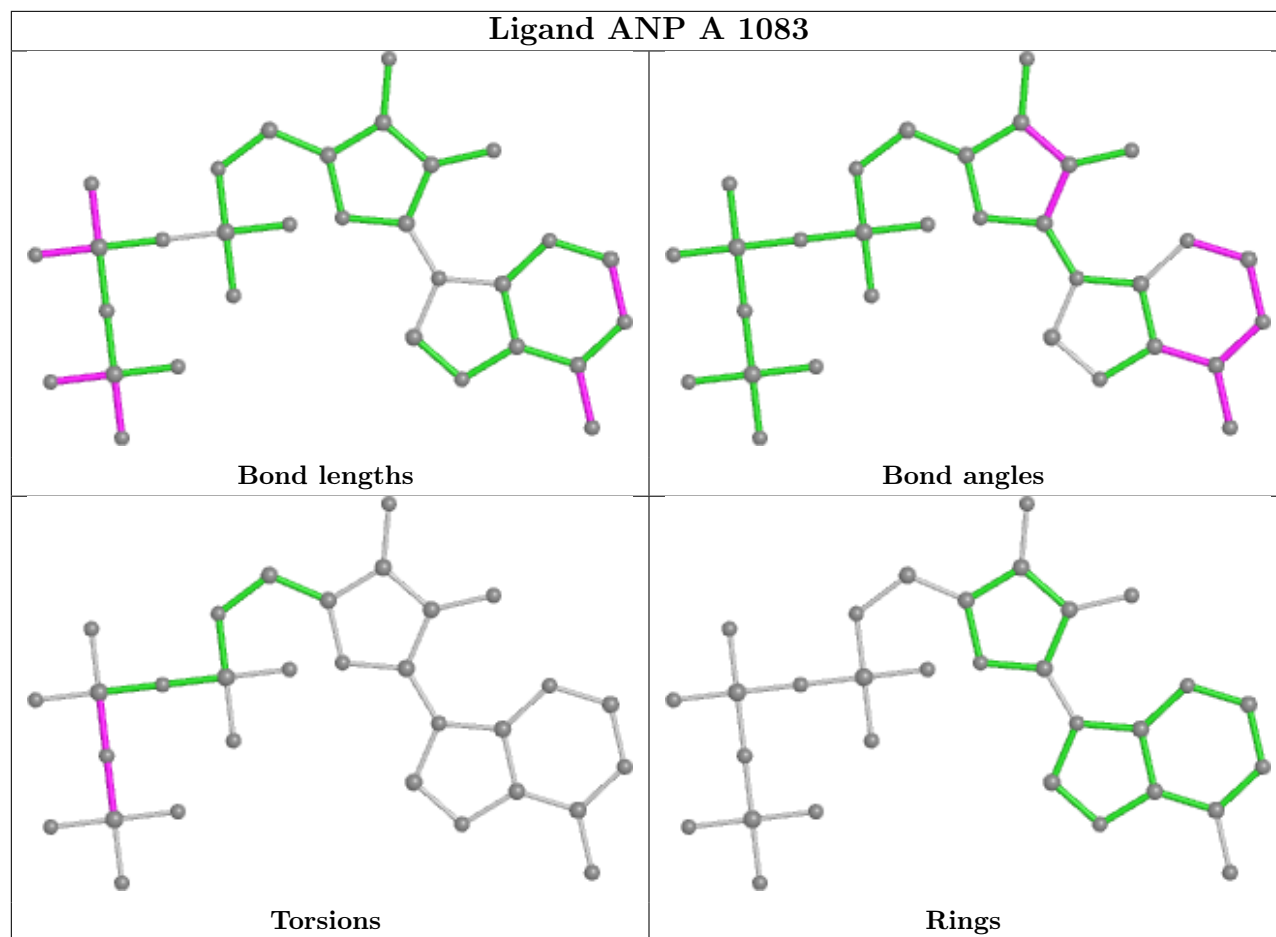
Mol	Chain	Res	Type	Atoms
6	A	1083	ANP	PB-N3B-PG-O1G
6	A	1083	ANP	PG-N3B-PB-O1B
6	A	1083	ANP	PG-N3B-PB-O3A
6	A	1084	ANP	PB-N3B-PG-O1G
6	A	1084	ANP	PG-N3B-PB-O1B

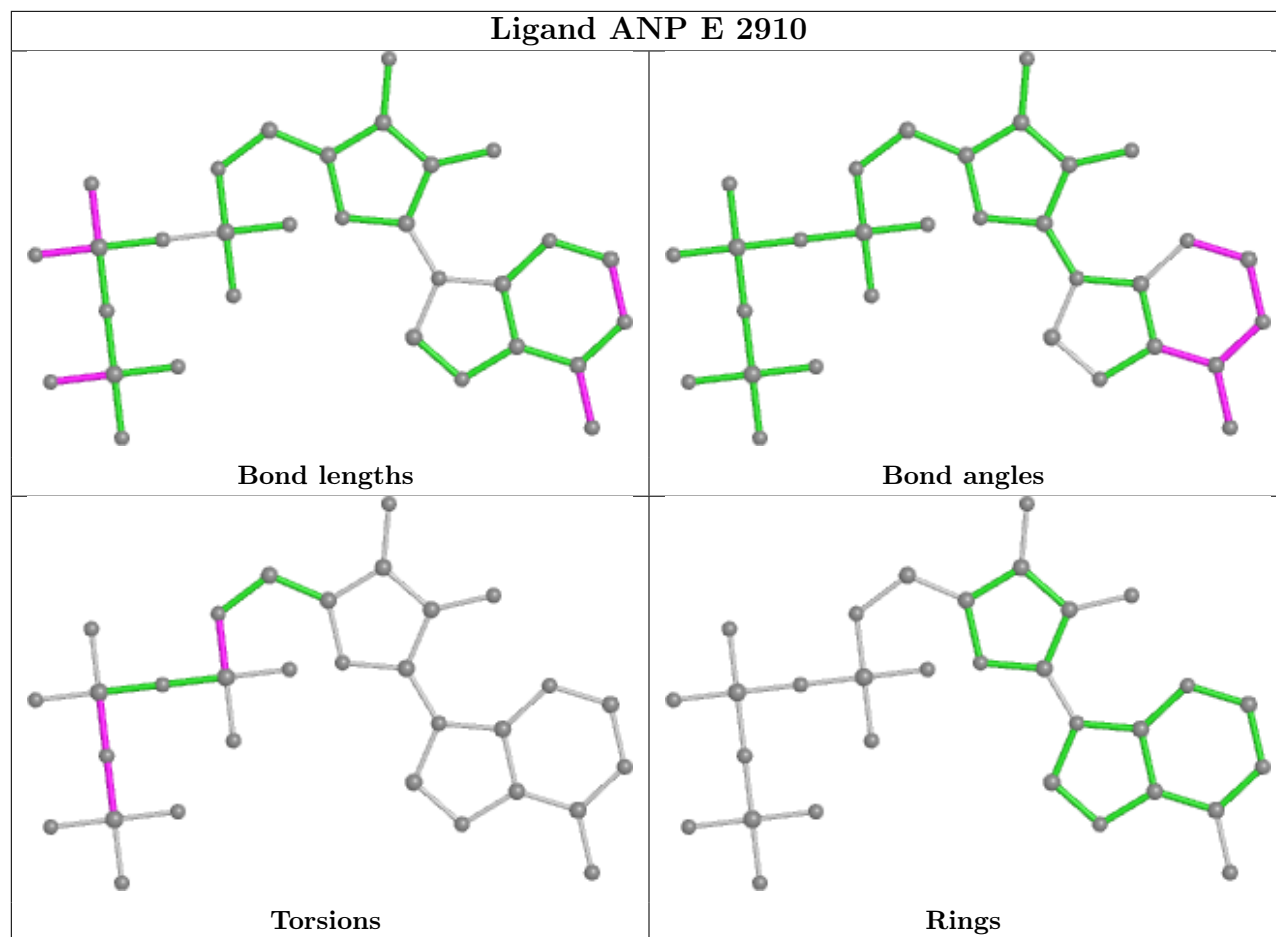
There are no ring outliers.

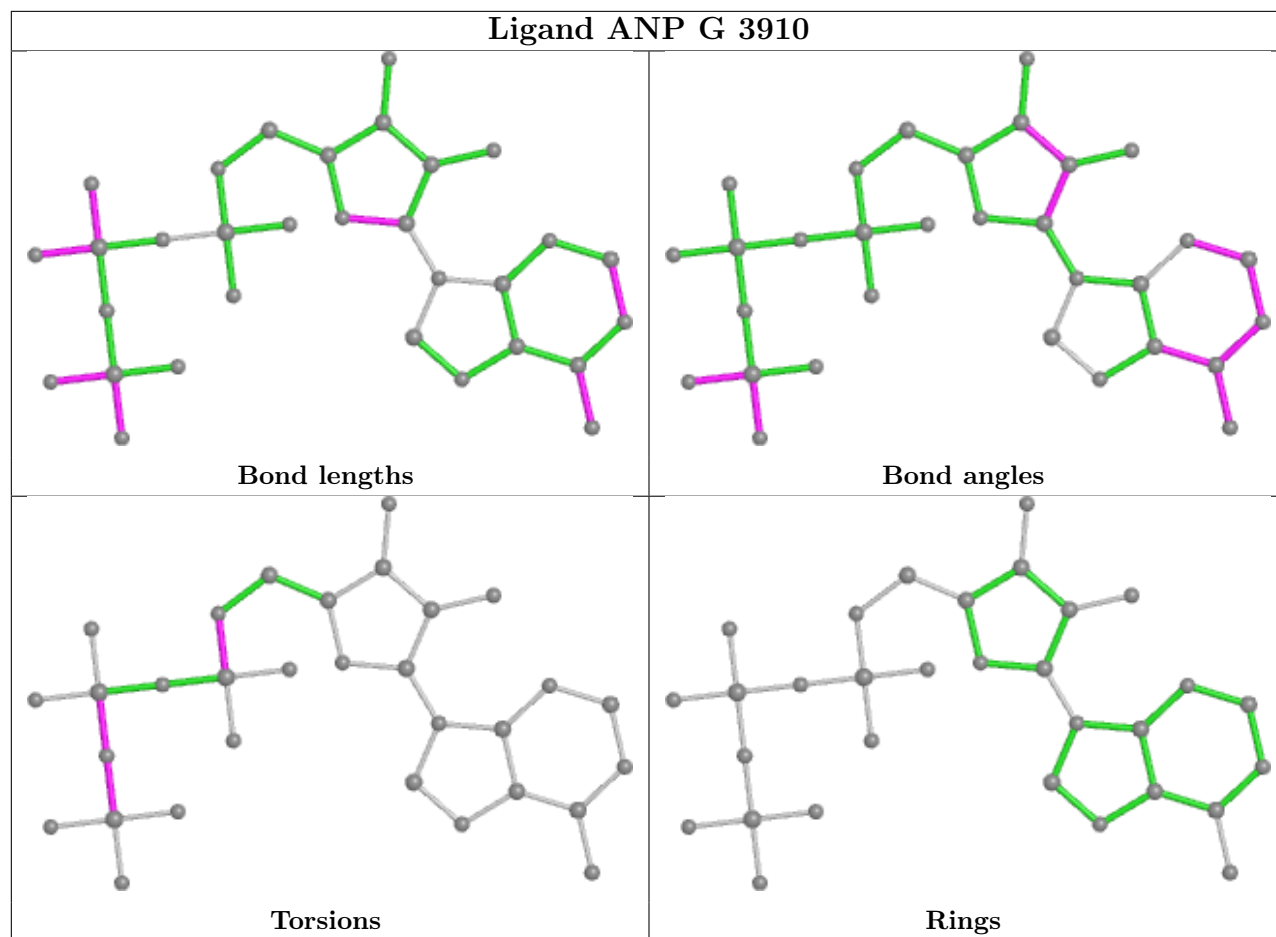
13 monomers are involved in 35 short contacts:

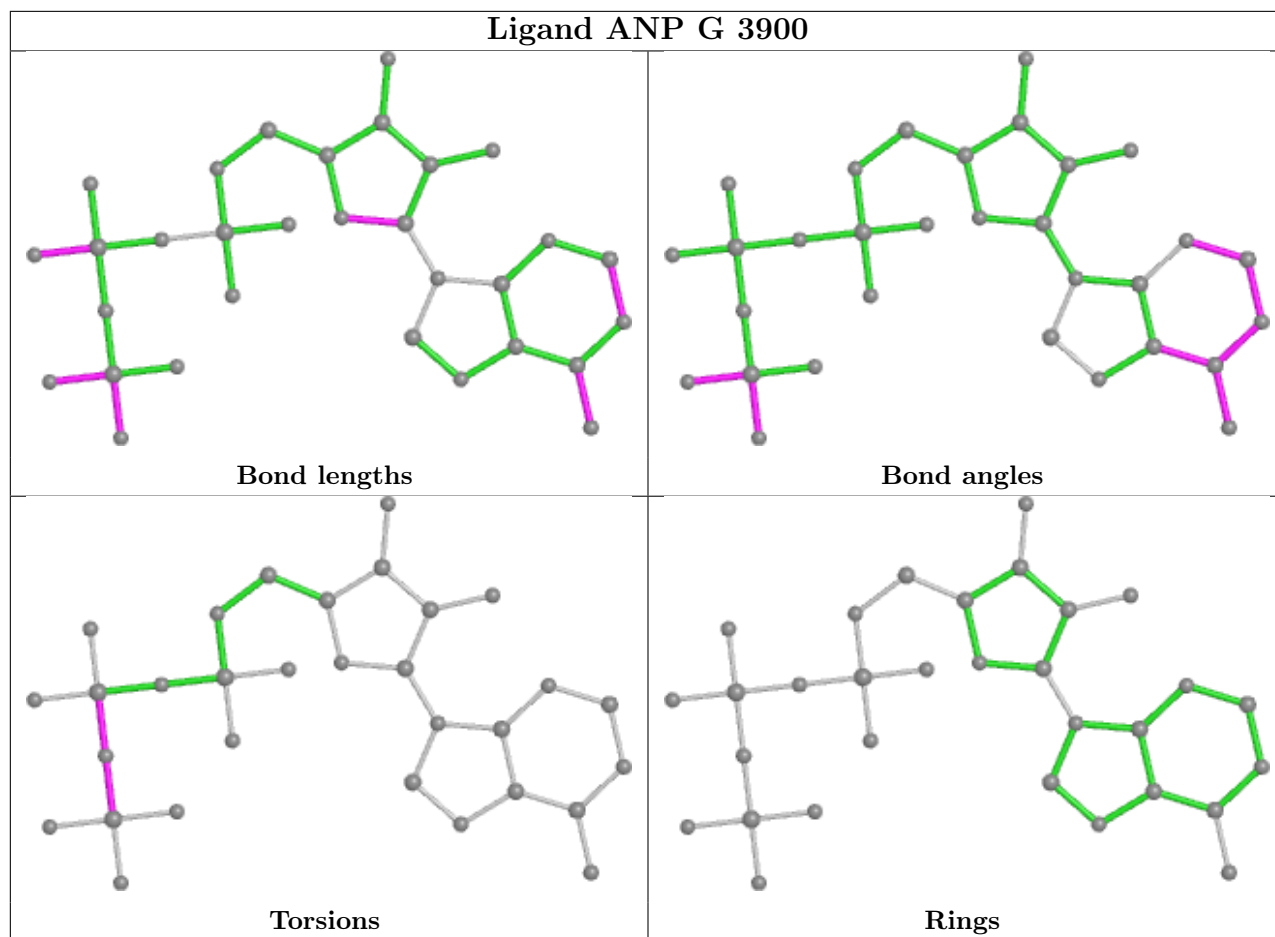
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1083	ANP	3	0
7	A	1085	ORN	1	0
6	E	2910	ANP	3	0
7	C	1920	ORN	1	0
7	E	2920	ORN	1	0
7	G	3920	ORN	1	0
8	C	1950	NET	4	0
8	E	2950	NET	6	0
6	G	3910	ANP	2	0
6	G	3900	ANP	2	0
8	A	1086	NET	6	0
6	C	1910	ANP	1	0
8	G	3950	NET	4	0

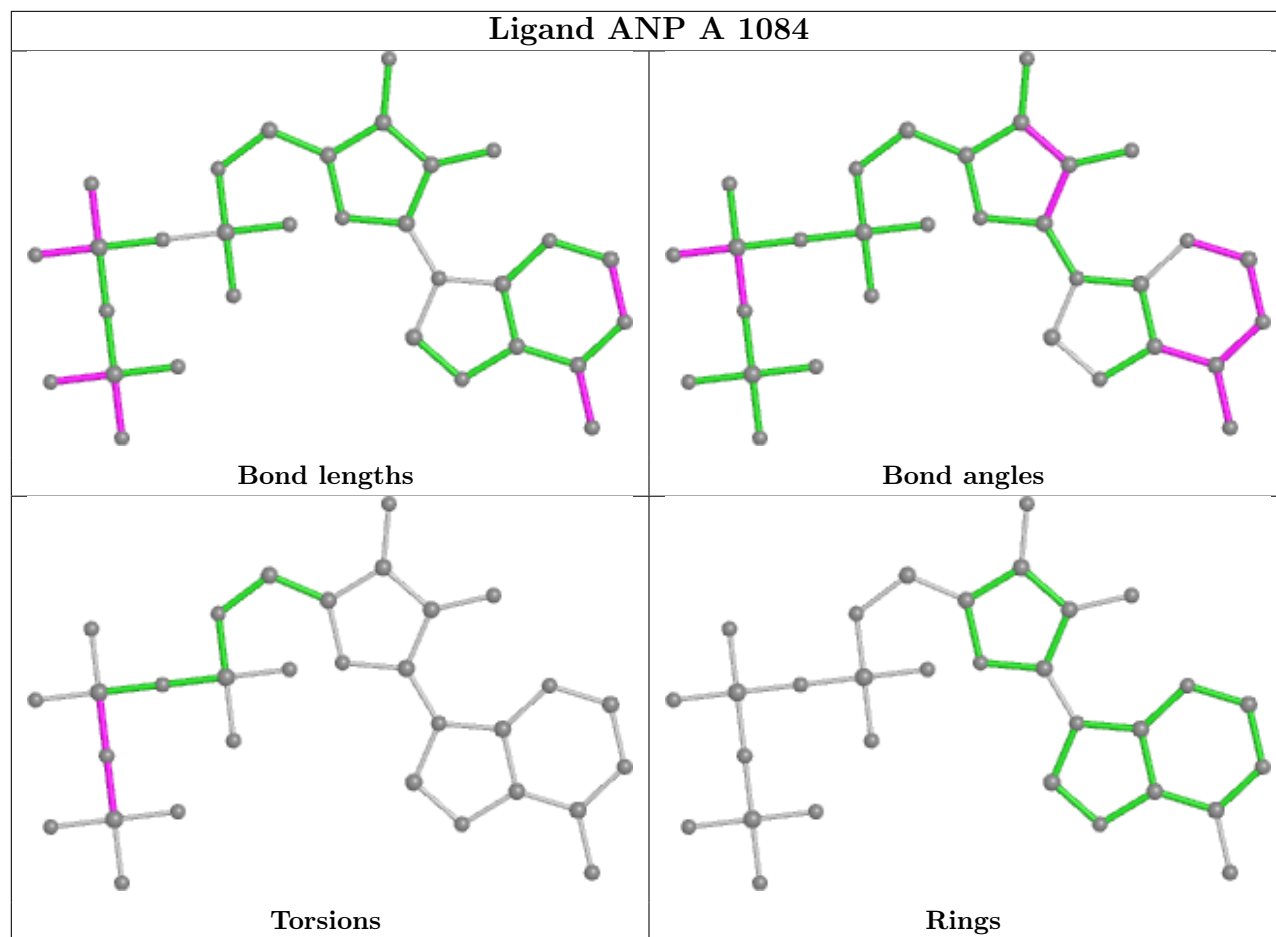
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 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.

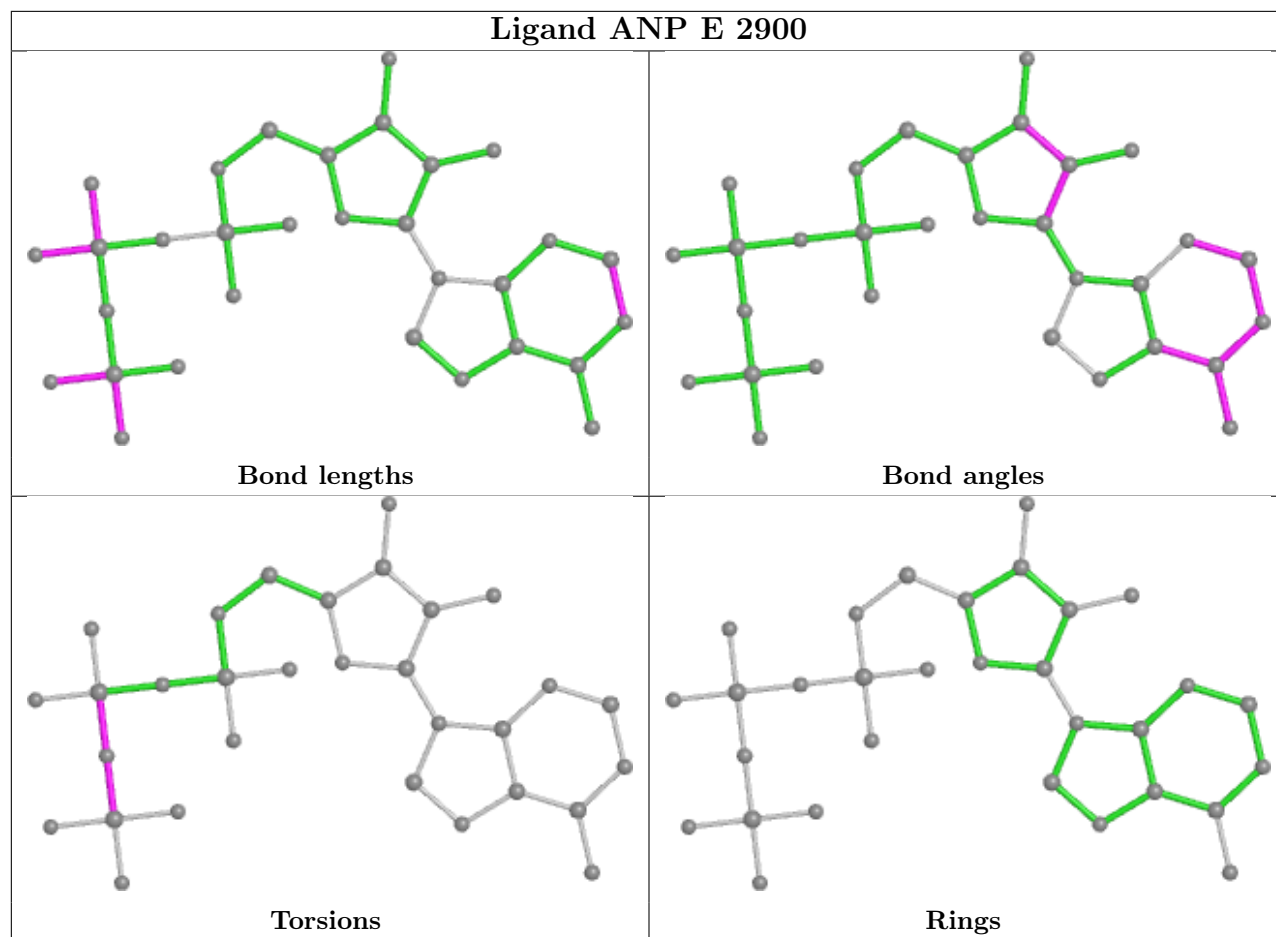


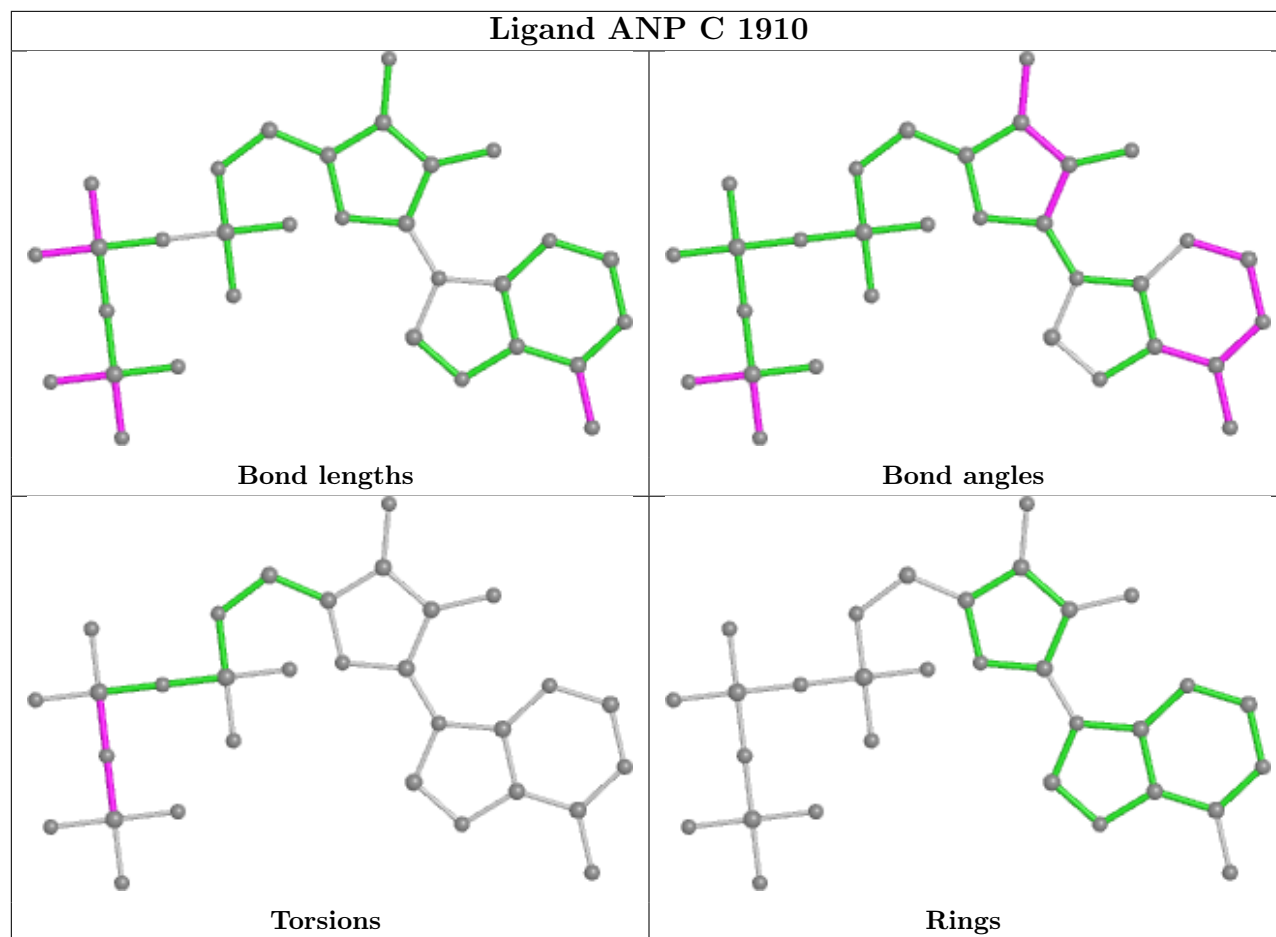


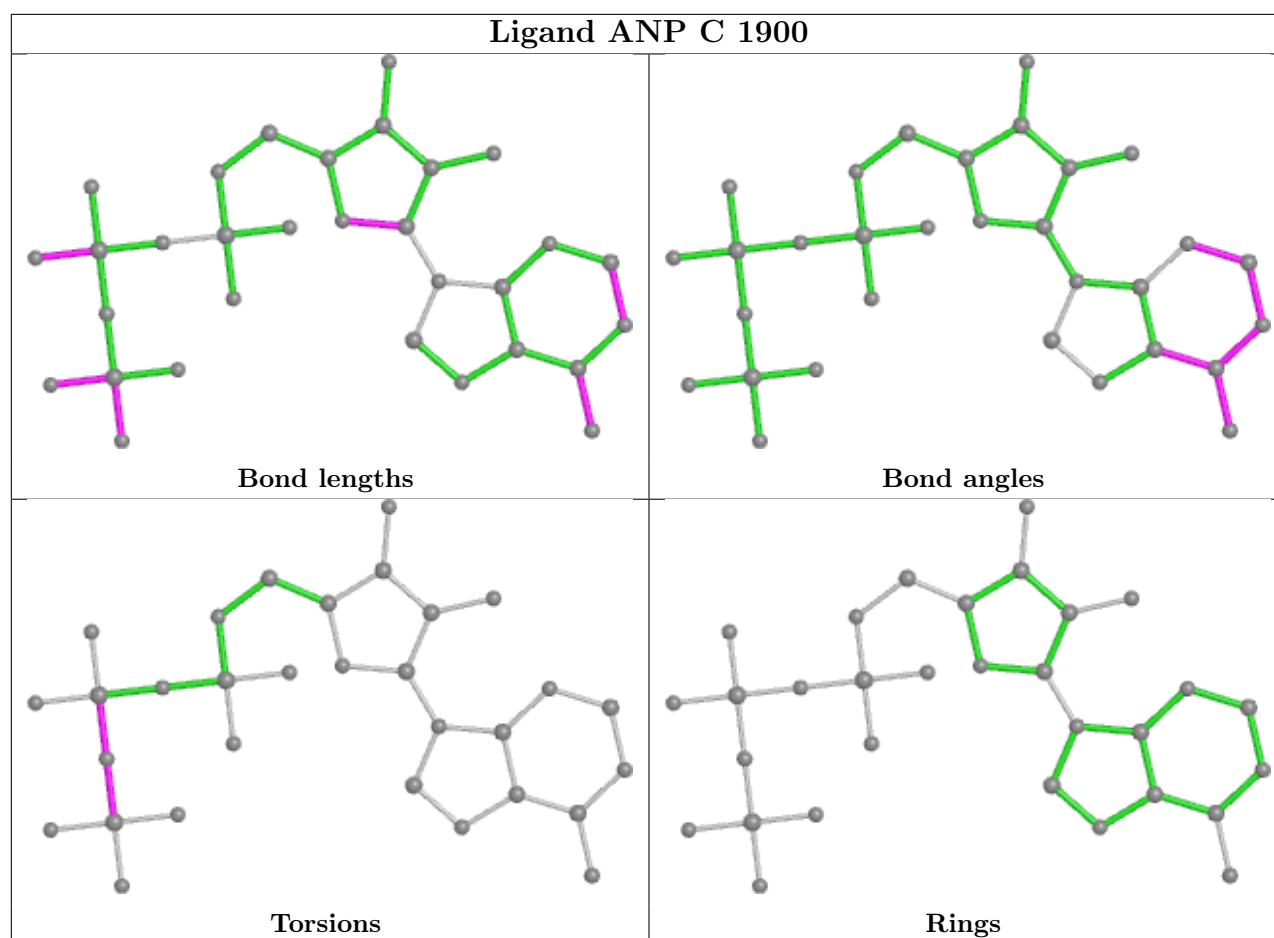












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.