wwPDB X-ray Structure Validation Summary Report (i)

Feb 4, 2024 – 03:23 PM EST

PDB ID	:	1RAF
Title	:	CRYSTAL STRUCTURE OF CTP-LIGATED T STATE ASPARTATE TRANSCARBAMOYLASE AT 2.5 ANGSTROMS RESOLUTION: IMPLICATIONS FOR ATCASE MUTANTS AND THE MECHANISM OF NEGATIVE COOPERATIVITY
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Deposited on	:	1992-08-14
Resolution	:	2.50 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:

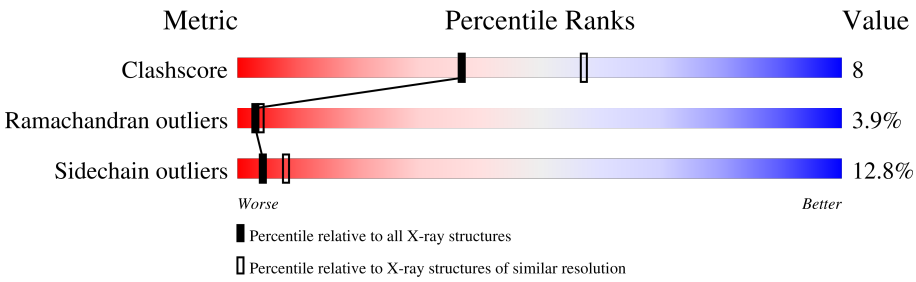
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.50 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	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)

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	310	67% 25% 7% •
1	C	310	69% 21% 8% •
2	B	153	65% 23% 10% •
2	D	153	59% 27% 8% 7%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7375 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 Aspartate carbamoyltransferase catalytic chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	310	2415	1527	423	456	9	0	0	0
1	C	310	2415	1527	423	456	9	0	0	0

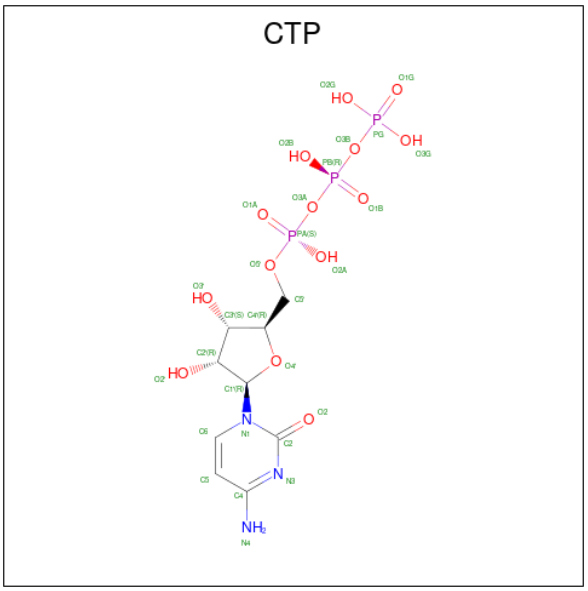
- Molecule 2 is a protein called Aspartate carbamoyltransferase regulatory chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	153	1196	749	212	229	6	0	0	0
2	D	153	1196	749	212	229	6	0	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
3	B	1	1	1	0	0
3	D	1	1	1	0	0

- Molecule 4 is CYTIDINE-5'-TRIPHOSPHATE (three-letter code: CTP) (formula: $C_9H_{16}N_3O_{14}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	B	1	29	9	3	14	3	0	0
4	D	1	29	9	3	14	3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	29	29	29	0	0
5	B	11	11	11	0	0
5	C	44	44	44	0	0
5	D	9	9	9	0	0

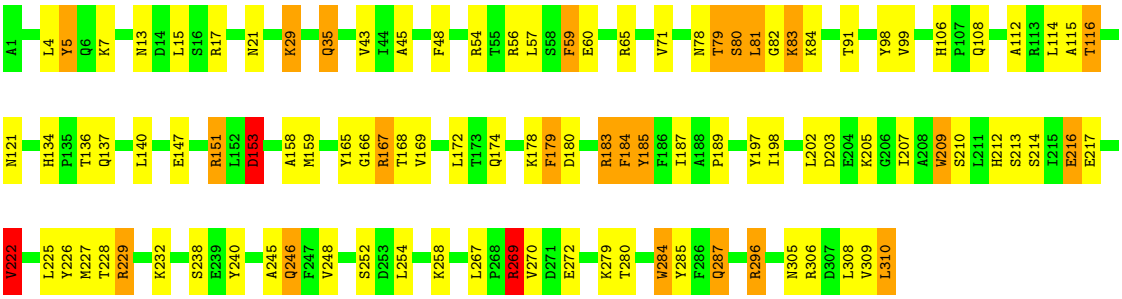
3 Residue-property plots (i)

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.

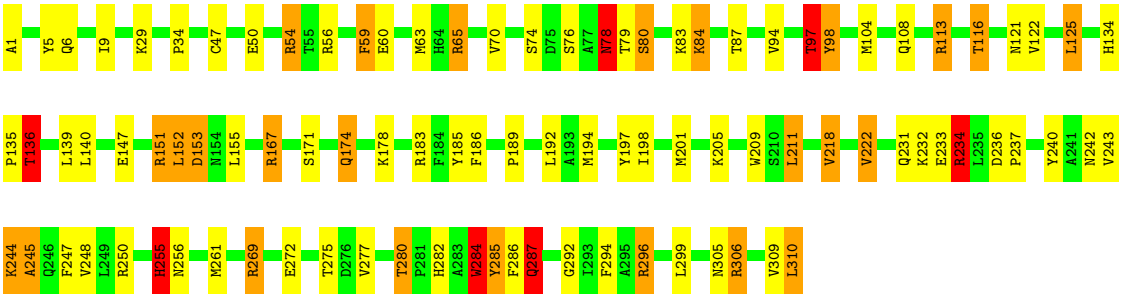
• Molecule 1: Aspartate carbamoyltransferase catalytic chain

Chain A: 67% 25% 7% •



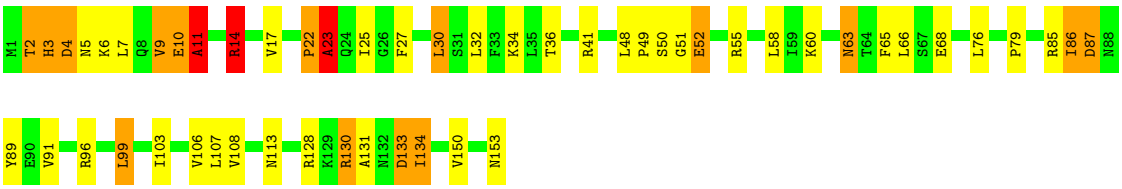
• Molecule 1: Aspartate carbamoyltransferase catalytic chain

Chain C: 69% 21% 8% •



• Molecule 2: Aspartate carbamoyltransferase regulatory chain

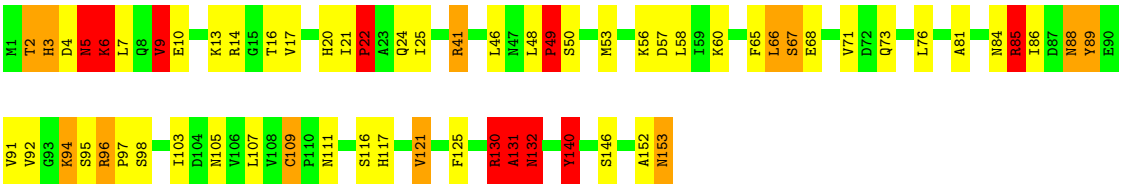
Chain B: 65% 23% 10% •



• Molecule 2: Aspartate carbamoyltransferase regulatory chain

Chain D:

59%
27%
8%
7%


M1 T2 H3 D4 N5 K6 L7 Q8 Y9 E10 K13 R14 G15 T16 V17 H20 I21 P22 A23 Q24 I25 R41 L46 N47 L48 P49 S50 M53 K56 D57 L58 I59 K60 F65 L66 S67 E68 V71 D72 Q73 L76 A81 N84 R85 I86 D87 N88 Y89 E90
V91 V92 G93 K94 S95 R96 P97 S98 I103 D104 N105 V106 L107 Y108 C109 P110 N111 S116 H117 V121 F125 R130 A131 N132 Y140 S146 A152 N153

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α, β, γ	122.13Å 122.13Å 142.51Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.188 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7375	wwPDB-VP
Average B, all atoms ($Å^2$)	25.0	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: CTP, ZN

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	0.96	2/2461 (0.1%)	1.74	43/3339 (1.3%)
1	C	1.01	3/2461 (0.1%)	1.82	56/3339 (1.7%)
2	B	0.88	0/1214	1.73	17/1640 (1.0%)
2	D	0.90	0/1214	1.79	28/1640 (1.7%)
All	All	0.96	5/7350 (0.1%)	1.77	144/9958 (1.4%)

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	0	7
1	C	0	5
2	B	0	1
2	D	0	2
All	All	0	15

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	147	GLU	CD-OE1	8.06	1.34	1.25
1	A	147	GLU	CD-OE2	7.19	1.33	1.25
1	A	60	GLU	CD-OE2	7.01	1.33	1.25
1	C	56	ARG	CA-CB	-5.18	1.42	1.53
1	C	60	GLU	CD-OE2	5.00	1.31	1.25

The worst 5 of 144 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	269	ARG	NE-CZ-NH1	15.85	128.23	120.30
1	C	296	ARG	NE-CZ-NH1	15.83	128.22	120.30
1	C	269	ARG	NE-CZ-NH2	-14.01	113.30	120.30
1	C	269	ARG	NE-CZ-NH1	13.76	127.18	120.30
1	A	56	ARG	NE-CZ-NH2	-11.69	114.45	120.30

There are no chirality outliers.

5 of 15 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	184	PHE	Sidechain
1	A	185	TYR	Sidechain
1	A	48	PHE	Sidechain
1	A	59	PHE	Sidechain
1	A	98	TYR	Sidechain

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	2415	0	2422	33	0
1	C	2415	0	2422	35	0
2	B	1196	0	1212	23	0
2	D	1196	0	1212	28	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
4	B	29	0	12	1	0
4	D	29	0	12	0	0
5	A	29	0	0	0	0
5	B	11	0	0	0	0
5	C	44	0	0	2	0
5	D	9	0	0	1	0
All	All	7375	0	7292	114	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 8.

The worst 5 of 114 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:4:ASP:HA	2:B:10:GLU:HB2	1.56	0.87
1:A:308:LEU:HG	1:A:310:LEU:HD22	1.58	0.86
1:A:81:LEU:HD13	1:A:91:THR:HG23	1.57	0.84
1:A:205:LYS:HB2	1:A:207:ILE:HD12	1.58	0.84
1:A:45:ALA:HB2	1:A:99:VAL:HG11	1.61	0.83

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	308/310 (99%)	288 (94%)	13 (4%)	7 (2%)	6 10
1	C	308/310 (99%)	283 (92%)	19 (6%)	6 (2%)	8 13
2	B	151/153 (99%)	120 (80%)	19 (13%)	12 (8%)	1 1
2	D	151/153 (99%)	124 (82%)	16 (11%)	11 (7%)	1 1
All	All	918/926 (99%)	815 (89%)	67 (7%)	36 (4%)	3 4

5 of 36 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	80	SER
1	A	245	ALA
1	A	270	VAL
2	B	3	HIS
2	B	11	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	261/261 (100%)	232 (89%)	29 (11%)	6 11
1	C	261/261 (100%)	228 (87%)	33 (13%)	4 8
2	B	136/137 (99%)	117 (86%)	19 (14%)	3 6
2	D	136/137 (99%)	115 (85%)	21 (15%)	2 5
All	All	794/796 (100%)	692 (87%)	102 (13%)	4 8

5 of 102 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	121	ASN
1	C	236	ASP
2	D	132	ASN
1	C	134	HIS
1	C	171	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	149	GLN
2	D	73	GLN
1	C	174	GLN
2	D	117	HIS
2	D	5	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)

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 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	$\#\|Z\| > 2$
4	CTP	B	999	-	26,30,30	1.36	6 (23%)	39,47,47	1.93	5 (12%)
4	CTP	D	999	-	26,30,30	1.27	5 (19%)	39,47,47	1.81	5 (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
4	CTP	B	999	-	-	7/22/38/38	0/2/2/2
4	CTP	D	999	-	-	3/22/38/38	0/2/2/2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	999	CTP	PG-O1G	2.65	1.59	1.50
4	D	999	CTP	C5-C4	-2.45	1.37	1.42
4	B	999	CTP	C6-N1	-2.37	1.32	1.38
4	B	999	CTP	C2-N3	-2.37	1.31	1.36
4	B	999	CTP	PG-O1G	2.37	1.58	1.50

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	999	CTP	PB-O3A-PA	-6.87	109.27	132.83
4	B	999	CTP	PB-O3A-PA	-6.48	110.59	132.83
4	B	999	CTP	PB-O3B-PG	-5.23	114.89	132.83
4	B	999	CTP	O2-C2-N3	-5.10	114.04	122.33
4	D	999	CTP	PB-O3B-PG	-4.77	116.47	132.83

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

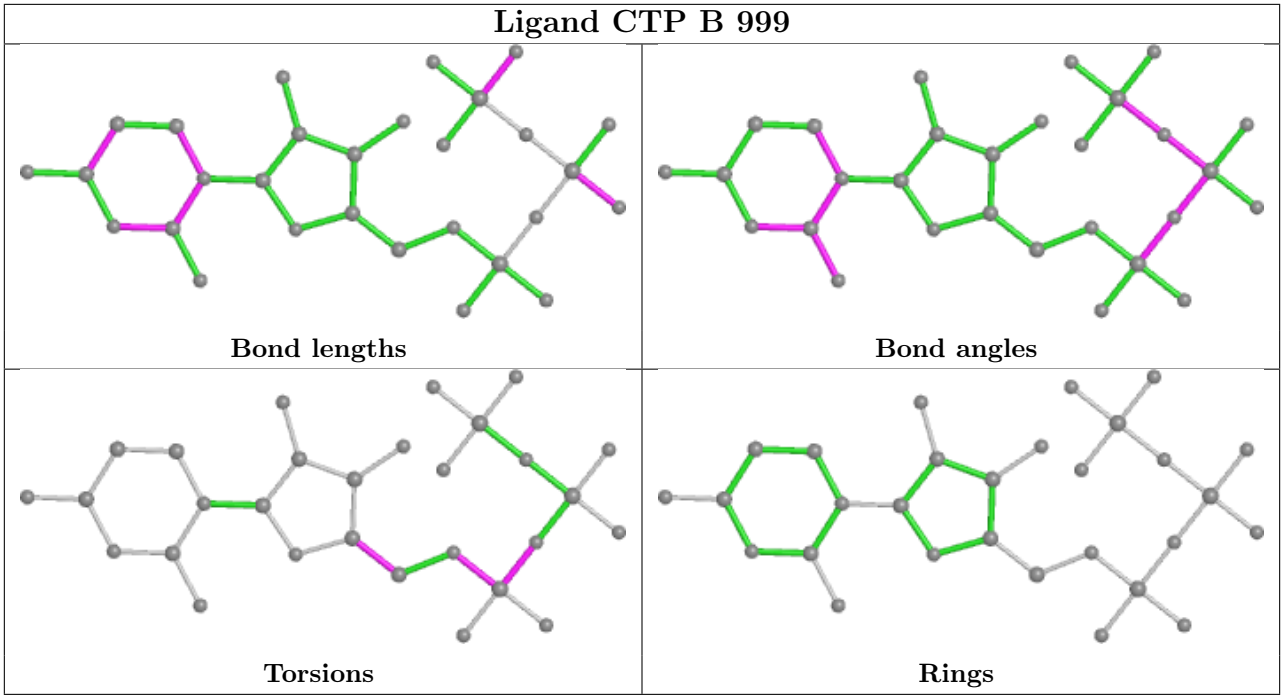
Mol	Chain	Res	Type	Atoms
4	B	999	CTP	O4'-C4'-C5'-O5'
4	B	999	CTP	C5'-O5'-PA-O1A
4	B	999	CTP	C5'-O5'-PA-O2A
4	B	999	CTP	C5'-O5'-PA-O3A
4	B	999	CTP	C3'-C4'-C5'-O5'

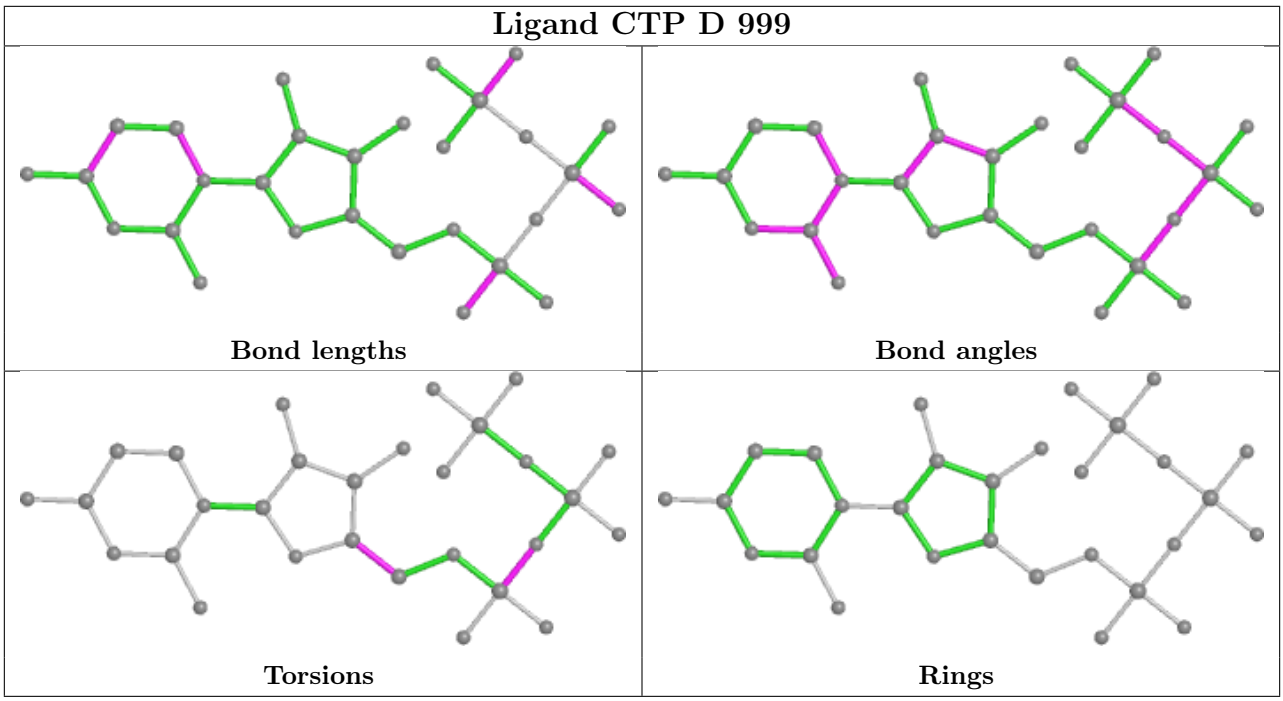
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	999	CTP	1	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.





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.