WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

May 29, 2024 – 02:23 PM EDT

PDB ID	:	4RUB
Title	:	A CRYSTAL FORM OF RIBULOSE-1,5-BISPHOSPHATE CARBOXY LASE(SLASH)OXYGENASE FROM NICOTIANA TABACUM IN THE ACTIVATED STATE
Authors	:	Schreuder, H.; Cascio, D.; Curmi, P.M.G.; Eisenberg, D.
Deposited on	:	1990-05-25
Resolution	:	2.70 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 (i)) were used in the production of this report:

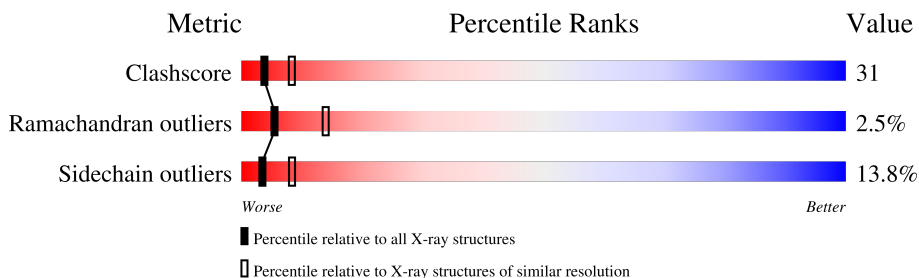|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.70 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	Percentile Ranks	Value
Clashscore		31
Ramachandran outliers		2.5%
Sidechain outliers		13.8%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)

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	477	35% 39% 19% · ·
1	B	477	34% 42% 17% 5% ·
1	C	477	31% 41% 21% 5% ·
1	D	477	36% 38% 18% 5% ·
2	S	123	30% 46% 20% 5%
2	T	123	34% 43% 17% 6%
2	U	123	20% 43% 33% 5%
2	V	123	27% 41% 25% 7%

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
4	CAP	A	490	-	X	-	-
4	CAP	B	490	-	X	-	-
4	CAP	C	490	-	X	-	-

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 18708 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 RIBULOSE 1,5-BISPHOSPHATE CARBOXYLASE/OXYG ENASE (FORM IV).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	465	Total 3628	C 2307	N 641	O 664	S 16	0	0	1
1	B	465	Total 3628	C 2307	N 641	O 664	S 16	0	0	1
1	C	465	Total 3628	C 2307	N 641	O 664	S 16	0	0	1
1	D	465	Total 3628	C 2307	N 641	O 664	S 16	0	0	1

- Molecule 2 is a protein called RIBULOSE 1,5-BISPHOSPHATE CARBOXYLASE/OXYG ENASE (FORM IV).

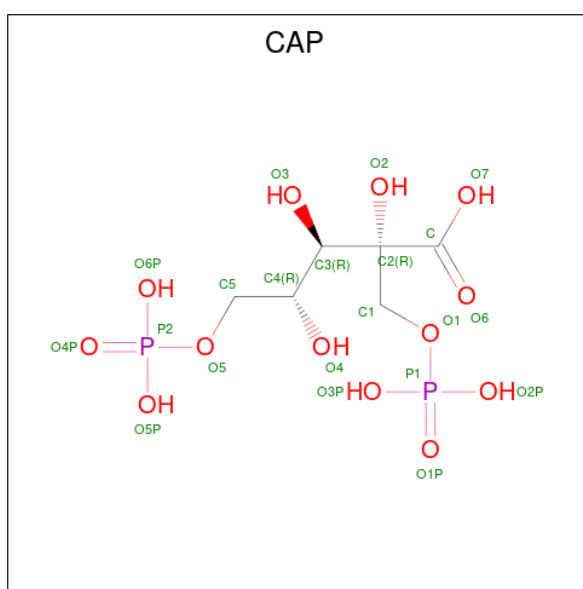| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	S	123	Total 1024	C 669	N 163	O 186	S 6	0	0	0
2	T	123	Total 1024	C 669	N 163	O 186	S 6	0	0	0
2	U	123	Total 1024	C 669	N 163	O 186	S 6	0	0	0
2	V	123	Total 1024	C 669	N 163	O 186	S 6	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	88	GLY	GLU	conflict	UNP P69249
T	88	GLY	GLU	conflict	UNP P69249
U	88	GLY	GLU	conflict	UNP P69249
V	88	GLY	GLU	conflict	UNP P69249

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Mg 1	0	0
3	B	1	Total 1	Mg 1	0	0
3	C	1	Total 1	Mg 1	0	0
3	D	1	Total 1	Mg 1	0	0

- Molecule 4 is 2-CARBOXYARABINITOL-1,5-DIPHOSPHATE (three-letter code: CAP) (formula: $C_6H_{14}O_{13}P_2$).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total 21	C 6	O 13	P 2	0	0
4	B	1	Total 21	C 6	O 13	P 2	0	0
4	C	1	Total 21	C 6	O 13	P 2	0	0
4	D	1	Total 21	C 6	O 13	P 2	0	0

- Molecule 5 is FORMIC ACID (three-letter code: FMT) (formula: CH_2O_2).

FMT

C

OH O2

O

O1

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 3	C 1	O 2	0	0
5	B	1	Total 3	C 1	O 2	0	0
5	C	1	Total 3	C 1	O 2	0	0
5	D	1	Total 3	C 1	O 2	0	0

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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.
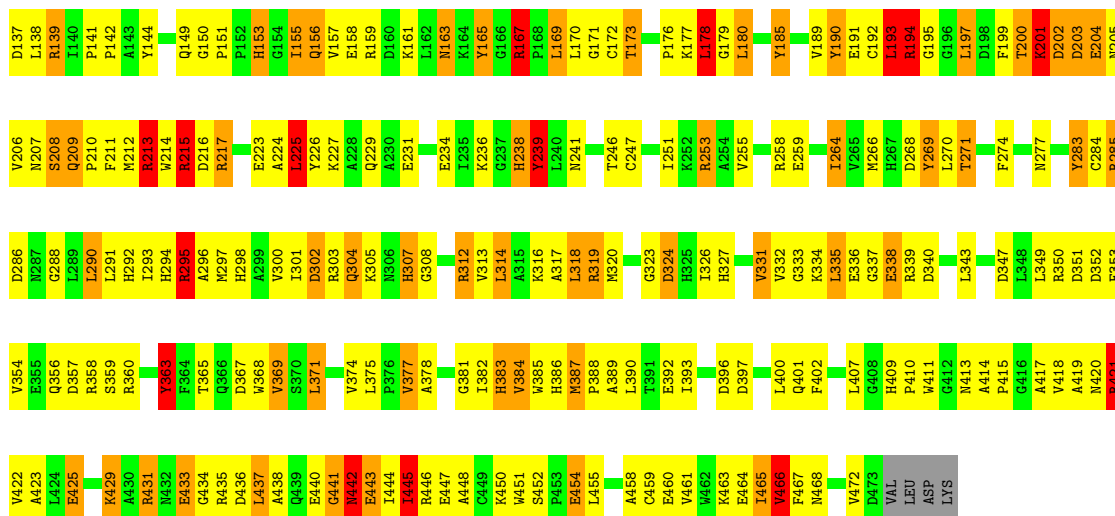
Note EDS was not executed.

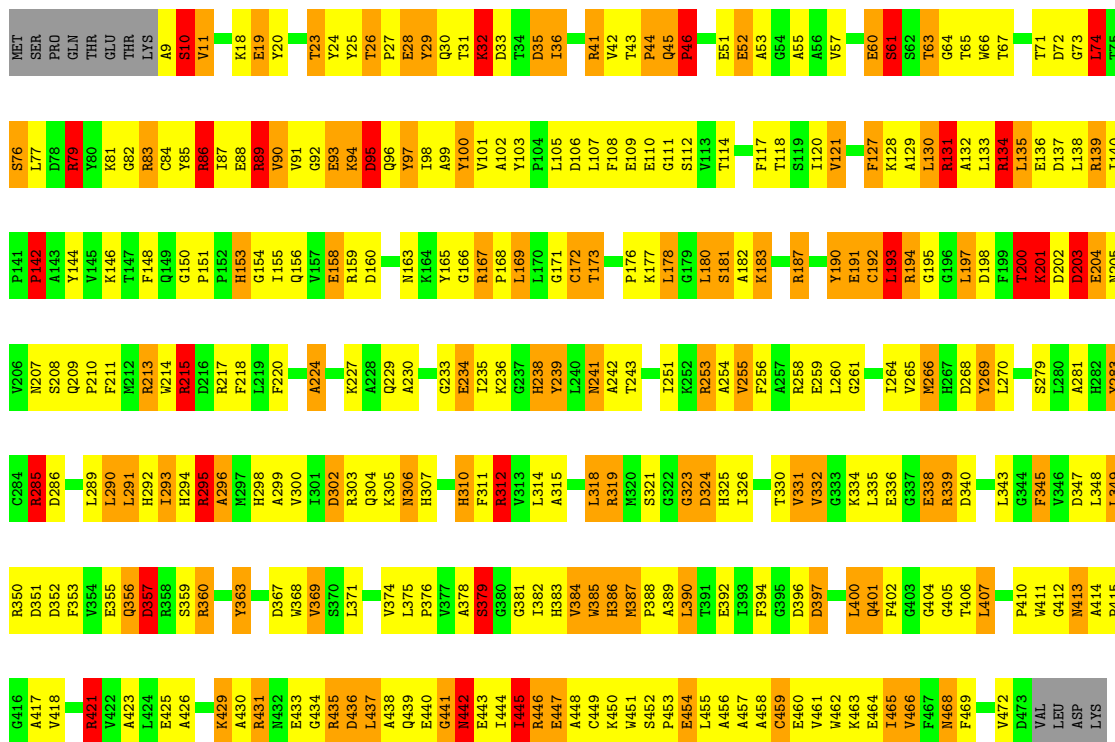• Molecule 1: RIBULOSE 1,5-BISPHOSPHATE CARBOXYLASE/OXYGENASE (FORM IV)
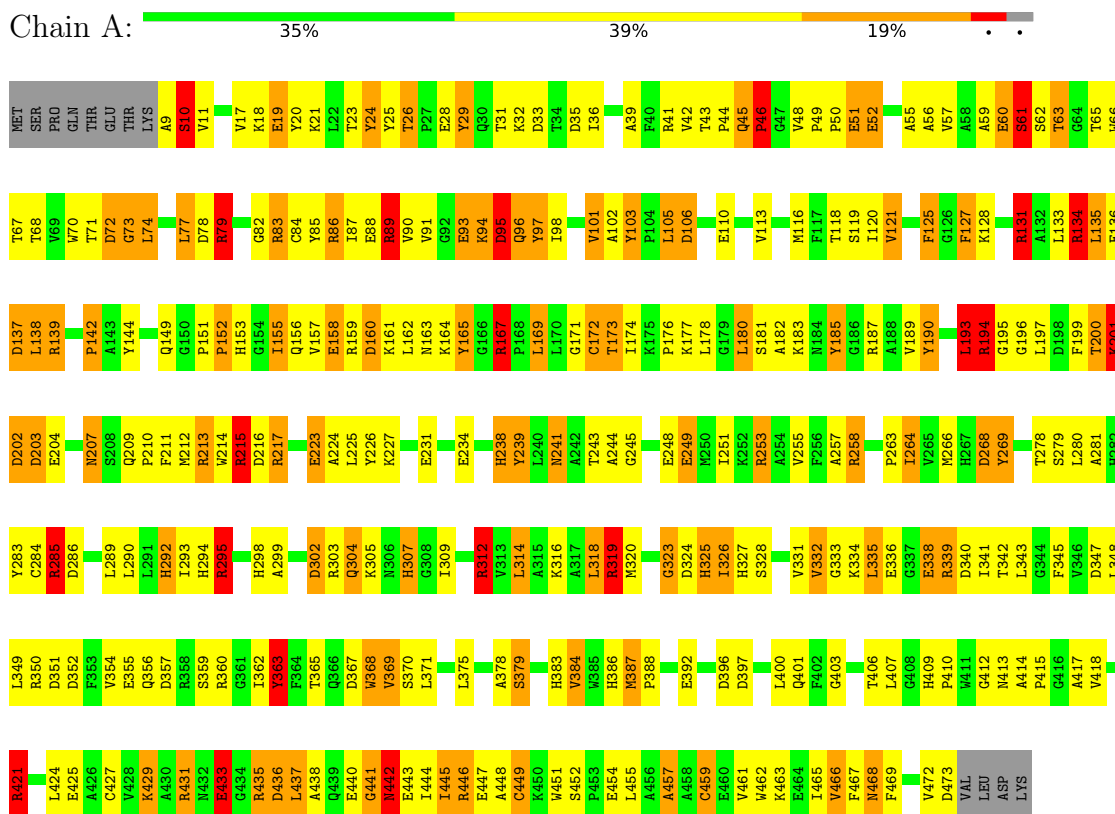
Chain A:

• Molecule 1: RIBULOSE 1,5-BISPHOSPHATE CARBOXYLASE/OXYGENASE (FORM IV)

Chain B:

• Molecule 1: RIBULOSE 1,5-BISPHOSPHATE CARBOXYLASE/OXYGENASE (FORM IV)

Chain C:

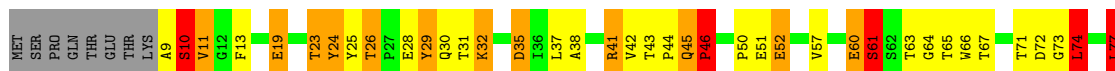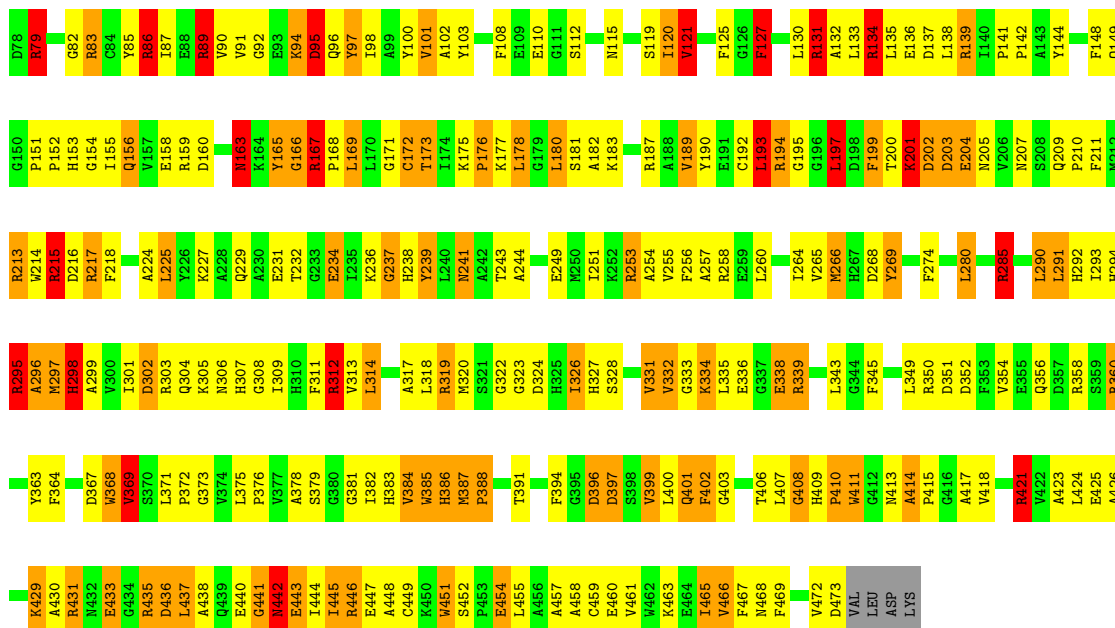• Molecule 1: RIBULOSE 1,5-BISPHOSPHATE CARBOXYLASE/OXYGENASE (FORM IV)

Chain D:
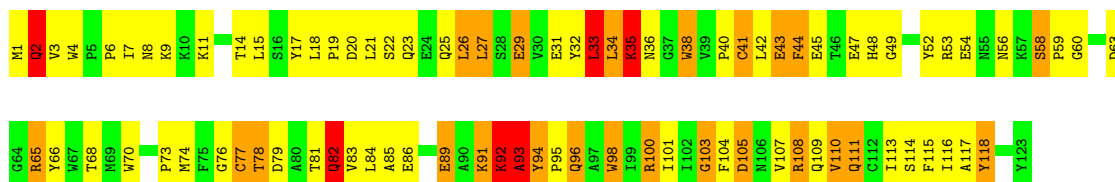
• Molecule 2: RIBULOSE 1,5-BISPHOSPHATE CARBOXYLASE/OXYGENASE (FORM IV)

• Molecule 2: RIBULOSE 1,5-BISPHOSPHATE CARBOXYLASE/OXYGENASE (FORM IV)

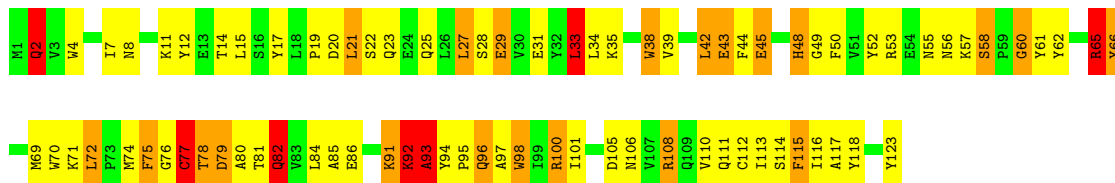• Molecule 2: RIBULOSE 1,5-BISPHOSPHATE CARBOXYLASE/OXYGENASE (FORM IV)

R65 Y66 W67 T68 M69 L72 P73 M74 F75 G76 C77 T78 D79 A80 T81 Q82 V83 L84 A85 E86 V87 G88 E89 A90 K91 K92 A93 Y94 P95 Q96 A97 W98 I99 R100 I101 I102 G103 F104 D105 N106 V107 R108 Q109 V110 Q111 C112 I113 S114 F115 I116 A117 Y118 K119 P120 E121 G122 Y123

• Molecule 2: RIBULOSE 1,5-BISPHOSPHATE CARBOXYLASE/OXYGENASE (FORM IV)

Chain V:

27%   41%   25%   7%

M1 Q2 V3 W4 P5 P6 I7 N8 K11 Y12 E13 S16 Y17 L18 P19 D20 L21 S22 Q23 E24 Q25 L26 L27 S28 E29 V30 E31 Y32 L33 L34 K35 N36 G37 W38 V39 L42 E43 F44 E47 H48 Y52 R53 E54 N55 N56 K57 S58 P59 G60 Y61 Y62 D63 G64 R65 Y66

W67 T68 M69 W70 K71 L72 F75 G76 C77 T78 D79 A80 T81 Q82 V83 L84 A85 E86 V87 G88 E89 A90 K91 K92 A93 Y94 P95 Q96 A97 W98 I99 R100 I101 I102 G103 F104 D105 N106 V107 R108 Q109 V110 Q111 C112 I113 S114 F115 I116 P120 E121 G122 Y123

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	204.60Å 204.60Å 117.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 2.70	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROFFT	Depositor
R, R_{free}	0.202 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	18708	wwPDB-VP
Average B, all atoms (Å^2)	21.0	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: MG, CAP, FMT

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	1.69	30/3716 (0.8%)	2.59	253/5038 (5.0%)
1	B	1.66	24/3716 (0.6%)	2.57	227/5038 (4.5%)
1	C	1.75	46/3716 (1.2%)	2.66	253/5038 (5.0%)
1	D	1.69	39/3716 (1.0%)	2.60	235/5038 (4.7%)
2	S	1.57	8/1057 (0.8%)	2.51	71/1435 (4.9%)
2	T	1.48	3/1057 (0.3%)	2.25	56/1435 (3.9%)
2	U	1.79	13/1057 (1.2%)	2.53	70/1435 (4.9%)
2	V	1.70	14/1057 (1.3%)	2.50	80/1435 (5.6%)
All	All	1.68	177/19092 (0.9%)	2.57	1245/25892 (4.8%)

The worst 5 of 177 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	S	58	SER	CB-OG	-9.13	1.30	1.42
1	C	181	SER	CB-OG	8.99	1.53	1.42
1	C	323	GLY	N-CA	8.87	1.59	1.46
1	A	459	CYS	CB-SG	-8.49	1.67	1.82
1	A	134	ARG	CZ-NH1	8.02	1.43	1.33

The worst 5 of 1245 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	350	ARG	NE-CZ-NH2	-35.79	102.40	120.30
1	A	319	ARG	CD-NE-CZ	25.36	159.11	123.60
1	C	319	ARG	CD-NE-CZ	23.95	157.13	123.60
1	D	139	ARG	NE-CZ-NH1	-23.24	108.68	120.30
1	A	139	ARG	NE-CZ-NH2	23.20	131.90	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	3628	0	3559	200	0
1	B	3628	0	3558	225	1
1	C	3628	0	3556	246	1
1	D	3628	0	3557	242	0
2	S	1024	0	991	67	0
2	T	1024	0	991	85	0
2	U	1024	0	991	95	0
2	V	1024	0	991	93	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	21	0	6	2	0
4	B	21	0	5	0	0
4	C	21	0	6	1	0
4	D	21	0	6	3	0
5	A	3	0	0	1	0
5	B	3	0	0	0	0
5	C	3	0	0	1	0
5	D	3	0	0	1	0
All	All	18708	0	18217	1145	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 31.

The worst 5 of 1145 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:U:79:ASP:HB3	2:U:82:GLN:HE21	1.13	1.10
1:A:79:ARG:HH11	1:A:79:ARG:HG2	1.18	1.09
2:V:79:ASP:HB3	2:V:82:GLN:HE21	1.14	1.09
1:D:79:ARG:HG2	1:D:79:ARG:HH11	1.15	1.06
1:C:26:THR:HG22	1:C:29:TYR:HB2	1.37	1.05

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:446:ARG:NH2	1:C:30:GLN:NE2[3_654]	2.00	0.20

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	463/477 (97%)	402 (87%)	48 (10%)	13 (3%)	5	11
1	B	463/477 (97%)	399 (86%)	52 (11%)	12 (3%)	5	13
1	C	463/477 (97%)	388 (84%)	63 (14%)	12 (3%)	5	13
1	D	463/477 (97%)	400 (86%)	52 (11%)	11 (2%)	6	15
2	S	121/123 (98%)	104 (86%)	14 (12%)	3 (2%)	5	14
2	T	121/123 (98%)	102 (84%)	17 (14%)	2 (2%)	9	23
2	U	121/123 (98%)	99 (82%)	19 (16%)	3 (2%)	5	14
2	V	121/123 (98%)	100 (83%)	19 (16%)	2 (2%)	9	23
All	All	2336/2400 (97%)	1994 (85%)	284 (12%)	58 (2%)	5	14

5 of 58 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	46	PRO
1	A	95	ASP
1	A	167	ARG
2	S	93	ALA
1	B	46	PRO

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	373/386 (97%)	326 (87%)	47 (13%)	4	10
1	B	373/386 (97%)	321 (86%)	52 (14%)	3	8
1	C	373/386 (97%)	322 (86%)	51 (14%)	3	8
1	D	373/386 (97%)	325 (87%)	48 (13%)	4	10
2	S	109/109 (100%)	94 (86%)	15 (14%)	3	8
2	T	109/109 (100%)	93 (85%)	16 (15%)	3	7
2	U	109/109 (100%)	91 (84%)	18 (16%)	2	5
2	V	109/109 (100%)	90 (83%)	19 (17%)	2	5
All	All	1928/1980 (97%)	1662 (86%)	266 (14%)	3	8

5 of 266 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	312	ARG
1	D	384	VAL
2	V	91	LYS
1	B	319	ARG
1	B	312	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 53 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	229	GLN
2	U	36	ASN
2	V	25	GLN
1	C	238	HIS
1	C	356	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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	$\#|Z| > 2$
5	FMT	B	492	3,1	2,2,2	0.46	0	1,1,1	0.27	0
4	CAP	D	490	3	17,20,20	1.85	4 (23%)	22,31,31	5.42	12 (54%)
5	FMT	A	492	3,1	2,2,2	0.78	0	1,1,1	1.51	0
4	CAP	C	490	3	17,20,20	2.44	9 (52%)	22,31,31	6.52	13 (59%)
5	FMT	C	492	3,1	2,2,2	1.30	0	1,1,1	0.67	0
4	CAP	B	490	3	17,20,20	3.07	7 (41%)	22,31,31	5.53	12 (54%)
4	CAP	A	490	3	17,20,20	2.93	10 (58%)	22,31,31	5.14	12 (54%)
5	FMT	D	492	3,1	2,2,2	1.11	0	1,1,1	0.30	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
4	CAP	A	490	3	-	16/29/29/29	-
4	CAP	B	490	3	-	17/29/29/29	-
4	CAP	C	490	3	-	12/29/29/29	-
4	CAP	D	490	3	-	13/29/29/29	-

The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	490	CAP	C5-C4	-7.22	1.41	1.51
4	A	490	CAP	C4-C3	-6.23	1.48	1.54
4	C	490	CAP	C4-C3	-5.96	1.48	1.54
4	B	490	CAP	O2-C2	-4.80	1.32	1.42
4	B	490	CAP	P1-O1P	4.47	1.65	1.50

The worst 5 of 49 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	490	CAP	O3-C3-C4	-15.43	76.08	109.13
4	C	490	CAP	C5-C4-C3	-14.67	81.95	111.94
4	C	490	CAP	O2-C2-C	-14.36	82.72	108.97
4	D	490	CAP	C5-C4-C3	-13.08	85.20	111.94
4	A	490	CAP	O2-C2-C	-12.84	85.51	108.97

There are no chirality outliers.

5 of 58 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	490	CAP	C1-C2-C3-O3
4	A	490	CAP	O2-C2-C3-C4
4	A	490	CAP	O2-C2-C3-O3
4	A	490	CAP	O6-C-C2-O2
4	A	490	CAP	C2-C3-C4-C5

There are no ring outliers.

6 monomers are involved in 8 short contacts:

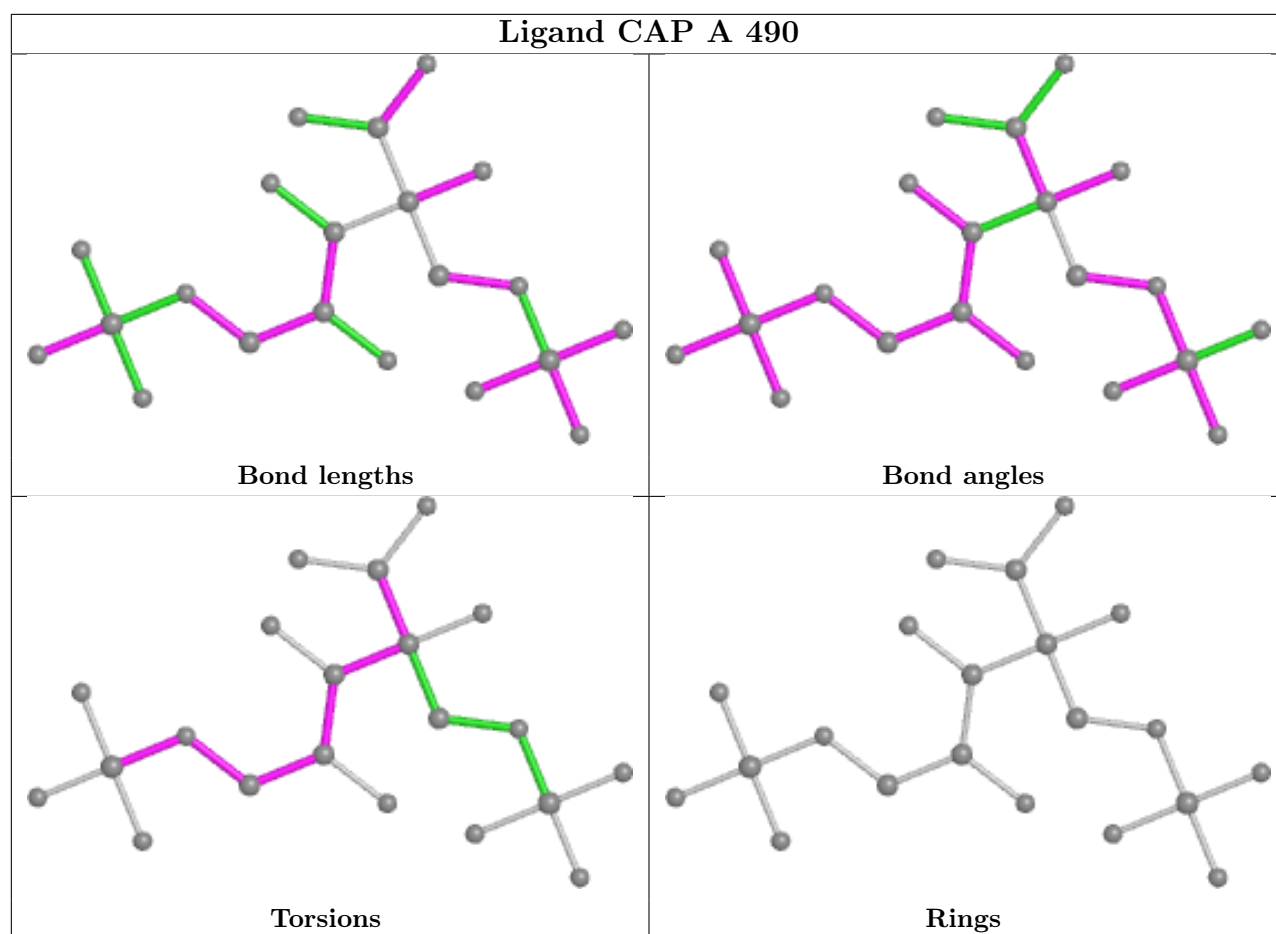| Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	490	CAP	3	0
5	A	492	FMT	1	0
4	C	490	CAP	1	0
5	C	492	FMT	1	0
4	A	490	CAP	2	0
5	D	492	FMT	1	0

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.

Ligand CAP D 490

Bond lengths

Bond angles

Torsions

Rings

Ligand CAP C 490

Bond lengths

Bond angles

Torsions

Rings

Ligand CAP B 490

Bond lengths

Bond angles

Torsions

Rings

Ligand CAP A 490

Bond lengths

Bond angles

Torsions

Rings
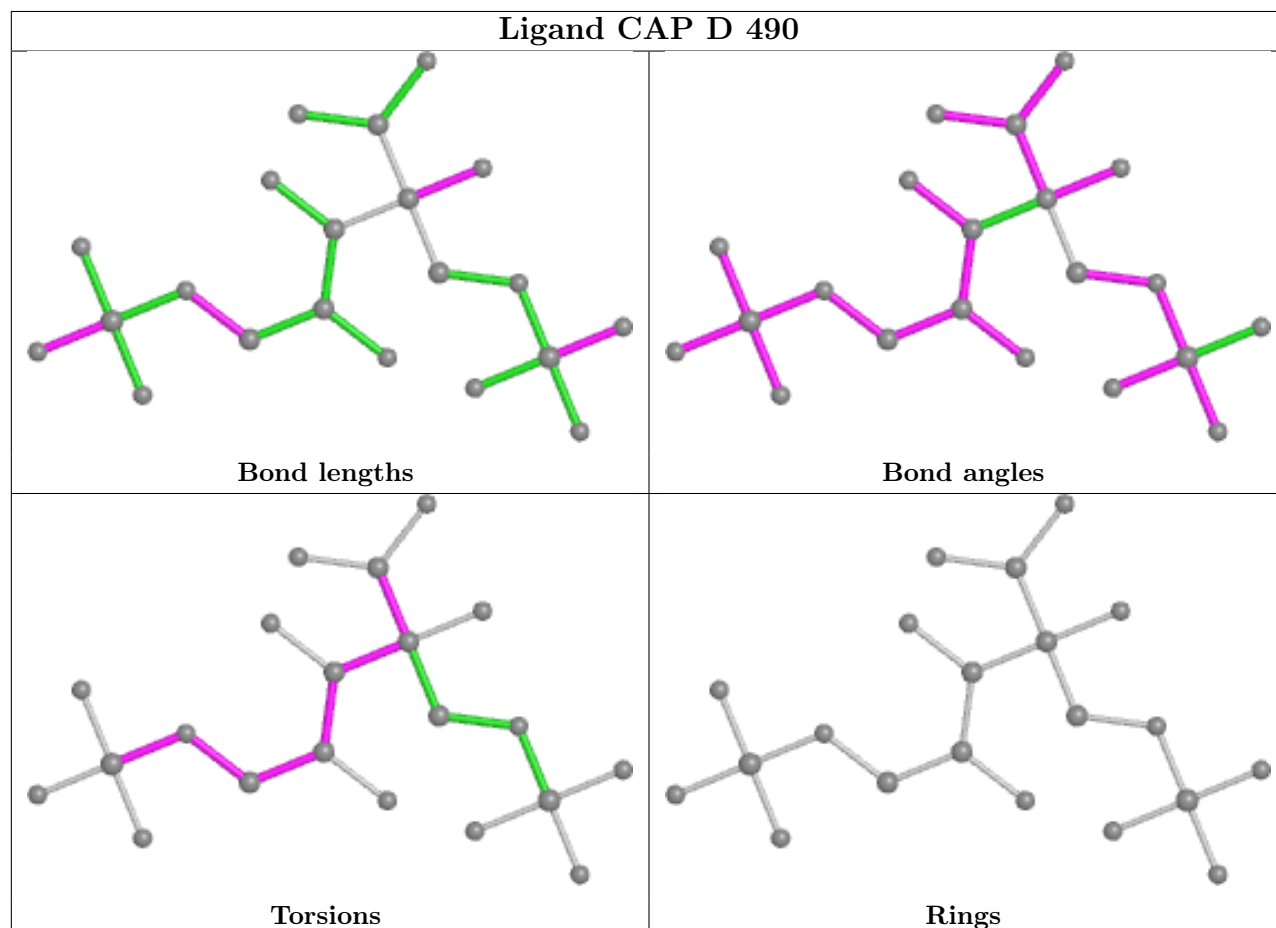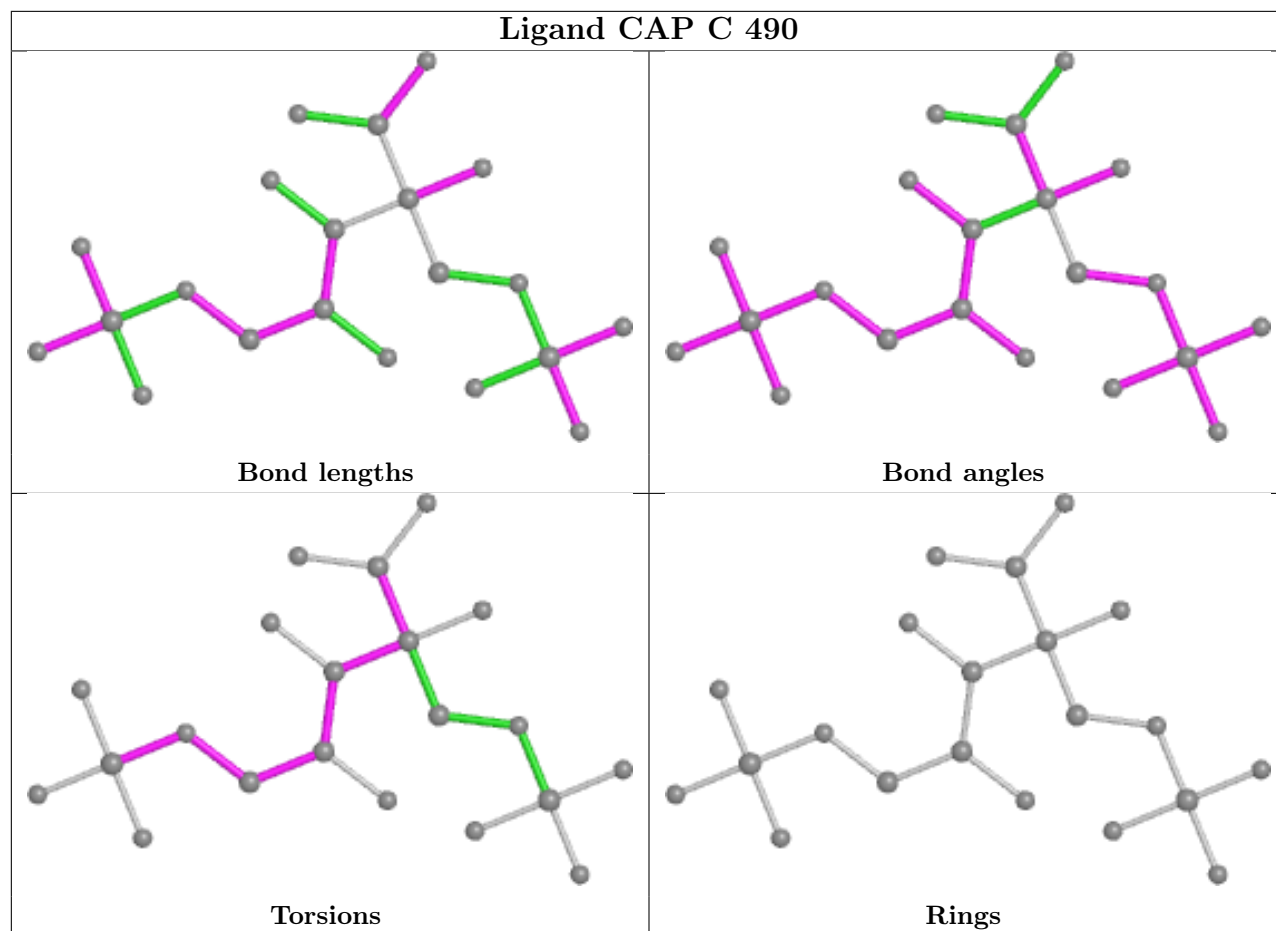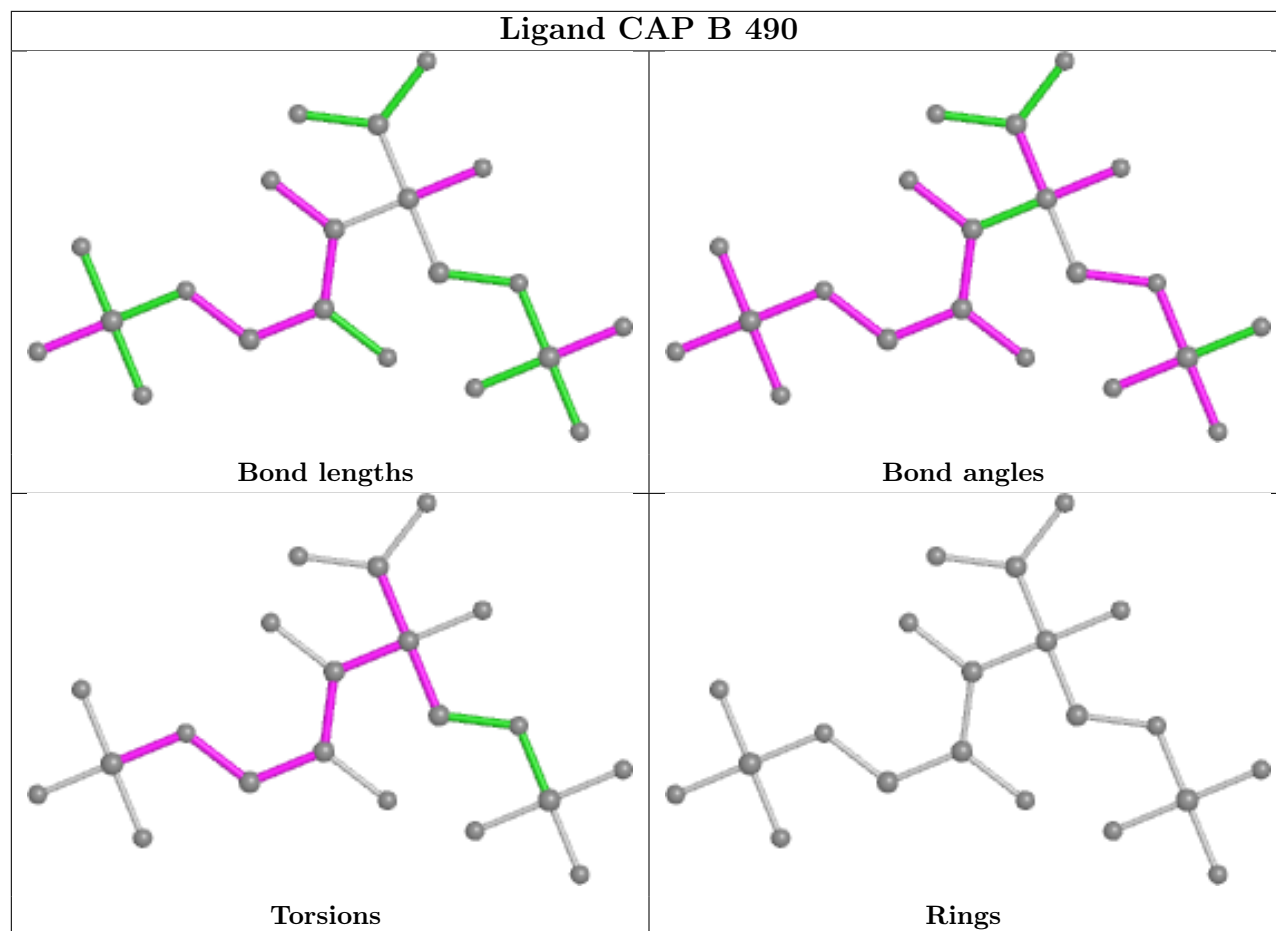
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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.