wwPDB X-ray Structure Validation Summary Report (i)

Jan 30, 2024 – 10:23 PM EST

PDB ID	:	1JYL
Title	:	Catalytic Mechanism of CTP:phosphocholine Cytidylyltransferase from Streptococcus pneumoniae (LicC)
Authors	:	Kwak, B.-Y.; Yun, M.; Park, H.-w.
Deposited on	:	2001-09-12
Resolution	:	2.40 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:

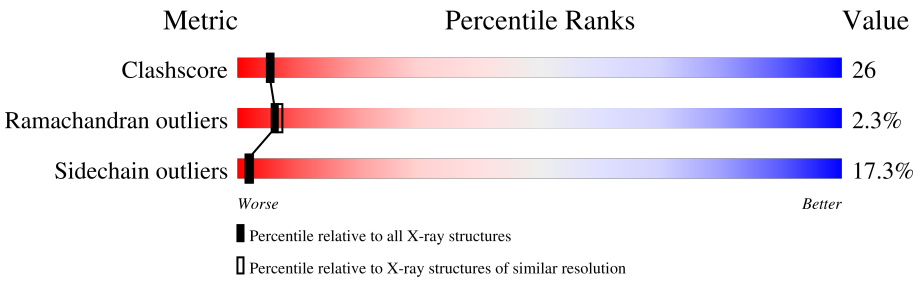
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.40 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	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)

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	254	51% 28% 10% • 10%
1	B	254	39% 42% 9% 10%
1	C	254	43% 36% 10% 10%
1	D	254	44% 36% 9% 10%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7904 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 CTP:phosphocholine Cytidylyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	228	1905	1237	301	364	3	0	1	0
			Total	C	N	O	S			
1	B	228	1894	1231	297	363	3	0	0	0
			Total	C	N	O	S			
1	C	228	1905	1237	301	364	3	0	1	0
			Total	C	N	O	S			
1	D	228	1894	1231	297	363	3	0	0	0

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP Q97QE9
A	-18	GLY	-	expression tag	UNP Q97QE9
A	-17	SER	-	expression tag	UNP Q97QE9
A	-16	SER	-	expression tag	UNP Q97QE9
A	-15	HIS	-	expression tag	UNP Q97QE9
A	-14	HIS	-	expression tag	UNP Q97QE9
A	-13	HIS	-	expression tag	UNP Q97QE9
A	-12	HIS	-	expression tag	UNP Q97QE9
A	-11	HIS	-	expression tag	UNP Q97QE9
A	-10	HIS	-	expression tag	UNP Q97QE9
A	-9	SER	-	expression tag	UNP Q97QE9
A	-8	SER	-	expression tag	UNP Q97QE9
A	-7	GLY	-	expression tag	UNP Q97QE9
A	-6	LEU	-	expression tag	UNP Q97QE9
A	-5	VAL	-	expression tag	UNP Q97QE9
A	-4	PRO	-	expression tag	UNP Q97QE9
A	-3	ARG	-	expression tag	UNP Q97QE9
A	-2	GLY	-	expression tag	UNP Q97QE9
A	-1	SER	-	expression tag	UNP Q97QE9
A	0	HIS	-	expression tag	UNP Q97QE9
A	1	MET	-	expression tag	UNP Q97QE9

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	LYS	-	expression tag	UNP Q97QE9
A	3	GLU	-	expression tag	UNP Q97QE9
A	4	ILE	-	expression tag	UNP Q97QE9
A	5	ARG	-	expression tag	UNP Q97QE9
A	6	VAL	-	expression tag	UNP Q97QE9
A	22	LEU	MET	conflict	UNP Q97QE9
B	-19	MET	-	expression tag	UNP Q97QE9
B	-18	GLY	-	expression tag	UNP Q97QE9
B	-17	SER	-	expression tag	UNP Q97QE9
B	-16	SER	-	expression tag	UNP Q97QE9
B	-15	HIS	-	expression tag	UNP Q97QE9
B	-14	HIS	-	expression tag	UNP Q97QE9
B	-13	HIS	-	expression tag	UNP Q97QE9
B	-12	HIS	-	expression tag	UNP Q97QE9
B	-11	HIS	-	expression tag	UNP Q97QE9
B	-10	HIS	-	expression tag	UNP Q97QE9
B	-9	SER	-	expression tag	UNP Q97QE9
B	-8	SER	-	expression tag	UNP Q97QE9
B	-7	GLY	-	expression tag	UNP Q97QE9
B	-6	LEU	-	expression tag	UNP Q97QE9
B	-5	VAL	-	expression tag	UNP Q97QE9
B	-4	PRO	-	expression tag	UNP Q97QE9
B	-3	ARG	-	expression tag	UNP Q97QE9
B	-2	GLY	-	expression tag	UNP Q97QE9
B	-1	SER	-	expression tag	UNP Q97QE9
B	0	HIS	-	expression tag	UNP Q97QE9
B	1	MET	-	expression tag	UNP Q97QE9
B	2	LYS	-	expression tag	UNP Q97QE9
B	3	GLU	-	expression tag	UNP Q97QE9
B	4	ILE	-	expression tag	UNP Q97QE9
B	5	ARG	-	expression tag	UNP Q97QE9
B	6	VAL	-	expression tag	UNP Q97QE9
B	22	LEU	MET	conflict	UNP Q97QE9
C	-19	MET	-	expression tag	UNP Q97QE9
C	-18	GLY	-	expression tag	UNP Q97QE9
C	-17	SER	-	expression tag	UNP Q97QE9
C	-16	SER	-	expression tag	UNP Q97QE9
C	-15	HIS	-	expression tag	UNP Q97QE9
C	-14	HIS	-	expression tag	UNP Q97QE9
C	-13	HIS	-	expression tag	UNP Q97QE9
C	-12	HIS	-	expression tag	UNP Q97QE9
C	-11	HIS	-	expression tag	UNP Q97QE9

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	-10	HIS	-	expression tag	UNP Q97QE9
C	-9	SER	-	expression tag	UNP Q97QE9
C	-8	SER	-	expression tag	UNP Q97QE9
C	-7	GLY	-	expression tag	UNP Q97QE9
C	-6	LEU	-	expression tag	UNP Q97QE9
C	-5	VAL	-	expression tag	UNP Q97QE9
C	-4	PRO	-	expression tag	UNP Q97QE9
C	-3	ARG	-	expression tag	UNP Q97QE9
C	-2	GLY	-	expression tag	UNP Q97QE9
C	-1	SER	-	expression tag	UNP Q97QE9
C	0	HIS	-	expression tag	UNP Q97QE9
C	1	MET	-	expression tag	UNP Q97QE9
C	2	LYS	-	expression tag	UNP Q97QE9
C	3	GLU	-	expression tag	UNP Q97QE9
C	4	ILE	-	expression tag	UNP Q97QE9
C	5	ARG	-	expression tag	UNP Q97QE9
C	6	VAL	-	expression tag	UNP Q97QE9
C	22	LEU	MET	conflict	UNP Q97QE9
D	-19	MET	-	expression tag	UNP Q97QE9
D	-18	GLY	-	expression tag	UNP Q97QE9
D	-17	SER	-	expression tag	UNP Q97QE9
D	-16	SER	-	expression tag	UNP Q97QE9
D	-15	HIS	-	expression tag	UNP Q97QE9
D	-14	HIS	-	expression tag	UNP Q97QE9
D	-13	HIS	-	expression tag	UNP Q97QE9
D	-12	HIS	-	expression tag	UNP Q97QE9
D	-11	HIS	-	expression tag	UNP Q97QE9
D	-10	HIS	-	expression tag	UNP Q97QE9
D	-9	SER	-	expression tag	UNP Q97QE9
D	-8	SER	-	expression tag	UNP Q97QE9
D	-7	GLY	-	expression tag	UNP Q97QE9
D	-6	LEU	-	expression tag	UNP Q97QE9
D	-5	VAL	-	expression tag	UNP Q97QE9
D	-4	PRO	-	expression tag	UNP Q97QE9
D	-3	ARG	-	expression tag	UNP Q97QE9
D	-2	GLY	-	expression tag	UNP Q97QE9
D	-1	SER	-	expression tag	UNP Q97QE9
D	0	HIS	-	expression tag	UNP Q97QE9
D	1	MET	-	expression tag	UNP Q97QE9
D	2	LYS	-	expression tag	UNP Q97QE9
D	3	GLU	-	expression tag	UNP Q97QE9
D	4	ILE	-	expression tag	UNP Q97QE9

Continued on next page...

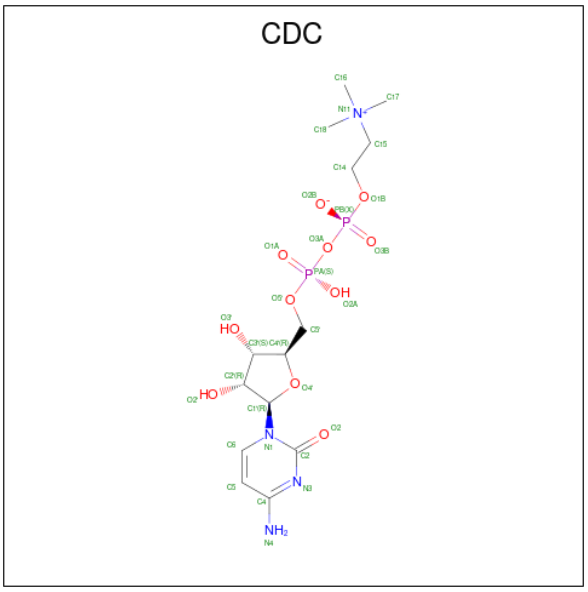
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	5	ARG	-	expression tag	UNP Q97QE9
D	6	VAL	-	expression tag	UNP Q97QE9
D	22	LEU	MET	conflict	UNP Q97QE9

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is [2-CYTIDYLATE-O'-PHOSPHONYLOXYL]-ETHYL-TRIMETHYL-AMMONIUM (three-letter code: CDC) (formula: $C_{14}H_{26}N_4O_{11}P_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O P 31 14 4 11 2	0	0
3	B	1	Total C N O P 31 14 4 11 2	0	0
3	C	1	Total C N O P 31 14 4 11 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	D	1	31	14	4	11	2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	51	51	51	0	0
			Total	O		
4	B	33	33	33	0	0
			Total	O		
4	C	50	50	50	0	0
			Total	O		
4	D	44	44	44	0	0

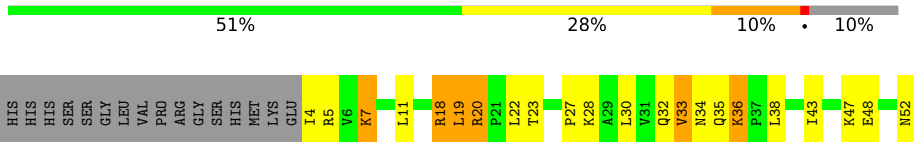
3 Residue-property plots (i)

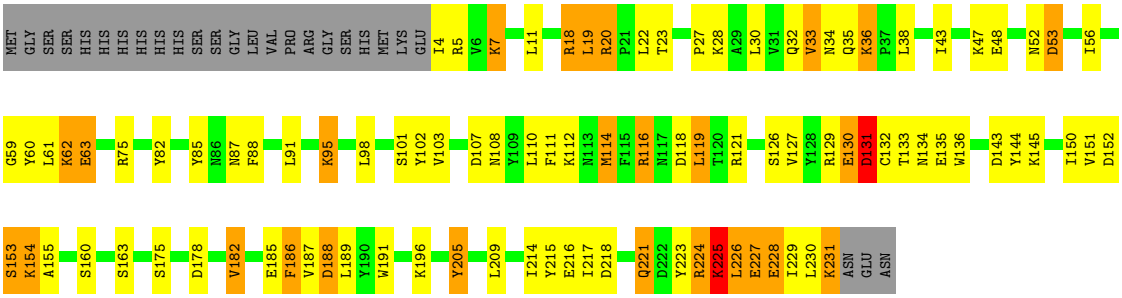
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

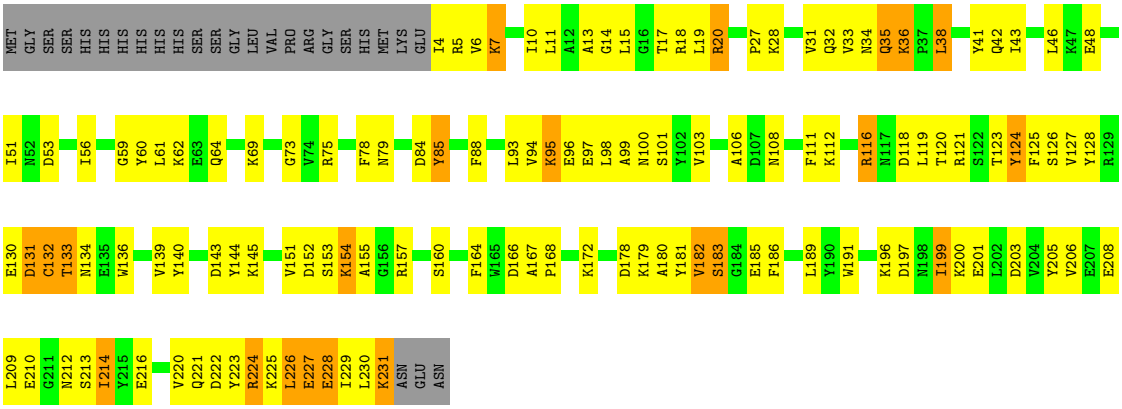
Chain A:





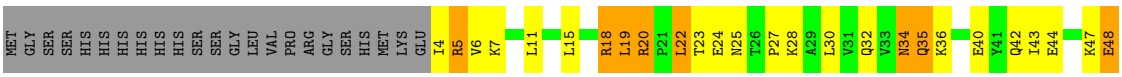
• Molecule 1: CTP:phosphocholine Cytidylyltransferase

Chain B:



• Molecule 1: CTP:phosphocholine Cytidylyltransferase

Chain C:



K49 G50 I51 N52 D53 I56 G59 Y60 L61 K62 E63 Q64 L68 K69 E70 K71 Y72 F78 K81 Y85 F88 Y89 S90 L91 Y92 L93 E97 S101 D107 N108 F111 K112 N113 M114 F115 R116 L119 T120 R121 S122 T123 Y124 F125 S126 V127 Y128 D131

C132 T133 N134 E135 W136 F137 L138 V139 Y140 I150 V151 D152 S153 K154 A155 G156 R157 S160 A170 V174 S175 F176 I177 D178 K179 V182 F186 V187 D188 L189 Y190 W191 D192 K196 D197 N198 I199 K200 E201 L202 Y205 V206 E207 E210 Y215 E216 I217 D218 S219 V220

Q221 D222 Y223 R224 K225 L226 E227 E228 I229 L230 K231 ASN GLU ASN

- Molecule 1: CTP:phosphocholine Cytidylyltransferase

Chain D: 44% 36% 9% 10%

MET GLY SER SER HIS HIS HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET LYS GLU I4 K7 A13 G14 L15 R18 L19 R20 P21 L22 T23 E24 N25 T26 P27 K28 V31 Q32 V33 N34 Q35 K36 P37 Y41 Q42 I43 K47 E48 K49 I56

G59 Y60 L61 K62 E63 L68 K69 E70 V74 R75 F78 D84 Y85 N86 N87 F88 L91 Y92 K95 E96 N100 N108 K112 N113 M114 F115 R116 N117 D118 L119 T120 R121 S122 F125 S126 V127 Y128 R129 E130 D131 C132 T133 N134 E135 W136 F137 Y140

D143 Y144 K145 D148 I149 I150 V151 D152 S153 K154 A155 G156 R157 I158 F164 W165 A170 E171 K172 I173 V174 S175 D178 K179 A180 Y181 V182 S183 F186 V187 D188 L189 Y190 W191 K196 D197 Y205 V206 E207 E208 L209 E210 S213 I214 Y215 E216 I217 D218 S219 V220 Q221

R224 K225 L226 E227 E228 I229 L230 K231 ASN GLU ASN

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	48.20Å 69.00Å 81.60Å 93.40° 92.80° 97.10°	Depositor
Resolution (Å)	20.00 – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
Refinement program	XTALVIEW	Depositor
R, R_{free}	0.208 , 0.239	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7904	wwPDB-VP
Average B, all atoms (Å^2)	36.0	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: CDC, MG

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	0.50	0/1944	0.72	0/2631
1	B	0.50	0/1933	0.73	0/2616
1	C	0.48	0/1944	0.69	0/2631
1	D	0.47	0/1933	0.72	0/2616
All	All	0.49	0/7754	0.71	0/10494

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	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	205	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	1905	0	1884	101	0
1	B	1894	0	1871	103	1
1	C	1905	0	1884	109	1
1	D	1894	0	1871	93	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	31	0	25	1	0
3	B	31	0	25	4	0
3	C	31	0	25	3	0
3	D	31	0	25	3	0
4	A	51	0	0	1	0
4	B	33	0	0	2	0
4	C	50	0	0	3	0
4	D	44	0	0	5	0
All	All	7904	0	7610	404	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 26.

The worst 5 of 404 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:231:LYS:O	1:C:231:LYS:HG2	1.63	0.99
1:A:223:TYR:O	1:A:227:GLU:HG2	1.67	0.95
1:A:116:ARG:HG3	1:A:119:LEU:HD23	1.47	0.93
1:A:28:LYS:HD3	1:A:107:ASP:HB2	1.52	0.91
1:D:225:LYS:O	1:D:228:GLU:HG3	1.71	0.91

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)
1:B:128:TYR:OH	1:C:128:TYR:OH[1_554]	2.12	0.08

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	227/254 (89%)	200 (88%)	21 (9%)	6 (3%)	5 5
1	B	226/254 (89%)	201 (89%)	21 (9%)	4 (2%)	8 10
1	C	227/254 (89%)	199 (88%)	22 (10%)	6 (3%)	5 5
1	D	226/254 (89%)	206 (91%)	15 (7%)	5 (2%)	6 7
All	All	906/1016 (89%)	806 (89%)	79 (9%)	21 (2%)	6 7

5 of 21 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	226	LEU
1	C	131	ASP
1	A	87	ASN
1	A	131	ASP
1	A	225	LYS

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	208/230 (90%)	173 (83%)	35 (17%)	2 2
1	B	207/230 (90%)	170 (82%)	37 (18%)	2 2
1	C	208/230 (90%)	173 (83%)	35 (17%)	2 2
1	D	207/230 (90%)	169 (82%)	38 (18%)	1 2
All	All	830/920 (90%)	685 (82%)	145 (18%)	2 2

5 of 145 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	33	VAL
1	D	221	GLN
1	D	62	LYS
1	D	130	GLU
1	B	112	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	32	GLN
1	C	64	GLN
1	D	134	ASN
1	C	221	GLN
1	D	64	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 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	CDC	A	1991	2	30,32,32	1.06	1 (3%)	43,49,49	1.51	8 (18%)
3	CDC	B	2991	2	30,32,32	1.06	1 (3%)	43,49,49	1.58	9 (20%)
3	CDC	C	3991	2	30,32,32	1.00	1 (3%)	43,49,49	1.43	7 (16%)
3	CDC	D	4991	2	30,32,32	1.05	1 (3%)	43,49,49	1.57	8 (18%)

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
3	CDC	A	1991	2	-	11/24/40/40	0/2/2/2
3	CDC	B	2991	2	-	10/24/40/40	0/2/2/2
3	CDC	C	3991	2	-	11/24/40/40	0/2/2/2
3	CDC	D	4991	2	-	10/24/40/40	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1991	CDC	C6-C5	2.51	1.40	1.35
3	D	4991	CDC	C6-C5	2.29	1.40	1.35
3	C	3991	CDC	C6-C5	2.22	1.40	1.35
3	B	2991	CDC	C6-C5	2.09	1.39	1.35

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	2991	CDC	O2-C2-N3	-4.96	114.26	122.33
3	A	1991	CDC	O2-C2-N3	-4.84	114.46	122.33
3	D	4991	CDC	O2-C2-N3	-4.81	114.51	122.33
3	C	3991	CDC	O2-C2-N3	-4.74	114.62	122.33
3	B	2991	CDC	C5'-C4'-C3'	-4.63	97.83	115.18

There are no chirality outliers.

5 of 42 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1991	CDC	O4'-C4'-C5'-O5'
3	A	1991	CDC	C5'-O5'-PA-O2A
3	A	1991	CDC	C5'-O5'-PA-O3A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	A	1991	CDC	O1B-C14-C15-N11
3	B	2991	CDC	O4'-C4'-C5'-O5'

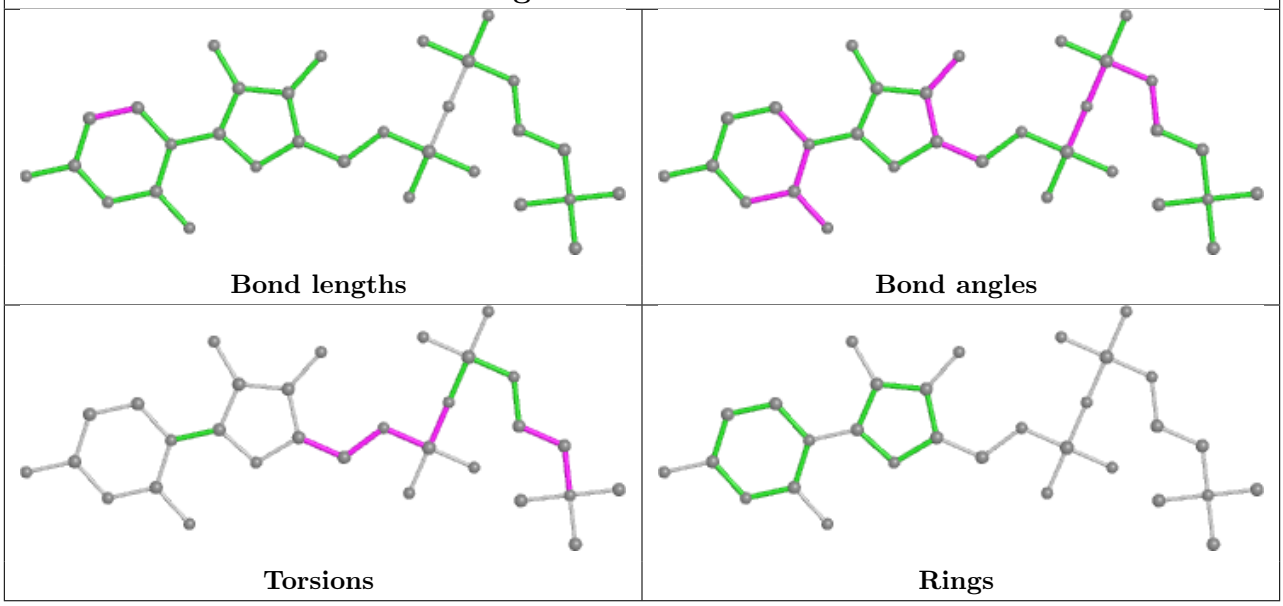
There are no ring outliers.

4 monomers are involved in 11 short contacts:

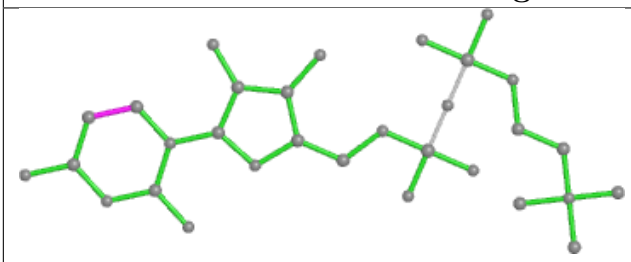
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1991	CDC	1	0
3	B	2991	CDC	4	0
3	C	3991	CDC	3	0
3	D	4991	CDC	3	0

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.

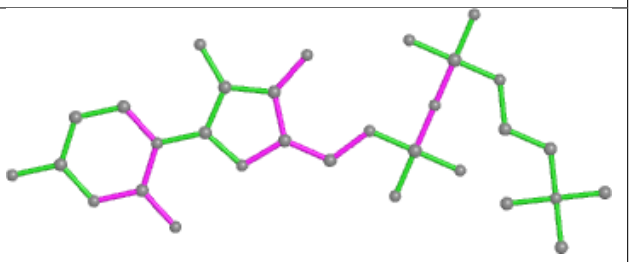
Ligand CDC A 1991



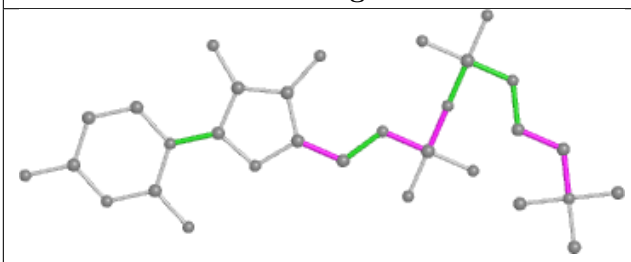
Ligand CDC B 2991



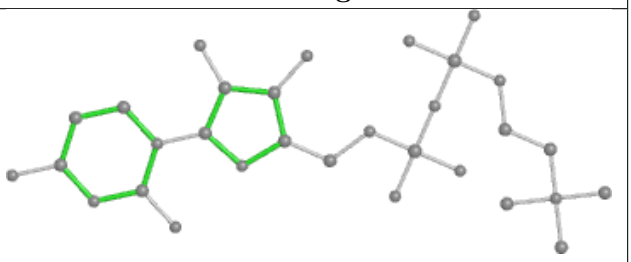
Bond lengths



Bond angles

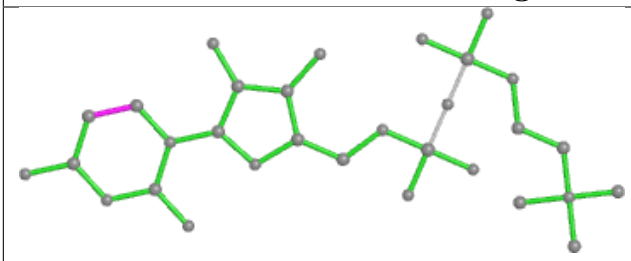


Torsions

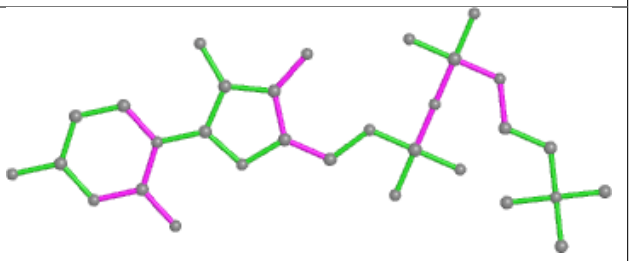


Rings

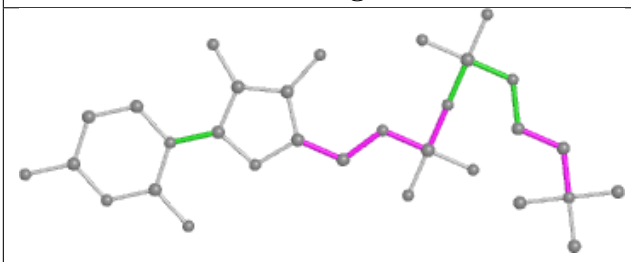
Ligand CDC C 3991



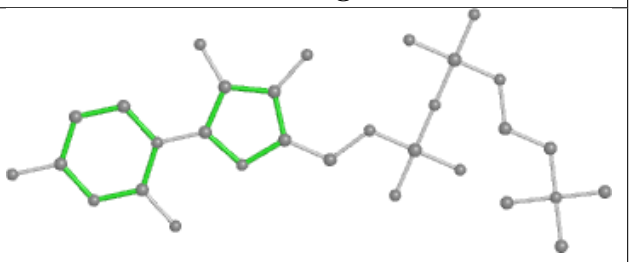
Bond lengths



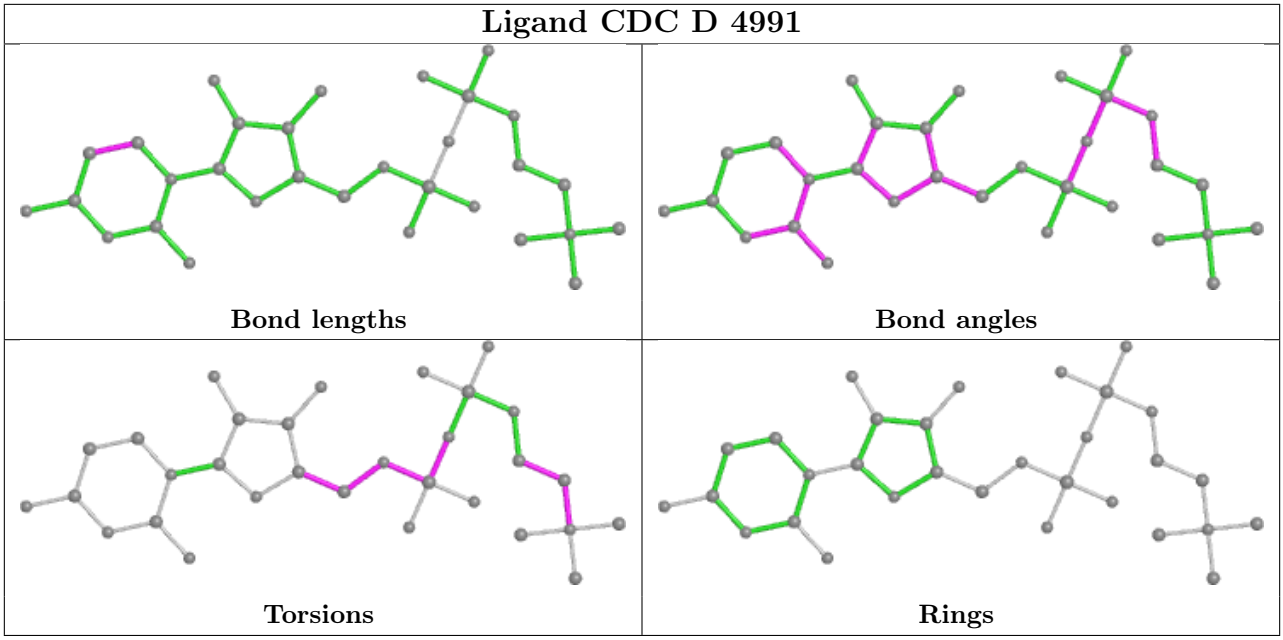
Bond angles



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 (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.