Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2023 – 02:03 AM EDT

PDB ID	:	7SFF
Title	:	Human DNMT1(729-1600) Bound to Zebularine-Containing 12mer dsDNA and Inhibitor GSK3852279B
Authors	:	Horton, J.R.; Pathuri, S.; Cheng, X.
Deposited on	:	2021-10-03
Resolution	:	2.05 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 ⓘ 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:

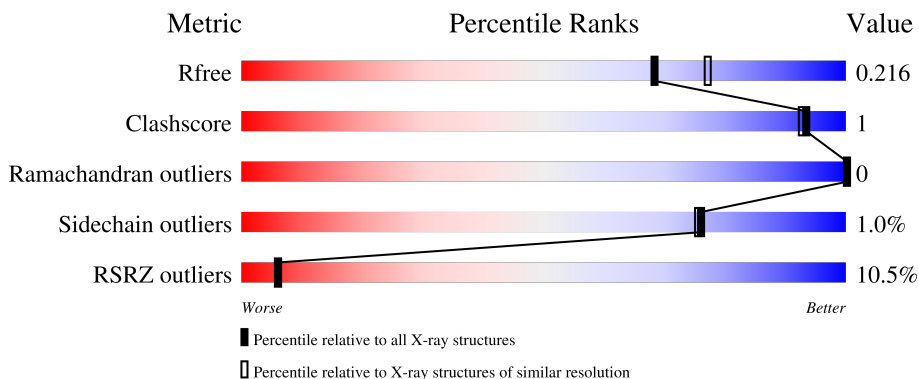|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
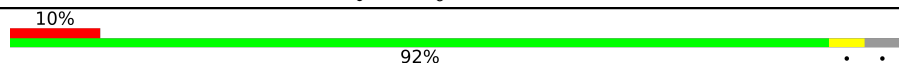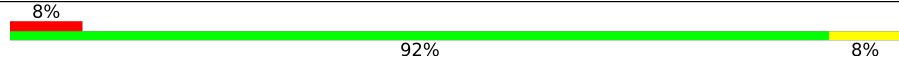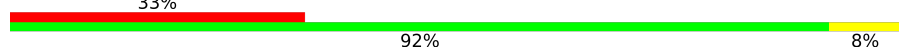*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.05 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
Rfree		0.216
Clashscore		1
Ramachandran outliers		0
Sidechain outliers		1.0%
RSRZ outliers		10.5%

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))
R_{free}	130704	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	874	10% / 92% · ·
2	C	12	8% / 92% 8%
3	D	12	33% / 92% 8%

2 Entry composition ⓘ

There are 8 unique types of molecules in this entry. The entry contains 7425 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 DNA (cytosine-5)-methyltransferase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	842	Total	C	N	O	S	0	7	0
			6518	4145	1137	1193	43			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	727	HIS	-	expression tag	UNP P26358
A	728	MET	-	expression tag	UNP P26358

- Molecule 2 is a DNA chain called DNA (12-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	12	Total	C	N	O	P	0	0	0
			244	116	47	70	11			

- Molecule 3 is a DNA chain called DNA (12-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	12	Total	C	N	O	P	0	0	0
			243	115	46	71	11			

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Zn	0	0
			2	2		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).

EDO
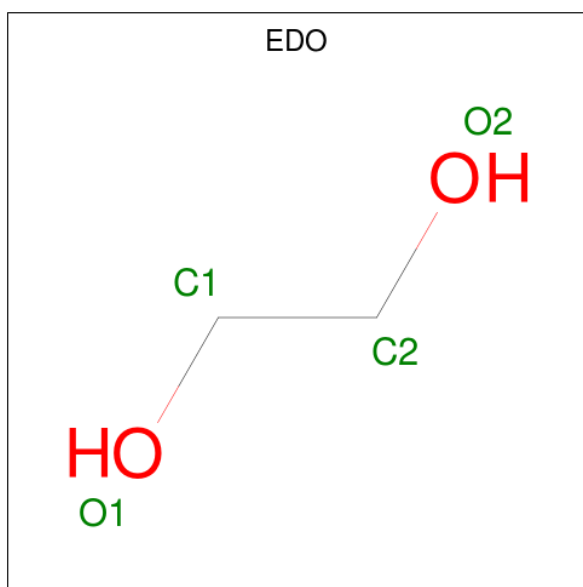
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

GOL
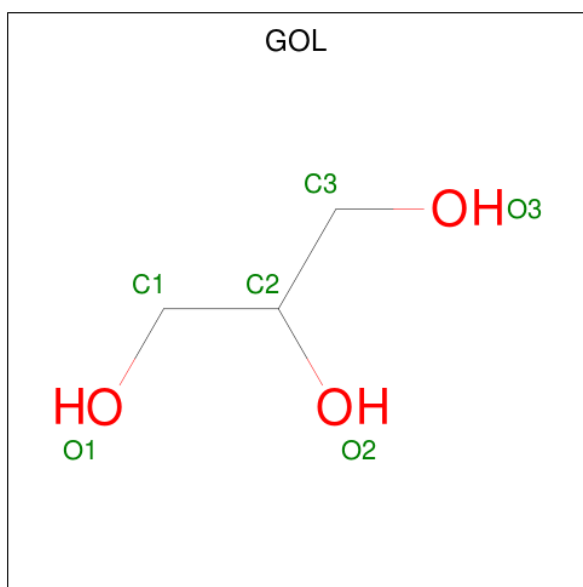
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total 6	C 3	O 3	0	0

- Molecule 7 is (2R)-2-{[6-(4-aminopiperidin-1-yl)-3,5-dicyano-4-ethylpyridin-2-yl]sulfanyl}-2-[4-(trifluoromethyl)phenyl]acetamide (three-letter code: C79) (formula: $C_{23}H_{23}F_3N_6OS$) (labeled as "Ligand of Interest" by depositor).

C79
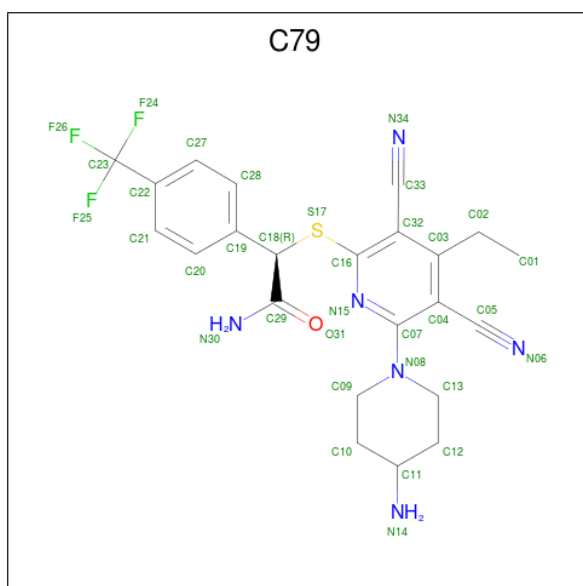
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
7	C	1	Total 34	C 23	F 3	N 6	O 1	S 1	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	344	Total 344	O 344	0	0
8	C	3	Total 3	O 3	0	0
8	D	3	Total 3	O 3	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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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.
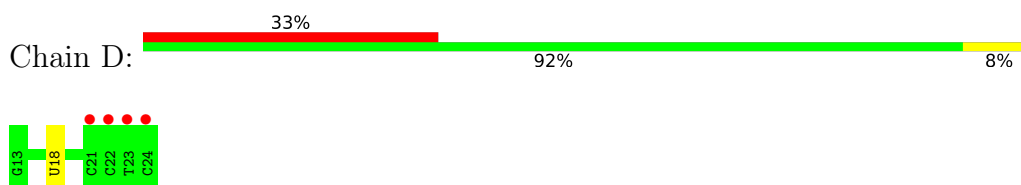
- Molecule 1: DNA (cytosine-5)-methyltransferase 1
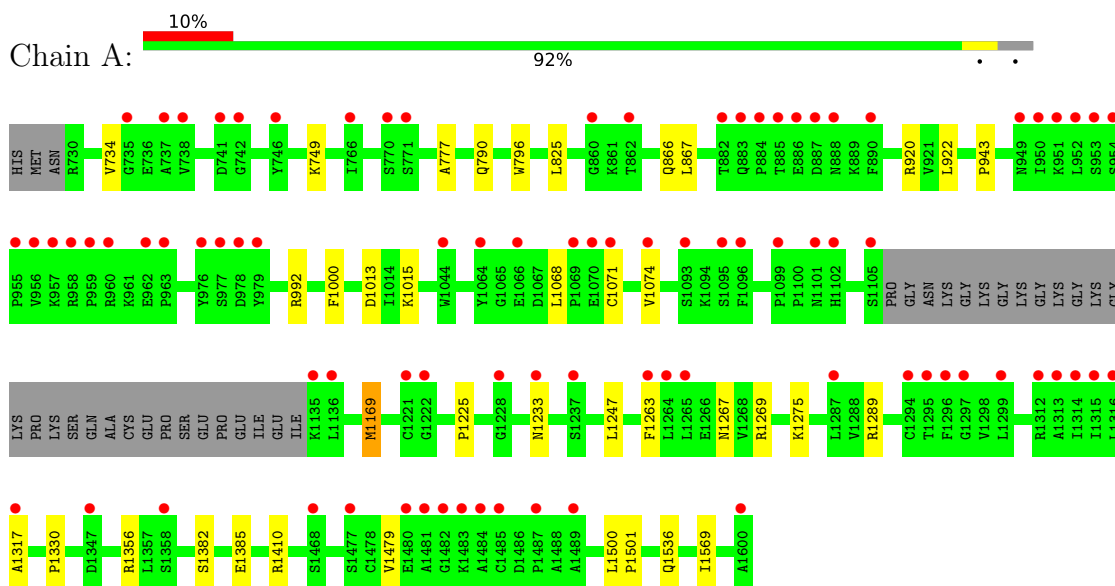
- Molecule 2: DNA (12-MER)
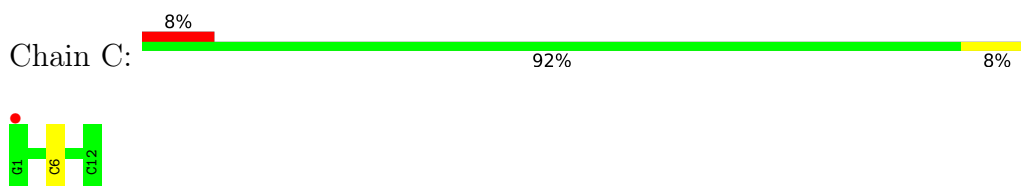
- Molecule 3: DNA (12-MER)

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	161.72Å 78.24Å 117.06Å 90.00° 125.93° 90.00°	Depositor
Resolution (Å)	38.75 – 2.05 38.75 – 2.05	Depositor EDS
% Data completeness (in resolution range)	96.8 (38.75-2.05) 96.8 (38.75-2.05)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.65 (at 2.05Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.181 , 0.217 0.181 , 0.216	Depositor DCC
R_{free} test set	1996 reflections (2.79%)	wwPDB-VP
Wilson B-factor (Å^2)	36.7	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 49.1	EDS
L-test for twinning[2]	$< \lvert L \rvert > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7425	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.38% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< \lvert L \rvert >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5   Model quality ⓘ

5.1   Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 5CM, EDO, PYO, C79, GOL

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	0.26	0/6704	0.52	0/9119
2	C	0.52	0/250	0.78	0/382
3	D	0.51	0/250	0.81	0/382
All	All	0.29	0/7204	0.54	0/9883

There are no bond length outliers.

There are no bond angle outliers.

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	6518	0	6208	19	0
2	C	244	0	137	0	0
3	D	243	0	134	0	0
4	A	2	0	0	0	0
5	A	28	0	42	3	0
6	A	6	0	8	0	0
7	C	34	0	0	0	0
8	A	344	0	0	1	0
8	C	3	0	0	0	0
8	D	3	0	0	0	0
All	All	7425	0	6529	19	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 1.

All (19) 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:1263:PHE:HB3	1:A:1317:ALA:HB3	1.81	0.62
1:A:790:GLN:HB3	1:A:825:LEU:HD12	1.82	0.61
1:A:1013:ASP:OD1	1:A:1015:LYS:NZ	2.39	0.54
1:A:1385:GLU:OE1	1:A:1410[A]:ARG:NH1	2.42	0.53
1:A:1169:MET:SD	8:A:1960:HOH:O	2.60	0.48
1:A:943:PRO:HA	1:A:992:ARG:HG2	1.96	0.48
1:A:734:VAL:HB	1:A:749:LYS:HB3	1.95	0.47
1:A:1500:LEU:HB2	1:A:1501:PRO:HD3	1.96	0.46
1:A:1225:PRO:HG2	1:A:1247:LEU:HD12	1.97	0.46
1:A:1330:PRO:HD2	1:A:1356:ARG:HB2	1.98	0.45
1:A:777:ALA:HB2	1:A:796:TRP:CE3	2.52	0.44
1:A:866:GLN:HG3	1:A:867:LEU:HG	1.98	0.44
1:A:922:LEU:HD23	1:A:1000:PHE:HB3	1.99	0.44
1:A:1569:ILE:HD12	5:A:1708:EDO:H12	2.00	0.43
1:A:1289:ARG:HA	5:A:1705:EDO:H22	2.00	0.43
1:A:1071:CYS:SG	1:A:1074:VAL:HG22	2.59	0.42
1:A:1233:ASN:O	1:A:1275:LYS:HD3	2.19	0.41
1:A:1382:SER:HA	5:A:1708:EDO:H11	2.02	0.41
1:A:1233:ASN:O	1:A:1275:LYS:HA	2.21	0.41

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	845/874 (97%)	823 (97%)	22 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	675/753 (90%)	668 (99%)	7 (1%)	76	75

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	920	ARG
1	A	1068	LEU
1	A	1169	MET
1	A	1267	ASN
1	A	1269	ARG
1	A	1479	VAL
1	A	1536	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1493	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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
3	PYO	D	18	3,2	16,20,21	1.29	2 (12%)	22,28,31	0.60	0
2	5CM	C	6	3,2	17,21,22	1.66	5 (29%)	24,30,33	1.90	8 (33%)

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	PYO	D	18	3,2	-	3/7/25/26	0/2/2/2
2	5CM	C	6	3,2	-	4/7/21/22	0/2/2/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	18	PYO	C2-N1	3.58	1.47	1.40
2	C	6	5CM	O2-C2	-3.55	1.17	1.23
2	C	6	5CM	C2-N1	3.45	1.47	1.40
2	C	6	5CM	C6-C5	2.63	1.38	1.34
3	D	18	PYO	O2-C2	-2.61	1.18	1.23
2	C	6	5CM	C4-N3	2.36	1.38	1.34
2	C	6	5CM	C6-N1	2.09	1.41	1.38

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	6	5CM	O4'-C1'-N1	3.77	114.60	107.86
2	C	6	5CM	C6-N1-C2	-3.48	116.06	120.87
2	C	6	5CM	C1'-N1-C2	3.45	123.80	117.74
2	C	6	5CM	C5A-C5-C6	-3.24	118.53	122.85
2	C	6	5CM	C4-N3-C2	-3.14	116.44	120.69
2	C	6	5CM	N1-C2-N3	2.63	123.59	118.81
2	C	6	5CM	C5-C6-N1	-2.32	120.95	123.34
2	C	6	5CM	O2-C2-N3	-2.17	118.81	122.33

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	18	PYO	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
3	D	18	PYO	C3'-C4'-C5'-O5'
2	C	6	5CM	C2'-C1'-N1-C6
2	C	6	5CM	O4'-C1'-N1-C6
2	C	6	5CM	O4'-C1'-N1-C2
2	C	6	5CM	C2'-C1'-N1-C2
3	D	18	PYO	C4'-C5'-O5'-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 11 ligands modelled in this entry, 2 are monoatomic - leaving 9 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	EDO	A	1705	-	3,3,3	0.50	0	2,2,2	0.22	0
5	EDO	A	1703	-	3,3,3	0.52	0	2,2,2	0.22	0
7	C79	C	101	-	35,36,36	0.77	1 (2%)	44,52,52	1.01	0
6	GOL	A	1710	-	5,5,5	1.11	0	5,5,5	0.80	0
5	EDO	A	1706	-	3,3,3	0.50	0	2,2,2	0.27	0
5	EDO	A	1704	-	3,3,3	0.50	0	2,2,2	0.25	0
5	EDO	A	1708	-	3,3,3	0.48	0	2,2,2	0.21	0
5	EDO	A	1709	-	3,3,3	0.42	0	2,2,2	0.47	0
5	EDO	A	1707	-	3,3,3	0.46	0	2,2,2	0.35	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
5	EDO	A	1705	-	-	1/1/1/1	-
5	EDO	A	1703	-	-	1/1/1/1	-
7	C79	C	101	-	-	1/24/38/38	0/3/3/3
6	GOL	A	1710	-	-	2/4/4/4	-
5	EDO	A	1706	-	-	0/1/1/1	-
5	EDO	A	1704	-	-	0/1/1/1	-
5	EDO	A	1708	-	-	0/1/1/1	-
5	EDO	A	1709	-	-	0/1/1/1	-
5	EDO	A	1707	-	-	0/1/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	101	C79	C32-C03	-2.38	1.38	1.40

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1710	GOL	O1-C1-C2-C3
6	A	1710	GOL	O1-C1-C2-O2
7	C	101	C79	S17-C18-C29-O31
5	A	1703	EDO	O1-C1-C2-O2
5	A	1705	EDO	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1705	EDO	1	0
5	A	1708	EDO	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 C79 C 101

Bond lengths

Bond angles

Torsions

Rings
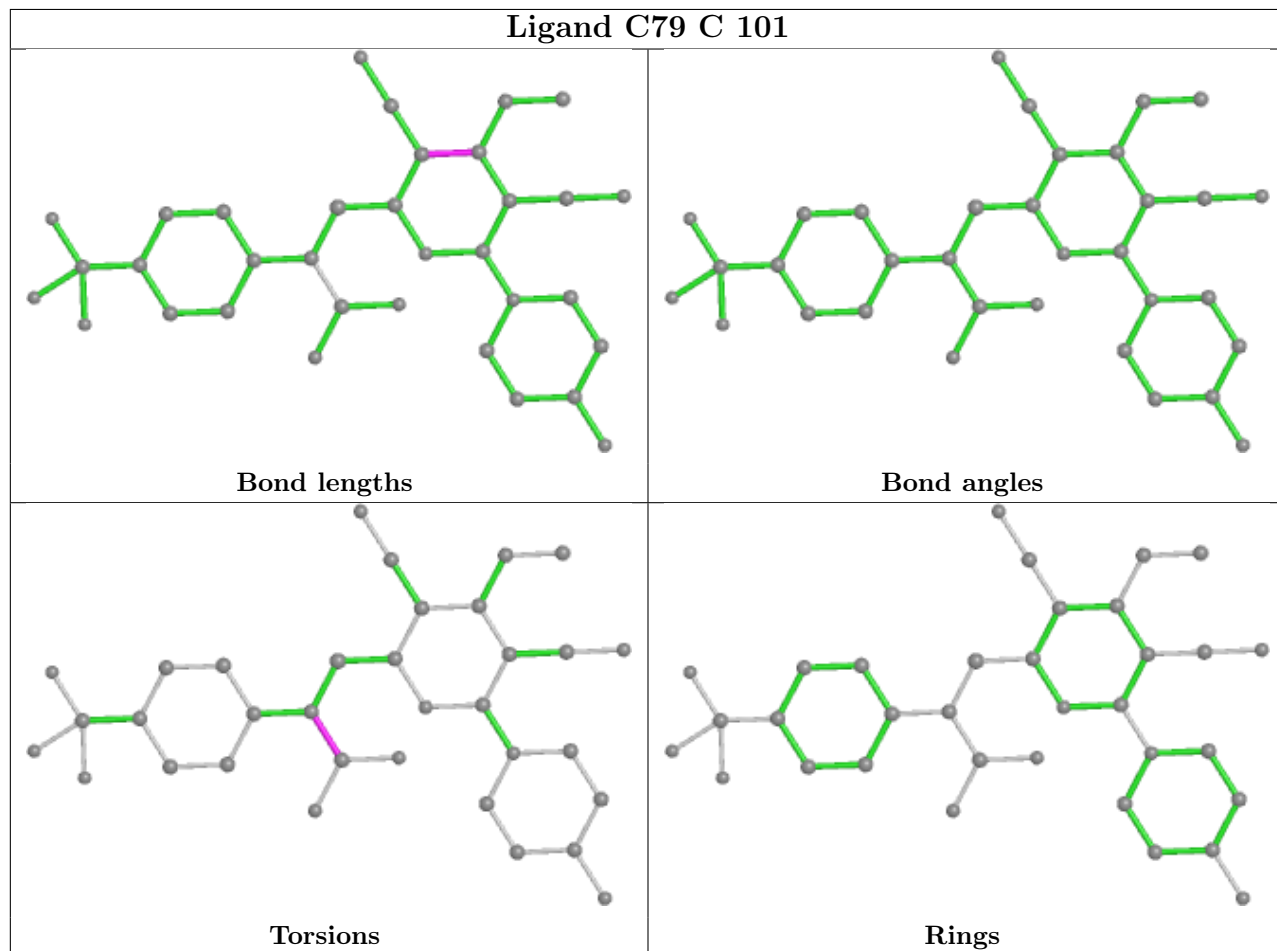
5.7 Other polymers ⓘ

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 ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	842/874 (96%)	0.49	86 (10%)	6	7	23, 47, 94, 159	0
2	C	11/12 (91%)	0.90	1 (9%)	9	9	73, 89, 156, 177	0
3	D	11/12 (91%)	1.58	4 (36%)	0	0	75, 87, 149, 174	0
All	All	864/898 (96%)	0.51	91 (10%)	6	6	23, 48, 100, 177	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	956	VAL	10.2
1	A	955	PRO	9.3
1	A	959	PRO	8.4
1	A	953	SER	8.0
1	A	957	LYS	7.8
1	A	952	LEU	7.3
1	A	954	SER	6.9
1	A	951	LYS	6.9
1	A	1481	ALA	6.4
1	A	885	THR	6.3
1	A	960	ARG	6.1
1	A	958	ARG	5.9
1	A	737	ALA	5.7
1	A	771	SER	5.3
1	A	884	PRO	5.0
1	A	976	TYR	4.7
1	A	1600	ALA	4.6
1	A	738	VAL	4.5
1	A	1101	ASN	4.4
1	A	1136	LEU	4.3
1	A	890	PHE	4.3
1	A	883	GLN	4.3
2	C	1	DG	4.3

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Mol	Chain	Res	Type	RSRZ
3	D	24	DC	4.2
1	A	1044	TRP	4.1
1	A	860	GLY	4.1
1	A	963	PRO	4.0
1	A	1096	PHE	4.0
1	A	1069	PRO	3.9
1	A	886	GLU	3.9
1	A	979	TYR	3.9
1	A	1482	GLY	3.8
1	A	741	ASP	3.8
1	A	1264	LEU	3.8
1	A	1485	CYS	3.7
1	A	1071	CYS	3.7
3	D	22	DC	3.6
1	A	742	GLY	3.4
1	A	1265	LEU	3.4
1	A	1135	LYS	3.3
1	A	1093	SER	3.3
1	A	1487	PRO	3.3
3	D	23	DT	3.2
1	A	887	ASP	3.2
1	A	978	ASP	3.2
1	A	1315	ILE	3.2
1	A	1480	GLU	3.1
1	A	1064	TYR	3.1
1	A	1102	HIS	3.0
1	A	1314	ILE	3.0
3	D	21	DC	3.0
1	A	1099	PRO	3.0
1	A	862	THR	2.9
1	A	1066	GLU	2.9
1	A	735	GLY	2.8
1	A	1233	ASN	2.8
1	A	1489	ALA	2.8
1	A	1237	SER	2.8
1	A	1347	ASP	2.7
1	A	1358	SER	2.6
1	A	1299	LEU	2.6
1	A	882	THR	2.6
1	A	770	SER	2.5
1	A	1313	ALA	2.5
1	A	949	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	1222	GLY	2.5
1	A	1317	ALA	2.4
1	A	1484	ALA	2.4
1	A	1477	SER	2.4
1	A	1312[A]	ARG	2.4
1	A	1074	VAL	2.4
1	A	746	TYR	2.4
1	A	1483	LYS	2.3
1	A	950	ILE	2.3
1	A	977	SER	2.3
1	A	888	ASN	2.3
1	A	1295	THR	2.3
1	A	1095	SER	2.3
1	A	1263	PHE	2.2
1	A	1316	LEU	2.2
1	A	1296	PHE	2.2
1	A	1468	SER	2.1
1	A	766	ILE	2.1
1	A	1287	LEU	2.1
1	A	1105	SER	2.1
1	A	962	GLU	2.1
1	A	1228	GLY	2.1
1	A	1294	CYS	2.1
1	A	1221	CYS	2.0
1	A	1070	GLU	2.0
1	A	1297	GLY	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

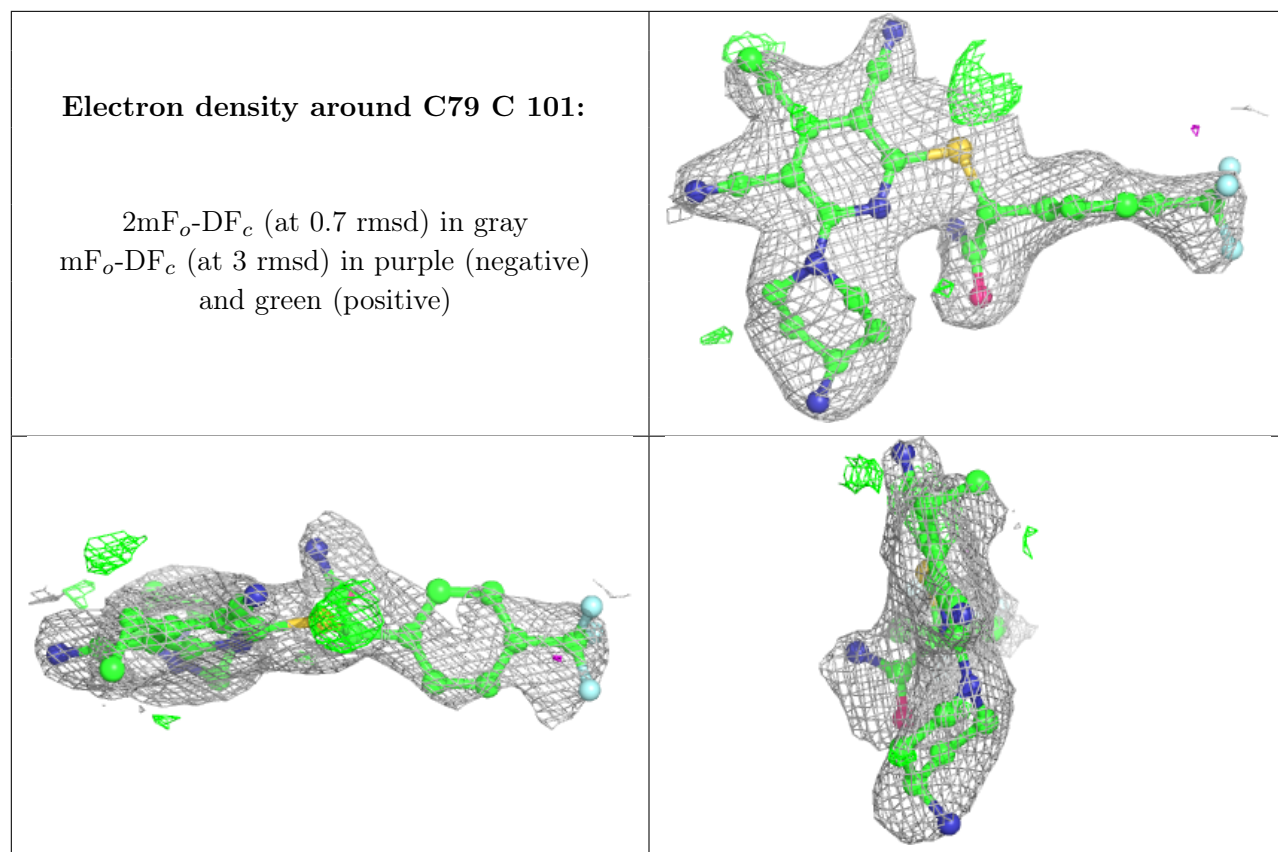| Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
3	PYO	D	18	19/20	0.82	0.16	79,95,110,120	0
2	5CM	C	6	20/21	0.93	0.11	57,67,75,75	0

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	EDO	A	1705	4/4	0.66	0.24	47,56,57,66	0
5	EDO	A	1706	4/4	0.77	0.20	52,62,64,70	0
6	GOL	A	1710	6/6	0.85	0.20	39,49,61,62	0
7	C79	C	101	34/34	0.85	0.20	63,79,117,122	0
5	EDO	A	1704	4/4	0.88	0.14	44,45,47,56	0
5	EDO	A	1703	4/4	0.89	0.17	38,41,47,54	0
5	EDO	A	1707	4/4	0.92	0.16	43,51,51,55	0
5	EDO	A	1709	4/4	0.93	0.17	34,49,49,60	0
5	EDO	A	1708	4/4	0.94	0.26	47,47,51,56	0
4	ZN	A	1701	1/1	0.95	0.04	72,72,72,72	0
4	ZN	A	1702	1/1	0.98	0.05	45,45,45,45	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around C79 C 101:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

6.5 Other polymers (i)

There are no such residues in this entry.