



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:49 AM UTC

PDB ID : 6X9J / pdb_00006x9j
Title : Human DNMT1(729-1600) Bound to Zebularine-Containing 12mer dsDNA and Inhibitor GSK3830052
Authors : Pathuri, S.; Horton, J.R.; Cheng, X.
Deposited on : 2020-06-02
Resolution : 1.79 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

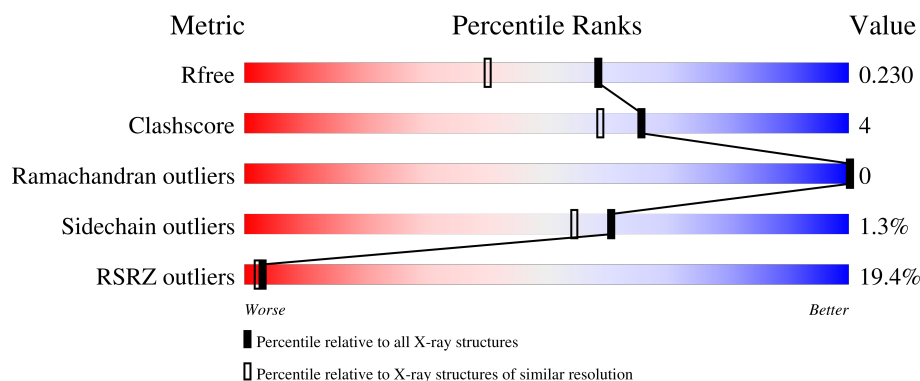
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.79 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))
R_{free}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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 $\leq 5\%$. 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	18% 88% 7% • •
2	C	12	8% 58% 42%
3	D	12	58% 33% 8%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7497 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	6	0
			6518	4139	1136	1200	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 (5'-D(*GP*AP*GP*GP*CP*(5CM)P*GP*CP*CP*TP*GP*C)-3').

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 (5'-D(*GP*CP*AP*GP*G)-R(P*(PYO))-D(P*GP*GP*CP*CP*TP*C)-3').

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 (CCD ID: ZN) (formula: Zn).

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

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



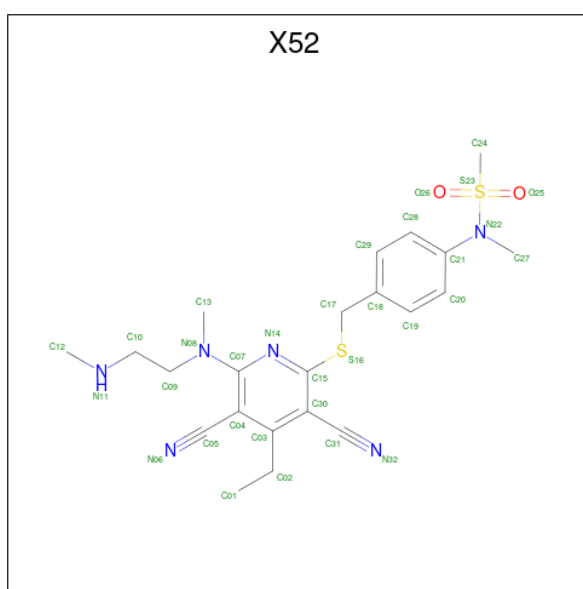
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total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

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

- Molecule 6 is N-(4-{[(3,5-dicyano-4-ethyl-6-{methyl[2-(methylamino)ethyl]amino}pyridin-2-yl)sulfanyl]methyl}phenyl)-N-methylmethanesulfonamide (CCD ID: X52) (formula: C₂₂H₂₈N₆O₂S₂) (labeled as "Ligand of Interest" by depositor).

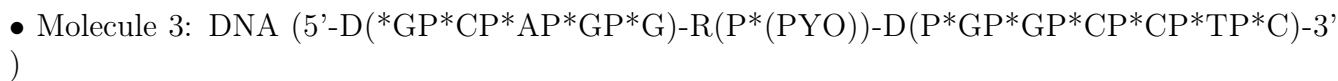


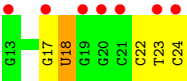
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	D	1	Total	C	N	O	S	0	0
			32	22	6	2	2		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	381	Total	O	0	0
			381	381		
7	C	4	Total	O	0	0
			4	4		
7	D	5	Total	O	0	0
			5	5		

- Molecule 1: DNA (cytosine-5)-methyltransferase 1





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	160.06Å 77.77Å 116.72Å 90.00° 125.35° 90.00°	Depositor
Resolution (Å)	34.92 – 1.79 34.92 – 1.79	Depositor EDS
% Data completeness (in resolution range)	94.2 (34.92-1.79) 94.2 (34.92-1.79)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.32 (at 1.79Å)	Xtriage
Refinement program	PHENIX 1.17.1 _3660	Depositor
R, R_{free}	0.200 , 0.229 0.201 , 0.230	Depositor DCC
R_{free} test set	2000 reflections (1.82%)	wwPDB-VP
Wilson B-factor (Å ²)	33.2	Xtriage
Anisotropy	0.129	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 54.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7497	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.69% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: PYO, X52, 5CM, EDO, 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	0.20	0/6704	0.43	0/9120
2	C	0.24	0/250	0.49	0/382
3	D	0.27	0/250	0.49	0/382
All	All	0.20	0/7204	0.44	0/9884

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	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1098	ASP	Peptide
1	A	752	ILE	Peptide

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	6187	46	0
2	C	244	0	137	4	0
3	D	243	0	134	5	0
4	A	2	0	0	0	0
5	A	64	0	96	2	0
5	C	4	0	6	1	0
6	D	32	0	0	2	0
7	A	381	0	0	1	0
7	C	4	0	0	0	0
7	D	5	0	0	0	0
All	All	7497	0	6560	52	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 4.

All (52) 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:1088:ALA:HB3	1:A:1098:ASP:H	1.46	0.78
1:A:1443:GLU:HA	1:A:1452:ALA:O	1.86	0.75
1:A:1535[A]:LYS:HD3	1:A:1536:GLN:HG2	1.73	0.71
1:A:885:THR:HG22	1:A:887:ASP:H	1.57	0.69
1:A:998:GLU:HB2	1:A:1017:ARG:HB3	1.81	0.62
1:A:1169[A]:MET:HE3	1:A:1169[A]:MET:H	1.62	0.62
1:A:1476:CYS:SG	1:A:1478:CYS:HB2	2.41	0.61
1:A:790:GLN:HB3	1:A:825:LEU:HD12	1.83	0.61
3:D:23:DT:H4'	3:D:24:DC:OP1	2.01	0.60
1:A:1385:GLU:OE2	1:A:1410:ARG:NH1	2.36	0.59
1:A:1207[B]:ARG:NH1	7:A:1805:HOH:O	2.35	0.59
1:A:1457:TYR:CD2	1:A:1472:LEU:HB2	2.40	0.57
1:A:777:ALA:HB2	1:A:796:TRP:CE3	2.41	0.56
1:A:1088:ALA:O	1:A:1096:PHE:HA	2.06	0.55
1:A:1145:PHE:HD1	1:A:1169[A]:MET:HE1	1.73	0.53
3:D:22:DC:H2''	3:D:23:DT:C6	2.43	0.53
3:D:17:DG:H2''	3:D:18:PYO:H5'	1.89	0.53
1:A:1500:LEU:HB2	1:A:1501:PRO:HD3	1.93	0.50
1:A:752:ILE:HG22	1:A:753:ASP:H	1.77	0.49
1:A:1263:PHE:HB3	1:A:1317:ALA:HB3	1.96	0.48
1:A:1195:LEU:HG	1:A:1199:MET:HE2	1.96	0.48
1:A:1467:SER:OG	1:A:1471:ALA:N	2.45	0.48
1:A:1004:LYS:C	1:A:1006:ASN:H	2.21	0.47
1:A:1154:GLY:HA3	1:A:1585:ALA:HB3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1506:ARG:HH12	2:C:7:DG:P	2.37	0.47
1:A:1270:ASN:N	3:D:18:PYO:OP1	2.45	0.47
1:A:1004:LYS:HD3	1:A:1006:ASN:HD21	1.80	0.46
1:A:1519:TRP:CH2	5:A:1708:EDO:H12	2.50	0.46
1:A:835:ILE:O	1:A:864:PHE:HA	2.14	0.46
1:A:1092:LYS:N	1:A:1092:LYS:HD2	2.31	0.45
1:A:885:THR:H	1:A:888:ASN:HB2	1.81	0.45
1:A:1015:LYS:C	1:A:1016:ILE:HD12	2.41	0.45
1:A:1392:PRO:HG3	1:A:1401:ARG:HD2	1.98	0.45
1:A:981:LYS:HE2	1:A:981:LYS:HB2	1.75	0.44
1:A:1506:ARG:NH1	2:C:7:DG:OP2	2.51	0.44
1:A:1004:LYS:C	1:A:1006:ASN:N	2.75	0.43
1:A:1415:LYS:HG2	5:C:4201:EDO:H12	2.01	0.43
2:C:1:DG:H2"	2:C:2:DA:C8	2.54	0.43
1:A:1091:ALA:C	1:A:1092:LYS:HD2	2.45	0.42
2:C:3:DG:N2	3:D:23:DT:O2	2.53	0.42
1:A:1232:MET:HE1	1:A:1273[B]:SER:HB3	2.00	0.42
1:A:1461:ASP:HA	1:A:1479:VAL:CG1	2.50	0.42
1:A:1426:ARG:HG3	1:A:1545:HIS:CD2	2.55	0.42
6:D:101:X52:C13	6:D:101:X52:C05	2.98	0.41
1:A:1491:GLN:HE21	1:A:1491:GLN:HB2	1.64	0.41
1:A:1535[A]:LYS:HD2	6:D:101:X52:N32	2.35	0.41
1:A:943:PRO:HA	1:A:992:ARG:HG2	2.03	0.41
1:A:1142:LEU:HD13	1:A:1165:TRP:HB2	2.03	0.41
1:A:1138:LYS:HD2	1:A:1162:ASP:CG	2.46	0.40
1:A:873:TYR:HE2	5:A:1716:EDO:H11	1.87	0.40
1:A:1187:PHE:HB3	1:A:1194:LEU:HD11	2.04	0.40

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	844/874 (97%)	816 (97%)	28 (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	676/753 (90%)	665 (98%)	11 (2%)	55	47

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	790	GLN
1	A	1045	SER
1	A	1063	GLU
1	A	1092	LYS
1	A	1169[A]	MET
1	A	1169[B]	MET
1	A	1267	ASN
1	A	1475	VAL
1	A	1478	CYS
1	A	1535[A]	LYS
1	A	1535[B]	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	829	HIS
1	A	972	HIS

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	1.30	2 (12%)	21,28,31	0.63	0
2	5CM	C	6	3,2	18,21,22	1.69	5 (27%)	24,30,33	1.92	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	-	2/7/25/26	0/2/2/2
2	5CM	C	6	3,2	-	2/7/21/22	0/2/2/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	6	5CM	C2-N1	3.66	1.47	1.40
2	C	6	5CM	O2-C2	-3.51	1.17	1.23
3	D	18	PYO	C2-N1	3.38	1.47	1.40
2	C	6	5CM	C6-C5	2.78	1.39	1.34
3	D	18	PYO	O2-C2	-2.62	1.18	1.23
2	C	6	5CM	C4-N3	2.30	1.37	1.34
2	C	6	5CM	C6-N1	2.24	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	5.21	117.11	107.86
2	C	6	5CM	C6-N1-C2	-3.36	116.47	120.95
2	C	6	5CM	C1'-N1-C2	3.31	123.51	117.83
2	C	6	5CM	C5A-C5-C6	-3.03	118.75	122.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	6	5CM	C4-N3-C2	-2.27	117.66	120.81
2	C	6	5CM	O2-C2-N3	-2.22	118.83	122.33
2	C	6	5CM	N1-C2-N3	2.12	122.49	118.80
2	C	6	5CM	C5-C6-N1	-2.12	121.01	123.31

There are no chirality outliers.

All (4) torsion outliers are listed below:

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

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	18	PYO	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 2 are monoatomic - leaving 18 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	1703	-	3,3,3	0.50	0	2,2,2	0.18	0
5	EDO	A	1705	-	3,3,3	0.41	0	2,2,2	0.55	0
5	EDO	A	1704	-	3,3,3	0.45	0	2,2,2	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	EDO	A	1713	-	3,3,3	0.43	0	2,2,2	0.37	0
5	EDO	A	1714	-	3,3,3	0.41	0	2,2,2	0.43	0
5	EDO	A	1715	-	3,3,3	0.44	0	2,2,2	0.34	0
5	EDO	A	1716	-	3,3,3	0.42	0	2,2,2	0.34	0
5	EDO	A	1706	-	3,3,3	0.43	0	2,2,2	0.60	0
5	EDO	C	4201	-	3,3,3	0.48	0	2,2,2	0.21	0
5	EDO	A	1711	-	3,3,3	0.46	0	2,2,2	0.34	0
5	EDO	A	1709	-	3,3,3	0.43	0	2,2,2	0.39	0
5	EDO	A	1717	-	3,3,3	0.44	0	2,2,2	0.37	0
5	EDO	A	1712	-	3,3,3	0.40	0	2,2,2	0.37	0
5	EDO	A	1710	-	3,3,3	0.41	0	2,2,2	0.44	0
6	X52	D	101	-	31,33,33	0.90	2 (6%)	37,46,46	0.82	0
5	EDO	A	1707	-	3,3,3	0.43	0	2,2,2	0.30	0
5	EDO	A	1708	-	3,3,3	0.43	0	2,2,2	0.30	0
5	EDO	A	1718	-	3,3,3	0.42	0	2,2,2	0.41	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	1703	-	-	0/1/1/1	-
5	EDO	A	1705	-	-	1/1/1/1	-
5	EDO	A	1704	-	-	0/1/1/1	-
5	EDO	A	1713	-	-	0/1/1/1	-
5	EDO	A	1714	-	-	0/1/1/1	-
5	EDO	A	1715	-	-	0/1/1/1	-
5	EDO	A	1716	-	-	1/1/1/1	-
5	EDO	A	1706	-	-	0/1/1/1	-
5	EDO	C	4201	-	-	0/1/1/1	-
5	EDO	A	1711	-	-	0/1/1/1	-
5	EDO	A	1709	-	-	0/1/1/1	-
5	EDO	A	1717	-	-	0/1/1/1	-
5	EDO	A	1712	-	-	0/1/1/1	-
5	EDO	A	1710	-	-	0/1/1/1	-
6	X52	D	101	-	-	6/27/29/29	0/2/2/2
5	EDO	A	1707	-	-	0/1/1/1	-
5	EDO	A	1708	-	-	0/1/1/1	-
5	EDO	A	1718	-	-	0/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	101	X52	C30-C03	-3.20	1.37	1.40
6	D	101	X52	C04-C03	-2.19	1.38	1.40

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

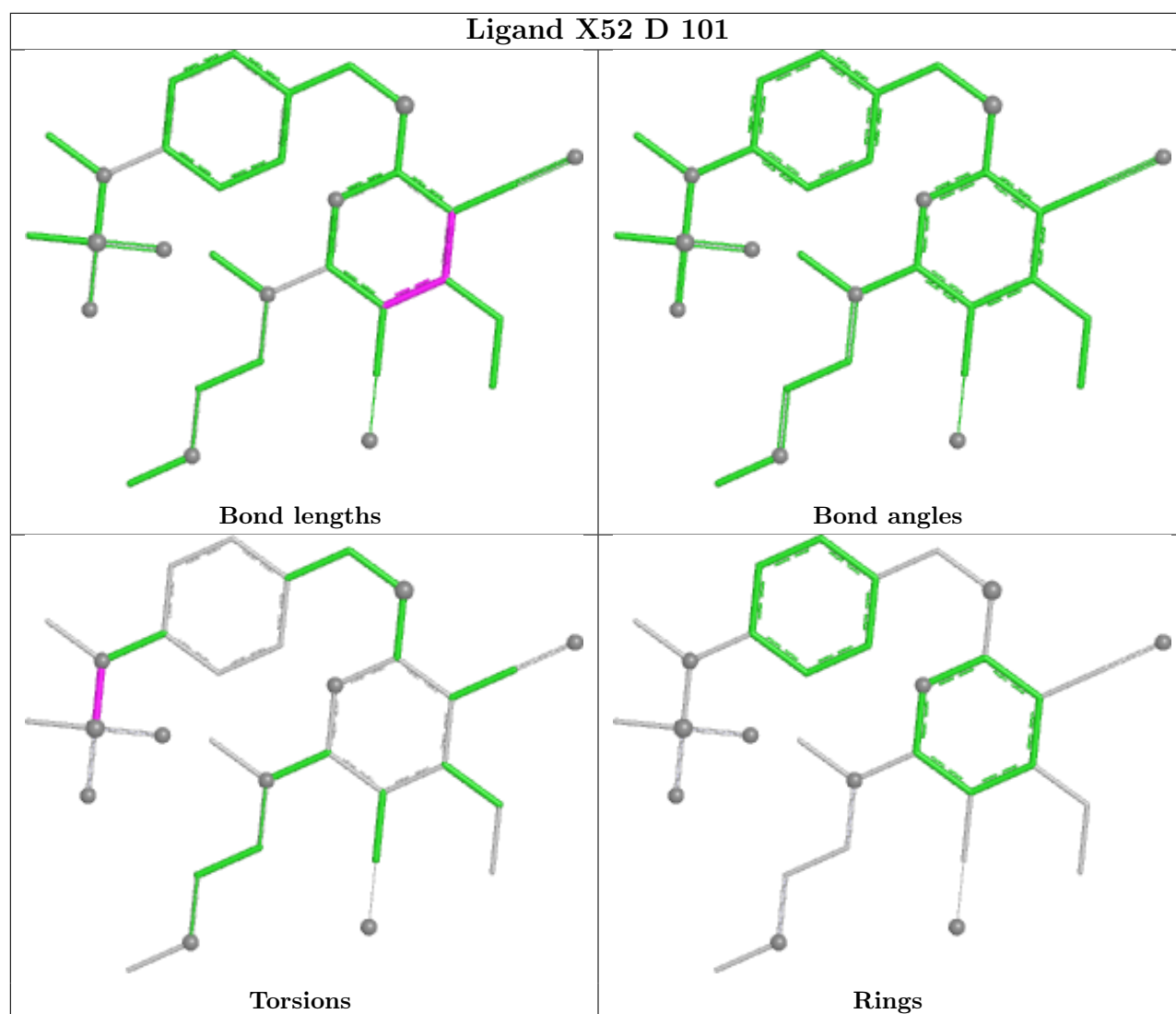
Mol	Chain	Res	Type	Atoms
6	D	101	X52	C21-N22-S23-C24
6	D	101	X52	C21-N22-S23-O25
6	D	101	X52	C21-N22-S23-O26
6	D	101	X52	C27-N22-S23-C24
6	D	101	X52	C27-N22-S23-O26
6	D	101	X52	C27-N22-S23-O25
5	A	1705	EDO	O1-C1-C2-O2
5	A	1716	EDO	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1716	EDO	1	0
5	C	4201	EDO	1	0
6	D	101	X52	2	0
5	A	1708	EDO	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 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 ⓘ

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(Å ²)	Q<0.9
1	A	842/874 (96%)	0.87	160 (19%) 3 2	17, 47, 106, 150	6 (0%)
2	C	11/12 (91%)	1.23	1 (9%) 15 13	76, 84, 141, 177	0
3	D	11/12 (91%)	2.00	7 (63%) 0 0	75, 99, 220, 228	0
All	All	864/898 (96%)	0.88	168 (19%) 3 2	17, 47, 109, 228	6 (0%)

All (168) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	950	ILE	7.0
1	A	1457	TYR	7.0
1	A	979	TYR	6.0
1	A	1489	ALA	5.8
1	A	1099	PRO	5.6
1	A	1044	TRP	5.5
1	A	1475	VAL	5.3
1	A	1096	PHE	5.1
1	A	1492	PHE	4.9
1	A	959	PRO	4.8
1	A	952	LEU	4.7
1	A	955	PRO	4.6
1	A	1100	PRO	4.6
1	A	980	ILE	4.5
1	A	1098	ASP	4.5
1	A	1005	SER	4.5
1	A	1490	ARG	4.5
1	A	1103	ALA	4.5
1	A	976	TYR	4.4
1	A	1478	CYS	4.3
1	A	1481	ALA	4.2
1	A	1479	VAL	4.2
1	A	1091	ALA	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	1484	ALA	4.0
1	A	956	VAL	3.7
1	A	954	SER	3.7
1	A	1502	HIS	3.7
1	A	982	GLY	3.7
1	A	1064	TYR	3.7
1	A	731	ILE	3.6
1	A	1476	CYS	3.6
1	A	1102	HIS	3.6
1	A	1491	GLN	3.5
1	A	1488	ALA	3.5
1	A	967	ASP	3.4
1	A	981	LYS	3.4
1	A	1498	TRP	3.4
1	A	754	ALA	3.3
1	A	1455	LEU	3.3
1	A	1472	LEU	3.3
1	A	1085	PHE	3.3
1	A	1068	LEU	3.3
1	A	960	ARG	3.3
1	A	1462	ARG	3.3
1	A	1470	GLY	3.2
1	A	1030	SER	3.2
1	A	1468	SER	3.2
1	A	890	PHE	3.2
1	A	882	THR	3.1
1	A	738	VAL	3.1
3	D	19	DG	3.1
1	A	1136	LEU	3.1
1	A	1503	THR	3.1
1	A	1043	TYR	3.1
1	A	1067	ASP	3.1
1	A	1460	HIS	3.0
1	A	884	PRO	3.0
1	A	1069	PRO	3.0
1	A	1487	PRO	3.0
1	A	1097	GLU	3.0
1	A	1022	TYR	3.0
1	A	1092	LYS	3.0
1	A	1499	CYS	3.0
1	A	1101	ASN	3.0
1	A	1095	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	1086	LEU	2.9
1	A	752	ILE	2.9
1	A	907	ILE	2.9
1	A	963	PRO	2.9
1	A	1469	SER	2.9
1	A	729	ASN	2.9
1	A	964	VAL	2.9
1	A	1089	TYR	2.9
1	A	1474	GLY	2.9
1	A	1090	ASN	2.9
1	A	860	GLY	2.8
1	A	1021	PHE	2.8
1	A	734	VAL	2.8
1	A	1007	GLY	2.8
1	A	1088	ALA	2.7
1	A	1072	VAL	2.7
1	A	917	LEU	2.7
1	A	766	ILE	2.7
1	A	1459	HIS	2.7
1	A	953	SER	2.7
1	A	773	PRO	2.7
1	A	1071	CYS	2.7
1	A	1458	THR	2.7
1	A	1494	THR	2.7
1	A	1471	ALA	2.7
1	A	1029	LYS	2.6
1	A	849	MET	2.6
1	A	922	LEU	2.6
1	A	741	ASP	2.6
1	A	1480	GLU	2.6
1	A	772	LYS	2.6
1	A	958	ARG	2.6
1	A	887	ASP	2.6
1	A	1046	ASP	2.6
3	D	24	DC	2.6
1	A	1600	ALA	2.6
1	A	1066	GLU	2.6
1	A	948	PHE	2.6
1	A	1467	SER	2.6
1	A	1006	ASN	2.6
1	A	1065	GLY	2.5
1	A	774	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	957	LYS	2.5
1	A	968	LEU	2.5
1	A	1093	SER	2.5
1	A	1485	CYS	2.5
1	A	911	LEU	2.5
1	A	973	TYR	2.5
1	A	767	PRO	2.5
1	A	1062	VAL	2.5
1	A	1466	ARG	2.5
1	A	951	LYS	2.5
1	A	949	ASN	2.4
1	A	1104	ARG	2.4
1	A	1461	ASP	2.4
1	A	885	THR	2.4
1	A	913	GLN	2.4
1	A	886	GLU	2.4
1	A	966	GLU	2.4
1	A	788	ASN	2.3
1	A	733	TRP	2.3
1	A	924	TYR	2.3
1	A	1500	LEU	2.3
1	A	1441	ASN	2.3
1	A	1477	SER	2.3
1	A	765	VAL	2.3
1	A	1050	VAL	2.3
1	A	965	ASP	2.3
3	D	20	DG	2.3
1	A	740	THR	2.3
1	A	756	THR	2.3
1	A	914	LEU	2.3
1	A	753	ASP	2.3
1	A	768	ASP	2.3
1	A	918	ASP	2.3
1	A	883	GLN	2.2
1	A	1016	ILE	2.2
1	A	1404	GLN	2.2
1	A	1493	ASN	2.2
1	A	961	LYS	2.2
3	D	23	DT	2.2
2	C	3	DG	2.2
1	A	1008	ARG	2.2
1	A	1347	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
3	D	21	DC	2.2
1	A	861	LYS	2.2
1	A	1019	ASN	2.2
1	A	1535[A]	LYS	2.2
1	A	1045	SER	2.2
3	D	13	DG	2.1
1	A	1465	GLY	2.1
1	A	1534	GLY	2.1
1	A	1486	ASP	2.1
1	A	969	TYR	2.1
1	A	1454	LYS	2.1
1	A	970	PRO	2.1
1	A	1453	ARG	2.1
1	A	1456	ARG	2.1
1	A	1049	ALA	2.0
1	A	977	SER	2.0
1	A	1074	VAL	2.0
1	A	1463	LYS	2.0
3	D	17	DG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
2	5CM	C	6	20/21	0.91	0.13	68,74,84,85	0
3	PYO	D	18	19/20	0.92	0.14	66,77,81,90	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

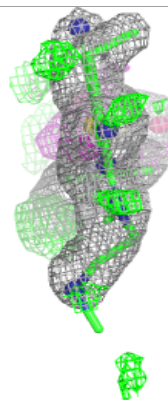
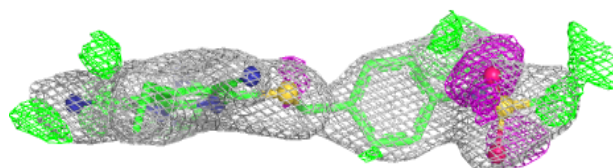
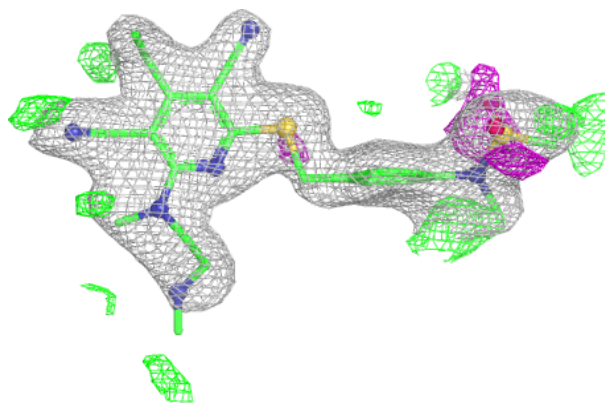
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	EDO	C	4201	4/4	0.78	0.17	52,60,64,67	0
5	EDO	A	1718	4/4	0.79	0.17	69,69,69,70	0
5	EDO	A	1710	4/4	0.80	0.18	62,63,63,65	0
5	EDO	A	1716	4/4	0.80	0.17	69,69,70,70	0
6	X52	D	101	32/32	0.80	0.20	52,66,71,78	0
5	EDO	A	1708	4/4	0.82	0.15	56,57,58,59	0
5	EDO	A	1704	4/4	0.83	0.13	68,70,72,74	0
5	EDO	A	1705	4/4	0.84	0.17	59,61,61,61	0
5	EDO	A	1707	4/4	0.85	0.17	63,63,65,65	0
5	EDO	A	1711	4/4	0.88	0.14	43,43,44,49	0
5	EDO	A	1709	4/4	0.89	0.10	61,61,62,62	0
5	EDO	A	1712	4/4	0.89	0.13	62,63,65,67	0
5	EDO	A	1717	4/4	0.90	0.12	52,53,54,56	0
5	EDO	A	1713	4/4	0.90	0.15	65,65,65,67	0
5	EDO	A	1714	4/4	0.91	0.10	55,57,59,60	0
5	EDO	A	1703	4/4	0.92	0.12	38,44,45,52	0
5	EDO	A	1715	4/4	0.93	0.10	46,49,52,55	0
5	EDO	A	1706	4/4	0.94	0.09	43,45,45,45	0
4	ZN	A	1701	1/1	0.95	0.13	69,69,69,69	0
4	ZN	A	1702	1/1	0.99	0.04	40,40,40,40	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 X52 D 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.