



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 11, 2022 – 12:11 PM EST

PDB ID : 6X9J
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 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 : 2.25
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) : 2.25

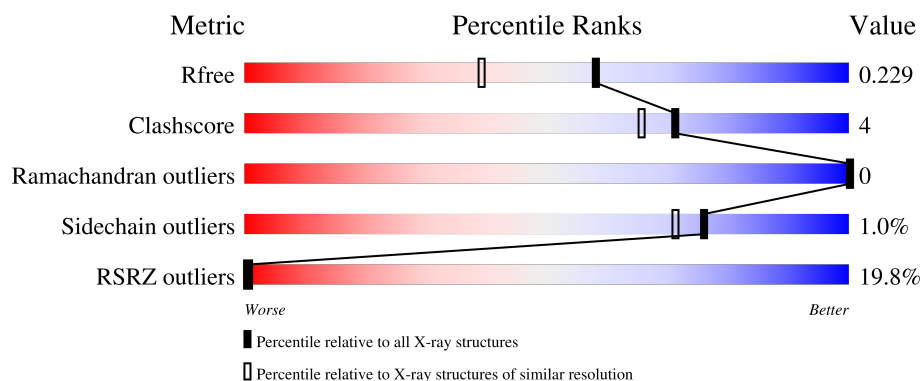
1 Overall quality at a glance

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}	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (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	<div> <div>19%</div> <div>89%</div> <div>7%</div> <div>• •</div> </div>
2	C	12	<div> <div>17%</div> <div>67%</div> <div>33%</div> </div>
3	D	12	<div> <div>25%</div> <div>58%</div> <div>42%</div> </div>

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 (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: C₂H₆O₂).



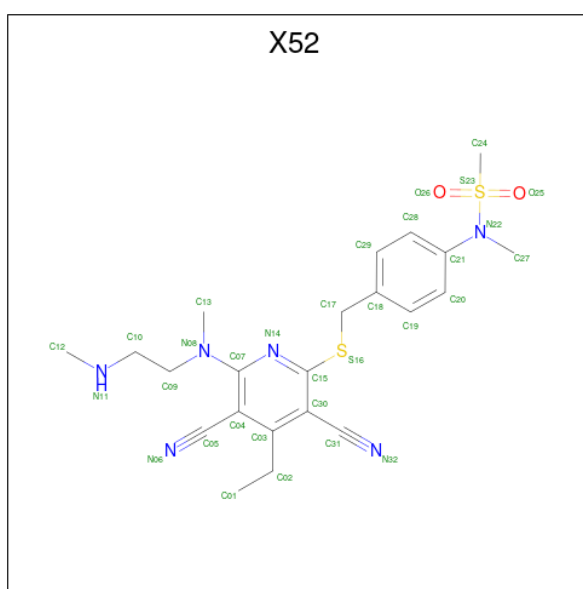
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
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 (three-letter code: 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		

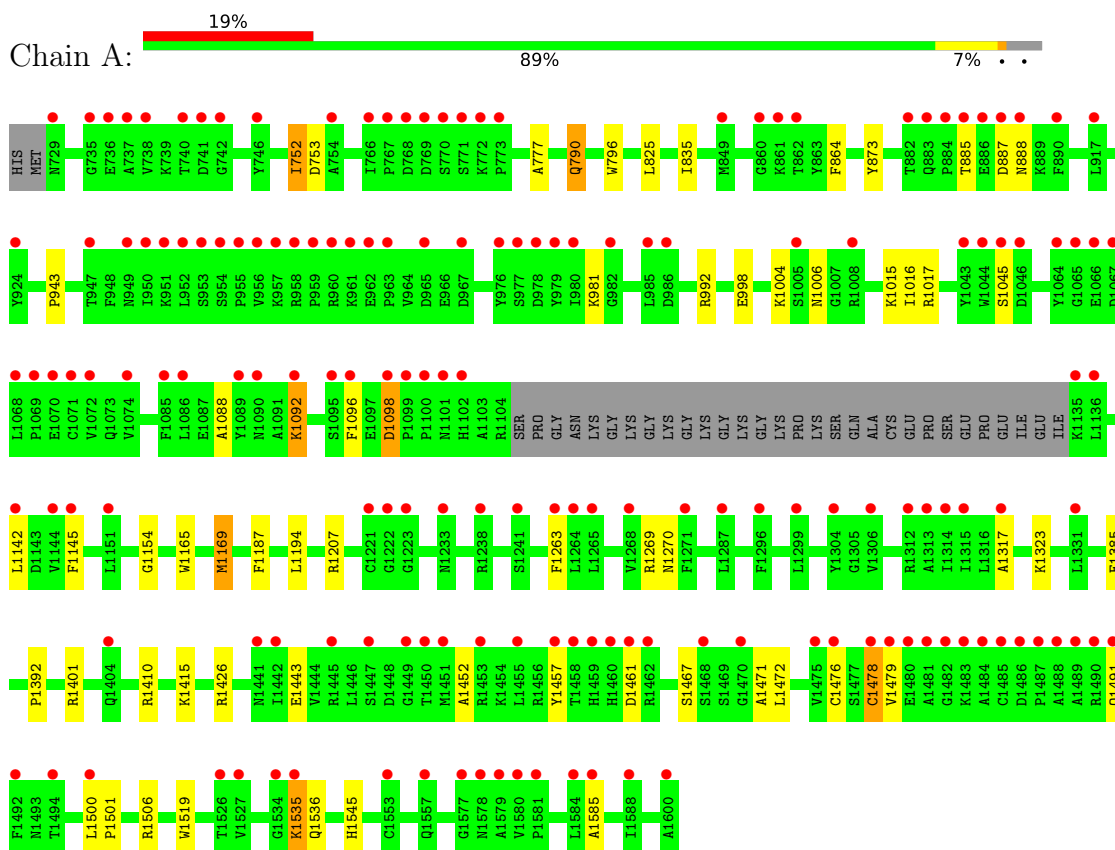
- Molecule 7 is water.

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		

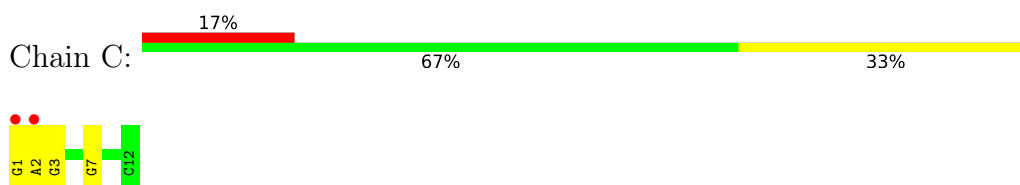
3 Residue-property plots [i](#)

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 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

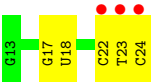


- Molecule 2: DNA (5'-D(*GP*AP*GP*GP*CP*(5CM)P*GP*CP*CP*TP*GP*C)-3')



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





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 0.200 , 0.229	Depositor DCC
R_{free} test set	1999 reflections (1.93%)	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)	0.32 , 56.8	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: EDO, ZN, X52, 5CM, PYO

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	0.30	0/6704	0.49	0/9120
2	C	0.64	0/250	0.89	0/382
3	D	0.62	0/250	0.92	0/382
All	All	0.33	0/7204	0.53	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	42	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	2	0
7	C	4	0	0	0	0
7	D	5	0	0	0	0
All	All	7497	0	6560	48	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 (48) 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: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
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:1467:SER:OG	1:A:1471:ALA:N	2.45	0.48
1:A:1154:GLY:HA3	1:A:1585:ALA:HB3	1.95	0.47
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:835:ILE:O	1:A:864:PHE:HA	2.14	0.46
1:A:1145:PHE:HD1	1:A:1169[A]:MET:HE1	1.81	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: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:1323:LYS:NZ	7:A:1822:HOH:O	2.51	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:1004:LYS:C	1:A:1006:ASN:H	2.21	0.43
1:A:1145:PHE:CD1	1:A:1169[A]:MET:HE1	2.54	0.42
2:C:3:DG:N2	3:D:23:DT:O2	2.53	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:1015:LYS:C	1:A:1016:ILE:HD12	2.41	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 ⓘ

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	844/874 (97%)	816 (97%)	28 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	676/753 (90%)	667 (99%)	9 (1%)	69 62

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	790	GLN
1	A	1045	SER
1	A	1092	LYS
1	A	1169[A]	MET
1	A	1169[B]	MET
1	A	1269	ARG
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. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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	14,20,21	0.76	0	16,28,31	0.71	0
2	5CM	C	6	3,2	15,21,22	0.70	0	19,30,33	0.86	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
3	PYO	D	18	3,2	-	2/5/25/26	0/2/2/2
2	5CM	C	6	3,2	-	1/4/21/22	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

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

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

There are no monosaccharides in this entry.

5.6 Ligand geometry

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	1712	-	3,3,3	0.44	0	2,2,2	0.33	0
5	EDO	A	1717	-	3,3,3	0.47	0	2,2,2	0.32	0
5	EDO	A	1711	-	3,3,3	0.50	0	2,2,2	0.29	0
5	EDO	A	1718	-	3,3,3	0.45	0	2,2,2	0.37	0
5	EDO	C	4201	-	3,3,3	0.51	0	2,2,2	0.16	0
5	EDO	A	1715	-	3,3,3	0.47	0	2,2,2	0.29	0
5	EDO	A	1703	-	3,3,3	0.53	0	2,2,2	0.16	0
5	EDO	A	1710	-	3,3,3	0.44	0	2,2,2	0.40	0
5	EDO	A	1714	-	3,3,3	0.44	0	2,2,2	0.38	0
6	X52	D	101	-	31,33,33	0.87	2 (6%)	37,46,46	0.83	1 (2%)
5	EDO	A	1706	-	3,3,3	0.46	0	2,2,2	0.57	0
5	EDO	A	1709	-	3,3,3	0.46	0	2,2,2	0.34	0
5	EDO	A	1716	-	3,3,3	0.45	0	2,2,2	0.29	0
5	EDO	A	1707	-	3,3,3	0.47	0	2,2,2	0.25	0
5	EDO	A	1704	-	3,3,3	0.48	0	2,2,2	0.32	0
5	EDO	A	1713	-	3,3,3	0.46	0	2,2,2	0.33	0
5	EDO	A	1705	-	3,3,3	0.44	0	2,2,2	0.51	0
5	EDO	A	1708	-	3,3,3	0.46	0	2,2,2	0.26	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	1712	-	-	0/1/1/1	-
5	EDO	A	1717	-	-	0/1/1/1	-
5	EDO	A	1711	-	-	0/1/1/1	-
5	EDO	A	1718	-	-	0/1/1/1	-
5	EDO	C	4201	-	-	0/1/1/1	-
5	EDO	A	1715	-	-	0/1/1/1	-
5	EDO	A	1703	-	-	0/1/1/1	-
5	EDO	A	1710	-	-	0/1/1/1	-
5	EDO	A	1714	-	-	0/1/1/1	-
6	X52	D	101	-	-	7/27/29/29	0/2/2/2
5	EDO	A	1706	-	-	0/1/1/1	-
5	EDO	A	1709	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	A	1716	-	-	1/1/1/1	-
5	EDO	A	1707	-	-	0/1/1/1	-
5	EDO	A	1704	-	-	0/1/1/1	-
5	EDO	A	1713	-	-	0/1/1/1	-
5	EDO	A	1705	-	-	1/1/1/1	-
5	EDO	A	1708	-	-	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	-3.12	1.37	1.40
6	D	101	X52	C04-C03	-2.11	1.38	1.40

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	101	X52	N14-C07-N08	-2.43	112.24	115.81

There are no chirality outliers.

All (9) torsion outliers are listed below:

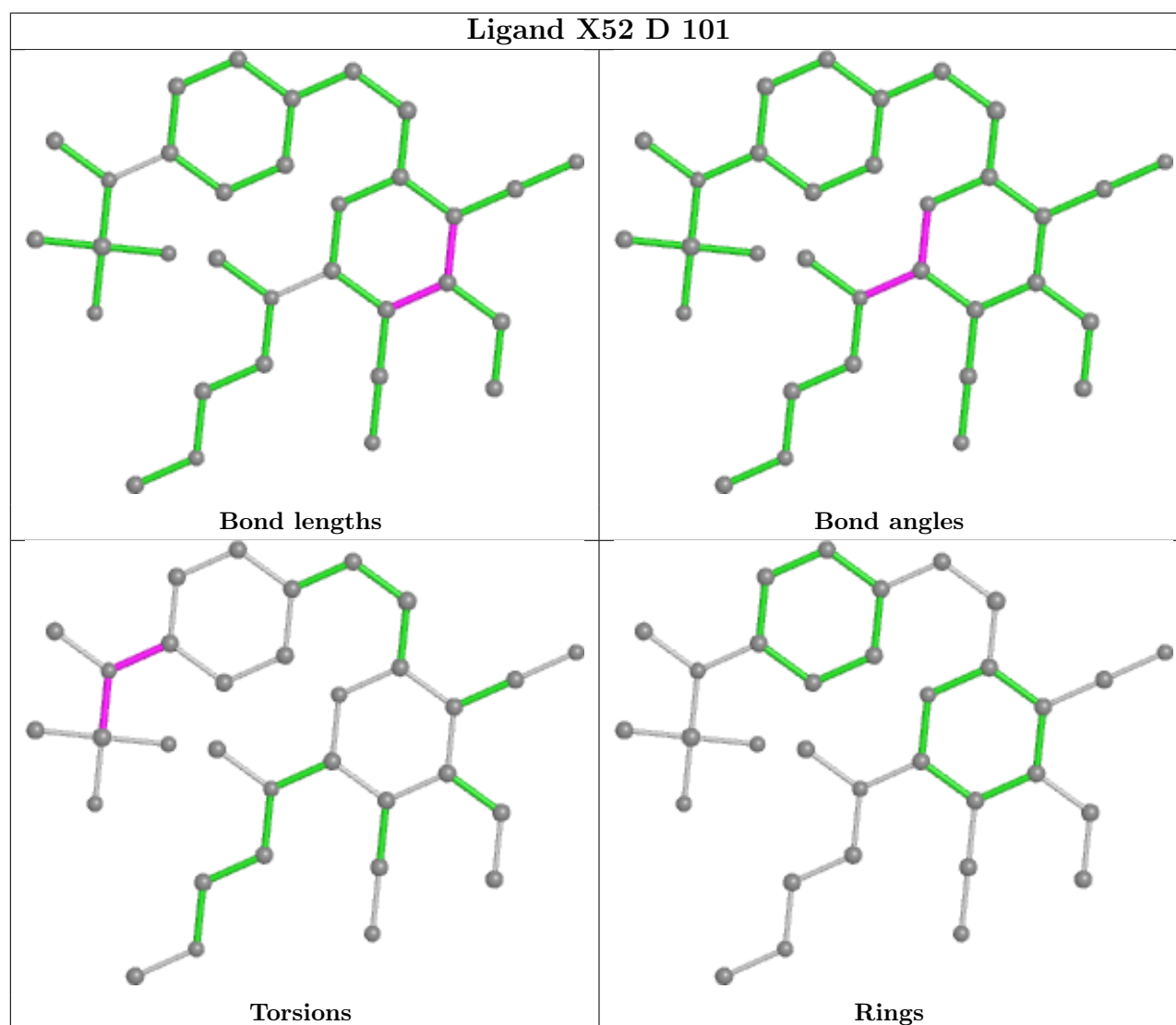
Mol	Chain	Res	Type	Atoms
6	D	101	X52	C21-N22-S23-C24
6	D	101	X52	C21-N22-S23-O25
6	D	101	X52	C21-N22-S23-O26
6	D	101	X52	C27-N22-S23-C24
6	D	101	X52	C27-N22-S23-O26
6	D	101	X52	C20-C21-N22-C27
6	D	101	X52	C28-C21-N22-C27
5	A	1716	EDO	O1-C1-C2-O2
5	A	1705	EDO	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 5 short contacts:

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

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(Å ²)	Q<0.9
1	A	842/874 (96%)	1.06	166 (19%)  	22, 47, 106, 150	0
2	C	11/12 (91%)	1.42	2 (18%)  	76, 84, 141, 177	0
3	D	11/12 (91%)	3.07	3 (27%)  	75, 99, 220, 228	0
All	All	864/898 (96%)	1.09	171 (19%)  	22, 47, 109, 228	0

All (171) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	959	PRO	13.3
3	D	23	DT	12.4
1	A	1489	ALA	12.1
1	A	1481	ALA	10.9
1	A	979	TYR	10.8
1	A	956	VAL	10.7
1	A	957	LYS	10.6
1	A	885	THR	10.1
1	A	958	ARG	9.0
1	A	729	ASN	8.9
1	A	1482	GLY	8.8
1	A	954	SER	8.7
1	A	955	PRO	8.5
1	A	1069	PRO	8.0
1	A	771	SER	7.8
3	D	24	DC	7.8
1	A	1044	TRP	7.7
1	A	1096	PHE	7.7
1	A	1484	ALA	7.5
1	A	976	TYR	6.9
1	A	887	ASP	6.9
1	A	738	VAL	6.5
1	A	884	PRO	6.3

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Mol	Chain	Res	Type	RSRZ
2	C	1	DG	6.2
1	A	890	PHE	5.9
1	A	1478	CYS	5.9
1	A	1457	TYR	5.8
1	A	888	ASN	5.7
1	A	1485	CYS	5.7
1	A	1100	PRO	5.5
1	A	952	LEU	5.4
1	A	1480	GLU	5.3
1	A	960	ARG	5.1
1	A	980	ILE	5.0
1	A	1064	TYR	5.0
1	A	963	PRO	4.9
1	A	862	THR	4.9
1	A	1492	PHE	4.8
1	A	962	GLU	4.8
3	D	22	DC	4.8
1	A	961	LYS	4.8
1	A	883	GLN	4.8
1	A	1462	ARG	4.7
1	A	1600	ALA	4.7
1	A	1265	LEU	4.7
1	A	882	THR	4.6
1	A	1479	VAL	4.6
1	A	770	SER	4.5
1	A	1005	SER	4.5
1	A	1264	LEU	4.4
1	A	1102	HIS	4.4
1	A	737	ALA	4.4
1	A	978	ASP	4.4
1	A	1483	LYS	4.4
1	A	741	ASP	4.4
1	A	1099	PRO	4.4
1	A	1074	VAL	4.3
1	A	742	GLY	4.2
1	A	1488	ALA	4.2
1	A	772	LYS	4.2
1	A	1459	HIS	4.2
1	A	917	LEU	4.1
1	A	953	SER	4.1
1	A	1313	ALA	4.0
1	A	951	LYS	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	1580	VAL	3.9
1	A	1314	ILE	3.9
1	A	860	GLY	3.8
1	A	1460	HIS	3.7
1	A	1315	ILE	3.7
1	A	1151	LEU	3.7
1	A	1487	PRO	3.7
1	A	1066	GLU	3.7
1	A	977	SER	3.7
1	A	1455	LEU	3.7
1	A	1475	VAL	3.6
1	A	950	ILE	3.5
1	A	1527	VAL	3.5
1	A	740	THR	3.5
1	A	1584	LEU	3.5
1	A	1086	LEU	3.5
1	A	1136	LEU	3.4
1	A	1071	CYS	3.4
1	A	1233	ASN	3.4
1	A	1101	ASN	3.3
1	A	1263	PHE	3.3
1	A	1238	ARG	3.3
1	A	1312[A]	ARG	3.2
1	A	1221	CYS	3.2
1	A	949	ASN	3.2
1	A	1535[A]	LYS	3.1
1	A	1135	LYS	3.1
1	A	1458	THR	3.1
1	A	1072	VAL	3.1
1	A	1299	LEU	3.1
1	A	1145	PHE	3.1
1	A	886	GLU	3.1
1	A	1085	PHE	3.0
1	A	985	LEU	3.0
1	A	1222	GLY	2.9
1	A	766	ILE	2.9
1	A	1476	CYS	2.9
1	A	947	THR	2.9
1	A	1526	THR	2.9
1	A	1065	GLY	2.8
1	A	1588	ILE	2.8
1	A	1577	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	769	ASP	2.8
1	A	1491	GLN	2.7
1	A	736	GLU	2.7
1	A	1095	SER	2.7
1	A	1098	ASP	2.7
1	A	1144	VAL	2.7
1	A	1296	PHE	2.7
1	A	1579	ALA	2.6
1	A	1404	GLN	2.6
1	A	965	ASP	2.6
1	A	1090	ASN	2.6
1	A	1461	ASP	2.5
1	A	1304	TYR	2.5
1	A	1468	SER	2.5
1	A	1271	PHE	2.5
1	A	1441	ASN	2.5
1	A	1450	THR	2.5
1	A	1442	ILE	2.5
1	A	773	PRO	2.4
1	A	1268	VAL	2.4
1	A	1581	PRO	2.4
1	A	861	LYS	2.4
1	A	1070	GLU	2.4
1	A	1445	ARG	2.4
1	A	1490	ARG	2.4
1	A	735	GLY	2.4
1	A	1447	SER	2.4
1	A	1046	ASP	2.4
1	A	746	TYR	2.3
1	A	982	GLY	2.3
2	C	2	DA	2.3
1	A	1451	MET	2.3
1	A	1453	ARG	2.3
1	A	1092	LYS	2.3
1	A	1585	ALA	2.3
1	A	768	ASP	2.3
1	A	1045	SER	2.3
1	A	1142	LEU	2.3
1	A	1089	TYR	2.3
1	A	849	MET	2.3
1	A	1068	LEU	2.2
1	A	1317	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	1534	GLY	2.2
1	A	1008	ARG	2.2
1	A	967	ASP	2.2
1	A	1306	VAL	2.2
1	A	1578	ASN	2.2
1	A	1241	SER	2.2
1	A	986	ASP	2.2
1	A	767	PRO	2.2
1	A	924	TYR	2.1
1	A	1067	ASP	2.1
1	A	1500	LEU	2.1
1	A	1494	THR	2.1
1	A	1557	GLN	2.1
1	A	1553	CYS	2.1
1	A	754	ALA	2.1
1	A	1449	GLY	2.1
1	A	1470	GLY	2.1
1	A	1043	TYR	2.1
1	A	1223	GLY	2.0
1	A	1486	ASP	2.0
1	A	1287	LEU	2.0
1	A	1331	LEU	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(\AA^2)	Q<0.9
2	5CM	C	6	20/21	0.88	0.13	68,74,84,85	0
3	PYO	D	18	19/20	0.92	0.20	66,77,81,90	0

6.3 Carbohydrates

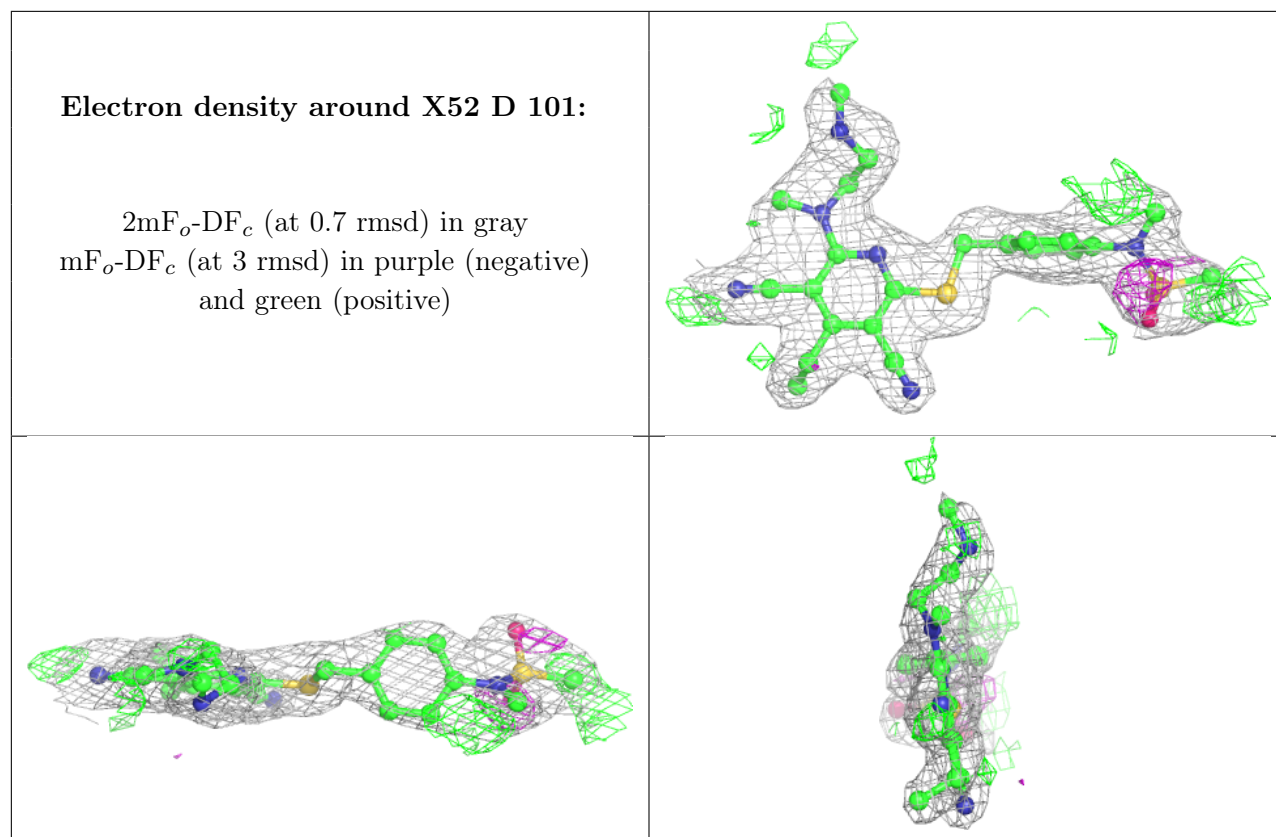
There are no monosaccharides in this entry.

6.4 Ligands

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(\AA^2)	Q<0.9
5	EDO	A	1707	4/4	0.69	0.20	63,63,65,65	0
5	EDO	A	1704	4/4	0.73	0.18	68,70,72,74	0
5	EDO	A	1718	4/4	0.75	0.14	69,69,69,70	0
5	EDO	C	4201	4/4	0.81	0.18	52,60,64,67	0
6	X52	D	101	32/32	0.81	0.15	52,66,71,78	0
5	EDO	A	1703	4/4	0.82	0.24	38,44,45,52	0
5	EDO	A	1708	4/4	0.84	0.11	56,57,58,59	0
5	EDO	A	1711	4/4	0.84	0.16	43,43,44,49	0
5	EDO	A	1713	4/4	0.84	0.16	65,65,65,67	0
5	EDO	A	1705	4/4	0.85	0.16	59,61,61,61	0
5	EDO	A	1716	4/4	0.86	0.17	69,69,70,70	0
5	EDO	A	1710	4/4	0.89	0.14	62,63,63,65	0
5	EDO	A	1706	4/4	0.91	0.07	43,45,45,45	0
5	EDO	A	1715	4/4	0.91	0.12	46,49,52,55	0
5	EDO	A	1709	4/4	0.91	0.21	61,61,62,62	0
5	EDO	A	1717	4/4	0.92	0.10	52,53,54,56	0
5	EDO	A	1712	4/4	0.93	0.14	62,63,65,67	0
4	ZN	A	1701	1/1	0.95	0.11	69,69,69,69	0
5	EDO	A	1714	4/4	0.95	0.16	55,57,59,60	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.