



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 15, 2022 – 04:09 PM EDT

PDB ID : 7KQN
Title : Ternary complex of TERT (telomerase reverse transcriptase) with RNA template, DNA primer, an incoming dGTP and a downstream hybrid duplex
Authors : Choi, W.S.; Weng, P.J.; Yang, W.
Deposited on : 2020-11-17
Resolution : 2.02 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 ⓘ 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 : 2.27
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) : 2.27

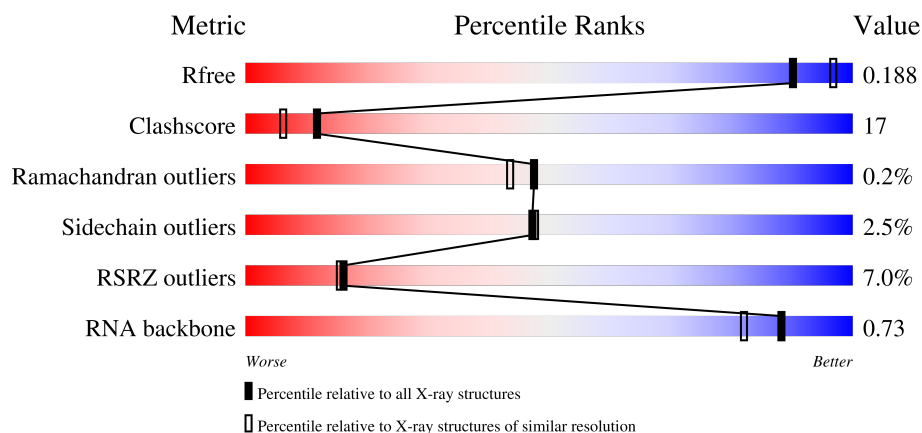
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.02 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.






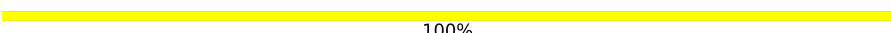
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	10434 (2.04-2.00)
Clashscore	141614	11643 (2.04-2.00)
Ramachandran outliers	138981	11493 (2.04-2.00)
Sidechain outliers	138945	11492 (2.04-2.00)
RSRZ outliers	127900	10220 (2.04-2.00)
RNA backbone	3102	1039 (2.50-1.54)

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	596	<div> <div>7%</div> <div>77%</div> <div>21%</div> <div>.</div> </div>
1	D	596	<div> <div>7%</div> <div>78%</div> <div>21%</div> <div>.</div> </div>
2	B	18	<div> <div>67%</div> <div>22%</div> <div>11%</div> </div>
2	E	18	<div> <div>61%</div> <div>39%</div> </div>

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Mol	Chain	Length	Quality of chain
3	C	7	 86% 14%
3	F	7	 57% 43%
4	I	7	 14% 86%
4	J	7	 100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	EDO	A	605	-	-	X	-
5	EDO	A	606	-	-	X	-
5	EDO	A	609	-	-	X	-
5	EDO	D	604	-	-	X	-
5	EDO	D	607	-	-	X	-
5	EDO	D	608	-	-	X	-
5	EDO	D	609	-	-	X	-
5	EDO	D	610	-	-	X	-
6	MES	A	612	-	-	X	-
7	PEG	A	613	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 12874 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 Telomerase reverse transcriptase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	596	Total	C	N	O	S	0	14	0
			5059	3307	868	861	23			
1	D	596	Total	C	N	O	S	0	8	0
			5002	3270	858	851	23			

- Molecule 2 is a RNA chain called RNA (5'-R(*CP*AP*AP*AP*GP*AP*AP*AP*UP*CP*CP*AP*GP*GP*UP*GP*CP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	18	Total	C	N	O	P	0	0	0
			384	174	76	117	17			
2	E	18	Total	C	N	O	P	0	0	0
			385	174	76	118	17			

- Molecule 3 is a DNA chain called DNA (5'-D(*GP*CP*AP*CP*CP*TP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	7	Total	C	N	O	P	0	0	0
			139	67	26	40	6			
3	F	7	Total	C	N	O	P	0	0	0
			139	67	26	40	6			

- Molecule 4 is a DNA chain called DNA (5'-D(*TP*TP*CP*TP*TP*TP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	I	7	Total	C	N	O	P	0	0	0
			138	69	18	45	6			
4	J	7	Total	C	N	O	P	0	0	0
			138	69	18	45	6			

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



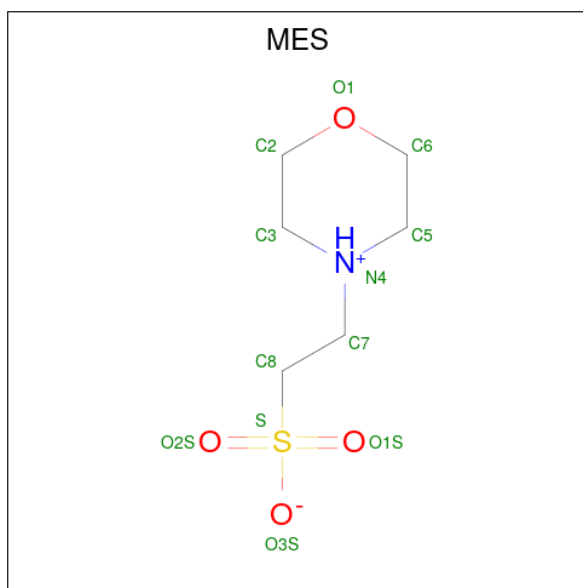
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total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

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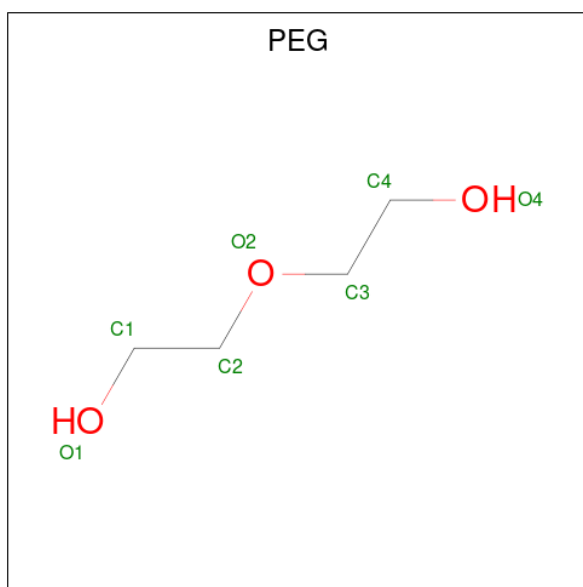
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	E	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
6	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 7 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).

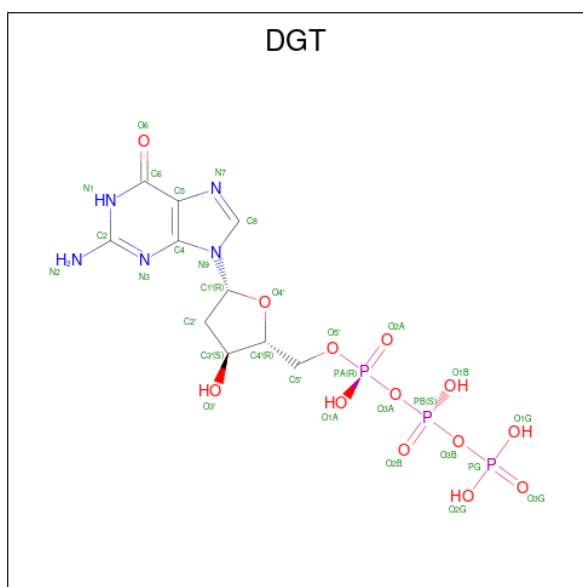


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			7	4	3		
7	D	1	Total	C	O	0	0
			7	4	3		

- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Ca	0	0
			1	1		
8	D	1	Total	Ca	0	0
			1	1		

- Molecule 9 is 2'-DEOXYGUANOSINE-5'-TRIPHOSPHATE (three-letter code: DGT) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	A	1	Total 31	C 10	N 5	O 13	P 3	0	0
9	D	1	Total 31	C 10	N 5	O 13	P 3	0	0

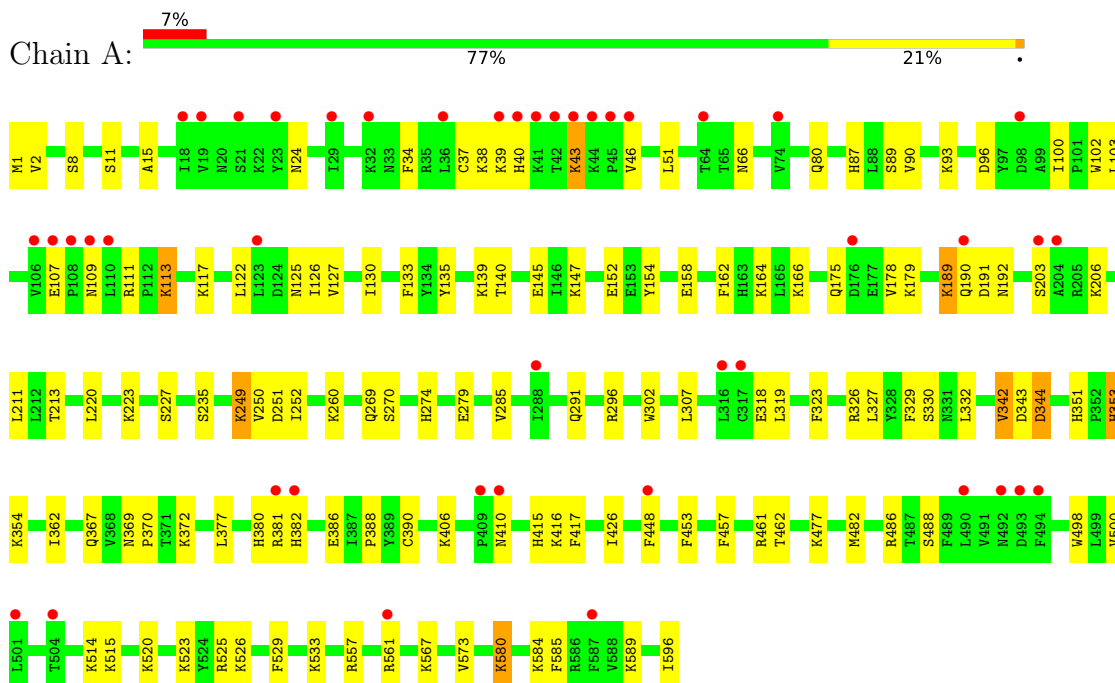
- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	571	Total O 571 571	0	0
10	B	80	Total O 80 80	0	0
10	C	39	Total O 39 39	0	0
10	D	496	Total O 496 496	0	0
10	E	83	Total O 83 83	0	0
10	F	32	Total O 32 32	0	0
10	I	2	Total O 2 2	0	0
10	J	1	Total O 1 1	0	0

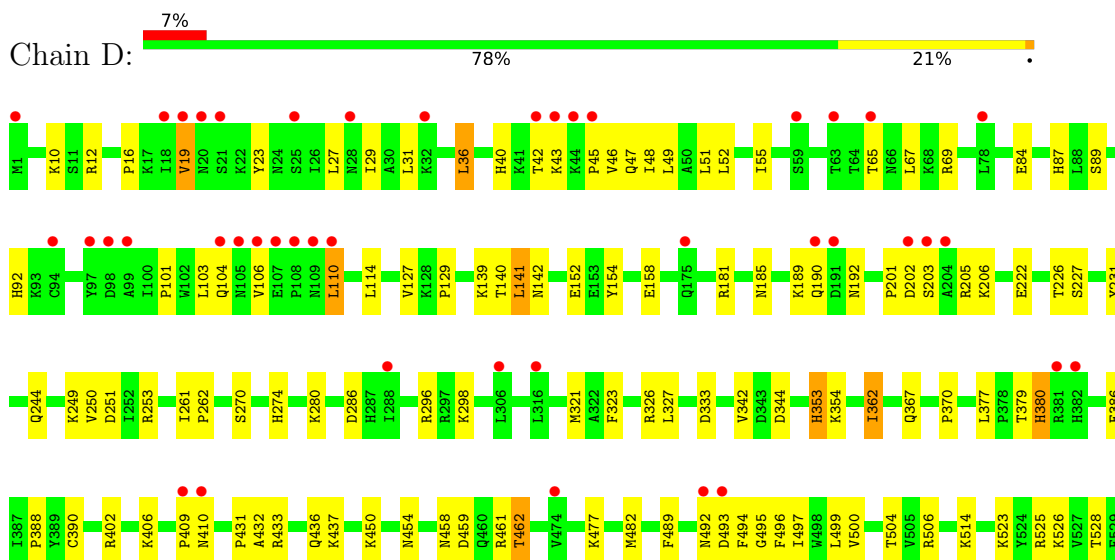
3 Residue-property plots [i](#)

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 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: Telomerase reverse transcriptase

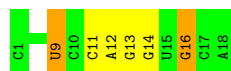


• Molecule 1: Telomerase reverse transcriptase

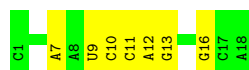




- Molecule 2: RNA (5'-R(*CP*AP*AP*AP*GP*AP*AP*AP*UP*CP*CP*AP*GP*GP*UP*GP*CP*A)-3')



- Molecule 2: RNA (5'-R(*CP*AP*AP*AP*GP*AP*AP*AP*UP*CP*CP*AP*GP*GP*UP*GP*CP*A)-3')



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



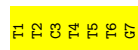
- Molecule 3: DNA (5'-D(*GP*CP*AP*CP*CP*TP*G)-3')



- Molecule 4: DNA (5'-D(*TP*TP*CP*TP*TP*TP*G)-3')



- Molecule 4: DNA (5'-D(*TP*TP*CP*TP*TP*TP*G)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	71.86Å 164.04Å 95.36Å 90.00° 111.91° 90.00°	Depositor
Resolution (Å)	29.65 – 2.02 29.65 – 2.02	Depositor EDS
% Data completeness (in resolution range)	98.0 (29.65-2.02) 98.0 (29.65-2.02)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 2.03Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.168 , 0.188 0.168 , 0.188	Depositor DCC
R_{free} test set	1007 reflections (0.77%)	wwPDB-VP
Wilson B-factor (Å ²)	42.3	Xtriage
Anisotropy	0.340	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 49.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.078 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	12874	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.55% 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: CA, PEG, MES, EDO, DGT

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	0.48	0/5192	0.66	3/7005 (0.0%)
1	D	0.47	0/5134	0.66	5/6930 (0.1%)
2	B	0.64	0/431	1.05	3/671 (0.4%)
2	E	0.57	0/432	1.00	0/672
3	C	1.23	0/155	1.07	0/237
3	F	1.17	0/155	1.17	1/237 (0.4%)
4	I	0.75	0/152	1.18	0/233
4	J	0.74	0/152	1.19	0/233
All	All	0.53	0/11803	0.74	12/16218 (0.1%)

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	6
1	D	0	3
All	All	0	9

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	36	LEU	CA-CB-CG	9.22	136.51	115.30
2	B	9	U	O5'-P-OP1	-7.98	98.52	105.70
1	D	10	LYS	CB-CG-CD	7.83	131.96	111.60
1	D	141	LEU	CB-CG-CD2	7.14	123.13	111.00
1	A	164	LYS	CA-CB-CG	6.26	127.17	113.40

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	329	PHE	Mainchain
1	A	330[A]	SER	Mainchain
1	A	330[B]	SER	Mainchain
1	A	344[B]	ASP	Mainchain
1	A	353[B]	HIS	Mainchain

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	5059	0	5151	141	0
1	D	5002	0	5077	178	1
2	B	384	0	195	2	0
2	E	385	0	198	5	0
3	C	139	0	80	2	0
3	F	139	0	80	3	0
4	I	138	0	84	6	0
4	J	138	0	84	6	0
5	A	40	0	60	24	0
5	D	40	0	60	39	0
5	E	4	0	6	0	0
6	A	24	0	26	9	0
7	A	7	0	10	4	1
7	D	7	0	10	2	0
8	A	1	0	0	0	0
8	D	1	0	0	0	0
9	A	31	0	12	0	0
9	D	31	0	12	0	0
10	A	571	0	0	117	3
10	B	80	0	0	0	0
10	C	39	0	0	0	0
10	D	496	0	0	139	3
10	E	83	0	0	11	0
10	F	32	0	0	1	0
10	I	2	0	0	2	0
10	J	1	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	12874	0	11145	396	4

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 17.

The worst 5 of 396 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)
5:A:605:EDO:H11	10:A:1030:HOH:O	1.31	1.31
1:A:381:ARG:HB3	10:A:1121:HOH:O	1.32	1.30
1:A:525:ARG:NH1	10:A:701:HOH:O	1.67	1.28
1:A:1:MET:HG2	10:A:1203:HOH:O	1.14	1.27
1:A:367:GLN:HG2	10:A:1138:HOH:O	1.30	1.25

All (4) 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:D:205:ARG:CB	10:D:785:HOH:O[1_455]	1.97	0.23
10:A:832:HOH:O	10:D:1121:HOH:O[2_655]	2.13	0.07
7:A:613:PEG:C4	10:A:716:HOH:O[1_455]	2.18	0.02
10:A:1125:HOH:O	10:D:738:HOH:O[2_555]	2.18	0.02

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	608/596 (102%)	584 (96%)	23 (4%)	1 (0%)	47	43
1	D	602/596 (101%)	586 (97%)	15 (2%)	1 (0%)	47	43
All	All	1210/1192 (102%)	1170 (97%)	38 (3%)	2 (0%)	47	43

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	342	VAL
1	A	342	VAL

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	558/552 (101%)	545 (98%)	13 (2%)	50	51
1	D	549/552 (100%)	532 (97%)	17 (3%)	40	38
All	All	1107/1104 (100%)	1077 (97%)	30 (3%)	47	44

5 of 30 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	42	THR
1	D	390	CYS
1	D	69	ARG
1	D	567	LYS
1	D	362[A]	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	125	ASN
1	A	303	ASN
1	D	40	HIS
1	D	185	ASN
1	D	380	HIS

5.3.3 RNA [i](#)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	17/18 (94%)	2 (11%)	0
2	E	17/18 (94%)	2 (11%)	0
All	All	34/36 (94%)	4 (11%)	0

All (4) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	9	U
2	B	16	G
2	E	9	U
2	E	16	G

There are no RNA pucker outliers to report.

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 29 ligands modelled in this entry, 2 are monoatomic - leaving 27 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	606	-	3,3,3	0.07	0	2,2,2	0.16	0
5	EDO	D	603	-	3,3,3	0.06	0	2,2,2	0.17	0
9	DGT	A	615	8	26,33,33	1.94	6 (23%)	32,52,52	1.72	4 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	EDO	A	602	-	3,3,3	0.47	0	2,2,2	0.54	0
5	EDO	D	610	-	3,3,3	0.07	0	2,2,2	0.13	0
6	MES	A	611	-	12,12,12	0.71	0	14,16,16	0.38	0
7	PEG	A	613	-	6,6,6	0.12	0	5,5,5	0.08	0
5	EDO	D	602	-	3,3,3	0.62	0	2,2,2	0.24	0
5	EDO	D	607	-	3,3,3	0.07	0	2,2,2	0.16	0
5	EDO	A	610	-	3,3,3	0.08	0	2,2,2	0.14	0
5	EDO	D	601	-	3,3,3	0.41	0	2,2,2	0.95	0
5	EDO	A	607	-	3,3,3	0.05	0	2,2,2	0.16	0
5	EDO	A	605	-	3,3,3	0.06	0	2,2,2	0.17	0
5	EDO	D	604	-	3,3,3	0.07	0	2,2,2	0.15	0
5	EDO	D	608	-	3,3,3	0.06	0	2,2,2	0.11	0
5	EDO	A	609	-	3,3,3	0.07	0	2,2,2	0.16	0
5	EDO	A	603	-	3,3,3	0.55	0	2,2,2	0.33	0
5	EDO	D	609	-	3,3,3	0.07	0	2,2,2	0.12	0
5	EDO	A	601	-	3,3,3	0.52	0	2,2,2	0.33	0
5	EDO	E	101	-	3,3,3	0.50	0	2,2,2	0.36	0
5	EDO	D	606	-	3,3,3	0.05	0	2,2,2	0.16	0
6	MES	A	612	-	12,12,12	0.72	0	14,16,16	0.36	0
5	EDO	A	608	-	3,3,3	0.06	0	2,2,2	0.15	0
5	EDO	A	604	-	3,3,3	0.56	0	2,2,2	0.18	0
5	EDO	D	605	-	3,3,3	0.07	0	2,2,2	0.16	0
9	DGT	D	613	8	26,33,33	1.97	5 (19%)	32,52,52	1.67	3 (9%)
7	PEG	D	611	-	6,6,6	0.11	0	5,5,5	0.08	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	606	-	-	0/1/1/1	-
5	EDO	D	603	-	-	1/1/1/1	-
9	DGT	A	615	8	-	3/18/34/34	0/3/3/3
5	EDO	A	602	-	-	0/1/1/1	-
5	EDO	D	610	-	-	1/1/1/1	-
6	MES	A	611	-	-	4/6/14/14	0/1/1/1
7	PEG	A	613	-	-	2/4/4/4	-
5	EDO	D	602	-	-	1/1/1/1	-
5	EDO	D	607	-	-	1/1/1/1	-
5	EDO	A	610	-	-	1/1/1/1	-
5	EDO	D	601	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	A	607	-	-	1/1/1/1	-
5	EDO	A	605	-	-	1/1/1/1	-
5	EDO	D	604	-	-	1/1/1/1	-
5	EDO	D	608	-	-	1/1/1/1	-
5	EDO	A	609	-	-	0/1/1/1	-
5	EDO	A	603	-	-	0/1/1/1	-
5	EDO	D	609	-	-	1/1/1/1	-
5	EDO	A	601	-	-	1/1/1/1	-
5	EDO	E	101	-	-	0/1/1/1	-
5	EDO	D	606	-	-	1/1/1/1	-
6	MES	A	612	-	-	2/6/14/14	0/1/1/1
5	EDO	A	608	-	-	1/1/1/1	-
5	EDO	A	604	-	-	1/1/1/1	-
5	EDO	D	605	-	-	1/1/1/1	-
9	DGT	D	613	8	-	5/18/34/34	0/3/3/3
7	PEG	D	611	-	-	2/4/4/4	-

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	D	613	DGT	PA-O5'	5.80	1.82	1.59
9	A	615	DGT	PA-O5'	5.58	1.81	1.59
9	A	615	DGT	O6-C6	4.60	1.36	1.24
9	D	613	DGT	O6-C6	4.58	1.36	1.24
9	D	613	DGT	C2-N2	3.06	1.40	1.33

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	613	DGT	C4-C5-C6	-6.61	114.48	120.80
9	A	615	DGT	C4-C5-C6	-6.52	114.57	120.80
9	A	615	DGT	O5'-PA-O2A	-3.84	94.07	109.07
9	D	613	DGT	O5'-PA-O2A	-3.74	94.46	109.07
9	D	613	DGT	O1A-PA-O5'	-2.54	95.94	107.75

There are no chirality outliers.

5 of 33 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	611	MES	C8-C7-N4-C5
6	A	611	MES	N4-C7-C8-S

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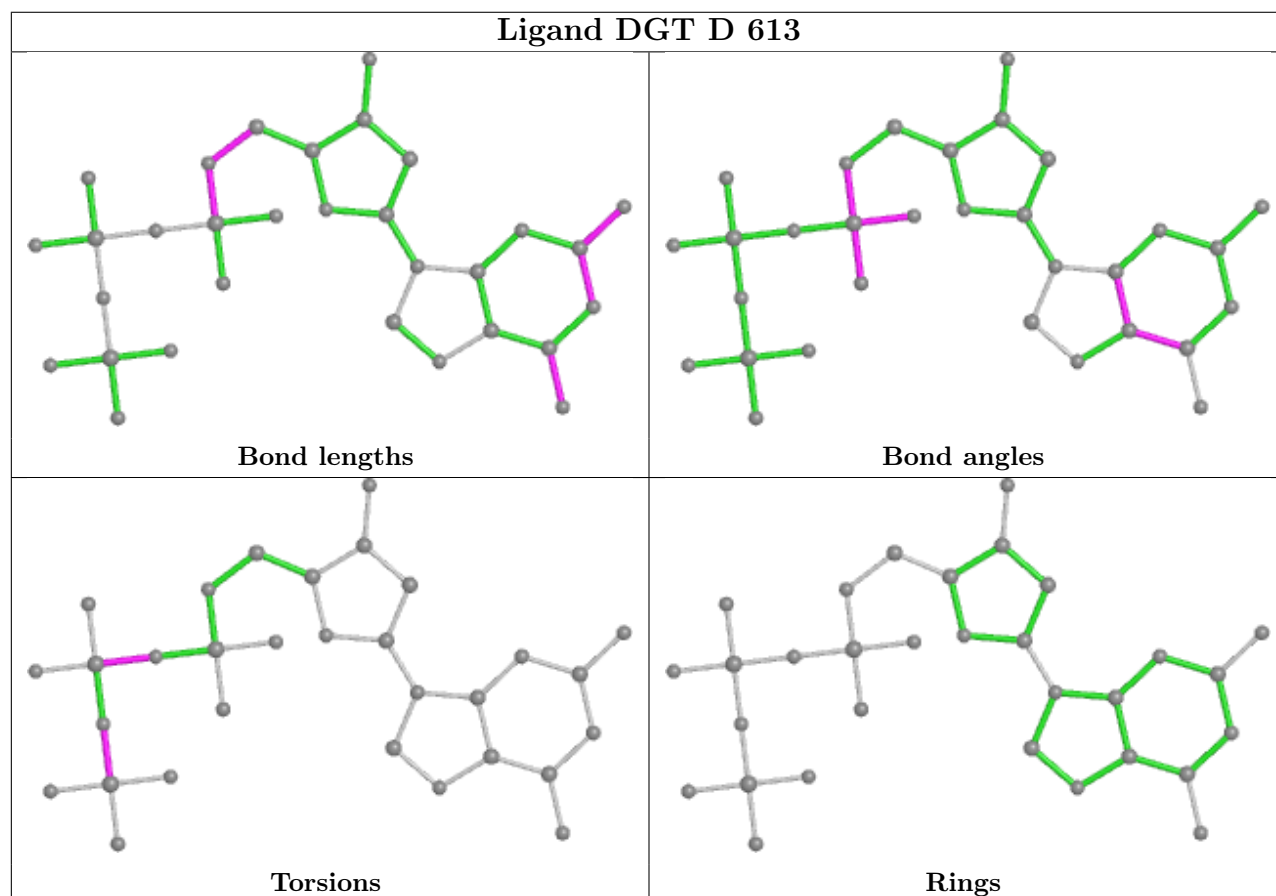
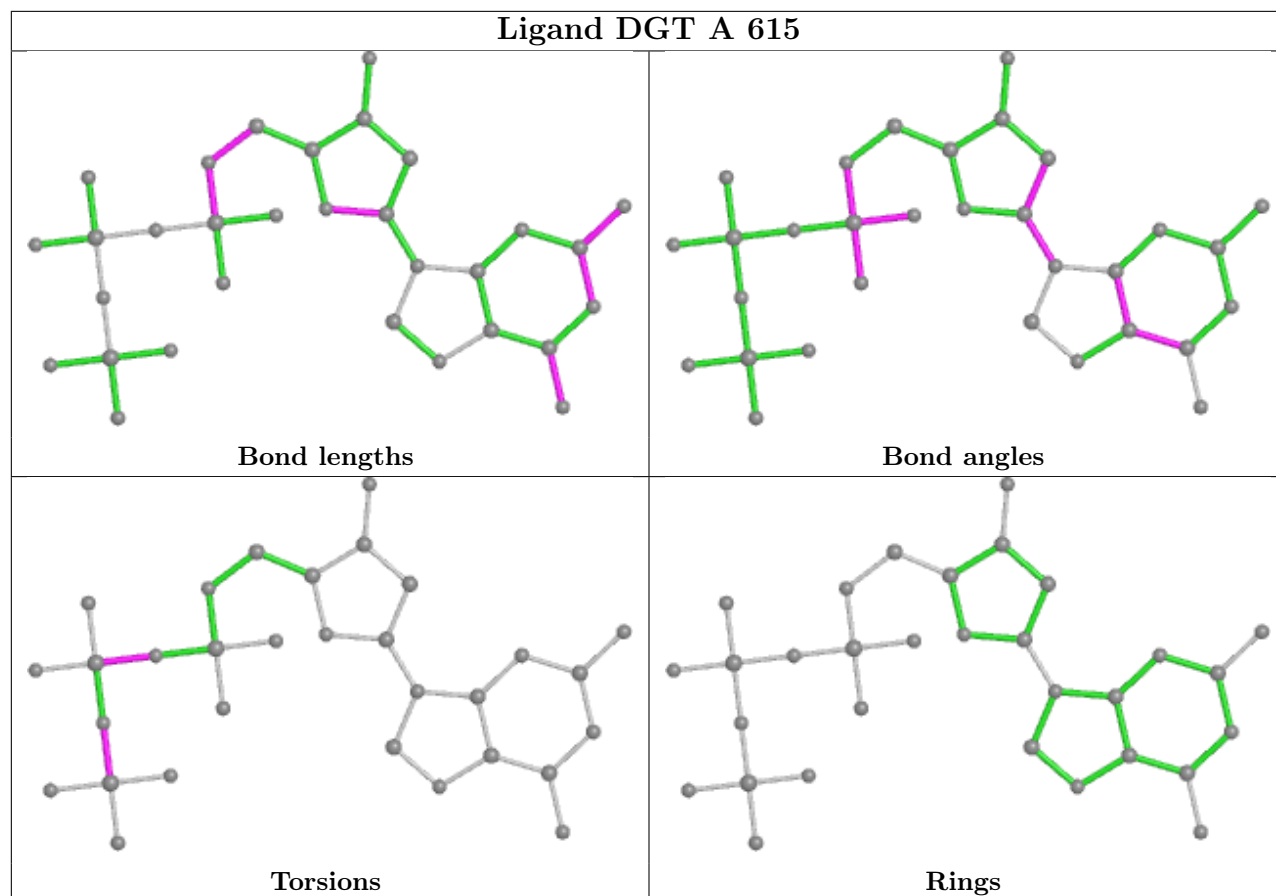
Mol	Chain	Res	Type	Atoms
6	A	612	MES	C8-C7-N4-C5
9	A	615	DGT	PB-O3B-PG-O2G
9	D	613	DGT	PB-O3B-PG-O2G

There are no ring outliers.

19 monomers are involved in 79 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	606	EDO	4	0
5	D	603	EDO	1	0
5	D	610	EDO	6	0
6	A	611	MES	3	0
7	A	613	PEG	4	1
5	D	602	EDO	3	0
5	D	607	EDO	5	0
5	D	601	EDO	2	0
5	A	607	EDO	3	0
5	A	605	EDO	9	0
5	D	604	EDO	4	0
5	D	608	EDO	5	0
5	A	609	EDO	4	0
5	A	603	EDO	2	0
5	D	609	EDO	10	0
6	A	612	MES	8	0
5	A	604	EDO	2	0
5	D	605	EDO	3	0
7	D	611	PEG	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 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	596/596 (100%)	0.24	44 (7%) 14 14	28, 52, 100, 131	0
1	D	596/596 (100%)	0.25	44 (7%) 14 14	29, 55, 105, 157	0
2	B	18/18 (100%)	-0.87	0 100 100	33, 45, 106, 110	0
2	E	18/18 (100%)	-1.02	0 100 100	33, 53, 82, 83	0
3	C	7/7 (100%)	-0.46	0 100 100	33, 35, 39, 42	0
3	F	7/7 (100%)	-0.45	0 100 100	36, 39, 45, 48	0
4	I	7/7 (100%)	0.30	0 100 100	92, 95, 101, 106	0
4	J	7/7 (100%)	0.75	0 100 100	112, 112, 118, 118	0
All	All	1256/1256 (100%)	0.20	88 (7%) 16 15	28, 53, 106, 157	0

The worst 5 of 88 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	20	ASN	7.5
1	D	108	PRO	6.0
1	A	42	THR	6.0
1	D	110	LEU	5.8
1	A	110	LEU	5.2

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

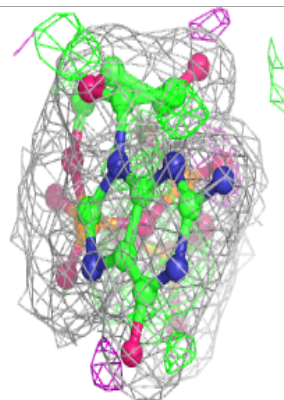
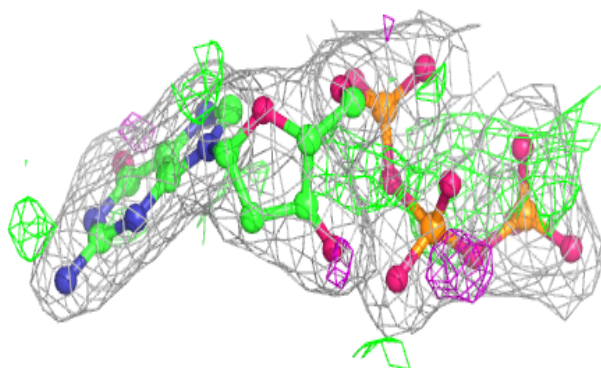
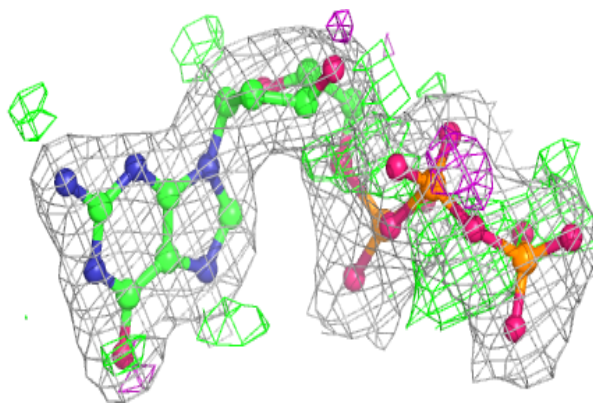
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	EDO	A	604	4/4	0.44	0.36	72,79,83,83	0
5	EDO	D	603	4/4	0.71	0.15	72,73,74,75	0
5	EDO	D	607	4/4	0.71	0.15	73,76,81,82	0
5	EDO	A	609	4/4	0.73	0.29	56,71,73,80	0
5	EDO	A	605	4/4	0.77	0.16	67,73,74,76	0
5	EDO	A	608	4/4	0.78	0.24	54,59,62,69	0
5	EDO	A	601	4/4	0.78	0.27	64,66,68,75	0
7	PEG	A	613	7/7	0.80	0.13	53,63,73,76	0
5	EDO	A	606	4/4	0.82	0.19	67,69,72,72	0
5	EDO	D	602	4/4	0.83	0.26	63,71,72,72	0
6	MES	A	612	12/12	0.84	0.24	71,80,98,103	0
5	EDO	D	604	4/4	0.85	0.22	65,65,70,75	0
5	EDO	E	101	4/4	0.85	0.36	74,76,80,84	0
7	PEG	D	611	7/7	0.85	0.18	65,71,77,78	0
5	EDO	D	606	4/4	0.86	0.26	61,65,65,69	0
5	EDO	D	609	4/4	0.86	0.25	64,65,69,78	0
5	EDO	D	608	4/4	0.87	0.24	65,67,70,74	0
5	EDO	A	607	4/4	0.87	0.18	51,53,64,74	0
6	MES	A	611	12/12	0.88	0.20	59,69,103,122	0
5	EDO	D	605	4/4	0.91	0.18	55,56,57,59	0
5	EDO	D	610	4/4	0.92	0.17	51,54,54,65	0
5	EDO	A	610	4/4	0.92	0.13	46,52,59,61	0
5	EDO	A	602	4/4	0.94	0.14	45,49,51,62	0
5	EDO	D	601	4/4	0.94	0.17	59,61,63,67	0
5	EDO	A	603	4/4	0.95	0.27	61,65,68,71	0
9	DGT	A	615	31/31	0.98	0.12	28,33,40,46	0
9	DGT	D	613	31/31	0.98	0.12	29,35,41,47	0
8	CA	A	614	1/1	1.00	0.10	30,30,30,30	0
8	CA	D	612	1/1	1.00	0.08	29,29,29,29	0

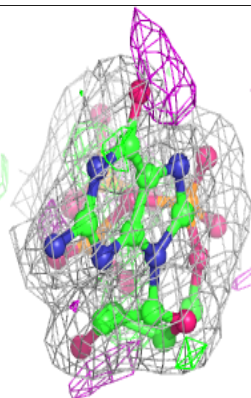
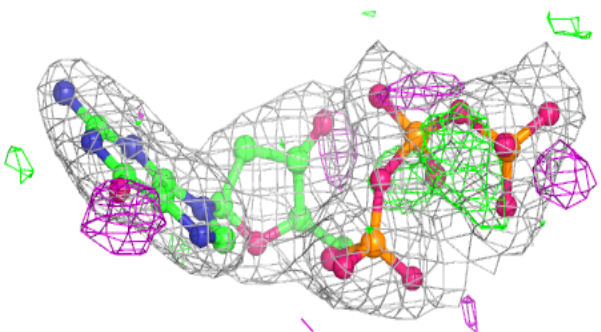
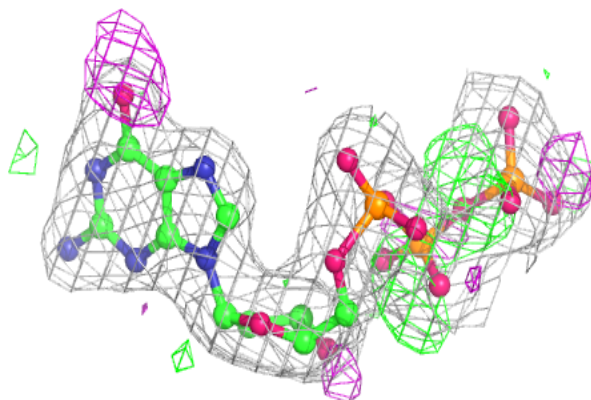
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DGT A 615:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

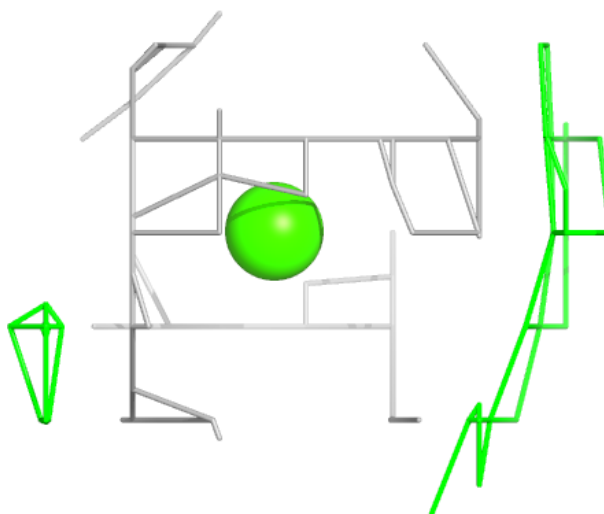
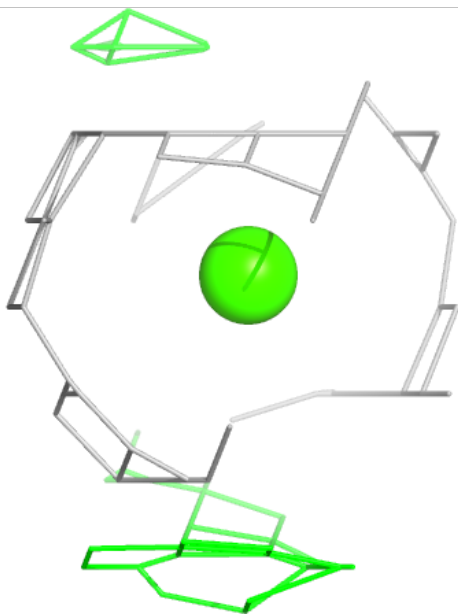
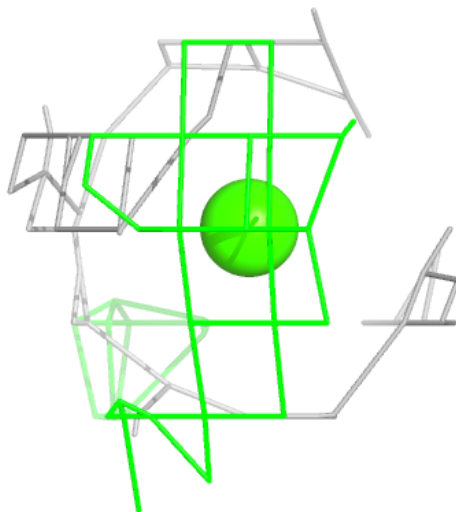
**Electron density around DGT D 613:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



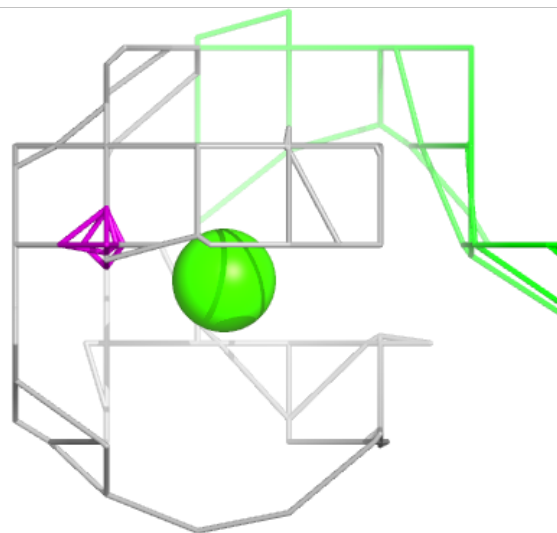
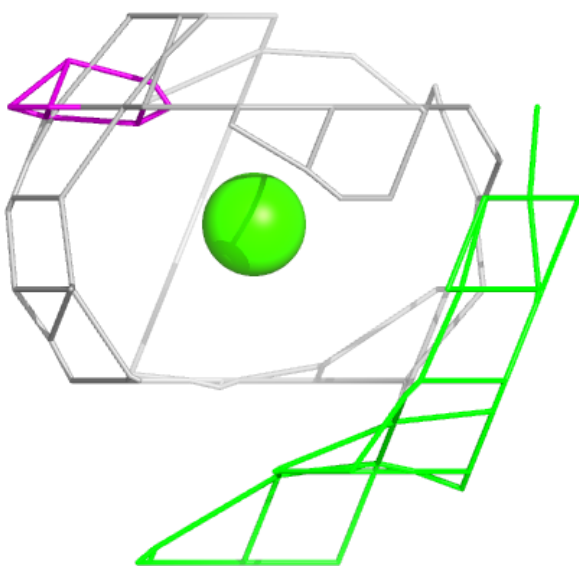
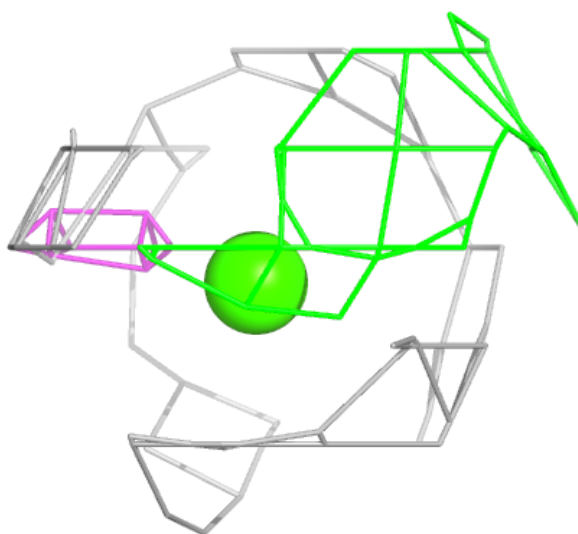
Electron density around CA A 614:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CA D 612:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers ⓘ

There are no such residues in this entry.