



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2020 – 03:43 am BST

PDB ID : 3RBD  
Title : Dpo4 extension ternary complex with 3'-terminal primer C base opposite the 3-methylcytosine (m3c) lesion  
Authors : Rechkoblit, O.; Patel, D.J.  
Deposited on : 2011-03-29  
Resolution : 2.50 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](mailto: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.

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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 : 2.11  
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) : 2.11

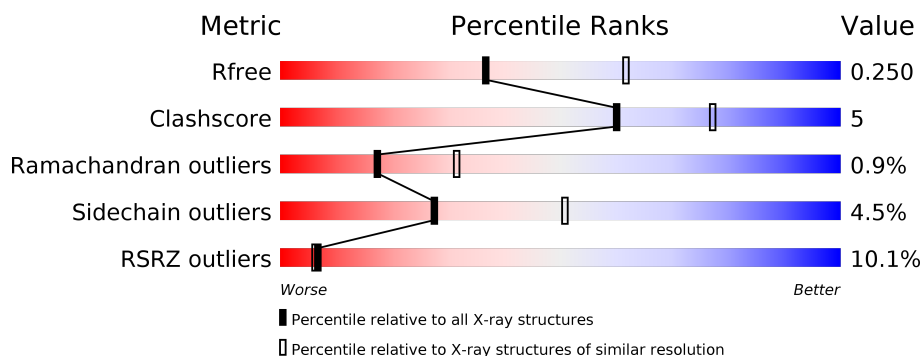
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	341	<div> <div>87%</div> <div>13%</div> <div>•</div> </div>
1	B	341	<div> <div>18%</div> <div>82%</div> <div>17%</div> <div>•</div> </div>
2	D	13	<div> <div>8%</div> <div>62%</div> <div>23%</div> <div>15%</div> </div>
2	H	13	<div> <div>23%</div> <div>54%</div> <div>8%</div> <div>23%</div> <div>15%</div> </div>
3	E	20	<div> <div>10%</div> <div>55%</div> <div>40%</div> <div>5%</div> </div>
3	J	20	<div> <div>15%</div> <div>45%</div> <div>10%</div> <div>45%</div> </div>

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 6772 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 polymerase IV.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	341	Total	C	N	O	S	0	0	0
			2740	1757	472	505	6			
1	B	341	Total	C	N	O	S	0	0	0
			2740	1757	472	505	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	EXPRESSION TAG	UNP Q97W02
B	1001	GLY	-	EXPRESSION TAG	UNP Q97W02

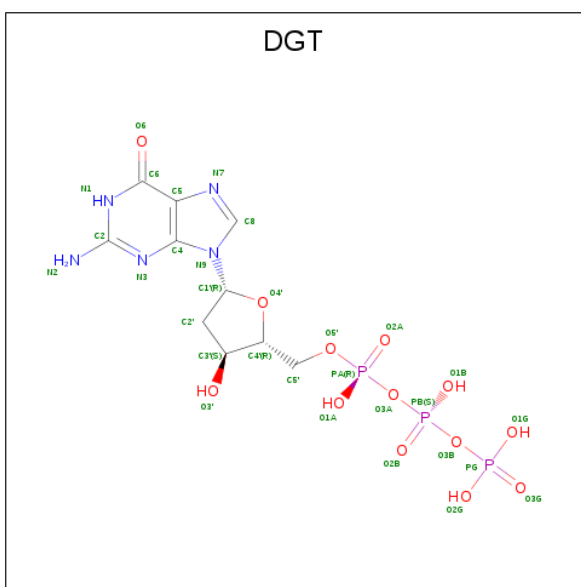
- Molecule 2 is a DNA chain called DNA (5'-D(\*GP\*TP\*TP\*GP\*GP\*AP\*TP\*GP\*GP\*TP\*AP\*GP\*(DOC))-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	13	Total	C	N	O	P	0	0	0
			269	129	51	77	12			
2	H	11	Total	C	N	O	P	0	0	0
			230	109	44	66	11			

- Molecule 3 is a DNA chain called DNA (5'-D(\*C\*CP\*TP\*AP\*AP\*CP\*(ME6)P\*CP\*TP\*AP\*CP\*CP\*AP\*TP\*CP\*CP\*AP\*AP\*CP\*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	19	Total	C	N	O	P	0	0	0
			374	181	66	109	18			
3	J	11	Total	C	N	O	P	0	0	0
			216	104	35	66	11			

- Molecule 4 is 2'-DEOXYGUANOSINE-5'-TRIPHOSPHATE (three-letter code: DGT) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).

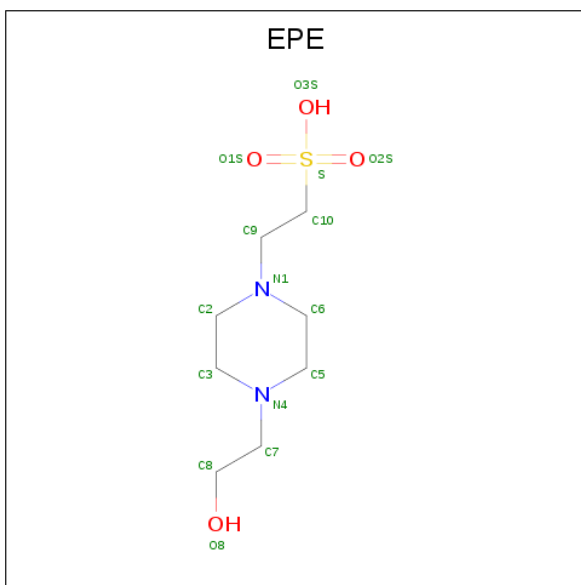


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	3	Total	Ca	0	0
			3	3		
5	A	3	Total	Ca	0	0
			3	3		

- Molecule 6 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C<sub>8</sub>H<sub>18</sub>N<sub>2</sub>O<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	D	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

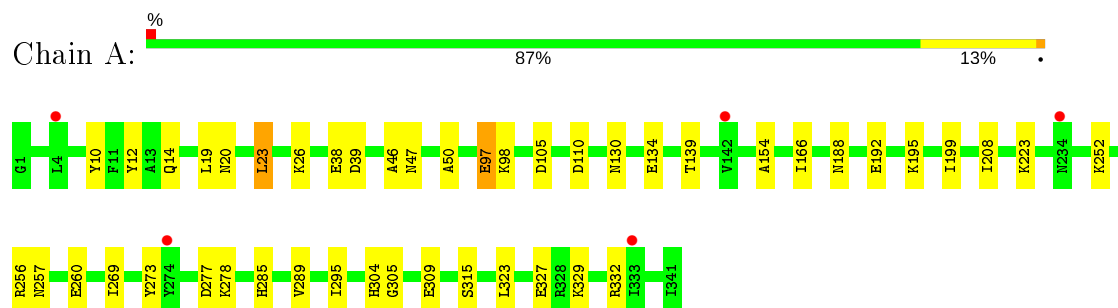
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	59	Total	O	0	0
			59	59		
7	D	8	Total	O	0	0
			8	8		
7	E	11	Total	O	0	0
			11	11		
7	B	37	Total	O	0	0
			37	37		
7	H	4	Total	O	0	0
			4	4		
7	J	1	Total	O	0	0
			1	1		

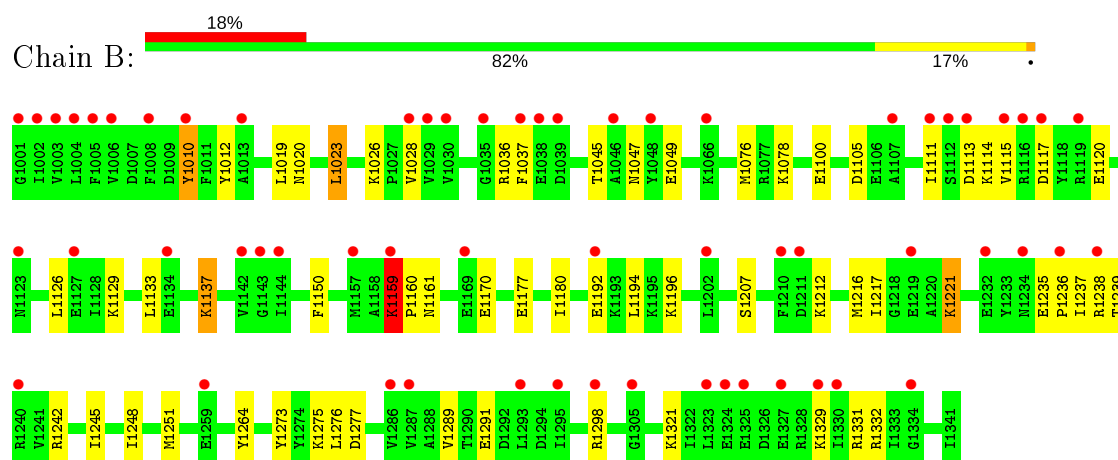
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

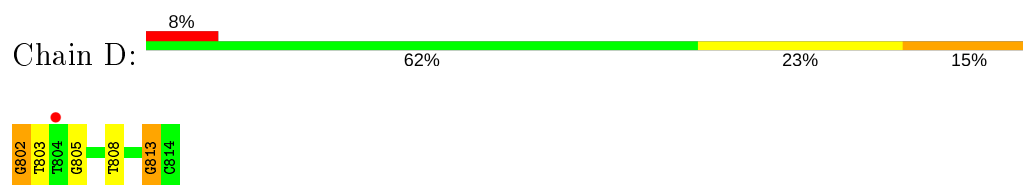
#### • Molecule 1: DNA polymerase IV



#### • Molecule 1: DNA polymerase IV

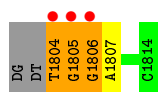


#### • Molecule 2: DNA (5'-D(\*GP\*TP\*TP\*GP\*GP\*AP\*TP\*GP\*GP\*TP\*AP\*GP\*(DOC))-3')

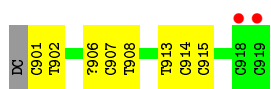


#### • Molecule 2: DNA (5'-D(\*GP\*TP\*TP\*GP\*GP\*AP\*TP\*GP\*GP\*TP\*AP\*GP\*(DOC))-3')

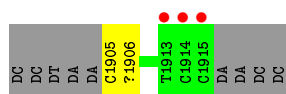
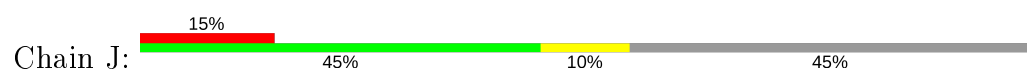




- Molecule 3: DNA (5'-D(\*C\*CP\*TP\*AP\*AP\*CP\*(ME6)P\*CP\*TP\*AP\*CP\*CP\*AP\*TP\*CP\*CP\*AP\*AP\*CP\*C)-3')



- Molecule 3: DNA (5'-D(\*C\*CP\*TP\*AP\*AP\*CP\*(ME6)P\*CP\*TP\*AP\*CP\*CP\*AP\*TP\*CP\*CP\*AP\*AP\*CP\*C)-3')



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	52.85Å 109.34Å 100.68Å 90.00° 101.12° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50 20.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	96.5 (20.00-2.50) 96.5 (20.00-2.50)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.78 (at 2.50Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.204 , 0.238 0.216 , 0.250	Depositor DCC
$R_{free}$ test set	1866 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	56.6	Xtriage
Anisotropy	0.345	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 59.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6772	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.37% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: EPE, DOC, CA, ME6, 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	0.51	0/2779	0.61	0/3731
1	B	0.39	0/2779	0.51	0/3731
2	D	0.80	0/282	1.56	4/436 (0.9%)
2	H	0.69	0/238	1.34	3/367 (0.8%)
3	E	0.91	0/394	1.44	7/600 (1.2%)
3	J	0.77	0/216	1.26	0/326
All	All	0.53	0/6688	0.80	14/9191 (0.2%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	813	DG	O4'-C1'-N9	12.60	116.82	108.00
2	D	805	DG	O4'-C1'-N9	7.49	113.24	108.00
3	E	913	DT	P-O3'-C3'	7.45	128.64	119.70
2	D	802	DG	O4'-C1'-N9	6.88	112.81	108.00
3	E	901	DC	C1'-O4'-C4'	-6.81	103.29	110.10
2	H	1806	DG	P-O3'-C3'	6.11	127.03	119.70
2	H	1805	DG	O4'-C1'-N9	5.97	112.18	108.00
2	H	1804	DT	P-O3'-C3'	5.84	126.70	119.70
2	D	808	DT	C1'-O4'-C4'	-5.74	104.36	110.10
3	E	908	DT	P-O3'-C3'	5.64	126.47	119.70
3	E	902	DT	P-O3'-C3'	5.58	126.40	119.70
3	E	914	DC	O4'-C1'-N1	5.57	111.90	108.00
3	E	915	DC	O4'-C1'-N1	5.39	111.77	108.00
3	E	901	DC	O4'-C1'-N1	5.29	111.70	108.00

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	2740	0	2883	22	0
1	B	2740	0	2880	28	0
2	D	269	0	149	4	0
2	H	230	0	125	2	0
3	E	374	0	217	1	0
3	J	216	0	127	3	0
4	A	31	0	12	1	0
4	B	31	0	12	1	0
5	A	3	0	0	0	0
5	B	3	0	0	0	0
6	D	15	0	17	2	0
7	A	59	0	0	3	0
7	B	37	0	0	4	0
7	D	8	0	0	0	0
7	E	11	0	0	0	0
7	H	4	0	0	1	0
7	J	1	0	0	0	0
All	All	6772	0	6422	60	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 5.

All (60) 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:14:GLN:HE22	1:A:139:THR:H	1.20	0.85
1:A:285:HIS:HD2	7:A:346:HOH:O	1.64	0.80
1:B:1289:VAL:HB	1:B:1332:ARG:HB2	1.66	0.77
1:B:1177:GLU:HB2	7:B:32:HOH:O	1.85	0.75
1:B:1049:GLU:HG3	7:B:25:HOH:O	1.96	0.65
1:B:1111:ILE:HG23	1:B:1114:LYS:HB2	1.79	0.64
1:B:1100:GLU:HB2	1:B:1237:ILE:HG23	1.80	0.62
2:D:802:DG:H2'	2:D:803:DT:H72	1.80	0.62
1:B:1036:ARG:NH2	1:B:1331:ARG:HG3	2.16	0.61
1:A:289:VAL:HB	1:A:332:ARG:HB2	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1028:VAL:H	1:B:1047:ASN:HB2	1.67	0.60
1:A:14:GLN:NE2	1:A:139:THR:H	1.97	0.59
1:B:1117:ASP:HB3	1:B:1120:GLU:HG3	1.86	0.57
1:B:1159:LYS:HB3	1:B:1160:PRO:HD3	1.87	0.56
3:E:906:ME6:H2'A	3:E:907:DC:O5'	2.05	0.56
2:H:1804:DT:H2''	2:H:1805:DG:OP2	2.05	0.56
1:A:130:ASN:O	1:A:134:GLU:HG3	2.06	0.56
1:B:1026:LYS:O	1:B:1047:ASN:ND2	2.39	0.55
1:A:97:GLU:H	1:A:97:GLU:CD	2.09	0.54
1:B:1159:LYS:CB	1:B:1160:PRO:HD3	2.38	0.54
1:B:1020:ASN:HB3	1:B:1023:LEU:HD22	1.90	0.53
1:A:269:ILE:HD11	1:A:315:SER:OG	2.09	0.53
7:H:73:HOH:O	3:J:1906:ME6:H20	2.08	0.53
1:B:1298:ARG:HD2	1:B:1321:LYS:HD3	1.90	0.53
1:A:38:GLU:O	1:A:39:ASP:HB2	2.09	0.52
1:A:20:ASN:HB3	1:A:23:LEU:HD22	1.91	0.51
1:A:256:ARG:HG3	1:A:329:LYS:HG2	1.93	0.50
1:B:1180:ILE:HG12	1:B:1194:LEU:HD13	1.93	0.50
1:A:195:LYS:HE2	7:A:355:HOH:O	2.11	0.50
1:B:1217:ILE:HD12	1:B:1221:LYS:HB3	1.93	0.50
1:B:1192:GLU:O	1:B:1196:LYS:HG2	2.12	0.49
1:A:188:ASN:O	1:A:192:GLU:HG2	2.13	0.48
1:B:1036:ARG:HH21	1:B:1331:ARG:HG3	1.79	0.47
1:B:1150:PHE:HB2	7:B:105:HOH:O	2.14	0.47
1:B:1245:ILE:HG21	1:B:1275:LYS:HB3	1.97	0.47
1:A:199:ILE:HD11	1:A:208:ILE:HG21	1.96	0.46
2:H:1806:DG:H2''	2:H:1807:DA:OP2	2.16	0.46
1:A:154:ALA:HB2	1:A:166:ILE:HG13	1.98	0.46
1:B:1010:TYR:HA	4:B:1414:DGT:O3B	2.16	0.46
1:A:46:ALA:HB1	1:A:50:ALA:HB3	1.99	0.45
1:A:98:LYS:HE3	1:A:110:ASP:OD2	2.17	0.45
2:D:813:DG:H21	6:D:1:EPE:H62	1.82	0.45
1:A:47:ASN:HB2	7:A:358:HOH:O	2.17	0.45
1:B:1133:LEU:O	1:B:1137:LYS:HA	2.18	0.44
1:A:304:HIS:HD2	1:A:305:GLY:O	2.00	0.43
1:B:1129:LYS:NZ	1:B:1161:ASN:OD1	2.45	0.43
1:B:1291:GLU:HB2	1:B:1329:LYS:HB2	2.00	0.43
1:B:1235:GLU:HA	1:B:1236:PRO:HD3	1.89	0.43
1:B:1273:TYR:HA	1:B:1276:LEU:HD12	2.00	0.42
1:A:257:ASN:HD22	1:A:260:GLU:H	1.67	0.42
1:A:277:ASP:O	1:A:278:LYS:HB2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:802:DG:H2'	2:D:803:DT:C7	2.49	0.42
7:B:55:HOH:O	3:J:1905:DC:H5"	2.19	0.42
1:B:1251:MET:HG2	1:B:1264:TYR:CG	2.55	0.42
1:A:12:TYR:CD2	4:A:414:DGT:H2'	2.55	0.41
1:B:1076:MET:CE	1:B:1078:LYS:HB2	2.50	0.41
3:J:1906:ME6:HN4	3:J:1906:ME6:H20	1.75	0.41
1:B:1012:TYR:HB2	1:B:1045:THR:CG2	2.50	0.41
1:A:289:VAL:HG22	1:A:295:ILE:HG12	2.03	0.40
2:D:813:DG:N2	6:D:1:EPE:H62	2.37	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	339/341 (99%)	328 (97%)	10 (3%)	1 (0%)	41	61
1	B	339/341 (99%)	313 (92%)	21 (6%)	5 (2%)	10	18
All	All	678/682 (99%)	641 (94%)	31 (5%)	6 (1%)	17	31

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1010	TYR
1	B	1159	LYS
1	B	1115	VAL
1	A	10	TYR
1	B	1277	ASP
1	B	1239	THR

### 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	299/299 (100%)	288 (96%)	11 (4%)	34	60
1	B	299/299 (100%)	283 (95%)	16 (5%)	22	42
All	All	598/598 (100%)	571 (96%)	27 (4%)	27	51

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	LEU
1	A	23	LEU
1	A	26	LYS
1	A	97	GLU
1	A	105	ASP
1	A	223	LYS
1	A	252	LYS
1	A	273	TYR
1	A	309	GLU
1	A	323	LEU
1	A	327	GLU
1	B	1019	LEU
1	B	1023	LEU
1	B	1037	PHE
1	B	1105	ASP
1	B	1113	ASP
1	B	1126	LEU
1	B	1137	LYS
1	B	1159	LYS
1	B	1170	GLU
1	B	1207	SER
1	B	1212	LYS
1	B	1216	MET
1	B	1221	LYS
1	B	1238	ARG
1	B	1242	ARG
1	B	1248	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	188	ASN
1	A	254	ASN
1	A	257	ASN
1	A	285	HIS
1	A	304	HIS
1	B	1047	ASN
1	B	1304	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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	ME6	J	1906	3	15,21,22	0.61	0	17,30,33	1.04	1 (5%)
3	ME6	E	906	3	15,21,22	0.82	0	17,30,33	1.09	1 (5%)
2	DOC	D	814	2	14,19,20	0.75	0	13,26,29	1.71	1 (7%)
2	DOC	H	1814	2	14,19,20	0.80	0	13,26,29	1.71	2 (15%)

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	ME6	J	1906	3	-	0/4/21/22	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ME6	E	906	3	-	3/4/21/22	0/2/2/2
2	DOC	D	814	2	-	0/4/18/19	0/2/2/2
2	DOC	H	1814	2	-	0/4/18/19	0/2/2/2

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	814	DOC	C2-N3-C4	4.94	121.34	116.34
2	H	1814	DOC	C2-N3-C4	4.21	120.61	116.34
3	E	906	ME6	C5-C4-N3	2.70	121.14	118.20
3	J	1906	ME6	C5-C4-N3	2.57	121.00	118.20
2	H	1814	DOC	C3'-C2'-C1'	2.43	105.58	102.78

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	906	ME6	O4'-C1'-N1-C6
3	E	906	ME6	O4'-C4'-C5'-O5'
3	E	906	ME6	C3'-C4'-C5'-O5'

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	J	1906	ME6	2	0
3	E	906	ME6	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 6 are monoatomic - leaving 3 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
4	DGT	B	1414	5	26,33,33	1.03	2 (7%)	32,52,52	3.43	14 (43%)
4	DGT	A	414	5	26,33,33	1.03	2 (7%)	32,52,52	3.26	13 (40%)
6	EPE	D	1	-	15,15,15	0.91	1 (6%)	18,20,20	2.28	6 (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
4	DGT	B	1414	5	-	4/18/34/34	0/3/3/3
4	DGT	A	414	5	-	4/18/34/34	0/3/3/3
6	EPE	D	1	-	-	6/9/19/19	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	414	DGT	C6-N1	3.94	1.39	1.33
4	B	1414	DGT	C6-N1	3.90	1.39	1.33
6	D	1	EPE	C10-S	3.11	1.81	1.77
4	A	414	DGT	C8-N7	-2.09	1.31	1.34
4	B	1414	DGT	C8-N7	-2.04	1.31	1.34

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1414	DGT	O1G-PG-O3G	-8.57	77.13	110.68
4	B	1414	DGT	C5-C6-N1	-7.94	112.57	123.43
4	A	414	DGT	C5-C6-N1	-7.79	112.78	123.43
4	B	1414	DGT	C6-N1-C2	6.87	126.84	115.93
4	A	414	DGT	O2G-PG-O3G	-6.80	84.06	110.68
4	A	414	DGT	O1G-PG-O3G	-6.66	84.61	110.68
4	B	1414	DGT	O2G-PG-O3G	-6.55	85.06	110.68
4	A	414	DGT	C6-N1-C2	5.93	125.35	115.93
4	B	1414	DGT	N3-C2-N1	-5.43	119.98	127.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	414	DGT	PB-O3B-PG	-5.35	114.45	132.83
6	D	1	EPE	C5-N4-C3	5.19	120.51	108.83
4	B	1414	DGT	O2G-PG-O1G	4.83	126.11	107.64
4	A	414	DGT	O3B-PG-O3G	-4.49	86.26	111.19
4	A	414	DGT	O1G-PG-O3B	4.43	119.49	104.64
4	B	1414	DGT	O1G-PG-O3B	4.05	118.23	104.64
4	B	1414	DGT	PA-O3A-PB	-4.03	118.99	132.83
6	D	1	EPE	O3S-S-C10	4.01	112.26	105.77
4	A	414	DGT	N3-C2-N1	-3.99	121.89	127.22
4	A	414	DGT	O2G-PG-O3B	3.72	117.13	104.64
4	B	1414	DGT	PB-O3B-PG	-3.68	120.21	132.83
6	D	1	EPE	C7-N4-C5	3.58	120.39	111.23
4	A	414	DGT	O2G-PG-O1G	3.52	121.10	107.64
4	B	1414	DGT	C6-C5-C4	-3.45	117.50	120.80
4	B	1414	DGT	O3B-PG-O3G	-3.34	92.64	111.19
4	A	414	DGT	C2'-C1'-N9	-3.34	106.57	114.27
4	A	414	DGT	C6-C5-C4	-3.17	117.77	120.80
4	A	414	DGT	PA-O3A-PB	-2.91	122.84	132.83
6	D	1	EPE	C7-N4-C3	2.71	118.16	111.23
6	D	1	EPE	C9-N1-C2	-2.64	104.48	111.23
6	D	1	EPE	C3-C2-N1	2.64	116.05	110.64
4	B	1414	DGT	O2G-PG-O3B	2.48	112.97	104.64
4	B	1414	DGT	N2-C2-N3	2.46	121.80	117.79
4	B	1414	DGT	C2'-C1'-N9	-2.28	109.00	114.27

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1414	DGT	C5'-O5'-PA-O2A
6	D	1	EPE	C9-C10-S-O2S
6	D	1	EPE	C9-C10-S-O3S
4	A	414	DGT	PG-O3B-PB-O2B
6	D	1	EPE	S-C10-C9-N1
6	D	1	EPE	C10-C9-N1-C6
4	B	1414	DGT	C5'-O5'-PA-O3A
4	A	414	DGT	PA-O3A-PB-O1B
6	D	1	EPE	C8-C7-N4-C5
4	B	1414	DGT	C5'-O5'-PA-O1A
6	D	1	EPE	C9-C10-S-O1S
4	A	414	DGT	PG-O3B-PB-O1B
4	B	1414	DGT	PA-O3A-PB-O1B

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Mol	Chain	Res	Type	Atoms
4	A	414	DGT	PB-O3B-PG-O2G

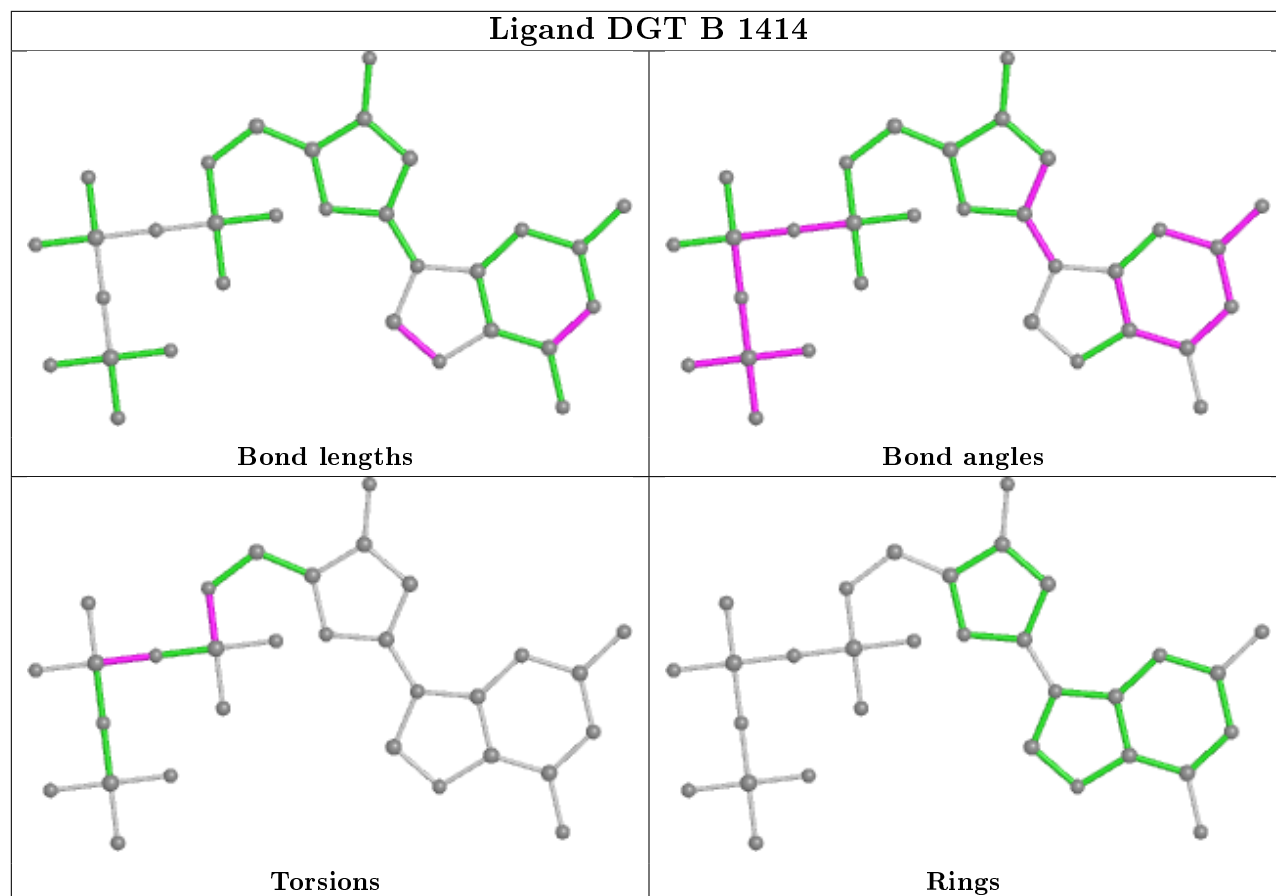
There are no ring outliers.

3 monomers are involved in 4 short contacts:

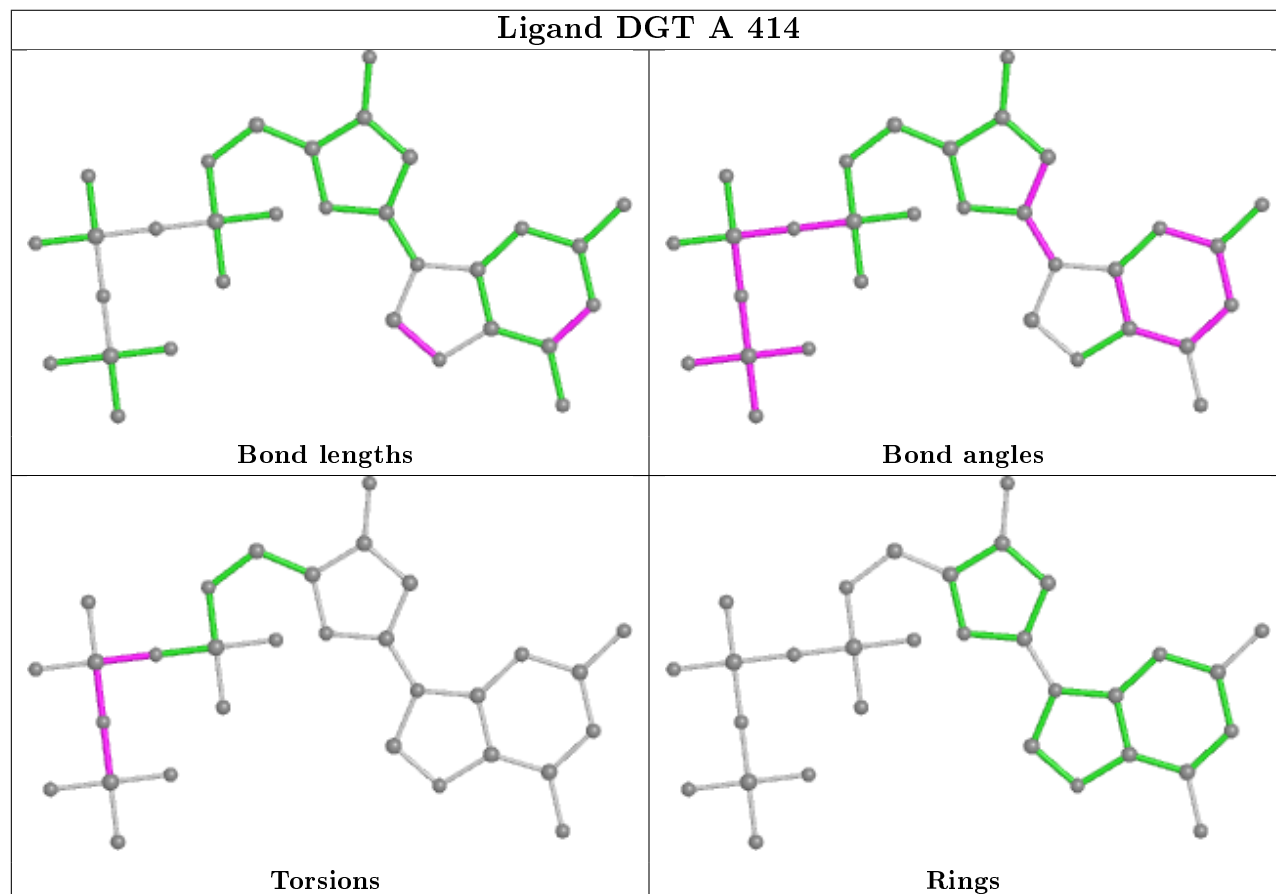
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1414	DGT	1	0
4	A	414	DGT	1	0
6	D	1	EPE	2	0

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.

## Ligand DGT B 1414



## Ligand DGT A 414



## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	341/341 (100%)	0.24	5 (1%) 73 75	34, 54, 76, 93	0
1	B	341/341 (100%)	0.96	60 (17%) 1 1	58, 97, 132, 158	0
2	D	12/13 (92%)	-0.05	1 (8%) 11 11	41, 61, 127, 134	0
2	H	10/13 (76%)	1.36	3 (30%) 0 0	75, 116, 168, 208	0
3	E	18/20 (90%)	0.24	2 (11%) 5 5	38, 66, 142, 163	0
3	J	10/20 (50%)	1.32	3 (30%) 0 0	74, 101, 172, 201	0
All	All	732/748 (97%)	0.60	74 (10%) 7 6	34, 72, 127, 208	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1115	VAL	7.3
2	H	1804	DT	6.2
1	B	1116	ARG	6.0
1	B	1004	LEU	5.9
2	H	1805	DG	5.7
3	J	1915	DC	5.6
1	B	1006	VAL	5.5
1	B	1143	GLY	5.1
1	B	1293	LEU	5.0
1	B	1324	GLU	4.9
3	E	919	DC	4.9
1	B	1001	GLY	4.4
3	J	1914	DC	4.3
1	B	1005	PHE	4.3
1	B	1037	PHE	4.3
1	B	1144	ILE	4.2
1	B	1119	ARG	4.0
1	B	1113	ASP	3.9
1	B	1329	LYS	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	1159	LYS	3.7
1	B	1142	VAL	3.6
1	A	234	ASN	3.6
1	B	1238	ARG	3.5
1	B	1286	VAL	3.5
1	B	1157	MET	3.3
1	B	1232	GLU	3.3
1	B	1234	ASN	3.2
1	B	1111	ILE	3.2
1	B	1046	ALA	3.1
1	B	1323	LEU	3.0
1	B	1210	PHE	2.9
2	H	1806	DG	2.9
1	B	1240	ARG	2.9
1	B	1330	ILE	2.8
3	J	1913	DT	2.8
1	B	1048	TYR	2.8
1	B	1169	GLU	2.7
1	B	1219	GLU	2.6
1	B	1013	ALA	2.6
1	A	4	LEU	2.5
1	B	1008	PHE	2.5
1	B	1259	GLU	2.5
1	B	1334	GLY	2.5
1	B	1236	PRO	2.5
1	B	1127	GLU	2.5
1	B	1325	GLU	2.5
1	B	1211	ASP	2.5
1	A	274	TYR	2.4
1	B	1035	GLY	2.4
1	B	1298	ARG	2.4
1	B	1192	GLU	2.4
1	B	1029	VAL	2.4
1	B	1038	GLU	2.4
1	B	1117	ASP	2.3
1	B	1134	GLU	2.3
3	E	918	DC	2.3
1	B	1305	GLY	2.3
1	B	1327	GLU	2.3
1	B	1003	VAL	2.2
1	B	1002	ILE	2.2
1	B	1107	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	1066	LYS	2.2
1	A	333	ILE	2.2
1	B	1123	ASN	2.2
1	B	1030	VAL	2.1
1	B	1202	LEU	2.1
1	B	1295	ILE	2.1
1	B	1039	ASP	2.1
2	D	804	DT	2.1
1	A	142	VAL	2.0
1	B	1287	VAL	2.0
1	B	1112	SER	2.0
1	B	1010	TYR	2.0
1	B	1028	VAL	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, 95<sup>th</sup> 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
2	DOC	H	1814	18/19	0.92	0.26	86,88,90,92	0
3	ME6	J	1906	20/21	0.94	0.11	78,85,102,103	0
2	DOC	D	814	18/19	0.98	0.12	45,47,48,48	0
3	ME6	E	906	20/21	0.98	0.12	40,45,49,51	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates 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, 95<sup>th</sup> 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	CA	B	1415	1/1	0.81	0.09	64,64,64,64	0

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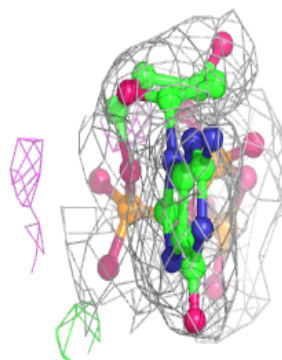
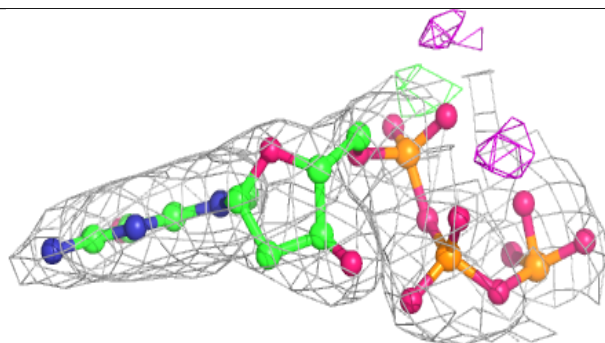
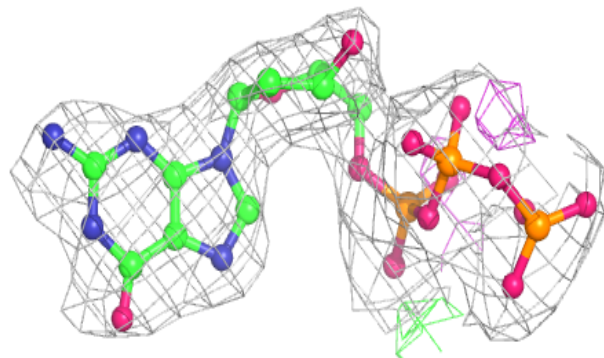
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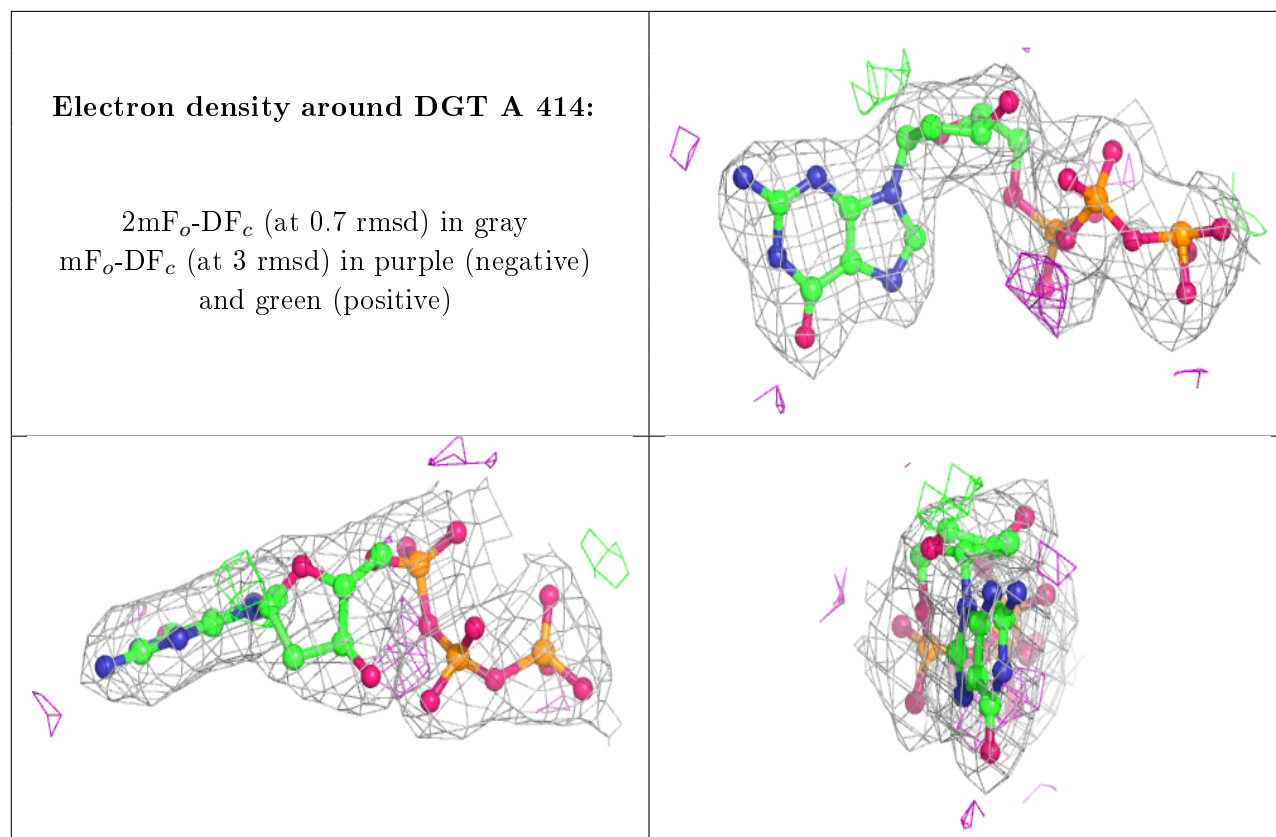
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	CA	B	1417	1/1	0.88	0.06	61,61,61,61	0
4	DGT	B	1414	31/31	0.95	0.12	62,65,83,88	0
5	CA	A	415	1/1	0.95	0.07	53,53,53,53	0
5	CA	B	1416	1/1	0.96	0.04	53,53,53,53	0
6	EPE	D	1	15/15	0.96	0.19	48,49,59,61	0
5	CA	A	416	1/1	0.97	0.15	35,35,35,35	0
5	CA	A	417	1/1	0.97	0.05	48,48,48,48	0
4	DGT	A	414	31/31	0.98	0.14	31,34,39,42	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 B 1414:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.