



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 02:07 pm BST

PDB ID : 3RB6
Title : Dpo4 extension ternary complex with 3'-terminal primer A base opposite the 3-methylcytosine (m3c) lesion
Authors : Rechkoblit, O.; Patel, D.J.
Deposited on : 2011-03-28
Resolution : 2.70 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 : 2.11
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

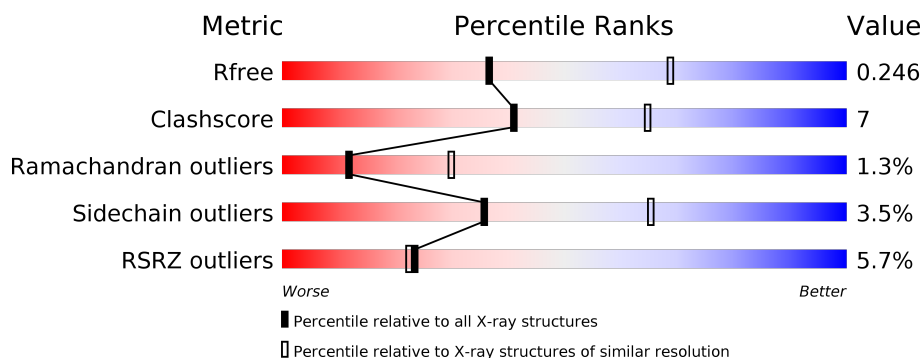
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 ≥ 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>100%</div> <div> <div>83%</div> <div>16%</div> <div>•</div> </div> </div>
1	B	341	<div> <div>10%</div> <div> <div>82%</div> <div>16%</div> <div>•</div> </div> </div>
2	D	13	<div> <div>8%</div> <div> <div>77%</div> <div>23%</div> </div> </div>
2	H	13	<div> <div>15%</div> <div> <div>38%</div> <div>31%</div> <div>8%</div> <div>23%</div> </div> </div>
3	E	20	<div> <div>5%</div> <div> <div>50%</div> <div>45%</div> <div>5%</div> </div> </div>
3	J	20	<div> <div>15%</div> <div> <div>40%</div> <div>10%</div> <div>5%</div> <div>45%</div> </div> </div>

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
2	2DA	D	814	-	-	X	-
3	ME6	E	906	-	-	X	-
3	ME6	J	1906	-	-	X	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 6694 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

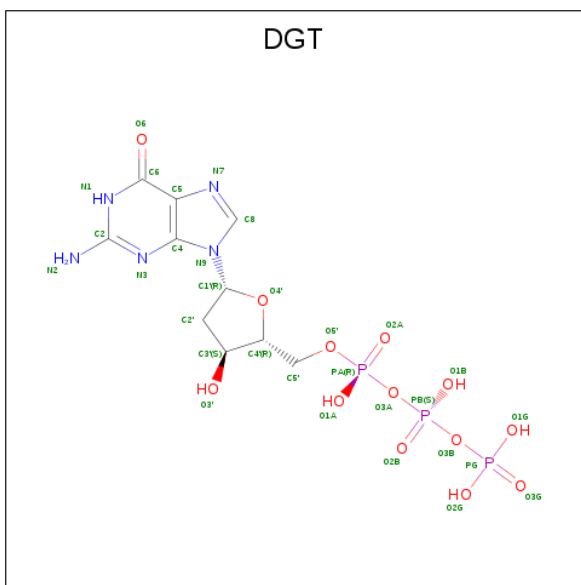
- Molecule 2 is a DNA chain called DNA (5'-D(*GP*TP*TP*GP*GP*AP*TP*GP*GP*TP*AP*GP*(2DA))-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	13	Total	C	N	O	P	0	0	0
			271	130	53	76	12			
2	H	10	Total	C	N	O	P	0	0	0
			212	100	44	58	10			

- 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').

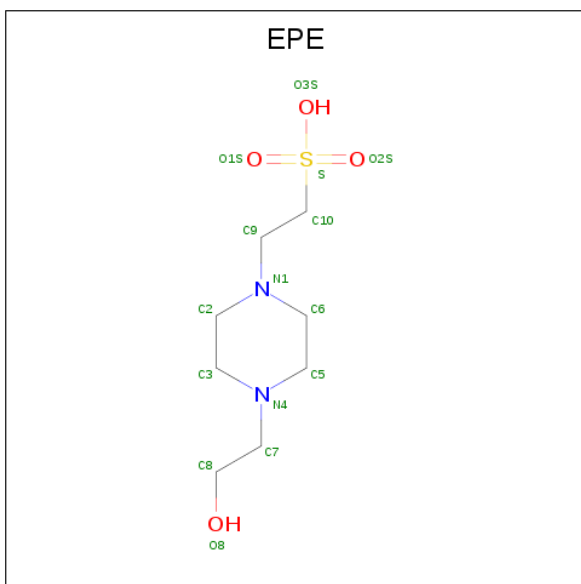
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	19	Total	C	N	O	P	0	0	0
			374	181	66	109	18			
3	J	11	Total	C	N	O	P	0	0	0
			216	104	35	66	11			

- Molecule 4 is 2'-DEOXYGUANOSINE-5'-TRIPHOSPHATE (three-letter code: DGT) (formula: C₁₀H₁₆N₅O₁₃P₃).



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

- Molecule 5 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).



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

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

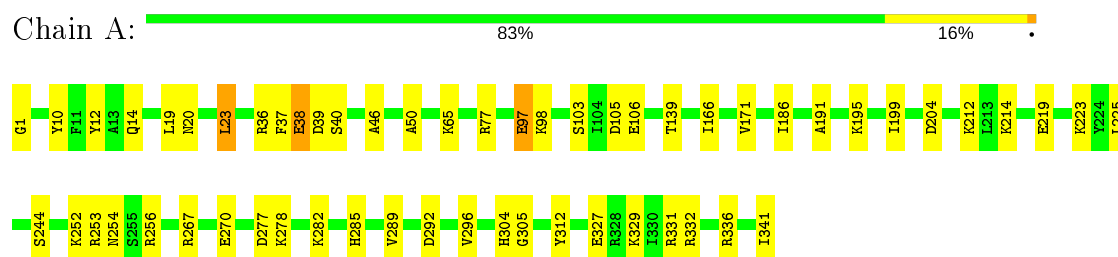
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	29	Total 29	O 29	0	0
7	D	6	Total 6	O 6	0	0
7	E	5	Total 5	O 5	0	0
7	B	14	Total 14	O 14	0	0
7	H	3	Total 3	O 3	0	0
7	J	1	Total 1	O 1	0	0

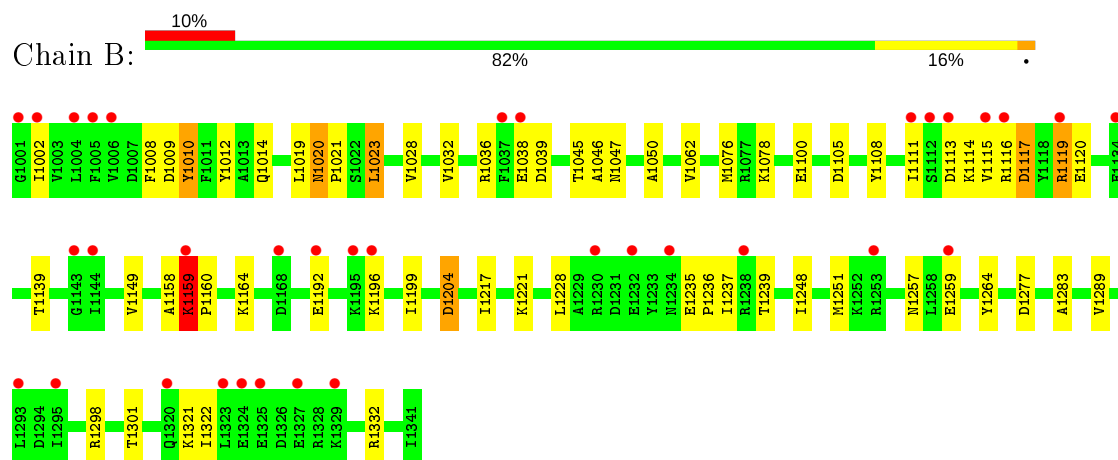
3 Residue-property plots

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.

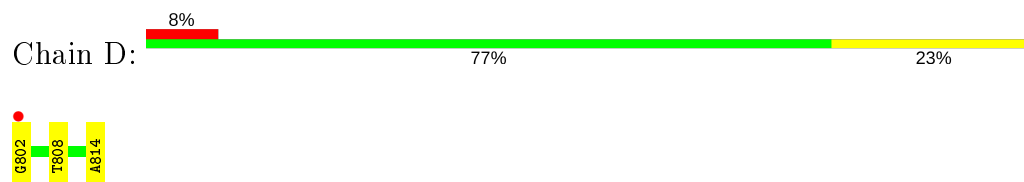
• Molecule 1: DNA polymerase IV



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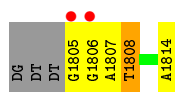


• Molecule 2: DNA (5'-D(*GP*TP*TP*GP*GP*AP*TP*GP*GP*TP*AP*GP*(2DA))-3')



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

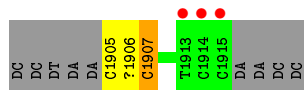
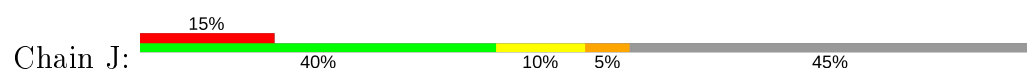




- Molecule 3: DNA (5'-D(*C*CP*TP*AP*AP*CP*(ME6)P*CP*TP*AP*CP*CP*AP*TP*CP*CP*AP*AP*CP*C)-3')



- 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, α , β , γ	52.91Å 109.33Å 100.83Å 90.00° 101.07° 90.00°	Depositor
Resolution (Å)	20.00 – 2.70 19.92 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.0 (20.00-2.70) 98.3 (19.92-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.36 (at 2.71Å)	Xtriage
Refinement program	REFMAC 5.6.0107	Depositor
R, R_{free}	0.203 , 0.247 0.202 , 0.246	Depositor DCC
R_{free} test set	1531 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	60.3	Xtriage
Anisotropy	0.478	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 42.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6694	wwPDB-VP
Average B, all atoms (Å ²)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.61% 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: EPE, CA, ME6, 2DA, 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	0.50	0/2779	0.60	0/3731
1	B	0.40	0/2779	0.52	0/3731
2	D	0.34	0/282	0.93	1/436 (0.2%)
2	H	0.25	0/216	1.09	4/333 (1.2%)
3	E	0.36	0/394	1.03	4/600 (0.7%)
3	J	0.30	0/216	0.96	1/326 (0.3%)
All	All	0.43	0/6666	0.67	10/9157 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	E	913	DT	P-O3'-C3'	8.22	129.56	119.70
2	H	1806	DG	P-O3'-C3'	7.31	128.48	119.70
2	H	1805	DG	P-O3'-C3'	7.02	128.13	119.70
3	E	902	DT	P-O3'-C3'	6.77	127.83	119.70
2	H	1808	DT	C1'-O4'-C4'	-6.47	103.63	110.10
3	E	901	DC	C1'-O4'-C4'	-5.48	104.62	110.10
2	H	1807	DA	P-O3'-C3'	5.44	126.23	119.70
3	E	908	DT	P-O3'-C3'	5.35	126.12	119.70
3	J	1907	DC	C1'-O4'-C4'	-5.29	104.81	110.10
2	D	808	DT	P-O3'-C3'	5.20	125.94	119.70

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	36	0
1	B	2740	0	2880	35	0
2	D	271	0	149	8	0
2	H	212	0	113	4	0
3	E	374	0	217	10	0
3	J	216	0	127	9	0
4	A	31	0	12	1	0
4	B	31	0	12	1	0
5	A	15	0	18	1	0
6	A	3	0	0	0	0
6	B	3	0	0	0	0
7	A	29	0	0	4	0
7	B	14	0	0	1	0
7	D	6	0	0	0	0
7	E	5	0	0	0	0
7	H	3	0	0	0	0
7	J	1	0	0	0	0
All	All	6694	0	6411	92	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 7.

All (92) 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	1.07	0.94
1:B:1159:LYS:HB3	1:B:1160:PRO:HD3	1.50	0.92
1:A:285:HIS:HD2	7:A:356:HOH:O	1.54	0.91
2:D:814:2DA:O5'	2:D:814:2DA:H8	1.86	0.74
3:J:1905:DC:H2''	3:J:1906:ME6:H5'A	1.71	0.71
1:A:14:GLN:NE2	1:A:139:THR:H	1.87	0.71
1:B:1192:GLU:O	1:B:1196:LYS:HG2	1.91	0.70
2:D:814:2DA:H2	3:E:906:ME6:H20B	1.73	0.69
1:B:1117:ASP:HB3	1:B:1120:GLU:HG3	1.75	0.68
2:D:814:2DA:C2	3:E:906:ME6:H20B	2.24	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1100:GLU:HB2	1:B:1237:ILE:HG23	1.75	0.67
1:A:103:SER:OG	1:A:106:GLU:HG2	1.95	0.67
1:B:1159:LYS:HB3	1:B:1160:PRO:CD	2.25	0.65
1:A:97:GLU:H	1:A:97:GLU:CD	1.99	0.64
1:B:1014:GLN:HE22	1:B:1139:THR:H	1.45	0.63
1:B:1159:LYS:CB	1:B:1160:PRO:HD3	2.26	0.62
1:B:1289:VAL:HB	1:B:1332:ARG:HB2	1.81	0.62
1:B:1298:ARG:HG3	1:B:1322:ILE:HG12	1.82	0.62
3:E:915:DC:H2'	3:E:916:DA:C8	2.35	0.62
2:H:1814:2DA:N1	3:J:1906:ME6:H20B	2.14	0.61
2:D:802:DG:H2'	2:D:802:DG:N3	2.15	0.61
1:A:186:ILE:HD11	1:A:225:LEU:HD21	1.82	0.59
1:B:1217:ILE:HD12	1:B:1221:LYS:HB3	1.84	0.59
2:D:814:2DA:N1	3:E:906:ME6:C20	2.66	0.59
1:A:36:ARG:HH22	1:A:254:ASN:ND2	2.00	0.58
1:B:1298:ARG:HG3	1:B:1322:ILE:CG1	2.34	0.57
1:B:1028:VAL:H	1:B:1047:ASN:HB2	1.69	0.56
2:D:814:2DA:N1	3:E:906:ME6:H20B	2.23	0.54
1:A:214:LYS:HE2	1:A:219:GLU:HB2	1.90	0.54
7:B:56:HOH:O	3:J:1905:DC:H5'	2.09	0.52
1:B:1199:ILE:HG23	1:B:1204:ASP:HB2	1.93	0.51
4:B:1414:DGT:O1B	4:B:1414:DGT:H5'A	2.12	0.50
3:E:906:ME6:H2'A	3:E:907:DC:O5'	2.12	0.49
1:A:166:ILE:HG22	1:A:171:VAL:HG23	1.93	0.49
1:B:1111:ILE:HG23	1:B:1114:LYS:HB2	1.95	0.49
2:D:814:2DA:C2	3:E:906:ME6:C20	2.90	0.48
1:A:270:GLU:HG2	1:A:312:TYR:OH	2.13	0.48
2:D:814:2DA:H2	3:E:906:ME6:C20	2.42	0.48
1:A:1:GLY:N	7:A:349:HOH:O	2.46	0.48
1:A:277:ASP:O	1:A:278:LYS:HB2	2.13	0.48
1:B:1298:ARG:HD2	1:B:1321:LYS:HE3	1.95	0.48
1:B:1251:MET:HA	1:B:1264:TYR:CE1	2.49	0.48
1:B:1038:GLU:O	1:B:1039:ASP:HB2	2.14	0.47
1:B:1020:ASN:HD22	1:B:1020:ASN:C	2.18	0.47
1:A:191:ALA:O	1:A:195:LYS:HG2	2.14	0.47
1:B:1298:ARG:HA	2:H:1808:DT:OP2	2.14	0.47
1:A:103:SER:HA	5:A:342:EPE:O2S	2.14	0.46
2:H:1814:2DA:N1	3:J:1906:ME6:C20	2.78	0.46
1:A:254:ASN:HD22	1:A:254:ASN:H	1.64	0.46
1:B:1100:GLU:HB3	1:B:1108:TYR:HB2	1.98	0.46
1:B:1046:ALA:HB1	1:B:1050:ALA:HB3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1235:GLU:HA	1:B:1236:PRO:HD3	1.86	0.45
1:A:20:ASN:HB3	1:A:23:LEU:HD22	1.98	0.45
1:B:1283:ALA:HB2	1:B:1301:THR:HG23	1.99	0.45
1:A:254:ASN:ND2	1:A:254:ASN:H	2.15	0.45
1:A:289:VAL:HB	1:A:332:ARG:HB2	1.99	0.45
1:A:39:ASP:CG	1:A:65:LYS:HE3	2.37	0.45
1:A:199:ILE:HG23	1:A:204:ASP:HB2	1.99	0.44
1:B:1257:ASN:HD21	1:B:1259:GLU:HG3	1.81	0.44
2:H:1814:2DA:C2	3:J:1906:ME6:H20B	2.47	0.44
3:E:906:ME6:HN4	3:E:906:ME6:H20	1.65	0.44
1:A:285:HIS:CD2	7:A:356:HOH:O	2.43	0.44
1:A:37:PHE:CE2	1:A:40:SER:HB3	2.53	0.44
1:B:1002:ILE:HB	1:B:1111:ILE:HB	2.00	0.44
3:E:916:DA:H2''	3:E:917:DA:C8	2.52	0.44
1:A:267:ARG:HD2	7:A:350:HOH:O	2.18	0.43
1:A:36:ARG:HH22	1:A:254:ASN:CG	2.21	0.43
1:A:46:ALA:HB1	1:A:50:ALA:HB3	1.99	0.43
1:B:1332:ARG:HH12	3:J:1906:ME6:H5	1.84	0.43
1:A:14:GLN:HE22	1:A:139:THR:N	1.91	0.43
1:A:38:GLU:O	1:A:39:ASP:HB2	2.19	0.43
1:A:12:TYR:CD2	4:A:414:DGT:H2'	2.54	0.43
1:A:256:ARG:HG3	1:A:329:LYS:HG2	2.01	0.42
1:A:292:ASP:N	1:A:292:ASP:OD1	2.39	0.42
1:B:1116:ARG:O	1:B:1117:ASP:HB2	2.19	0.42
3:J:1906:ME6:H20	3:J:1906:ME6:HN4	1.65	0.42
1:A:36:ARG:NH2	1:A:331:ARG:HG3	2.35	0.42
3:J:1906:ME6:H2'A	3:J:1907:DC:O5'	2.19	0.42
1:B:1158:ALA:HB2	1:B:1164:LYS:HB2	2.02	0.42
1:B:1021:PRO:C	1:B:1023:LEU:H	2.24	0.41
1:A:304:HIS:HD2	1:A:305:GLY:O	2.03	0.41
1:B:1008:PHE:CD1	1:B:1008:PHE:N	2.87	0.41
1:A:19:LEU:HD23	1:A:77:ARG:HH22	1.86	0.41
1:A:19:LEU:HD23	1:A:77:ARG:NH2	2.36	0.41
1:B:1149:VAL:HG21	1:B:1228:LEU:HD21	2.03	0.41
1:A:282:LYS:HE3	1:A:341:ILE:HG12	2.01	0.41
1:A:244:SER:OG	1:A:336:ARG:HD3	2.21	0.40
1:B:1076:MET:HE3	1:B:1078:LYS:HB2	2.03	0.40
1:B:1009:ASP:O	1:B:1010:TYR:C	2.59	0.40
1:B:1012:TYR:HB2	1:B:1045:THR:CG2	2.52	0.40
1:B:1119:ARG:HE	1:B:1119:ARG:HA	1.85	0.40
3:J:1906:ME6:H6	3:J:1906:ME6:H2'	1.72	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%)	324 (96%)	13 (4%)	2 (1%)	25	50
1	B	339/341 (99%)	307 (91%)	25 (7%)	7 (2%)	7	18
All	All	678/682 (99%)	631 (93%)	38 (6%)	9 (1%)	12	30

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1277	ASP
1	B	1036	ARG
1	B	1115	VAL
1	B	1117	ASP
1	A	38	GLU
1	A	10	TYR
1	B	1010	TYR
1	B	1159	LYS
1	B	1239	THR

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	299/299 (100%)	289 (97%)	10 (3%)	38	67
1	B	299/299 (100%)	288 (96%)	11 (4%)	34	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	598/598 (100%)	577 (96%)	21 (4%)	36 65

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LEU
1	A	97	GLU
1	A	98	LYS
1	A	105	ASP
1	A	212	LYS
1	A	223	LYS
1	A	252	LYS
1	A	253	ARG
1	A	296	VAL
1	A	327	GLU
1	B	1019	LEU
1	B	1020	ASN
1	B	1023	LEU
1	B	1032	VAL
1	B	1062	VAL
1	B	1105	ASP
1	B	1113	ASP
1	B	1119	ARG
1	B	1159	LYS
1	B	1204	ASP
1	B	1248	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	254	ASN
1	A	257	ASN
1	A	304	HIS
1	B	1014	GLN
1	B	1020	ASN

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
2	2DA	H	1814	2	17,22,23	1.02	1 (5%)	13,31,34	1.89	4 (30%)
3	ME6	J	1906	3	15,21,22	0.62	0	17,30,33	1.05	2 (11%)
3	ME6	E	906	3	15,21,22	0.83	0	17,30,33	0.96	1 (5%)
2	2DA	D	814	2	17,22,23	1.10	1 (5%)	13,31,34	2.09	7 (53%)

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
2	2DA	H	1814	2	-	0/3/18/19	0/3/3/3
3	ME6	J	1906	3	-	2/4/21/22	0/2/2/2
3	ME6	E	906	3	-	3/4/21/22	0/2/2/2
2	2DA	D	814	2	-	0/3/18/19	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	814	2DA	C5-C4	2.71	1.48	1.40
2	H	1814	2DA	C5-C4	2.70	1.48	1.40

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	814	2DA	C2'-C1'-N9	-3.38	106.12	112.48
2	H	1814	2DA	N3-C2-N1	-3.35	123.44	128.68
2	D	814	2DA	N3-C2-N1	-2.63	124.56	128.68
2	D	814	2DA	C2-N1-C6	2.63	123.26	118.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	814	2DA	C4-C5-N7	-2.62	106.67	109.40
2	H	1814	2DA	C3'-C2'-C1'	2.53	105.71	102.78
2	H	1814	2DA	C2-N1-C6	2.37	122.81	118.75
2	H	1814	2DA	O4'-C4'-C3'	2.29	108.60	104.80
2	D	814	2DA	C5-C6-N1	-2.28	115.19	120.35
3	E	906	ME6	C5-C4-N3	2.17	120.56	118.20
2	D	814	2DA	O4'-C4'-C3'	2.14	108.35	104.80
2	D	814	2DA	C3'-C2'-C1'	2.11	105.22	102.78
3	J	1906	ME6	C5-C4-N3	2.08	120.46	118.20
3	J	1906	ME6	C2'-C1'-N1	-2.03	109.59	114.27

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	J	1906	ME6	O4'-C1'-N1-C6
3	E	906	ME6	O4'-C1'-N1-C6
3	E	906	ME6	O4'-C4'-C5'-O5'
3	E	906	ME6	C3'-C4'-C5'-O5'
3	J	1906	ME6	O4'-C4'-C5'-O5'

There are no ring outliers.

4 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	1814	2DA	3	0
3	J	1906	ME6	8	0
3	E	906	ME6	8	0
2	D	814	2DA	7	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
5	EPE	A	342	-	15,15,15	2.56	6 (40%)	18,20,20	5.29	10 (55%)
4	DGT	B	1414	6	26,33,33	1.08	2 (7%)	32,52,52	3.39	15 (46%)
4	DGT	A	414	6	26,33,33	1.04	1 (3%)	32,52,52	3.47	14 (43%)

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	EPE	A	342	-	-	5/9/19/19	0/1/1/1
4	DGT	B	1414	6	-	6/18/34/34	0/3/3/3
4	DGT	A	414	6	-	3/18/34/34	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	342	EPE	C10-S	-6.19	1.68	1.77
5	A	342	EPE	O3S-S	4.84	1.64	1.47
4	A	414	DGT	C6-N1	4.15	1.40	1.33
4	B	1414	DGT	C6-N1	3.97	1.40	1.33
5	A	342	EPE	C6-N1	3.87	1.57	1.46
5	A	342	EPE	C9-N1	2.61	1.53	1.47
5	A	342	EPE	C6-C5	2.45	1.60	1.51
4	B	1414	DGT	C8-N7	-2.44	1.30	1.34
5	A	342	EPE	C9-C10	2.02	1.58	1.52

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	342	EPE	O2S-S-C10	10.94	120.08	106.92
5	A	342	EPE	O3S-S-O2S	-10.39	85.88	111.27
5	A	342	EPE	O3S-S-O1S	-9.37	88.37	111.27
4	A	414	DGT	C5-C6-N1	-8.66	111.58	123.43
5	A	342	EPE	O1S-S-C10	8.08	116.65	106.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1414	DGT	C5-C6-N1	-8.01	112.47	123.43
5	A	342	EPE	O3S-S-C10	-7.66	93.39	105.77
4	A	414	DGT	PB-O3B-PG	-7.27	107.87	132.83
4	B	1414	DGT	O1G-PG-O3G	-6.90	83.68	110.68
4	A	414	DGT	C6-N1-C2	6.67	126.54	115.93
4	B	1414	DGT	C6-N1-C2	6.66	126.52	115.93
4	B	1414	DGT	O2G-PG-O3G	-6.58	84.92	110.68
4	A	414	DGT	O2G-PG-O3G	-6.31	85.98	110.68
4	A	414	DGT	O1G-PG-O3G	-5.59	88.80	110.68
4	B	1414	DGT	N3-C2-N1	-5.15	120.36	127.22
4	A	414	DGT	O3B-PG-O3G	-5.04	83.26	111.19
4	A	414	DGT	O2G-PG-O3B	5.03	121.50	104.64
4	B	1414	DGT	PA-O3A-PB	-4.99	115.70	132.83
4	B	1414	DGT	O3B-PG-O3G	-4.47	86.40	111.19
4	A	414	DGT	N3-C2-N1	-4.40	121.35	127.22
4	A	414	DGT	PA-O3A-PB	-4.36	117.87	132.83
4	B	1414	DGT	O2G-PG-O3B	4.24	118.85	104.64
4	B	1414	DGT	PB-O3B-PG	-4.14	118.61	132.83
4	B	1414	DGT	O2G-PG-O1G	4.08	123.21	107.64
5	A	342	EPE	C5-C6-N1	-4.06	102.32	110.64
4	A	414	DGT	O1G-PG-O3B	3.96	117.90	104.64
5	A	342	EPE	C5-N4-C3	3.70	117.15	108.83
4	A	414	DGT	C2'-C1'-N9	-3.56	106.06	114.27
4	B	1414	DGT	O1G-PG-O3B	3.29	115.66	104.64
5	A	342	EPE	C6-N1-C2	3.19	116.01	108.83
5	A	342	EPE	C3-C2-N1	3.07	116.95	110.64
4	A	414	DGT	O2G-PG-O1G	3.01	119.14	107.64
4	B	1414	DGT	C2'-C1'-N9	-2.94	107.48	114.27
4	B	1414	DGT	C6-C5-C4	-2.70	118.22	120.80
5	A	342	EPE	O2S-S-O1S	2.67	123.20	113.95
4	B	1414	DGT	N2-C2-N3	2.64	122.10	117.79
4	A	414	DGT	N2-C2-N3	2.35	121.62	117.79
4	B	1414	DGT	C4-C5-N7	2.13	111.62	109.40
4	A	414	DGT	C6-C5-C4	-2.05	118.84	120.80

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1414	DGT	PB-O3B-PG-O2G
4	B	1414	DGT	C5'-O5'-PA-O2A
5	A	342	EPE	C10-C9-N1-C2

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Mol	Chain	Res	Type	Atoms
5	A	342	EPE	C10-C9-N1-C6
4	A	414	DGT	PB-O3A-PA-O5'
5	A	342	EPE	C8-C7-N4-C3
4	B	1414	DGT	C5'-O5'-PA-O3A
4	B	1414	DGT	C5'-O5'-PA-O1A
4	A	414	DGT	C5'-O5'-PA-O1A
5	A	342	EPE	C9-C10-S-O2S
4	B	1414	DGT	PA-O3A-PB-O1B
4	B	1414	DGT	PA-O3A-PB-O2B
5	A	342	EPE	C8-C7-N4-C5
4	A	414	DGT	C5'-O5'-PA-O3A

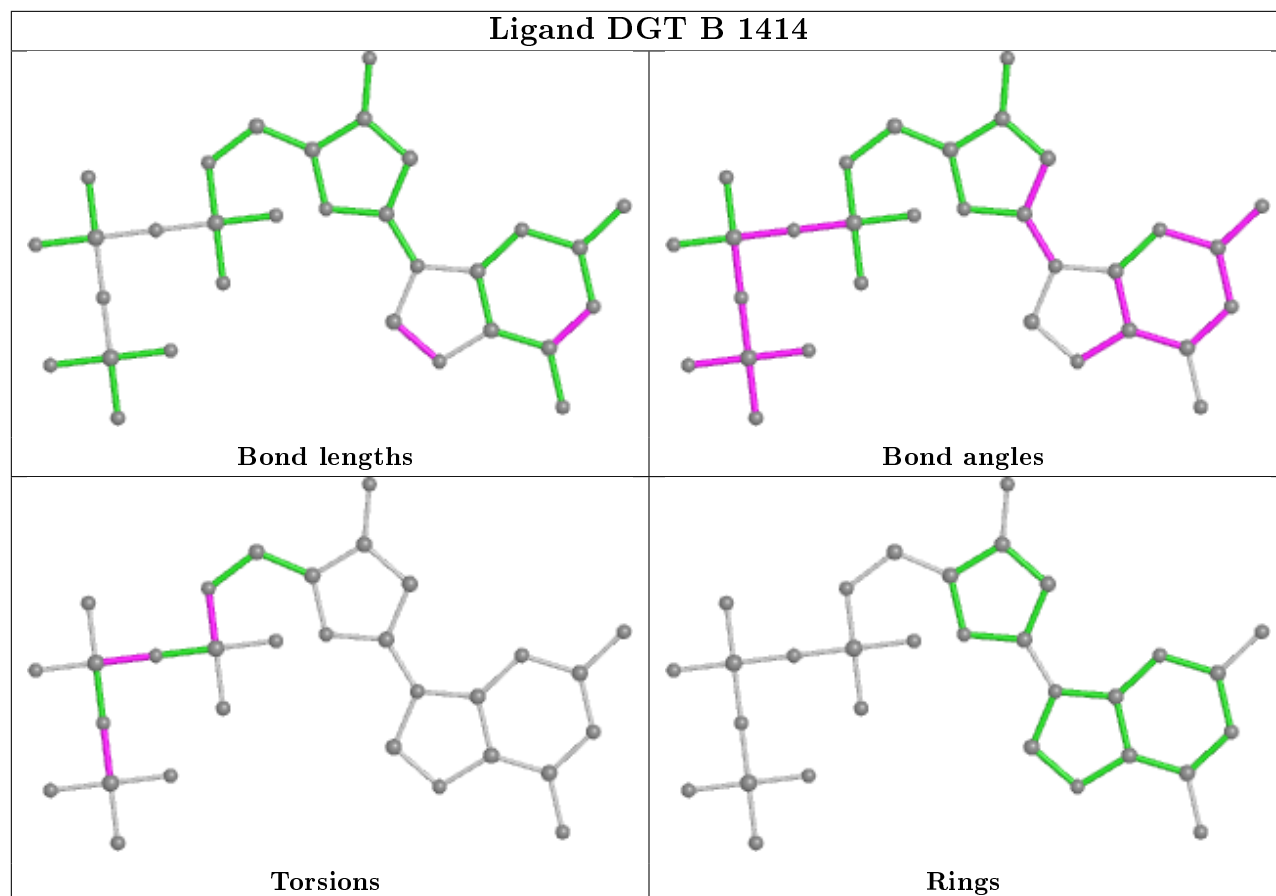
There are no ring outliers.

3 monomers are involved in 3 short contacts:

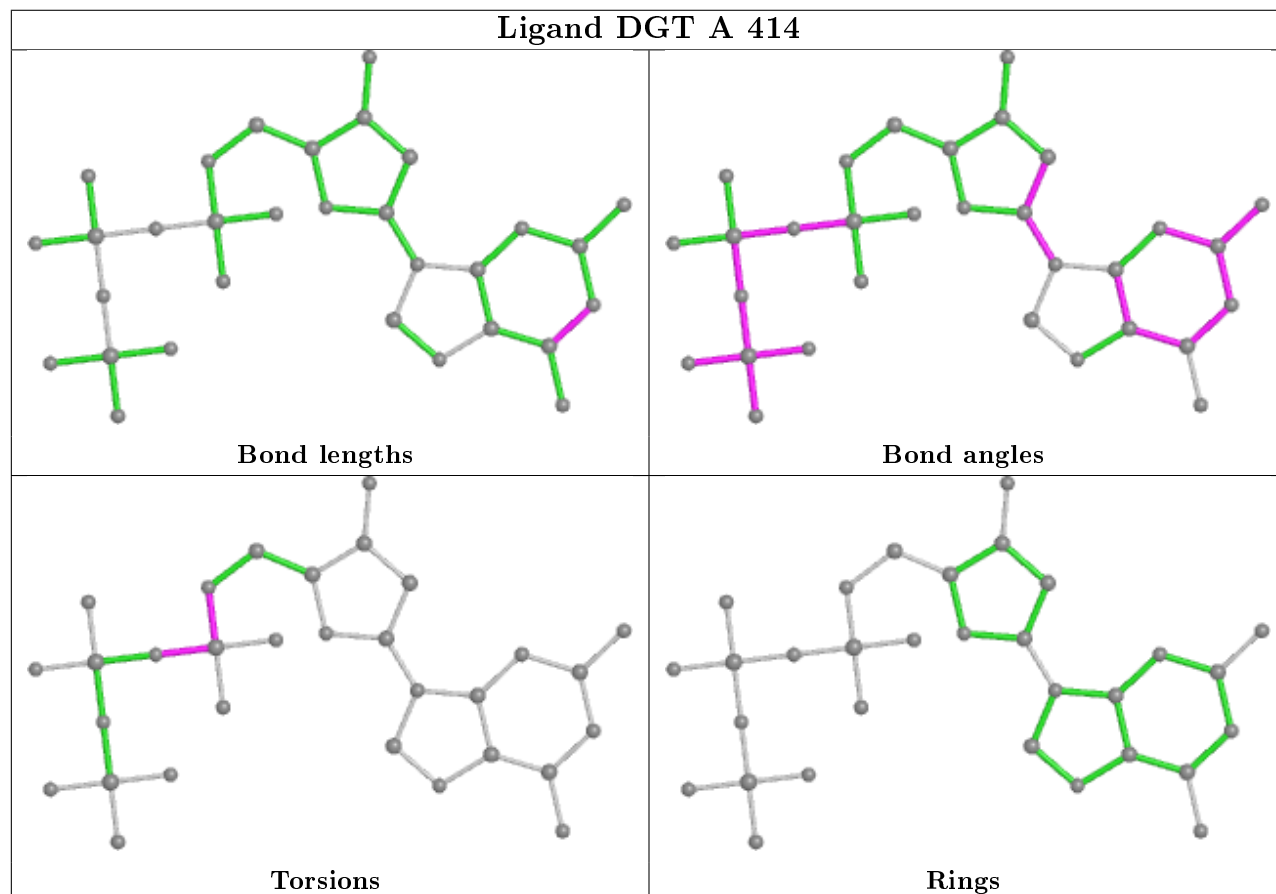
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	342	EPE	1	0
4	B	1414	DGT	1	0
4	A	414	DGT	1	0

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.

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, 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	341/341 (100%)	-0.11	0 100 100	36, 58, 84, 107	0
1	B	341/341 (100%)	0.55	35 (10%) 6 5	62, 104, 144, 166	0
2	D	12/13 (92%)	-0.20	1 (8%) 11 9	43, 64, 135, 147	0
2	H	9/13 (69%)	0.46	2 (22%) 0 0	96, 123, 198, 218	0
3	E	18/20 (90%)	-0.11	1 (5%) 24 23	40, 67, 148, 171	0
3	J	10/20 (50%)	1.09	3 (30%) 0 0	93, 119, 197, 225	0
All	All	731/748 (97%)	0.22	42 (5%) 23 22	36, 78, 138, 225	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1143	GLY	6.0
1	B	1115	VAL	5.3
1	B	1001	GLY	5.0
1	B	1116	ARG	4.9
3	J	1915	DC	4.6
1	B	1113	ASP	4.4
2	H	1805	DG	4.4
1	B	1329	LYS	4.2
1	B	1037	PHE	4.1
1	B	1159	LYS	3.5
1	B	1005	PHE	3.3
3	E	919	DC	3.3
1	B	1004	LEU	3.1
1	B	1134	GLU	3.1
1	B	1232	GLU	3.1
1	B	1324	GLU	2.9
3	J	1914	DC	2.8
1	B	1144	ILE	2.8
1	B	1327	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	1168	ASP	2.8
3	J	1913	DT	2.8
1	B	1293	LEU	2.8
1	B	1259	GLU	2.7
1	B	1238	ARG	2.6
1	B	1002	ILE	2.6
1	B	1295	ILE	2.6
2	H	1806	DG	2.5
1	B	1192	GLU	2.4
1	B	1234	ASN	2.4
1	B	1325	GLU	2.3
1	B	1006	VAL	2.3
1	B	1196	LYS	2.3
1	B	1230	ARG	2.3
1	B	1195	LYS	2.3
1	B	1320	GLN	2.2
1	B	1111	ILE	2.2
1	B	1112	SER	2.2
1	B	1119	ARG	2.2
1	B	1253	ARG	2.1
1	B	1038	GLU	2.0
2	D	802	DG	2.0
1	B	1323	LEU	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(\AA^2)	Q<0.9
2	2DA	H	1814	20/21	0.89	0.30	105,111,113,113	0
3	ME6	J	1906	20/21	0.93	0.12	99,105,113,113	0
2	2DA	D	814	20/21	0.94	0.24	48,52,59,60	0
3	ME6	E	906	20/21	0.97	0.14	40,46,55,60	0

6.3 Carbohydrates [i](#)

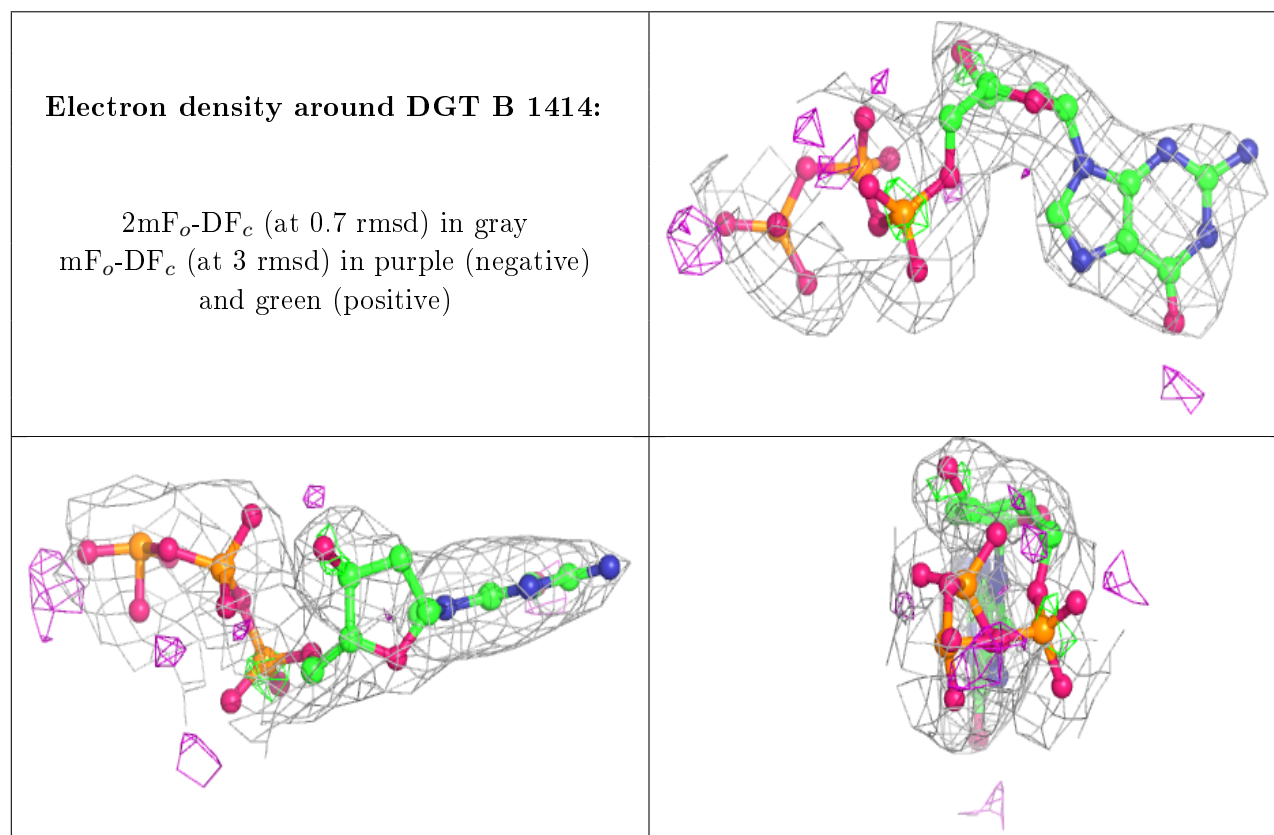
There are no carbohydrates in this entry.

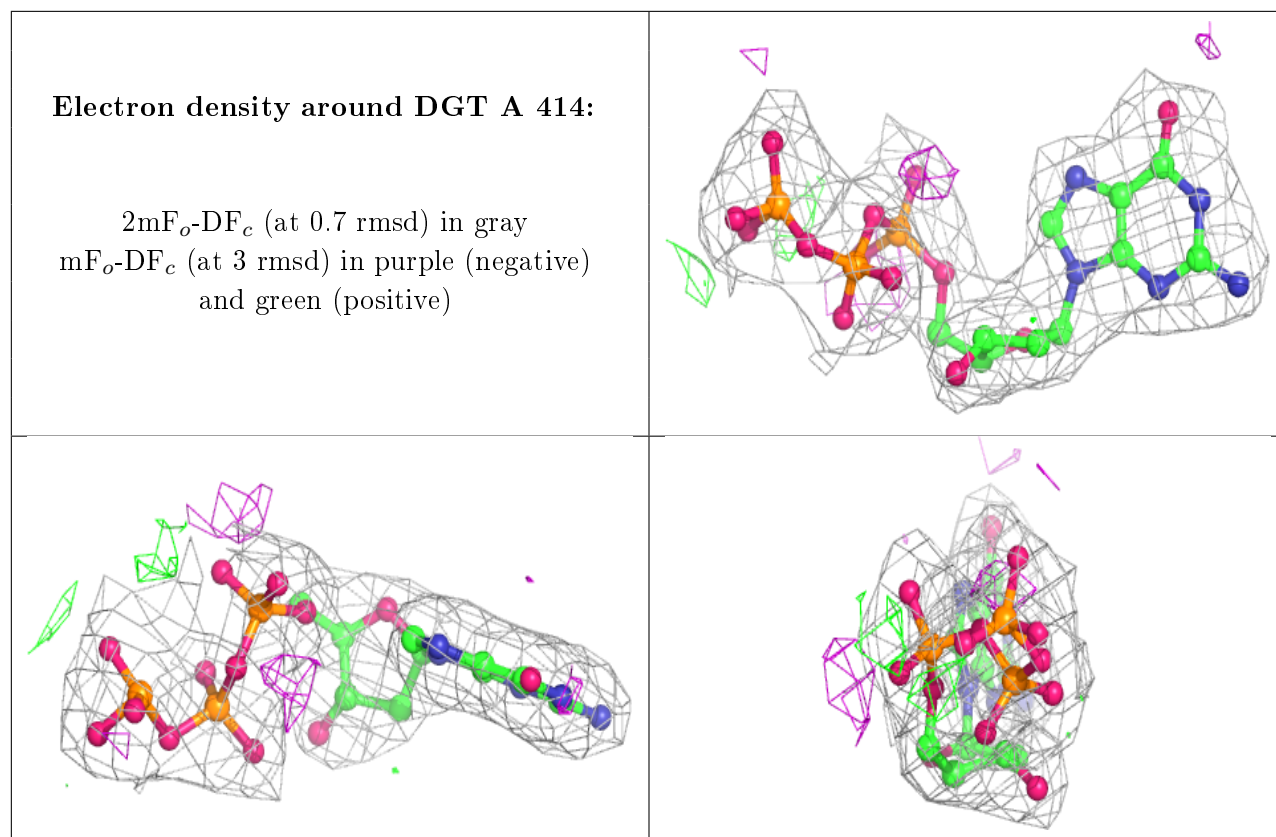
6.4 Ligands [i](#)

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, 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
6	CA	A	415	1/1	0.86	0.11	53,53,53,53	0
6	CA	B	1415	1/1	0.89	0.10	73,73,73,73	0
4	DGT	B	1414	31/31	0.92	0.16	84,90,101,103	0
5	EPE	A	342	15/15	0.96	0.19	52,56,64,64	0
6	CA	B	1416	1/1	0.96	0.03	63,63,63,63	0
6	CA	A	417	1/1	0.97	0.04	58,58,58,58	0
6	CA	B	1417	1/1	0.98	0.07	68,68,68,68	0
4	DGT	A	414	31/31	0.98	0.11	32,35,43,47	0
6	CA	A	416	1/1	0.98	0.15	39,39,39,39	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.