Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:56 AM GMT

PDB ID	:	3GIL
Title	:	Dpo4 extension ternary complex with oxoG(anti)-T(anti) pair
Authors	:	Rechkoblit, O.; Malinina, L.; Patel, D.J.
Deposited on	:	2009-03-05
Resolution	:	2.71 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

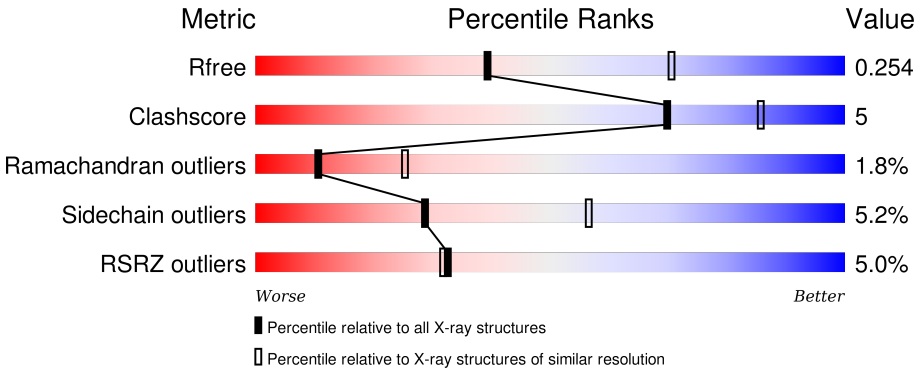
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.71 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}	91344	2439 (2.74-2.70)
Clashscore	102246	2771 (2.74-2.70)
Ramachandran outliers	100387	2726 (2.74-2.70)
Sidechain outliers	100360	2727 (2.74-2.70)
RSRZ outliers	91569	2443 (2.74-2.70)

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. 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 <=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	89% 8%
1	B	341	7% 79% 18%
2	D	13	8% 62% 31% 8%
2	H	13	31% 69% 23% 8%
3	E	18	67% 28% 6%

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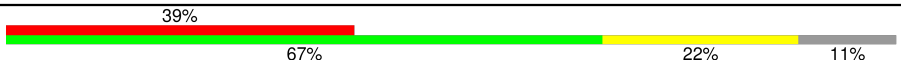
Mol	Chain	Length	Quality of chain
3	J	18	

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
3	8OG	E	906	X	-	-	-
3	8OG	J	1906	X	-	-	-
5	CA	B	1417	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6894 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	1	0
			2750	1763	475	506	6			

There are 2 discrepancies between the modelled and reference sequences:

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

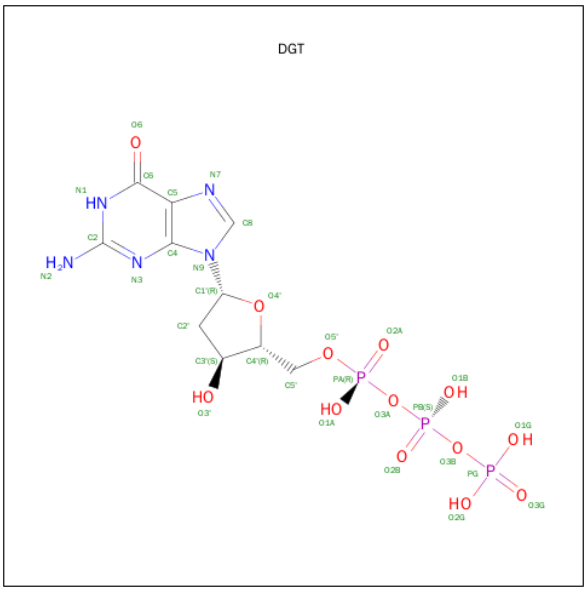
- Molecule 2 is a DNA chain called 5'-D(*GP*TP*TP*GP*GP*AP*TP*GP*GP*TP*AP*GP*(2DT))-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	13	Total	C	N	O	P	0	0	0
			270	130	50	78	12			
2	H	13	Total	C	N	O	P	0	0	0
			270	130	50	78	12			

- Molecule 3 is a DNA chain called 5'-D(*CP*TP*AP*AP*CP*(8OG)P*CP*TP*AP*CP*CP*AP*TP*CP*CP*AP*AP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	18	Total	C	N	O	P	0	0	0
			358	172	65	104	17			
3	J	16	Total	C	N	O	P	0	0	0
			319	153	60	91	15			

- Molecule 4 is 2'-DEOXYGUANOSINE-5'-TRIPHOSPHATE (three-letter code: DGT) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

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

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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	74	Total O 74 74	0	0
6	B	21	Total O 21 21	0	0
6	D	13	Total O 13 13	0	0
6	E	6	Total O 6 6	0	0
6	H	2	Total O 2 2	0	0

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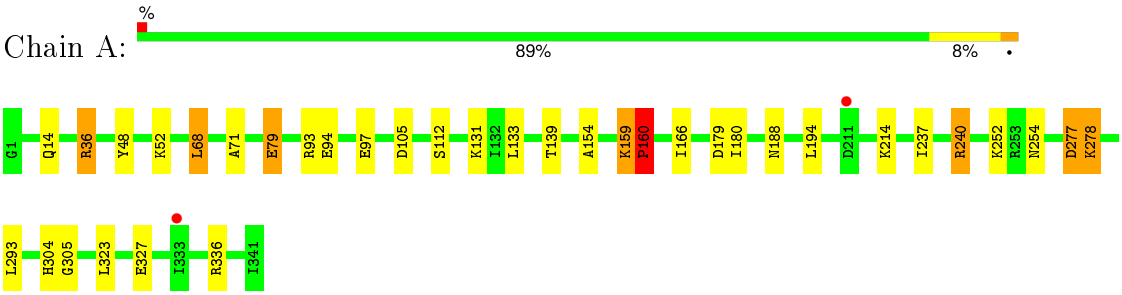
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	J	3	Total O 3 3	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

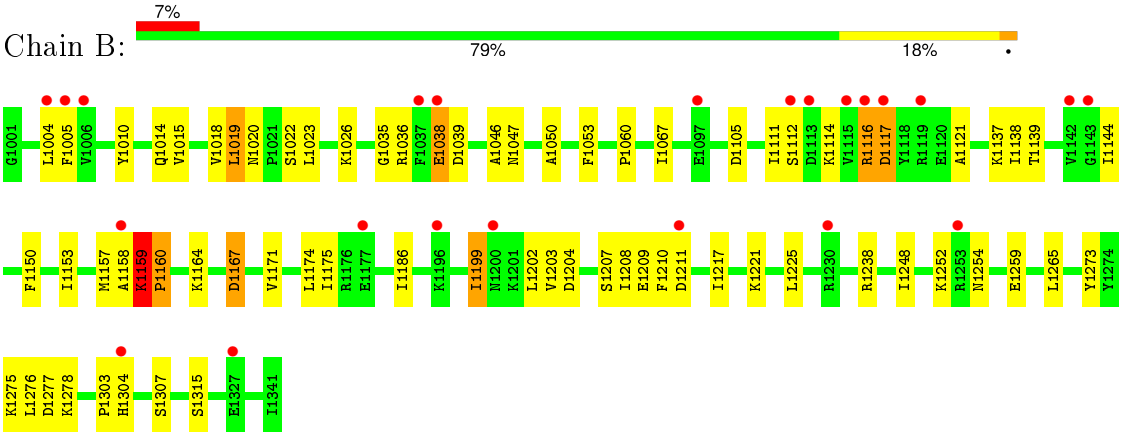
- Molecule 1: DNA polymerase IV

Chain A:



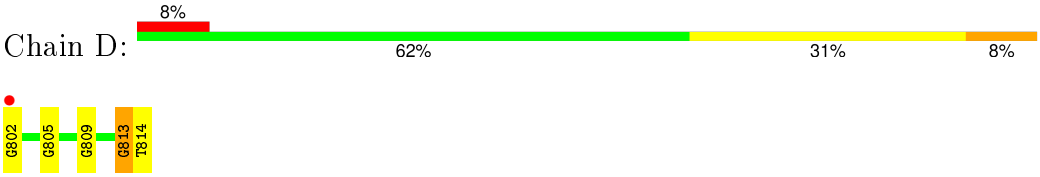
- Molecule 1: DNA polymerase IV

Chain B:



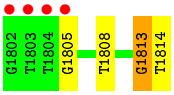
- Molecule 2: 5'-D(*GP*TP*TP*GP*GP*AP*TP*GP*GP*TP*AP*GP*(2DT))-3'

Chain D:



- Molecule 2: 5'-D(*GP*TP*TP*GP*GP*AP*TP*GP*GP*TP*AP*GP*(2DT))-3'

Chain H:

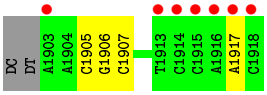


• Molecule 3: 5'-D(*CP*TP*AP*AP*CP*(8OG)P*CP*TP*AP*CP*CP*AP*TP*CP*CP*AP*AP*C)-3'

Chain E:

• Molecule 3: 5'-D(*CP*TP*AP*AP*CP*(8OG)P*CP*TP*AP*CP*CP*AP*TP*CP*CP*AP*AP*C)-3'

Chain J:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	53.29Å 110.68Å 102.19Å 90.00° 99.22° 90.00°	Depositor
Resolution (Å)	20.00 – 2.71 19.99 – 2.71	Depositor EDS
% Data completeness (in resolution range)	98.8 (20.00-2.71) 98.7 (19.99-2.71)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.20 (at 2.71Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.200 , 0.259 0.200 , 0.254	Depositor DCC
R_{free} test set	1583 reflections (5.31%)	DCC
Wilson B-factor (Å^2)	52.1	Xtriage
Anisotropy	0.275	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 50.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	1 of 31370 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6894	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.07% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: 2DT, CA, DGT, 8OG

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	0.59	0/2779	0.64	3/3731 (0.1%)
1	B	0.45	0/2790	0.59	0/3746
2	D	0.86	0/282	1.51	4/436 (0.9%)
2	H	0.72	0/282	1.45	5/436 (1.1%)
3	E	0.93	0/373	1.64	8/568 (1.4%)
3	J	0.81	0/330	1.43	2/502 (0.4%)
All	All	0.60	0/6836	0.88	22/9419 (0.2%)

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	1
1	B	0	2
3	E	1	0
3	J	1	0
All	All	2	3

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	907	DC	O4'-C4'-C3'	-10.53	99.68	106.00
3	E	907	DC	C1'-O4'-C4'	-8.73	101.37	110.10
1	A	159	LYS	C-N-CD	-8.20	102.55	120.60
2	D	802	DG	O4'-C4'-C3'	-8.13	101.12	106.00
3	J	1917	DA	O4'-C1'-N9	7.83	113.48	108.00
2	H	1813	DG	O4'-C1'-N9	7.81	113.47	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	813	DG	O4'-C1'-N9	7.71	113.40	108.00
2	H	1805	DG	P-O3'-C3'	7.29	128.44	119.70
3	E	905	DC	O4'-C1'-N1	-6.88	103.19	108.00
3	E	907	DC	P-O5'-C5'	-6.51	110.48	120.90
1	A	159	LYS	C-N-CA	6.22	148.13	122.00
2	H	1805	DG	O4'-C1'-N9	5.95	112.16	108.00
2	H	1805	DG	C1'-O4'-C4'	-5.87	104.23	110.10
3	E	902	DT	P-O3'-C3'	5.84	126.71	119.70
3	J	1905	DC	O4'-C1'-N1	-5.81	103.94	108.00
2	H	1808	DT	C1'-O4'-C4'	-5.75	104.35	110.10
2	D	805	DG	O4'-C1'-N9	5.73	112.01	108.00
3	E	903	DA	P-O5'-C5'	-5.60	111.94	120.90
3	E	907	DC	O4'-C1'-C2'	-5.50	101.50	105.90
1	A	160	PRO	CA-N-CD	-5.43	103.89	111.50
3	E	907	DC	C4'-C3'-C2'	-5.36	98.28	103.10
2	D	809	DG	O4'-C1'-N9	5.28	111.69	108.00

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	E	906	8OG	C1'
3	J	1906	8OG	C1'

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	159	LYS	Peptide
1	B	1159	LYS	Peptide
1	B	1303	PRO	Peptide

5.2 Too-close contacts (i)

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	21	0
1	B	2750	0	2886	34	0
2	D	270	0	150	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	270	0	150	2	0
3	E	358	0	201	3	0
3	J	319	0	178	2	0
4	A	31	0	12	0	0
4	B	31	0	12	1	0
5	A	3	0	0	0	0
5	B	3	0	0	0	0
6	A	74	0	0	1	0
6	B	21	0	0	0	0
6	D	13	0	0	0	0
6	E	6	0	0	0	0
6	H	2	0	0	0	0
6	J	3	0	0	1	0
All	All	6894	0	6472	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:68:LEU:HD13	1:A:71:ALA:HB2	1.44	0.97
1:B:1014:GLN:HE22	1:B:1139:THR:H	1.17	0.91
1:A:14:GLN:HE22	1:A:139:THR:H	1.24	0.85
1:B:1158:ALA:HB2	1:B:1164:LYS:HB2	1.73	0.71
1:A:293:LEU:HD11	3:E:904:DA:C8	2.25	0.71
1:A:180:ILE:HD13	1:A:194:LEU:HD13	1.72	0.70
1:A:133:LEU:CD1	1:A:139:THR:HG22	2.24	0.68
1:B:1111:ILE:CG2	1:B:1114:LYS:O	2.45	0.65
1:B:1026:LYS:O	1:B:1047:ASN:ND2	2.33	0.62
1:A:133:LEU:HD11	1:A:139:THR:HG22	1.82	0.60
1:B:1046:ALA:HB1	1:B:1050:ALA:HB3	1.83	0.60
1:B:1111:ILE:HG22	1:B:1114:LYS:O	2.01	0.60
1:B:1020:ASN:OD1	1:B:1022:SER:OG	2.20	0.59
1:A:14:GLN:NE2	1:A:139:THR:H	1.98	0.59
1:B:1167:ASP:O	1:B:1171:VAL:HG23	2.03	0.58
1:B:1111:ILE:HG23	1:B:1114:LYS:HB2	1.87	0.56
1:B:1121:ALA:HB1	1:B:1144:ILE:HD13	1.88	0.56
1:B:1159:LYS:HB3	1:B:1160:PRO:CD	2.37	0.54
1:B:1199:ILE:HG23	1:B:1204:ASP:HB2	1.88	0.54
1:B:1014:GLN:HE22	1:B:1139:THR:N	1.96	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1038:GLU:O	1:B:1039:ASP:HB2	2.09	0.53
1:A:277:ASP:O	1:A:278:LYS:HB2	2.11	0.50
1:B:1150:PHE:HA	1:B:1153:ILE:HD12	1.93	0.50
1:B:1265:LEU:HD21	1:B:1315:SER:HB2	1.92	0.50
2:D:813:DG:H2"	2:D:814:2DT:H5"	1.95	0.49
1:B:1014:GLN:NE2	1:B:1138:ILE:HA	2.27	0.48
1:A:240:ARG:HB3	6:A:506:HOH:O	2.14	0.48
1:B:1207:SER:O	1:B:1208:ILE:HD12	2.15	0.47
1:A:48:TYR:OH	1:A:160:PRO:HD3	2.15	0.47
1:B:1248:ILE:CG2	3:J:1906:8OG:H2"	2.44	0.47
3:J:1906:8OG:H2'	3:J:1907:DC:O4'	2.15	0.46
1:B:1116:ARG:O	1:B:1117:ASP:CB	2.63	0.46
3:E:907:DC:H2'	3:E:908:DT:C6	2.51	0.46
1:B:1116:ARG:O	1:B:1117:ASP:HB2	2.16	0.46
1:B:1175:ILE:HG22	1:B:1203:VAL:HB	1.97	0.46
1:B:1004:LEU:HD23	1:B:1004:LEU:C	2.36	0.46
1:A:304:HIS:HD2	1:A:305:GLY:O	1.99	0.45
1:B:1018:VAL:HG13	1:B:1137:LYS:HD2	1.98	0.45
1:B:1186:ILE:HD11	1:B:1225:LEU:HD21	1.98	0.45
1:A:48:TYR:CE2	1:A:160:PRO:HG3	2.52	0.44
1:A:48:TYR:CZ	1:A:160:PRO:HD3	2.53	0.44
1:A:36:ARG:NH2	1:A:254:ASN:OD1	2.50	0.44
1:B:1004:LEU:HD23	1:B:1005:PHE:N	2.33	0.43
1:A:277:ASP:O	1:A:277:ASP:CG	2.57	0.43
1:B:1060:PRO:HB3	6:J:599:HOH:O	2.19	0.43
1:B:1217:ILE:HD12	1:B:1221:LYS:HB3	2.01	0.43
1:B:1254:ASN:HD22	1:B:1254:ASN:H	1.67	0.43
4:B:1414:DGT:N7	2:H:1814:2DT:H2'	2.34	0.42
1:B:1273:TYR:HA	1:B:1276:LEU:HD12	2.00	0.42
1:A:79:GLU:H	1:A:79:GLU:CD	2.22	0.42
2:H:1813:DG:H2"	2:H:1814:2DT:H6	2.02	0.42
1:A:154:ALA:HB2	1:A:166:ILE:HD12	2.01	0.41
1:B:1035:GLY:O	1:B:1036:ARG:C	2.58	0.41
1:A:188:ASN:N	1:A:188:ASN:HD22	2.19	0.41
1:A:336:ARG:NH2	3:E:908:DT:OP2	2.54	0.41
1:B:1053:PHE:O	1:B:1067:ILE:HG21	2.21	0.41
1:B:1015:VAL:HG12	1:B:1019:LEU:HD22	2.03	0.41
1:A:237:ILE:N	1:A:237:ILE:HD12	2.36	0.40
1:B:1157:MET:CE	1:B:1174:LEU:HD21	2.52	0.40
1:A:277:ASP:O	1:A:278:LYS:CB	2.70	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	339/341 (99%)	332 (98%)	5 (2%)	2 (1%)	30 58
1	B	340/341 (100%)	316 (93%)	14 (4%)	10 (3%)	6 13
All	All	679/682 (100%)	648 (95%)	19 (3%)	12 (2%)	11 25

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	160	PRO
1	B	1117	ASP
1	B	1159	LYS
1	B	1160	PRO
1	B	1210	PHE
1	B	1277	ASP
1	B	1112	SER
1	B	1209	GLU
1	A	278	LYS
1	B	1010	TYR
1	B	1278	LYS
1	B	1199	ILE

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%)	282 (94%)	17 (6%)	25 52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	300/299 (100%)	285 (95%)	15 (5%)	30 59
All	All	599/598 (100%)	567 (95%)	32 (5%)	29 56

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	ARG
1	A	52	LYS
1	A	68	LEU
1	A	79	GLU
1	A	93	ARG
1	A	94	GLU
1	A	97	GLU
1	A	105	ASP
1	A	112	SER
1	A	131	LYS
1	A	179	ASP
1	A	214	LYS
1	A	240	ARG
1	A	252	LYS
1	A	277	ASP
1	A	323	LEU
1	A	327	GLU
1	B	1019	LEU
1	B	1023	LEU
1	B	1038	GLU
1	B	1105	ASP
1	B	1116	ARG
1	B	1167	ASP
1	B	1202	LEU
1	B	1211	ASP
1	B	1238	ARG
1	B	1252	LYS
1	B	1259	GLU
1	B	1275	LYS
1	B	1304[A]	HIS
1	B	1304[B]	HIS
1	B	1307	SER

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	188	ASN
1	A	304	HIS
1	B	1014	GLN
1	B	1047	ASN
1	B	1254	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	2DT	D	814	3,2	11,20,21	1.30	2 (18%)	12,28,31	4.62	4 (33%)
3	8OG	E	906	3,2	16,25,26	3.30	4 (25%)	21,37,40	4.80	15 (71%)
2	2DT	H	1814	3,2	11,20,21	1.41	2 (18%)	12,28,31	4.26	2 (16%)
3	8OG	J	1906	3,2	16,25,26	3.26	4 (25%)	21,37,40	4.79	14 (66%)

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	2DT	D	814	3,2	-	0/3/18/19	0/2/2/2
3	8OG	E	906	3,2	1/1/4/4	0/3/21/22	0/3/3/3
2	2DT	H	1814	3,2	-	0/3/18/19	0/2/2/2
3	8OG	J	1906	3,2	1/1/4/4	0/3/21/22	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	906	8OG	O3'-C3'	-9.60	1.21	1.43
3	J	1906	8OG	O3'-C3'	-9.36	1.22	1.43
3	J	1906	8OG	C3'-C4'	-7.34	1.32	1.53
3	E	906	8OG	C3'-C4'	-7.23	1.32	1.53
3	J	1906	8OG	C6-C5	2.46	1.46	1.41
2	D	814	2DT	C6-N1	2.49	1.38	1.35
2	H	1814	2DT	C4-N3	2.78	1.38	1.33
2	D	814	2DT	C4-N3	2.92	1.38	1.33
3	E	906	8OG	C5-C4	3.00	1.47	1.40
2	H	1814	2DT	C6-N1	3.12	1.39	1.35
3	E	906	8OG	C6-C5	3.54	1.48	1.41
3	J	1906	8OG	C5-C4	3.88	1.49	1.40

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	1814	2DT	C5-C4-N3	-8.31	115.89	125.14
2	D	814	2DT	C5-C4-N3	-8.19	116.02	125.14
3	J	1906	8OG	C5-C6-N1	-5.32	116.31	123.59
3	E	906	8OG	C6-C5-C4	-5.17	114.72	120.90
2	D	814	2DT	C3'-C2'-C1'	-4.84	97.29	102.71
3	E	906	8OG	C5-C6-N1	-4.23	117.80	123.59
3	J	1906	8OG	C6-C5-C4	-3.87	116.27	120.90
3	E	906	8OG	C1'-N9-C4	-3.85	121.40	127.37
3	E	906	8OG	N3-C2-N1	-3.67	121.86	127.44
3	E	906	8OG	C4'-O4'-C1'	-3.49	100.63	109.47
3	J	1906	8OG	C4'-O4'-C1'	-3.36	100.97	109.47
3	J	1906	8OG	N3-C2-N1	-3.20	122.57	127.44
3	J	1906	8OG	C1'-N9-C4	-2.96	122.78	127.37
3	J	1906	8OG	O5'-C5'-C4'	-2.25	100.86	109.12
3	E	906	8OG	N2-C2-N1	2.01	120.52	117.20
3	E	906	8OG	C2'-C3'-C4'	2.03	106.99	102.77
3	E	906	8OG	O4'-C4'-C3'	2.18	111.14	105.67
3	E	906	8OG	O3'-C3'-C4'	2.18	118.85	110.05
2	D	814	2DT	C5M-C5-C6	2.30	123.25	118.62
3	J	1906	8OG	O4'-C4'-C5'	2.43	118.00	109.32
3	E	906	8OG	O4'-C4'-C5'	2.63	118.73	109.32
3	E	906	8OG	O3'-C3'-C2'	2.76	119.86	110.74
3	E	906	8OG	O4'-C1'-C2'	2.77	111.79	106.27
3	J	1906	8OG	C2'-C3'-C4'	2.98	108.95	102.77
3	J	1906	8OG	O4'-C4'-C3'	3.07	113.38	105.67
3	J	1906	8OG	O4'-C1'-C2'	3.19	112.63	106.27
3	J	1906	8OG	O3'-C3'-C2'	3.28	121.59	110.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	906	8OG	C6-N1-C2	5.33	123.34	115.94
3	J	1906	8OG	C6-N1-C2	6.19	124.53	115.94
3	E	906	8OG	O4'-C1'-N9	11.12	117.62	108.22
2	H	1814	2DT	C4-N3-C2	11.79	125.44	115.25
3	J	1906	8OG	O4'-C1'-N9	12.32	118.64	108.22
2	D	814	2DT	C4-N3-C2	12.37	125.94	115.25
3	J	1906	8OG	C2'-C1'-N9	12.63	128.49	115.83
3	E	906	8OG	C2'-C1'-N9	14.11	129.98	115.83

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	E	906	8OG	C1'
3	J	1906	8OG	C1'

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	814	2DT	1	0
2	H	1814	2DT	2	0
3	J	1906	8OG	2	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 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	A	414	5	25,33,33	0.97	1 (4%)	35,52,52	3.40	13 (37%)
4	DGT	B	1414	5	25,33,33	1.07	1 (4%)	35,52,52	3.43	14 (40%)

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	A	414	5	-	0/18/34/34	0/3/3/3
4	DGT	B	1414	5	-	0/18/34/34	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	414	DGT	C6-N1	3.05	1.38	1.33
4	B	1414	DGT	C6-N1	3.69	1.40	1.33

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	414	DGT	C5-C6-N1	-9.29	110.89	123.59
4	B	1414	DGT	C5-C6-N1	-8.84	111.51	123.59
4	A	414	DGT	O1G-PG-O3G	-8.20	84.19	110.58
4	B	1414	DGT	PB-O3B-PG	-7.67	106.94	132.67
4	B	1414	DGT	O1G-PG-O3G	-7.49	86.46	110.58
4	A	414	DGT	O2G-PG-O3G	-7.07	87.83	110.58
4	A	414	DGT	PB-O3B-PG	-6.63	110.45	132.67
4	B	1414	DGT	O2G-PG-O3G	-6.05	91.10	110.58
4	B	1414	DGT	N3-C2-N1	-4.84	120.08	127.44
4	A	414	DGT	PA-O3A-PB	-4.23	120.85	132.73
4	B	1414	DGT	C2'-C1'-N9	-3.21	106.35	114.16
4	B	1414	DGT	PA-O3A-PB	-3.20	123.75	132.73
4	A	414	DGT	N3-C2-N1	-2.94	122.97	127.44
4	A	414	DGT	C2'-C1'-N9	-2.84	107.25	114.16
4	B	1414	DGT	C6-C5-C4	-2.44	117.98	120.90
4	A	414	DGT	O1B-PB-O3A	2.28	115.44	105.09
4	B	1414	DGT	O1B-PB-O3A	2.34	115.72	105.09
4	A	414	DGT	O2G-PG-O3B	2.99	118.66	105.09
4	A	414	DGT	O3A-PA-O5'	3.05	111.03	102.94
4	B	1414	DGT	O2G-PG-O3B	3.24	119.77	105.09
4	B	1414	DGT	O1G-PG-O3B	3.25	119.86	105.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	414	DGT	O1G-PG-O3B	3.28	119.96	105.09
4	B	1414	DGT	O2G-PG-O1G	3.32	120.03	107.38
4	A	414	DGT	O2G-PG-O1G	3.43	120.43	107.38
4	B	1414	DGT	O4'-C1'-N9	3.48	113.73	107.72
4	A	414	DGT	C6-N1-C2	7.42	126.24	115.94
4	B	1414	DGT	C6-N1-C2	7.96	126.99	115.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1414	DGT	1	0

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, 95^{th} 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%)	0.17	2 (0%) 90 91	40, 49, 61, 68	0
1	B	341/341 (100%)	0.46	23 (6%) 21 20	37, 50, 65, 70	0
2	D	12/13 (92%)	0.22	1 (8%) 14 12	38, 50, 77, 79	0
2	H	12/13 (92%)	1.83	4 (33%) 0 0	39, 49, 85, 87	0
3	E	17/18 (94%)	0.08	0 100 100	45, 51, 67, 68	0
3	J	15/18 (83%)	2.17	7 (46%) 0 0	31, 45, 82, 84	0
All	All	738/744 (99%)	0.37	37 (5%) 32 32	31, 50, 66, 87	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	J	1918	DC	9.1
2	H	1802	DG	7.2
3	J	1916	DA	5.9
2	H	1803	DT	5.1
3	J	1917	DA	4.8
3	J	1903	DA	4.6
1	B	1327	GLU	3.7
3	J	1914	DC	3.6
2	H	1804	DT	3.4
1	B	1113	ASP	3.4
3	J	1915	DC	3.4
1	B	1112	SER	3.3
1	B	1006	VAL	3.2
1	B	1097	GLU	3.2
1	B	1115	VAL	3.2
1	B	1117	ASP	3.2
2	H	1805	DG	3.2
1	B	1196	LYS	3.0
1	B	1119	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
2	D	802	DG	2.9
1	B	1005	PHE	2.8
1	B	1038	GLU	2.7
1	B	1211	ASP	2.6
1	B	1253	ARG	2.5
1	B	1004	LEU	2.5
1	B	1143	GLY	2.4
1	B	1116	ARG	2.3
1	B	1158	ALA	2.3
1	B	1037	PHE	2.3
1	B	1177	GLU	2.3
3	J	1913	DT	2.3
1	B	1142	VAL	2.2
1	B	1304[A]	HIS	2.1
1	A	211	ASP	2.1
1	B	1200	ASN	2.1
1	A	333	ILE	2.1
1	B	1230	ARG	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
2	2DT	H	1814	19/20	0.90	0.23	-	48,51,54,54	0
3	8OG	E	906	23/24	0.97	0.15	-	41,47,48,49	0
2	2DT	D	814	19/20	0.95	0.17	-	43,46,48,50	0
3	8OG	J	1906	23/24	0.96	0.12	-	31,33,34,36	0

6.3 Carbohydrates (i)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
5	CA	B	1417	1/1	0.70	0.29	2.79	64,64,64,64	0
5	CA	A	417	1/1	0.97	0.17	0.33	60,60,60,60	0
5	CA	B	1415	1/1	0.95	0.18	-0.27	47,47,47,47	0
4	DGT	B	1414	31/31	0.94	0.15	-0.75	23,25,37,40	0
5	CA	B	1416	1/1	0.98	0.13	-0.85	40,40,40,40	0
4	DGT	A	414	31/31	0.97	0.14	-1.44	34,37,40,43	0
5	CA	A	416	1/1	0.91	0.08	-2.89	38,38,38,38	0
5	CA	A	415	1/1	0.95	0.07	-	37,37,37,37	0

6.5 Other polymers

There are no such residues in this entry.