



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 04:48 am GMT

PDB ID : 2VA3  
Title : COMPLEX STRUCTURE OF SULFOLOBUS SOLFATARICUS DPO4 AND  
DNA DUPLEX CONTAINING A HYDROPHOBIC THYMINE ISOSTERE  
2,4-DIFLUOROTOLUENE NUCLEOTIDE IN THE TEMPLATE STRAND  
Authors : Irimia, A.; Pallan, P.S.; Egli, M.  
Deposited on : 2007-08-28  
Resolution : 2.98 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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

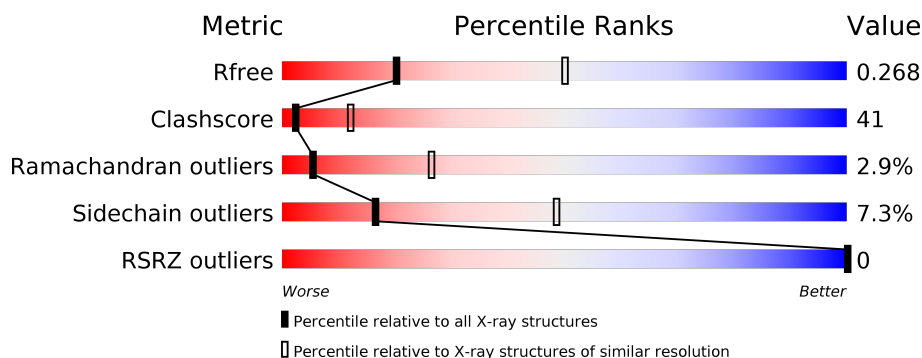
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.98 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))
$R_{free}$	100719	2168 (3.00-2.96)
Clashscore	112137	2535 (3.00-2.96)
Ramachandran outliers	110173	2451 (3.00-2.96)
Sidechain outliers	110143	2454 (3.00-2.96)
RSRZ outliers	101464	2192 (3.00-2.96)

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. 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	358	
2	P	13	
3	T	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	DFT	T	5	-	-	X	-
4	DGT	A	1344	-	-	X	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 3441 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	343	Total	C	N	O	S	0	0	1
			2753	1765	474	507	7			

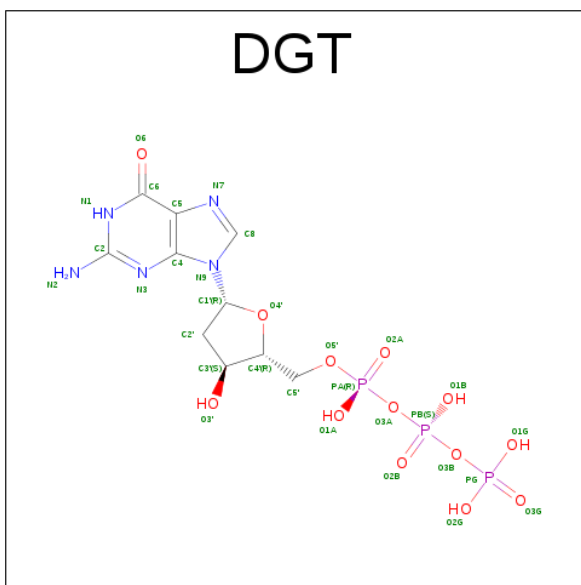
- Molecule 2 is a DNA chain called 5'-D(\*GP\*GP\*GP\*GP\*GP\*AP\*AP\*GP\*GP\*AP\*CP\*TP\*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	13	Total	C	N	O	P	0	0	0
			274	129	60	73	12			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	T	16	Total	C	F	N	O	P	0	0	0
			317	154	2	47	98	16			

- 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 31	C 10	N 5	O 13	P 3	0	0

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

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

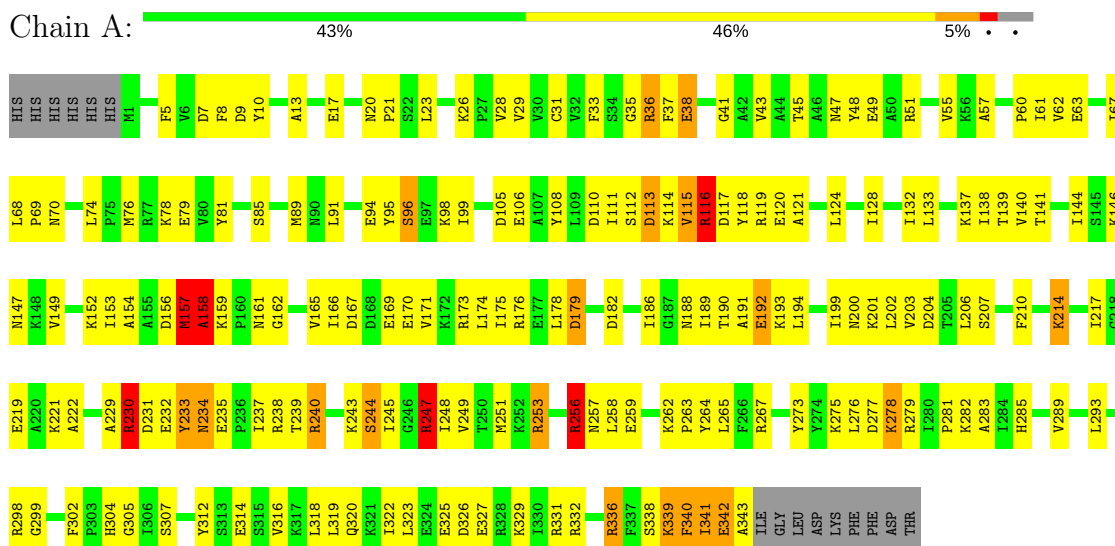
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	46	Total O 46 46	0	0
6	P	11	Total O 11 11	0	0
6	T	6	Total O 6 6	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.

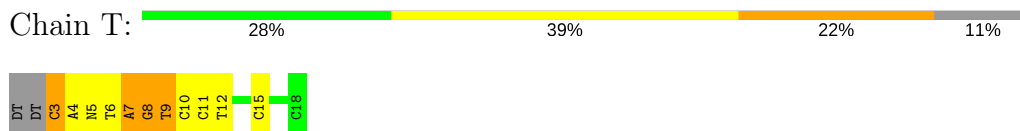
#### • Molecule 1: DNA POLYMERASE IV



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



#### • Molecule 3: 5'-D(\*TP\*TP\*CP\*AP\*DFTP\*TP\*AP\*GP\*TP\*CP\*CP \*TP\*TP\*CP\*CP\*CP\*C P\*C)-3'



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	94.62Å 103.57Å 52.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.17 – 2.98 30.17 – 2.75	Depositor EDS
% Data completeness (in resolution range)	84.5 (30.17-2.98) 77.5 (30.17-2.75)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.76 (at 2.76Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.231 , 0.282 0.219 , 0.268	Depositor DCC
$R_{free}$ test set	500 reflections (5.64%)	DCC
Wilson B-factor (Å <sup>2</sup> )	69.2	Xtriage
Anisotropy	0.241	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 45.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	3441	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.71% 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: DFT, CA, 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	0.57	1/2792 (0.0%)	0.99	19/3750 (0.5%)
2	P	0.56	0/310	0.84	0/479
3	T	1.10	3/328 (0.9%)	1.61	6/497 (1.2%)
All	All	0.64	4/3430 (0.1%)	1.06	25/4726 (0.5%)

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	3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	T	3	DC	OP3-P	-7.44	1.52	1.61
3	T	8	DG	C3'-O3'	-6.37	1.35	1.44
1	A	230	ARG	CZ-NH1	6.26	1.41	1.33
3	T	9	DT	P-OP1	5.95	1.59	1.49

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	230	ARG	NE-CZ-NH2	-23.04	108.78	120.30
1	A	230	ARG	NE-CZ-NH1	18.20	129.40	120.30
3	T	8	DG	OP1-P-O3'	12.89	133.55	105.20
3	T	8	DG	O3'-P-O5'	-12.63	80.00	104.00
3	T	7	DA	OP1-P-O3'	-12.56	77.56	105.20
1	A	247	ARG	NE-CZ-NH1	11.26	125.93	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	247	ARG	NE-CZ-NH2	-10.50	115.05	120.30
3	T	3	DC	OP2-P-O3'	10.28	127.82	105.20
1	A	230	ARG	NH1-CZ-NH2	-9.39	109.07	119.40
1	A	256	ARG	NE-CZ-NH1	9.30	124.95	120.30
1	A	158	ALA	N-CA-C	-9.05	86.56	111.00
1	A	115	VAL	C-N-CA	8.73	143.52	121.70
3	T	9	DT	O5'-P-OP2	8.22	120.56	110.70
1	A	116	ARG	N-CA-CB	-7.67	96.79	110.60
1	A	115	VAL	CA-C-N	-7.51	100.68	117.20
1	A	234	ASN	N-CA-CB	7.17	123.51	110.60
1	A	233	TYR	C-N-CA	-6.70	104.96	121.70
1	A	256	ARG	NE-CZ-NH2	-6.53	117.03	120.30
1	A	112	SER	C-N-CA	-6.10	106.44	121.70
1	A	247	ARG	CG-CD-NE	-5.86	99.50	111.80
1	A	341	ILE	C-N-CA	-5.64	107.61	121.70
1	A	230	ARG	CG-CD-NE	-5.63	99.98	111.80
1	A	342	GLU	N-CA-CB	-5.47	100.75	110.60
1	A	247	ARG	NH1-CZ-NH2	-5.41	113.45	119.40
3	T	7	DA	OP2-P-O3'	5.09	116.40	105.20

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	230	ARG	Sidechain
1	A	247	ARG	Sidechain
1	A	256	ARG	Sidechain

## 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	2753	0	2894	232	0
2	P	274	0	146	8	0
3	T	317	0	182	46	0
4	A	31	0	12	9	0
5	A	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	46	0	0	18	0
6	P	11	0	0	1	0
6	T	6	0	0	5	0
All	All	3441	0	3234	273	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 41.

All (273) 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:256:ARG:NH2	1:A:327:GLU:HA	1.29	1.39
1:A:116:ARG:HG3	1:A:120:GLU:CG	1.68	1.23
1:A:207:SER:HB3	6:A:2024:HOH:O	1.36	1.22
1:A:256:ARG:HH21	1:A:327:GLU:CA	1.57	1.17
1:A:115:VAL:HG13	1:A:116:ARG:HG3	1.30	1.13
1:A:115:VAL:HG13	1:A:116:ARG:CG	1.81	1.11
1:A:256:ARG:NH2	1:A:327:GLU:CA	2.15	1.08
3:T:8:DG:C8	3:T:9:DT:H72	1.96	1.00
1:A:33:PHE:HB3	6:A:2006:HOH:O	1.63	0.98
1:A:256:ARG:HH21	1:A:327:GLU:C	1.68	0.96
1:A:119:ARG:HD2	1:A:119:ARG:H	1.28	0.96
1:A:158:ALA:O	1:A:162:GLY:HA3	1.68	0.93
1:A:256:ARG:HH22	1:A:327:GLU:HA	1.27	0.90
1:A:116:ARG:HD2	1:A:120:GLU:HG2	1.51	0.90
1:A:115:VAL:HA	1:A:116:ARG:HG2	1.53	0.89
1:A:340:PHE:HD1	6:A:2041:HOH:O	1.54	0.89
1:A:116:ARG:HG3	1:A:120:GLU:HG3	1.52	0.89
1:A:115:VAL:CA	1:A:116:ARG:HG2	2.03	0.89
1:A:116:ARG:HG3	1:A:120:GLU:HG2	1.52	0.89
4:A:1344:DGT:H5'A	4:A:1344:DGT:O2B	1.74	0.87
1:A:147:ASN:HB2	1:A:234:ASN:OD1	1.75	0.86
3:T:4:DA:H2''	3:T:5:DFT:H5'	1.56	0.86
1:A:146:LYS:HG3	6:A:2019:HOH:O	1.73	0.86
1:A:256:ARG:HH21	1:A:327:GLU:HA	1.04	0.86
2:P:4:DG:H2''	2:P:5:DG:H5''	1.57	0.86
2:P:11:DC:O2	3:T:8:DG:N2	2.08	0.86
1:A:247:ARG:HH21	1:A:249:VAL:HG12	1.41	0.85
1:A:153:ILE:O	1:A:156:ASP:HB2	1.77	0.84
1:A:36:ARG:HH11	1:A:331:ARG:NH1	1.77	0.83
1:A:214:LYS:HG2	1:A:219:GLU:HA	1.60	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:GLU:CD	1:A:173:ARG:HH21	1.80	0.82
1:A:116:ARG:HG3	1:A:120:GLU:CB	2.09	0.82
1:A:91:LEU:HD23	1:A:91:LEU:O	1.78	0.81
3:T:3:DC:O2	3:T:3:DC:H2'	1.80	0.81
1:A:115:VAL:CG1	1:A:116:ARG:CG	2.59	0.80
1:A:116:ARG:CG	1:A:120:GLU:CG	2.57	0.80
4:A:1344:DGT:N1	3:T:4:DA:C2	2.48	0.80
1:A:217:ILE:HD12	1:A:221:LYS:HG3	1.63	0.80
1:A:116:ARG:CG	1:A:120:GLU:HG2	2.13	0.78
1:A:116:ARG:CD	1:A:120:GLU:HG2	2.14	0.77
1:A:115:VAL:HG13	1:A:120:GLU:HG3	1.68	0.76
1:A:186:ILE:HG22	1:A:191:ALA:HB2	1.67	0.76
1:A:302:PHE:HZ	1:A:314:GLU:HG3	1.51	0.75
3:T:4:DA:H2''	3:T:5:DFT:C5'	2.16	0.75
3:T:7:DA:C6	3:T:8:DG:O6	2.40	0.74
4:A:1344:DGT:C3'	6:A:2044:HOH:O	2.35	0.74
1:A:115:VAL:HG13	1:A:116:ARG:HG2	1.71	0.72
1:A:119:ARG:N	1:A:119:ARG:HD2	2.05	0.72
1:A:318:LEU:O	1:A:322:ILE:HG13	1.90	0.71
3:T:4:DA:OP1	6:T:2002:HOH:O	2.06	0.71
2:P:4:DG:H1	3:T:15:DC:H42	1.39	0.71
4:A:1344:DGT:H3'	6:A:2044:HOH:O	1.90	0.71
1:A:336:ARG:NH2	3:T:7:DA:H5'	2.04	0.71
1:A:158:ALA:O	1:A:162:GLY:CA	2.39	0.71
1:A:115:VAL:CG1	1:A:116:ARG:HG2	2.21	0.71
1:A:312:TYR:O	1:A:316:VAL:HG23	1.91	0.71
3:T:7:DA:C6	3:T:8:DG:C6	2.79	0.70
1:A:338:SER:HB2	6:A:2028:HOH:O	1.89	0.70
1:A:67:ILE:O	1:A:68:LEU:HD23	1.91	0.70
1:A:240:ARG:NH1	1:A:243:LYS:NZ	2.40	0.70
1:A:256:ARG:HG3	1:A:323:LEU:HD22	1.74	0.70
1:A:108:TYR:OH	1:A:152:LYS:HE3	1.93	0.68
1:A:113:ASP:O	1:A:115:VAL:N	2.27	0.67
1:A:98:LYS:CB	1:A:110:ASP:HB3	2.24	0.67
1:A:233:TYR:CZ	1:A:235:GLU:HG2	2.30	0.67
1:A:283:ALA:CB	1:A:339:LYS:HD3	2.24	0.67
1:A:76:MET:CE	1:A:78:LYS:HB2	2.26	0.66
4:A:1344:DGT:O6	3:T:4:DA:N1	2.28	0.66
3:T:8:DG:H2''	3:T:9:DT:C6	2.30	0.65
1:A:247:ARG:NH2	1:A:249:VAL:HG12	2.12	0.65
1:A:199:ILE:HG23	1:A:204:ASP:HB2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:LYS:HB2	1:A:110:ASP:HB3	1.79	0.64
1:A:283:ALA:HB2	1:A:339:LYS:HD3	1.79	0.64
1:A:342:GLU:HG3	1:A:343:ALA:N	2.13	0.64
1:A:119:ARG:CD	1:A:119:ARG:H	2.07	0.64
1:A:230:ARG:HD3	1:A:232:GLU:OE1	1.97	0.63
1:A:31:CYS:HB3	1:A:61:ILE:HD11	1.80	0.63
1:A:256:ARG:NH2	1:A:326:ASP:O	2.31	0.63
1:A:279:ARG:HB3	1:A:340:PHE:CD2	2.34	0.62
1:A:341:ILE:O	1:A:341:ILE:HG13	1.98	0.62
1:A:146:LYS:HE3	6:A:2019:HOH:O	2.00	0.61
1:A:200:ASN:O	1:A:201:LYS:HD3	1.99	0.61
1:A:113:ASP:C	1:A:115:VAL:H	2.03	0.61
1:A:113:ASP:C	1:A:115:VAL:N	2.53	0.61
1:A:244:SER:O	1:A:245:ILE:HD13	1.99	0.61
1:A:279:ARG:HB3	1:A:340:PHE:HD2	1.64	0.61
3:T:6:DT:H1'	3:T:7:DA:H5''	1.82	0.61
1:A:171:VAL:O	1:A:175:ILE:HG13	2.02	0.60
1:A:302:PHE:CZ	1:A:314:GLU:HG3	2.34	0.60
1:A:116:ARG:HG3	1:A:120:GLU:HB3	1.84	0.60
3:T:8:DG:H2''	3:T:9:DT:H6	1.65	0.60
1:A:89:MET:C	1:A:91:LEU:H	2.05	0.60
1:A:234:ASN:ND2	1:A:235:GLU:O	2.35	0.59
1:A:256:ARG:HG2	1:A:256:ARG:O	2.01	0.59
1:A:115:VAL:HG13	1:A:120:GLU:CG	2.33	0.59
1:A:147:ASN:CB	1:A:234:ASN:OD1	2.48	0.59
1:A:259:GLU:OE2	1:A:262:LYS:HE3	2.02	0.59
1:A:60:PRO:HG3	3:T:3:DC:H5''	1.84	0.59
1:A:76:MET:HE3	1:A:78:LYS:HB2	1.85	0.59
1:A:186:ILE:O	6:A:2022:HOH:O	2.17	0.58
1:A:307:SER:HB2	6:A:2039:HOH:O	2.03	0.58
1:A:233:TYR:CE1	1:A:235:GLU:HG2	2.39	0.58
3:T:7:DA:C5	3:T:8:DG:C6	2.92	0.57
4:A:1344:DGT:H16	3:T:4:DA:H2	1.43	0.57
2:P:4:DG:C2'	2:P:5:DG:H5''	2.32	0.57
1:A:36:ARG:NH1	1:A:331:ARG:NH1	2.50	0.56
1:A:251:MET:HG2	1:A:264:TYR:CD2	2.39	0.56
1:A:36:ARG:HH21	1:A:253:ARG:HA	1.71	0.56
2:P:11:DC:N3	3:T:8:DG:N1	2.49	0.56
1:A:45:THR:HG21	6:A:2044:HOH:O	2.06	0.56
1:A:238:ARG:HB2	6:A:2026:HOH:O	2.06	0.56
1:A:265:LEU:HD22	1:A:319:LEU:HD22	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:ASN:O	1:A:192:GLU:HB2	2.06	0.55
1:A:259:GLU:OE2	1:A:262:LYS:CE	2.55	0.55
3:T:8:DG:C2'	3:T:9:DT:C7	2.85	0.55
3:T:8:DG:H2'	3:T:9:DT:H72	1.89	0.55
3:T:8:DG:N9	3:T:9:DT:H72	2.21	0.55
3:T:7:DA:C5	3:T:8:DG:O6	2.59	0.55
1:A:20:ASN:ND2	6:A:2002:HOH:O	2.40	0.55
1:A:10:TYR:HD1	1:A:13:ALA:HB3	1.71	0.55
1:A:230:ARG:HB3	1:A:232:GLU:OE2	2.06	0.55
1:A:98:LYS:HB3	1:A:110:ASP:HB3	1.89	0.54
1:A:149:VAL:O	1:A:153:ILE:HG13	2.08	0.54
1:A:8:PHE:HD1	1:A:140:VAL:HG11	1.73	0.54
1:A:256:ARG:CG	1:A:256:ARG:O	2.56	0.54
1:A:23:LEU:O	1:A:26:LYS:HG2	2.08	0.54
3:T:4:DA:C2'	3:T:5:DFT:C5'	2.86	0.54
1:A:28:VAL:HG23	1:A:47:ASN:ND2	2.22	0.54
1:A:210:PHE:CE2	1:A:214:LYS:HG3	2.43	0.54
1:A:115:VAL:CG1	1:A:116:ARG:N	2.70	0.53
1:A:76:MET:HE2	1:A:78:LYS:HB2	1.90	0.53
1:A:60:PRO:HB3	6:T:2001:HOH:O	2.07	0.53
1:A:31:CYS:HB3	1:A:61:ILE:CD1	2.38	0.53
3:T:4:DA:C2'	3:T:5:DFT:H5''	2.39	0.53
1:A:8:PHE:CD2	1:A:105:ASP:HA	2.43	0.53
1:A:245:ILE:HG23	1:A:275:LYS:HD2	1.90	0.53
3:T:8:DG:C2'	3:T:9:DT:H72	2.38	0.53
1:A:67:ILE:HG22	1:A:68:LEU:CD2	2.39	0.53
1:A:91:LEU:C	1:A:91:LEU:HD23	2.28	0.52
1:A:200:ASN:HB3	6:A:2023:HOH:O	2.08	0.52
3:T:4:DA:H1'	3:T:5:DFT:H5''	1.92	0.52
1:A:240:ARG:NH1	1:A:243:LYS:HZ3	2.08	0.52
1:A:178:LEU:HD12	1:A:179:ASP:H	1.76	0.51
1:A:248:ILE:HG22	3:T:5:DFT:H3'	1.93	0.51
1:A:35:GLY:O	1:A:36:ARG:C	2.47	0.51
1:A:8:PHE:CE2	1:A:105:ASP:HA	2.46	0.51
3:T:10:DC:H2''	3:T:11:DC:H5'	1.93	0.51
1:A:144:ILE:HB	1:A:165:VAL:HG22	1.92	0.50
1:A:5:PHE:CD2	1:A:152:LYS:HA	2.47	0.50
1:A:85:SER:O	1:A:89:MET:HG2	2.10	0.50
1:A:118:TYR:CE1	1:A:167:ASP:HA	2.46	0.50
1:A:186:ILE:HG23	1:A:190:THR:HG22	1.92	0.50
1:A:170:GLU:OE2	1:A:173:ARG:NH2	2.38	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:ARG:HD3	6:A:2033:HOH:O	2.10	0.50
1:A:95:TYR:O	1:A:96:SER:HB2	2.12	0.50
2:P:4:DG:H1	3:T:15:DC:N4	2.06	0.50
2:P:13:DA:OP2	6:P:2007:HOH:O	2.19	0.50
1:A:234:ASN:CG	1:A:235:GLU:N	2.65	0.49
1:A:239:THR:HA	6:A:2027:HOH:O	2.11	0.49
1:A:282:LYS:HD3	1:A:341:ILE:HG21	1.93	0.49
4:A:1344:DGT:N1	3:T:4:DA:H2	2.02	0.49
3:T:11:DC:C6	3:T:12:DT:H72	2.47	0.49
1:A:267:ARG:NH1	6:A:2032:HOH:O	2.45	0.49
1:A:7:ASP:OD1	1:A:106:GLU:HG2	2.13	0.49
1:A:62:VAL:HG13	6:T:2001:HOH:O	2.12	0.48
1:A:35:GLY:O	1:A:37:PHE:N	2.46	0.48
1:A:262:LYS:N	1:A:263:PRO:HD2	2.28	0.48
1:A:141:THR:HA	1:A:162:GLY:O	2.14	0.48
1:A:113:ASP:N	1:A:113:ASP:OD2	2.46	0.48
1:A:115:VAL:HG12	1:A:116:ARG:N	2.28	0.48
1:A:166:ILE:HG23	1:A:170:GLU:HB3	1.95	0.47
3:T:7:DA:C4	3:T:8:DG:C5	3.03	0.47
1:A:189:ILE:HG22	1:A:193:LYS:HE2	1.97	0.47
1:A:37:PHE:HZ	3:T:3:DC:OP1	1.96	0.47
1:A:115:VAL:HG11	1:A:121:ALA:N	2.30	0.47
1:A:240:ARG:NH1	1:A:243:LYS:HZ1	2.13	0.47
1:A:137:LYS:HE2	1:A:137:LYS:HA	1.96	0.47
1:A:116:ARG:HB2	1:A:120:GLU:HB3	1.97	0.47
1:A:175:ILE:HG22	1:A:175:ILE:O	2.15	0.47
1:A:141:THR:OG1	1:A:159:LYS:HA	2.16	0.46
1:A:41:GLY:HA2	3:T:4:DA:H5'	1.97	0.46
1:A:190:THR:HB	2:P:12:DT:OP1	2.14	0.46
1:A:276:LEU:HD22	1:A:340:PHE:HE2	1.80	0.46
1:A:8:PHE:HA	1:A:140:VAL:HG12	1.98	0.46
1:A:67:ILE:HG22	1:A:68:LEU:HG	1.96	0.46
1:A:37:PHE:CD1	1:A:37:PHE:O	2.68	0.46
1:A:329:LYS:HE3	6:A:2031:HOH:O	2.15	0.46
1:A:244:SER:HB3	6:T:2005:HOH:O	2.15	0.45
1:A:336:ARG:HH22	3:T:6:DT:H2''	1.80	0.45
1:A:115:VAL:CB	1:A:116:ARG:HG2	2.47	0.45
1:A:316:VAL:O	1:A:320:GLN:HG3	2.16	0.45
1:A:68:LEU:C	1:A:70:ASN:H	2.19	0.45
1:A:132:ILE:HG22	1:A:138:ILE:O	2.17	0.45
1:A:178:LEU:HD12	1:A:179:ASP:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:ARG:O	1:A:231:ASP:HB3	2.16	0.45
1:A:302:PHE:C	1:A:304:HIS:H	2.20	0.45
1:A:8:PHE:HD1	1:A:140:VAL:CG1	2.28	0.45
1:A:340:PHE:O	1:A:341:ILE:HG23	2.16	0.45
1:A:304:HIS:ND1	1:A:305:GLY:O	2.48	0.45
1:A:116:ARG:HB2	1:A:117:ASP:H	1.46	0.45
1:A:174:LEU:C	1:A:176:ARG:H	2.20	0.45
1:A:214:LYS:HD3	1:A:219:GLU:HG3	1.99	0.45
1:A:167:ASP:O	1:A:170:GLU:N	2.47	0.44
1:A:133:LEU:O	1:A:137:LYS:HA	2.17	0.44
1:A:203:VAL:O	1:A:203:VAL:HG22	2.16	0.44
1:A:203:VAL:O	1:A:206:LEU:HD12	2.17	0.44
1:A:217:ILE:HD11	1:A:222:ALA:HA	2.00	0.44
1:A:31:CYS:HB2	1:A:33:PHE:CE1	2.52	0.44
1:A:10:TYR:HD2	1:A:48:TYR:HE1	1.66	0.44
1:A:124:LEU:O	1:A:128:ILE:HG13	2.17	0.44
1:A:170:GLU:CD	1:A:173:ARG:NH2	2.61	0.44
1:A:214:LYS:NZ	1:A:214:LYS:HB3	2.32	0.44
1:A:279:ARG:HD2	1:A:340:PHE:CE2	2.52	0.44
1:A:167:ASP:OD2	1:A:169:GLU:HG2	2.17	0.44
3:T:6:DT:H2''	3:T:7:DA:H5'	1.98	0.44
1:A:156:ASP:O	1:A:157:MET:HB2	2.16	0.44
1:A:23:LEU:HD11	1:A:74:LEU:HD11	1.99	0.44
1:A:174:LEU:C	1:A:176:ARG:N	2.70	0.44
1:A:285:HIS:CD2	1:A:299:GLY:HA3	2.52	0.44
1:A:29:VAL:HG13	1:A:43:VAL:HG13	2.00	0.44
1:A:230:ARG:O	1:A:231:ASP:CB	2.66	0.44
1:A:233:TYR:CD2	1:A:233:TYR:C	2.91	0.44
1:A:298:ARG:HG3	1:A:322:ILE:HG12	2.00	0.44
1:A:214:LYS:HD3	1:A:219:GLU:CG	2.48	0.43
1:A:67:ILE:C	1:A:68:LEU:HD23	2.38	0.43
1:A:89:MET:C	1:A:91:LEU:N	2.71	0.43
1:A:336:ARG:NH2	3:T:7:DA:OP2	2.51	0.43
1:A:276:LEU:CD2	1:A:340:PHE:HE2	2.32	0.43
1:A:289:VAL:HB	1:A:332:ARG:HB2	1.99	0.43
1:A:202:LEU:HD22	1:A:229:ALA:HB2	1.99	0.43
1:A:282:LYS:HG3	1:A:339:LYS:O	2.19	0.43
1:A:43:VAL:O	1:A:57:ALA:HA	2.19	0.43
1:A:115:VAL:HG13	1:A:120:GLU:HB3	1.99	0.42
1:A:257:ASN:OD1	1:A:259:GLU:N	2.52	0.42
3:T:8:DG:H2'	3:T:9:DT:C7	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:ARG:CG	1:A:120:GLU:CB	2.91	0.42
1:A:166:ILE:O	1:A:166:ILE:HG22	2.18	0.42
1:A:23:LEU:CD1	1:A:74:LEU:HD11	2.49	0.42
1:A:203:VAL:HG13	1:A:204:ASP:OD1	2.19	0.42
1:A:276:LEU:HD13	1:A:281:PRO:HD3	2.01	0.42
1:A:332:ARG:HH12	3:T:5:DFT:H6	1.84	0.42
1:A:332:ARG:NH1	3:T:5:DFT:H71	2.34	0.42
1:A:62:VAL:HG22	6:T:2001:HOH:O	2.18	0.42
1:A:154:ALA:C	1:A:156:ASP:N	2.72	0.42
1:A:186:ILE:HD12	1:A:190:THR:HG21	2.01	0.42
1:A:293:LEU:N	1:A:293:LEU:CD2	2.82	0.42
1:A:141:THR:CG2	1:A:158:ALA:HB3	2.50	0.42
1:A:158:ALA:O	1:A:162:GLY:N	2.52	0.42
4:A:1344:DGT:C6	3:T:4:DA:N1	2.83	0.42
1:A:204:ASP:N	1:A:204:ASP:OD1	2.53	0.41
1:A:37:PHE:O	1:A:38:GLU:HB3	2.19	0.41
1:A:233:TYR:CD2	1:A:234:ASN:HA	2.55	0.41
3:T:10:DC:C2'	3:T:11:DC:H5'	2.49	0.41
1:A:105:ASP:CG	4:A:1344:DGT:H5'	2.40	0.41
1:A:178:LEU:HD11	1:A:182:ASP:HB2	2.03	0.41
1:A:233:TYR:CD2	1:A:233:TYR:O	2.74	0.41
1:A:166:ILE:HD13	1:A:174:LEU:HD11	2.03	0.41
1:A:17:GLU:O	1:A:21:PRO:HA	2.21	0.41
1:A:10:TYR:HE1	1:A:17:GLU:OE2	2.04	0.41
1:A:240:ARG:HD3	1:A:240:ARG:HA	1.80	0.41
1:A:278:LYS:CD	1:A:278:LYS:N	2.84	0.41
1:A:282:LYS:HD3	1:A:341:ILE:CG2	2.51	0.41
1:A:29:VAL:HG21	1:A:55:VAL:HG11	2.02	0.41
1:A:293:LEU:H	1:A:293:LEU:HD22	1.86	0.40
1:A:51:ARG:HA	1:A:55:VAL:O	2.21	0.40
1:A:133:LEU:HD13	1:A:139:THR:HG22	2.03	0.40
1:A:190:THR:O	1:A:194:LEU:HG	2.21	0.40
1:A:9:ASP:CG	1:A:161:ASN:H	2.25	0.40
1:A:331:ARG:HH21	3:T:4:DA:P	2.44	0.40
1:A:332:ARG:HH12	3:T:5:DFT:H71	1.86	0.40
3:T:6:DT:H2''	3:T:7:DA:C5'	2.51	0.40
1:A:111:ILE:CD1	1:A:111:ILE:O	2.70	0.40
1:A:237:ILE:N	1:A:237:ILE:HD12	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	341/358 (95%)	286 (84%)	45 (13%)	10 (3%)	5	26

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	114	LYS
1	A	340	PHE
1	A	36	ARG
1	A	96	SER
1	A	157	MET
1	A	277	ASP
1	A	38	GLU
1	A	116	ARG
1	A	158	ALA
1	A	69	PRO

### 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	301/315 (96%)	279 (93%)	22 (7%)	16	48

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	GLU

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Mol	Chain	Res	Type
1	A	63	GLU
1	A	79	GLU
1	A	81	TYR
1	A	94	GLU
1	A	99	ILE
1	A	113	ASP
1	A	116	ARG
1	A	157	MET
1	A	179	ASP
1	A	192	GLU
1	A	214	LYS
1	A	240	ARG
1	A	244	SER
1	A	253	ARG
1	A	256	ARG
1	A	258	LEU
1	A	273	TYR
1	A	278	LYS
1	A	325	GLU
1	A	336	ARG
1	A	339	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	GLN
1	A	285	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	DFT	T	5	3	18,21,22	0.73	0	25,30,33	2.37	7 (28%)

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	DFT	T	5	3	-	0/7/21/22	0/2/2/2

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	T	5	DFT	C3-C4-C5	-6.29	119.55	124.38
3	T	5	DFT	C3'-C2'-C1'	-4.92	98.08	102.69
3	T	5	DFT	C3-C2-C1	-2.76	120.05	123.66
3	T	5	DFT	C2'-C1'-C1	-2.63	110.88	114.71
3	T	5	DFT	C6-C1-C2	2.73	119.48	116.15
3	T	5	DFT	O4'-C1'-C1	3.14	112.99	109.76
3	T	5	DFT	C6-C5-C4	5.50	119.83	116.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	T	5	DFT	9	0

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 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	1344	5	26,33,33	1.29	2 (7%)	28,52,52	2.12	6 (21%)

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	1344	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	1344	DGT	C2-N1	3.08	1.41	1.35
4	A	1344	DGT	C6-N1	4.07	1.40	1.33

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1344	DGT	N3-C2-N1	-5.69	119.15	127.46
4	A	1344	DGT	C5-C6-N1	-3.92	117.90	123.48
4	A	1344	DGT	C2'-C1'-N9	-3.58	105.77	114.23
4	A	1344	DGT	O4'-C1'-N9	2.91	112.69	107.78
4	A	1344	DGT	C6-N1-C2	3.11	120.53	116.06
4	A	1344	DGT	C2-N3-C4	5.43	121.49	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1344	DGT	9	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	343/358 (95%)	-0.24	0 100 100	32, 54, 78, 88	17 (4%)
2	P	13/13 (100%)	-0.32	0 100 100	42, 53, 69, 72	0
3	T	15/18 (83%)	0.02	0 100 100	59, 78, 109, 125	0
All	All	371/389 (95%)	-0.23	0 100 100	32, 55, 79, 125	17 (4%)

There are no RSRZ outliers to report.

### 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<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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	DFT	T	5	20/21	0.92	0.20	-	89,91,102,102	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. 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<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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	CA	A	1346	1/1	0.95	0.26	1.47	46,46,46,46	0
4	DGT	A	1344	31/31	0.90	0.22	0.76	64,69,72,74	0
5	CA	A	1345	1/1	0.75	0.34	-	88,88,88,88	0
5	CA	A	1347	1/1	0.96	0.06	-	125,125,125,125	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.