



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:32 AM GMT

PDB ID : 3F2C
Title : DNA Polymerase PolC from *Geobacillus kaustophilus* complex with DNA, dGTP and Mn
Authors : Davies, D.R.; Evans, R.J.; Bullard, J.M.; Christensen, J.; Green, L.S.; Guiles, J.W.; Ribble, W.K.; Janjic, N.; Jarvis, T.C.
Deposited on : 2008-10-29
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/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 : 1.7 (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

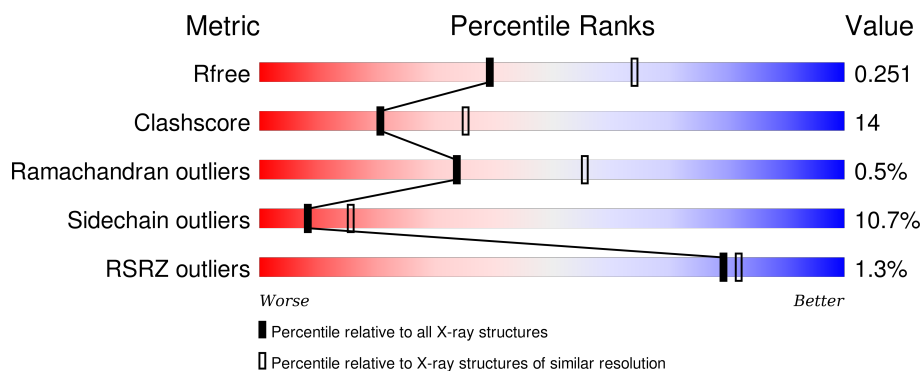
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	1041	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> % 68% 23% • 5% </div> </div>
2	P	17	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> 6% 24% 41% 12% 24% </div> </div>
3	T	22	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> 45% 14% 23% 18% </div> </div>

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 8622 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 GEOBACILLUS KAUSTOPHILUS DNA POLC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	993	Total	C	N	O	S	0	0	0
			7796	4961	1318	1481	36			

There are 17 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	227	MET	-	EXPRESSION TAG	UNP Q5L0J3
A	425	GLY	-	LINKER	UNP Q5L0J3
A	426	SER	-	LINKER	UNP Q5L0J3
A	427	GLY	-	LINKER	UNP Q5L0J3
A	428	SER	-	LINKER	UNP Q5L0J3
A	429	GLY	-	LINKER	UNP Q5L0J3
A	1445	SER	-	EXPRESSION TAG	UNP Q5L0J3
A	1446	GLY	-	EXPRESSION TAG	UNP Q5L0J3
A	1447	GLY	-	EXPRESSION TAG	UNP Q5L0J3
A	1448	HIS	-	EXPRESSION TAG	UNP Q5L0J3
A	1449	HIS	-	EXPRESSION TAG	UNP Q5L0J3
A	1450	HIS	-	EXPRESSION TAG	UNP Q5L0J3
A	1451	HIS	-	EXPRESSION TAG	UNP Q5L0J3
A	1452	HIS	-	EXPRESSION TAG	UNP Q5L0J3
A	1453	HIS	-	EXPRESSION TAG	UNP Q5L0J3
A	1454	HIS	-	EXPRESSION TAG	UNP Q5L0J3
A	1455	HIS	-	EXPRESSION TAG	UNP Q5L0J3

- Molecule 2 is a DNA chain called 5'-D(*DCP*DAP*DGP*DTP*DGP*DAP*DGP*DAP*DCP*DGP*DGP*DGP*DCP*DAP*DAP*DCP*DC)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	13	Total	C	N	O	P	0	0	0
			269	126	57	73	13			

- Molecule 3 is a DNA chain called 5'-D(*DAP*DTP*DAP*DAP*DCP*DGP*DGP*DTP*D

TP*DGP*DCP*DCP*DCP*DGP*DTP*DCP*DTP*DCP*DAP*DCP*DTP*DG)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	T	18	Total	C	N	O	P	0	0	0
			362	174	63	108	17			

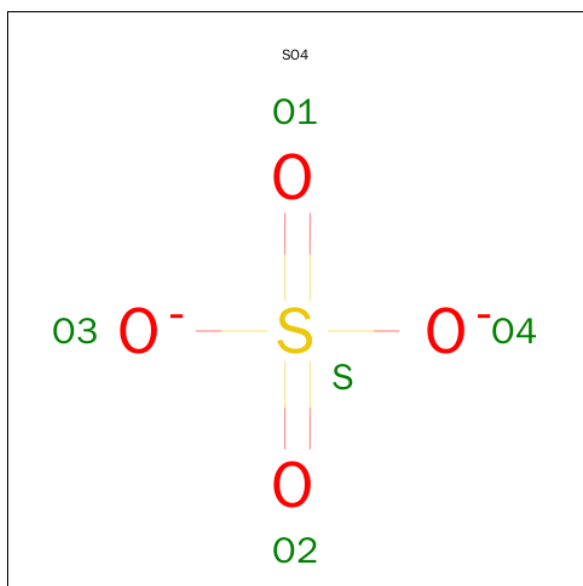
- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	Mn	0	0
			3	3		

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

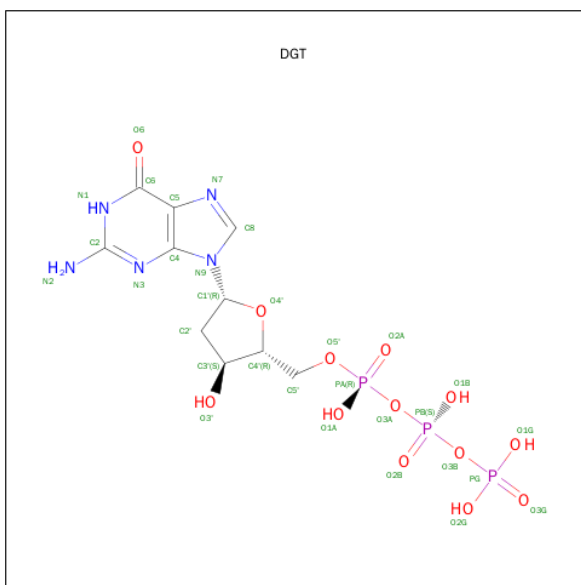
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Zn	0	0
			1	1		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is 2'-DEOXYGUANOSINE-5'-TRIPHOSPHATE (three-letter code: DGT) (formula: C₁₀H₁₆N₅O₁₃P₃).



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

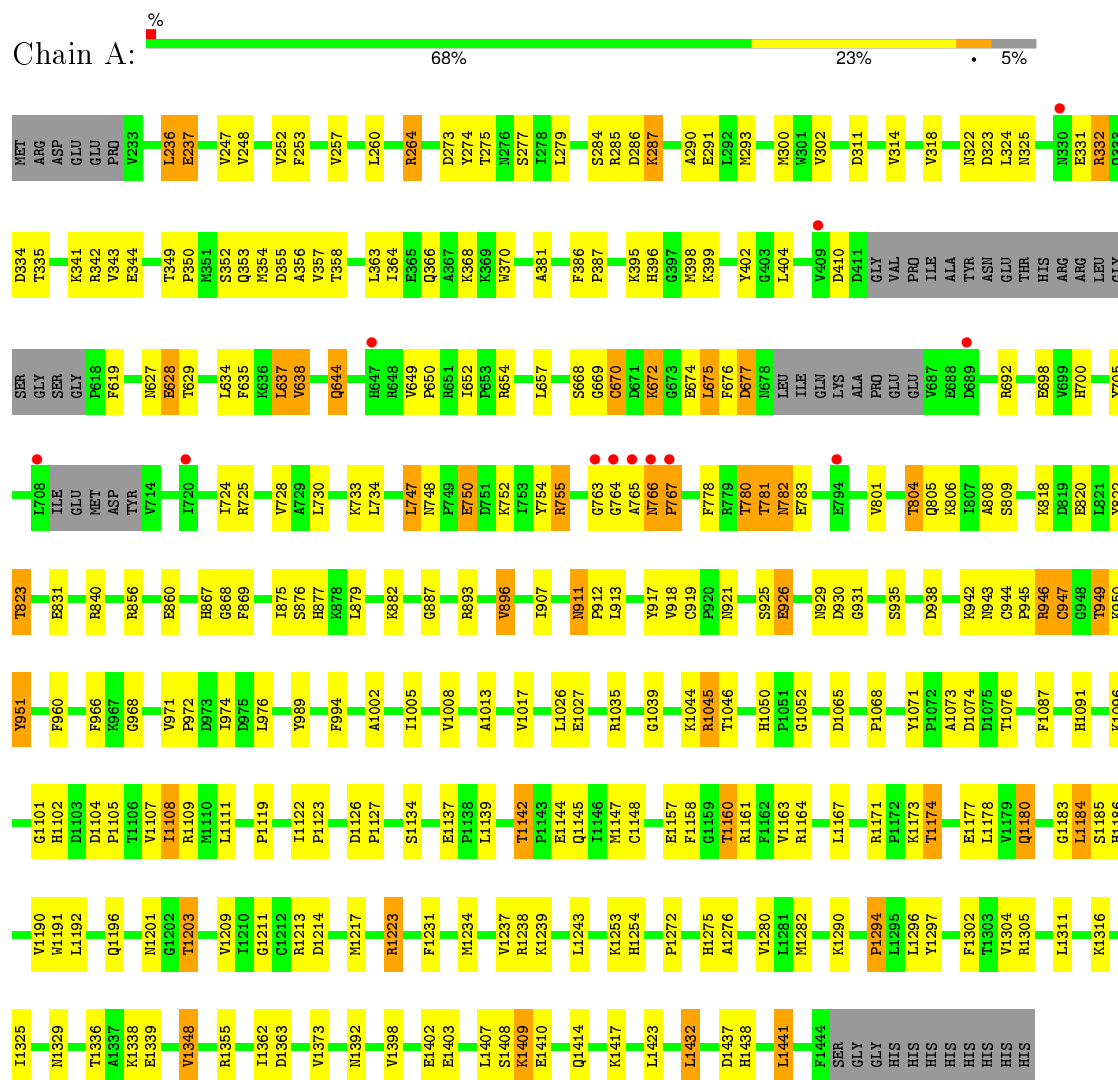
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	142	Total O 142 142	0	0
8	P	7	Total O 7 7	0	0
8	T	6	Total O 6 6	0	0

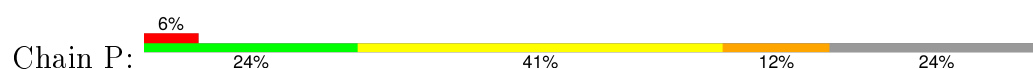
3 Residue-property plots

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



• Molecule 2: 5'-D(*DCP*DAP*DGP*DTP*DGP*DAP*DGP*DAP*DCP*DGP*DGP*DGP*D CP*DAP*DAP*DCP*DC)-3'





- Molecule 3: 5'-D(*DAP*DTP*DAP*DAP*DCP*DGP*DGP*DTP*DTP*DGP*DCP*DCP*DCP*DGP*DTP*DCP*DTP*DCP*DAP*DCP*DTP*DG)-3'

Chain T: 45% 14% 23% 18%



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	115.89Å 141.19Å 184.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.60 – 2.50 43.60 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (43.60-2.50) 98.9 (43.60-2.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.43 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.4.0069	Depositor
R, R_{free}	0.210 , 0.255 0.209 , 0.251	Depositor DCC
R_{free} test set	2641 reflections (5.37%)	DCC
Wilson B-factor (Å ²)	41.9	Xtriage
Anisotropy	0.068	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 41.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 51789 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8622	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% 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, 0.375 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: ZN, MN, SO4, 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	0.52	4/7960 (0.1%)	0.66	3/10776 (0.0%)
2	P	1.10	2/303 (0.7%)	1.84	7/465 (1.5%)
3	T	1.32	2/404 (0.5%)	2.25	20/621 (3.2%)
All	All	0.61	8/8667 (0.1%)	0.89	30/11862 (0.3%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	T	8	DT	C4'-O4'	-17.10	1.27	1.45
1	A	725	ARG	CZ-NH1	9.41	1.45	1.33
1	A	725	ARG	CZ-NH2	9.02	1.44	1.33
1	A	725	ARG	CD-NE	8.91	1.61	1.46
1	A	725	ARG	NE-CZ	8.89	1.44	1.33
3	T	8	DT	O4'-C1'	7.57	1.51	1.42
2	P	16	DC	O4'-C1'	-6.10	1.34	1.42
2	P	7	DG	N3-C4	5.42	1.39	1.35

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	T	8	DT	O4'-C1'-N1	29.39	128.57	108.00
2	P	16	DC	O4'-C1'-N1	18.40	120.88	108.00
3	T	8	DT	N1-C1'-C2'	-12.45	88.94	112.60
3	T	8	DT	O4'-C4'-C3'	11.65	112.99	106.00
3	T	17	DT	O4'-C1'-N1	10.03	115.02	108.00
1	A	725	ARG	NE-CZ-NH2	-9.71	115.44	120.30
3	T	18	DC	N1-C2-O2	7.88	123.63	118.90
3	T	17	DT	C4'-C3'-C2'	-7.65	96.21	103.10
3	T	15	DT	C4-C5-C7	7.40	123.44	119.00
3	T	16	DC	P-O3'-C3'	7.27	128.43	119.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	12	DG	O4'-C1'-N9	6.68	112.67	108.00
3	T	8	DT	O5'-P-OP2	-6.38	99.96	105.70
2	P	7	DG	O4'-C1'-N9	6.31	112.42	108.00
1	A	1441	LEU	CA-CB-CG	6.26	129.69	115.30
3	T	8	DT	C5'-C4'-O4'	6.19	121.06	109.30
3	T	15	DT	C6-C5-C7	-6.14	119.22	122.90
3	T	8	DT	N3-C4-O4	6.11	123.57	119.90
3	T	16	DC	O4'-C1'-N1	-5.94	103.84	108.00
3	T	8	DT	C5-C4-O4	-5.64	120.95	124.90
2	P	16	DC	C5'-C4'-O4'	5.52	119.78	109.30
2	P	10	DG	O4'-C1'-N9	-5.47	104.17	108.00
3	T	9	DT	C4-C5-C7	5.45	122.27	119.00
2	P	5	DG	P-O3'-C3'	5.37	126.14	119.70
1	A	725	ARG	NE-CZ-NH1	5.33	122.96	120.30
2	P	8	DA	O4'-C1'-N9	-5.17	104.38	108.00
3	T	6	DG	P-O3'-C3'	5.16	125.89	119.70
3	T	9	DT	C6-C5-C7	-5.16	119.80	122.90
3	T	3	DA	O4'-C1'-N9	-5.16	104.39	108.00
3	T	16	DC	P-O5'-C5'	-5.03	112.86	120.90
3	T	17	DT	N3-C4-O4	5.01	122.91	119.90

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	7796	0	7707	223	0
2	P	269	0	142	6	0
3	T	362	0	205	8	0
4	A	3	0	0	0	0
5	A	1	0	0	0	0
6	A	5	0	0	0	0
7	A	31	0	12	8	0
8	A	142	0	0	12	0
8	P	7	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	T	6	0	0	1	0
All	All	8622	0	8066	239	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 14.

All (239) 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:947:CYS:SG	1:A:949:THR:OG1	2.05	1.15
1:A:877:HIS:CA	1:A:907:ILE:HD11	1.79	1.12
1:A:966:PHE:HE2	1:A:1217:MET:HE2	1.19	1.06
1:A:1217:MET:CE	1:A:1231:PHE:HB2	1.86	1.06
1:A:342:ARG:HB2	1:A:781:THR:HB	1.34	1.05
1:A:780:THR:HG22	1:A:783:GLU:HG2	1.33	1.04
1:A:877:HIS:HA	1:A:907:ILE:HD11	1.36	1.03
1:A:1217:MET:HE3	1:A:1231:PHE:HB2	1.44	1.00
1:A:1174:THR:HG22	1:A:1177:GLU:H	1.30	0.96
1:A:1398:VAL:O	1:A:1402:GLU:HG3	1.66	0.96
7:A:1456:DGT:H8	7:A:1456:DGT:C5'	1.97	0.94
1:A:335:THR:H	1:A:782:ASN:ND2	1.66	0.93
1:A:1142:THR:HG22	1:A:1145:GLN:H	1.32	0.92
1:A:1160:THR:HG21	3:T:6:DG:OP1	1.71	0.91
1:A:644:GLN:HE21	1:A:644:GLN:H	1.17	0.91
1:A:877:HIS:HA	1:A:907:ILE:CD1	2.02	0.89
1:A:877:HIS:N	1:A:907:ILE:HD11	1.85	0.89
1:A:966:PHE:HE2	1:A:1217:MET:CE	1.86	0.89
1:A:343:VAL:H	1:A:804:THR:HG21	1.38	0.89
1:A:780:THR:HG22	1:A:783:GLU:H	1.39	0.87
1:A:966:PHE:CE2	1:A:1217:MET:HE2	2.11	0.84
7:A:1456:DGT:H8	7:A:1456:DGT:H5'A	1.62	0.82
1:A:342:ARG:CB	1:A:781:THR:HB	2.08	0.82
1:A:1217:MET:HE1	1:A:1231:PHE:HB2	1.62	0.81
1:A:1102:HIS:HA	3:T:8:DT:H5'	1.63	0.81
1:A:1223:ARG:HD3	8:A:53:HOH:O	1.79	0.81
7:A:1456:DGT:H8	7:A:1456:DGT:H5'	1.61	0.80
1:A:368:LYS:HD3	1:A:398:MET:HE2	1.64	0.80
1:A:334:ASP:OD2	1:A:781:THR:HG22	1.83	0.79
1:A:1160:THR:HG22	1:A:1163:VAL:H	1.47	0.78
1:A:628:GLU:HG3	8:A:87:HOH:O	1.83	0.78
1:A:343:VAL:H	1:A:804:THR:CG2	1.96	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:780:THR:CG2	1:A:783:GLU:HG2	2.11	0.77
7:A:1456:DGT:H5'A	2:P:17:DC:C2'	2.14	0.77
1:A:896:VAL:HG22	8:A:39:HOH:O	1.86	0.75
1:A:1201:ASN:HB3	1:A:1203:THR:HG22	1.69	0.75
3:T:8:DT:H2'	3:T:9:DT:H71	1.69	0.75
1:A:942:LYS:O	1:A:951:TYR:HB2	1.87	0.74
1:A:911:ASN:C	1:A:911:ASN:HD22	1.91	0.74
1:A:1217:MET:HE3	1:A:1231:PHE:CB	2.17	0.73
1:A:724:ILE:O	1:A:728:VAL:HG23	1.88	0.73
1:A:237:GLU:HG2	1:A:275:THR:HB	1.71	0.72
1:A:1102:HIS:HD2	1:A:1104:ASP:H	1.39	0.71
1:A:335:THR:H	1:A:782:ASN:HD21	1.38	0.70
1:A:237:GLU:HG2	1:A:275:THR:CB	2.22	0.70
1:A:820:GLU:HG2	8:A:15:HOH:O	1.91	0.70
1:A:1201:ASN:CB	1:A:1203:THR:HG22	2.21	0.69
7:A:1456:DGT:H5'A	2:P:17:DC:H2'	1.73	0.68
1:A:1282:MET:HE1	8:A:36:HOH:O	1.94	0.68
1:A:669:GLY:HA2	1:A:698:GLU:OE2	1.94	0.67
1:A:1102:HIS:CD2	1:A:1104:ASP:H	2.12	0.66
1:A:637:LEU:HG	1:A:652:ILE:HD13	1.75	0.66
1:A:877:HIS:CA	1:A:907:ILE:CD1	2.66	0.66
1:A:355:ASP:O	1:A:755:ARG:HD2	1.96	0.66
1:A:343:VAL:HB	1:A:804:THR:HG23	1.78	0.66
1:A:287:LYS:O	1:A:291:GLU:HG2	1.95	0.66
1:A:279:LEU:HB3	1:A:318:VAL:HG22	1.77	0.65
1:A:1161:ARG:HH12	1:A:1329:ASN:HD21	1.43	0.65
1:A:766:ASN:N	1:A:767:PRO:HD2	2.11	0.65
1:A:966:PHE:CE2	1:A:1217:MET:CE	2.76	0.64
1:A:342:ARG:NH2	1:A:344:GLU:OE1	2.29	0.64
1:A:764:GLY:O	1:A:767:PRO:HD3	1.98	0.64
1:A:366:GLN:HG2	1:A:747:LEU:HD21	1.81	0.63
1:A:764:GLY:O	1:A:767:PRO:CD	2.47	0.63
1:A:368:LYS:HA	1:A:398:MET:CE	2.29	0.62
1:A:675:LEU:HD23	1:A:676:PHE:H	1.65	0.62
1:A:237:GLU:HG2	1:A:275:THR:OG1	2.00	0.61
1:A:1414:GLN:HG3	8:A:68:HOH:O	2.00	0.61
1:A:856:ARG:O	1:A:860:GLU:HB2	2.00	0.61
1:A:896:VAL:HG11	1:A:974:ILE:HG12	1.83	0.61
3:T:8:DT:C2'	3:T:9:DT:H71	2.30	0.60
1:A:334:ASP:OD2	1:A:781:THR:CG2	2.49	0.60
1:A:1102:HIS:CD2	1:A:1104:ASP:HB2	2.37	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1456:DGT:C5'	7:A:1456:DGT:C8	2.77	0.59
3:T:8:DT:H2'	3:T:9:DT:C7	2.33	0.59
1:A:911:ASN:ND2	1:A:913:LEU:H	2.01	0.58
1:A:349:THR:O	1:A:356:ALA:HB3	2.03	0.58
1:A:1142:THR:HG22	1:A:1145:GLN:N	2.13	0.58
1:A:1409:LYS:HG3	1:A:1437:ASP:HA	1.86	0.58
1:A:368:LYS:HA	1:A:398:MET:HE1	1.86	0.58
1:A:253:PHE:CZ	1:A:1035:ARG:HB3	2.39	0.57
1:A:644:GLN:HE21	1:A:644:GLN:N	1.94	0.57
1:A:896:VAL:CG1	1:A:974:ILE:HG12	2.35	0.57
1:A:1005:ILE:HG23	1:A:1044:LYS:HG3	1.86	0.57
1:A:1104:ASP:O	1:A:1108:ILE:HG23	2.04	0.57
1:A:669:GLY:HA2	1:A:698:GLU:CD	2.25	0.57
7:A:1456:DGT:H5'A	2:P:17:DC:H2"	1.86	0.57
1:A:780:THR:CG2	1:A:783:GLU:H	2.15	0.57
1:A:670:CYS:HB3	1:A:672:LYS:H	1.70	0.56
1:A:368:LYS:HD3	1:A:398:MET:CE	2.35	0.56
1:A:1410:GLU:OE1	1:A:1438:HIS:HB3	2.06	0.56
1:A:668:SER:HB2	1:A:675:LEU:HD22	1.87	0.56
1:A:335:THR:N	1:A:782:ASN:ND2	2.48	0.56
1:A:766:ASN:N	1:A:767:PRO:CD	2.69	0.55
1:A:806:LYS:HD3	8:A:76:HOH:O	2.06	0.55
1:A:634:LEU:O	1:A:638:VAL:HG12	2.05	0.55
1:A:619:PHE:CD2	1:A:674:GLU:HB2	2.41	0.55
1:A:1217:MET:HE3	1:A:1231:PHE:CA	2.36	0.55
1:A:747:LEU:HD13	1:A:748:ASN:ND2	2.22	0.55
1:A:818:LYS:HE2	1:A:1065:ASP:O	2.08	0.54
1:A:944:CYS:C	1:A:946:ARG:H	2.11	0.54
1:A:675:LEU:HD23	1:A:676:PHE:N	2.22	0.54
1:A:938:ASP:OD1	1:A:1174:THR:HG23	2.07	0.54
1:A:1407:LEU:O	1:A:1408:SER:HB3	2.08	0.54
1:A:823:THR:HG21	1:A:868:GLY:HA3	1.91	0.53
1:A:1161:ARG:NH1	1:A:1329:ASN:HD21	2.06	0.53
1:A:634:LEU:O	1:A:638:VAL:CG1	2.57	0.52
1:A:1087:PHE:CZ	1:A:1096:LYS:HE2	2.44	0.52
1:A:1223:ARG:CD	8:A:53:HOH:O	2.48	0.52
1:A:1002:ALA:HB3	1:A:1050:HIS:CB	2.40	0.52
1:A:277:SER:OG	1:A:1035:ARG:HG2	2.09	0.52
2:P:5:DG:H4'	2:P:6:DA:O5'	2.09	0.52
1:A:1157:GLU:OE2	1:A:1186:HIS:NE2	2.36	0.52
3:T:8:DT:H2"	3:T:9:DT:C6	2.44	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1160:THR:HG23	8:A:75:HOH:O	2.11	0.51
1:A:1045:ARG:HG3	1:A:1046:THR:HG23	1.91	0.51
2:P:10:DG:H2"	2:P:11:DG:OP2	2.09	0.51
1:A:334:ASP:OD1	1:A:341:LYS:NZ	2.43	0.51
1:A:1398:VAL:O	1:A:1402:GLU:CG	2.52	0.51
3:T:16:DC:H2"	3:T:17:DT:H5"	1.92	0.51
1:A:386:PHE:HB2	1:A:387:PRO:HD3	1.93	0.50
1:A:869:PHE:CZ	1:A:972:PRO:HD2	2.46	0.50
1:A:381:ALA:HB1	1:A:650:PRO:HG2	1.93	0.50
1:A:917:TYR:HB3	1:A:951:TYR:CD1	2.46	0.50
1:A:879:LEU:HD23	1:A:989:TYR:HD2	1.76	0.50
1:A:635:PHE:HA	1:A:1068:PRO:HG3	1.93	0.50
1:A:911:ASN:HD22	1:A:913:LEU:H	1.58	0.49
1:A:1254:HIS:HE1	8:A:71:HOH:O	1.95	0.49
1:A:1158:PHE:HA	1:A:1163:VAL:HG11	1.95	0.49
1:A:368:LYS:CA	1:A:398:MET:HE3	2.42	0.49
1:A:1363:ASP:C	1:A:1363:ASP:OD1	2.51	0.49
1:A:1148:CYS:SG	1:A:1164:ARG:HD3	2.51	0.49
1:A:1336:THR:HG23	1:A:1339:GLU:OE1	2.12	0.49
1:A:290:ALA:O	1:A:293:MET:HB2	2.13	0.49
1:A:1046:THR:HB	8:T:67:HOH:O	2.11	0.49
1:A:1174:THR:HG22	1:A:1177:GLU:N	2.13	0.49
7:A:1456:DGT:C8	7:A:1456:DGT:H5'A	2.37	0.48
1:A:692:ARG:HG3	1:A:734:LEU:HD13	1.95	0.48
1:A:1282:MET:CE	8:A:36:HOH:O	2.59	0.48
1:A:1180:GLN:HA	1:A:1180:GLN:HE21	1.78	0.48
1:A:804:THR:HG22	1:A:805:GLN:N	2.27	0.48
1:A:1302:PHE:CZ	1:A:1348:VAL:HG22	2.48	0.48
1:A:754:TYR:CD1	1:A:1039:GLY:HA3	2.48	0.48
1:A:1201:ASN:HB2	1:A:1203:THR:CG2	2.43	0.48
1:A:911:ASN:C	1:A:911:ASN:ND2	2.62	0.48
1:A:1102:HIS:HD2	1:A:1104:ASP:HB2	1.76	0.48
1:A:1408:SER:O	1:A:1409:LYS:C	2.49	0.48
1:A:399:LYS:NZ	1:A:808:ALA:O	2.46	0.48
1:A:1104:ASP:HB2	1:A:1105:PRO:HD3	1.95	0.48
1:A:1101:GLY:O	3:T:8:DT:H4'	2.14	0.47
1:A:1108:ILE:HD11	1:A:1119:PRO:HG3	1.97	0.47
1:A:875:ILE:HG12	1:A:994:PHE:CZ	2.49	0.47
1:A:1201:ASN:CB	1:A:1203:THR:CG2	2.91	0.47
1:A:822:TYR:CD2	1:A:822:TYR:N	2.83	0.47
1:A:324:LEU:HD23	1:A:325:ASN:N	2.30	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1213:ARG:O	1:A:1234:MET:HG3	2.14	0.47
1:A:917:TYR:HB2	1:A:926:GLU:HG3	1.98	0.46
1:A:1163:VAL:HG22	1:A:1185:SER:HB2	1.96	0.46
1:A:1108:ILE:HD11	1:A:1119:PRO:CG	2.45	0.46
1:A:368:LYS:CA	1:A:398:MET:CE	2.93	0.46
1:A:1073:ALA:O	1:A:1074:ASP:HB2	2.15	0.46
1:A:355:ASP:O	1:A:755:ARG:CD	2.64	0.46
1:A:860:GLU:HG2	1:A:960:PHE:CE1	2.51	0.46
1:A:236:LEU:HD23	1:A:277:SER:HA	1.98	0.46
1:A:1002:ALA:HB3	1:A:1050:HIS:HB2	1.98	0.46
1:A:1147:MET:CE	1:A:1325:ILE:HG21	2.46	0.46
1:A:1142:THR:CG2	1:A:1144:GLU:HB3	2.46	0.46
1:A:334:ASP:OD1	1:A:781:THR:HG23	2.17	0.45
1:A:386:PHE:CZ	1:A:402:TYR:HB3	2.51	0.45
1:A:1338:LYS:HA	1:A:1338:LYS:HD3	1.60	0.45
1:A:1201:ASN:HB2	1:A:1203:THR:HG22	1.97	0.45
1:A:1409:LYS:HD3	1:A:1432:LEU:HB3	1.98	0.45
1:A:273:ASP:O	1:A:274:TYR:HB2	2.16	0.45
1:A:1184:LEU:HA	1:A:1190:VAL:HG11	1.98	0.45
1:A:867:HIS:NE2	1:A:968:GLY:HA3	2.31	0.45
1:A:929:ASN:C	1:A:931:GLY:N	2.69	0.45
1:A:1045:ARG:CG	1:A:1046:THR:HG23	2.47	0.45
1:A:264:ARG:HG3	1:A:284:SER:O	2.17	0.45
1:A:1294:PRO:O	1:A:1297:TYR:HB3	2.17	0.45
1:A:341:LYS:HE3	1:A:370:TRP:O	2.17	0.45
1:A:1147:MET:HE1	1:A:1325:ILE:HG21	1.98	0.45
1:A:1108:ILE:CD1	1:A:1119:PRO:CB	2.94	0.45
1:A:352:SER:O	1:A:353:GLN:C	2.55	0.45
1:A:1290:LYS:O	1:A:1355:ARG:NH1	2.30	0.45
1:A:1142:THR:HB	1:A:1145:GLN:HG3	1.99	0.44
1:A:311:ASP:HB3	1:A:314:VAL:HG12	1.99	0.44
1:A:1091:HIS:HB3	8:A:114:HOH:O	2.16	0.44
1:A:1142:THR:HG22	1:A:1144:GLU:N	2.33	0.44
1:A:1013:ALA:O	1:A:1017:VAL:HG23	2.18	0.44
1:A:1104:ASP:OD1	1:A:1305:ARG:NH2	2.38	0.44
1:A:1276:ALA:O	1:A:1280:VAL:HG23	2.18	0.43
1:A:1087:PHE:CE2	1:A:1096:LYS:HE2	2.53	0.43
1:A:324:LEU:C	1:A:324:LEU:HD23	2.39	0.43
1:A:368:LYS:HE3	1:A:396:HIS:O	2.18	0.43
1:A:343:VAL:N	1:A:804:THR:CG2	2.72	0.43
1:A:358:THR:HG21	1:A:747:LEU:HB2	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1238:ARG:HD2	1:A:1239:LYS:HG3	2.00	0.43
1:A:929:ASN:C	1:A:931:GLY:H	2.21	0.42
1:A:627:ASN:OD1	1:A:629:THR:HB	2.19	0.42
1:A:1107:VAL:HG23	1:A:1304:VAL:HG11	2.01	0.42
1:A:876:SER:HB3	1:A:907:ILE:HG13	2.01	0.42
1:A:1213:ARG:HG2	1:A:1272:PRO:HA	2.00	0.42
1:A:700:HIS:HB2	1:A:705:TYR:CE1	2.54	0.42
1:A:893:ARG:HG3	1:A:1275:HIS:CE1	2.54	0.42
1:A:944:CYS:C	1:A:946:ARG:N	2.72	0.42
1:A:1071:TYR:CD2	1:A:1076:THR:HA	2.55	0.42
1:A:754:TYR:CE1	1:A:1039:GLY:HA3	2.54	0.42
1:A:331:GLU:O	1:A:332:ARG:C	2.58	0.42
2:P:5:DG:H1'	2:P:6:DA:C8	2.55	0.42
1:A:350:PRO:HD3	1:A:358:THR:O	2.19	0.42
1:A:921:ASN:OD1	1:A:947:CYS:SG	2.78	0.42
1:A:343:VAL:N	1:A:804:THR:HG21	2.20	0.41
1:A:354:MET:HE3	1:A:1008:VAL:CG2	2.50	0.41
1:A:882:LYS:HD2	1:A:989:TYR:CD2	2.55	0.41
1:A:1183:GLY:HA3	1:A:1211:GLY:O	2.19	0.41
1:A:919:CYS:SG	1:A:921:ASN:HB3	2.60	0.41
1:A:780:THR:CB	1:A:783:GLU:HG2	2.50	0.41
1:A:236:LEU:HD11	1:A:248:VAL:HG11	2.02	0.41
1:A:1409:LYS:HE2	1:A:1432:LEU:O	2.20	0.41
1:A:252:VAL:HG13	1:A:300:MET:O	2.20	0.41
1:A:804:THR:CG2	1:A:805:GLN:N	2.83	0.41
1:A:364:ILE:HG23	1:A:398:MET:HG2	2.03	0.41
1:A:1126:ASP:HA	1:A:1127:PRO:HD3	1.89	0.41
1:A:1102:HIS:HD2	1:A:1104:ASP:N	2.11	0.41
1:A:943:ASN:HD22	1:A:950:LYS:HA	1.86	0.41
1:A:1005:ILE:CG2	1:A:1044:LYS:HG3	2.51	0.41
1:A:763:GLY:C	1:A:765:ALA:H	2.24	0.41
1:A:911:ASN:HD22	1:A:912:PRO:N	2.19	0.41
1:A:1311:LEU:HA	1:A:1311:LEU:HD23	1.94	0.41
1:A:750:GLU:C	1:A:752:LYS:H	2.23	0.41
1:A:1173:LYS:HB2	1:A:1173:LYS:HE2	1.97	0.40
1:A:1134:SER:O	1:A:1171:ARG:NH1	2.54	0.40
1:A:1296:LEU:HD12	1:A:1296:LEU:N	2.35	0.40
1:A:1122:ILE:HA	1:A:1123:PRO:HD3	1.79	0.40
1:A:1191:TRP:CE2	1:A:1196:GLN:HB2	2.56	0.40
1:A:747:LEU:HD13	1:A:748:ASN:HD21	1.86	0.40
1:A:1108:ILE:HD12	1:A:1119:PRO:HB3	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:354:MET:HE3	1:A:1045:ARG:HB2	2.04	0.40
1:A:887:GLY:O	1:A:1109:ARG:HD2	2.22	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	985/1041 (95%)	933 (95%)	47 (5%)	5 (0%)	34 55

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	767	PRO
1	A	670	CYS
1	A	1052	GLY
1	A	677	ASP
1	A	945	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	850/904 (94%)	759 (89%)	91 (11%)	8 15

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	236	LEU
1	A	237	GLU
1	A	247	VAL
1	A	257	VAL
1	A	260	LEU
1	A	264	ARG
1	A	285	ARG
1	A	286	ASP
1	A	287	LYS
1	A	302	VAL
1	A	322	ASN
1	A	323	ASP
1	A	332	ARG
1	A	357	VAL
1	A	363	LEU
1	A	395	LYS
1	A	404	LEU
1	A	410	ASP
1	A	628	GLU
1	A	637	LEU
1	A	638	VAL
1	A	644	GLN
1	A	649	VAL
1	A	654	ARG
1	A	657	LEU
1	A	672	LYS
1	A	675	LEU
1	A	677	ASP
1	A	730	LEU
1	A	733	LYS
1	A	747	LEU
1	A	750	GLU
1	A	755	ARG
1	A	766	ASN
1	A	778	PHE
1	A	780	THR
1	A	781	THR
1	A	782	ASN
1	A	801	VAL
1	A	804	THR
1	A	809	SER
1	A	823	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	831	GLU
1	A	840	ARG
1	A	896	VAL
1	A	911	ASN
1	A	918	VAL
1	A	925	SER
1	A	926	GLU
1	A	930	ASP
1	A	935	SER
1	A	946	ARG
1	A	947	CYS
1	A	949	THR
1	A	951	TYR
1	A	971	VAL
1	A	976	LEU
1	A	1026	LEU
1	A	1027	GLU
1	A	1045	ARG
1	A	1108	ILE
1	A	1111	LEU
1	A	1137	GLU
1	A	1139	LEU
1	A	1142	THR
1	A	1160	THR
1	A	1167	LEU
1	A	1174	THR
1	A	1178	LEU
1	A	1180	GLN
1	A	1184	LEU
1	A	1192	LEU
1	A	1203	THR
1	A	1209	VAL
1	A	1214	ASP
1	A	1223	ARG
1	A	1237	VAL
1	A	1243	LEU
1	A	1253	LYS
1	A	1294	PRO
1	A	1316	LYS
1	A	1348	VAL
1	A	1362	ILE
1	A	1373	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1392	ASN
1	A	1403	GLU
1	A	1409	LYS
1	A	1417	LYS
1	A	1423	LEU
1	A	1432	LEU
1	A	1441	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	322	ASN
1	A	380	HIS
1	A	633	ASN
1	A	644	GLN
1	A	647	HIS
1	A	766	ASN
1	A	782	ASN
1	A	803	ASN
1	A	805	GLN
1	A	911	ASN
1	A	921	ASN
1	A	924	HIS
1	A	943	ASN
1	A	1093	ASN
1	A	1102	HIS
1	A	1180	GLN
1	A	1200	GLN
1	A	1254	HIS
1	A	1329	ASN
1	A	1414	GLN
1	A	1439	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 4 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	$\# Z > 2$
7	DGT	A	1456	4	25,33,33	1.15	2 (8%)	35,52,52	2.43	11 (31%)
6	SO4	A	5	-	4,4,4	0.19	0	6,6,6	0.12	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	DGT	A	1456	4	-	0/18/34/34	0/3/3/3
6	SO4	A	5	-	-	0/0/0/0	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1456	DGT	C5-C4	2.70	1.46	1.40
7	A	1456	DGT	C6-C5	3.55	1.48	1.41

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1456	DGT	C2'-C1'-N9	-6.23	99.02	114.16
7	A	1456	DGT	C5-C6-N1	-3.98	118.15	123.59
7	A	1456	DGT	N3-C2-N1	-3.92	121.47	127.44
7	A	1456	DGT	C6-C5-C4	-3.76	116.41	120.90
7	A	1456	DGT	C4-C5-N7	-3.62	106.14	109.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1456	DGT	O5'-PA-O2A	-2.75	98.93	109.62
7	A	1456	DGT	C1'-N9-C4	-2.70	122.59	127.16
7	A	1456	DGT	O4'-C4'-C5'	-2.39	100.76	109.32
7	A	1456	DGT	C5'-C4'-C3'	-2.23	100.47	114.64
7	A	1456	DGT	C6-N1-C2	4.93	122.78	115.94
7	A	1456	DGT	O4'-C1'-N9	5.92	117.97	107.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1456	DGT	8	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, 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	993/1041 (95%)	-0.08	12 (1%) 81 83	25, 38, 52, 73	0
2	P	13/17 (76%)	0.29	1 (7%) 16 18	25, 39, 73, 78	0
3	T	18/22 (81%)	-0.04	0 100 100	26, 41, 60, 60	0
All	All	1024/1080 (94%)	-0.08	13 (1%) 79 82	25, 38, 53, 78	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	767	PRO	5.7
1	A	765	ALA	3.7
1	A	708	LEU	3.5
1	A	647	HIS	3.4
1	A	330	ASN	3.4
2	P	5	DG	3.3
1	A	794	GLU	2.9
1	A	689	ASP	2.6
1	A	766	ASN	2.5
1	A	764	GLY	2.4
1	A	409	VAL	2.3
1	A	763	GLY	2.2
1	A	720	ILE	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

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, 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	LLDF	B-factors(Å ²)	Q<0.9
6	SO4	A	5	5/5	0.88	0.17	-0.07	100,100,100,100	0
5	ZN	A	4	1/1	0.97	0.08	-1.72	67,67,67,67	0
7	DGT	A	1456	31/31	0.99	0.06	-4.20	20,23,25,26	0
4	MN	A	3	1/1	0.99	0.04	-6.37	61,61,61,61	0
4	MN	A	2	1/1	0.95	0.06	-	105,105,105,105	0
4	MN	A	1	1/1	0.99	0.02	-	23,23,23,23	0

6.5 Other polymers [i](#)

There are no such residues in this entry.