Full wwPDB X-ray Structure Validation Report

Jan 31, 2016 – 10:25 PM GMT

PDB ID	:	1TK0
Title	:	T7 DNA polymerase ternary complex with 8 oxo guanosine and ddCTP at the insertion site
Authors	:	Brieba, L.G.; Eichman, B.F.; Kokoska, R.J.; Doublie, S.; Kunkel, T.A.; Ellenberger, T.
Deposited on	:	2004-06-07
Resolution	:	2.30 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 ①) were used in the production of this report:

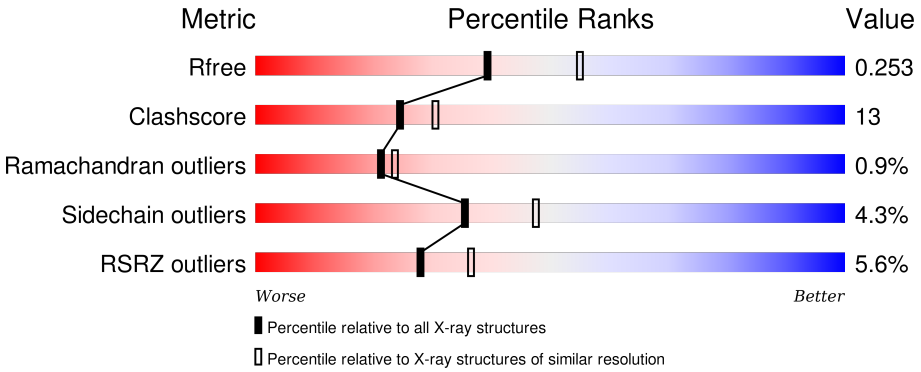
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	P	22	18% 18% 32% 9% 41%
2	T	26	12% 31% 27% · 38%
3	A	698	5% 74% 22% · ·
4	B	108	3% 67% 28% · ·

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
6	SO4	A	995	-	-	-	X
8	1PE	A	901	-	-	-	X
9	MES	A	902	-	-	-	X

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 7428 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 DNA chain called 5'-D(*CP*GP*AP*AP*AP*AP*CP*GP*A*CP*GP*GP*CP*CP*AP*GP*TP*GP*CP*CP*AP*(DDG))-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	P	13	262	125	52	73	12	0	0	0

- Molecule 2 is a DNA chain called 5'-D(*CP*CP*CP*(8OG)P*CP*TP*GP*GP*CP*AP*CP*TP*GP*GP*CP*CP*GP*TP*CP*GP*TP*TP*TP*TP*CP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	T	16	319	149	57	97	16	0	0	0

- Molecule 3 is a protein called DNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	A	686	5444	3468	939	1013	24	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	LYS	DELETION	UNP P00581
A	?	-	ARG	DELETION	UNP P00581
A	?	-	PHE	DELETION	UNP P00581
A	?	-	GLY	DELETION	UNP P00581
A	?	-	SER	DELETION	UNP P00581
A	?	-	HIS	DELETION	UNP P00581

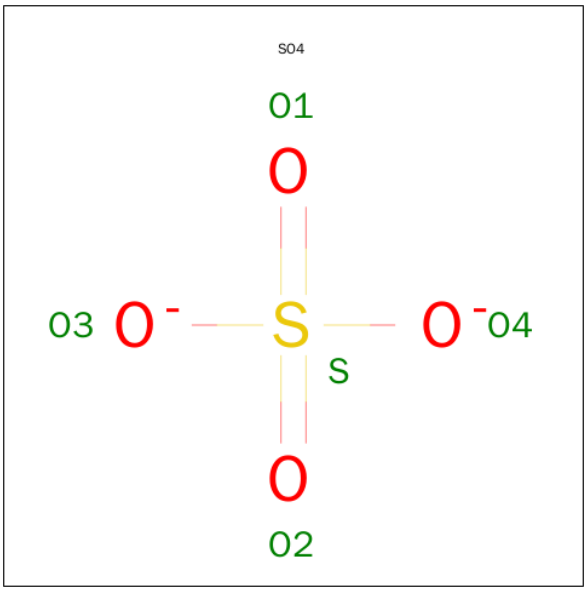
- Molecule 4 is a protein called Thioredoxin 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	B	105	802	518	129	152	3	0	0	0

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

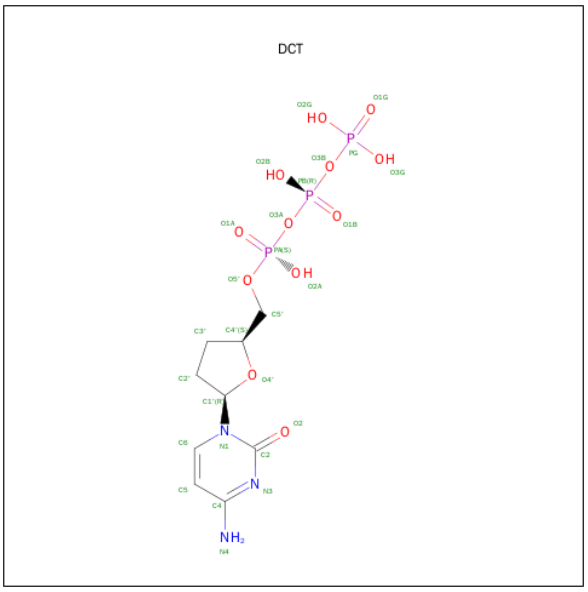
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	3	Total Mg 3 3	0	0

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



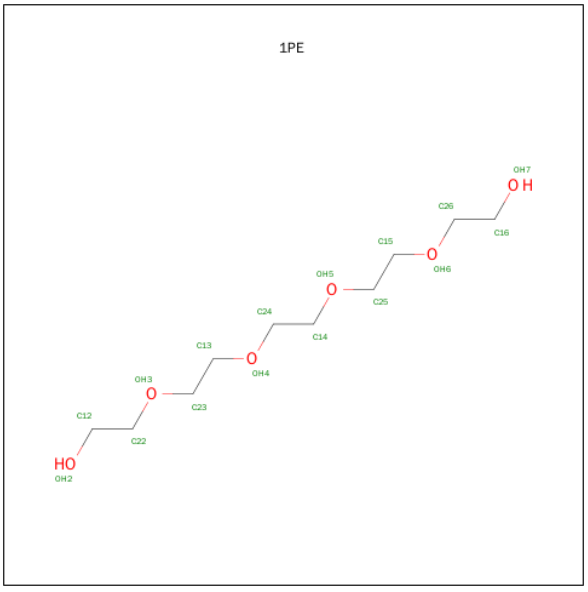
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0

- Molecule 7 is 2',3'-DIDEOXYCYTIDINE 5'-TRIPHOSPHATE (three-letter code: DCT) (formula: $C_9H_{16}N_3O_{12}P_3$).



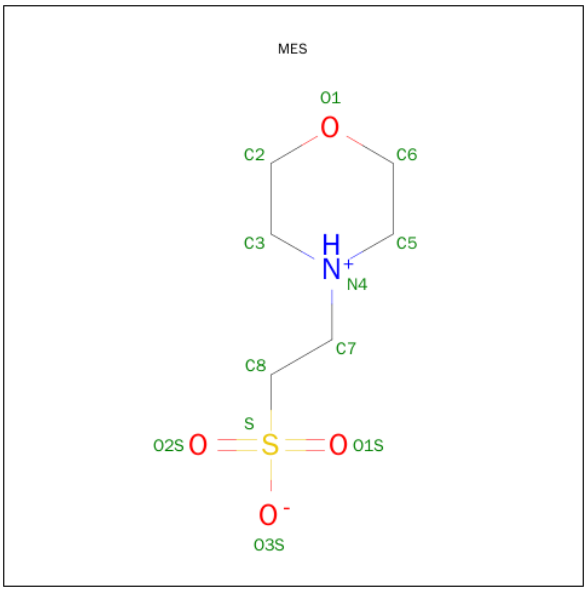
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	P	0	0
			27	9	3	12	3		

- Molecule 8 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			16	10	6		

- Molecule 9 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 10 is water.

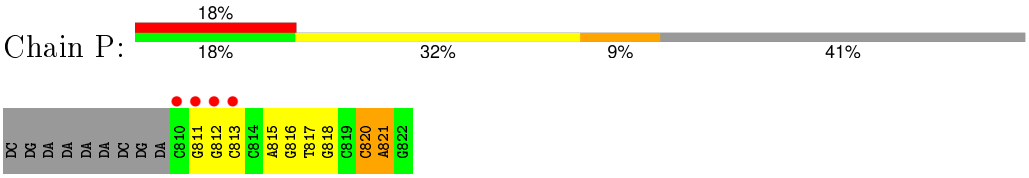
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	461	Total	O	0	0
			461	461		
10	B	27	Total	O	0	0
			27	27		
10	P	18	Total	O	0	0
			18	18		
10	T	27	Total	O	0	0
			27	27		

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.

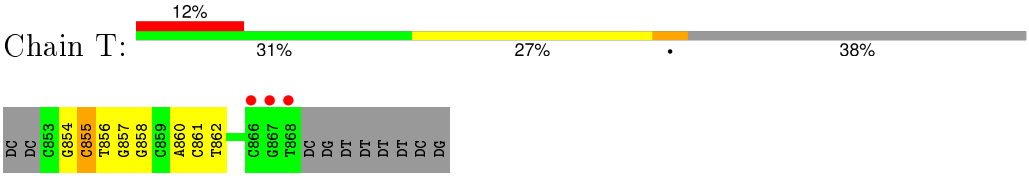
• Molecule 1: 5'-D(*CP*GP*AP*AP*AP*AP*CP*GP*A*CP*GP*GP*CP*CP*AP*GP*TP*GP*CP*CP*AP*(DDG))-3'

Chain P:



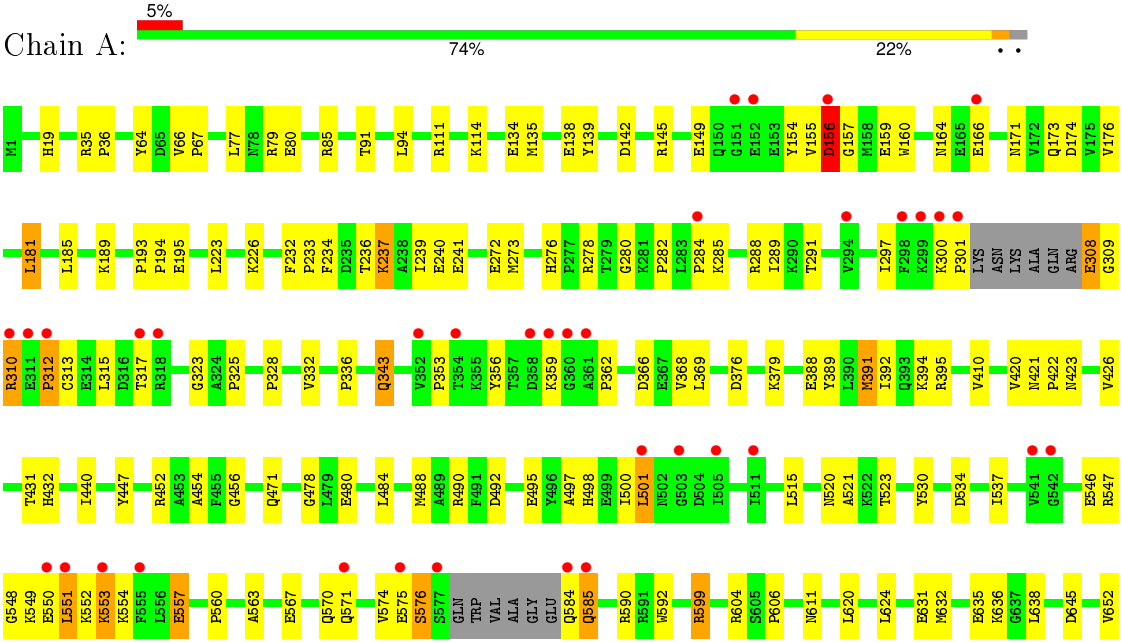
• Molecule 2: 5'-D(*CP*CP*CP*(8OG)P*CP*TP*GP*GP*CP*AP*CP*TP*GP*GP*CP*CP*GP*TP*CP*GP*TP*TP*TP*TP*CP*G)-3'

Chain T:

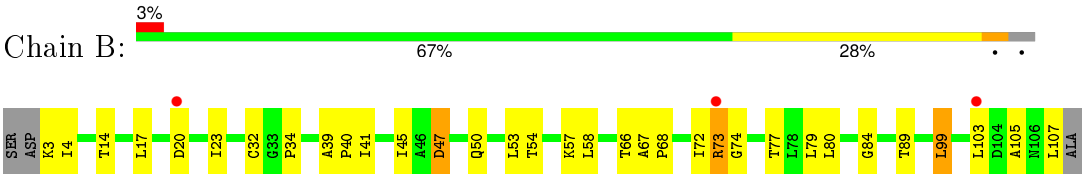


• Molecule 3: DNA polymerase

Chain A:



- Molecule 4: Thioredoxin 1



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	106.23Å 215.10Å 52.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.85 – 2.30 35.85 – 2.29	Depositor EDS
% Data completeness (in resolution range)	94.0 (35.85-2.30) 93.5 (35.85-2.29)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	3.33 (at 2.29Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.217 , 0.263 0.211 , 0.253	Depositor DCC
R_{free} test set	2456 reflections (5.07%)	DCC
Wilson B-factor (Å^2)	32.1	Xtriage
Anisotropy	0.509	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 49.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 51068 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7428	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.04% 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: MG, 1PE, 8OG, SO4, MES, DCT, DDG

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	P	0.45	0/270	0.87	0/415
2	T	0.48	0/329	0.87	0/502
3	A	0.33	0/5577	0.58	0/7547
4	B	0.29	0/817	0.57	0/1108
All	All	0.34	0/6993	0.61	0/9572

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	P	0	2
2	T	0	2
All	All	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	P	820	DC	Sidechain
1	P	821	DA	Sidechain
2	T	855	DC	Sidechain
2	T	857	DG	Sidechain

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	P	262	0	143	17	0
2	T	319	0	174	8	0
3	A	5444	0	5317	131	0
4	B	802	0	816	22	0
5	A	3	0	0	0	0
6	A	10	0	0	0	0
7	A	27	0	12	2	0
8	A	16	0	22	0	0
9	A	12	0	13	2	0
10	A	461	0	0	6	0
10	B	27	0	0	1	0
10	P	18	0	0	2	0
10	T	27	0	0	0	0
All	All	7428	0	6497	173	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 13.

All (173) 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:P:816:DG:H2"	1:P:817:DT:H5'	1.38	1.01
1:P:812:DG:H2"	1:P:813:DC:H5'	1.38	1.00
3:A:111:ARG:HH21	3:A:114:LYS:HD2	1.32	0.94
1:P:812:DG:H2"	1:P:813:DC:C5'	1.98	0.93
3:A:297:ILE:HD12	3:A:297:ILE:H	1.34	0.91
3:A:570:GLN:HE22	3:A:606:PRO:HB3	1.38	0.88
1:P:815:DA:H2"	1:P:816:DG:H5'	1.54	0.88
3:A:164:ASN:OD1	3:A:166:GLU:HG2	1.79	0.83
1:P:816:DG:H2"	1:P:817:DT:C5'	2.08	0.82
3:A:35:ARG:HB3	3:A:36:PRO:HD2	1.62	0.80
1:P:815:DA:H2"	1:P:816:DG:C5'	2.11	0.80
3:A:301:PRO:HA	3:A:308:GLU:HG2	1.65	0.79
4:B:39:ALA:HB3	4:B:40:PRO:HD3	1.65	0.78
3:A:300:LYS:HG3	3:A:301:PRO:HD2	1.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:817:DT:H2"	1:P:818:DG:H5'	1.66	0.76
3:A:570:GLN:NE2	3:A:606:PRO:HB3	2.04	0.72
3:A:328:PRO:HB3	4:B:73:ARG:HH12	1.56	0.70
3:A:480:GLU:CD	7:A:823:DCT:H2"	2.12	0.70
3:A:79:ARG:HD3	10:A:1108:HOH:O	1.92	0.69
2:T:860:DA:H2"	2:T:861:DC:H5'	1.74	0.68
3:A:343:GLN:HG3	3:A:362:PRO:HG3	1.77	0.67
3:A:546:GLU:H	3:A:546:GLU:CD	1.99	0.66
3:A:284:PRO:HA	3:A:288:ARG:NH2	2.10	0.66
4:B:45:ILE:HG13	4:B:99:LEU:HD13	1.77	0.65
3:A:563:ALA:O	3:A:567:GLU:HG3	1.96	0.65
3:A:391:MET:HE2	3:A:392:ILE:HA	1.78	0.65
3:A:678:ARG:NH1	3:A:691:ASP:OD1	2.23	0.65
4:B:3:LYS:HE3	4:B:50:GLN:CD	2.18	0.64
3:A:276:HIS:CD2	3:A:278:ARG:HB3	2.32	0.63
3:A:484:LEU:O	3:A:488:MET:HG2	1.99	0.63
4:B:23:ILE:HD13	4:B:54:THR:HB	1.78	0.63
3:A:91:THR:HB	3:A:181:LEU:HD13	1.80	0.62
3:A:94:LEU:HB3	3:A:185:LEU:HD13	1.80	0.62
3:A:285:LYS:HA	3:A:285:LYS:HE2	1.81	0.62
3:A:276:HIS:O	3:A:280:GLY:HA2	2.00	0.62
1:P:817:DT:H2"	1:P:818:DG:C5'	2.30	0.62
3:A:631:GLU:O	3:A:635:GLU:HG2	1.99	0.61
3:A:139:TYR:HE1	3:A:166:GLU:HG3	1.65	0.61
3:A:154:TYR:OH	3:A:157:GLY:HA2	2.00	0.61
3:A:276:HIS:HD2	3:A:278:ARG:H	1.47	0.61
3:A:145:ARG:O	3:A:149:GLU:HB2	2.02	0.60
3:A:85:ARG:HD3	10:A:1180:HOH:O	2.01	0.60
1:P:820:DC:H2"	1:P:821:DA:H5'	1.83	0.59
2:T:858:DG:H4'	3:A:432:HIS:O	2.03	0.59
3:A:64:TYR:O	3:A:67:PRO:HD2	2.03	0.58
3:A:584:GLN:O	3:A:585:GLN:O	2.21	0.58
3:A:237:LYS:O	3:A:241:GLU:HG3	2.04	0.58
3:A:135:MET:HG3	3:A:174:ASP:OD1	2.04	0.57
1:P:812:DG:H2"	1:P:813:DC:H5"	1.86	0.57
3:A:297:ILE:HD12	3:A:297:ILE:N	2.14	0.57
3:A:667:GLN:O	3:A:671:GLU:HG3	2.05	0.57
10:P:1650:HOH:O	3:A:394:LYS:HE2	2.07	0.55
3:A:19:HIS:O	3:A:36:PRO:HD3	2.06	0.55
4:B:14:THR:HG21	10:B:1190:HOH:O	2.07	0.54
4:B:23:ILE:CD1	4:B:54:THR:HB	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:599:ARG:HD3	3:A:620:LEU:HD11	1.90	0.54
3:A:391:MET:HE3	3:A:391:MET:O	2.08	0.54
3:A:575:GLU:O	3:A:576:SER:HB3	2.08	0.54
4:B:77:THR:HG22	4:B:79:LEU:HD13	1.90	0.53
3:A:343:GLN:HG3	3:A:362:PRO:CG	2.38	0.53
3:A:282:PRO:O	3:A:284:PRO:HD3	2.08	0.53
3:A:515:LEU:HD12	3:A:521:ALA:HA	1.90	0.52
3:A:421:ASN:HB3	3:A:431:THR:OG1	2.10	0.52
4:B:32:CYS:SG	4:B:34:PRO:HD2	2.50	0.52
3:A:134:GLU:O	3:A:138:GLU:HB2	2.10	0.51
3:A:557:GLU:O	3:A:560:PRO:HD3	2.10	0.51
3:A:391:MET:HE2	3:A:392:ILE:HD13	1.92	0.51
2:T:855:DC:C6	2:T:856:DT:H72	2.46	0.51
3:A:315:LEU:HD21	4:B:105:ALA:HB1	1.91	0.51
1:P:816:DG:C2'	1:P:817:DT:C5'	2.86	0.51
3:A:173:GLN:O	3:A:176:VAL:HG22	2.11	0.51
3:A:195:GLU:H	3:A:195:GLU:CD	2.13	0.51
4:B:73:ARG:O	4:B:73:ARG:HD2	2.11	0.51
3:A:189:LYS:HD2	3:A:194:PRO:HG2	1.93	0.50
4:B:74:GLY:O	4:B:77:THR:OG1	2.29	0.50
3:A:234:PHE:CZ	3:A:239:ILE:HG13	2.46	0.50
1:P:815:DA:H2"	1:P:816:DG:H5"	1.92	0.50
4:B:41:ILE:O	4:B:45:ILE:HG12	2.11	0.50
3:A:368:VAL:HG23	3:A:369:LEU:N	2.26	0.49
4:B:17:LEU:HA	4:B:84:GLY:HA2	1.94	0.49
3:A:478:GLY:HA2	7:A:823:DCT:O1B	2.12	0.49
2:T:855:DC:H2'	2:T:856:DT:H72	1.94	0.49
3:A:698:PRO:HD2	3:A:702:ILE:HD12	1.94	0.49
3:A:328:PRO:HB3	4:B:73:ARG:NH1	2.24	0.49
3:A:645:ASP:HB3	3:A:665:ILE:HD13	1.95	0.49
3:A:552:LYS:HE3	10:A:1412:HOH:O	2.12	0.48
3:A:549:LYS:O	3:A:553:LYS:HG2	2.12	0.48
3:A:550:GLU:O	3:A:554:LYS:HB2	2.13	0.48
3:A:391:MET:HE1	3:A:447:TYR:CD2	2.48	0.48
3:A:456:GLY:HA2	3:A:471:GLN:OE1	2.14	0.48
4:B:3:LYS:CD	4:B:47:ASP:HA	2.44	0.48
3:A:66:VAL:HB	3:A:67:PRO:HD3	1.96	0.47
3:A:272:GLU:CD	3:A:291:THR:H	2.17	0.47
3:A:282:PRO:C	3:A:284:PRO:HD3	2.35	0.47
3:A:530:TYR:CE1	3:A:611:ASN:HA	2.50	0.47
1:P:820:DC:H2"	1:P:821:DA:C5'	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:811:DG:H2"	1:P:812:DG:C8	2.50	0.47
3:A:111:ARG:HH21	3:A:114:LYS:CD	2.14	0.47
3:A:77:LEU:HD13	9:A:902:MES:O2S	2.15	0.47
4:B:103:LEU:O	4:B:107:LEU:HD13	2.14	0.47
4:B:3:LYS:HE3	4:B:50:GLN:NE2	2.29	0.46
3:A:77:LEU:O	9:A:902:MES:H31	2.14	0.46
3:A:284:PRO:HA	3:A:288:ARG:HH21	1.81	0.46
3:A:189:LYS:HD2	3:A:194:PRO:CG	2.46	0.46
3:A:548:GLY:O	3:A:552:LYS:HG2	2.15	0.46
3:A:420:VAL:O	3:A:422:PRO:HD3	2.16	0.46
3:A:111:ARG:NH2	3:A:114:LYS:HD2	2.14	0.46
3:A:297:ILE:CD1	3:A:297:ILE:H	2.12	0.46
3:A:368:VAL:CG2	3:A:369:LEU:N	2.78	0.46
1:P:816:DG:H1'	1:P:817:DT:H5"	1.97	0.46
3:A:35:ARG:HG3	3:A:35:ARG:HH11	1.80	0.46
3:A:79:ARG:HG2	3:A:80:GLU:N	2.31	0.46
3:A:574:VAL:HG12	3:A:576:SER:H	1.80	0.46
3:A:388:GLU:O	3:A:392:ILE:HG12	2.16	0.45
3:A:239:ILE:HD11	3:A:454:ALA:CB	2.46	0.45
2:T:854:8OG:H2"	2:T:855:DC:C6	2.51	0.45
3:A:223:LEU:O	3:A:226:LYS:HB3	2.16	0.45
3:A:376:ASP:OD2	3:A:379:LYS:HG3	2.16	0.45
3:A:35:ARG:HB3	3:A:36:PRO:CD	2.41	0.45
3:A:410:VAL:HG23	3:A:410:VAL:O	2.16	0.45
3:A:276:HIS:CD2	3:A:278:ARG:H	2.32	0.45
3:A:155:VAL:O	3:A:157:GLY:N	2.50	0.45
3:A:423:ASN:OD1	3:A:599:ARG:NH2	2.50	0.44
3:A:273:MET:CE	3:A:284:PRO:HG3	2.47	0.44
3:A:574:VAL:HG12	3:A:575:GLU:N	2.32	0.44
3:A:537:ILE:HG13	3:A:552:LYS:HD3	2.00	0.44
3:A:534:ASP:CG	3:A:549:LYS:HG2	2.38	0.44
3:A:233:PRO:HB2	3:A:456:GLY:O	2.17	0.44
3:A:236:THR:O	3:A:240:GLU:HG3	2.17	0.44
3:A:497:ALA:O	3:A:500:ILE:HG22	2.18	0.44
3:A:276:HIS:HD2	3:A:278:ARG:N	2.15	0.44
3:A:520:ASN:HA	3:A:523:THR:HG22	1.99	0.44
3:A:336:PRO:HB2	3:A:389:TYR:CD1	2.53	0.44
3:A:391:MET:HE3	3:A:395:ARG:HG2	2.00	0.44
2:T:861:DC:H2'	2:T:862:DT:H71	1.99	0.43
3:A:490:ARG:HD3	10:A:1146:HOH:O	2.17	0.43
3:A:193:PRO:HA	3:A:194:PRO:HD3	1.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:58:LEU:HD21	4:B:66:THR:HB	2.00	0.43
3:A:155:VAL:CG1	3:A:156:ASP:N	2.81	0.43
3:A:574:VAL:HG12	3:A:576:SER:N	2.34	0.43
2:T:854:8OG:H5"	2:T:854:8OG:O8	2.19	0.43
3:A:155:VAL:O	3:A:156:ASP:C	2.57	0.43
3:A:145:ARG:HH11	3:A:145:ARG:HB2	1.83	0.43
3:A:632:MET:O	3:A:636:LYS:HG3	2.19	0.43
3:A:590:ARG:HD2	3:A:592:TRP:O	2.19	0.43
3:A:391:MET:HE2	3:A:392:ILE:CA	2.46	0.42
3:A:547:ARG:O	3:A:551:LEU:HD22	2.19	0.42
2:T:855:DC:H2'	2:T:856:DT:C7	2.49	0.42
3:A:554:LYS:HD3	3:A:554:LYS:O	2.19	0.42
3:A:492:ASP:OD2	3:A:495:GLU:HB3	2.19	0.42
3:A:343:GLN:CG	3:A:362:PRO:HG3	2.46	0.42
3:A:276:HIS:O	3:A:280:GLY:CA	2.66	0.42
3:A:155:VAL:HG12	3:A:156:ASP:N	2.33	0.42
3:A:323:GLY:O	3:A:325:PRO:HD3	2.20	0.42
3:A:570:GLN:HG2	10:A:1272:HOH:O	2.19	0.42
4:B:67:ALA:HB3	4:B:68:PRO:HD3	2.01	0.42
3:A:426:VAL:CG1	3:A:604:ARG:NH2	2.83	0.42
3:A:652:VAL:HB	3:A:655:GLU:HG2	2.02	0.42
1:P:821:DA:H5"	3:A:440:ILE:O	2.20	0.42
4:B:4:ILE:HG21	4:B:57:LYS:HG3	2.01	0.41
3:A:353:PRO:HB2	3:A:356:TYR:OH	2.20	0.41
3:A:309:GLY:O	3:A:310:ARG:CB	2.68	0.41
3:A:317:THR:HG22	3:A:317:THR:O	2.20	0.41
3:A:159:GLU:HG2	3:A:160:TRP:CD1	2.56	0.41
3:A:308:GLU:HG3	3:A:313:CYS:SG	2.61	0.41
3:A:410:VAL:HG22	10:A:1178:HOH:O	2.21	0.41
3:A:135:MET:CE	3:A:135:MET:HA	2.51	0.41
3:A:452:ARG:HG3	3:A:700:TRP:HB3	2.01	0.41
3:A:391:MET:HE1	3:A:447:TYR:HD2	1.84	0.41
3:A:498:HIS:O	3:A:501:LEU:HD12	2.21	0.41
1:P:815:DA:H5'	10:P:1478:HOH:O	2.20	0.41
4:B:72:ILE:CD1	4:B:77:THR:HG21	2.51	0.40
3:A:289:ILE:HD12	3:A:325:PRO:HB2	2.03	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
3	A	680/698 (97%)	648 (95%)	25 (4%)	7 (1%)	19 21
4	B	103/108 (95%)	99 (96%)	4 (4%)	0	100 100
All	All	783/806 (97%)	747 (95%)	29 (4%)	7 (1%)	21 24

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	156	ASP
3	A	312	PRO
3	A	585	GLN
3	A	310	ARG
3	A	359	LYS
3	A	576	SER
3	A	653	HIS

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
3	A	564/579 (97%)	543 (96%)	21 (4%)	41 55
4	B	85/87 (98%)	78 (92%)	7 (8%)	14 17
All	All	649/666 (97%)	621 (96%)	28 (4%)	35 47

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	142	ASP
3	A	156	ASP
3	A	171	ASN
3	A	181	LEU
3	A	232	PHE
3	A	237	LYS
3	A	308	GLU
3	A	312	PRO
3	A	332	VAL
3	A	343	GLN
3	A	366	ASP
3	A	391	MET
3	A	501	LEU
3	A	551	LEU
3	A	553	LYS
3	A	557	GLU
3	A	571	GLN
3	A	599	ARG
3	A	624	LEU
3	A	638	LEU
3	A	686	PHE
4	B	20	ASP
4	B	47	ASP
4	B	53	LEU
4	B	73	ARG
4	B	80	LEU
4	B	89	THR
4	B	99	LEU

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

Mol	Chain	Res	Type
3	A	266	GLN
3	A	276	HIS
3	A	343	GLN
3	A	347	GLN
3	A	570	GLN
4	B	50	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

2 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	$\#\|Z\| > 2$
1	DDG	P	822	1,2	15,23,24	1.30	2 (13%)	16,33,36	3.00	4 (25%)
2	8OG	T	854	2	16,25,26	1.23	2 (12%)	21,37,40	3.19	5 (23%)

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
1	DDG	P	822	1,2	-	0/3/18/19	0/3/3/3
2	8OG	T	854	2	-	0/3/21/22	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	854	8OG	C8-N7	-2.82	1.31	1.34
1	P	822	DDG	C6-C5	2.23	1.45	1.41
2	T	854	8OG	C6-N1	3.45	1.39	1.33
1	P	822	DDG	C6-N1	3.53	1.39	1.33

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	P	822	DDG	C5-C6-N1	-9.11	111.14	123.59
2	T	854	8OG	C5-C6-N1	-8.73	111.66	123.59
2	T	854	8OG	C2'-C1'-N9	-7.93	107.87	115.83
1	P	822	DDG	C6-C5-C4	-2.31	118.14	120.90
2	T	854	8OG	N3-C2-N1	-2.30	123.94	127.44
2	T	854	8OG	C1'-N9-C4	-2.07	124.16	127.37
1	P	822	DDG	N3-C2-N1	-2.01	124.39	127.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	P	822	DDG	C6-N1-C2	6.47	124.93	115.94
2	T	854	8OG	C6-N1-C2	6.54	125.02	115.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	T	854	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, 3 are monoatomic - leaving 5 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	DCT	A	823	5	20,28,28	0.85	0	29,43,43	1.22	3 (10%)
8	1PE	A	901	-	15,15,15	1.03	0	14,14,14	0.90	0
9	MES	A	902	-	11,12,12	0.49	0	14,16,16	0.81	1 (7%)
6	SO4	A	994	-	4,4,4	0.23	0	6,6,6	0.08	0
6	SO4	A	995	-	4,4,4	0.35	0	6,6,6	0.17	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	DCT	A	823	5	-	0/18/31/31	0/2/2/2
8	1PE	A	901	-	-	0/13/13/13	0/0/0/0
9	MES	A	902	-	-	0/6/14/14	0/1/1/1
6	SO4	A	994	-	-	0/0/0/0	0/0/0/0
6	SO4	A	995	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	902	MES	O1S-S-C8	-2.20	105.03	106.91
7	A	823	DCT	PB-O3B-PG	-2.11	125.61	132.67
7	A	823	DCT	O2G-PG-O1G	2.82	119.65	110.58
7	A	823	DCT	C2-N3-C4	3.14	120.04	115.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	823	DCT	2	0
9	A	902	MES	2	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	P	12/22 (54%)	1.55	4 (33%)	0	0	29, 46, 97, 98	0
2	T	15/26 (57%)	1.12	3 (20%)	1	2	24, 39, 97, 100	0
3	A	686/698 (98%)	0.18	36 (5%)	31	39	16, 30, 64, 83	0
4	B	105/108 (97%)	0.34	3 (2%)	55	64	28, 45, 64, 67	0
All	All	818/854 (95%)	0.23	46 (5%)	28	36	16, 33, 66, 100	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	300	LYS	8.9
2	T	867	DG	6.7
1	P	811	DG	5.6
2	T	868	DT	5.6
1	P	810	DC	5.4
3	A	294	VAL	5.3
3	A	542	GLY	5.2
3	A	551	LEU	5.1
3	A	312	PRO	4.8
1	P	812	DG	4.1
3	A	584	GLN	4.0
3	A	577	SER	3.9
3	A	317	THR	3.8
3	A	550	GLU	3.8
3	A	358	ASP	3.8
3	A	298	PHE	3.7
3	A	301	PRO	3.7
4	B	73	ARG	3.7
3	A	511	ILE	3.5
3	A	151	GLY	3.5
3	A	166	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
3	A	156	ASP	3.3
3	A	311	GLU	3.2
3	A	352	VAL	3.2
4	B	20	ASP	3.1
3	A	318	ARG	3.0
3	A	361	ALA	3.0
3	A	501	LEU	2.9
3	A	585	GLN	2.8
2	T	866	DC	2.8
3	A	360	GLY	2.6
3	A	503	GLY	2.6
3	A	359	LYS	2.6
3	A	553	LYS	2.5
3	A	299	LYS	2.5
3	A	354	THR	2.4
3	A	575	GLU	2.4
3	A	541	VAL	2.4
3	A	571	GLN	2.4
3	A	505	ILE	2.4
3	A	555	PHE	2.4
3	A	284	PRO	2.4
3	A	152	GLU	2.3
3	A	310	ARG	2.3
4	B	103	LEU	2.1
1	P	813	DC	2.1

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	8OG	T	854	23/24	0.90	0.14	-	38,42,51,53	0
1	DDG	P	822	21/22	0.97	0.17	-	24,28,29,32	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
8	1PE	A	901	16/16	0.81	0.27	5.14	54,58,63,63	0
6	SO4	A	995	5/5	0.95	0.17	4.93	65,66,66,67	0
9	MES	A	902	12/12	0.96	0.20	2.11	46,48,49,50	0
7	DCT	A	823	27/27	0.94	0.14	-0.70	28,35,37,39	0
5	MG	A	993	1/1	0.96	0.09	-2.78	29,29,29,29	0
5	MG	A	991	1/1	0.81	0.07	-3.04	42,42,42,42	0
6	SO4	A	994	5/5	0.95	0.16	-	63,64,65,65	0
5	MG	A	992	1/1	0.92	0.10	-	33,33,33,33	0

6.5 Other polymers

There are no such residues in this entry.