



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 15, 2023 – 04:49 PM EDT

PDB ID : 1TK5  
Title : T7 DNA polymerase binary complex with 8 oxo guanosine in the templating strand  
Authors : Brieba, L.G.; Eichman, B.F.; Kokoska, R.J.; Doublet, S.; Kunkel, T.A.; Ellenberger, T.  
Deposited on : 2004-06-08  
Resolution : 2.20 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : 1.13  
EDS : 2.35  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35

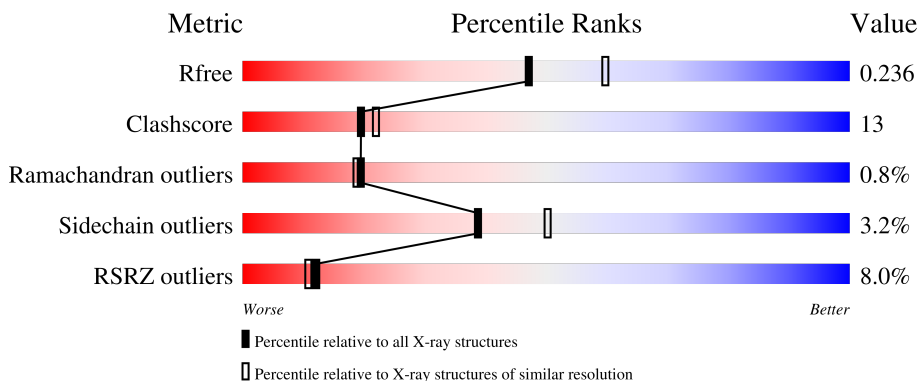
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	P	22	
2	T	26	
3	A	698	
4	B	108	

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 7441 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\*A\*GP\*CP\*CP\*AP\*GP\*TP\*GP\*CP\*CP\*AP\*(DDG)P\*TP\*GP\*CP\*AP\*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	P	11	222	106	44	62	10	0	0	0

- Molecule 2 is a DNA chain called 5'-D(\*CP\*CP\*CP\*(8OG)P\*CP\*TP\*GP\*GP\*CP\*AP\*C P\*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	13	266	125	49	79	13	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	681	5340	3405	923	988	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	1	Total Mg 1 1	0	0

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



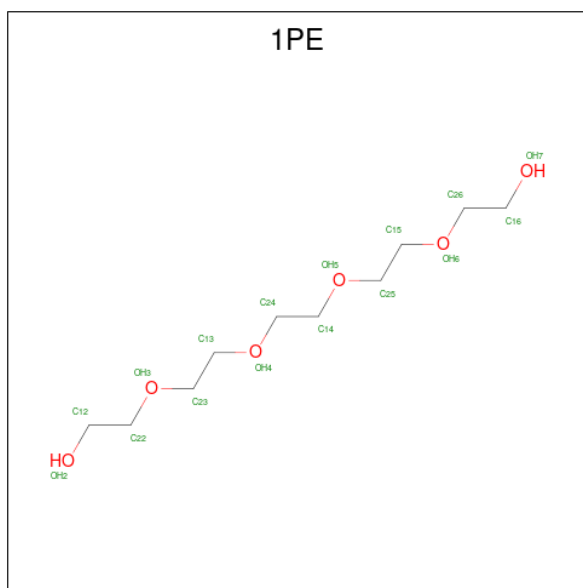
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0

- Molecule 7 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



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

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



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

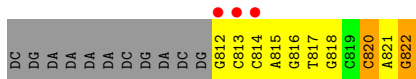
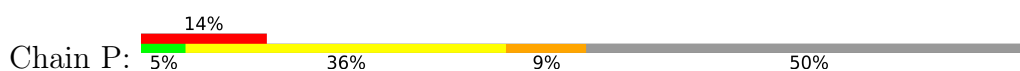
- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	P	27	Total O 27 27	0	0
9	T	48	Total O 48 48	0	0
9	A	649	Total O 649 649	0	0
9	B	48	Total O 48 48	0	0

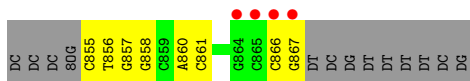
### 3 Residue-property plots i

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

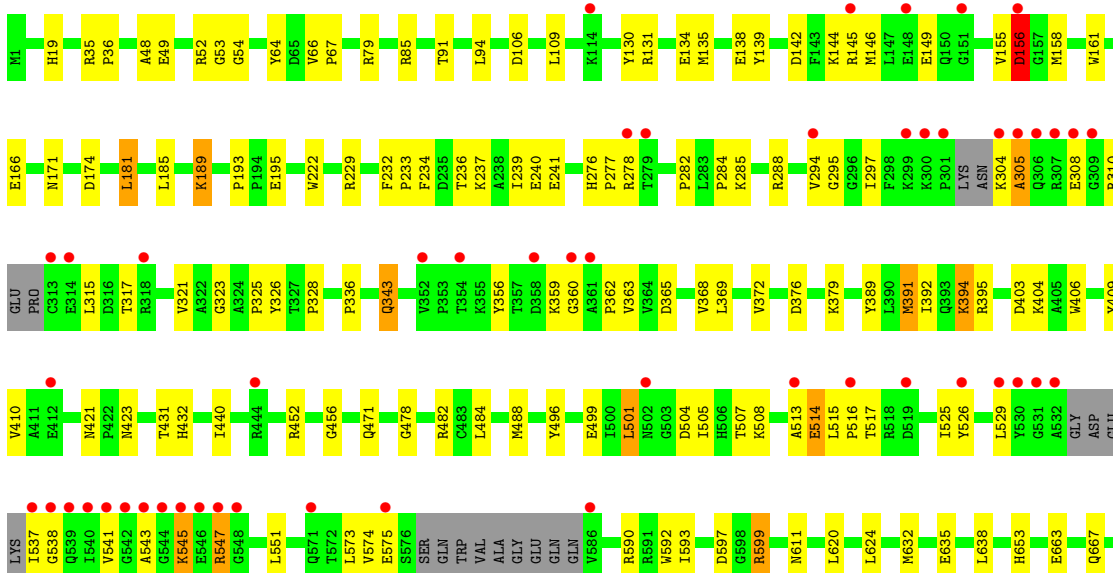
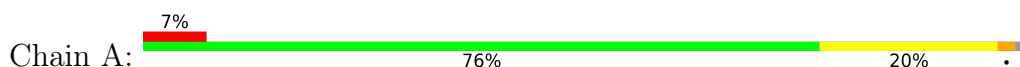
- Molecule 1: 5'-D(\*CP\*GP\*AP\*AP\*A\*GP\*CP\*CP\*AP\*GP\*TP\*GP\*CP\*CP\*AP\*(DDG)P\*TP\*GP\*CP\*AP\*A)-3'



- 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\*CP\*G)-3'



- Molecule 3: DNA polymerase





● Molecule 4: Thioredoxin 1





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.31Å 213.26Å 52.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	26.33 – 2.20 26.33 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.5 (26.33-2.20) 99.0 (26.33-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.34 (at 1.99Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.214 , 0.246 0.202 , 0.236	Depositor DCC
$R_{free}$ test set	3873 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.5	Xtrriage
Anisotropy	0.269	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 65.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7441	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% 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: 1PE, SO4, MG, DDG, MES

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	0.37	0/225	0.89	0/345
2	T	0.46	0/297	0.85	0/456
3	A	0.32	0/5470	0.55	0/7413
4	B	0.28	0/817	0.55	0/1108
All	All	0.33	0/6809	0.59	0/9322

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	1
2	T	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	P	820	DC	Sidechain
2	T	857	DG	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	P	222	0	124	23	0
2	T	266	0	146	7	0
3	A	5340	0	5156	123	0
4	B	802	0	816	20	0
5	A	1	0	0	0	0
6	A	10	0	0	0	0
7	A	12	0	13	0	0
8	A	16	0	22	0	0
9	A	649	0	0	8	0
9	B	48	0	0	0	0
9	P	27	0	0	0	0
9	T	48	0	0	1	0
All	All	7441	0	6277	165	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 (165) 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:815:DA:H2''	1:P:816:DG:H5'	1.39	1.04
3:A:537:ILE:HG13	3:A:538:GLY:H	1.27	0.97
1:P:820:DC:H2''	1:P:821:DA:H5'	1.49	0.93
1:P:817:DT:H2''	1:P:818:DG:H5'	1.53	0.91
3:A:391:MET:HE1	3:A:392:ILE:HA	1.56	0.88
1:P:820:DC:H2''	1:P:821:DA:C5'	2.03	0.88
3:A:343:GLN:HG3	3:A:362:PRO:HG3	1.55	0.86
1:P:816:DG:H2''	1:P:817:DT:C5'	2.13	0.78
2:T:866:DC:H2''	2:T:867:DG:C8	2.19	0.76
4:B:39:ALA:HB3	4:B:40:PRO:HD3	1.67	0.75
3:A:343:GLN:HG3	3:A:362:PRO:CG	2.15	0.75
1:P:812:DG:H2'	1:P:813:DC:H5''	1.69	0.74
3:A:285:LYS:HA	3:A:285:LYS:HE2	1.68	0.73
3:A:537:ILE:HG13	3:A:538:GLY:N	2.03	0.72
1:P:816:DG:H2''	1:P:817:DT:H5''	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:145:ARG:O	3:A:149:GLU:HG3	1.92	0.70
3:A:504:ASP:OD2	3:A:507:THR:HG23	1.90	0.70
3:A:547:ARG:O	3:A:547:ARG:HD3	1.91	0.70
3:A:632:MET:HA	3:A:635:GLU:HG2	1.73	0.70
3:A:35:ARG:HB3	3:A:36:PRO:HD2	1.73	0.68
4:B:95:SER:OG	4:B:98:GLN:HG3	1.94	0.68
1:P:815:DA:C2'	1:P:816:DG:H5'	2.23	0.67
3:A:376:ASP:OD2	3:A:379:LYS:HG3	1.97	0.65
1:P:821:DA:H5'	1:P:821:DA:H8	1.61	0.65
3:A:667:GLN:HG2	3:A:696:MET:HE1	1.79	0.65
4:B:77:THR:HG22	4:B:79:LEU:HD13	1.80	0.64
1:P:816:DG:C2'	1:P:817:DT:H5''	2.28	0.63
1:P:816:DG:H2''	1:P:817:DT:H5'	1.81	0.63
3:A:315:LEU:HD21	4:B:105:ALA:HB1	1.81	0.62
4:B:32:CYS:SG	4:B:34:PRO:HD2	2.40	0.62
3:A:66:VAL:HB	3:A:67:PRO:HD3	1.80	0.61
2:T:860:DA:H2''	2:T:861:DC:H5'	1.82	0.61
3:A:484:LEU:O	3:A:488:MET:HG2	2.01	0.61
2:T:855:DC:H2''	2:T:856:DT:H5'	1.82	0.61
1:P:817:DT:H2''	1:P:818:DG:C5'	2.28	0.60
4:B:100:LYS:NZ	4:B:100:LYS:HB3	2.17	0.60
3:A:525:ILE:HG23	3:A:526:TYR:N	2.15	0.60
3:A:499:GLU:HG2	3:A:508:LYS:HD2	1.84	0.60
3:A:156:ASP:HB2	9:A:1366:HOH:O	2.01	0.60
1:P:814:DC:H2''	1:P:815:DA:H5''	1.85	0.59
3:A:135:MET:HG3	3:A:174:ASP:OD1	2.03	0.59
3:A:391:MET:HE3	3:A:395:ARG:HG3	1.85	0.59
3:A:667:GLN:O	3:A:671:GLU:HG3	2.03	0.59
4:B:45:ILE:HG13	4:B:99:LEU:HD13	1.84	0.59
3:A:391:MET:HE1	3:A:392:ILE:CA	2.30	0.59
3:A:321:VAL:HG23	4:B:90:LYS:HD2	1.84	0.58
3:A:574:VAL:HG12	3:A:575:GLU:N	2.19	0.58
1:P:812:DG:C2'	1:P:813:DC:H5''	2.32	0.58
3:A:504:ASP:HB3	3:A:507:THR:OG1	2.04	0.58
3:A:663:GLU:HG2	3:A:696:MET:SD	2.44	0.58
3:A:236:THR:O	3:A:240:GLU:HG3	2.04	0.57
3:A:336:PRO:HB2	3:A:389:TYR:CD1	2.40	0.56
3:A:155:VAL:HG12	9:A:1366:HOH:O	2.05	0.56
3:A:234:PHE:CD2	3:A:410:VAL:HG11	2.41	0.56
3:A:229:ARG:HD2	9:A:1039:HOH:O	2.06	0.56
3:A:597:ASP:OD1	3:A:599:ARG:CD	2.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:49:GLU:OE2	3:A:54:GLY:HA3	2.07	0.55
3:A:496:TYR:CE1	3:A:505:ILE:HD11	2.42	0.54
3:A:304:LYS:O	3:A:305:ALA:HB2	2.06	0.54
3:A:19:HIS:O	3:A:36:PRO:HD3	2.06	0.54
1:P:815:DA:H2''	1:P:816:DG:C5'	2.27	0.54
3:A:142:ASP:O	3:A:146:MET:HG3	2.08	0.54
3:A:237:LYS:O	3:A:237:LYS:HD3	2.08	0.54
3:A:308:GLU:C	3:A:310:ARG:H	2.10	0.54
3:A:64:TYR:O	3:A:67:PRO:HD2	2.08	0.53
3:A:496:TYR:CZ	3:A:505:ILE:HD11	2.44	0.53
3:A:131:ARG:O	3:A:135:MET:HG2	2.09	0.53
3:A:297:ILE:CD1	4:B:101:GLU:HB2	2.38	0.53
3:A:391:MET:CE	3:A:395:ARG:HG3	2.39	0.52
3:A:276:HIS:CD2	3:A:278:ARG:H	2.27	0.52
3:A:501:LEU:HD21	9:A:1535:HOH:O	2.09	0.52
4:B:37:MET:O	4:B:40:PRO:HD2	2.10	0.51
1:P:821:DA:H5'	1:P:821:DA:C8	2.44	0.51
3:A:106:ASP:OD2	3:A:109:LEU:HD12	2.10	0.51
3:A:135:MET:HE1	3:A:138:GLU:OE2	2.10	0.51
3:A:79:ARG:HD3	9:A:1127:HOH:O	2.11	0.51
1:P:814:DC:H2''	1:P:815:DA:C5'	2.41	0.50
1:P:816:DG:H1'	1:P:817:DT:H5''	1.93	0.50
1:P:820:DC:H2''	1:P:821:DA:H5''	1.89	0.50
3:A:284:PRO:HA	3:A:288:ARG:NH2	2.27	0.50
3:A:308:GLU:C	3:A:310:ARG:N	2.65	0.49
3:A:478:GLY:O	3:A:482:ARG:HG3	2.12	0.49
3:A:94:LEU:HB3	3:A:185:LEU:HD13	1.93	0.49
4:B:58:LEU:HD21	4:B:66:THR:HB	1.93	0.49
1:P:814:DC:C2'	1:P:815:DA:H5''	2.43	0.49
3:A:499:GLU:HG2	3:A:508:LYS:CD	2.42	0.48
3:A:234:PHE:CZ	3:A:239:ILE:HG13	2.49	0.48
3:A:297:ILE:HD13	4:B:101:GLU:HB2	1.94	0.48
2:T:858:DG:H4'	3:A:432:HIS:O	2.13	0.48
3:A:391:MET:O	3:A:391:MET:HE2	2.13	0.48
3:A:323:GLY:O	3:A:325:PRO:HD3	2.14	0.48
3:A:49:GLU:HA	3:A:52:ARG:HH11	1.79	0.48
3:A:139:TYR:HE1	3:A:166:GLU:HG3	1.79	0.48
3:A:365:ASP:O	3:A:368:VAL:HG22	2.14	0.48
3:A:440:ILE:O	3:A:452:ARG:NH1	2.47	0.48
3:A:233:PRO:HB2	3:A:456:GLY:O	2.14	0.47
3:A:599:ARG:HD3	3:A:620:LEU:HD11	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:537:ILE:CD1	3:A:545:LYS:H	2.28	0.47
1:P:817:DT:OP1	3:A:359:LYS:HB3	2.14	0.47
3:A:488:MET:HE1	3:A:496:TYR:CD1	2.50	0.47
3:A:195:GLU:H	3:A:195:GLU:CD	2.18	0.47
3:A:513:ALA:O	3:A:514:GLU:C	2.53	0.47
3:A:574:VAL:CG1	3:A:575:GLU:N	2.78	0.47
3:A:678:ARG:NH2	3:A:689:LEU:HD21	2.29	0.47
1:P:821:DA:H2'	1:P:822:DDG:C8	2.44	0.46
3:A:541:VAL:HG23	3:A:543:ALA:H	1.80	0.46
3:A:237:LYS:O	3:A:241:GLU:HG3	2.15	0.46
3:A:91:THR:HB	3:A:181:LEU:HD13	1.97	0.46
3:A:48:ALA:O	3:A:52:ARG:HG3	2.15	0.46
3:A:193:PRO:HG3	9:A:1232:HOH:O	2.15	0.46
3:A:237:LYS:HD3	3:A:237:LYS:C	2.35	0.46
3:A:356:TYR:HD2	3:A:360:GLY:O	1.99	0.46
3:A:391:MET:HE2	3:A:395:ARG:HG2	1.98	0.46
3:A:130:TYR:CZ	3:A:134:GLU:HG3	2.50	0.46
3:A:597:ASP:OD1	3:A:599:ARG:HD2	2.15	0.46
3:A:234:PHE:CD2	3:A:410:VAL:CG1	2.99	0.45
3:A:368:VAL:O	3:A:372:VAL:HG23	2.16	0.45
3:A:516:PRO:HG2	3:A:517:THR:H	1.81	0.45
3:A:638:LEU:CD1	3:A:638:LEU:N	2.80	0.45
3:A:189:LYS:HD3	3:A:189:LYS:C	2.38	0.45
3:A:328:PRO:HB3	4:B:73:ARG:HH12	1.82	0.44
3:A:529:LEU:O	3:A:611:ASN:HB2	2.17	0.44
3:A:158:MET:HA	3:A:161:TRP:CE2	2.51	0.44
3:A:85:ARG:HG3	3:A:222:TRP:CG	2.53	0.44
3:A:513:ALA:O	3:A:515:LEU:HG	2.17	0.44
3:A:525:ILE:CG2	3:A:526:TYR:N	2.79	0.44
1:P:821:DA:H2'	1:P:822:DDG:H8	2.00	0.43
3:A:525:ILE:HG23	3:A:526:TYR:H	1.81	0.43
3:A:638:LEU:N	3:A:638:LEU:HD12	2.33	0.43
3:A:404:LYS:HA	3:A:409:TYR:HE2	1.82	0.43
3:A:406:TRP:O	3:A:410:VAL:HG13	2.18	0.43
3:A:597:ASP:OD1	3:A:599:ARG:HD3	2.19	0.43
3:A:49:GLU:HA	3:A:52:ARG:NH1	2.34	0.43
4:B:103:LEU:O	4:B:107:LEU:HD22	2.18	0.43
4:B:49:TYR:HB3	4:B:53:LEU:HB3	2.00	0.43
3:A:421:ASN:HB3	3:A:431:THR:OG1	2.19	0.43
2:T:860:DA:H2''	2:T:861:DC:C5'	2.48	0.42
3:A:590:ARG:HD3	3:A:592:TRP:CE2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:155:VAL:O	3:A:156:ASP:C	2.57	0.42
3:A:391:MET:HE2	3:A:395:ARG:CG	2.50	0.42
2:T:856:DT:H2'	9:T:1070:HOH:O	2.20	0.42
3:A:573:LEU:HD21	3:A:593:ILE:CD1	2.49	0.42
3:A:590:ARG:HD2	3:A:592:TRP:O	2.19	0.42
3:A:452:ARG:HG3	3:A:700:TRP:HB3	2.01	0.42
4:B:27:PHE:CE1	4:B:79:LEU:HD22	2.55	0.42
4:B:17:LEU:HA	4:B:84:GLY:HA2	2.02	0.42
4:B:22:ALA:O	4:B:23:ILE:HD13	2.20	0.42
3:A:505:ILE:HD12	3:A:508:LYS:HD3	2.02	0.41
3:A:363:VAL:O	3:A:368:VAL:HG21	2.20	0.41
3:A:456:GLY:HA2	3:A:471:GLN:OE1	2.20	0.41
3:A:674:GLN:NE2	3:A:678:ARG:HH11	2.18	0.41
3:A:317:THR:HG22	3:A:317:THR:O	2.20	0.41
3:A:547:ARG:CD	3:A:551:LEU:HG	2.51	0.41
2:T:855:DC:C2'	2:T:856:DT:H5'	2.48	0.41
3:A:326:TYR:HB3	4:B:92:GLY:HA2	2.03	0.41
4:B:67:ALA:HB3	4:B:68:PRO:HD3	2.01	0.41
3:A:53:GLY:HA2	9:A:1095:HOH:O	2.20	0.41
3:A:394:LYS:HA	3:A:394:LYS:HD3	1.91	0.41
3:A:423:ASN:OD1	3:A:599:ARG:NH2	2.53	0.41
3:A:368:VAL:HG23	3:A:369:LEU:N	2.36	0.41
3:A:294:VAL:HG12	3:A:295:GLY:N	2.36	0.40
3:A:144:LYS:HE2	3:A:144:LYS:HB3	1.88	0.40
3:A:282:PRO:C	3:A:284:PRO:HD3	2.41	0.40
3:A:452:ARG:NH2	9:A:1716:HOH:O	2.48	0.40
3:A:276:HIS:HD2	3:A:277:PRO:HD2	1.86	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	
3	A	671/698 (96%)	643 (96%)	23 (3%)	5 (1%)	22	22
4	B	103/108 (95%)	99 (96%)	3 (3%)	1 (1%)	15	14
All	All	774/806 (96%)	742 (96%)	26 (3%)	6 (1%)	19	19

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	156	ASP
3	A	305	ALA
3	A	545	LYS
3	A	653	HIS
4	B	50	GLN
3	A	514	GLU

### 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	
3	A	542/579 (94%)	527 (97%)	15 (3%)	43	56
4	B	85/87 (98%)	80 (94%)	5 (6%)	19	23
All	All	627/666 (94%)	607 (97%)	20 (3%)	39	50

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	156	ASP
3	A	171	ASN
3	A	181	LEU
3	A	189	LYS
3	A	232	PHE
3	A	343	GLN
3	A	391	MET
3	A	394	LYS
3	A	403	ASP
3	A	501	LEU

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Mol	Chain	Res	Type
3	A	547	ARG
3	A	599	ARG
3	A	624	LEU
3	A	686	PHE
3	A	704	HIS
4	B	20	ASP
4	B	73	ARG
4	B	89	THR
4	B	99	LEU
4	B	107	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	276	HIS
3	A	343	GLN
3	A	347	GLN
3	A	510	GLN
4	B	50	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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$
1	DDG	P	822	2,1	17,23,24	1.08	2 (11%)	15,33,36	0.83	1 (6%)

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	2,1	-	0/3/18/19	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	822	DDG	C8-N7	-2.44	1.30	1.35
1	P	822	DDG	C5-C6	-2.37	1.42	1.47

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	822	DDG	O6-C6-C5	2.16	128.59	124.37

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
1	P	822	DDG	2	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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
8	1PE	A	992	-	15,15,15	0.90	0	14,14,14	0.95	0
6	SO4	A	905	-	4,4,4	0.26	0	6,6,6	0.08	0
6	SO4	A	904	-	4,4,4	0.22	0	6,6,6	0.06	0
7	MES	A	991	-	12,12,12	0.55	0	14,16,16	0.73	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
8	1PE	A	992	-	-	4/13/13/13	-
7	MES	A	991	-	-	3/6/14/14	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	991	MES	C7-C8-S-O1S
7	A	991	MES	C7-C8-S-O3S
8	A	992	1PE	C13-C23-OH3-C22
8	A	992	1PE	C25-C15-OH6-C26
7	A	991	MES	C7-C8-S-O2S
8	A	992	1PE	OH2-C12-C22-OH3
8	A	992	1PE	OH4-C13-C23-OH3

There are no ring outliers.

No monomer is involved in short contacts.

## 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<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	P	10/22 (45%)	0.91	3 (30%) <b>0</b> <b>0</b>	25, 40, 96, 97	0
2	T	13/26 (50%)	0.84	4 (30%) <b>0</b> <b>0</b>	20, 35, 95, 99	0
3	A	681/698 (97%)	0.11	52 (7%) <b>13</b> <b>12</b>	11, 26, 69, 89	0
4	B	105/108 (97%)	0.32	6 (5%) <b>23</b> <b>22</b>	21, 36, 53, 59	0
All	All	809/854 (94%)	0.16	65 (8%) <b>12</b> <b>11</b>	11, 27, 69, 99	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	T	867	DG	6.3
3	A	545	LYS	6.0
3	A	301	PRO	4.9
3	A	156	ASP	4.7
2	T	866	DC	4.5
3	A	358	ASP	4.5
3	A	151	GLY	4.4
3	A	544	GLY	4.2
3	A	278	ARG	4.1
3	A	300	LYS	4.1
3	A	313	CYS	4.0
3	A	294	VAL	3.9
3	A	444	ARG	3.8
1	P	813	DC	3.7
3	A	314	GLU	3.6
3	A	546	GLU	3.6
1	P	812	DG	3.6
3	A	306	GLN	3.5
3	A	538	GLY	3.5
3	A	531	GLY	3.5
4	B	20	ASP	3.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	A	704	HIS	3.4
3	A	304	LYS	3.3
3	A	532	ALA	3.2
3	A	148	GLU	3.2
3	A	513	ALA	3.2
3	A	354	THR	3.1
3	A	114	LYS	3.1
3	A	548	GLY	3.1
3	A	360	GLY	3.1
4	B	82	LYS	3.0
3	A	542	GLY	2.9
3	A	539	GLN	2.9
3	A	305	ALA	2.9
3	A	541	VAL	2.9
3	A	145	ARG	2.9
3	A	308	GLU	2.9
3	A	540	ILE	2.8
3	A	575	GLU	2.8
3	A	318	ARG	2.8
4	B	50	GLN	2.7
3	A	352	VAL	2.5
4	B	3	LYS	2.5
2	T	865	DC	2.5
3	A	543	ALA	2.5
3	A	309	GLY	2.5
3	A	529	LEU	2.4
3	A	361	ALA	2.4
4	B	47	ASP	2.3
3	A	412	GLU	2.2
4	B	78	LEU	2.2
3	A	526	TYR	2.2
3	A	502	ASN	2.2
2	T	864	DG	2.2
1	P	814	DC	2.1
3	A	516	PRO	2.1
3	A	571	GLN	2.1
3	A	299	LYS	2.1
3	A	547	ARG	2.1
3	A	279	THR	2.1
3	A	586	VAL	2.1
3	A	530	TYR	2.1
3	A	307	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
3	A	537	ILE	2.0
3	A	519	ASP	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	B-factors(Å <sup>2</sup> )	Q<0.9
1	DDG	P	822	21/22	0.97	0.09	22,25,26,26	0

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	B-factors(Å <sup>2</sup> )	Q<0.9
8	1PE	A	992	16/16	0.82	0.21	45,51,60,62	0
6	SO4	A	905	5/5	0.90	0.17	77,77,78,78	0
6	SO4	A	904	5/5	0.90	0.17	74,74,76,76	0
5	MG	A	903	1/1	0.94	0.16	30,30,30,30	0
7	MES	A	991	12/12	0.96	0.13	39,41,45,45	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.