



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:26 PM GMT

PDB ID : 1TK5
Title : T7 DNA polymerase binary complex with 8 oxo guanosine in the templating strand
Authors : Briebe, L.G.; Eichman, B.F.; Kokoska, R.J.; Doublié, 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
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

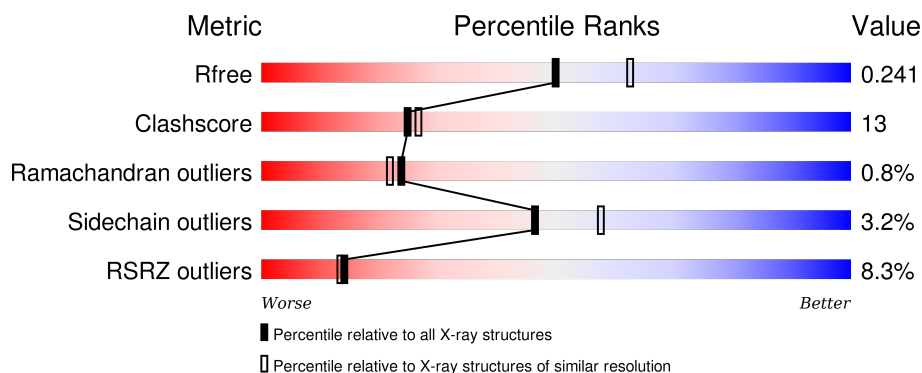
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (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 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	P	22	
2	T	26	
3	A	698	
4	B	108	

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	905	-	-	-	X
8	1PE	A	992	-	-	-	X

2 Entry composition [i](#)

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
1	P	11	Total	C	N	O	P	0	0	0
			222	106	44	62	10			

- 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
2	T	13	Total	C	N	O	P	0	0	0
			266	125	49	79	13			

- Molecule 3 is a protein called DNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	681	Total	C	N	O	S	0	0	0
			5340	3405	923	988	24			

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
4	B	105	Total	C	N	O	S	0	0	0
			802	518	129	152	3			

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

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

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



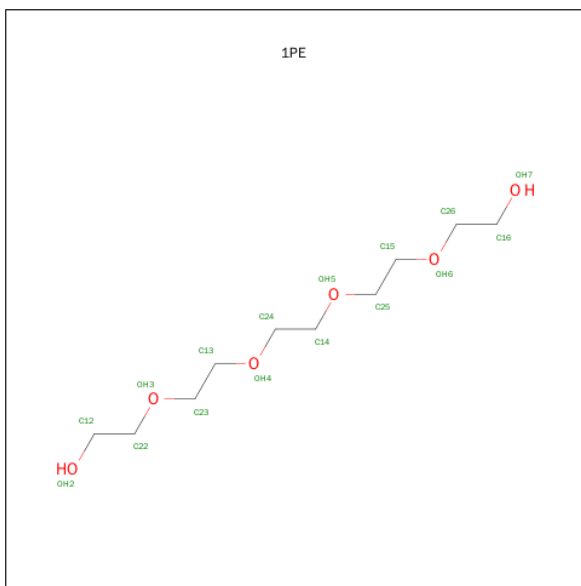
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



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

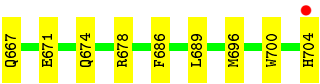
- Molecule 8 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C₁₀H₂₂O₆).



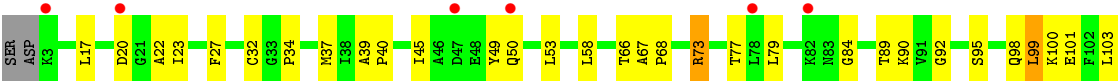
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			16	10	6		

- Molecule 9 is water.

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



● Molecule 4: Thioredoxin 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	5.34 (at 1.99Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.214 , 0.246 0.209 , 0.241	Depositor DCC
R_{free} test set	2891 reflections (4.78%)	DCC
Wilson B-factor (Å ²)	25.5	Xtriage
Anisotropy	0.269	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 65.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 79909 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7441	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage'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.*

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: MG, DDG, SO4, MES, 1PE

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:HE2	3:A:285:LYS:HA	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:HD3	3:A:547:ARG:O	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:H8	1:P:821:DA:H5'	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:HB3	4:B:100:LYS:NZ	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: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
3:A:135:MET:HG3	3:A:174:ASP:OD1	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:237:LYS:O	3:A:237:LYS:HD3	2.08	0.54
3:A:142:ASP:O	3:A:146:MET:HG3	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:C8	1:P:821:DA:H5'	2.44	0.51
3:A:135:MET:HE1	3:A:138:GLU:OE2	2.10	0.51
3:A:106:ASP:OD2	3:A:109:LEU:HD12	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
3:A:391:MET:HE2	3:A:391:MET:O	2.13	0.48
2:T:858:DG:H4'	3:A:432:HIS:O	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:440:ILE:O	3:A:452:ARG:NH1	2.47	0.48
3:A:365:ASP:O	3:A:368:VAL:HG22	2.14	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:574:VAL:CG1	3:A:575:GLU:N	2.78	0.47
3:A:513:ALA:O	3:A:514:GLU:C	2.53	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:237:LYS:HD3	3:A:237:LYS:C	2.35	0.46
3:A:193:PRO:HG3	9:A:1232:HOH:O	2.15	0.46
3:A:391:MET:HE2	3:A:395:ARG:HG2	1.98	0.46
3:A:356:TYR:HD2	3:A:360:GLY:O	1.99	0.46
3:A:597:ASP:OD1	3:A:599:ARG:HD2	2.15	0.46
3:A:130:TYR:CZ	3:A:134:GLU:HG3	2.50	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:HD12	3:A:638:LEU:N	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:391:MET:HE2	3:A:395:ARG:CG	2.50	0.42
3:A:155:VAL:O	3:A:156:ASP:C	2.57	0.42
2:T:856:DT:H2'	9:T:1070:HOH:O	2.20	0.42
3:A:590:ARG:HD2	3:A:592:TRP:O	2.19	0.42
3:A:573:LEU:HD21	3:A:593:ILE:CD1	2.49	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:547:ARG:CD	3:A:551:LEU:HG	2.51	0.41
3:A:317:THR:HG22	3:A:317:THR:O	2.20	0.41
2:T:855:DC:C2'	2:T:856:DT:H5'	2.48	0.41
4:B:67:ALA:HB3	4:B:68:PRO:HD3	2.01	0.41
3:A:326:TYR:HB3	4:B:92:GLY:HA2	2.03	0.41
3:A:53:GLY:HA2	9:A:1095:HOH:O	2.20	0.41
3:A:423:ASN:OD1	3:A:599:ARG:NH2	2.53	0.41
3:A:394:LYS:HA	3:A:394:LYS:HD3	1.91	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 ⓘ

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	671/698 (96%)	643 (96%)	23 (3%)	5 (1%)	26	25
4	B	103/108 (95%)	99 (96%)	3 (3%)	1 (1%)	19	16
All	All	774/806 (96%)	742 (96%)	26 (3%)	6 (1%)	24	22

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 ⓘ

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%)	51	63
4	B	85/87 (98%)	80 (94%)	5 (6%)	24	27
All	All	627/666 (94%)	607 (97%)	20 (3%)	46	57

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

Some 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 ⓘ

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$
1	DDG	P	822	1,2	15,23,24	1.18	1 (6%)	16,33,36	2.90	3 (18%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	822	DDG	C6-N1	3.46	1.39	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	822	DDG	C5-C6-N1	-8.80	111.55	123.59
1	P	822	DDG	N3-C2-N1	-2.26	124.01	127.44
1	P	822	DDG	C6-N1-C2	6.54	125.01	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
1	P	822	DDG	2	0

5.5 Carbohydrates [i](#)

There are no carbohydrates 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
6	SO4	A	904	-	4,4,4	0.16	0	6,6,6	0.09	0
6	SO4	A	905	-	4,4,4	0.20	0	6,6,6	0.11	0
7	MES	A	991	-	11,12,12	0.54	0	14,16,16	0.75	0
8	1PE	A	992	-	15,15,15	0.90	0	14,14,14	0.96	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
6	SO4	A	904	-	-	0/0/0/0	0/0/0/0
6	SO4	A	905	-	-	0/0/0/0	0/0/0/0
7	MES	A	991	-	-	0/6/14/14	0/1/1/1
8	1PE	A	992	-	-	0/13/13/13	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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, 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	P	10/22 (45%)	0.98	3 (30%) 1 0	25, 40, 96, 97	0
2	T	13/26 (50%)	0.90	4 (30%) 1 0	20, 35, 95, 99	0
3	A	681/698 (97%)	0.16	54 (7%) 15 15	11, 26, 69, 89	0
4	B	105/108 (97%)	0.38	6 (5%) 27 27	21, 36, 53, 59	0
All	All	809/854 (94%)	0.21	67 (8%) 14 13	11, 27, 69, 99	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	T	867	DG	6.4
3	A	545	LYS	6.1
3	A	301	PRO	5.1
3	A	156	ASP	4.8
2	T	866	DC	4.6
3	A	358	ASP	4.6
3	A	151	GLY	4.6
3	A	544	GLY	4.4
3	A	313	CYS	4.2
3	A	278	ARG	4.2
3	A	300	LYS	4.2
3	A	294	VAL	4.1
3	A	444	ARG	3.9
1	P	813	DC	3.8
3	A	546	GLU	3.7
3	A	314	GLU	3.7
3	A	538	GLY	3.7
3	A	306	GLN	3.6
1	P	812	DG	3.6
3	A	531	GLY	3.6
4	B	20	ASP	3.6

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Mol	Chain	Res	Type	RSRZ
3	A	704	HIS	3.5
3	A	532	ALA	3.4
3	A	304	LYS	3.4
3	A	148	GLU	3.3
3	A	513	ALA	3.3
3	A	548	GLY	3.3
3	A	354	THR	3.3
3	A	360	GLY	3.2
3	A	114	LYS	3.2
3	A	305	ALA	3.1
3	A	541	VAL	3.1
3	A	542	GLY	3.0
4	B	82	LYS	3.0
3	A	539	GLN	3.0
3	A	308	GLU	3.0
3	A	145	ARG	3.0
3	A	540	ILE	2.9
3	A	575	GLU	2.9
3	A	318	ARG	2.9
4	B	50	GLN	2.8
3	A	352	VAL	2.7
3	A	543	ALA	2.6
2	T	865	DC	2.6
4	B	3	LYS	2.5
3	A	529	LEU	2.5
3	A	309	GLY	2.5
3	A	361	ALA	2.5
4	B	47	ASP	2.4
3	A	412	GLU	2.3
4	B	78	LEU	2.3
3	A	526	TYR	2.3
3	A	502	ASN	2.3
3	A	516	PRO	2.3
1	P	814	DC	2.2
2	T	864	DG	2.2
3	A	571	GLN	2.2
3	A	586	VAL	2.2
3	A	299	LYS	2.2
3	A	279	THR	2.2
3	A	537	ILE	2.1
3	A	547	ARG	2.1
3	A	530	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
3	A	307	ARG	2.1
3	A	519	ASP	2.1
3	A	153	GLU	2.0
3	A	525	ILE	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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
1	DDG	P	822	21/22	0.97	0.09	-	22,25,26,26	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, 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
8	1PE	A	992	16/16	0.82	0.21	6.50	45,51,60,62	0
6	SO4	A	905	5/5	0.90	0.17	2.04	77,77,78,78	0
5	MG	A	903	1/1	0.94	0.16	0.77	30,30,30,30	0
7	MES	A	991	12/12	0.96	0.13	0.42	39,41,45,45	0
6	SO4	A	904	5/5	0.90	0.18	-	74,74,76,76	0

6.5 Other polymers [i](#)

There are no such residues in this entry.