Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 08:03 PM GMT

PDB ID	:	1IG9
Title	:	Structure of the Replicating Complex of a Pol Alpha Family DNA Polymerase
Authors	:	Franklin, M.C.; Wang, J.; Steitz, T.A.
Deposited on	:	2001-04-17
Resolution	:	2.60 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

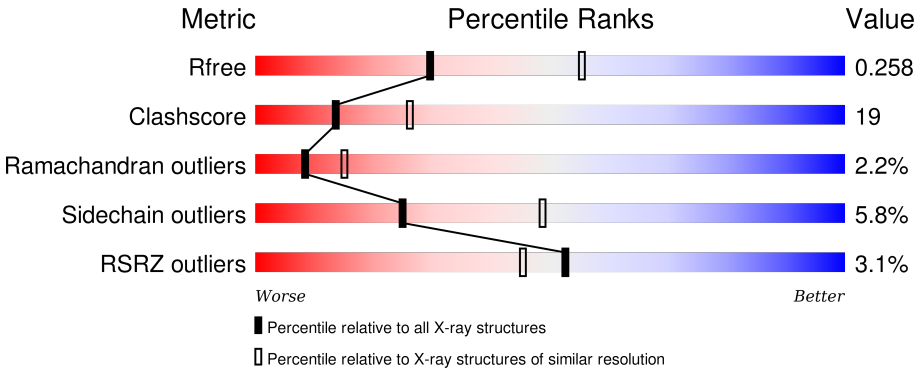
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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	T	18	6%, 22%, 67%, 11%
2	P	14	14%, 86%
3	A	903	3%, 66%, 30%, ·

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8394 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(*AP*CP*AP*GP*GP*TP*AP*AP*GP*CP*AP*GP*TP*CP*CP*GP*CP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	T	18	369	175	74	103	17	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	P	14	281	135	51	82	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	901	7355	4724	1224	1374	33	0	0	0

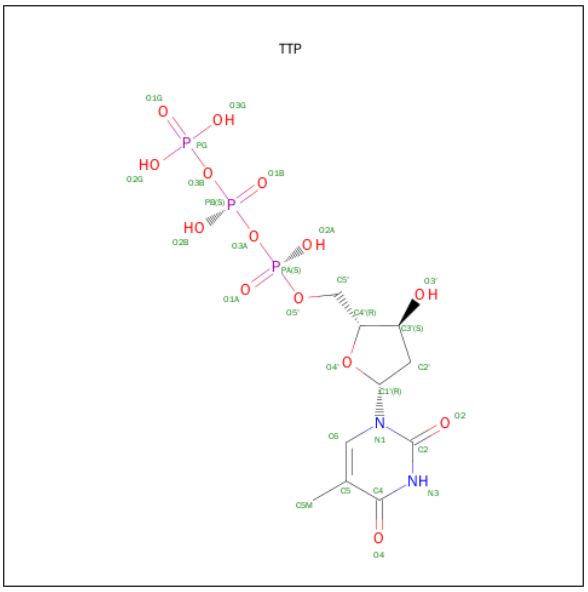
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	222	ALA	ASP	ENGINEERED	UNP Q38087
A	327	ALA	ASP	ENGINEERED	UNP Q38087

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
4	A	4	4	4	0	0

- Molecule 5 is THYMIDINE-5'-TRIPHOSPHATE (three-letter code: TTP) (formula: $C_{10}H_{17}N_2O_{14}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			29	10	2	14	3		

- Molecule 6 is water.

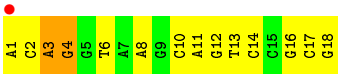
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	306	Total	O	0	0
			306	306		
6	P	19	Total	O	0	0
			19	19		
6	T	31	Total	O	0	0
			31	31		

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(*AP*CP*AP*GP*GP*TP*AP*AP*GP*CP*AP*GP*TP*CP*CP*GP*CP*G)-3'

Chain T:

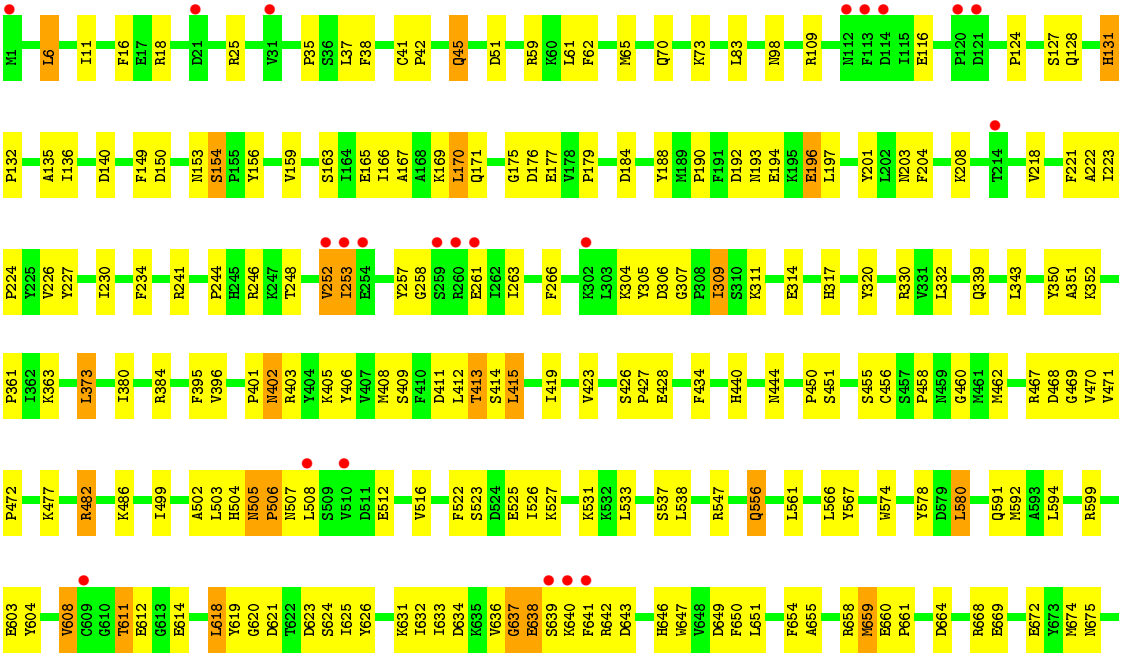


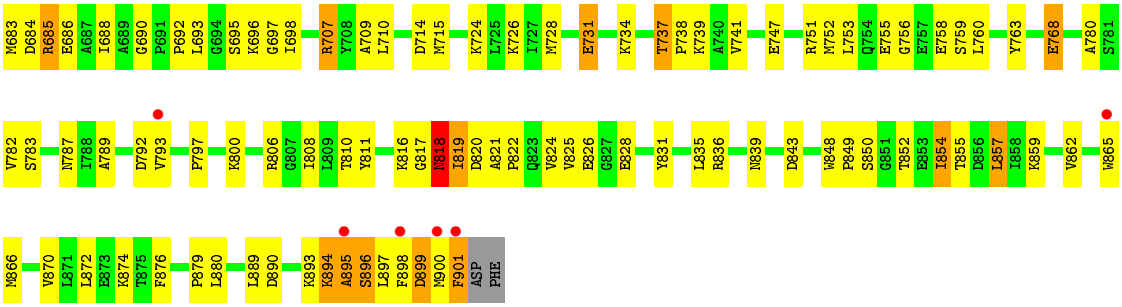
• Molecule 2: 5'-D(*GP*CP*GP*GP*AP*CP*TP*GP*CP*TP*TP*AP*CP*(DOC))-3'

Chain P:

• Molecule 3: DNA POLYMERASE

Chain A:




M683 D684 R685 E686 A687 I688 A689 G690 P691 P692 L693 G694 S695 K696 G697 I698 R707 Y708 A709 L710 D714 M715 K724 L725 K726 I727 M728 E731 K734 T737 P738 K739 A740 V741 E747 R751 M752 L753 Q754 E755 G756 E757 E758 S759 L760 Y763 E768 A780 S781
V782 S783 N787 I788 A789 D792 V793 P797 K800 R806 G807 I808 L809 T810 Y811 K816 G817 M818 I819 D820 A821 P822 Q823 V824 V825 E826 G827 E828 Y831 L835 R836 N839 D843 W848 P849 S850 G851 T852 E853 I854 T855 D856 L857 I858 K859 V862 W865
M866 V870 L871 L872 E873 K874 T875 F876 P879 L880 L889 D890 K893 K894 A895 S896 L897 F898 D899 M900 F901 ASP PHE

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	80.79Å 118.60Å 128.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.75 – 2.60 29.75 – 2.60	Depositor EDS
% Data completeness (in resolution range)	96.7 (29.75-2.60) 96.8 (29.75-2.60)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.17 (at 2.61Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.197 , 0.258 0.197 , 0.258	Depositor DCC
R_{free} test set	3622 reflections (9.72%)	DCC
Wilson B-factor (Å^2)	57.4	Xtriage
Anisotropy	0.171	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 63.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	1 of 38439 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8394	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.40% 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: DOC, CA, TTP

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	T	0.47	0/415	0.78	0/639
2	P	0.40	0/294	0.68	0/452
3	A	0.36	0/7535	0.58	0/10182
All	All	0.37	0/8244	0.60	0/11273

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	T	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	T	3	DA	Sidechain
1	T	4	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	T	369	0	202	22	0
2	P	281	0	159	13	0
3	A	7355	0	7254	265	0
4	A	4	0	0	0	0
5	A	29	0	13	2	0
6	A	306	0	0	17	0
6	P	19	0	0	0	0
6	T	31	0	0	2	0
All	All	8394	0	7628	290	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 19.

All (290) 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)
3:A:415:LEU:HD22	3:A:623:ASP:HB3	1.37	1.04
2:P:114:DC:H2"	2:P:115:DOC:H5'	1.36	1.03
3:A:402:ASN:ND2	3:A:403:ARG:H	1.57	1.01
3:A:402:ASN:HD22	3:A:403:ARG:N	1.59	1.00
2:P:105:DG:H4'	2:P:106:DA:OP1	1.64	0.96
3:A:402:ASN:HD22	3:A:403:ARG:H	0.92	0.91
3:A:614:GLU:HG2	3:A:631:LYS:HE3	1.53	0.91
3:A:373:LEU:CD1	3:A:470:VAL:HG11	2.03	0.88
3:A:642:ARG:HH11	3:A:642:ARG:HB2	1.38	0.86
2:P:113:DA:C5'	3:A:734:LYS:HG2	2.07	0.84
3:A:894:LYS:HE3	3:A:894:LYS:HA	1.57	0.84
3:A:822:PRO:HD2	3:A:855:THR:CG2	2.10	0.81
3:A:258:GLY:HA3	6:A:1251:HOH:O	1.81	0.80
3:A:408:MET:HE1	3:A:651:LEU:HB3	1.62	0.80
1:T:16:DG:H2"	1:T:17:DC:C5'	2.13	0.79
3:A:405:LYS:HZ2	3:A:406:TYR:HE1	1.32	0.77
2:P:113:DA:H5"	3:A:734:LYS:HG2	1.66	0.77
3:A:193:ASN:HD21	3:A:196:GLU:CD	1.88	0.76
3:A:373:LEU:HD11	3:A:470:VAL:HG11	1.68	0.75
3:A:822:PRO:HD2	3:A:855:THR:HG22	1.68	0.75
3:A:170:LEU:HD22	3:A:170:LEU:H	1.52	0.74
2:P:114:DC:C2'	2:P:115:DOC:H5'	2.18	0.72
1:T:10:DC:H5'	1:T:10:DC:H6	1.54	0.72
1:T:16:DG:H2"	1:T:17:DC:H5"	1.72	0.71
3:A:618:LEU:HD13	3:A:618:LEU:H	1.56	0.71
3:A:642:ARG:NH1	3:A:642:ARG:HB2	2.05	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:685:ARG:HH22	3:A:714:ASP:HB3	1.56	0.71
3:A:373:LEU:HD23	3:A:380:ILE:HG22	1.75	0.69
3:A:373:LEU:HD13	3:A:470:VAL:HG11	1.73	0.69
3:A:223:ILE:HB	3:A:224:PRO:HD3	1.75	0.69
2:P:103:DC:H2"	2:P:104:DG:C8	2.28	0.69
1:T:10:DC:H2"	1:T:11:DA:O5'	1.92	0.69
3:A:825:VAL:HB	3:A:828:GLU:HG3	1.74	0.68
3:A:188:TYR:CE2	3:A:190:PRO:HG3	2.28	0.68
3:A:505:ASN:O	3:A:505:ASN:CG	2.31	0.68
3:A:252:VAL:HG23	3:A:253:ILE:H	1.59	0.67
3:A:241:ARG:HA	3:A:246:ARG:NH1	2.09	0.67
3:A:428:GLU:OE2	3:A:470:VAL:HG22	1.94	0.67
3:A:508:LEU:HD22	3:A:508:LEU:H	1.60	0.67
3:A:408:MET:CE	3:A:651:LEU:HB3	2.25	0.66
3:A:632:ILE:HD13	3:A:654:PHE:HE1	1.60	0.66
3:A:599:ARG:O	3:A:603:GLU:HG3	1.95	0.66
3:A:685:ARG:HH22	3:A:714:ASP:CB	2.10	0.65
3:A:149:PHE:HB3	3:A:197:LEU:HD21	1.78	0.65
3:A:41:CYS:HB2	3:A:42:PRO:HD2	1.79	0.65
3:A:222:ALA:O	3:A:226:VAL:HG12	1.97	0.65
3:A:128:GLN:HA	3:A:128:GLN:HE21	1.61	0.64
3:A:738:PRO:HB3	3:A:780:ALA:O	1.96	0.64
2:P:114:DC:H2"	2:P:115:DOC:C5'	2.23	0.63
3:A:471:VAL:HB	3:A:472:PRO:HD3	1.79	0.63
3:A:647:TRP:HA	3:A:650:PHE:HB3	1.79	0.63
1:T:16:DG:H2"	1:T:17:DC:H5'	1.80	0.63
3:A:412:LEU:N	3:A:412:LEU:HD12	2.14	0.62
3:A:618:LEU:HD13	3:A:626:TYR:O	2.00	0.62
3:A:471:VAL:HG13	3:A:566:LEU:HD21	1.80	0.62
3:A:808:ILE:HD13	3:A:824:VAL:HG11	1.81	0.61
1:T:1:DA:H2"	1:T:2:DC:O5'	1.99	0.61
3:A:685:ARG:NH2	3:A:714:ASP:HB3	2.14	0.61
3:A:395:PHE:HB2	3:A:591:GLN:HG2	1.83	0.60
3:A:642:ARG:H	3:A:646:HIS:CD2	2.19	0.60
6:T:32:HOH:O	3:A:874:LYS:HD2	2.02	0.60
2:P:113:DA:H5'	3:A:734:LYS:HG2	1.83	0.60
3:A:304:LYS:HB3	3:A:304:LYS:NZ	2.17	0.60
3:A:862:VAL:O	3:A:866:MET:HG3	2.01	0.60
1:T:3:DA:OP2	3:A:361:PRO:HD2	2.02	0.60
3:A:751:ARG:HD3	3:A:759:SER:OG	2.02	0.59
1:T:10:DC:C6	1:T:10:DC:H5'	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:128:GLN:HA	3:A:128:GLN:NE2	2.17	0.59
3:A:405:LYS:HB3	3:A:405:LYS:NZ	2.17	0.59
3:A:793:VAL:O	3:A:793:VAL:HG12	2.03	0.59
3:A:505:ASN:ND2	3:A:531:LYS:O	2.36	0.58
3:A:894:LYS:CE	3:A:894:LYS:HA	2.32	0.58
3:A:599:ARG:HH11	3:A:599:ARG:HG2	1.69	0.58
3:A:309:ILE:O	3:A:309:ILE:HD13	2.03	0.58
3:A:604:TYR:OH	3:A:658:ARG:HB3	2.04	0.58
3:A:707:ARG:HH11	3:A:707:ARG:HB3	1.69	0.58
3:A:165:GLU:H	3:A:165:GLU:CD	2.07	0.58
3:A:855:THR:HB	3:A:857:LEU:CD2	2.33	0.58
3:A:685:ARG:HD2	6:A:1123:HOH:O	2.03	0.57
3:A:724:LYS:NZ	3:A:724:LYS:HB2	2.20	0.57
3:A:896:SER:C	3:A:898:PHE:H	2.08	0.57
3:A:817:GLY:O	3:A:819:ILE:N	2.38	0.57
1:T:16:DG:C2'	1:T:17:DC:H5"	2.35	0.56
3:A:428:GLU:OE1	3:A:428:GLU:N	2.34	0.56
3:A:11:ILE:HD12	3:A:16:PHE:CD2	2.40	0.55
3:A:632:ILE:HD13	3:A:654:PHE:CE1	2.41	0.55
3:A:731:GLU:O	3:A:737:THR:HG21	2.05	0.55
3:A:692:PRO:HB2	3:A:695:SER:OG	2.06	0.55
3:A:611:THR:HG23	3:A:612:GLU:N	2.22	0.55
3:A:854:ILE:HD12	3:A:862:VAL:HG11	1.88	0.55
3:A:456:CYS:O	3:A:674:MET:HG3	2.06	0.55
3:A:163:SER:HB3	3:A:166:ILE:HD12	1.89	0.55
3:A:631:LYS:HA	3:A:634:ASP:HB2	1.89	0.55
1:T:8:DA:H4'	3:A:707:ARG:HD2	1.89	0.55
3:A:664:ASP:HB3	6:A:1023:HOH:O	2.07	0.54
3:A:395:PHE:HD2	3:A:594:LEU:HD12	1.73	0.54
3:A:642:ARG:HH11	3:A:642:ARG:CB	2.17	0.54
3:A:604:TYR:O	3:A:608:VAL:HG23	2.07	0.54
3:A:159:VAL:HG21	3:A:317:HIS:CD2	2.43	0.54
1:T:17:DC:H2"	1:T:18:DG:O5'	2.08	0.54
3:A:806:ARG:O	3:A:810:THR:HG23	2.08	0.54
2:P:106:DA:H2"	2:P:107:DC:O5'	2.06	0.53
3:A:768:GLU:HG2	3:A:872:LEU:HD21	1.90	0.53
3:A:696:LYS:HB3	3:A:756:GLY:HA3	1.90	0.53
1:T:3:DA:H2"	1:T:4:DG:H5'	1.90	0.53
1:T:12:DG:H2"	1:T:13:DT:H5'	1.90	0.53
1:T:11:DA:OP1	3:A:874:LYS:HE3	2.09	0.53
3:A:825:VAL:HB	3:A:828:GLU:CG	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:655:ALA:HA	3:A:659:MET:HB2	1.91	0.53
3:A:686:GLU:HG3	3:A:715:MET:CE	2.38	0.53
3:A:633:ILE:HD11	3:A:651:LEU:HD21	1.91	0.52
3:A:451:SER:HB3	3:A:456:CYS:SG	2.48	0.52
3:A:821:ALA:HB1	3:A:855:THR:HG21	1.92	0.52
3:A:505:ASN:N	3:A:506:PRO:CD	2.73	0.52
3:A:306:ASP:OD2	3:A:307:GLY:N	2.43	0.52
3:A:697:GLY:HA3	3:A:753:LEU:O	2.09	0.52
3:A:620:GLY:HA2	3:A:624:SER:O	2.10	0.52
3:A:817:GLY:O	3:A:819:ILE:HG13	2.10	0.52
3:A:664:ASP:O	3:A:668:ARG:HG3	2.09	0.52
3:A:637:GLY:O	3:A:639:SER:N	2.43	0.52
3:A:167:ALA:HA	3:A:176:ASP:HB2	1.92	0.52
1:T:11:DA:H2"	1:T:12:DG:C8	2.45	0.52
3:A:504:HIS:C	3:A:506:PRO:HD2	2.30	0.51
3:A:658:ARG:O	3:A:661:PRO:HD2	2.11	0.51
2:P:105:DG:C4'	2:P:106:DA:OP1	2.50	0.51
3:A:224:PRO:HG3	6:A:1072:HOH:O	2.10	0.51
3:A:482:ARG:NH2	5:A:1005:TTP:O2G	2.44	0.51
3:A:525:GLU:CD	3:A:525:GLU:H	2.14	0.51
3:A:203:ASN:ND2	3:A:241:ARG:HH12	2.09	0.50
3:A:384:ARG:HD3	6:A:1253:HOH:O	2.11	0.50
3:A:818:ASN:HD22	3:A:818:ASN:H	1.59	0.50
3:A:197:LEU:HD13	3:A:197:LEU:C	2.32	0.50
3:A:797:PRO:HD3	6:A:1146:HOH:O	2.12	0.50
3:A:170:LEU:N	3:A:170:LEU:HD22	2.24	0.50
3:A:618:LEU:HD22	3:A:619:TYR:N	2.27	0.50
3:A:685:ARG:HH22	3:A:714:ASP:CG	2.15	0.50
3:A:351:ALA:O	3:A:352:LYS:HB2	2.12	0.50
3:A:83:LEU:HD12	3:A:83:LEU:H	1.77	0.49
3:A:660:GLU:HB2	3:A:661:PRO:HD3	1.93	0.49
3:A:726:LYS:HG2	6:A:1164:HOH:O	2.12	0.49
1:T:2:DC:H5'	3:A:574:TRP:CD1	2.47	0.49
3:A:758:GLU:HB2	6:A:1137:HOH:O	2.12	0.49
3:A:153:ASN:HB2	3:A:192:ASP:O	2.12	0.49
3:A:855:THR:HB	3:A:857:LEU:HD21	1.94	0.49
3:A:611:THR:HG21	3:A:614:GLU:CB	2.42	0.49
3:A:350:TYR:OH	3:A:477:LYS:HE3	2.12	0.48
3:A:898:PHE:O	3:A:901:PHE:HB2	2.14	0.48
3:A:636:VAL:O	3:A:637:GLY:O	2.31	0.48
3:A:686:GLU:HG3	3:A:715:MET:HE3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:643:ASP:C	3:A:693:LEU:HD12	2.33	0.48
3:A:824:VAL:HG22	3:A:849:PRO:HD3	1.96	0.48
3:A:533:LEU:HD12	3:A:537:SER:CB	2.44	0.48
3:A:642:ARG:H	3:A:646:HIS:HD2	1.59	0.48
3:A:857:LEU:HD23	3:A:857:LEU:H	1.79	0.48
3:A:707:ARG:NH2	3:A:731:GLU:OE2	2.46	0.48
3:A:440:HIS:O	3:A:444:ASN:ND2	2.47	0.48
3:A:797:PRO:HG3	3:A:806:ARG:NH1	2.29	0.47
3:A:244:PRO:HD2	3:A:266:PHE:O	2.14	0.47
3:A:894:LYS:HE3	3:A:894:LYS:CA	2.39	0.47
3:A:561:LEU:HD23	6:A:1172:HOH:O	2.13	0.47
3:A:859:LYS:O	3:A:862:VAL:HG13	2.15	0.47
3:A:684:ASP:HB3	6:A:1261:HOH:O	2.15	0.47
3:A:486:LYS:HB2	3:A:556:GLN:HG3	1.97	0.47
3:A:685:ARG:HG2	3:A:686:GLU:N	2.29	0.46
3:A:132:PRO:HB3	3:A:194:GLU:OE2	2.15	0.46
3:A:599:ARG:NH1	3:A:599:ARG:HG2	2.31	0.46
3:A:697:GLY:HA2	3:A:755:GLU:O	2.16	0.46
3:A:405:LYS:O	3:A:690:GLY:HA2	2.16	0.46
3:A:499:ILE:O	3:A:503:LEU:HG	2.16	0.46
3:A:808:ILE:O	3:A:811:TYR:HB3	2.16	0.46
3:A:625:ILE:HG12	3:A:683:MET:HE2	1.98	0.46
2:P:109:DG:O4'	3:A:800:LYS:HE2	2.15	0.46
3:A:839:ASN:HA	3:A:865:TRP:CD2	2.51	0.46
3:A:131:HIS:ND1	3:A:131:HIS:N	2.64	0.45
3:A:128:GLN:CA	3:A:128:GLN:NE2	2.79	0.45
3:A:406:TYR:CD1	3:A:406:TYR:N	2.84	0.45
3:A:578:TYR:CE2	3:A:580:LEU:HD13	2.51	0.45
3:A:413:THR:O	3:A:414:SER:C	2.55	0.45
3:A:415:LEU:O	3:A:419:ILE:HG13	2.16	0.45
1:T:2:DC:H2"	1:T:3:DA:OP1	2.15	0.45
3:A:163:SER:CB	3:A:166:ILE:HD12	2.45	0.45
2:P:110:DC:H2"	2:P:111:DT:C5'	2.47	0.45
3:A:502:ALA:C	3:A:504:HIS:H	2.20	0.45
3:A:876:PHE:O	3:A:879:PRO:HG2	2.17	0.45
3:A:870:VAL:CG1	3:A:874:LYS:HD3	2.47	0.45
1:T:3:DA:P	3:A:361:PRO:HD2	2.57	0.45
3:A:793:VAL:HG12	6:A:1111:HOH:O	2.17	0.45
1:T:11:DA:H2"	1:T:12:DG:H8	1.80	0.45
3:A:409:SER:OG	3:A:686:GLU:HB3	2.17	0.45
3:A:402:ASN:ND2	3:A:403:ARG:N	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:848:TRP:CE2	3:A:854:ILE:HG12	2.51	0.45
3:A:136:ILE:HB	3:A:149:PHE:HB2	1.99	0.44
3:A:612:GLU:OE1	3:A:612:GLU:HA	2.17	0.44
3:A:116:GLU:HB2	3:A:135:ALA:HB3	1.99	0.44
3:A:523:SER:O	3:A:527:LYS:HG3	2.18	0.44
3:A:363:LYS:HE3	6:A:1110:HOH:O	2.17	0.44
3:A:751:ARG:NH1	3:A:763:TYR:HB2	2.32	0.44
3:A:889:LEU:HD23	3:A:890:ASP:H	1.82	0.44
3:A:787:ASN:N	3:A:826:GLU:OE2	2.50	0.44
3:A:578:TYR:CZ	3:A:580:LEU:HD13	2.53	0.44
3:A:127:SER:HA	3:A:261:GLU:OE2	2.17	0.44
3:A:241:ARG:HG2	3:A:246:ARG:NH1	2.33	0.44
3:A:61:LEU:HD13	3:A:62:PHE:N	2.33	0.44
3:A:401:PRO:O	3:A:402:ASN:HB2	2.18	0.44
3:A:599:ARG:HA	6:A:1248:HOH:O	2.17	0.44
3:A:639:SER:C	3:A:641:PHE:H	2.21	0.44
3:A:816:LYS:C	3:A:816:LYS:HD3	2.37	0.44
3:A:547:ARG:NH2	6:A:1205:HOH:O	2.50	0.44
3:A:304:LYS:HZ3	3:A:305:TYR:H	1.66	0.43
3:A:405:LYS:NZ	3:A:406:TYR:HE1	2.09	0.43
3:A:263:ILE:N	3:A:263:ILE:HD12	2.33	0.43
3:A:415:LEU:HD22	3:A:623:ASP:CB	2.27	0.43
1:T:12:DG:H1'	1:T:13:DT:H5"	2.00	0.43
3:A:25:ARG:HD2	6:A:1113:HOH:O	2.16	0.43
3:A:512:GLU:O	3:A:512:GLU:HG3	2.19	0.43
3:A:633:ILE:O	3:A:637:GLY:N	2.51	0.43
2:P:108:DT:H1'	3:A:800:LYS:NZ	2.33	0.43
3:A:426:SER:HB2	3:A:472:PRO:HD3	2.01	0.43
3:A:482:ARG:HH22	5:A:1005:TTP:PG	2.42	0.43
3:A:70:GLN:NE2	3:A:73:LYS:HE2	2.34	0.43
3:A:169:LYS:HB2	3:A:175:GLY:HA3	2.00	0.43
3:A:171:GLN:HG2	3:A:177:GLU:OE2	2.19	0.43
3:A:412:LEU:HD22	3:A:415:LEU:HD13	2.01	0.43
3:A:402:ASN:ND2	3:A:403:ARG:HG2	2.33	0.43
3:A:516:VAL:HG21	3:A:522:PHE:CE1	2.53	0.43
3:A:458:PRO:HG3	3:A:592:MET:SD	2.59	0.43
3:A:37:LEU:C	3:A:38:PHE:CD1	2.92	0.43
3:A:836:ARG:HB2	3:A:836:ARG:HE	1.59	0.43
3:A:154:SER:C	3:A:156:TYR:H	2.23	0.42
3:A:455:SER:HA	3:A:675:ASN:O	2.19	0.42
3:A:395:PHE:CB	3:A:591:GLN:HG2	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:889:LEU:HD23	3:A:890:ASP:N	2.34	0.42
3:A:35:PRO:HG3	3:A:65:MET:HA	2.01	0.42
3:A:412:LEU:HG	3:A:683:MET:HB2	2.01	0.42
3:A:70:GLN:HE22	3:A:73:LYS:CE	2.32	0.42
3:A:747:GLU:OE2	3:A:747:GLU:HA	2.20	0.42
3:A:789:ALA:O	3:A:792:ASP:HB2	2.20	0.42
3:A:611:THR:HG21	3:A:614:GLU:HB3	2.00	0.42
3:A:738:PRO:HG2	3:A:741:VAL:CG2	2.49	0.42
3:A:150:ASP:OD2	3:A:317:HIS:CE1	2.73	0.42
3:A:468:ASP:CG	3:A:469:GLY:H	2.23	0.42
3:A:505:ASN:O	3:A:506:PRO:C	2.58	0.42
3:A:203:ASN:HD22	3:A:241:ARG:HH12	1.67	0.42
3:A:899:ASP:O	3:A:901:PHE:N	2.53	0.42
3:A:831:TYR:CD2	3:A:850:SER:HA	2.55	0.42
3:A:405:LYS:NZ	3:A:406:TYR:CE1	2.84	0.42
3:A:163:SER:OG	3:A:165:GLU:HG2	2.20	0.42
3:A:547:ARG:HD3	3:A:547:ARG:HA	1.87	0.42
3:A:38:PHE:CD1	3:A:38:PHE:N	2.88	0.42
3:A:38:PHE:CE2	3:A:59:ARG:HB2	2.54	0.42
3:A:201:TYR:O	3:A:204:PHE:HB3	2.20	0.42
3:A:895:ALA:O	3:A:897:LEU:N	2.52	0.42
3:A:6:LEU:HB2	3:A:18:ARG:O	2.19	0.42
3:A:460:GLY:HA3	6:A:1141:HOH:O	2.18	0.42
3:A:373:LEU:HD12	3:A:373:LEU:HA	1.78	0.42
3:A:434:PHE:CE2	3:A:450:PRO:HB3	2.55	0.42
3:A:611:THR:CG2	3:A:614:GLU:HB3	2.50	0.41
1:T:13:DT:H2"	1:T:14:DC:C6	2.55	0.41
3:A:252:VAL:HG23	3:A:253:ILE:N	2.32	0.41
3:A:116:GLU:HB3	3:A:320:TYR:OH	2.20	0.41
3:A:782:VAL:HG12	3:A:783:SER:N	2.35	0.41
3:A:870:VAL:HG13	3:A:874:LYS:HD3	2.01	0.41
3:A:226:VAL:O	3:A:230:ILE:HG13	2.20	0.41
3:A:503:LEU:HD23	3:A:538:LEU:HD13	2.03	0.41
3:A:423:VAL:HG12	3:A:423:VAL:O	2.19	0.41
3:A:234:PHE:N	3:A:234:PHE:CD1	2.88	0.41
3:A:508:LEU:HD22	3:A:508:LEU:N	2.31	0.41
3:A:311:LYS:O	3:A:314:GLU:HG2	2.21	0.41
3:A:396:VAL:HG22	3:A:621:ASP:OD1	2.20	0.41
3:A:408:MET:HE2	3:A:688:ILE:HG12	2.03	0.41
3:A:619:TYR:CG	3:A:620:GLY:N	2.89	0.41
3:A:455:SER:O	3:A:462:MET:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:412:LEU:N	3:A:412:LEU:CD1	2.82	0.41
3:A:647:TRP:O	3:A:650:PHE:HB3	2.20	0.41
3:A:227:TYR:CE1	3:A:248:THR:HG21	2.56	0.41
3:A:221:PHE:O	3:A:224:PRO:HD2	2.21	0.41
3:A:51:ASP:HB2	6:A:1183:HOH:O	2.20	0.41
3:A:668:ARG:NH1	3:A:668:ARG:HG2	2.36	0.40
3:A:669:GLU:O	3:A:672:GLU:HB3	2.21	0.40
1:T:6:DT:H73	6:T:36:HOH:O	2.21	0.40
3:A:426:SER:OG	3:A:427:PRO:HD2	2.20	0.40
3:A:751:ARG:CZ	3:A:763:TYR:HB2	2.51	0.40
3:A:850:SER:O	3:A:852:THR:HG23	2.21	0.40
3:A:698:ILE:HG12	3:A:752:MET:O	2.20	0.40
3:A:709:ALA:O	3:A:710:LEU:HD23	2.21	0.40
3:A:505:ASN:O	3:A:507:ASN:N	2.54	0.40
3:A:150:ASP:OD2	3:A:317:HIS:HE1	2.04	0.40
3:A:686:GLU:HG3	3:A:715:MET:HE1	2.02	0.40
3:A:523:SER:H	3:A:526:ILE:HD12	1.86	0.40
3:A:109:ARG:HD3	3:A:140:ASP:OD2	2.22	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	899/903 (100%)	815 (91%)	64 (7%)	20 (2%)	8 15

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	818	ASN
3	A	893	LYS
3	A	899	ASP

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Mol	Chain	Res	Type
3	A	252	VAL
3	A	415	LEU
3	A	467	ARG
3	A	637	GLY
3	A	820	ASP
3	A	895	ALA
3	A	896	SER
3	A	900	MET
3	A	640	LYS
3	A	506	PRO
3	A	638	GLU
3	A	819	ILE
3	A	45	GLN
3	A	253	ILE
3	A	124	PRO
3	A	179	PRO
3	A	608	VAL

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	798/800 (100%)	752 (94%)	46 (6%)	25 49

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	6	LEU
3	A	45	GLN
3	A	98	ASN
3	A	131	HIS
3	A	154	SER
3	A	170	LEU
3	A	184	ASP
3	A	196	GLU
3	A	208	LYS

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Mol	Chain	Res	Type
3	A	218	VAL
3	A	257	TYR
3	A	309	ILE
3	A	330	ARG
3	A	332	LEU
3	A	339	GLN
3	A	343	LEU
3	A	373	LEU
3	A	402	ASN
3	A	411	ASP
3	A	413	THR
3	A	482	ARG
3	A	505	ASN
3	A	556	GLN
3	A	567	TYR
3	A	580	LEU
3	A	611	THR
3	A	618	LEU
3	A	638	GLU
3	A	649	ASP
3	A	659	MET
3	A	685	ARG
3	A	707	ARG
3	A	728	MET
3	A	731	GLU
3	A	737	THR
3	A	739	LYS
3	A	760	LEU
3	A	768	GLU
3	A	818	ASN
3	A	835	LEU
3	A	843	ASP
3	A	854	ILE
3	A	857	LEU
3	A	880	LEU
3	A	894	LYS
3	A	901	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	40	HIS

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Mol	Chain	Res	Type
3	A	70	GLN
3	A	112	ASN
3	A	128	GLN
3	A	158	ASN
3	A	171	GLN
3	A	193	ASN
3	A	203	ASN
3	A	317	HIS
3	A	333	GLN
3	A	402	ASN
3	A	424	ASN
3	A	539	ASN
3	A	546	GLN
3	A	556	GLN
3	A	564	ASN
3	A	646	HIS
3	A	773	GLN
3	A	786	ASN
3	A	787	ASN
3	A	818	ASN
3	A	823	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	$\#\|Z\| > 2$
2	DOC	P	115	1,2	11,19,20	0.77	0	14,26,29	1.01	1 (7%)

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
2	DOC	P	115	1,2	-	0/3/18/19	0/2/2/2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	P	115	DOC	C2-N3-C4	3.07	119.94	115.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	P	115	DOC	3	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	TTP	A	1005	4	21,30,30	1.96	8 (38%)	31,47,47	3.12	5 (16%)

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
5	TTP	A	1005	4	-	0/18/34/34	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1005	TTP	PG-O1G	-3.63	1.39	1.51
5	A	1005	TTP	PA-O2A	-2.74	1.43	1.54
5	A	1005	TTP	C6-C5	-2.50	1.33	1.40
5	A	1005	TTP	PB-O2B	-2.42	1.44	1.54
5	A	1005	TTP	PB-O1B	-2.35	1.42	1.51
5	A	1005	TTP	O4-C4	-2.26	1.19	1.24
5	A	1005	TTP	C4-N3	3.46	1.39	1.33
5	A	1005	TTP	C6-N1	3.87	1.40	1.35

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1005	TTP	C5-C4-N3	-7.48	116.81	125.14
5	A	1005	TTP	O4'-C1'-N1	2.07	111.31	107.72
5	A	1005	TTP	O2G-PG-O1G	2.29	117.95	110.58
5	A	1005	TTP	C5M-C5-C6	2.40	123.45	118.62
5	A	1005	TTP	C4-N3-C2	14.48	127.76	115.25

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
5	A	1005	TTP	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	T	18/18 (100%)	-0.19	1 (5%) 28 21	34, 53, 94, 135	0
2	P	13/14 (92%)	-0.28	0 100 100	43, 60, 84, 85	0
3	A	901/903 (99%)	0.00	28 (3%) 52 45	28, 58, 101, 138	0
All	All	932/935 (99%)	-0.01	29 (3%) 52 45	28, 58, 101, 138	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	640	LYS	5.0
1	T	1	DA	4.4
3	A	901	PHE	3.4
3	A	900	MET	3.4
3	A	508	LEU	3.3
3	A	895	ALA	3.2
3	A	112	ASN	3.0
3	A	121	ASP	3.0
3	A	639	SER	2.8
3	A	1	MET	2.7
3	A	252	VAL	2.7
3	A	214	THR	2.6
3	A	259	SER	2.6
3	A	254	GLU	2.6
3	A	114	ASP	2.5
3	A	302	LYS	2.4
3	A	113	PHE	2.3
3	A	793	VAL	2.3
3	A	253	ILE	2.3
3	A	120	PRO	2.3
3	A	865	TRP	2.2
3	A	510	VAL	2.2
3	A	260	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
3	A	898	PHE	2.1
3	A	609	CYS	2.1
3	A	641	PHE	2.1
3	A	21	ASP	2.1
3	A	261	GLU	2.0
3	A	31	VAL	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, 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	DOC	P	115	18/19	0.96	0.19	-	40,46,56,61	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{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
5	TTP	A	1005	29/29	0.97	0.22	0.51	15,40,52,55	0
4	CA	A	1003	1/1	0.68	0.19	-0.63	105,105,105,105	0
4	CA	A	1004	1/1	0.94	0.26	-	99,99,99,99	0
4	CA	A	1001	1/1	0.96	0.25	-	44,44,44,44	0
4	CA	A	1002	1/1	0.94	0.43	-	79,79,79,79	0

6.5 Other polymers (i)

There are no such residues in this entry.