



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 10, 2023 – 10:00 AM EDT

PDB ID : 4KLT  
Title : DNA polymerase beta mismatched product complex with Mn<sup>2+</sup>, 30 min  
Authors : Freudenthal, B.D.; Beard, W.A.; Shock, D.D.; Wilson, S.H.  
Deposited on : 2013-05-07  
Resolution : 1.98 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>.

---

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 : 2.35.1  
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

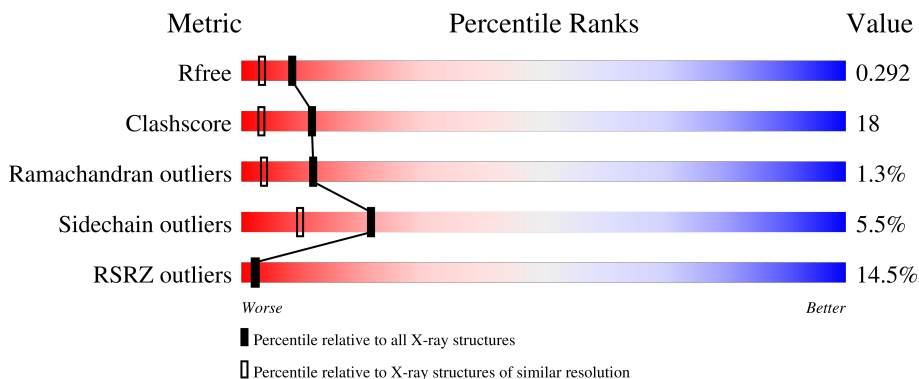
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.98 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	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

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	A	335	 14% 67% 22% 6%
2	D	5	 60% 40%
3	P	11	 9% 27% 64% 9%
4	T	16	 6% 56% 44%

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 3484 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA polymerase beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	314	2543	1607	445	482	9	0	4	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	D	5	106	49	20	32	5	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	P	11	224	107	43	64	10	0	1	0

- Molecule 4 is a DNA chain called 5'-D(\*CP\*CP\*GP\*AP\*CP\*GP\*GP\*CP\*GP\*CP\*AP\*TP\*CP\*AP\*GP\*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
4	T	16	323	153	63	92	15	0	0	0

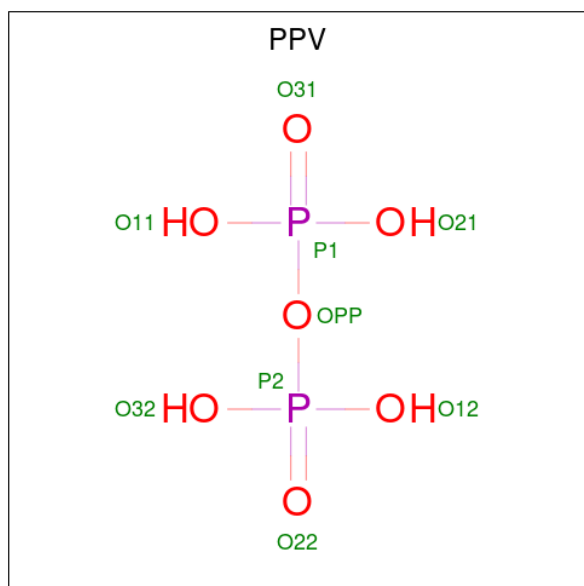
- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Na	0	0
			2	2		

- Molecule 6 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	3	Total Mn 4 4	0	1

- Molecule 7 is PYROPHOSPHATE (three-letter code: PPV) (formula:  $H_4O_7P_2$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total O P 9 7 2	0	1

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total Cl 1 1	0	0

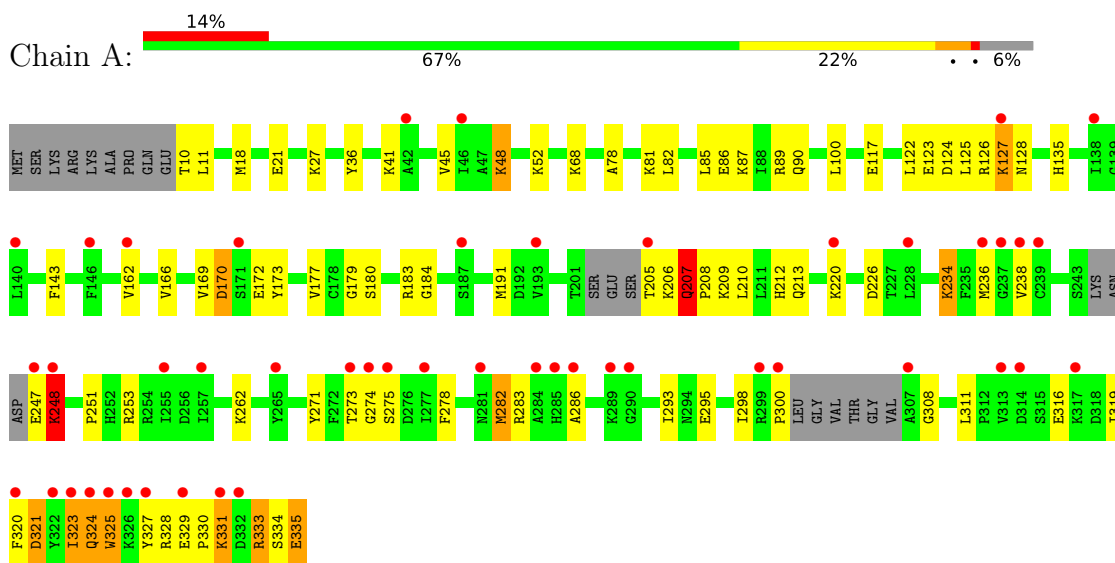
- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	187	Total O 187 187	0	0
9	D	12	Total O 12 12	0	0
9	P	29	Total O 29 29	0	0
9	T	44	Total O 44 44	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: DNA polymerase beta



- Molecule 2: 5'-D(P\*GP\*TP\*CP\*GP\*G)-3'

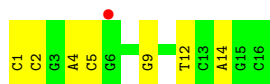


- Molecule 3: 5'-D(\*GP\*CP\*TP\*GP\*AP\*TP\*GP\*CP\*GP\*CP\*A)-3'



- Molecule 4: 5'-D(\*CP\*CP\*GP\*AP\*CP\*GP\*GP\*CP\*GP\*CP\*AP\*TP\*CP\*AP\*GP\*C)-3'





## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	55.08Å 78.60Å 54.98Å 90.00° 112.43° 90.00°	Depositor
Resolution (Å)	25.76 – 1.98 25.76 – 1.98	Depositor EDS
% Data completeness (in resolution range)	86.8 (25.76-1.98) 85.4 (25.76-1.98)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.96 (at 1.98Å)	Xtrriage
Refinement program	PHENIX 1.7_650	Depositor
R, $R_{free}$	0.229 , 0.292 0.236 , 0.292	Depositor DCC
$R_{free}$ test set	1486 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.3	Xtrriage
Anisotropy	0.186	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 56.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.038 for l,-k,h	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	3484	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.84% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PPV, MN, CL, NA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.43	0/2592	0.61	3/3481 (0.1%)
2	D	0.93	0/118	1.57	1/179 (0.6%)
3	P	0.86	0/251	1.30	1/386 (0.3%)
4	T	1.39	1/362 (0.3%)	1.38	4/556 (0.7%)
All	All	0.66	1/3323 (0.0%)	0.87	9/4602 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	T	12	DT	C4'-O4'	-5.83	1.39	1.45

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	207	GLN	N-CA-CB	-5.69	100.35	110.60
4	T	14	DA	O4'-C1'-N9	-5.62	104.06	108.00
2	D	2	DT	O4'-C1'-N1	-5.55	104.11	108.00
3	P	5	DA	O4'-C1'-N9	-5.55	104.12	108.00
1	A	170[A]	ASP	C-N-CA	5.38	135.15	121.70
1	A	170[B]	ASP	C-N-CA	5.38	135.15	121.70
4	T	4	DA	O4'-C1'-N9	-5.35	104.26	108.00
4	T	5	DC	O4'-C4'-C3'	-5.32	102.37	104.50
4	T	12	DT	O4'-C1'-C2'	-5.16	101.77	105.90

There are no chirality outliers.

There are no planarity outliers.



## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2543	0	2531	92	0
2	D	106	0	57	2	0
3	P	224	0	125	14	0
4	T	323	0	179	3	0
5	A	2	0	0	0	0
6	A	4	0	0	0	0
7	A	9	0	0	0	0
8	A	1	0	0	0	0
9	A	187	0	0	7	0
9	D	12	0	0	0	0
9	P	29	0	0	1	0
9	T	44	0	0	0	0
All	All	3484	0	2892	107	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 18.

All (107) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:THR:CG2	1:A:206:LYS:H	1.60	1.11
1:A:205:THR:HG22	1:A:206:LYS:N	1.57	1.05
1:A:183:ARG:NH1	1:A:275:SER:H	1.59	1.00
1:A:205:THR:HG22	1:A:206:LYS:H	0.86	0.98
3:P:10:DC:H5''	9:P:128:HOH:O	1.63	0.97
1:A:184:GLY:HA2	1:A:331:LYS:HE2	1.49	0.94
1:A:184:GLY:CA	1:A:331:LYS:HE2	2.09	0.81
1:A:183:ARG:NH1	1:A:275:SER:N	2.28	0.81
1:A:293:ILE:HD11	1:A:298:ILE:HD12	1.64	0.79
3:P:5:DA:H1'	3:P:6:DT:H5'	1.65	0.78
1:A:286:ALA:HA	1:A:323:ILE:HG21	1.65	0.78
3:P:10:DC:H2''	3:P:11[A]:DA:OP1	1.86	0.75
1:A:183:ARG:C	1:A:331:LYS:HG2	2.07	0.74
1:A:180:SER:HA	1:A:183:ARG:HH21	1.54	0.72
1:A:205:THR:CG2	1:A:206:LYS:N	2.30	0.70

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:ASP:HA	1:A:127:LYS:CG	2.24	0.68
3:P:1:DG:H2'	3:P:2:DC:C6	2.29	0.68
1:A:124:ASP:HA	1:A:127:LYS:HG2	1.76	0.68
3:P:6:DT:H2''	3:P:7:DG:OP2	1.96	0.66
1:A:209:LYS:HA	1:A:212:HIS:HB3	1.76	0.66
1:A:330:PRO:O	1:A:333:ARG:HG3	1.96	0.65
1:A:124:ASP:HA	1:A:127:LYS:HD3	1.79	0.65
3:P:2:DC:H2''	3:P:3:DT:H5'	1.79	0.65
1:A:127:LYS:O	1:A:128:ASN:ND2	2.31	0.63
1:A:11:LEU:O	1:A:52:LYS:HE2	1.99	0.61
1:A:180:SER:CA	1:A:183:ARG:HH21	2.12	0.61
1:A:21:GLU:OE2	1:A:89:ARG:HD3	2.01	0.60
4:T:1:DC:H1'	4:T:2:DC:H5'	1.82	0.60
1:A:300:PRO:HG2	1:A:308:GLY:HA3	1.84	0.59
1:A:124:ASP:CA	1:A:127:LYS:HG2	2.32	0.59
1:A:117:GLU:HG3	9:A:658:HOH:O	2.02	0.58
1:A:177:VAL:HG11	1:A:191:MET:HE2	1.84	0.58
1:A:234:LYS:HD3	1:A:236:MET:HG3	1.85	0.58
1:A:275:SER:OG	1:A:334:SER:HA	2.04	0.58
1:A:274:GLY:HA2	3:P:11[A]:DA:O3'	2.05	0.57
1:A:179:GLY:O	1:A:273:THR:O	2.22	0.56
1:A:282:MET:HE1	1:A:320:PHE:CZ	2.41	0.56
1:A:124:ASP:HA	1:A:127:LYS:CD	2.36	0.55
1:A:226:ASP:HB2	1:A:238:VAL:HB	1.90	0.54
1:A:320:PHE:HB3	1:A:325:TRP:O	2.07	0.54
1:A:208:PRO:O	1:A:209:LYS:HB2	2.08	0.53
1:A:293:ILE:HD11	1:A:319:ILE:HG23	1.91	0.53
1:A:180:SER:HA	1:A:183:ARG:HE	1.73	0.53
1:A:183:ARG:O	1:A:331:LYS:HG2	2.09	0.53
1:A:329:GLU:O	1:A:333:ARG:HG2	2.10	0.52
1:A:81:LYS:HE3	9:A:608:HOH:O	2.09	0.52
1:A:86:GLU:O	1:A:90:GLN:HG3	2.10	0.51
1:A:282:MET:CE	1:A:320:PHE:CE2	2.94	0.51
1:A:300:PRO:HD3	1:A:311:LEU:HG	1.92	0.51
3:P:5:DA:C1'	3:P:6:DT:H5'	2.38	0.51
1:A:234:LYS:NZ	4:T:9:DG:H1'	2.25	0.51
1:A:41:LYS:O	1:A:45:VAL:HG23	2.12	0.50
3:P:11[A]:DA:OP1	3:P:11[A]:DA:O4'	2.30	0.50
1:A:293:ILE:HG12	1:A:298:ILE:HG13	1.94	0.50
1:A:170[B]:ASP:HB3	1:A:173:TYR:CD2	2.47	0.49
1:A:68:LYS:HE2	2:D:1:DG:OP2	2.12	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:LYS:O	1:A:90:GLN:HB2	2.13	0.49
1:A:271:TYR:CD2	1:A:295:GLU:HB3	2.48	0.48
1:A:275:SER:CB	1:A:333:ARG:O	2.61	0.48
1:A:170[A]:ASP:HB3	1:A:173:TYR:CD2	2.47	0.48
1:A:248:LYS:CB	1:A:248:LYS:NZ	2.77	0.48
1:A:251:PRO:HG2	1:A:253:ARG:CZ	2.43	0.48
3:P:5:DA:C2'	3:P:6:DT:H5'	2.44	0.47
1:A:234:LYS:HZ2	4:T:9:DG:H1'	1.80	0.47
1:A:184:GLY:N	1:A:331:LYS:HG2	2.30	0.47
9:A:514:HOH:O	2:D:1:DG:H5''	2.15	0.47
9:A:686:HOH:O	3:P:11[A]:DA:C5'	2.62	0.46
1:A:78:ALA:HB2	9:A:510:HOH:O	2.15	0.46
1:A:123:GLU:O	1:A:127:LYS:HG2	2.15	0.46
1:A:282:MET:HE1	1:A:320:PHE:CE2	2.51	0.46
3:P:5:DA:H2''	3:P:6:DT:H5'	1.98	0.46
1:A:180:SER:HA	1:A:183:ARG:NH2	2.26	0.46
1:A:184:GLY:HA3	1:A:331:LYS:HG2	1.96	0.46
1:A:206:LYS:HG3	1:A:207:GLN:N	2.31	0.45
1:A:124:ASP:C	1:A:127:LYS:HG2	2.37	0.45
1:A:172:GLU:HG3	9:A:535:HOH:O	2.16	0.45
1:A:122:LEU:HD11	1:A:143:PHE:CD2	2.52	0.45
1:A:169:VAL:HG11	1:A:213:GLN:HB3	1.99	0.45
1:A:183:ARG:HH11	1:A:275:SER:N	2.12	0.44
1:A:48:LYS:HE3	1:A:335:GLU:OE2	2.17	0.44
1:A:282:MET:HE2	1:A:320:PHE:CE2	2.53	0.44
1:A:275:SER:HB3	1:A:278:PHE:HB3	2.00	0.44
1:A:293:ILE:CD1	1:A:319:ILE:HG23	2.48	0.44
1:A:27:LYS:HB2	1:A:36:TYR:CD1	2.52	0.43
1:A:324:GLN:HB3	1:A:325:TRP:H	1.60	0.43
1:A:180:SER:HB3	1:A:183:ARG:HH21	1.84	0.43
1:A:184:GLY:CA	1:A:331:LYS:HG2	2.48	0.43
1:A:247:GLU:O	1:A:248:LYS:C	2.56	0.43
1:A:278:PHE:CE2	1:A:333:ARG:HB3	2.53	0.43
1:A:278:PHE:CE1	1:A:282:MET:HE3	2.53	0.43
1:A:127:LYS:HG3	1:A:128:ASN:ND2	2.33	0.43
1:A:135:HIS:CD2	1:A:135:HIS:C	2.92	0.43
3:P:1:DG:H2'	3:P:2:DC:H6	1.80	0.43
1:A:320:PHE:O	1:A:321:ASP:C	2.57	0.43
1:A:162:VAL:O	1:A:166:VAL:HG23	2.18	0.42
1:A:21:GLU:HG2	1:A:85:LEU:HD22	2.01	0.42
1:A:126:ARG:HD2	9:A:531:HOH:O	2.19	0.42

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:LEU:HD22	1:A:125:LEU:HD11	2.01	0.42
3:P:6:DT:C2'	3:P:7:DG:OP2	2.67	0.42
1:A:316:GLU:HB2	1:A:327:TYR:HE2	1.84	0.42
1:A:210:LEU:HA	1:A:210:LEU:HD12	1.79	0.42
1:A:18:MET:SD	1:A:82:LEU:HD22	2.60	0.41
1:A:177:VAL:CG1	1:A:191:MET:HE2	2.48	0.41
1:A:48:LYS:NZ	1:A:335:GLU:HG2	2.36	0.41
1:A:180:SER:CB	1:A:183:ARG:HH21	2.34	0.41
1:A:183:ARG:NH1	1:A:275:SER:CA	2.83	0.40
1:A:124:ASP:O	1:A:127:LYS:HG2	2.22	0.40

There are no symmetry-related clashes.

### 5.3 Torsion angles [i](#)

#### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	310/335 (92%)	282 (91%)	24 (8%)	4 (1%)	<b>12</b>   <b>4</b>

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	248	LYS
1	A	331	LYS
1	A	321	ASP
1	A	323	ILE

#### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	276/295 (94%)	261 (95%)	15 (5%)	22	10

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	THR
1	A	48	LYS
1	A	127	LYS
1	A	207	GLN
1	A	220	LYS
1	A	234	LYS
1	A	248	LYS
1	A	262	LYS
1	A	282	MET
1	A	283	ARG
1	A	324	GLN
1	A	325	TRP
1	A	328	ARG
1	A	333	ARG
1	A	335	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	128	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 7 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
7	PPV	A	406[B]	6	6,8,8	0.69	0	13,13,13	1.10	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
7	PPV	A	406[B]	6	-	0/6/6/6	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
7	A	406[B]	PPV	O21-P1-OPP	2.25	112.20	104.64

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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	A	314/335 (93%)	0.87	48 (15%) 2 2	15, 34, 72, 89	0
2	D	5/5 (100%)	-0.24	0 100 100	22, 25, 38, 48	0
3	P	11/11 (100%)	0.09	1 (9%) 9 10	20, 31, 39, 56	0
4	T	16/16 (100%)	0.17	1 (6%) 20 22	20, 37, 54, 68	0
All	All	346/367 (94%)	0.80	50 (14%) 2 2	15, 34, 72, 89	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	323	ILE	10.7
1	A	274	GLY	8.5
1	A	322	TYR	5.6
1	A	273	THR	5.5
1	A	307	ALA	5.5
1	A	325	TRP	5.3
1	A	281	ASN	5.2
1	A	324	GLN	4.7
1	A	205	THR	4.7
1	A	331	LYS	4.7
1	A	317	LYS	4.6
1	A	285	HIS	4.6
1	A	284	ALA	4.6
1	A	255	ILE	4.5
1	A	127	LYS	3.9
1	A	247	GLU	3.7
1	A	326	LYS	3.7
1	A	257	ILE	3.6
1	A	286	ALA	3.5
1	A	275	SER	3.3
1	A	320	PHE	3.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	238	VAL	3.0
1	A	313	VAL	2.9
1	A	228	LEU	2.9
1	A	193	VAL	2.8
1	A	237	GLY	2.8
1	A	329	GLU	2.8
1	A	332	ASP	2.7
1	A	300	PRO	2.7
1	A	236	MET	2.7
1	A	277	ILE	2.6
1	A	299	ARG	2.5
3	P	11[A]	DA	2.4
1	A	314	ASP	2.3
1	A	265[A]	TYR	2.3
1	A	248	LYS	2.3
1	A	327	TYR	2.3
1	A	289	LYS	2.3
1	A	290	GLY	2.2
4	T	6	DG	2.2
1	A	171	SER	2.2
1	A	46	ILE	2.2
1	A	146	PHE	2.2
1	A	220	LYS	2.1
1	A	42	ALA	2.1
1	A	162	VAL	2.1
1	A	140	LEU	2.1
1	A	239	CYS	2.1
1	A	138	ILE	2.0
1	A	187	SER	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no 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
7	PPV	A	406[B]	9/9	0.78	0.19	25,34,44,52	9
8	CL	A	407	1/1	0.82	0.15	30,30,30,30	0
5	NA	A	401	1/1	0.86	0.27	49,49,49,49	0
6	MN	A	405[A]	1/1	0.89	0.33	32,32,32,32	1
6	MN	A	405[B]	1/1	0.89	0.33	29,29,29,29	1
6	MN	A	404	1/1	0.91	0.26	52,52,52,52	1
6	MN	A	403	1/1	0.92	0.12	65,65,65,65	0
5	NA	A	402	1/1	0.95	0.13	30,30,30,30	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.