



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:20 PM UTC

PDB ID : 352D / pdb_0000352d
Title : THE CRYSTAL STRUCTURE OF A PARALLEL-STRANDED PARALLEL-STRANDED GUANINE TETRAPLEX AT 0.95 ANGSTROM RESOLUTION
Authors : Phillips, K.; Dauter, Z.; Murchie, A.I.H.; Lilley, D.M.J.; Luisi, B.
Deposited on : 1997-09-04
Resolution : 0.95 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

<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 : 4-5-2 with Phenix2.0
Xtrriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

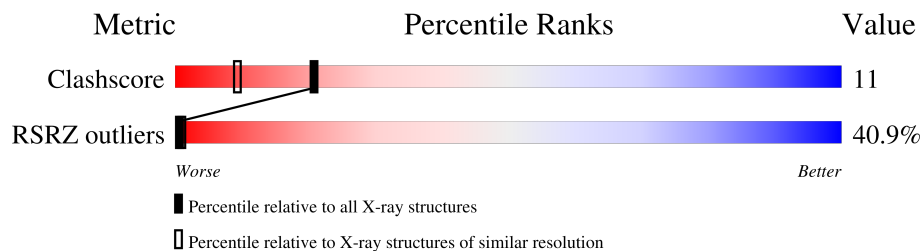
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 0.95 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))
Clashescore	190562	1090 (1.00-0.92)
RSRZ outliers	180081	1043 (1.00-0.92)

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 ≥ 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	6	
1	B	6	
1	C	6	
1	D	6	
1	E	6	
1	F	6	
1	G	6	
1	H	6	
1	I	6	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	J	6	
1	K	6	
1	L	6	
1	M	6	
1	N	6	
1	O	6	
1	P	6	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2490 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 DNA (5'-D(*TP*GP*GP*GP*GP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	A	6	Total 125	C 60	N 24	O 36	P 5	0	0	0
1	B	6	Total 111	C 51	N 22	O 32	P 6	0	2	1
1	C	5	Total 105	C 50	N 22	O 29	P 4	0	0	0
1	D	6	Total 125	C 60	N 24	O 36	P 5	0	0	0
1	E	6	Total 109	C 50	N 22	O 32	P 5	0	0	0
1	F	6	Total 125	C 60	N 24	O 36	P 5	0	0	0
1	G	6	Total 124	C 56	N 24	O 38	P 6	0	2	0
1	H	6	Total 124	C 56	N 24	O 38	P 6	0	2	0
1	I	6	Total 125	C 60	N 24	O 36	P 5	0	0	0
1	J	6	Total 131	C 61	N 24	O 40	P 6	0	2	0
1	K	4	Total 94	C 41	N 20	O 28	P 5	0	2	0
1	L	6	Total 129	C 60	N 24	O 39	P 6	0	2	0
1	M	6	Total 125	C 60	N 24	O 36	P 5	0	0	0
1	N	6	Total 118	C 55	N 24	O 34	P 5	0	0	0
1	O	6	Total 107	C 49	N 22	O 31	P 5	0	0	0
1	P	6	Total 130	C 61	N 24	O 39	P 6	0	2	0

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	3	Total Na 3 3	0	0
2	B	1	Total Na 1 1	0	0
2	E	2	Total Na 2 2	0	0
2	G	1	Total Na 1 1	0	0
2	I	3	Total Na 3 3	0	0
2	K	1	Total Na 1 1	0	0
2	M	3	Total Na 3 3	0	0

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Ca 2 2	0	0
3	B	1	Total Ca 1 1	0	0
3	C	1	Total Ca 1 1	0	0
3	G	1	Total Ca 1 1	0	0
3	K	1	Total Ca 1 1	0	0
3	M	1	Total Ca 1 1	0	0
3	N	1	Total Ca 1 1	0	0
3	O	1	Total Ca 1 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	46	Total O 46 46	0	0
4	B	35	Total O 35 35	0	0

Continued on next page...


Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	26	Total 26	O 26	0	0
4	D	41	Total 41	O 41	0	0
4	E	34	Total 34	O 34	0	0
4	F	37	Total 37	O 37	0	0
4	G	35	Total 35	O 35	0	0
4	H	28	Total 28	O 28	0	0
4	I	36	Total 36	O 36	0	0
4	J	34	Total 34	O 34	0	0
4	K	25	Total 25	O 25	0	0
4	L	24	Total 24	O 24	0	0
4	M	38	Total 38	O 38	0	0
4	N	40	Total 40	O 40	0	0
4	O	45	Total 45	O 45	0	0
4	P	36	Total 36	O 36	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 (5'-D(*TP*GP*GP*GP*GP*T)-3')

Chain A: 



- Molecule 1: DNA (5'-D(*TP*GP*GP*GP*GP*T)-3')

Chain B: 



- Molecule 1: DNA (5'-D(*TP*GP*GP*GP*GP*T)-3')

Chain C: 



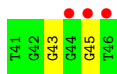
- Molecule 1: DNA (5'-D(*TP*GP*GP*GP*GP*T)-3')

Chain D: 



- Molecule 1: DNA (5'-D(*TP*GP*GP*GP*GP*T)-3')

Chain E: 



- Molecule 1: DNA (5'-D(*TP*GP*GP*GP*GP*T)-3')

Chain F:  67% 33%

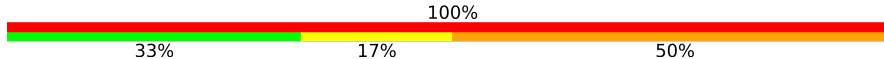


- Molecule 1: DNA (5'-D(*TP*GP*GP*GP*GP*T)-3')

Chain G:  17% 67% 83%




- Molecule 1: DNA (5'-D(*TP*GP*GP*GP*GP*T)-3')

Chain H:  33% 100% 17% 50%



- Molecule 1: DNA (5'-D(*TP*GP*GP*GP*GP*T)-3')

Chain I:  17% 83% 17%



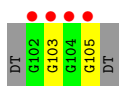
- Molecule 1: DNA (5'-D(*TP*GP*GP*GP*GP*T)-3')

Chain J:  33% 33% 67%




- Molecule 1: DNA (5'-D(*TP*GP*GP*GP*GP*T)-3')

Chain K:  33% 67% 33% 33%



- Molecule 1: DNA (5'-D(*TP*GP*GP*GP*GP*T)-3')

Chain L:  83% 83% 17%




- Molecule 1: DNA (5'-D(*TP*GP*GP*GP*GP*T)-3')

Chain M:  67% 33%



- Molecule 1: DNA (5'-D(*TP*GP*GP*GP*GP*T)-3')

Chain N:  17% 83% 17%



- Molecule 1: DNA (5'-D(*TP*GP*GP*GP*GP*T)-3')

Chain O:  67% 67% 33%



- Molecule 1: DNA (5'-D(*TP*GP*GP*GP*GP*T)-3')

Chain P:  33% 67% 33%



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	28.28Å 34.78Å 56.23Å 74.31° 77.68° 89.81°	Depositor
Resolution (Å)	(Not available) – 0.95 52.80 – 0.95	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-0.95) 89.3 (52.80-0.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.75 (at 0.95Å)	Xtrriage
Refinement program	SHELXL93, SHELXL-93	Depositor
R, R_{free}	0.152 , (Not available) 0.202 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	49.1	Xtrriage
Anisotropy	0.299	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.47 , 55.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.020 for h,-k,h-l	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	2490	wwPDB-VP
Average B, all atoms (Å ²)	11.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 61.18 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.3619e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical 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: CA, 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	0.67	0/140	1.25	0/216
1	B	0.72	0/168	1.76	7/260 (2.7%)
1	C	0.64	0/118	2.06	5/182 (2.7%)
1	D	0.66	0/140	1.38	1/216 (0.5%)
1	E	0.72	0/122	1.79	4/189 (2.1%)
1	F	0.68	0/140	1.40	1/216 (0.5%)
1	G	0.70	0/166	1.81	7/255 (2.7%)
1	H	0.73	0/175	2.55	14/270 (5.2%)
1	I	0.65	0/140	1.39	0/216
1	J	0.64	0/184	1.61	5/285 (1.8%)
1	K	0.65	0/149	1.52	1/230 (0.4%)
1	L	0.80	0/188	1.89	11/291 (3.8%)
1	M	0.69	0/140	1.29	1/216 (0.5%)
1	N	0.75	0/131	1.31	0/201
1	O	0.80	0/120	1.71	3/186 (1.6%)
1	P	2.17	2/186 (1.1%)	1.80	8/285 (2.8%)
All	All	0.91	2/2407 (0.1%)	1.71	68/3714 (1.8%)

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	A	0	1
1	H	0	3
1	I	0	1
1	L	0	1
1	M	0	1
1	N	0	1
1	O	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	9

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	156[A]	DT	P-OP1	20.04	1.88	1.48
1	P	156[B]	DT	P-OP1	20.04	1.88	1.48

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	71[A]	DT	C4'-C3'-O3'	-16.09	85.86	110.00
1	H	71[B]	DT	C4'-C3'-O3'	-16.09	85.86	110.00
1	C	24	DG	C2'-C3'-O3'	12.32	129.99	111.50
1	E	45	DG	O5'-C5'-C4'	-10.49	95.06	110.80
1	C	25	DG	O5'-C5'-C4'	-9.77	96.15	110.80
1	H	75	DG	C4'-C3'-O3'	-8.64	97.04	110.00
1	C	24	DG	C4'-C3'-O3'	-8.51	97.23	110.00
1	E	45	DG	P-O5'-C5'	-8.11	107.83	120.00
1	H	75	DG	C5'-C4'-O4'	-7.98	97.43	109.40
1	G	62[A]	DG	C5'-C4'-C3'	-7.86	103.11	114.90
1	G	62[B]	DG	C5'-C4'-C3'	-7.86	103.11	114.90
1	B	12[A]	DG	C4'-C3'-O3'	-7.81	98.28	110.00
1	B	12[B]	DG	C4'-C3'-O3'	-7.81	98.28	110.00
1	H	75	DG	C5'-C4'-C3'	-7.30	103.95	114.90
1	K	105	DG	C2'-C3'-O3'	-7.29	100.56	111.50
1	J	96	DT	N1-C1'-C2'	-7.09	102.86	113.50
1	L	112	DG	O5'-C5'-C4'	-7.09	100.17	110.80
1	L	116	DT	O5'-C5'-C4'	-7.01	100.29	110.80
1	O	145	DG	C4'-C3'-C2'	6.95	112.82	102.40
1	D	36	DT	O5'-C5'-C4'	-6.88	100.49	110.80
1	C	25	DG	C5'-C4'-C3'	6.86	125.19	114.90
1	G	66	DT	C4'-C3'-O3'	-6.81	99.78	110.00
1	E	45	DG	C2'-C3'-O3'	-6.71	101.43	111.50
1	J	96	DT	O4'-C1'-N1	-6.69	98.36	108.40
1	H	72[A]	DG	O5'-C5'-C4'	6.68	120.82	110.80
1	H	72[B]	DG	O5'-C5'-C4'	6.68	120.82	110.80
1	B	15	DG	P-O3'-C3'	6.64	130.16	120.20
1	P	155[A]	DG	O4'-C1'-C2'	-6.50	96.64	106.40
1	P	155[B]	DG	O4'-C1'-C2'	-6.50	96.64	106.40
1	P	155[A]	DG	O5'-C5'-C4'	-6.50	101.05	110.80
1	P	155[B]	DG	O5'-C5'-C4'	-6.50	101.05	110.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	74	DG	O5'-C5'-C4'	-6.49	101.06	110.80
1	C	26	DT	O5'-C5'-C4'	-6.44	101.14	110.80
1	L	116	DT	O4'-C4'-C3'	-6.43	95.75	105.40
1	B	15	DG	C4'-C3'-C2'	6.24	111.76	102.40
1	O	145	DG	C3'-C2'-C1'	-6.19	92.31	101.60
1	L	111	DT	C1'-O4'-C4'	6.19	118.98	109.70
1	J	96	DT	C4'-C3'-O3'	6.09	119.14	110.00
1	O	145	DG	C5'-C4'-C3'	5.98	123.87	114.90
1	L	115	DG	O5'-C5'-C4'	-5.95	101.88	110.80
1	G	65	DG	C4'-C3'-O3'	-5.84	101.24	110.00
1	E	45	DG	C5'-C4'-O4'	5.77	118.06	109.40
1	B	13[A]	DG	C4'-C3'-O3'	-5.74	101.39	110.00
1	B	13[B]	DG	C4'-C3'-O3'	-5.74	101.39	110.00
1	L	111	DT	O4'-C1'-C2'	-5.73	97.80	106.40
1	H	75	DG	C4'-C3'-C2'	5.62	110.83	102.40
1	L	114[A]	DG	O5'-C5'-C4'	-5.58	102.42	110.80
1	L	114[B]	DG	O5'-C5'-C4'	-5.58	102.42	110.80
1	H	74	DG	C4'-C3'-O3'	-5.57	101.64	110.00
1	H	75	DG	C2'-C3'-O3'	-5.49	103.27	111.50
1	J	96	DT	O5'-C5'-C4'	-5.45	102.62	110.80
1	G	64	DG	C2'-C3'-O3'	5.45	119.68	111.50
1	P	156[A]	DT	C2'-C3'-O3'	-5.41	103.39	111.50
1	P	156[B]	DT	C2'-C3'-O3'	-5.41	103.39	111.50
1	M	126	DT	O5'-C5'-C4'	-5.39	102.71	110.80
1	B	15	DG	C2'-C3'-O3'	-5.35	103.48	111.50
1	J	95	DG	C2'-C3'-O3'	-5.32	103.53	111.50
1	H	74	DG	O4'-C1'-N9	-5.31	100.43	108.40
1	P	156[A]	DT	OP1-P-OP2	5.29	135.88	120.00
1	P	156[B]	DT	OP1-P-OP2	5.29	135.88	120.00
1	F	51	DT	C3'-C2'-C1'	5.24	109.47	101.60
1	L	111	DT	C3'-C2'-C1'	5.24	109.45	101.60
1	G	63	DG	C4'-C3'-O3'	-5.23	102.16	110.00
1	G	64	DG	O5'-C5'-C4'	-5.15	103.08	110.80
1	H	71[A]	DT	P-O3'-C3'	-5.12	112.52	120.20
1	H	71[B]	DT	P-O3'-C3'	-5.12	112.52	120.20
1	L	113[A]	DG	C4'-C3'-O3'	5.09	117.64	110.00
1	L	113[B]	DG	C4'-C3'-O3'	5.09	117.64	110.00

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	6	DT	Sidechain
1	H	71[A]	DT	Sidechain
1	H	71[B]	DT	Sidechain
1	H	74	DG	Sidechain
1	I	86	DT	Sidechain
1	L	114[A]	DG	Sidechain
1	M	124	DG	Sidechain
1	N	136	DT	Sidechain
1	O	142	DG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	125	0	70	0	0
1	B	111	0	40	1	0
1	C	105	0	58	0	0
1	D	125	0	70	1	0
1	E	109	0	57	1	0
1	F	125	0	70	2	0
1	G	124	0	52	0	0
1	H	124	0	46	10	0
1	I	125	0	70	0	0
1	J	131	0	54	3	0
1	K	94	0	31	3	0
1	L	129	0	52	2	0
1	M	125	0	70	0	0
1	N	118	0	62	0	0
1	O	107	0	53	0	0
1	P	130	0	54	9	0
2	A	3	0	0	0	0
2	B	1	0	0	0	0
2	E	2	0	0	0	0
2	G	1	0	0	0	0
2	I	3	0	0	0	0
2	K	1	0	0	0	0
2	M	3	0	0	0	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1	0	0	0	0
3	G	1	0	0	0	0
3	K	1	0	0	0	0
3	M	1	0	0	0	0
3	N	1	0	0	0	0
3	O	1	0	0	0	0
4	A	46	0	0	0	0
4	B	35	0	0	2	0
4	C	26	0	0	0	0
4	D	41	0	0	1	0
4	E	34	0	0	1	0
4	F	37	0	0	0	0
4	G	35	0	0	1	0
4	H	28	0	0	1	0
4	I	36	0	0	0	0
4	J	34	0	0	1	0
4	K	25	0	0	0	0
4	L	24	0	0	0	0
4	M	38	0	0	0	0
4	N	40	0	0	0	0
4	O	45	0	0	0	0
4	P	36	0	0	0	0
All	All	2490	0	909	33	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 11.

All (33) 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:H:72[B]:DG:OP1	1:H:72[B]:DG:P	1.14	1.51
1:P:156[B]:DT:P	1:P:156[B]:DT:OP2	1.04	1.43
1:P:155[B]:DG:O3'	1:P:156[B]:DT:OP2	1.98	0.78
1:H:72[B]:DG:C5'	1:H:72[B]:DG:H4'	1.25	0.76
1:H:72[B]:DG:OP1	1:H:72[B]:DG:OP2	2.07	0.73
1:P:156[B]:DT:OP2	1:P:156[B]:DT:O5'	2.14	0.65
1:H:72[B]:DG:OP1	4:H:336:HOH:O	2.12	0.65
1:E:43:DG:H5''	4:E:711:HOH:O	1.96	0.65
1:D:31:DT:H1'	4:D:726:HOH:O	1.99	0.63
1:F:56:DT:H73	4:G:729:HOH:O	2.06	0.54
1:B:14:DG:H5''	4:B:547:HOH:O	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:156[B]:DT:OP2	1:P:156[B]:DT:C5'	2.58	0.52
1:F:56:DT:H71	4:J:642:HOH:O	2.13	0.48
1:P:156[B]:DT:OP2	1:P:156[B]:DT:H5'	2.19	0.43

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein molecules in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein molecules in this entry.

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 23 ligands modelled in this entry, 23 are monoatomic - leaving 0 for Mogul analysis.

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

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	H	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	71[B]:DT	O3'	72[B]:DG	P	1.33

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, 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	A	6/6 (100%)	1.08	0 100 100	5, 7, 8, 8	0
1	B	6/6 (100%)	2.43	3 (50%) 0 1	5, 8, 12, 17	1 (16%)
1	C	5/6 (83%)	2.08	2 (40%) 1 1	6, 7, 11, 13	0
1	D	6/6 (100%)	1.41	1 (16%) 4 3	6, 7, 8, 10	0
1	E	6/6 (100%)	3.16	3 (50%) 0 1	6, 7, 13, 19	0
1	F	6/6 (100%)	1.02	0 100 100	6, 7, 9, 9	0
1	G	6/6 (100%)	2.14	4 (66%) 0 0	7, 10, 10, 12	1 (16%)
1	H	6/6 (100%)	3.20	6 (100%) 0 0	8, 13, 14, 16	1 (16%)
1	I	6/6 (100%)	1.25	1 (16%) 4 3	6, 7, 9, 10	0
1	J	6/6 (100%)	1.88	2 (33%) 1 1	6, 8, 9, 18	1 (16%)
1	K	4/6 (66%)	2.64	4 (100%) 0 0	10, 10, 11, 12	1 (25%)
1	L	6/6 (100%)	2.76	5 (83%) 0 0	8, 9, 11, 16	1 (16%)
1	M	6/6 (100%)	1.02	0 100 100	5, 7, 8, 10	0
1	N	6/6 (100%)	1.49	1 (16%) 4 3	6, 6, 8, 16	0
1	O	6/6 (100%)	2.95	4 (66%) 0 0	6, 8, 11, 18	0
1	P	6/6 (100%)	1.78	2 (33%) 1 1	5, 8, 10, 12	1 (16%)
All	All	93/96 (96%)	2.00	38 (40%) 0 1	5, 8, 16, 19	7 (7%)

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	46	DT	9.7
1	O	146	DT	6.5
1	N	131	DT	5.2
1	H	74	DG	5.0
1	B	16	DT	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	J	96	DT	4.0
1	C	25	DG	3.9
1	E	44	DG	3.8
1	L	111	DT	3.6
1	E	45	DG	3.5
1	B	15	DG	3.4
1	B	14	DG	3.3
1	P	155[A]	DG	3.3
1	H	73	DG	3.2
1	P	156[A]	DT	3.1
1	H	75	DG	3.1
1	G	61[A]	DT	3.1
1	O	141	DT	3.0
1	H	72[A]	DG	3.0
1	L	112	DG	2.9
1	L	114[A]	DG	2.9
1	O	145	DG	2.9
1	K	103[A]	DG	2.9
1	K	104[A]	DG	2.8
1	H	76	DT	2.7
1	K	102	DG	2.6
1	L	113[A]	DG	2.5
1	L	115	DG	2.5
1	K	105	DG	2.3
1	G	64	DG	2.3
1	J	95	DG	2.3
1	O	144	DG	2.3
1	G	62[A]	DG	2.2
1	H	71[A]	DT	2.2
1	C	24	DG	2.2
1	I	85	DG	2.2
1	G	65	DG	2.1
1	D	36	DT	2.1

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 oligosaccharides 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, 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	B-factors(Å ²)	Q<0.9
3	CA	A	179	1/1	0.97	0.05	8,8,8,8	0
3	CA	O	175	1/1	0.97	0.07	7,7,7,7	0
2	NA	E	169	1/1	0.98	0.05	7,7,7,7	0
2	NA	I	167	1/1	0.98	0.05	7,7,7,7	0
2	NA	M	163	1/1	0.98	0.04	7,7,7,7	0
2	NA	A	170	1/1	0.98	0.05	7,7,7,7	0
3	CA	C	176	1/1	0.98	0.05	6,6,6,6	0
3	CA	G	174	1/1	0.98	0.05	6,6,6,6	0
2	NA	E	165	1/1	0.98	0.06	7,7,7,7	0
2	NA	M	168	1/1	0.99	0.04	6,6,6,6	0
3	CA	A	177	1/1	0.99	0.04	5,5,5,5	0
2	NA	I	166	1/1	0.99	0.04	7,7,7,7	0
2	NA	B	164	1/1	0.99	0.04	7,7,7,7	0
2	NA	K	162	1/1	0.99	0.03	5,5,5,5	0
3	CA	K	172	1/1	0.99	0.04	7,7,7,7	0
3	CA	N	173	1/1	0.99	0.03	5,5,5,5	0
2	NA	G	161	1/1	0.99	0.03	5,5,5,5	0
2	NA	A	160	1/1	1.00	0.03	4,4,4,4	0
2	NA	A	159	1/1	1.00	0.06	4,4,4,4	0
2	NA	I	158	1/1	1.00	0.03	4,4,4,4	0
3	CA	M	171	1/1	1.00	0.03	5,5,5,5	0
2	NA	M	157	1/1	1.00	0.07	4,4,4,4	0
3	CA	B	178	1/1	1.00	0.02	4,4,4,4	0

6.5 Other polymers [i](#)

There are no such residues in this entry.