



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:50 PM GMT

PDB ID : 3V6H
Title : Replication of N2,3-Ethenoguanine by DNA Polymerases
Authors : Zhao, L.
Deposited on : 2011-12-19
Resolution : 2.30 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

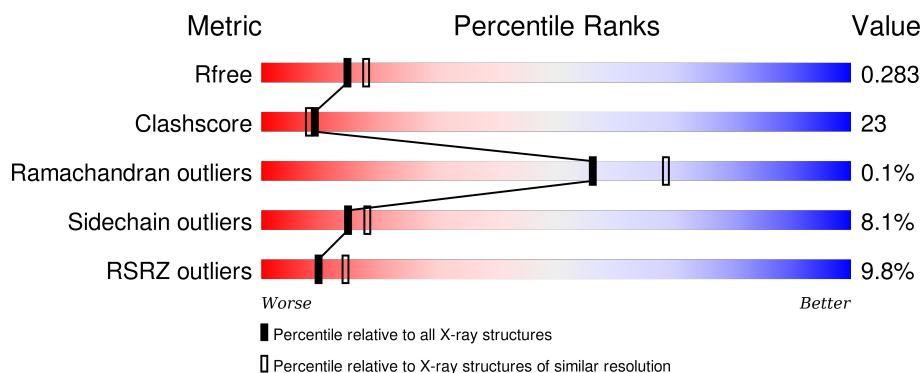
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	C	18	<div> <div>17%</div> <div>17% 67% 11% 6%</div> </div>
1	T	18	<div> <div>28%</div> <div>6% 56% 11% 28%</div> </div>
2	D	13	<div> <div>15%</div> <div>31% 46% 15% 8%</div> </div>
2	P	13	<div> <div>38%</div> <div>46% 38% 15%</div> </div>
3	A	348	<div> <div>3%</div> <div>80% 16% ..</div> </div>

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Mol	Chain	Length	Quality of chain
3	B	348	

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
2	DOC	P	13	-	-	X	-
6	MG	B	402	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6867 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*CP*AP*CP*(EFG)P*GP*AP*AP*TP*CP*CP*TP*TP*CP*CP*CP*CP*C)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	T	13	Total	C	F	N	O	P	0	0	0
			263	126	1	44	79	13			
1	C	17	Total	C	F	N	O	P	0	0	0
			339	164	1	57	101	16			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	11	Total	C	N	O	P	0	0	0
			228	109	47	62	10			
2	D	12	Total	C	N	O	P	0	0	0
			250	119	52	68	11			

- Molecule 3 is a protein called DNA polymerase IV.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	343	Total	C	N	O	S	0	0	0
			2762	1771	476	508	7			
3	B	342	Total	C	N	O	S	0	0	0
			2752	1765	473	507	7			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	EXPRESSION TAG	UNP Q97W02
A	-4	HIS	-	EXPRESSION TAG	UNP Q97W02
A	-3	HIS	-	EXPRESSION TAG	UNP Q97W02
A	-2	HIS	-	EXPRESSION TAG	UNP Q97W02
A	-1	HIS	-	EXPRESSION TAG	UNP Q97W02
A	0	HIS	-	EXPRESSION TAG	UNP Q97W02

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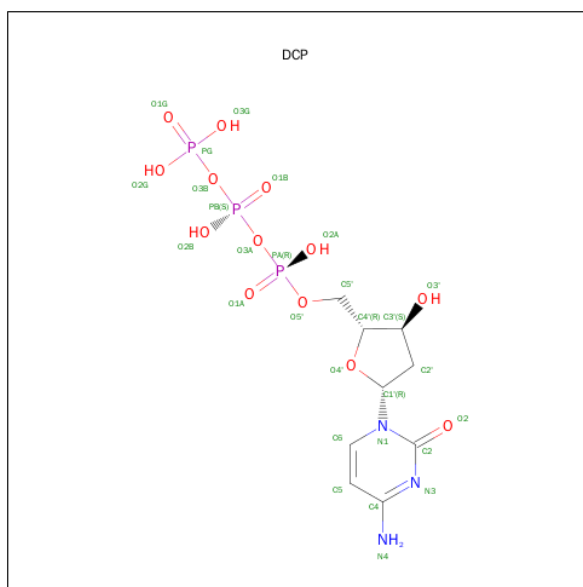
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	HIS	-	EXPRESSION TAG	UNP Q97W02
B	-4	HIS	-	EXPRESSION TAG	UNP Q97W02
B	-3	HIS	-	EXPRESSION TAG	UNP Q97W02
B	-2	HIS	-	EXPRESSION TAG	UNP Q97W02
B	-1	HIS	-	EXPRESSION TAG	UNP Q97W02
B	0	HIS	-	EXPRESSION TAG	UNP Q97W02

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Ca 1 1	0	0
4	A	1	Total Ca 1 1	0	0
4	D	1	Total Ca 1 1	0	0

- Molecule 5 is 2'-DEOXYCYTIDINE-5'-TRIPHOSPHATE (three-letter code: DCP) (formula: C₉H₁₆N₃O₁₃P₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O P 28 9 3 13 3	0	0
5	B	1	Total C N O P 28 9 3 13 3	0	0

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

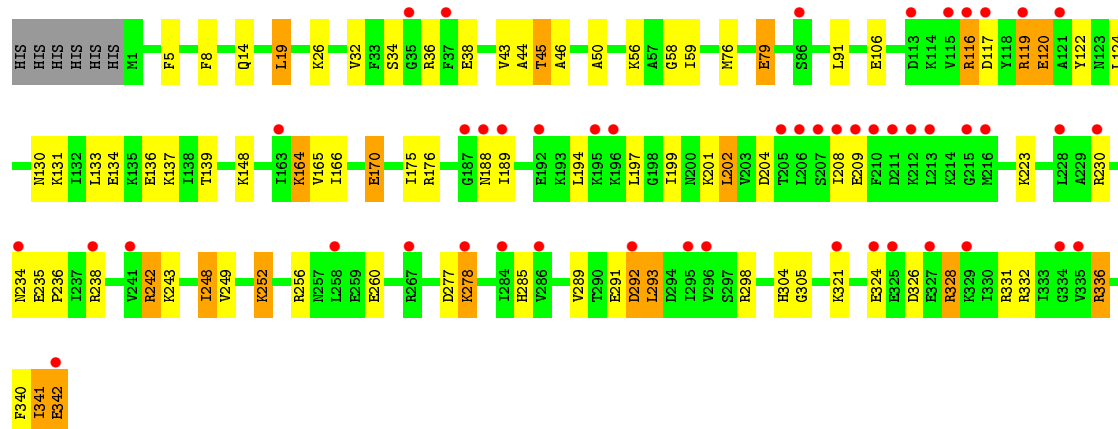
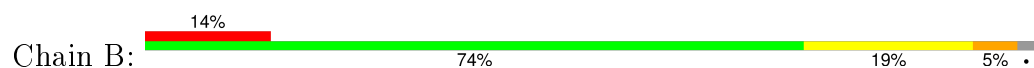
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	2	Total 2	Mg 2	0	0
6	A	2	Total 2	Mg 2	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	T	8	Total 8	O 8	0	0
7	P	4	Total 4	O 4	0	0
7	C	15	Total 15	O 15	0	0
7	D	7	Total 7	O 7	0	0
7	A	115	Total 115	O 115	0	0
7	B	61	Total 61	O 61	0	0



• Molecule 3: DNA polymerase IV



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	52.53Å 111.27Å 98.94Å 90.00° 102.68° 90.00°	Depositor
Resolution (Å)	27.80 – 2.30 29.80 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.0 (27.80-2.30) 98.1 (29.80-2.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.215 , 0.267 0.230 , 0.283	Depositor DCC
R_{free} test set	2441 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	51.5	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 51.8	EDS
Estimated twinning fraction	0.030 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	2 of 48486 reflections (0.004%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6867	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.10% 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: DOC, MG, CA, DCP, EFG

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	C	0.75	2/348 (0.6%)	1.09	3/530 (0.6%)
1	T	0.36	0/263	0.98	2/399 (0.5%)
2	D	0.55	1/262 (0.4%)	1.05	3/405 (0.7%)
2	P	1.23	3/237 (1.3%)	1.28	5/366 (1.4%)
3	A	0.42	0/2802	0.60	0/3763
3	B	0.36	0/2791	0.57	0/3748
All	All	0.48	6/6703 (0.1%)	0.71	13/9211 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	8	DG	O3'-P	-12.50	1.46	1.61
2	P	4	DG	O3'-P	9.41	1.72	1.61
1	C	1	DT	O3'-P	-6.91	1.52	1.61
1	C	3	DA	O3'-P	-6.88	1.52	1.61
2	D	11	DT	O3'-P	6.27	1.68	1.61
2	P	6	DA	O3'-P	-5.03	1.55	1.61

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	14	DC	P-O3'-C3'	7.40	128.58	119.70
2	D	11	DT	P-O3'-C3'	7.25	128.40	119.70
1	C	6	DG	C1'-O4'-C4'	-6.91	103.19	110.10
2	D	3	DG	P-O3'-C3'	6.20	127.14	119.70
2	P	12	DT	O5'-P-OP1	-5.90	100.39	105.70
1	T	10	DC	P-O3'-C3'	5.84	126.71	119.70
2	P	4	DG	P-O3'-C3'	-5.79	112.75	119.70
2	P	10	DA	P-O3'-C3'	5.58	126.40	119.70
2	P	9	DG	OP1-P-O3'	5.55	117.41	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	12	DT	O5'-P-OP1	-5.38	100.85	105.70
2	P	4	DG	O3'-P-O5'	5.37	114.19	104.00
1	C	1	DT	P-O3'-C3'	-5.33	113.30	119.70
1	T	6	DG	P-O3'-C3'	5.28	126.03	119.70

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	C	339	0	192	24	0
1	T	263	0	146	76	0
2	D	250	0	136	28	0
2	P	228	0	125	79	0
3	A	2762	0	2902	50	0
3	B	2752	0	2895	71	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
5	A	28	0	12	2	0
5	B	28	0	12	4	0
6	A	2	0	0	0	0
6	B	2	0	0	0	0
7	A	115	0	0	19	0
7	B	61	0	0	19	0
7	C	15	0	0	2	0
7	D	7	0	0	2	0
7	P	4	0	0	0	0
7	T	8	0	0	0	0
All	All	6867	0	6420	298	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 23.

All (298) 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:T:11:DC:H2'	1:T:12:DT:C6	1.42	1.51
1:T:11:DC:C6	1:T:11:DC:H5''	1.59	1.37
1:T:11:DC:H3'	1:T:12:DT:C7	1.54	1.35
2:P:5:DG:H5''	2:P:5:DG:C8	1.68	1.27
2:P:12:DT:H2'	2:P:13:DOC:C5	1.64	1.25
1:T:11:DC:H2'	1:T:12:DT:C5	1.76	1.21
2:P:11:DT:C6	2:P:12:DT:H72	1.79	1.16
3:B:164:LYS:HE3	3:B:165:VAL:O	1.46	1.15
1:T:11:DC:C2'	1:T:12:DT:C6	2.30	1.14
2:P:7:DA:C4	2:P:8:DG:C8	2.35	1.14
2:D:2:DG:C2'	2:D:3:DG:H2'	1.76	1.13
1:T:15:DC:H1'	1:T:16:DC:O5'	1.49	1.11
2:P:13:DOC:H5''	2:P:13:DOC:H6	1.17	1.11
1:T:11:DC:H3'	1:T:12:DT:H73	1.11	1.10
2:P:12:DT:H2'	2:P:13:DOC:H5	1.11	1.09
2:P:13:DOC:H2'	5:B:401:DCP:H1'	1.35	1.08
1:T:11:DC:H6	1:T:11:DC:C5'	1.65	1.08
1:T:11:DC:H2''	1:T:12:DT:OP1	1.36	1.07
1:T:11:DC:C3'	1:T:12:DT:C7	2.32	1.06
2:P:3:DG:H2''	2:P:4:DG:O5'	1.51	1.06
2:P:12:DT:H2''	2:P:13:DOC:H5''	1.28	1.05
3:A:36:ARG:HH22	3:A:254:ASN:ND2	1.54	1.05
1:C:2:DC:O2	1:C:2:DC:H2'	1.54	1.05
1:T:12:DT:H2''	1:T:13:DT:H5'	1.36	1.05
3:B:341:ILE:HA	7:B:505:HOH:O	1.57	1.04
2:P:12:DT:H2''	2:P:13:DOC:C6	1.86	1.03
2:P:12:DT:H2''	2:P:13:DOC:H6	1.34	1.03
1:T:14:DC:H2''	1:T:15:DC:O5'	1.58	1.03
2:D:2:DG:H2'	2:D:3:DG:H2'	1.37	1.03
2:D:2:DG:O3'	2:D:3:DG:H3'	1.60	1.02
1:T:11:DC:H3'	1:T:12:DT:H72	1.42	1.02
2:P:12:DT:C2'	2:P:13:DOC:C5	2.37	1.01
2:P:5:DG:C5'	2:P:5:DG:H8	1.71	1.01
3:B:14:GLN:HE22	3:B:139:THR:H	1.06	1.01
2:P:10:DA:H2'	2:P:11:DT:H71	1.43	1.01
1:T:15:DC:H2''	1:T:16:DC:OP2	1.63	0.99
1:T:11:DC:H6	1:T:11:DC:H5''	0.81	0.98
2:P:12:DT:C2'	2:P:13:DOC:C6	2.42	0.97
3:B:248:ILE:HD11	3:B:332:ARG:HB3	1.44	0.97
2:P:7:DA:C2	2:P:8:DG:C4	2.53	0.97
3:A:67:ILE:HG13	7:A:609:HOH:O	1.62	0.97
1:T:14:DC:H1'	1:T:15:DC:H5''	1.46	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:43:VAL:HB	7:B:561:HOH:O	1.63	0.95
2:P:5:DG:H5''	2:P:5:DG:H8	0.80	0.94
2:P:7:DA:N3	2:P:8:DG:C8	2.35	0.94
3:B:242:ARG:HG3	3:B:242:ARG:HH11	1.32	0.93
1:T:8:DA:H2	2:P:11:DT:H3	1.17	0.93
2:P:7:DA:C5	2:P:8:DG:N7	2.36	0.93
2:P:7:DA:C6	2:P:8:DG:C5	2.56	0.92
2:P:5:DG:C5'	2:P:5:DG:C8	2.50	0.92
3:A:319:LEU:HD12	7:A:580:HOH:O	1.70	0.92
2:P:12:DT:H2''	2:P:13:DOC:C5'	2.00	0.90
1:T:11:DC:C6	1:T:11:DC:C5'	2.48	0.89
2:P:7:DA:N1	2:P:8:DG:C5	2.39	0.89
1:T:11:DC:C3'	1:T:12:DT:H73	1.98	0.89
3:B:164:LYS:CE	3:B:165:VAL:O	2.21	0.89
2:D:6:DA:H4'	2:D:7:DA:OP1	1.72	0.89
1:T:11:DC:C3'	1:T:12:DT:H72	1.98	0.88
2:D:2:DG:H2''	2:D:3:DG:H2'	1.53	0.88
3:B:164:LYS:HE2	3:B:166:ILE:HG12	1.54	0.88
2:P:7:DA:H2''	2:P:8:DG:O5'	1.75	0.87
1:T:11:DC:H2'	1:T:12:DT:H6	1.36	0.87
3:A:14:GLN:HE22	3:A:139:THR:H	1.20	0.87
1:T:7:DA:C2	2:P:12:DT:N3	2.43	0.86
1:T:14:DC:H1'	1:T:15:DC:C5'	2.06	0.86
1:T:12:DT:O2	1:T:13:DT:C2	2.30	0.84
3:A:36:ARG:NH2	3:A:254:ASN:ND2	2.26	0.84
3:A:1:MET:C	3:A:2:ILE:HD13	1.97	0.84
2:P:5:DG:H2''	2:P:6:DA:O4'	1.79	0.83
2:P:7:DA:C2	2:P:8:DG:N9	2.47	0.82
1:T:7:DA:H2	2:P:12:DT:H3	1.25	0.82
2:D:6:DA:H2'	2:D:7:DA:C8	2.16	0.81
3:B:201:LYS:HE2	7:B:501:HOH:O	1.82	0.80
1:T:15:DC:C1'	1:T:16:DC:O5'	2.30	0.79
1:T:14:DC:C2'	1:T:15:DC:O5'	2.31	0.79
2:P:7:DA:C6	2:P:8:DG:N7	2.51	0.79
3:A:2:ILE:N	3:A:2:ILE:HD13	1.94	0.79
3:B:201:LYS:CE	7:B:501:HOH:O	2.31	0.79
2:D:2:DG:H2''	2:D:3:DG:C2'	2.13	0.78
1:C:3:DA:H5''	1:C:3:DA:H8	1.48	0.78
7:D:204:HOH:O	3:A:285:HIS:HE1	1.67	0.77
1:C:2:DC:O2	1:C:2:DC:C2'	2.30	0.77
3:A:79:GLU:H	3:A:79:GLU:CD	1.87	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:248:ILE:CD1	3:B:332:ARG:HB3	2.14	0.76
2:P:7:DA:C2	2:P:8:DG:C8	2.72	0.76
1:T:11:DC:C2'	1:T:12:DT:H6	1.90	0.76
1:C:7:DA:C2	2:D:12:DT:N3	2.52	0.76
2:P:13:DOC:H2'	5:B:401:DCP:C1'	2.15	0.75
3:A:275:LYS:HE3	7:A:563:HOH:O	1.85	0.75
3:A:31:CYS:SG	7:A:581:HOH:O	2.43	0.75
2:P:13:DOC:H5''	2:P:13:DOC:C6	2.09	0.75
2:P:13:DOC:H6	2:P:13:DOC:C5'	2.09	0.75
3:B:164:LYS:HE2	3:B:166:ILE:CG1	2.17	0.74
3:B:175:ILE:HG23	7:B:542:HOH:O	1.87	0.74
2:D:2:DG:C2'	2:D:3:DG:C2'	2.61	0.74
3:B:341:ILE:HG22	3:B:342:GLU:H	1.53	0.73
1:T:14:DC:H1'	1:T:15:DC:OP1	1.87	0.73
3:B:166:ILE:HG23	3:B:170:GLU:HB3	1.71	0.73
2:P:11:DT:C6	2:P:12:DT:C7	2.69	0.73
2:P:7:DA:C4	2:P:8:DG:N7	2.57	0.72
1:T:7:DA:H2	2:P:12:DT:C2	2.07	0.72
2:P:3:DG:C2'	2:P:4:DG:O5'	2.35	0.71
1:T:7:DA:H2	2:P:12:DT:N3	1.82	0.71
1:T:11:DC:C2'	1:T:12:DT:C7	2.69	0.71
2:P:13:DOC:C2'	5:B:401:DCP:H1'	2.19	0.71
1:C:7:DA:H2	2:D:12:DT:C2	2.09	0.70
3:B:292:ASP:OD2	3:B:328:ARG:NH1	2.20	0.70
1:T:11:DC:C2'	1:T:12:DT:C5	2.62	0.69
1:C:3:DA:H5''	1:C:3:DA:C8	2.27	0.69
1:C:5:EFG:H1	5:A:401:DCP:HN41	1.41	0.69
2:P:7:DA:C2	2:P:8:DG:C5	2.79	0.69
1:C:5:EFG:H1'	1:C:5:EFG:H10	1.73	0.69
2:P:4:DG:N7	2:P:5:DG:C2	2.62	0.68
2:D:3:DG:P	2:D:3:DG:H3'	2.34	0.68
1:C:7:DA:H2	2:D:12:DT:O2	1.76	0.68
3:A:52:LYS:HE3	7:A:561:HOH:O	1.92	0.68
1:T:14:DC:C1'	1:T:15:DC:C5'	2.71	0.68
3:A:342:GLU:C	7:A:538:HOH:O	2.32	0.67
1:T:13:DT:C6	1:T:14:DC:N4	2.62	0.67
3:A:43:VAL:HA	7:A:581:HOH:O	1.95	0.67
1:T:5:EFG:H1'	1:T:5:EFG:H10	1.76	0.67
2:D:6:DA:C2'	2:D:7:DA:C8	2.77	0.66
3:B:119:ARG:O	3:B:122:TYR:HB3	1.96	0.66
3:B:289:VAL:HB	3:B:332:ARG:HB2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:11:DC:H2'	1:T:12:DT:C7	2.27	0.65
3:A:97:GLU:HA	7:A:569:HOH:O	1.95	0.65
3:B:59:ILE:N	7:B:561:HOH:O	2.29	0.65
3:A:0:HIS:O	3:A:0:HIS:ND1	2.30	0.65
3:B:292:ASP:OD1	3:B:292:ASP:N	2.30	0.65
1:T:14:DC:H2''	1:T:15:DC:C5'	2.26	0.65
3:B:285:HIS:HD2	7:B:523:HOH:O	1.78	0.64
2:P:12:DT:C2'	2:P:13:DOC:H6	2.13	0.64
1:T:14:DC:N4	2:P:5:DG:H22	1.96	0.63
2:P:12:DT:C2'	2:P:13:DOC:H5''	2.18	0.63
3:B:238:ARG:HG3	3:B:238:ARG:O	1.98	0.63
2:P:7:DA:C6	2:P:8:DG:C6	2.87	0.62
3:A:277:ASP:O	3:A:278:LYS:HB2	1.99	0.62
1:T:6:DG:N7	2:P:13:DOC:O2	2.33	0.62
1:T:14:DC:H1'	1:T:15:DC:P	2.40	0.61
3:B:202:LEU:HB2	7:B:535:HOH:O	1.99	0.61
2:P:7:DA:N1	2:P:8:DG:C4	2.66	0.61
2:P:4:DG:C8	2:P:5:DG:C6	2.89	0.61
3:A:199:ILE:HG23	3:A:204:ASP:HB2	1.82	0.61
1:T:15:DC:H1'	1:T:16:DC:C5'	2.31	0.60
3:A:285:HIS:HD2	7:A:550:HOH:O	1.83	0.60
3:A:241:VAL:HB	7:A:560:HOH:O	2.01	0.60
2:D:13:DOC:C5'	7:A:614:HOH:O	2.48	0.60
1:T:9:DT:H2'	1:T:10:DC:C6	2.36	0.60
3:B:164:LYS:HE3	3:B:165:VAL:C	2.20	0.60
1:T:5:EFG:H9	3:B:32:VAL:HG21	1.82	0.60
2:P:5:DG:H2'	2:P:6:DA:C8	2.37	0.60
3:B:130:ASN:O	3:B:134:GLU:HG2	2.02	0.60
2:P:10:DA:H4'	2:P:11:DT:OP1	2.00	0.59
3:B:341:ILE:CA	7:B:505:HOH:O	2.32	0.59
2:P:12:DT:C2'	2:P:13:DOC:H5	2.04	0.59
3:A:130:ASN:O	3:A:134:GLU:HG2	2.02	0.59
3:B:56:LYS:HB2	7:B:546:HOH:O	2.01	0.59
3:B:194:LEU:HB3	3:B:199:ILE:HB	1.86	0.58
1:T:11:DC:C2'	1:T:12:DT:OP1	2.30	0.57
1:T:14:DC:N4	2:P:5:DG:N2	2.53	0.57
1:T:7:DA:H2	2:P:12:DT:O2	1.87	0.57
3:B:14:GLN:NE2	3:B:139:THR:H	1.90	0.57
3:A:49:GLU:HA	3:A:52:LYS:HE2	1.86	0.57
3:B:277:ASP:O	3:B:278:LYS:HD3	2.04	0.57
2:P:11:DT:C5	2:P:12:DT:H72	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:201:LYS:HE3	7:B:501:HOH:O	2.00	0.57
1:T:5:EFG:H4'	3:B:34:SER:HB3	1.86	0.57
3:A:341:ILE:O	3:A:342:GLU:C	2.43	0.56
3:B:148:LYS:HE3	7:B:557:HOH:O	2.05	0.56
3:B:252:LYS:HE3	7:B:503:HOH:O	2.06	0.56
1:C:7:DA:H2	2:D:12:DT:N3	1.99	0.56
1:C:6:DG:H21	3:A:332:ARG:NH1	2.02	0.56
2:P:4:DG:C2'	2:P:5:DG:O5'	2.53	0.56
3:B:14:GLN:HE22	3:B:139:THR:N	1.89	0.55
2:P:7:DA:N3	2:P:8:DG:N9	2.50	0.55
2:P:11:DT:H2''	2:P:12:DT:H6	1.72	0.55
3:B:326:ASP:OD1	3:B:328:ARG:HG3	2.07	0.55
3:B:46:ALA:HB1	3:B:50:ALA:HB3	1.89	0.55
2:D:2:DG:C4	2:D:3:DG:C8	2.95	0.54
3:B:79:GLU:H	3:B:79:GLU:CD	2.09	0.54
1:C:11:DC:H4'	7:A:519:HOH:O	2.07	0.54
2:P:6:DA:H2''	2:P:7:DA:H8	1.71	0.54
3:B:208:ILE:HG13	3:B:209:GLU:H	1.71	0.54
3:B:326:ASP:OD2	3:B:328:ARG:HG3	2.07	0.54
2:D:2:DG:C4	2:D:3:DG:N7	2.76	0.54
3:B:58:GLY:N	7:B:561:HOH:O	2.40	0.54
3:B:242:ARG:HH11	3:B:242:ARG:CG	2.12	0.54
3:B:291:GLU:HG3	3:B:292:ASP:OD1	2.08	0.53
3:B:44:ALA:O	5:B:401:DCP:H2'1	2.09	0.53
2:D:2:DG:C3'	2:D:3:DG:H3'	2.37	0.53
2:D:13:DOC:H5''	7:A:614:HOH:O	2.07	0.53
1:T:14:DC:C1'	1:T:15:DC:P	2.95	0.53
3:A:186:ILE:HD11	3:A:225:LEU:HD21	1.90	0.53
1:T:13:DT:O2	2:P:7:DA:C2	2.62	0.52
3:A:289:VAL:HB	3:A:332:ARG:HB2	1.90	0.52
1:T:11:DC:C2'	1:T:12:DT:H72	2.38	0.52
2:D:2:DG:H2''	2:D:3:DG:C3'	2.39	0.52
1:T:14:DC:C1'	1:T:15:DC:H5''	2.27	0.52
2:P:4:DG:C8	2:P:5:DG:C5	2.98	0.52
3:B:340:PHE:CD1	3:B:340:PHE:N	2.77	0.52
1:T:12:DT:C2'	1:T:13:DT:H5'	2.26	0.51
2:P:11:DT:H2''	2:P:12:DT:C6	2.46	0.51
2:P:11:DT:C2'	2:P:12:DT:C6	2.94	0.51
1:T:14:DC:C2'	1:T:15:DC:C5'	2.87	0.51
7:D:204:HOH:O	3:A:285:HIS:CE1	2.51	0.51
1:C:5:EFG:C9	3:A:32:VAL:HG21	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:6:DA:H2''	2:P:7:DA:C8	2.46	0.51
1:T:15:DC:C6	1:T:16:DC:H5'	2.46	0.50
1:T:8:DA:P	3:B:336:ARG:HH22	2.35	0.50
1:T:15:DC:P	1:T:15:DC:H3'	2.52	0.50
1:C:3:DA:N6	1:C:4:DC:N4	2.60	0.50
3:B:199:ILE:HG23	3:B:204:ASP:HB2	1.93	0.49
2:P:4:DG:H2'	2:P:5:DG:C8	2.48	0.49
1:T:13:DT:C5	1:T:14:DC:N4	2.81	0.49
3:B:292:ASP:O	3:B:293:LEU:HB2	2.12	0.49
3:A:242:ARG:NH1	7:A:597:HOH:O	2.46	0.49
1:T:11:DC:C4'	1:T:11:DC:C6	2.95	0.49
1:T:12:DT:OP1	1:T:12:DT:O4'	2.30	0.49
1:T:15:DC:C2'	1:T:16:DC:O5'	2.60	0.49
2:P:11:DT:H2'	2:P:12:DT:C7	2.43	0.49
1:C:7:DA:C2	2:D:12:DT:C2	2.95	0.49
3:B:331:ARG:HG2	3:B:332:ARG:HG3	1.95	0.49
3:A:67:ILE:CG1	7:A:609:HOH:O	2.40	0.49
2:P:10:DA:H2'	2:P:11:DT:C7	2.29	0.48
1:T:5:EFG:C10	3:B:32:VAL:HG21	2.44	0.48
3:A:273:TYR:HA	3:A:276:LEU:HD12	1.93	0.48
2:D:12:DT:H2''	2:D:13:DOC:H6	1.96	0.48
3:B:136:GLU:O	3:B:137:LYS:CB	2.62	0.48
2:P:7:DA:N6	2:P:8:DG:C6	2.81	0.48
1:T:11:DC:O2	2:P:8:DG:N2	2.34	0.48
3:A:322:ILE:HB	7:A:580:HOH:O	2.12	0.48
3:B:298:ARG:NH1	3:B:321:LYS:HG2	2.29	0.48
1:T:14:DC:C1'	1:T:15:DC:OP1	2.59	0.47
3:B:326:ASP:CG	3:B:328:ARG:HG3	2.35	0.47
2:P:3:DG:N2	2:P:4:DG:C2	2.82	0.47
3:B:136:GLU:O	3:B:137:LYS:HB2	2.15	0.47
3:B:248:ILE:HD13	3:B:249:VAL:N	2.29	0.47
1:C:6:DG:H5'	3:A:32:VAL:HG11	1.97	0.47
3:B:304:HIS:HD2	3:B:305:GLY:O	1.98	0.47
3:B:8:PHE:HZ	7:B:522:HOH:O	1.97	0.47
3:B:5:PHE:CZ	3:B:106:GLU:HG2	2.50	0.47
1:C:9:DT:H2''	1:C:10:DC:H5'	1.95	0.46
2:P:7:DA:N1	2:P:8:DG:C6	2.82	0.46
1:T:15:DC:C1'	1:T:16:DC:C5'	2.93	0.46
1:T:13:DT:H2''	1:T:14:DC:C2	2.49	0.46
1:C:12:DT:H2'	7:C:111:HOH:O	2.15	0.46
2:P:4:DG:N7	2:P:5:DG:N1	2.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:5:EFG:H1'	1:T:5:EFG:C9	2.43	0.46
3:A:233:TYR:CD1	3:A:233:TYR:C	2.89	0.46
3:B:341:ILE:C	7:B:505:HOH:O	2.54	0.45
3:B:116:ARG:HG2	3:B:120:GLU:OE1	2.16	0.45
2:P:11:DT:C2'	2:P:12:DT:H6	2.29	0.45
3:A:298:ARG:HD2	3:A:321:LYS:HD3	1.99	0.45
3:B:235:GLU:HG3	3:B:236:PRO:HD2	1.99	0.45
1:C:5:EFG:H10	3:A:32:VAL:HG21	1.99	0.44
3:B:260:GLU:HA	7:B:532:HOH:O	2.18	0.44
2:P:3:DG:H1'	2:P:4:DG:O4'	2.17	0.44
1:T:14:DC:C4	2:P:5:DG:N2	2.85	0.44
1:T:15:DC:H3'	1:T:15:DC:OP2	2.18	0.44
1:C:5:EFG:C9	1:C:5:EFG:H1'	2.42	0.44
3:A:1:MET:SD	3:A:234:ASN:ND2	2.88	0.44
3:A:55:VAL:HG21	3:A:68:LEU:HD12	2.00	0.44
1:T:15:DC:H1'	1:T:16:DC:P	2.56	0.43
1:T:15:DC:C2'	1:T:16:DC:OP2	2.46	0.43
3:B:242:ARG:NH1	3:B:242:ARG:CG	2.77	0.43
3:B:117:ASP:OD1	3:B:119:ARG:HB2	2.18	0.43
1:T:14:DC:H41	2:P:5:DG:H22	1.67	0.43
1:T:11:DC:C5'	1:T:12:DT:H72	2.49	0.43
1:T:13:DT:H6	1:T:13:DT:H2'	1.69	0.43
3:A:46:ALA:HB1	3:A:50:ALA:HB3	2.00	0.43
3:A:242:ARG:HH11	3:A:242:ARG:CG	2.32	0.42
1:T:11:DC:C6	1:T:12:DT:H72	2.54	0.42
2:P:10:DA:O3'	3:B:189:ILE:HB	2.19	0.42
2:D:6:DA:H2''	2:D:7:DA:O5'	2.20	0.42
3:A:95:TYR:HD2	3:A:124:LEU:HD11	1.84	0.42
2:P:7:DA:N6	2:P:8:DG:O6	2.53	0.42
3:B:45:THR:HG21	7:B:559:HOH:O	2.19	0.42
3:B:326:ASP:OD1	3:B:328:ARG:CG	2.67	0.42
3:A:173:ARG:NH1	3:A:177:GLU:OE1	2.52	0.42
2:D:5:DG:C2'	2:D:6:DA:C8	3.02	0.42
7:A:562:HOH:O	3:B:19:LEU:HG	2.20	0.42
1:C:8:DA:P	3:A:336:ARG:HH22	2.43	0.42
1:T:9:DT:OP1	3:B:243:LYS:N	2.38	0.42
2:D:13:DOC:H5'	7:A:614:HOH:O	2.15	0.42
3:A:241:VAL:HG13	7:A:592:HOH:O	2.20	0.42
1:C:10:DC:H1'	7:C:102:HOH:O	2.20	0.42
3:B:124:LEU:HD12	7:B:513:HOH:O	2.19	0.42
1:C:6:DG:H21	3:A:332:ARG:CZ	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:15:DC:OP2	1:C:15:DC:H2'	2.20	0.41
2:D:2:DG:H2'	2:D:3:DG:H8	1.86	0.41
2:D:6:DA:C4'	2:D:7:DA:OP1	2.56	0.41
3:A:2:ILE:HD12	3:A:2:ILE:HA	1.84	0.41
3:A:10:TYR:HA	5:A:401:DCP:PB	2.61	0.41
3:A:6:VAL:O	3:A:106:GLU:HA	2.21	0.41
3:A:206:LEU:HD21	3:A:230:ARG:HG3	2.02	0.41
2:P:12:DT:C2'	2:P:13:DOC:C5'	2.84	0.40
3:A:116:ARG:HE	3:A:116:ARG:HB2	1.66	0.40
2:D:5:DG:H2''	2:D:6:DA:C8	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	341/348 (98%)	329 (96%)	12 (4%)	0	100	100
3	B	340/348 (98%)	326 (96%)	13 (4%)	1 (0%)	46	57
All	All	681/696 (98%)	655 (96%)	25 (4%)	1 (0%)	56	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	B	341	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	
3	A	302/307 (98%)	286 (95%)	16 (5%)	28	37
3	B	301/307 (98%)	268 (89%)	33 (11%)	8	8
All	All	603/614 (98%)	554 (92%)	49 (8%)	15	18

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	0	HIS
3	A	2	ILE
3	A	19	LEU
3	A	56	LYS
3	A	62	VAL
3	A	97	GLU
3	A	105	ASP
3	A	116	ARG
3	A	192	GLU
3	A	195	LYS
3	A	242	ARG
3	A	253	ARG
3	A	267	ARG
3	A	323	LEU
3	A	336	ARG
3	A	342	GLU
3	B	19	LEU
3	B	26	LYS
3	B	36	ARG
3	B	38	GLU
3	B	45	THR
3	B	76	MET
3	B	79	GLU
3	B	91	LEU
3	B	116	ARG
3	B	119	ARG
3	B	120	GLU
3	B	131	LYS
3	B	133	LEU
3	B	164	LYS
3	B	170	GLU
3	B	176	ARG
3	B	188	ASN

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Mol	Chain	Res	Type
3	B	197	LEU
3	B	202	LEU
3	B	223	LYS
3	B	230	ARG
3	B	234	ASN
3	B	242	ARG
3	B	248	ILE
3	B	252	LYS
3	B	256	ARG
3	B	278	LYS
3	B	292	ASP
3	B	293	LEU
3	B	324	GLU
3	B	328	ARG
3	B	336	ARG
3	B	342	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	14	GLN
3	A	254	ASN
3	A	304	HIS
3	A	320	GLN
3	B	14	GLN
3	B	82	GLN
3	B	188	ASN
3	B	234	ASN
3	B	304	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

4 non-standard protein/DNA/RNA residues are 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	EFG	C	5	1	16,28,29	1.86	4 (25%)	17,42,45	1.65	5 (29%)
2	DOC	D	13	1,2	11,19,20	1.09	1 (9%)	14,26,29	1.79	4 (28%)
2	DOC	P	13	2	11,19,20	1.13	1 (9%)	14,26,29	1.96	5 (35%)
1	EFG	T	5	1	16,28,29	1.98	4 (25%)	17,42,45	1.19	1 (5%)

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	EFG	C	5	1	-	0/3/25/26	0/4/4/4
2	DOC	D	13	1,2	-	0/3/18/19	0/2/2/2
2	DOC	P	13	2	-	0/3/18/19	0/2/2/2
1	EFG	T	5	1	-	0/3/25/26	0/4/4/4

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	T	5	EFG	C6-C5	-3.01	1.35	1.41
1	C	5	EFG	C6-C5	-2.81	1.35	1.41
1	C	5	EFG	C5-C4	-2.55	1.34	1.40
1	T	5	EFG	C5-C4	-2.52	1.34	1.40
2	P	13	DOC	C6-N1	-2.44	1.32	1.35
2	D	13	DOC	C6-N1	-2.20	1.32	1.35
1	C	5	EFG	C6-N1	3.19	1.39	1.33
1	T	5	EFG	C6-N1	4.04	1.40	1.33
1	T	5	EFG	O4'-C1'	4.60	1.47	1.41
1	C	5	EFG	O4'-C1'	4.64	1.47	1.41

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	5	EFG	C5-C6-N1	-2.72	119.87	123.59
1	C	5	EFG	F-C2'-C3'	-2.69	102.56	109.07
2	P	13	DOC	O4'-C1'-C2'	-2.46	104.00	106.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	5	EFG	C5-C6-N1	-2.33	120.40	123.59
1	C	5	EFG	C4-C5-N7	-2.29	107.38	109.48
2	P	13	DOC	C5-C4-N3	-2.14	119.10	121.80
2	D	13	DOC	O4'-C1'-N1	2.03	111.24	107.72
2	P	13	DOC	N4-C4-N3	2.20	120.51	116.50
1	C	5	EFG	F-C2'-C1'	2.21	114.89	109.54
1	C	5	EFG	C2'-C1'-N9	2.26	117.80	113.76
2	D	13	DOC	C2-N3-C4	2.41	119.02	115.61
2	D	13	DOC	O4'-C4'-C5'	2.76	113.62	109.54
2	P	13	DOC	C3'-C2'-C1'	3.11	106.18	102.71
2	P	13	DOC	C2-N3-C4	4.02	121.28	115.61
2	D	13	DOC	C2'-C1'-N1	4.19	120.97	112.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	5	EFG	5	0
2	D	13	DOC	4	0
2	P	13	DOC	19	0
1	T	5	EFG	5	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 7 are monoatomic - leaving 2 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	DCP	A	401	6	21,29,29	0.58	0	33,45,45	1.46	4 (12%)
5	DCP	B	401	6	21,29,29	0.67	0	33,45,45	1.74	6 (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
5	DCP	A	401	6	-	0/18/34/34	0/2/2/2
5	DCP	B	401	6	-	0/18/34/34	0/2/2/2

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	401	DCP	PB-O3B-PG	-3.91	119.57	132.67
5	A	401	DCP	PB-O3A-PA	-3.08	124.07	132.73
5	A	401	DCP	PB-O3B-PG	-2.95	122.78	132.67
5	B	401	DCP	O3G-PG-O2G	2.23	115.86	107.38
5	B	401	DCP	O5'-C5'-C4'	2.73	119.17	109.12
5	B	401	DCP	O4'-C4'-C5'	2.77	119.22	109.32
5	A	401	DCP	C2-N3-C4	2.92	119.73	115.61
5	B	401	DCP	C2-N3-C4	3.58	120.66	115.61
5	A	401	DCP	O4'-C1'-N1	3.87	114.42	107.72
5	B	401	DCP	O4'-C1'-N1	4.31	115.19	107.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	401	DCP	2	0
5	B	401	DCP	4	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, 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	C	16/18 (88%)	0.52	3 (18%)	2 2	47, 66, 135, 137	2 (12%)
1	T	12/18 (66%)	1.89	5 (41%)	0 0	61, 99, 137, 139	4 (33%)
2	D	11/13 (84%)	0.74	2 (18%)	2 3	61, 70, 126, 133	2 (18%)
2	P	10/13 (76%)	3.08	5 (50%)	0 0	50, 99, 123, 127	4 (40%)
3	A	343/348 (98%)	0.37	9 (2%)	59 68	28, 53, 82, 103	3 (0%)
3	B	342/348 (98%)	0.84	48 (14%)	4 6	43, 79, 114, 137	8 (2%)
All	All	734/758 (96%)	0.66	72 (9%)	10 14	28, 64, 112, 139	23 (3%)

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	B	213	LEU	8.0
3	B	116	ARG	7.9
2	P	4	DG	7.7
1	T	13	DT	6.6
1	T	16	DC	6.0
3	B	207	SER	5.8
2	P	6	DA	5.6
2	P	8	DG	5.3
2	P	3	DG	5.2
2	P	5	DG	4.0
2	D	2	DG	4.0
3	B	119	ARG	3.9
3	A	0	HIS	3.9
3	B	209	GLU	3.9
3	B	212	LYS	3.9
3	B	295	ILE	3.8
3	B	115	VAL	3.7
3	B	327	GLU	3.6
3	B	296	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
3	B	188	ASN	3.6
3	B	189	ILE	3.5
3	B	278	LYS	3.4
1	T	12	DT	3.2
3	B	292	ASP	3.2
1	C	17	DC	3.1
3	B	195	LYS	3.1
3	B	258	LEU	3.0
1	T	14	DC	3.0
3	B	241	VAL	3.0
3	B	187	GLY	2.9
3	B	321	LYS	2.8
1	C	16	DC	2.8
3	B	210	PHE	2.8
3	A	274	TYR	2.8
3	B	113	ASP	2.8
2	D	3	DG	2.8
1	T	15	DC	2.6
3	B	196	LYS	2.6
3	B	192	GLU	2.6
3	B	37	PHE	2.5
3	B	121	ALA	2.5
3	A	318	LEU	2.5
3	B	215	GLY	2.4
3	A	286	VAL	2.4
3	B	206	LEU	2.4
3	B	267	ARG	2.4
3	A	253	ARG	2.4
3	B	216	MET	2.4
3	B	335	VAL	2.4
3	B	205	THR	2.4
3	A	210	PHE	2.3
3	B	117	ASP	2.3
3	B	35	GLY	2.3
3	B	228	LEU	2.3
3	B	211	ASP	2.3
3	B	208	ILE	2.3
3	A	4	LEU	2.3
3	B	284	ILE	2.2
3	B	230	ARG	2.2
3	B	234	ASN	2.2
3	B	342	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
3	A	284	ILE	2.1
3	B	325	GLU	2.1
3	B	163	ILE	2.1
3	B	86	SER	2.1
3	A	312	TYR	2.1
1	C	15	DC	2.1
3	B	324	GLU	2.1
3	B	238	ARG	2.1
3	B	286	VAL	2.0
3	B	334	GLY	2.0
3	B	329	LYS	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	EFG	T	5	25/26	0.88	0.14	-0.25	72,79,100,107	0
1	EFG	C	5	25/26	0.96	0.12	-0.84	44,50,56,59	0
2	DOC	P	13	18/19	0.76	0.26	-	85,87,89,91	1
2	DOC	D	13	18/19	0.70	0.26	-	51,57,77,78	3

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(\AA^2)	Q<0.9
6	MG	B	402	1/1	0.98	0.23	2.47	40,40,40,40	0
6	MG	B	404	1/1	0.53	0.21	1.16	52,52,52,52	0
4	CA	A	404	1/1	0.83	0.15	0.91	117,117,117,117	0
6	MG	A	402	1/1	0.97	0.17	-0.09	19,19,19,19	0
5	DCP	B	401	28/28	0.93	0.14	-0.18	59,67,74,79	0
5	DCP	A	401	28/28	0.97	0.12	-1.07	31,46,52,53	0
6	MG	A	403	1/1	0.90	0.28	-	29,29,29,29	0
4	CA	D	101	1/1	0.92	0.22	-	73,73,73,73	0
4	CA	B	403	1/1	0.84	0.27	-	77,77,77,77	0

6.5 Other polymers [i](#)

There are no such residues in this entry.