



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 08:56 PM GMT

PDB ID : 3V6J
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 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/ValidationPDFNotes.html>

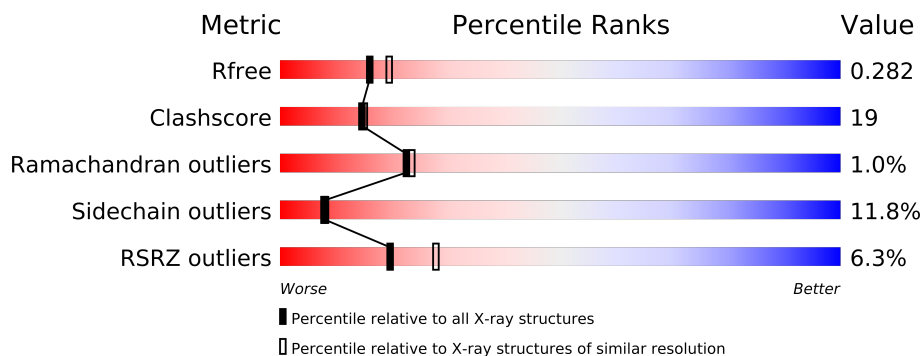
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	348	
1	J	348	
2	K	12	
2	P	12	
3	B	17	
3	M	17	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
5	MG	J	402	-	X
5	MG	J	403	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6824 atoms, of which 0 are hydrogen and 0 are deuterium.

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 IV.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	343	Total	C	N	O	S	2	0	0
			2762	1771	476	508	7			
1	J	343	Total	C	N	O	S	1	0	0
			2754	1765	474	508	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
J	-5	HIS	-	EXPRESSION TAG	UNP Q97W02
J	-4	HIS	-	EXPRESSION TAG	UNP Q97W02
J	-3	HIS	-	EXPRESSION TAG	UNP Q97W02
J	-2	HIS	-	EXPRESSION TAG	UNP Q97W02
J	-1	HIS	-	EXPRESSION TAG	UNP Q97W02
J	0	HIS	-	EXPRESSION TAG	UNP Q97W02

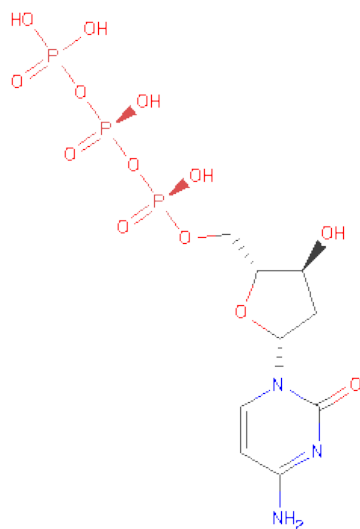
- Molecule 2 is a DNA chain called DNA (5'-D(*GP*GP*GP*GP*AP*AP*GP*GP*AP*TP*TP*(DOC))-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	12	Total	C	N	O	P	0	0	0
			250	119	52	68	11			
2	K	11	Total	C	N	O	P	0	0	0
			231	109	47	64	11			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	B	17	Total	C	F	N	O	P	0	0	0
			340	165	1	56	102	16			
3	M	13	Total	C	F	N	O	P	0	0	0
			264	127	1	43	80	13			

- Molecule 4 is 2'-DEOXYCYTIDINE-5'-TRIPHOSPHATE (three-letter code: DCP) (formula: C₉H₁₆N₃O₁₃P₃).



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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	J	2	Total	Mg	0	0
			2	2		
5	A	2	Total	Mg	0	0
			2	2		
5	K	1	Total	Mg	0	0
			1	1		

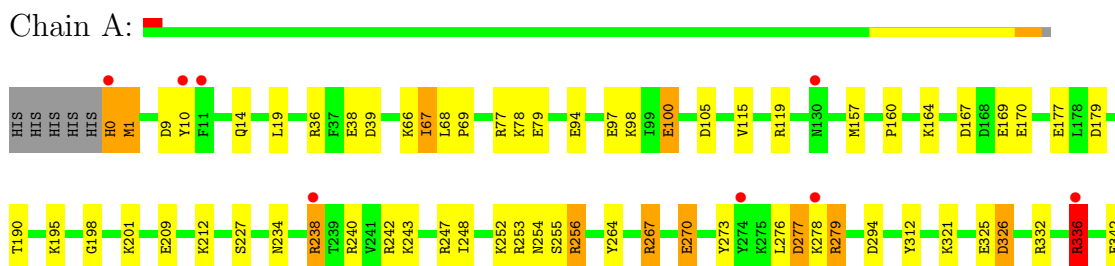
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	99	Total 99	O 99	0	0
6	J	43	Total 43	O 43	0	0
6	P	7	Total 7	O 7	0	0
6	B	8	Total 8	O 8	0	0
6	K	3	Total 3	O 3	0	0
6	M	2	Total 2	O 2	0	0

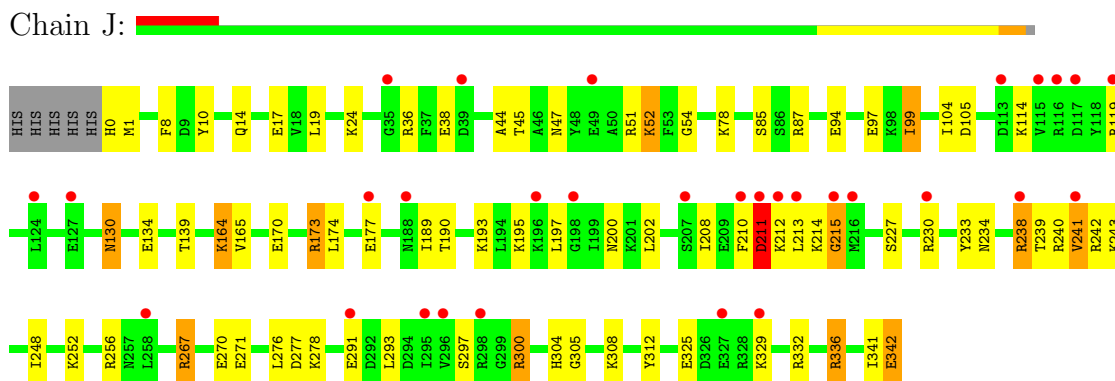
3 Residue-property plots

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: DNA polymerase IV



- Molecule 1: DNA polymerase IV



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



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



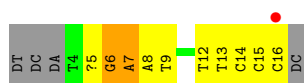
- Molecule 3: DNA (5'-D(*TP*CP*AP*TP*(EFG)P*GP*AP*AP*TP*CP*CP*TP*TP*CP*CP*CP*C)-3')

Chain B:



- Molecule 3: DNA (5'-D(*TP*CP*AP*TP*(EFG)P*GP*AP*AP*TP*CP*CP*TP*TP*CP*CP*CP*C)-3')

Chain M:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	52.70Å 111.42Å 98.81Å 90.00° 102.57° 90.00°	Depositor
Resolution (Å)	29.84 – 2.30 29.84 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.7 (29.84-2.30) 97.8 (29.84-2.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.45 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.210 , 0.273 0.221 , 0.282	Depositor DCC
R_{free} test set	2456 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	47.5	Xtriage
Anisotropy	0.072	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 43.4	EDS
Estimated twinning fraction	0.026 for h,-k,-h-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 48557 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6824	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.86% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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, 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	A	0.93	0/2802	1.08	9/3763 (0.2%)
1	J	0.73	0/2794	0.86	1/3755 (0.0%)
2	K	0.49	0/240	1.16	3/370 (0.8%)
2	P	1.00	2/262 (0.8%)	1.45	9/405 (2.2%)
3	B	0.79	1/349 (0.3%)	1.54	11/532 (2.1%)
3	M	0.92	2/264 (0.8%)	1.29	4/401 (1.0%)
All	All	0.83	5/6711 (0.1%)	1.07	37/9226 (0.4%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	4	DG	O3'-P	-10.61	1.48	1.61
3	M	7	DA	O3'-P	-10.01	1.49	1.61
3	M	6	DG	O3'-P	8.39	1.71	1.61
2	P	3	DG	O3'-P	5.85	1.68	1.61
3	B	3	DA	O3'-P	-5.06	1.55	1.61

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	6	DG	P-O3'-C3'	13.44	135.83	119.70
2	P	3	DG	P-O3'-C3'	11.50	133.50	119.70
3	B	1	DT	P-O3'-C3'	10.28	132.04	119.70
2	P	12	DT	O5'-P-OP1	-9.60	97.06	105.70
2	P	2	DG	P-O3'-C3'	8.59	130.00	119.70
1	A	336	ARG	NE-CZ-NH2	-8.30	116.15	120.30
2	K	11	DT	P-O3'-C3'	8.03	129.33	119.70
2	P	11	DT	P-O3'-C3'	7.79	129.06	119.70
3	M	14	DC	P-O3'-C3'	7.45	128.64	119.70
2	K	12	DT	O5'-P-OP1	-7.30	99.13	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	10	DA	P-O3'-C3'	6.94	128.03	119.70
3	B	10	DC	P-O3'-C3'	-6.93	111.38	119.70
3	B	2	DC	O3'-P-O5'	6.71	116.75	104.00
3	B	7	DA	O5'-P-OP2	-6.65	99.72	105.70
2	K	11	DT	O5'-P-OP1	-6.58	99.78	105.70
2	P	5	DG	P-O3'-C3'	6.50	127.50	119.70
1	J	240	ARG	N-CA-C	6.48	128.50	111.00
1	A	167	ASP	CB-CG-OD1	6.43	124.09	118.30
3	B	6	DG	C1'-O4'-C4'	-6.24	103.86	110.10
3	M	15	DC	P-O3'-C3'	6.10	127.02	119.70
3	B	3	DA	P-O3'-C3'	6.07	126.98	119.70
3	B	11	DC	O5'-P-OP2	-6.03	100.27	105.70
2	P	7	DA	P-O3'-C3'	6.02	126.93	119.70
2	P	8	DG	P-O3'-C3'	6.00	126.90	119.70
3	B	8	DA	O3'-P-O5'	-5.88	92.83	104.00
3	M	12	DT	P-O3'-C3'	5.83	126.69	119.70
1	A	336	ARG	CG-CD-NE	-5.62	99.99	111.80
2	P	2	DG	O3'-P-O5'	5.48	114.41	104.00
3	B	14	DC	P-O3'-C3'	5.42	126.21	119.70
1	A	336	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	A	67	ILE	CB-CA-C	-5.36	100.88	111.60
3	B	11	DC	O3'-P-O5'	-5.36	93.83	104.00
1	A	179	ASP	CB-CG-OD1	5.31	123.08	118.30
1	A	77	ARG	NE-CZ-NH2	5.26	122.93	120.30
1	A	100	GLU	OE1-CD-OE2	-5.17	117.10	123.30
1	A	270	GLU	CB-CA-C	-5.12	100.17	110.40
3	B	6	DG	P-O3'-C3'	5.10	125.82	119.70

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2762	0	9	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J	2754	0	9	42	0
2	K	231	0	0	17	0
2	P	250	0	0	10	0
3	B	340	0	0	16	0
3	M	264	0	0	13	0
4	A	28	0	12	0	0
4	J	28	0	12	3	0
5	A	2	0	0	0	0
5	J	2	0	0	0	0
5	K	1	0	0	0	0
6	A	99	0	0	8	0
6	B	8	0	0	2	0
6	J	43	0	0	6	0
6	K	3	0	0	1	0
6	M	2	0	0	0	0
6	P	7	0	0	0	0
All	All	6824	0	42	113	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 19.

All (113) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:P:12:DT:N3	3:B:7:DA:C2	2.28	1.01
3:B:10:DC:OP1	3:B:10:DC:C4'	2.10	0.99
1:J:211:ASP:C	1:J:211:ASP:OD1	2.00	0.97
2:K:4:DG:C1'	2:K:5:DG:C5'	2.46	0.94
1:J:341:ILE:CG2	1:J:342:GLU:N	2.27	0.94
1:J:164:LYS:CD	1:J:165:VAL:O	2.20	0.90
1:A:248:ILE:CD1	6:A:512:HOH:O	2.21	0.87
2:K:4:DG:C2'	2:K:5:DG:O5'	2.23	0.86
4:J:401:DCP:H5'2	6:J:503:HOH:O	1.75	0.86
3:B:10:DC:C6	3:B:10:DC:C5'	2.59	0.85
1:J:211:ASP:O	1:J:211:ASP:OD1	1.97	0.82
3:M:16:DC:O2	3:M:16:DC:C2'	2.29	0.81
1:J:164:LYS:CE	1:J:165:VAL:O	2.29	0.81
1:A:264:TYR:O	1:A:267:ARG:CG	2.30	0.80
2:K:12:DT:N3	3:M:7:DA:C2	2.50	0.80
2:K:12:DT:C2'	2:K:13:DOC:C6	2.61	0.79
2:K:9:DG:C2'	6:K:202:HOH:O	2.31	0.79
1:A:0:HIS:O	1:A:1:MET:CB	2.32	0.78
1:A:195:LYS:CE	6:A:585:HOH:O	2.33	0.77

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:173:ARG:CG	1:J:173:ARG:NH1	2.46	0.77
1:A:66:LYS:CA	6:A:573:HOH:O	2.33	0.75
2:K:12:DT:C2'	2:K:13:DOC:C5	2.64	0.75
1:J:243:LYS:N	3:M:9:DT:OP1	2.21	0.74
1:J:342:GLU:CG	1:J:342:GLU:O	2.36	0.72
1:J:277:ASP:O	1:J:278:LYS:CB	2.34	0.72
3:B:1:DT:C6	3:B:1:DT:C5'	2.74	0.71
2:K:11:DT:N3	3:M:8:DA:C2	2.58	0.70
1:J:238:ARG:CG	1:J:238:ARG:O	2.40	0.70
1:J:267:ARG:NH1	1:J:271:GLU:OE2	2.24	0.70
1:J:336:ARG:NH2	3:M:8:DA:OP2	2.26	0.69
2:P:3:DG:C2'	2:P:4:DG:C8	2.76	0.69
2:K:12:DT:O2	3:M:7:DA:C2	2.47	0.67
2:K:12:DT:C2	3:M:7:DA:C2	2.83	0.67
3:B:10:DC:C3'	6:B:101:HOH:O	2.43	0.67
1:A:270:GLU:CD	1:A:312:TYR:OH	2.32	0.67
1:J:332:ARG:NH2	3:M:6:DG:OP2	2.28	0.66
1:J:300:ARG:CG	6:J:530:HOH:O	2.42	0.66
2:P:2:DG:N2	2:P:3:DG:C6	2.67	0.63
1:A:248:ILE:CD1	6:A:565:HOH:O	2.46	0.62
2:K:13:DOC:O2	3:M:6:DG:N7	2.33	0.62
1:A:195:LYS:O	1:A:198:GLY:N	2.35	0.60
1:A:234:ASN:N	6:A:539:HOH:O	2.35	0.60
2:P:11:DT:N3	3:B:8:DA:C2	2.70	0.59
1:A:10:TYR:CZ	1:A:14:GLN:CG	2.86	0.58
1:J:130:ASN:O	1:J:130:ASN:ND2	2.36	0.58
1:A:10:TYR:CE2	1:A:14:GLN:CB	2.87	0.57
1:A:67:ILE:O	1:A:67:ILE:CG2	2.52	0.57
1:A:0:HIS:N	1:A:0:HIS:CD2	2.72	0.57
1:J:341:ILE:O	1:J:342:GLU:C	2.43	0.57
1:A:332:ARG:NH1	3:B:6:DG:N2	2.53	0.56
2:K:11:DT:O4	3:M:8:DA:N1	2.38	0.56
1:J:241:VAL:CG1	1:J:242:ARG:N	2.69	0.55
1:J:210:PHE:O	1:J:213:LEU:N	2.40	0.55
1:A:169:GLU:N	1:A:169:GLU:OE2	2.40	0.55
2:K:4:DG:C1'	2:K:5:DG:O5'	2.53	0.54
2:P:2:DG:C2'	2:P:3:DG:O4'	2.55	0.54
1:J:51:ARG:O	1:J:54:GLY:N	2.41	0.54
2:K:7:DA:N1	3:M:13:DT:O2	2.41	0.53
2:P:2:DG:C2'	2:P:3:DG:C4'	2.87	0.53
2:P:11:DT:O4	3:B:8:DA:N1	2.43	0.52
1:J:211:ASP:OD1	1:J:212:LYS:CD	2.58	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:210:PHE:CD1	1:J:211:ASP:N	2.79	0.51
1:J:210:PHE:CD1	1:J:210:PHE:C	2.84	0.50
1:A:276:LEU:O	1:A:279:ARG:CD	2.59	0.50
1:J:190:THR:OG1	2:K:11:DT:OP1	2.29	0.49
1:A:336:ARG:NH2	3:B:8:DA:OP2	2.45	0.49
2:K:11:DT:C6	2:K:12:DT:C7	2.96	0.49
1:A:238:ARG:CG	6:A:566:HOH:O	2.60	0.49
1:A:9:ASP:O	1:A:10:TYR:C	2.51	0.49
3:B:9:DT:C5'	3:B:9:DT:C6	2.96	0.49
1:A:157:MET:CE	1:A:164:LYS:CE	2.92	0.48
1:J:17:GLU:OE2	1:J:47:ASN:ND2	2.46	0.48
1:J:270:GLU:OE2	1:J:312:TYR:OH	2.31	0.48
4:J:401:DCP:H1'	2:K:13:DOC:C2'	2.43	0.48
1:J:24:LYS:CA	6:J:521:HOH:O	2.60	0.48
1:J:170:GLU:O	1:J:174:LEU:N	2.47	0.48
1:J:304:HIS:CD2	1:J:305:GLY:O	2.67	0.47
2:P:12:DT:C2	3:B:7:DA:C2	3.00	0.47
1:A:247:ARG:NH1	6:A:547:HOH:O	2.48	0.47
1:J:336:ARG:NH2	3:M:8:DA:P	2.88	0.47
2:K:9:DG:C2'	2:K:10:DA:C8	2.98	0.47
1:J:213:LEU:O	1:J:215:GLY:N	2.48	0.46
1:A:277:ASP:O	1:A:278:LYS:CB	2.63	0.46
1:A:38:GLU:O	1:A:39:ASP:CB	2.63	0.46
1:A:10:TYR:O	1:A:10:TYR:CD2	2.69	0.46
3:B:1:DT:C6	3:B:1:DT:C4'	2.98	0.46
1:A:270:GLU:OE1	1:A:312:TYR:OH	2.33	0.46
1:A:68:LEU:O	1:A:69:PRO:C	2.52	0.46
1:J:52:LYS:CD	6:J:537:HOH:O	2.62	0.46
1:J:227:SER:O	1:J:233:TYR:N	2.49	0.46
1:A:243:LYS:N	3:B:9:DT:OP1	2.48	0.45
3:M:5:EFG:C9	3:M:5:EFG:C1'	2.94	0.45
1:A:256:ARG:NH2	1:A:326:ASP:O	2.50	0.45
1:J:14:GLN:NE2	1:J:139:THR:N	2.66	0.44
1:A:100:GLU:OE2	1:A:240:ARG:NE	2.51	0.44
1:J:238:ARG:NH2	6:J:514:HOH:O	2.50	0.44
1:A:209:GLU:O	1:A:212:LYS:N	2.51	0.44
1:J:173:ARG:NH1	1:J:177:GLU:OE2	2.51	0.43
1:J:238:ARG:CD	1:J:239:THR:O	2.66	0.43
3:B:8:DA:N6	6:B:108:HOH:O	2.52	0.43
1:A:177:GLU:O	1:A:201:LYS:NZ	2.52	0.43
1:A:190:THR:OG1	2:P:11:DT:OP1	2.36	0.43
1:J:189:ILE:O	1:J:193:LYS:CG	2.67	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:B:1:DT:O5'	3:B:1:DT:C6	2.71	0.43
1:J:213:LEU:O	1:J:214:LYS:C	2.56	0.43
1:J:87:ARG:NH1	6:J:538:HOH:O	2.52	0.42
1:J:164:LYS:CD	1:J:164:LYS:C	2.86	0.42
1:A:10:TYR:O	1:A:10:TYR:CG	2.72	0.42
1:A:10:TYR:OH	1:A:14:GLN:CG	2.68	0.42
1:J:44:ALA:O	4:J:401:DCP:H2'1	2.20	0.41
1:J:85:SER:OG	1:J:104:ILE:O	2.37	0.41
2:P:11:DT:C4	3:B:8:DA:N1	2.88	0.41
1:A:254:ASN:ND2	6:A:599:HOH:O	2.55	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	
1	A	341/348 (98%)	323 (95%)	16 (5%)	2 (1%)	33	39
1	J	341/348 (98%)	300 (88%)	36 (11%)	5 (2%)	15	13
All	All	682/696 (98%)	623 (91%)	52 (8%)	7 (1%)	22	23

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	J	241	VAL
1	A	277	ASP
1	J	211	ASP
1	J	215	GLY
1	J	10	TYR
1	J	99	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	302/307 (98%)	273 (90%)	29 (10%)	12	13
1	J	300/307 (98%)	258 (86%)	42 (14%)	5	5
All	All	602/614 (98%)	531 (88%)	71 (12%)	8	8

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	0	HIS
1	A	19	LEU
1	A	36	ARG
1	A	78	LYS
1	A	79	GLU
1	A	94	GLU
1	A	97	GLU
1	A	98	LYS
1	A	105	ASP
1	A	115	VAL
1	A	119	ARG
1	A	160	PRO
1	A	170	GLU
1	A	227	SER
1	A	238	ARG
1	A	242	ARG
1	A	252	LYS
1	A	253	ARG
1	A	255	SER
1	A	256	ARG
1	A	267	ARG
1	A	273	TYR
1	A	279	ARG
1	A	294	ASP
1	A	321	LYS
1	A	325	GLU
1	A	326	ASP
1	A	336	ARG
1	A	342	GLU

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Mol	Chain	Res	Type
1	J	0	HIS
1	J	1	MET
1	J	8	PHE
1	J	19	LEU
1	J	36	ARG
1	J	38	GLU
1	J	45	THR
1	J	52	LYS
1	J	78	LYS
1	J	94	GLU
1	J	97	GLU
1	J	99	ILE
1	J	105	ASP
1	J	114	LYS
1	J	119	ARG
1	J	130	ASN
1	J	134	GLU
1	J	164	LYS
1	J	173	ARG
1	J	195	LYS
1	J	197	LEU
1	J	200	ASN
1	J	202	LEU
1	J	208	ILE
1	J	211	ASP
1	J	230	ARG
1	J	234	ASN
1	J	238	ARG
1	J	248	ILE
1	J	252	LYS
1	J	256	ARG
1	J	267	ARG
1	J	276	LEU
1	J	291	GLU
1	J	293	LEU
1	J	297	SER
1	J	300	ARG
1	J	308	LYS
1	J	325	GLU
1	J	329	LYS
1	J	336	ARG
1	J	342	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	0	HIS
1	J	0	HIS

5.3.3 RNA ⓘ

There are no RNA chains 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	$\# Z > 2$
3	EFG	B	5	3	26,28,29	3.99	17 (65%)	32,42,45	3.85	14 (43%)
2	DOC	K	13	2	17,19,20	1.10	3 (17%)	20,26,29	4.05	10 (50%)
3	EFG	M	5	3	26,28,29	2.67	11 (42%)	32,42,45	3.67	10 (31%)
2	DOC	P	13	3,2	17,19,20	1.34	2 (11%)	20,26,29	2.13	4 (20%)

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
3	EFG	B	5	3	-	0/8/25/26	0/1/4/4
2	DOC	K	13	2	-	0/5/18/19	0/2/2/2
3	EFG	M	5	3	-	0/8/25/26	0/1/4/4
2	DOC	P	13	3,2	-	0/5/18/19	0/2/2/2

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	5	EFG	C4-N3	-9.29	1.29	1.39
3	B	5	EFG	C2-N3	-7.31	1.30	1.39
3	M	5	EFG	C4-N3	-6.42	1.32	1.39
3	B	5	EFG	C9-N3	-6.07	1.28	1.37
3	B	5	EFG	P-OP1	-5.90	1.40	1.46
3	M	5	EFG	O4'-C1'	5.39	1.49	1.41
3	B	5	EFG	C2-N2	-5.32	1.29	1.36
3	B	5	EFG	C6-C5	-5.28	1.32	1.41
3	B	5	EFG	C8-N9	-4.77	1.29	1.36
3	B	5	EFG	C5-C4	-4.63	1.30	1.40
3	B	5	EFG	C2'-C1'	-4.23	1.46	1.53
3	M	5	EFG	C2-N3	-4.22	1.33	1.39
2	P	13	DOC	P-OP1	4.14	1.51	1.46
3	M	5	EFG	P-OP1	3.99	1.51	1.46
3	B	5	EFG	C4-N9	-3.86	1.31	1.38
3	M	5	EFG	C2'-C1'	3.84	1.58	1.53
3	B	5	EFG	C2'-C3'	-3.70	1.46	1.52
3	M	5	EFG	C1'-N9	3.60	1.59	1.48
3	M	5	EFG	C9-N3	-3.51	1.32	1.37
3	B	5	EFG	O4'-C1'	-3.51	1.35	1.41
3	M	5	EFG	C2-N2	-3.00	1.32	1.36
2	P	13	DOC	C2-N1	2.96	1.41	1.38
3	B	5	EFG	C5-N7	-2.86	1.29	1.40
2	K	13	DOC	C2-N1	2.85	1.41	1.38
3	B	5	EFG	C6-N1	-2.64	1.32	1.37
3	B	5	EFG	C2-N1	-2.52	1.32	1.37
3	M	5	EFG	C6-C5	-2.30	1.37	1.41
3	B	5	EFG	C8-N7	-2.22	1.30	1.34
3	M	5	EFG	O3'-C3'	2.15	1.48	1.43
3	B	5	EFG	O3'-C3'	-2.14	1.37	1.43
3	M	5	EFG	C4-N9	-2.07	1.34	1.38
2	K	13	DOC	C6-N1	-2.05	1.32	1.35
2	K	13	DOC	C5'-C4'	2.01	1.56	1.50

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	13	DOC	C4'-O4'-C1'	14.33	116.02	110.05
3	B	5	EFG	O4'-C1'-N9	-12.27	97.03	108.44
3	M	5	EFG	O4'-C1'-N9	11.63	119.26	108.44
3	B	5	EFG	C6-C5-N7	-10.57	132.72	134.14
3	M	5	EFG	C10-N2-C2	9.30	107.09	104.92
3	M	5	EFG	C6-C5-N7	-9.16	132.91	134.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	5	EFG	C10-N2-C2	7.37	106.64	104.92
3	B	5	EFG	C6-N1-C2	-6.17	115.92	120.28
3	M	5	EFG	C4'-O4'-C1'	-5.83	103.42	109.75
2	P	13	DOC	C6-C5-C4	5.50	119.75	117.47
2	K	13	DOC	C6-C5-C4	4.90	119.51	117.47
2	K	13	DOC	C3'-C2'-C1'	4.64	107.95	102.80
2	K	13	DOC	C2-N1-C1'	4.48	124.47	119.25
2	K	13	DOC	C2-N3-C4	4.34	121.85	115.57
3	B	5	EFG	C3'-C2'-C1'	4.25	108.75	103.30
2	P	13	DOC	C4'-O4'-C1'	4.13	111.77	110.05
3	B	5	EFG	C5-C4-N3	-3.82	115.52	124.96
3	B	5	EFG	F-C2'-C3'	-3.76	99.22	109.39
3	M	5	EFG	C8-N9-C1'	3.64	133.56	126.38
3	M	5	EFG	N2-C2-N3	-3.42	109.32	111.58
3	B	5	EFG	C4-C5-N7	-3.38	106.63	109.52
3	M	5	EFG	C1'-N9-C4	-3.34	120.96	126.46
2	P	13	DOC	C2-N3-C4	3.27	120.30	115.57
3	B	5	EFG	C1'-N9-C4	3.23	131.78	126.46
3	M	5	EFG	C6-N1-C2	-3.23	117.99	120.28
3	B	5	EFG	N2-C2-N3	-3.13	109.51	111.58
2	P	13	DOC	C3'-C2'-C1'	3.06	106.19	102.80
2	K	13	DOC	O4'-C1'-C2'	-2.79	103.04	106.37
3	M	5	EFG	C4-C5-N7	-2.70	107.21	109.52
2	K	13	DOC	O4'-C4'-C5'	2.61	113.31	109.67
3	B	5	EFG	C5-C6-N1	2.54	122.82	115.39
2	K	13	DOC	C2'-C1'-N1	2.48	117.62	112.66
3	B	5	EFG	C9-N3-C4	-2.33	126.06	130.10
3	M	5	EFG	C5-C4-N3	-2.29	119.31	124.96
2	K	13	DOC	C5-C4-N3	-2.28	118.60	121.68
3	B	5	EFG	C8-N9-C1'	-2.12	122.20	126.38
3	B	5	EFG	C4'-O4'-C1'	2.07	112.00	109.75
2	K	13	DOC	N4-C4-N3	2.07	120.55	116.59

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 7 ligands modelled in this entry, 5 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$
4	DCP	A	401	5	29,29,29	1.73	3 (10%)	42,45,45	1.87	8 (19%)
4	DCP	J	401	5	29,29,29	1.33	3 (10%)	42,45,45	1.78	7 (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
4	DCP	A	401	5	-	0/19/34/34	0/2/2/2
4	DCP	J	401	5	-	0/19/34/34	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	401	DCP	C2-N1	6.97	1.45	1.38
4	J	401	DCP	C2-N1	4.96	1.43	1.38
4	J	401	DCP	PA-O3A	2.76	1.64	1.59
4	J	401	DCP	PB-O3A	2.31	1.64	1.59
4	A	401	DCP	PA-O3A	-2.22	1.55	1.59
4	A	401	DCP	PG-O3B	2.08	1.63	1.60

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	401	DCP	C6-C5-C4	8.60	121.04	117.47
4	J	401	DCP	C6-C5-C4	6.47	120.16	117.47
4	J	401	DCP	PB-O3B-PG	-5.29	116.18	131.68
4	A	401	DCP	O2B-PB-O3A	2.91	118.95	105.14
4	J	401	DCP	C2-N1-C1'	2.76	122.46	119.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	401	DCP	O3G-PG-O2G	2.54	117.51	107.61
4	A	401	DCP	O3'-C3'-C4'	2.53	120.53	110.14
4	J	401	DCP	C2'-C3'-C4'	2.37	108.03	102.73
4	A	401	DCP	O3B-PB-O3A	-2.36	96.85	101.66
4	J	401	DCP	O2G-PG-O3B	-2.35	93.97	105.14
4	A	401	DCP	O4'-C1'-N1	2.35	112.10	107.68
4	A	401	DCP	C5-C6-N1	-2.20	118.72	121.21
4	A	401	DCP	O2G-PG-O1G	2.15	117.48	110.44
4	J	401	DCP	C2-N3-C4	2.05	118.54	115.57
4	A	401	DCP	C2-N3-C4	2.04	118.52	115.57

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	A	343/348 (98%)	0.10	8 (2%) 57 67	23, 43, 70, 88	23 (6%)
1	J	343/348 (98%)	0.56	31 (9%) 10 16	33, 69, 102, 118	14 (4%)
2	K	11/12 (91%)	1.45	3 (27%) 1 1	63, 99, 152, 154	3 (27%)
2	P	12/12 (100%)	0.62	2 (16%) 2 4	49, 56, 119, 139	1 (8%)
3	B	17/17 (100%)	0.27	2 (11%) 5 8	37, 56, 105, 120	2 (11%)
3	M	13/17 (76%)	0.97	1 (7%) 13 20	51, 92, 171, 172	1 (7%)
All	All	739/754 (98%)	0.36	47 (6%) 19 27	23, 55, 102, 172	44 (5%)

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	P	2	DG	6.5
2	K	3	DG	6.4
2	K	4	DG	6.3
1	J	241	VAL	6.1
1	J	212	LYS	6.0
1	J	216	MET	5.1
1	A	336	ARG	5.1
1	J	213	LEU	4.8
1	J	207	SER	4.8
1	J	49	GLU	4.6
1	J	116	ARG	4.5
1	J	211	ASP	3.7
3	M	16	DC	3.7
1	J	115	VAL	3.6
1	J	119	ARG	3.4
1	A	10	TYR	3.3
1	A	130	ASN	3.0
1	A	0	HIS	2.9
1	J	295	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	J	329	LYS	2.7
1	J	117	ASP	2.7
2	K	5	DG	2.7
1	A	274	TYR	2.7
1	A	11	PHE	2.7
1	A	278	LYS	2.6
1	J	124	LEU	2.5
1	A	238	ARG	2.5
1	J	230	ARG	2.5
1	J	188	ASN	2.4
1	J	198	GLY	2.4
3	B	17	DC	2.3
1	J	39	ASP	2.3
2	P	3	DG	2.3
1	J	215	GLY	2.2
1	J	327	GLU	2.2
1	J	296	VAL	2.1
1	J	35	GLY	2.1
1	J	127	GLU	2.1
1	J	113	ASP	2.1
1	J	298	ARG	2.1
1	J	177	GLU	2.1
1	J	210	PHE	2.1
1	J	238	ARG	2.0
1	J	258	LEU	2.0
1	J	291	GLU	2.0
1	J	196	LYS	2.0
3	B	15	DC	2.0

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

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	RSR	LLDF	B-factors(Å ²)	Q < 0.9
2	DOC	P	13	18/19	0.24	1.88	35,43,87,90	0
2	DOC	K	13	18/19	0.19	1.22	61,76,86,87	0
3	EFG	M	5	25/26	0.17	0.38	48,70,96,98	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	EFG	B	5	25/26	0.12	-0.04	35,40,51,58	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	MG	J	402	1/1	0.27	4.33	43,43,43,43	0
5	MG	J	403	1/1	0.22	2.53	28,28,28,28	0
5	MG	A	402	1/1	0.25	1.50	19,19,19,19	0
4	DCP	J	401	28/28	0.15	0.18	45,57,72,90	0
5	MG	A	403	1/1	0.20	0.00	13,13,13,13	0
4	DCP	A	401	28/28	0.13	-0.50	24,37,46,47	0
5	MG	K	101	1/1	0.34	-	49,49,49,49	0

6.5 Other polymers ⓘ

There are no such residues in this entry.