



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2014 – 01:00 AM GMT

PDB ID : 3V6K
Title : Replication of N2,3-Ethenoguanine by DNA Polymerases
Authors : Zhao, L.
Deposited on : 2011-12-20
Resolution : 3.60 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>

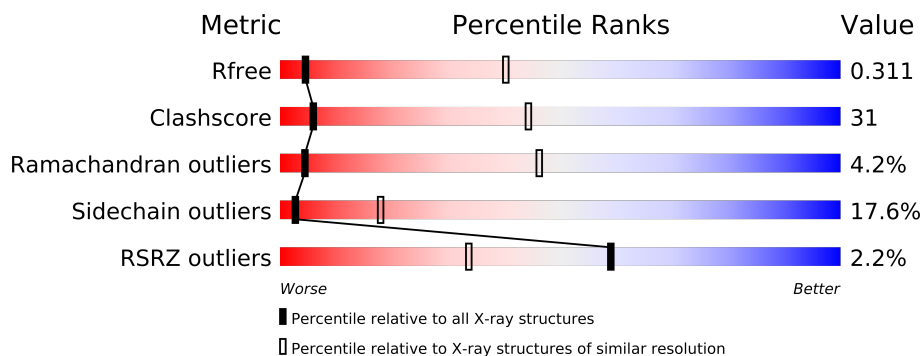
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1020 (3.86-3.34)
Clashscore	79885	1155 (3.80-3.40)
Ramachandran outliers	78287	1109 (3.80-3.40)
Sidechain outliers	78261	1108 (3.80-3.40)
RSRZ outliers	66119	1000 (3.84-3.36)

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	347	
1	J	347	
2	K	10	
2	P	10	
3	B	14	
3	M	14	

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

Mol	Type	Chain	Res	Geometry	Electron density
4	MG	A	401	-	X
4	MG	A	402	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
4	MG	J	401	-	X
5	CA	A	403	-	X
5	CA	J	402	-	X
5	CA	J	405	-	X
5	CA	J	406	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6100 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	342	Total	C	N	O	S	0	0	0
			2729	1752	467	503	7			
1	J	334	Total	C	N	O	S	0	0	1
			2368	1498	412	451	7			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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	-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(P*GP*AP*AP*GP*GP*AP*TP*TP*CP*(2 DT))-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	10	Total	C	N	O	P	0	0	0
			207	99	39	59	10			
2	K	10	Total	C	N	O	P	0	0	0
			207	99	39	59	10			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	B	14	Total	C	F	N	O	P	0	0	0
			282	137	1	48	83	13			
3	M	13	Total	C	F	N	O	P	0	0	0
			262	127	1	46	76	12			

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	J	2	Total	Mg	0	0
			2	2		
4	A	2	Total	Mg	0	0
			2	2		

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	J	4	Total	Ca	0	0
			4	4		
5	A	3	Total	Ca	0	0
			3	3		

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	P	1	Total	Na	0	0
			1	1		
6	J	1	Total	Na	0	0
			1	1		
6	A	1	Total	Na	0	0
			1	1		
6	B	1	Total	Na	0	0
			1	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	9	Total	O	0	0
			9	9		
7	J	15	Total	O	0	0
			15	15		
7	P	2	Total	O	0	0
			2	2		

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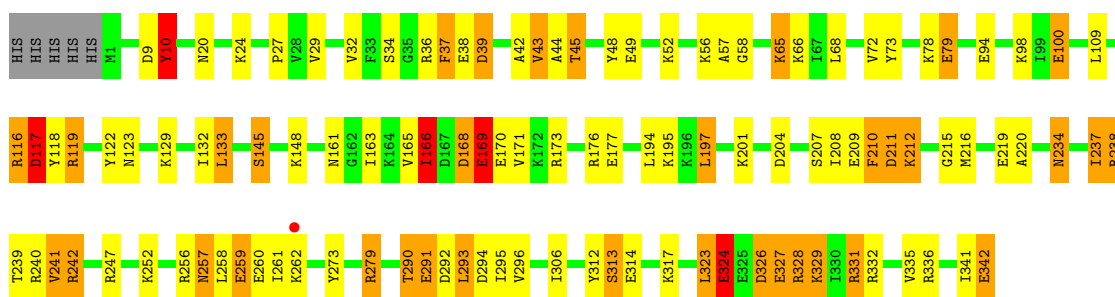
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	3	Total	O	0	0
			3	3		
7	M	1	Total	O	0	0
			1	1		

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.

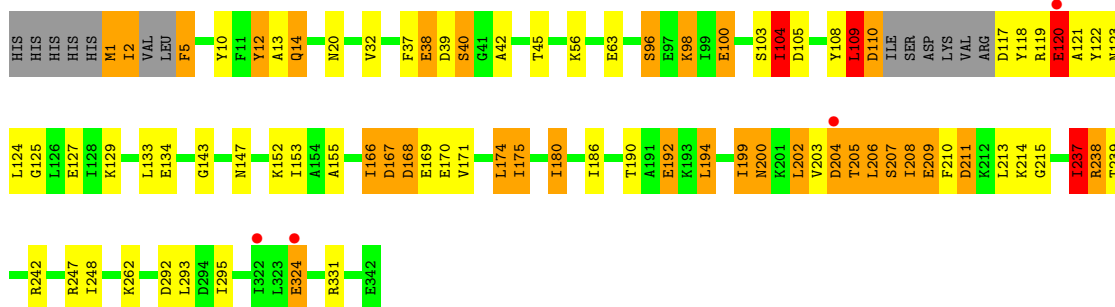
- Molecule 1: DNA polymerase IV

Chain A: 



- Molecule 1: DNA polymerase IV

Chain J: 



- Molecule 2: DNA (5'-D(P*GP*AP*AP*GP*GP*AP*TP*TP*CP*(2DT))-3')

Chain P: 



- Molecule 2: DNA (5'-D(P*GP*AP*AP*GP*GP*AP*TP*TP*CP*(2DT))-3')

Chain K: 

There are no outlier residues recorded for this chain.

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

Chain B: 



- Molecule 3: DNA (5'-D(*TP*CP*AP*CP*(EFG)P*GP*AP*AP*TP*CP*CP*TP*TP*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	51.85Å 110.95Å 100.24Å 90.00° 102.70° 90.00°	Depositor
Resolution (Å)	48.90 – 3.60 48.89 – 3.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.90-3.60) 99.9 (48.89-3.60)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.99 (at 3.57Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.229 , 0.303 0.246 , 0.311	Depositor DCC
R_{free} test set	1026 reflections (8.61%)	DCC
Wilson B-factor (Å ²)	89.0	Xtriage
Anisotropy	0.069	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 77.3	EDS
Estimated twinning fraction	0.042 for h,-k,-h-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	1 of 12937 reflections (0.008%)	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	6100	wwPDB-VP
Average B, all atoms (Å ²)	111.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.60% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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: 2DT, MG, EFG, 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	0.68	1/2768 (0.0%)	0.83	3/3720 (0.1%)
1	J	0.48	0/2396	0.83	9/3257 (0.3%)
2	K	0.32	0/211	0.80	0/324
2	P	0.42	0/211	0.83	1/324 (0.3%)
3	B	0.53	1/285 (0.4%)	0.88	1/434 (0.2%)
3	M	0.37	0/263	0.92	1/400 (0.2%)
All	All	0.57	2/6134 (0.0%)	0.84	15/8459 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	79	GLU	CD-OE1	5.52	1.31	1.25
3	B	3	DA	O3'-P	5.33	1.67	1.61

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	38	GLU	N-CA-CB	13.70	135.26	110.60
1	J	37	PHE	N-CA-C	9.59	136.90	111.00
1	J	38	GLU	N-CA-C	-8.03	89.31	111.00
1	J	210	PHE	N-CA-C	7.33	130.78	111.00
2	P	11	DT	P-O3'-C3'	6.83	127.90	119.70
1	J	215	GLY	N-CA-C	6.71	129.88	113.10
3	M	9	DT	P-O3'-C3'	5.77	126.63	119.70
1	A	109	LEU	CB-CG-CD2	-5.65	101.40	111.00
1	J	42	ALA	CB-CA-C	5.64	118.55	110.10
1	J	120	GLU	N-CA-C	-5.59	95.91	111.00
1	J	109	LEU	N-CA-C	-5.44	96.32	111.00
3	B	9	DT	P-O3'-C3'	5.43	126.21	119.70
1	J	134	GLU	N-CA-CB	-5.30	101.07	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	197	LEU	CA-CB-CG	5.27	127.42	115.30
1	A	314	GLU	N-CA-CB	-5.16	101.31	110.60

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	2729	0	3	83	0
1	J	2368	0	7	73	0
2	K	207	0	0	0	0
2	P	207	0	0	3	0
3	B	282	0	0	16	0
3	M	262	0	0	18	0
4	A	2	0	0	0	0
4	J	2	0	0	0	0
5	A	3	0	0	0	0
5	J	4	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	J	1	0	0	0	0
6	P	1	0	0	0	0
7	A	9	0	0	1	0
7	B	3	0	0	0	0
7	J	15	0	0	0	0
7	M	1	0	0	0	0
7	P	2	0	0	0	0
All	All	6100	0	10	184	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 31.

All (184) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:B:4:DC:C6	3:B:4:DC:C5'	2.41	1.03
1:J:205:THR:CG2	1:J:206:LEU:N	2.20	1.01
1:A:119:ARG:NH1	1:A:119:ARG:CG	2.27	0.97
1:A:210:PHE:CD1	1:A:210:PHE:N	2.30	0.96
1:J:199:ILE:CG1	1:J:200:ASN:N	2.31	0.94
1:A:145:SER:CB	1:A:166:ILE:CG2	2.48	0.91
1:A:43:VAL:CG1	1:A:57:ALA:CA	2.49	0.91
1:J:166:ILE:CD1	1:J:170:GLU:CB	2.51	0.88
1:J:204:ASP:CA	1:J:205:THR:C	2.42	0.88
1:A:292:ASP:O	1:A:293:LEU:CB	2.22	0.87
1:J:98:LYS:CD	1:J:110:ASP:OD2	2.23	0.87
1:A:312:TYR:O	1:A:313:SER:OG	1.93	0.87
1:J:5:PHE:CA	1:J:109:LEU:CD2	2.53	0.87
1:J:204:ASP:CA	1:J:206:LEU:N	2.43	0.81
3:M:2:DC:C1'	3:M:3:DA:OP2	2.27	0.81
1:A:44:ALA:O	1:A:45:THR:CG2	2.29	0.80
1:A:326:ASP:O	1:A:327:GLU:CG	2.30	0.80
3:B:11:DC:C2'	3:B:12:DT:OP2	2.30	0.80
1:A:328:ARG:CG	1:A:328:ARG:NH1	2.45	0.80
1:A:44:ALA:C	1:A:45:THR:CG2	2.50	0.78
3:M:3:DA:C2	3:M:4:DC:C5	2.72	0.78
1:A:326:ASP:O	1:A:327:GLU:CB	2.30	0.77
1:A:37:PHE:O	1:A:37:PHE:CD1	2.38	0.77
3:B:13:DT:C4	3:B:14:DC:N4	2.53	0.77
1:J:175:ILE:CA	1:J:202:LEU:CB	2.64	0.76
3:M:4:DC:P	3:M:4:DC:C3'	2.74	0.76
1:A:65:LYS:C	1:A:65:LYS:CD	2.55	0.76
1:A:323:LEU:O	1:A:324:GLU:CB	2.35	0.75
3:M:4:DC:OP1	3:M:4:DC:C3'	2.35	0.74
3:M:3:DA:C3'	3:M:3:DA:OP1	2.36	0.74
1:J:237:ILE:O	1:J:237:ILE:CG2	2.36	0.73
1:J:211:ASP:OD1	1:J:214:LYS:CD	2.38	0.71
2:P:5:DG:C2'	2:P:6:DA:C8	2.73	0.71
1:J:117:ASP:CB	1:J:120:GLU:OE1	2.39	0.70
1:J:204:ASP:CG	1:J:204:ASP:O	2.30	0.70
1:A:234:ASN:ND2	1:A:234:ASN:C	2.45	0.70
1:A:36:ARG:O	1:A:37:PHE:CB	2.40	0.70
3:M:5:EFG:F	3:M:5:EFG:C8	2.30	0.69
1:A:259:GLU:OE1	1:A:259:GLU:CA	2.41	0.69
3:M:4:DC:OP2	3:M:4:DC:C2'	2.41	0.68
1:J:204:ASP:N	1:J:205:THR:CG2	2.56	0.68
1:J:5:PHE:N	1:J:143:GLY:O	2.27	0.68
3:M:4:DC:C2'	3:M:5:EFG:OP1	2.39	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:10:TYR:CD2	1:A:48:TYR:CD1	2.82	0.68
1:A:294:ASP:CB	1:A:328:ARG:NH2	2.56	0.67
3:M:5:EFG:C5'	3:M:5:EFG:F	2.30	0.67
1:A:331:ARG:NH2	3:B:5:EFG:P	2.69	0.66
1:A:237:ILE:CD1	1:A:237:ILE:N	2.59	0.66
1:A:331:ARG:NH2	3:B:5:EFG:OP1	2.29	0.66
1:A:116:ARG:O	1:A:117:ASP:CB	2.44	0.66
1:J:121:ALA:C	1:J:123:ASN:N	2.48	0.66
1:J:206:LEU:O	1:J:207:SER:CB	2.44	0.65
3:B:3:DA:C2'	3:B:4:DC:C5'	2.75	0.64
1:J:103:SER:O	1:J:105:ASP:N	2.32	0.63
1:J:324:GLU:CG	1:J:324:GLU:O	2.46	0.63
1:J:12:TYR:CD1	1:J:12:TYR:N	2.67	0.62
1:A:257:ASN:OD1	1:A:257:ASN:C	2.37	0.62
1:A:117:ASP:CG	1:A:117:ASP:O	2.37	0.62
1:A:119:ARG:O	1:A:123:ASN:ND2	2.32	0.62
1:J:167:ASP:O	1:J:169:GLU:N	2.33	0.62
1:A:65:LYS:O	1:A:65:LYS:CD	2.48	0.61
1:J:192:GLU:CA	1:J:192:GLU:OE2	2.48	0.61
1:J:5:PHE:N	1:J:109:LEU:CD2	2.63	0.61
1:J:125:GLY:O	1:J:129:LYS:N	2.33	0.61
1:J:175:ILE:CG2	1:J:202:LEU:HD12	2.30	0.60
1:A:79:GLU:OE1	1:A:79:GLU:N	2.34	0.60
1:A:36:ARG:O	1:A:37:PHE:CD2	2.53	0.60
1:J:109:LEU:O	1:J:110:ASP:C	2.38	0.60
1:A:100:GLU:OE2	1:A:148:LYS:NZ	2.35	0.60
1:A:239:THR:O	1:A:239:THR:CG2	2.47	0.60
1:J:180:ILE:CB	1:J:200:ASN:O	2.50	0.60
1:A:273:TYR:OH	1:A:306:ILE:O	2.20	0.60
1:J:109:LEU:CD2	1:J:109:LEU:N	2.65	0.59
1:J:118:TYR:O	1:J:120:GLU:N	2.35	0.59
1:J:190:THR:CG2	1:J:194:LEU:CD1	2.81	0.59
3:M:4:DC:P	3:M:4:DC:C2'	2.90	0.59
1:J:5:PHE:CD2	1:J:108:TYR:CE1	2.91	0.59
1:J:175:ILE:O	1:J:202:LEU:CB	2.51	0.59
1:A:168:ASP:O	1:A:171:VAL:N	2.36	0.58
1:J:38:GLU:O	1:J:40:SER:N	2.36	0.58
1:A:10:TYR:O	1:A:10:TYR:CD1	2.57	0.57
1:A:166:ILE:O	1:A:166:ILE:CG2	2.52	0.57
1:J:117:ASP:OD1	1:J:118:TYR:N	2.38	0.57
1:A:100:GLU:CB	1:A:238:ARG:O	2.52	0.57
1:J:203:VAL:CG1	1:J:203:VAL:O	2.52	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:38:GLU:O	1:A:39:ASP:CB	2.53	0.56
3:M:5:EFG:C5'	3:M:5:EFG:C8	2.83	0.56
1:J:207:SER:O	1:J:208:ILE:CB	2.53	0.55
1:A:68:LEU:O	1:A:73:TYR:OH	2.25	0.55
1:J:207:SER:C	1:J:209:GLU:N	2.59	0.55
1:J:5:PHE:CD1	1:J:5:PHE:C	2.79	0.55
3:B:4:DC:C6	3:B:4:DC:C4'	2.89	0.54
1:A:241:VAL:O	1:A:242:ARG:C	2.46	0.54
1:A:177:GLU:O	1:A:201:LYS:NZ	2.40	0.54
1:J:167:ASP:O	1:J:168:ASP:C	2.45	0.54
1:A:239:THR:O	1:A:240:ARG:C	2.46	0.54
1:A:49:GLU:OE2	1:A:52:LYS:CE	2.57	0.53
1:A:117:ASP:OD1	1:A:117:ASP:O	2.27	0.53
1:A:324:GLU:O	1:A:324:GLU:CG	2.55	0.53
1:J:174:LEU:CD2	1:J:174:LEU:N	2.71	0.53
1:J:190:THR:O	1:J:194:LEU:CD1	2.57	0.52
1:A:342:GLU:N	1:A:342:GLU:CD	2.62	0.52
1:A:9:ASP:O	1:A:10:TYR:C	2.46	0.52
3:M:3:DA:C2	3:M:4:DC:C4	2.98	0.52
1:A:258:LEU:O	1:A:262:LYS:N	2.42	0.52
1:J:238:ARG:O	1:J:239:THR:C	2.48	0.52
1:J:100:GLU:CB	1:J:237:ILE:CG2	2.88	0.52
1:J:12:TYR:O	1:J:13:ALA:CB	2.56	0.51
1:A:336:ARG:NH2	3:B:8:DA:OP2	2.43	0.51
3:B:13:DT:O4	3:B:14:DC:N4	2.43	0.51
1:J:118:TYR:C	1:J:120:GLU:N	2.63	0.51
1:A:10:TYR:CE2	1:A:48:TYR:CD1	2.98	0.51
1:A:165:VAL:CG1	1:A:166:ILE:N	2.73	0.50
1:A:258:LEU:O	1:A:261:ILE:N	2.44	0.50
1:A:43:VAL:CG1	1:A:56:LYS:O	2.60	0.50
1:J:204:ASP:O	1:J:204:ASP:OD1	2.30	0.50
1:J:208:ILE:O	1:J:209:GLU:O	2.28	0.50
1:J:124:LEU:O	1:J:127:GLU:N	2.45	0.50
1:J:203:VAL:O	1:J:204:ASP:OD2	2.30	0.50
1:A:212:LYS:O	1:A:215:GLY:N	2.45	0.50
1:J:104:ILE:CG1	1:J:105:ASP:N	2.74	0.49
1:A:290:THR:C	1:A:292:ASP:N	2.65	0.49
1:A:168:ASP:O	1:A:169:GLU:C	2.51	0.49
1:J:1:MET:O	1:J:2:ILE:O	2.30	0.49
1:A:43:VAL:CG1	1:A:58:GLY:N	2.77	0.48
1:A:328:ARG:NH1	1:A:328:ARG:CB	2.75	0.48
1:J:5:PHE:CB	1:J:108:TYR:CD1	2.97	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:171:VAL:O	1:J:174:LEU:CD2	2.62	0.47
1:A:170:GLU:OE2	1:A:173:ARG:NH2	2.47	0.47
1:J:32:VAL:CG2	1:J:32:VAL:O	2.61	0.47
1:J:293:LEU:CD2	3:M:4:DC:C2	2.97	0.47
3:M:4:DC:O2	3:M:4:DC:O4'	2.30	0.47
3:B:10:DC:C2'	3:B:11:DC:C6	2.98	0.47
1:A:49:GLU:CA	1:A:49:GLU:OE2	2.63	0.46
1:A:10:TYR:N	1:A:10:TYR:CD1	2.80	0.46
1:A:331:ARG:NH2	3:B:5:EFG:OP2	2.48	0.46
1:A:211:ASP:N	1:A:211:ASP:OD1	2.48	0.46
1:A:43:VAL:CG1	1:A:44:ALA:N	2.75	0.46
1:A:279:ARG:NE	1:A:279:ARG:CA	2.78	0.46
1:A:195:LYS:NZ	7:A:508:HOH:O	2.48	0.46
1:A:324:GLU:C	1:A:327:GLU:OE2	2.54	0.46
1:J:110:ASP:O	1:J:237:ILE:CB	2.64	0.46
1:J:121:ALA:O	1:J:123:ASN:N	2.48	0.46
1:A:118:TYR:O	1:A:119:ARG:C	2.54	0.46
3:M:2:DC:C2'	3:M:3:DA:OP2	2.62	0.45
1:J:103:SER:O	1:J:104:ILE:C	2.55	0.45
1:J:175:ILE:O	1:J:202:LEU:CA	2.64	0.45
1:J:205:THR:O	1:J:207:SER:N	2.50	0.45
1:A:258:LEU:O	1:A:259:GLU:C	2.55	0.45
2:P:14:2DT:N3	3:B:5:EFG:N1	2.65	0.45
1:J:10:TYR:O	1:J:12:TYR:O	2.35	0.45
1:A:259:GLU:OE1	1:A:259:GLU:O	2.35	0.45
1:A:219:GLU:CG	1:A:220:ALA:N	2.79	0.45
1:A:291:GLU:N	1:A:329:LYS:O	2.50	0.44
1:J:110:ASP:O	1:J:237:ILE:CG1	2.66	0.44
1:J:152:LYS:O	1:J:155:ALA:N	2.51	0.44
1:A:132:ILE:O	1:A:133:LEU:C	2.54	0.44
1:A:34:SER:O	1:A:36:ARG:N	2.50	0.43
1:J:174:LEU:CD2	1:J:175:ILE:N	2.81	0.43
1:J:248:ILE:N	3:M:7:DA:OP2	2.51	0.43
1:J:166:ILE:O	1:J:166:ILE:CG2	2.66	0.43
3:B:5:EFG:F	3:B:5:EFG:C8	2.56	0.43
1:J:293:LEU:CD1	3:M:4:DC:C6	3.01	0.43
1:A:208:ILE:C	1:A:209:GLU:O	2.56	0.43
1:A:10:TYR:C	1:A:10:TYR:CD1	2.90	0.43
1:A:279:ARG:NH2	1:A:341:ILE:O	2.51	0.43
3:B:12:DT:C2'	3:B:13:DT:OP2	2.67	0.42
1:A:122:TYR:CD1	1:A:122:TYR:C	2.92	0.42
1:A:256:ARG:NH2	1:A:327:GLU:OE1	2.52	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:279:ARG:CZ	1:A:341:ILE:O	2.67	0.42
1:J:166:ILE:C	1:J:166:ILE:CD1	2.87	0.41
1:J:12:TYR:O	1:J:14:GLN:N	2.53	0.41
1:J:213:LEU:O	1:J:214:LYS:C	2.59	0.41
1:J:121:ALA:O	1:J:122:TYR:C	2.58	0.41
1:A:43:VAL:CG1	1:A:57:ALA:C	2.89	0.41
1:J:199:ILE:O	1:J:200:ASN:CB	2.69	0.41
3:B:3:DA:C2'	3:B:4:DC:O5'	2.69	0.41
1:A:42:ALA:C	1:A:43:VAL:O	2.56	0.41
1:J:96:SER:OG	1:J:110:ASP:CB	2.69	0.41
3:M:3:DA:C2'	3:M:4:DC:O5'	2.69	0.41
1:A:29:VAL:N	1:A:72:VAL:O	2.55	0.40
1:J:186:ILE:CG2	1:J:190:THR:CG2	2.99	0.40
1:A:332:ARG:NE	3:B:6:DG:OP2	2.54	0.40
2:P:8:DG:C2	2:P:9:DG:C4	3.09	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	340/347 (98%)	283 (83%)	44 (13%)	13 (4%)	5	50
1	J	328/347 (94%)	267 (81%)	46 (14%)	15 (5%)	4	43
All	All	668/694 (96%)	550 (82%)	90 (14%)	28 (4%)	4	46

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	10	TYR
1	A	37	PHE
1	A	39	ASP
1	A	293	LEU
1	A	324	GLU

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Mol	Chain	Res	Type
1	A	327	GLU
1	J	39	ASP
1	J	96	SER
1	J	104	ILE
1	J	168	ASP
1	J	200	ASN
1	J	206	LEU
1	J	207	SER
1	J	208	ILE
1	J	209	GLU
1	J	242	ARG
1	A	27	PRO
1	A	117	ASP
1	A	291	GLU
1	J	133	LEU
1	A	161	ASN
1	A	313	SER
1	A	169	GLU
1	J	292	ASP
1	J	199	ILE
1	J	262	LYS
1	A	166	ILE
1	J	237	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	296/306 (97%)	242 (82%)	54 (18%)	2	16
1	J	216/306 (71%)	180 (83%)	36 (17%)	3	21
All	All	512/612 (84%)	422 (82%)	90 (18%)	3	18

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	TYR
1	A	20	ASN

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Mol	Chain	Res	Type
1	A	24	LYS
1	A	32	VAL
1	A	43	VAL
1	A	45	THR
1	A	65	LYS
1	A	66	LYS
1	A	78	LYS
1	A	94	GLU
1	A	98	LYS
1	A	100	GLU
1	A	116	ARG
1	A	117	ASP
1	A	119	ARG
1	A	129	LYS
1	A	133	LEU
1	A	145	SER
1	A	163	ILE
1	A	166	ILE
1	A	168	ASP
1	A	169	GLU
1	A	176	ARG
1	A	194	LEU
1	A	197	LEU
1	A	204	ASP
1	A	207	SER
1	A	210	PHE
1	A	211	ASP
1	A	212	LYS
1	A	216	MET
1	A	234	ASN
1	A	237	ILE
1	A	238	ARG
1	A	241	VAL
1	A	242	ARG
1	A	247	ARG
1	A	252	LYS
1	A	257	ASN
1	A	259	GLU
1	A	260	GLU
1	A	279	ARG
1	A	290	THR
1	A	295	ILE

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Mol	Chain	Res	Type
1	A	296	VAL
1	A	317	LYS
1	A	323	LEU
1	A	324	GLU
1	A	326	ASP
1	A	328	ARG
1	A	329	LYS
1	A	331	ARG
1	A	335	VAL
1	A	342	GLU
1	J	1	MET
1	J	2	ILE
1	J	5	PHE
1	J	12	TYR
1	J	14	GLN
1	J	20	ASN
1	J	40	SER
1	J	45	THR
1	J	56	LYS
1	J	63	GLU
1	J	98	LYS
1	J	100	GLU
1	J	104	ILE
1	J	109	LEU
1	J	110	ASP
1	J	119	ARG
1	J	120	GLU
1	J	147	ASN
1	J	153	ILE
1	J	166	ILE
1	J	167	ASP
1	J	174	LEU
1	J	175	ILE
1	J	180	ILE
1	J	192	GLU
1	J	194	LEU
1	J	202	LEU
1	J	204	ASP
1	J	205	THR
1	J	211	ASP
1	J	237	ILE
1	J	238	ARG

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Mol	Chain	Res	Type
1	J	247	ARG
1	J	295	ILE
1	J	324	GLU
1	J	331	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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	2.36	10 (38%)	32,42,45	5.01	10 (31%)
2	2DT	K	14	2,4	18,20,21	1.48	3 (16%)	20,28,31	2.44	3 (15%)
3	EFG	M	5	3	26,28,29	2.63	10 (38%)	32,42,45	5.68	12 (37%)
2	2DT	P	14	2	18,20,21	1.61	3 (16%)	20,28,31	2.20	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	2DT	K	14	2,4	-	0/5/18/19	0/2/2/2
3	EFG	M	5	3	-	0/8/25/26	0/1/4/4
2	2DT	P	14	2	-	0/5/18/19	0/2/2/2

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	5	EFG	C4-N3	-6.98	1.32	1.39
3	B	5	EFG	C4-N3	-6.44	1.32	1.39
3	M	5	EFG	C2-N3	-5.82	1.31	1.39
3	B	5	EFG	C2-N3	-5.24	1.32	1.39
3	M	5	EFG	C6-C5	-4.92	1.33	1.41
2	P	14	2DT	P-OP1	4.76	1.52	1.46
2	K	14	2DT	P-OP1	4.11	1.51	1.46
3	M	5	EFG	C9-N3	-3.71	1.31	1.37
3	B	5	EFG	C6-C5	-3.36	1.35	1.41
3	M	5	EFG	C5-C4	-3.36	1.32	1.40
2	P	14	2DT	C4-C5	3.35	1.50	1.42
3	M	5	EFG	C2-N2	-3.28	1.32	1.36
3	M	5	EFG	C2'-C3'	-3.23	1.46	1.52
2	K	14	2DT	C4-C5	2.92	1.49	1.42
3	B	5	EFG	O4'-C1'	2.87	1.45	1.41
3	B	5	EFG	O4'-C4'	2.86	1.51	1.45
3	B	5	EFG	C4-N9	-2.86	1.33	1.38
3	M	5	EFG	C8-N9	-2.75	1.32	1.36
3	B	5	EFG	C5-C4	-2.64	1.34	1.40
3	B	5	EFG	C9-N3	-2.63	1.33	1.37
3	M	5	EFG	C4-N9	-2.57	1.33	1.38
2	K	14	2DT	C2-N1	2.51	1.41	1.38
2	P	14	2DT	C2-N1	2.31	1.40	1.38
3	B	5	EFG	C8-N9	-2.15	1.33	1.36
3	M	5	EFG	C5-N7	-2.07	1.32	1.40
3	B	5	EFG	C2'-C1'	-2.02	1.50	1.53

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	5	EFG	C6-C5-N7	-27.25	130.47	134.14
3	B	5	EFG	C6-C5-N7	-20.53	131.38	134.14
3	B	5	EFG	C10-N2-C2	16.38	108.74	104.92
3	M	5	EFG	C10-N2-C2	10.25	107.31	104.92
3	M	5	EFG	F-C2'-C3'	-7.54	89.02	109.39
2	K	14	2DT	C6-N1-C2	-7.04	120.41	122.41
2	P	14	2DT	C6-N1-C2	-6.78	120.48	122.41
2	K	14	2DT	N3-C2-N1	6.22	121.16	115.97
2	P	14	2DT	N3-C2-N1	4.99	120.14	115.97
3	M	5	EFG	C6-N1-C2	-4.69	116.96	120.28
3	B	5	EFG	N2-C2-N3	-4.68	108.48	111.58
3	M	5	EFG	C1'-N9-C4	4.40	133.70	126.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	5	EFG	C8-N9-C1'	-3.78	118.94	126.38
3	B	5	EFG	C3'-C2'-C1'	3.71	108.06	103.30
3	M	5	EFG	N2-C2-N3	-3.69	109.14	111.58
2	P	14	2DT	C3'-C2'-C1'	3.53	106.71	102.80
3	B	5	EFG	O4'-C1'-N9	-3.47	105.21	108.44
2	K	14	2DT	C3'-C2'-C1'	3.23	106.37	102.80
3	B	5	EFG	C10-C9-N3	3.13	109.61	106.86
3	M	5	EFG	C5-C4-N3	-3.01	117.52	124.96
3	M	5	EFG	O4'-C1'-N9	2.83	111.07	108.44
3	B	5	EFG	C6-N1-C2	-2.74	118.34	120.28
3	M	5	EFG	P-O5'-C5'	-2.60	113.05	123.19
3	B	5	EFG	F-C2'-C3'	-2.48	102.69	109.39
3	B	5	EFG	C4-C5-N7	-2.47	107.41	109.52
3	B	5	EFG	C5-C4-N3	-2.42	118.98	124.96
3	M	5	EFG	C3'-C2'-C1'	2.08	105.97	103.30
3	M	5	EFG	N7-C8-N9	-2.06	108.54	114.36
2	P	14	2DT	O4'-C4'-C3'	2.01	108.17	104.80

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 15 ligands modelled in this entry, 15 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.

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	342/347 (98%)	0.05	1 (0%) 91 81	43, 78, 126, 154	16 (4%)
1	J	334/347 (96%)	0.14	4 (1%) 75 49	64, 121, 201, 254	25 (7%)
2	K	10/10 (100%)	0.45	0 100 100	118, 158, 205, 221	1 (10%)
2	P	10/10 (100%)	0.25	1 (10%) 8 6	99, 127, 193, 233	2 (20%)
3	B	14/14 (100%)	0.49	2 (14%) 3 3	65, 111, 209, 221	2 (14%)
3	M	13/14 (92%)	0.64	2 (15%) 3 3	86, 171, 219, 226	0
All	All	723/742 (97%)	0.12	10 (1%) 59 45	43, 98, 193, 254	46 (6%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	B	11	DC	2.5
1	J	322	ILE	2.4
1	J	324	GLU	2.4
1	J	120	GLU	2.2
3	M	13	DT	2.2
2	P	5	DG	2.2
1	A	262	LYS	2.2
3	B	12	DT	2.2
3	M	2	DC	2.1
1	J	204	ASP	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(\AA^2)	Q<0.9
2	2DT	K	14	19/20	0.31	3.49	131,150,178,178	0
2	2DT	P	14	19/20	0.23	0.11	76,96,142,152	0
3	EFG	M	5	25/26	0.19	-0.71	94,110,166,171	0
3	EFG	B	5	25/26	0.15	-1.01	65,70,73,75	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
4	MG	A	401	1/1	1.15	31.36	210,210,210,210	0
4	MG	A	402	1/1	1.50	28.48	210,210,210,210	0
5	CA	J	406	1/1	0.98	28.03	209,209,209,209	0
5	CA	A	403	1/1	0.75	7.81	210,210,210,210	0
5	CA	J	402	1/1	0.86	6.82	210,210,210,210	0
4	MG	J	401	1/1	0.39	3.58	210,210,210,210	0
5	CA	J	405	1/1	0.31	2.10	209,209,209,209	0
4	MG	J	403	1/1	0.36	1.56	210,210,210,210	0
6	NA	P	101	1/1	0.42	1.13	209,209,209,209	0
5	CA	A	404	1/1	0.20	-0.20	209,209,209,209	0
5	CA	J	404	1/1	0.18	-0.42	209,209,209,209	0
5	CA	A	405	1/1	0.47	-	209,209,209,209	0
6	NA	B	101	1/1	0.66	-	148,148,148,148	0
6	NA	A	406	1/1	0.24	-	209,209,209,209	0
6	NA	J	407	1/1	0.21	-	209,209,209,209	0

6.5 Other polymers

There are no such residues in this entry.