



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 11:28 AM GMT

PDB ID : 4F5R  
Title : Open and closed ternary complex of R283K DNA polymerase beta with a dCTP analog in the same asymmetric unit  
Authors : Freudenthal, B.D.; Beard, W.A.; Wilson, S.H.  
Deposited on : 2012-05-13  
Resolution : 2.20 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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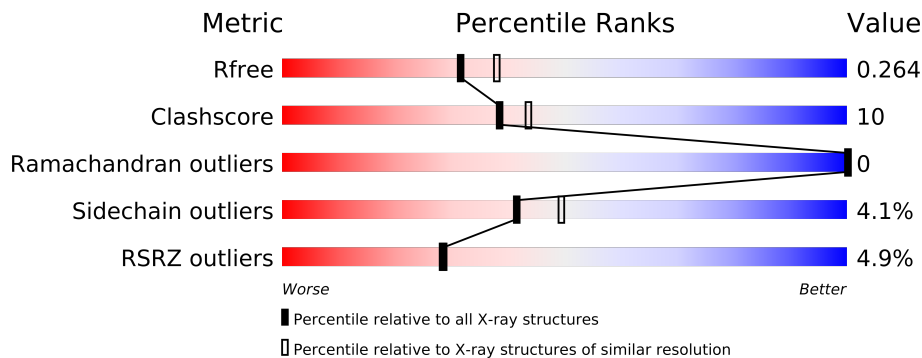
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.20 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	2938 (2.20-2.20)
Clashscore	79885	3751 (2.20-2.20)
Ramachandran outliers	78287	3681 (2.20-2.20)
Sidechain outliers	78261	3682 (2.20-2.20)
RSRZ outliers	66119	2939 (2.20-2.20)

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  $\geq 3$ , 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	335	
1	B	335	
2	C	5	
2	D	5	
3	G	10	
3	P	10	
4	F	16	
4	T	16	

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 6910 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 beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	325	Total	C	N	O	S	0	0	0
			2581	1635	450	487	9			
1	B	321	Total	C	N	O	S	0	1	0
			2583	1636	449	489	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	283	LYS	ARG	ENGINEERED MUTATION	UNP P06746
B	283	LYS	ARG	ENGINEERED MUTATION	UNP P06746

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	P	10	Total	C	N	O	P	0	0	0
			203	97	38	59	9			
3	G	10	Total	C	N	O	P	0	0	0
			203	97	38	59	9			

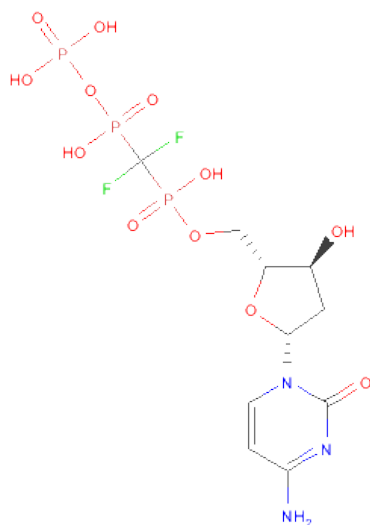
- Molecule 4 is a DNA chain called DNA (5'-D(\*CP\*CP\*GP\*AP\*CP\*GP\*GP\*CP\*GP\*CP\*AP\*TP\*CP\*AP\*GP\*C)-3').

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	1	Total	Na	0	0
			1	1		
5	B	1	Total	Na	0	0
			1	1		
5	A	1	Total	Na	0	0
			1	1		
5	T	1	Total	Na	0	0
			1	1		

- Molecule 6 is 2'-DEOXY-5'-O-[(S)-{DIFLUORO[(S)-HYDROXY(PHOSPHONOOXY)PHOSPHORYL]METHYL}(HYDROXY)PHOSPHORYL]CYTIDINE (three-letter code: 6CF) (formula: C<sub>10</sub>H<sub>16</sub>F<sub>2</sub>N<sub>3</sub>O<sub>12</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	A	1	Total	C	F	N	O	P	0	0
			30	10	2	3	12	3		
6	B	1	Total	C	F	N	O	P	0	0
			30	10	2	3	12	3		

- Molecule 7 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	T	1	Total 1	Mn 1	0	0
7	B	2	Total 2	Mn 2	0	0
7	D	1	Total 1	Mn 1	0	0

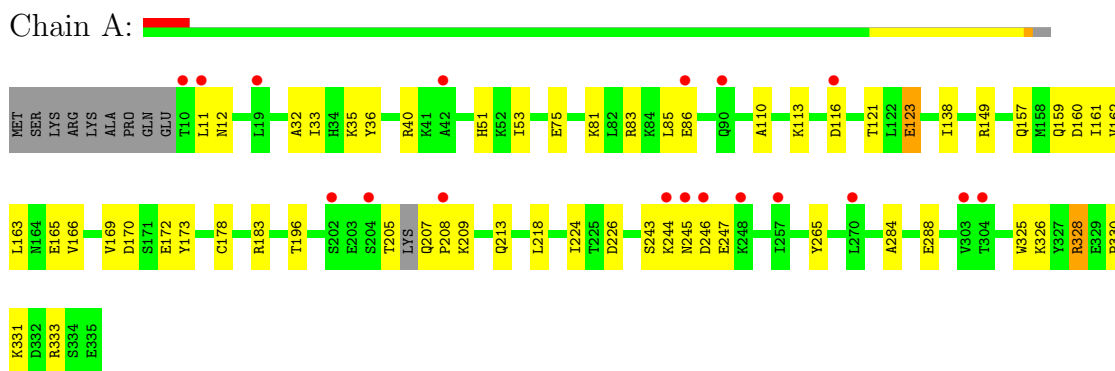
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	184	Total 184	O 184	0	0
8	B	120	Total 120	O 120	0	0
8	D	17	Total 17	O 17	0	0
8	P	19	Total 19	O 19	0	0
8	T	41	Total 41	O 41	0	0
8	C	4	Total 4	O 4	0	0
8	G	12	Total 12	O 12	0	0
8	F	17	Total 17	O 17	0	0

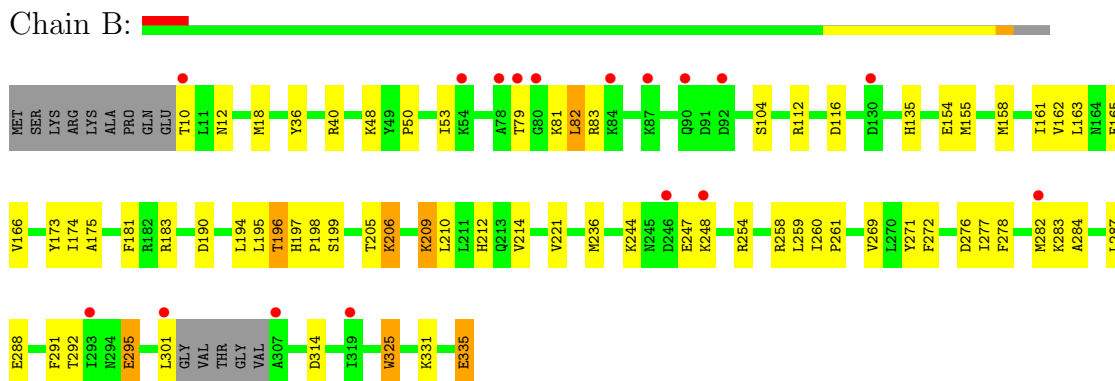
### 3 Residue-property plots

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 beta



- Molecule 1: DNA polymerase beta



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

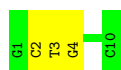


- Molecule 2: DNA (5'-D(P\*GP\*TP\*CP\*GP\*G)-3')



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

Chain P: 



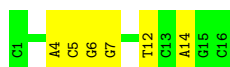
- Molecule 3: DNA (5'-D(\*GP\*CP\*TP\*GP\*AP\*TP\*GP\*CP\*GP\*C)-3')

Chain G: 



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

Chain T: 



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

Chain F: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	55.03Å 79.45Å 102.09Å 90.00° 96.96° 90.00°	Depositor
Resolution (Å)	21.36 – 2.20 21.36 – 2.20	Depositor EDS
% Data completeness (in resolution range)	85.8 (21.36-2.20) 84.9 (21.36-2.20)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.38 (at 2.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, $R_{free}$	0.210 , 0.278 0.199 , 0.264	Depositor DCC
$R_{free}$ test set	1394 reflections (3.65%)	DCC
Wilson B-factor (Å <sup>2</sup> )	33.2	Xtriage
Anisotropy	0.367	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 38.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 44093 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6910	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.56% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities 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: NA, MN, 6CF

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	0.38	0/2629	0.53	0/3534
1	B	0.38	1/2632 (0.0%)	0.51	0/3538
2	C	1.17	1/118 (0.8%)	1.35	2/179 (1.1%)
2	D	1.15	1/118 (0.8%)	1.42	2/179 (1.1%)
3	G	0.78	1/227 (0.4%)	1.13	0/349
3	P	0.80	0/227	1.33	1/349 (0.3%)
4	F	0.67	0/362	1.25	1/556 (0.2%)
4	T	0.73	0/362	1.30	4/556 (0.7%)
All	All	0.51	4/6675 (0.1%)	0.77	10/9240 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	DG	OP3-P	-10.17	1.49	1.61
2	D	1	DG	OP3-P	-9.94	1.49	1.61
3	G	9	DG	O3'-P	5.91	1.68	1.61
1	B	190	ASP	C-N	5.76	1.47	1.34

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2	DT	O4'-C1'-N1	-7.29	102.90	108.00
3	P	4	DG	O4'-C1'-N9	-7.13	103.01	108.00
4	T	4	DA	O4'-C1'-N9	-6.76	103.27	108.00
4	T	14	DA	O4'-C1'-N9	-6.10	103.73	108.00
4	T	7	DG	O4'-C1'-N9	5.55	111.89	108.00
4	F	12	DT	N3-C4-O4	5.45	123.17	119.90
4	T	12	DT	P-O5'-C5'	-5.37	112.31	120.90
2	D	1	DG	O4'-C1'-N9	-5.21	104.35	108.00
2	D	2	DT	O4'-C1'-N1	-5.12	104.42	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	DG	O4'-C1'-N9	-5.10	104.43	108.00

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	2581	0	2590	42	0
1	B	2583	0	2587	66	0
2	C	106	0	57	4	0
2	D	106	0	57	0	0
3	G	203	0	113	1	0
3	P	203	0	114	1	0
4	F	323	0	179	7	0
4	T	323	0	179	3	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	G	1	0	0	0	0
5	T	1	0	0	0	0
6	A	30	0	12	3	0
6	B	30	0	12	0	0
7	B	2	0	0	0	0
7	D	1	0	0	0	0
7	T	1	0	0	0	0
8	A	184	0	0	8	0
8	B	120	0	0	3	0
8	C	4	0	0	1	0
8	D	17	0	0	0	0
8	F	17	0	0	0	0
8	G	12	0	0	0	0
8	P	19	0	0	1	0
8	T	41	0	0	1	0
All	All	6910	0	5900	121	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 10.

All (121) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:292:THR:HB	1:B:301:LEU:HD21	1.49	0.95
1:B:287:LEU:HD23	1:B:301:LEU:CD1	1.98	0.93
1:B:10:THR:O	1:B:10:THR:HG22	1.68	0.91
1:B:174:ILE:HB	1:B:196:THR:HG22	1.54	0.89
1:B:292:THR:CB	1:B:301:LEU:HD21	2.10	0.81
1:A:328:ARG:HH11	1:A:328:ARG:HB2	1.46	0.79
1:B:287:LEU:CD2	1:B:301:LEU:CD1	2.60	0.79
1:B:292:THR:CG2	1:B:301:LEU:HD21	2.13	0.79
1:B:282:MET:HB2	1:B:325:TRP:CZ3	2.17	0.79
1:A:36:TYR:CE1	1:A:40:ARG:HD2	2.20	0.76
1:B:287:LEU:HD23	1:B:301:LEU:HD11	1.69	0.72
1:A:116:ASP:HB2	8:A:667:HOH:O	1.90	0.71
1:A:33:ILE:HG22	8:A:664:HOH:O	1.91	0.71
4:F:2:DC:H4'	4:F:3:DG:OP1	1.92	0.69
4:T:6:DG:N7	8:T:201:HOH:O	2.26	0.68
1:B:244:LYS:O	1:B:247:GLU:HB2	1.94	0.66
4:F:2:DC:H2''	4:F:3:DG:C8	2.30	0.66
1:A:207:GLN:N	1:A:208:PRO:HD3	2.10	0.66
1:B:83:ARG:NH1	1:B:83:ARG:HB3	2.11	0.65
1:B:10:THR:CG2	1:B:10:THR:O	2.42	0.64
1:A:75:GLU:OE2	1:A:83:ARG:HG2	1.96	0.64
1:A:81:LYS:NZ	1:A:86:GLU:HG3	2.12	0.64
1:B:174:ILE:HB	1:B:196:THR:CG2	2.28	0.64
1:B:206:LYS:HB3	1:B:206:LYS:NZ	2.13	0.64
1:B:194:LEU:HD11	1:B:260:ILE:HG12	1.81	0.62
1:B:12:ASN:HD21	1:B:53:ILE:H	1.48	0.61
1:A:36:TYR:CZ	1:A:40:ARG:CD	2.85	0.60
1:A:196:THR:HB	1:A:265:TYR:CD1	2.36	0.60
1:A:245:ASN:O	8:A:614:HOH:O	2.17	0.59
1:B:194:LEU:HD11	1:B:260:ILE:CG1	2.33	0.58
1:B:287:LEU:CD2	1:B:301:LEU:HD13	2.32	0.58
3:P:2:DC:H2'	3:P:3:DT:H71	1.84	0.58
1:B:36:TYR:CZ	1:B:40:ARG:HD2	2.39	0.58
1:B:36:TYR:CE1	1:B:40:ARG:HD2	2.39	0.57
1:B:206:LYS:HZ3	1:B:206:LYS:HB3	1.68	0.57
1:B:194:LEU:CD1	1:B:260:ILE:HG12	2.35	0.57
6:A:402:6CF:O5'	6:A:402:6CF:H6	2.04	0.57
1:A:244:LYS:CB	1:A:247:GLU:H	2.18	0.57
1:B:195:LEU:O	1:B:259:LEU:HD12	2.04	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:12:ASN:ND2	1:B:53:ILE:H	2.02	0.56
1:A:36:TYR:CZ	1:A:40:ARG:HD2	2.40	0.56
1:A:328:ARG:HB2	1:A:328:ARG:NH1	2.18	0.56
1:B:287:LEU:CD2	1:B:301:LEU:HD11	2.31	0.55
1:B:195:LEU:HD21	1:B:214:VAL:HG21	1.87	0.55
2:C:5:DG:H1	4:F:1:DC:H42	1.53	0.55
1:B:18:MET:SD	1:B:82:LEU:HG	2.47	0.55
1:A:244:LYS:O	1:A:245:ASN:CB	2.55	0.54
1:A:36:TYR:CE1	1:A:40:ARG:CD	2.92	0.53
1:B:292:THR:HB	1:B:301:LEU:HD11	1.90	0.53
1:B:199:SER:OG	1:B:210:LEU:HD11	2.09	0.52
3:G:3:DT:H2"	3:G:4:DG:C8	2.45	0.52
1:B:292:THR:HB	1:B:301:LEU:CD2	2.31	0.52
1:A:159:GLN:O	1:A:163:LEU:HG	2.10	0.52
1:A:32:ALA:HB1	1:A:35:LYS:HG3	1.91	0.52
1:B:163:LEU:HD22	1:B:175:ALA:HB3	1.93	0.51
1:B:161:ILE:O	1:B:165:GLU:HG2	2.11	0.50
1:A:51:HIS:NE2	8:A:647:HOH:O	2.34	0.50
1:B:260:ILE:HG23	1:B:261:PRO:HD2	1.93	0.50
1:B:135:HIS:HD2	8:B:556:HOH:O	1.93	0.50
1:A:165:GLU:O	1:A:169:VAL:HG23	2.12	0.49
1:A:121:THR:HB	8:A:668:HOH:O	2.12	0.49
1:B:284:ALA:O	1:B:288:GLU:HG3	2.13	0.48
1:A:288:GLU:HG3	8:A:644:HOH:O	2.13	0.48
1:B:209:LYS:HB3	1:B:212:HIS:HB3	1.93	0.48
1:A:218:LEU:HB2	1:A:224:ILE:HD12	1.95	0.48
1:B:48:LYS:O	1:B:50:PRO:HD3	2.14	0.48
2:C:4:DG:N7	8:C:102:HOH:O	2.34	0.48
1:B:278:PHE:HB2	1:B:335:GLU:HG3	1.96	0.48
1:A:209:LYS:O	1:A:213:GLN:HG3	2.14	0.48
1:B:287:LEU:HD22	1:B:301:LEU:HD13	1.96	0.47
1:A:33:ILE:O	1:A:36:TYR:HB3	2.15	0.47
1:A:81:LYS:HZ3	1:A:86:GLU:HG3	1.79	0.47
1:B:206:LYS:CB	1:B:206:LYS:NZ	2.77	0.47
1:A:162:VAL:O	1:A:166:VAL:HG23	2.15	0.47
1:B:236:MET:HE3	1:B:254:ARG:NH2	2.29	0.47
1:B:258:ARG:NH2	8:B:577:HOH:O	2.48	0.47
6:A:402:6CF:O2	4:T:6:DG:N2	2.45	0.46
1:B:291:PHE:C	1:B:301:LEU:CD1	2.84	0.46
1:B:155:MET:HE2	1:B:181:PHE:HB2	1.98	0.46
1:A:157:GLN:O	1:A:161:ILE:HG13	2.14	0.46
1:B:314:ASP:HB2	8:B:616:HOH:O	2.17	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:158:MET:O	1:B:162:VAL:HG23	2.16	0.45
2:C:5:DG:H1	4:F:1:DC:N4	2.15	0.45
1:A:110:ALA:HB2	8:P:103:HOH:O	2.16	0.45
1:B:283:LYS:HE3	4:F:6:DG:H21	1.82	0.45
1:B:197:HIS:CG	1:B:198:PRO:HD2	2.51	0.45
1:B:248:LYS:HE3	1:B:248:LYS:HB2	1.68	0.45
2:C:3:DC:H2'	2:C:4:DG:C8	2.51	0.44
1:B:292:THR:HG22	1:B:301:LEU:HD21	1.96	0.44
1:B:79:THR:OG1	1:B:81:LYS:HG2	2.18	0.44
1:B:104:SER:OG	1:B:135:HIS:HE1	1.99	0.44
1:B:83:ARG:CZ	1:B:83:ARG:HB3	2.47	0.43
1:B:12:ASN:HD21	1:B:53:ILE:N	2.15	0.43
1:B:82:LEU:HA	1:B:82:LEU:HD23	1.80	0.43
1:B:83:ARG:CB	1:B:83:ARG:NH1	2.80	0.43
1:A:81:LYS:HE3	1:A:83:ARG:HD2	2.00	0.43
1:A:178:CYS:O	8:A:502:HOH:O	2.22	0.43
1:B:83:ARG:CB	1:B:83:ARG:HH11	2.31	0.43
1:B:165:GLU:OE1	1:B:221:VAL:HG11	2.19	0.43
4:F:1:DC:H2''	4:F:2:DC:O5'	2.19	0.42
1:B:154:GLU:O	1:B:158:MET:HG3	2.19	0.42
1:B:166:VAL:CG1	1:B:173:TYR:CB	2.97	0.42
1:A:284:ALA:HA	8:A:589:HOH:O	2.19	0.42
1:A:11:LEU:HA	1:A:11:LEU:HD23	1.84	0.42
1:A:149:ARG:NH2	6:A:402:6CF:O2G	2.50	0.42
1:A:138:ILE:HD13	1:A:226:ASP:HB3	2.01	0.42
1:B:166:VAL:CG1	1:B:173:TYR:HB3	2.49	0.42
1:A:183:ARG:O	1:A:331:LYS:HA	2.20	0.42
1:A:170:ASP:HB3	1:A:173:TYR:CD2	2.55	0.42
1:B:295:GLU:OE1	4:F:8:DC:H4'	2.20	0.41
1:A:123:GLU:HG3	1:A:123:GLU:H	1.64	0.41
1:A:81:LYS:HZ2	1:A:86:GLU:HG3	1.82	0.41
1:B:221:VAL:O	1:B:221:VAL:HG23	2.21	0.41
1:B:183:ARG:O	1:B:331:LYS:HD3	2.21	0.41
1:A:330:PRO:HA	1:A:333:ARG:HD2	2.02	0.41
1:A:12:ASN:ND2	1:A:53:ILE:HD12	2.35	0.41
4:T:5:DC:H2''	4:T:6:DG:OP1	2.21	0.41
1:B:287:LEU:HD23	1:B:301:LEU:HD12	1.94	0.40
1:A:244:LYS:C	1:A:246:ASP:H	2.23	0.40
1:A:81:LYS:CE	1:A:83:ARG:HD2	2.52	0.40
1:B:276:ASP:OD2	1:B:277:ILE:N	2.54	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	321/335 (96%)	310 (97%)	11 (3%)	0	100	100
1	B	318/335 (95%)	308 (97%)	10 (3%)	0	100	100
All	All	639/670 (95%)	618 (97%)	21 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	280/295 (95%)	270 (96%)	10 (4%)	47	56
1	B	282/295 (96%)	269 (95%)	13 (5%)	37	43
All	All	562/590 (95%)	539 (96%)	23 (4%)	41	49

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	85	LEU
1	A	113	LYS
1	A	123	GLU
1	A	160	ASP
1	A	172	GLU
1	A	205	THR
1	A	243	SER
1	A	325	TRP
1	A	326	LYS
1	A	328	ARG
1	B	82	LEU

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Mol	Chain	Res	Type
1	B	112	ARG
1	B	116	ASP
1	B	196	THR
1	B	205	THR
1	B	206	LYS
1	B	209	LYS
1	B	269	VAL
1	B	271	TYR
1	B	272	PHE
1	B	295	GLU
1	B	325	TRP
1	B	335	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	264	GLN
1	B	12	ASN
1	B	135	HIS
1	B	213	GLN
1	B	264	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 8 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	$\# Z  > 2$
6	6CF	A	402	-	31,31,31	2.08	10 (32%)	46,50,50	2.23	9 (19%)
6	6CF	B	404	7	31,31,31	2.04	10 (32%)	46,50,50	2.59	10 (21%)

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
6	6CF	A	402	-	-	0/28/46/46	0/2/2/2
6	6CF	B	404	7	-	0/28/46/46	0/2/2/2

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	402	6CF	O2-C2	6.82	1.37	1.23
6	B	404	6CF	O2-C2	6.59	1.37	1.23
6	B	404	6CF	P2-O1B	3.52	1.57	1.51
6	A	402	6CF	C6-N1	3.31	1.41	1.35
6	A	402	6CF	C4-N4	3.23	1.45	1.35
6	B	404	6CF	P1-O2A	3.04	1.56	1.51
6	A	402	6CF	F2A-C3A	-3.00	1.33	1.36
6	B	404	6CF	C4-N4	2.98	1.44	1.35
6	B	404	6CF	C6-N1	2.96	1.40	1.35
6	A	402	6CF	P1-O2A	2.75	1.56	1.51
6	B	404	6CF	F2A-C3A	-2.71	1.33	1.36
6	A	402	6CF	P2-O1B	2.61	1.55	1.51
6	A	402	6CF	O3'-C3'	-2.52	1.37	1.43
6	B	404	6CF	C2-N3	2.47	1.42	1.35
6	A	402	6CF	C2-N3	2.40	1.42	1.35
6	B	404	6CF	O3'-C3'	-2.36	1.38	1.43
6	B	404	6CF	F1A-C3A	-2.24	1.34	1.36
6	A	402	6CF	O4'-C4'	-2.22	1.39	1.45
6	B	404	6CF	O4'-C4'	-2.21	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	402	6CF	F1A-C3A	-2.17	1.34	1.36

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	404	6CF	O1A-P1-C3A	10.17	112.22	105.23
6	B	404	6CF	O2B-P2-C3A	8.56	111.12	105.23
6	A	402	6CF	O2B-P2-C3A	8.42	111.02	105.23
6	B	404	6CF	F2A-C3A-F1A	6.19	111.18	105.53
6	A	402	6CF	O1A-P1-C3A	6.13	109.44	105.23
6	B	404	6CF	O5'-P1-O2A	-4.54	106.52	115.00
6	A	402	6CF	O5'-P1-O2A	-4.36	106.86	115.00
6	A	402	6CF	F2A-C3A-F1A	3.96	109.15	105.53
6	A	402	6CF	C2-N3-C4	3.28	120.32	115.57
6	A	402	6CF	P3-O3B-P2	-3.27	120.63	131.81
6	A	402	6CF	O1B-P2-C3A	-3.17	107.06	112.80
6	B	404	6CF	O1B-P2-C3A	-2.82	107.69	112.80
6	A	402	6CF	P1-O5'-C5'	-2.78	118.43	122.09
6	B	404	6CF	P3-O3B-P2	-2.76	122.37	131.81
6	B	404	6CF	C2-N3-C4	2.71	119.49	115.57
6	A	402	6CF	P2-C3A-P1	-2.60	107.47	114.26
6	B	404	6CF	O2G-P3-O3G	-2.42	102.52	110.44
6	B	404	6CF	O4'-C1'-N1	2.26	111.93	107.68
6	B	404	6CF	O1G-P3-O3B	2.17	115.41	105.14

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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	325/335 (97%)	0.24	18 (5%) 24 24	18, 31, 51, 80	0
1	B	321/335 (95%)	0.35	17 (5%) 25 25	23, 37, 56, 68	0
2	C	5/5 (100%)	0.08	0 100 100	35, 37, 48, 51	0
2	D	5/5 (100%)	-0.48	0 100 100	22, 26, 31, 32	0
3	G	10/10 (100%)	-0.28	0 100 100	29, 39, 49, 49	0
3	P	10/10 (100%)	-0.35	0 100 100	24, 31, 36, 41	0
4	F	16/16 (100%)	0.18	0 100 100	31, 46, 63, 65	0
4	T	16/16 (100%)	-0.36	0 100 100	24, 34, 41, 44	0
All	All	708/732 (96%)	0.25	35 (4%) 28 28	18, 34, 55, 80	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	245	ASN	5.9
1	A	10	THR	5.3
1	B	10	THR	5.3
1	B	301	LEU	5.2
1	B	78	ALA	4.2
1	A	244	LYS	3.8
1	A	11	LEU	3.7
1	B	307	ALA	3.6
1	B	79	THR	3.5
1	A	42	ALA	3.4
1	A	208	PRO	3.4
1	B	246	ASP	3.3
1	A	116	ASP	3.2
1	A	303	VAL	3.1
1	B	293	ILE	3.0
1	A	246	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	304	THR	2.7
1	A	90	GLN	2.7
1	B	282	MET	2.7
1	B	248	LYS	2.7
1	B	130	ASP	2.7
1	A	270	LEU	2.5
1	A	202	SER	2.5
1	A	204	SER	2.4
1	A	248	LYS	2.4
1	B	84	LYS	2.4
1	B	90	GLN	2.4
1	B	92	ASP	2.3
1	A	257	ILE	2.2
1	B	319	ILE	2.2
1	B	54	LYS	2.2
1	B	80	GLY	2.2
1	A	19	LEU	2.1
1	A	86	GLU	2.1
1	B	87	LYS	2.1

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

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

## 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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
6	6CF	A	402	30/30	0.14	0.08	27,40,54,62	0
5	NA	G	101	1/1	0.14	-0.58	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	6CF	B	404	30/30	0.12	-0.59	26,32,37,41	0
5	NA	B	403	1/1	0.12	-0.85	33,33,33,33	0
5	NA	T	102	1/1	0.10	-1.36	54,54,54,54	0
7	MN	B	402	1/1	0.07	-1.72	29,29,29,29	0
5	NA	A	401	1/1	0.06	-2.22	22,22,22,22	0
7	MN	B	401	1/1	0.06	-2.87	27,27,27,27	0
7	MN	T	101	1/1	0.05	-5.21	39,39,39,39	0
7	MN	D	101	1/1	0.05	-5.69	36,36,36,36	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.