



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:46 AM GMT

PDB ID : 2E9T  
Title : Foot-and-mouth disease virus RNA-polymerase RNA dependent in complex with a template-primer RNA and 5F-UTP  
Authors : Ferrer-Orta, C.; Arias, A.; Perez-Luque, R.; Escarmis, C.; Domingo, E.; Verdaguier, N.  
Deposited on : 2007-01-26  
Resolution : 2.60 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](mailto: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.

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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 : 1.7 (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

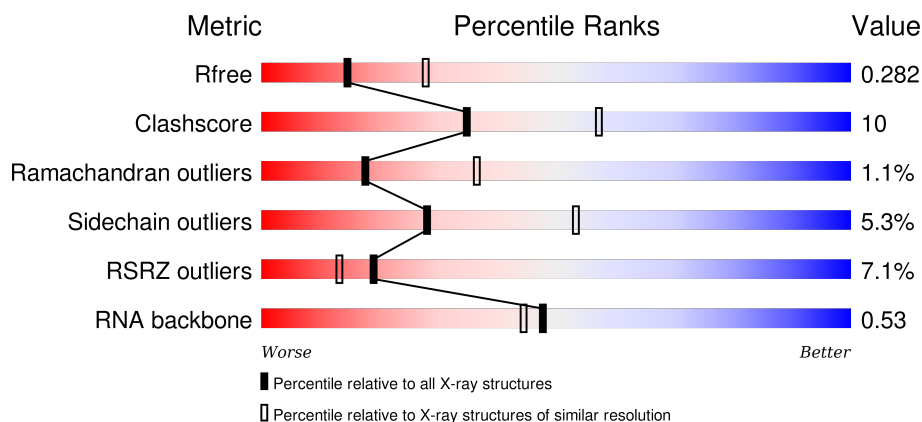
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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))
$R_{free}$	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)
RNA backbone	2183	1022 (3.00-2.20)

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. 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	B	8	<div> <div>38%</div> <div> <div>13%</div> <div>63%</div> <div>13%</div> <div>13%</div> </div> </div>
1	E	8	<div> <div>25%</div> <div> <div>13%</div> <div>50%</div> <div>38%</div> </div> </div>
2	C	7	<div> <div>43%</div> <div> <div>29%</div> <div>57%</div> <div>14%</div> </div> </div>
2	F	7	<div> <div>43%</div> <div> <div>29%</div> <div>71%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
3	A	476	 6% 81% 16% •
3	D	476	 6% 80% 17% •

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
5	PPV	A	930	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8205 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 RNA chain called 5'-R(P\*UP\*AP\*GP\*GP\*GP\*CP\*CP\*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	8	Total	C	N	O	P	0	0	0
			171	76	31	56	8			
1	E	8	Total	C	N	O	P	0	0	0
			171	76	31	56	8			

- Molecule 2 is a RNA chain called 5'-R(\*GP\*GP\*GP\*CP\*CP\*CP\*(5FU))-3'.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	7	Total	C	F	N	O	P	0	0	0
			147	66	1	26	48	6			
2	F	7	Total	C	F	N	O	P	0	0	0
			147	66	1	26	48	6			

- Molecule 3 is a protein called RNA-dependent RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	474	Total	C	N	O	S	0	0	0
			3741	2378	647	695	21			
3	D	474	Total	C	N	O	S	0	0	0
			3741	2378	647	695	21			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	471	ALA	-	CLONING ARTIFACT	UNP Q0QEE1
A	472	ALA	-	CLONING ARTIFACT	UNP Q0QEE1
A	473	LEU	-	CLONING ARTIFACT	UNP Q0QEE1
A	474	GLU	-	CLONING ARTIFACT	UNP Q0QEE1
A	475	HIS	-	CLONING ARTIFACT	UNP Q0QEE1
A	476	HIS	-	CLONING ARTIFACT	UNP Q0QEE1
D	471	ALA	-	CLONING ARTIFACT	UNP Q0QEE1
D	472	ALA	-	CLONING ARTIFACT	UNP Q0QEE1

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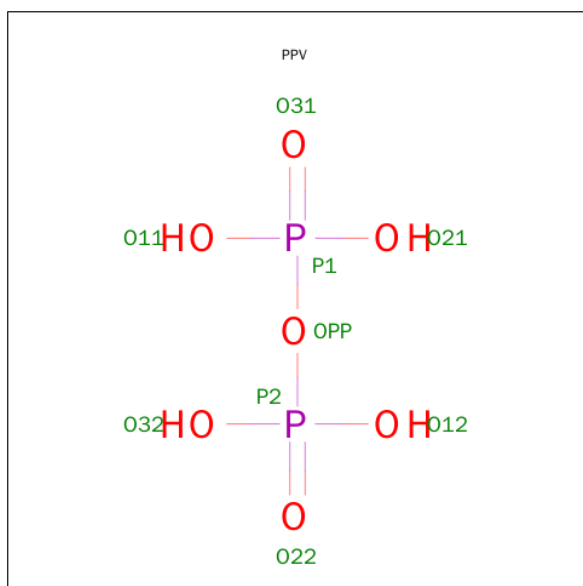
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Chain	Residue	Modelled	Actual	Comment	Reference
D	473	LEU	-	CLONING ARTIFACT	UNP Q0QEE1
D	474	GLU	-	CLONING ARTIFACT	UNP Q0QEE1
D	475	HIS	-	CLONING ARTIFACT	UNP Q0QEE1
D	476	HIS	-	CLONING ARTIFACT	UNP Q0QEE1

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

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

- Molecule 5 is PYROPHOSPHATE (three-letter code: PPV) (formula: H<sub>4</sub>O<sub>7</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O P 9 7 2	0	0
5	D	1	Total O P 9 7 2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	35	Total O 35 35	0	0

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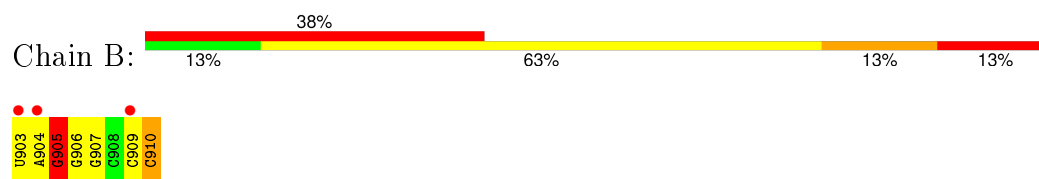
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	2	Total 2	O 2	0	0
6	C	1	Total 1	O 1	0	0
6	D	24	Total 24	O 24	0	0
6	E	2	Total 2	O 2	0	0
6	F	1	Total 1	O 1	0	0

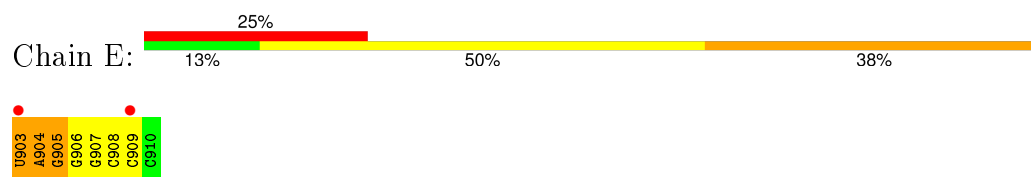
### 3 Residue-property plots [i](#)

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.

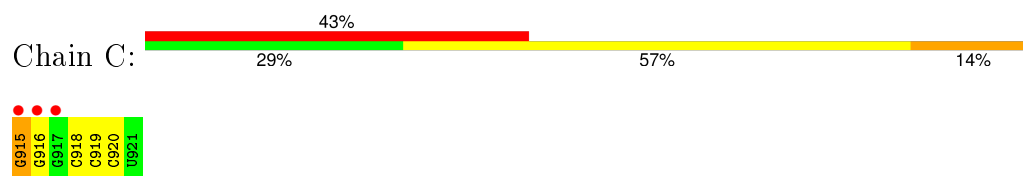
- Molecule 1: 5'-R(P\*UP\*AP\*GP\*GP\*GP\*CP\*CP\*C)-3'



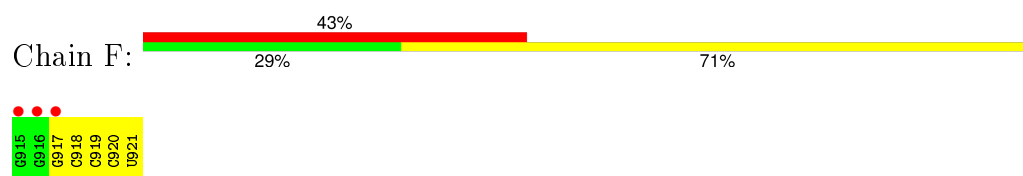
- Molecule 1: 5'-R(P\*UP\*AP\*GP\*GP\*GP\*CP\*CP\*C)-3'



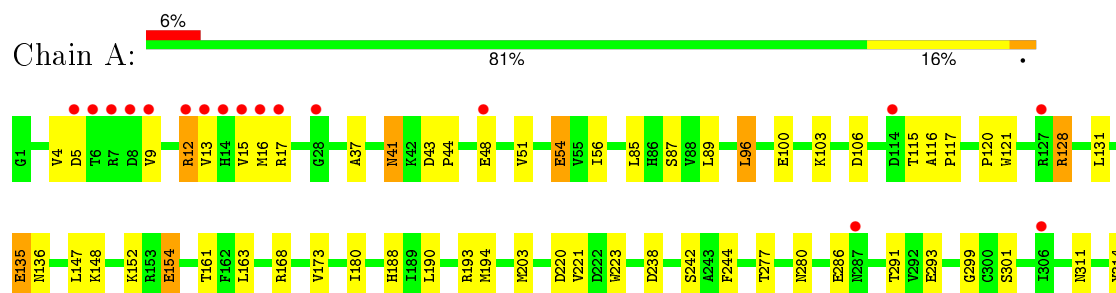
- Molecule 2: 5'-R(\*GP\*GP\*GP\*CP\*CP\*CP\*(5FU))-3'



- Molecule 2: 5'-R(\*GP\*GP\*GP\*CP\*CP\*CP\*(5FU))-3'

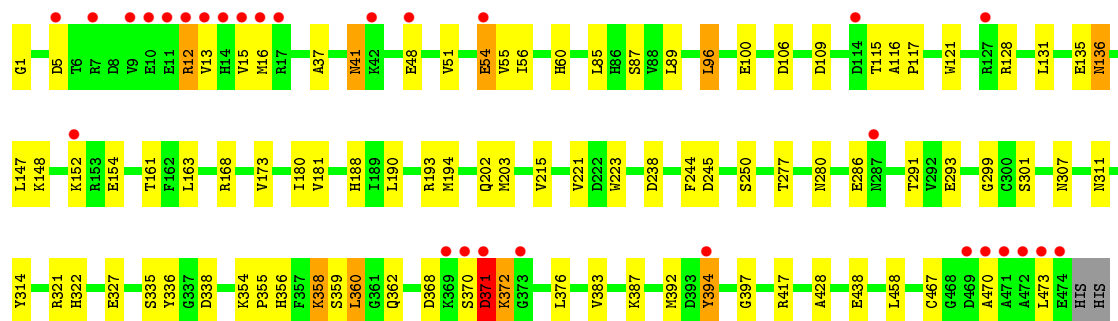
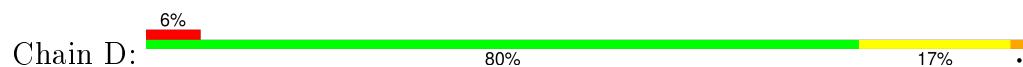


- Molecule 3: RNA-dependent RNA polymerase





● Molecule 3: RNA-dependent RNA polymerase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	95.60Å 95.60Å 201.16Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.60 29.88 – 2.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-2.60) 100.0 (29.88-2.60)	Depositor EDS
$R_{merge}$	0.90	Depositor
$R_{sym}$	0.74	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.19 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.233 , 0.289 0.229 , 0.282	Depositor DCC
$R_{free}$ test set	1691 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	45.2	Xtriage
Anisotropy	0.080	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 54.9	EDS
Estimated twinning fraction	0.028 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 33529 reflections (0.003%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8205	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 81.22 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 3.7341e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical 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: MG, 5FU, PPV

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	B	1.01	0/190	1.71	4/294 (1.4%)
1	E	1.06	0/190	1.72	3/294 (1.0%)
2	C	0.84	0/140	1.37	0/217
2	F	0.87	0/140	1.50	0/217
3	A	0.64	0/3830	0.69	0/5186
3	D	0.65	0/3830	0.70	0/5186
All	All	0.67	0/8320	0.82	7/11394 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	D	0	1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	910	C	C1'-O4'-C4'	-6.98	104.31	109.90
1	E	909	C	O4'-C1'-N1	6.64	113.51	108.20
1	B	909	C	O4'-C1'-N1	6.59	113.48	108.20
1	E	908	C	O4'-C1'-N1	6.33	113.27	108.20
1	B	910	C	O4'-C1'-N1	6.12	113.09	108.20
1	E	903	U	O4'-C1'-N1	5.70	112.76	108.20
1	B	905	G	C1'-O4'-C4'	-5.21	105.74	109.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	371	ASP	Peptide

## 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	B	171	0	88	14	0
1	E	171	0	88	11	0
2	C	147	0	77	6	0
2	F	147	0	77	6	0
3	A	3741	0	3669	72	0
3	D	3741	0	3669	68	0
4	A	2	0	0	0	0
4	D	2	0	0	0	0
5	A	9	0	0	0	0
5	D	9	0	0	0	0
6	A	35	0	0	7	0
6	B	2	0	0	0	0
6	C	1	0	0	0	0
6	D	24	0	0	1	0
6	E	2	0	0	0	0
6	F	1	0	0	0	0
All	All	8205	0	7668	156	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 10.

All (156) 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)
3:D:467:CYS:SG	3:D:470:ALA:HB3	1.64	1.37
3:A:467:CYS:SG	3:A:470:ALA:HB3	1.74	1.26
3:A:85:LEU:HD11	3:A:203:MET:CE	1.72	1.19
3:D:85:LEU:HD11	3:D:203:MET:CE	1.83	1.08
3:D:85:LEU:HD11	3:D:203:MET:HE1	1.01	1.01
3:D:467:CYS:SG	3:D:470:ALA:CB	2.49	1.00
3:A:85:LEU:CD1	3:A:203:MET:HE1	1.94	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:85:LEU:HD11	3:A:203:MET:HE1	0.97	0.95
3:A:120:PRO:HD2	6:A:979:HOH:O	1.65	0.94
3:D:12:ARG:HH11	3:D:12:ARG:HG2	1.33	0.93
3:A:121:TRP:CD2	6:A:979:HOH:O	2.23	0.91
3:D:85:LEU:CD1	3:D:203:MET:HE1	1.97	0.90
3:A:12:ARG:HH11	3:A:12:ARG:HG2	1.33	0.90
3:D:467:CYS:O	3:D:467:CYS:SG	2.32	0.88
3:D:12:ARG:HH11	3:D:12:ARG:CG	1.87	0.87
3:A:467:CYS:SG	3:A:470:ALA:CB	2.62	0.85
3:A:121:TRP:CE2	6:A:979:HOH:O	2.30	0.85
3:A:12:ARG:HH11	3:A:12:ARG:CG	1.90	0.84
3:D:89:LEU:HD11	3:D:203:MET:CE	2.13	0.78
3:A:321:ARG:HH11	3:A:356:HIS:HD2	1.32	0.77
3:A:467:CYS:SG	3:A:467:CYS:O	2.42	0.76
3:D:89:LEU:HD11	3:D:203:MET:HE2	1.68	0.75
1:E:904:A:O4'	3:D:299:GLY:HA2	1.88	0.74
3:A:121:TRP:CG	6:A:979:HOH:O	2.39	0.73
1:B:903:U:H5''	3:A:115:THR:HB	1.70	0.72
2:F:919:C:H2'	2:F:920:C:C6	2.25	0.72
3:A:56:ILE:HG23	3:A:180:ILE:HG21	1.72	0.71
2:F:919:C:H2'	2:F:920:C:H6	1.56	0.70
3:D:322:HIS:ND1	3:D:356:HIS:HE1	1.91	0.69
3:D:280:ASN:ND2	3:D:293:GLU:HG2	2.08	0.68
3:D:56:ILE:HG23	3:D:180:ILE:HG21	1.75	0.68
3:D:321:ARG:HH11	3:D:356:HIS:HD2	1.40	0.67
1:E:904:A:C1'	3:D:299:GLY:HA2	2.24	0.66
3:A:322:HIS:ND1	3:A:356:HIS:HE1	1.94	0.66
3:A:89:LEU:HD11	3:A:203:MET:CE	2.26	0.65
2:C:918:C:H2'	2:C:919:C:C6	2.31	0.65
3:A:467:CYS:HG	3:A:470:ALA:HB3	1.62	0.64
1:B:904:A:O4'	3:A:299:GLY:HA2	1.98	0.63
3:D:12:ARG:HG2	3:D:12:ARG:NH1	2.07	0.63
3:D:250:SER:HB2	6:D:1967:HOH:O	1.99	0.62
3:A:89:LEU:HD11	3:A:203:MET:HE2	1.80	0.62
3:A:37:ALA:HA	3:A:173:VAL:HG22	1.82	0.62
3:A:121:TRP:CD1	6:A:979:HOH:O	2.52	0.62
3:A:85:LEU:CD1	3:A:203:MET:CE	2.65	0.61
3:A:115:THR:O	3:A:128:ARG:HD3	2.00	0.61
3:D:37:ALA:HA	3:D:173:VAL:HG22	1.81	0.61
3:A:327:GLU:OE1	3:A:327:GLU:HA	2.00	0.61
3:A:12:ARG:HG2	3:A:12:ARG:NH1	2.09	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:238:ASP:HB2	3:D:383:VAL:HG12	1.83	0.61
1:B:910:C:H42	2:C:915:G:H1	1.49	0.60
3:A:9:VAL:HG11	6:A:982:HOH:O	2.01	0.60
1:B:903:U:H5'	3:A:116:ALA:H	1.67	0.60
3:D:12:ARG:NH1	3:D:12:ARG:CG	2.58	0.59
3:A:13:VAL:O	3:A:286:GLU:HA	2.03	0.59
3:D:89:LEU:HD11	3:D:203:MET:HE3	1.84	0.59
1:B:904:A:O2'	3:A:301:SER:HA	2.02	0.58
2:C:915:G:H5''	2:C:915:G:C8	2.38	0.58
3:D:13:VAL:O	3:D:286:GLU:HA	2.04	0.58
2:C:918:C:H2'	2:C:919:C:H6	1.69	0.57
3:D:115:THR:O	3:D:128:ARG:HD3	2.04	0.57
3:A:120:PRO:CD	6:A:979:HOH:O	2.37	0.56
2:F:918:C:H2'	2:F:919:C:C6	2.41	0.56
3:D:152:LYS:HB3	3:D:154:GLU:HG3	1.87	0.56
3:D:15:VAL:HG11	3:D:161:THR:O	2.06	0.56
3:A:280:ASN:ND2	3:A:293:GLU:HG2	2.21	0.55
3:D:15:VAL:HG23	3:D:16:MET:H	1.71	0.54
3:D:48:GLU:OE1	3:D:48:GLU:HA	2.06	0.54
3:D:96:LEU:HG	3:D:100:GLU:HB3	1.89	0.54
3:A:56:ILE:HD11	3:A:163:LEU:HD21	1.90	0.54
3:D:356:HIS:O	3:D:359:SER:OG	2.19	0.53
3:D:355:PRO:HA	3:D:358:LYS:HB2	1.90	0.53
3:D:314:TYR:CD1	3:D:360:LEU:HD13	2.43	0.53
3:A:188:HIS:HE1	3:A:277:THR:OG1	1.92	0.53
3:A:96:LEU:HG	3:A:100:GLU:HB3	1.89	0.53
1:E:905:G:H2'	1:E:906:G:C8	2.44	0.53
3:D:368:ASP:O	3:D:368:ASP:OD1	2.27	0.53
3:A:392:MET:SD	3:A:397:GLY:O	2.67	0.53
3:A:398:PHE:HE2	3:A:467:CYS:SG	2.31	0.52
3:A:48:GLU:HA	3:A:48:GLU:OE1	2.10	0.52
3:D:327:GLU:OE1	3:D:327:GLU:HA	2.10	0.51
3:D:280:ASN:HD21	3:D:293:GLU:HG2	1.74	0.51
3:D:51:VAL:HB	3:D:54:GLU:HB2	1.92	0.51
3:A:355:PRO:HA	3:A:358:LYS:HB2	1.93	0.51
3:A:56:ILE:HD11	3:A:163:LEU:CD2	2.41	0.51
3:A:314:TYR:CD1	3:A:360:LEU:HD13	2.45	0.51
3:A:56:ILE:CD1	3:A:163:LEU:HD21	2.42	0.50
1:E:903:U:H5'	3:D:116:ALA:H	1.76	0.50
3:A:238:ASP:HB2	3:A:383:VAL:HG12	1.93	0.50
3:A:152:LYS:HB3	3:A:154:GLU:HG3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:392:MET:SD	3:D:397:GLY:O	2.69	0.49
2:F:921:5FU:O3'	3:D:338:ASP:OD1	2.26	0.49
1:B:904:A:C1'	3:A:299:GLY:HA2	2.43	0.49
1:B:906:G:H2'	1:B:907:G:O4'	2.13	0.49
3:A:370:SER:O	3:A:372:LYS:N	2.46	0.49
3:D:188:HIS:HE1	3:D:277:THR:OG1	1.96	0.48
3:A:4:VAL:CG2	3:A:291:THR:HG22	2.44	0.48
1:E:904:A:O4'	3:D:299:GLY:CA	2.59	0.48
3:A:51:VAL:HB	3:A:54:GLU:HB2	1.94	0.48
3:A:244:PHE:HA	3:A:362:GLN:HE22	1.78	0.48
2:C:920:C:H5''	3:A:387:LYS:HE2	1.95	0.48
3:D:244:PHE:HA	3:D:362:GLN:HE22	1.79	0.48
3:D:168:ARG:HB2	3:D:173:VAL:HG23	1.96	0.48
1:E:903:U:H1'	3:D:181:VAL:HG11	1.96	0.48
3:D:85:LEU:CD1	3:D:203:MET:CE	2.74	0.47
3:A:220:ASP:OD1	3:A:433:HIS:HE1	1.97	0.47
3:A:15:VAL:HG11	3:A:161:THR:O	2.13	0.47
3:A:368:ASP:OD1	3:A:368:ASP:O	2.33	0.47
3:A:168:ARG:HB2	3:A:173:VAL:HG23	1.96	0.46
3:A:89:LEU:HD11	3:A:203:MET:HE3	1.96	0.46
1:B:903:U:H5'	3:A:116:ALA:CB	2.46	0.46
3:A:96:LEU:HD22	3:A:193:ARG:O	2.15	0.46
3:D:121:TRP:CD2	3:D:131:LEU:HD21	2.51	0.46
3:D:245:ASP:CG	3:D:307:ASN:HD21	2.19	0.46
3:A:117:PRO:HA	3:A:128:ARG:HD2	1.99	0.45
1:B:904:A:H2'	1:B:905:G:O4'	2.15	0.45
1:E:904:A:C8	3:D:299:GLY:HA2	2.52	0.45
1:E:905:G:H2'	1:E:906:G:H8	1.82	0.45
3:A:354:LYS:HB2	3:A:355:PRO:HD3	1.99	0.45
3:D:215:VAL:HA	3:D:336:TYR:CE1	2.51	0.45
3:A:121:TRP:CD2	3:A:131:LEU:HD21	2.53	0.44
3:A:96:LEU:HB2	3:A:194:MET:HA	1.99	0.44
1:B:904:A:C8	3:A:299:GLY:HA2	2.53	0.44
3:D:438:GLU:HA	3:D:438:GLU:OE1	2.17	0.44
3:D:354:LYS:HB2	3:D:355:PRO:HD3	2.00	0.44
3:D:56:ILE:HG23	3:D:180:ILE:CG2	2.47	0.44
3:D:51:VAL:O	3:D:55:VAL:HG23	2.18	0.44
3:D:96:LEU:HB2	3:D:194:MET:HA	2.00	0.43
3:D:89:LEU:HB3	3:D:202:GLN:HG2	2.01	0.43
2:C:915:G:N3	2:C:915:G:H2'	2.32	0.43
3:D:117:PRO:HA	3:D:128:ARG:HD2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:16:MET:CE	3:D:41:ASN:OD1	2.66	0.43
3:D:96:LEU:HD22	3:D:193:ARG:O	2.19	0.43
3:D:428:ALA:HB1	3:D:458:LEU:HD11	2.01	0.43
3:D:5:ASP:HB3	3:D:291:THR:HB	2.01	0.43
3:D:370:SER:O	3:D:372:LYS:N	2.52	0.42
3:D:371:ASP:HA	3:D:372:LYS:HE2	2.01	0.42
1:B:903:U:C5'	3:A:116:ALA:H	2.33	0.42
3:A:56:ILE:HG23	3:A:180:ILE:CG2	2.45	0.42
3:A:56:ILE:CD1	3:A:163:LEU:CD2	2.97	0.42
2:F:920:C:H5''	3:D:387:LYS:HE2	2.00	0.42
1:E:906:G:OP2	3:D:109:ASP:OD2	2.38	0.42
3:A:12:ARG:CG	3:A:12:ARG:NH1	2.60	0.41
1:B:903:U:H2'	1:B:904:A:C8	2.54	0.41
2:F:918:C:H2'	2:F:919:C:H6	1.85	0.41
3:A:5:ASP:HB3	3:A:291:THR:HB	2.01	0.41
3:A:103:LYS:NZ	3:A:135:GLU:O	2.48	0.41
1:E:904:A:O2'	3:D:301:SER:HA	2.20	0.41
1:E:906:G:H2'	1:E:907:G:O4'	2.21	0.41
3:A:17:ARG:HE	3:A:17:ARG:HB2	1.68	0.41
1:B:905:G:H2'	1:B:906:G:C8	2.55	0.41
3:D:56:ILE:HD11	3:D:163:LEU:CD2	2.50	0.41
3:D:1:GLY:N	3:D:60:HIS:HD2	2.19	0.41
3:A:16:MET:CE	3:A:41:ASN:OD1	2.70	0.40
3:A:43:ASP:HA	3:A:44:PRO:HD3	1.89	0.40
1:B:904:A:O4'	3:A:299:GLY:CA	2.68	0.40
3:D:136:ASN:HD22	3:D:136:ASN:HA	1.65	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	
3	A	472/476 (99%)	449 (95%)	17 (4%)	6 (1%)	15	30
3	D	472/476 (99%)	446 (94%)	22 (5%)	4 (1%)	24	46
All	All	944/952 (99%)	895 (95%)	39 (4%)	10 (1%)	17	36

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	371	ASP
3	D	371	ASP
3	A	106	ASP
3	A	468	GLY
3	D	106	ASP
3	A	372	LYS
3	A	394	TYR
3	D	372	LYS
3	A	370	SER
3	D	394	TYR

### 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	
3	A	397/399 (100%)	375 (94%)	22 (6%)	27	51
3	D	397/399 (100%)	377 (95%)	20 (5%)	30	56
All	All	794/798 (100%)	752 (95%)	42 (5%)	28	53

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	12	ARG
3	A	41	ASN
3	A	54	GLU
3	A	87	SER
3	A	96	LEU
3	A	128	ARG

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Mol	Chain	Res	Type
3	A	135	GLU
3	A	136	ASN
3	A	147	LEU
3	A	148	LYS
3	A	154	GLU
3	A	190	LEU
3	A	221	VAL
3	A	223	TRP
3	A	242	SER
3	A	311	ASN
3	A	358	LYS
3	A	360	LEU
3	A	376	LEU
3	A	394	TYR
3	A	417	ARG
3	A	473	LEU
3	D	12	ARG
3	D	41	ASN
3	D	54	GLU
3	D	87	SER
3	D	96	LEU
3	D	135	GLU
3	D	136	ASN
3	D	147	LEU
3	D	148	LYS
3	D	190	LEU
3	D	221	VAL
3	D	223	TRP
3	D	311	ASN
3	D	335	SER
3	D	358	LYS
3	D	360	LEU
3	D	376	LEU
3	D	394	TYR
3	D	417	ARG
3	D	473	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	60	HIS
3	A	86	HIS

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Mol	Chain	Res	Type
3	A	136	ASN
3	A	160	GLN
3	A	188	HIS
3	A	254	ASN
3	A	307	ASN
3	A	311	ASN
3	A	356	HIS
3	A	362	GLN
3	D	60	HIS
3	D	124	GLN
3	D	136	ASN
3	D	160	GLN
3	D	188	HIS
3	D	254	ASN
3	D	307	ASN
3	D	311	ASN
3	D	356	HIS
3	D	362	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	B	7/8 (87%)	1 (14%)	1 (14%)
1	E	7/8 (87%)	1 (14%)	1 (14%)
2	C	7/7 (100%)	1 (14%)	1 (14%)
2	F	6/7 (85%)	1 (16%)	0
All	All	27/30 (90%)	4 (14%)	3 (11%)

All (4) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	B	905	G
2	C	916	G
1	E	905	G
2	F	917	G

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	B	905	G
2	C	915	G

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Mol	Chain	Res	Type
1	E	904	A

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

2 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
2	5FU	C	921	1,2	13,22,23	1.22	1 (7%)	13,32,35	1.90	2 (15%)
2	5FU	F	921	1,2	13,22,23	1.17	1 (7%)	13,32,35	2.27	3 (23%)

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
2	5FU	C	921	1,2	-	0/3/25/26	0/2/2/2
2	5FU	F	921	1,2	-	0/3/25/26	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	921	5FU	C4-C5	2.90	1.42	1.38
2	F	921	5FU	C4-C5	2.92	1.42	1.38

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	921	5FU	C5-C4-N3	-2.73	119.30	122.34
2	C	921	5FU	C5-C4-N3	-2.69	119.35	122.34
2	F	921	5FU	O4'-C1'-N1	4.80	118.19	108.08
2	C	921	5FU	C4-N3-C2	5.87	120.32	115.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	921	5FU	C4-N3-C2	5.89	120.34	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	921	5FU	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 4 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	PPV	A	930	4	6,8,8	0.64	0	11,13,13	1.13	0
5	PPV	D	1930	4	6,8,8	0.65	0	11,13,13	1.09	0

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	PPV	A	930	4	-	0/6/6/6	0/0/0/0
5	PPV	D	1930	4	-	0/6/6/6	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

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	B	8/8 (100%)	1.55	3 (37%) 0 0	46, 55, 70, 88	8 (100%)
1	E	8/8 (100%)	1.53	2 (25%) 1 0	51, 53, 67, 91	8 (100%)
2	C	6/7 (85%)	1.47	3 (50%) 0 0	41, 48, 73, 78	6 (100%)
2	F	6/7 (85%)	1.57	3 (50%) 0 0	43, 47, 68, 68	6 (100%)
3	A	474/476 (99%)	0.25	29 (6%) 25 18	34, 39, 44, 47	0
3	D	474/476 (99%)	0.25	29 (6%) 25 18	34, 39, 44, 47	0
All	All	976/982 (99%)	0.28	69 (7%) 19 13	34, 39, 46, 91	28 (2%)

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	371	ASP	7.0
3	A	370	SER	6.6
3	A	371	ASP	6.5
1	B	903	U	5.1
3	D	13	VAL	5.1
3	D	16	MET	5.0
3	A	469	ASP	4.9
1	E	903	U	4.9
3	D	469	ASP	4.7
3	D	471	ALA	4.6
3	D	14	HIS	4.5
3	A	287	ASN	4.3
3	D	473	LEU	4.3
3	D	369	LYS	4.2
3	D	15	VAL	4.2
3	D	474	GLU	4.1
2	C	915	G	4.1
3	D	370	SER	4.1
3	A	9	VAL	3.8

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Mol	Chain	Res	Type	RSRZ
3	A	471	ALA	3.8
2	F	916	G	3.8
3	A	394	TYR	3.8
3	A	473	LEU	3.7
3	D	12	ARG	3.7
3	A	472	ALA	3.6
3	D	5	ASP	3.6
3	A	14	HIS	3.4
3	A	8	ASP	3.4
3	A	127	ARG	3.3
3	D	287	ASN	3.3
3	A	16	MET	3.2
3	D	127	ARG	3.2
3	A	15	VAL	3.0
3	A	5	ASP	3.0
2	F	915	G	3.0
3	A	369	LYS	3.0
3	D	394	TYR	3.0
3	A	470	ALA	2.9
3	A	7	ARG	2.9
2	C	916	G	2.8
3	D	152	LYS	2.8
3	D	42	LYS	2.7
3	D	17	ARG	2.7
3	D	470	ALA	2.7
3	A	13	VAL	2.6
3	D	373	GLY	2.6
3	D	9	VAL	2.5
2	F	917	G	2.5
3	A	468	GLY	2.5
3	A	114	ASP	2.5
3	D	54	GLU	2.5
3	D	114	ASP	2.5
3	A	6	THR	2.4
3	D	10	GLU	2.4
3	D	7	ARG	2.4
3	D	472	ALA	2.4
1	B	904	A	2.4
3	A	28	GLY	2.4
3	A	48	GLU	2.4
1	B	909	C	2.4
3	D	48	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
3	A	12	ARG	2.3
3	A	17	ARG	2.2
3	A	373	GLY	2.2
3	A	474	GLU	2.2
3	A	306	ILE	2.1
1	E	909	C	2.1
2	C	917	G	2.1
3	D	11	GLU	2.1

## 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, 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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	5FU	F	921	21/22	0.84	0.25	-	20,48,52,53	21
2	5FU	C	921	21/22	0.89	0.20	-	20,42,44,46	21

## 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, 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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	PPV	A	930	9/9	0.73	0.25	2.16	80,81,84,84	9
5	PPV	D	1930	9/9	0.82	0.23	1.31	78,79,79,80	9
4	MG	A	780	1/1	0.89	0.19	0.38	41,41,41,41	0
4	MG	D	1780	1/1	0.76	0.14	-1.92	38,38,38,38	0
4	MG	A	781	1/1	0.80	0.18	-	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	MG	D	1781	1/1	0.72	0.21	-	66,66,66,66	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.