



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:16 AM UTC

PDB ID : 2E9T / pdb_00002e9t
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

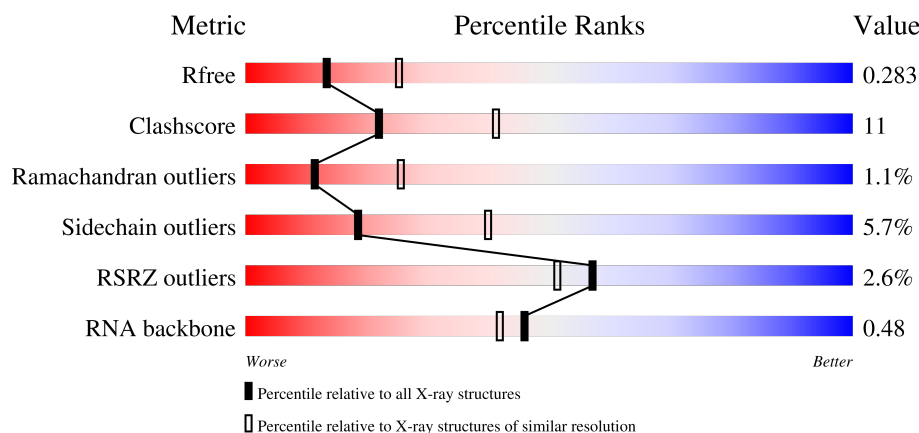
1 Overall quality at a glance

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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)
RNA backbone	3983	1014 (2.84-2.36)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	
1	E	8	
2	C	7	
2	F	7	

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Mol	Chain	Length	Quality of chain
3	A	476	2% 81% 15%
3	D	476	2% 78% 18%

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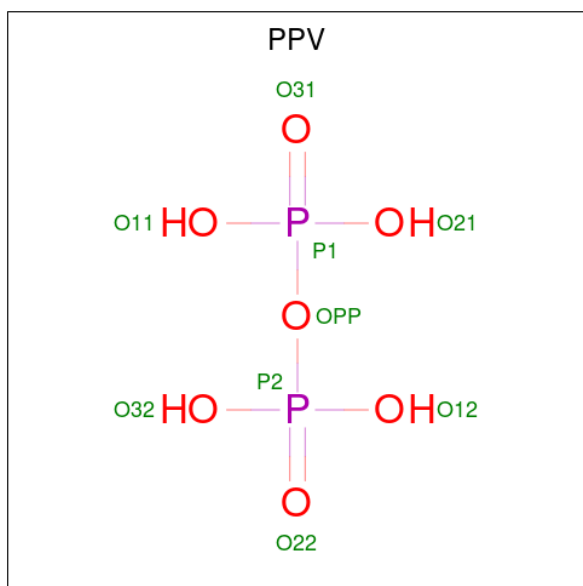
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Chain	Residue	Modelled	Actual	Comment	Reference
D	473	LEU	-	cloning artifact	UNP Q0QEE1
D	474	GLU	-	cloning artifact	UNP Q0QEE1
D	475	HIS	-	cloning artifact	UNP Q0QEE1
D	476	HIS	-	cloning artifact	UNP Q0QEE1

- Molecule 4 is MAGNESIUM ION (CCD ID: 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 (CCD ID: PPV) (formula: $H_4O_7P_2$).



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	B	2	Total O 2 2	0	0

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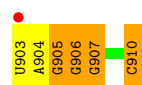
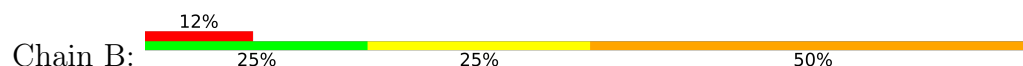
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	1	Total 1	O 1	0	0
6	E	2	Total 2	O 2	0	0
6	F	1	Total 1	O 1	0	0
6	A	35	Total 35	O 35	0	0
6	D	24	Total 24	O 24	0	0

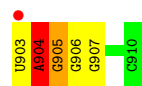
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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'



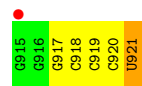
- Molecule 1: 5'-R(P*UP*AP*GP*GP*GP*CP*CP*C)-3'



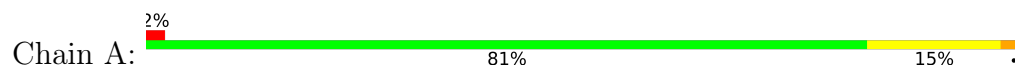
- Molecule 2: 5'-R(*GP*GP*GP*CP*CP*CP*(5FU))-3'

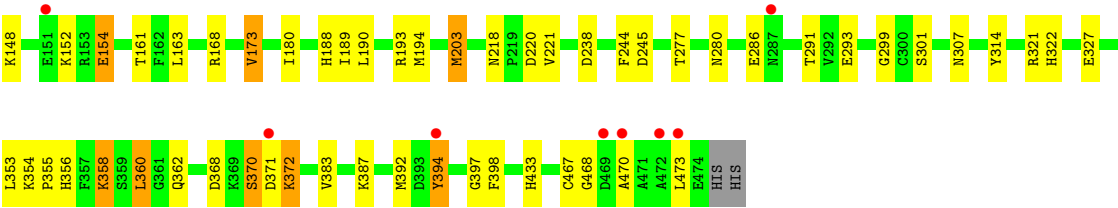


- Molecule 2: 5'-R(*GP*GP*GP*CP*CP*CP*(5FU))-3'

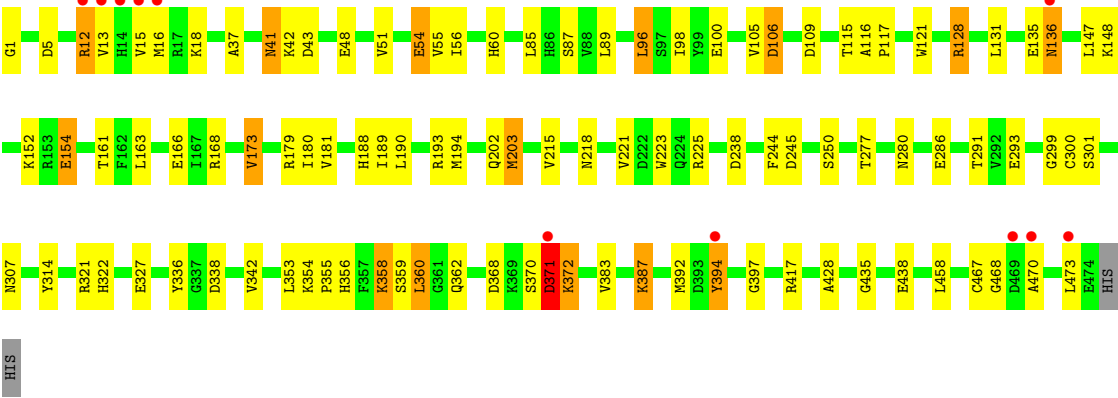
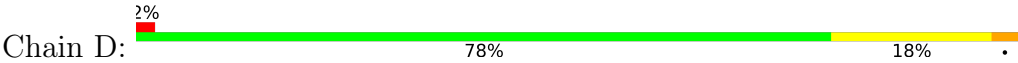


- Molecule 3: RNA-dependent RNA polymerase





● 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, α , β , γ	95.60Å 95.60Å 201.16Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.60 20.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-2.60) 99.7 (20.00-2.60)	Depositor EDS
R_{merge}	0.90	Depositor
R_{sym}	0.74	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.19 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.233 , 0.289 0.229 , 0.283	Depositor DCC
R_{free} test set	1694 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	45.2	Xtriage
Anisotropy	0.080	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 47.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.028 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8205	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: PPV, MG, 5FU

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	0.72	0/190	1.48	4/294 (1.4%)
1	E	0.79	0/190	1.45	1/294 (0.3%)
2	C	0.57	0/140	1.05	0/217
2	F	0.61	0/140	1.19	0/217
3	A	0.77	0/3830	0.92	0/5186
3	D	0.78	1/3830 (0.0%)	0.92	5/5186 (0.1%)
All	All	0.77	1/8320 (0.0%)	0.96	10/11394 (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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	468	GLY	N-CA	5.07	1.52	1.45

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	904	A	C4'-C3'-O3'	-5.93	104.10	113.00
1	B	906	G	C1'-C2'-O2'	-5.50	100.15	108.40
3	D	435	GLY	CA-C-N	5.47	125.12	119.05
3	D	435	GLY	C-N-CA	5.47	125.12	119.05
1	B	910	C	C1'-O4'-C4'	-5.39	104.31	109.70
1	B	907	G	O5'-C5'-C4'	-5.36	103.45	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	18	LYS	N-CA-C	-5.29	102.69	110.52
3	D	300	CYS	N-CA-C	-5.20	102.37	110.42
1	B	910	C	O4'-C4'-C3'	-5.14	100.96	106.10
3	D	342	VAL	CB-CA-C	-5.03	103.08	110.82

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	12	0
2	C	147	0	77	6	0
2	F	147	0	77	6	0
3	A	3741	0	3669	78	0
3	D	3741	0	3669	74	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	168	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 11.

All (168) 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:A:85:LEU:CD1	3:A:203:MET:HE1	1.89	1.02
3:D:467:CYS:SG	3:D:470:ALA:CB	2.49	1.00
3:D:85:LEU:CD1	3:D:203:MET:HE1	1.91	0.99
3:A:120:PRO:HD2	6:A:979:HOH:O	1.65	0.94
3:D:85:LEU:HD11	3:D:203:MET:HE1	0.95	0.94
3:D:12:ARG:HG2	3:D:12:ARG:HH11	1.33	0.93
3:A:85:LEU:HD11	3:A:203:MET:HE1	0.92	0.91
3:A:121:TRP:CD2	6:A:979:HOH:O	2.23	0.91
3:A:12:ARG:HG2	3:A:12:ARG:HH11	1.33	0.90
3:D:467:CYS:SG	3:D:467:CYS:O	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:16:MET:HE1	3:D:41:ASN:OD1	1.80	0.81
3:D:89:LEU:HD11	3:D:203:MET:CE	2.13	0.78
3:A:16:MET:HE1	3:A:41:ASN:OD1	1.84	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:HE3	1.69	0.74
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
2:C:918:C:H2'	2:C:919:C:C6	2.31	0.65
3:A:89:LEU:HD11	3:A:203:MET:CE	2.26	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:37:ALA:HA	3:A:173:VAL:HG22	1.82	0.62
3:A:89:LEU:HD11	3:A:203:MET:HE3	1.80	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:HA	3:A:327:GLU:OE1	2.00	0.61
3:A:12:ARG:HG2	3:A:12:ARG:NH1	2.09	0.61
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:CG	3:D:12:ARG:NH1	2.58	0.59
3:A:13:VAL:O	3:A:286:GLU:HA	2.03	0.59
1:B:904:A:O2'	3:A:301:SER:HA	2.02	0.58
2:C:915:G:C8	2:C:915:G:H5''	2.38	0.58
3:D:89:LEU:HD11	3:D:203:MET:HE2	1.83	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:96:LEU:HG	3:D:100:GLU:HB3	1.89	0.54
3:D:48:GLU:HA	3:D:48:GLU:OE1	2.06	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:OD1	3:D:368:ASP:O	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:HA	3:D:327:GLU:OE1	2.10	0.51
3:D:280:ASN:HD21	3:D:293:GLU:HG2	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:D:245:ASP:CG	3:D:307:ASN:HD21	2.19	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
2:F:921:5FU:O3'	3:D:338:ASP:OD1	2.26	0.49
3:D:392:MET:SD	3:D:397:GLY:O	2.69	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
2:C:920:C:H5''	3:A:387:LYS:HE2	1.95	0.48
3:A:244:PHE:HA	3:A:362:GLN:HE22	1.78	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:A:15:VAL:HG11	3:A:161:THR:O	2.13	0.47
3:A:220:ASP:OD1	3:A:433:HIS:HE1	1.97	0.47
3:A:368:ASP:O	3:A:368:ASP:OD1	2.33	0.47
3:A:89:LEU:HD11	3:A:203:MET:HE2	1.95	0.47
3:A:168:ARG:HB2	3:A:173:VAL:HG23	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: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:D:166:GLU:CD	3:D:179:ARG:HH21	2.23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:353:LEU:O	3:A:354:LYS:C	2.60	0.44
3:D:354:LYS:HB2	3:D:355:PRO:HD3	2.00	0.44
3:D:51:VAL:O	3:D:55:VAL:HG23	2.18	0.44
3:D:56:ILE:HG23	3:D:180:ILE:CG2	2.47	0.44
3:D:438:GLU:HA	3:D:438:GLU:OE1	2.17	0.44
1:E:904:A:O4'	3:D:299:GLY:C	2.61	0.43
3:D:85:LEU:CD1	3:D:203:MET:CE	2.74	0.43
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
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:A:368:ASP:C	3:A:370:SER:N	2.75	0.42
3:A:218:ASN:OD1	3:A:218:ASN:C	2.63	0.42
3:D:42:LYS:O	3:D:43:ASP:C	2.61	0.42
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:105:VAL:O	3:A:106:ASP:C	2.62	0.42
3:D:353:LEU:O	3:D:354:LYS:C	2.63	0.42
3:A:56:ILE:CD1	3:A:163:LEU:CD2	2.97	0.42
1:E:906:G:OP2	3:D:109:ASP:OD2	2.38	0.42
2:F:920:C:H5''	3:D:387:LYS:HE2	2.00	0.42
1:B:903:U:H2'	1:B:904:A:C8	2.54	0.41
3:A:12:ARG:CG	3:A:12:ARG:NH1	2.60	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
3:D:218:ASN:OD1	3:D:218:ASN:C	2.63	0.41
3:D:105:VAL:O	3:D:106:ASP:C	2.63	0.41
1:E:904:A:O2'	3:D:301:SER:HA	2.20	0.41
3:A:370:SER:C	3:A:372:LYS:H	2.28	0.41
1:E:906:G:H2'	1:E:907:G:O4'	2.21	0.41
3:A:245:ASP:CG	3:A:307:ASN:HD21	2.29	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:1:GLY:N	3:D:60:HIS:HD2	2.19	0.41
3:D:56:ILE:HD11	3:D:163:LEU:CD2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	472/476 (99%)	449 (95%)	17 (4%)	6 (1%)	9	21
3	D	472/476 (99%)	446 (94%)	22 (5%)	4 (1%)	16	34
All	All	944/952 (99%)	895 (95%)	39 (4%)	10 (1%)	11	25

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%)	377 (95%)	20 (5%)	22	46
3	D	397/399 (100%)	372 (94%)	25 (6%)	16	36
All	All	794/798 (100%)	749 (94%)	45 (6%)	18	40

All (45) 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	96	LEU
3	A	98	ILE
3	A	128	ARG
3	A	135	GLU
3	A	136	ASN
3	A	147	LEU
3	A	148	LYS
3	A	154	GLU
3	A	173	VAL
3	A	189	ILE
3	A	190	LEU
3	A	203	MET
3	A	221	VAL
3	A	358	LYS
3	A	360	LEU
3	A	394	TYR
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	98	ILE
3	D	128	ARG

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Mol	Chain	Res	Type
3	D	135	GLU
3	D	136	ASN
3	D	147	LEU
3	D	148	LYS
3	D	154	GLU
3	D	173	VAL
3	D	189	ILE
3	D	190	LEU
3	D	203	MET
3	D	221	VAL
3	D	223	TRP
3	D	225	ARG
3	D	358	LYS
3	D	360	LEU
3	D	387	LYS
3	D	394	TYR
3	D	417	ARG
3	D	473	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	60	HIS
3	A	86	HIS
3	A	136	ASN
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	A	378	HIS
3	A	464	ASN
3	D	60	HIS
3	D	86	HIS
3	D	136	ASN
3	D	188	HIS
3	D	254	ASN
3	D	307	ASN
3	D	311	ASN
3	D	356	HIS
3	D	362	GLN

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Mol	Chain	Res	Type
3	D	464	ASN

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%)	2 (28%)	1 (14%)
2	C	7/7 (100%)	1 (14%)	1 (14%)
2	F	6/7 (85%)	1 (16%)	0
All	All	27/30 (90%)	5 (18%)	3 (11%)

All (5) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	B	905	G
2	C	916	G
1	E	904	A
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
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	F	921	2,1	19,22,23	1.03	1 (5%)	27,32,35	2.98	11 (40%)
2	5FU	C	921	2,1	19,22,23	1.16	2 (10%)	27,32,35	2.67	7 (25%)

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	F	921	2,1	-	0/7/25/26	0/2/2/2
2	5FU	C	921	2,1	-	0/7/25/26	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	921	5FU	C2-N1	-2.28	1.34	1.38
2	C	921	5FU	C2-N1	-2.25	1.34	1.38
2	C	921	5FU	C1'-N1	-2.12	1.41	1.47

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	921	5FU	C5-C4-N3	7.33	119.35	112.64
2	F	921	5FU	C5-C4-N3	7.28	119.30	112.64
2	C	921	5FU	O4-C4-C5	-6.20	120.41	125.69
2	F	921	5FU	O4-C4-C5	-6.17	120.44	125.69
2	C	921	5FU	C4-N3-C2	-5.35	120.32	127.34
2	F	921	5FU	C4-N3-C2	-5.34	120.34	127.34
2	F	921	5FU	N3-C2-N1	4.70	121.02	114.89
2	C	921	5FU	N3-C2-N1	4.69	121.00	114.89
2	C	921	5FU	F5-C5-C4	4.47	120.38	116.47
2	F	921	5FU	F5-C5-C4	4.45	120.37	116.47
2	F	921	5FU	O4'-C1'-N1	4.34	118.19	108.36
2	F	921	5FU	C2'-C1'-N1	-4.12	101.77	113.25
2	C	921	5FU	C6-C5-C4	-3.76	119.14	122.57
2	F	921	5FU	C6-C5-C4	-3.73	119.17	122.57
2	F	921	5FU	C1'-N1-C6	-3.16	115.95	121.15
2	F	921	5FU	C1'-N1-C2	2.79	122.60	117.59
2	F	921	5FU	O2-C2-N1	-2.58	119.44	122.80
2	C	921	5FU	O2-C2-N1	-2.56	119.46	122.80

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 oligosaccharides 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	0.65	0	12,13,13	1.01	0
5	PPV	D	1930	4	6,8,8	0.69	0	12,13,13	0.97	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	-	2/6/6/6	-
5	PPV	D	1930	4	-	0/6/6/6	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	930	PPV	P1-OPP-P2-O32
5	A	930	PPV	P1-OPP-P2-O22

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, 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	B	8/8 (100%)	1.03	1 (12%) 8 6	37, 44, 55, 70	8 (100%)
1	E	8/8 (100%)	1.09	1 (12%) 8 6	40, 42, 53, 73	8 (100%)
2	C	6/7 (85%)	1.06	1 (16%) 4 3	33, 37, 59, 63	6 (100%)
2	F	6/7 (85%)	0.91	1 (16%) 4 3	35, 37, 55, 55	6 (100%)
3	A	474/476 (99%)	0.13	10 (2%) 63 58	34, 39, 44, 47	0
3	D	474/476 (99%)	0.01	11 (2%) 61 55	34, 39, 44, 47	0
All	All	976/982 (99%)	0.10	25 (2%) 57 51	33, 39, 45, 73	28 (2%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	469	ASP	4.0
3	D	473	LEU	3.5
3	A	470	ALA	3.1
3	D	16	MET	3.1
1	E	903	U	3.1
2	F	915	G	2.9
1	B	903	U	2.9
3	A	371	ASP	2.8
2	C	915	G	2.7
3	A	473	LEU	2.7
3	D	14	HIS	2.6
3	D	13	VAL	2.6
3	D	371	ASP	2.6
3	A	394	TYR	2.6
3	A	151	GLU	2.4
3	D	394	TYR	2.4
3	D	15	VAL	2.3
3	D	469	ASP	2.2
3	A	8	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
3	A	472	ALA	2.2
3	D	136	ASN	2.2
3	D	470	ALA	2.2
3	D	12	ARG	2.1
3	A	9	VAL	2.1
3	A	287	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	5FU	F	921	21/22	0.83	0.16	20,48,52,53	21
2	5FU	C	921	21/22	0.87	0.12	20,42,44,46	21

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MG	A	781	1/1	0.54	0.11	57,57,57,57	0
4	MG	A	780	1/1	0.67	0.10	41,41,41,41	0
5	PPV	A	930	9/9	0.67	0.13	80,81,84,84	9
4	MG	D	1781	1/1	0.69	0.09	66,66,66,66	0
5	PPV	D	1930	9/9	0.70	0.11	78,79,79,80	9
4	MG	D	1780	1/1	0.77	0.08	38,38,38,38	0

6.5 Other polymers [i](#)

There are no such residues in this entry.