



# Full wwPDB X-ray Structure Validation Report ⓘ

May 27, 2020 – 07:25 pm BST

PDB ID : 2E9Z  
Title : Foot-and-mouth disease virus RNA-polymerase in complex with a template-primer RNA, ATP and UTP  
Authors : Ferrer-Orta, C.; Arias, A.; Perez-Luque, R.; Escarmis, C.; Domingo, E.; Verdaguier, N.  
Deposited on : 2007-01-29  
Resolution : 3.00 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

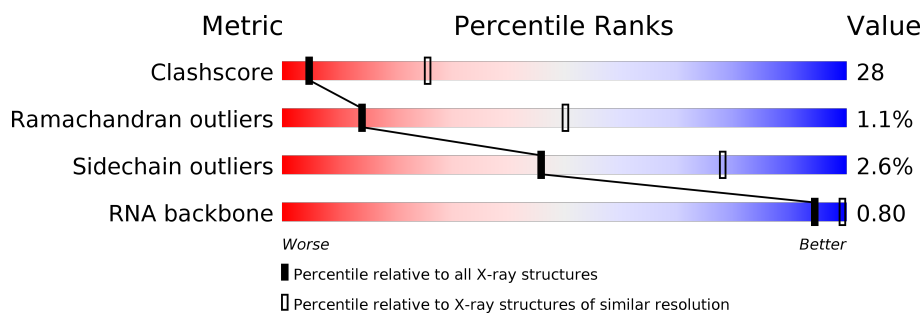
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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))
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RNA backbone	3102	1173 (3.30-2.70)

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 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	B	9	<div> <div style="width: 11%; background-color: green;"></div> <div style="width: 89%; background-color: yellow;"></div> </div> <div>11% 89%</div>
2	C	7	<div> <div style="width: 29%; background-color: green;"></div> <div style="width: 71%; background-color: yellow;"></div> </div> <div>29% 71%</div>
3	A	476	<div> <div style="width: 51%; background-color: green;"></div> <div style="width: 46%; background-color: yellow;"></div> <div style="width: 3%; background-color: orange;"></div> <div style="width: 2%; background-color: red;"></div> </div> <div>51% 46% .</div>

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 4127 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(\*CP\*AP\*UP\*GP\*GP\*GP\*CP\*CP\*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	9	Total	C	N	O	P	0	0	0
			188	85	34	61	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	7	Total	C	N	O	P	0	0	0
			148	67	29	46	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	476	Total	C	N	O	S	0	0	0
			3731	2369	652	689	21			

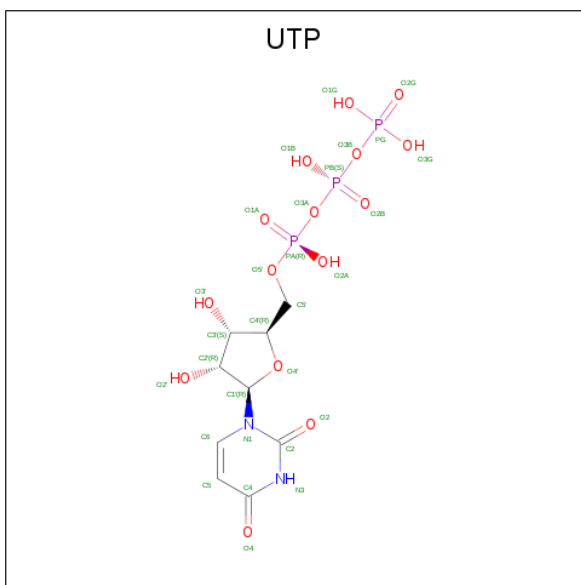
There are 6 discrepancies between the modelled and reference sequences:

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

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

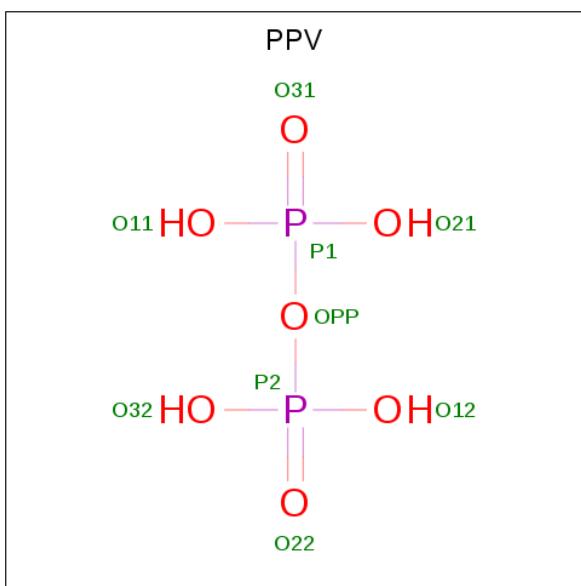
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Mg	0	0
			2	2		

- Molecule 5 is URIDINE 5'-TRIPHOSPHATE (three-letter code: UTP) (formula: C<sub>9</sub>H<sub>15</sub>N<sub>2</sub>O<sub>15</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			29	9	2	15	3		

- Molecule 6 is PYROPHOSPHATE (three-letter code: PPV) (formula:  $\text{H}_4\text{O}_7\text{P}_2$ ).



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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	2	Total 2	O 2	0	0
7	C	3	Total 3	O 3	0	0
7	A	15	Total 15	O 15	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 the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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(\*CP\*AP\*UP\*GP\*GP\*GP\*CP\*CP\*C)-3'

Chain B: 



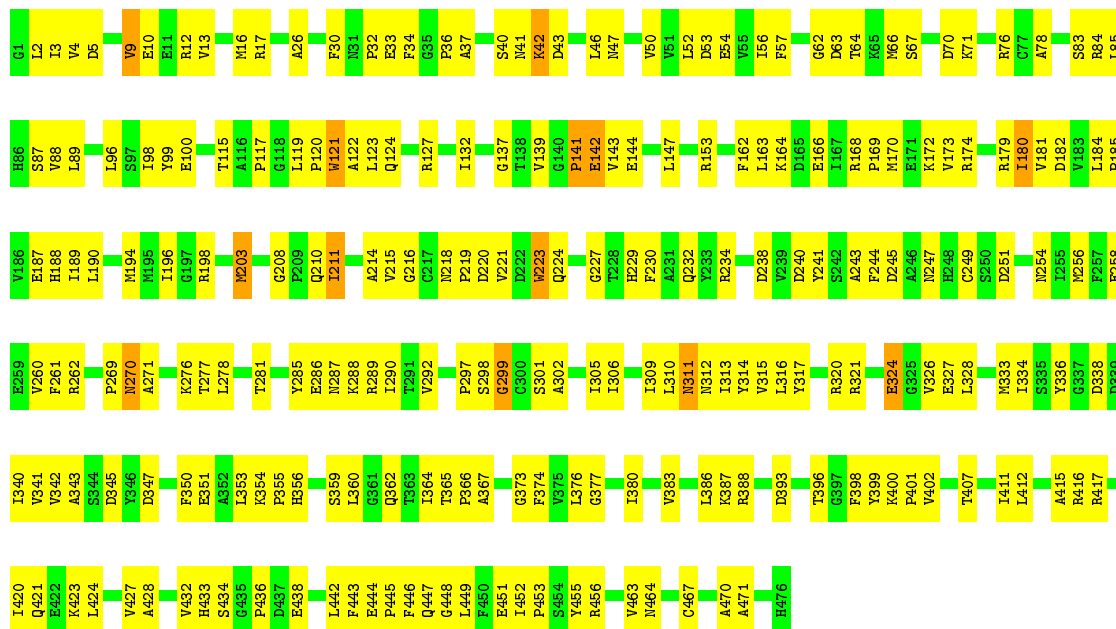
- Molecule 2: 5'-R(\*GP\*GP\*GP\*CP\*CP\*CP\*A)-3'

Chain C: 



- Molecule 3: RNA-dependent RNA polymerase

Chain A: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	94.11Å 94.11Å 99.36Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 3.00 29.42 – 3.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (30.00-3.00) 100.0 (29.42-3.00)	Depositor EDS
$R_{merge}$	0.80	Depositor
$R_{sym}$	0.56	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.32 (at 3.00Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.227 , 0.290 0.348 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	68.7	Xtriage
Anisotropy	0.243	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 57.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.037 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.82	EDS
Total number of atoms	4127	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% of the height of the origin peak. No significant pseudotranslation is detected.*

<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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 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: UTP, MG, 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	0.15	0/209	0.61	0/324
2	C	0.15	0/165	0.61	0/256
3	A	0.25	0/3820	0.43	0/5174
All	All	0.24	0/4194	0.45	0/5754

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	188	0	100	13	3
2	C	148	0	79	12	0
3	A	3731	0	3646	214	14
4	A	2	0	0	0	0
5	A	29	0	11	1	0
6	A	9	0	0	0	0
7	A	15	0	0	2	0
7	B	2	0	0	0	0
7	C	3	0	0	0	0
All	All	4127	0	3836	221	14



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 28.

All (221) 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:A:388:ARG:HD3	3:A:401:PRO:HB3	1.45	0.97
3:A:189:ILE:HG23	3:A:301:SER:HB2	1.46	0.94
3:A:12:ARG:HG2	3:A:287:ASN:HB3	1.48	0.92
3:A:89:LEU:HD11	3:A:203:MET:HE3	1.52	0.90
3:A:180:ILE:H	3:A:180:ILE:HD13	1.34	0.90
3:A:230:PHE:HB2	3:A:380:ILE:HD12	1.61	0.83
3:A:172:LYS:HA	3:A:172:LYS:HE2	1.61	0.82
3:A:78:ALA:HA	3:A:313:ILE:HD12	1.62	0.82
2:C:920:C:H5''	3:A:387:LYS:HG3	1.64	0.79
3:A:37:ALA:HA	3:A:173:VAL:HG13	1.65	0.79
3:A:443:PHE:HB3	3:A:452:ILE:HD13	1.65	0.77
3:A:153:ARG:HH12	3:A:270:ASN:HA	1.52	0.75
3:A:98:ILE:HD11	3:A:139:VAL:HG13	1.69	0.72
3:A:281:THR:HG21	3:A:297:PRO:HG3	1.73	0.70
3:A:290:ILE:H	3:A:290:ILE:HD12	1.58	0.69
1:B:906:G:H4'	3:A:216:GLY:HA2	1.75	0.69
3:A:350:PHE:HA	3:A:353:LEU:HD12	1.75	0.69
3:A:354:LYS:HB2	3:A:355:PRO:HD3	1.73	0.68
3:A:43:ASP:HB3	3:A:46:LEU:HG	1.74	0.68
3:A:96:LEU:HD11	3:A:198:ARG:N	2.09	0.67
3:A:96:LEU:HD11	3:A:198:ARG:H	1.60	0.66
1:B:902:C:H5'	3:A:17:ARG:HH22	1.58	0.66
3:A:314:TYR:CD1	3:A:360:LEU:HD13	2.31	0.66
3:A:163:LEU:HD23	3:A:180:ILE:HG22	1.77	0.66
3:A:234:ARG:HB3	3:A:234:ARG:NH1	2.11	0.66
3:A:185:PRO:HB2	3:A:187:GLU:OE1	1.97	0.65
3:A:85:LEU:HD11	3:A:203:MET:HE1	1.79	0.63
3:A:444:GLU:HB3	3:A:445:PRO:HD3	1.81	0.63
3:A:9:VAL:HG12	3:A:10:GLU:H	1.64	0.63
1:B:903:A:H5'	3:A:115:THR:HB	1.79	0.63
3:A:436:PRO:HG3	3:A:455:TYR:CE2	2.34	0.62
3:A:256:MET:HG3	3:A:310:LEU:HD23	1.82	0.62
3:A:290:ILE:HD12	3:A:290:ILE:N	2.14	0.61
3:A:227:GLY:HA2	3:A:380:ILE:HD13	1.82	0.61
3:A:52:LEU:O	3:A:56:ILE:HD13	2.00	0.61
3:A:12:ARG:HB3	3:A:12:ARG:NH1	2.15	0.61
3:A:9:VAL:HG12	3:A:10:GLU:N	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:84:ARG:HG2	3:A:84:ARG:HH11	1.67	0.59
3:A:276:LYS:C	3:A:278:LEU:H	2.07	0.58
3:A:85:LEU:HD11	3:A:203:MET:CE	2.34	0.58
3:A:208:GLY:N	3:A:211:ILE:HD11	2.18	0.58
3:A:351:GLU:HG2	3:A:374:PHE:HB2	1.86	0.57
3:A:211:ILE:H	3:A:211:ILE:HD13	1.70	0.57
3:A:463:VAL:HG12	3:A:471:ALA:HB2	1.86	0.57
3:A:123:LEU:HD12	3:A:124:GLN:HG3	1.87	0.57
3:A:144:GLU:HA	3:A:147:LEU:HD23	1.85	0.57
3:A:229:HIS:O	3:A:232:GLN:HG2	2.04	0.57
3:A:305:ILE:O	3:A:309:ILE:HG13	2.05	0.57
3:A:321:ARG:HH11	3:A:356:HIS:HA	1.69	0.57
3:A:316:LEU:HD22	3:A:328:LEU:HD21	1.87	0.57
3:A:420:ILE:HG22	3:A:424:LEU:HD11	1.87	0.56
1:B:903:A:N3	3:A:299:GLY:HA2	2.20	0.56
3:A:43:ASP:H	3:A:46:LEU:HD12	1.69	0.56
3:A:238:ASP:HB2	3:A:383:VAL:HG12	1.88	0.56
1:B:902:C:N3	3:A:164:LYS:HE2	2.21	0.56
3:A:141:PRO:HG2	3:A:142:GLU:H	1.71	0.55
3:A:432:VAL:HG13	3:A:433:HIS:CD2	2.41	0.55
3:A:71:LYS:HE2	3:A:251:ASP:OD2	2.06	0.55
3:A:184:LEU:HD23	3:A:188:HIS:CD2	2.42	0.55
3:A:376:LEU:HD12	3:A:376:LEU:N	2.21	0.55
3:A:214:ALA:HB2	3:A:334:ILE:HG12	1.89	0.54
3:A:180:ILE:N	3:A:180:ILE:HD13	2.13	0.54
3:A:3:ILE:HD13	3:A:292:VAL:HG22	1.89	0.54
3:A:2:LEU:HD13	3:A:62:GLY:HA2	1.90	0.53
3:A:211:ILE:N	3:A:211:ILE:HD13	2.23	0.53
3:A:56:ILE:HG22	3:A:57:PHE:CD1	2.44	0.53
3:A:211:ILE:CD1	3:A:211:ILE:H	2.21	0.53
3:A:36:PRO:HA	3:A:166:GLU:O	2.09	0.53
3:A:119:LEU:HD23	3:A:122:ALA:HB3	1.90	0.53
3:A:64:THR:O	3:A:249:CYS:HB2	2.08	0.53
3:A:184:LEU:HB3	3:A:185:PRO:HD2	1.91	0.52
3:A:219:PRO:O	3:A:223:TRP:HB2	2.09	0.52
3:A:311:ASN:O	3:A:315:VAL:HG23	2.09	0.52
3:A:240:ASP:HB2	3:A:365:THR:HG23	1.90	0.52
3:A:456:ARG:HH11	3:A:456:ARG:HG3	1.75	0.52
3:A:13:VAL:O	3:A:286:GLU:HG2	2.09	0.52
3:A:99:TYR:CD1	3:A:137:GLY:HA3	2.45	0.52
3:A:340:ILE:HG12	3:A:341:VAL:N	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:288:LYS:N	3:A:288:LYS:HD2	2.25	0.52
3:A:2:LEU:HB2	3:A:63:ASP:N	2.26	0.51
3:A:121:TRP:CH2	3:A:142:GLU:HB3	2.45	0.51
3:A:141:PRO:HG2	3:A:142:GLU:OE1	2.11	0.51
3:A:88:VAL:HG21	3:A:210:GLN:HE21	1.76	0.51
3:A:153:ARG:HH11	3:A:153:ARG:HG2	1.75	0.51
3:A:290:ILE:CD1	3:A:290:ILE:H	2.24	0.51
3:A:350:PHE:HA	3:A:353:LEU:CD1	2.41	0.51
3:A:386:LEU:O	3:A:388:ARG:HG3	2.09	0.51
1:B:908:C:H2'	1:B:909:C:C6	2.45	0.50
2:C:918:C:H2'	2:C:919:C:C6	2.46	0.50
1:B:903:A:H62	3:A:164:LYS:NZ	2.09	0.50
3:A:420:ILE:O	3:A:424:LEU:HG	2.12	0.50
3:A:190:LEU:O	3:A:194:MET:HG3	2.11	0.50
3:A:84:ARG:HG2	3:A:84:ARG:NH1	2.26	0.50
3:A:99:TYR:HD1	3:A:137:GLY:HA3	1.77	0.49
3:A:132:ILE:HD11	3:A:143:VAL:HG11	1.95	0.49
3:A:447:GLN:NE2	3:A:447:GLN:HA	2.27	0.49
3:A:117:PRO:HB3	3:A:127:ARG:HA	1.95	0.49
3:A:215:VAL:HA	3:A:336:TYR:CE1	2.47	0.49
3:A:467:CYS:HB3	3:A:470:ALA:HB2	1.94	0.49
1:B:906:G:H2'	1:B:907:G:C8	2.48	0.49
3:A:302:ALA:O	3:A:306:ILE:HG12	2.12	0.49
3:A:40:SER:C	3:A:52:LEU:HD22	2.33	0.49
2:C:918:C:O3'	3:A:423:LYS:HE2	2.13	0.49
3:A:66:MET:O	3:A:71:LYS:HE3	2.12	0.48
3:A:184:LEU:N	3:A:184:LEU:HD12	2.28	0.48
2:C:918:C:H5''	3:A:423:LYS:HE3	1.94	0.48
3:A:223:TRP:CG	3:A:401:PRO:HG3	2.48	0.48
3:A:132:ILE:CG1	3:A:143:VAL:HG21	2.43	0.48
3:A:434:SER:O	3:A:438:GLU:HB2	2.14	0.48
3:A:227:GLY:HA2	3:A:380:ILE:CD1	2.43	0.48
2:C:921:A:O3'	3:A:338:ASP:OD1	2.32	0.48
3:A:449:LEU:HD12	3:A:449:LEU:N	2.29	0.48
3:A:9:VAL:CG1	3:A:10:GLU:H	2.25	0.47
3:A:40:SER:OG	3:A:42:LYS:HD2	2.14	0.47
3:A:96:LEU:HD12	3:A:96:LEU:N	2.28	0.47
3:A:98:ILE:HD11	3:A:139:VAL:HG22	1.96	0.47
3:A:245:ASP:HB2	5:A:993:UTP:O2'	2.14	0.47
3:A:53:ASP:OD1	3:A:285:TYR:HE2	1.98	0.47
3:A:180:ILE:H	3:A:180:ILE:CD1	2.16	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:185:PRO:HG2	3:A:188:HIS:HB2	1.95	0.47
3:A:324:GLU:OE1	3:A:324:GLU:N	2.43	0.47
3:A:342:VAL:HG12	3:A:343:ALA:N	2.30	0.47
3:A:386:LEU:HD23	7:A:1034:HOH:O	2.14	0.47
3:A:407:THR:O	3:A:411:ILE:HG13	2.15	0.47
3:A:47:ASN:O	3:A:50:VAL:HG12	2.15	0.47
2:C:920:C:H5''	3:A:387:LYS:CG	2.40	0.47
3:A:234:ARG:HB2	3:A:345:ASP:HA	1.97	0.47
3:A:386:LEU:HA	7:A:1034:HOH:O	2.15	0.47
3:A:366:PRO:HD3	3:A:374:PHE:CE1	2.50	0.47
3:A:320:ARG:HG2	3:A:326:VAL:HB	1.98	0.46
3:A:33:GLU:C	3:A:170:MET:HG2	2.36	0.46
3:A:354:LYS:HG2	3:A:364:ILE:HG13	1.98	0.46
3:A:447:GLN:CD	3:A:452:ILE:HD12	2.36	0.46
3:A:309:ILE:O	3:A:313:ILE:HG12	2.15	0.46
2:C:918:C:OP1	3:A:416:ARG:HG2	2.16	0.46
3:A:88:VAL:CG2	3:A:210:GLN:HE21	2.29	0.46
3:A:448:GLY:C	3:A:449:LEU:HD12	2.36	0.46
3:A:4:VAL:HG23	3:A:5:ASP:N	2.32	0.46
3:A:321:ARG:NH1	3:A:359:SER:HB3	2.31	0.45
3:A:16:MET:HA	3:A:163:LEU:HD12	1.98	0.45
3:A:351:GLU:OE1	3:A:373:GLY:HA2	2.16	0.45
3:A:415:ALA:HB3	3:A:420:ILE:HD13	1.97	0.45
3:A:241:TYR:HB3	3:A:244:PHE:HB2	1.97	0.45
3:A:244:PHE:HA	3:A:362:GLN:HE22	1.81	0.45
3:A:132:ILE:HD13	3:A:139:VAL:HG12	1.99	0.45
1:B:903:A:C2	3:A:299:GLY:HA2	2.52	0.45
2:C:918:C:H5''	3:A:423:LYS:CE	2.46	0.45
3:A:256:MET:O	3:A:260:VAL:HG23	2.16	0.45
1:B:903:A:H1'	3:A:181:VAL:HG11	1.97	0.45
3:A:401:PRO:HD2	3:A:433:HIS:CE1	2.52	0.45
3:A:432:VAL:O	3:A:455:TYR:HE1	1.99	0.45
3:A:123:LEU:HD12	3:A:124:GLN:N	2.32	0.45
3:A:241:TYR:CB	3:A:244:PHE:HB2	2.46	0.45
3:A:56:ILE:CG2	3:A:180:ILE:HG21	2.47	0.44
3:A:182:ASP:HB2	3:A:298:SER:N	2.32	0.44
3:A:185:PRO:HB2	3:A:187:GLU:CD	2.37	0.44
3:A:26:ALA:HB1	3:A:30:PHE:CE2	2.53	0.44
3:A:396:THR:HG1	3:A:398:PHE:HD2	1.62	0.44
3:A:120:PRO:O	3:A:123:LEU:HG	2.18	0.44
3:A:168:ARG:NH1	3:A:179:ARG:HG3	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:67:SER:O	3:A:71:LYS:HG3	2.17	0.44
2:C:917:G:O2'	2:C:918:C:H5'	2.17	0.44
3:A:218:ASN:HD22	3:A:221:VAL:HG22	1.83	0.44
3:A:421:GLN:HA	3:A:424:LEU:HD12	2.00	0.44
3:A:400:LYS:O	3:A:402:VAL:HG23	2.17	0.44
3:A:256:MET:HG3	3:A:310:LEU:CD2	2.47	0.44
3:A:132:ILE:HG13	3:A:143:VAL:HG21	2.00	0.43
3:A:47:ASN:OD1	3:A:174:ARG:HG2	2.18	0.43
3:A:412:LEU:HD21	3:A:427:VAL:HG11	2.00	0.43
3:A:123:LEU:CD1	3:A:124:GLN:HG3	2.48	0.43
3:A:26:ALA:HB2	3:A:446:PHE:CE1	2.53	0.43
3:A:289:ARG:HH11	3:A:289:ARG:HG2	1.84	0.43
3:A:412:LEU:O	3:A:446:PHE:HZ	2.02	0.43
3:A:312:ASN:HA	3:A:333:MET:HE1	2.00	0.43
3:A:456:ARG:HG3	3:A:456:ARG:NH1	2.33	0.43
2:C:920:C:O2'	3:A:386:LEU:HD22	2.19	0.43
3:A:143:VAL:HG12	3:A:147:LEU:HD21	2.00	0.43
2:C:919:C:H2'	2:C:920:C:C6	2.54	0.42
3:A:243:ALA:HB3	3:A:247:ASN:ND2	2.34	0.42
3:A:417:ARG:HH21	3:A:417:ARG:HG3	1.85	0.42
3:A:447:GLN:HE21	3:A:447:GLN:HA	1.85	0.42
3:A:321:ARG:HD3	3:A:356:HIS:CD2	2.55	0.42
1:B:905:G:N2	2:C:920:C:O2	2.52	0.42
3:A:16:MET:SD	3:A:41:ASN:ND2	2.92	0.42
3:A:276:LYS:C	3:A:278:LEU:N	2.71	0.42
3:A:162:PHE:HB2	3:A:181:VAL:HB	2.02	0.42
3:A:215:VAL:HG22	3:A:336:TYR:CD1	2.55	0.42
3:A:393:ASP:HB2	3:A:400:LYS:HD3	2.01	0.42
3:A:42:LYS:HD2	3:A:42:LYS:H	1.83	0.42
3:A:240:ASP:OD1	3:A:367:ALA:HB2	2.20	0.42
3:A:3:ILE:CD1	3:A:292:VAL:HG22	2.50	0.42
3:A:56:ILE:HG23	3:A:180:ILE:HG21	2.01	0.42
3:A:340:ILE:CG1	3:A:341:VAL:N	2.82	0.41
3:A:52:LEU:C	3:A:54:GLU:H	2.23	0.41
3:A:234:ARG:HH11	3:A:234:ARG:HB3	1.84	0.41
3:A:254:ASN:O	3:A:258:GLU:HG3	2.21	0.41
3:A:288:LYS:H	3:A:288:LYS:HD2	1.84	0.41
3:A:240:ASP:HB2	3:A:365:THR:O	2.20	0.41
3:A:190:LEU:C	3:A:190:LEU:HD13	2.41	0.41
3:A:224:GLN:HA	3:A:399:TYR:HB2	2.02	0.41
3:A:278:LEU:O	3:A:281:THR:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:32:PRO:C	3:A:34:PHE:H	2.23	0.41
1:B:906:G:H2'	1:B:907:G:O4'	2.19	0.41
3:A:142:GLU:OE1	3:A:142:GLU:N	2.54	0.41
3:A:243:ALA:HB3	3:A:247:ASN:HD21	1.85	0.41
3:A:70:ASP:HB3	3:A:317:TYR:OH	2.21	0.41
3:A:119:LEU:CD2	3:A:122:ALA:HB3	2.50	0.41
3:A:3:ILE:HD12	3:A:290:ILE:CG2	2.51	0.41
3:A:12:ARG:HH11	3:A:12:ARG:CB	2.33	0.41
3:A:143:VAL:HG12	3:A:147:LEU:CD2	2.51	0.41
3:A:172:LYS:CA	3:A:172:LYS:HE2	2.40	0.41
3:A:208:GLY:H	3:A:211:ILE:HD11	1.85	0.41
3:A:182:ASP:HB2	3:A:298:SER:H	1.86	0.40
3:A:196:ILE:HG21	3:A:261:PHE:CD2	2.56	0.40
1:B:903:A:N6	3:A:164:LYS:HZ2	2.20	0.40
3:A:428:ALA:HA	3:A:443:PHE:CZ	2.55	0.40
3:A:438:GLU:O	3:A:442:LEU:HG	2.20	0.40
3:A:234:ARG:HH11	3:A:234:ARG:CB	2.34	0.40
3:A:269:PRO:C	3:A:271:ALA:H	2.25	0.40
3:A:347:ASP:HB3	3:A:376:LEU:CD2	2.51	0.40
3:A:34:PHE:CE2	3:A:169:PRO:HG3	2.57	0.40

All (14) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:910:C:OP2	3:A:327:GLU:OE1[6_665]	1.56	0.64
1:B:910:C:OP2	3:A:327:GLU:CD[6_665]	1.69	0.51
3:A:83:SER:OG	3:A:453:PRO:CA[6_655]	1.72	0.48
3:A:87:SER:OG	3:A:451:GLU:CA[6_655]	1.75	0.45
3:A:377:GLY:O	3:A:417:ARG:NH1[5_665]	1.76	0.44
3:A:100:GLU:CD	3:A:100:GLU:CD[4_556]	1.77	0.43
3:A:100:GLU:OE1	3:A:100:GLU:OE1[4_556]	2.00	0.20
1:B:910:C:C5'	3:A:327:GLU:CG[6_665]	2.02	0.18
3:A:76:ARG:NH2	3:A:464:ASN:ND2[6_655]	2.06	0.14
3:A:100:GLU:CG	3:A:100:GLU:OE2[4_556]	2.10	0.10
3:A:100:GLU:CD	3:A:100:GLU:OE2[4_556]	2.13	0.07
3:A:84:ARG:CD	3:A:451:GLU:OE1[6_655]	2.17	0.03
3:A:100:GLU:CD	3:A:100:GLU:OE1[4_556]	2.17	0.03
3:A:262:ARG:CZ	3:A:456:ARG:CD[6_655]	2.18	0.02

## 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	474/476 (100%)	410 (86%)	59 (12%)	5 (1%)	14	50

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	9	VAL
3	A	299	GLY
3	A	141	PRO
3	A	270	ASN
3	A	277	THR

### 5.3.2 Protein sidechains [i](#)

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	392/399 (98%)	382 (97%)	10 (3%)	46	78

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	42	LYS
3	A	121	TRP
3	A	142	GLU
3	A	180	ILE
3	A	203	MET
3	A	211	ILE

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Mol	Chain	Res	Type
3	A	220	ASP
3	A	223	TRP
3	A	311	ASN
3	A	324	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	31	ASN
3	A	124	GLN
3	A	160	GLN
3	A	188	HIS
3	A	210	GLN
3	A	247	ASN
3	A	311	ASN
3	A	356	HIS
3	A	362	GLN
3	A	447	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	B	8/9 (88%)	0	0
2	C	6/7 (85%)	0	0
All	All	14/16 (87%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

## 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 4 ligands modelled in this entry, 2 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	PPV	A	665	-	6,8,8	1.74	1 (16%)	13,13,13	1.03	0
5	UTP	A	993	4	26,30,30	2.03	4 (15%)	34,47,47	2.26	10 (29%)

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	PPV	A	665	-	-	2/6/6/6	-
5	UTP	A	993	4	-	4/22/38/38	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	993	UTP	C2-N1	6.08	1.44	1.35
5	A	993	UTP	C6-C5	-5.74	1.37	1.52
6	A	665	PPV	P1-O31	3.59	1.62	1.50
5	A	993	UTP	C4-N3	2.75	1.42	1.37
5	A	993	UTP	PA-O1A	2.21	1.58	1.50

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	993	UTP	O2A-PA-O5'	-6.29	78.54	107.75
5	A	993	UTP	PA-O5'-C5'	4.55	148.33	121.68
5	A	993	UTP	C3'-C2'-C1'	4.16	109.32	101.43
5	A	993	UTP	O3'-C3'-C2'	3.88	124.36	111.82
5	A	993	UTP	O2A-PA-O1A	3.45	129.31	112.24
5	A	993	UTP	PB-O3A-PA	-3.25	121.66	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	993	UTP	C5-C6-N1	3.24	122.31	111.61
5	A	993	UTP	O4'-C4'-C3'	2.99	111.04	105.11
5	A	993	UTP	O5'-PA-O1A	-2.29	100.13	109.07
5	A	993	UTP	O2-C2-N1	2.05	125.68	123.11

There are no chirality outliers.

All (6) torsion outliers are listed below:

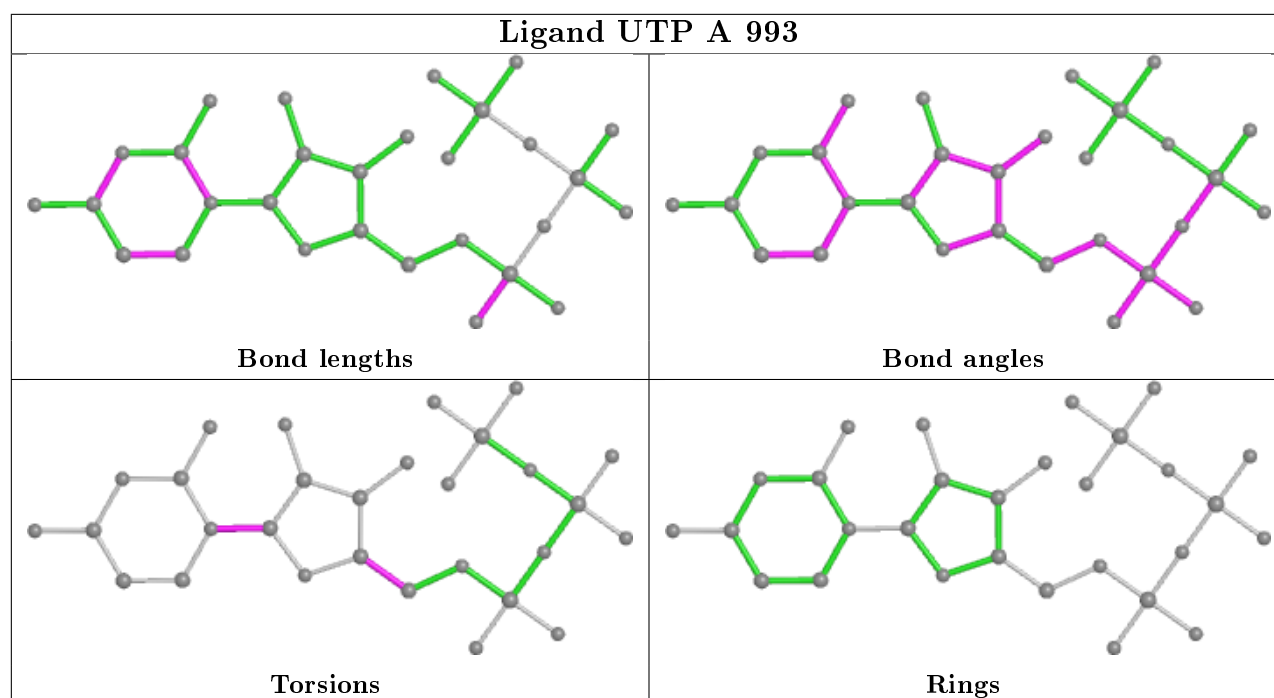
Mol	Chain	Res	Type	Atoms
6	A	665	PPV	P1-OPP-P2-O32
5	A	993	UTP	O4'-C4'-C5'-O5'
5	A	993	UTP	C3'-C4'-C5'-O5'
6	A	665	PPV	P1-OPP-P2-O12
5	A	993	UTP	O4'-C1'-N1-C6
5	A	993	UTP	C2'-C1'-N1-C2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	993	UTP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 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 ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

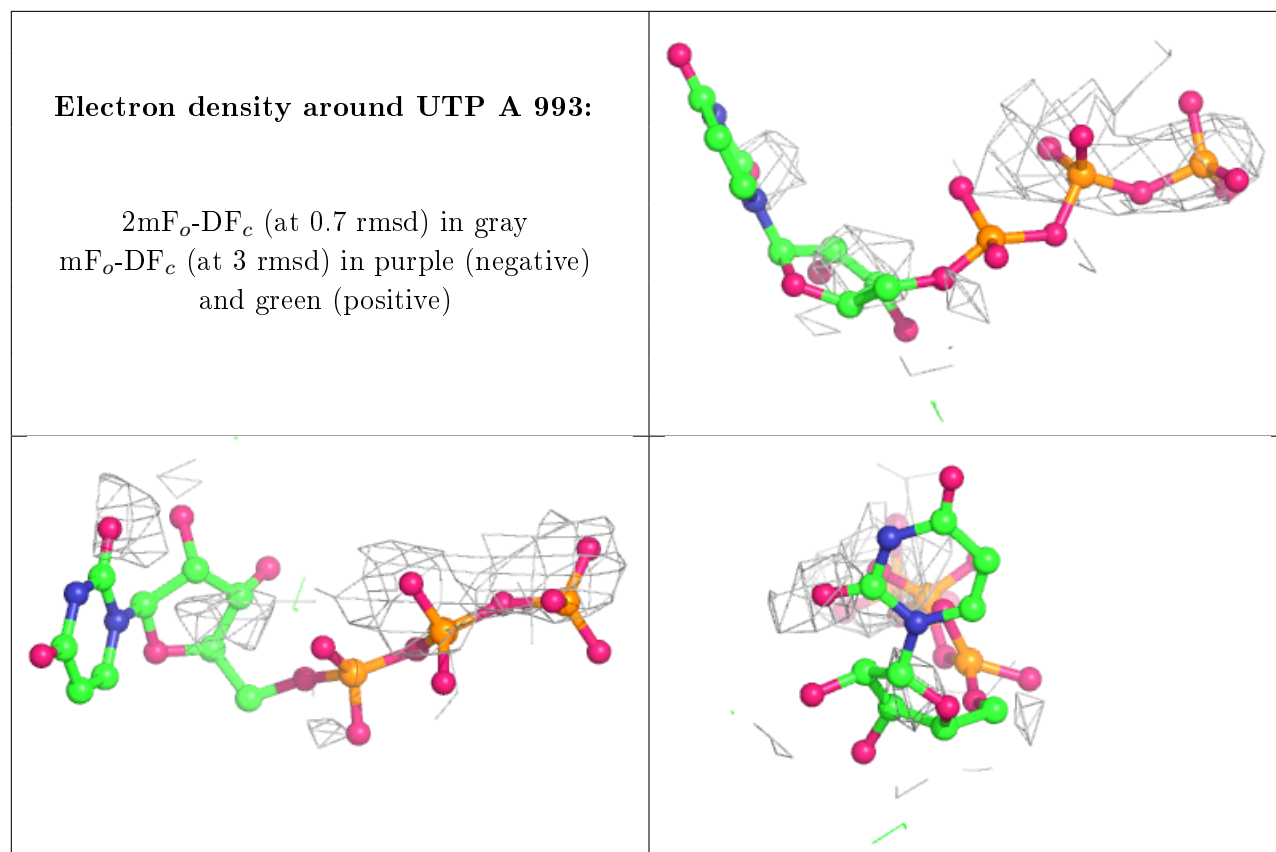
### 6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



## 6.5 Other polymers [i](#)

Unable to reproduce the depositor's R factor - this section is therefore empty.