



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 16, 2023 – 10:26 PM EDT

PDB ID : 4RY5  
Title : C-terminal mutant (W550N) of HCV/J4 RNA polymerase  
Authors : Jaeger, J.; Cherry, A.; Dennis, C.  
Deposited on : 2014-12-13  
Resolution : 2.71 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.

The types of validation reports are described at

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

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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 : 2.35.1  
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) : 2.35.1

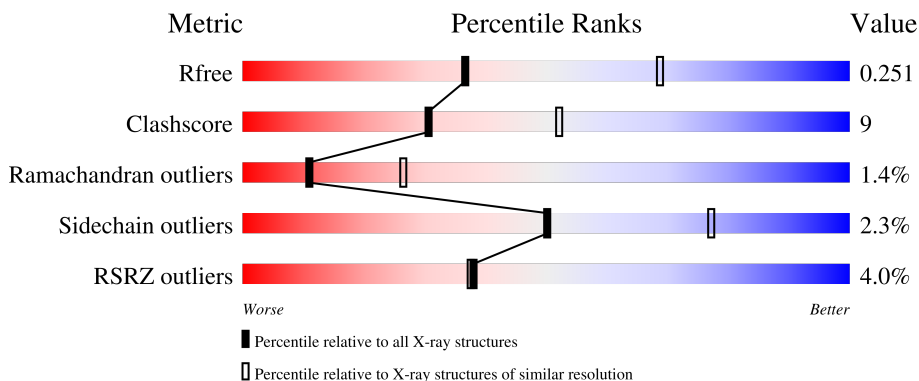
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


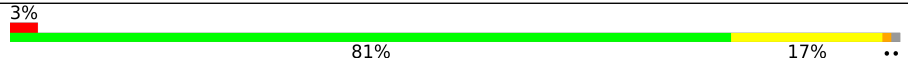
The reported resolution of this entry is 2.71 Å.

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))
$R_{free}$	130704	3359 (2.74-2.70)
Clashscore	141614	3686 (2.74-2.70)
Ramachandran outliers	138981	3622 (2.74-2.70)
Sidechain outliers	138945	3623 (2.74-2.70)
RSRZ outliers	127900	3276 (2.74-2.70)

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 of 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  $\leq 5\%$ . 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	A	570	 5% 79% 18% ..
1	B	570	 3% 81% 17% ..

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9328 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 protein called HCV J4 RNA polymerase (NS5B).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	565	4392	2762	777	821	32	0	0	0
1	B	565	4392	2762	777	821	32	0	0	0

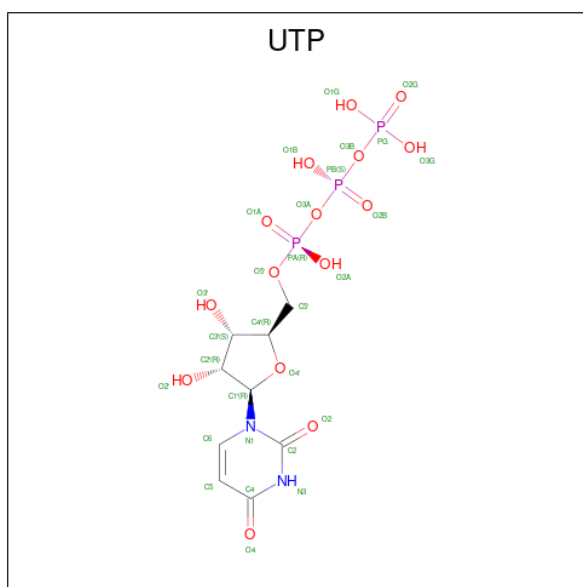
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	550	ASN	TRP	ENGINEERED MUTATION	UNP O92972
B	550	ASN	TRP	ENGINEERED MUTATION	UNP O92972

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Mn	0	0
			2	2		
2	B	2	Total	Mn	0	0
			2	2		

- Molecule 3 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
			Total	C	N	O	P		
3	A	1	58	18	4	30	6	0	1
3	B	1	58	18	4	30	6	0	1

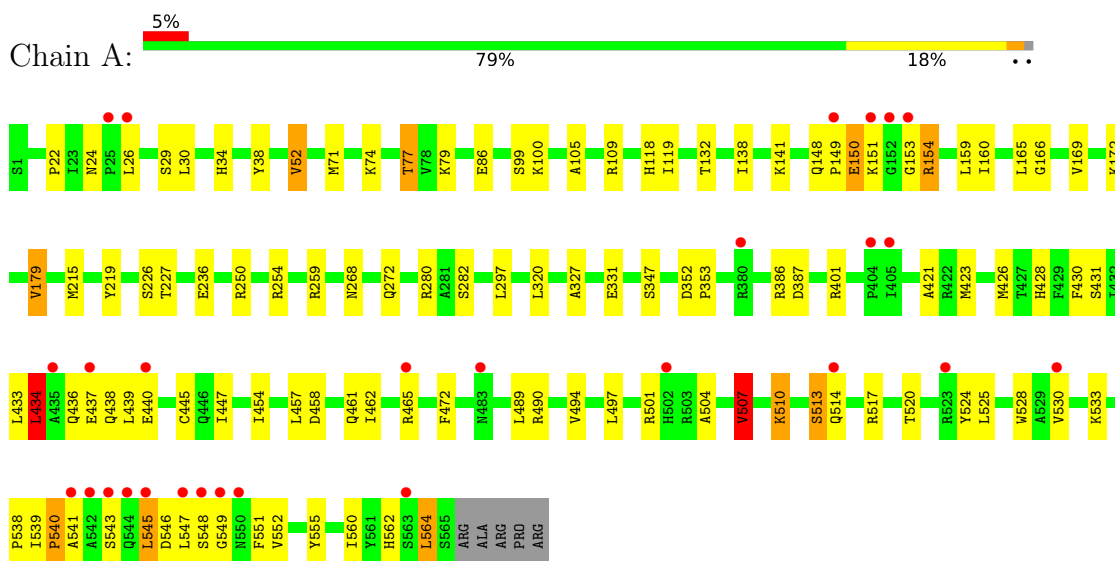
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	247	247	247	0	0
4	B	177	177	177	0	0

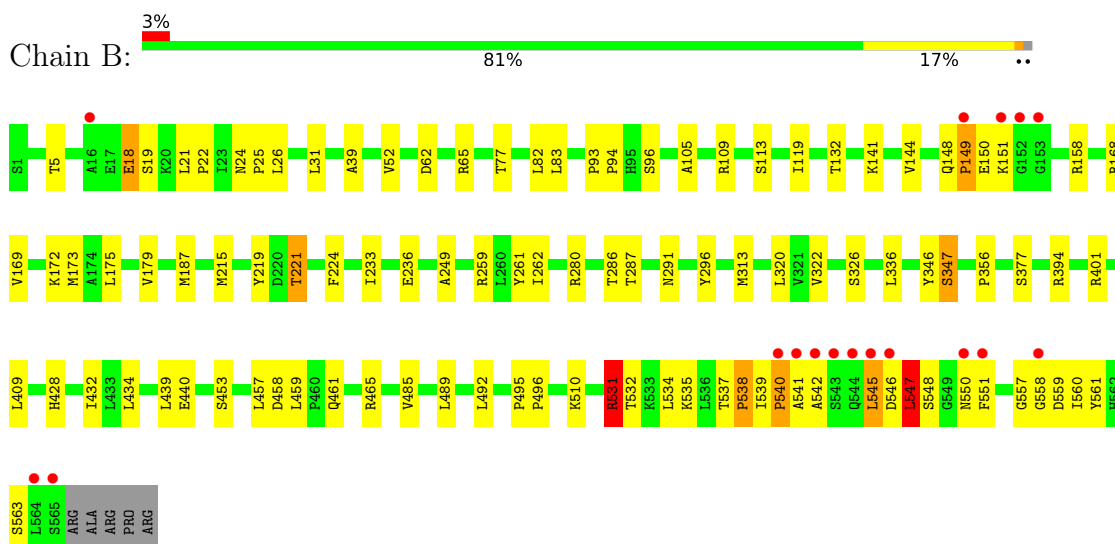
### 3 Residue-property plots [i](#)

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: HCV J4 RNA polymerase (NS5B)



- Molecule 1: HCV J4 RNA polymerase (NS5B)



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.49Å 107.95Å 133.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.98 – 2.71 21.88 – 2.71	Depositor EDS
% Data completeness (in resolution range)	96.9 (19.98-2.71) 96.9 (21.88-2.71)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.14	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.21 (at 2.71Å)	Xtrriage
Refinement program	PHENIX 1.8.4	Depositor
R, $R_{free}$	0.166 , 0.248 0.170 , 0.251	Depositor DCC
$R_{free}$ test set	2706 reflections (6.66%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.8	Xtrriage
Anisotropy	0.669	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 48.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	0.035 for k,h,-l	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	9328	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% 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, MN

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	0.44	1/4486 (0.0%)	0.63	1/6087 (0.0%)
1	B	0.46	0/4486	0.62	1/6087 (0.0%)
All	All	0.45	1/8972 (0.0%)	0.62	2/12174 (0.0%)

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
1	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	507	VAL	CB-CG1	6.00	1.65	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	547	LEU	CA-CB-CG	7.75	133.13	115.30
1	A	434	LEU	CA-CB-CG	-7.11	98.94	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	545	LEU	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	A	4392	0	4409	90	0
1	B	4392	0	4409	71	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	58	0	22	3	0
3	B	58	0	22	5	0
4	A	247	0	0	11	0
4	B	177	0	0	2	0
All	All	9328	0	8862	163	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 9.

All (163) 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)
1:A:148:GLN:HE21	1:A:153:GLY:HA3	1.50	0.77
1:B:546:ASP:OD1	1:B:547:LEU:N	2.16	0.76
1:A:166:GLY:HA3	4:A:1223:HOH:O	1.88	0.74
1:B:561:TYR:CE2	1:B:563:SER:HB3	2.24	0.72
1:B:540:PRO:O	1:B:542:ALA:N	2.22	0.72
1:A:562:HIS:HB3	1:A:564:LEU:HB2	1.72	0.71
1:B:219:TYR:HE2	1:B:221:THR:HG22	1.56	0.71
1:A:517:ARG:NH2	4:A:1161:HOH:O	2.25	0.70
1:A:236:GLU:OE1	1:A:280:ARG:NH2	2.24	0.70
1:A:434:LEU:HD12	1:A:510:LYS:HE3	1.74	0.70
1:A:148:GLN:HE21	1:A:153:GLY:CA	2.05	0.69
1:B:93:PRO:HG2	1:B:96:SER:HB2	1.74	0.69
1:A:541:ALA:HB1	1:A:545:LEU:HD13	1.74	0.68
1:B:82:LEU:HD13	1:B:249:ALA:HB2	1.76	0.68
1:A:530:VAL:O	1:A:533:LYS:NZ	2.27	0.67
1:B:31:LEU:HD11	1:B:492:LEU:HD22	1.78	0.66
1:A:490:ARG:NH2	4:A:1198:HOH:O	2.28	0.66
1:A:148:GLN:HG3	1:A:150:GLU:HB3	1.79	0.65
1:B:558:GLY:O	1:B:560:ILE:N	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:504:ALA:HA	1:A:507:VAL:HB	1.79	0.65
1:B:132:THR:O	1:B:259:ARG:HD2	1.97	0.64
1:B:236:GLU:OE1	1:B:280:ARG:NH2	2.30	0.64
1:B:280:ARG:HD3	1:B:287:THR:HG23	1.80	0.64
1:A:148:GLN:CG	1:A:150:GLU:HB3	2.28	0.63
1:B:148:GLN:O	1:B:150:GLU:N	2.31	0.63
1:A:219:TYR:HB3	1:A:320:LEU:HD23	1.80	0.63
1:B:18:GLU:HG2	1:B:401:ARG:CZ	2.30	0.62
1:B:148:GLN:NE2	1:B:150:GLU:HG2	2.14	0.61
1:A:138:ILE:HD11	1:A:159:LEU:HD13	1.82	0.61
1:A:227:THR:HB	1:A:347:SER:O	1.99	0.61
1:B:534:LEU:HD12	1:B:535:LYS:H	1.64	0.61
1:A:433:LEU:HB3	1:A:439:LEU:HD13	1.81	0.60
1:B:224:PHE:N	3:B:1003[A]:UTP:O1A	2.32	0.60
1:B:336:LEU:HD23	1:B:356:PRO:HD3	1.83	0.60
1:B:434:LEU:HD12	1:B:439:LEU:HD11	1.84	0.60
1:B:21:LEU:HD12	1:B:22:PRO:HD2	1.82	0.60
1:B:18:GLU:HG2	1:B:401:ARG:NH2	2.18	0.59
1:A:434:LEU:HG	1:A:439:LEU:HD21	1.85	0.59
1:B:215:MET:HB2	1:B:326:SER:HB2	1.84	0.59
1:B:105:ALA:O	1:B:109:ARG:HG3	2.03	0.59
1:B:347:SER:O	1:B:347:SER:OG	2.15	0.59
1:A:79:LYS:NZ	4:A:1208:HOH:O	2.35	0.59
1:B:96:SER:OG	1:B:168:ARG:NH1	2.36	0.59
1:A:436:GLN:O	1:A:438:GLN:HG3	2.04	0.57
1:A:118:HIS:CD2	4:A:1223:HOH:O	2.56	0.57
1:B:144:VAL:HG22	1:B:394:ARG:HG2	1.86	0.57
1:A:119:ILE:HD13	1:A:169:VAL:HG11	1.86	0.57
1:A:507:VAL:HA	1:A:510:LYS:HD3	1.86	0.57
1:A:430:PHE:O	1:A:510:LYS:NZ	2.31	0.56
1:B:547:LEU:HD23	1:B:550:ASN:ND2	2.20	0.56
1:A:457:LEU:HB3	1:A:517:ARG:HG3	1.88	0.56
1:B:119:ILE:HD13	1:B:169:VAL:HG11	1.88	0.55
1:B:313:MET:HE2	1:B:322:VAL:HG22	1.88	0.55
1:A:513:SER:O	1:A:513:SER:OG	2.23	0.55
1:B:158:ARG:NE	3:B:1003[B]:UTP:H2'	2.22	0.55
1:A:431:SER:HA	1:A:510:LYS:NZ	2.21	0.55
1:A:148:GLN:NE2	1:A:153:GLY:HA3	2.18	0.55
1:A:132:THR:O	1:A:259:ARG:HD2	2.07	0.54
1:B:96:SER:HG	1:B:168:ARG:HH11	1.55	0.53
1:B:141:LYS:HZ2	3:B:1003[B]:UTP:H5	1.56	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:LYS:NZ	3:B:1003[B]:UTP:H5	2.06	0.53
1:A:268:ASN:HD21	1:A:272:GLN:HE21	1.55	0.53
1:A:141:LYS:HD2	3:A:1003[B]:UTP:O4	2.09	0.53
1:B:280:ARG:NH1	1:B:291:ASN:OD1	2.33	0.53
1:A:327:ALA:O	1:A:331:GLU:HG3	2.08	0.53
1:A:179:VAL:HG13	4:A:1112:HOH:O	2.10	0.52
1:A:74:LYS:O	1:A:77:THR:HB	2.08	0.52
1:A:437:GLU:HB2	4:A:1341:HOH:O	2.10	0.52
1:B:346:TYR:O	1:B:347:SER:HB3	2.08	0.51
1:B:550:ASN:ND2	1:B:551:PHE:CD1	2.78	0.51
1:A:440:GLU:HG3	4:A:1268:HOH:O	2.09	0.51
1:A:86:GLU:H	1:A:86:GLU:CD	2.14	0.50
1:A:436:GLN:O	1:A:437:GLU:HB2	2.11	0.50
1:A:26:LEU:O	1:A:29:SER:HB3	2.12	0.50
1:A:172:LYS:HE3	1:A:560:ILE:HD13	1.93	0.50
1:A:465:ARG:NH1	1:A:546:ASP:O	2.45	0.49
1:B:557:GLY:N	4:B:1165:HOH:O	2.45	0.49
1:A:541:ALA:O	1:A:545:LEU:HD22	2.12	0.49
1:B:219:TYR:CE2	1:B:221:THR:HG22	2.42	0.49
1:A:268:ASN:HD21	1:A:272:GLN:HG3	1.78	0.49
1:A:489:LEU:HD22	1:A:494:VAL:HB	1.95	0.49
1:A:148:GLN:CD	1:A:150:GLU:HB3	2.33	0.49
1:A:148:GLN:HG2	1:A:153:GLY:O	2.13	0.48
1:A:520:THR:HG23	1:A:524:TYR:CD1	2.49	0.48
1:A:447:ILE:HG21	1:A:551:PHE:CZ	2.48	0.48
1:B:26:LEU:HD22	1:B:432:ILE:HD12	1.96	0.48
1:A:457:LEU:HB2	1:A:517:ARG:HE	1.79	0.47
1:B:141:LYS:HZ2	3:B:1003[A]:UTP:H5	1.62	0.47
1:A:148:GLN:HE21	1:A:153:GLY:C	2.17	0.47
1:B:440:GLU:HG2	4:B:1216:HOH:O	2.14	0.47
1:B:545:LEU:HD12	1:B:546:ASP:H	1.78	0.47
1:B:546:ASP:OD1	1:B:547:LEU:HD12	2.14	0.47
1:A:100:LYS:HB2	1:A:100:LYS:HE3	1.72	0.47
1:A:386:ARG:HG2	1:A:387:ASP:N	2.29	0.47
1:A:347:SER:O	1:A:347:SER:OG	2.30	0.47
1:B:465:ARG:NE	1:B:546:ASP:OD2	2.45	0.46
1:A:38:TYR:CE1	1:A:154:ARG:HB3	2.50	0.46
1:A:539:ILE:HA	1:A:540:PRO:HD2	1.62	0.46
1:A:268:ASN:ND2	1:A:272:GLN:HG3	2.30	0.45
1:B:148:GLN:C	1:B:150:GLU:H	2.19	0.45
3:A:1003[B]:UTP:O3B	3:A:1003[B]:UTP:O1A	2.33	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:507:VAL:HG22	1:A:510:LYS:HZ3	1.81	0.45
1:A:105:ALA:O	1:A:109:ARG:HG3	2.17	0.45
1:A:548:SER:OG	1:A:549:GLY:N	2.49	0.45
1:A:24:ASN:HD21	1:A:26:LEU:HB2	1.82	0.45
1:A:22:PRO:HG3	1:A:401:ARG:CZ	2.47	0.44
1:A:501:ARG:NH2	4:A:1118:HOH:O	2.45	0.44
1:A:434:LEU:HD13	1:A:510:LYS:HB2	1.99	0.44
1:B:531:ARG:HB2	1:B:532:THR:H	1.55	0.44
1:A:423:MET:HA	1:A:528:TRP:CH2	2.53	0.44
1:B:93:PRO:HA	1:B:94:PRO:HD3	1.76	0.44
1:A:160:ILE:HD12	1:A:282:SER:OG	2.17	0.44
1:A:439:LEU:HB3	1:A:457:LEU:HD21	1.99	0.44
1:B:151:LYS:HE2	1:B:151:LYS:HB3	1.74	0.44
1:A:30:LEU:HB2	1:A:428:HIS:NE2	2.33	0.43
1:A:497:LEU:HD23	1:A:497:LEU:HA	1.85	0.43
1:B:485:VAL:O	1:B:489:LEU:HG	2.19	0.43
1:A:148:GLN:OE1	1:A:150:GLU:HB3	2.19	0.43
3:A:1003[A]:UTP:H4 <sup>+</sup>	3:A:1003[A]:UTP:O2A	2.18	0.43
1:B:148:GLN:HG2	1:B:149:PRO:HD2	2.01	0.43
1:B:434:LEU:HD21	1:B:510:LYS:HB3	2.01	0.43
1:B:537:THR:HG22	1:B:538:PRO:O	2.18	0.43
1:B:439:LEU:O	1:B:457:LEU:HG	2.19	0.43
1:A:52:VAL:HG22	1:A:226:SER:OG	2.19	0.43
1:A:547:LEU:O	1:A:548:SER:HB2	2.19	0.42
1:A:148:GLN:HA	1:A:149:PRO:HD3	1.84	0.42
1:A:458:ASP:HA	1:A:461:GLN:NE2	2.34	0.42
1:A:462:ILE:HA	1:A:465:ARG:HD3	2.01	0.42
1:B:233:ILE:HD13	1:B:261:TYR:O	2.19	0.42
1:B:531:ARG:H	1:B:531:ARG:HG3	1.40	0.42
1:A:99:SER:HB2	1:A:165:LEU:HB3	2.01	0.42
1:B:175:LEU:O	1:B:179:VAL:HB	2.19	0.42
1:B:495:PRO:HA	1:B:496:PRO:HD2	1.85	0.42
1:B:62:ASP:OD1	1:B:65:ARG:NH1	2.51	0.42
1:A:352:ASP:HA	1:A:353:PRO:HD3	1.95	0.42
1:A:423:MET:HA	1:A:528:TRP:CZ2	2.54	0.42
1:B:148:GLN:CD	1:B:150:GLU:HG2	2.40	0.42
1:B:428:HIS:O	1:B:432:ILE:HG12	2.19	0.42
1:B:539:ILE:H	1:B:539:ILE:HG13	1.64	0.42
1:A:421:ALA:O	1:A:426:MET:HG3	2.20	0.42
1:A:30:LEU:HB2	1:A:428:HIS:CD2	2.55	0.41
1:A:250:ARG:NH2	4:A:1132:HOH:O	2.31	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:409:LEU:HD11	1:B:459:LEU:HD21	2.02	0.41
1:A:254:ARG:HA	1:A:254:ARG:HD2	1.83	0.41
1:A:445:CYS:SG	1:A:454:ILE:HD12	2.61	0.41
1:A:472:PHE:CE2	1:A:525:LEU:HD23	2.55	0.41
1:B:534:LEU:HD12	1:B:535:LYS:N	2.33	0.41
1:A:71:MET:SD	1:A:297:LEU:HB2	2.59	0.41
1:A:507:VAL:HG22	1:A:510:LYS:NZ	2.35	0.41
1:A:540:PRO:HB2	1:A:541:ALA:H	1.46	0.41
1:A:555:TYR:CD2	1:A:560:ILE:HG13	2.55	0.41
1:B:458:ASP:OD1	1:B:461:GLN:NE2	2.54	0.41
1:B:550:ASN:ND2	1:B:551:PHE:HD1	2.18	0.41
1:A:507:VAL:HG22	1:A:510:LYS:CE	2.50	0.41
1:B:546:ASP:CG	1:B:547:LEU:N	2.71	0.41
1:A:434:LEU:CD1	1:A:510:LYS:HE3	2.49	0.41
1:B:24:ASN:HA	1:B:25:PRO:HD3	1.94	0.41
1:A:552:VAL:O	4:A:1228:HOH:O	2.22	0.40
1:B:83:LEU:HB2	1:B:173:MET:HA	2.03	0.40
1:B:219:TYR:HB3	1:B:320:LEU:HD23	2.02	0.40
1:B:187:MET:HE3	1:B:296:TYR:CD1	2.56	0.40
1:B:19:SER:HA	1:B:39:ALA:HB3	2.03	0.40
1:B:172:LYS:HE3	1:B:560:ILE:HD13	2.04	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
1	A	563/570 (99%)	520 (92%)	34 (6%)	9 (2%)	9 23
1	B	563/570 (99%)	530 (94%)	26 (5%)	7 (1%)	13 30
All	All	1126/1140 (99%)	1050 (93%)	60 (5%)	16 (1%)	11 26

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	540	PRO
1	B	149	PRO
1	B	531	ARG
1	B	540	PRO
1	B	541	ALA
1	B	559	ASP
1	A	150	GLU
1	A	543	SER
1	A	545	LEU
1	B	547	LEU
1	A	514	GLN
1	A	564	LEU
1	A	513	SER
1	A	538	PRO
1	A	34	HIS
1	B	548	SER

### 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	
1	A	481/485 (99%)	472 (98%)	9 (2%)	57	81
1	B	481/485 (99%)	468 (97%)	13 (3%)	44	72
All	All	962/970 (99%)	940 (98%)	22 (2%)	50	77

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	VAL
1	A	77	THR
1	A	151	LYS
1	A	154	ARG
1	A	179	VAL
1	A	215	MET
1	A	434	LEU

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Mol	Chain	Res	Type
1	A	507	VAL
1	A	510	LYS
1	B	5	THR
1	B	18	GLU
1	B	52	VAL
1	B	77	THR
1	B	113	SER
1	B	221	THR
1	B	262	ILE
1	B	286	THR
1	B	347	SER
1	B	377	SER
1	B	453	SER
1	B	531	ARG
1	B	538	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	148	GLN
1	A	272	GLN
1	B	550	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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
3	UTP	B	1003[A]	2	22,30,30	1.60	4 (18%)	27,47,47	1.33	2 (7%)
3	UTP	A	1003[B]	2	22,30,30	1.51	3 (13%)	27,47,47	1.35	4 (14%)
3	UTP	A	1003[A]	2	22,30,30	1.83	2 (9%)	27,47,47	1.27	2 (7%)
3	UTP	B	1003[B]	2	22,30,30	1.15	3 (13%)	27,47,47	1.49	5 (18%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	UTP	B	1003[A]	2	-	6/20/38/38	0/2/2/2
3	UTP	A	1003[B]	2	-	9/20/38/38	0/2/2/2
3	UTP	A	1003[A]	2	-	10/20/38/38	0/2/2/2
3	UTP	B	1003[B]	2	-	7/20/38/38	0/2/2/2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1003[A]	UTP	O4-C4	-6.83	1.07	1.24
3	A	1003[B]	UTP	C4-N3	5.08	1.41	1.33
3	B	1003[A]	UTP	C6-N1	-5.05	1.29	1.35
3	A	1003[A]	UTP	C6-N1	-4.23	1.30	1.35
3	A	1003[B]	UTP	C2-N3	-3.66	1.30	1.38
3	B	1003[A]	UTP	O4'-C1'	-3.25	1.36	1.41
3	B	1003[B]	UTP	O4-C4	-3.07	1.16	1.24
3	B	1003[B]	UTP	C6-N1	2.58	1.39	1.35
3	B	1003[A]	UTP	C2'-C1'	2.54	1.57	1.53
3	A	1003[B]	UTP	O4'-C1'	2.38	1.44	1.41
3	B	1003[A]	UTP	C4-N3	2.17	1.36	1.33
3	B	1003[B]	UTP	C2-N3	-2.01	1.34	1.38

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1003[B]	UTP	C6-N1-C2	-3.53	115.59	121.20
3	A	1003[B]	UTP	C3'-C2'-C1'	3.41	106.11	100.98
3	A	1003[A]	UTP	PB-O3B-PG	-3.29	121.52	132.83
3	B	1003[A]	UTP	C6-N1-C2	-3.25	116.04	121.20
3	B	1003[B]	UTP	C3'-C2'-C1'	2.83	105.23	100.98
3	B	1003[B]	UTP	PB-O3B-PG	-2.67	123.68	132.83
3	B	1003[A]	UTP	C3'-C2'-C1'	2.60	104.89	100.98
3	A	1003[B]	UTP	PB-O3A-PA	-2.44	124.45	132.83
3	B	1003[B]	UTP	PB-O3A-PA	-2.44	124.47	132.83
3	A	1003[B]	UTP	C6-N1-C2	-2.41	117.37	121.20
3	A	1003[A]	UTP	PB-O3A-PA	-2.38	124.67	132.83
3	A	1003[B]	UTP	O5'-C5'-C4'	2.17	116.46	108.99
3	B	1003[B]	UTP	C5-C4-N3	-2.16	118.56	123.31

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1003[A]	UTP	C5'-O5'-PA-O1A
3	A	1003[A]	UTP	C5'-O5'-PA-O2A
3	A	1003[A]	UTP	C5'-O5'-PA-O3A
3	A	1003[A]	UTP	C4'-C5'-O5'-PA
3	A	1003[A]	UTP	C3'-C4'-C5'-O5'
3	A	1003[A]	UTP	O4'-C1'-N1-C6
3	A	1003[A]	UTP	C2'-C1'-N1-C6
3	A	1003[B]	UTP	C4'-C5'-O5'-PA
3	A	1003[B]	UTP	O4'-C4'-C5'-O5'
3	A	1003[B]	UTP	O4'-C1'-N1-C6
3	A	1003[B]	UTP	C2'-C1'-N1-C6
3	B	1003[A]	UTP	C5'-O5'-PA-O3A
3	B	1003[A]	UTP	PB-O3B-PG-O1G
3	B	1003[A]	UTP	C2'-C1'-N1-C6
3	B	1003[B]	UTP	C5'-O5'-PA-O3A
3	B	1003[B]	UTP	PB-O3B-PG-O1G
3	A	1003[B]	UTP	C3'-C4'-C5'-O5'
3	B	1003[B]	UTP	O4'-C4'-C5'-O5'
3	A	1003[A]	UTP	O4'-C4'-C5'-O5'
3	B	1003[B]	UTP	C3'-C4'-C5'-O5'
3	A	1003[A]	UTP	PB-O3A-PA-O1A
3	B	1003[B]	UTP	C4'-C5'-O5'-PA
3	A	1003[B]	UTP	PG-O3B-PB-O2B
3	B	1003[A]	UTP	C5'-O5'-PA-O2A
3	B	1003[B]	UTP	C5'-O5'-PA-O1A

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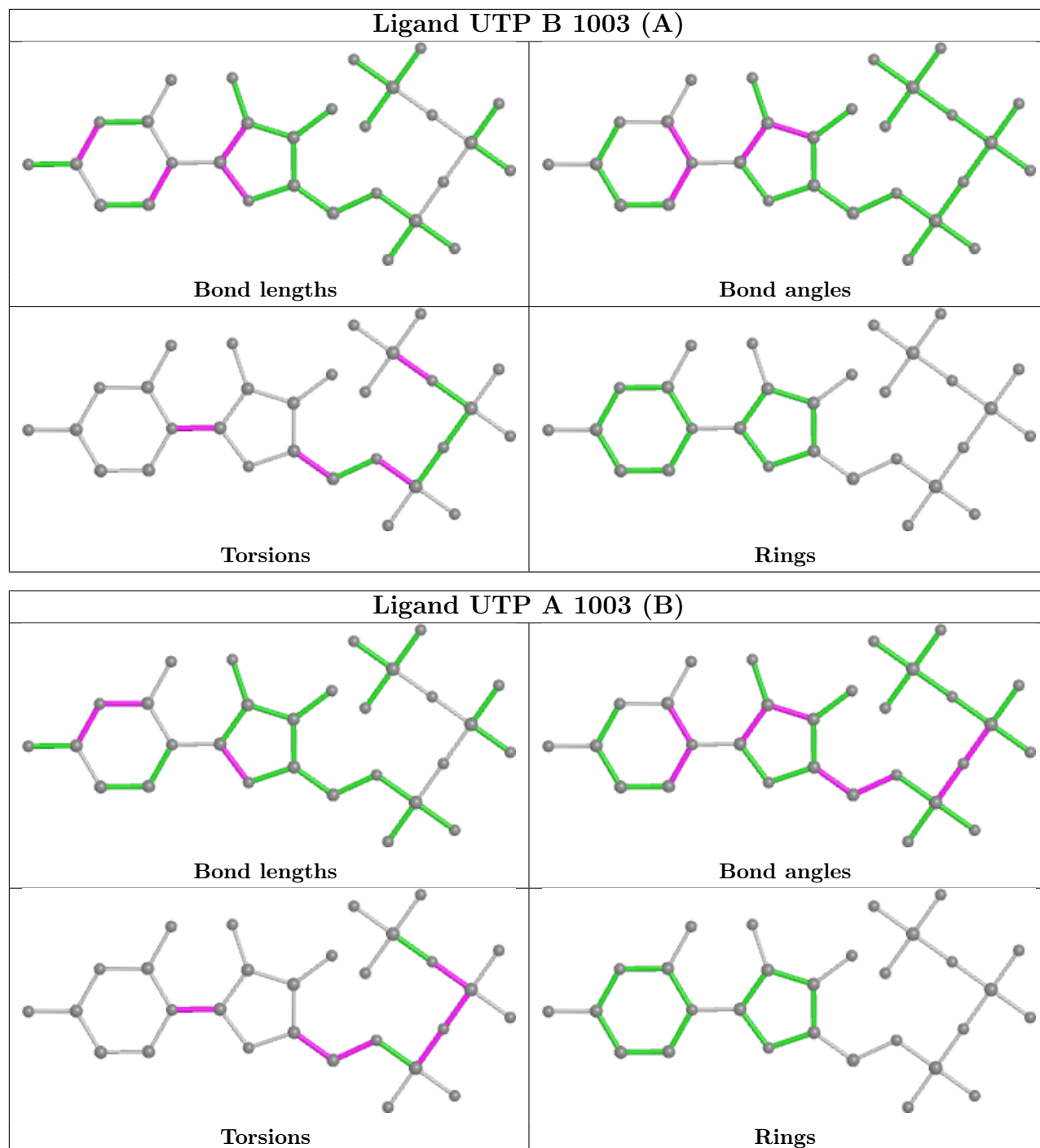
Mol	Chain	Res	Type	Atoms
3	A	1003[B]	UTP	PA-O3A-PB-O3B
3	B	1003[A]	UTP	PB-O3B-PG-O2G
3	A	1003[A]	UTP	PB-O3A-PA-O2A
3	A	1003[B]	UTP	PG-O3B-PB-O1B
3	B	1003[B]	UTP	PB-O3B-PG-O2G
3	B	1003[A]	UTP	O4'-C4'-C5'-O5'
3	A	1003[B]	UTP	PB-O3A-PA-O1A

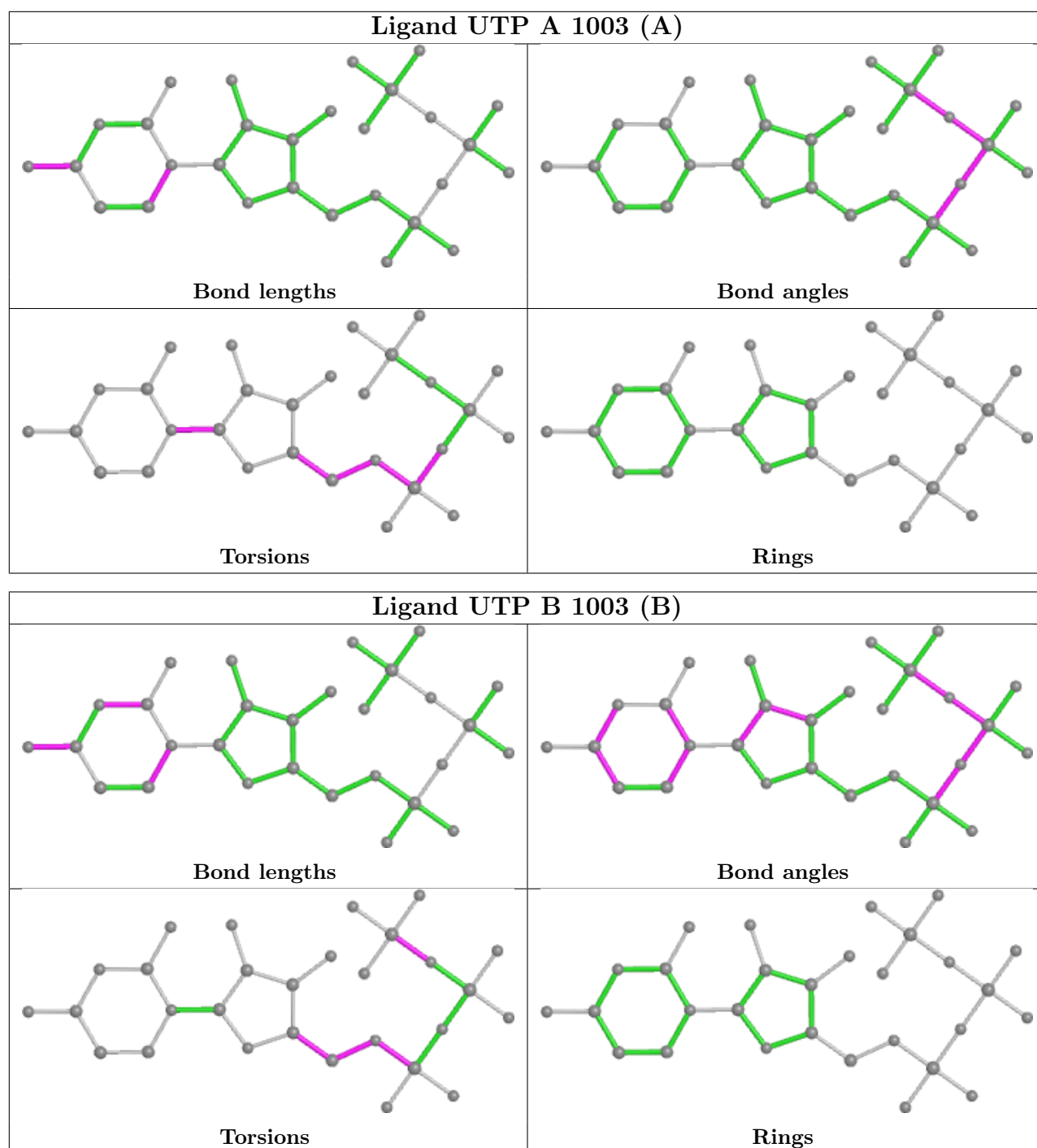
There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1003[A]	UTP	2	0
3	A	1003[B]	UTP	2	0
3	A	1003[A]	UTP	1	0
3	B	1003[B]	UTP	3	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

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	565/570 (99%)	-0.24	28 (4%) 28 28	11, 37, 104, 168	0
1	B	565/570 (99%)	-0.51	17 (3%) 50 51	9, 23, 67, 159	0
All	All	1130/1140 (99%)	-0.38	45 (3%) 38 37	9, 28, 96, 168	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	544	GLN	9.2
1	A	152	GLY	7.5
1	B	545	LEU	7.4
1	B	543	SER	6.1
1	A	543	SER	5.5
1	A	25	PRO	5.4
1	A	544	GLN	4.8
1	B	151	LYS	4.5
1	A	149	PRO	4.5
1	B	542	ALA	4.4
1	A	549	GLY	4.3
1	A	547	LEU	4.3
1	A	404	PRO	3.9
1	A	151	LYS	3.9
1	B	541	ALA	3.8
1	A	542	ALA	3.8
1	A	153	GLY	3.7
1	B	152	GLY	3.4
1	B	565	SER	3.3
1	B	550	ASN	3.3
1	A	523	ARG	3.2
1	B	149	PRO	3.2
1	B	564	LEU	3.2
1	A	541	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	540	PRO	2.8
1	A	26	LEU	2.8
1	B	153	GLY	2.7
1	A	502	HIS	2.7
1	A	548	SER	2.6
1	B	546	ASP	2.5
1	A	440	GLU	2.4
1	A	465	ARG	2.4
1	A	550	ASN	2.3
1	A	405	ILE	2.3
1	A	545	LEU	2.2
1	B	16	ALA	2.2
1	A	380	ARG	2.2
1	A	563	SER	2.2
1	A	530	VAL	2.1
1	B	558	GLY	2.1
1	A	483	ASN	2.1
1	B	551	PHE	2.1
1	A	437	GLU	2.0
1	A	514	GLN	2.0
1	A	435	ALA	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides 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, 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	B-factors(Å <sup>2</sup> )	Q<0.9
3	UTP	B	1003[A]	29/29	0.85	0.31	24,66,83,84	29
3	UTP	B	1003[B]	29/29	0.85	0.31	24,72,83,87	29

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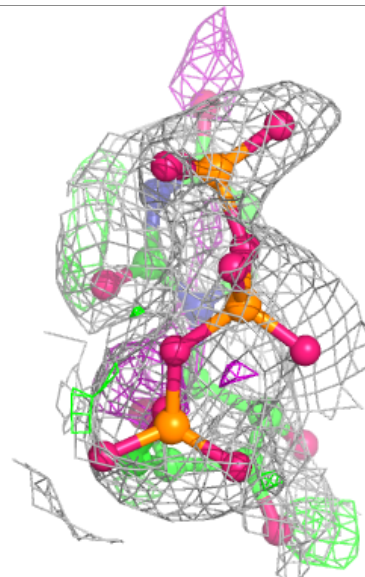
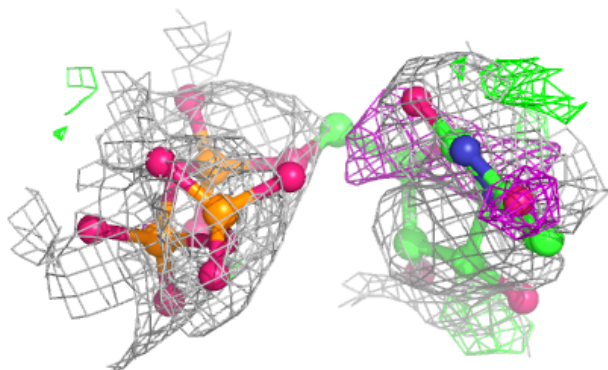
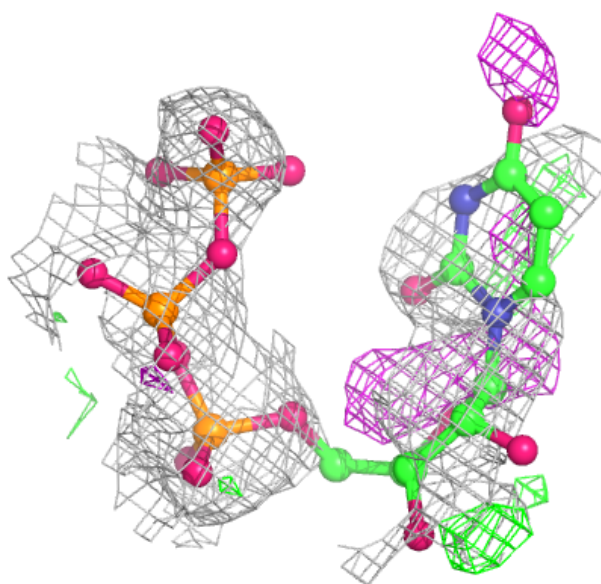
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	UTP	A	1003[A]	29/29	0.87	0.26	21,64,77,80	29
3	UTP	A	1003[B]	29/29	0.87	0.26	38,64,77,79	29
2	MN	A	1001	1/1	0.94	0.09	30,30,30,30	1
2	MN	B	1002	1/1	0.95	0.10	21,21,21,21	1
2	MN	A	1002	1/1	0.98	0.06	31,31,31,31	1
2	MN	B	1001	1/1	0.99	0.03	25,25,25,25	1

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.

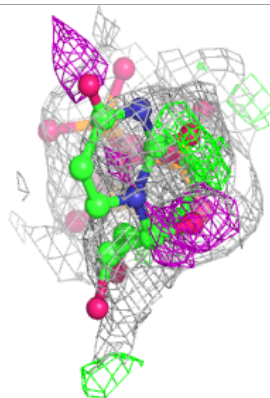
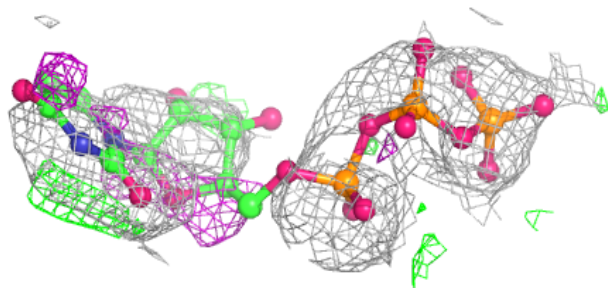
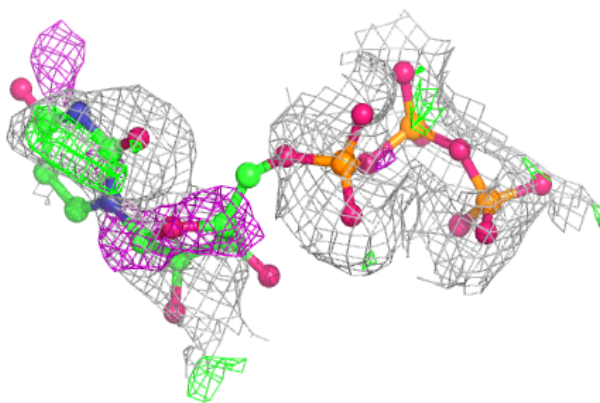
**Electron density around UTP B 1003 (A):**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
 mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
 and green (positive)

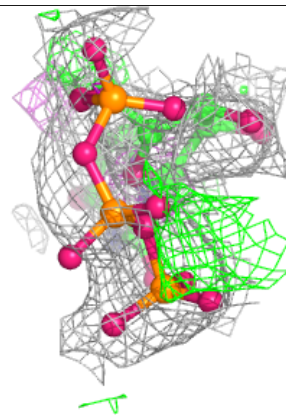
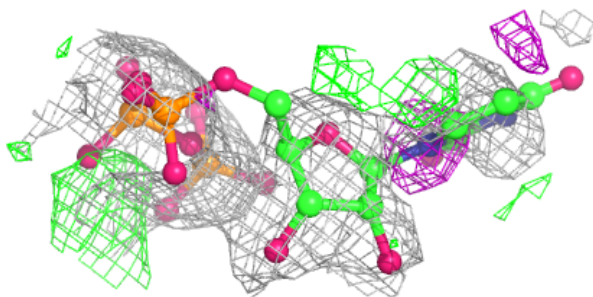
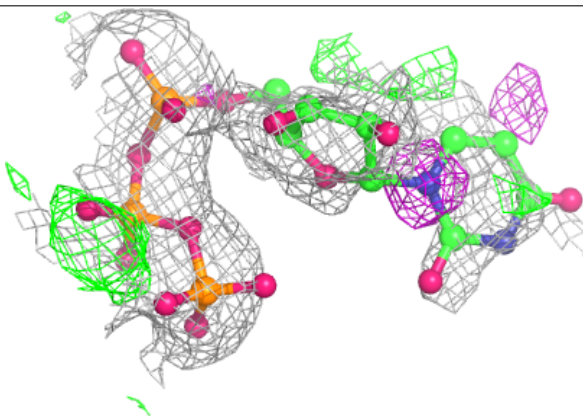


**Electron density around UTP B 1003 (B):**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

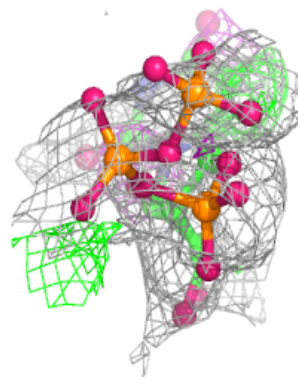
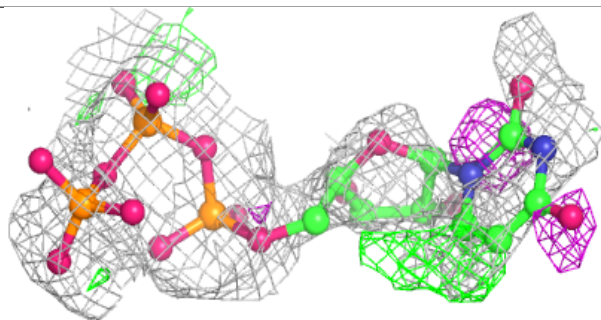
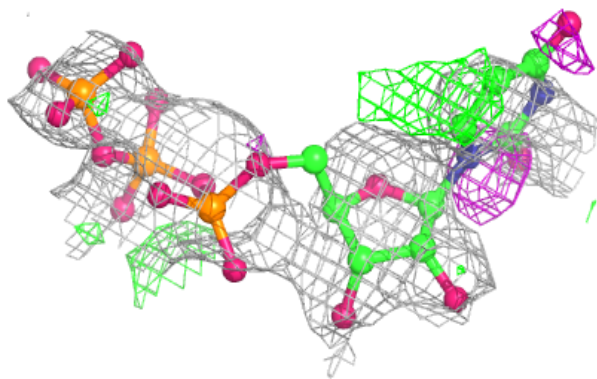
**Electron density around UTP A 1003 (A):**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around UTP A 1003 (B):**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.