



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:00 AM UTC

PDB ID : 4RY5 / pdb_00004ry5
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

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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

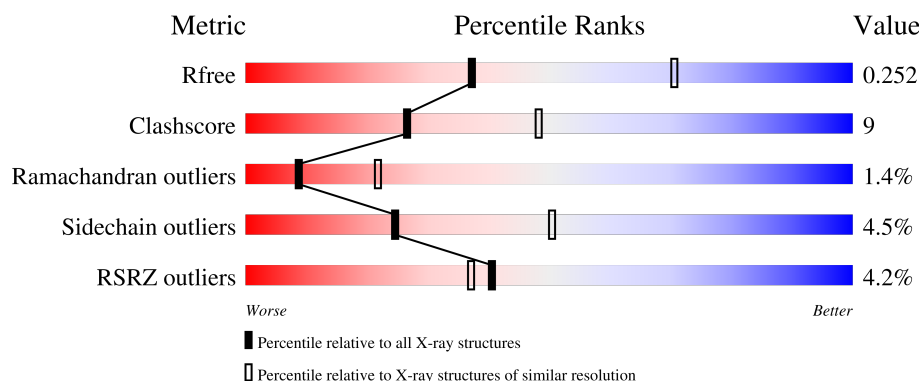
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.71 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}	180053	4348 (2.74-2.70)
Clashscore	190562	4665 (2.74-2.70)
Ramachandran outliers	187476	4584 (2.74-2.70)
Sidechain outliers	187428	4585 (2.74-2.70)
RSRZ outliers	180081	4348 (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 ≥ 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% 77% 19% ..
1	B	570	4% 79% 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
1	A	565	Total	C	N	O	S	0	0	0
			4392	2762	777	821	32			
1	B	565	Total	C	N	O	S	0	0	0
			4392	2762	777	821	32			

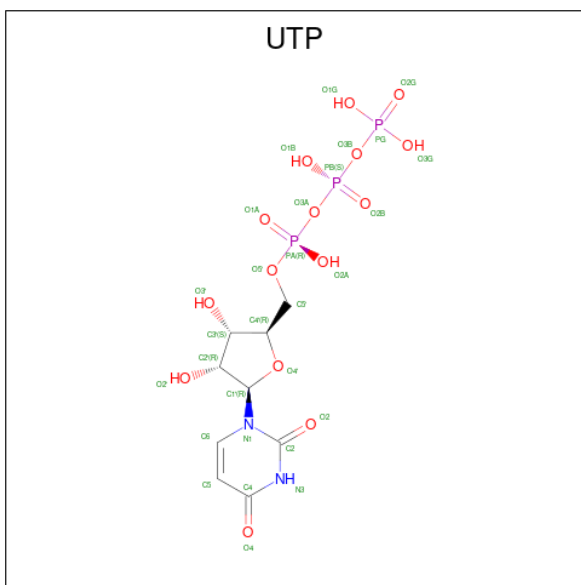
There are 2 discrepancies between the modelled and reference sequences:

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 (CCD ID: 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 (CCD ID: UTP) (formula: C₉H₁₅N₂O₁₅P₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
3	A	1	Total 58	C 18	N 4	O 30	P 6	0	1
3	B	1	Total 58	C 18	N 4	O 30	P 6	0	1

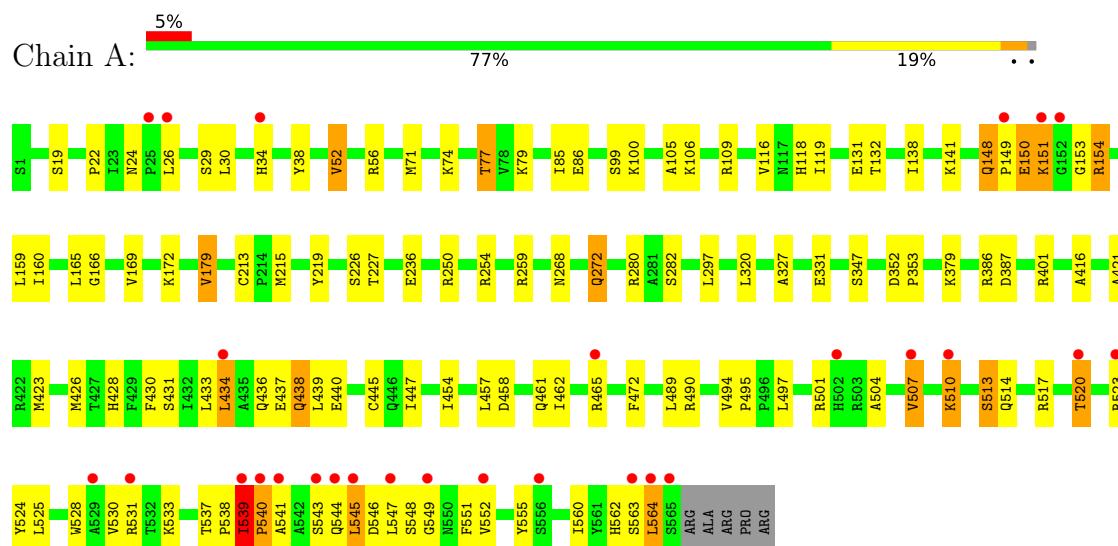
- Molecule 4 is water.

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

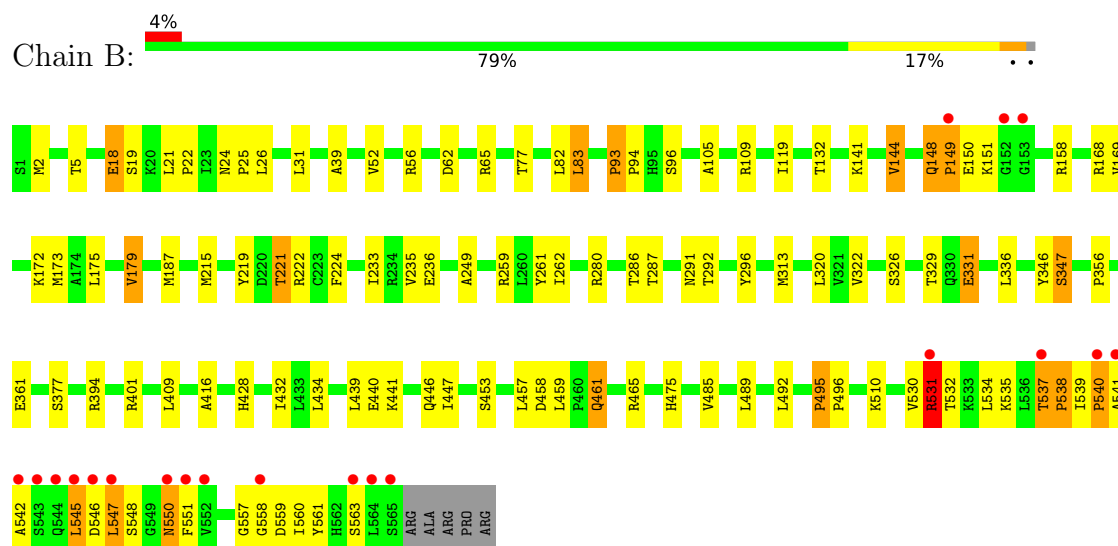
3 Residue-property plots

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, α , β , γ	105.49Å 107.95Å 133.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.98 – 2.71 19.98 – 2.71	Depositor EDS
% Data completeness (in resolution range)	96.9 (19.98-2.71) 96.6 (19.98-2.71)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.21 (at 2.71Å)	Xtriage
Refinement program	PHENIX 1.8.4	Depositor
R, R_{free}	0.166 , 0.248 0.171 , 0.252	Depositor DCC
R_{free} test set	2706 reflections (6.66%)	wwPDB-VP
Wilson B-factor (Å ²)	25.8	Xtriage
Anisotropy	0.669	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 49.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.035 for k,h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9328	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage'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.*

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: MN, UTP

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	0.56	0/4486	0.97	17/6087 (0.3%)
1	B	0.59	1/4486 (0.0%)	0.91	13/6087 (0.2%)
All	All	0.58	1/8972 (0.0%)	0.94	30/12174 (0.2%)

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	B	235	VAL	C-N	-7.14	1.24	1.33

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	539	ILE	CA-C-N	9.07	131.18	119.84
1	A	539	ILE	C-N-CA	9.07	131.18	119.84
1	A	151	LYS	CB-CA-C	-8.52	105.64	117.23
1	A	148	GLN	CA-C-N	7.55	127.26	119.56
1	A	148	GLN	C-N-CA	7.55	127.26	119.56
1	B	416	ALA	CA-C-N	-7.13	112.34	120.04
1	B	416	ALA	C-N-CA	-7.13	112.34	120.04
1	A	416	ALA	CA-C-N	-7.07	112.40	120.04
1	A	416	ALA	C-N-CA	-7.07	112.40	120.04
1	A	544	GLN	N-CA-C	-6.76	104.78	113.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	213	CYS	CA-C-N	6.42	126.79	119.92
1	A	213	CYS	C-N-CA	6.42	126.79	119.92
1	B	93	PRO	CA-C-N	6.14	125.82	119.56
1	B	93	PRO	C-N-CA	6.14	125.82	119.56
1	B	530	VAL	N-CA-C	6.12	118.19	108.89
1	A	563	SER	N-CA-C	-5.94	105.80	113.16
1	A	537	THR	CA-C-N	5.58	126.81	119.84
1	A	537	THR	C-N-CA	5.58	126.81	119.84
1	B	475	HIS	CA-C-N	-5.42	115.77	123.03
1	B	475	HIS	C-N-CA	-5.42	115.77	123.03
1	B	495	PRO	CA-C-N	5.32	125.31	119.89
1	B	495	PRO	C-N-CA	5.32	125.31	119.89
1	B	148	GLN	CA-C-N	5.27	126.43	119.84
1	B	148	GLN	C-N-CA	5.27	126.43	119.84
1	B	537	THR	CA-C-N	-5.12	114.34	120.13
1	B	537	THR	C-N-CA	-5.12	114.34	120.13
1	A	438	GLN	N-CA-C	5.09	116.54	110.44
1	A	510	LYS	CB-CG-CD	5.03	122.88	111.30
1	A	495	PRO	CA-C-N	5.01	126.10	119.84
1	A	495	PRO	C-N-CA	5.01	126.10	119.84

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	89	0
1	B	4392	0	4409	75	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	247	0	0	11	0
4	B	177	0	0	2	0
All	All	9328	0	8862	166	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 (166) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:86:GLU:H	1:A:86:GLU:CD	2.14	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:141:LYS:HZ1	3:B:1003[B]:UTP:H5	1.55	0.54
1:A:148:GLN:CD	1:A:150:GLU:HB3	2.33	0.54
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:148:GLN:HE21	1:A:153:GLY:C	2.17	0.52
1:B:313:MET:HE2	1:B:322:VAL:HG22	1.90	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:436:GLN:O	1:A:437:GLU:HB2	2.11	0.50
1:B:148:GLN:C	1:B:150:GLU:H	2.19	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:HG2	1:A:153:GLY:O	2.13	0.48
1:B:187:MET:HE3	1:B:296:TYR:CD1	2.47	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:B:141:LYS:HZ1	3:B:1003[A]:UTP:H5	1.61	0.48
1:A:457:LEU:HB2	1:A:517:ARG:HE	1.79	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:B:546:ASP:CG	1:B:547:LEU:H	2.18	0.47
1:B:148:GLN:CD	1:B:150:GLU:HG2	2.40	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:B:546:ASP:CG	1:B:547:LEU:N	2.71	0.45
1:A:268:ASN:ND2	1:A:272:GLN:HG3	2.30	0.45
3:A:1003[B]:UTP:O3B	3:A:1003[B]:UTP:O1A	2.33	0.45
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:446:GLN:C	1:B:447:ILE:HD12	2.42	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'	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:B:187:MET:HE1	1:B:292:THR:HG22	2.00	0.42
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:A:513:SER:O	1:A:513:SER:OG	2.23	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: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
1:B:2:MET:HE3	1:B:2:MET:HB3	1.88	0.41
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
1:B:331:GLU:CD	1:B:331:GLU:H	2.30	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	563/570 (99%)	520 (92%)	34 (6%)	9 (2%)	7	18
1	B	563/570 (99%)	530 (94%)	26 (5%)	7 (1%)	10	25
All	All	1126/1140 (99%)	1050 (93%)	60 (5%)	16 (1%)	9	22

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

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Mol	Chain	Res	Type
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 ⓘ

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%)	461 (96%)	20 (4%)	26	53
1	B	481/485 (99%)	458 (95%)	23 (5%)	23	48
All	All	962/970 (99%)	919 (96%)	43 (4%)	24	50

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	SER
1	A	52	VAL
1	A	56	ARG
1	A	77	THR
1	A	85	ILE
1	A	106	LYS
1	A	116	VAL
1	A	131	GLU
1	A	151	LYS
1	A	154	ARG
1	A	179	VAL
1	A	215	MET
1	A	272	GLN

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Mol	Chain	Res	Type
1	A	379	LYS
1	A	434	LEU
1	A	507	VAL
1	A	520	THR
1	A	523	ARG
1	A	531	ARG
1	A	539	ILE
1	B	5	THR
1	B	18	GLU
1	B	52	VAL
1	B	56	ARG
1	B	77	THR
1	B	83	LEU
1	B	144	VAL
1	B	179	VAL
1	B	221	THR
1	B	222	ARG
1	B	262	ILE
1	B	286	THR
1	B	329	THR
1	B	331	GLU
1	B	347	SER
1	B	361	GLU
1	B	377	SER
1	B	441	LYS
1	B	453	SER
1	B	461	GLN
1	B	531	ARG
1	B	538	PRO
1	B	550	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	ASN
1	A	148	GLN
1	A	272	GLN
1	A	527	ASN
1	B	63	HIS
1	B	273	ASN
1	B	550	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	A	1003[B]	2	29,30,30	1.74	6 (20%)	43,47,47	2.07	10 (23%)
3	UTP	B	1003[A]	2	29,30,30	2.34	7 (24%)	43,47,47	2.25	7 (16%)
3	UTP	A	1003[A]	2	29,30,30	2.20	6 (20%)	43,47,47	1.70	5 (11%)
3	UTP	B	1003[B]	2	29,30,30	1.53	7 (24%)	43,47,47	1.87	8 (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	A	1003[B]	2	-	10/22/38/38	0/2/2/2
3	UTP	B	1003[A]	2	-	9/22/38/38	0/2/2/2
3	UTP	A	1003[A]	2	-	12/22/38/38	0/2/2/2
3	UTP	B	1003[B]	2	-	10/22/38/38	0/2/2/2

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1003[A]	UTP	O4-C4	-8.79	1.07	1.24
3	B	1003[A]	UTP	C2-N1	7.89	1.50	1.38
3	B	1003[A]	UTP	C5-C4	-5.86	1.31	1.43
3	A	1003[B]	UTP	C5-C4	-5.25	1.32	1.43
3	A	1003[B]	UTP	C2-N3	-4.05	1.30	1.38
3	A	1003[A]	UTP	C2-N1	3.96	1.44	1.38
3	B	1003[B]	UTP	O4-C4	-3.93	1.16	1.24
3	B	1003[A]	UTP	PA-O3A	3.66	1.63	1.59
3	B	1003[A]	UTP	C6-N1	-3.56	1.29	1.38
3	B	1003[B]	UTP	PA-O3A	3.30	1.63	1.59
3	A	1003[A]	UTP	C6-N1	-3.14	1.30	1.38
3	B	1003[B]	UTP	C2-N1	3.06	1.43	1.38
3	B	1003[A]	UTP	PB-O3B	3.02	1.62	1.59
3	A	1003[A]	UTP	C4-N3	-2.97	1.33	1.38
3	B	1003[A]	UTP	PB-O3A	2.93	1.62	1.59
3	A	1003[B]	UTP	PA-O3A	2.89	1.62	1.59
3	A	1003[B]	UTP	PB-O3B	2.77	1.62	1.59
3	A	1003[B]	UTP	PB-O3A	2.67	1.62	1.59
3	B	1003[B]	UTP	PB-O3A	2.66	1.62	1.59
3	B	1003[B]	UTP	C4-N3	-2.62	1.34	1.38
3	A	1003[A]	UTP	O2-C2	2.50	1.27	1.23
3	B	1003[A]	UTP	O4'-C1'	-2.36	1.36	1.42
3	A	1003[A]	UTP	PA-O3A	2.33	1.62	1.59
3	B	1003[B]	UTP	C2-N3	-2.17	1.34	1.38
3	A	1003[B]	UTP	C2-N1	2.14	1.41	1.38
3	B	1003[B]	UTP	PB-O3B	2.03	1.61	1.59

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1003[B]	UTP	C4-N3-C2	-6.63	118.38	126.61
3	B	1003[A]	UTP	O4'-C1'-N1	6.48	123.05	108.36
3	B	1003[A]	UTP	C4-N3-C2	-6.47	118.58	126.61
3	B	1003[A]	UTP	C5-C4-N3	6.35	123.69	114.80
3	A	1003[B]	UTP	N3-C2-N1	6.21	122.97	114.89
3	B	1003[B]	UTP	N3-C2-N1	5.70	122.31	114.89
3	A	1003[A]	UTP	C4-N3-C2	-5.49	119.80	126.61
3	B	1003[B]	UTP	C6-N1-C2	-4.44	115.59	121.00
3	A	1003[B]	UTP	O2-C2-N3	-4.42	113.34	121.49
3	A	1003[A]	UTP	O4'-C1'-N1	4.40	118.32	108.36
3	B	1003[B]	UTP	C4-N3-C2	-4.31	121.26	126.61
3	B	1003[A]	UTP	O4-C4-C5	-4.10	118.09	125.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1003[A]	UTP	C6-N1-C2	-4.07	116.04	121.00
3	A	1003[A]	UTP	N3-C2-N1	3.85	119.90	114.89
3	A	1003[B]	UTP	C5-C4-N3	3.54	119.76	114.80
3	A	1003[A]	UTP	C5-C4-N3	3.39	119.55	114.80
3	B	1003[B]	UTP	C1'-N1-C2	3.06	123.09	117.59
3	A	1003[B]	UTP	C1'-N1-C2	3.05	123.07	117.59
3	A	1003[B]	UTP	C6-N1-C2	-2.98	117.37	121.00
3	B	1003[B]	UTP	O2-C2-N3	-2.91	116.12	121.49
3	B	1003[B]	UTP	O4-C4-C5	-2.89	120.18	125.16
3	B	1003[B]	UTP	C5-C4-N3	2.69	118.56	114.80
3	A	1003[A]	UTP	O4-C4-C5	-2.64	120.61	125.16
3	B	1003[B]	UTP	O4'-C1'-N1	2.61	114.27	108.36
3	B	1003[A]	UTP	N3-C2-N1	2.54	118.20	114.89
3	A	1003[B]	UTP	C3'-C2'-C1'	2.46	106.11	101.46
3	B	1003[A]	UTP	O2-C2-N3	-2.28	117.29	121.49
3	A	1003[B]	UTP	O4'-C1'-N1	2.20	113.33	108.36
3	A	1003[B]	UTP	O5'-C5'-C4'	2.19	116.46	108.99
3	A	1003[B]	UTP	O4-C4-C5	-2.19	121.39	125.16

There are no chirality outliers.

All (41) 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[B]	UTP	C4'-C5'-O5'-PA
3	B	1003[A]	UTP	C5'-O5'-PA-O2A
3	B	1003[A]	UTP	C5'-O5'-PA-O3A
3	B	1003[A]	UTP	PB-O3B-PG-O1G
3	B	1003[A]	UTP	O4'-C1'-N1-C6
3	B	1003[A]	UTP	O4'-C1'-N1-C2
3	B	1003[B]	UTP	C5'-O5'-PA-O3A
3	B	1003[B]	UTP	PB-O3B-PG-O1G
3	B	1003[B]	UTP	O4'-C1'-N1-C6
3	B	1003[B]	UTP	O4'-C1'-N1-C2
3	A	1003[A]	UTP	C3'-C4'-C5'-O5'
3	A	1003[A]	UTP	O4'-C4'-C5'-O5'
3	B	1003[B]	UTP	O4'-C4'-C5'-O5'
3	B	1003[B]	UTP	C3'-C4'-C5'-O5'
3	A	1003[B]	UTP	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
3	A	1003[B]	UTP	C3'-C4'-C5'-O5'
3	A	1003[A]	UTP	PB-O3A-PA-O1A
3	A	1003[B]	UTP	PG-O3B-PB-O2B
3	B	1003[B]	UTP	C5'-O5'-PA-O1A
3	B	1003[B]	UTP	C4'-C5'-O5'-PA
3	B	1003[A]	UTP	PB-O3B-PG-O2G
3	A	1003[A]	UTP	O4'-C1'-N1-C6
3	A	1003[B]	UTP	PA-O3A-PB-O3B
3	A	1003[A]	UTP	PB-O3A-PA-O2A
3	A	1003[B]	UTP	PG-O3B-PB-O1B
3	A	1003[A]	UTP	O4'-C1'-N1-C2
3	B	1003[B]	UTP	PB-O3B-PG-O2G
3	A	1003[A]	UTP	C2'-C1'-N1-C6
3	A	1003[B]	UTP	PB-O3A-PA-O1A
3	B	1003[A]	UTP	O4'-C4'-C5'-O5'
3	A	1003[B]	UTP	O4'-C1'-N1-C6
3	A	1003[A]	UTP	C2'-C1'-N1-C2
3	A	1003[B]	UTP	PB-O3A-PA-O2A
3	A	1003[B]	UTP	PA-O3A-PB-O1B
3	B	1003[A]	UTP	PA-O3A-PB-O1B
3	B	1003[A]	UTP	PG-O3B-PB-O1B
3	B	1003[B]	UTP	PB-O3A-PA-O2A

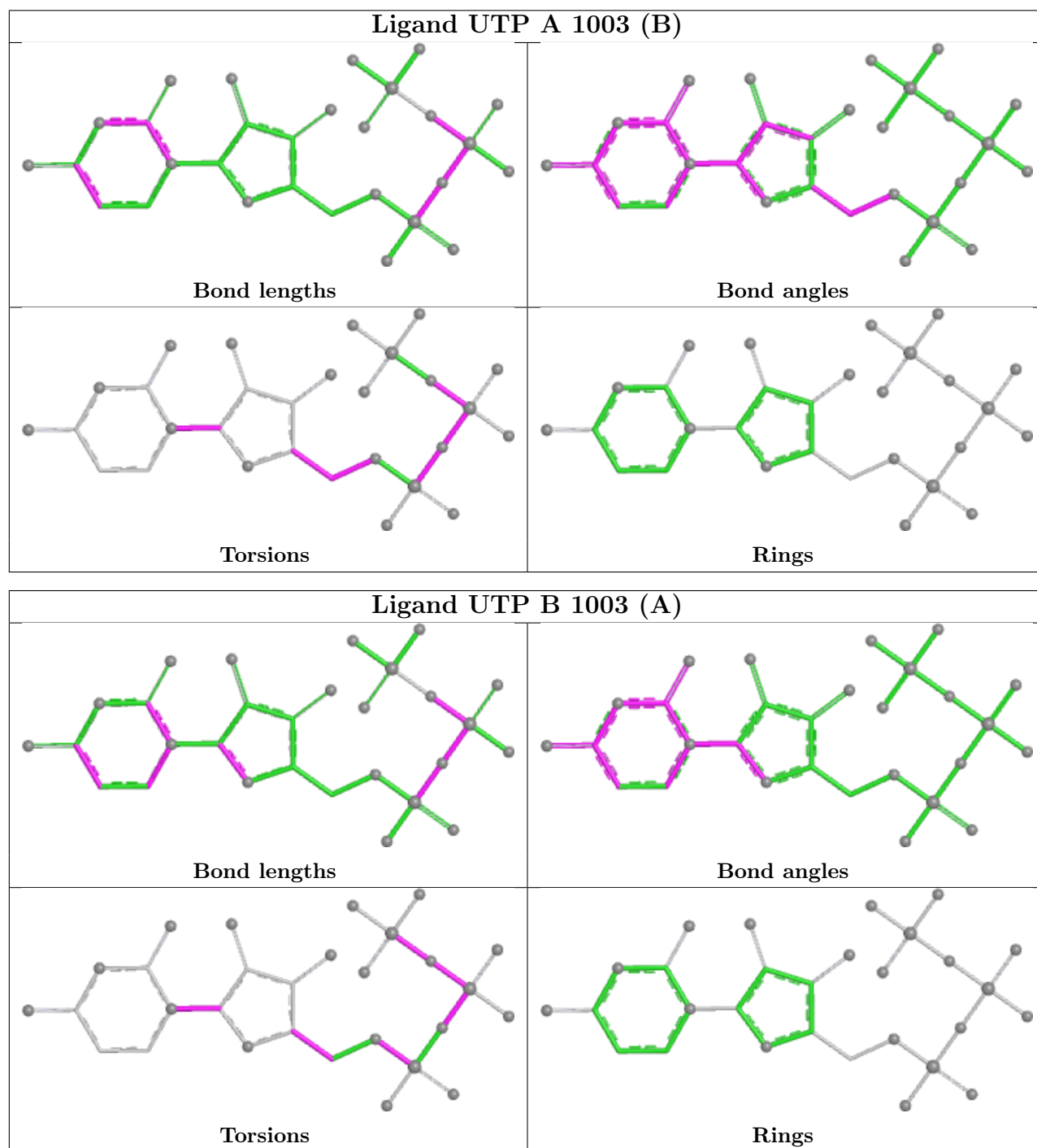
There are no ring outliers.

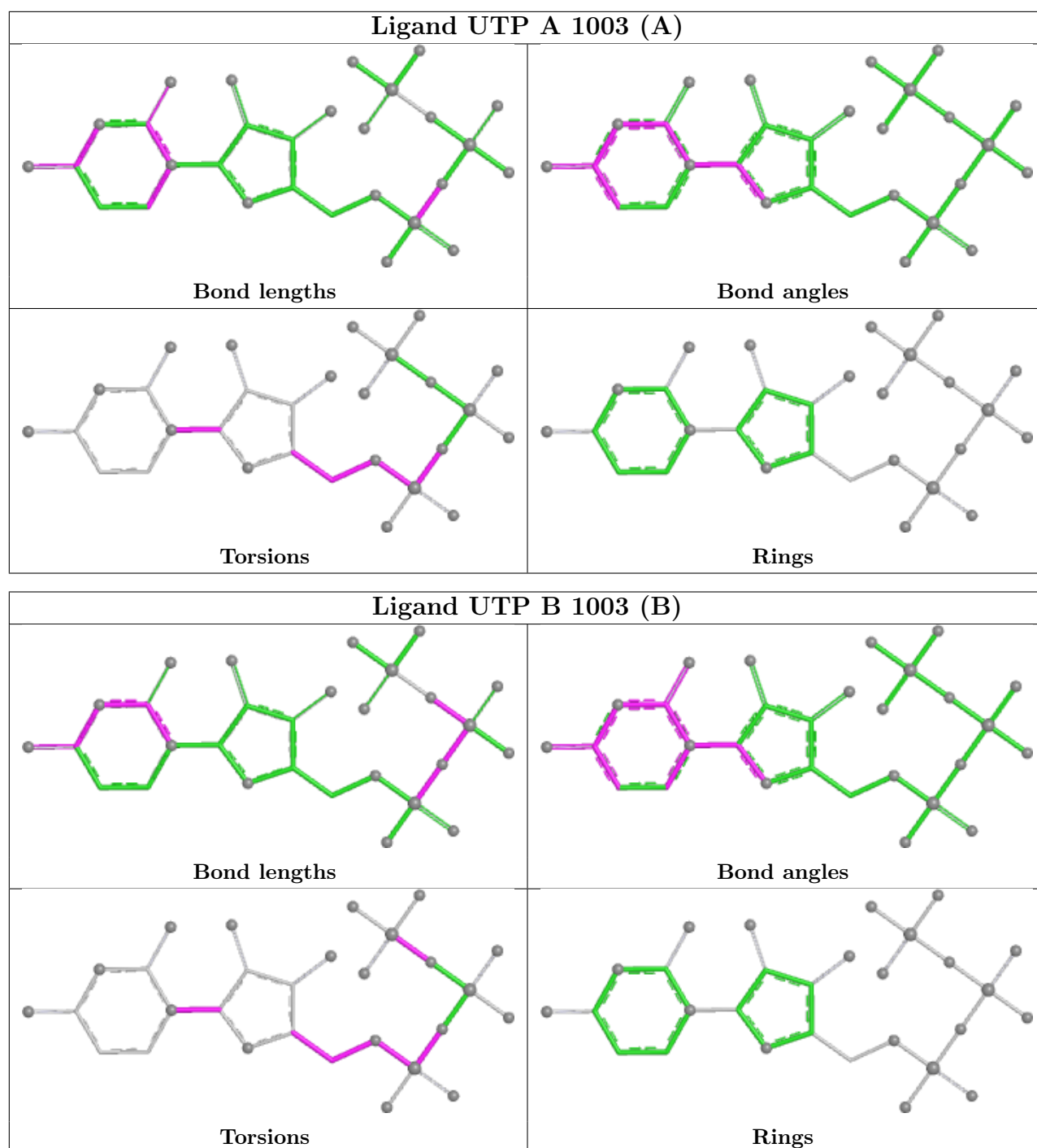
4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1003[B]	UTP	2	0
3	B	1003[A]	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, 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	A	565/570 (99%)	-0.30	28 (4%) 34 31	11, 37, 104, 168	0
1	B	565/570 (99%)	-0.68	20 (3%) 47 43	9, 23, 67, 159	0
All	All	1130/1140 (99%)	-0.49	48 (4%) 40 37	9, 28, 96, 168	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	564	LEU	4.5
1	B	550	ASN	4.4
1	A	549	GLY	4.1
1	B	540	PRO	3.8
1	B	551	PHE	3.8
1	B	545	LEU	3.6
1	B	153	GLY	3.6
1	A	541	ALA	3.4
1	B	552	VAL	3.4
1	A	26	LEU	3.3
1	B	152	GLY	3.2
1	A	149	PRO	3.2
1	A	545	LEU	3.0
1	A	510	LYS	3.0
1	A	547	LEU	2.9
1	A	544	GLN	2.9
1	B	537	THR	2.9
1	B	565	SER	2.8
1	A	34	HIS	2.8
1	A	531	ARG	2.7
1	A	465	ARG	2.7
1	B	546	ASP	2.6
1	B	541	ALA	2.6
1	A	151	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	565	SER	2.6
1	B	563	SER	2.6
1	B	543	SER	2.5
1	A	152	GLY	2.5
1	A	539	ILE	2.5
1	B	531	ARG	2.5
1	B	544	GLN	2.5
1	A	543	SER	2.5
1	A	552	VAL	2.5
1	A	25	PRO	2.4
1	B	558	GLY	2.4
1	A	502	HIS	2.4
1	B	149	PRO	2.4
1	A	434	LEU	2.4
1	B	547	LEU	2.4
1	A	563	SER	2.3
1	A	520	THR	2.3
1	A	523	ARG	2.3
1	A	556	SER	2.1
1	A	529	ALA	2.1
1	B	542	ALA	2.1
1	A	564	LEU	2.1
1	A	507	VAL	2.1
1	A	540	PRO	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

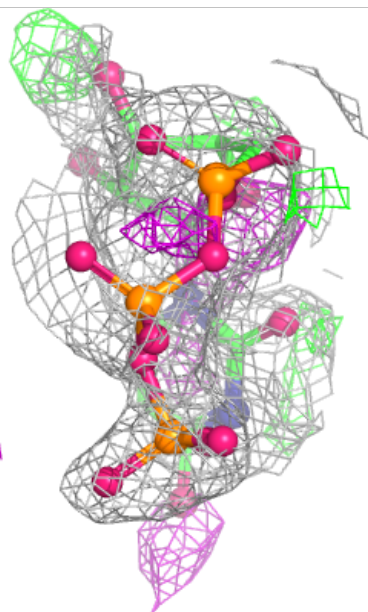
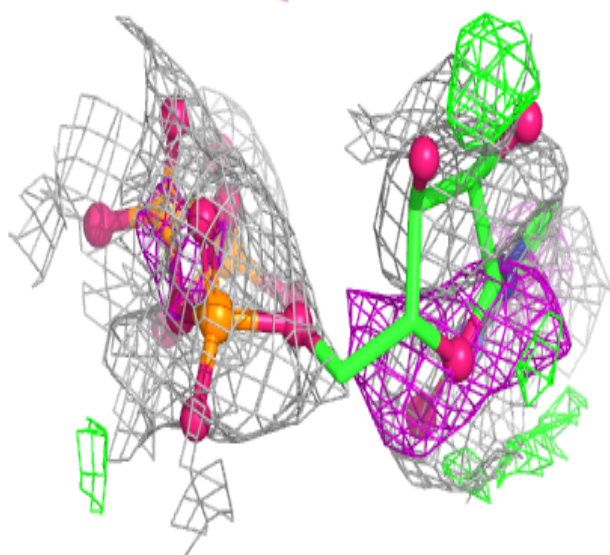
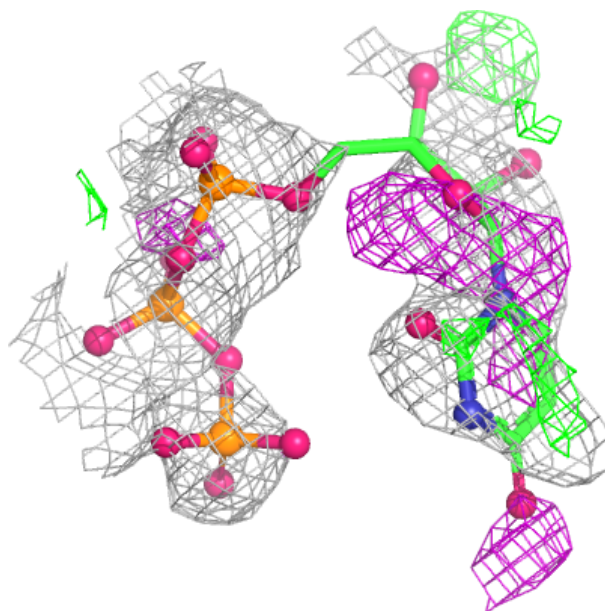
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	UTP	B	1003[A]	29/29	0.80	0.20	24,66,83,84	29
3	UTP	B	1003[B]	29/29	0.80	0.20	24,72,83,87	29
3	UTP	A	1003[A]	29/29	0.84	0.18	21,64,77,80	29
3	UTP	A	1003[B]	29/29	0.84	0.18	38,64,77,79	29
2	MN	A	1001	1/1	0.90	0.07	30,30,30,30	1
2	MN	B	1002	1/1	0.97	0.04	21,21,21,21	1
2	MN	A	1002	1/1	0.99	0.02	31,31,31,31	1
2	MN	B	1001	1/1	1.00	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.

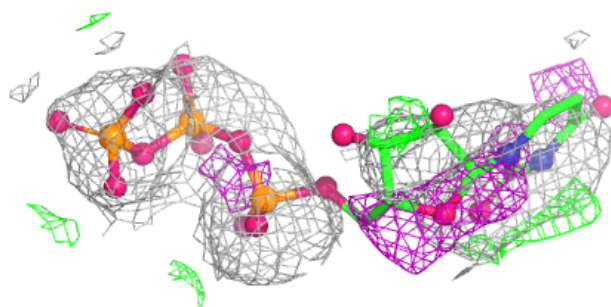
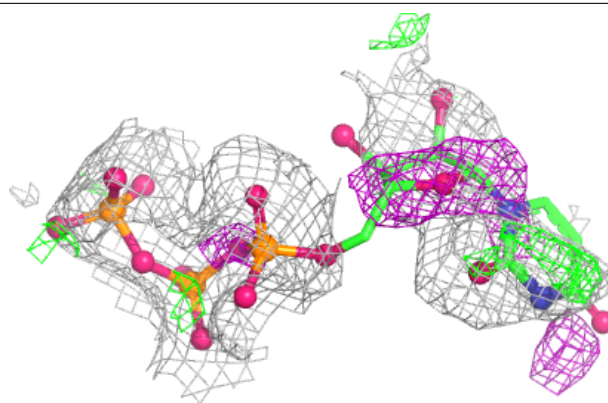
Electron density around UTP B 1003 (A):

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

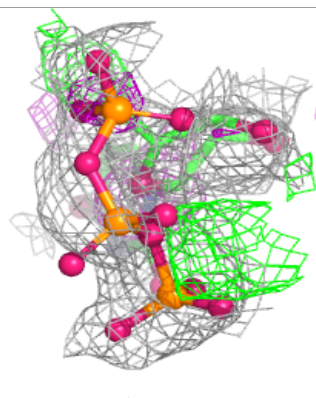
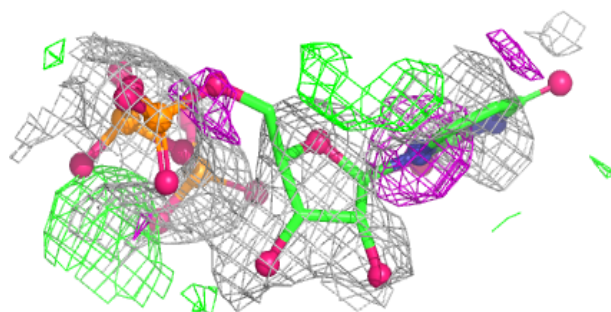
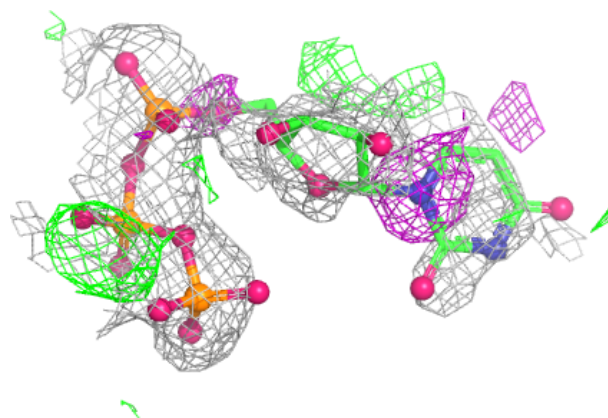


Electron density around UTP B 1003 (B):

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

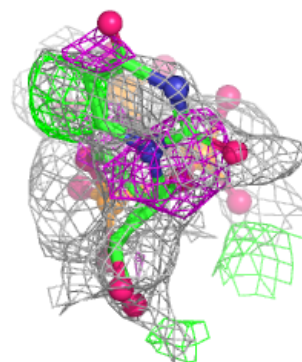
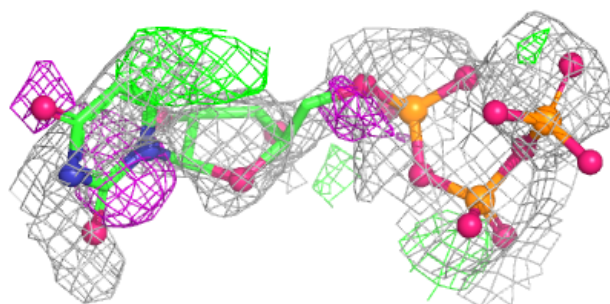
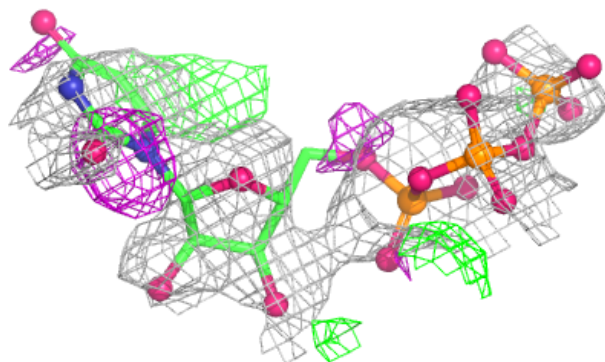
**Electron density around UTP A 1003 (A):**

$2mF_o-DF_c$ (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.