



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:35 PM UTC

PDB ID : 4E80 / pdb_00004e80
Title : Structural Basis for the Activity of a Cytoplasmic RNA Terminal U-transferase
Authors : Yates, L.A.; Fleurdepine, S.; Rissland, O.S.; DeColibus, L.; Harlos, K.; Norbury, C.J.; Gilbert, R.J.C.
Deposited on : 2012-03-19
Resolution : 3.02 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

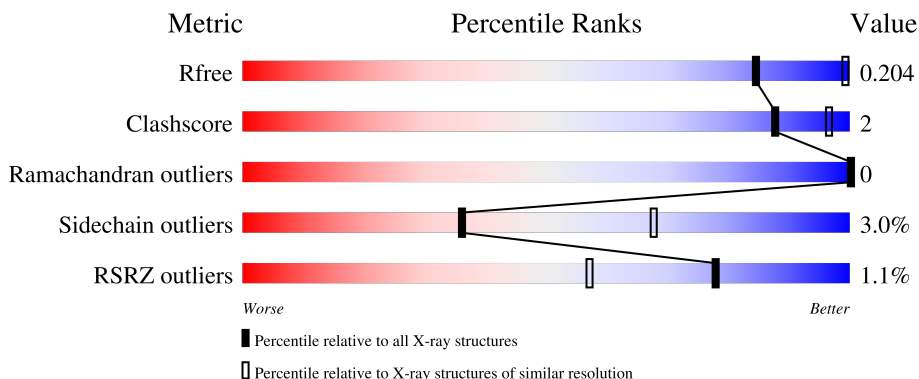
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.02 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	3131 (3.04-3.00)
Clashscore	190562	3444 (3.04-3.00)
Ramachandran outliers	187476	3319 (3.04-3.00)
Sidechain outliers	187428	3322 (3.04-3.00)
RSRZ outliers	180081	3130 (3.04-3.00)

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	405	 72% 6% 22%
1	B	405	 70% 6% 23%
1	C	405	 74% 6% 19%
1	D	405	 74% 6% 20%

2 Entry composition [i](#)

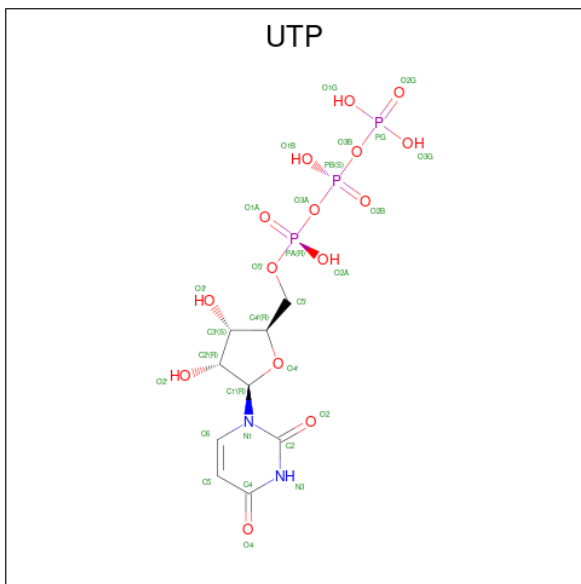
There are 3 unique types of molecules in this entry. The entry contains 10472 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Poly(A) RNA polymerase protein cid1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	317	Total 2563	C 1667	N 425	O 462	S 9	0	0	0
1	B	311	Total 2520	C 1641	N 416	O 454	S 9	0	0	0
1	C	330	Total 2653	C 1719	N 439	O 486	S 9	0	0	0
1	D	324	Total 2603	C 1686	N 434	O 474	S 9	0	0	0

- Molecule 2 is URIDINE 5'-TRIPHOSPHATE (CCD ID: UTP) (formula: C₉H₁₅N₂O₁₅P₃).



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

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

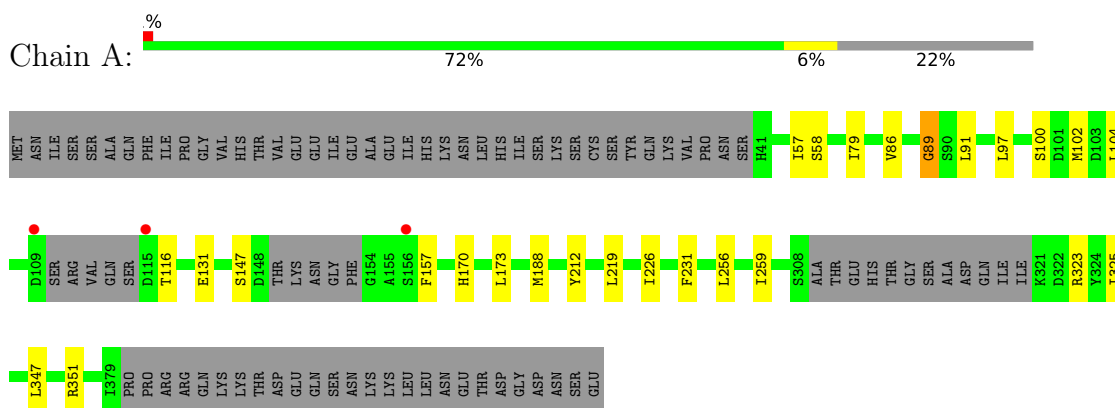
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	O	0	0
			3	3		
3	B	7	Total	O	0	0
			7	7		
3	C	2	Total	O	0	0
			2	2		
3	D	5	Total	O	0	0
			5	5		

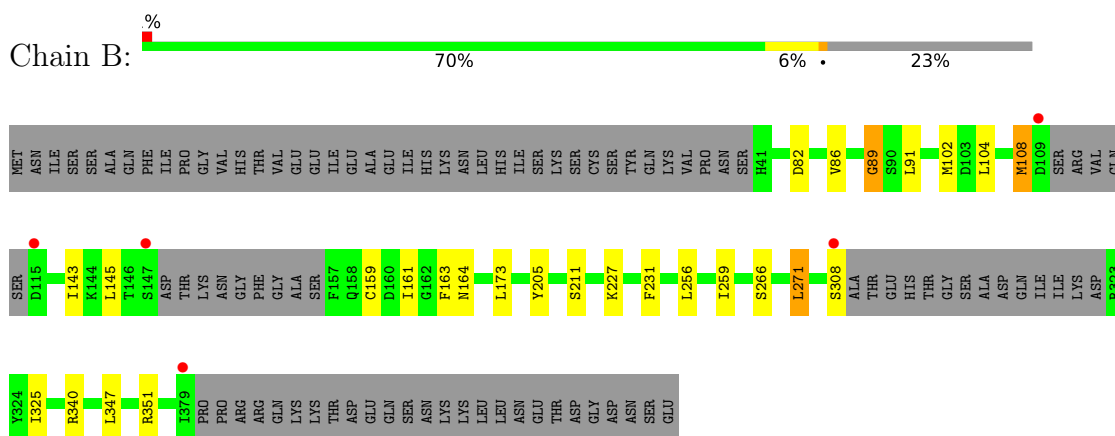
3 Residue-property plots [i](#)

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.

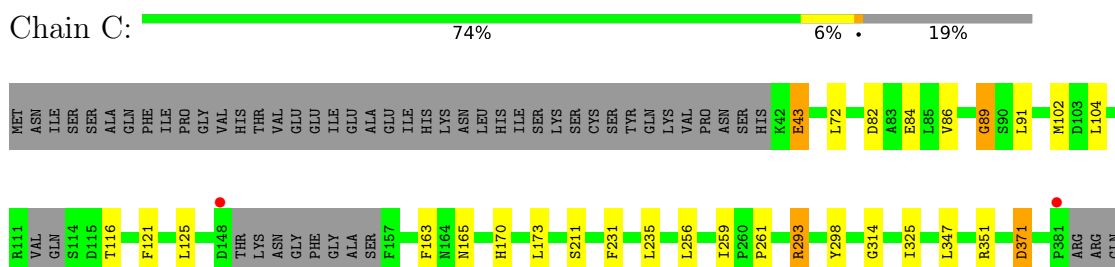
- Molecule 1: Poly(A) RNA polymerase protein cid1



- Molecule 1: Poly(A) RNA polymerase protein cid1

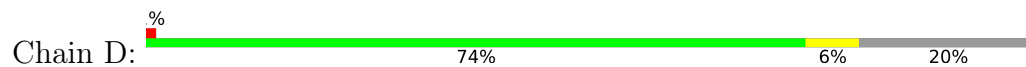


- Molecule 1: Poly(A) RNA polymerase protein cid1



LYS
LYS
THR
SER
GLU
GLN
SER
ASN
LYS
LYS
LEU
LEU
ASN
GLU
THR
ASP
GLY
ASP
ASN
SER
GLU

- Molecule 1: Poly(A) RNA polymerase protein cid1



MET
ASN
ILE
SER
SER
ALA
GLN
PHE
ILE
PRO
GLY
VAL
HIS
THR
VAL
GLY
GLU
ILE
GLU
ALA
GLU
ILE
HIS
HIS
LYS
ASN
LEU
HIS
ILE
SER
LYS
SER
CYS
TYR
GLN
LYS
VAL
PRO
ASN
SER
H41
L72
V86
G89
S90
L91
M102
D103
L104
M108
D109
SER
ARG
VAL
GLN

SER
D115
T116
L125
R139
I143
S147
ASP
THR
LYS
ASN
GLY
PHE
GLY
ALA
S156
I161
H170
L173
Y212
F231
L256
I259
E311
S315
A316
D317
GLN
ILE
ILE
K321
I325
L347
R351
P380
PRO
ARG
ARG
GLN
LYS
LYS
THR
ASP

GLU
GLN
SER
ASN
LYS
LEU
LEU
ASN
THR
GLY
ASP
ASP
ASN
SER
GLU

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	164.69Å 77.96Å 151.68Å 90.00° 109.29° 90.00°	Depositor
Resolution (Å)	28.72 – 3.02 28.72 – 3.02	Depositor EDS
% Data completeness (in resolution range)	99.1 (28.72-3.02) 99.1 (28.72-3.02)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.84 (at 3.01Å)	Xtrriage
Refinement program	BUSTER 2.11.2	Depositor
R, R_{free}	0.176 , 0.201 0.182 , 0.204	Depositor DCC
R_{free} test set	1784 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	57.1	Xtrriage
Anisotropy	0.131	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 63.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10472	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% 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 i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.79	0/2623	1.22	5/3538 (0.1%)
1	B	0.79	0/2579	1.21	5/3480 (0.1%)
1	C	0.80	0/2715	1.24	10/3669 (0.3%)
1	D	0.78	0/2662	1.23	6/3592 (0.2%)
All	All	0.79	0/10579	1.22	26/14279 (0.2%)

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	371	ASP	CA-CB-CG	8.12	120.72	112.60
1	D	380	PRO	N-CA-CB	6.33	109.97	103.00
1	D	116	THR	CA-C-N	5.86	128.49	120.46
1	D	116	THR	C-N-CA	5.86	128.49	120.46
1	A	231	PHE	CA-CB-CG	5.62	119.42	113.80
1	A	89	GLY	CA-C-N	5.50	127.97	120.54
1	A	89	GLY	C-N-CA	5.50	127.97	120.54
1	B	231	PHE	CA-CB-CG	5.41	119.21	113.80
1	D	89	GLY	CA-C-N	5.39	127.82	120.54
1	D	89	GLY	C-N-CA	5.39	127.82	120.54
1	D	231	PHE	CA-CB-CG	5.38	119.18	113.80
1	C	116	THR	CA-C-N	5.36	127.80	120.46
1	C	116	THR	C-N-CA	5.36	127.80	120.46
1	A	116	THR	CA-C-N	5.28	127.70	120.46
1	A	116	THR	C-N-CA	5.28	127.70	120.46
1	C	314	GLY	CA-C-N	5.26	127.27	120.44
1	C	314	GLY	C-N-CA	5.26	127.27	120.44
1	B	89	GLY	CA-C-N	5.24	127.61	120.54
1	B	89	GLY	C-N-CA	5.24	127.61	120.54
1	C	231	PHE	CA-CB-CG	5.22	119.02	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	C	163	PHE	CA-C-N	5.08	129.95	122.63
1	C	163	PHE	C-N-CA	5.08	129.95	122.63
1	C	89	GLY	CA-C-N	5.08	127.40	120.54
1	C	89	GLY	C-N-CA	5.08	127.40	120.54
1	B	163	PHE	CA-C-N	5.05	129.90	122.63
1	B	163	PHE	C-N-CA	5.05	129.90	122.63

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	A	2563	0	2573	12	0
1	B	2520	0	2533	10	0
1	C	2653	0	2650	14	0
1	D	2603	0	2600	7	0
2	A	29	0	11	2	0
2	B	29	0	11	3	0
2	C	29	0	11	3	0
2	D	29	0	11	1	0
3	A	3	0	0	0	0
3	B	7	0	0	0	0
3	C	2	0	0	0	0
3	D	5	0	0	0	0
All	All	10472	0	10400	41	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 2.

All (41) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (\AA)	Clash overlap (\AA)
1:D:256:LEU:HA	1:D:259:ILE:HD12	1.75	0.69
1:A:58:SER:CB	1:C:261:PRO:HG3	2.23	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:256:LEU:HA	1:C:259:ILE:HD12	1.75	0.68
1:A:256:LEU:HA	1:A:259:ILE:HD12	1.75	0.67
1:B:256:LEU:HA	1:B:259:ILE:HD12	1.74	0.67
1:A:58:SER:HB3	1:C:261:PRO:HG3	1.77	0.66
1:B:102:MET:HE2	1:B:104:LEU:HD21	1.78	0.65
1:A:102:MET:HE2	1:A:104:LEU:HD21	1.79	0.63
1:D:212:TYR:HB2	2:D:500:UTP:H5'2	1.79	0.62
1:C:102:MET:HE2	1:C:104:LEU:HD21	1.83	0.61
1:D:102:MET:HE2	1:D:104:LEU:HD21	1.84	0.59
1:B:211:SER:HB2	2:B:501:UTP:O3A	2.06	0.55
1:A:58:SER:HB2	1:C:261:PRO:HG3	1.89	0.54
1:C:211:SER:HB2	2:C:501:UTP:O3A	2.07	0.54
2:C:501:UTP:H5'1	2:C:501:UTP:H6	1.74	0.53
2:B:501:UTP:H5'1	2:B:501:UTP:H6	1.74	0.52
1:C:72:LEU:HD23	1:C:125:LEU:HD22	1.92	0.52
1:D:170:HIS:HA	1:D:173:LEU:HD12	1.92	0.51
1:A:170:HIS:HA	1:A:173:LEU:HD12	1.92	0.51
1:A:325:ILE:HG22	1:A:347:LEU:HD22	1.92	0.51
1:B:89:GLY:HA2	2:B:501:UTP:O3'	2.11	0.51
1:B:325:ILE:HG22	1:B:347:LEU:HD22	1.92	0.51
1:C:170:HIS:HA	1:C:173:LEU:HD12	1.93	0.51
1:C:235:LEU:HD23	1:C:293:ARG:HH11	1.76	0.50
1:A:89:GLY:HA2	2:A:501:UTP:O3'	2.11	0.49
1:A:323:ARG:HG2	1:A:325:ILE:HG12	1.95	0.49
1:C:89:GLY:HA2	2:C:501:UTP:O3'	2.12	0.49
1:C:325:ILE:HG22	1:C:347:LEU:HD22	1.95	0.48
1:D:325:ILE:HG22	1:D:347:LEU:HD22	1.97	0.47
1:C:43:GLU:CD	1:C:43:GLU:H	2.23	0.46
1:A:212:TYR:HB2	2:A:501:UTP:H5'2	1.97	0.46
1:A:131:GLU:HB2	1:A:147:SER:HB3	1.99	0.45
1:D:72:LEU:HD23	1:D:125:LEU:HD22	2.00	0.44
1:B:266:SER:HB2	1:B:271:LEU:HD13	2.00	0.44
1:B:227:LYS:HB3	1:C:298:TYR:CE1	2.54	0.43
1:B:143:ILE:HB	1:B:161:ILE:HB	2.00	0.42
1:B:108:MET:HG2	1:B:164:ASN:HD21	1.85	0.42
1:C:121:PHE:CE1	1:C:125:LEU:HD21	2.54	0.42
1:B:145:LEU:HB2	1:B:159:CYS:HB3	2.02	0.42
1:A:97:LEU:O	1:A:100:SER:HB2	2.20	0.41
1:D:143:ILE:HB	1:D:161:ILE:HB	2.02	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	309/405 (76%)	299 (97%)	10 (3%)	0	100	100
1	B	303/405 (75%)	298 (98%)	5 (2%)	0	100	100
1	C	324/405 (80%)	314 (97%)	10 (3%)	0	100	100
1	D	316/405 (78%)	309 (98%)	7 (2%)	0	100	100
All	All	1252/1620 (77%)	1220 (97%)	32 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	279/363 (77%)	270 (97%)	9 (3%)	34	66
1	B	275/363 (76%)	265 (96%)	10 (4%)	31	64
1	C	289/363 (80%)	280 (97%)	9 (3%)	35	67
1	D	282/363 (78%)	276 (98%)	6 (2%)	47	74
All	All	1125/1452 (78%)	1091 (97%)	34 (3%)	36	68

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	ILE
1	A	79	ILE

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Mol	Chain	Res	Type
1	A	86	VAL
1	A	91	LEU
1	A	157	PHE
1	A	188	MET
1	A	219	LEU
1	A	226	ILE
1	A	351	ARG
1	B	82	ASP
1	B	86	VAL
1	B	91	LEU
1	B	108	MET
1	B	173	LEU
1	B	205	TYR
1	B	271	LEU
1	B	308	SER
1	B	340	ARG
1	B	351	ARG
1	C	43	GLU
1	C	82	ASP
1	C	84	GLU
1	C	86	VAL
1	C	91	LEU
1	C	165	ASN
1	C	293	ARG
1	C	351	ARG
1	C	371	ASP
1	D	86	VAL
1	D	91	LEU
1	D	108	MET
1	D	139	ARG
1	D	311	GLU
1	D	351	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	ASN
1	A	120	GLN
1	A	200	GLN
1	A	362	ASN
1	B	164	ASN
1	C	120	GLN

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Mol	Chain	Res	Type
1	C	158	GLN
1	D	120	GLN
1	D	164	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	UTP	D	500	-	29,30,30	1.81	3 (10%)	43,47,47	1.68	9 (20%)
2	UTP	B	501	-	29,30,30	1.70	3 (10%)	43,47,47	1.77	10 (23%)
2	UTP	A	501	-	29,30,30	1.90	3 (10%)	43,47,47	1.96	12 (27%)
2	UTP	C	501	-	29,30,30	1.66	2 (6%)	43,47,47	1.70	11 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	UTP	D	500	-	-	7/22/38/38	0/2/2/2
2	UTP	B	501	-	-	7/22/38/38	0/2/2/2
2	UTP	A	501	-	-	6/22/38/38	0/2/2/2
2	UTP	C	501	-	-	7/22/38/38	0/2/2/2

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	UTP	PB-O3A	6.54	1.66	1.59
2	D	500	UTP	PB-O3A	6.25	1.66	1.59
2	C	501	UTP	PB-O3A	6.03	1.66	1.59
2	A	501	UTP	PB-O3B	5.43	1.65	1.59
2	D	500	UTP	PB-O3B	5.42	1.65	1.59
2	A	501	UTP	PB-O3A	5.27	1.65	1.59
2	A	501	UTP	PA-O3A	4.69	1.64	1.59
2	C	501	UTP	PB-O3B	4.51	1.64	1.59
2	B	501	UTP	PB-O3B	3.93	1.63	1.59
2	D	500	UTP	PA-O3A	3.05	1.62	1.59
2	B	501	UTP	PG-O3G	2.01	1.62	1.54

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	UTP	C4-N3-C2	-5.38	119.94	126.61
2	A	501	UTP	C4-N3-C2	-5.20	120.16	126.61
2	C	501	UTP	C4-N3-C2	-4.90	120.53	126.61
2	D	500	UTP	C4-N3-C2	-4.87	120.57	126.61
2	A	501	UTP	C5'-C4'-C3'	-4.48	99.07	115.21
2	A	501	UTP	N3-C2-N1	4.45	120.69	114.89
2	B	501	UTP	N3-C2-N1	4.29	120.48	114.89
2	D	500	UTP	N3-C2-N1	4.16	120.31	114.89
2	C	501	UTP	N3-C2-N1	4.15	120.29	114.89
2	B	501	UTP	C5-C4-N3	3.42	119.60	114.80
2	A	501	UTP	O4'-C4'-C5'	3.36	120.09	109.33
2	D	500	UTP	O4-C4-C5	-3.34	119.40	125.16
2	B	501	UTP	O4-C4-C5	-3.27	119.52	125.16
2	C	501	UTP	C3'-C2'-C1'	3.25	107.61	101.46
2	C	501	UTP	O4-C4-C5	-3.22	119.62	125.16
2	A	501	UTP	C5-C4-N3	3.21	119.30	114.80
2	C	501	UTP	C5-C4-N3	3.21	119.29	114.80
2	A	501	UTP	C3'-C2'-C1'	3.13	107.38	101.46
2	D	500	UTP	C5-C4-N3	3.09	119.12	114.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	UTP	O4-C4-C5	-3.06	119.88	125.16
2	B	501	UTP	C3'-C2'-C1'	3.05	107.24	101.46
2	D	500	UTP	C3'-C2'-C1'	3.02	107.18	101.46
2	D	500	UTP	O4'-C4'-C3'	3.02	111.15	105.15
2	B	501	UTP	O2-C2-N1	-2.88	119.04	122.80
2	C	501	UTP	O4'-C4'-C3'	2.86	110.83	105.15
2	B	501	UTP	O4'-C4'-C3'	2.79	110.68	105.15
2	B	501	UTP	O1B-PB-O3A	2.62	114.36	107.27
2	C	501	UTP	O1B-PB-O3A	2.55	114.17	107.27
2	A	501	UTP	O4'-C4'-C3'	2.49	110.10	105.15
2	A	501	UTP	O3G-PG-O3B	2.46	112.88	104.64
2	D	500	UTP	O3G-PG-O3B	2.46	112.88	104.64
2	C	501	UTP	O3G-PG-O3B	2.43	112.77	104.64
2	C	501	UTP	O2-C2-N1	-2.43	119.64	122.80
2	B	501	UTP	O3G-PG-O3B	2.35	112.52	104.64
2	D	500	UTP	PA-O5'-C5'	-2.23	108.58	121.35
2	A	501	UTP	O2-C2-N1	-2.21	119.91	122.80
2	C	501	UTP	PA-O5'-C5'	-2.21	108.66	121.35
2	A	501	UTP	PA-O5'-C5'	-2.17	108.92	121.35
2	A	501	UTP	C2'-C1'-N1	-2.14	107.29	113.25
2	B	501	UTP	PA-O5'-C5'	-2.14	109.09	121.35
2	C	501	UTP	C2'-C1'-N1	-2.05	107.53	113.25
2	D	500	UTP	O2A-PA-O3A	2.01	112.71	107.27

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	UTP	C5'-O5'-PA-O2A
2	A	501	UTP	PB-O3B-PG-O3G
2	B	501	UTP	PB-O3B-PG-O3G
2	C	501	UTP	PB-O3B-PG-O3G
2	D	500	UTP	PB-O3B-PG-O1G
2	D	500	UTP	PB-O3B-PG-O3G
2	B	501	UTP	C3'-C4'-C5'-O5'
2	C	501	UTP	C3'-C4'-C5'-O5'
2	B	501	UTP	O4'-C4'-C5'-O5'
2	C	501	UTP	O4'-C4'-C5'-O5'
2	A	501	UTP	C5'-O5'-PA-O3A
2	D	500	UTP	C5'-O5'-PA-O1A
2	D	500	UTP	C5'-O5'-PA-O2A
2	D	500	UTP	C5'-O5'-PA-O3A

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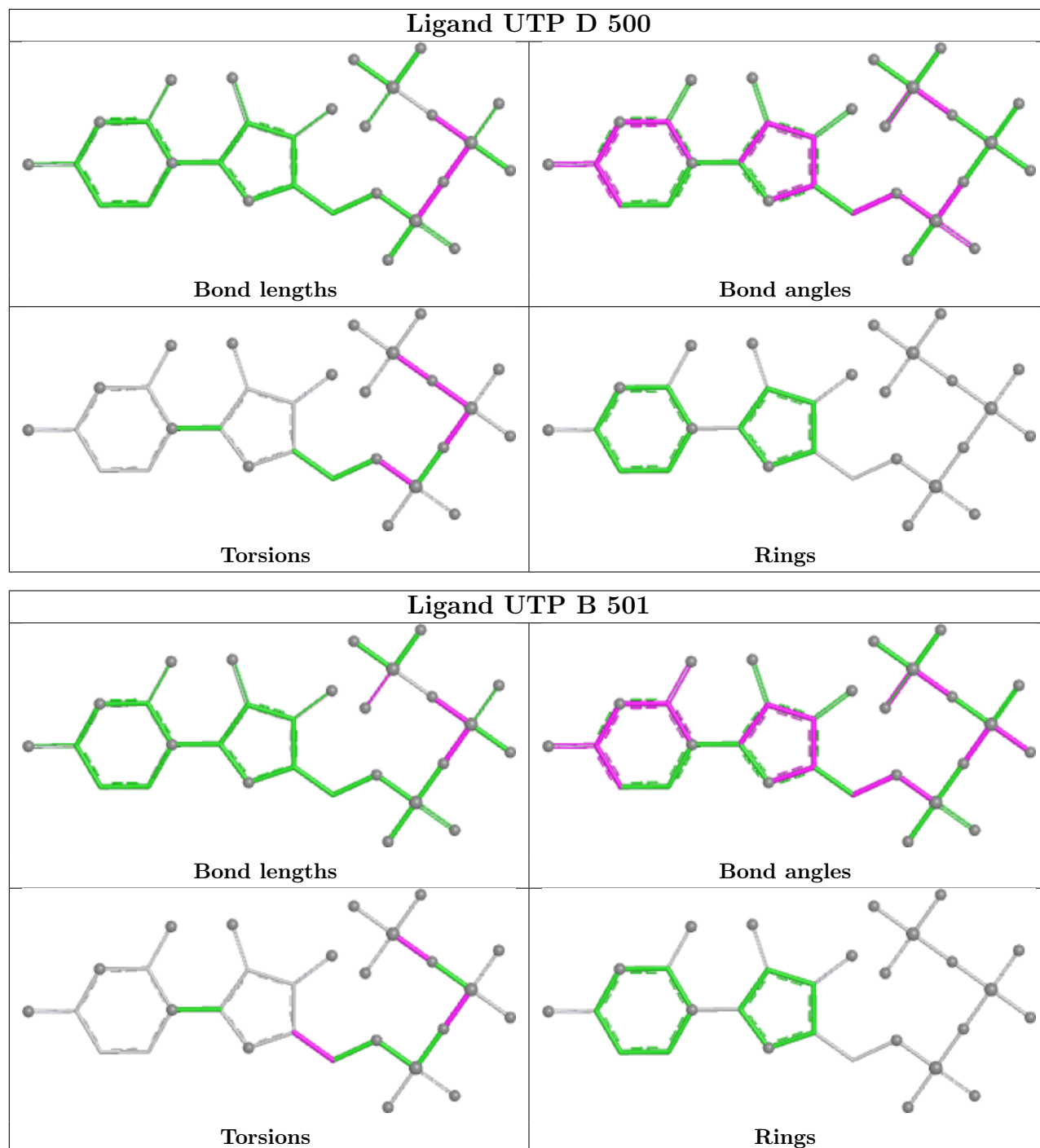
Mol	Chain	Res	Type	Atoms
2	A	501	UTP	PA-O3A-PB-O1B
2	A	501	UTP	PB-O3B-PG-O1G
2	B	501	UTP	PB-O3B-PG-O1G
2	C	501	UTP	PB-O3B-PG-O1G
2	B	501	UTP	PA-O3A-PB-O1B
2	C	501	UTP	PA-O3A-PB-O1B
2	D	500	UTP	PA-O3A-PB-O1B
2	A	501	UTP	PB-O3B-PG-O2G
2	B	501	UTP	PB-O3B-PG-O2G
2	C	501	UTP	PB-O3B-PG-O2G
2	B	501	UTP	PA-O3A-PB-O2B
2	C	501	UTP	PA-O3A-PB-O2B
2	D	500	UTP	PG-O3B-PB-O1B

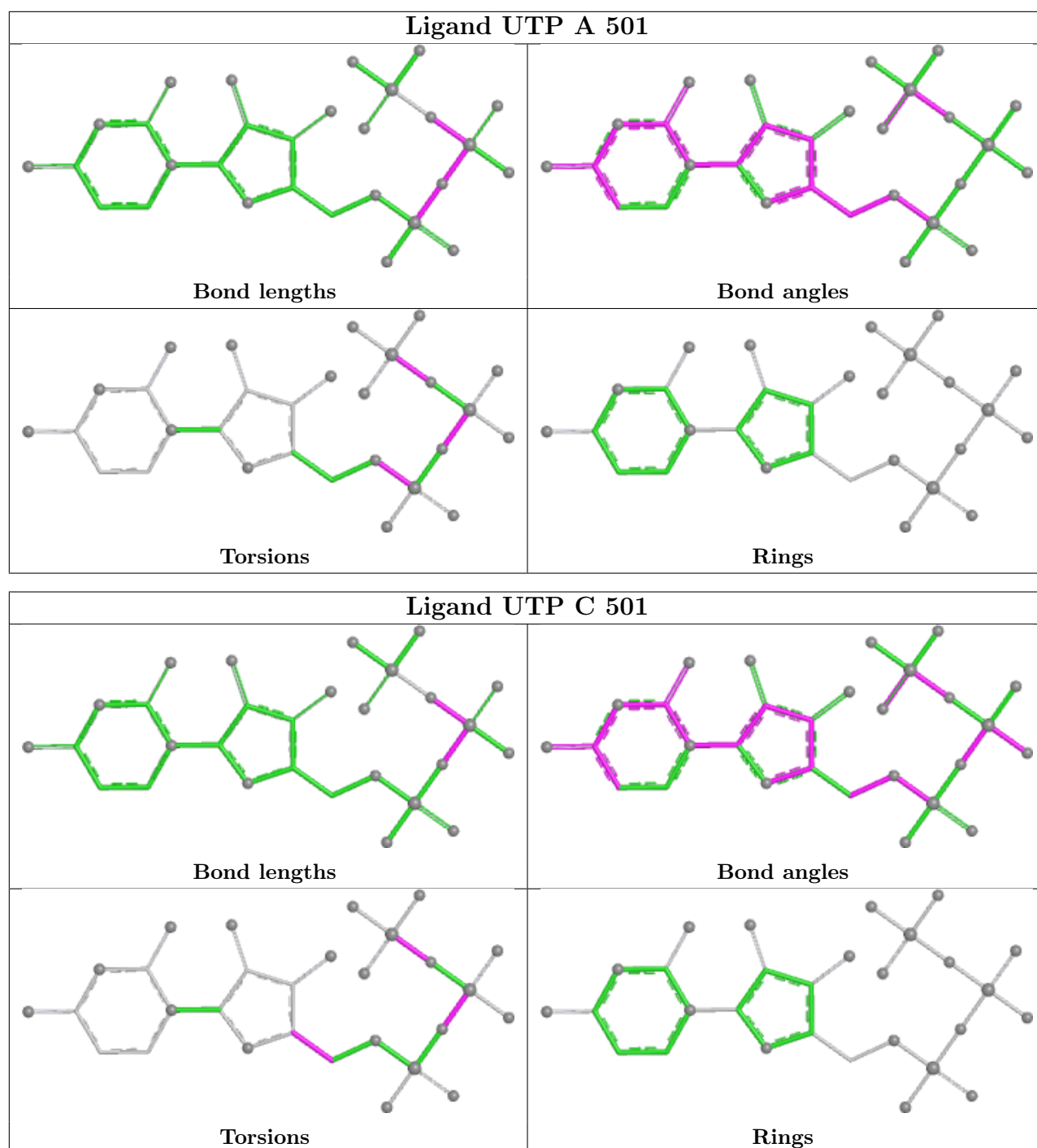
There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	500	UTP	1	0
2	B	501	UTP	3	0
2	A	501	UTP	2	0
2	C	501	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	317/405 (78%)	-0.21	3 (0%) 81 61	38, 66, 110, 140	0
1	B	311/405 (76%)	-0.53	5 (1%) 70 47	23, 41, 76, 108	0
1	C	330/405 (81%)	-0.29	2 (0%) 85 69	35, 56, 98, 122	0
1	D	324/405 (80%)	-0.29	4 (1%) 76 55	29, 58, 113, 146	0
All	All	1282/1620 (79%)	-0.33	14 (1%) 78 57	23, 56, 105, 146	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	148	ASP	5.0
1	B	109	ASP	3.7
1	A	115	ASP	3.6
1	D	115	ASP	3.6
1	A	109	ASP	3.3
1	B	147	SER	3.2
1	B	379	ILE	3.1
1	D	156	SER	2.8
1	B	308	SER	2.6
1	D	147	SER	2.6
1	D	315	SER	2.3
1	A	156	SER	2.2
1	C	381	PRO	2.1
1	B	115	ASP	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](#)

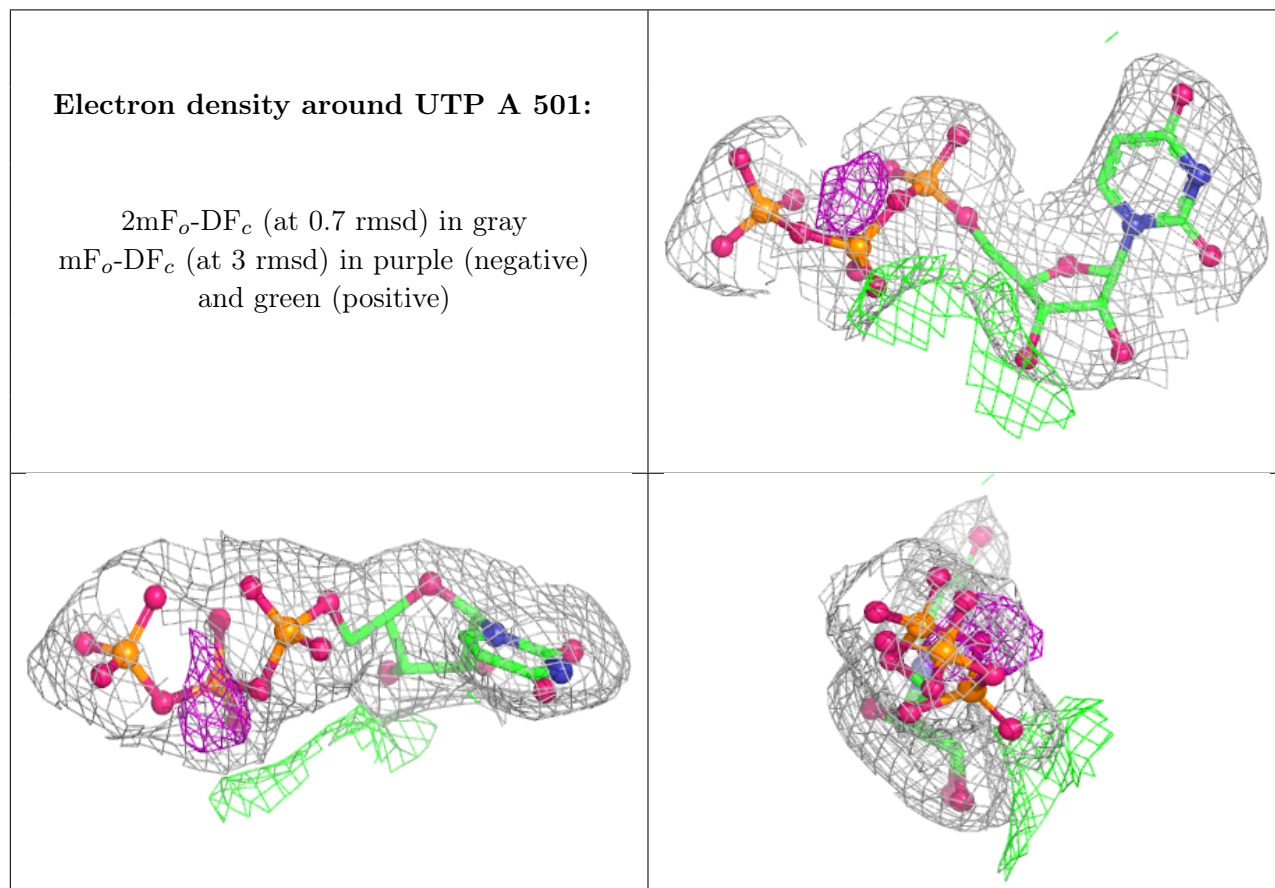
There are no oligosaccharides in this entry.

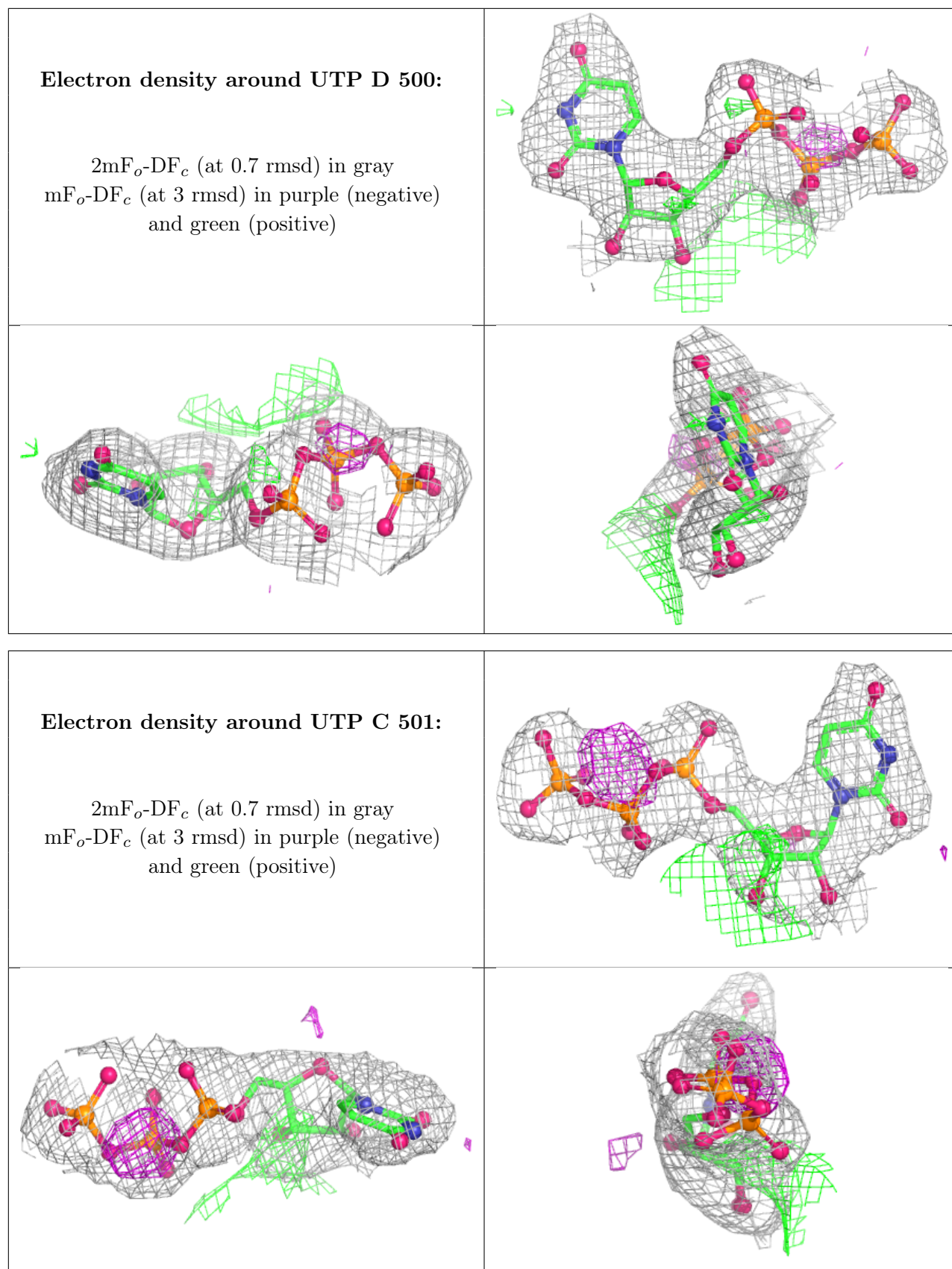
6.4 Ligands [i](#)

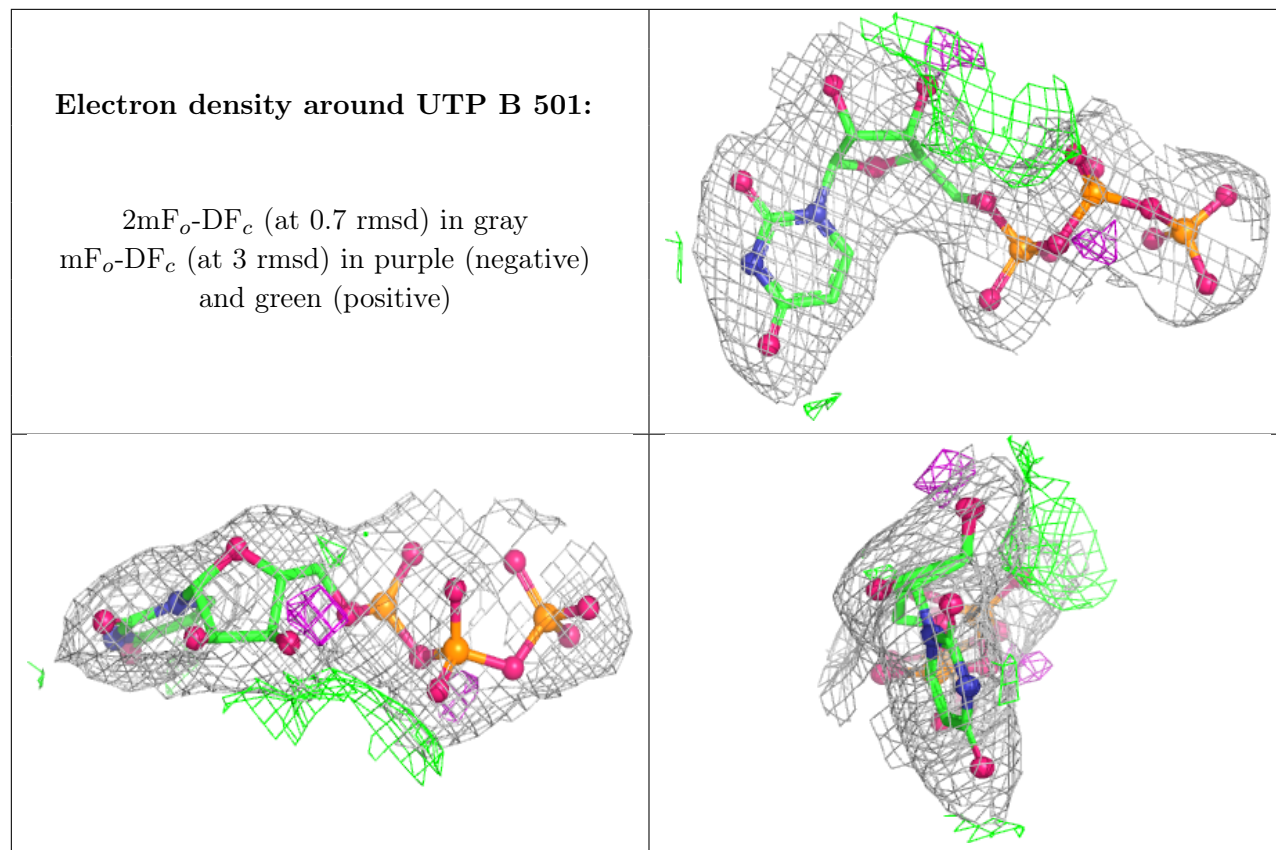
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	UTP	A	501	29/29	0.90	0.11	70,76,92,94	0
2	UTP	D	500	29/29	0.91	0.10	43,65,84,86	0
2	UTP	C	501	29/29	0.92	0.09	45,53,77,79	0
2	UTP	B	501	29/29	0.94	0.08	38,43,55,58	0

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](#)

There are no such residues in this entry.