



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 01:16 AM UTC

PDB ID : 6SU6 / pdb_00006su6
Title : Complex between a UDP-glucosyltransferase from *Polygonum tinctorium* capable of glucosylating indoxyl and UDP-glucose
Authors : Fredslund, F.; Teze, D.; Svensson, B.; Adams, P.D.; Welner, D.H.
Deposited on : 2019-09-13
Resolution : 2.40 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

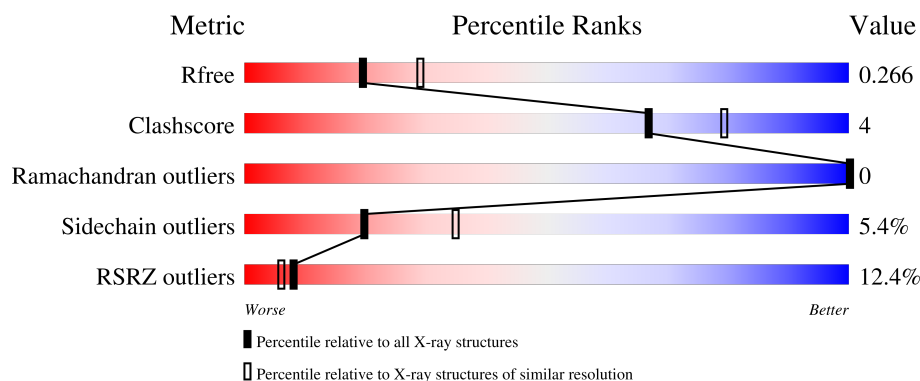
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	499	
1	B	499	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14439 atoms, of which 7165 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 Glycosyltransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	467	Total	C	H	N	O	S	0	0	0
			7182	2291	3599	613	665	14			
1	B	455	Total	C	H	N	O	S	0	0	0
			7021	2238	3524	600	646	13			

There are 42 discrepancies between the modelled and reference sequences:

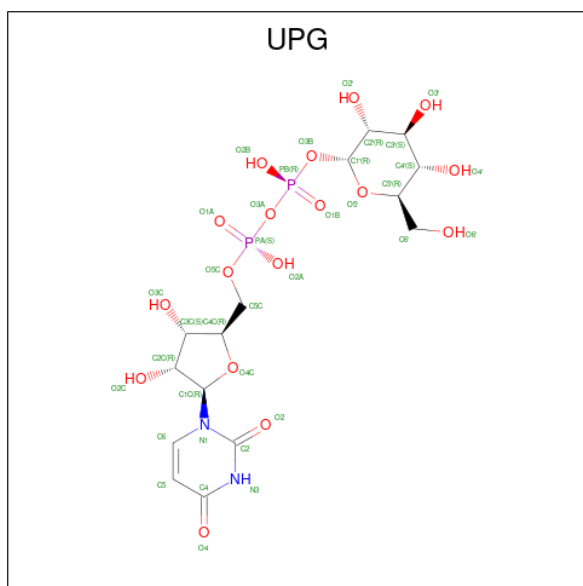
Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	initiating methionine	UNP A0A2R2JFJ4
A	-20	GLY	-	expression tag	UNP A0A2R2JFJ4
A	-19	HIS	-	expression tag	UNP A0A2R2JFJ4
A	-18	HIS	-	expression tag	UNP A0A2R2JFJ4
A	-17	HIS	-	expression tag	UNP A0A2R2JFJ4
A	-16	HIS	-	expression tag	UNP A0A2R2JFJ4
A	-15	HIS	-	expression tag	UNP A0A2R2JFJ4
A	-14	HIS	-	expression tag	UNP A0A2R2JFJ4
A	-13	ASP	-	expression tag	UNP A0A2R2JFJ4
A	-12	TYR	-	expression tag	UNP A0A2R2JFJ4
A	-11	ASP	-	expression tag	UNP A0A2R2JFJ4
A	-10	ILE	-	expression tag	UNP A0A2R2JFJ4
A	-9	PRO	-	expression tag	UNP A0A2R2JFJ4
A	-8	THR	-	expression tag	UNP A0A2R2JFJ4
A	-7	THR	-	expression tag	UNP A0A2R2JFJ4
A	-6	GLU	-	expression tag	UNP A0A2R2JFJ4
A	-5	ASN	-	expression tag	UNP A0A2R2JFJ4
A	-4	LEU	-	expression tag	UNP A0A2R2JFJ4
A	-3	TYR	-	expression tag	UNP A0A2R2JFJ4
A	-2	PHE	-	expression tag	UNP A0A2R2JFJ4
A	-1	GLN	-	expression tag	UNP A0A2R2JFJ4
B	-21	MET	-	initiating methionine	UNP A0A2R2JFJ4
B	-20	GLY	-	expression tag	UNP A0A2R2JFJ4
B	-19	HIS	-	expression tag	UNP A0A2R2JFJ4
B	-18	HIS	-	expression tag	UNP A0A2R2JFJ4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-17	HIS	-	expression tag	UNP A0A2R2JFJ4
B	-16	HIS	-	expression tag	UNP A0A2R2JFJ4
B	-15	HIS	-	expression tag	UNP A0A2R2JFJ4
B	-14	HIS	-	expression tag	UNP A0A2R2JFJ4
B	-13	ASP	-	expression tag	UNP A0A2R2JFJ4
B	-12	TYR	-	expression tag	UNP A0A2R2JFJ4
B	-11	ASP	-	expression tag	UNP A0A2R2JFJ4
B	-10	ILE	-	expression tag	UNP A0A2R2JFJ4
B	-9	PRO	-	expression tag	UNP A0A2R2JFJ4
B	-8	THR	-	expression tag	UNP A0A2R2JFJ4
B	-7	THR	-	expression tag	UNP A0A2R2JFJ4
B	-6	GLU	-	expression tag	UNP A0A2R2JFJ4
B	-5	ASN	-	expression tag	UNP A0A2R2JFJ4
B	-4	LEU	-	expression tag	UNP A0A2R2JFJ4
B	-3	TYR	-	expression tag	UNP A0A2R2JFJ4
B	-2	PHE	-	expression tag	UNP A0A2R2JFJ4
B	-1	GLN	-	expression tag	UNP A0A2R2JFJ4

- Molecule 2 is URIDINE-5'-DIPHOSPHATE-GLUCOSE (CCD ID: UPG) (formula: $C_{15}H_{24}N_2O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



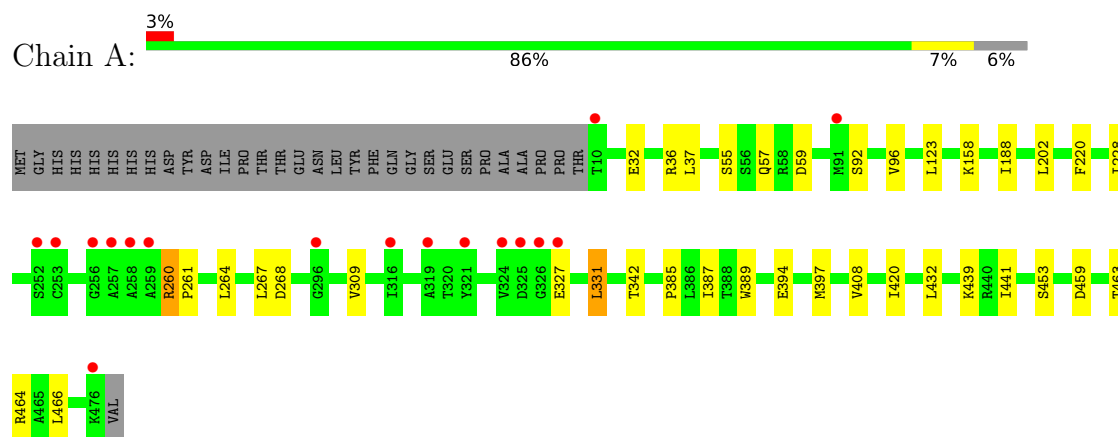
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	99	Total 99	O 99	0	0
3	B	23	Total 23	O 23	0	0

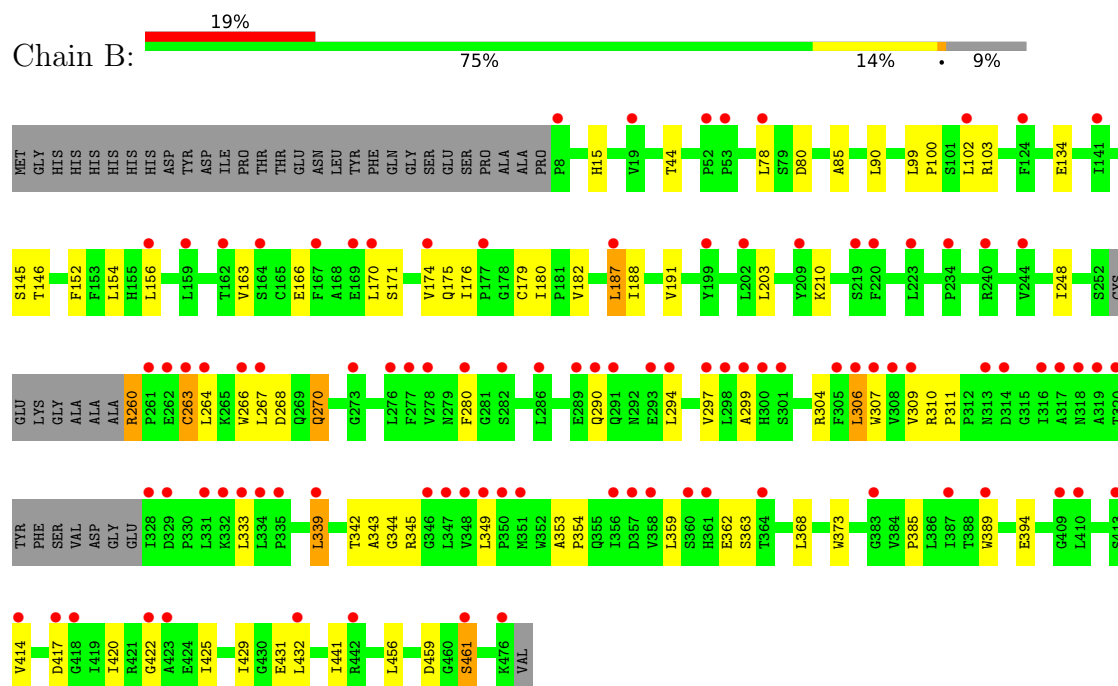
3 Residue-property plots [i](#)

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: Glycosyltransferase



• Molecule 1: Glycosyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	121.24Å 174.17Å 48.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	57.25 – 2.40 57.25 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.8 (57.25-2.40) 98.8 (57.25-2.40)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.37 (at 2.32Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.231 , 0.263 0.234 , 0.266	Depositor DCC
R_{free} test set	2196 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	47.2	Xtriage
Anisotropy	0.403	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 55.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	14439	wwPDB-VP
Average B, all atoms (Å ²)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.57% 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: UPG

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	0.15	0/3670	0.31	0/4990
1	B	0.12	0/3581	0.29	0/4868
All	All	0.14	0/7251	0.30	0/9858

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	3583	3599	3605	17	2
1	B	3497	3524	3531	35	2
2	A	36	21	22	0	0
2	B	36	21	22	2	0
3	A	99	0	0	0	0
3	B	23	0	0	0	0
All	All	7274	7165	7180	53	2

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 4.

All (53) 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:188:ILE:HG23	1:A:397:MET:HE3	1.55	0.89
1:A:260:ARG:NH2	1:A:268:ASP:OD2	2.13	0.81
1:B:420:ILE:HD11	1:B:425:ILE:HD11	1.76	0.67
1:B:260:ARG:NH2	1:B:268:ASP:OD2	2.31	0.64
1:A:385:PRO:HB2	1:A:432:LEU:HD11	1.83	0.61
1:A:92:SER:O	1:A:96:VAL:HG23	2.04	0.58
1:A:188:ILE:HG23	1:A:397:MET:CE	2.32	0.58
1:B:266:TRP:O	1:B:270:GLN:NE2	2.39	0.56
1:A:261:PRO:HD2	1:A:264:LEU:HD12	1.87	0.56
1:B:339:LEU:O	1:B:343:ALA:N	2.39	0.56
1:B:152:PHE:HE2	1:B:188:ILE:HD11	1.71	0.55
1:B:290:GLN:O	1:B:290:GLN:NE2	2.40	0.55
1:B:385:PRO:HB2	1:B:432:LEU:HD11	1.89	0.54
1:B:103:ARG:NH1	1:B:134:GLU:OE1	2.40	0.53
1:B:270:GLN:OE1	1:B:304:ARG:NH1	2.41	0.53
1:B:394:GLU:OE1	2:B:501:UPG:O4'	2.20	0.52
1:A:188:ILE:HG22	1:A:394:GLU:CB	2.39	0.52
1:B:299:ALA:O	1:B:345:ARG:NH2	2.42	0.52
1:B:263:CYS:CB	1:B:349:LEU:HD11	2.40	0.52
2:B:501:UPG:O1B	2:B:501:UPG:O2'	2.25	0.51
1:B:294:LEU:HA	1:B:425:ILE:HD13	1.91	0.51
1:A:408:VAL:HA	1:A:441:ILE:HG23	1.91	0.51
1:B:306:LEU:HD11	1:B:349:LEU:HD12	1.93	0.50
1:A:387:ILE:HG13	1:A:432:LEU:HD22	1.93	0.50
1:B:146:THR:HG22	1:B:373:TRP:CH2	2.46	0.50
1:B:175:GLN:NE2	1:B:176:ILE:O	2.45	0.50
1:B:304:ARG:NH2	1:B:344:GLY:O	2.43	0.49
1:B:297:VAL:HG21	1:B:422:GLY:O	2.11	0.49
1:B:85:ALA:HB3	1:B:90:LEU:HD21	1.93	0.48
1:B:99:LEU:N	1:B:100:PRO:HD2	2.29	0.48
1:A:264:LEU:HD23	1:A:267:LEU:HD12	1.95	0.48
1:B:15:HIS:NE2	1:B:44:THR:OG1	2.43	0.47
1:B:145:SER:OG	1:B:146:THR:N	2.46	0.47
1:A:37:LEU:HD21	1:A:466:LEU:HD22	1.97	0.46
1:A:188:ILE:HG22	1:A:394:GLU:HA	1.97	0.46
1:A:331:LEU:HD23	1:A:331:LEU:N	2.31	0.46
1:B:425:ILE:HG22	1:B:429:ILE:HD12	1.97	0.46
1:A:389:TRP:CE2	1:A:420:ILE:HD12	2.52	0.45
1:B:311:PRO:HA	1:B:333:LEU:HD13	1.98	0.45
1:B:146:THR:HG22	1:B:373:TRP:CZ3	2.53	0.44
1:B:264:LEU:HA	1:B:267:LEU:HD12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:ILE:HD11	1:A:202:LEU:HD21	2.00	0.43
1:A:32:GLU:O	1:A:36:ARG:HG2	2.18	0.43
1:B:353:ALA:HB1	1:B:354:PRO:HD2	2.01	0.43
1:B:389:TRP:CD1	1:B:389:TRP:O	2.72	0.43
1:B:307:TRP:CE2	1:B:309:VAL:HG12	2.53	0.42
1:B:368:LEU:HD23	1:B:368:LEU:C	2.45	0.42
1:A:220:PHE:C	1:A:228:ILE:HD12	2.45	0.41
1:B:280:PHE:CD1	1:B:280:PHE:N	2.89	0.41
1:B:414:VAL:HG23	1:B:420:ILE:HG23	2.02	0.41
1:B:156:LEU:HD23	1:B:203:LEU:HA	2.03	0.40
1:B:187:LEU:HD13	1:B:191:VAL:CG2	2.51	0.40
1:B:417:ASP:OD1	1:B:417:ASP:N	2.55	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:459:ASP:OD2	1:B:461:SER:OG[1_554]	2.10	0.10
1:A:464:ARG:NH1	1:B:459:ASP:OD1[1_554]	2.11	0.09

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	465/499 (93%)	446 (96%)	19 (4%)	0	100	100
1	B	449/499 (90%)	415 (92%)	34 (8%)	0	100	100
All	All	914/998 (92%)	861 (94%)	53 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	391/419 (93%)	378 (97%)	13 (3%)	33	55
1	B	384/419 (92%)	355 (92%)	29 (8%)	12	21
All	All	775/838 (92%)	733 (95%)	42 (5%)	20	35

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	SER
1	A	57	GLN
1	A	59	ASP
1	A	123	LEU
1	A	158	LYS
1	A	260	ARG
1	A	309	VAL
1	A	327	GLU
1	A	331	LEU
1	A	342	THR
1	A	439	LYS
1	A	453	SER
1	A	463	THR
1	B	78	LEU
1	B	80	ASP
1	B	102	LEU
1	B	154	LEU
1	B	163	VAL
1	B	166	GLU
1	B	170	LEU
1	B	171	SER
1	B	174	VAL
1	B	179	CYS
1	B	180	ILE
1	B	182	VAL
1	B	187	LEU
1	B	210	LYS

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Mol	Chain	Res	Type
1	B	248	ILE
1	B	260	ARG
1	B	263	CYS
1	B	270	GLN
1	B	306	LEU
1	B	310	ARG
1	B	339	LEU
1	B	342	THR
1	B	359	LEU
1	B	362	GLU
1	B	363	SER
1	B	431	GLU
1	B	441	ILE
1	B	456	LEU
1	B	461	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	183	HIS
1	A	270	GLN
1	A	374	ASN
1	A	446	GLN
1	B	175	GLN
1	B	249	GLN
1	B	291	GLN
1	B	300	HIS
1	B	303	GLN
1	B	374	ASN
1	B	395	GLN
1	B	446	GLN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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	UPG	A	501	-	37,38,38	3.78	16 (43%)	55,58,58	1.42	8 (14%)
2	UPG	B	501	-	37,38,38	3.81	16 (43%)	55,58,58	1.26	5 (9%)

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	UPG	A	501	-	-	4/23/59/59	0/3/3/3
2	UPG	B	501	-	-	5/23/59/59	0/3/3/3

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	UPG	C2-N1	9.05	1.52	1.38
2	A	501	UPG	C3C-C4C	-8.89	1.30	1.53
2	A	501	UPG	C2-N1	8.87	1.52	1.38
2	B	501	UPG	C3C-C4C	-8.74	1.30	1.53
2	A	501	UPG	C2-N3	8.40	1.52	1.38
2	B	501	UPG	C2-N3	8.26	1.52	1.38
2	A	501	UPG	C2C-C1C	-6.89	1.31	1.53
2	B	501	UPG	C2C-C1C	-6.80	1.32	1.53
2	A	501	UPG	O4C-C1C	6.66	1.57	1.42
2	B	501	UPG	O4C-C1C	6.58	1.57	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	UPG	O4C-C4C	6.23	1.58	1.45
2	B	501	UPG	O4C-C4C	6.05	1.58	1.45
2	B	501	UPG	PB-O3A	5.89	1.65	1.59
2	B	501	UPG	PA-O3A	5.83	1.65	1.59
2	A	501	UPG	C3C-C2C	5.14	1.67	1.53
2	A	501	UPG	PB-O3A	5.09	1.65	1.59
2	A	501	UPG	PA-O3A	5.05	1.65	1.59
2	B	501	UPG	C3C-C2C	4.94	1.66	1.53
2	B	501	UPG	C6-C5	4.63	1.45	1.35
2	A	501	UPG	C6-C5	4.58	1.45	1.35
2	A	501	UPG	C4-N3	4.15	1.45	1.38
2	B	501	UPG	C4-N3	3.97	1.45	1.38
2	A	501	UPG	C6-N1	3.47	1.46	1.38
2	B	501	UPG	C6-N1	3.37	1.46	1.38
2	A	501	UPG	O5'-C1'	3.11	1.49	1.41
2	B	501	UPG	O5'-C1'	3.11	1.49	1.41
2	B	501	UPG	O4-C4	-2.84	1.19	1.24
2	A	501	UPG	O4-C4	-2.78	1.19	1.24
2	B	501	UPG	O2-C2	-2.40	1.18	1.23
2	A	501	UPG	O2-C2	-2.33	1.18	1.23
2	B	501	UPG	PB-O3B	2.21	1.66	1.59
2	A	501	UPG	PB-O3B	2.21	1.66	1.59

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	UPG	O5'-C1'-O3B	-4.68	105.25	111.36
2	B	501	UPG	C5-C4-N3	4.36	120.90	114.80
2	A	501	UPG	C5-C4-N3	4.27	120.78	114.80
2	A	501	UPG	O4-C4-C5	-3.70	118.78	125.16
2	B	501	UPG	C4-N3-C2	-3.42	122.37	126.61
2	B	501	UPG	O4-C4-C5	-3.40	119.30	125.16
2	A	501	UPG	C4-N3-C2	-3.37	122.44	126.61
2	B	501	UPG	C3C-C2C-C1C	2.63	106.45	101.46
2	B	501	UPG	O5'-C1'-O3B	-2.51	108.09	111.36
2	A	501	UPG	C1'-O5'-C5'	-2.18	109.47	113.72
2	A	501	UPG	C4C-O4C-C1C	-2.09	104.84	109.47
2	A	501	UPG	C3C-C2C-C1C	2.08	105.40	101.46
2	A	501	UPG	O3B-C1'-C2'	2.06	112.16	108.38

There are no chirality outliers.

All (9) torsion outliers are listed below:

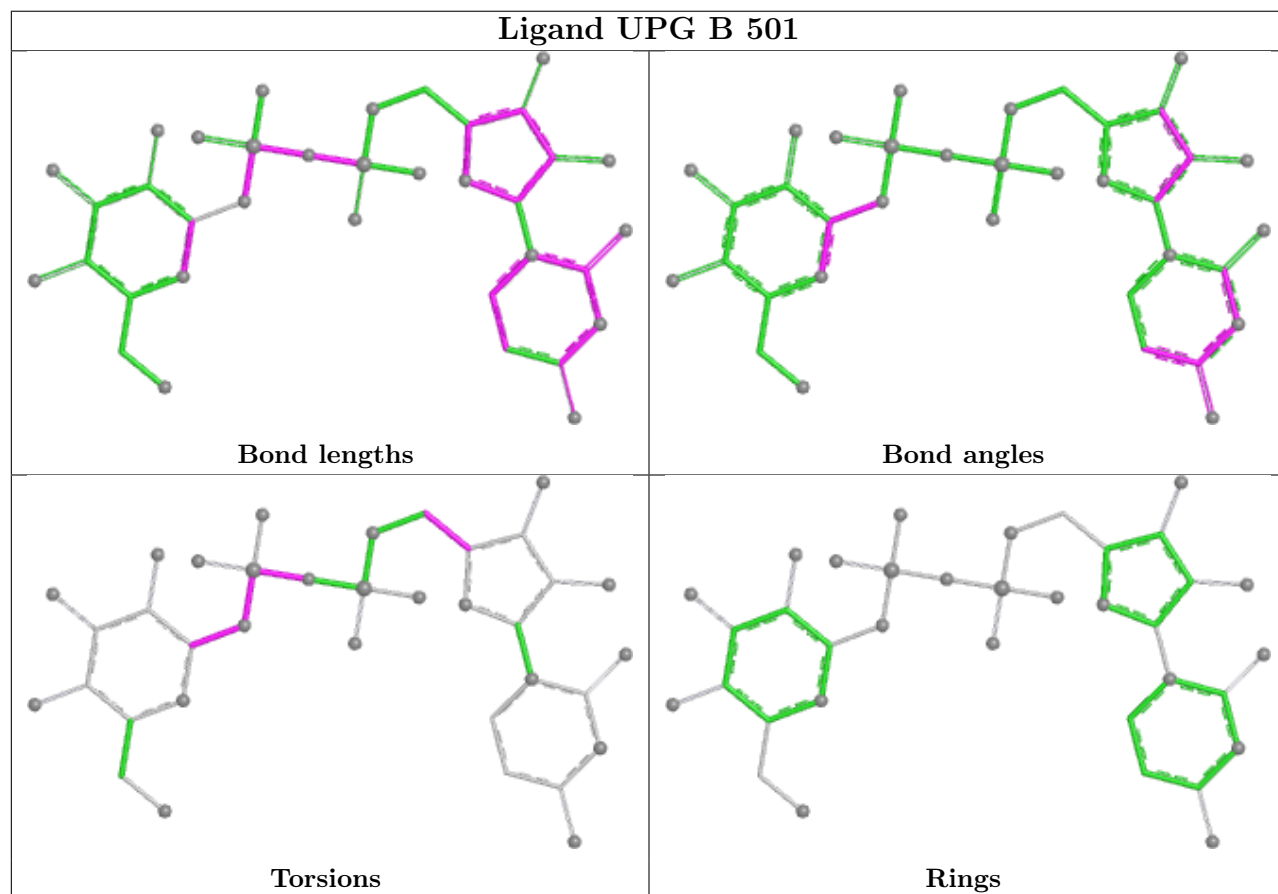
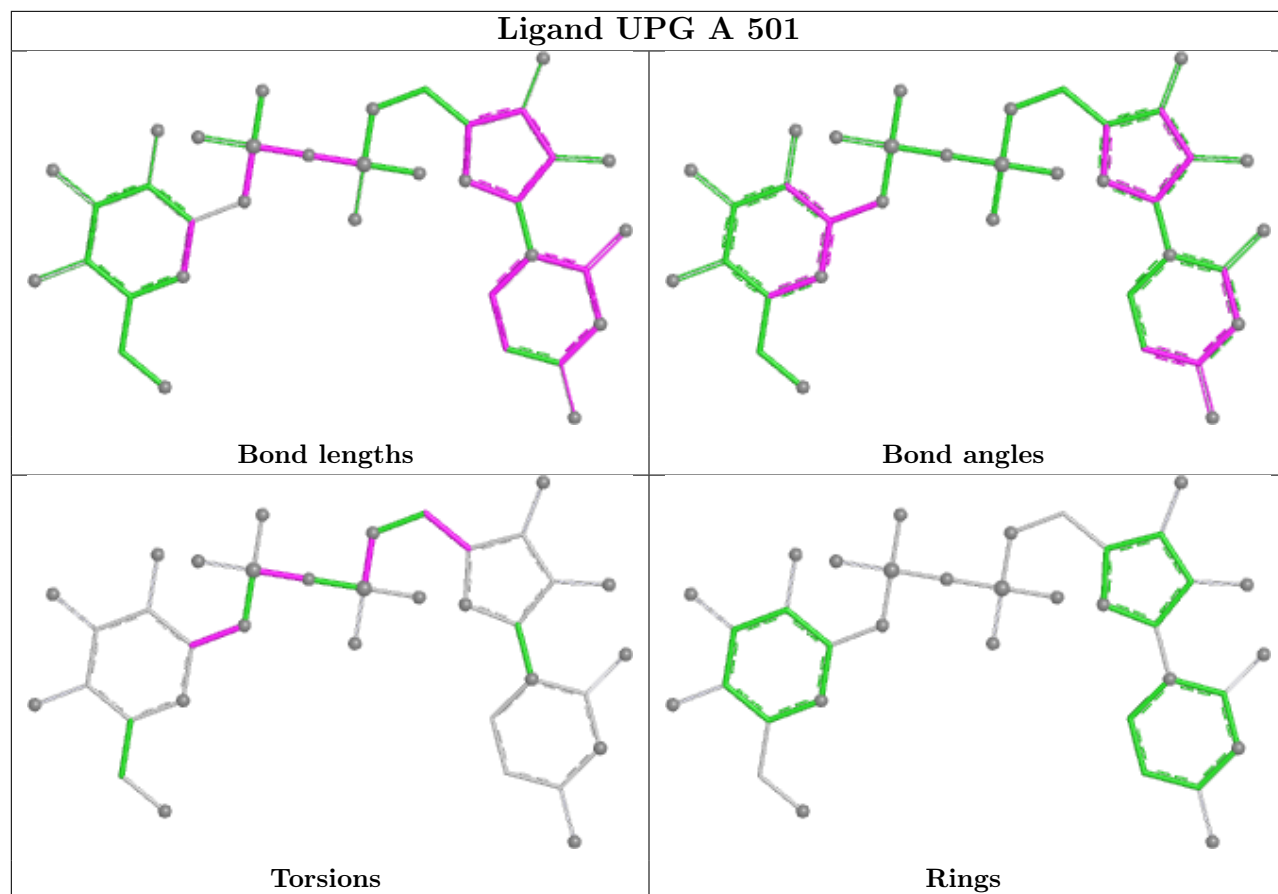
Mol	Chain	Res	Type	Atoms
2	A	501	UPG	PA-O3A-PB-O3B
2	A	501	UPG	O5'-C1'-O3B-PB
2	B	501	UPG	PA-O3A-PB-O3B
2	B	501	UPG	O5'-C1'-O3B-PB
2	B	501	UPG	C3C-C4C-C5C-O5C
2	B	501	UPG	O4C-C4C-C5C-O5C
2	A	501	UPG	C5C-O5C-PA-O1A
2	B	501	UPG	C1'-O3B-PB-O1B
2	A	501	UPG	O4C-C4C-C5C-O5C

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	UPG	2	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	467/499 (93%)	0.12	17 (3%) 46 42	28, 52, 104, 202	0
1	B	455/499 (91%)	1.35	97 (21%) 2 2	48, 115, 173, 239	0
All	All	922/998 (92%)	0.72	114 (12%) 8 6	28, 77, 164, 239	0

All (114) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	316	ILE	5.9
1	B	263	CYS	5.0
1	B	8	PRO	4.8
1	B	358	VAL	4.3
1	B	423	ALA	4.3
1	B	305	PHE	4.2
1	B	262	GLU	4.1
1	A	257	ALA	4.1
1	B	331	LEU	4.1
1	B	364	THR	3.8
1	B	317	ALA	3.8
1	B	339	LEU	3.8
1	A	259	ALA	3.8
1	B	328	ILE	3.7
1	B	167	PHE	3.6
1	A	324	VAL	3.6
1	A	10	THR	3.5
1	B	266	TRP	3.4
1	B	273	GLY	3.4
1	A	258	ALA	3.4
1	B	293	GLU	3.4
1	B	410	LEU	3.3
1	B	349	LEU	3.3
1	A	325	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	291	GLN	3.2
1	B	476	LYS	3.2
1	B	297	VAL	3.2
1	B	319	ALA	3.1
1	B	413	SER	3.1
1	B	159	LEU	3.1
1	B	124	PHE	3.0
1	B	409	GLY	3.0
1	B	442	ARG	3.0
1	B	348	VAL	3.0
1	B	320	THR	3.0
1	B	52	PRO	3.0
1	B	294	LEU	3.0
1	B	461	SER	3.0
1	B	240	ARG	2.9
1	B	187	LEU	2.9
1	B	346	GLY	2.9
1	B	306	LEU	2.9
1	B	244	VAL	2.8
1	B	78	LEU	2.8
1	B	264	LEU	2.8
1	B	209	TYR	2.7
1	B	234	PRO	2.7
1	B	19	VAL	2.7
1	B	308	VAL	2.7
1	A	253	CYS	2.7
1	B	156	LEU	2.7
1	B	299	ALA	2.7
1	B	356	ILE	2.7
1	B	307	TRP	2.7
1	B	170	LEU	2.6
1	B	164	SER	2.6
1	B	267	LEU	2.6
1	A	321	TYR	2.6
1	B	347	LEU	2.6
1	B	418	GLY	2.5
1	B	280	PHE	2.5
1	B	298	LEU	2.5
1	A	252	SER	2.5
1	A	91	MET	2.5
1	B	417	ASP	2.5
1	B	309	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	333	LEU	2.5
1	B	289	GLU	2.5
1	A	327	GLU	2.4
1	B	290	GLN	2.4
1	B	286	LEU	2.4
1	B	313	ASN	2.4
1	B	162	THR	2.4
1	B	53	PRO	2.4
1	A	319	ALA	2.4
1	B	329	ASP	2.4
1	B	318	ASN	2.4
1	B	387	ILE	2.3
1	B	278	VAL	2.3
1	A	256	GLY	2.3
1	B	300	HIS	2.3
1	B	351	MET	2.3
1	B	220	PHE	2.3
1	B	350	PRO	2.3
1	B	223	LEU	2.3
1	B	261	PRO	2.3
1	A	296	GLY	2.3
1	A	316	ILE	2.3
1	A	476	LYS	2.3
1	B	277	PHE	2.3
1	B	219	SER	2.2
1	B	334	LEU	2.2
1	B	360	SER	2.2
1	B	422	GLY	2.2
1	B	276	LEU	2.2
1	B	282	SER	2.2
1	B	301	SER	2.2
1	B	174	VAL	2.2
1	B	332	LYS	2.2
1	B	202	LEU	2.2
1	B	383	GLY	2.2
1	B	169	GLU	2.2
1	B	432	LEU	2.2
1	B	177	PRO	2.2
1	B	361	HIS	2.1
1	B	199	TYR	2.1
1	B	414	VAL	2.1
1	A	326	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	102	LEU	2.1
1	B	314	ASP	2.1
1	B	389	TRP	2.1
1	B	335	PRO	2.0
1	B	141	ILE	2.0
1	B	357	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](#)

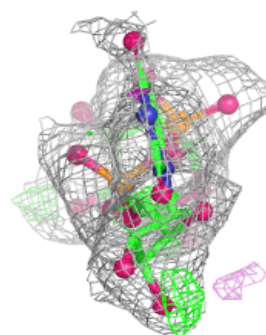
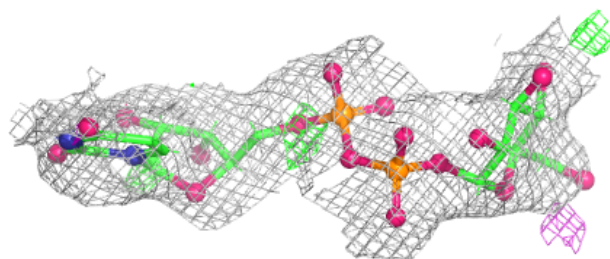
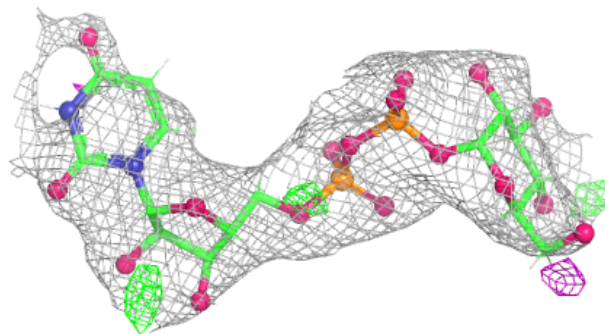
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	UPG	B	501	36/36	0.86	0.13	99,116,142,147	0
2	UPG	A	501	36/36	0.94	0.08	36,46,59,65	0

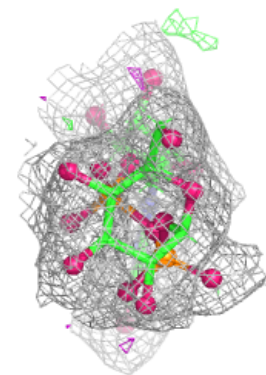
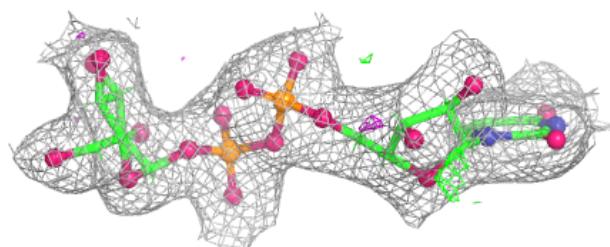
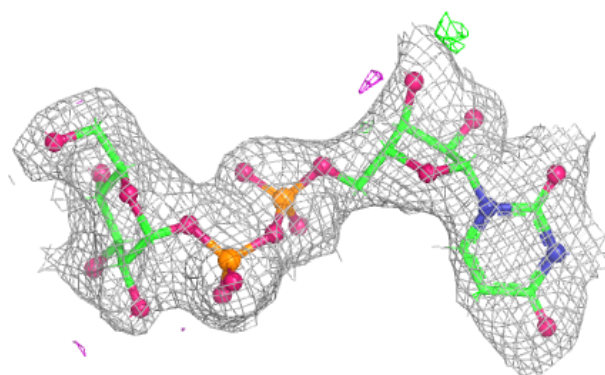
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around UPG B 501:

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

**Electron density around UPG A 501:**

$2mF_o-DF_c$ (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.