



Full wwPDB X-ray Structure Validation Report i

Nov 22, 2023 – 10:52 PM JST

PDB ID : 7XX4
Title : designed glycosyltransferase
Authors : Lu, M.; Wu, X.
Deposited on : 2022-05-28
Resolution : 2.43 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 i 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](#) ①) 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 : 2.36
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) : 2.36

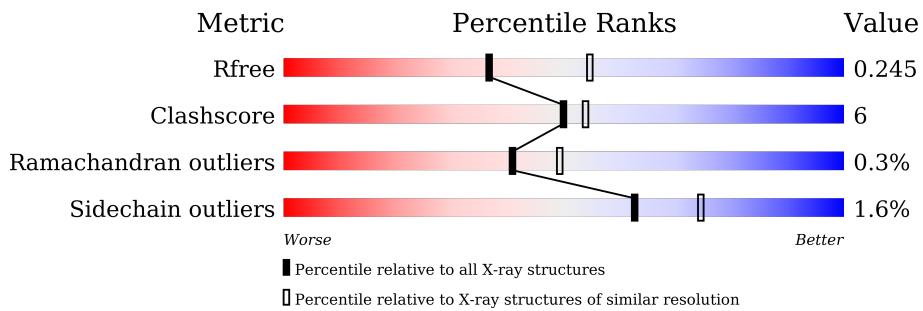
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.43 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	1564 (2.46-2.42)
Clashscore	141614	1631 (2.46-2.42)
Ramachandran outliers	138981	1617 (2.46-2.42)
Sidechain outliers	138945	1617 (2.46-2.42)

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain		
1	A	408	<div style="width: 81%; background-color: green;"></div> 81%	<div style="width: 15%; background-color: yellow;"></div> 15%	.
1	B	408	<div style="width: 81%; background-color: green;"></div> 81%	<div style="width: 15%; background-color: yellow;"></div> 15%	.

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6166 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 Oleandomycin glycosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	395	Total	C 3049	N 1933	O 539	S 567	10	0	0
1	B	393	Total	C 3026	N 1919	O 536	S 561	10	0	0

There are 86 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	MET	-	initiating methionine	UNP Q3HTL6
A	-4	THR	-	expression tag	UNP Q3HTL6
A	-3	SER	-	expression tag	UNP Q3HTL6
A	-2	GLU	-	expression tag	UNP Q3HTL6
A	-1	HIS	-	expression tag	UNP Q3HTL6
A	0	ARG	-	expression tag	UNP Q3HTL6
A	1	SER	-	expression tag	UNP Q3HTL6
A	2	ALA	-	expression tag	UNP Q3HTL6
A	3	SER	-	expression tag	UNP Q3HTL6
A	4	VAL	-	expression tag	UNP Q3HTL6
A	65	LYS	GLY	engineered mutation	UNP Q3HTL6
A	67	SER	ASP	engineered mutation	UNP Q3HTL6
A	68	ASN	ALA	engineered mutation	UNP Q3HTL6
A	69	PRO	ASP	engineered mutation	UNP Q3HTL6
A	70	GLU	PRO	engineered mutation	UNP Q3HTL6
A	72	SER	ALA	engineered mutation	UNP Q3HTL6
A	74	PRO	GLY	engineered mutation	UNP Q3HTL6
A	75	GLU	SER	engineered mutation	UNP Q3HTL6
A	76	ASP	THR	engineered mutation	UNP Q3HTL6
A	77	GLN	LEU	engineered mutation	UNP Q3HTL6
A	78	GLU	LEU	engineered mutation	UNP Q3HTL6
A	79	SER	ASP	engineered mutation	UNP Q3HTL6
A	80	ALA	ASN	engineered mutation	UNP Q3HTL6
A	81	MET	VAL	engineered mutation	UNP Q3HTL6
A	82	GLY	GLU	engineered mutation	UNP Q3HTL6

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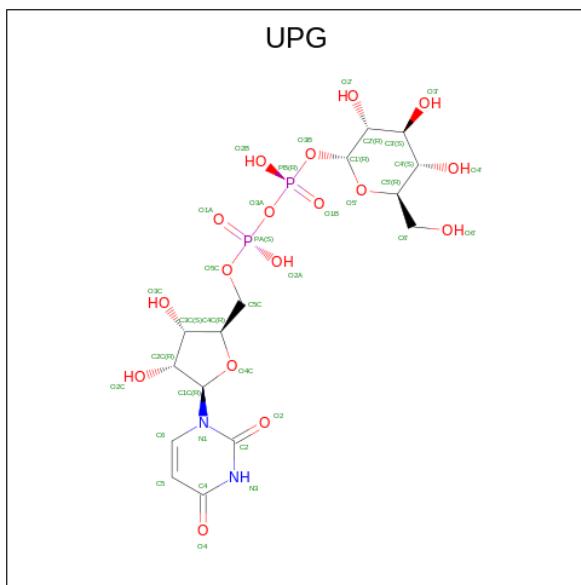
Chain	Residue	Modelled	Actual	Comment	Reference
A	83	LEU	PRO	engineered mutation	UNP Q3HTL6
A	282	PRO	ASP	engineered mutation	UNP Q3HTL6
A	288	GLN	ASP	engineered mutation	UNP Q3HTL6
A	294	ASP	ALA	engineered mutation	UNP Q3HTL6
A	297	THR	ARG	engineered mutation	UNP Q3HTL6
A	298	LYS	GLN	engineered mutation	UNP Q3HTL6
A	300	SER	ASP	engineered mutation	UNP Q3HTL6
A	301	ALA	LEU	engineered mutation	UNP Q3HTL6
A	303	ILE	VAL	engineered mutation	UNP Q3HTL6
A	308	MET	ALA	engineered mutation	UNP Q3HTL6
A	310	SER	GLY	engineered mutation	UNP Q3HTL6
A	311	THR	SER	engineered mutation	UNP Q3HTL6
A	312	MET	GLN	engineered mutation	UNP Q3HTL6
A	314	ALA	GLY	engineered mutation	UNP Q3HTL6
A	316	SER	ALA	engineered mutation	UNP Q3HTL6
A	317	ASN	THR	engineered mutation	UNP Q3HTL6
A	319	VAL	THR	engineered mutation	UNP Q3HTL6
A	402	GLY	-	expression tag	UNP Q3HTL6
B	-5	MET	-	initiating methionine	UNP Q3HTL6
B	-4	THR	-	expression tag	UNP Q3HTL6
B	-3	SER	-	expression tag	UNP Q3HTL6
B	-2	GLU	-	expression tag	UNP Q3HTL6
B	-1	HIS	-	expression tag	UNP Q3HTL6
B	0	ARG	-	expression tag	UNP Q3HTL6
B	1	SER	-	expression tag	UNP Q3HTL6
B	2	ALA	-	expression tag	UNP Q3HTL6
B	3	SER	-	expression tag	UNP Q3HTL6
B	4	VAL	-	expression tag	UNP Q3HTL6
B	65	LYS	GLY	engineered mutation	UNP Q3HTL6
B	67	SER	ASP	engineered mutation	UNP Q3HTL6
B	68	ASN	ALA	engineered mutation	UNP Q3HTL6
B	69	PRO	ASP	engineered mutation	UNP Q3HTL6
B	70	GLU	PRO	engineered mutation	UNP Q3HTL6
B	72	SER	ALA	engineered mutation	UNP Q3HTL6
B	74	PRO	GLY	engineered mutation	UNP Q3HTL6
B	75	GLU	SER	engineered mutation	UNP Q3HTL6
B	76	ASP	THR	engineered mutation	UNP Q3HTL6
B	77	GLN	LEU	engineered mutation	UNP Q3HTL6
B	78	GLU	LEU	engineered mutation	UNP Q3HTL6
B	79	SER	ASP	engineered mutation	UNP Q3HTL6
B	80	ALA	ASN	engineered mutation	UNP Q3HTL6
B	81	MET	VAL	engineered mutation	UNP Q3HTL6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	82	GLY	GLU	engineered mutation	UNP Q3HTL6
B	83	LEU	PRO	engineered mutation	UNP Q3HTL6
B	282	PRO	ASP	engineered mutation	UNP Q3HTL6
B	288	GLN	ASP	engineered mutation	UNP Q3HTL6
B	294	ASP	ALA	engineered mutation	UNP Q3HTL6
B	297	THR	ARG	engineered mutation	UNP Q3HTL6
B	298	LYS	GLN	engineered mutation	UNP Q3HTL6
B	300	SER	ASP	engineered mutation	UNP Q3HTL6
B	301	ALA	LEU	engineered mutation	UNP Q3HTL6
B	303	ILE	VAL	engineered mutation	UNP Q3HTL6
B	308	MET	ALA	engineered mutation	UNP Q3HTL6
B	310	SER	GLY	engineered mutation	UNP Q3HTL6
B	311	THR	SER	engineered mutation	UNP Q3HTL6
B	312	MET	GLN	engineered mutation	UNP Q3HTL6
B	314	ALA	GLY	engineered mutation	UNP Q3HTL6
B	316	SER	ALA	engineered mutation	UNP Q3HTL6
B	317	ASN	THR	engineered mutation	UNP Q3HTL6
B	319	VAL	THR	engineered mutation	UNP Q3HTL6
B	402	GLY	-	expression tag	UNP Q3HTL6

- Molecule 2 is URIDINE-5'-DIPHOSPHATE-GLUCOSE (three-letter code: UPG) (formula: C₁₅H₂₄N₂O₁₇P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			36	15	2	17	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	B	1	36	15	2	17	2	0	0

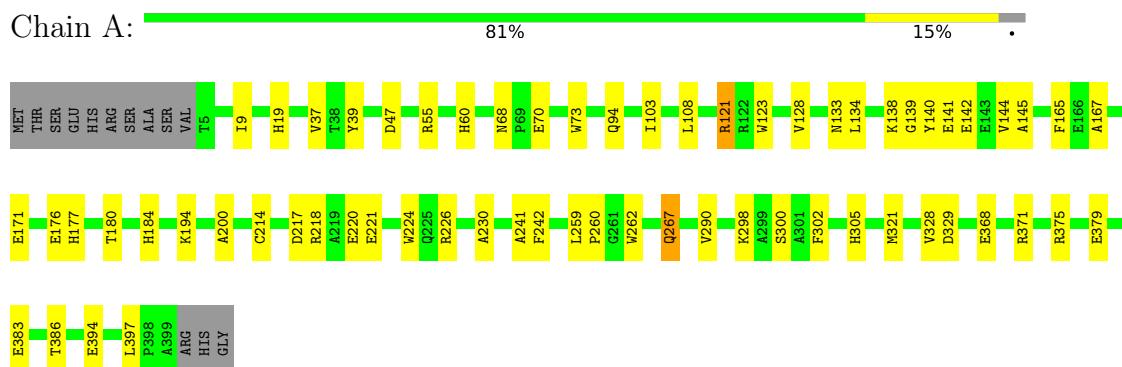
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	12	12	12	0	0
3	B	7	7	7	0	0

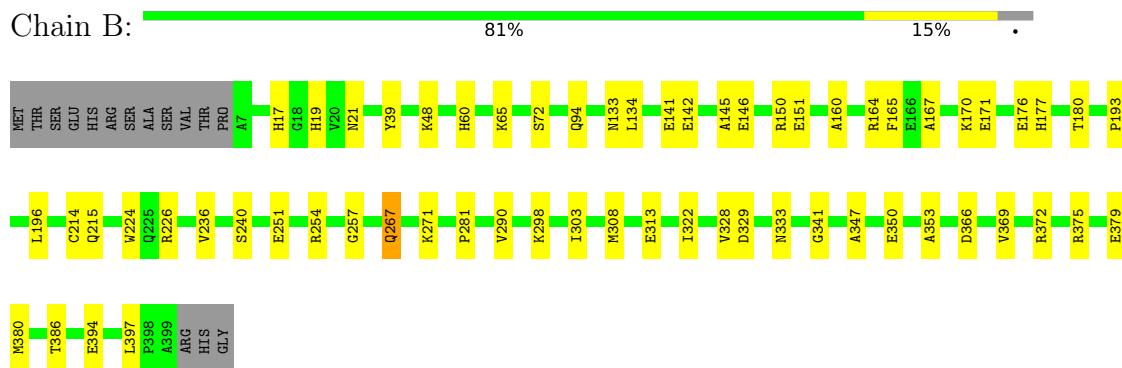
3 Residue-property plots [\(i\)](#)

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. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Oleandomycin glycosyltransferase



- Molecule 1: Oleandomycin glycosyltransferase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 1 21	Depositor
Cell constants a, b, c, α , β , γ	65.72Å 92.28Å 191.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.37 – 2.43 30.95 – 1.49	Depositor EDS
% Data completeness (in resolution range)	99.5 (30.37-2.43) 43.7 (30.95-1.49)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ ¹	0.89 (at 1.48Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R , R_{free}	(Not available), 0.239 0.216, 0.245	Depositor DCC
R_{free} test set	1718 reflections (1.41%)	wwPDB-VP
Wilson B-factor (Å ²)	27.8	Xtriage
Anisotropy	0.177	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39, 69.5	EDS
L-test for twinning ²	$< L > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6166	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 37.38 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.3268e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $< |L| >$, $< L^2 >$ 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: 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	0.38	0/3128	0.60	1/4272 (0.0%)
1	B	0.36	0/3104	0.62	1/4238 (0.0%)
All	All	0.37	0/6232	0.61	2/8510 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	138	LYS	CD-CE-NZ	8.10	130.32	111.70
1	B	254	ARG	CA-CB-CG	5.64	125.80	113.40

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	3049	0	2996	37	0
1	B	3026	0	2971	34	0
2	A	36	0	22	5	0
2	B	36	0	22	3	0
3	A	12	0	0	3	0
3	B	7	0	0	0	0
All	All	6166	0	6011	71	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 6.

All (71) 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:305:HIS:NE2	2:A:501:UPG:O2B	2.13	0.82
1:B:60:HIS:H	1:B:94:GLN:HE22	1.35	0.72
1:B:193:PRO:HB3	1:B:380:MET:HG2	1.72	0.70
1:A:60:HIS:H	1:A:94:GLN:HE22	1.37	0.70
1:A:214:CYS:HB3	1:A:386:THR:OG1	1.94	0.67
1:A:375:ARG:O	1:A:379:GLU:HG3	1.96	0.66
1:B:341:GLY:O	1:B:372:ARG:NH2	2.21	0.64
1:A:68:ASN:HB3	1:A:70:GLU:OE2	2.01	0.61
1:B:375:ARG:O	1:B:379:GLU:HG3	2.01	0.60
1:A:368:GLU:CD	1:A:371:ARG:HH12	2.04	0.60
1:B:196:LEU:HD23	1:B:196:LEU:O	2.02	0.60
1:A:224:TRP:O	1:A:298:LYS:NZ	2.36	0.58
1:B:167:ALA:O	1:B:171:GLU:HB2	2.03	0.58
1:A:55:ARG:NH1	3:A:602:HOH:O	2.28	0.58
1:B:21:ASN:OD1	1:B:48:LYS:NZ	2.37	0.57
1:B:366:ASP:HB3	1:B:369:VAL:HG22	1.86	0.56
1:A:9:ILE:O	1:A:37:VAL:HA	2.06	0.56
1:A:108:LEU:HD23	1:A:128:VAL:HB	1.90	0.54
1:B:19:HIS:NE2	2:B:501:UPG:H6'1	2.23	0.54
1:A:220:GLU:H	1:A:220:GLU:CD	2.10	0.54
1:A:259:LEU:HD22	1:A:262:TRP:CD1	2.44	0.52
1:A:242:PHE:HE2	2:A:501:UPG:O2'	1.92	0.51
1:B:141:GLU:HA	1:B:145:ALA:HB3	1.92	0.51
1:B:240:SER:OG	2:B:501:UPG:O1B	2.29	0.51
1:B:215:GLN:HE22	1:B:313:GLU:HG3	1.76	0.50
1:A:259:LEU:HD23	1:A:260:PRO:HD2	1.93	0.50
1:B:72:SER:HB3	1:B:271:LYS:NZ	2.27	0.50
1:A:103:ILE:HG23	1:A:123:TRP:CD2	2.49	0.48
1:B:366:ASP:O	1:B:369:VAL:HG22	2.13	0.48
1:A:133:ASN:OD1	1:A:134:LEU:N	2.39	0.47
1:B:142:GLU:OE1	1:B:142:GLU:N	2.43	0.47
1:B:308:MET:HE1	1:B:333:ASN:OD1	2.14	0.47
1:A:302:PHE:O	1:A:321:MET:HA	2.14	0.47
1:B:146:GLU:HG2	1:B:150:ARG:HH21	1.79	0.47
1:A:300:SER:OG	3:A:601:HOH:O	2.21	0.47
1:B:146:GLU:O	1:B:151:GLU:HG3	2.15	0.47
1:B:251:GLU:OE1	1:B:353:ALA:N	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:GLN:HG3	1:A:290:VAL:HG22	1.95	0.46
1:B:160:ALA:O	1:B:164:ARG:HG3	2.16	0.46
1:A:218:ARG:HD2	1:A:221:GLU:OE2	2.16	0.46
1:A:140:TYR:CE2	1:A:144:VAL:HG21	2.51	0.46
1:B:224:TRP:O	1:B:298:LYS:NZ	2.41	0.46
1:A:329:ASP:OD1	1:A:329:ASP:N	2.48	0.45
1:B:214:CYS:HB3	1:B:386:THR:OG1	2.16	0.45
1:A:394:GLU:O	1:A:397:LEU:HB2	2.17	0.45
1:B:176:GLU:N	1:B:176:GLU:OE1	2.50	0.45
1:A:167:ALA:O	1:A:171:GLU:HB2	2.17	0.45
1:B:267:GLN:HG3	1:B:290:VAL:HG22	1.98	0.44
1:A:141:GLU:HA	1:A:145:ALA:HB3	1.98	0.44
1:A:19:HIS:NE2	2:A:501:UPG:H6'1	2.32	0.44
1:A:177:HIS:HB3	1:A:180:THR:HG23	1.99	0.44
1:A:226:ARG:HD3	1:A:230:ALA:O	2.17	0.44
1:A:139:GLY:HA2	1:A:142:GLU:OE1	2.18	0.44
1:B:133:ASN:OD1	1:B:134:LEU:N	2.42	0.44
1:A:141:GLU:OE2	1:A:184:HIS:HE1	2.01	0.43
1:B:303:ILE:HG12	1:B:322:ILE:HB	2.00	0.43
1:B:394:GLU:O	1:B:397:LEU:HB2	2.18	0.43
1:B:257:GLY:HA3	1:B:281:PRO:HG3	2.01	0.42
1:A:383:GLU:OE1	1:A:383:GLU:HA	2.18	0.42
1:B:177:HIS:HB3	1:B:180:THR:HG23	2.00	0.42
1:B:17:HIS:CE1	1:B:48:LYS:HE3	2.55	0.42
1:B:329:ASP:OD2	1:B:329:ASP:N	2.47	0.42
1:A:73:TRP:CG	2:A:501:UPG:H3'	2.55	0.42
1:A:217:ASP:N	1:A:217:ASP:OD1	2.53	0.41
1:A:121:ARG:NH1	1:A:176:GLU:OE1	2.41	0.41
1:A:47:ASP:HB2	3:A:606:HOH:O	2.21	0.41
1:A:241:ALA:CB	2:A:501:UPG:H2'	2.50	0.41
1:B:236:VAL:HG22	1:B:303:ILE:HB	2.01	0.41
1:B:347:ALA:HB3	1:B:350:GLU:HG2	2.03	0.40
1:B:19:HIS:CD2	2:B:501:UPG:H6'1	2.57	0.40
1:A:194:LYS:HE3	1:A:200:ALA:HB1	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	393/408 (96%)	382 (97%)	10 (2%)	1 (0%)	41 49
1	B	391/408 (96%)	377 (96%)	13 (3%)	1 (0%)	41 49
All	All	784/816 (96%)	759 (97%)	23 (3%)	2 (0%)	41 49

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	328	VAL
1	A	328	VAL

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	313/325 (96%)	309 (99%)	4 (1%)	69 80
1	B	309/325 (95%)	303 (98%)	6 (2%)	57 69
All	All	622/650 (96%)	612 (98%)	10 (2%)	62 74

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

Mol	Chain	Res	Type
1	A	39	TYR
1	A	121	ARG
1	A	165	PHE
1	A	267	GLN

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Mol	Chain	Res	Type
1	B	39	TYR
1	B	65	LYS
1	B	165	PHE
1	B	170	LYS
1	B	226	ARG
1	B	267	GLN

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	94	GLN
1	A	184	HIS
1	B	94	GLN

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)

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	B	501	-	35,38,38	2.69	11 (31%)	53,58,58	1.94	13 (24%)
2	UPG	A	501	-	35,38,38	2.27	8 (22%)	53,58,58	1.99	13 (24%)

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	B	501	-	-	9/23/59/59	0/3/3/3
2	UPG	A	501	-	-	8/23/59/59	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	UPG	PB-O3B	10.88	1.89	1.60
2	A	501	UPG	PB-O3B	9.04	1.84	1.60
2	B	501	UPG	PA-O5C	5.28	1.80	1.59
2	A	501	UPG	PA-O5C	4.49	1.77	1.59
2	B	501	UPG	C2-N3	4.04	1.45	1.38
2	B	501	UPG	C1C-N1	3.83	1.58	1.47
2	A	501	UPG	C1C-N1	3.31	1.57	1.47
2	A	501	UPG	C2-N3	3.21	1.43	1.38
2	B	501	UPG	C4'-C5'	3.10	1.59	1.53
2	B	501	UPG	O5'-C1'	3.09	1.49	1.41
2	A	501	UPG	C4'-C5'	2.94	1.59	1.53
2	B	501	UPG	C1'-C2'	2.86	1.60	1.52
2	A	501	UPG	O5C-C5C	-2.80	1.34	1.44
2	B	501	UPG	O5C-C5C	-2.58	1.34	1.44
2	B	501	UPG	C2-N1	2.54	1.42	1.38
2	A	501	UPG	C2-N1	2.26	1.42	1.38
2	B	501	UPG	C5-C4	2.09	1.48	1.43
2	A	501	UPG	O5'-C1'	2.07	1.47	1.41
2	B	501	UPG	C6'-C5'	2.03	1.58	1.51

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	UPG	C1'-O5'-C5'	5.32	124.13	113.69
2	A	501	UPG	C1'-O5'-C5'	5.22	123.93	113.69
2	A	501	UPG	O3A-PB-O3B	4.89	112.34	102.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	UPG	O3A-PB-O3B	4.41	111.38	102.48
2	A	501	UPG	C4-N3-C2	-4.27	120.95	126.58
2	A	501	UPG	O5'-C5'-C4'	4.21	117.34	109.69
2	B	501	UPG	C4-N3-C2	-4.16	121.09	126.58
2	A	501	UPG	N3-C2-N1	3.98	120.18	114.89
2	B	501	UPG	O5'-C5'-C6'	3.84	115.99	106.44
2	B	501	UPG	N3-C2-N1	3.77	119.89	114.89
2	B	501	UPG	O5'-C5'-C4'	3.37	115.81	109.69
2	A	501	UPG	O5'-C5'-C6'	3.29	114.62	106.44
2	B	501	UPG	O5'-C1'-O3B	3.01	115.30	111.36
2	A	501	UPG	C6'-C5'-C4'	-2.98	106.03	113.00
2	A	501	UPG	O5C-PA-O1A	-2.91	97.70	109.07
2	B	501	UPG	O3B-C1'-C2'	2.90	113.69	108.38
2	A	501	UPG	PB-O3B-C1'	2.82	130.65	119.74
2	B	501	UPG	PB-O3B-C1'	2.77	130.46	119.74
2	B	501	UPG	O5C-PA-O1A	-2.71	98.49	109.07
2	B	501	UPG	C1'-C2'-C3'	-2.63	104.52	110.00
2	A	501	UPG	C1'-C2'-C3'	-2.61	104.55	110.00
2	B	501	UPG	C6'-C5'-C4'	-2.54	107.06	113.00
2	A	501	UPG	O2B-PB-O3B	-2.45	97.12	106.78
2	A	501	UPG	C4'-C3'-C2'	-2.27	106.86	110.82
2	B	501	UPG	O2-C2-N1	-2.17	119.91	122.79
2	A	501	UPG	O5'-C1'-O3B	2.15	114.17	111.36

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	UPG	C5C-O5C-PA-O3A
2	B	501	UPG	O4C-C4C-C5C-O5C
2	B	501	UPG	C2'-C1'-O3B-PB
2	B	501	UPG	O5'-C1'-O3B-PB
2	A	501	UPG	C4'-C5'-C6'-O6'
2	A	501	UPG	O4C-C4C-C5C-O5C
2	A	501	UPG	O5'-C5'-C6'-O6'
2	B	501	UPG	O5'-C5'-C6'-O6'
2	B	501	UPG	C4'-C5'-C6'-O6'
2	B	501	UPG	C3C-C4C-C5C-O5C
2	A	501	UPG	C3C-C4C-C5C-O5C
2	B	501	UPG	PB-O3A-PA-O5C
2	B	501	UPG	PA-O3A-PB-O3B
2	A	501	UPG	C5C-O5C-PA-O1A

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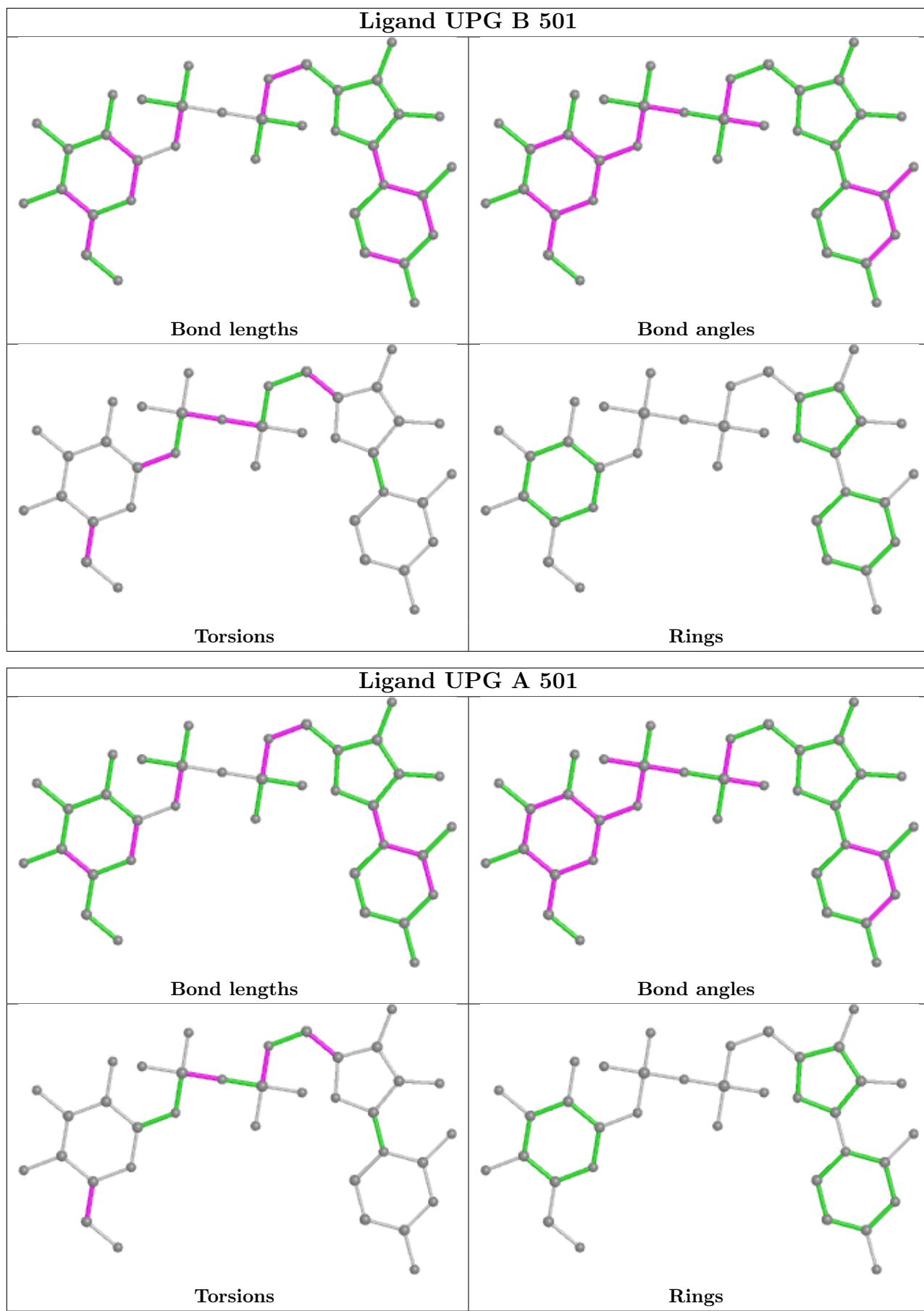
Mol	Chain	Res	Type	Atoms
2	A	501	UPG	C5C-O5C-PA-O2A
2	B	501	UPG	PB-O3A-PA-O1A
2	A	501	UPG	PA-O3A-PB-O2B

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	UPG	3	0
2	A	501	UPG	5	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 [\(i\)](#)

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

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

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

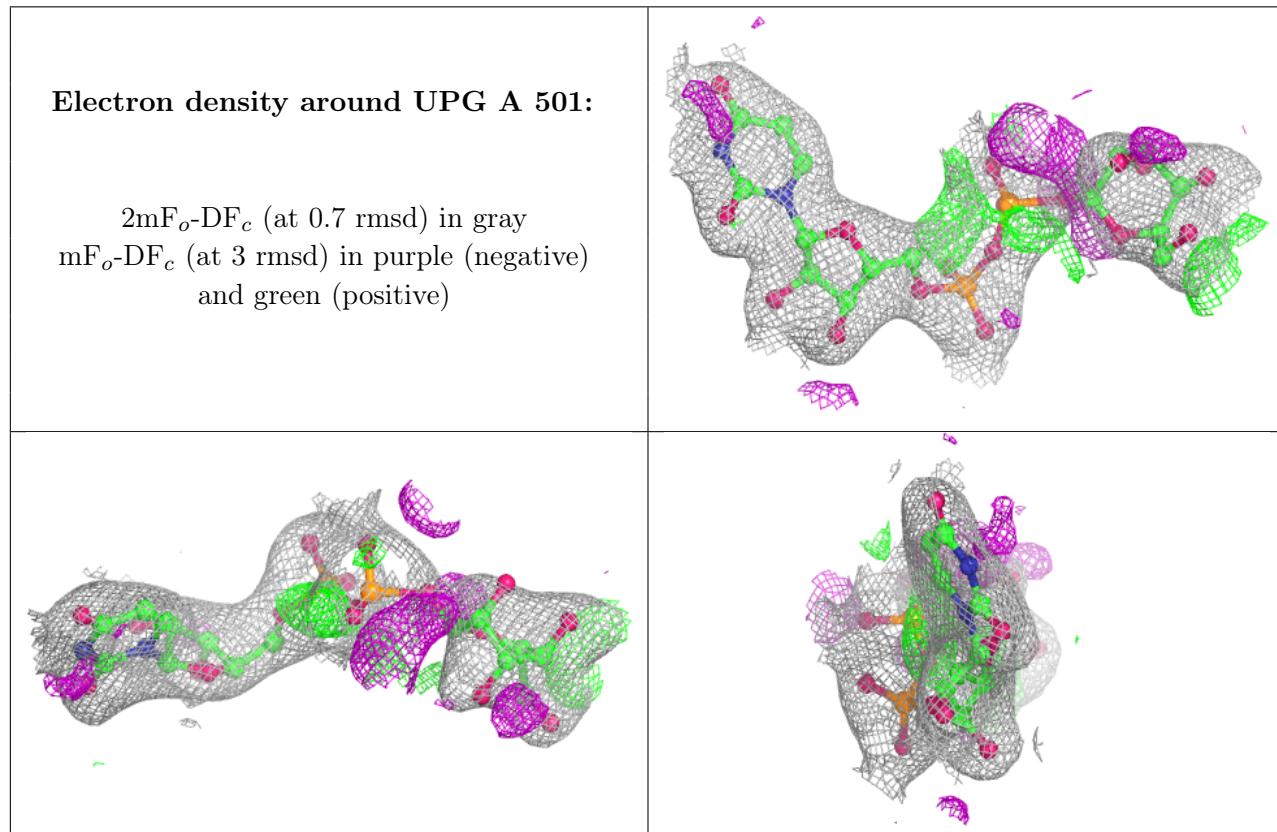
6.3 Carbohydrates [\(i\)](#)

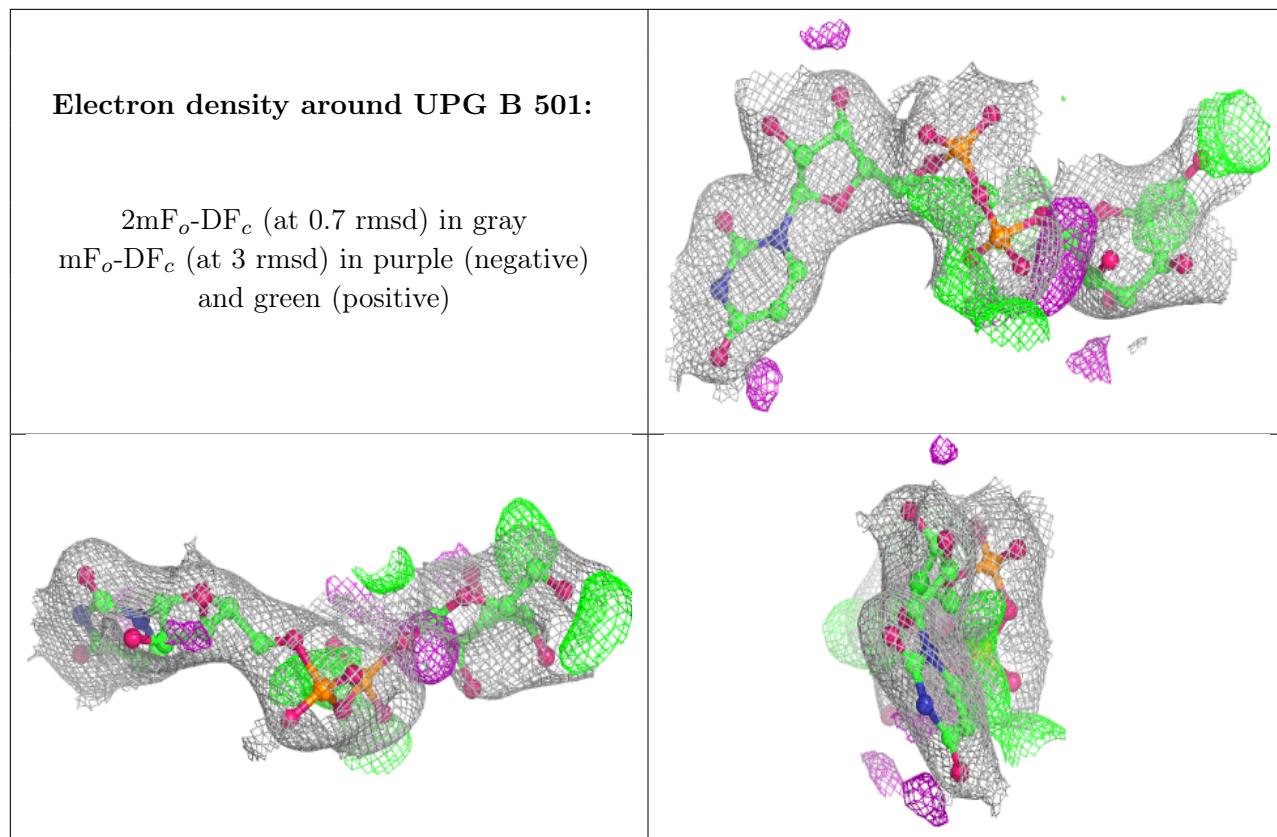
Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands [\(i\)](#)

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

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





6.5 Other polymers [\(i\)](#)

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