



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 25, 2024 – 12:14 PM JST

PDB ID : 8IXQ
Title : Structure of glycosyltransferase LmbT in complex with GDP and ergothioneine
Authors : Mori, T.; Sun, X.; Abe, I.
Deposited on : 2023-04-02
Resolution : 2.10 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

<https://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 : 4.02b-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

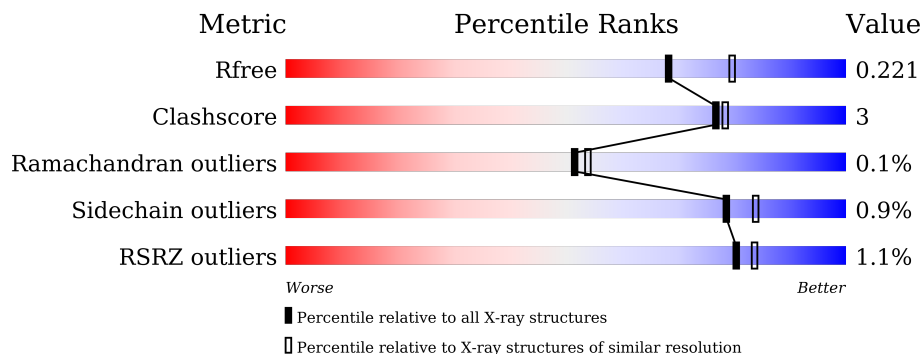
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	451	 3% 86% 8% 6%
1	B	451	 87% 8% 5%
1	C	451	 3% 88% 6% 6%
1	D	451	 86% 9% 5%

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 14312 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 Glycosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	425	3204	2009	600	588	7	0	0	0
1	B	429	3245	2032	608	598	7	0	0	0
1	C	424	3184	1996	593	588	7	0	0	0
1	D	429	3257	2037	612	601	7	0	1	0

There are 60 discrepancies between the modelled and reference sequences:

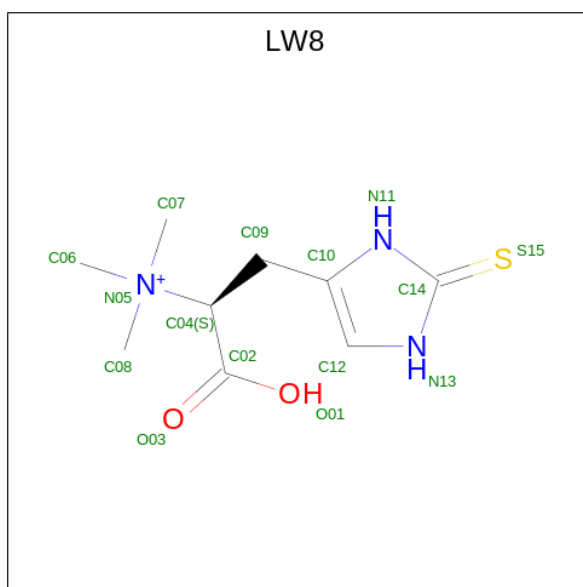
Chain	Residue	Modelled	Actual	Comment	Reference
A	437	LYS	-	expression tag	UNP A9Y8T1
A	438	LEU	-	expression tag	UNP A9Y8T1
A	439	ALA	-	expression tag	UNP A9Y8T1
A	440	ALA	-	expression tag	UNP A9Y8T1
A	441	ALA	-	expression tag	UNP A9Y8T1
A	442	LEU	-	expression tag	UNP A9Y8T1
A	443	GLU	-	expression tag	UNP A9Y8T1
A	444	HIS	-	expression tag	UNP A9Y8T1
A	445	HIS	-	expression tag	UNP A9Y8T1
A	446	HIS	-	expression tag	UNP A9Y8T1
A	447	HIS	-	expression tag	UNP A9Y8T1
A	448	HIS	-	expression tag	UNP A9Y8T1
A	449	HIS	-	expression tag	UNP A9Y8T1
A	450	HIS	-	expression tag	UNP A9Y8T1
A	451	HIS	-	expression tag	UNP A9Y8T1
B	437	LYS	-	expression tag	UNP A9Y8T1
B	438	LEU	-	expression tag	UNP A9Y8T1
B	439	ALA	-	expression tag	UNP A9Y8T1
B	440	ALA	-	expression tag	UNP A9Y8T1
B	441	ALA	-	expression tag	UNP A9Y8T1
B	442	LEU	-	expression tag	UNP A9Y8T1

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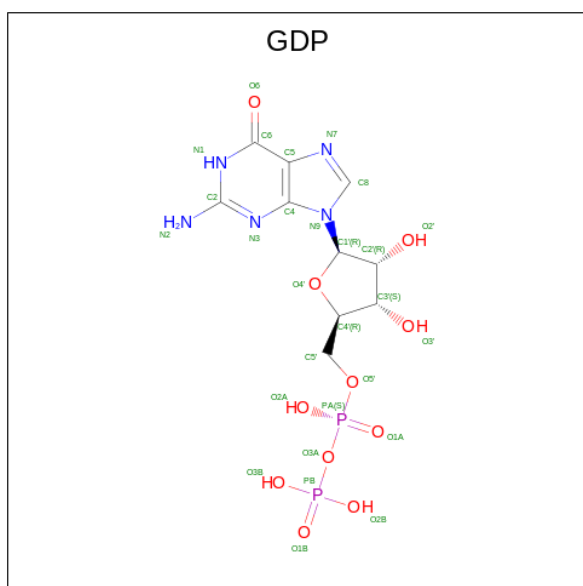
Chain	Residue	Modelled	Actual	Comment	Reference
B	443	GLU	-	expression tag	UNP A9Y8T1
B	444	HIS	-	expression tag	UNP A9Y8T1
B	445	HIS	-	expression tag	UNP A9Y8T1
B	446	HIS	-	expression tag	UNP A9Y8T1
B	447	HIS	-	expression tag	UNP A9Y8T1
B	448	HIS	-	expression tag	UNP A9Y8T1
B	449	HIS	-	expression tag	UNP A9Y8T1
B	450	HIS	-	expression tag	UNP A9Y8T1
B	451	HIS	-	expression tag	UNP A9Y8T1
C	437	LYS	-	expression tag	UNP A9Y8T1
C	438	LEU	-	expression tag	UNP A9Y8T1
C	439	ALA	-	expression tag	UNP A9Y8T1
C	440	ALA	-	expression tag	UNP A9Y8T1
C	441	ALA	-	expression tag	UNP A9Y8T1
C	442	LEU	-	expression tag	UNP A9Y8T1
C	443	GLU	-	expression tag	UNP A9Y8T1
C	444	HIS	-	expression tag	UNP A9Y8T1
C	445	HIS	-	expression tag	UNP A9Y8T1
C	446	HIS	-	expression tag	UNP A9Y8T1
C	447	HIS	-	expression tag	UNP A9Y8T1
C	448	HIS	-	expression tag	UNP A9Y8T1
C	449	HIS	-	expression tag	UNP A9Y8T1
C	450	HIS	-	expression tag	UNP A9Y8T1
C	451	HIS	-	expression tag	UNP A9Y8T1
D	437	LYS	-	expression tag	UNP A9Y8T1
D	438	LEU	-	expression tag	UNP A9Y8T1
D	439	ALA	-	expression tag	UNP A9Y8T1
D	440	ALA	-	expression tag	UNP A9Y8T1
D	441	ALA	-	expression tag	UNP A9Y8T1
D	442	LEU	-	expression tag	UNP A9Y8T1
D	443	GLU	-	expression tag	UNP A9Y8T1
D	444	HIS	-	expression tag	UNP A9Y8T1
D	445	HIS	-	expression tag	UNP A9Y8T1
D	446	HIS	-	expression tag	UNP A9Y8T1
D	447	HIS	-	expression tag	UNP A9Y8T1
D	448	HIS	-	expression tag	UNP A9Y8T1
D	449	HIS	-	expression tag	UNP A9Y8T1
D	450	HIS	-	expression tag	UNP A9Y8T1
D	451	HIS	-	expression tag	UNP A9Y8T1

- Molecule 2 is trimethyl-[(2S)-1-oxidanyl-1-oxidanylidene-3-(2-sulfanylidene-1,3-dihydroimidazol-4-yl)propan-2-yl]azanium (three-letter code: LW8) (formula: C₉H₁₆N₃O₂S) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	B	1	28	10	5	11	2	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	D	1	28	10	5	11	2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	276	Total 276	O 276	0	0
4	B	388	Total 388	O 388	0	0
4	C	268	Total 268	O 268	0	0
4	D	404	Total 404	O 404	0	0

V349		
V357		
I358		
A359		
L365		
I376		
R390		
R391		
V392		
R393		
V411		
R412		
S436		
LYS		
LEU		
ALA		
ALA		
ALA		
ALA		
LEU		
GLU		
HIS		
HIS		
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	97.63Å 139.48Å 158.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.82 – 2.10 48.82 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.82-2.10) 100.0 (48.82-2.10)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.96 (at 2.10Å)	Xtrriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.184 , 0.221 0.184 , 0.221	Depositor DCC
R_{free} test set	2000 reflections (1.58%)	wwPDB-VP
Wilson B-factor (Å ²)	22.5	Xtrriage
Anisotropy	0.231	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 48.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.54$, $\langle L^2 \rangle = 0.38$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14312	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 47.16 % 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 1.0327e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: LW8, GDP

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	0/3269	0.63	1/4449 (0.0%)
1	B	0.41	0/3313	0.63	0/4511
1	C	0.38	0/3248	0.61	0/4422
1	D	0.40	0/3325	0.64	0/4526
All	All	0.39	0/13155	0.63	1/17908 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	35	LEU	CA-CB-CG	5.28	127.43	115.30

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	3204	0	3156	22	0
1	B	3245	0	3194	19	0
1	C	3184	0	3129	16	0
1	D	3257	0	3201	22	0
2	B	15	0	0	0	0
2	D	15	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	28	0	12	0	0
3	D	28	0	12	0	0
4	A	276	0	0	0	0
4	B	388	0	0	2	0
4	C	268	0	0	0	0
4	D	404	0	0	4	0
All	All	14312	0	12704	78	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 3.

The worst 5 of 78 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:D:187:THR:HG21	1:D:212:ILE:HG23	1.78	0.65
1:A:290:ARG:HH21	1:A:291:ARG:HH12	1.47	0.61
1:A:75:ARG:O	1:A:79:GLU:HG3	2.00	0.61
1:D:376:ILE:HD13	1:D:392:VAL:HG22	1.83	0.59
1:A:237:GLU:O	1:A:241:GLU:HG2	2.03	0.59

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	421/451 (93%)	410 (97%)	11 (3%)	0	100	100
1	B	427/451 (95%)	414 (97%)	13 (3%)	0	100	100
1	C	420/451 (93%)	409 (97%)	11 (3%)	0	100	100
1	D	428/451 (95%)	416 (97%)	11 (3%)	1 (0%)	47	49
All	All	1696/1804 (94%)	1649 (97%)	46 (3%)	1 (0%)	51	54

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	161	PHE

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	308/335 (92%)	306 (99%)	2 (1%)	86	90
1	B	314/335 (94%)	310 (99%)	4 (1%)	69	75
1	C	306/335 (91%)	304 (99%)	2 (1%)	84	88
1	D	315/335 (94%)	312 (99%)	3 (1%)	76	82
All	All	1243/1340 (93%)	1232 (99%)	11 (1%)	78	84

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	410	ARG
1	D	9	ARG
1	D	188	ARG
1	D	105	ARG
1	B	387	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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](#)

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	LW8	B	501	-	14,15,15	2.22	5 (35%)	18,22,22	2.39	5 (27%)
3	GDP	D	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.13	3 (10%)
3	GDP	B	502	-	24,30,30	0.99	2 (8%)	30,47,47	1.16	2 (6%)
2	LW8	D	502	-	14,15,15	2.15	6 (42%)	18,22,22	2.50	5 (27%)

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	LW8	B	501	-	-	3/14/14/14	0/1/1/1
3	GDP	D	501	-	-	3/12/32/32	0/3/3/3
3	GDP	B	502	-	-	3/12/32/32	0/3/3/3
2	LW8	D	502	-	-	0/14/14/14	0/1/1/1

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	LW8	C14-S15	5.54	1.81	1.68
2	D	502	LW8	C14-S15	4.10	1.77	1.68
2	D	502	LW8	C10-N11	-3.17	1.32	1.37
2	D	502	LW8	C14-N11	-2.84	1.32	1.37
2	B	501	LW8	C10-N11	-2.82	1.33	1.37

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	502	LW8	N13-C14-N11	5.66	110.47	106.08
2	B	501	LW8	N13-C14-N11	5.52	110.36	106.08
2	D	502	LW8	C12-C10-N11	4.91	110.60	106.00
2	B	501	LW8	C12-C10-N11	4.54	110.25	106.00
2	D	502	LW8	C12-N13-C14	-4.39	106.75	110.68

There are no chirality outliers.

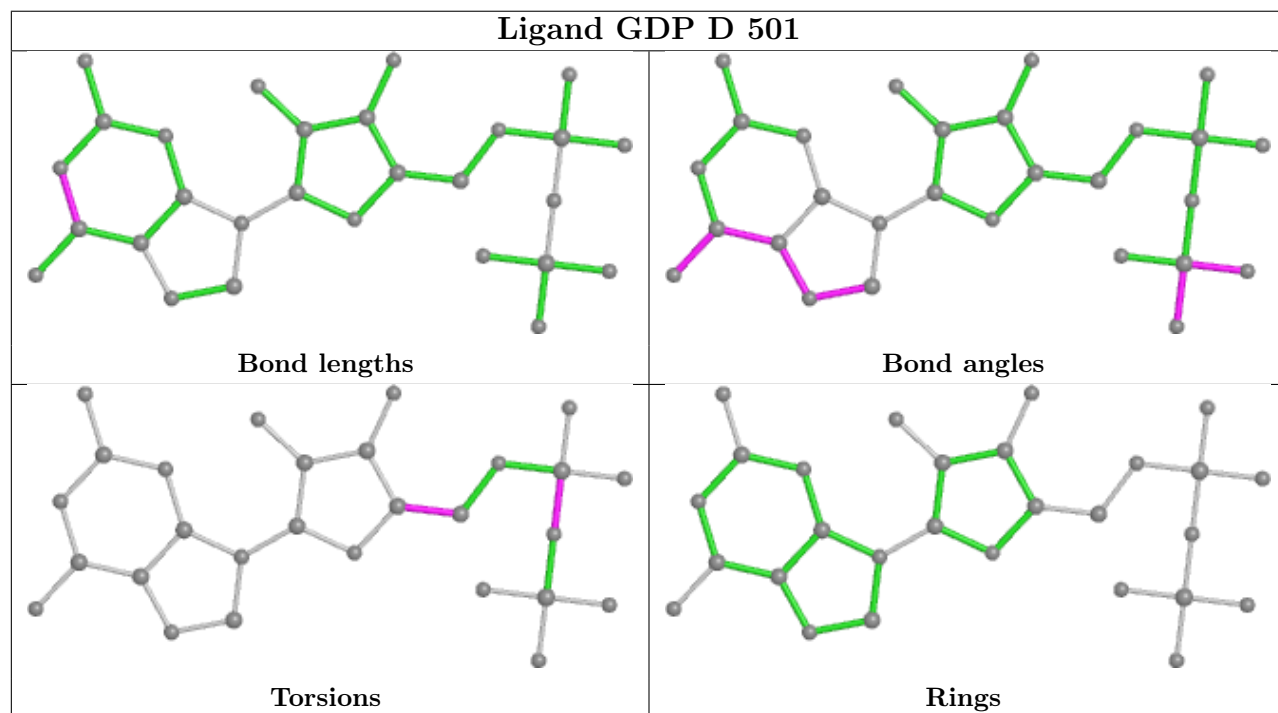
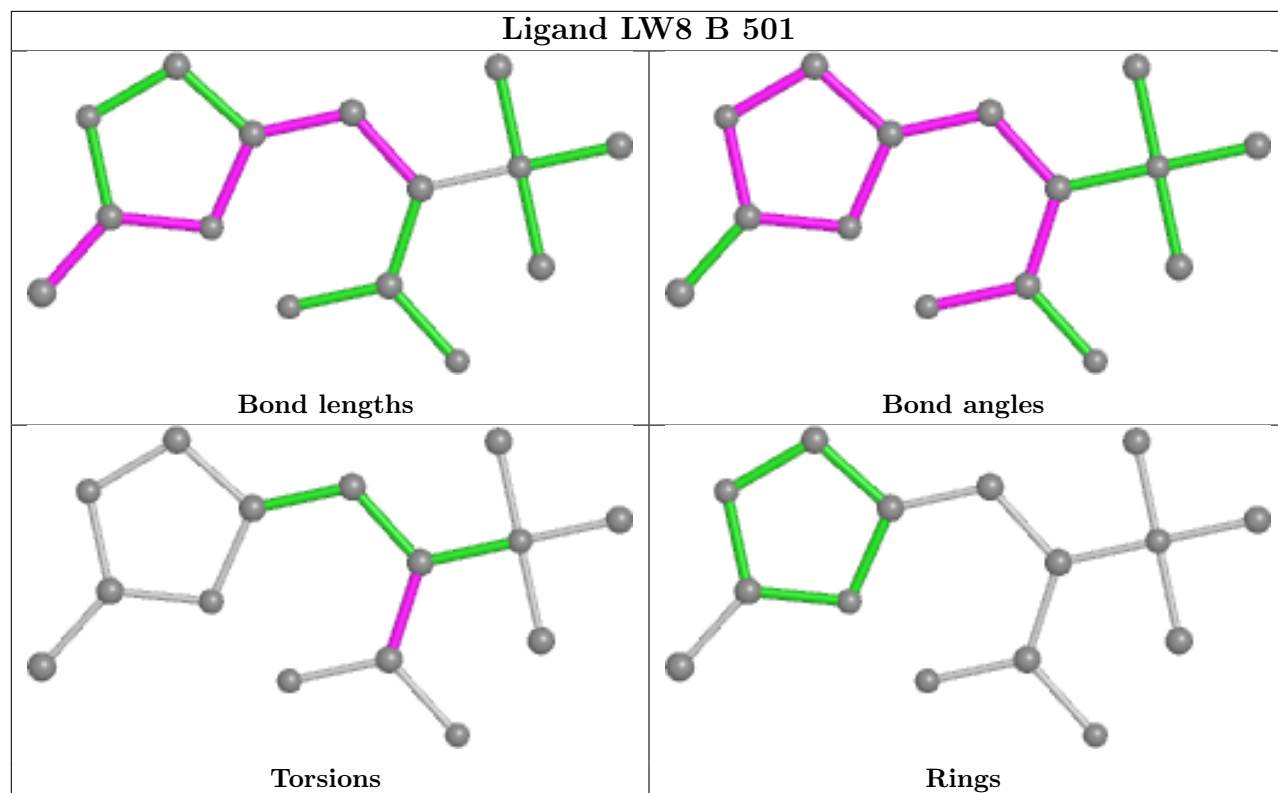
5 of 9 torsion outliers are listed below:

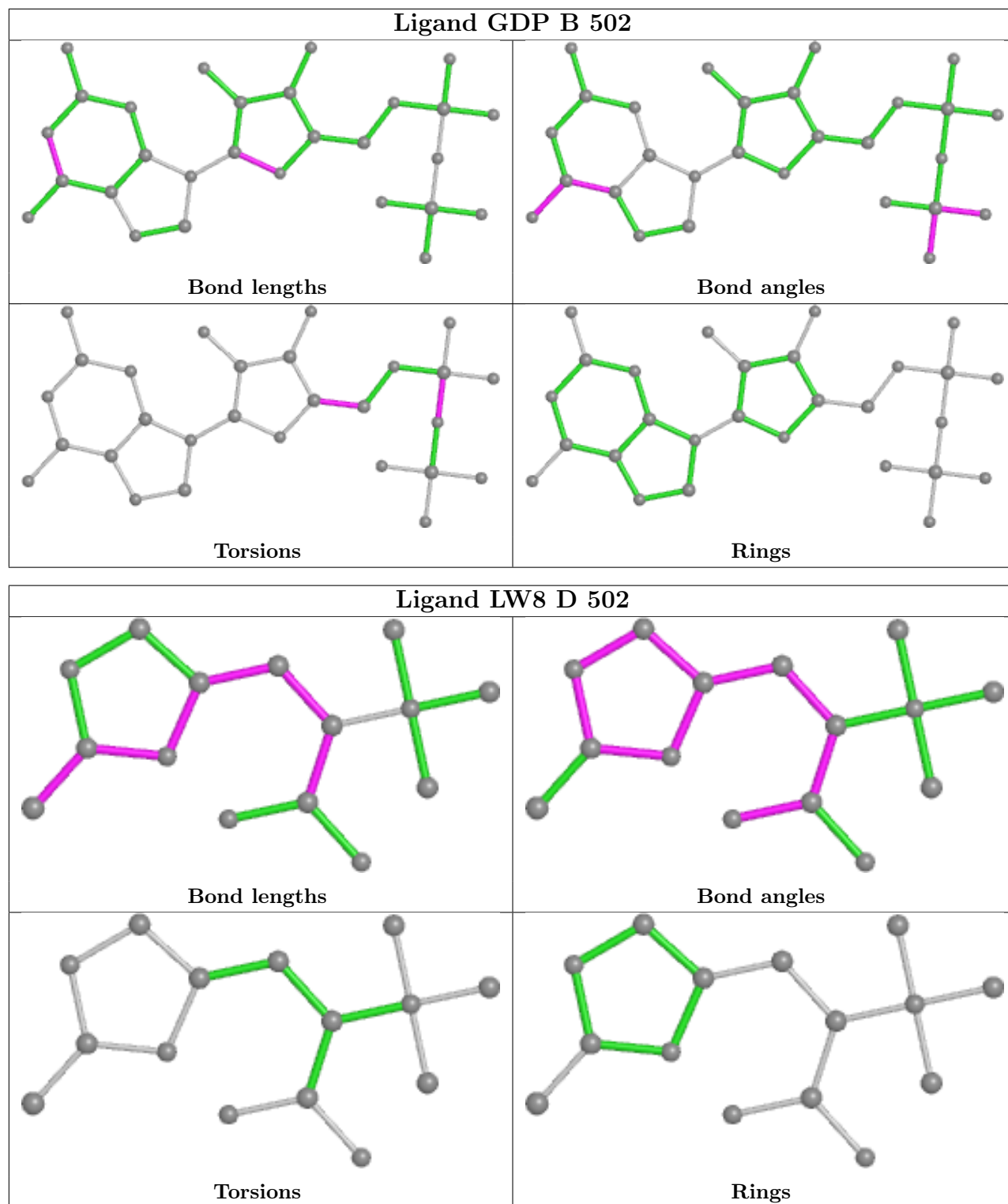
Mol	Chain	Res	Type	Atoms
3	B	502	GDP	PB-O3A-PA-O5'
3	B	502	GDP	O4'-C4'-C5'-O5'
3	D	501	GDP	PB-O3A-PA-O5'
3	B	502	GDP	C3'-C4'-C5'-O5'
3	D	501	GDP	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

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

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	425/451 (94%)	-0.34	6 (1%) 75 78	13, 25, 44, 60	0
1	B	429/451 (95%)	-0.47	0 100 100	12, 19, 35, 47	0
1	C	424/451 (94%)	-0.15	12 (2%) 53 59	12, 26, 49, 69	0
1	D	429/451 (95%)	-0.44	0 100 100	12, 20, 34, 47	0
All	All	1707/1804 (94%)	-0.35	18 (1%) 80 84	12, 22, 42, 69	0

The worst 5 of 18 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	265	GLY	5.0
1	A	303	TYR	4.6
1	C	266	LEU	3.5
1	C	8	GLY	3.4
1	C	264	PRO	3.3

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

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

6.3 Carbohydrates [i](#)

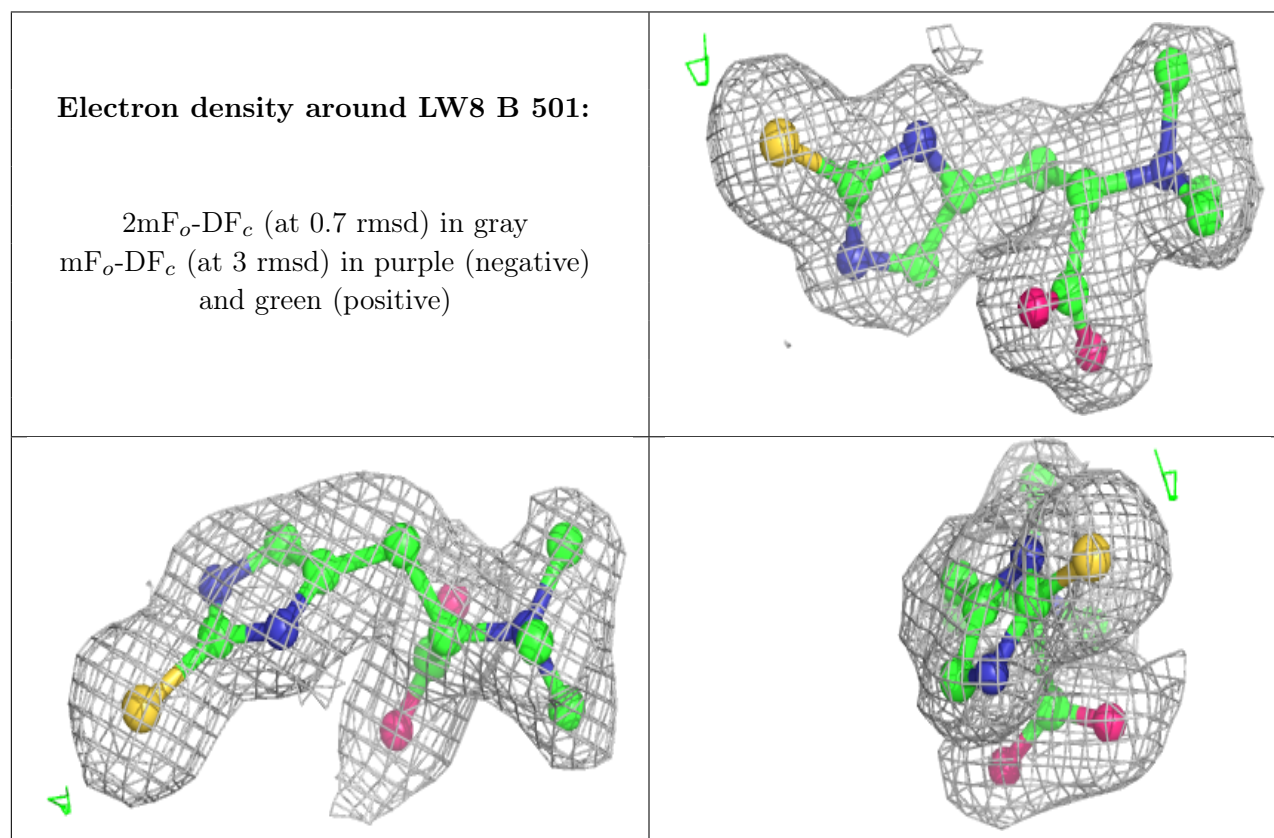
There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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.

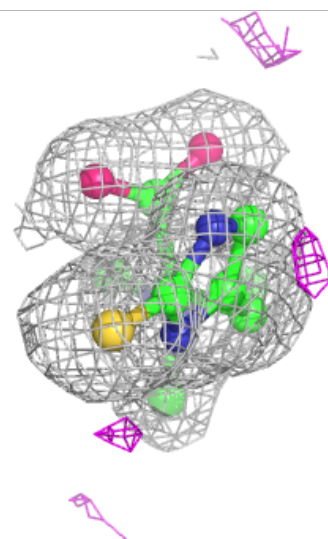
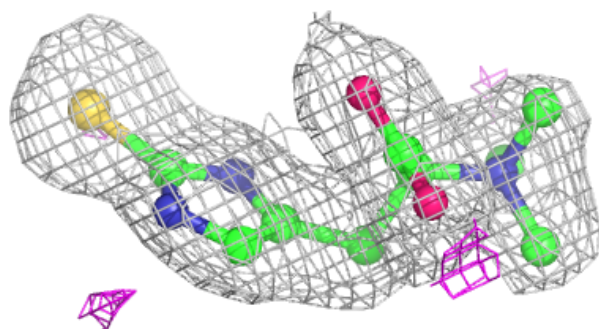
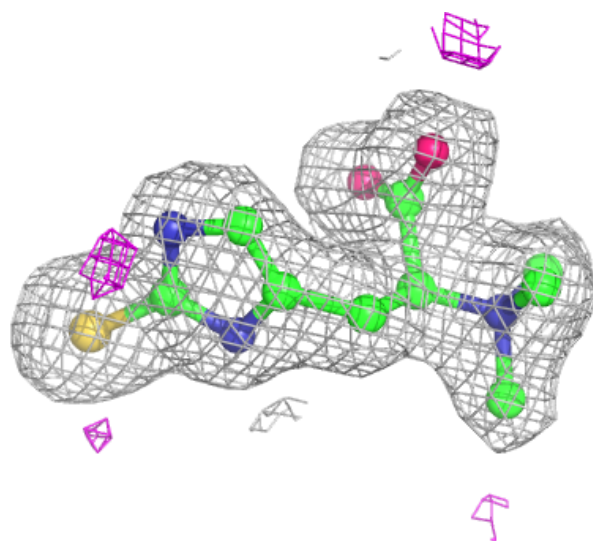
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	LW8	B	501	15/15	0.97	0.09	14,20,24,25	0
2	LW8	D	502	15/15	0.97	0.09	17,21,25,25	0
3	GDP	B	502	28/28	0.98	0.09	12,15,18,20	0
3	GDP	D	501	28/28	0.99	0.08	11,15,18,18	0

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.



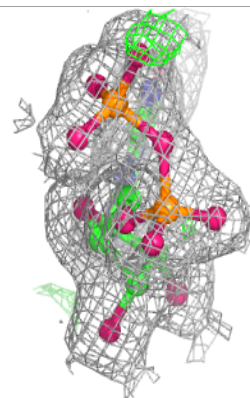
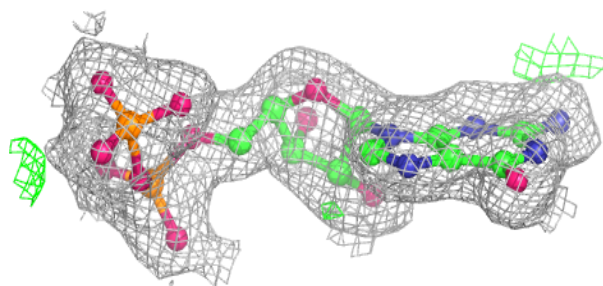
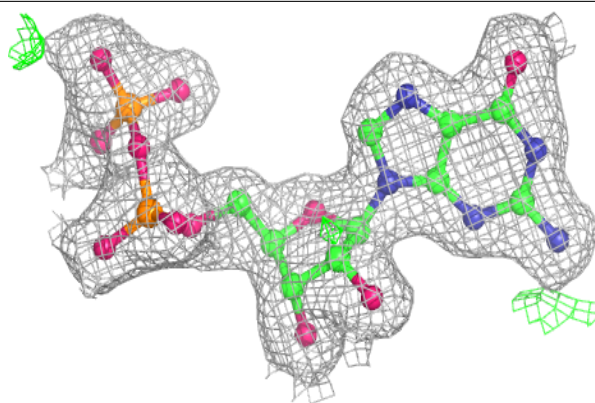
Electron density around LW8 D 502:

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

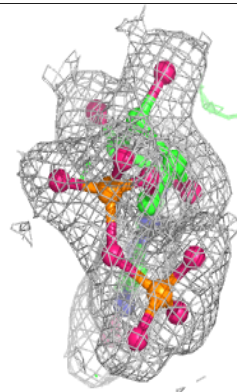
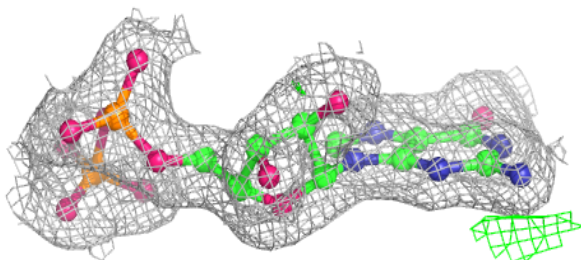
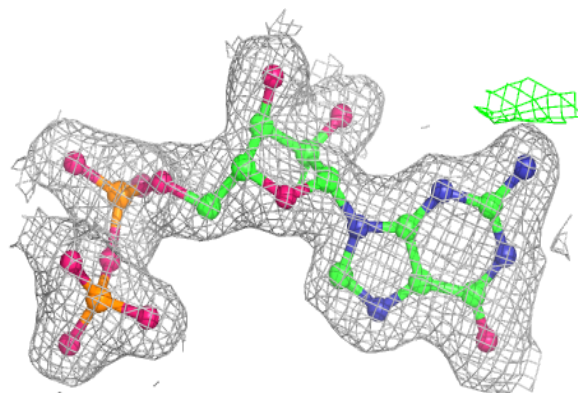


Electron density around GDP B 502:

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

**Electron density around GDP D 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.