



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 11:37 AM EDT

PDB ID : 6B9D / pdb_00006b9d
Title : Human ATL1 mutant - R77A bound to GDP
Authors : O'Donnell, J.P.; Sondermann, H.
Deposited on : 2017-10-10
Resolution : 1.95 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

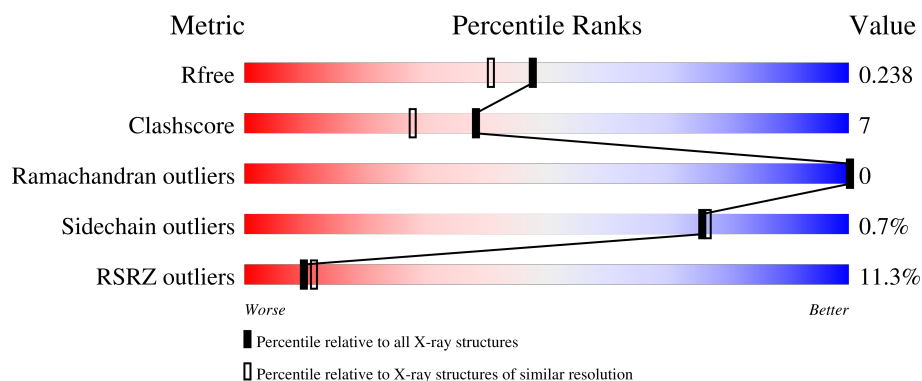
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	458	9% 70% 13% 17%
1	B	458	10% 69% 14% 17%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6247 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 Atlastin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	379	Total	C	N	O	S	0	0	0
			2929	1879	487	550	13			
1	B	380	Total	C	N	O	S	0	0	0
			2943	1893	491	546	13			

There are 26 discrepancies between the modelled and reference sequences:

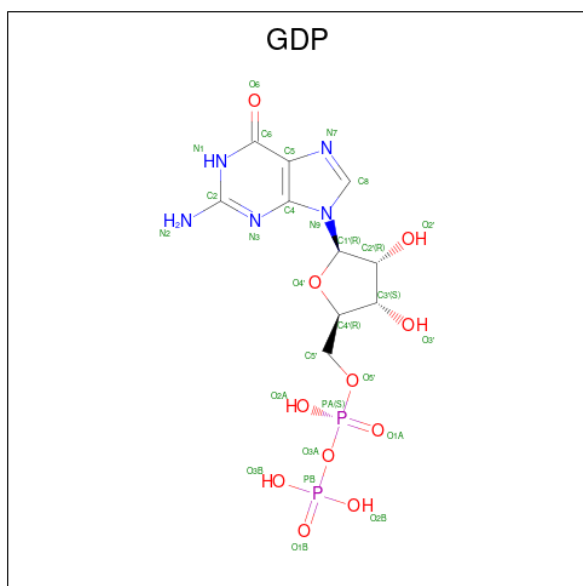
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP Q8WXF7
A	77	ALA	ARG	engineered mutation	UNP Q8WXF7
A	447	ALA	-	expression tag	UNP Q8WXF7
A	448	ALA	-	expression tag	UNP Q8WXF7
A	449	ALA	-	expression tag	UNP Q8WXF7
A	450	LEU	-	expression tag	UNP Q8WXF7
A	451	GLU	-	expression tag	UNP Q8WXF7
A	452	HIS	-	expression tag	UNP Q8WXF7
A	453	HIS	-	expression tag	UNP Q8WXF7
A	454	HIS	-	expression tag	UNP Q8WXF7
A	455	HIS	-	expression tag	UNP Q8WXF7
A	456	HIS	-	expression tag	UNP Q8WXF7
A	457	HIS	-	expression tag	UNP Q8WXF7
B	0	SER	-	expression tag	UNP Q8WXF7
B	77	ALA	ARG	engineered mutation	UNP Q8WXF7
B	447	ALA	-	expression tag	UNP Q8WXF7
B	448	ALA	-	expression tag	UNP Q8WXF7
B	449	ALA	-	expression tag	UNP Q8WXF7
B	450	LEU	-	expression tag	UNP Q8WXF7
B	451	GLU	-	expression tag	UNP Q8WXF7
B	452	HIS	-	expression tag	UNP Q8WXF7
B	453	HIS	-	expression tag	UNP Q8WXF7
B	454	HIS	-	expression tag	UNP Q8WXF7
B	455	HIS	-	expression tag	UNP Q8WXF7
B	456	HIS	-	expression tag	UNP Q8WXF7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	457	HIS	-	expression tag	UNP Q8WXF7

- Molecule 2 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	147	Total O 147 147	0	0
5	B	134	Total O 134 134	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	51.06Å 68.43Å 75.88Å 117.00° 89.81° 99.04°	Depositor
Resolution (Å)	25.18 – 1.95 25.18 – 1.95	Depositor EDS
% Data completeness (in resolution range)	96.3 (25.18-1.95) 89.8 (25.18-1.95)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.42 (at 1.79Å)	Xtriage
Refinement program	PHENIX (1.12_2829)	Depositor
R, R_{free}	0.204 , 0.239 0.204 , 0.238	Depositor DCC
R_{free} test set	1980 reflections (2.48%)	wwPDB-VP
Wilson B-factor (Å ²)	24.3	Xtriage
Anisotropy	0.467	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 63.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6247	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.84% 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: MG, GDP, GOL

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	0.31	0/2983	0.51	0/4033
1	B	0.32	0/2998	0.51	0/4049
All	All	0.32	0/5981	0.51	0/8082

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	2929	0	2819	39	0
1	B	2943	0	2851	42	0
2	A	28	0	12	0	0
2	B	28	0	12	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	18	0	24	2	0
4	B	18	0	24	3	0
5	A	147	0	0	3	0
5	B	134	0	0	1	0
All	All	6247	0	5742	81	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 7.

All (81) 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:B:125:ILE:HG22	1:B:145:MET:HG2	1.68	0.74
1:A:68:VAL:HG21	1:A:310:LEU:HB3	1.72	0.71
1:B:243:SER:HB3	1:B:250:LEU:HD23	1.72	0.70
1:B:68:VAL:HG21	1:B:310:LEU:HB3	1.77	0.66
1:B:330:LYS:HB2	4:B:505:GOL:H31	1.79	0.64
1:A:271:HIS:CD2	1:A:273:GLY:H	2.17	0.63
1:B:71:SER:HB2	1:B:145:MET:HE3	1.81	0.63
1:B:271:HIS:CD2	1:B:273:GLY:H	2.17	0.62
1:A:125:ILE:HG22	1:A:145:MET:HG2	1.84	0.60
1:A:87:MET:HE3	1:A:305:LEU:HD11	1.85	0.59
1:B:323:ARG:NH1	5:B:603:HOH:O	2.32	0.59
1:B:355:ASN:HD21	1:B:407:LYS:HA	1.68	0.58
1:A:48:LEU:HD11	1:A:329:PHE:HB3	1.87	0.56
1:B:35:VAL:HG21	1:B:56:ILE:HD11	1.88	0.56
1:B:94:GLN:HB2	4:B:504:GOL:H32	1.87	0.55
1:B:386:ASP:OD2	1:B:390:LYS:NZ	2.40	0.55
1:A:372:GLU:HG2	1:A:432:TYR:OH	2.08	0.54
1:B:355:ASN:ND2	1:B:407:LYS:HA	2.23	0.54
1:A:270:PRO:HG2	1:A:293:PHE:HA	1.90	0.54
1:B:204:THR:HB	1:B:316:ASN:HD22	1.73	0.52
1:B:271:HIS:HD2	1:B:273:GLY:H	1.57	0.52
1:A:200:ALA:HB1	4:A:504:GOL:H31	1.91	0.52
1:A:91:MET:CE	1:A:94:GLN:HE21	2.23	0.51
1:A:271:HIS:HD2	1:A:273:GLY:H	1.56	0.51
1:B:437:ASP:OD1	1:B:438:SER:N	2.44	0.51
1:A:419:GLN:NE2	5:A:607:HOH:O	2.38	0.51
1:B:48:LEU:HD11	1:B:53:LEU:HD22	1.93	0.51
1:A:91:MET:HE1	1:A:94:GLN:HE21	1.77	0.50
1:A:243:SER:HB3	1:A:246:GLN:N	2.27	0.50
1:A:395:LYS:HG3	1:A:425:ILE:HG21	1.92	0.50
1:A:248:GLU:H	1:A:248:GLU:CD	2.21	0.49
1:A:206:LEU:O	4:A:504:GOL:O3	2.31	0.49
1:A:364:LYS:HE3	1:A:424:GLU:HB3	1.94	0.49
1:A:219:TRP:CE2	1:A:268:LEU:HD13	2.48	0.49
1:A:364:LYS:HE2	1:A:428:LEU:HD11	1.95	0.48
1:A:323:ARG:NH1	5:A:609:HOH:O	2.39	0.48
1:B:41:LYS:N	1:B:45:SER:O	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:VAL:HG21	1:A:56:ILE:HD11	1.95	0.48
1:B:169:MET:HE2	1:B:209:PHE:HE1	1.79	0.48
1:B:199:LEU:HB3	1:B:348:LEU:HD22	1.95	0.48
1:B:257:ILE:HG22	1:B:264:ILE:CD1	2.43	0.48
1:B:169:MET:HE1	1:B:196:TYR:CE2	2.50	0.47
1:A:363:ALA:HA	1:A:401:LEU:HD23	1.98	0.46
1:B:367:TYR:CZ	1:B:371:MET:HG3	2.51	0.46
1:A:78:LYS:HD2	1:A:179:SER:HB2	1.98	0.45
1:A:412:GLU:O	5:A:601:HOH:O	2.21	0.45
1:B:204:THR:HB	1:B:316:ASN:ND2	2.31	0.45
1:B:363:ALA:HA	1:B:401:LEU:HD23	1.99	0.45
1:A:210:GLN:NE2	1:A:312:ILE:O	2.44	0.44
1:B:162:THR:HG23	1:B:336:TYR:HD1	1.82	0.44
1:A:332:TYR:O	1:A:336:TYR:HD2	1.99	0.44
1:A:89:ARG:HH21	1:A:107:LEU:HA	1.82	0.44
1:A:308:GLU:H	1:A:308:GLU:CD	2.25	0.44
1:B:90:TYR:CD2	1:B:91:MET:CE	3.00	0.44
1:B:41:LYS:CB	1:B:44:HIS:H	2.31	0.43
1:B:86:PHE:CG	1:B:297:LEU:HD21	2.53	0.43
1:B:55:ARG:HA	4:B:503:GOL:H11	2.01	0.43
1:B:91:MET:HE1	1:B:305:LEU:HB3	2.00	0.43
1:B:80:LYS:O	1:B:84:MET:HG3	2.19	0.43
1:A:165:ALA:O	1:A:169:MET:HG2	2.19	0.43
1:A:90:TYR:CD2	1:A:91:MET:CE	3.02	0.43
1:B:72:VAL:HG21	1:B:87:MET:HE1	2.01	0.42
1:B:84:MET:HA	1:B:87:MET:HE2	2.01	0.42
1:A:386:ASP:OD2	1:A:390:LYS:NZ	2.52	0.42
1:A:429:TYR:CZ	1:A:433:ILE:HD11	2.54	0.42
1:B:219:TRP:CE2	1:B:268:LEU:HD13	2.54	0.42
1:A:86:PHE:CG	1:A:297:LEU:HD21	2.55	0.42
1:B:270:PRO:HG2	1:B:293:PHE:HA	2.02	0.42
1:A:91:MET:HE1	1:A:305:LEU:HB3	2.03	0.41
1:A:66:GLU:OE2	1:A:312:ILE:HD13	2.19	0.41
1:B:84:MET:HA	1:B:87:MET:CE	2.50	0.41
1:B:429:TYR:CZ	1:B:433:ILE:HD11	2.55	0.41
1:B:429:TYR:CE2	1:B:433:ILE:HD11	2.56	0.41
1:A:162:THR:HG23	1:A:336:TYR:CD1	2.55	0.41
1:B:401:LEU:O	1:B:405:VAL:HG23	2.20	0.41
1:A:239:ARG:HH11	1:A:239:ARG:HD3	1.75	0.40
1:B:323:ARG:CZ	1:B:361:ALA:HB1	2.51	0.40
1:B:210:GLN:HE22	1:B:313:LYS:HD2	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:MET:HE3	1:A:305:LEU:HD13	2.03	0.40
1:B:381:PHE:HB2	1:B:439:LYS:C	2.47	0.40
1:A:84:MET:HE2	1:A:84:MET:HB3	1.99	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	365/458 (80%)	356 (98%)	9 (2%)	0	100	100
1	B	364/458 (80%)	356 (98%)	8 (2%)	0	100	100
All	All	729/916 (80%)	712 (98%)	17 (2%)	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	303/402 (75%)	302 (100%)	1 (0%)	86	87
1	B	306/402 (76%)	303 (99%)	3 (1%)	68	67
All	All	609/804 (76%)	605 (99%)	4 (1%)	76	76

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	375	CYS
1	B	97	VAL
1	B	203	GLU
1	B	375	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	ASN
1	A	94	GLN
1	A	191	GLN
1	A	258	HIS
1	A	271	HIS
1	A	318	ASN
1	A	356	ASN
1	A	419	GLN
1	B	54	ASN
1	B	124	GLN
1	B	180	GLN
1	B	210	GLN
1	B	271	HIS
1	B	316	ASN
1	B	349	GLN
1	B	355	ASN
1	B	356	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	B	505	-	5,5,5	1.17	0	5,5,5	0.92	0
4	GOL	A	505	-	5,5,5	0.94	0	5,5,5	1.18	1 (20%)
4	GOL	A	504	-	5,5,5	0.81	0	5,5,5	1.11	0
2	GDP	A	501	-	29,30,30	1.07	1 (3%)	45,47,47	1.75	6 (13%)
2	GDP	B	501	-	29,30,30	1.03	1 (3%)	45,47,47	1.80	8 (17%)
4	GOL	B	503	-	5,5,5	1.02	0	5,5,5	0.93	0
4	GOL	A	503	-	5,5,5	0.87	0	5,5,5	1.13	0
4	GOL	B	504	-	5,5,5	1.12	0	5,5,5	1.07	0

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
4	GOL	B	505	-	-	2/4/4/4	-
4	GOL	A	505	-	-	0/4/4/4	-
4	GOL	A	504	-	-	3/4/4/4	-
2	GDP	A	501	-	-	2/16/32/32	0/3/3/3
2	GDP	B	501	-	-	1/16/32/32	0/3/3/3
4	GOL	B	503	-	-	4/4/4/4	-
4	GOL	A	503	-	-	2/4/4/4	-
4	GOL	B	504	-	-	2/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	GDP	C5-C4	2.95	1.46	1.38
2	A	501	GDP	C5-C4	2.90	1.46	1.38

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	GDP	C5-C4-N3	-5.62	119.44	128.39
2	A	501	GDP	C5-C4-N3	-5.44	119.73	128.39
2	B	501	GDP	C2-N3-C4	5.21	121.27	112.30
2	A	501	GDP	C2-N3-C4	4.94	120.81	112.30
2	B	501	GDP	N9-C4-N3	4.25	134.45	125.95
2	A	501	GDP	C6-C5-N7	3.77	137.14	130.29
2	A	501	GDP	N9-C4-N3	3.65	133.25	125.95
2	B	501	GDP	C6-C5-N7	3.42	136.51	130.29
2	B	501	GDP	O6-C6-C5	-2.73	119.32	126.53
2	A	501	GDP	C4-C5-N7	-2.64	106.48	110.67
2	B	501	GDP	C4-C5-N7	-2.31	107.02	110.67
2	A	501	GDP	O6-C6-C5	-2.30	120.46	126.53
4	A	505	GOL	C3-C2-C1	-2.12	104.00	111.80
2	B	501	GDP	C5-C6-N1	2.04	118.44	113.25
2	B	501	GDP	O3B-PB-O3A	2.00	111.36	104.64

There are no chirality outliers.

All (16) torsion outliers are listed below:

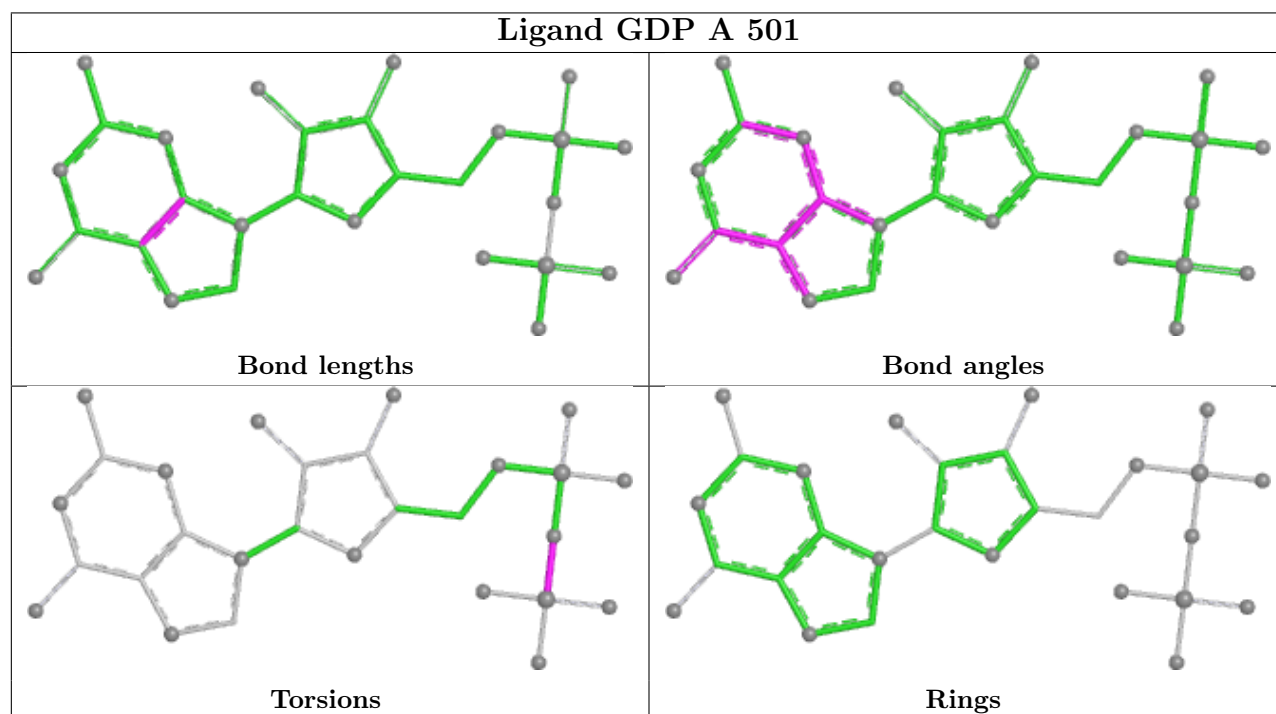
Mol	Chain	Res	Type	Atoms
4	B	503	GOL	C1-C2-C3-O3
4	B	503	GOL	O2-C2-C3-O3
4	B	505	GOL	C1-C2-C3-O3
4	A	503	GOL	O1-C1-C2-C3
4	A	504	GOL	O1-C1-C2-C3
4	A	504	GOL	C1-C2-C3-O3
4	B	503	GOL	O1-C1-C2-C3
4	B	504	GOL	O1-C1-C2-C3
4	B	505	GOL	O2-C2-C3-O3
4	A	504	GOL	O1-C1-C2-O2
4	B	504	GOL	O1-C1-C2-O2
2	B	501	GDP	PA-O3A-PB-O1B
2	A	501	GDP	PA-O3A-PB-O3B
4	A	503	GOL	O1-C1-C2-O2
4	B	503	GOL	O1-C1-C2-O2
2	A	501	GDP	PA-O3A-PB-O2B

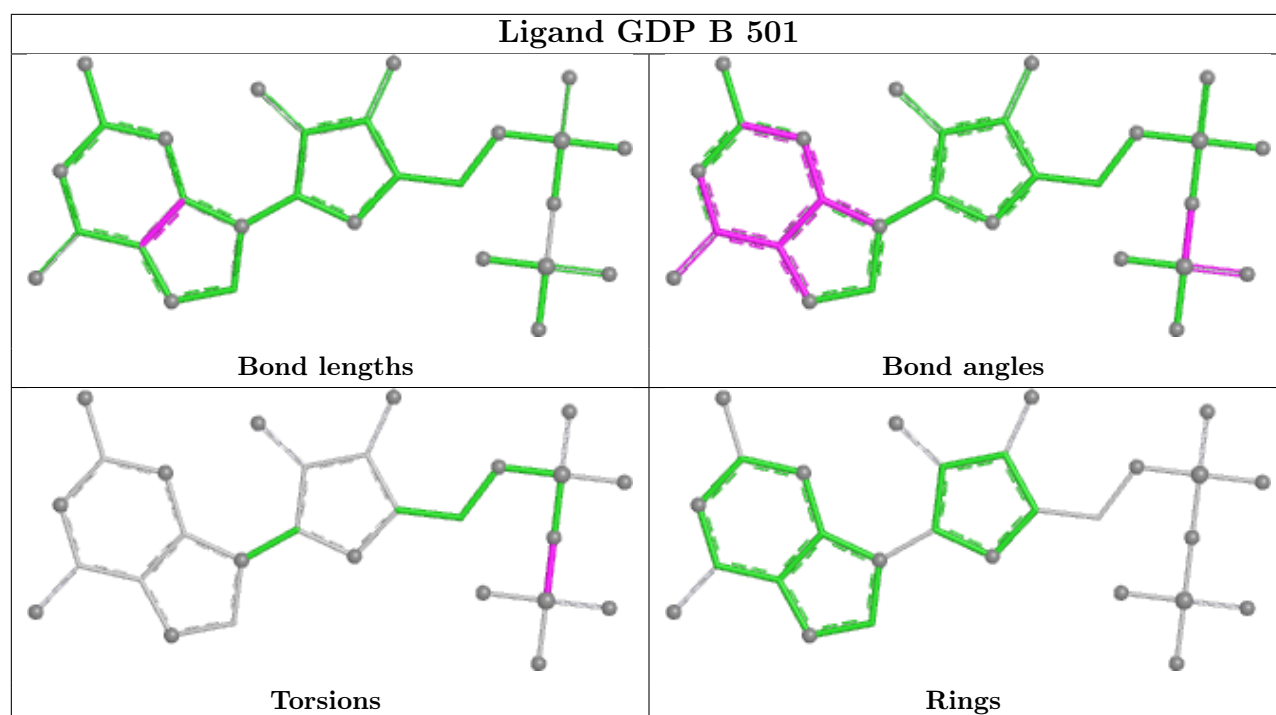
There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	505	GOL	1	0
4	A	504	GOL	2	0
4	B	503	GOL	1	0
4	B	504	GOL	1	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	379/458 (82%)	0.69	40 (10%)	11 13	22, 40, 74, 91	0
1	B	380/458 (82%)	0.71	46 (12%)	8 10	22, 40, 76, 100	0
All	All	759/916 (82%)	0.70	86 (11%)	10 11	22, 40, 76, 100	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	381	PHE	6.3
1	A	29	VAL	5.5
1	B	157	LEU	5.1
1	A	376	GLY	4.6
1	B	382	LEU	4.5
1	A	438	SER	4.4
1	B	383	ALA	4.2
1	B	380	PRO	4.1
1	A	107	LEU	4.0
1	B	120	THR	4.0
1	B	43	ASP	3.9
1	B	244	GLY	3.9
1	A	282	PHE	3.7
1	A	284	GLY	3.7
1	B	280	PRO	3.5
1	A	243	SER	3.5
1	A	374	ILE	3.4
1	A	120	THR	3.3
1	A	106	PRO	3.3
1	A	40	VAL	3.2
1	A	39	ILE	3.2
1	B	384	PRO	3.2
1	B	279	ASN	3.2
1	A	76	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	281	ASN	3.1
1	B	76	PHE	3.0
1	A	383	ALA	3.0
1	B	381	PHE	2.9
1	B	242	VAL	2.9
1	B	437	ASP	2.9
1	A	341	LEU	2.9
1	B	436	ASN	2.8
1	B	29	VAL	2.8
1	B	108	THR	2.8
1	B	46	PHE	2.7
1	B	374	ILE	2.7
1	B	435	HIS	2.7
1	B	282	PHE	2.7
1	B	121	THR	2.7
1	B	246	GLN	2.7
1	B	40	VAL	2.7
1	A	286	LEU	2.7
1	B	111	SER	2.7
1	B	439	LYS	2.6
1	A	343	HIS	2.6
1	A	283	ASP	2.6
1	B	149	GLY	2.6
1	B	97	VAL	2.6
1	A	382	LEU	2.5
1	A	274	LEU	2.5
1	B	240	LEU	2.5
1	A	279	ASN	2.5
1	A	375	CYS	2.5
1	B	375	CYS	2.4
1	A	48	LEU	2.4
1	A	160	SER	2.4
1	B	438	SER	2.4
1	B	281	ASN	2.4
1	A	309	SER	2.3
1	A	433	ILE	2.3
1	B	158	ARG	2.3
1	A	435	HIS	2.3
1	A	436	ASN	2.3
1	A	38	LEU	2.2
1	B	203	GLU	2.2
1	B	373	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	243	SER	2.2
1	B	110	PHE	2.2
1	B	371	MET	2.2
1	A	97	VAL	2.2
1	B	286	LEU	2.2
1	B	386	ASP	2.2
1	A	111	SER	2.2
1	B	101	GLY	2.2
1	A	161	ALA	2.2
1	B	430	ILE	2.1
1	A	166	LEU	2.1
1	B	41	LYS	2.1
1	A	280	PRO	2.1
1	A	384	PRO	2.1
1	B	283	ASP	2.1
1	A	41	LYS	2.0
1	B	285	LYS	2.0
1	B	434	LYS	2.0
1	A	336	TYR	2.0
1	A	194	THR	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
4	GOL	B	504	6/6	0.81	0.18	46,54,58,66	0
4	GOL	B	503	6/6	0.83	0.13	55,63,63,69	0
3	MG	B	502	1/1	0.85	0.23	59,59,59,59	0

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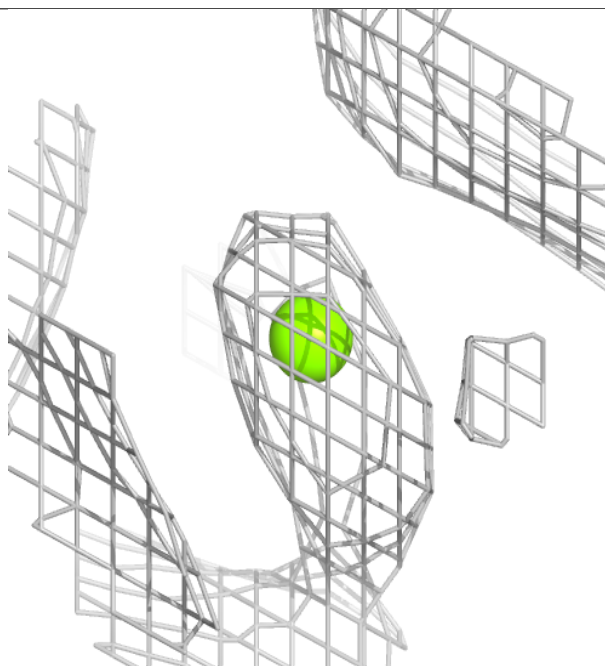
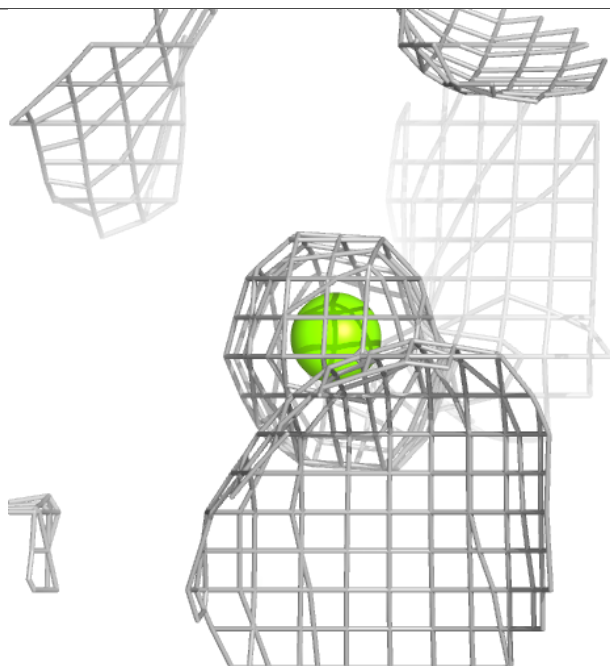
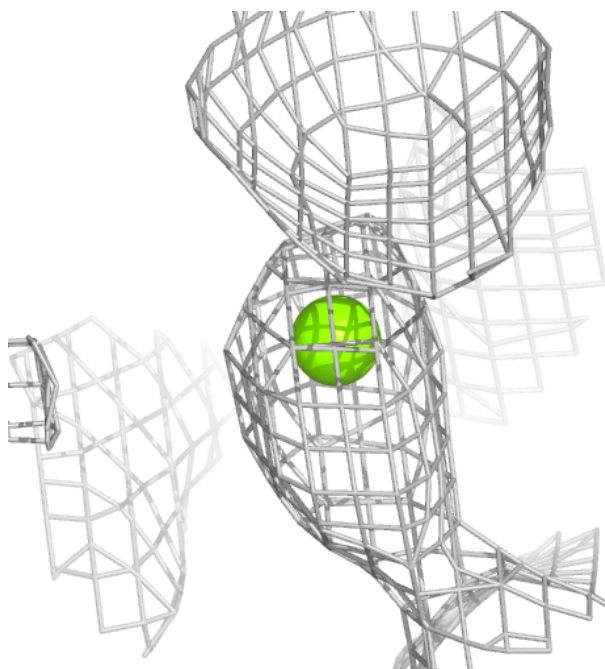
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	GOL	A	505	6/6	0.87	0.14	36,41,51,53	0
4	GOL	A	504	6/6	0.88	0.14	50,58,59,61	0
4	GOL	A	503	6/6	0.88	0.14	26,40,49,49	0
4	GOL	B	505	6/6	0.90	0.12	34,53,58,60	0
3	MG	A	502	1/1	0.93	0.10	55,55,55,55	0
2	GDP	A	501	28/28	0.95	0.07	22,31,39,41	0
2	GDP	B	501	28/28	0.95	0.08	26,34,39,48	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.

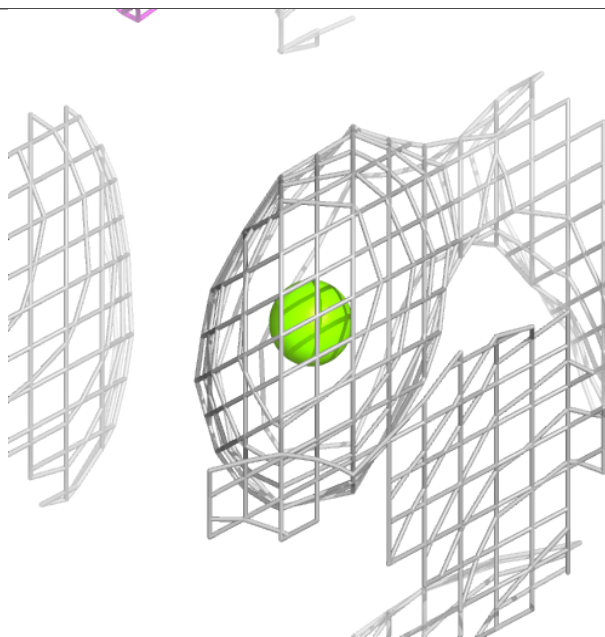
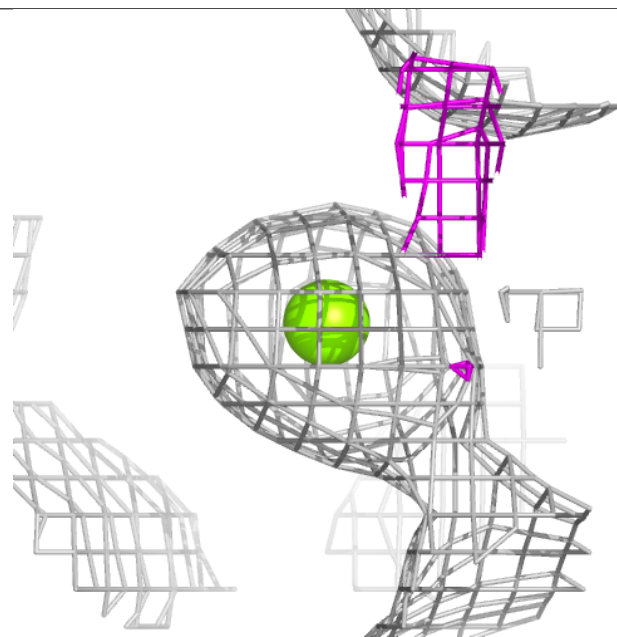
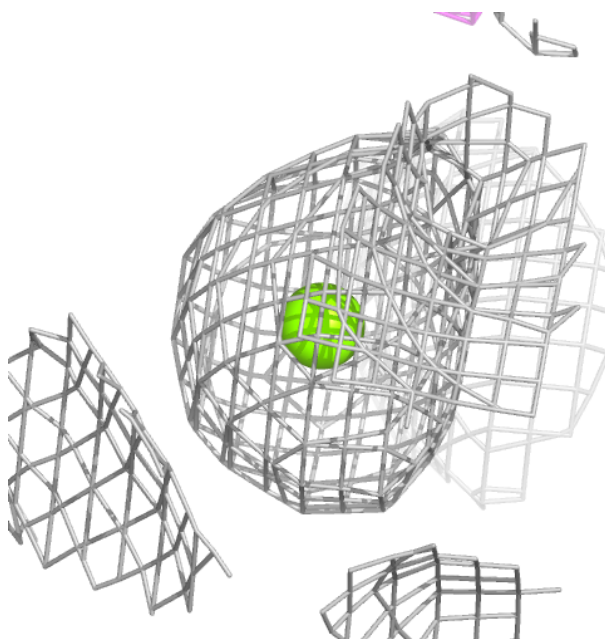
Electron density around MG B 502:

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



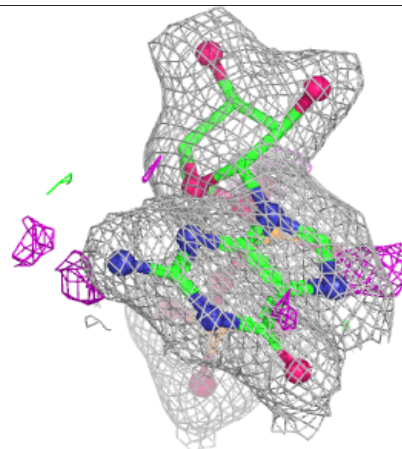
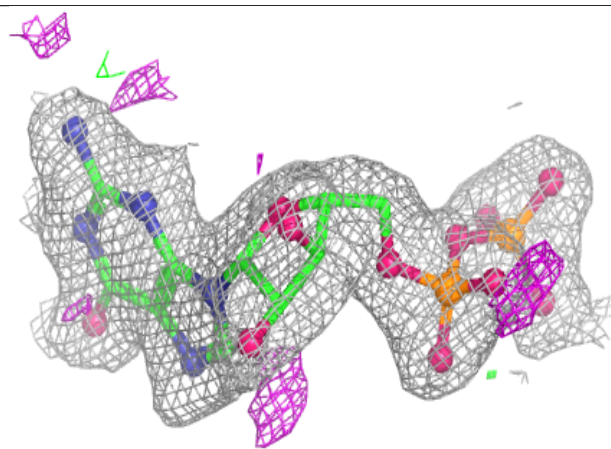
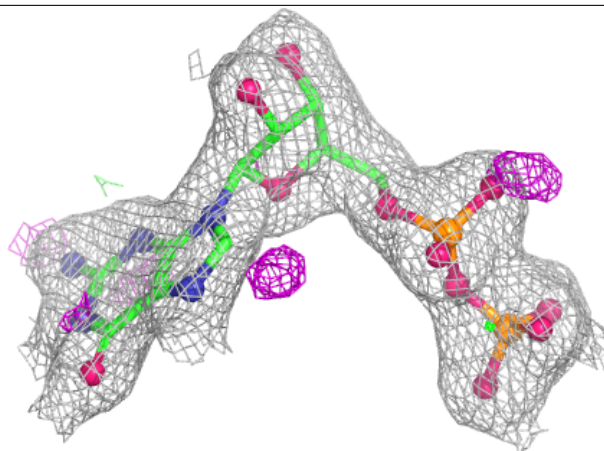
Electron density around MG A 502:

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



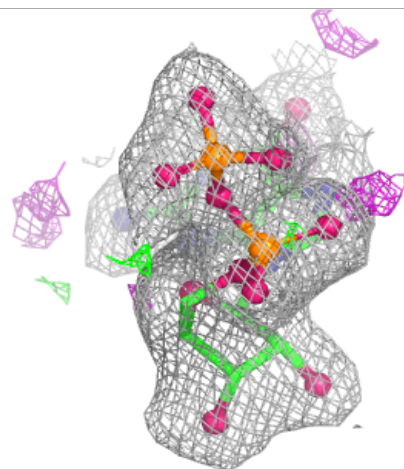
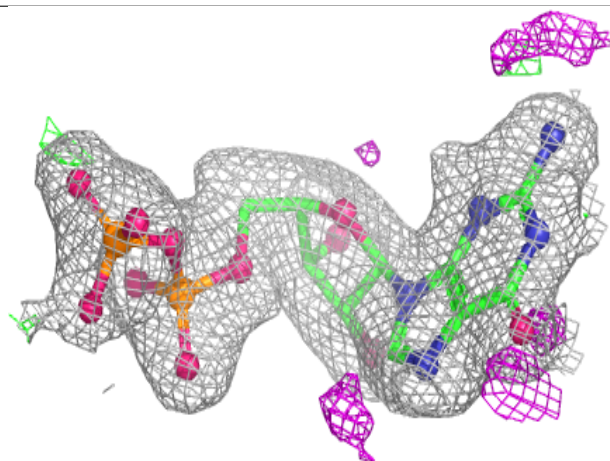
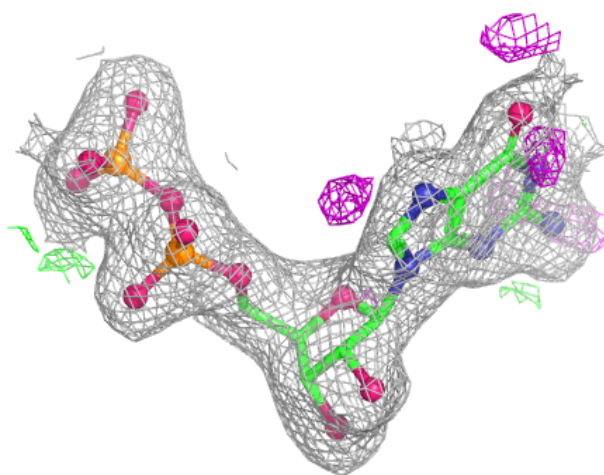
Electron density around GDP A 501:

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



Electron density around GDP 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.