



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 12:16 PM UTC

PDB ID : 7CDW / pdb\_00007cdw  
Title : Crystal Structure of Mycobacterium Tuberculosis Elongation Factor G1  
Authors : Gao, X.; Cui, S.  
Deposited on : 2020-06-20  
Resolution : 3.00 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](mailto: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>.

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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)  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

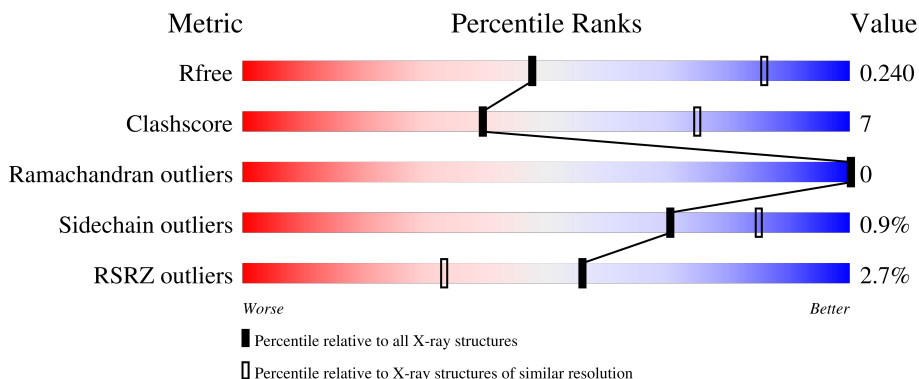
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*



The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	710	 82% 14% 4%
1	B	710	 78% 17% 5%

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 20963 atoms, of which 10370 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.

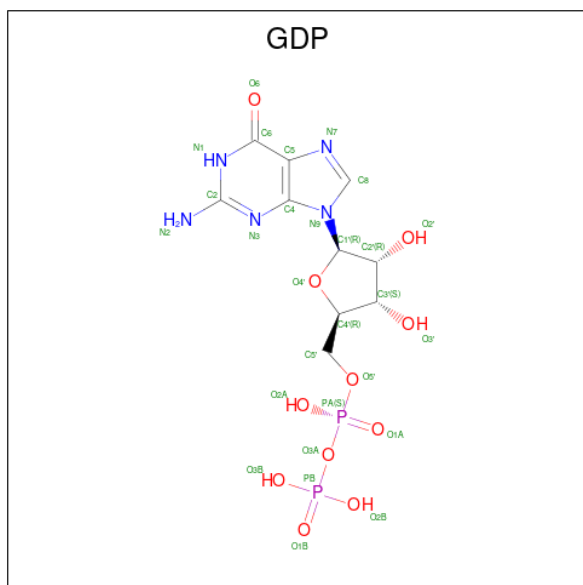
- Molecule 1 is a protein called Elongation factor G.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S	Se			
1	A	683	10493	3336	5208	892	1039	2	16	0	0	0
1	B	678	10394	3319	5142	886	1029	2	16	0	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	702	LEU	-	expression tag	UNP P9WNM7
A	703	GLU	-	expression tag	UNP P9WNM7
A	704	GLY	-	expression tag	UNP P9WNM7
A	705	HIS	-	expression tag	UNP P9WNM7
A	706	HIS	-	expression tag	UNP P9WNM7
A	707	HIS	-	expression tag	UNP P9WNM7
A	708	HIS	-	expression tag	UNP P9WNM7
A	709	HIS	-	expression tag	UNP P9WNM7
A	710	HIS	-	expression tag	UNP P9WNM7
B	702	LEU	-	expression tag	UNP P9WNM7
B	703	GLU	-	expression tag	UNP P9WNM7
B	704	GLY	-	expression tag	UNP P9WNM7
B	705	HIS	-	expression tag	UNP P9WNM7
B	706	HIS	-	expression tag	UNP P9WNM7
B	707	HIS	-	expression tag	UNP P9WNM7
B	708	HIS	-	expression tag	UNP P9WNM7
B	709	HIS	-	expression tag	UNP P9WNM7
B	710	HIS	-	expression tag	UNP P9WNM7

- Molecule 2 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>11</sub>P<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).

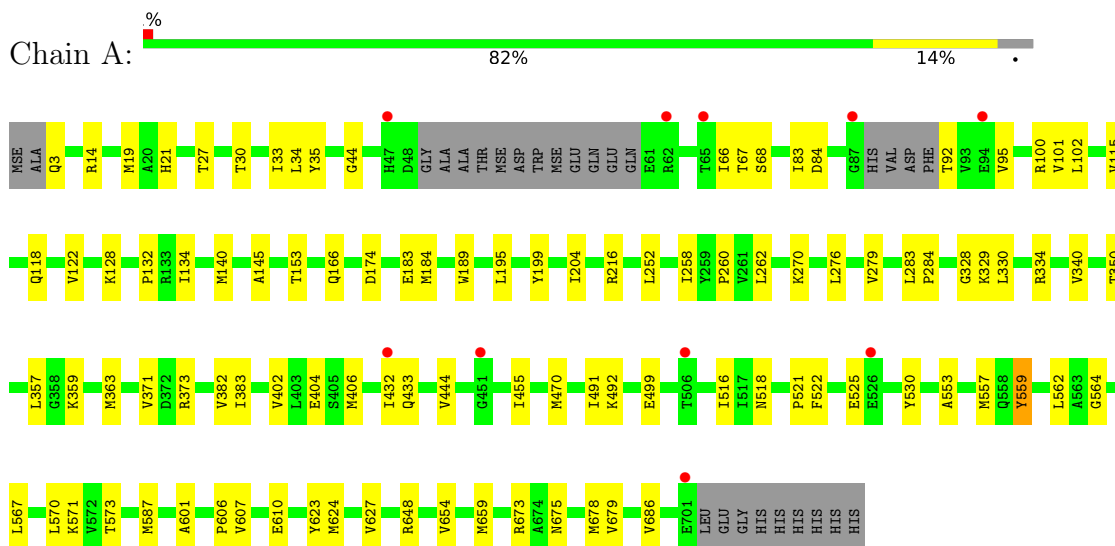


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	H	N	O			P
2	A	1	Total	C	H	N	O	P	0	0
			38	10	10	5	11	2		
2	B	1	Total	C	H	N	O	P	0	0
			38	10	10	5	11	2		

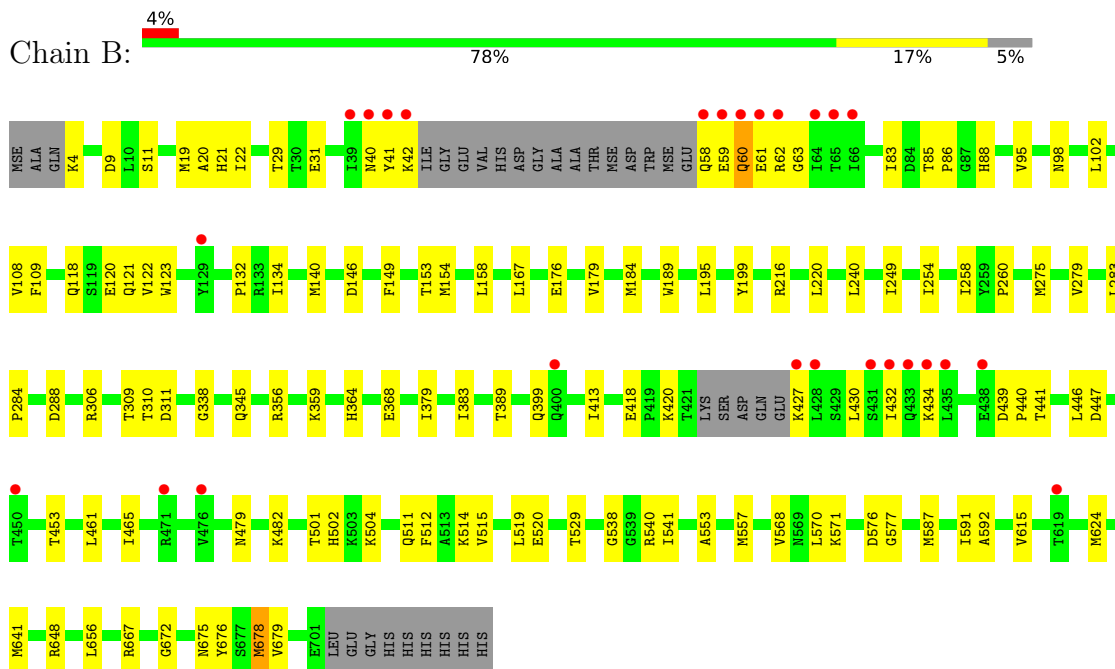
### 3 Residue-property plots [i](#)

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: Elongation factor G



#### • Molecule 1: Elongation factor G



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	101.54Å 301.52Å 145.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.95 – 3.00 47.95 – 3.00	Depositor EDS
% Data completeness (in resolution range)	96.7 (47.95-3.00) 89.8 (47.95-3.00)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.80 (at 3.01Å)	Xtrriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, $R_{free}$	0.206 , 0.241 0.211 , 0.240	Depositor DCC
$R_{free}$ test set	1958 reflections (4.46%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	55.8	Xtrriage
Anisotropy	0.621	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 39.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	20963	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	75.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.53% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: 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	0.27	2/5361 (0.0%)	0.60	6/7232 (0.1%)
1	B	0.25	1/5329 (0.0%)	0.50	3/7190 (0.0%)
All	All	0.26	3/10690 (0.0%)	0.55	9/14422 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	27	THR	C-N	7.15	1.43	1.34
1	A	340	VAL	C-O	-5.82	1.18	1.23
1	B	679	VAL	C-O	-5.03	1.19	1.24

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	559	TYR	N-CA-C	29.92	143.98	111.36
1	A	340	VAL	CA-C-O	-6.33	114.58	121.28
1	A	27	THR	O-C-N	5.68	127.92	122.07
1	B	420	LYS	CB-CA-C	-5.44	110.32	116.63
1	B	447	ASP	N-CA-C	-5.33	106.77	113.28
1	A	559	TYR	CB-CA-C	-5.30	101.83	110.85
1	A	678	MSE	CG-SE-CE	5.24	110.45	98.92
1	B	140	MSE	CG-SE-CE	5.23	110.44	98.92
1	A	679	VAL	CA-C-O	-5.19	116.22	121.67

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	5285	5208	5269	67	3
1	B	5252	5142	5236	81	4
2	A	28	10	12	0	0
2	B	28	10	12	0	0
All	All	10593	10370	10529	142	5

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 (142) 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:557:MSE:HE3	1:A:570:LEU:HD12	1.32	1.06
1:B:19:MSE:HE3	1:B:122:VAL:HB	1.50	0.92
1:B:624:MSE:HE3	1:B:641:MSE:SE	2.24	0.88
1:B:624:MSE:HE1	1:B:641:MSE:HE1	1.60	0.83
1:B:60:GLN:O	1:B:61:GLU:HG3	1.78	0.82
1:B:427:LYS:HA	1:B:430:LEU:HD23	1.60	0.81
1:B:309:THR:HG22	1:B:311:ASP:H	1.50	0.73
1:B:624:MSE:CE	1:B:641:MSE:SE	2.87	0.73
1:A:330:LEU:HD21	1:A:363:MSE:HE3	1.75	0.68
1:A:14:ARG:HG3	1:A:14:ARG:HH11	1.57	0.68
1:A:553:ALA:O	1:A:557:MSE:HG3	1.94	0.67
1:B:62:ARG:HG2	1:B:63:GLY:N	2.10	0.66
1:B:413:ILE:HG12	1:B:656:LEU:HD21	1.77	0.65
1:B:624:MSE:HE1	1:B:641:MSE:CE	2.26	0.64
1:A:68:SER:HA	1:B:61:GLU:OE2	1.97	0.64
1:A:610:GLU:HB2	1:A:686:VAL:HG22	1.81	0.63
1:A:140:MSE:HE2	1:A:145:ALA:HB1	1.81	0.63
1:A:432:ILE:HD12	1:A:444:VAL:HG21	1.81	0.63
1:B:667:ARG:HG3	1:B:672:GLY:HA2	1.80	0.63
1:A:329:LYS:N	1:B:31:GLU:OE2	2.31	0.62
1:A:522:PHE:HB2	1:A:571:LYS:HB2	1.80	0.62
1:B:146:ASP:HB3	1:B:149:PHE:HB3	1.81	0.61
1:B:345:GLN:HG3	1:B:356:ARG:HG2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:654:VAL:HG11	1:A:659:MSE:HE3	1.84	0.59
1:B:184:MSE:SE	1:B:216:ARG:HD3	2.53	0.59
1:A:101:VAL:HG13	1:A:334:ARG:HB2	1.85	0.58
1:B:359:LYS:HB2	1:B:383:ILE:HG13	1.85	0.58
1:B:19:MSE:HE1	1:B:123:TRP:N	2.19	0.58
1:B:519:LEU:HD11	1:B:570:LEU:HD23	1.88	0.56
1:A:623:TYR:O	1:A:627:VAL:HG23	2.04	0.56
1:A:67:THR:O	1:B:61:GLU:CD	2.50	0.55
1:A:3:GLN:HG3	1:A:371:VAL:HB	1.89	0.55
1:B:220:LEU:HD22	1:B:240:LEU:HD12	1.90	0.54
1:A:132:PRO:HG2	1:A:284:PRO:HG3	1.89	0.54
1:B:389:THR:HG21	1:B:440:PRO:HD3	1.90	0.53
1:A:33:ILE:HG23	1:A:276:LEU:HD21	1.90	0.53
1:B:249:ILE:HG23	1:B:258:ILE:HD11	1.90	0.53
1:A:624:MSE:HE1	1:A:648:ARG:NH1	2.24	0.53
1:A:557:MSE:HE3	1:A:570:LEU:CD1	2.22	0.53
1:B:41:TYR:O	1:B:42:LYS:C	2.52	0.53
1:A:499:GLU:HB2	1:A:516:ILE:HG12	1.91	0.52
1:A:559:TYR:O	1:A:564:GLY:HA2	2.10	0.52
1:A:567:LEU:HB3	1:A:570:LEU:HD11	1.92	0.52
1:A:189:TRP:CE2	1:A:199:TYR:HB3	2.45	0.52
1:B:19:MSE:CE	1:B:122:VAL:HB	2.31	0.51
1:A:562:LEU:HG	1:A:606:PRO:HB2	1.93	0.51
1:A:184:MSE:SE	1:A:216:ARG:HD3	2.60	0.51
1:A:491:ILE:HG13	1:A:521:PRO:HG3	1.92	0.51
1:B:624:MSE:SE	1:B:648:ARG:HD3	2.62	0.50
1:B:501:THR:HG23	1:B:514:LYS:HB2	1.94	0.49
1:A:128:LYS:HG3	1:A:675:ASN:HD21	1.77	0.49
1:A:83:ILE:HD12	1:A:102:LEU:HD23	1.93	0.49
1:A:328:GLY:HA2	1:B:195:LEU:HD11	1.94	0.49
1:B:615:VAL:HG22	1:B:678:MSE:HG3	1.94	0.49
1:A:30:THR:HG22	1:A:66:ILE:HG21	1.95	0.49
1:B:254:ILE:HD13	1:B:288:ASP:HB3	1.94	0.49
1:B:504:LYS:HD2	1:B:511:GLN:HE21	1.77	0.49
1:B:553:ALA:O	1:B:557:MSE:HG3	2.12	0.49
1:A:455:ILE:HD13	1:A:470:MSE:HE1	1.95	0.49
1:B:62:ARG:HG2	1:B:63:GLY:H	1.77	0.49
1:A:350:THR:O	1:A:406:MSE:HE3	2.13	0.48
1:B:62:ARG:CG	1:B:63:GLY:N	2.76	0.48
1:B:434:LYS:HA	1:B:434:LYS:HE2	1.94	0.48
1:A:184:MSE:HE3	1:A:204:ILE:CD1	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:189:TRP:CE2	1:B:199:TYR:HB3	2.49	0.48
1:A:189:TRP:HB2	1:A:270:LYS:HG2	1.95	0.47
1:B:29:THR:CG2	1:B:275:MSE:HE1	2.44	0.47
1:B:541:ILE:HD11	1:B:577:GLY:HA3	1.96	0.47
1:A:357:LEU:HD22	1:A:382:VAL:HG11	1.95	0.47
1:A:166:GLN:HG2	1:A:262:LEU:HA	1.97	0.47
1:B:515:VAL:HG22	1:B:592:ALA:HB1	1.96	0.47
1:A:14:ARG:HG3	1:A:14:ARG:NH1	2.25	0.46
1:B:482:LYS:HA	1:B:482:LYS:HD3	1.73	0.46
1:A:433:GLN:NE2	1:B:368:GLU:OE2	2.49	0.46
1:B:29:THR:HG23	1:B:275:MSE:HE1	1.98	0.46
1:B:85:THR:HG23	1:B:86:PRO:HD2	1.97	0.46
1:A:279:VAL:HG13	1:A:283:LEU:HD12	1.98	0.46
1:B:120:GLU:HA	1:B:158:LEU:HD21	1.97	0.46
1:B:86:PRO:HG3	1:B:95:VAL:HA	1.98	0.46
1:B:432:ILE:HG23	1:B:434:LYS:HG3	1.97	0.45
1:B:83:ILE:HB	1:B:102:LEU:HD21	1.98	0.45
1:A:100:ARG:HH12	1:A:404:GLU:HG2	1.82	0.45
1:A:623:TYR:CE2	1:A:673:ARG:HG3	2.51	0.45
1:A:92:THR:HG23	1:A:95:VAL:H	1.82	0.45
1:A:559:TYR:O	1:A:564:GLY:C	2.60	0.45
1:A:19:MSE:O	1:A:19:MSE:HG3	2.16	0.45
1:B:9:ASP:OD1	1:B:11:SER:OG	2.31	0.45
1:A:359:LYS:HB2	1:A:383:ILE:HG13	1.99	0.45
1:B:88:HIS:CE1	1:B:465:ILE:HD12	2.52	0.45
1:B:109:PHE:CD2	1:B:154:MSE:HE2	2.51	0.45
1:B:83:ILE:HD11	1:B:379:ILE:CD1	2.47	0.44
1:B:624:MSE:HE1	1:B:641:MSE:SE	2.66	0.44
1:A:66:ILE:HD12	1:A:84:ASP:OD2	2.17	0.44
1:B:4:LYS:HB3	1:B:364:HIS:CE1	2.52	0.44
1:B:21:HIS:HD2	1:B:22:ILE:O	1.98	0.44
1:B:134:ILE:HG22	1:B:260:PRO:HD2	1.99	0.44
1:A:19:MSE:HE3	1:A:122:VAL:CG1	2.47	0.44
1:B:461:LEU:O	1:B:465:ILE:HG12	2.17	0.44
1:A:34:LEU:HD12	1:A:66:ILE:HG22	1.98	0.44
1:A:66:ILE:O	1:A:66:ILE:HG13	2.17	0.44
1:A:252:LEU:HB3	1:A:258:ILE:HG12	1.99	0.44
1:A:530:TYR:CD1	1:A:557:MSE:SE	3.21	0.44
1:A:562:LEU:HD23	1:A:562:LEU:HA	1.85	0.44
1:A:19:MSE:HE3	1:A:122:VAL:HB	2.00	0.43
1:B:86:PRO:HD3	1:B:98:ASN:OD1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:402:VAL:HG11	1:A:406:MSE:HG3	2.00	0.43
1:A:67:THR:O	1:B:61:GLU:OE1	2.36	0.43
1:A:115:VAL:HG22	1:A:153:THR:HB	2.01	0.43
1:B:19:MSE:O	1:B:19:MSE:HG3	2.17	0.43
1:B:306:ARG:NH2	1:B:399:GLN:HB3	2.33	0.43
1:A:21:HIS:ND1	1:A:118:GLN:HB2	2.34	0.43
1:B:21:HIS:ND1	1:B:118:GLN:HB3	2.34	0.43
1:B:149:PHE:O	1:B:153:THR:HG23	2.18	0.43
1:B:283:LEU:HD23	1:B:283:LEU:HA	1.89	0.42
1:B:83:ILE:HD11	1:B:379:ILE:HD13	2.00	0.42
1:B:538:GLY:C	1:B:540:ARG:H	2.27	0.42
1:B:167:LEU:HB2	1:B:179:VAL:HB	2.01	0.42
1:A:134:ILE:HG22	1:A:260:PRO:HD2	2.01	0.42
1:B:279:VAL:O	1:B:283:LEU:HB2	2.20	0.42
1:B:154:MSE:O	1:B:158:LEU:HB2	2.20	0.42
1:B:418:GLU:HG3	1:B:479:ASN:HB2	2.02	0.42
1:A:492:LYS:HE3	1:A:607:VAL:HG21	2.01	0.42
1:B:587:MSE:HE2	1:B:591:ILE:HD11	2.02	0.41
1:B:310:THR:HA	1:B:338:GLY:HA2	2.02	0.41
1:B:439:ASP:HB3	1:B:441:THR:HG23	2.02	0.41
1:B:520:GLU:HG3	1:B:571:LYS:HB3	2.02	0.41
1:A:3:GLN:OE1	1:A:373:ARG:HG2	2.21	0.41
1:A:128:LYS:HG3	1:A:675:ASN:ND2	2.35	0.41
1:A:30:THR:CG2	1:A:66:ILE:HG21	2.51	0.41
1:A:601:ALA:O	1:A:606:PRO:HG3	2.21	0.41
1:B:504:LYS:HB2	1:B:504:LYS:HE3	1.93	0.41
1:A:34:LEU:CD1	1:A:66:ILE:HG22	2.50	0.41
1:B:132:PRO:HG2	1:B:284:PRO:HG3	2.03	0.41
1:B:60:GLN:O	1:B:61:GLU:CG	2.60	0.40
1:B:121:GLN:HA	1:B:675:ASN:HD21	1.86	0.40
1:A:518:ASN:HB3	1:A:573:THR:HB	2.03	0.40
1:B:109:PHE:CE2	1:B:154:MSE:HE2	2.56	0.40
1:B:529:THR:HG23	1:B:568:VAL:HA	2.01	0.40
1:A:35:TYR:CE2	1:A:195:LEU:HG	2.55	0.40
1:B:20:ALA:HB2	1:B:108:VAL:HB	2.02	0.40
1:B:502:HIS:O	1:B:512:PHE:HA	2.22	0.40
1:A:525:GLU:H	1:A:525:GLU:HG3	1.72	0.40

All (5) 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:174:ASP:OD2	1:A:174:ASP:OD2[3_656]	1.30	0.90
1:B:624:MSE:CE	1:B:641:MSE:HE1[3_555]	0.73	0.87
1:B:624:MSE:CE	1:B:641:MSE:CE[3_555]	1.64	0.56
1:A:648:ARG:HH22	1:B:576:ASP:OD2[6_565]	1.46	0.14
1:A:44:GLY:H	1:B:176:GLU:OE1[4_566]	1.54	0.06

## 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	677/710 (95%)	664 (98%)	13 (2%)	0	100	100
1	B	672/710 (95%)	653 (97%)	19 (3%)	0	100	100
All	All	1349/1420 (95%)	1317 (98%)	32 (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	569/572 (100%)	567 (100%)	2 (0%)	84	90
1	B	565/572 (99%)	557 (99%)	8 (1%)	59	80
All	All	1134/1144 (99%)	1124 (99%)	10 (1%)	70	85

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

Mol	Chain	Res	Type
1	A	183	GLU
1	A	587	MSE
1	B	40	ASN
1	B	58	GLN
1	B	59	GLU
1	B	60	GLN
1	B	446	LEU
1	B	453	THR
1	B	676	TYR
1	B	678	MSE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	185	ASN
1	A	433	GLN
1	B	58	GLN
1	B	81	ASN
1	B	166	GLN
1	B	348	ASN
1	B	445	HIS
1	B	496	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 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	GDP	A	801	-	29,30,30	1.22	4 (13%)	45,47,47	1.83	6 (13%)
2	GDP	B	801	-	29,30,30	1.16	3 (10%)	45,47,47	1.83	7 (15%)

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	GDP	A	801	-	-	0/16/32/32	0/3/3/3
2	GDP	B	801	-	-	0/16/32/32	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	GDP	C5-C4	3.03	1.47	1.38
2	B	801	GDP	C5-C4	2.94	1.46	1.38
2	A	801	GDP	PA-O3A	2.59	1.62	1.59
2	A	801	GDP	C6-N1	-2.28	1.34	1.38
2	B	801	GDP	PA-O3A	2.15	1.61	1.59
2	A	801	GDP	C5-N7	-2.14	1.34	1.39
2	B	801	GDP	C6-N1	-2.12	1.34	1.38

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	GDP	C5-C4-N3	-5.99	118.86	128.39
2	B	801	GDP	C2-N3-C4	5.32	121.46	112.30
2	A	801	GDP	C2-N3-C4	5.30	121.42	112.30
2	B	801	GDP	C5-C4-N3	-5.24	120.05	128.39
2	A	801	GDP	N9-C4-N3	4.46	134.86	125.95
2	B	801	GDP	C6-C5-N7	4.20	137.94	130.29
2	B	801	GDP	N9-C4-N3	3.67	133.30	125.95
2	A	801	GDP	C6-C5-N7	3.40	136.47	130.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	GDP	C4-C5-N7	-2.72	106.36	110.67
2	A	801	GDP	C4-C5-N7	-2.58	106.59	110.67
2	A	801	GDP	O6-C6-C5	-2.31	120.45	126.53
2	B	801	GDP	O6-C6-C5	-2.21	120.69	126.53
2	B	801	GDP	C6-C5-C4	-2.08	115.71	118.83

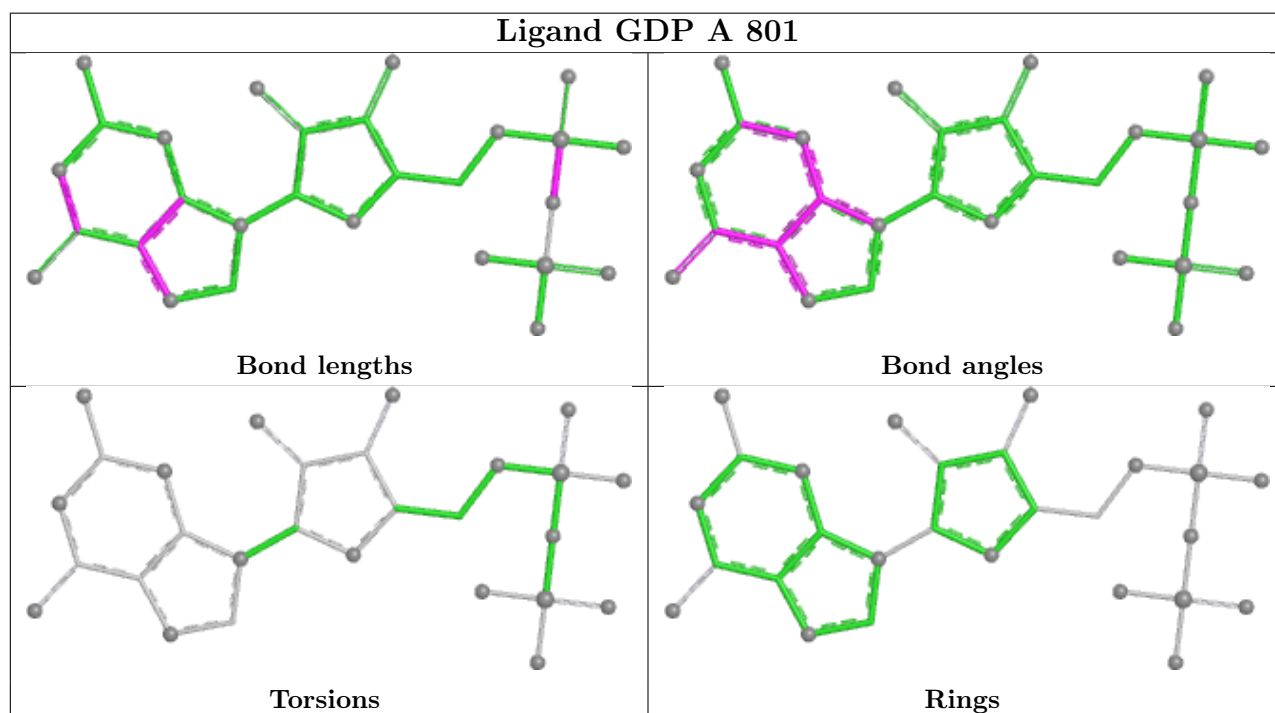
There are no chirality outliers.

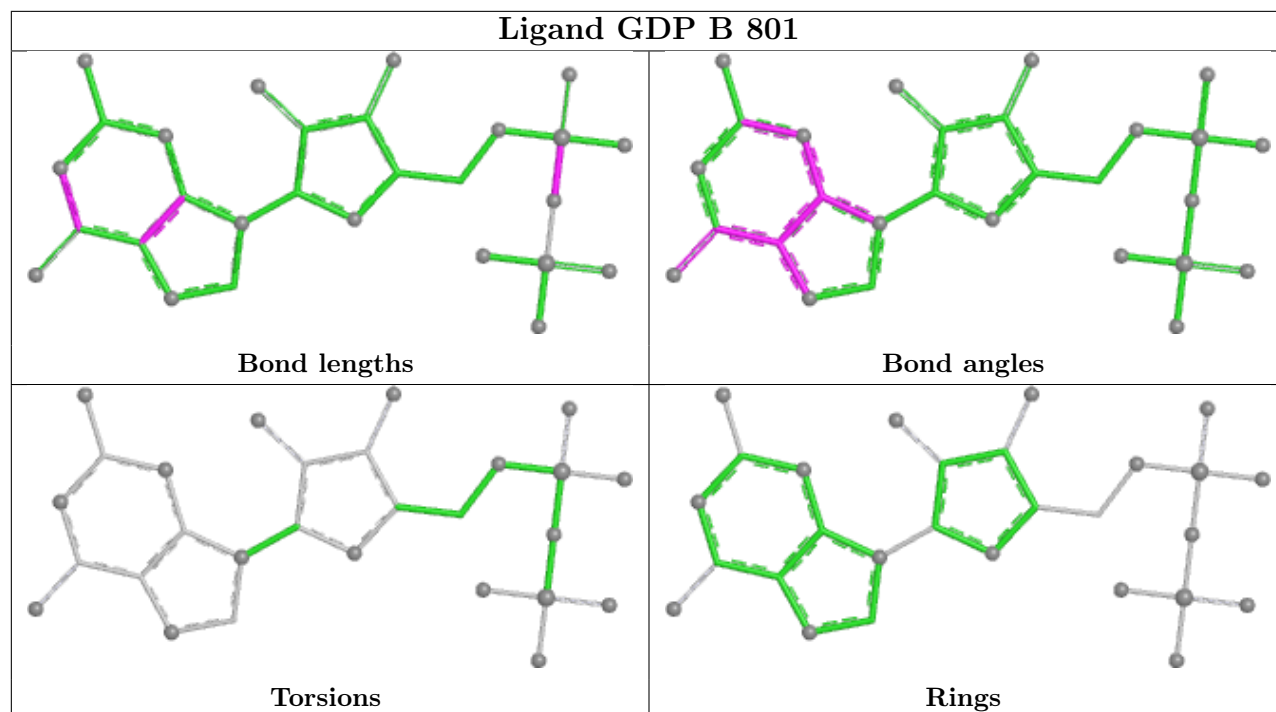
There are no torsion outliers.

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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	667/710 (93%)	0.05	10 (1%) 72 49	42, 68, 116, 153	0
1	B	662/710 (93%)	0.17	26 (3%) 43 24	42, 71, 129, 161	0
All	All	1329/1420 (93%)	0.11	36 (2%) 56 33	42, 69, 123, 161	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	87	GLY	5.4
1	B	39	ILE	4.2
1	B	59	GLU	3.9
1	B	60	GLN	3.6
1	B	61	GLU	3.5
1	B	435	LEU	3.2
1	B	64	ILE	3.1
1	B	427	LYS	3.0
1	B	431	SER	3.0
1	B	42	LYS	3.0
1	B	434	LYS	2.8
1	B	41	TYR	2.8
1	B	476	VAL	2.7
1	B	428	LEU	2.6
1	B	400	GLN	2.5
1	A	526	GLU	2.5
1	B	432	ILE	2.5
1	B	65	THR	2.5
1	B	471	ARG	2.5
1	B	450	THR	2.4
1	A	432	ILE	2.4
1	A	65	THR	2.3
1	A	62	ARG	2.3
1	B	438	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	40	ASN	2.2
1	B	58	GLN	2.2
1	B	62	ARG	2.2
1	A	94	GLU	2.1
1	A	701	GLU	2.1
1	A	47	HIS	2.1
1	A	506	THR	2.1
1	B	66	ILE	2.1
1	B	129	TYR	2.1
1	B	433	GLN	2.1
1	A	451	GLY	2.0
1	B	619	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](#)

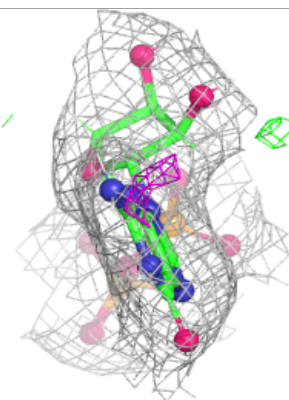
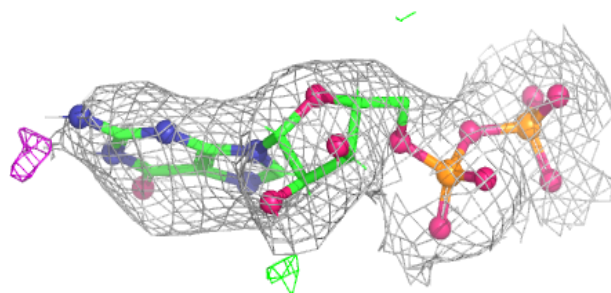
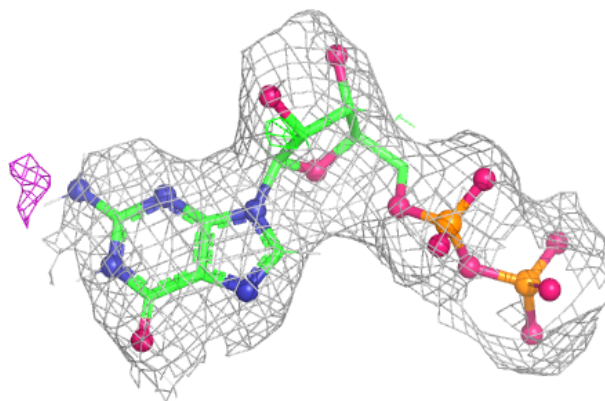
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	GDP	A	801	28/28	0.96	0.08	39,63,89,95	0
2	GDP	B	801	28/28	0.97	0.07	37,45,59,68	0

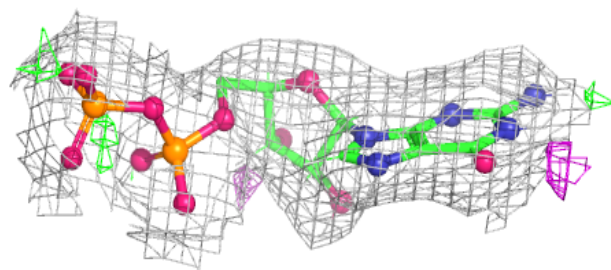
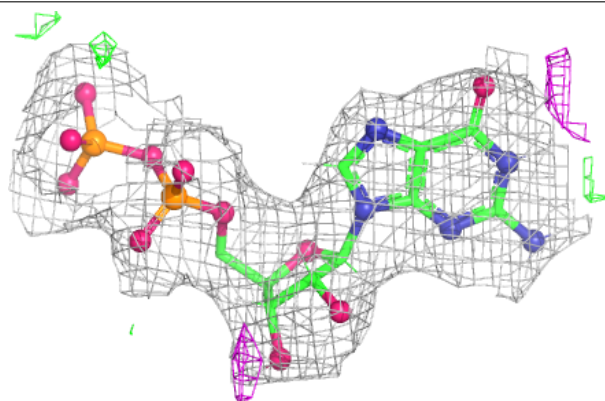
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around GDP A 801:**

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

**Electron density around GDP B 801:**

$2mF_o-DF_c$  (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.