



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:39 AM UTC

PDB ID : 9N2T / pdb_00009n2t
Title : Structure of GDP-bound GM4951_D125G mutant
Authors : Raj, R.; Beutler, B.
Deposited on : 2025-01-29
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

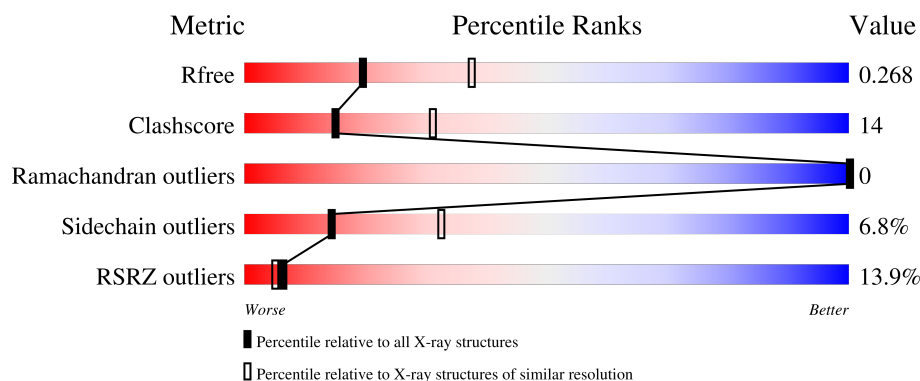
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	416	10% 67% 26% • 5%
1	B	416	16% 60% 31% • 7%
1	C	416	14% 68% 22% • 7%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9390 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 Interferon inducible GTPase 1C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	388	Total	C	N	O	S	0	0	0
			3095	1988	518	573	16			
1	A	395	Total	C	N	O	S	0	0	0
			3120	1994	520	591	15			
1	C	388	Total	C	N	O	S	0	0	0
			3078	1979	517	566	16			

There are 33 discrepancies between the modelled and reference sequences:

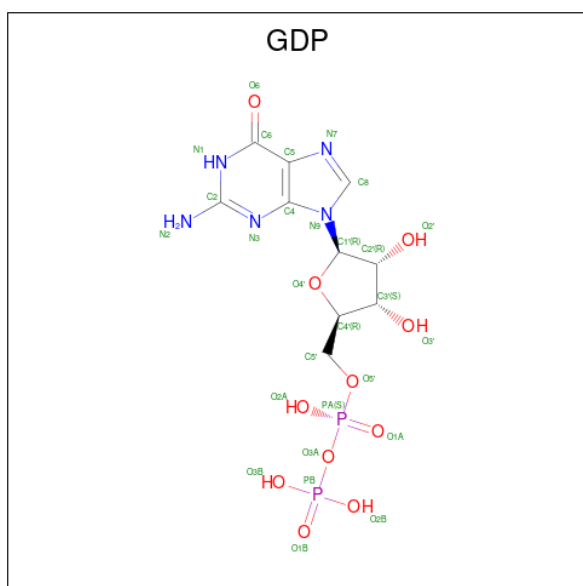
Chain	Residue	Modelled	Actual	Comment	Reference
B	-9	HIS	-	expression tag	UNP Q3UED7
B	-8	HIS	-	expression tag	UNP Q3UED7
B	-7	HIS	-	expression tag	UNP Q3UED7
B	-6	HIS	-	expression tag	UNP Q3UED7
B	-5	HIS	-	expression tag	UNP Q3UED7
B	-4	HIS	-	expression tag	UNP Q3UED7
B	-3	SER	-	expression tag	UNP Q3UED7
B	-2	GLN	-	expression tag	UNP Q3UED7
B	-1	ASP	-	expression tag	UNP Q3UED7
B	0	PRO	-	expression tag	UNP Q3UED7
B	125	GLY	ASP	engineered mutation	UNP Q3UED7
A	-9	HIS	-	expression tag	UNP Q3UED7
A	-8	HIS	-	expression tag	UNP Q3UED7
A	-7	HIS	-	expression tag	UNP Q3UED7
A	-6	HIS	-	expression tag	UNP Q3UED7
A	-5	HIS	-	expression tag	UNP Q3UED7
A	-4	HIS	-	expression tag	UNP Q3UED7
A	-3	SER	-	expression tag	UNP Q3UED7
A	-2	GLN	-	expression tag	UNP Q3UED7
A	-1	ASP	-	expression tag	UNP Q3UED7
A	0	PRO	-	expression tag	UNP Q3UED7
A	125	GLY	ASP	engineered mutation	UNP Q3UED7
C	-9	HIS	-	expression tag	UNP Q3UED7

Continued on next page...

Continued from previous page...

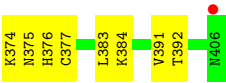
Chain	Residue	Modelled	Actual	Comment	Reference
C	-8	HIS	-	expression tag	UNP Q3UED7
C	-7	HIS	-	expression tag	UNP Q3UED7
C	-6	HIS	-	expression tag	UNP Q3UED7
C	-5	HIS	-	expression tag	UNP Q3UED7
C	-4	HIS	-	expression tag	UNP Q3UED7
C	-3	SER	-	expression tag	UNP Q3UED7
C	-2	GLN	-	expression tag	UNP Q3UED7
C	-1	ASP	-	expression tag	UNP Q3UED7
C	0	PRO	-	expression tag	UNP Q3UED7
C	125	GLY	ASP	engineered mutation	UNP Q3UED7

- 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).

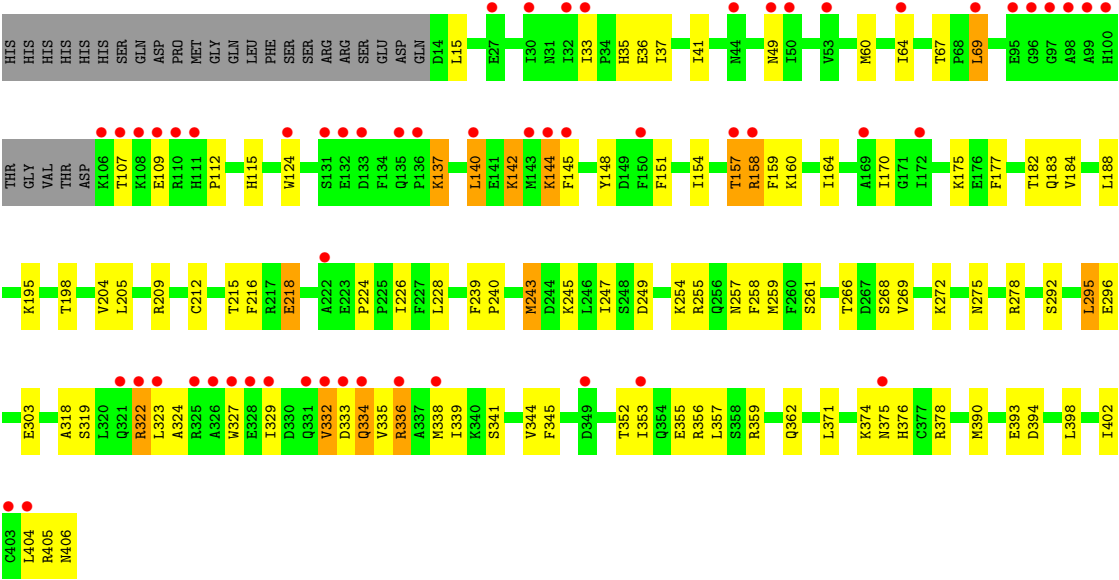


Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	7	Total	O	0	0
			7	7		
3	C	2	Total	O	0	0
			2	2		



● Molecule 1: Interferon inducible GTPase 1C



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	297.82Å 58.91Å 100.68Å 90.00° 92.03° 90.00°	Depositor
Resolution (Å)	50.01 – 2.60 50.01 – 2.60	Depositor EDS
% Data completeness (in resolution range)	71.0 (50.01-2.60) 71.0 (50.01-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.11 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0349	Depositor
R, R_{free}	0.233 , 0.267 0.230 , 0.268	Depositor DCC
R_{free} test set	1860 reflections (3.43%)	wwPDB-VP
Wilson B-factor (Å ²)	41.3	Xtriage
Anisotropy	0.157	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 41.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.005 for -h,-k,l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	9390	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.05% 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 [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	0.59	2/3185 (0.1%)	0.91	2/4314 (0.0%)
1	B	0.58	2/3162 (0.1%)	0.88	0/4275
1	C	0.56	1/3144 (0.0%)	0.85	0/4253
All	All	0.58	5/9491 (0.1%)	0.88	2/12842 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	35	HIS	CE1-NE2	6.47	1.39	1.32
1	A	35	HIS	CE1-NE2	6.26	1.38	1.32
1	C	376	HIS	CE1-NE2	6.15	1.38	1.32
1	A	376	HIS	CE1-NE2	5.63	1.38	1.32
1	B	376	HIS	CE1-NE2	5.41	1.38	1.32

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	138	THR	N-CA-C	-7.14	104.19	113.12
1	A	98	ALA	N-CA-C	6.19	118.70	110.53

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	3120	0	3012	83	0
1	B	3095	0	3011	101	0
1	C	3078	0	3000	75	0
2	A	28	0	12	5	0
2	B	28	0	12	6	0
2	C	28	0	12	1	0
3	A	7	0	0	0	0
3	B	4	0	0	0	0
3	C	2	0	0	0	0
All	All	9390	0	9059	252	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 14.

All (252) 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:C:341:SER:HA	1:C:390:MET:HE1	1.47	0.96
1:A:96:GLY:HA3	1:A:113:TYR:HE2	1.37	0.88
1:B:127:PRO:HD2	1:B:143:MET:HE3	1.56	0.88
1:B:277:LEU:O	1:B:281:THR:HG23	1.78	0.84
1:B:348:THR:HG22	1:B:350:GLU:H	1.41	0.83
1:B:69:LEU:HD22	1:B:258:PHE:HB2	1.61	0.82
1:C:341:SER:HA	1:C:390:MET:CE	2.09	0.81
1:B:237:TYR:HA	1:A:101:THR:HG21	1.64	0.79
1:A:134:PHE:CE2	1:A:136:PRO:HD3	2.19	0.77
1:B:145:PHE:HE1	1:B:170:ILE:HG12	1.51	0.76
1:C:335:VAL:HA	1:C:338:MET:SD	2.26	0.76
1:C:266:THR:HG22	1:C:268:SER:H	1.50	0.76
1:C:160:LYS:O	1:C:164:ILE:HD12	1.87	0.75
1:B:67:THR:HG21	1:B:254:LYS:HG3	1.68	0.73
1:C:140:LEU:HD11	1:C:170:ILE:HG12	1.70	0.73
1:B:183:GLN:HG2	2:B:501:GDP:C5	2.24	0.73
1:C:37:ILE:O	1:C:41:ILE:HG12	1.90	0.72
1:C:212:CYS:HB3	1:C:226:ILE:HD13	1.71	0.72
1:A:375:ASN:HD22	1:A:377:CYS:HB3	1.56	0.71
1:C:159:PHE:O	1:C:215:THR:HG21	1.90	0.70
1:C:359:ARG:HA	1:C:362:GLN:HE21	1.57	0.70
1:C:332:VAL:HB	1:C:336:ARG:NH1	2.06	0.70
1:C:324:ALA:HB2	1:C:332:VAL:HG13	1.72	0.69
1:C:332:VAL:HB	1:C:336:ARG:HH12	1.58	0.67
1:B:338:MET:HE1	1:B:401:GLU:HG3	1.75	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:154:ILE:HD11	1:C:182:THR:HG21	1.77	0.67
1:B:140:LEU:HD22	1:B:145:PHE:HD1	1.60	0.67
1:A:213:VAL:HG21	1:C:371:LEU:HD22	1.76	0.66
1:B:348:THR:HG22	1:B:349:ASP:N	2.11	0.66
1:A:145:PHE:HE1	1:A:175:LYS:HG3	1.61	0.65
1:B:243:MET:HE1	1:B:265:ILE:HG13	1.79	0.65
1:B:145:PHE:CE2	1:B:175:LYS:HG3	2.32	0.65
1:B:266:THR:HG22	1:B:268:SER:H	1.62	0.64
1:A:87:THR:HG21	1:A:234:VAL:HG11	1.80	0.64
1:B:74:THR:HG22	1:B:126:LEU:HB2	1.79	0.63
1:C:319:SER:HA	1:C:322:ARG:HD2	1.78	0.63
1:C:359:ARG:HA	1:C:362:GLN:NE2	2.14	0.62
1:C:353:ILE:O	1:C:357:LEU:HG	1.98	0.62
1:C:398:LEU:O	1:C:402:ILE:HD12	2.00	0.61
1:A:292:SER:HA	1:A:295:LEU:HD22	1.82	0.61
1:B:242:LEU:O	1:B:246:LEU:HD13	2.00	0.61
1:B:183:GLN:HG2	2:B:501:GDP:C6	2.36	0.61
1:A:104:THR:O	1:A:108:LYS:HB2	2.00	0.60
1:A:96:GLY:HA3	1:A:113:TYR:CE2	2.29	0.60
1:C:205:LEU:O	1:C:209:ARG:HG3	2.01	0.60
1:B:353:ILE:O	1:B:357:LEU:HG	2.02	0.60
1:B:375:ASN:HD22	1:B:378:ARG:H	1.48	0.60
1:C:183:GLN:HG2	2:C:501:GDP:C5	2.37	0.60
1:B:69:LEU:CD2	1:B:258:PHE:HB2	2.31	0.59
1:A:205:LEU:O	1:A:209:ARG:HG3	2.02	0.59
1:C:184:VAL:HG21	1:C:228:LEU:HB3	1.85	0.59
1:B:332:VAL:O	1:B:335:VAL:HG22	2.02	0.59
1:C:67:THR:HB	1:C:257:ASN:OD1	2.02	0.59
1:B:348:THR:HG22	1:B:349:ASP:H	1.67	0.58
1:C:353:ILE:HD12	1:C:356:ARG:HE	1.68	0.58
1:C:35:HIS:CE1	1:C:36:GLU:HG3	2.38	0.58
1:B:241:VAL:HG13	1:A:97:GLY:O	2.03	0.58
1:B:259:MET:HA	1:B:262:LEU:HD21	1.86	0.58
1:A:20:ILE:HG22	1:A:24:LYS:HE3	1.84	0.58
1:B:127:PRO:CD	1:B:143:MET:HE3	2.32	0.58
1:A:164:ILE:HG12	1:A:216:PHE:CE1	2.39	0.57
1:B:134:PHE:CE2	1:B:162:ASN:HB3	2.39	0.57
1:C:151:PHE:CG	1:C:170:ILE:HD13	2.40	0.57
1:B:164:ILE:HD12	1:B:216:PHE:CE1	2.40	0.57
1:B:236:HIS:CE1	1:B:406:ASN:HD22	2.23	0.57
1:C:15:LEU:HD21	1:C:41:ILE:CD1	2.35	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:THR:HG22	1:A:268:SER:H	1.70	0.56
1:B:115:HIS:CD2	1:B:261:SER:HB2	2.41	0.56
1:A:89:ARG:HB3	1:A:91:ILE:HG13	1.86	0.56
1:A:145:PHE:CE1	1:A:175:LYS:HG3	2.40	0.56
1:A:148:TYR:O	1:A:175:LYS:HE3	2.05	0.56
1:A:291:LEU:O	1:A:295:LEU:HD13	2.06	0.56
1:B:31:ASN:HB2	1:A:325:ARG:HH22	1.71	0.56
1:A:96:GLY:CA	1:A:113:TYR:HE2	2.14	0.56
1:C:145:PHE:CE1	1:C:175:LYS:HG3	2.41	0.56
1:C:195:LYS:HB3	1:C:198:THR:CG2	2.36	0.56
1:B:145:PHE:CE1	1:B:170:ILE:HG12	2.37	0.56
1:C:212:CYS:CB	1:C:226:ILE:HD13	2.36	0.55
1:B:303:GLU:HG2	1:B:307:LYS:HE2	1.89	0.55
1:B:184:VAL:HG21	1:B:228:LEU:HB3	1.89	0.55
1:B:320:LEU:HD13	1:B:336:ARG:HG2	1.87	0.54
1:B:57:VAL:CG1	1:B:287:ALA:HB2	2.38	0.54
1:C:140:LEU:HD13	1:C:145:PHE:CD1	2.43	0.54
1:A:134:PHE:HB3	1:A:162:ASN:HD22	1.73	0.54
1:A:164:ILE:CD1	1:A:215:THR:HG22	2.37	0.54
1:B:327:TRP:CD1	1:B:405:ARG:HD3	2.43	0.54
1:A:66:ASN:HA	1:A:120:ASN:ND2	2.24	0.53
1:B:146:TYR:HA	1:B:175:LYS:HZ1	1.73	0.53
1:B:371:LEU:HB3	1:B:374:LYS:NZ	2.22	0.53
1:A:72:ALA:HB2	1:A:148:TYR:CD2	2.44	0.53
1:C:334:GLN:O	1:C:338:MET:HG3	2.09	0.53
1:B:80:GLY:N	2:B:501:GDP:O1A	2.41	0.53
1:C:341:SER:CA	1:C:390:MET:CE	2.84	0.53
1:B:323:LEU:HD22	1:B:327:TRP:CZ2	2.43	0.52
1:C:327:TRP:CD1	1:C:405:ARG:HD3	2.45	0.52
1:C:352:THR:HG22	1:C:355:GLU:CD	2.34	0.52
1:B:216:PHE:HB3	1:B:221:ILE:O	2.09	0.52
1:C:69:LEU:HD21	1:C:258:PHE:HB2	1.90	0.52
1:B:266:THR:HB	1:B:269:VAL:HG22	1.92	0.51
1:C:148:TYR:O	1:C:175:LYS:HE2	2.09	0.51
1:B:146:TYR:HA	1:B:175:LYS:NZ	2.25	0.51
1:B:348:THR:HG21	1:B:350:GLU:HG2	1.92	0.51
1:B:129:THR:HB	1:B:134:PHE:CE2	2.45	0.51
1:B:371:LEU:HB3	1:B:374:LYS:HZ3	1.76	0.51
1:B:151:PHE:CG	1:B:170:ILE:HD13	2.46	0.51
1:B:399:LEU:HD23	1:B:399:LEU:C	2.36	0.50
1:A:152:ILE:HG22	1:A:154:ILE:HG13	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:310:ARG:NH2	1:B:342:PRO:HB3	2.26	0.50
1:B:145:PHE:CZ	1:B:175:LYS:HG3	2.46	0.49
1:B:264:ASN:OD1	1:B:273:LYS:HE3	2.12	0.49
1:A:18:SER:HB3	1:A:37:ILE:HG12	1.93	0.49
1:B:112:PRO:HB3	1:B:124:TRP:CZ3	2.47	0.49
1:A:213:VAL:HG21	1:C:371:LEU:CD2	2.42	0.49
1:B:124:TRP:CD1	1:B:148:TYR:HE1	2.31	0.49
1:B:241:VAL:CG1	1:A:97:GLY:O	2.60	0.49
1:B:348:THR:CG2	1:B:349:ASP:N	2.74	0.49
1:B:268:SER:O	1:B:272:LYS:HG3	2.13	0.49
1:A:252:VAL:O	1:A:256:GLN:OE1	2.31	0.49
1:B:348:THR:CG2	1:B:349:ASP:H	2.25	0.48
1:A:184:VAL:HG21	1:A:228:LEU:HB3	1.95	0.48
1:B:25:GLU:OE2	1:B:28:LYS:HE2	2.13	0.48
1:B:57:VAL:HG11	1:B:287:ALA:HB2	1.95	0.48
1:A:170:ILE:HD13	1:A:170:ILE:HA	1.73	0.48
1:C:15:LEU:HD11	1:C:41:ILE:HD11	1.95	0.48
1:B:167:ALA:HB2	1:B:179:PHE:CZ	2.48	0.48
1:A:309:TYR:HB3	1:A:391:VAL:HG21	1.95	0.48
1:B:63:GLU:CG	1:B:253:PHE:HD2	2.27	0.48
1:C:303:GLU:HA	1:C:345:PHE:CZ	2.48	0.48
1:B:137:LYS:HA	1:B:137:LYS:HD3	1.58	0.48
1:C:239:PHE:HB3	1:C:240:PRO:HD3	1.95	0.48
1:B:288:ASP:HB3	1:B:295:LEU:HD11	1.95	0.48
1:B:80:GLY:HA2	2:B:501:GDP:O1A	2.13	0.48
1:A:80:GLY:HA2	2:A:501:GDP:C8	2.49	0.48
1:C:151:PHE:O	1:C:177:PHE:HA	2.14	0.47
1:B:147:GLU:HG2	1:B:147:GLU:O	2.14	0.47
1:C:216:PHE:CE2	1:C:224:PRO:HG3	2.48	0.47
1:C:247:ILE:HG23	1:C:255:ARG:HG3	1.96	0.47
1:B:405:ARG:O	1:B:406:ASN:C	2.58	0.47
1:B:64:ILE:HD11	1:B:279:TRP:HH2	1.80	0.47
1:B:210:LEU:HD12	1:B:213:VAL:HB	1.97	0.47
1:B:82:SER:HB3	1:B:99:ALA:O	2.15	0.47
1:A:164:ILE:HD13	1:A:216:PHE:HA	1.96	0.47
1:A:188:LEU:HD12	1:A:188:LEU:HA	1.74	0.47
1:A:142:LYS:HB3	1:A:142:LYS:HE2	1.55	0.46
1:A:149:ASP:OD1	1:A:254:LYS:HE2	2.16	0.46
1:B:41:ILE:O	1:B:45:MET:HG2	2.16	0.46
1:A:256:GLN:HG2	1:A:276:PHE:CD1	2.51	0.46
1:B:60:MET:HE3	1:B:60:MET:HB2	1.80	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:LYS:O	1:A:28:LYS:HG3	2.16	0.46
1:A:357:LEU:HD13	1:A:383:LEU:HD13	1.97	0.46
1:B:162:ASN:N	1:B:162:ASN:HD22	2.14	0.46
1:C:137:LYS:H	1:C:137:LYS:HD3	1.81	0.46
1:A:20:ILE:CG2	1:A:24:LYS:HE3	2.46	0.46
1:C:247:ILE:O	1:C:255:ARG:HD3	2.16	0.46
1:B:77:THR:HA	2:B:501:GDP:O1B	2.16	0.46
1:A:265:ILE:HD13	1:A:265:ILE:H	1.81	0.45
1:A:258:PHE:CZ	1:A:262:LEU:HD21	2.51	0.45
1:C:112:PRO:HB3	1:C:124:TRP:CE2	2.51	0.45
1:B:129:THR:HB	1:B:134:PHE:CZ	2.51	0.45
1:B:151:PHE:O	1:B:177:PHE:HA	2.16	0.45
1:A:245:LYS:HE3	1:A:249:ASP:OD2	2.17	0.45
1:A:86:ASN:HB3	1:A:92:GLY:HA2	1.97	0.45
1:C:188:LEU:HD23	1:C:204:VAL:HG11	1.99	0.45
1:A:341:SER:OG	1:A:342:PRO:HD3	2.16	0.45
1:B:110:ARG:HB3	1:B:126:LEU:HD22	1.98	0.45
1:A:80:GLY:HA2	2:A:501:GDP:H8	1.82	0.45
1:A:91:ILE:HD11	1:A:116:PRO:HD3	1.99	0.45
1:C:154:ILE:HD11	1:C:182:THR:CG2	2.45	0.45
1:C:268:SER:O	1:C:272:LYS:HG3	2.16	0.45
1:B:320:LEU:CD1	1:B:336:ARG:HG2	2.47	0.45
1:B:332:VAL:HG22	1:B:336:ARG:HG3	1.98	0.45
1:A:164:ILE:HD11	1:A:215:THR:HG22	1.99	0.45
1:C:115:HIS:CD2	1:C:261:SER:HB2	2.52	0.44
1:C:218:GLU:HA	1:C:218:GLU:OE2	2.17	0.44
1:C:333:ASP:HA	1:C:336:ARG:HG3	1.98	0.44
1:C:393:GLU:OE2	1:C:393:GLU:HA	2.16	0.44
1:A:41:ILE:O	1:A:45:MET:HG3	2.16	0.44
1:A:159:PHE:O	1:A:215:THR:HG21	2.17	0.44
1:A:226:ILE:HD12	1:A:226:ILE:O	2.18	0.44
1:B:70:ASN:OD1	1:B:122:VAL:CG1	2.65	0.44
1:B:225:PRO:HB2	1:B:227:PHE:CE2	2.53	0.44
1:A:134:PHE:HB3	1:A:162:ASN:ND2	2.32	0.44
1:C:359:ARG:O	1:C:362:GLN:HG2	2.16	0.44
1:B:153:ILE:HG22	1:B:159:PHE:CE1	2.53	0.44
1:A:86:ASN:O	1:A:91:ILE:O	2.36	0.44
1:B:180:VAL:CG1	1:B:229:ILE:HG12	2.48	0.44
1:A:323:LEU:HD11	1:A:327:TRP:CZ2	2.53	0.44
1:C:157:THR:OG1	1:C:158:ARG:N	2.51	0.44
1:A:80:GLY:HA2	2:A:501:GDP:O2A	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:GLN:HG2	2:A:501:GDP:C6	2.53	0.44
1:C:145:PHE:CZ	1:C:175:LYS:HG3	2.51	0.44
1:C:275:ASN:HA	1:C:278:ARG:HD2	2.00	0.44
1:C:243:MET:HE3	1:C:269:VAL:HG21	2.00	0.43
1:B:140:LEU:HG	1:B:166:LEU:HD21	1.99	0.43
1:A:371:LEU:HD23	1:A:371:LEU:HA	1.87	0.43
1:C:318:ALA:HB1	1:C:322:ARG:NH2	2.33	0.43
1:A:268:SER:O	1:A:272:LYS:HG3	2.18	0.43
1:C:137:LYS:H	1:C:137:LYS:CD	2.31	0.43
1:B:167:ALA:HB2	1:B:179:PHE:HZ	1.83	0.43
1:C:259:MET:HE2	1:C:272:LYS:HB3	2.00	0.43
1:A:331:GLN:HG3	1:A:333:ASP:HB2	2.00	0.43
1:C:341:SER:CA	1:C:390:MET:HE3	2.48	0.43
1:A:183:GLN:HG2	2:A:501:GDP:C5	2.53	0.43
1:B:17:SER:O	1:B:21:GLU:HG3	2.19	0.43
1:A:320:LEU:HD11	1:A:339:ILE:HD11	2.00	0.43
1:C:124:TRP:CZ3	1:C:144:LYS:HE3	2.54	0.43
1:A:34:PRO:O	1:A:38:ILE:HG13	2.19	0.43
1:A:87:THR:CG2	1:A:234:VAL:HG11	2.49	0.43
1:A:89:ARG:NH1	1:A:113:TYR:HB3	2.34	0.43
1:A:270:ILE:HG22	1:A:392:THR:HG23	2.01	0.43
1:C:341:SER:N	1:C:390:MET:HE3	2.34	0.43
1:B:126:LEU:HB3	1:B:139:TYR:OH	2.19	0.42
1:A:58:ARG:CZ	1:A:287:ALA:HB1	2.49	0.42
1:B:86:ASN:ND2	1:B:98:ALA:HB1	2.34	0.42
1:A:19:PHE:HD1	1:A:37:ILE:HD13	1.84	0.42
1:C:292:SER:HA	1:C:295:LEU:HD13	2.02	0.42
1:A:98:ALA:HB2	1:A:111:HIS:CD2	2.54	0.42
1:A:110:ARG:HH22	1:A:147:GLU:CD	2.26	0.42
1:A:279:TRP:CZ2	1:A:283:LEU:HD22	2.55	0.42
1:A:301:THR:HG22	1:A:384:LYS:HE2	2.00	0.42
1:C:60:MET:HE3	1:C:60:MET:HB2	1.71	0.42
1:B:80:GLY:CA	2:B:501:GDP:O1A	2.67	0.42
1:C:109:GLU:OE1	1:C:109:GLU:HA	2.20	0.42
1:B:34:PRO:O	1:B:38:ILE:HG13	2.18	0.42
1:A:226:ILE:HD12	1:A:226:ILE:C	2.45	0.42
1:C:140:LEU:HD11	1:C:170:ILE:CG1	2.47	0.42
1:A:132:GLU:O	1:A:133:ASP:C	2.63	0.41
1:B:30:ILE:HD12	1:A:322:ARG:HD2	2.01	0.41
1:B:188:LEU:HD23	1:B:188:LEU:HA	1.88	0.41
1:A:136:PRO:O	1:A:137:LYS:CB	2.68	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:142:LYS:HE3	1:C:142:LYS:HB2	1.77	0.41
1:B:61:LEU:HD23	1:B:61:LEU:HA	1.91	0.41
1:B:388:LEU:HD23	1:B:388:LEU:HA	1.94	0.41
1:C:245:LYS:HE3	1:C:249:ASP:OD2	2.19	0.41
1:C:405:ARG:O	1:C:406:ASN:C	2.62	0.41
1:A:151:PHE:O	1:A:177:PHE:HA	2.21	0.41
1:C:353:ILE:HD12	1:C:356:ARG:NE	2.35	0.41
1:A:164:ILE:HD12	1:A:215:THR:HG22	2.01	0.41
1:B:129:THR:CG2	1:B:166:LEU:HD12	2.51	0.41
1:B:260:PHE:HZ	1:B:276:PHE:HD2	1.68	0.41
1:B:306:MET:HE2	1:B:344:VAL:HG21	2.03	0.41
1:A:210:LEU:CD1	1:A:214:ASN:HD21	2.34	0.41
1:B:86:ASN:HD21	1:B:98:ALA:HB1	1.86	0.40
1:B:112:PRO:HB3	1:B:124:TRP:CH2	2.57	0.40
1:B:262:LEU:HB2	1:B:263:PRO:HD2	2.02	0.40
1:B:239:PHE:HB3	1:B:240:PRO:HD3	2.02	0.40
1:A:164:ILE:HG12	1:A:216:PHE:CD1	2.57	0.40
1:C:339:ILE:CG2	1:C:394:ASP:HB3	2.51	0.40
1:B:31:ASN:HB3	1:B:370:TYR:OH	2.22	0.40
1:A:73:LEU:HB2	1:A:81:LYS:HD2	2.03	0.40
1:A:145:PHE:HB2	1:A:151:PHE:HZ	1.87	0.40
1:C:158:ARG:H	1:C:158:ARG:HG3	1.57	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	393/416 (94%)	382 (97%)	11 (3%)	0	100	100
1	B	384/416 (92%)	370 (96%)	14 (4%)	0	100	100
1	C	384/416 (92%)	372 (97%)	12 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1161/1248 (93%)	1124 (97%)	37 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	335/381 (88%)	315 (94%)	20 (6%)	17	37
1	B	332/381 (87%)	311 (94%)	21 (6%)	16	36
1	C	329/381 (86%)	302 (92%)	27 (8%)	10	24
All	All	996/1143 (87%)	928 (93%)	68 (7%)	14	32

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	52	GLU
1	B	110	ARG
1	B	137	LYS
1	B	138	THR
1	B	154	ILE
1	B	166	LEU
1	B	173	MET
1	B	176	GLU
1	B	189	ARG
1	B	198	THR
1	B	252	VAL
1	B	255	ARG
1	B	259	MET
1	B	262	LEU
1	B	325	ARG
1	B	332	VAL
1	B	352	THR
1	B	366	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	374	LYS
1	B	375	ASN
1	B	377	CYS
1	A	32	ILE
1	A	60	MET
1	A	69	LEU
1	A	81	LYS
1	A	91	ILE
1	A	122	VAL
1	A	138	THR
1	A	142	LYS
1	A	144	LYS
1	A	145	PHE
1	A	170	ILE
1	A	192	GLU
1	A	207	ASP
1	A	221	ILE
1	A	243	MET
1	A	265	ILE
1	A	299	LEU
1	A	325	ARG
1	A	350	GLU
1	A	374	LYS
1	C	33	ILE
1	C	49	ASN
1	C	64	ILE
1	C	69	LEU
1	C	107	THR
1	C	137	LYS
1	C	140	LEU
1	C	142	LYS
1	C	144	LYS
1	C	157	THR
1	C	158	ARG
1	C	218	GLU
1	C	243	MET
1	C	254	LYS
1	C	295	LEU
1	C	296	GLU
1	C	322	ARG
1	C	323	LEU
1	C	329	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	332	VAL
1	C	334	GLN
1	C	336	ARG
1	C	344	VAL
1	C	374	LYS
1	C	375	ASN
1	C	378	ARG
1	C	404	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	54	ASN
1	B	93	HIS
1	B	375	ASN
1	B	406	ASN
1	A	54	ASN
1	A	111	HIS
1	A	214	ASN
1	A	236	HIS
1	A	368	ASN
1	A	375	ASN
1	C	35	HIS
1	C	44	ASN
1	C	49	ASN
1	C	66	ASN
1	C	361	ASN
1	C	362	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

3 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	501	-	29,30,30	0.51	0	45,47,47	0.55	0
2	GDP	B	501	-	29,30,30	0.45	0	45,47,47	0.77	1 (2%)
2	GDP	C	501	-	29,30,30	0.51	0	45,47,47	0.71	1 (2%)

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	501	-	-	6/16/32/32	0/3/3/3
2	GDP	B	501	-	-	8/16/32/32	0/3/3/3
2	GDP	C	501	-	-	1/16/32/32	0/3/3/3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	GDP	O3'-C3'-C2'	-2.90	102.52	111.82
2	B	501	GDP	O3A-PB-O1B	-2.17	99.61	111.04

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	501	GDP	PA-O3A-PB-O3B
2	B	501	GDP	C5'-O5'-PA-O3A
2	B	501	GDP	C5'-O5'-PA-O1A
2	A	501	GDP	PA-O3A-PB-O3B

Continued on next page...

Continued from previous page...

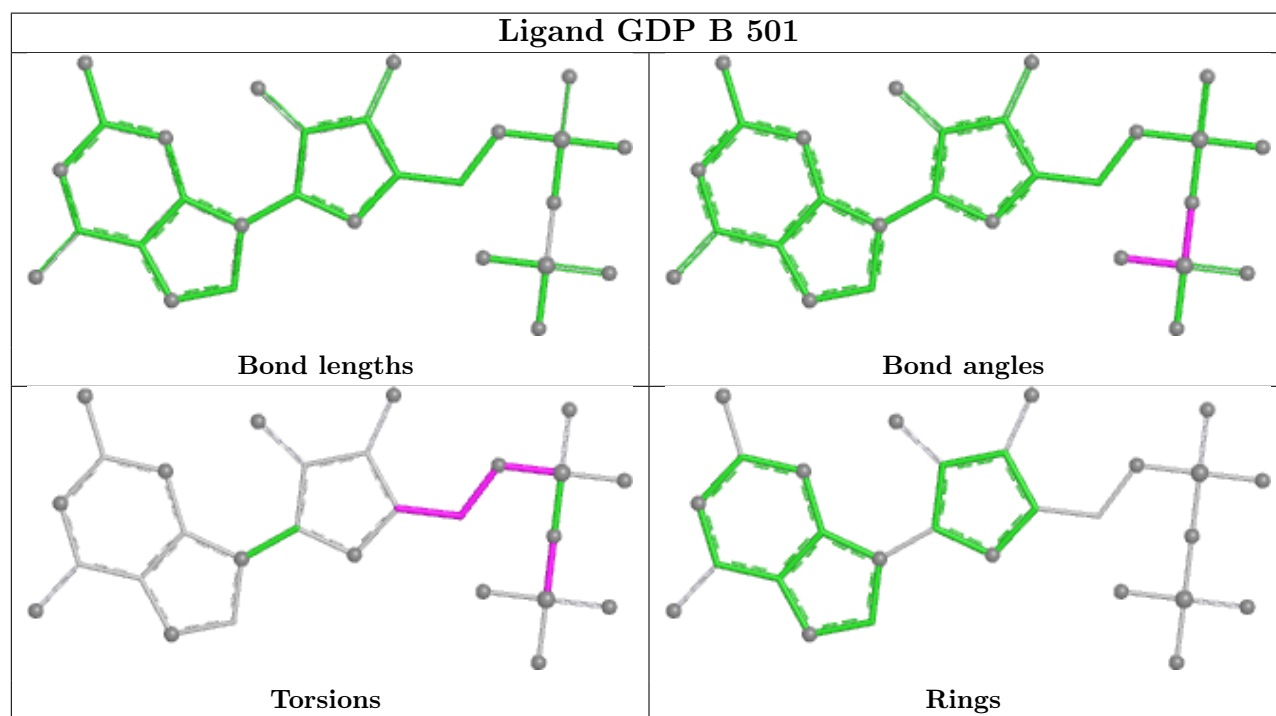
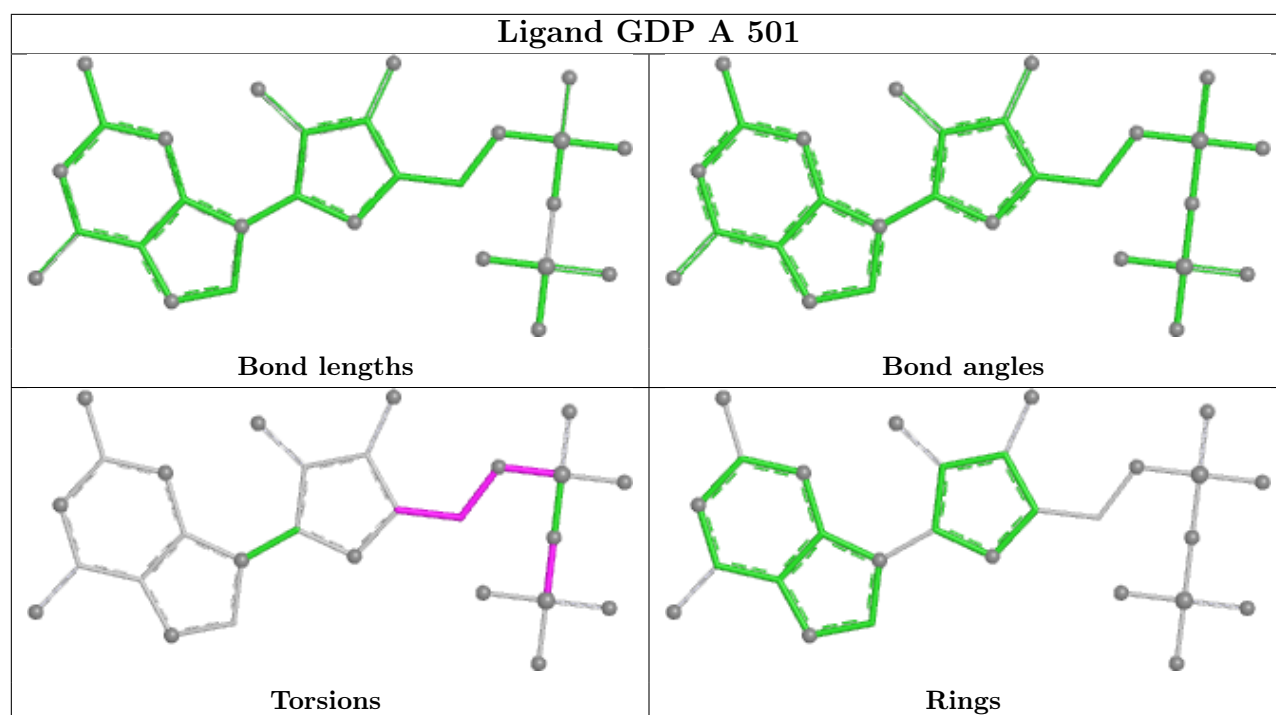
Mol	Chain	Res	Type	Atoms
2	A	501	GDP	C5'-O5'-PA-O3A
2	A	501	GDP	C5'-O5'-PA-O1A
2	B	501	GDP	O4'-C4'-C5'-O5'
2	B	501	GDP	C3'-C4'-C5'-O5'
2	C	501	GDP	PB-O3A-PA-O1A
2	A	501	GDP	C4'-C5'-O5'-PA
2	B	501	GDP	C5'-O5'-PA-O2A
2	A	501	GDP	C3'-C4'-C5'-O5'
2	B	501	GDP	C4'-C5'-O5'-PA
2	B	501	GDP	PA-O3A-PB-O1B
2	A	501	GDP	PA-O3A-PB-O2B

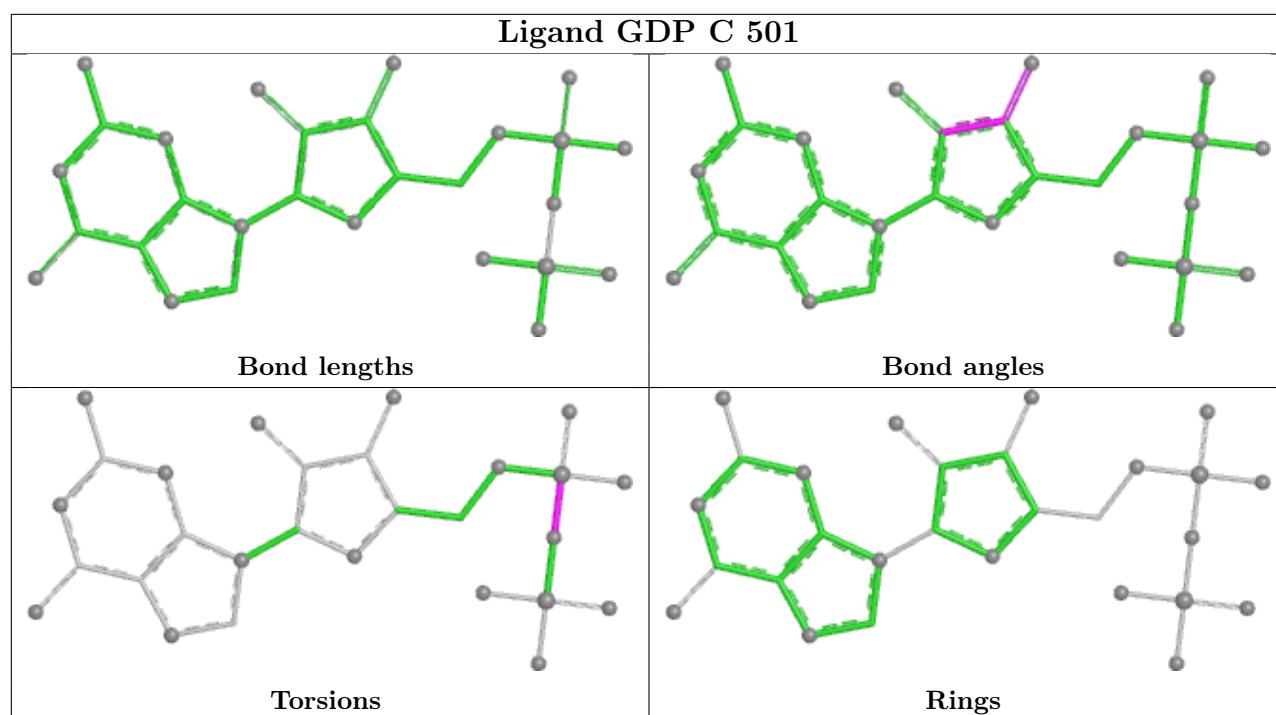
There are no ring outliers.

3 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	GDP	5	0
2	B	501	GDP	6	0
2	C	501	GDP	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	395/416 (94%)	0.61	40 (10%) 12 9	11, 49, 95, 137	0
1	B	388/416 (93%)	0.74	66 (17%) 4 3	14, 47, 103, 138	0
1	C	388/416 (93%)	0.84	57 (14%) 6 4	18, 52, 103, 120	0
All	All	1171/1248 (93%)	0.73	163 (13%) 6 5	11, 50, 103, 138	0

All (163) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	97	GLY	7.7
1	A	132	GLU	4.6
1	B	139	TYR	4.5
1	B	145	PHE	4.5
1	B	138	THR	4.4
1	B	159	PHE	4.4
1	A	133	ASP	4.3
1	C	145	PHE	4.1
1	C	99	ALA	4.1
1	B	223	GLU	4.0
1	B	135	GLN	3.9
1	C	100	HIS	3.9
1	A	12	ASP	3.9
1	A	197	GLN	3.8
1	B	134	PHE	3.7
1	B	259	MET	3.7
1	C	97	GLY	3.7
1	B	132	GLU	3.7
1	C	331	GLN	3.7
1	B	225	PRO	3.6
1	B	374	LYS	3.6
1	A	30	ILE	3.6
1	C	157	THR	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	322	ARG	3.6
1	B	226	ILE	3.5
1	A	107	THR	3.5
1	A	173	MET	3.5
1	C	95	GLU	3.5
1	B	331	GLN	3.5
1	B	133	ASP	3.5
1	C	98	ALA	3.5
1	A	131	SER	3.4
1	B	221	ILE	3.4
1	C	336	ARG	3.4
1	A	145	PHE	3.4
1	C	106	LYS	3.3
1	C	32	ILE	3.3
1	B	76	GLU	3.3
1	A	143	MET	3.3
1	B	98	ALA	3.3
1	A	163	ASP	3.3
1	C	329	ILE	3.3
1	C	133	ASP	3.2
1	C	323	LEU	3.2
1	B	68	PRO	3.1
1	C	140	LEU	3.1
1	C	132	GLU	3.1
1	C	107	THR	3.1
1	B	166	LEU	3.0
1	A	140	LEU	3.0
1	A	120	ASN	3.0
1	C	144	LYS	3.0
1	C	27	GLU	3.0
1	B	136	PRO	3.0
1	A	80	GLY	3.0
1	A	170	ILE	3.0
1	B	219	ASN	3.0
1	B	351	GLU	2.9
1	B	224	PRO	2.9
1	B	143	MET	2.9
1	C	321	GLN	2.9
1	B	99	ALA	2.9
1	C	108	LYS	2.9
1	C	96	GLY	2.8
1	C	375	ASN	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	129	THR	2.8
1	A	93	HIS	2.8
1	B	352	THR	2.8
1	C	135	GLN	2.7
1	B	137	LYS	2.7
1	C	169	ALA	2.7
1	A	139	TYR	2.7
1	B	333	ASP	2.7
1	A	188	LEU	2.7
1	B	216	PHE	2.7
1	B	222	ALA	2.7
1	A	136	PRO	2.7
1	C	403	CYS	2.7
1	C	327	TRP	2.7
1	B	260	PHE	2.6
1	C	404	LEU	2.6
1	B	189	ARG	2.6
1	B	130	GLY	2.6
1	B	131	SER	2.6
1	C	131	SER	2.6
1	B	353	ILE	2.6
1	C	325	ARG	2.6
1	B	348	THR	2.5
1	C	333	ASP	2.5
1	C	338	MET	2.5
1	B	108	LYS	2.5
1	A	108	LYS	2.5
1	C	353	ILE	2.5
1	B	107	THR	2.5
1	C	33	ILE	2.5
1	A	330	ASP	2.5
1	B	75	GLY	2.5
1	C	136	PRO	2.5
1	A	99	ALA	2.4
1	C	326	ALA	2.4
1	B	217	ARG	2.4
1	B	163	ASP	2.4
1	B	332	VAL	2.4
1	C	334	GLN	2.4
1	B	215	THR	2.4
1	A	154	ILE	2.4
1	A	92	GLY	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	158	ARG	2.4
1	A	169	ALA	2.4
1	C	49	ASN	2.4
1	C	349	ASP	2.4
1	B	403	CYS	2.4
1	C	53	VAL	2.4
1	B	172	ILE	2.3
1	B	120	ASN	2.3
1	C	69	LEU	2.3
1	A	91	ILE	2.3
1	C	50	ILE	2.3
1	B	198	THR	2.3
1	B	111	HIS	2.3
1	A	111	HIS	2.3
1	A	31	ASN	2.3
1	A	157	THR	2.3
1	B	257	ASN	2.3
1	B	354	GLN	2.3
1	A	184	VAL	2.3
1	B	346	THR	2.2
1	C	124	TRP	2.2
1	C	332	VAL	2.2
1	B	164	ILE	2.2
1	B	300	GLU	2.2
1	B	210	LEU	2.2
1	A	134	PHE	2.2
1	B	377	CYS	2.2
1	B	322	ARG	2.2
1	B	100	HIS	2.2
1	B	253	PHE	2.2
1	A	239	PHE	2.2
1	C	64	ILE	2.2
1	C	172	ILE	2.2
1	B	177	PHE	2.2
1	C	150	PHE	2.2
1	B	110	ARG	2.1
1	C	158	ARG	2.1
1	C	222	ALA	2.1
1	A	129	THR	2.1
1	B	142	LYS	2.1
1	C	143	MET	2.1
1	A	76	GLU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	225	PRO	2.1
1	B	144	LYS	2.1
1	A	224	PRO	2.1
1	C	44	ASN	2.1
1	B	114	GLU	2.0
1	C	109	GLU	2.0
1	C	328	GLU	2.0
1	C	111	HIS	2.0
1	C	30	ILE	2.0
1	B	72	ALA	2.0
1	A	222	ALA	2.0
1	A	96	GLY	2.0
1	A	406	ASN	2.0
1	C	110	ARG	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](#)

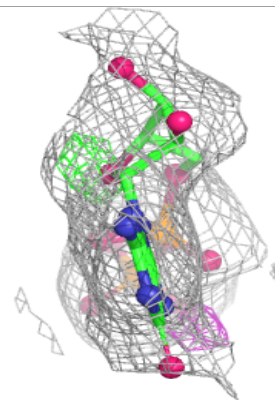
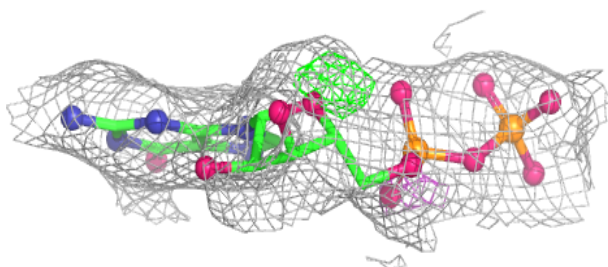
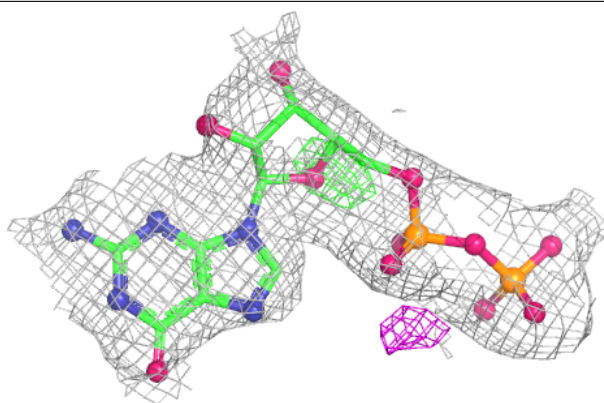
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GDP	A	501	28/28	0.91	0.11	49,67,80,82	0
2	GDP	B	501	28/28	0.92	0.08	28,39,55,63	0
2	GDP	C	501	28/28	0.95	0.08	31,39,47,48	0

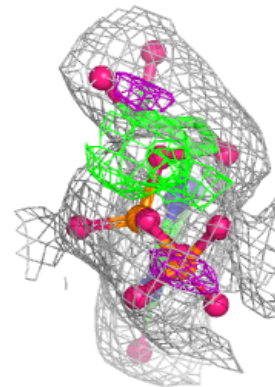
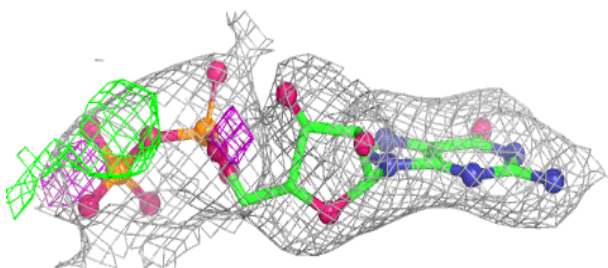
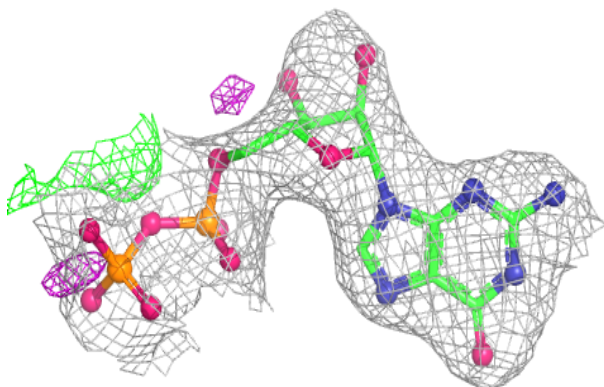
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

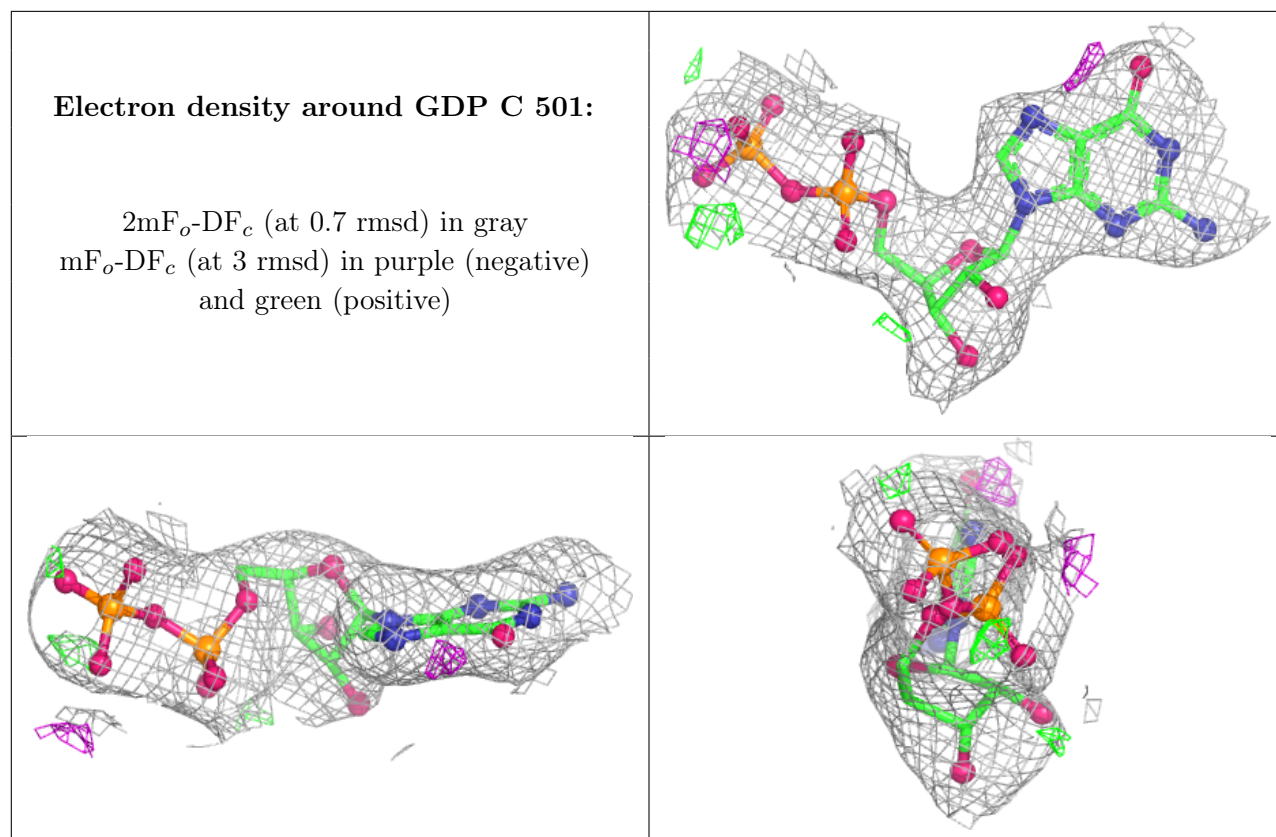
Electron density around GDP A 501:

$2mF_o - DF_c$ (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.