



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:53 AM UTC

PDB ID : 6S8K / pdb_00006s8k
Title : Structure, Thermodynamics, and Kinetics of Plinabulin Binding to two Tubulin Isotypes
Authors : Sharma, A.; Olieric, N.; Steinmetz, M.
Deposited on : 2019-07-10
Resolution : 1.52 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

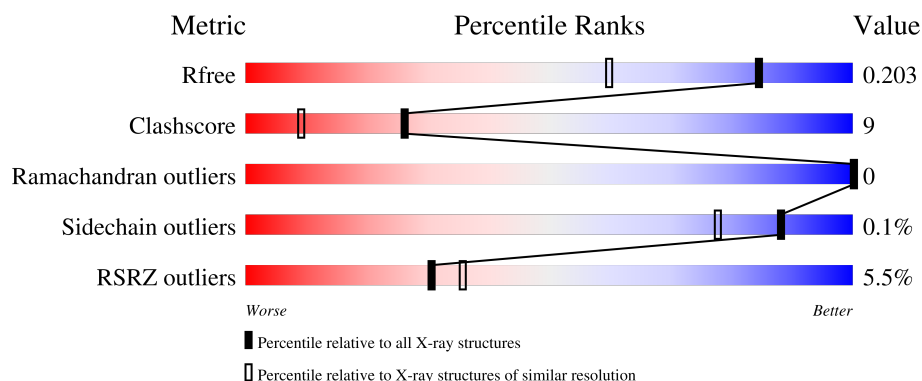
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.52 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	5890 (1.54-1.50)
Clashscore	190562	6116 (1.54-1.50)
Ramachandran outliers	187476	6002 (1.54-1.50)
Sidechain outliers	187428	5999 (1.54-1.50)
RSRZ outliers	180081	5891 (1.54-1.50)

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	437	6% 85% 14%
2	B	445	6% 74% 22%
3	F	155	% 90% 10%

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 9056 atoms, of which 44 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 Tubulin alpha-1B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	437	Total	C	N	O	S	0	11	0
			3471	2202	587	657	25			

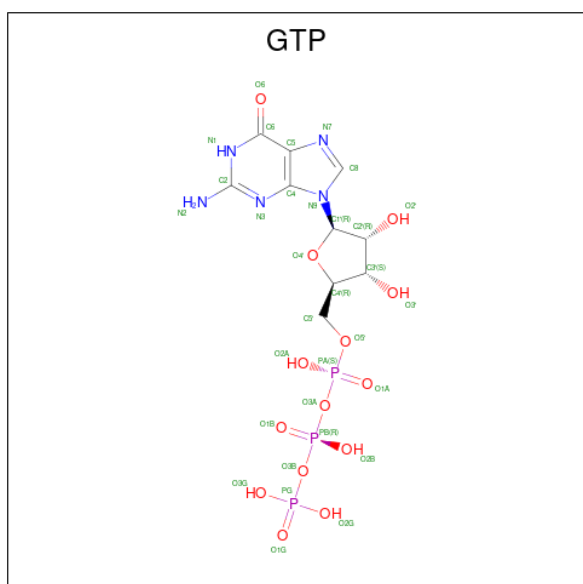
- Molecule 2 is a protein called Tubulin beta-2B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	425	Total	C	N	O	S	0	11	0
			3410	2145	583	654	28			

- Molecule 3 is a protein called Designed ankyrin repeat protein (DARPIN) D1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	155	Total	C	N	O	S	0	3	0
			1175	745	199	228	3			

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

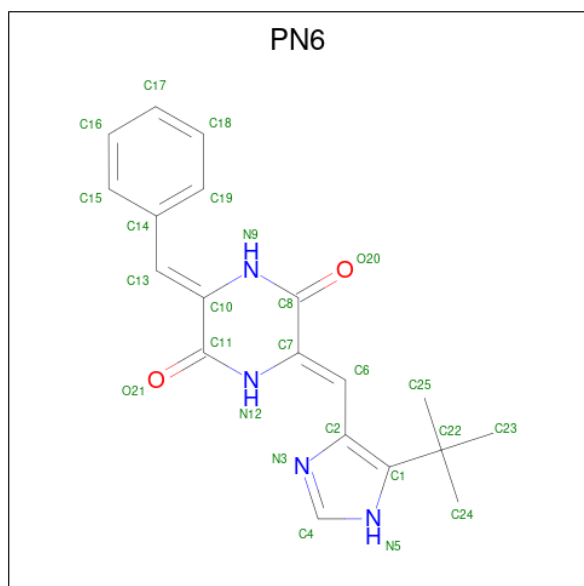


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	P	
			44	10	12	5	14	3	
								0	0

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

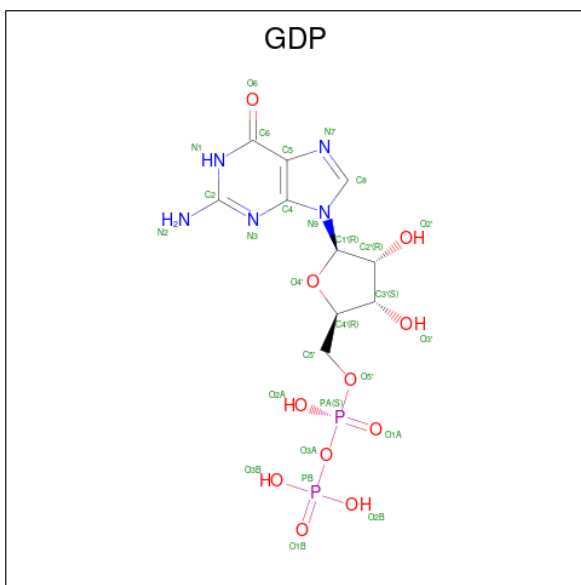
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		

- Molecule 6 is (3Z,6Z)-3-benzylidene-6-[(5-tert-butyl-1H-imidazol-4-yl)methylidene]piperazine-2,5-dione (CCD ID: PN6) (formula: C₁₉H₂₀N₄O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	H	N	O		
			45	19	20	4	2		
								0	0

- Molecule 7 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
7	B	1	Total	C	H	N	O	P	0	0
			40	10	12	5	11	2		

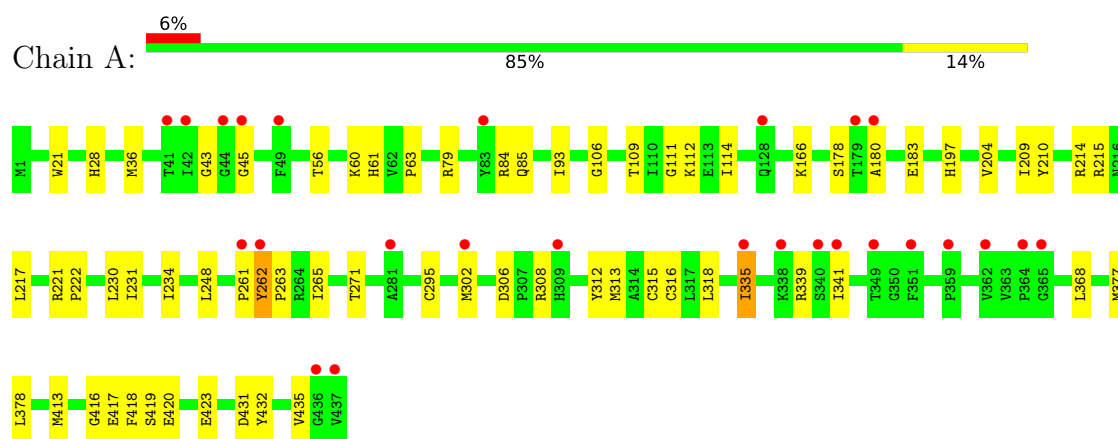
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	442	Total O 442 442	0	0
8	B	239	Total O 239 239	0	0
8	F	189	Total O 189 189	0	0

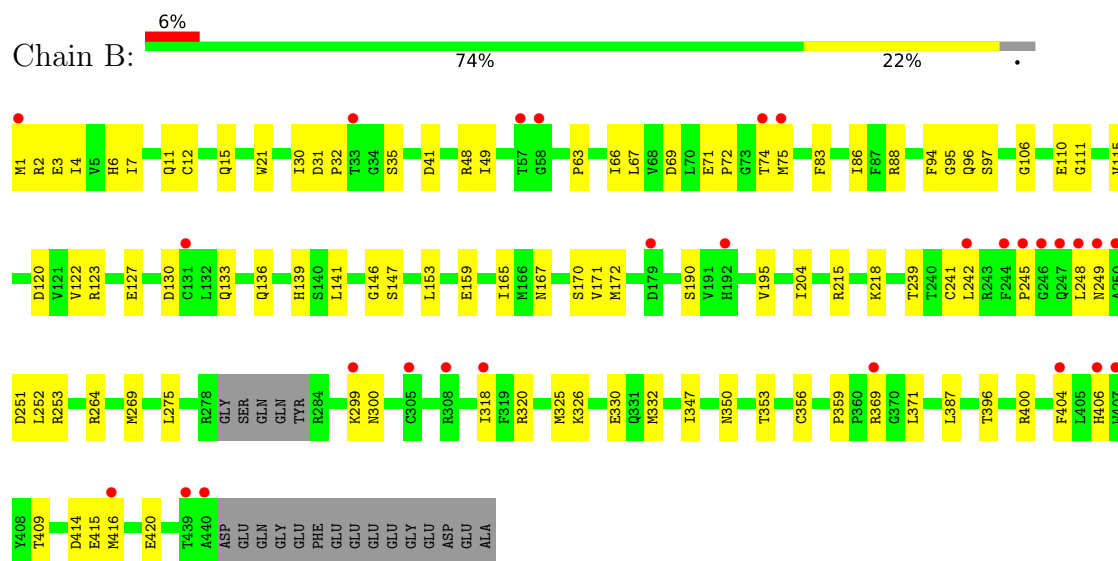
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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: Tubulin alpha-1B chain



• Molecule 2: Tubulin beta-2B chain



• Molecule 3: Designed ankyrin repeat protein (DARPIN) D1





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	73.56Å 91.35Å 83.22Å 90.00° 96.85° 90.00°	Depositor
Resolution (Å)	45.02 – 1.52 45.02 – 1.52	Depositor EDS
% Data completeness (in resolution range)	98.4 (45.02-1.52) 99.2 (45.02-1.52)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.35 (at 1.52Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.177 , 0.203 0.178 , 0.203	Depositor DCC
R_{free} test set	8319 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	23.2	Xtriage
Anisotropy	0.360	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 41.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	9056	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.16% 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, GTP, MG, PN6

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	0.19	0/3579	0.43	0/4857
2	B	0.16	0/3505	0.36	0/4744
3	F	0.17	0/1198	0.36	0/1629
All	All	0.17	0/8282	0.39	0/11230

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	262	TYR	Peptide

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	3471	0	3415	50	0
2	B	3410	0	3313	92	0
3	F	1175	0	1184	14	0
4	A	32	12	11	0	0
5	A	1	0	0	0	0
6	B	25	20	20	3	0
7	B	28	12	11	1	0
8	A	442	0	0	6	0
8	B	239	0	0	7	0
8	F	189	0	0	0	0
All	All	9012	44	7954	151	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 9.

All (151) 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)
2:B:1:MET:HG3	2:B:133:GLN:HG2	1.40	0.98
1:A:308:ARG:HH22	1:A:339:ARG:HH11	1.16	0.90
1:A:234:ILE:HD13	1:A:302:MET:SD	2.15	0.87
2:B:165:ILE:HD11	2:B:253[B]:ARG:HG3	1.70	0.74
2:B:72:PRO:HG3	2:B:96:GLN:HA	1.70	0.73
2:B:241[A]:CYS:SG	2:B:318:ILE:HD12	2.28	0.73
2:B:97:SER:OG	2:B:110:GLU:HG2	1.89	0.72
2:B:1:MET:SD	2:B:253[B]:ARG:NH2	2.64	0.70
2:B:248:LEU:HD12	2:B:249:ASN:H	1.55	0.69
2:B:147[B]:SER:HG	2:B:190:SER:HG	1.18	0.69
2:B:275:LEU:HD11	2:B:300:ASN:HA	1.75	0.67
2:B:242:LEU:HD11	2:B:252:LEU:CD2	2.24	0.67
2:B:11[B]:GLN:HG2	2:B:74:THR:HG21	1.76	0.66
2:B:15:GLN:NE2	8:B:605:HOH:O	2.28	0.66
2:B:332:MET:HG3	2:B:353:THR:HG21	1.77	0.66
2:B:71:GLU:HG3	8:B:607:HOH:O	1.96	0.66
2:B:11[B]:GLN:HG2	2:B:74:THR:CG2	2.26	0.65
3:F:23:ARG:NH1	3:F:57[B]:TYR:OH	2.30	0.64
1:A:315:CYS:SG	1:A:377[B]:MET:HE1	2.39	0.63
2:B:396:THR:O	2:B:400:ARG:HG3	1.98	0.63
3:F:167:LYS:HE2	3:F:167:LYS:HA	1.80	0.62
2:B:400:ARG:HD2	3:F:112:TRP:NE1	2.13	0.62
1:A:180:ALA:HB3	1:A:183:GLU:HG3	1.83	0.60
2:B:120:ASP:OD2	8:B:601:HOH:O	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:11[B]:GLN:CG	2:B:74:THR:HG21	2.32	0.59
2:B:83:PHE:O	2:B:86:ILE:HG22	2.03	0.59
2:B:242:LEU:HD11	2:B:252:LEU:HD23	1.83	0.59
2:B:88:ARG:NH2	8:B:608:HOH:O	2.37	0.58
2:B:239:THR:HG22	6:B:501:PN6:C17	2.33	0.58
2:B:48:ARG:HG3	2:B:245:PRO:HG3	1.85	0.56
1:A:318[B]:LEU:HD21	8:A:773:HOH:O	2.05	0.56
1:A:316[B]:CYS:SG	1:A:378:LEU:HB2	2.45	0.56
3:F:34:MET:HE1	3:F:69:HIS:HB2	1.88	0.55
2:B:318:ILE:HD11	6:B:501:PN6:H1	1.89	0.54
2:B:404[A]:PHE:HE2	3:F:90:ILE:HD12	1.73	0.54
2:B:72:PRO:CG	2:B:96:GLN:HA	2.38	0.54
2:B:326:LYS:HE3	2:B:330:GLU:OE2	2.08	0.54
1:A:215:ARG:NH1	8:A:602:HOH:O	2.23	0.53
1:A:416:GLY:O	1:A:420[B]:GLU:HG3	2.08	0.53
2:B:416:MET:O	2:B:420:GLU:HG3	2.08	0.53
2:B:241[A]:CYS:HG	2:B:318:ILE:HD12	1.73	0.53
2:B:406:HIS:HA	2:B:409:THR:OG1	2.09	0.52
2:B:123:ARG:O	2:B:127:GLU:HG2	2.10	0.52
2:B:400:ARG:HD2	3:F:112:TRP:CE2	2.44	0.52
2:B:248:LEU:HD12	2:B:249:ASN:N	2.23	0.52
1:A:180:ALA:HB3	1:A:183:GLU:CG	2.39	0.52
2:B:21:TRP:CZ3	2:B:63:PRO:HB3	2.45	0.52
2:B:2:ARG:HG3	2:B:3:GLU:OE2	2.09	0.52
2:B:75:MET:HG3	2:B:94:PHE:HB3	1.93	0.51
2:B:4:ILE:HD11	2:B:242:LEU:HD13	1.93	0.50
2:B:106:GLY:O	2:B:111:GLY:HA3	2.11	0.50
1:A:210:TYR:CE2	1:A:214:ARG:HD3	2.47	0.50
3:F:34:MET:HE3	3:F:40:VAL:CG2	2.42	0.50
2:B:1:MET:CG	2:B:133:GLN:HG2	2.28	0.50
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.47	0.50
2:B:67:LEU:HD12	2:B:67:LEU:N	2.27	0.50
2:B:400:ARG:HD3	8:B:788:HOH:O	2.11	0.49
1:A:306:ASP:OD1	8:A:601:HOH:O	2.19	0.49
3:F:30:VAL:O	3:F:34:MET:HG3	2.12	0.49
2:B:69:ASP:O	2:B:94:PHE:HA	2.13	0.48
3:F:61:GLU:O	3:F:65:VAL:HG23	2.13	0.48
1:A:28:HIS:O	1:A:36:MET:HE3	2.13	0.48
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.48	0.48
1:A:377[B]:MET:HG3	8:A:719:HOH:O	2.14	0.48
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:31:ASP:OD2	2:B:35[B]:SER:HB2	2.14	0.48
2:B:97:SER:HG	2:B:110:GLU:HG2	1.78	0.48
1:A:79:ARG:O	1:A:84:ARG:HB2	2.14	0.47
2:B:1:MET:HE2	2:B:251:ASP:HB2	1.96	0.47
2:B:41:ASP:HB2	8:B:796:HOH:O	2.13	0.47
2:B:299:LYS:HB3	8:B:604:HOH:O	2.13	0.47
2:B:115:VAL:HG23	2:B:153[A]:LEU:HD23	1.96	0.47
2:B:387[A]:LEU:C	2:B:387[A]:LEU:HD23	2.39	0.47
2:B:242:LEU:HD12	6:B:501:PN6:H18	1.96	0.47
1:A:217:LEU:HD21	1:A:368:LEU:HD23	1.96	0.47
2:B:139:HIS:HE1	2:B:170:SER:OG	1.97	0.47
1:A:180:ALA:O	1:A:183:GLU:HG3	2.15	0.47
1:A:262:TYR:HB2	1:A:263:PRO:CD	2.44	0.47
2:B:414:ASP:OD1	2:B:415:GLU:N	2.48	0.47
2:B:66:ILE:CD1	2:B:122:VAL:HG22	2.45	0.47
2:B:195:VAL:CG1	2:B:264[A]:ARG:HG2	2.45	0.47
2:B:139:HIS:HD2	2:B:146:GLY:O	1.98	0.46
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.32	0.46
1:A:312:TYR:CE2	1:A:341:ILE:HG23	2.51	0.46
1:A:261:PRO:HG2	1:A:313:MET:HB3	1.98	0.46
1:A:43:GLY:HA2	1:A:56:THR:O	2.16	0.46
1:A:93:ILE:HG22	1:A:114:ILE:HD11	1.97	0.46
2:B:7:ILE:HG21	2:B:153[B]:LEU:HD21	1.98	0.46
2:B:165:ILE:CD1	2:B:253[B]:ARG:HG3	2.44	0.45
2:B:66:ILE:HD12	2:B:122:VAL:HG22	1.98	0.45
1:A:60:LYS:HE3	8:A:680:HOH:O	2.17	0.45
2:B:165:ILE:HD11	2:B:253[B]:ARG:CG	2.43	0.45
3:F:34:MET:HE3	3:F:40:VAL:HG22	1.98	0.45
1:A:262:TYR:HB2	1:A:263:PRO:HD3	1.99	0.45
1:A:210:TYR:CE1	1:A:222:PRO:HD2	2.52	0.45
2:B:215:ARG:NH2	3:F:160:ASP:OD1	2.46	0.45
2:B:1:MET:HE2	2:B:251:ASP:CG	2.41	0.45
2:B:242:LEU:HD11	2:B:252:LEU:HD21	1.95	0.45
1:A:413:MET:HE2	1:A:418:PHE:CE2	2.53	0.44
2:B:2:ARG:HG3	2:B:3:GLU:CD	2.42	0.44
2:B:218:LYS:HA	2:B:218:LYS:HE2	1.99	0.44
1:A:265:ILE:HD11	1:A:431:ASP:HB3	2.00	0.44
2:B:31:ASP:OD2	2:B:35[A]:SER:HB3	2.17	0.44
1:A:45:GLY:HA3	8:A:660:HOH:O	2.18	0.44
2:B:30:ILE:HD11	2:B:49:ILE:HD11	2.00	0.44
2:B:172:MET:HG3	2:B:387[A]:LEU:HD11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:79:MET:O	3:F:111:THR:HG22	2.18	0.44
2:B:359:PRO:HB2	2:B:371:LEU:O	2.18	0.43
1:A:109:THR:O	1:A:112:LYS:HG2	2.17	0.43
1:A:178:SER:OG	1:A:183:GLU:OE2	2.28	0.43
2:B:147[A]:SER:HB2	2:B:190:SER:HG	1.83	0.43
2:B:172:MET:HG3	2:B:387[B]:LEU:HD21	2.00	0.43
2:B:69:ASP:OD2	2:B:74:THR:OG1	2.31	0.43
1:A:248:LEU:HD21	1:A:316[B]:CYS:HB2	2.01	0.43
1:A:413:MET:HE3	1:A:417:GLU:HB3	2.01	0.43
1:A:335:ILE:HD13	1:A:335:ILE:HA	1.87	0.43
1:A:221:ARG:CZ	2:B:325:MET:HB3	2.49	0.43
1:A:312:TYR:CD2	1:A:341:ILE:HG23	2.54	0.43
2:B:48:ARG:HG3	2:B:245:PRO:CG	2.48	0.43
2:B:1:MET:HE3	2:B:133:GLN:HB3	2.00	0.43
2:B:369:ARG:HB2	2:B:369:ARG:HH11	1.83	0.43
3:F:34:MET:CE	3:F:69:HIS:HB2	2.49	0.43
2:B:406:HIS:HA	2:B:409:THR:HG1	1.83	0.42
2:B:171:VAL:HA	2:B:204:ILE:O	2.19	0.42
1:A:217:LEU:HD21	1:A:368:LEU:CD2	2.49	0.42
2:B:67:LEU:O	2:B:75:MET:HE1	2.20	0.42
2:B:141:LEU:HD12	2:B:172:MET:SD	2.58	0.42
1:A:180:ALA:CB	1:A:183:GLU:HG3	2.48	0.42
2:B:72:PRO:HG3	2:B:95:GLY:O	2.18	0.42
1:A:419:SER:O	1:A:423:GLU:HG3	2.20	0.42
1:A:166:LYS:HE2	1:A:197:HIS:O	2.21	0.41
1:A:271:THR:HG21	1:A:295:CYS:O	2.21	0.41
1:A:56:THR:OG1	1:A:60:LYS:HB3	2.21	0.41
2:B:299:LYS:HB3	2:B:299:LYS:HE2	1.95	0.41
1:A:106:GLY:O	1:A:111:GLY:HA3	2.21	0.41
2:B:2:ARG:HD2	2:B:130:ASP:HB3	2.03	0.41
2:B:31:ASP:HB2	2:B:32:PRO:CD	2.51	0.41
1:A:313:MET:SD	1:A:435:VAL:HG11	2.61	0.41
2:B:12:CYS:HB2	7:B:502:GDP:C8	2.55	0.40
1:A:21:TRP:CE3	1:A:63:PRO:HB3	2.56	0.40
1:A:209:ILE:HG23	1:A:230:LEU:HD23	2.04	0.40
2:B:215:ARG:O	2:B:218:LYS:HE3	2.20	0.40
2:B:136:GLN:HA	2:B:167:ASN:O	2.22	0.40
2:B:269:MET:HE2	2:B:269:MET:HB3	1.94	0.40
1:A:60:LYS:NZ	1:A:85:GLN:O	2.42	0.40
1:A:204:VAL:HG11	1:A:231:ILE:HG12	2.04	0.40
2:B:320:ARG:HA	2:B:356:CYS:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:121:ALA:HB1	3:F:161:LEU:HD21	2.02	0.40
2:B:347:ILE:HG22	2:B:350:ASN:HB3	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	446/437 (102%)	438 (98%)	8 (2%)	0	100	100
2	B	432/445 (97%)	424 (98%)	8 (2%)	0	100	100
3	F	156/155 (101%)	156 (100%)	0	0	100	100
All	All	1034/1037 (100%)	1018 (98%)	16 (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	379/368 (103%)	378 (100%)	1 (0%)	86	75
2	B	378/383 (99%)	378 (100%)	0	100	100
3	F	123/120 (102%)	123 (100%)	0	100	100
All	All	880/871 (101%)	879 (100%)	1 (0%)	88	78

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	335	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	233	GLN
1	A	393	HIS
2	B	139	HIS
2	B	331	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](#)

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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	$\# Z > 2$
6	PN6	B	501	-	26,27,27	2.63	13 (50%)	34,39,39	2.35	12 (35%)
7	GDP	B	502	-	29,30,30	3.65	18 (62%)	45,47,47	2.07	14 (31%)
4	GTP	A	501	5	33,34,34	3.05	15 (45%)	50,54,54	2.02	14 (28%)

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
6	PN6	B	501	-	-	0/14/14/14	0/3/3/3
7	GDP	B	502	-	-	3/16/32/32	0/3/3/3
4	GTP	A	501	5	-	6/22/38/38	0/3/3/3

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	502	GDP	C2'-C3'	-10.57	1.24	1.53
4	A	501	GTP	O4'-C1'	8.13	1.60	1.42
4	A	501	GTP	C2'-C1'	-6.99	1.31	1.53
7	B	502	GDP	C4-N3	6.56	1.49	1.34
6	B	501	PN6	C6-C2	6.53	1.55	1.40
7	B	502	GDP	C3'-C4'	5.85	1.67	1.53
7	B	502	GDP	C1'-N9	-5.83	1.31	1.47
4	A	501	GTP	PB-O3B	5.32	1.65	1.59
7	B	502	GDP	C2-N3	5.31	1.46	1.33
7	B	502	GDP	O4'-C4'	-5.06	1.33	1.45
4	A	501	GTP	O4'-C4'	-5.01	1.33	1.45
4	A	501	GTP	C4-N3	5.00	1.45	1.34
7	B	502	GDP	O4'-C1'	4.42	1.52	1.42
6	B	501	PN6	C1-N5	-4.36	1.31	1.37
7	B	502	GDP	C2-N2	4.34	1.44	1.34
6	B	501	PN6	C8-N9	4.25	1.46	1.38
4	A	501	GTP	C2-N3	4.18	1.43	1.33
6	B	501	PN6	C14-C13	4.18	1.54	1.46
4	A	501	GTP	C2-N2	4.08	1.43	1.34
6	B	501	PN6	C10-N9	3.80	1.46	1.38
4	A	501	GTP	C4-N9	-3.63	1.28	1.38
6	B	501	PN6	C7-N12	3.50	1.46	1.38
6	B	501	PN6	C11-N12	3.34	1.45	1.38
7	B	502	GDP	PA-O3A	3.19	1.62	1.59
6	B	501	PN6	C22-C1	3.12	1.55	1.52
6	B	501	PN6	C2-N3	-2.92	1.31	1.39
7	B	502	GDP	C5-N7	-2.88	1.33	1.39
4	A	501	GTP	C2-N1	2.86	1.44	1.37
7	B	502	GDP	C2-N1	2.73	1.44	1.37
4	A	501	GTP	C5-C6	2.69	1.54	1.44
4	A	501	GTP	PA-O3A	2.59	1.62	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	502	GDP	C5-C6	2.58	1.54	1.44
6	B	501	PN6	C10-C11	2.54	1.53	1.48
6	B	501	PN6	C7-C8	2.52	1.53	1.48
4	A	501	GTP	C6-N1	2.51	1.43	1.38
6	B	501	PN6	O20-C8	-2.42	1.19	1.23
4	A	501	GTP	O6-C6	-2.42	1.19	1.23
7	B	502	GDP	O2'-C2'	2.42	1.48	1.43
6	B	501	PN6	O21-C11	-2.40	1.19	1.23
4	A	501	GTP	O2'-C2'	2.35	1.48	1.43
7	B	502	GDP	C2'-C1'	2.30	1.60	1.53
7	B	502	GDP	O3'-C3'	2.22	1.48	1.43
4	A	501	GTP	O3'-C3'	-2.21	1.37	1.43
7	B	502	GDP	O6-C6	-2.18	1.19	1.23
7	B	502	GDP	C4-N9	-2.05	1.32	1.38
7	B	502	GDP	C6-N1	2.02	1.42	1.38

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	501	GTP	C1'-N9-C8	-5.99	109.71	126.73
7	B	502	GDP	C5-C4-N3	-5.85	119.08	128.39
4	A	501	GTP	C1'-N9-C4	5.61	143.07	126.49
6	B	501	PN6	N5-C4-N3	-5.23	106.91	112.98
6	B	501	PN6	C10-N9-C8	-4.97	119.87	125.51
7	B	502	GDP	C2-N3-C4	4.86	120.66	112.30
6	B	501	PN6	C10-C11-N12	4.66	120.60	116.02
6	B	501	PN6	C7-N12-C11	-4.53	120.37	125.51
6	B	501	PN6	C7-C8-N9	4.27	120.21	116.02
4	A	501	GTP	C6-C5-N7	4.15	137.83	130.29
7	B	502	GDP	C1'-N9-C4	-3.86	115.08	126.49
7	B	502	GDP	N9-C4-N3	3.68	133.31	125.95
4	A	501	GTP	C5-C4-N9	3.65	112.19	105.66
4	A	501	GTP	C4-C5-N7	-3.49	105.14	110.67
6	B	501	PN6	C7-C6-C2	-3.46	119.57	128.06
7	B	502	GDP	N9-C8-N7	-3.27	107.34	113.40
6	B	501	PN6	C14-C13-C10	-3.23	124.16	130.66
7	B	502	GDP	C1'-N9-C8	3.22	135.87	126.73
6	B	501	PN6	C8-C7-N12	3.21	119.54	116.65
4	A	501	GTP	N2-C2-N1	3.17	123.46	116.76
4	A	501	GTP	N9-C8-N7	-3.09	107.67	113.40
7	B	502	GDP	C2-N1-C6	-3.06	119.56	125.11
6	B	501	PN6	C11-C10-N9	3.04	119.38	116.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	502	GDP	C3'-C2'-C1'	2.96	107.07	101.46
6	B	501	PN6	C22-C1-C2	-2.76	129.31	135.52
7	B	502	GDP	O4'-C1'-C2'	-2.65	100.94	106.62
7	B	502	GDP	C8-N7-C5	2.64	108.96	104.26
7	B	502	GDP	C5-C6-N1	2.57	119.80	113.25
4	A	501	GTP	C2-N3-C4	2.50	116.60	112.30
7	B	502	GDP	O3'-C3'-C4'	-2.42	104.12	111.08
6	B	501	PN6	O20-C8-C7	-2.40	118.60	121.91
4	A	501	GTP	C2-N1-C6	-2.36	120.83	125.11
4	A	501	GTP	N2-C2-N3	-2.26	115.26	119.67
7	B	502	GDP	C4-C5-N7	-2.25	107.11	110.67
4	A	501	GTP	O3G-PG-O2G	2.23	116.17	107.80
7	B	502	GDP	C2'-C1'-N9	2.19	119.35	113.25
4	A	501	GTP	N9-C4-N3	-2.19	121.58	125.95
4	A	501	GTP	C4'-O4'-C1'	-2.18	104.66	109.47
6	B	501	PN6	C6-C7-N12	-2.13	119.77	122.75
4	A	501	GTP	C2'-C1'-N9	2.06	118.97	113.25

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	501	GTP	C5'-O5'-PA-O3A
4	A	501	GTP	C5'-O5'-PA-O1A
4	A	501	GTP	C5'-O5'-PA-O2A
7	B	502	GDP	C5'-O5'-PA-O3A
7	B	502	GDP	C5'-O5'-PA-O1A
7	B	502	GDP	C5'-O5'-PA-O2A
4	A	501	GTP	PB-O3B-PG-O1G
4	A	501	GTP	PB-O3B-PG-O2G
4	A	501	GTP	PB-O3B-PG-O3G

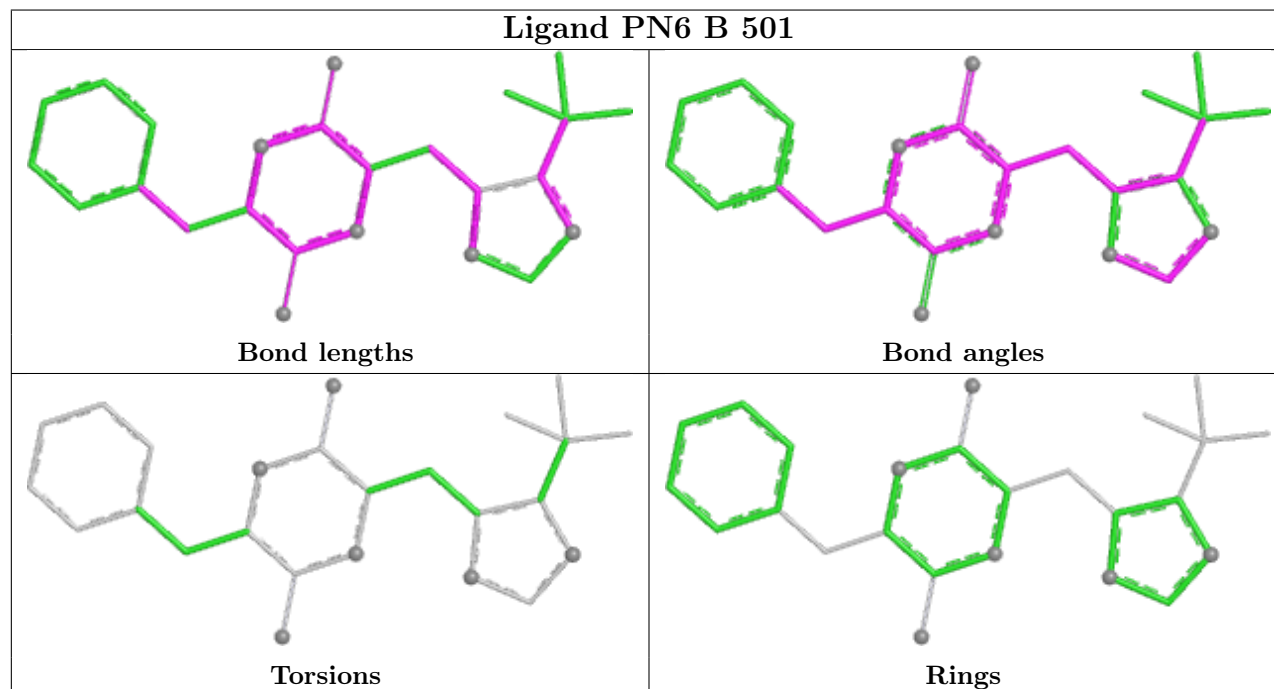
There are no ring outliers.

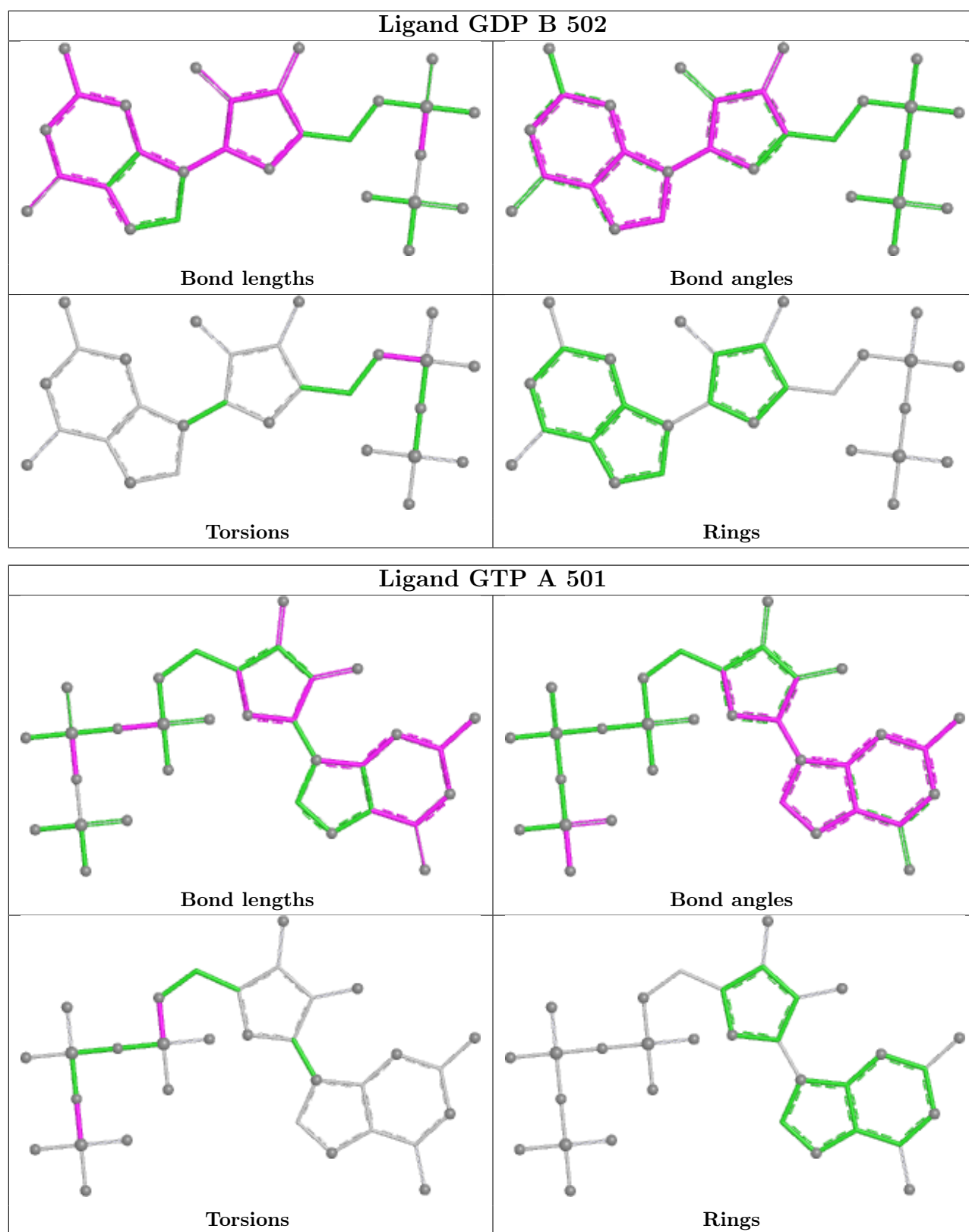
2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	501	PN6	3	0
7	B	502	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 ⓘ

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	437/437 (100%)	0.29	26 (5%)	28 33	14, 29, 57, 83	11 (2%)
2	B	425/445 (95%)	0.59	28 (6%)	24 29	11, 38, 70, 103	11 (2%)
3	F	155/155 (100%)	0.04	2 (1%)	75 79	15, 27, 54, 78	3 (1%)
All	All	1017/1037 (98%)	0.37	56 (5%)	30 36	11, 31, 64, 103	25 (2%)

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	262	TYR	6.6
2	B	248	LEU	4.9
1	A	335	ILE	4.8
2	B	250	ALA	4.8
2	B	440	ALA	4.8
1	A	437	VAL	4.8
1	A	83	TYR	4.7
2	B	246	GLY	4.3
1	A	364	PRO	3.8
1	A	341	ILE	3.7
1	A	362	VAL	3.7
2	B	1	MET	3.4
1	A	340	SER	3.2
2	B	75	MET	3.2
2	B	192	HIS	3.2
1	A	44	GLY	3.2
2	B	406	HIS	3.1
1	A	365	GLY	3.0
3	F	35	ALA	2.9
1	A	42	ILE	2.9
2	B	247	GLN	2.9
2	B	404[A]	PHE	2.8
2	B	308	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	369	ARG	2.8
1	A	351	PHE	2.7
1	A	349	THR	2.7
1	A	359	PRO	2.7
2	B	242	LEU	2.6
2	B	57	THR	2.6
2	B	179	ASP	2.6
1	A	436	GLY	2.6
2	B	249	ASN	2.6
1	A	179	THR	2.6
1	A	49	PHE	2.5
2	B	318	ILE	2.4
2	B	245	PRO	2.4
1	A	302	MET	2.4
3	F	32	ILE	2.4
2	B	33	THR	2.4
1	A	45	GLY	2.3
1	A	180	ALA	2.3
2	B	74	THR	2.3
1	A	41	THR	2.3
2	B	407	TRP	2.3
1	A	261	PRO	2.2
2	B	131	CYS	2.2
1	A	281	ALA	2.2
1	A	128	GLN	2.1
2	B	305	CYS	2.1
2	B	299	LYS	2.1
1	A	338	LYS	2.1
1	A	309	HIS	2.1
2	B	439	THR	2.0
2	B	58	GLY	2.0
2	B	244	PHE	2.0
2	B	416	MET	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](#)

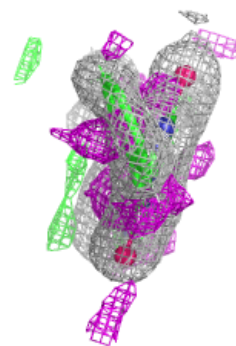
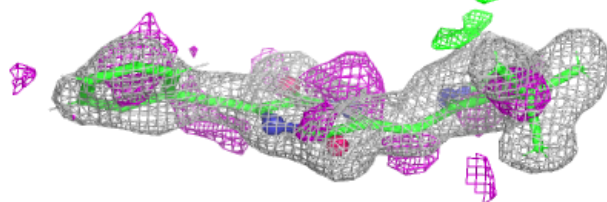
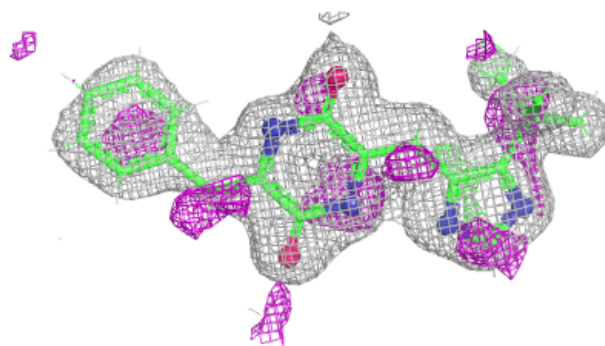
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
6	PN6	B	501	25/25	0.91	0.10	26,39,63,68	0
7	GDP	B	502	28/28	0.97	0.06	23,26,32,33	0
4	GTP	A	501	32/32	0.98	0.05	17,21,27,27	0
5	MG	A	502	1/1	1.00	0.02	19,19,19,19	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.

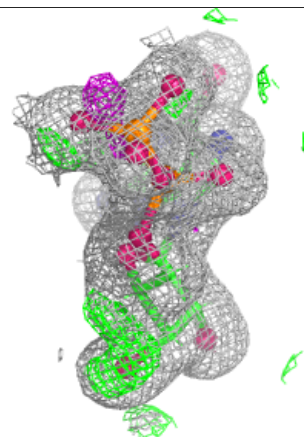
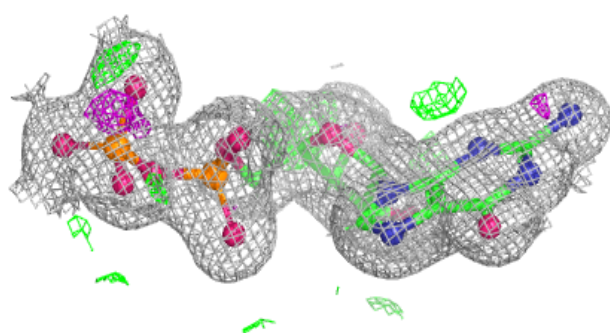
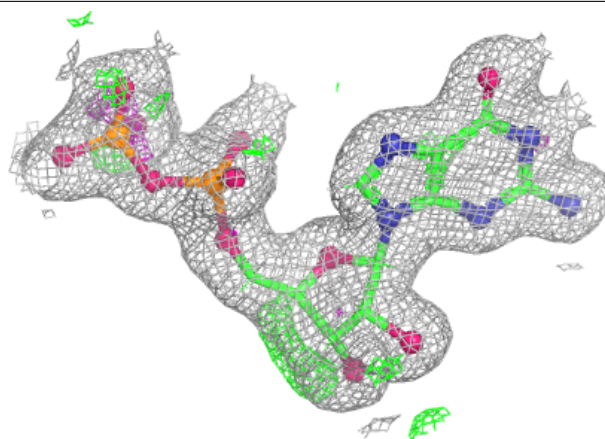
Electron density around PN6 B 501:

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

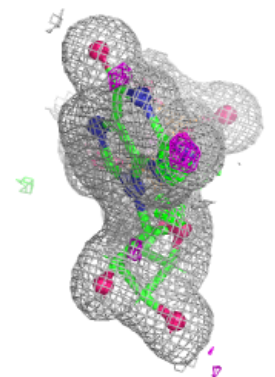
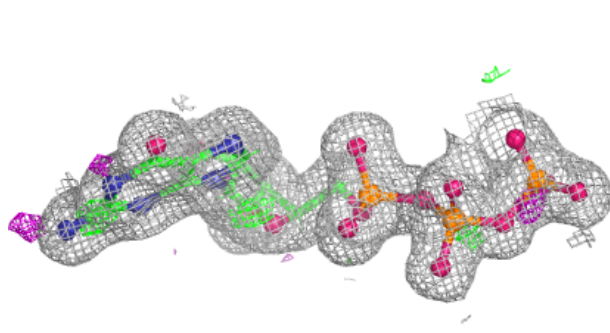
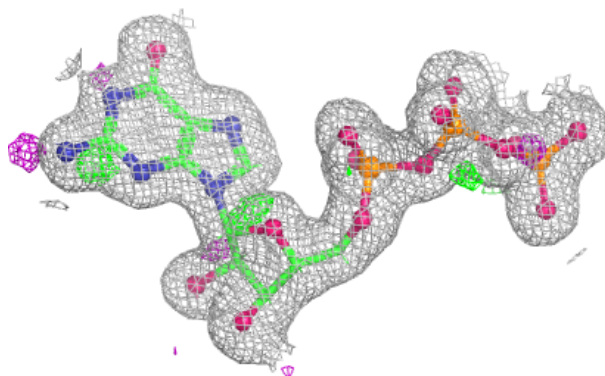


Electron density around GDP B 502:

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

**Electron density around GTP 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.