



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 05:32 PM EDT

PDB ID : 6TIS / pdb_00006tis
Title : DROSOPHILA GDP-TUBULIN
Authors : Gigant, B.
Deposited on : 2019-11-22
Resolution : 2.30 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

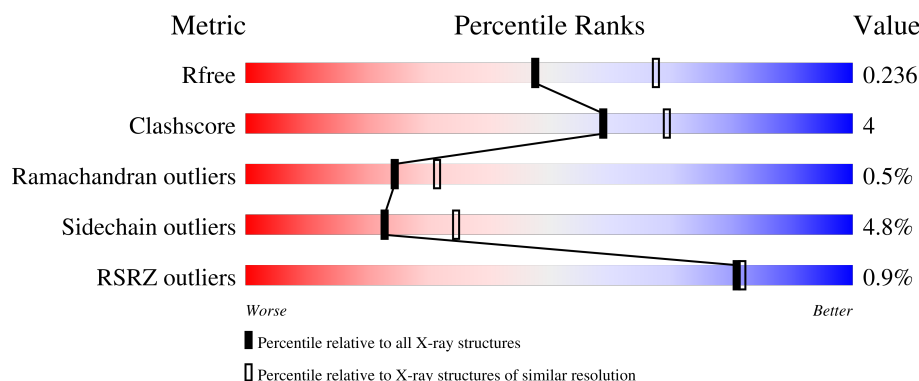
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	450	% 80% 14% • •
1	C	450	% 83% 10% • 5%
2	B	447	82% 13% •
2	D	447	% 86% 9% • •
3	E	143	% 78% 12% • 9%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 15255 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 Tubulin alpha-1 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	433	Total	C	N	O	S	0	0	0
			3388	2146	576	643	23			
1	C	428	Total	C	N	O	S	0	1	0
			3351	2123	568	637	23			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	40	ARG	LYS	engineered mutation	UNP P06603
C	40	ARG	LYS	engineered mutation	UNP P06603

- Molecule 2 is a protein called Tubulin beta-1 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	430	Total	C	N	O	S	0	0	0
			3361	2112	573	650	26			
2	D	429	Total	C	N	O	S	0	1	0
			3356	2108	574	648	26			

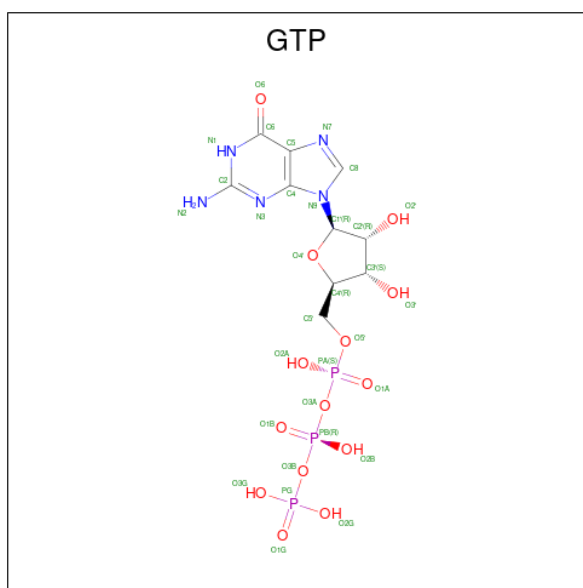
- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	130	Total	C	N	O	S	0	0	0
			1062	655	194	209	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	-	initiating methionine	UNP P63043
E	4	ALA	SER	engineered mutation	UNP P63043
E	14	ALA	CYS	engineered mutation	UNP P63043
E	20	TRP	PHE	engineered mutation	UNP P63043

- 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	N	O	P	0	0
			32	10	5	14	3		
4	C	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

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

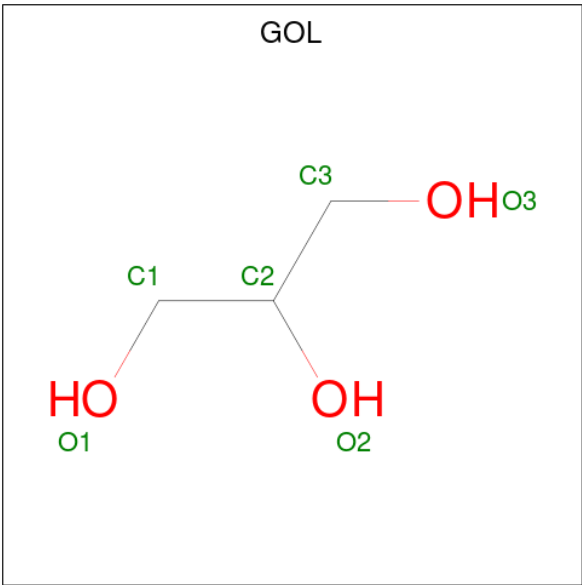
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		
5	C	1	Total	Mg	0	0
			1	1		

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



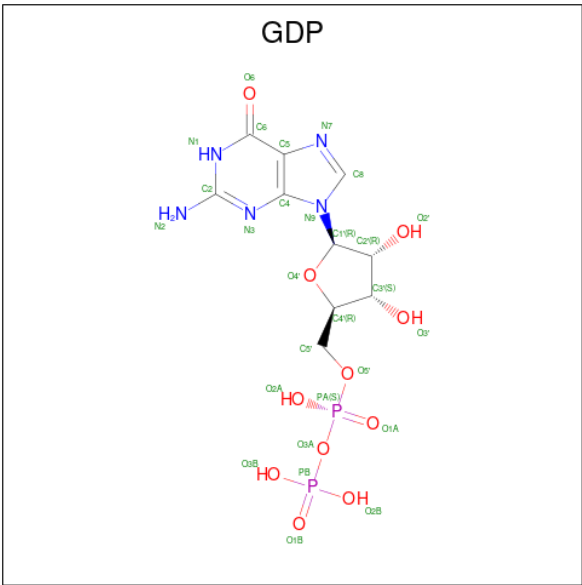
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	C	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



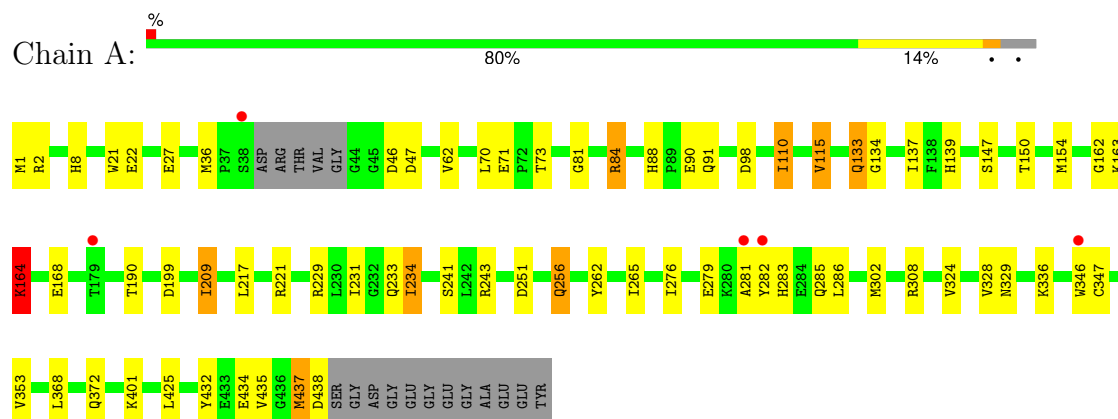
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	148	Total 148	O 148	0	0
9	B	113	Total 113	O 113	0	0
9	C	141	Total 141	O 141	0	0
9	D	120	Total 120	O 120	0	0
9	E	26	Total 26	O 26	0	0

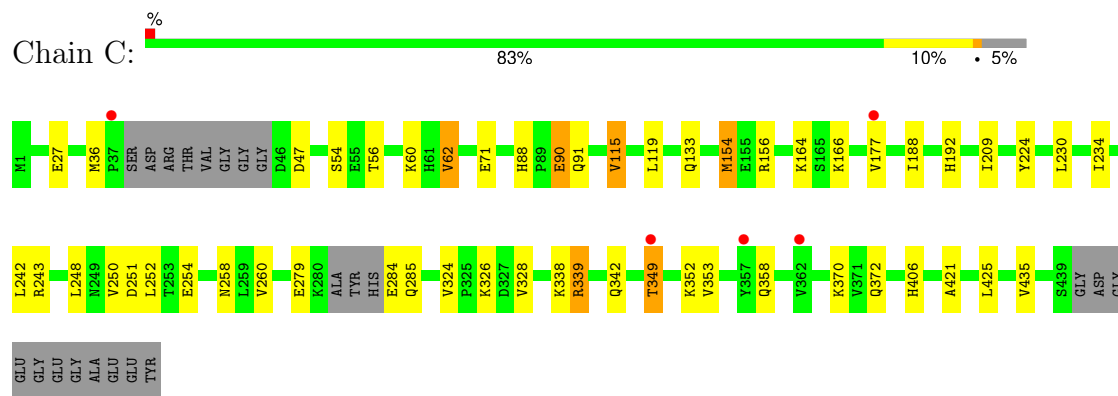
3 Residue-property plots

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.

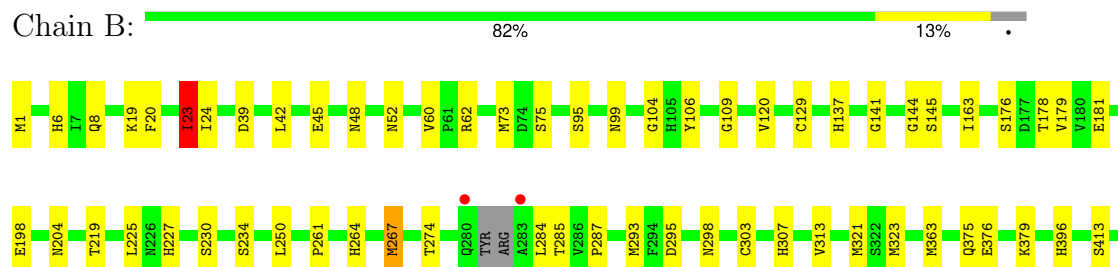
• Molecule 1: Tubulin alpha-1 chain



• Molecule 1: Tubulin alpha-1 chain

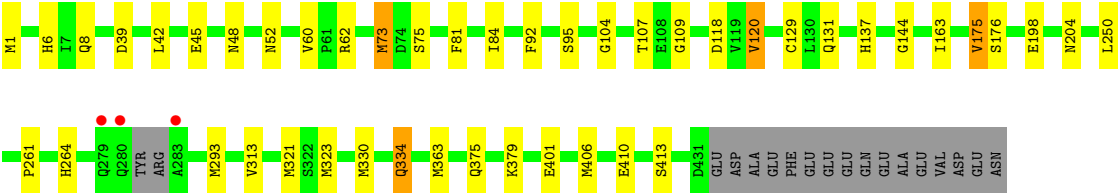
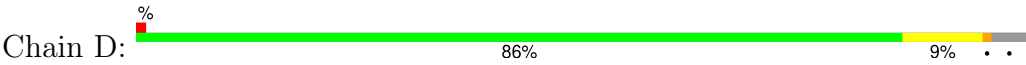


• Molecule 2: Tubulin beta-1 chain

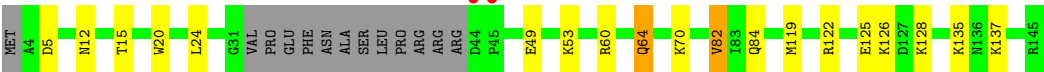
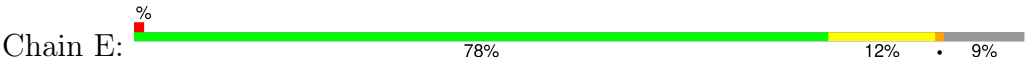


E432
ASP
ALA
GLU
PHE
GLU
GLU
GLN
ALA
ALA
GLU
VAL
ASP
GLU
ASN

• Molecule 2: Tubulin beta-1 chain



• Molecule 3: Stathmin-4



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	66.59Å 126.52Å 250.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.00 – 2.30 33.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	92.1 (33.00-2.30) 92.1 (33.00-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.18 (at 2.29Å)	Xtriage
Refinement program	BUSTER 2.10.3 (3-OCT-2019)	Depositor
R, R_{free}	0.183 , 0.218 0.197 , 0.236	Depositor DCC
R_{free} test set	4349 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	42.0	Xtriage
Anisotropy	1.232	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 54.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	15255	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, GTP, GDP, SO4, MG

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	0.71	0/3465	1.04	3/4703 (0.1%)
1	C	0.72	1/3428 (0.0%)	1.03	4/4653 (0.1%)
2	B	0.71	2/3433 (0.1%)	1.00	2/4650 (0.0%)
2	D	0.71	1/3436 (0.0%)	1.01	3/4653 (0.1%)
3	E	0.63	0/1072	1.14	1/1425 (0.1%)
All	All	0.71	4/14834 (0.0%)	1.03	13/20084 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	107	THR	CA-C	6.76	1.56	1.52
2	B	267	MET	SD-CE	-6.08	1.64	1.79
1	C	154	MET	SD-CE	-5.77	1.65	1.79
2	B	73	MET	SD-CE	-5.53	1.65	1.79

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	118	ASP	CA-CB-CG	7.44	120.04	112.60
1	C	115	VAL	N-CA-CB	6.97	118.70	110.55
2	B	23	ILE	N-CA-CB	6.77	118.47	110.55
1	C	338	LYS	CA-C-N	6.50	129.29	120.38
1	C	338	LYS	C-N-CA	6.50	129.29	120.38
1	C	90	GLU	CB-CG-CD	6.10	122.97	112.60
1	A	115	VAL	N-CA-CB	6.05	117.63	110.55
2	D	95	SER	N-CA-C	5.85	118.60	111.82
2	D	120	VAL	N-CA-CB	5.84	119.35	110.58
1	A	163	LYS	CA-C-N	5.74	132.50	121.54
1	A	163	LYS	C-N-CA	5.74	132.50	121.54
2	B	95	SER	N-CA-C	5.61	118.33	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	12	ASN	CA-CB-CG	5.57	118.17	112.60

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	3388	0	3298	47	0
1	C	3351	0	3261	27	0
2	B	3361	0	3237	40	0
2	D	3356	0	3231	21	0
3	E	1062	0	1067	9	0
4	A	32	0	12	0	0
4	C	32	0	12	0	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
6	A	20	0	0	1	0
6	B	15	0	0	0	0
6	C	5	0	0	0	0
6	D	15	0	0	0	0
7	A	6	0	8	0	0
7	B	6	0	8	0	0
8	B	28	0	12	1	0
8	D	28	0	12	1	0
9	A	148	0	0	1	0
9	B	113	0	0	0	0
9	C	141	0	0	0	0
9	D	120	0	0	0	0
9	E	26	0	0	0	0
All	All	15255	0	14158	128	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 4.

All (128) 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:6:HIS:HE1	2:B:8:GLN:HE21	1.06	0.99
2:D:6:HIS:HE1	2:D:8:GLN:HE21	1.15	0.93
1:A:81:GLY:O	1:A:84:ARG:HG3	1.72	0.90
2:B:6:HIS:CE1	2:B:8:GLN:HE21	1.92	0.86
2:D:204:ASN:HD21	8:D:501:GDP:HN22	1.20	0.86
2:B:204:ASN:HD21	8:B:501:GDP:HN22	1.21	0.85
1:C:339:ARG:H	1:C:339:ARG:HD3	1.44	0.83
2:D:6:HIS:CE1	2:D:8:GLN:HE21	1.99	0.81
2:B:99:ASN:HD22	1:C:258:ASN:HD21	1.30	0.77
1:A:71:GLU:OE2	1:A:73:THR:HB	1.84	0.76
3:E:60:ARG:O	3:E:64:GLN:HG2	1.86	0.74
1:A:133:GLN:HE22	1:A:251:ASP:HB2	1.53	0.74
2:D:261:PRO:O	2:D:264:HIS:HD2	1.72	0.72
1:C:328:VAL:HG11	1:C:353:VAL:HG11	1.72	0.71
1:A:329:ASN:HD21	3:E:20:TRP:HE1	1.40	0.69
2:B:261:PRO:O	2:B:264:HIS:HD2	1.76	0.69
2:B:48:ASN:O	2:B:62:ARG:NH2	2.26	0.67
1:C:27:GLU:OE2	1:C:243:ARG:NH2	2.27	0.65
1:A:401:LYS:NZ	2:B:432:GLU:HB3	2.12	0.65
2:B:285:THR:HG23	2:B:287:PRO:HD2	1.79	0.64
1:A:27:GLU:OE2	1:A:243:ARG:NH2	2.30	0.64
1:C:56:THR:CG2	1:C:60:LYS:HB3	2.28	0.63
2:D:73:MET:HE2	2:D:92:PHE:HB3	1.81	0.63
2:D:48:ASN:O	2:D:62:ARG:NH2	2.31	0.63
2:B:267:MET:CE	2:B:303:CYS:HB2	2.30	0.62
1:A:336:LYS:HD3	3:E:24:LEU:HD13	1.83	0.61
2:B:1:MET:N	2:B:129:CYS:SG	2.72	0.60
2:D:1:MET:N	2:D:129:CYS:SG	2.75	0.60
2:D:137:HIS:HD2	2:D:144:GLY:O	1.84	0.60
1:A:221:ARG:NH2	6:A:506:SO4:O3	2.34	0.59
2:B:227:HIS:HE1	2:B:274:THR:HG23	1.66	0.59
2:B:293:MET:HE3	2:B:313:VAL:HG11	1.84	0.58
2:D:131:GLN:NE2	2:D:250:LEU:H	2.01	0.58
2:D:293:MET:HE3	2:D:313:VAL:HG11	1.83	0.58
1:A:70:LEU:HD13	1:A:110:ILE:HG22	1.85	0.58
2:B:307:HIS:HD2	2:B:376:GLU:OE1	1.87	0.57
1:A:88:HIS:H	1:A:91:GLN:HE21	1.52	0.57
2:B:227:HIS:CE1	2:B:274:THR:HG23	2.39	0.57
1:A:134:GLY:HA2	1:A:164:LYS:HG2	1.86	0.57
1:C:56:THR:HG22	1:C:60:LYS:HB3	1.87	0.57
1:A:328:VAL:HG11	1:A:353:VAL:HG11	1.88	0.56
1:A:262:TYR:HE2	1:A:346:TRP:CH2	2.23	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:GLU:OE2	1:A:73:THR:CB	2.52	0.56
1:C:154:MET:HE3	1:C:166:LYS:HE2	1.89	0.54
1:A:88:HIS:H	1:A:91:GLN:NE2	2.06	0.54
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.43	0.54
2:B:23:ILE:HG12	2:B:230:SER:HB2	1.91	0.53
1:A:2:ARG:HB3	1:A:133:GLN:CD	2.34	0.53
1:C:209:ILE:HG23	1:C:230:LEU:HD23	1.91	0.53
2:B:267:MET:HE3	2:B:303:CYS:HB2	1.91	0.53
2:B:179:VAL:HG23	1:C:349:THR:O	2.09	0.52
2:B:99:ASN:ND2	1:C:258:ASN:HD21	2.05	0.52
1:A:285:GLN:NE2	1:A:372:GLN:H	2.08	0.52
1:C:285:GLN:NE2	1:C:372:GLN:H	2.08	0.52
1:A:46:ASP:O	1:A:47:ASP:HB3	2.08	0.52
1:A:62:VAL:HG11	1:A:88:HIS:HD2	1.76	0.51
2:B:137:HIS:HD2	2:B:144:GLY:O	1.94	0.51
1:A:401:LYS:HZ1	2:B:432:GLU:HB3	1.75	0.51
2:B:19:LYS:O	2:B:23:ILE:HG13	2.11	0.51
2:B:141:GLY:O	2:B:145:SER:OG	2.26	0.50
2:B:267:MET:HE1	2:B:303:CYS:HB2	1.93	0.50
1:A:209:ILE:HD13	1:A:231:ILE:HD11	1.92	0.50
1:A:346:TRP:CZ3	1:A:347:CYS:SG	3.04	0.50
3:E:125:GLU:HA	3:E:128:LYS:HD2	1.94	0.50
2:B:23:ILE:HD12	2:B:24:ILE:HG23	1.93	0.49
2:B:104:GLY:O	2:B:109:GLY:HA3	2.13	0.49
2:D:104:GLY:O	2:D:109:GLY:HA3	2.12	0.49
1:A:62:VAL:HG21	1:A:88:HIS:NE2	2.27	0.49
2:B:99:ASN:HB3	2:B:178:THR:HG21	1.95	0.49
2:D:330:MET:O	2:D:334:GLN:HG2	2.13	0.49
1:C:177:VAL:CG2	1:C:224:TYR:CE1	2.96	0.48
1:C:56:THR:HG21	1:C:60:LYS:HB3	1.96	0.48
1:A:71:GLU:HB2	1:A:98:ASP:HB3	1.94	0.48
2:B:52:ASN:OD1	2:B:62:ARG:NH1	2.47	0.48
1:A:329:ASN:HD21	3:E:20:TRP:NE1	2.07	0.48
2:D:52:ASN:OD1	2:D:62:ARG:NH1	2.47	0.47
1:A:262:TYR:CE2	1:A:346:TRP:CH2	3.01	0.47
1:C:188:ILE:HG13	1:C:425:LEU:HD22	1.96	0.47
1:A:276:ILE:HD11	1:A:286:LEU:HD13	1.96	0.47
1:A:70:LEU:HD13	1:A:110:ILE:CG2	2.44	0.46
1:C:88:HIS:H	1:C:91:GLN:NE2	2.14	0.46
1:C:88:HIS:H	1:C:91:GLN:HE21	1.62	0.46
1:C:133:GLN:HE22	1:C:252:LEU:H	1.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:23:ILE:HD13	2:B:234:SER:HB2	1.96	0.46
1:A:276:ILE:HD13	1:A:283:HIS:NE2	2.31	0.46
1:A:46:ASP:HB3	9:A:629:HOH:O	2.15	0.45
2:B:20:PHE:HA	2:B:23:ILE:HD11	1.98	0.45
2:D:375:GLN:HE21	2:D:379:LYS:HE3	1.80	0.45
3:E:49:GLU:O	3:E:53:LYS:HD2	2.16	0.45
1:A:137:ILE:HD13	1:A:154:MET:SD	2.56	0.45
1:A:150:THR:O	1:A:154:MET:HG2	2.17	0.45
2:D:406:MET:HE3	2:D:410:GLU:HG3	1.99	0.44
2:B:178:THR:HG23	2:B:181:GLU:HG3	2.00	0.44
1:C:406:HIS:CG	2:D:261:PRO:HD3	2.52	0.44
1:A:8:HIS:CE1	1:A:21:TRP:HE1	2.36	0.44
1:A:217:LEU:HD21	1:A:368:LEU:HD23	1.99	0.44
1:C:339:ARG:HD3	1:C:339:ARG:N	2.23	0.43
2:D:401:GLU:HA	3:E:137:LYS:HD3	2.00	0.43
2:B:295:ASP:HB3	2:B:298:ASN:HD22	1.82	0.43
1:A:139:HIS:HE1	1:A:168:GLU:OE1	2.01	0.43
2:B:163:ILE:HG21	2:B:250:LEU:HB3	2.01	0.43
2:B:285:THR:CG2	2:B:287:PRO:HD2	2.48	0.43
2:D:163:ILE:HG21	2:D:250:LEU:HB3	2.00	0.43
2:B:106:TYR:CD1	3:E:82:VAL:HG21	2.54	0.43
1:A:199:ASP:HB3	1:A:256:GLN:HG2	2.00	0.43
1:C:133:GLN:NE2	1:C:252:LEU:H	2.16	0.43
1:C:133:GLN:HE22	1:C:251:ASP:HB2	1.84	0.43
1:A:22:GLU:OE1	1:A:229:ARG:NH1	2.52	0.42
2:D:175:VAL:O	2:D:175:VAL:HG13	2.19	0.42
1:A:401:LYS:HZ2	2:B:432:GLU:HB3	1.83	0.42
1:A:62:VAL:HG11	1:A:88:HIS:CD2	2.54	0.42
1:A:434:GLU:HA	1:A:437:MET:HG2	2.01	0.42
2:B:219:THR:HG21	1:C:326:LYS:O	2.20	0.42
1:A:8:HIS:HE1	1:A:21:TRP:HE1	1.66	0.42
1:C:192:HIS:CG	1:C:421:ALA:HA	2.55	0.42
2:B:375:GLN:HE21	2:B:379:LYS:HE3	1.84	0.41
1:C:119:LEU:HD11	1:C:156:ARG:HB3	2.02	0.41
1:A:147:SER:HB2	1:A:190:THR:HB	2.03	0.41
1:C:54:SER:OG	1:C:62:VAL:HG13	2.19	0.41
2:B:396:HIS:HE1	1:C:260:VAL:O	2.03	0.41
2:D:137:HIS:CD2	2:D:144:GLY:O	2.68	0.41
1:A:209:ILE:CD1	1:A:231:ILE:HD11	2.51	0.41
2:B:99:ASN:ND2	1:C:254:GLU:HG2	2.36	0.40
2:B:106:TYR:CG	3:E:82:VAL:HG21	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:GLN:HG3	1:A:368:LEU:CD1	2.52	0.40
1:A:234:ILE:HD13	1:A:302:MET:SD	2.62	0.40
1:A:262:TYR:HB2	1:A:265:ILE:HD12	2.03	0.40
2:D:81:PHE:O	2:D:84:ILE:HG22	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	429/450 (95%)	414 (96%)	10 (2%)	5 (1%)	10	12
1	C	423/450 (94%)	412 (97%)	9 (2%)	2 (0%)	24	31
2	B	426/447 (95%)	417 (98%)	8 (2%)	1 (0%)	43	55
2	D	426/447 (95%)	419 (98%)	6 (1%)	1 (0%)	43	55
3	E	126/143 (88%)	122 (97%)	4 (3%)	0	100	100
All	All	1830/1937 (94%)	1784 (98%)	37 (2%)	9 (0%)	24	31

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	282	TYR
1	A	437	MET
1	A	164	LYS
1	C	47	ASP
1	C	279	GLU
1	A	162	GLY
1	A	281	ALA
2	B	284	LEU
2	D	175	VAL

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	364/375 (97%)	346 (95%)	18 (5%)	22	34
1	C	361/375 (96%)	342 (95%)	19 (5%)	20	30
2	B	364/382 (95%)	350 (96%)	14 (4%)	29	44
2	D	365/382 (96%)	351 (96%)	14 (4%)	29	44
3	E	112/126 (89%)	102 (91%)	10 (9%)	9	12
All	All	1566/1640 (96%)	1491 (95%)	75 (5%)	23	35

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	36	MET
1	A	84	ARG
1	A	90	GLU
1	A	110	ILE
1	A	115	VAL
1	A	133	GLN
1	A	164	LYS
1	A	209	ILE
1	A	234	ILE
1	A	241	SER
1	A	256	GLN
1	A	279	GLU
1	A	308	ARG
1	A	324	VAL
1	A	425	LEU
1	A	435	VAL
1	A	438	ASP
2	B	23	ILE
2	B	39	ASP
2	B	42	LEU
2	B	45	GLU
2	B	60	VAL

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Mol	Chain	Res	Type
2	B	75	SER
2	B	120	VAL
2	B	176	SER
2	B	198	GLU
2	B	225	LEU
2	B	321	MET
2	B	323	MET
2	B	363	MET
2	B	413	SER
1	C	36	MET
1	C	62	VAL
1	C	71	GLU
1	C	90	GLU
1	C	115	VAL
1	C	164	LYS
1	C	234	ILE
1	C	242	LEU
1	C	248	LEU
1	C	250	VAL
1	C	284	GLU
1	C	324	VAL
1	C	339	ARG
1	C	342	GLN
1	C	349	THR
1	C	352	LYS
1	C	358	GLN
1	C	370	LYS
1	C	435	VAL
2	D	39	ASP
2	D	42	LEU
2	D	45	GLU
2	D	60	VAL
2	D	73	MET
2	D	75	SER
2	D	120	VAL
2	D	176	SER
2	D	198	GLU
2	D	321	MET
2	D	323	MET
2	D	334	GLN
2	D	363	MET
2	D	413	SER

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Mol	Chain	Res	Type
3	E	5	ASP
3	E	15	THR
3	E	64	GLN
3	E	70	LYS
3	E	82	VAL
3	E	84	GLN
3	E	119	MET
3	E	122	ARG
3	E	126	LYS
3	E	135	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	11	GLN
1	A	15	GLN
1	A	88	HIS
1	A	91	GLN
1	A	133	GLN
1	A	139	HIS
1	A	249	ASN
1	A	285	GLN
1	A	301	GLN
1	A	329	ASN
2	B	6	HIS
2	B	11	GLN
2	B	37	HIS
2	B	99	ASN
2	B	137	HIS
2	B	165	ASN
2	B	204	ASN
2	B	227	HIS
2	B	245	GLN
2	B	264	HIS
2	B	292	GLN
2	B	298	ASN
2	B	307	HIS
2	B	332	ASN
2	B	375	GLN
2	B	423	GLN
2	B	424	GLN

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Mol	Chain	Res	Type
2	B	426	GLN
1	C	88	HIS
1	C	91	GLN
1	C	107	HIS
1	C	133	GLN
1	C	139	HIS
1	C	197	HIS
1	C	233	GLN
1	C	256	GLN
1	C	258	ASN
1	C	285	GLN
1	C	301	GLN
1	C	329	ASN
2	D	6	HIS
2	D	37	HIS
2	D	99	ASN
2	D	131	GLN
2	D	137	HIS
2	D	165	ASN
2	D	204	ASN
2	D	264	HIS
2	D	292	GLN
2	D	298	ASN
2	D	332	ASN
2	D	347	ASN
2	D	375	GLN
2	D	423	GLN
2	D	424	GLN
2	D	426	GLN
3	E	18	GLN
3	E	78	HIS
3	E	111	ASN
3	E	129	HIS

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 2 are monoatomic - leaving 17 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	SO4	B	502	-	4,4,4	0.31	0	6,6,6	0.13	0
6	SO4	D	503	-	4,4,4	0.18	0	6,6,6	0.19	0
8	GDP	D	501	-	29,30,30	0.64	1 (3%)	45,47,47	0.52	0
8	GDP	B	501	-	29,30,30	0.46	0	45,47,47	0.65	1 (2%)
6	SO4	A	504	-	4,4,4	0.25	0	6,6,6	0.22	0
6	SO4	B	504	-	4,4,4	0.24	0	6,6,6	0.22	0
4	GTP	C	501	5	33,34,34	0.40	0	50,54,54	0.52	0
6	SO4	A	505	-	4,4,4	0.25	0	6,6,6	0.17	0
6	SO4	A	503	-	4,4,4	0.36	0	6,6,6	0.21	0
6	SO4	C	503	-	4,4,4	0.26	0	6,6,6	0.19	0
6	SO4	D	504	-	4,4,4	0.32	0	6,6,6	0.15	0
4	GTP	A	501	5	33,34,34	0.46	0	50,54,54	0.50	0
6	SO4	D	502	-	4,4,4	0.21	0	6,6,6	0.26	0
7	GOL	A	507	-	5,5,5	0.12	0	5,5,5	0.16	0
6	SO4	A	506	-	4,4,4	0.24	0	6,6,6	0.17	0
6	SO4	B	503	-	4,4,4	0.22	0	6,6,6	0.08	0
7	GOL	B	505	-	5,5,5	0.08	0	5,5,5	0.17	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	GDP	D	501	-	-	3/16/32/32	0/3/3/3
8	GDP	B	501	-	-	3/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GTP	C	501	5	-	8/22/38/38	0/3/3/3
4	GTP	A	501	5	-	8/22/38/38	0/3/3/3
7	GOL	A	507	-	-	0/4/4/4	-
7	GOL	B	505	-	-	0/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	501	GDP	PB-O3B	-2.07	1.47	1.54

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	501	GDP	O3B-PB-O2B	2.64	117.69	107.80

There are no chirality outliers.

All (22) torsion outliers are listed below:

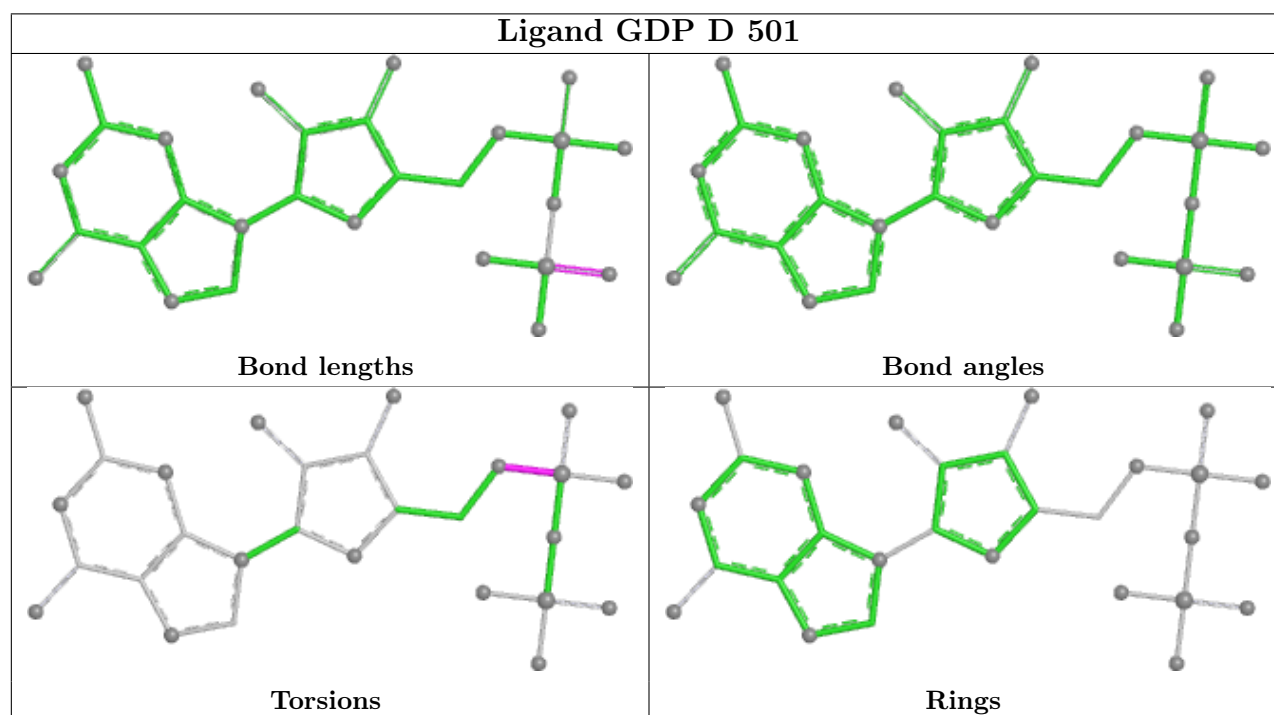
Mol	Chain	Res	Type	Atoms
4	A	501	GTP	C5'-O5'-PA-O3A
4	A	501	GTP	C5'-O5'-PA-O1A
4	A	501	GTP	C5'-O5'-PA-O2A
4	C	501	GTP	C5'-O5'-PA-O3A
4	C	501	GTP	C5'-O5'-PA-O1A
4	C	501	GTP	C5'-O5'-PA-O2A
8	B	501	GDP	C5'-O5'-PA-O3A
8	B	501	GDP	C5'-O5'-PA-O1A
8	B	501	GDP	C5'-O5'-PA-O2A
8	D	501	GDP	C5'-O5'-PA-O3A
8	D	501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

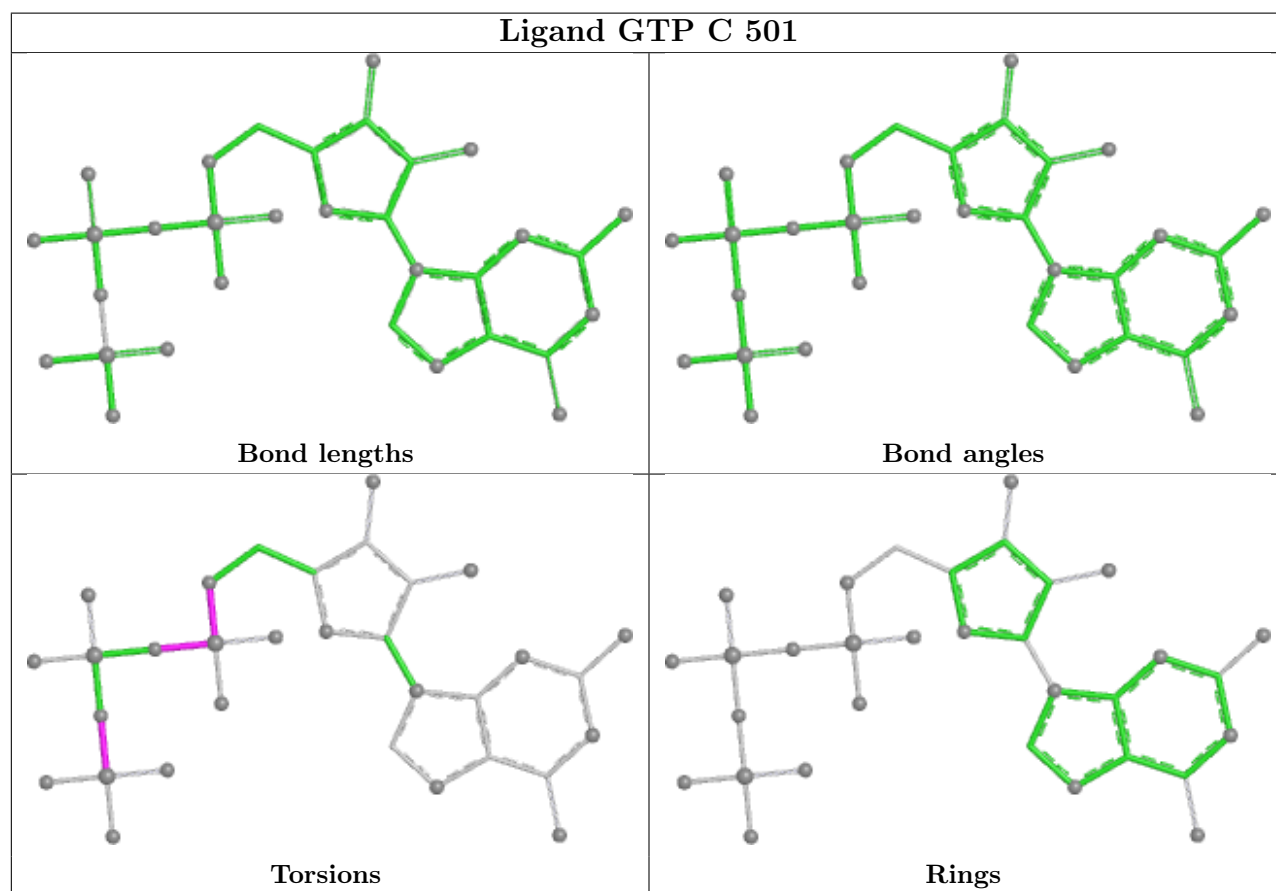
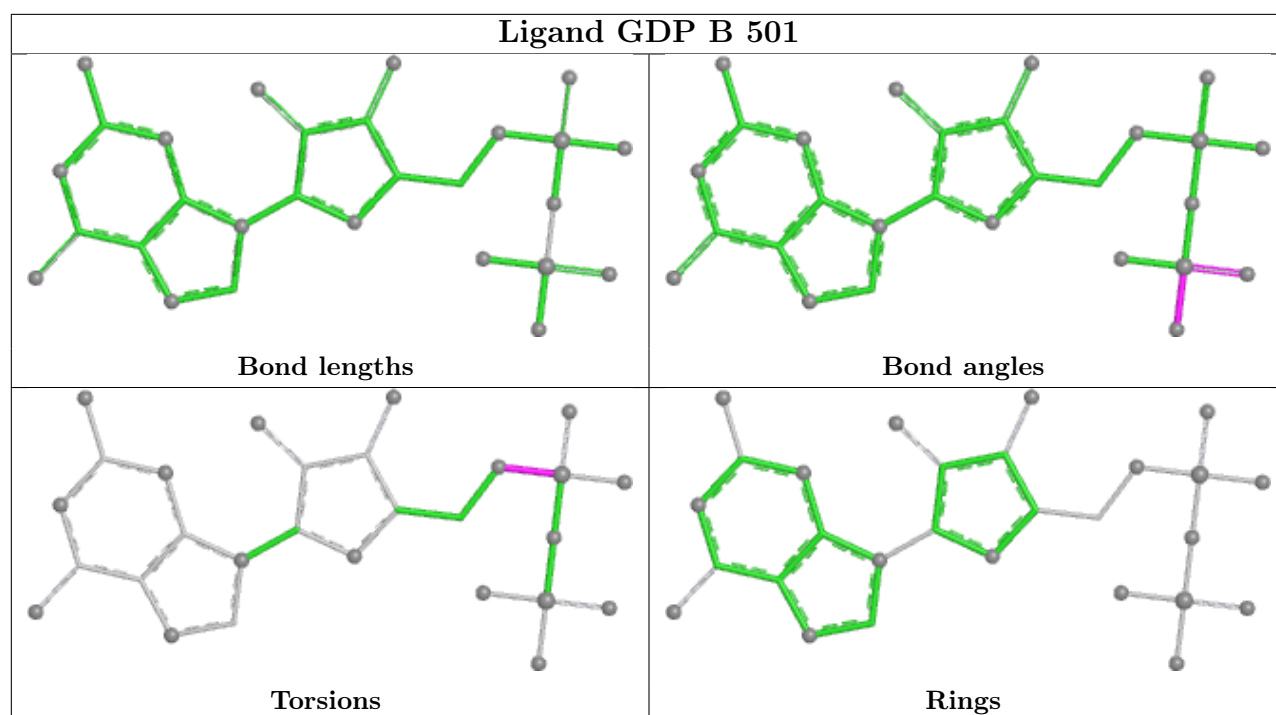
There are no ring outliers.

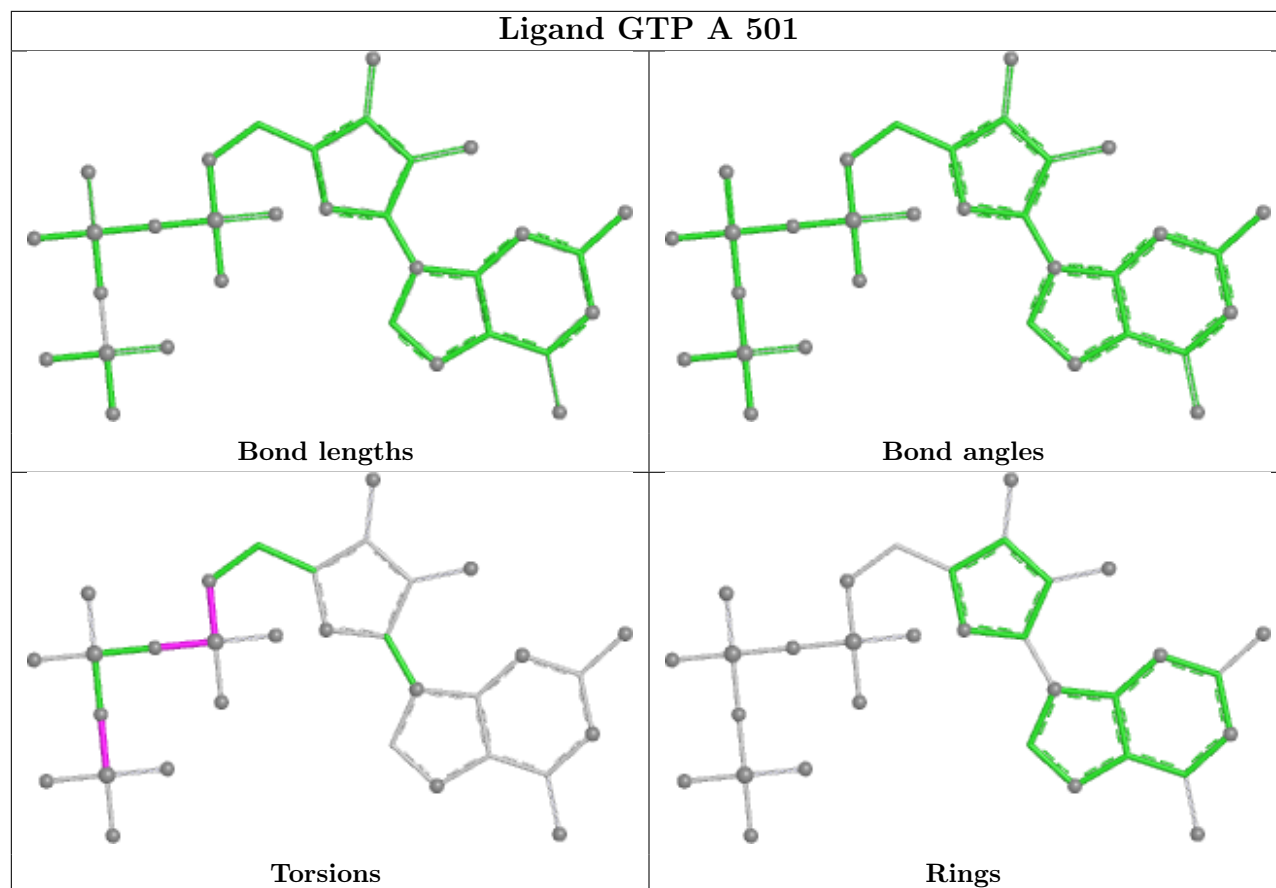
3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	D	501	GDP	1	0
8	B	501	GDP	1	0
6	A	506	SO4	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	433/450 (96%)	0.04	5 (1%) 76 77	48, 65, 87, 116	0
1	C	428/450 (95%)	0.15	5 (1%) 76 77	36, 69, 96, 104	1 (0%)
2	B	430/447 (96%)	0.01	2 (0%) 87 87	49, 63, 93, 114	0
2	D	429/447 (95%)	-0.00	3 (0%) 84 85	42, 61, 86, 97	1 (0%)
3	E	130/143 (90%)	0.27	2 (1%) 72 73	63, 78, 113, 135	0
All	All	1850/1937 (95%)	0.07	17 (0%) 81 82	36, 65, 94, 135	2 (0%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	281	ALA	3.8
2	D	280	GLN	3.7
2	B	283	ALA	3.2
1	C	357	TYR	3.2
2	B	280	GLN	3.1
1	A	282	TYR	2.9
1	A	346	TRP	2.9
1	C	37	PRO	2.6
1	C	349	THR	2.6
2	D	279	GLN	2.5
1	C	362	VAL	2.2
1	C	177	VAL	2.1
1	A	38	SER	2.1
3	E	45	PRO	2.1
2	D	283	ALA	2.1
3	E	44	ASP	2.0
1	A	179	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

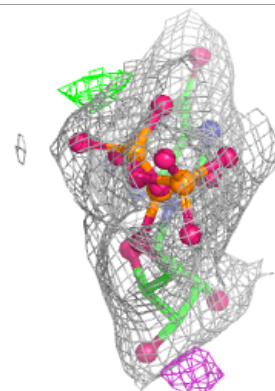
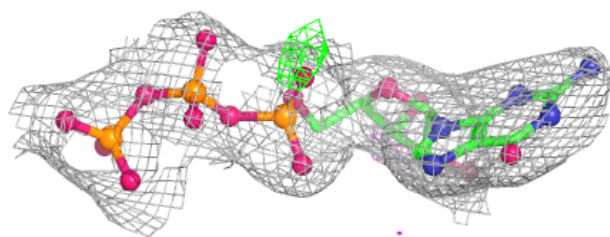
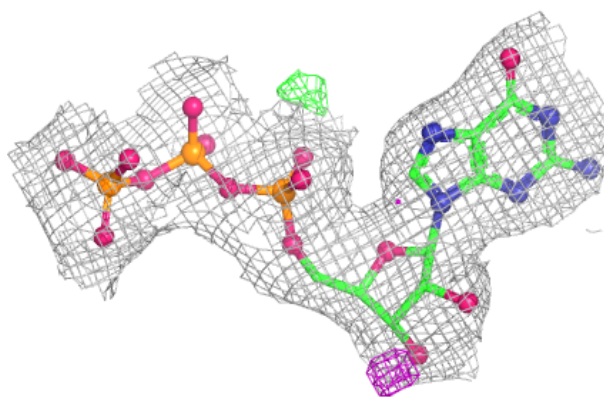
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	GOL	A	507	6/6	0.67	0.22	89,90,90,90	0
6	SO4	C	503	5/5	0.73	0.10	125,125,125,125	0
6	SO4	B	502	5/5	0.77	0.08	126,126,126,126	0
6	SO4	A	505	5/5	0.79	0.14	143,143,143,143	0
6	SO4	A	504	5/5	0.82	0.09	94,94,95,95	0
6	SO4	D	504	5/5	0.83	0.12	123,123,123,123	0
6	SO4	A	506	5/5	0.84	0.12	140,140,140,140	0
6	SO4	A	503	5/5	0.85	0.08	113,114,114,114	0
6	SO4	B	503	5/5	0.86	0.07	113,113,113,113	0
7	GOL	B	505	6/6	0.89	0.17	107,107,107,107	0
6	SO4	D	503	5/5	0.90	0.09	111,111,111,112	0
6	SO4	B	504	5/5	0.91	0.07	111,111,111,111	0
6	SO4	D	502	5/5	0.92	0.08	78,78,78,79	0
4	GTP	C	501	32/32	0.97	0.06	54,61,62,62	0
4	GTP	A	501	32/32	0.97	0.06	50,53,56,56	0
8	GDP	B	501	28/28	0.97	0.05	51,52,55,57	0
8	GDP	D	501	28/28	0.97	0.06	48,50,52,53	0
5	MG	C	502	1/1	0.99	0.04	61,61,61,61	0
5	MG	A	502	1/1	1.00	0.06	56,56,56,56	0

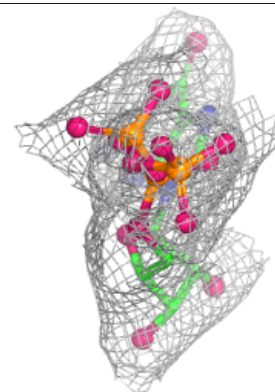
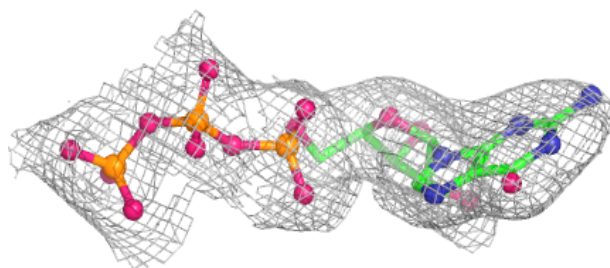
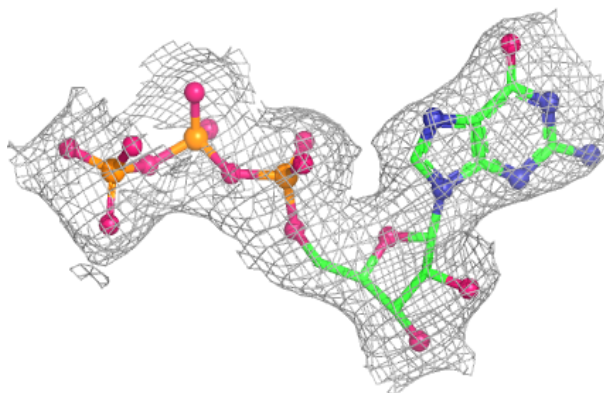
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GTP C 501:

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

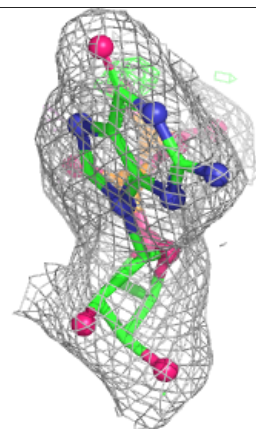
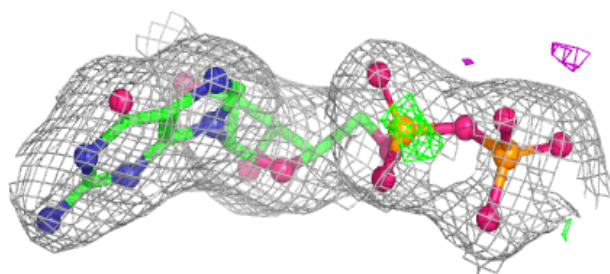
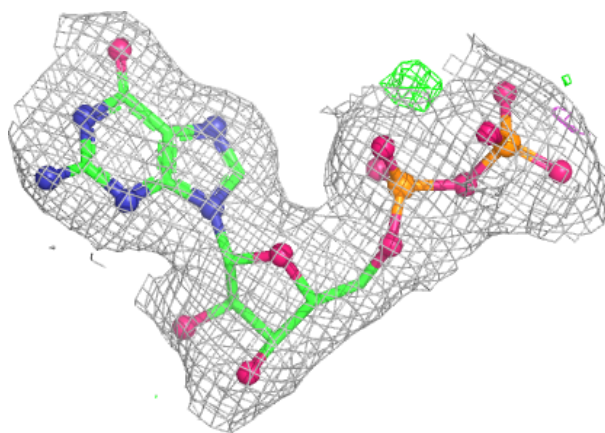
**Electron density around GTP A 501:**

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

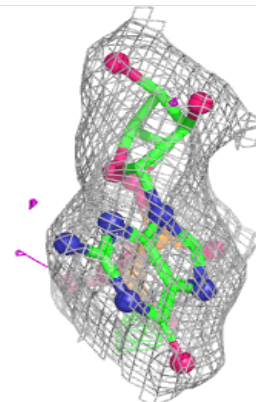
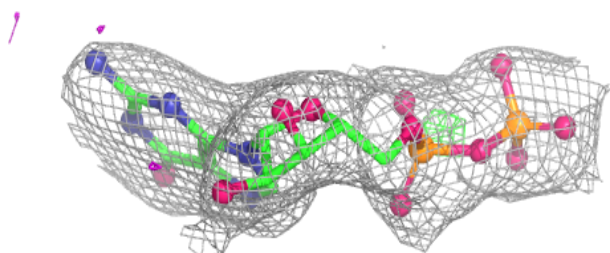
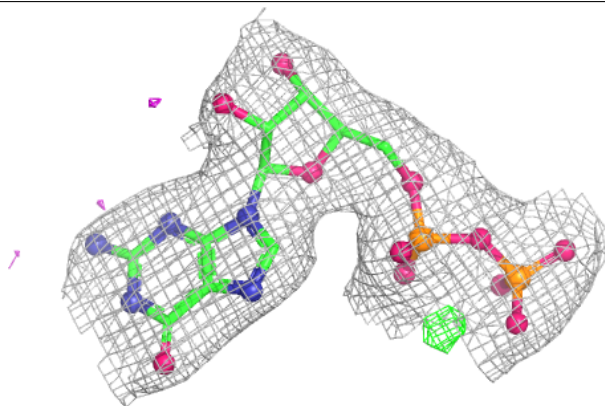


Electron density around GDP B 501:

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

**Electron density around GDP D 501:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.