



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:47 PM UTC

PDB ID : 9U6A / pdb_00009u6a
Title : Tubulin-DARPin D1 in complex with a flavone
Authors : Yan, W.; Yang, J.
Deposited on : 2025-03-22
Resolution : 1.92 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

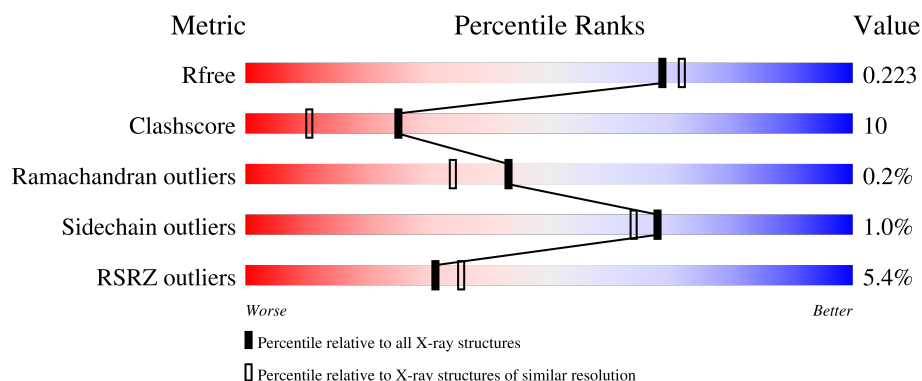
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.92 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	1188 (1.92-1.92)
Clashscore	190562	1209 (1.92-1.92)
Ramachandran outliers	187476	1195 (1.92-1.92)
Sidechain outliers	187428	1195 (1.92-1.92)
RSRZ outliers	180081	1188 (1.92-1.92)

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	451	5% 79% 16% 5%
2	B	431	7% 76% 23% .
3	F	169	% 83% 8% 8%

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 8452 atoms, of which 14 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	429	Total	C	N	O	S	0	1	0
			3341	2120	568	632	21			

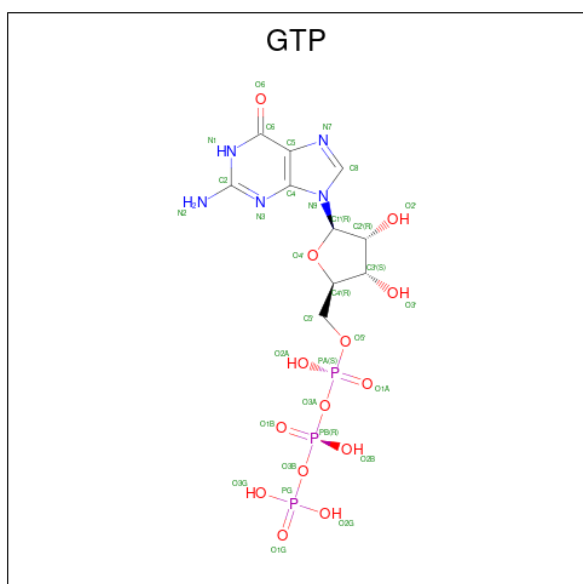
- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	431	Total	C	N	O	S	0	0	0
			3348	2103	571	648	26			

- 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	0	0
			1148	724	195	226	3			

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

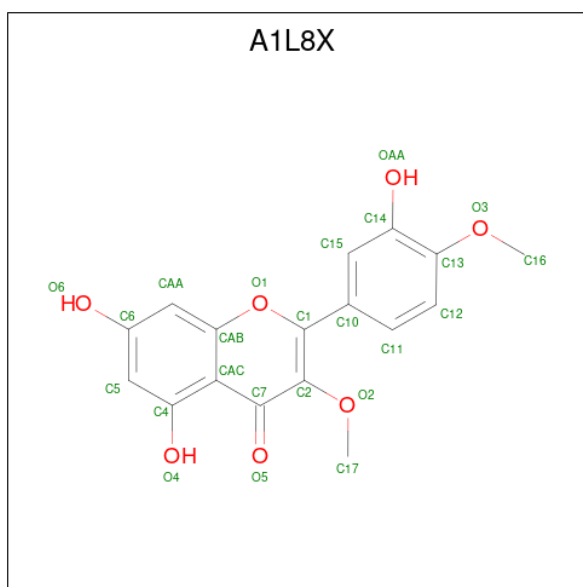


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
4	B	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

- 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	B	1	Total	Mg	0	0
			1	1		

- Molecule 6 is 3-methoxy-2-(4-methoxy-3-oxidanyl-phenyl)-5,7-bis(oxidanyl)chromen-4-one (CCD ID: A1L8X) (formula: C₁₇H₁₄O₇) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	H	O	0	0
			38	17	14	7		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	243	Total	O	0	0
			243	243		
7	B	150	Total	O	0	0
			150	150		

Continued on next page...

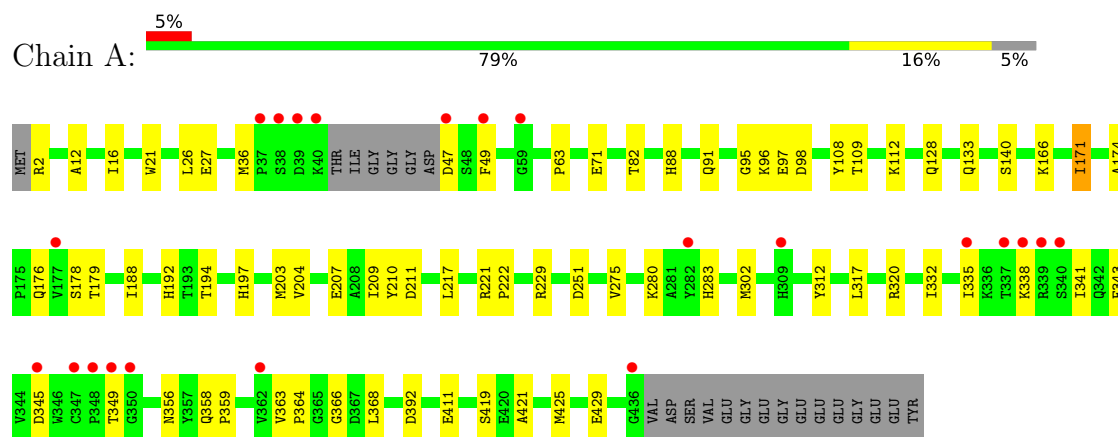
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	F	118	Total 118	O 118	0	0

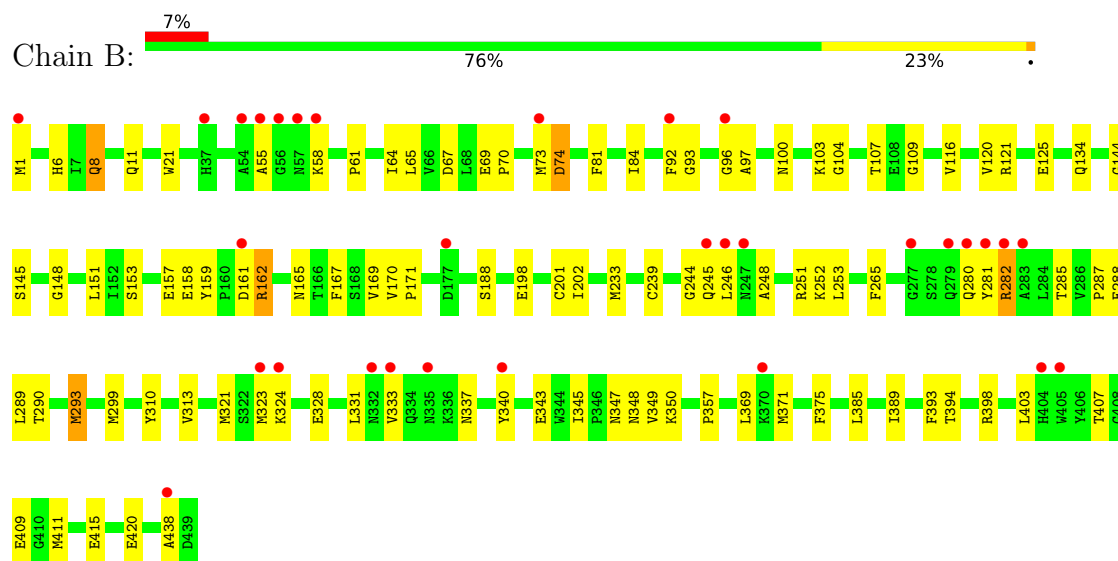
3 Residue-property plots [i](#)

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.

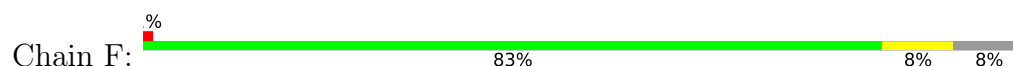
- Molecule 1: Tubulin alpha-1B chain



- Molecule 2: Tubulin beta chain



- Molecule 3: Designed Ankyrin Repeat Protein (DARPIN) D1



MET	ARG	GLY	SER	HIS	HIS	HIS	HIS	HIS	GLY	SER	D13	D28	E29	V30	F31	I32	L33	M34	V40	I62	V65	H69	M79	T111	W112	A121	K144	N156	L161	K167	LEU	ASN
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	-----	-----

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	73.60Å 91.08Å 83.17Å 90.00° 97.28° 90.00°	Depositor
Resolution (Å)	35.07 – 1.92 35.07 – 1.92	Depositor EDS
% Data completeness (in resolution range)	97.5 (35.07-1.92) 97.5 (35.07-1.92)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 1.92Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.183 , 0.224 0.183 , 0.223	Depositor DCC
R_{free} test set	2000 reflections (2.41%)	wwPDB-VP
Wilson B-factor (Å ²)	25.3	Xtriage
Anisotropy	0.397	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 39.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8452	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.43% 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: MG, A1L8X, GTP

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	0.15	0/3421	0.41	2/4648 (0.0%)
2	B	0.15	0/3422	0.38	0/4641
3	F	0.13	0/1164	0.32	0/1583
All	All	0.15	0/8007	0.38	2/10872 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	171	ILE	CA-C-N	5.68	131.73	120.94
1	A	171	ILE	C-N-CA	5.68	131.73	120.94

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	3341	0	3232	55	1
2	B	3348	0	3205	87	0
3	F	1148	0	1145	14	0
4	A	32	0	12	0	0
4	B	32	0	12	1	0
5	A	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	1	0	0	0	0
6	B	24	14	0	6	0
7	A	243	0	0	11	0
7	B	150	0	0	7	0
7	F	118	0	0	0	0
All	All	8438	14	7606	151	1

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 10.

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:6:HIS:HE2	2:B:8:GLN:HG2	1.22	0.99
2:B:73:MET:HE3	2:B:92:PHE:HB2	1.44	0.98
2:B:252:LYS:HB3	6:B:502:A1L8X:C17	2.00	0.92
2:B:6:HIS:NE2	2:B:8:GLN:HG2	1.88	0.88
2:B:170:VAL:HG11	2:B:385:LEU:HD11	1.56	0.88
3:F:34:MET:HE1	3:F:69:HIS:HB2	1.58	0.85
3:F:34:MET:HE3	3:F:40:VAL:CG2	2.10	0.81
2:B:73:MET:CE	2:B:92:PHE:HB2	2.10	0.81
1:A:275:VAL:HG13	1:A:368:LEU:HD21	1.61	0.80
2:B:170:VAL:CG1	2:B:389:ILE:HD11	2.12	0.79
2:B:350:LYS:HD3	6:B:502:A1L8X:O3	1.85	0.77
2:B:159:TYR:HB3	2:B:162:ARG:HG3	1.70	0.74
2:B:69:GLU:OE1	7:B:601:HOH:O	2.05	0.73
2:B:6:HIS:HE2	2:B:8:GLN:CG	2.02	0.72
3:F:111:THR:O	3:F:144:LYS:HE2	1.89	0.72
2:B:70:PRO:HG3	2:B:93:GLY:O	1.89	0.72
2:B:394:THR:O	2:B:398:ARG:HG3	1.91	0.70
2:B:170:VAL:HG13	2:B:389:ILE:HD11	1.75	0.68
4:B:501:GTP:O2G	7:B:602:HOH:O	2.11	0.68
2:B:107:THR:HG21	2:B:409:GLU:OE1	1.96	0.66
3:F:34:MET:HE3	3:F:40:VAL:HG22	1.76	0.66
1:A:95:GLY:O	1:A:96:LYS:HE2	1.97	0.65
1:A:176:GLN:HE22	1:A:207:GLU:HG3	1.61	0.65
1:A:128:GLN:NE2	7:A:604:HOH:O	2.29	0.65
2:B:280:GLN:O	2:B:282:ARG:N	2.30	0.65
2:B:324:LYS:O	2:B:328:GLU:HG3	1.97	0.65
7:A:726:HOH:O	2:B:347:ASN:HB3	2.01	0.61
2:B:121:ARG:O	2:B:125:GLU:HG2	1.99	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:79:MET:HE3	3:F:111:THR:HG21	1.81	0.61
2:B:347:ASN:HB3	7:B:736:HOH:O	1.99	0.61
1:A:95:GLY:C	1:A:96:LYS:HE2	2.25	0.61
2:B:290:THR:HG22	2:B:333:VAL:HG21	1.82	0.60
2:B:393:PHE:CE1	2:B:420:GLU:HB2	2.36	0.60
1:A:47:ASP:N	7:A:605:HOH:O	2.35	0.60
1:A:97:GLU:HG3	2:B:1:MET:HG2	1.83	0.60
2:B:285:THR:HB	2:B:287:PRO:HD2	1.83	0.60
3:F:34:MET:HE3	3:F:40:VAL:HG21	1.82	0.60
1:A:358:GLN:OE1	1:A:359:PRO:HD2	2.02	0.60
7:A:663:HOH:O	2:B:1:MET:HG3	2.02	0.59
3:F:34:MET:HE1	3:F:69:HIS:CB	2.33	0.59
2:B:246:LEU:CD2	2:B:248:ALA:HB2	2.33	0.59
2:B:170:VAL:HG11	2:B:389:ILE:HD11	1.85	0.58
1:A:317:LEU:CD1	1:A:332:ILE:HD11	2.33	0.57
1:A:211:ASP:HB2	7:A:621:HOH:O	2.05	0.57
2:B:350:LYS:HG2	6:B:502:A1L8X:C14	2.34	0.57
3:F:121:ALA:HB1	3:F:161:LEU:HD21	1.85	0.57
2:B:55:ALA:O	2:B:58:LYS:HG2	2.05	0.56
1:A:16:ILE:HD13	1:A:171:ILE:HD11	1.87	0.56
1:A:71:GLU:HG2	1:A:98:ASP:HB3	1.88	0.56
1:A:349:THR:O	1:A:349:THR:HG22	2.05	0.55
1:A:221:ARG:CZ	2:B:323:MET:HB3	2.36	0.55
2:B:96:GLY:HA3	7:B:602:HOH:O	2.07	0.55
3:F:62:ILE:HA	3:F:65:VAL:HG12	1.89	0.54
2:B:73:MET:HG2	2:B:92:PHE:CD1	2.42	0.53
3:F:30:VAL:O	3:F:34:MET:HG3	2.07	0.53
1:A:221:ARG:HD2	2:B:324:LYS:HD2	1.91	0.53
2:B:134:GLN:HA	2:B:165:ASN:O	2.07	0.53
2:B:371:MET:HA	2:B:371:MET:HE2	1.90	0.53
1:A:203:MET:O	1:A:302:MET:HE3	2.08	0.53
1:A:210:TYR:CZ	1:A:222:PRO:HD2	2.44	0.52
7:A:802:HOH:O	2:B:1:MET:HB2	2.10	0.52
2:B:245:GLN:NE2	7:B:605:HOH:O	2.27	0.52
2:B:289:LEU:HD11	2:B:371:MET:HB3	1.90	0.52
1:A:36:MET:HE1	1:A:49:PHE:CE2	2.45	0.52
1:A:210:TYR:CE1	1:A:222:PRO:HD2	2.45	0.52
1:A:317:LEU:HD13	1:A:332:ILE:HD11	1.90	0.52
2:B:81:PHE:O	2:B:84:ILE:HG22	2.10	0.52
2:B:104:GLY:O	2:B:109:GLY:HA3	2.11	0.51
2:B:407:THR:HA	2:B:411:MET:O	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:763:HOH:O	2:B:350:LYS:HG3	2.11	0.51
1:A:179:THR:HG21	7:A:710:HOH:O	2.11	0.50
2:B:169:VAL:HA	2:B:202:ILE:O	2.11	0.50
2:B:11:GLN:HB2	7:B:678:HOH:O	2.11	0.50
2:B:74:ASP:N	2:B:74:ASP:OD1	2.45	0.50
1:A:343:PHE:CD1	1:A:349:THR:HG23	2.47	0.50
2:B:161:ASP:O	2:B:251:ARG:NH2	2.44	0.50
1:A:109:THR:HG21	1:A:411:GLU:OE1	2.11	0.50
3:F:34:MET:CE	3:F:69:HIS:HB2	2.37	0.49
2:B:248:ALA:HB1	6:B:502:A1L8X:O4	2.12	0.49
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.48	0.49
2:B:253:LEU:HD13	6:B:502:A1L8X:CAB	2.42	0.49
2:B:343:GLU:HG2	2:B:438:ALA:HB2	1.95	0.49
7:A:601:HOH:O	2:B:350:LYS:HE2	2.11	0.49
2:B:116:VAL:HG11	2:B:151:LEU:HD11	1.94	0.48
2:B:321:MET:HE2	2:B:371:MET:CE	2.43	0.48
2:B:244:GLY:C	2:B:246:LEU:H	2.22	0.48
1:A:108:TYR:O	1:A:112:LYS:HB3	2.14	0.47
2:B:415:GLU:OE1	7:B:603:HOH:O	2.20	0.47
7:A:601:HOH:O	2:B:350:LYS:CE	2.63	0.47
1:A:217:LEU:HD21	1:A:368:LEU:HD23	1.96	0.47
1:A:363:VAL:HG12	1:A:364:PRO:O	2.15	0.47
2:B:67:ASP:HB3	2:B:92:PHE:CD2	2.50	0.47
1:A:335:ILE:HG23	1:A:341:ILE:HD12	1.97	0.46
2:B:285:THR:OG1	2:B:288:GLU:HG3	2.15	0.46
1:A:166:LYS:HE2	1:A:197:HIS:O	2.15	0.46
1:A:320:ARG:HA	1:A:356:ASN:O	2.16	0.46
2:B:246:LEU:HD22	2:B:248:ALA:HB2	1.97	0.46
2:B:64:ILE:HD12	2:B:120:VAL:HG22	1.97	0.46
2:B:67:ASP:O	2:B:92:PHE:HA	2.16	0.46
2:B:201:CYS:SG	2:B:265:PHE:HB3	2.56	0.46
2:B:246:LEU:HD23	2:B:248:ALA:HB2	1.97	0.46
1:A:174:ALA:O	1:A:178:SER:HB3	2.16	0.46
1:A:176:GLN:NE2	1:A:207:GLU:HG3	2.28	0.46
1:A:178:SER:C	7:A:601:HOH:O	2.58	0.46
2:B:285:THR:CB	2:B:287:PRO:HD2	2.45	0.46
1:A:312:TYR:CE2	1:A:341:ILE:HG23	2.50	0.46
2:B:310:TYR:CE1	2:B:375:PHE:HZ	2.33	0.45
2:B:398:ARG:HD2	3:F:112:TRP:NE1	2.31	0.45
2:B:145:SER:HB2	2:B:188:SER:OG	2.16	0.45
2:B:100:ASN:HB3	2:B:103:LYS:HD2	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:153:SER:O	2:B:157:GLU:HG3	2.18	0.44
2:B:65:LEU:N	2:B:65:LEU:HD12	2.33	0.44
2:B:144:GLY:O	2:B:148:GLY:HA3	2.18	0.44
1:A:27:GLU:CD	1:A:320:ARG:HH22	2.26	0.43
2:B:337:ASN:HB3	2:B:340:TYR:HD2	1.83	0.43
2:B:345:ILE:HG22	2:B:348:ASN:HB3	1.98	0.43
1:A:280:LYS:O	1:A:283:HIS:HD2	2.01	0.43
1:A:12:ALA:HB3	1:A:140:SER:HB3	2.00	0.43
2:B:167:PHE:CE2	2:B:233:MET:HG2	2.54	0.43
2:B:170:VAL:HG13	2:B:171:PRO:HD2	2.00	0.43
1:A:16:ILE:CD1	1:A:171:ILE:HD11	2.48	0.42
1:A:26:LEU:HD12	1:A:363:VAL:HG22	2.01	0.42
2:B:121:ARG:NH2	2:B:158:GLU:OE2	2.51	0.42
3:F:34:MET:CE	3:F:69:HIS:CB	2.97	0.42
1:A:392:ASP:OD2	1:A:429:GLU:OE2	2.37	0.42
1:A:88:HIS:HB2	1:A:91:GLN:HG2	2.01	0.42
1:A:358:GLN:CD	1:A:359:PRO:HD2	2.45	0.42
2:B:313:VAL:HB	2:B:349:VAL:HG22	2.01	0.42
2:B:97:ALA:O	2:B:103:LYS:HD2	2.20	0.41
1:A:2:ARG:HG2	1:A:2:ARG:HH21	1.85	0.41
3:F:28:ASP:O	3:F:32:ILE:HG12	2.19	0.41
1:A:188:ILE:HD12	1:A:425:MET:HG3	2.01	0.41
1:A:229[A]:ARG:HD2	1:A:366:GLY:HA2	2.01	0.41
2:B:244:GLY:C	2:B:246:LEU:N	2.77	0.41
2:B:21:TRP:CZ3	2:B:61:PRO:HB3	2.55	0.41
2:B:252:LYS:CB	6:B:502:A1L8X:C17	2.85	0.41
2:B:357:PRO:HB2	2:B:369:LEU:O	2.21	0.41
1:A:188:ILE:HG23	1:A:425:MET:HG3	2.02	0.41
1:A:209:ILE:HD11	1:A:302:MET:HG3	2.03	0.41
2:B:293:MET:O	2:B:299:MET:HE1	2.21	0.41
1:A:97:GLU:OE1	2:B:1:MET:HE2	2.21	0.41
1:A:192:HIS:CG	1:A:421:ALA:HA	2.56	0.41
1:A:204:VAL:HG22	1:A:302:MET:SD	2.61	0.41
2:B:239:CYS:O	2:B:248:ALA:HB3	2.21	0.41
1:A:194:THR:HG22	1:A:194:THR:O	2.20	0.40
1:A:204:VAL:HA	1:A:302:MET:HG2	2.03	0.40
1:A:221:ARG:HD3	2:B:323:MET:HB2	2.03	0.40
1:A:338:LYS:C	1:A:338:LYS:HD3	2.46	0.40
2:B:321:MET:HE2	2:B:371:MET:HE1	2.03	0.40
1:A:133:GLN:OE1	1:A:251:ASP:HB2	2.22	0.40
2:B:245:GLN:O	2:B:245:GLN:CG	2.69	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:THR:OG1	1:A:345:ASP:OD2[2_845]	1.81	0.39

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	426/451 (94%)	416 (98%)	10 (2%)	0	100	100
2	B	429/431 (100%)	415 (97%)	12 (3%)	2 (0%)	24	14
3	F	153/169 (90%)	150 (98%)	3 (2%)	0	100	100
All	All	1008/1051 (96%)	981 (97%)	25 (2%)	2 (0%)	43	34

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	281	TYR
2	B	282	ARG

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	356/379 (94%)	355 (100%)	1 (0%)	86	86
2	B	362/370 (98%)	355 (98%)	7 (2%)	50	37

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	F	119/132 (90%)	119 (100%)	0	100	100
All	All	837/881 (95%)	829 (99%)	8 (1%)	68	64

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	419	SER
2	B	8	GLN
2	B	74	ASP
2	B	162	ARG
2	B	198	GLU
2	B	293	MET
2	B	331	LEU
2	B	403	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	128	GLN
1	A	256	GLN
2	B	37	HIS
2	B	134	GLN
2	B	247	ASN
2	B	329	GLN
2	B	383	GLN
2	B	431	GLN
2	B	434	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

Of 5 ligands modelled in this entry, 2 are 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	A1L8X	B	502	-	26,26,26	1.83	4 (15%)	38,38,38	2.31	18 (47%)
4	GTP	A	501	5	33,34,34	0.97	2 (6%)	50,54,54	1.50	8 (16%)
4	GTP	B	501	5	33,34,34	0.85	1 (3%)	50,54,54	1.88	12 (24%)

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	A1L8X	B	502	-	-	2/8/8/8	0/3/3/3
4	GTP	A	501	5	-	6/22/38/38	0/3/3/3
4	GTP	B	501	5	-	4/22/38/38	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	502	A1L8X	C10-C1	5.26	1.55	1.47
6	B	502	A1L8X	CAA-CAB	3.81	1.45	1.38
6	B	502	A1L8X	O1-C1	3.29	1.41	1.37
6	B	502	A1L8X	C15-C14	2.94	1.43	1.38
4	A	501	GTP	C2-N3	2.21	1.38	1.33
4	A	501	GTP	PA-O3A	2.18	1.61	1.59
4	B	501	GTP	C2-N3	2.17	1.38	1.33

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	501	GTP	C2-N3-C4	5.82	122.32	112.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	501	GTP	C5-C4-N3	-5.30	119.95	128.39
6	B	502	A1L8X	O3-C13-C14	4.77	121.70	114.55
4	A	501	GTP	C5-C4-N3	-4.77	120.81	128.39
4	A	501	GTP	C2-N3-C4	4.42	119.91	112.30
6	B	502	A1L8X	C16-O3-C13	4.12	123.56	117.51
6	B	502	A1L8X	C11-C10-C15	-3.94	114.69	119.25
6	B	502	A1L8X	CAB-O1-C1	3.81	126.51	120.67
4	B	501	GTP	C2-N1-C6	-3.76	118.29	125.11
6	B	502	A1L8X	O4-C4-CAC	-3.51	114.64	121.14
4	B	501	GTP	C5-C6-N1	3.47	122.09	113.25
4	B	501	GTP	N9-C4-N3	3.44	132.83	125.95
6	B	502	A1L8X	O1-CAB-CAA	3.40	120.65	115.83
4	B	501	GTP	N9-C8-N7	-3.08	107.70	113.40
4	B	501	GTP	O6-C6-C5	-3.03	118.54	126.53
6	B	502	A1L8X	C1-C2-C7	-2.99	118.89	122.02
6	B	502	A1L8X	OAA-C14-C13	-2.98	113.14	120.13
6	B	502	A1L8X	C5-C4-CAC	2.97	124.24	120.92
6	B	502	A1L8X	C12-C11-C10	2.91	123.91	120.80
6	B	502	A1L8X	C15-C10-C1	2.85	124.67	120.65
4	A	501	GTP	C2-N1-C6	-2.81	120.02	125.11
6	B	502	A1L8X	C4-CAC-C7	2.78	125.55	121.45
4	A	501	GTP	N9-C4-N3	2.74	131.43	125.95
6	B	502	A1L8X	C12-C13-C14	-2.63	116.76	119.87
4	B	501	GTP	C8-N7-C5	2.63	108.94	104.26
4	A	501	GTP	N9-C8-N7	-2.62	108.53	113.40
6	B	502	A1L8X	C10-C15-C14	2.54	122.30	120.09
4	A	501	GTP	C5-C6-N1	2.47	119.53	113.25
4	A	501	GTP	C8-N7-C5	2.43	108.59	104.26
6	B	502	A1L8X	OAA-C14-C15	2.39	125.90	119.45
6	B	502	A1L8X	CAB-CAC-C7	-2.32	117.23	120.03
6	B	502	A1L8X	CAC-C7-C2	2.30	119.97	115.66
4	B	501	GTP	N2-C2-N1	2.27	121.54	116.76
4	B	501	GTP	O2B-PB-O3B	2.25	113.37	107.27
4	B	501	GTP	N1-C2-N3	-2.24	119.22	123.32
6	B	502	A1L8X	O1-C1-C10	2.12	113.84	110.87
4	B	501	GTP	C6-C5-N7	2.06	134.04	130.29
4	A	501	GTP	O6-C6-C5	-2.06	121.10	126.53

There are no chirality outliers.

All (12) torsion outliers are listed below:

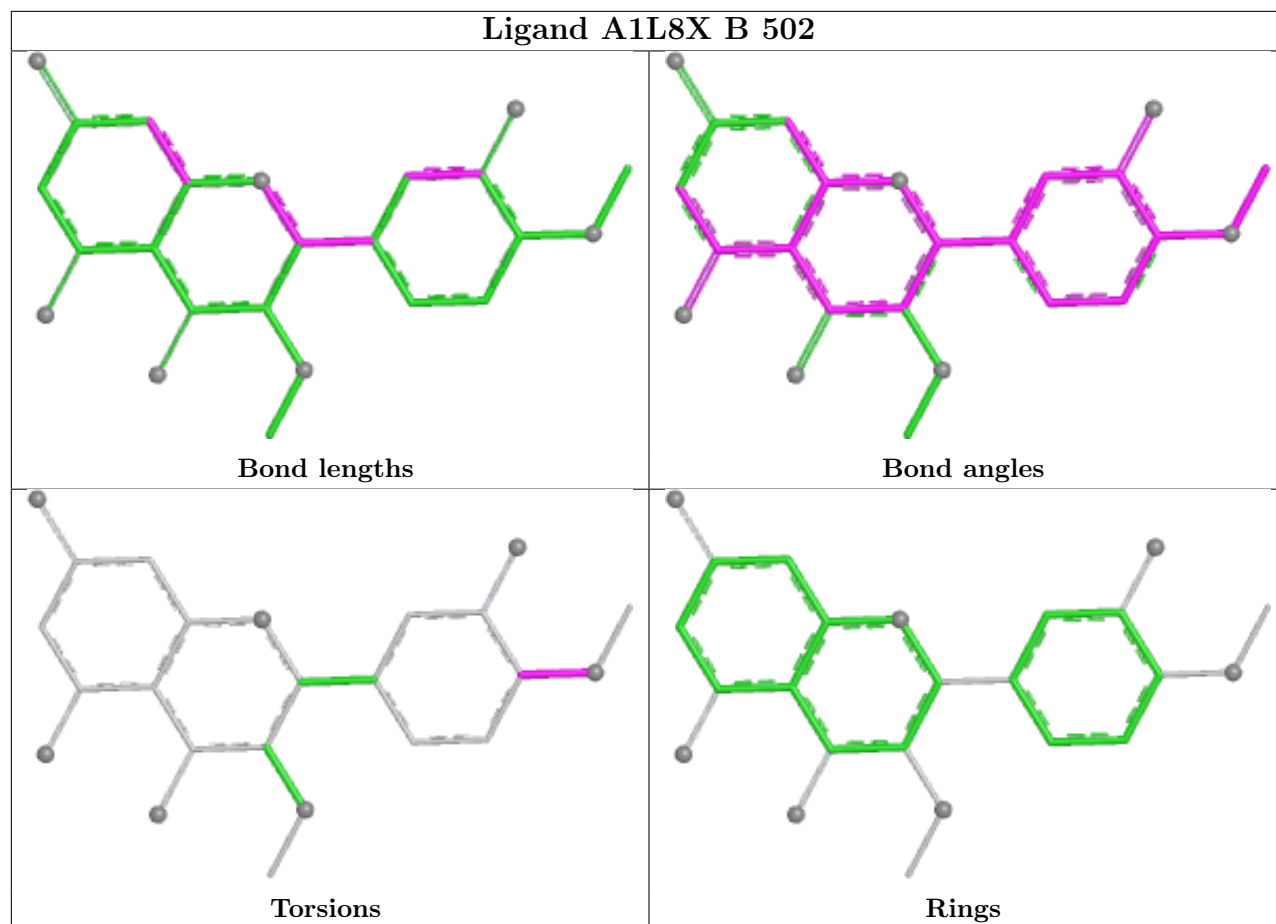
Mol	Chain	Res	Type	Atoms
4	A	501	GTP	C5'-O5'-PA-O3A
4	A	501	GTP	C5'-O5'-PA-O1A
4	A	501	GTP	C5'-O5'-PA-O2A
4	B	501	GTP	C5'-O5'-PA-O3A
4	B	501	GTP	C5'-O5'-PA-O1A
4	B	501	GTP	C5'-O5'-PA-O2A
6	B	502	A1L8X	C14-C13-O3-C16
6	B	502	A1L8X	C12-C13-O3-C16
4	B	501	GTP	PB-O3B-PG-O2G
4	A	501	GTP	PB-O3B-PG-O1G
4	A	501	GTP	PB-O3B-PG-O2G
4	A	501	GTP	PB-O3B-PG-O3G

There are no ring outliers.

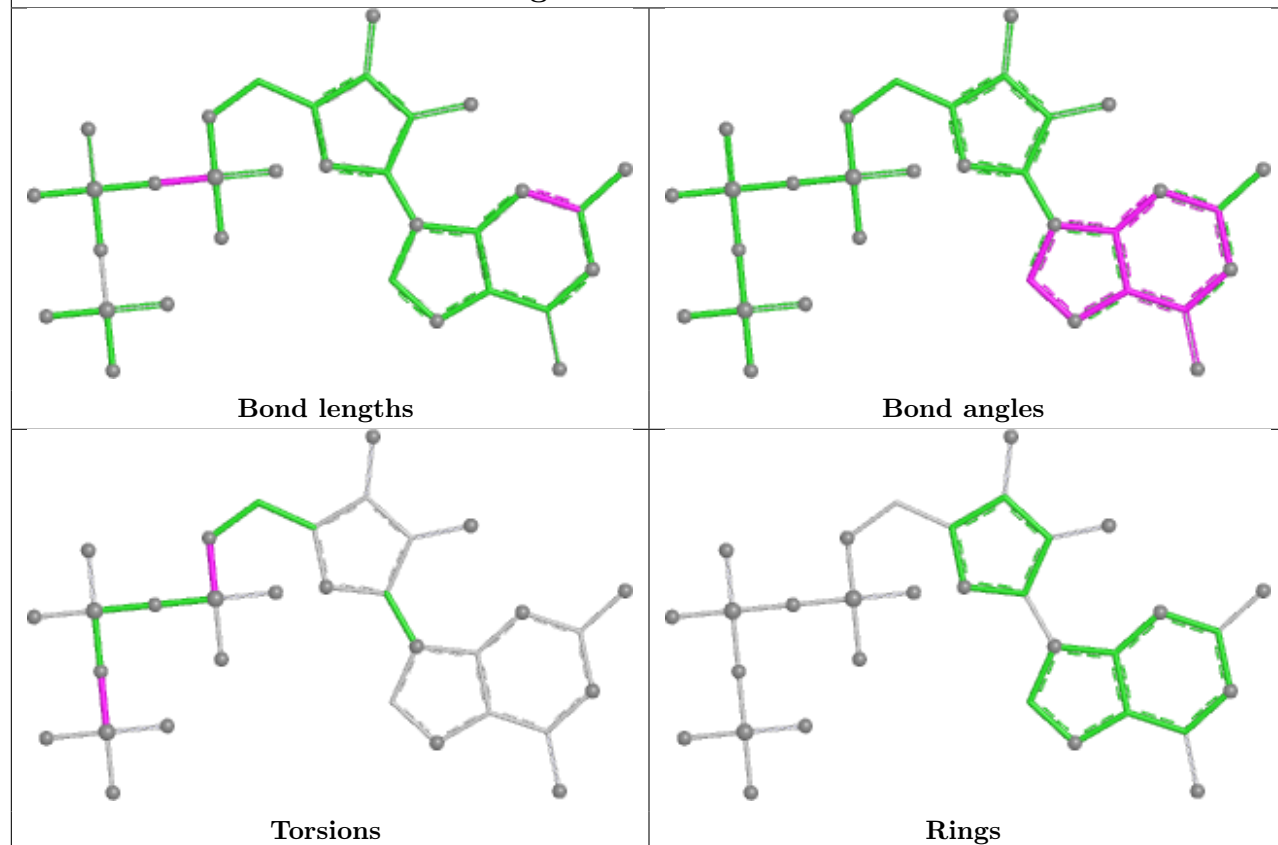
2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	502	A1L8X	6	0
4	B	501	GTP	1	0

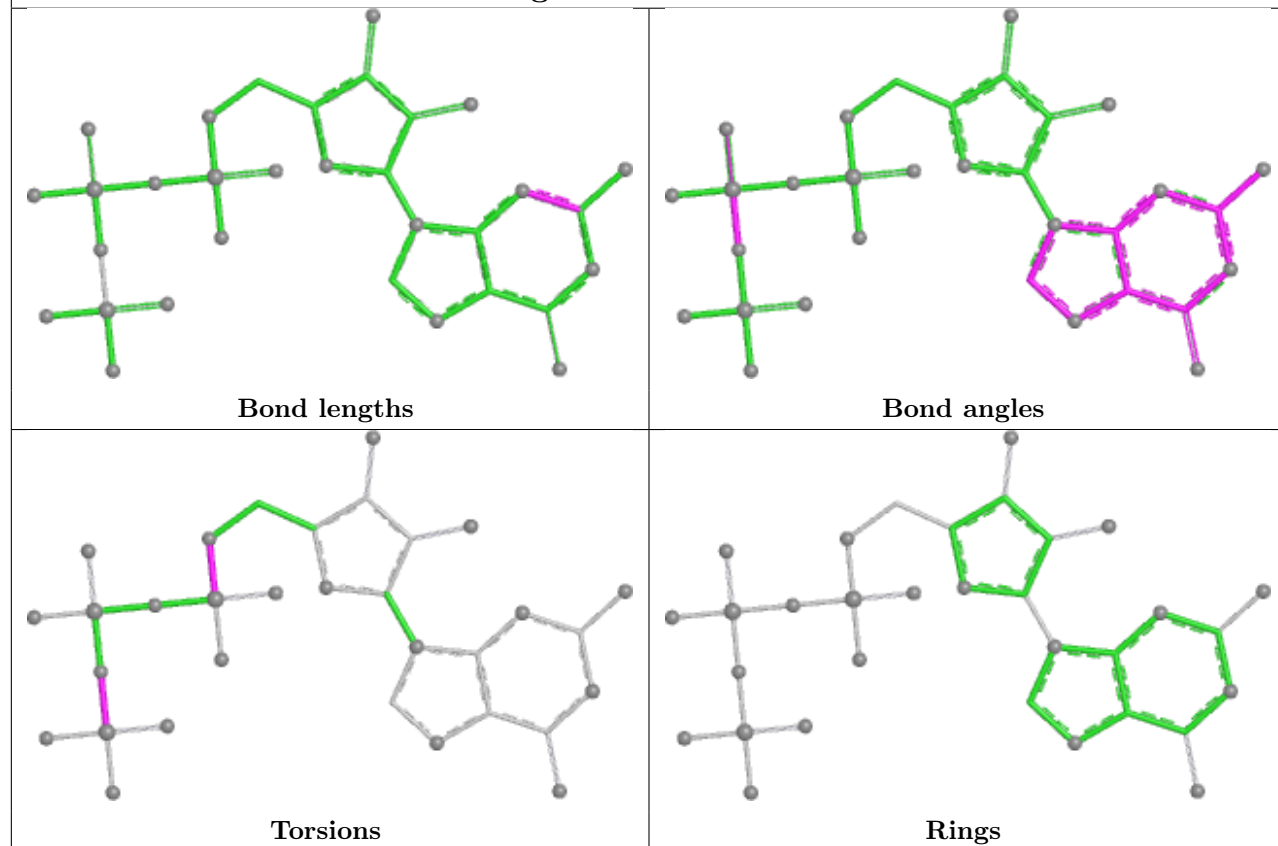
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



Ligand GTP A 501



Ligand GTP B 501



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	429/451 (95%)	0.01	22 (5%) 33 37	15, 25, 44, 83	2 (0%)
2	B	431/431 (100%)	0.44	31 (7%) 21 26	18, 32, 58, 89	0
3	F	155/169 (91%)	-0.17	2 (1%) 75 82	17, 23, 39, 58	0
All	All	1015/1051 (96%)	0.17	55 (5%) 31 35	15, 27, 52, 89	2 (0%)

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	281	TYR	5.2
2	B	283	ALA	5.2
2	B	1	MET	4.7
1	A	38	SER	4.2
1	A	337	THR	3.9
1	A	40	LYS	3.7
1	A	47	ASP	3.6
1	A	436	GLY	3.6
2	B	92	PHE	3.5
2	B	282	ARG	3.5
2	B	73	MET	3.3
2	B	279	GLN	3.3
2	B	54	ALA	3.2
1	A	347	CYS	3.2
2	B	246	LEU	3.2
2	B	438	ALA	3.2
1	A	362	VAL	3.2
2	B	177	ASP	3.1
1	A	349	THR	3.1
2	B	58	LYS	3.0
2	B	277	GLY	2.9
2	B	55	ALA	2.8
3	F	156	ASN	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	404	HIS	2.8
1	A	340	SER	2.7
1	A	339	ARG	2.7
2	B	405	TRP	2.7
1	A	345	ASP	2.6
2	B	245	GLN	2.6
2	B	280	GLN	2.6
1	A	39	ASP	2.5
1	A	49	PHE	2.5
2	B	37	HIS	2.5
1	A	335	ILE	2.5
3	F	167	LYS	2.5
1	A	177	VAL	2.4
2	B	335	ASN	2.4
1	A	37	PRO	2.4
2	B	57	ASN	2.4
1	A	348	PRO	2.3
2	B	324	LYS	2.3
1	A	309	HIS	2.3
2	B	340	TYR	2.3
2	B	56	GLY	2.2
2	B	247	ASN	2.2
2	B	161	ASP	2.2
1	A	59	GLY	2.2
2	B	332	ASN	2.1
1	A	350	GLY	2.1
1	A	282	TYR	2.1
2	B	370	LYS	2.1
2	B	96	GLY	2.1
2	B	323	MET	2.1
2	B	333	VAL	2.0
1	A	338	LYS	2.0

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

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

6.3 Carbohydrates ⓘ

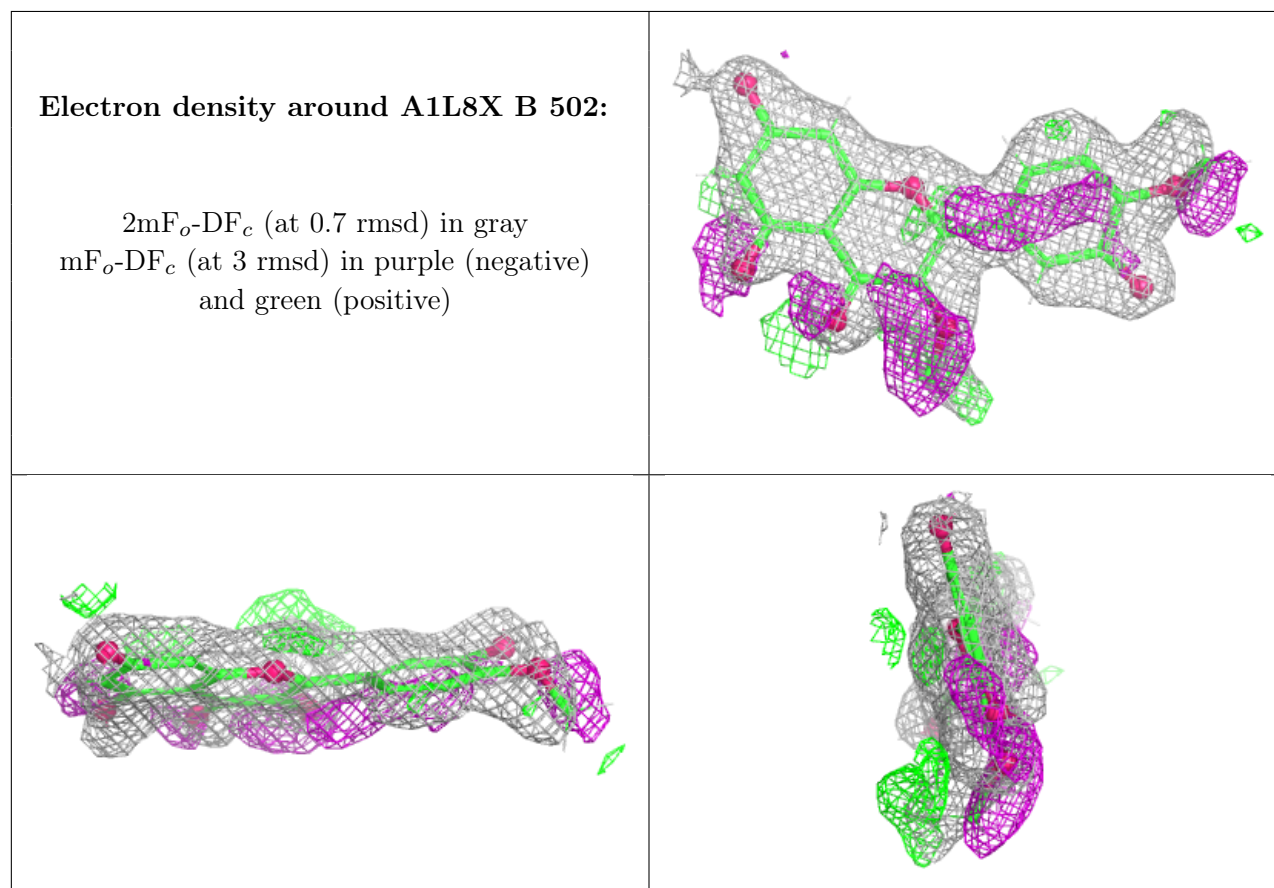
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

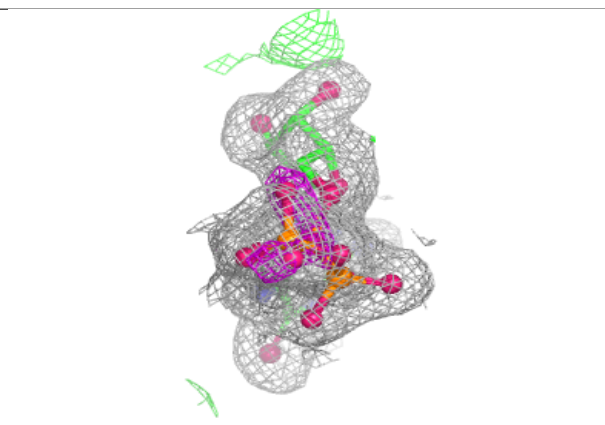
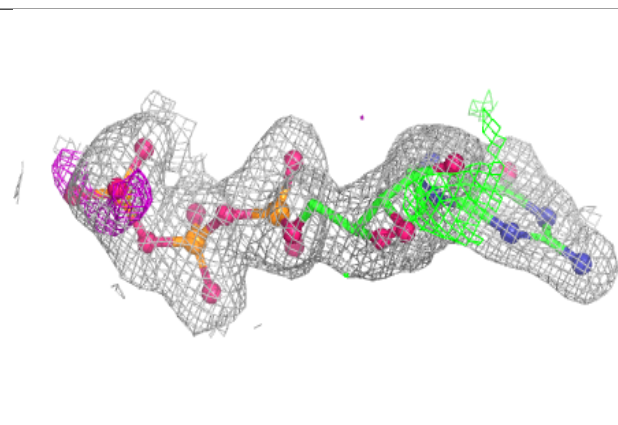
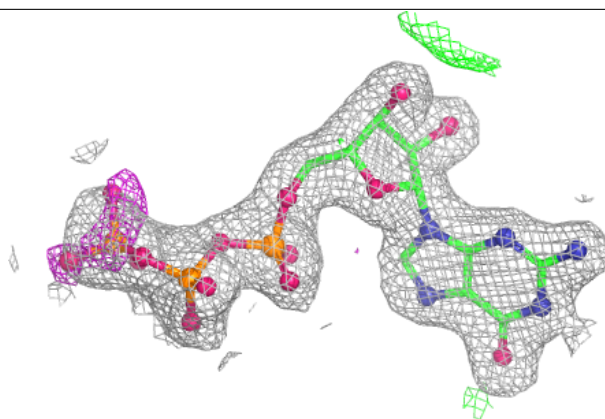
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	A1L8X	B	502	24/24	0.81	0.13	26,36,50,51	0
5	MG	B	503	1/1	0.96	0.09	43,43,43,43	0
4	GTP	B	501	32/32	0.97	0.06	19,25,44,47	0
5	MG	A	502	1/1	0.97	0.04	20,20,20,20	0
4	GTP	A	501	32/32	0.98	0.05	14,18,21,22	0

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.

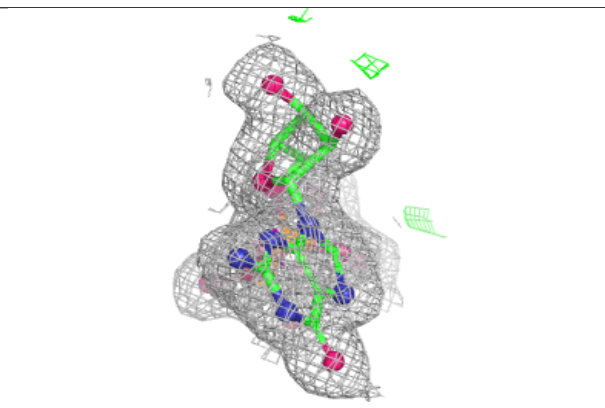
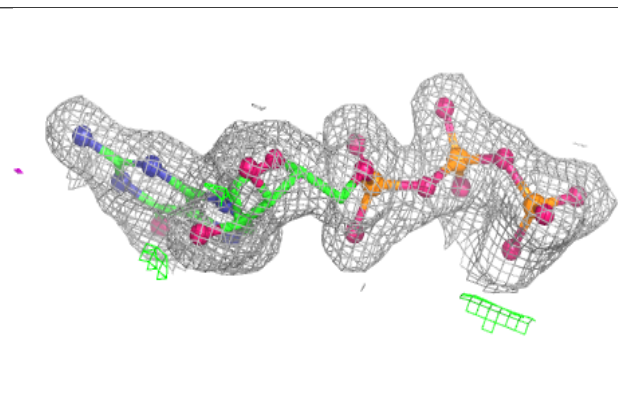
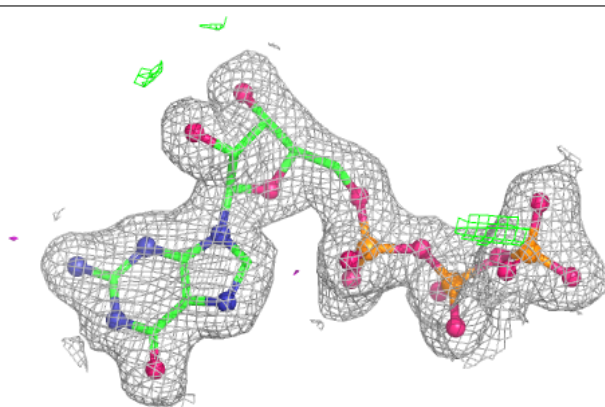


Electron density around GTP B 501:

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

**Electron density around 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.