



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:23 PM UTC

PDB ID : 2BTO / pdb_00002bto
Title : Structure of BtubA from Prosthecobacter dejongeii
Authors : Schlieper, D.; Lowe, J.
Deposited on : 2005-06-04
Resolution : 2.50 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

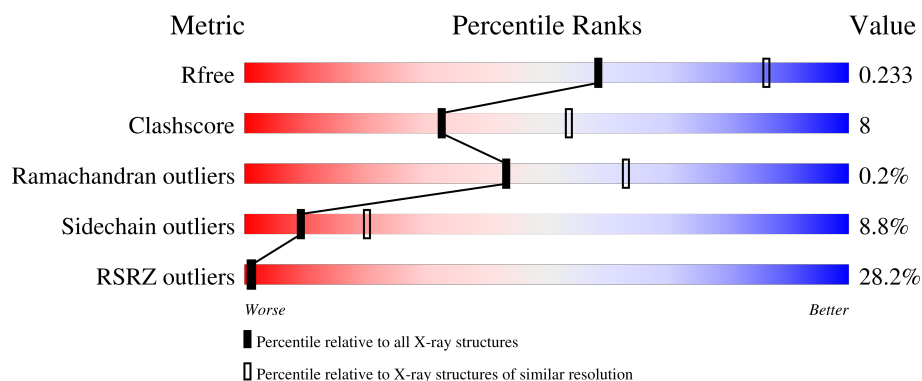
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	473	6% 69% 17% • 13%
1	B	473	29% 69% 18% • 11%
2	T	108	91% 74% 17% 5% 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7451 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 BTUBA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	413	Total	C	N	O	S	0	0	0
			3156	2012	531	597	16			
1	B	423	Total	C	N	O	S	0	0	0
			3230	2055	544	614	17			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	255	SER	THR	conflict	UNP Q8GCC5
B	255	SER	THR	conflict	UNP Q8GCC5

- Molecule 2 is a protein called THIOREDOXIN 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	103	Total	C	N	O	S	0	0	0
			785	506	126	150	3			

- Molecule 3 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).

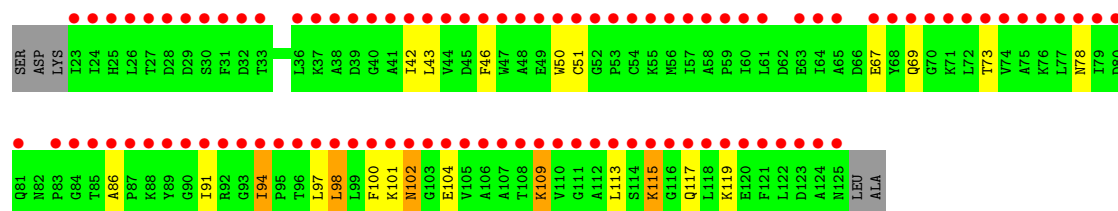
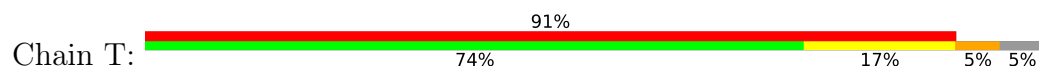


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
3	B	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	108	Total	O	0	0
			108	108		
4	B	93	Total	O	0	0
			93	93		
4	T	15	Total	O	0	0
			15	15		

- Molecule 2: THIOREDOXIN 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α , β , γ	180.54Å 180.54Å 84.23Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.50 50.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.00-2.50) 99.9 (50.00-2.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.79 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.200 , 0.235 0.198 , 0.233	Depositor DCC
R_{free} test set	2737 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	44.5	Xtriage
Anisotropy	0.449	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 67.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.025 for -h,-k,l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	7451	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.03% 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: 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	0.62	0/3219	0.90	3/4372 (0.1%)
1	B	0.94	7/3294 (0.2%)	0.91	7/4471 (0.2%)
2	T	0.62	1/800 (0.1%)	0.82	0/1086
All	All	0.78	8/7313 (0.1%)	0.90	10/9929 (0.1%)

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	B	0	2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	410	GLU	CD-OE1	29.47	1.81	1.25
1	B	411	GLU	CD-OE2	15.29	1.54	1.25
1	B	414	ASN	CG-OD1	13.70	1.49	1.23
1	B	411	GLU	CD-OE1	13.58	1.51	1.25
1	B	411	GLU	CB-CG	11.86	1.88	1.52
2	T	67	GLU	CD-OE2	8.17	1.40	1.25
1	B	410	GLU	CD-OE2	-5.86	1.14	1.25
1	B	407	GLY	C-N	5.25	1.40	1.33

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	100	GLY	N-CA-C	-7.22	101.47	112.89
1	A	223	SER	CA-C-N	6.38	126.40	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	223	SER	C-N-CA	6.38	126.40	119.90
1	B	414	ASN	OD1-CG-ND2	6.08	128.68	122.60
1	B	414	ASN	CB-CG-ND2	-5.64	107.93	116.40
1	B	411	GLU	OE1-CD-OE2	-5.43	109.86	122.90
1	A	348	TYR	N-CA-C	5.39	118.33	111.69
1	B	281	PRO	CA-C-N	5.36	126.54	119.84
1	B	281	PRO	C-N-CA	5.36	126.54	119.84
1	B	411	GLU	CB-CG-CD	-5.16	103.83	112.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	410	GLU	Sidechain
1	B	411	GLU	Sidechain

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	3156	0	3143	46	0
1	B	3230	0	3221	59	0
2	T	785	0	790	13	0
3	A	32	0	12	3	0
3	B	32	0	12	1	0
4	A	108	0	0	10	0
4	B	93	0	0	7	0
4	T	15	0	0	2	0
All	All	7451	0	7178	114	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 8.

All (114) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:411:GLU:CB	1:B:411:GLU:CG	1.88	1.51
1:B:410:GLU:CD	1:B:410:GLU:OE1	1.81	1.21
1:A:165:GLU:HG2	4:A:2055:HOH:O	1.36	1.21
3:A:1433:GTP:PB	4:A:2106:HOH:O	2.22	0.97
1:B:235:GLU:OE1	1:B:366:HIS:HE1	1.67	0.77
1:A:417:ARG:NH1	1:A:421:GLN:OE1	2.17	0.77
1:B:143:ILE:HG22	4:B:2038:HOH:O	1.87	0.74
1:A:295:MET:HG2	1:A:370:MET:HE2	1.69	0.73
1:A:152:GLY:O	1:A:156:ILE:HG12	1.90	0.72
1:B:399:PHE:O	1:B:402:TRP:HB2	1.92	0.69
3:A:1433:GTP:O3B	4:A:2106:HOH:O	2.08	0.68
2:T:42:ILE:HG23	2:T:100:PHE:HB2	1.74	0.68
1:A:376:ASN:HD22	1:A:378:GLU:H	1.40	0.68
1:A:376:ASN:ND2	1:A:378:GLU:H	1.91	0.67
1:B:366:HIS:HD2	4:B:2065:HOH:O	1.77	0.67
1:B:411:GLU:CB	1:B:411:GLU:CD	2.66	0.66
1:B:295:MET:HG2	1:B:370:MET:HE3	1.78	0.65
1:A:324:ARG:HD3	1:A:361:GLN:O	1.98	0.64
1:B:295:MET:HE1	1:B:368:LYS:HG3	1.79	0.64
1:A:257:ARG:HD2	4:A:2072:HOH:O	2.00	0.62
1:A:305:VAL:HG11	1:A:311:PRO:HG2	1.81	0.61
1:A:165:GLU:CG	4:A:2055:HOH:O	2.15	0.61
1:B:324:ARG:HG2	4:B:2087:HOH:O	2.00	0.60
1:B:411:GLU:HA	1:B:414:ASN:HD22	1.68	0.59
1:A:396:ARG:NH2	2:T:50:TRP:HB2	2.20	0.57
1:B:289:GLU:OE1	1:B:367:ARG:HB2	2.05	0.56
1:B:314:GLY:HA3	1:B:378:GLU:HG2	1.87	0.56
1:A:213:ASP:OD1	1:A:217:ARG:CZ	2.54	0.56
1:A:163:TYR:O	1:A:165:GLU:N	2.39	0.55
1:A:271:PHE:CE1	1:A:423:LEU:HD11	2.41	0.55
1:B:315:ARG:HD3	1:B:346:LEU:O	2.07	0.55
1:A:174:LEU:HD11	1:A:205:ILE:HG12	1.88	0.54
1:A:341:ARG:HG3	1:A:354:PHE:CG	2.43	0.54
1:B:281:PRO:HG2	1:B:284:ARG:HD2	1.89	0.54
1:B:47:GLY:HA2	4:B:2056:HOH:O	2.08	0.53
1:A:48:ASN:ND2	1:A:253:GLU:HB3	2.25	0.52
1:A:253:GLU:N	4:A:2069:HOH:O	2.43	0.51
1:B:292:ILE:HD13	1:B:368:LYS:HE3	1.92	0.51
1:B:108:GLY:O	1:B:113:GLY:HA3	2.10	0.51
1:A:197:ARG:HG3	1:A:423:LEU:HG	1.93	0.51
1:B:271:PHE:HB3	1:B:379:ILE:CD1	2.41	0.51
1:B:411:GLU:OE2	1:B:411:GLU:HB3	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:LEU:HD13	1:A:317:LEU:HD21	1.95	0.49
1:A:402:TRP:CH2	2:T:86:ALA:HB3	2.47	0.49
1:A:240:ILE:HD12	1:A:373:LEU:HG	1.94	0.49
4:A:2067:HOH:O	1:B:326:ILE:HD11	2.13	0.49
1:A:323:TYR:HD2	1:A:358:TYR:HD1	1.61	0.48
1:B:72:ASP:O	1:B:96:SER:HA	2.12	0.48
1:B:401:ASN:H	1:B:401:ASN:HD22	1.62	0.48
2:T:46:PHE:HE2	2:T:98:LEU:HD22	1.79	0.48
2:T:119:LYS:HD2	4:T:2005:HOH:O	2.12	0.48
1:B:295:MET:HG2	1:B:370:MET:CE	2.43	0.48
1:A:145:GLY:HA3	3:A:1433:GTP:O2B	2.14	0.47
1:B:411:GLU:CB	1:B:411:GLU:OE2	2.62	0.47
1:A:381:ARG:HB2	4:A:2096:HOH:O	2.14	0.47
1:B:295:MET:SD	1:B:370:MET:HE2	2.55	0.47
1:B:337:LEU:HD13	1:B:356:ILE:HD12	1.97	0.47
1:A:45:PRO:HG2	1:A:49:TRP:CD1	2.50	0.47
1:B:109:TYR:HD2	1:B:110:LEU:HG	1.80	0.47
1:B:215:ALA:O	1:B:219:TRP:HB2	2.15	0.47
1:A:236:ALA:O	1:A:240:ILE:HG12	2.15	0.46
1:A:317:LEU:O	1:A:352:THR:HG22	2.15	0.46
1:B:14:ALA:HB3	1:B:142:ALA:HB2	1.95	0.46
1:B:324:ARG:HA	1:B:359:VAL:O	2.16	0.46
1:B:58:GLU:HB2	2:T:104:GLU:HG3	1.97	0.46
1:B:140:LEU:HD12	1:B:171:CYS:HB2	1.98	0.46
1:A:44:ALA:HB1	1:A:45:PRO:HD2	1.98	0.45
1:B:269:LEU:HD13	1:B:317:LEU:HD21	1.97	0.45
1:B:391:ASP:O	1:B:395:GLN:HB2	2.16	0.45
1:A:390:PHE:CD2	1:A:390:PHE:C	2.95	0.45
2:T:46:PHE:CE2	2:T:98:LEU:HD22	2.52	0.45
1:B:148:GLY:O	1:B:152:GLY:HA3	2.17	0.45
1:A:406:GLU:O	1:A:406:GLU:HG3	2.16	0.45
1:B:271:PHE:HB3	1:B:379:ILE:HD13	1.97	0.45
2:T:51:CYS:HB2	2:T:94:ILE:CD1	2.47	0.44
2:T:102:ASN:OD1	2:T:102:ASN:N	2.43	0.44
1:A:79:ASP:OD2	1:B:33:ASP:OD2	2.35	0.44
1:A:72:ASP:O	1:A:96:SER:HA	2.18	0.43
1:A:7:ILE:HD12	1:A:127:GLU:HB3	1.99	0.43
1:B:11:ILE:HG22	1:B:147:THR:HG22	1.99	0.43
2:T:101:LYS:HE2	4:T:2009:HOH:O	2.18	0.43
1:A:324:ARG:HD2	1:A:362:PRO:HA	2.01	0.43
1:A:326:ILE:HA	4:A:2087:HOH:O	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:286:LYS:O	1:B:367:ARG:NH1	2.51	0.43
1:B:197:ARG:HG3	1:B:423:LEU:HG	2.01	0.43
1:A:289:GLU:OE1	1:A:367:ARG:HD2	2.19	0.42
1:B:274:CYS:HB3	1:B:373:LEU:HD23	2.00	0.42
1:B:292:ILE:HG12	4:B:2077:HOH:O	2.18	0.42
1:A:207:ASP:HB3	1:A:307:ALA:HA	2.01	0.42
1:A:226:VAL:HG12	4:A:2064:HOH:O	2.19	0.42
1:B:14:ALA:CB	1:B:142:ALA:HB2	2.50	0.42
1:A:157:GLU:O	1:A:161:GLU:HG3	2.20	0.42
1:A:228:ASP:OD1	1:B:367:ARG:NH2	2.46	0.42
1:B:292:ILE:HG12	1:B:292:ILE:H	1.73	0.42
2:T:43:LEU:HD11	2:T:97:LEU:HB3	2.00	0.42
1:B:390:PHE:CD2	1:B:390:PHE:C	2.98	0.41
1:B:352:THR:HG22	1:B:353:ALA:N	2.36	0.41
1:A:214:LEU:HD22	1:A:279:LEU:HD13	2.03	0.41
1:B:13:GLN:N	3:B:1433:GTP:O1B	2.42	0.41
1:B:411:GLU:CG	1:B:411:GLU:CA	2.85	0.41
1:B:296:ILE:HG13	1:B:370:MET:HE1	2.03	0.41
1:A:13:GLN:HG3	1:A:77:VAL:HG21	2.02	0.41
2:T:109:LYS:HE2	2:T:113:LEU:HD13	2.02	0.41
1:A:282:PRO:HB2	1:B:289:GLU:HG3	2.02	0.41
1:A:315:ARG:HG3	1:A:431:GLU:HG3	2.03	0.41
1:B:235:GLU:OE1	1:B:366:HIS:CE1	2.58	0.41
1:B:194:ASN:O	1:B:198:ARG:HG3	2.21	0.40
1:B:148:GLY:C	4:B:2038:HOH:O	2.63	0.40
1:B:274:CYS:HA	1:B:372:LEU:O	2.21	0.40
2:T:115:LYS:O	2:T:119:LYS:HG3	2.21	0.40
1:A:29:GLU:CD	1:A:324:ARG:HH12	2.28	0.40
1:B:112:ALA:HA	1:B:115:GLU:HG3	2.03	0.40
1:B:197:ARG:HD2	1:B:423:LEU:HB2	2.03	0.40
1:B:218:LYS:NZ	4:B:2051:HOH:O	2.54	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	403/473 (85%)	389 (96%)	14 (4%)	0	100	100
1	B	417/473 (88%)	399 (96%)	16 (4%)	2 (0%)	24	43
2	T	101/108 (94%)	99 (98%)	2 (2%)	0	100	100
All	All	921/1054 (87%)	887 (96%)	32 (4%)	2 (0%)	43	63

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	164	GLY
1	B	398	ALA

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	341/387 (88%)	313 (92%)	28 (8%)	10	23
1	B	350/387 (90%)	320 (91%)	30 (9%)	10	21
2	T	83/87 (95%)	73 (88%)	10 (12%)	5	10
All	All	774/861 (90%)	706 (91%)	68 (9%)	9	20

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

Mol	Chain	Res	Type
1	A	7	ILE
1	A	43	VAL
1	A	88	LEU
1	A	137	ILE
1	A	204	LEU
1	A	205	ILE
1	A	213	ASP
1	A	231	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	256	LEU
1	A	258	GLU
1	A	294	GLU
1	A	298	SER
1	A	299	LEU
1	A	318	SER
1	A	324	ARG
1	A	334	ASP
1	A	346	LEU
1	A	361	GLN
1	A	364	ILE
1	A	365	SER
1	A	371	VAL
1	A	372	LEU
1	A	379	ILE
1	A	402	TRP
1	A	404	LEU
1	A	417	ARG
1	A	423	LEU
1	A	432	GLU
1	B	56	LEU
1	B	63	SER
1	B	88	LEU
1	B	99	GLU
1	B	116	VAL
1	B	134	VAL
1	B	140	LEU
1	B	204	LEU
1	B	231	LEU
1	B	243	SER
1	B	247	SER
1	B	283	ASP
1	B	285	SER
1	B	292	ILE
1	B	297	LYS
1	B	299	LEU
1	B	328	GLU
1	B	347	THR
1	B	361	GLN
1	B	364	ILE
1	B	372	LEU
1	B	381	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	384	ASP
1	B	395	GLN
1	B	401	ASN
1	B	412	GLN
1	B	413	ILE
1	B	417	ARG
1	B	423	LEU
1	B	432	GLU
2	T	69	GLN
2	T	73	THR
2	T	78	ASN
2	T	91	ILE
2	T	94	ILE
2	T	98	LEU
2	T	102	ASN
2	T	109	LYS
2	T	115	LYS
2	T	117	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	GLN
1	A	16	ASN
1	A	17	GLN
1	A	48	ASN
1	A	262	ASN
1	A	266	GLN
1	A	375	ASN
1	A	376	ASN
1	A	389	ASN
1	A	401	ASN
1	A	412	GLN
1	B	5	ASN
1	B	17	GLN
1	B	133	ASN
1	B	262	ASN
1	B	361	GLN
1	B	366	HIS
1	B	388	HIS
1	B	389	ASN
1	B	401	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	405	ASN
1	B	414	ASN
1	B	421	GLN
2	T	78	ASN
2	T	82	ASN
2	T	125	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GTP	A	1433	-	33,34,34	1.00	2 (6%)	50,54,54	1.60	10 (20%)
3	GTP	B	1433	-	33,34,34	1.02	3 (9%)	50,54,54	1.59	10 (20%)

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
3	GTP	A	1433	-	-	3/22/38/38	0/3/3/3
3	GTP	B	1433	-	-	5/22/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1433	GTP	PA-O3A	3.00	1.62	1.59
3	B	1433	GTP	PB-O3B	2.60	1.62	1.59
3	B	1433	GTP	C2-N3	2.22	1.38	1.33
3	B	1433	GTP	PA-O3A	2.06	1.61	1.59
3	A	1433	GTP	C2-N3	2.06	1.38	1.33

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1433	GTP	C5-C4-N3	-4.64	121.01	128.39
3	B	1433	GTP	C2-N3-C4	4.37	119.83	112.30
3	A	1433	GTP	C2-N3-C4	4.35	119.79	112.30
3	A	1433	GTP	C5-C4-N3	-4.13	121.82	128.39
3	B	1433	GTP	O2B-PB-O3A	3.39	116.43	107.27
3	B	1433	GTP	N9-C4-N3	2.89	131.73	125.95
3	A	1433	GTP	N9-C8-N7	-2.80	108.21	113.40
3	A	1433	GTP	N9-C4-N3	2.77	131.49	125.95
3	B	1433	GTP	C8-N7-C5	2.60	108.89	104.26
3	B	1433	GTP	N9-C8-N7	-2.47	108.83	113.40
3	A	1433	GTP	O3G-PG-O3B	2.44	112.83	104.64
3	B	1433	GTP	C2-N1-C6	-2.42	120.72	125.11
3	B	1433	GTP	O2B-PB-O3B	2.33	113.56	107.27
3	A	1433	GTP	C5-C6-N1	2.27	119.04	113.25
3	A	1433	GTP	C2-N1-C6	-2.27	121.00	125.11
3	B	1433	GTP	C5-C6-N1	2.27	119.02	113.25
3	A	1433	GTP	O6-C6-C5	-2.26	120.56	126.53
3	A	1433	GTP	C8-N7-C5	2.23	108.24	104.26
3	B	1433	GTP	O6-C6-C5	-2.15	120.87	126.53
3	A	1433	GTP	O2B-PB-O1B	-2.11	102.62	112.44

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1433	GTP	C5'-O5'-PA-O1A
3	B	1433	GTP	C5'-O5'-PA-O3A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	B	1433	GTP	C5'-O5'-PA-O1A
3	A	1433	GTP	C5'-O5'-PA-O2A
3	B	1433	GTP	C5'-O5'-PA-O2A
3	A	1433	GTP	PB-O3A-PA-O1A
3	B	1433	GTP	PB-O3A-PA-O1A
3	B	1433	GTP	PB-O3A-PA-O2A

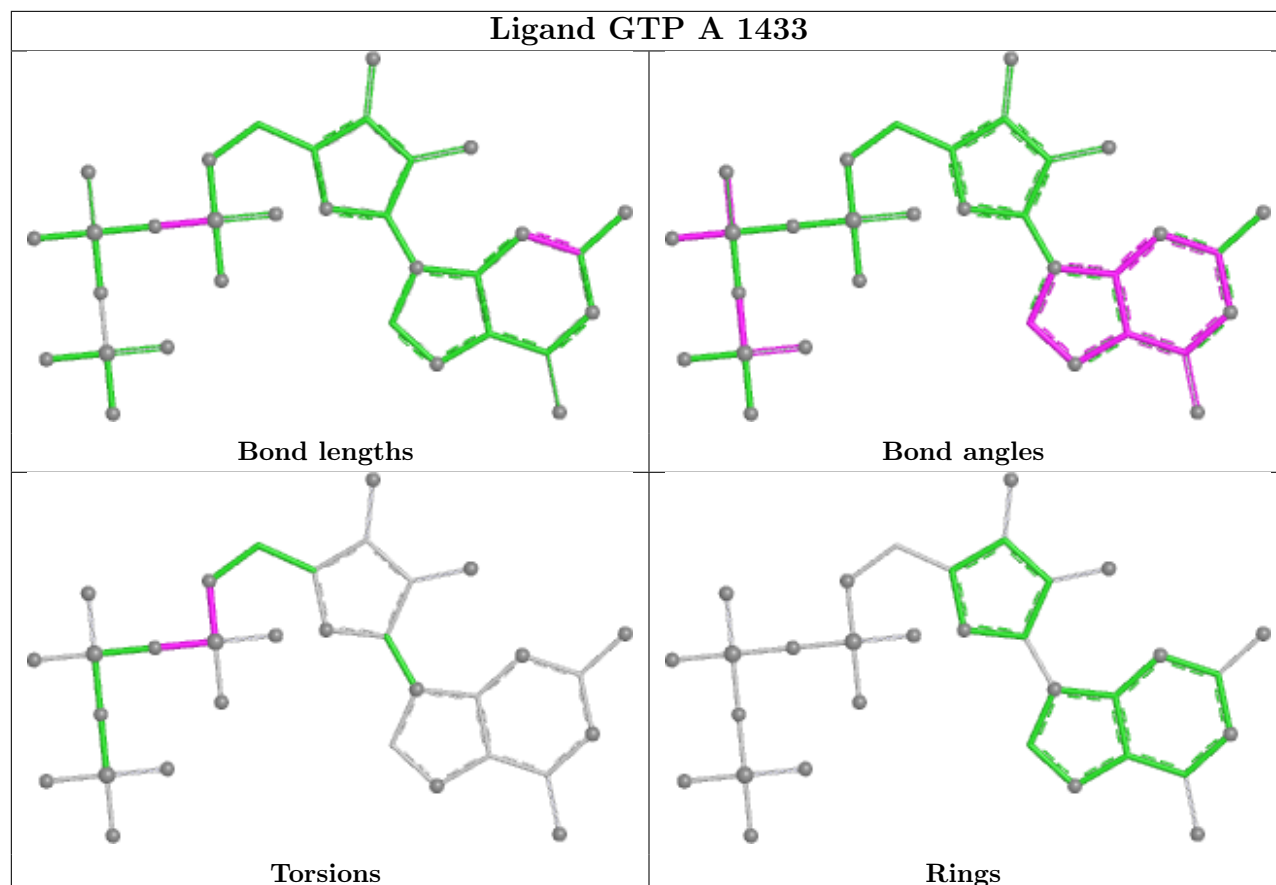
There are no ring outliers.

2 monomers are involved in 4 short contacts:

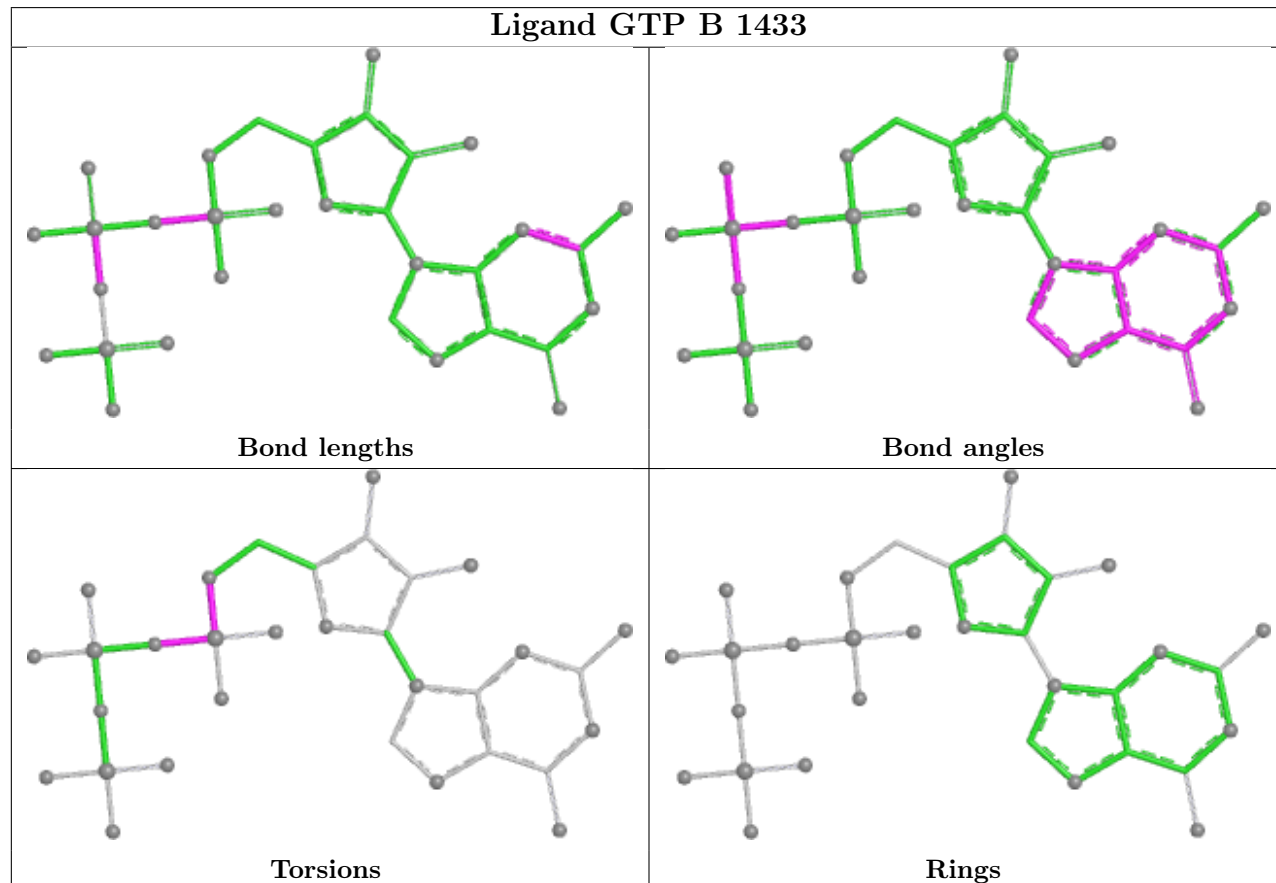
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1433	GTP	3	0
3	B	1433	GTP	1	0

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 1433



Ligand GTP B 1433



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	413/473 (87%)	0.77	28 (6%)	23 20	42, 51, 63, 76	0
1	B	423/473 (89%)	1.64	139 (32%)	1 1	39, 51, 66, 78	0
2	T	103/108 (95%)	3.74	98 (95%)	0 0	66, 71, 77, 78	0
All	All	939/1054 (89%)	1.49	265 (28%)	1 1	39, 52, 73, 78	0

All (265) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	T	72	LEU	6.9
2	T	23	ILE	6.8
2	T	101	LYS	6.7
2	T	91	ILE	6.3
2	T	92	ARG	6.2
2	T	125	ASN	6.1
2	T	102	ASN	6.1
2	T	56	MET	5.8
1	B	287	PHE	5.8
2	T	90	GLY	5.7
2	T	120	GLU	5.6
2	T	89	TYR	5.4
2	T	113	LEU	5.4
2	T	124	ALA	5.4
2	T	93	GLY	5.2
1	B	290	LEU	5.2
2	T	110	VAL	5.1
1	B	326	ILE	5.1
2	T	109	LYS	5.1
1	B	291	GLY	5.0
2	T	70	GLY	5.0
2	T	24	ILE	4.8
2	T	118	LEU	4.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	T	106	ALA	4.8
1	B	335	ALA	4.8
2	T	123	ASP	4.7
2	T	71	LYS	4.7
1	B	407	GLY	4.6
2	T	38	ALA	4.6
2	T	68	TYR	4.6
2	T	122	LEU	4.5
2	T	108	THR	4.5
2	T	100	PHE	4.5
1	B	333	ALA	4.5
2	T	105	VAL	4.4
2	T	107	ALA	4.4
2	T	37	LYS	4.4
2	T	117	GLN	4.4
2	T	121	PHE	4.4
1	B	411	GLU	4.4
2	T	40	GLY	4.3
2	T	116	GLY	4.3
2	T	88	LYS	4.3
1	B	250	LEU	4.3
2	T	63	GLU	4.3
1	B	61	SER	4.2
1	B	39	THR	4.2
2	T	53	PRO	4.2
2	T	112	ALA	4.2
2	T	77	LEU	4.1
1	B	414	ASN	4.1
2	T	119	LYS	4.1
1	B	416	LEU	4.1
1	B	285	SER	4.0
2	T	94	ILE	4.0
1	B	398	ALA	4.0
2	T	115	LYS	4.0
2	T	85	THR	4.0
2	T	46	PHE	3.9
2	T	86	ALA	3.9
1	B	55	LYS	3.9
1	B	40	ALA	3.9
2	T	99	LEU	3.9
2	T	87	PRO	3.8
2	T	60	ILE	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	T	65	ALA	3.8
1	B	351	PRO	3.8
1	B	365	SER	3.8
1	B	45	PRO	3.8
1	B	408	MET	3.8
2	T	73	THR	3.7
2	T	103	GLY	3.7
1	B	248	GLY	3.7
2	T	69	GLN	3.7
2	T	98	LEU	3.7
1	B	282	PRO	3.6
2	T	44	VAL	3.5
1	B	44	ALA	3.5
2	T	36	LEU	3.5
1	B	289	GLU	3.5
2	T	74	VAL	3.5
1	B	64	TYR	3.5
2	T	97	LEU	3.5
2	T	29	ASP	3.5
1	B	364	ILE	3.5
1	B	133	ASN	3.4
1	B	110	LEU	3.4
1	B	356	ILE	3.4
2	T	64	ILE	3.4
1	B	252	VAL	3.4
1	B	280	THR	3.4
1	B	111	GLY	3.4
1	B	363	GLY	3.4
1	B	56	LEU	3.3
1	B	218	LYS	3.3
1	B	359	VAL	3.3
1	B	102	GLY	3.3
1	B	251	THR	3.3
2	T	52	GLY	3.3
1	B	367	ARG	3.2
1	B	43	VAL	3.2
1	B	331	PRO	3.2
2	T	41	ALA	3.2
2	T	55	LYS	3.2
2	T	33	THR	3.2
2	T	49	GLU	3.2
1	B	336	ALA	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	T	61	LEU	3.1
1	B	3	VAL	3.1
1	B	292	ILE	3.1
2	T	25	HIS	3.1
1	A	403	TYR	3.1
1	B	425	GLN	3.1
2	T	75	ALA	3.1
1	B	404	LEU	3.1
2	T	32	ASP	3.1
1	B	106	ALA	3.0
1	B	32	ILE	3.0
1	B	254	ILE	3.0
2	T	96	THR	3.0
1	B	125	ASP	3.0
1	B	249	PHE	3.0
1	B	329	ASP	3.0
1	B	63	SER	3.0
2	T	104	GLU	3.0
1	A	59	SER	3.0
1	B	134	VAL	2.9
1	B	295	MET	2.9
1	B	103	GLY	2.9
2	T	27	THR	2.9
1	B	112	ALA	2.9
1	B	246	PHE	2.9
1	B	400	ALA	2.9
2	T	47	TRP	2.9
1	B	31	GLY	2.9
1	B	325	GLY	2.9
1	B	406	GLU	2.8
2	T	31	PHE	2.8
1	B	220	ASN	2.8
2	T	79	ILE	2.8
2	T	48	ALA	2.8
1	B	115	GLU	2.8
1	B	384	ASP	2.8
2	T	84	GLY	2.8
2	T	114	SER	2.8
1	A	331	PRO	2.8
2	T	95	PRO	2.8
2	T	59	PRO	2.8
2	T	26	LEU	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	48	ASN	2.7
1	B	163	TYR	2.7
1	B	328	GLU	2.7
2	T	80	ASP	2.7
1	B	421	GLN	2.7
1	A	78	ILE	2.7
1	B	298	SER	2.7
1	B	358	TYR	2.7
1	B	370	MET	2.7
1	A	40	ALA	2.7
1	B	323	TYR	2.7
2	T	67	GLU	2.7
2	T	43	LEU	2.6
1	B	281	PRO	2.6
1	B	327	MET	2.6
1	B	369	SER	2.6
1	B	52	PHE	2.6
1	B	191	PHE	2.6
1	B	279	LEU	2.6
1	B	393	LEU	2.6
1	B	126	TYR	2.6
1	A	402	TRP	2.6
1	A	290	LEU	2.6
1	A	179	VAL	2.6
1	B	321	VAL	2.6
1	B	57	GLY	2.5
1	B	177	PRO	2.5
1	B	337	LEU	2.5
1	B	412	GLN	2.5
1	B	277	ALA	2.5
1	B	418	ALA	2.5
2	T	57	ILE	2.5
1	B	368	LYS	2.5
1	B	165	GLU	2.5
1	B	151	PHE	2.5
2	T	81	GLN	2.5
2	T	111	GLY	2.5
1	B	402	TRP	2.4
1	B	415	VAL	2.4
2	T	78	ASN	2.4
1	B	62	GLY	2.4
1	B	391	ASP	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	88	LEU	2.4
1	A	339	ALA	2.4
1	B	395	GLN	2.4
1	B	403	TYR	2.4
1	A	82	LYS	2.4
1	A	253	GLU	2.4
1	B	409	SER	2.4
1	B	361	GLN	2.4
1	B	366	HIS	2.4
1	B	194	ASN	2.4
1	B	338	ALA	2.4
1	B	397	LYS	2.4
1	A	337	LEU	2.3
2	T	28	ASP	2.3
2	T	45	ASP	2.3
1	B	297	LYS	2.3
1	B	4	ASN	2.3
2	T	50	TRP	2.3
1	A	421	GLN	2.3
1	B	5	ASN	2.3
1	B	49	TRP	2.3
1	B	122	SER	2.3
1	B	332	LEU	2.3
1	B	350	ILE	2.3
1	B	286	LYS	2.3
1	B	26	VAL	2.3
1	B	92	ALA	2.3
1	B	148	GLY	2.3
1	B	357	GLY	2.3
1	B	353	ALA	2.2
1	A	57	GLY	2.2
1	B	299	LEU	2.2
1	A	79	ASP	2.2
1	A	58	GLU	2.2
2	T	54	CYS	2.2
1	B	28	LEU	2.2
1	A	74	GLU	2.2
1	B	128	ILE	2.2
1	A	389	ASN	2.2
1	B	215	ALA	2.2
1	B	187	TYR	2.2
1	B	214	LEU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	58	GLU	2.2
1	B	283	ASP	2.2
1	B	288	GLU	2.2
2	T	39	ASP	2.2
1	B	324	ARG	2.2
1	A	41	PRO	2.2
2	T	83	PRO	2.2
1	A	246	PHE	2.2
1	A	98	THR	2.1
1	A	222	GLU	2.1
2	T	30	SER	2.1
1	A	390	PHE	2.1
1	B	389	ASN	2.1
1	B	405	ASN	2.1
1	A	254	ILE	2.1
2	T	76	LYS	2.1
1	B	27	CYS	2.1
1	B	210	ALA	2.1
2	T	58	ALA	2.1
1	A	100	GLY	2.1
1	B	166	ILE	2.1
2	T	42	ILE	2.1
1	B	334	ASP	2.1
1	B	362	PRO	2.1
1	A	217	ARG	2.0
1	B	231	LEU	2.0
1	B	221	ILE	2.0
1	B	54	SER	2.0
1	B	60	SER	2.0
2	T	51	CYS	2.0
1	A	56	LEU	2.0
1	B	33	ASP	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](#)

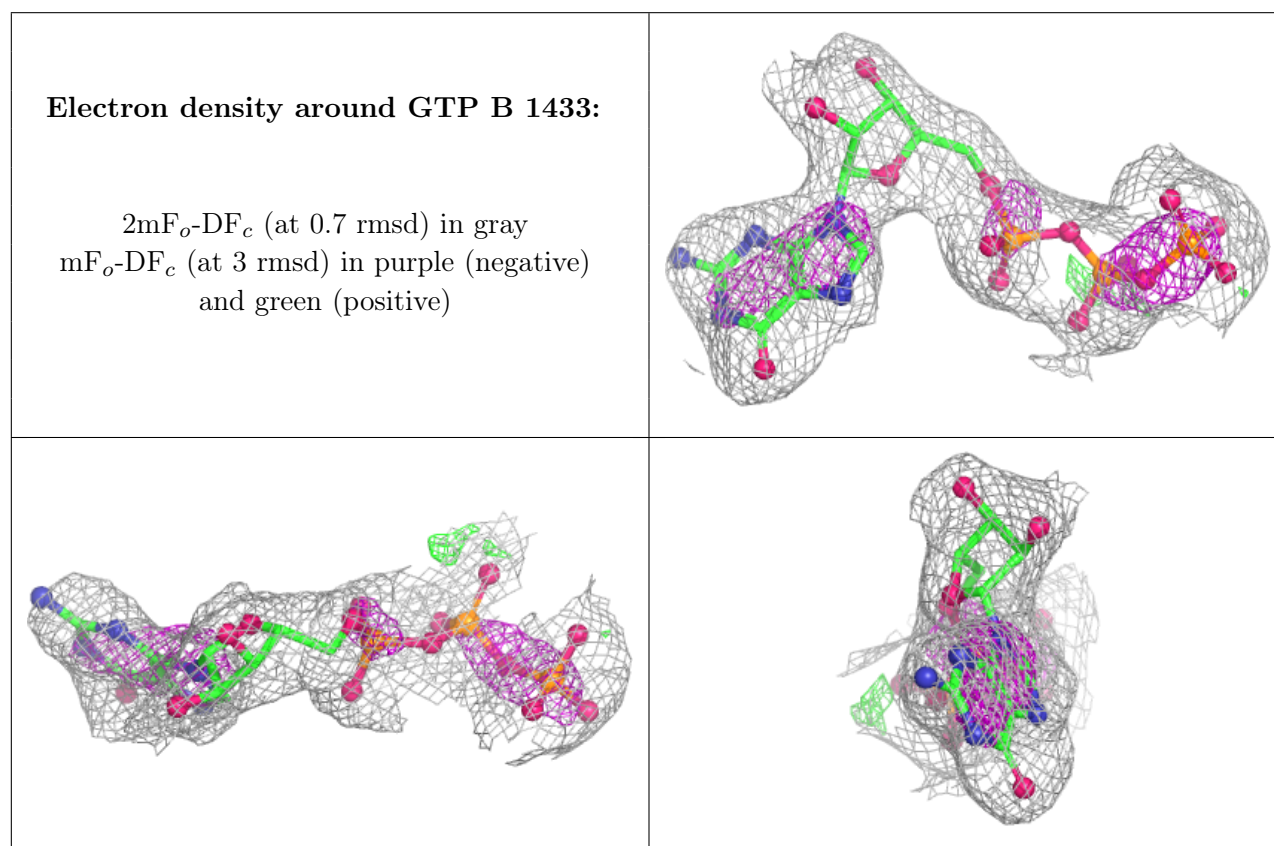
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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.

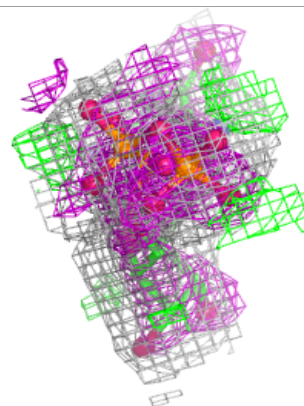
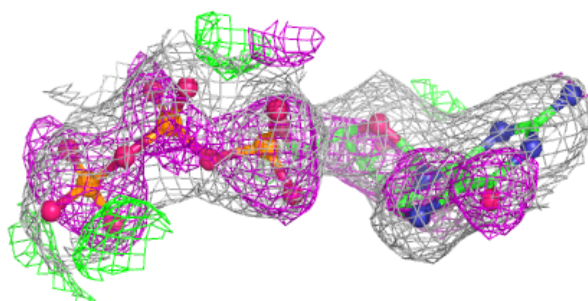
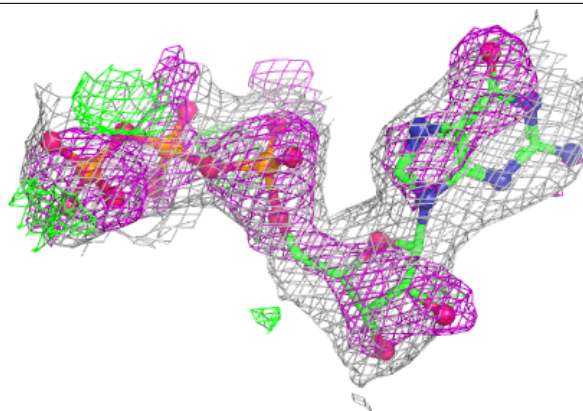
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GTP	B	1433	32/32	0.87	0.15	70,72,75,76	0
3	GTP	A	1433	32/32	0.90	0.14	48,54,57,58	0

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 A 1433:

$2mF_o-DF_c$ (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.