



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 19, 2022 – 04:10 PM JST

PDB ID : 7Y7T
Title : QDE-1 in complex with 12nt DNA template, ATP and 3'-dGTP
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Deposited on : 2022-06-22
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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.30
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.30

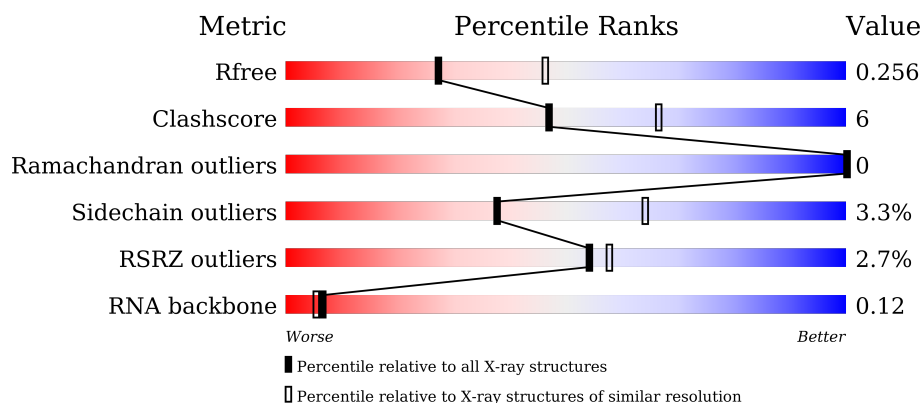
1 Overall quality at a glance

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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)
RNA backbone	3102	1008 (2.84-2.16)

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	1026	<div> <div>2%</div> <div>77%</div> <div>14%</div> <div>9%</div> </div>
1	B	1026	<div> <div>3%</div> <div>74%</div> <div>16%</div> <div>9%</div> </div>
2	C	12	<div> <div>25%</div> <div>25%</div> <div>50%</div> <div>25%</div> </div>
3	D	4	<div> <div>50%</div> <div>50%</div> </div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 15367 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 RNA-dependent RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	937	Total	C	N	O	S	0	0	0
			7450	4746	1288	1382	34			
1	B	930	Total	C	N	O	S	0	1	0
			7435	4746	1285	1369	35			

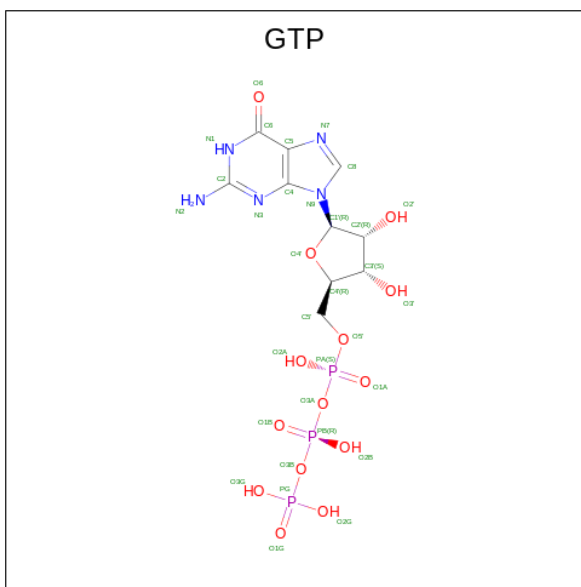
- Molecule 2 is a DNA chain called DNA (5'-D(*GP*AP*G*AP*GP*AP*CP*CP*TP*TP*TP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	9	Total	C	N	O	P	0	0	0
			168	83	24	53	8			

- Molecule 3 is a RNA chain called RNA (5'-R(P*AP*AP*AP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	4	Total	C	N	O	P	0	0	0
			88	40	20	24	4			

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃) (labeled as "Ligand of Interest" by depositor).

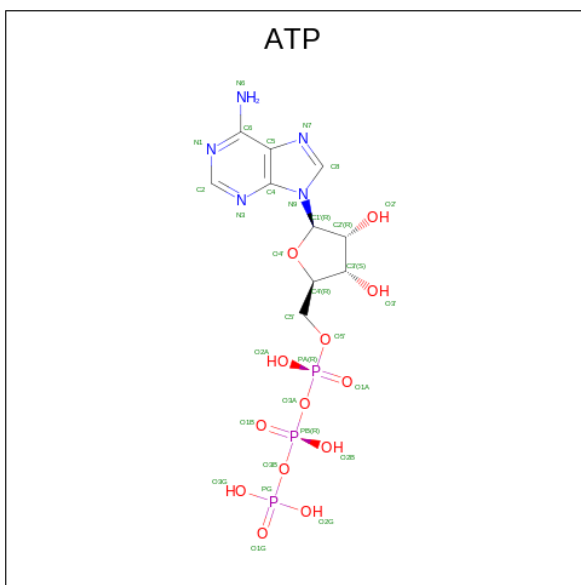


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	3	Total Mg 3 3	0	0
5	B	2	Total Mg 2 2	0	0

- Molecule 6 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{13}\text{P}_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total 31	C 10	N 5	O 13	P 3	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	81	Total O 81 81	0	0
7	B	75	Total O 75 75	0	0
7	C	3	Total O 3 3	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	81.50Å 85.79Å 101.28Å 102.38° 103.41° 94.13°	Depositor
Resolution (Å)	29.94 – 2.50 29.94 – 2.50	Depositor EDS
% Data completeness (in resolution range)	88.7 (29.94-2.50) 88.8 (29.94-2.50)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.53 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.221 , 0.257 0.221 , 0.256	Depositor DCC
R_{free} test set	3957 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	48.1	Xtriage
Anisotropy	0.466	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 39.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	15367	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.85% 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: ATP, MG, 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	0.37	0/7628	0.56	0/10310
1	B	0.35	0/7615	0.56	0/10290
2	C	0.47	0/186	1.00	0/285
3	D	0.16	0/99	0.64	0/152
All	All	0.36	0/15528	0.57	0/21037

There are no bond length outliers.

There are no bond angle outliers.

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	7450	0	7249	90	0
1	B	7435	0	7304	104	0
2	C	168	0	97	5	0
3	D	88	0	43	3	0
4	A	31	0	10	1	0
5	A	3	0	0	0	0
5	B	2	0	0	0	0
6	B	31	0	12	0	0
7	A	81	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	75	0	0	0	0
7	C	3	0	0	0	0
All	All	15367	0	14715	185	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 6.

All (185) 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:A:1075:PHE:HE2	1:A:1118:SER:HA	1.49	0.76
1:B:1133:ARG:HA	1:B:1137:LEU:HD12	1.67	0.75
1:B:540:ILE:HG13	1:B:541:PRO:HD2	1.68	0.74
1:B:406:PRO:HG2	1:B:409:LEU:HD12	1.73	0.69
1:B:583:PHE:HA	1:B:1069:ILE:HD13	1.73	0.69
1:A:860:ARG:NH1	1:B:1342:GLU:OE1	2.26	0.69
1:B:516:LYS:HG3	1:B:517:PRO:HD2	1.75	0.69
1:A:794:LEU:HD23	1:A:799:LEU:HD21	1.76	0.68
1:A:856:VAL:O	1:B:1369:ARG:NH2	2.26	0.68
1:B:904:ASP:OD1	1:B:907:LYS:NZ	2.27	0.68
1:B:687:PRO:HD3	1:B:778:ARG:NH1	2.09	0.67
1:B:796:LEU:HD11	1:B:910:LEU:HB3	1.76	0.67
1:B:1134:ARG:HA	1:B:1139:GLY:HA2	1.78	0.65
1:B:1226:THR:HG21	1:B:1273:MET:HB3	1.78	0.65
1:B:1091:ARG:NH1	1:B:1145:ASP:OD1	2.30	0.64
1:A:1089:LYS:NZ	1:A:1108:SER:OG	2.30	0.63
1:B:621:THR:OG1	1:B:640:GLU:O	2.17	0.62
1:B:450:VAL:HG11	1:B:472:PRO:HD2	1.80	0.62
1:A:1125:ASN:OD1	1:A:1128:SER:N	2.32	0.61
1:B:430:ASP:OD1	1:B:432:GLU:N	2.34	0.61
1:A:580:TRP:HB3	1:A:614:PHE:HB3	1.82	0.61
1:B:940:SER:HA	1:B:986:LYS:HD2	1.82	0.61
1:A:817:GLY:O	1:A:821:ILE:HG13	2.02	0.60
1:B:403:PRO:HG2	1:B:575:LEU:HD11	1.84	0.60
1:B:687:PRO:HD3	1:B:778:ARG:HH11	1.67	0.59
1:B:401:ILE:HG21	1:B:567:TRP:CZ2	2.37	0.59
1:A:784:SER:HA	1:B:1377:TYR:HE2	1.66	0.59
1:B:852:ARG:O	1:B:856:VAL:HG23	2.02	0.59
1:B:709:ASP:HB3	1:B:1007:ASP:HB2	1.85	0.58
1:B:808:ASP:HB3	1:B:811:LYS:HG2	1.85	0.58
1:A:397:ARG:HG2	1:A:508:ALA:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1075:PHE:CE2	1:A:1118:SER:HA	2.38	0.57
1:A:496:ALA:HB3	1:A:538:ILE:HG22	1.86	0.56
1:A:741:SER:HB3	1:A:770:CYS:HB2	1.86	0.56
1:A:1234:VAL:HG12	1:A:1261:VAL:HG12	1.86	0.56
1:A:683:MET:HE3	1:A:721:ARG:HG2	1.87	0.56
1:B:430:ASP:OD1	1:B:431:LEU:N	2.39	0.56
1:B:580:TRP:HB3	1:B:614:PHE:HB3	1.87	0.55
1:B:1050:LEU:HD11	1:B:1071:LYS:HE3	1.88	0.55
1:B:549:SER:HB2	1:B:607:ILE:HD11	1.87	0.55
1:B:665:HIS:HB2	1:B:1068:MET:HG3	1.88	0.55
1:B:440:TYR:HE1	1:B:444:TRP:HB2	1.71	0.55
1:A:824:LEU:HD11	1:A:1175:ILE:HG13	1.88	0.55
1:A:1257:ARG:O	1:A:1261:VAL:HG23	2.06	0.55
1:A:476:VAL:HG22	1:A:520:PHE:CD2	2.42	0.55
1:A:1270:PRO:HG2	1:A:1289:GLU:HG3	1.88	0.55
1:B:959:LEU:HG	1:B:1022:VAL:HG22	1.89	0.54
1:B:450:VAL:CG1	1:B:471:LYS:HB2	2.38	0.54
1:A:413:PRO:HG2	1:A:416:VAL:HG13	1.90	0.54
1:A:730:ASP:OD2	1:B:949:SER:HB2	2.07	0.54
1:A:1281:ASP:N	1:A:1281:ASP:OD1	2.37	0.54
1:B:1311:LYS:O	1:B:1311:LYS:HD2	2.08	0.54
1:A:1134:ARG:HA	1:A:1139:GLY:HA2	1.88	0.54
1:B:416:VAL:HG13	1:B:481:MET:CE	2.38	0.54
1:A:401:ILE:HD12	1:A:511:TYR:HB2	1.90	0.53
1:A:397:ARG:HB3	1:A:510:LEU:HB2	1.90	0.53
1:A:1089:LYS:HA	1:A:1107:LEU:HD13	1.91	0.53
1:A:1144:PRO:HA	2:C:4:DA:H2'	1.91	0.53
1:B:402:TRP:HE3	1:B:403:PRO:HD2	1.74	0.53
1:B:625:ASP:HB2	1:B:643:THR:HG23	1.90	0.53
1:A:673:GLN:NE2	3:D:2:A:OP1	2.42	0.52
1:A:940:SER:HA	1:A:986:LYS:HD2	1.91	0.52
1:B:1107:LEU:O	1:B:1111:VAL:HG22	2.10	0.52
1:A:575:LEU:HG	1:A:576:VAL:HG23	1.90	0.52
1:B:541:PRO:HD3	1:B:609:LYS:NZ	2.25	0.52
1:B:808:ASP:HB3	1:B:811:LYS:HE3	1.91	0.52
1:A:401:ILE:HD13	1:A:509:PRO:HB3	1.91	0.51
1:A:959:LEU:HG	1:A:1022:VAL:HG22	1.91	0.51
1:B:450:VAL:HG11	1:B:471:LYS:HB2	1.93	0.51
1:B:1075:PHE:HE2	1:B:1121:GLY:HA2	1.74	0.51
1:A:684:THR:HG21	1:A:775:LYS:HB2	1.92	0.51
1:A:397:ARG:HH21	1:A:510:LEU:HD12	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1224:PHE:CD1	1:A:1228:LYS:HD2	2.46	0.51
1:A:1348:MET:HG2	1:B:880:ASN:HB3	1.92	0.50
1:B:493:VAL:HG21	1:B:521:GLU:HB2	1.94	0.50
1:B:823:ASP:OD2	1:B:913:ARG:HD3	2.12	0.50
1:B:1075:PHE:CE2	1:B:1121:GLY:HA2	2.47	0.50
1:B:967:PHE:CD1	1:B:1031:PRO:HG3	2.47	0.50
1:B:1088:TYR:HD1	1:B:1107:LEU:HD11	1.76	0.50
1:B:904:ASP:HA	1:B:907:LYS:NZ	2.28	0.49
1:B:1132:LEU:HD23	1:B:1137:LEU:HD11	1.93	0.49
1:A:392:PRO:HA	1:A:394:VAL:N	2.28	0.48
1:A:1380:PRO:O	1:A:1384:GLU:HG3	2.14	0.48
1:B:565:ILE:HD13	1:B:1074:HIS:CD2	2.48	0.48
1:A:1036:LEU:HB2	1:A:1040:LEU:HD12	1.95	0.48
1:A:1290:LEU:HB2	1:A:1299:ASN:HB2	1.94	0.48
1:B:541:PRO:HD3	1:B:609:LYS:HZ3	1.77	0.48
1:A:1295:ASP:HA	1:B:1340:PRO:HG3	1.96	0.48
1:B:818:ASP:HA	1:B:821:ILE:HG22	1.95	0.48
1:B:406:PRO:CG	1:B:409:LEU:HD12	2.43	0.48
1:A:964:PRO:HG3	4:A:1501:GTP:HN22	1.78	0.47
2:C:8:DC:H2'	2:C:9:DT:C6	2.50	0.47
1:B:427:CYS:O	1:B:429:VAL:HG23	2.14	0.47
1:B:872:GLU:OE1	1:B:872:GLU:N	2.47	0.47
1:A:661:THR:HA	1:A:1047:PHE:HB3	1.96	0.47
2:C:7:DC:H2'	2:C:8:DC:C6	2.50	0.47
1:A:815:ALA:O	1:A:819:ARG:HG3	2.15	0.47
1:B:416:VAL:HG13	1:B:481:MET:HE1	1.97	0.47
1:A:416:VAL:O	1:A:420:VAL:HG13	2.15	0.47
1:B:837:ARG:NH1	1:B:840:GLU:OE1	2.48	0.47
1:A:770:CYS:HB3	1:A:772:PHE:CE1	2.49	0.46
1:A:922:MET:HE3	1:A:1003:LEU:HD12	1.96	0.46
1:B:744:GLY:HA2	1:B:1009:ASP:HB2	1.96	0.46
1:A:710:GLY:HA3	1:A:1009:ASP:HB3	1.96	0.46
1:A:611:ARG:NH2	3:D:0:A:H5''	2.31	0.46
1:A:719:ALA:HA	1:A:722:ILE:HD12	1.97	0.46
1:B:823:ASP:CG	1:B:913:ARG:HD3	2.36	0.46
1:B:1092:LEU:HD22	1:B:1107:LEU:HD12	1.97	0.46
1:B:884:ASP:HB3	1:B:887:LYS:HB2	1.97	0.46
1:A:1040:LEU:HD22	1:A:1122:ILE:HG21	1.97	0.46
1:A:784:SER:HA	1:B:1377:TYR:CE2	2.49	0.45
1:A:1222:LEU:O	1:A:1226:THR:OG1	2.33	0.45
1:A:794:LEU:HD13	1:A:914:VAL:HG21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:407:LYS:HA	1:B:410:HIS:ND1	2.30	0.45
1:B:694:LYS:HE2	1:B:694:LYS:HB3	1.79	0.45
1:A:418:TRP:HH2	1:A:536:PHE:HE1	1.65	0.45
1:A:1119:LYS:HB2	1:A:1119:LYS:HE3	1.63	0.45
1:A:1286:ARG:HH12	1:B:1212:GLU:HB2	1.81	0.45
1:A:1327:ARG:HD2	1:B:1344:ALA:HB1	1.99	0.45
1:B:1039:TYR:CD1	1:B:1132:LEU:HD12	2.51	0.45
1:A:860:ARG:HD3	1:B:1343:GLY:HA3	1.99	0.45
1:A:783:ARG:HD2	3:D:2:A:H4'	1.99	0.45
1:A:805:ARG:HD3	1:A:1026:VAL:O	2.17	0.45
1:A:820:LEU:HD11	1:A:1171:ALA:HB2	1.99	0.45
1:B:406:PRO:HB2	1:B:408:TRP:CD1	2.52	0.45
1:A:902:LYS:HA	1:A:902:LYS:HD2	1.78	0.44
1:A:867:LEU:HD22	1:A:874:THR:HG23	1.98	0.44
1:B:1230:ARG:HH12	1:B:1272:ALA:HB3	1.82	0.44
1:B:1379:ASP:N	1:B:1380:PRO:HD3	2.31	0.44
1:A:473:PRO:HB2	1:A:476:VAL:HG23	2.00	0.44
1:B:922:MET:SD	1:B:1013:ALA:HB2	2.57	0.44
1:A:561:VAL:O	1:A:565:ILE:HG13	2.17	0.44
1:A:958:VAL:HG12	1:A:1017:TRP:HB3	1.99	0.44
1:B:1070:GLN:OE1	1:B:1071:LYS:HG3	2.17	0.44
1:B:1203:LEU:HD13	1:B:1329:LEU:HD22	2.00	0.44
1:B:890:TYR:CE2	1:B:894:ILE:HD11	2.52	0.44
1:B:1187:LYS:HA	1:B:1187:LYS:HD2	1.83	0.44
1:B:421:THR:O	1:B:425:MET:HG3	2.18	0.43
1:B:1211:LYS:HE2	1:B:1211:LYS:HB3	1.86	0.43
1:A:1078:GLN:HG3	1:A:1079:PRO:HD2	2.00	0.43
1:A:1339:ARG:HA	1:A:1339:ARG:HD3	1.85	0.43
1:B:843:GLN:OE1	1:B:1360:LYS:HA	2.18	0.43
1:B:1172:ARG:O	1:B:1172:ARG:HD2	2.18	0.43
1:B:620:ILE:HD13	1:B:620:ILE:HA	1.86	0.43
1:B:710:GLY:HA3	1:B:1009:ASP:HB3	2.00	0.43
1:A:958:VAL:HG23	1:A:974:VAL:HG23	2.00	0.43
1:A:1343:GLY:HA3	1:B:860:ARG:HD2	1.99	0.43
1:B:661:THR:HA	1:B:1047:PHE:HB3	2.00	0.43
1:A:407:LYS:HB3	1:A:407:LYS:HE2	1.65	0.43
1:B:540:ILE:HG13	1:B:541:PRO:CD	2.45	0.43
1:B:569:THR:HG21	1:B:1070:GLN:HA	2.01	0.42
1:B:1081:PHE:HA	1:B:1084:MET:HE3	2.00	0.42
1:A:1399:ASN:N	7:A:1604:HOH:O	2.44	0.42
1:B:793:GLY:HA2	1:B:914:VAL:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1316:LYS:HE3	1:B:1316:LYS:HB2	1.90	0.42
2:C:10:DT:H2''	2:C:11:DT:H5''	2.01	0.42
1:B:883:PHE:HZ	1:B:1203:LEU:HD21	1.84	0.42
1:A:425:MET:HE1	1:A:515:LEU:H	1.85	0.42
1:A:1402:TYR:HE1	1:B:586:LYS:HD3	1.85	0.42
1:B:548:PRO:HA	1:B:551:PRO:HD3	2.01	0.42
1:B:839:VAL:HG22	1:B:1363:THR:HG23	2.02	0.42
1:B:1042:LYS:HE3	1:B:1122:ILE:HD11	2.02	0.42
1:A:679:THR:HB	1:A:781:GLU:HB3	2.02	0.42
1:A:744:GLY:HA2	1:A:1009:ASP:HB2	2.02	0.42
1:B:1224:PHE:HD1	1:B:1224:PHE:HA	1.78	0.42
1:A:824:LEU:HD21	1:A:906:LEU:HD23	2.02	0.42
1:A:946:GLU:HB3	1:A:947:GLU:H	1.59	0.41
1:A:1309:ALA:HB1	1:A:1321:VAL:HG12	2.01	0.41
1:B:403:PRO:CG	1:B:575:LEU:HD11	2.49	0.41
1:B:961:ALA:O	1:B:1014:TRP:N	2.50	0.41
1:A:550:VAL:HA	1:A:551:PRO:HD3	1.95	0.41
1:A:1083:GLY:HA2	2:C:7:DC:O4'	2.21	0.41
1:A:402:TRP:CD1	1:A:573:HIS:HB3	2.55	0.41
1:A:713:ARG:HE	1:A:713:ARG:HB2	1.76	0.41
1:B:662:TRP:CZ3	1:B:663:GLN:HG2	2.55	0.41
1:B:1227:LEU:HD13	1:B:1301:TRP:CZ2	2.55	0.41
1:A:1224:PHE:CE1	1:A:1228:LYS:HD2	2.55	0.41
1:B:811:LYS:HG3	1:B:812:MET:N	2.35	0.41
1:A:534:ARG:HD2	1:A:642:ARG:HD2	2.03	0.41
1:B:837:ARG:HA	1:B:838:PRO:HD3	1.95	0.41
1:B:1041:LYS:HB3	1:B:1041:LYS:HE2	1.85	0.40
1:A:579:GLN:HB2	1:A:618:THR:HG23	2.03	0.40
1:A:794:LEU:HD13	1:A:914:VAL:CG2	2.52	0.40
1:A:543:PRO:HG2	1:A:561:VAL:HG13	2.02	0.40
1:A:1245:LYS:O	1:A:1245:LYS:HG2	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	907/1026 (88%)	885 (98%)	22 (2%)	0	100	100
1	B	905/1026 (88%)	883 (98%)	22 (2%)	0	100	100
All	All	1812/2052 (88%)	1768 (98%)	44 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	796/894 (89%)	773 (97%)	23 (3%)	42	69
1	B	801/894 (90%)	771 (96%)	30 (4%)	34	60
All	All	1597/1788 (89%)	1544 (97%)	53 (3%)	38	64

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	407	LYS
1	A	410	HIS
1	A	416	VAL
1	A	428	LYS
1	A	430	ASP
1	A	474	ASN
1	A	545	SER
1	A	550	VAL
1	A	553	VAL
1	A	570	MET
1	A	618	THR
1	A	621	THR
1	A	743	LYS
1	A	778	ARG
1	A	812	MET

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Mol	Chain	Res	Type
1	A	813	ARG
1	A	1039	TYR
1	A	1078	GLN
1	A	1152	SER
1	A	1183	HIS
1	A	1311	LYS
1	A	1316	LYS
1	A	1373	ASP
1	B	398	LEU
1	B	399	ARG
1	B	401	ILE
1	B	407	LYS
1	B	448	ARG
1	B	475	ASP
1	B	504	ASN
1	B	505	SER
1	B	509	PRO
1	B	510	LEU
1	B	513	VAL
1	B	546	THR
1	B	549	SER
1	B	561	VAL
1	B	562	GLU
1	B	565	ILE
1	B	638	PRO
1	B	837	ARG
1	B	1075	PHE
1	B	1152	SER
1	B	1177	LYS
1	B	1178	GLU
1	B	1186	MET
1	B	1224	PHE
1	B	1273	MET
1	B	1285	ILE
1	B	1289	GLU
1	B	1291	SER
1	B	1296	ARG
1	B	1373	ASP

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	474	ASN
1	A	522	GLN
1	A	1078	GLN
1	A	1131	GLN
1	B	641	GLN
1	B	911	ASN
1	B	1074	HIS
1	B	1259	ASN
1	B	1260	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	D	2/4 (50%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 5 are monoatomic - leaving 2 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	$\# Z > 2$
4	GTP	A	1501	5	25,33,34	1.02	2 (8%)	29,52,54	0.80	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	ATP	B	1503	5	26,33,33	0.57	0	31,52,52	0.82	2 (6%)

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
4	GTP	A	1501	5	-	3/18/34/38	0/3/3/3
6	ATP	B	1503	5	-	9/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1501	GTP	C5-C6	-2.63	1.42	1.47
4	A	1501	GTP	C8-N7	-2.15	1.31	1.35

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1503	ATP	C5-C6-N6	2.39	123.98	120.35
6	B	1503	ATP	PB-O3B-PG	2.06	139.89	132.83

There are no chirality outliers.

All (12) torsion outliers are listed below:

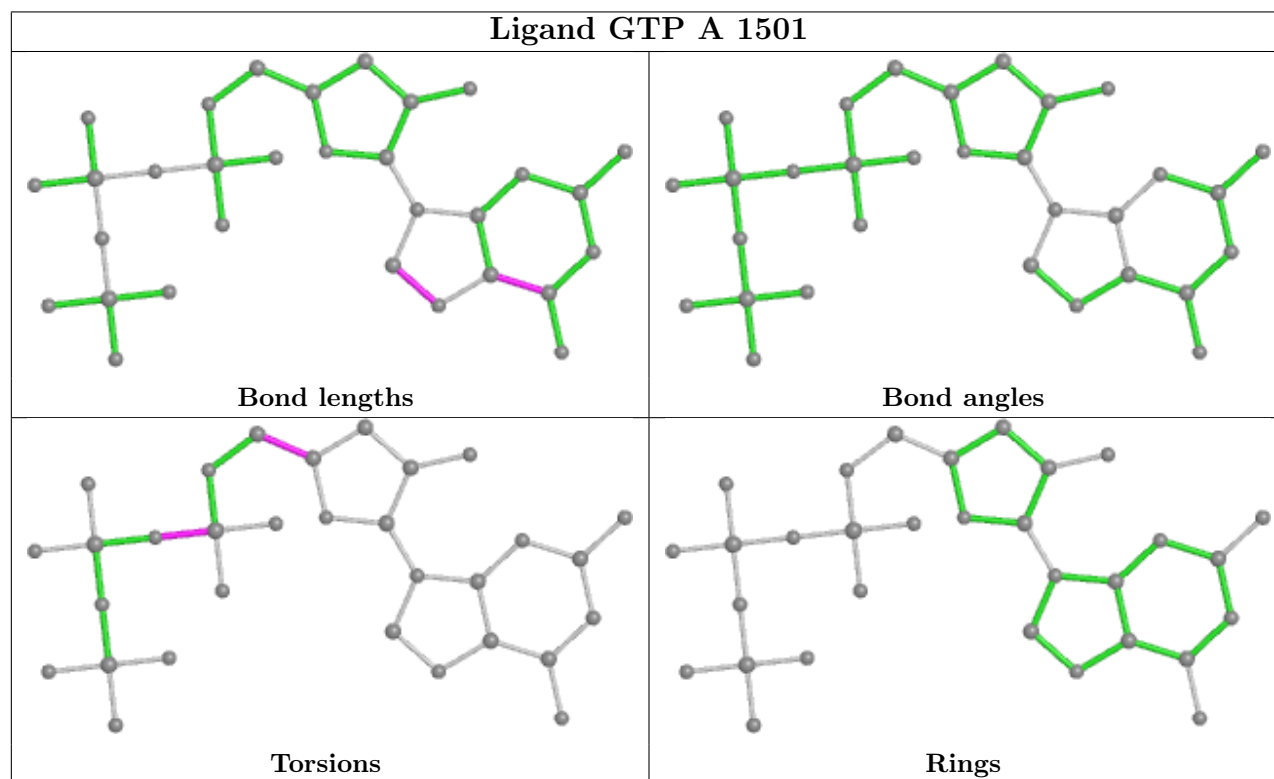
Mol	Chain	Res	Type	Atoms
4	A	1501	GTP	O4'-C4'-C5'-O5'
4	A	1501	GTP	C3'-C4'-C5'-O5'
6	B	1503	ATP	PB-O3B-PG-O3G
6	B	1503	ATP	C5'-O5'-PA-O1A
6	B	1503	ATP	C5'-O5'-PA-O2A
6	B	1503	ATP	O4'-C4'-C5'-O5'
6	B	1503	ATP	C3'-C4'-C5'-O5'
4	A	1501	GTP	PB-O3A-PA-O5'
6	B	1503	ATP	C4'-C5'-O5'-PA
6	B	1503	ATP	PB-O3B-PG-O1G
6	B	1503	ATP	PB-O3B-PG-O2G
6	B	1503	ATP	C5'-O5'-PA-O3A

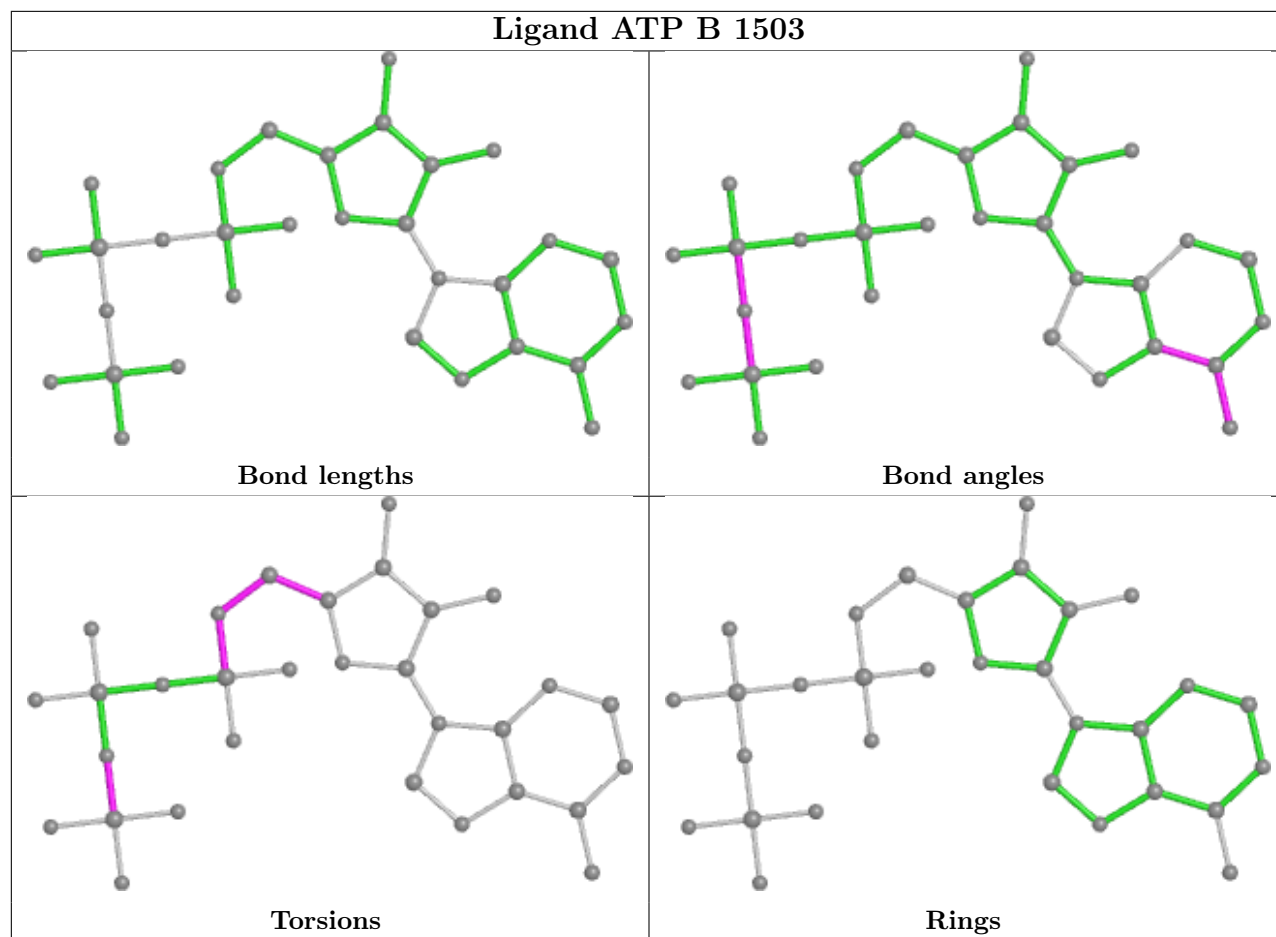
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1501	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.





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	937/1026 (91%)	-0.02	17 (1%) 68 71	29, 67, 117, 149	0
1	B	930/1026 (90%)	0.10	31 (3%) 46 50	28, 63, 122, 153	0
2	C	9/12 (75%)	1.08	3 (33%) 0 0	98, 114, 162, 164	0
3	D	4/4 (100%)	-0.24	0 100 100	93, 107, 141, 176	0
All	All	1880/2068 (90%)	0.04	51 (2%) 54 58	28, 66, 120, 176	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	477	PHE	3.9
1	B	606	PRO	3.9
1	B	416	VAL	3.8
1	A	409	LEU	3.6
1	B	398	LEU	3.4
1	B	1374	GLY	3.3
1	A	1218	ARG	3.3
1	A	444	TRP	3.2
2	C	12	DT	3.1
1	A	906	LEU	3.1
1	B	418	TRP	3.1
1	B	500	TYR	3.0
1	B	476	VAL	3.0
2	C	5	DG	3.0
1	B	608	ILE	2.9
1	A	427	CYS	2.9
1	B	1213	ILE	2.9
1	B	561	VAL	2.8
1	B	1251	LYS	2.8
1	B	1286	ARG	2.8
1	A	1154	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	454	TRP	2.7
1	B	1375	SER	2.7
1	A	455	LYS	2.6
2	C	4	DA	2.5
1	A	1282	SER	2.5
1	A	508	ALA	2.5
1	A	443	SER	2.4
1	B	540	ILE	2.4
1	B	512	LEU	2.4
1	B	504	ASN	2.4
1	B	570	MET	2.3
1	B	607	ILE	2.3
1	B	515	LEU	2.3
1	A	554	VAL	2.3
1	B	902	LYS	2.3
1	A	1122	ILE	2.2
1	B	510	LEU	2.2
1	B	947	GLU	2.2
1	B	1380	PRO	2.2
1	A	570	MET	2.1
1	B	560	ALA	2.1
1	B	506	PRO	2.1
1	B	513	VAL	2.1
1	A	405	PHE	2.1
1	B	625	ASP	2.1
1	A	454	TRP	2.1
1	A	1383	TYR	2.0
1	B	1288	LEU	2.0
1	B	1216	LYS	2.0
1	A	638	PRO	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 ⓘ

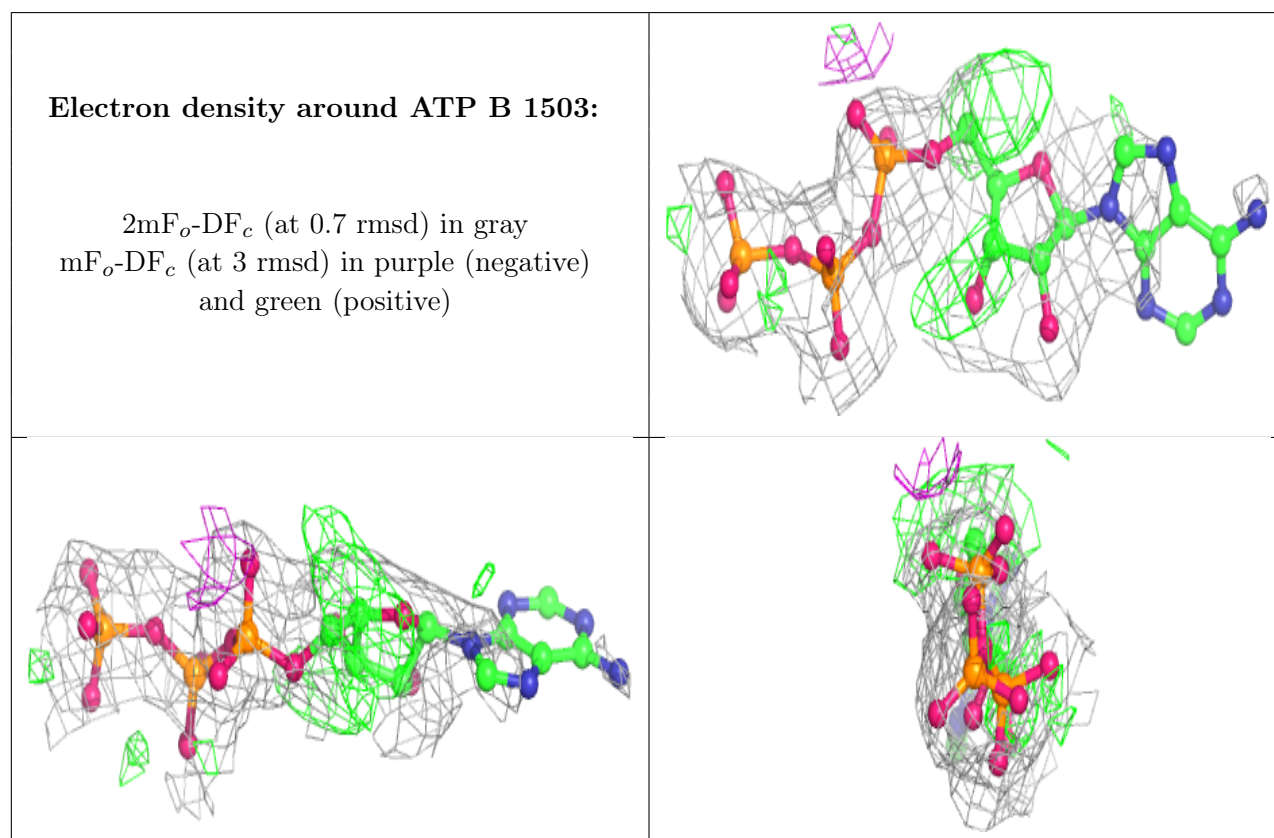
There are no monosaccharides in this entry.

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.

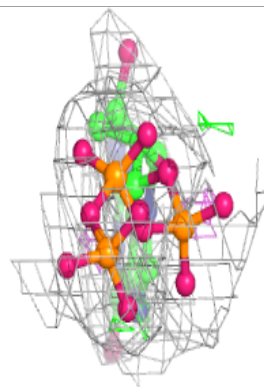
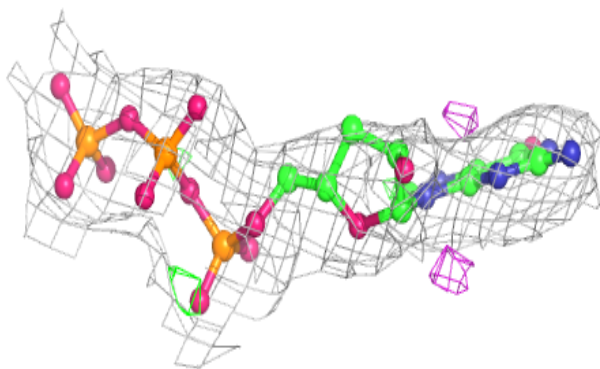
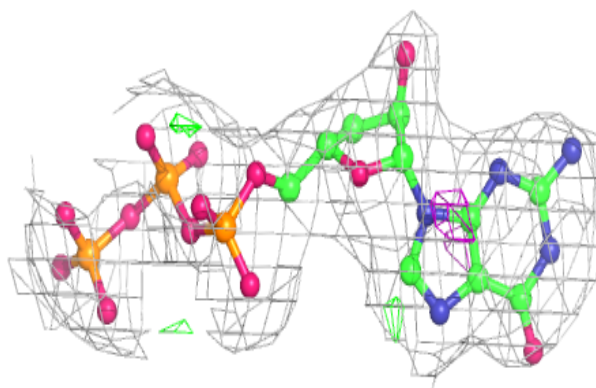
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	MG	A	1502	1/1	0.73	0.10	91,91,91,91	0
6	ATP	B	1503	31/31	0.84	0.21	44,74,105,109	13
5	MG	A	1503	1/1	0.92	0.12	62,62,62,62	0
5	MG	B	1501	1/1	0.93	0.23	67,67,67,67	0
4	GTP	A	1501	31/32	0.93	0.13	53,82,93,98	3
5	MG	A	1504	1/1	0.95	0.21	48,48,48,48	0
5	MG	B	1502	1/1	0.98	0.20	40,40,40,40	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 1501:

$2mF_o-DF_c$ (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.