



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 09:51 AM UTC

PDB ID : 7Y7Q / pdb_00007y7q
Title : QDE-1 in complex with RNA template, RNA primer and 3'-dGTP
Authors : Cui, R.X.; Gan, J.H.; Ma, J.B.
Deposited on : 2022-06-22
Resolution : 2.05 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

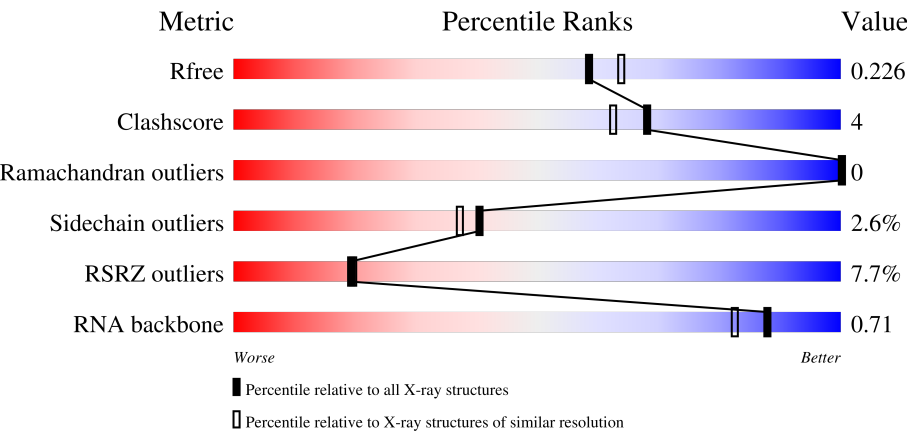
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)
RNA backbone	3983	1085 (2.40-1.68)

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	7% 82% 10% 7%
1	B	1026	7% 79% 9% 12%
2	C	14	64% 7% 29%
2	E	14	14% 29% 57%

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Mol	Chain	Length	Quality of chain
3	D	7	 100%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 16072 atoms, of which 18 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	951	Total	C	N	O	S	0	13	0
			7600	4864	1306	1394	36			
1	B	906	Total	C	N	O	S	0	1	0
			7213	4618	1254	1307	34			

- Molecule 2 is a RNA chain called RNA (5'-R(*GP*AP*AP*CP*UP*AP*CP*CP*GP*UP*CP*GP*GP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	10	Total	C	N	O	P	0	0	0
			213	95	38	70	10			
2	E	6	Total	C	N	O	P	0	2	0
			125	56	21	42	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	7	Total	C	N	O	P	0	0	0
			144	66	26	46	6			

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Ca	0	0
			2	2		
4	B	2	Total	Ca	0	0
			2	2		

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Mg 1 1	0	0
5	B	2	Total Mg 2 2	0	0

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



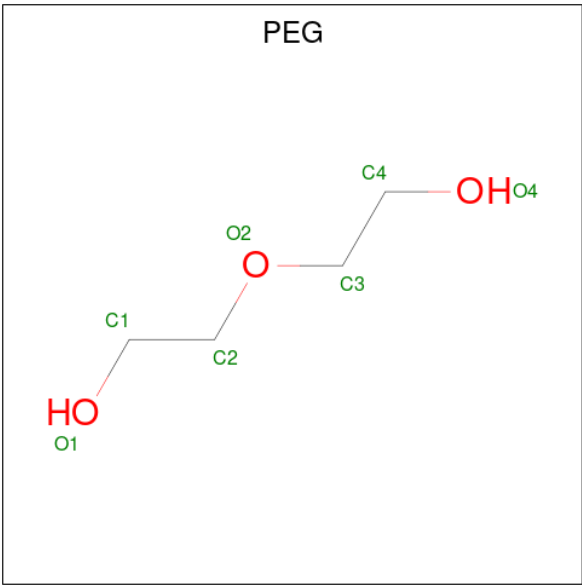
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C H O 14 3 8 3	0	0
6	B	1	Total C O 6 3 3	0	0
6	B	1	Total C O 6 3 3	0	0

- Molecule 7 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 8 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	B	1	Total	C	H	O	0	0
			17	4	10	3		

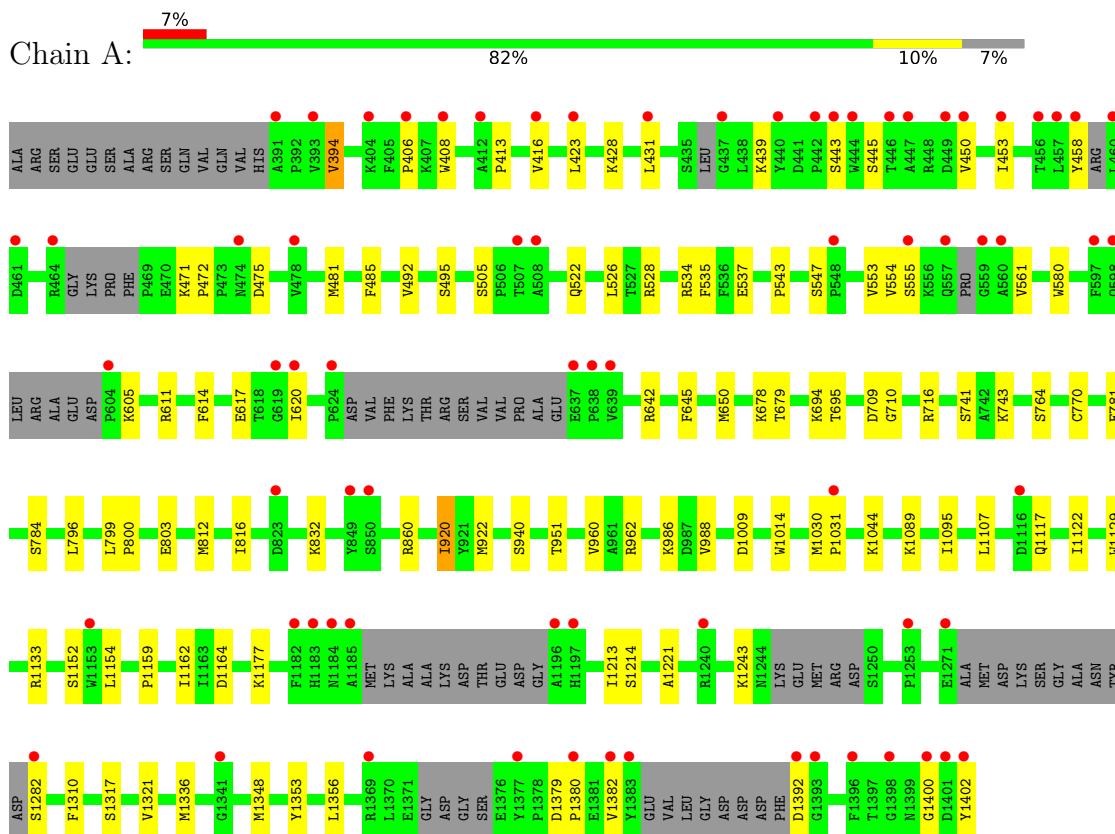
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	351	Total 351	O 351	0	0
9	B	245	Total 245	O 245	0	0
9	C	22	Total 22	O 22	0	0
9	D	12	Total 12	O 12	0	0
9	E	4	Total 4	O 4	0	0

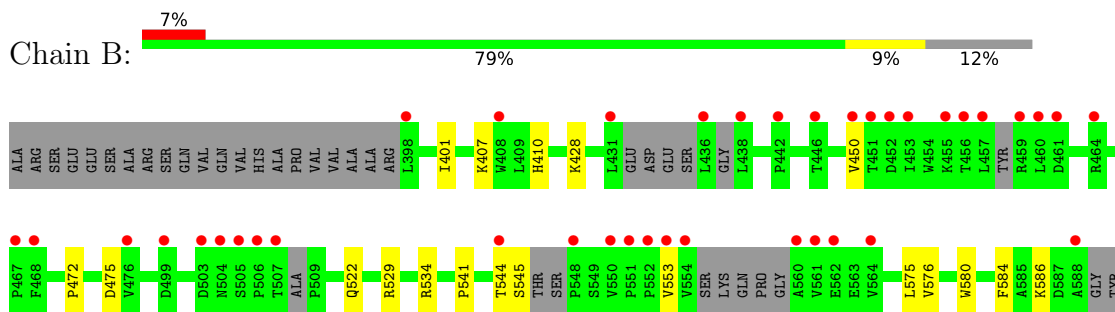
3 Residue-property plots [i](#)

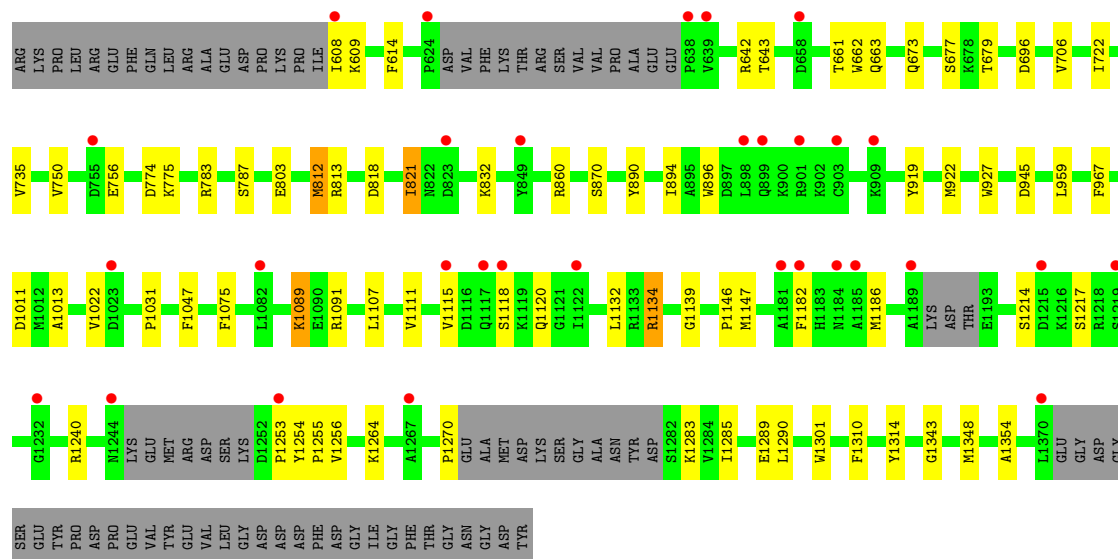
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



- Molecule 1: RNA-dependent RNA polymerase





- Molecule 2: RNA (5'-R(*GP*AP*AP*CP*UP*AP*CP*CP*GP*UP*CP*GP*GP*A)-3')

Chain C: 64% 7% 29%



- Molecule 2: RNA (5'-R(*GP*AP*AP*CP*UP*AP*CP*CP*GP*UP*CP*GP*GP*A)-3')

Chain E: 14% 14% 29% 57%



- Molecule 3: RNA (5'-R(*UP*CP*CP*GP*AP*CP*G)-3')

Chain D: 100%

There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	81.21Å 85.81Å 101.58Å 102.56° 104.05° 94.06°	Depositor
Resolution (Å)	29.31 – 2.05 29.31 – 2.05	Depositor EDS
% Data completeness (in resolution range)	94.1 (29.31-2.05) 94.1 (29.31-2.05)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.29 (at 2.06Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.196 , 0.226 0.196 , 0.226	Depositor DCC
R_{free} test set	7584 reflections (4.72%)	wwPDB-VP
Wilson B-factor (Å ²)	33.3	Xtriage
Anisotropy	0.373	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 42.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16072	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.75% 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, PEG, CA, 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	0.62	0/7791	0.86	2/10535 (0.0%)
1	B	0.59	0/7389	0.85	1/9985 (0.0%)
2	C	0.43	0/237	0.62	0/367
2	E	0.43	0/138	0.54	0/212
3	D	0.44	0/160	0.54	0/247
All	All	0.60	0/15715	0.85	3/21346 (0.0%)

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

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

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1154	LEU	N-CA-C	-6.68	104.71	112.92
1	A	951	THR	N-CA-C	-5.96	105.98	113.72
1	B	945	ASP	N-CA-C	-5.67	100.89	109.85

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	784[B]	SER	Mainchain

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	7600	0	7428	60	0
1	B	7213	0	7096	55	0
2	C	213	0	109	1	0
2	E	125	0	64	3	0
3	D	144	0	76	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	1	0	0	0	0
5	B	2	0	0	0	0
6	A	6	8	8	1	0
6	B	12	0	16	0	0
7	A	31	0	10	0	0
7	B	62	0	20	1	0
8	B	7	10	10	0	0
9	A	351	0	0	3	0
9	B	245	0	0	0	0
9	C	22	0	0	0	0
9	D	12	0	0	0	0
9	E	4	0	0	0	0
All	All	16054	18	14837	109	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 (109) 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:450:VAL:HG21	1:B:472:PRO:HG2	1.55	0.86
1:A:812[B]:MET:HE2	1:A:816:ILE:CD1	2.14	0.77
1:A:1348:MET:HE1	1:A:1356:LEU:HD12	1.77	0.66
1:B:1147:MET:HA	1:B:1147:MET:HE2	1.77	0.66
1:A:1400:GLY:H	1:B:783:ARG:HH12	1.41	0.66
1:B:1075:PHE:CE1	1:B:1118:SER:HA	2.31	0.65
1:A:526:LEU:HD13	1:A:650[B]:MET:HE3	1.76	0.65
1:B:575:LEU:HG	1:B:576:VAL:HG23	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1095:ILE:HA	6:A:2004:GOL:H31	1.80	0.64
1:A:528:ARG:NH1	9:A:2105:HOH:O	2.31	0.63
1:A:1402:TYR:HB2	1:B:677:SER:HA	1.81	0.63
1:A:1400:GLY:C	1:B:783:ARG:HH22	2.07	0.62
1:A:940:SER:HA	1:A:986:LYS:HD2	1.84	0.59
1:A:535:PHE:HE1	1:A:650[B]:MET:HE1	1.68	0.59
1:A:922[A]:MET:HE1	1:A:962:ARG:HD2	1.84	0.58
1:B:1270:PRO:HG2	1:B:1289:GLU:HG3	1.85	0.58
1:A:812[B]:MET:HE2	1:A:816:ILE:HD11	1.85	0.56
1:B:450:VAL:HG21	1:B:472:PRO:CG	2.31	0.56
1:B:584:PHE:CZ	1:B:673:GLN:HG3	2.41	0.56
1:A:1117:GLN:HG3	1:A:1122:ILE:HB	1.88	0.56
1:B:1111:VAL:O	1:B:1115:VAL:HG23	2.06	0.55
1:A:413:PRO:HG2	1:A:481:MET:HE1	1.88	0.54
1:B:1089:LYS:HG3	1:B:1107:LEU:HB3	1.89	0.53
1:A:812[B]:MET:HE2	1:A:816:ILE:HD12	1.89	0.53
1:B:896:TRP:HB3	1:B:1182:PHE:HE1	1.72	0.53
1:B:1253:PRO:HG2	1:B:1256:VAL:HG23	1.89	0.53
1:A:803:GLU:N	1:A:812[B]:MET:HE3	2.24	0.53
1:A:1089:LYS:HA	1:A:1107:LEU:HD13	1.90	0.52
1:B:967:PHE:CD1	1:B:1031:PRO:HG3	2.44	0.52
2:E:7:C:H2'	2:E:8:C:C6	2.45	0.52
1:A:423:LEU:HD11	1:A:458:TYR:HE1	1.74	0.51
1:A:450:VAL:HG11	1:A:471:LYS:HB2	1.93	0.50
1:B:541:PRO:HG3	1:B:609:LYS:HE2	1.92	0.50
1:B:1115:VAL:HG11	7:B:1509:GTP:C3'	2.42	0.50
1:A:694:LYS:HG2	1:A:695:THR:HG23	1.94	0.49
1:A:1348:MET:HE3	1:A:1353:TYR:HA	1.95	0.49
1:B:1134:ARG:HA	1:B:1139:GLY:HA2	1.94	0.49
1:A:741:SER:HB3	1:A:770:CYS:HB2	1.94	0.49
1:B:522:GLN:HE21	1:B:679:THR:C	2.20	0.49
1:B:812:MET:HE3	1:B:813:ARG:N	2.28	0.49
1:A:812[B]:MET:HE1	1:A:1162:ILE:CD1	2.43	0.49
1:B:922:MET:HE2	1:B:1011:ASP:HB3	1.95	0.49
1:A:534:ARG:HD2	1:A:642:ARG:HD2	1.95	0.48
1:B:959:LEU:HD13	1:B:1022:VAL:HG22	1.94	0.48
1:A:406:PRO:HB2	1:A:408:TRP:CD1	2.48	0.48
1:A:450:VAL:HG11	1:A:472:PRO:HD2	1.95	0.48
1:A:1379:ASP:HB3	1:A:1382:VAL:HB	1.95	0.47
1:A:709:ASP:OD1	1:A:764:SER:HB2	2.15	0.47
1:B:922:MET:SD	1:B:1013:ALA:HB2	2.53	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:543:PRO:HB2	1:A:561:VAL:HG13	1.97	0.47
1:B:750:VAL:HG22	1:B:927:TRP:CE2	2.49	0.47
1:B:774:ASP:OD1	1:B:775:LYS:N	2.47	0.47
1:B:803:GLU:HG3	1:B:812:MET:HE1	1.96	0.47
1:A:522[B]:GLN:HB3	1:A:678:LYS:HB3	1.97	0.46
1:B:529:ARG:O	1:B:529:ARG:NH1	2.36	0.46
1:B:544:THR:O	1:B:545:SER:C	2.58	0.46
1:A:832:LYS:NZ	9:A:2122:HOH:O	2.46	0.46
1:B:407:LYS:HA	1:B:410:HIS:CD2	2.51	0.46
1:B:1254:TYR:HB3	1:B:1255:PRO:HD3	1.96	0.46
1:B:1270:PRO:HB3	1:B:1285:ILE:CD1	2.46	0.45
1:A:799:LEU:HB2	1:A:800:PRO:HD3	1.98	0.45
1:A:526:LEU:HD13	1:A:650[B]:MET:CE	2.45	0.45
1:A:611[A]:ARG:NH2	9:A:2118:HOH:O	2.44	0.45
1:B:1310:PHE:O	1:B:1314:TYR:HB3	2.17	0.45
1:A:1392[A]:ASP:OD2	2:E:9:G:O3'	2.33	0.45
1:A:580:TRP:HB3	1:A:614:PHE:HB3	1.99	0.44
1:B:832:LYS:HB2	1:B:832:LYS:HE2	1.72	0.44
1:A:605:LYS:HE2	2:C:5:U:O4	2.18	0.44
1:B:696:ASP:HB3	1:B:706:VAL:HG13	1.99	0.44
1:A:416:VAL:HG22	1:A:453:ILE:HD13	2.00	0.44
1:A:450:VAL:CG1	1:A:471:LYS:HB2	2.48	0.44
1:A:413:PRO:HD2	1:A:416:VAL:HB	1.99	0.44
1:A:495:SER:HA	1:A:537:GLU:O	2.18	0.44
1:B:722:ILE:HD13	1:B:735:VAL:HG11	1.99	0.43
1:B:803:GLU:HG3	1:B:812:MET:CE	2.48	0.43
1:B:534:ARG:HD2	1:B:642:ARG:HD2	2.01	0.43
1:A:710:GLY:HA3	1:A:1009:ASP:HB3	2.01	0.43
1:B:662:TRP:CZ3	1:B:663:GLN:HG2	2.54	0.43
1:B:1089:LYS:HA	1:B:1107:LEU:HD13	2.01	0.43
1:A:679:THR:HB	1:A:781:GLU:HB3	2.01	0.43
1:B:890:TYR:CE2	1:B:894:ILE:HD11	2.54	0.42
1:A:1214:SER:HB2	1:A:1221:ALA:HA	2.01	0.42
1:B:860:ARG:HA	1:B:1354:ALA:HB2	2.00	0.42
1:B:919:TYR:CD2	2:E:10[B]:U:H5'	2.55	0.42
1:A:485:PHE:CD2	1:A:492:VAL:HB	2.54	0.42
1:A:860:ARG:HD2	1:B:1343:GLY:HA3	2.02	0.42
1:A:960:VAL:HA	1:A:1014:TRP:O	2.20	0.42
1:B:1186:MET:HE2	1:B:1186:MET:HB3	1.92	0.42
1:A:1336:MET:HE3	1:A:1336:MET:HB3	1.87	0.41
1:B:580:TRP:HB3	1:B:614:PHE:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1091:ARG:HG2	1:B:1146:PRO:HD3	2.01	0.41
1:A:1159:PRO:HB3	1:A:1164:ASP:HB3	2.02	0.41
1:B:1270:PRO:HG3	1:B:1301:TRP:CE3	2.56	0.41
1:A:796:LEU:O	1:A:800:PRO:HD3	2.20	0.41
1:A:1129:TRP:CE2	1:A:1133:ARG:HD2	2.56	0.41
1:A:1310:PHE:HA	1:A:1321:VAL:HG21	2.01	0.41
1:A:428:LYS:HA	1:A:428:LYS:HD2	1.83	0.41
1:A:1030:MET:HA	1:A:1031:PRO:HD3	1.93	0.41
1:B:1270:PRO:HG3	1:B:1301:TRP:CD2	2.56	0.41
1:B:1289:GLU:O	1:B:1290:LEU:C	2.64	0.41
1:A:920:ILE:HG22	1:A:988:VAL:HA	2.03	0.41
1:A:1380:PRO:HG3	1:B:787:SER:HB2	2.02	0.41
1:B:818:ASP:O	1:B:821:ILE:HG22	2.21	0.40
1:A:617:GLU:HA	1:A:645:PHE:O	2.21	0.40
1:A:1402:TYR:HE1	1:B:586:LYS:HD2	1.86	0.40
1:B:407:LYS:HG2	1:B:410:HIS:CE1	2.56	0.40
1:A:394:VAL:HG12	1:A:553:VAL:HG22	2.04	0.40
1:A:1402:TYR:CD1	1:B:673:GLN:HG2	2.57	0.40
1:B:661:THR:HA	1:B:1047:PHE:HB3	2.03	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	935/1026 (91%)	920 (98%)	15 (2%)	0	100	100
1	B	884/1026 (86%)	871 (98%)	13 (2%)	0	100	100
All	All	1819/2052 (89%)	1791 (98%)	28 (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	813/894 (91%)	791 (97%)	22 (3%)	39	36
1	B	770/894 (86%)	750 (97%)	20 (3%)	40	37
All	All	1583/1788 (88%)	1541 (97%)	42 (3%)	40	36

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	394	VAL
1	A	431	LEU
1	A	439	LYS
1	A	443	SER
1	A	445	SER
1	A	475	ASP
1	A	505	SER
1	A	547	SER
1	A	554	VAL
1	A	555	SER
1	A	620	ILE
1	A	716	ARG
1	A	743[A]	LYS
1	A	743[B]	LYS
1	A	920	ILE
1	A	1044	LYS
1	A	1152	SER
1	A	1177	LYS
1	A	1213	ILE
1	A	1243	LYS
1	A	1282	SER
1	A	1317	SER
1	B	401	ILE
1	B	428	LYS
1	B	475	ASP
1	B	553	VAL
1	B	608	ILE

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Mol	Chain	Res	Type
1	B	643	THR
1	B	756	GLU
1	B	812	MET
1	B	821	ILE
1	B	870	SER
1	B	1089	LYS
1	B	1120	GLN
1	B	1132	LEU
1	B	1134	ARG
1	B	1214	SER
1	B	1217	SER
1	B	1240	ARG
1	B	1264	LYS
1	B	1283	LYS
1	B	1348	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	484	ASN
1	A	673	GLN
1	A	831	GLN
1	A	858	HIS
1	A	876	ASN
1	A	1323	GLN
1	A	1335	GLN
1	B	410	HIS
1	B	522	GLN
1	B	613	HIS
1	B	814	GLN
1	B	1074	HIS
1	B	1078	GLN
1	B	1184	ASN
1	B	1259	ASN
1	B	1260	GLN
1	B	1335	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	C	9/14 (64%)	0	0
2	E	5/14 (35%)	0	0
3	D	5/7 (71%)	0	0
All	All	19/35 (54%)	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 7 are monoatomic - leaving 7 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	GOL	B	1506	-	5,5,5	0.07	0	5,5,5	0.33	0
7	GTP	B	1509	4,5	31,33,34	0.66	0	44,52,54	0.67	0
6	GOL	B	1507	-	5,5,5	0.08	0	5,5,5	0.29	0
8	PEG	B	1501	-	6,6,6	0.12	0	5,5,5	0.07	0
7	GTP	B	1502	-	31,33,34	0.65	0	44,52,54	0.64	0
7	GTP	A	2005	4	31,33,34	0.66	0	44,52,54	0.60	0
6	GOL	A	2004	-	5,5,5	0.08	0	5,5,5	0.26	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
6	GOL	B	1506	-	-	4/4/4/4	-
7	GTP	B	1509	4,5	-	4/22/34/38	0/3/3/3
6	GOL	B	1507	-	-	1/4/4/4	-
8	PEG	B	1501	-	-	2/4/4/4	-
7	GTP	B	1502	-	-	7/22/34/38	0/3/3/3
7	GTP	A	2005	4	-	3/22/34/38	0/3/3/3
6	GOL	A	2004	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (25) torsion outliers are listed below:

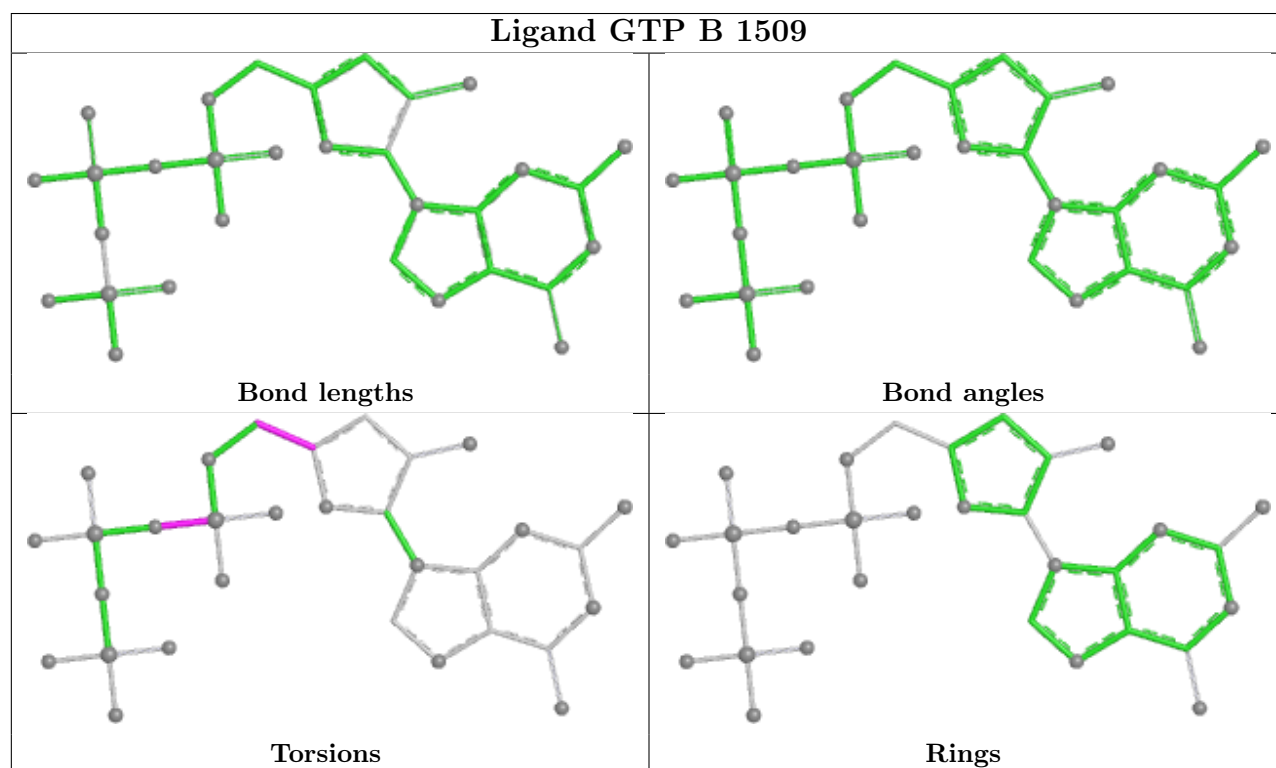
Mol	Chain	Res	Type	Atoms
6	A	2004	GOL	O1-C1-C2-C3
7	B	1502	GTP	C5'-O5'-PA-O3A
7	B	1502	GTP	C5'-O5'-PA-O2A
7	B	1502	GTP	O4'-C4'-C5'-O5'
7	B	1509	GTP	C3'-C4'-C5'-O5'
7	B	1509	GTP	O4'-C4'-C5'-O5'
8	B	1501	PEG	O1-C1-C2-O2
6	A	2004	GOL	C1-C2-C3-O3
6	B	1506	GOL	O1-C1-C2-C3
6	B	1506	GOL	C1-C2-C3-O3
6	B	1507	GOL	C1-C2-C3-O3
8	B	1501	PEG	O2-C3-C4-O4
6	B	1506	GOL	O1-C1-C2-O2
7	A	2005	GTP	C3'-C4'-C5'-O5'
7	B	1502	GTP	C3'-C4'-C5'-O5'
6	A	2004	GOL	O1-C1-C2-O2
6	B	1506	GOL	O2-C2-C3-O3
7	A	2005	GTP	PB-O3A-PA-O5'
7	B	1502	GTP	PB-O3A-PA-O5'
7	B	1509	GTP	PB-O3A-PA-O5'
7	B	1502	GTP	C5'-O5'-PA-O1A
7	B	1509	GTP	PB-O3A-PA-O1A
6	A	2004	GOL	O2-C2-C3-O3
7	A	2005	GTP	O4'-C4'-C5'-O5'
7	B	1502	GTP	PB-O3A-PA-O2A

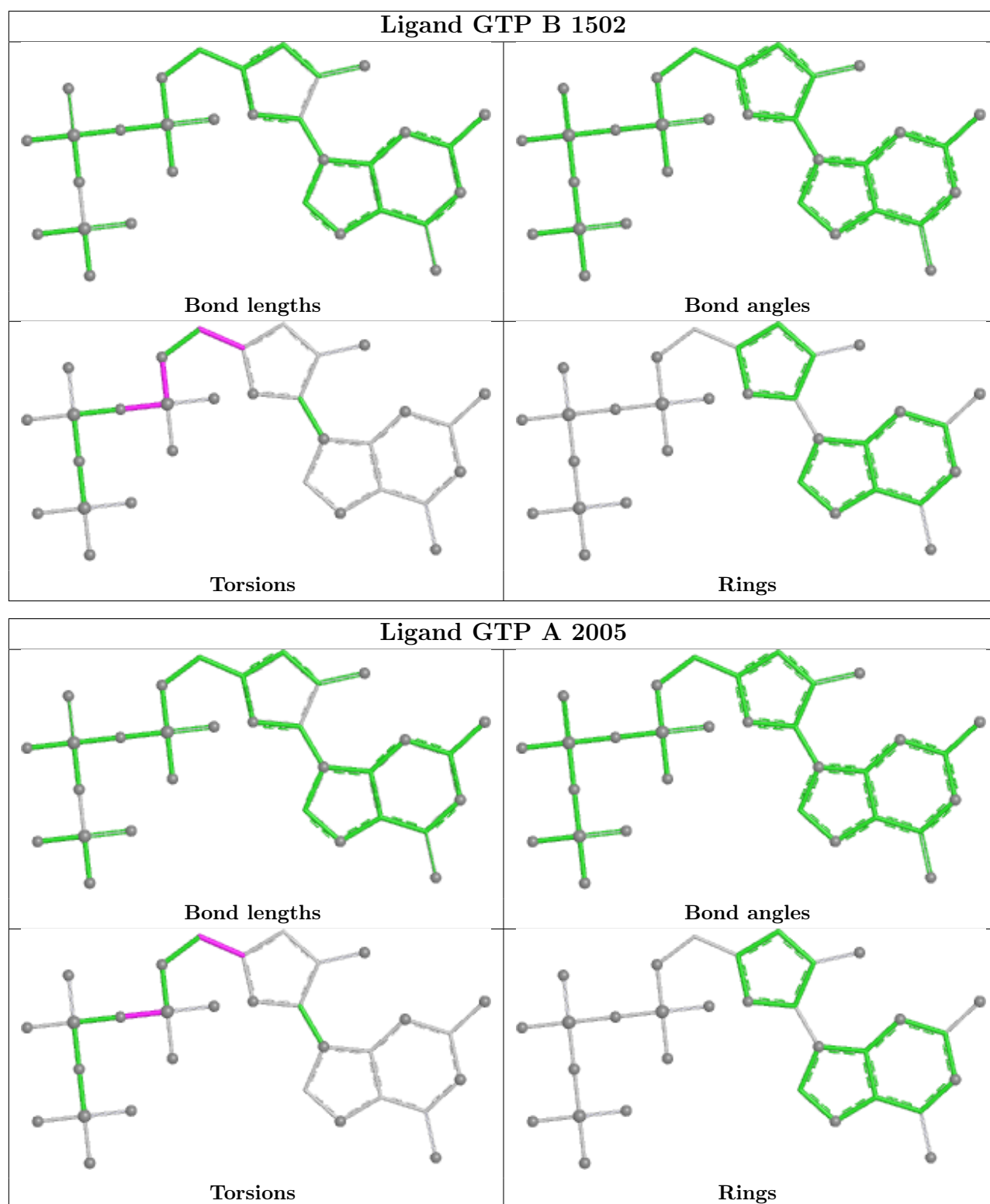
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	1509	GTP	1	0
6	A	2004	GOL	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	951/1026 (92%)	0.38	72 (7%)	20	20	12, 42, 77, 118	13 (1%)
1	B	906/1026 (88%)	0.47	70 (7%)	19	20	16, 45, 80, 100	1 (0%)
2	C	10/14 (71%)	-0.22	0	100	100	27, 43, 76, 101	0
2	E	6/14 (42%)	1.96	2 (33%)	1	0	26, 89, 98, 120	2 (33%)
3	D	7/7 (100%)	0.30	0	100	100	27, 46, 103, 130	0
All	All	1880/2087 (90%)	0.43	144 (7%)	19	20	12, 43, 80, 130	16 (0%)

All (144) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	559	GLY	5.6
1	B	561	VAL	5.2
1	A	444	TRP	5.0
1	A	508	ALA	4.7
1	A	620	ILE	4.7
1	A	1401	ASP	4.6
1	B	1244	ASN	4.6
2	E	11[B]	C	4.5
1	A	1396[A]	PHE	4.4
1	B	638	PRO	4.3
1	B	553	VAL	4.2
1	B	436	LEU	4.1
1	B	468	PHE	4.0
2	E	10[B]	U	3.8
1	B	507	THR	3.8
1	A	460	LEU	3.7
1	B	849	TYR	3.7
1	B	551	PRO	3.7
1	A	437	GLY	3.7
1	A	391	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	598	GLN	3.6
1	B	608	ILE	3.5
1	B	544	THR	3.5
1	A	1398	GLY	3.5
1	B	550	VAL	3.5
1	A	443	SER	3.4
1	A	458	TYR	3.4
1	A	1402	TYR	3.4
1	B	548	PRO	3.4
1	B	552	PRO	3.4
1	A	393	VAL	3.4
1	A	624	PRO	3.4
1	A	453	ILE	3.4
1	A	557	GLN	3.4
1	B	639	VAL	3.3
1	B	624	PRO	3.3
1	B	1185	ALA	3.2
1	B	1189	ALA	3.2
1	B	1182	PHE	3.2
1	A	1400	GLY	3.2
1	B	554	VAL	3.1
1	A	1116	ASP	3.1
1	A	637	GLU	3.1
1	B	451	THR	3.0
1	A	464	ARG	3.0
1	B	499	ASP	3.0
1	A	478	VAL	3.0
1	A	1185	ALA	3.0
1	B	456	THR	3.0
1	B	431	LEU	2.9
1	A	604	PRO	2.9
1	A	1383	TYR	2.9
1	B	398	LEU	2.9
1	A	1031	PRO	2.9
1	B	506	PRO	2.9
1	B	899	GLN	2.8
1	A	408	TRP	2.8
1	A	446	THR	2.8
1	A	1184	ASN	2.8
1	A	1382	VAL	2.8
1	A	412	ALA	2.7
1	A	447	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	1380	PRO	2.7
1	A	1271	GLU	2.7
1	A	1282	SER	2.7
1	B	467	PRO	2.7
1	A	1392[A]	ASP	2.7
1	A	849	TYR	2.6
1	B	450	VAL	2.6
1	A	1196	ALA	2.6
1	B	560	ALA	2.6
1	B	1181	ALA	2.6
1	B	460	LEU	2.6
1	B	898	LEU	2.6
1	B	1082	LEU	2.6
1	B	1118	SER	2.6
1	B	1253	PRO	2.5
1	B	562	GLU	2.5
1	A	619	GLY	2.5
1	B	453	ILE	2.5
1	A	423	LEU	2.5
1	A	597	PHE	2.5
1	A	850	SER	2.5
1	A	1240	ARG	2.4
1	B	823	ASP	2.4
1	B	588	ALA	2.4
1	B	1267	ALA	2.4
1	A	1153	TRP	2.4
1	B	505	SER	2.4
1	A	1183	HIS	2.4
1	B	455	LYS	2.4
1	A	431	LEU	2.3
1	B	564	VAL	2.3
1	A	406	PRO	2.3
1	A	1377	TYR	2.3
1	A	474	ASN	2.3
1	A	440	TYR	2.3
1	A	555	SER	2.3
1	B	1219	SER	2.3
1	A	638	PRO	2.3
1	B	459	ARG	2.3
1	B	464	ARG	2.3
1	A	461	ASP	2.3
1	A	1393[A]	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	503	ASP	2.2
1	A	1369	ARG	2.2
1	A	450	VAL	2.2
1	B	1023	ASP	2.2
1	A	560	ALA	2.2
1	B	901	ARG	2.2
1	A	507	THR	2.2
1	B	452	ASP	2.2
1	B	658	ASP	2.2
1	B	438	LEU	2.2
1	A	404	LYS	2.2
1	B	408	TRP	2.2
1	A	442	PRO	2.1
1	B	446	THR	2.2
1	A	1341	GLY	2.1
1	B	903	CYS	2.1
1	A	1253	PRO	2.1
1	B	442	PRO	2.1
1	A	1182	PHE	2.1
1	B	1122	ILE	2.1
1	A	1197	HIS	2.1
1	B	1115	VAL	2.1
1	B	461	ASP	2.1
1	B	755	ASP	2.1
1	A	548	PRO	2.1
1	A	416	VAL	2.1
1	B	476	VAL	2.1
1	B	1370	LEU	2.1
1	B	1184	ASN	2.1
1	A	456	THR	2.1
1	A	457	LEU	2.0
1	B	504	ASN	2.0
1	A	449	ASP	2.0
1	A	823	ASP	2.0
1	B	1117	GLN	2.0
1	B	1215	ASP	2.0
1	A	639	VAL	2.0
1	B	457	LEU	2.0
1	B	909	LYS	2.0
1	B	1232	GLY	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](#)

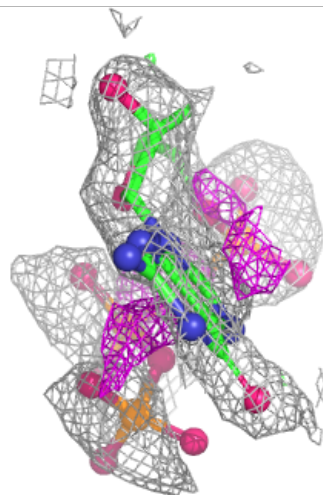
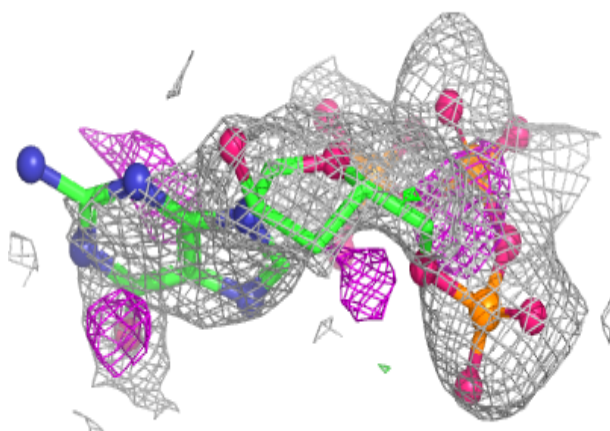
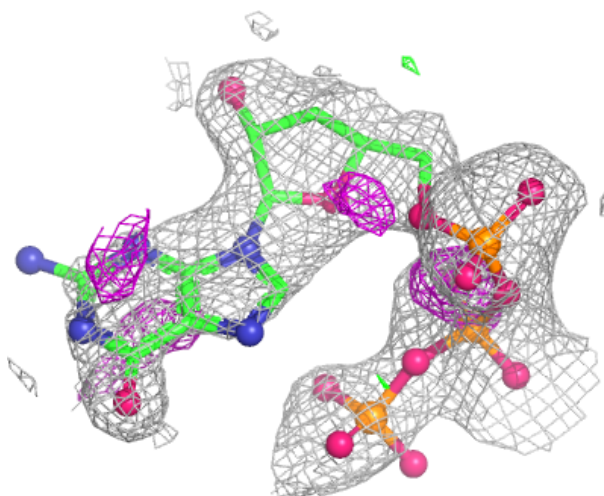
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	GTP	B	1502	31/32	0.79	0.17	68,94,106,115	6
8	PEG	B	1501	7/7	0.79	0.14	67,80,90,90	0
6	GOL	B	1507	6/6	0.80	0.11	45,53,57,58	0
6	GOL	A	2004	6/6	0.87	0.12	44,58,73,73	0
6	GOL	B	1506	6/6	0.89	0.11	44,52,56,57	0
7	GTP	B	1509	31/32	0.92	0.12	40,80,94,99	0
5	MG	B	1508	1/1	0.93	0.15	55,55,55,55	0
5	MG	B	1505	1/1	0.97	0.08	32,32,32,32	0
7	GTP	A	2005	31/32	0.98	0.06	23,28,40,46	0
5	MG	A	2003	1/1	0.98	0.04	22,22,22,22	0
4	CA	A	2002	1/1	0.99	0.02	31,31,31,31	0
4	CA	B	1504	1/1	0.99	0.04	39,39,39,39	0
4	CA	A	2001	1/1	0.99	0.03	30,30,30,30	0
4	CA	B	1503	1/1	1.00	0.02	34,34,34,34	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.

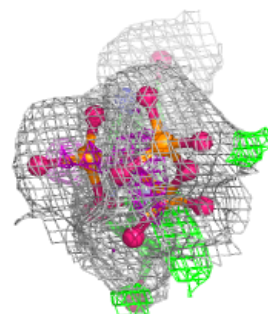
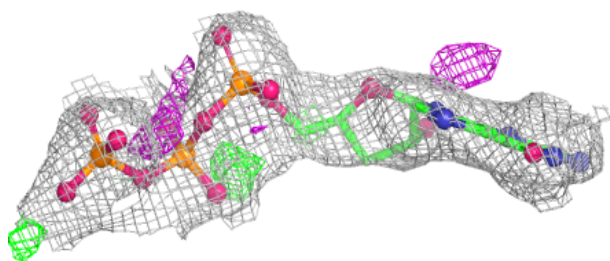
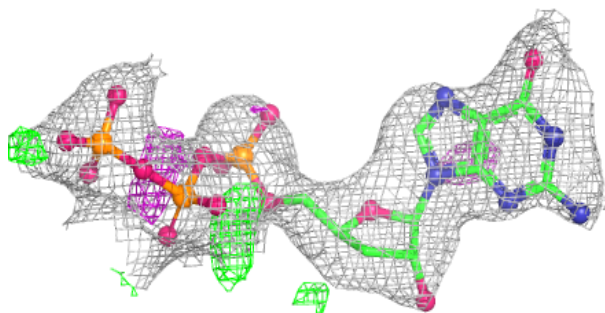
Electron density around GTP B 1502:

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

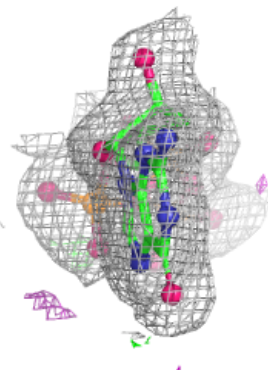
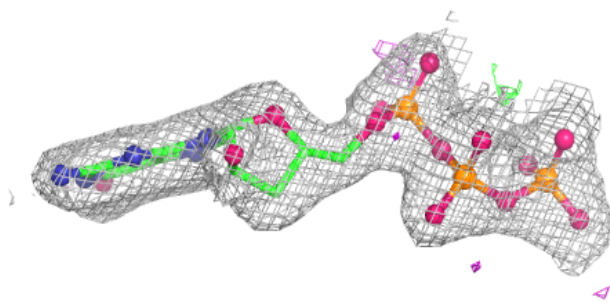
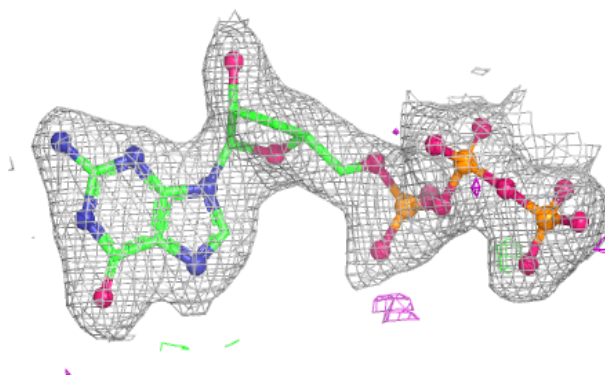


Electron density around GTP B 1509:

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

**Electron density around GTP A 2005:**

$2mF_o-DF_c$ (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.