wwPDB X-ray Structure Validation Summary Report (i)

Nov 22, 2023 – 11:42 AM JST

PDB ID	:	7VMG
Title	:	Crystal structure of tubulin with 17j
Authors	:	Jifa, Z.; Lun, T.
Deposited on	:	2021-10-08
Resolution	:	2.39 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (i)) were used in the production of this report:

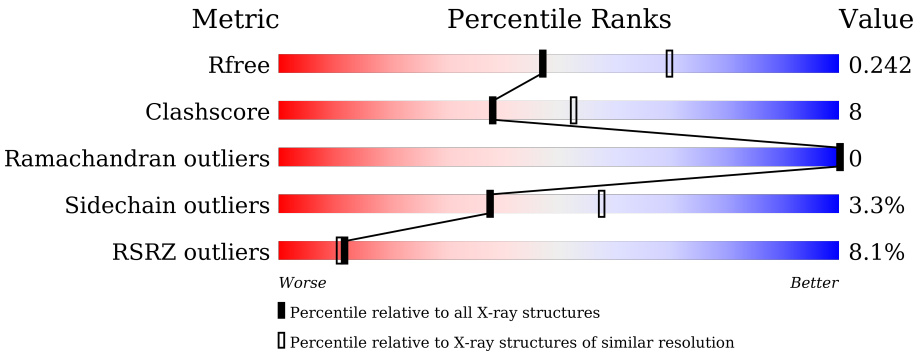
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.39 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	450	2% 85% 12% ·
1	C	450	2% 83% 14% ··
2	B	445	2% 82% 13% · 5%
2	D	445	13% 66% 27% · 6%
3	E	143	13% 65% 17% · 14%
4	F	384	20% 70% 18% · 10%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	CL	D	503	-	-	-	X

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 17851 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Tubulin alpha-1B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	437	Total	C	N	O	S	0	4	0
			3427	2170	580	653	24			
1	C	440	Total	C	N	O	S	0	9	0
			3468	2195	585	663	25			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	424	Total	C	N	O	S	0	4	0
			3364	2116	575	647	26			
2	D	420	Total	C	N	O	S	0	1	0
			3291	2069	557	639	26			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	123	Total	C	N	O	S	0	2	0
			1026	633	186	202	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	-	expression tag	UNP P63043
E	4	ALA	-	expression tag	UNP P63043

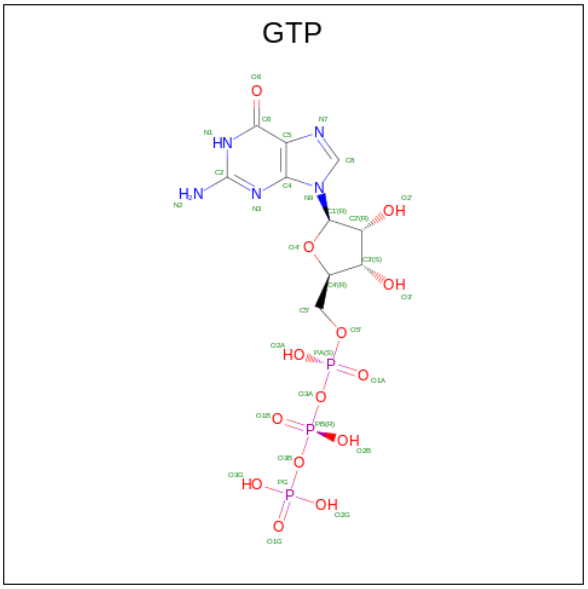
- Molecule 4 is a protein called TTL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	346	Total	C	N	O	S	0	5	0
			2856	1835	487	519	15			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	379	HIS	-	expression tag	UNP E1BQ43
F	380	HIS	-	expression tag	UNP E1BQ43
F	381	HIS	-	expression tag	UNP E1BQ43
F	382	HIS	-	expression tag	UNP E1BQ43
F	383	HIS	-	expression tag	UNP E1BQ43
F	384	HIS	-	expression tag	UNP E1BQ43

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

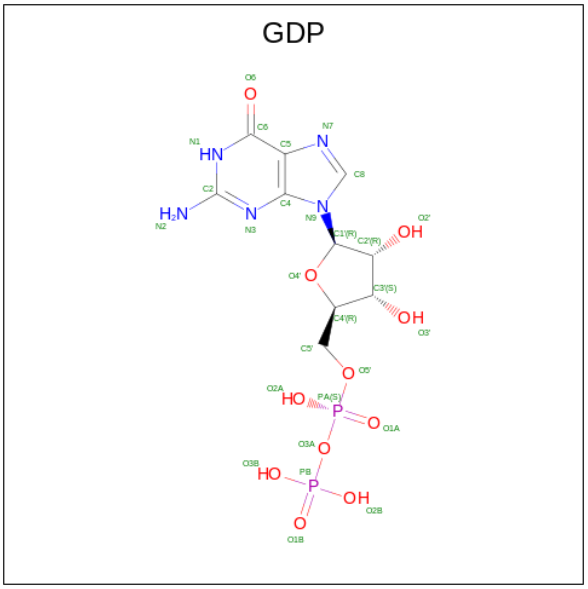
- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Ca 1 1	1	0
7	C	1	Total Ca 1 1	0	0

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

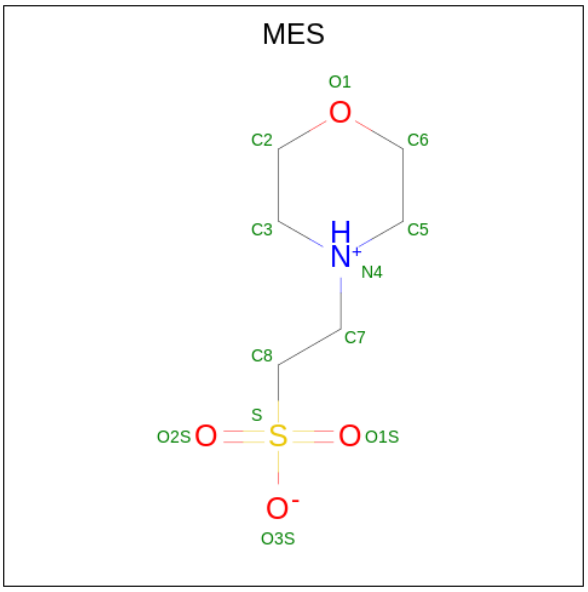
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total Cl 1 1	1	0
8	D	1	Total Cl 1 1	0	0

- Molecule 9 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



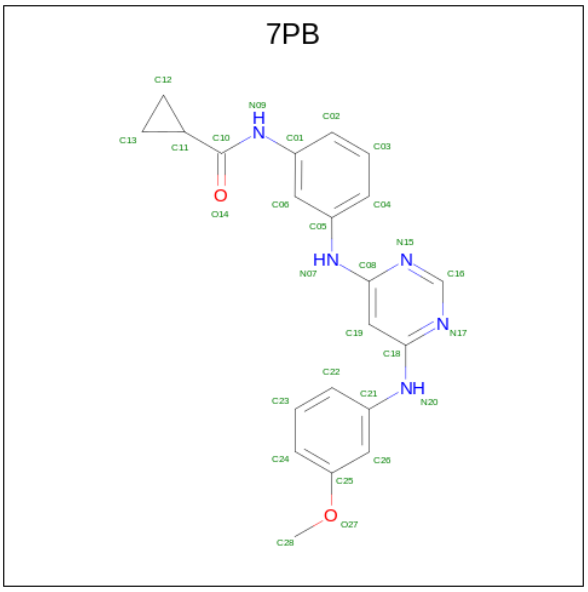
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total C N O P 28 10 5 11 2	0	0
9	D	1	Total C N O P 28 10 5 11 2	0	0

- Molecule 10 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
10	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 11 is N-[3-[[6-[(3-methoxyphenyl)amino]pyrimidin-4-yl]amino]phenyl]cyclopropanecarboxamide (three-letter code: 7PB) (formula: $C_{21}H_{21}N_5O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	B	1	Total	C	N	O	0	0
			28	21	5	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	D	1	Total	C	N	O	0	0
			28	21	5	2		

- Molecule 12 is water.

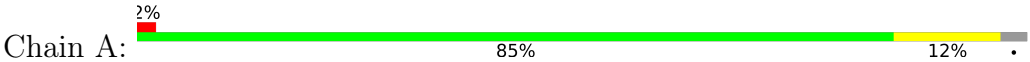
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	55	Total	O	0	0
			55	55		
12	B	51	Total	O	0	0
			51	51		
12	C	82	Total	O	0	0
			82	82		
12	D	4	Total	O	0	0
			4	4		
12	E	5	Total	O	0	0
			5	5		
12	F	15	Total	O	0	0
			15	15		

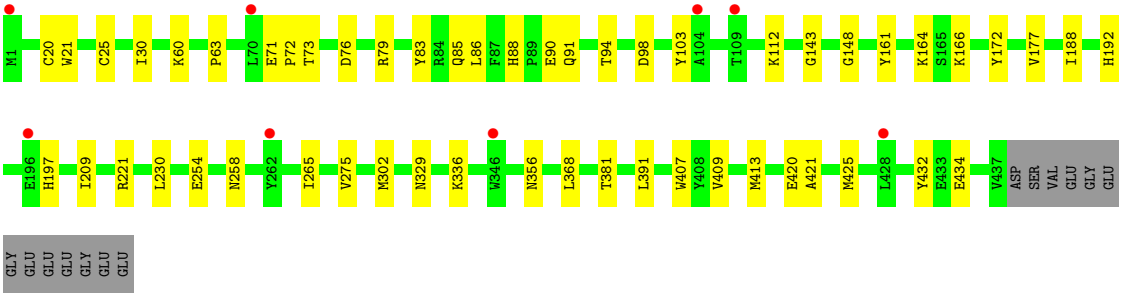
3 Residue-property plots (i)

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

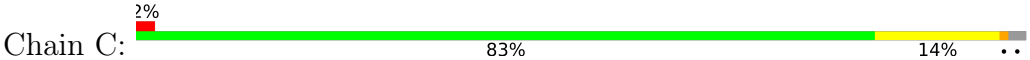
Chain A:

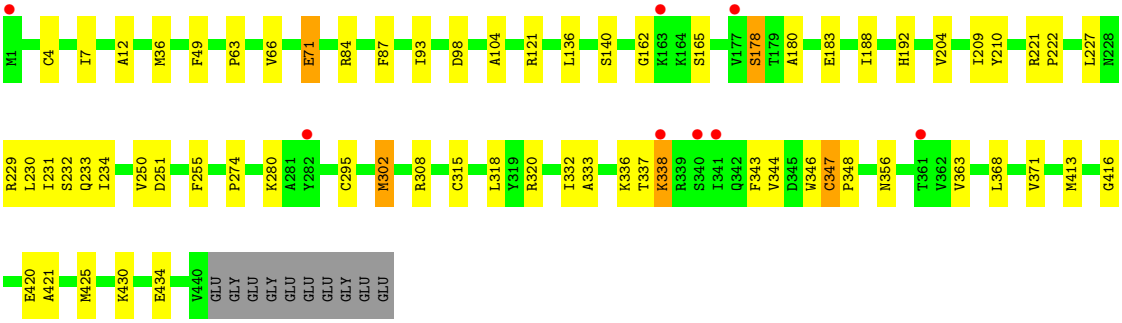




• Molecule 1: Tubulin alpha-1B chain

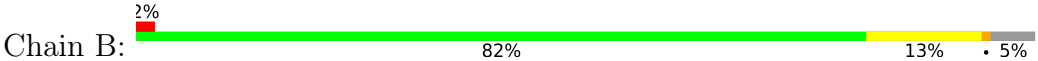
Chain C:

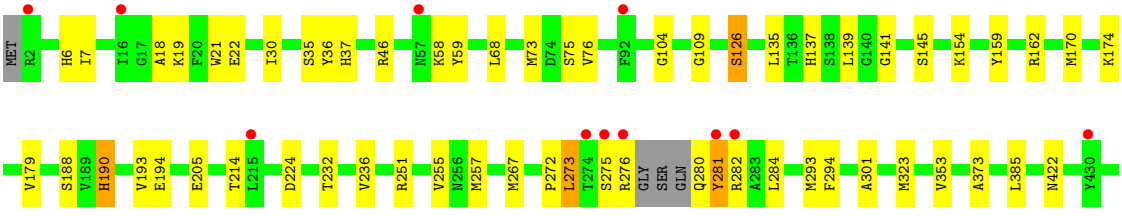




• Molecule 2: Tubulin beta-2B chain

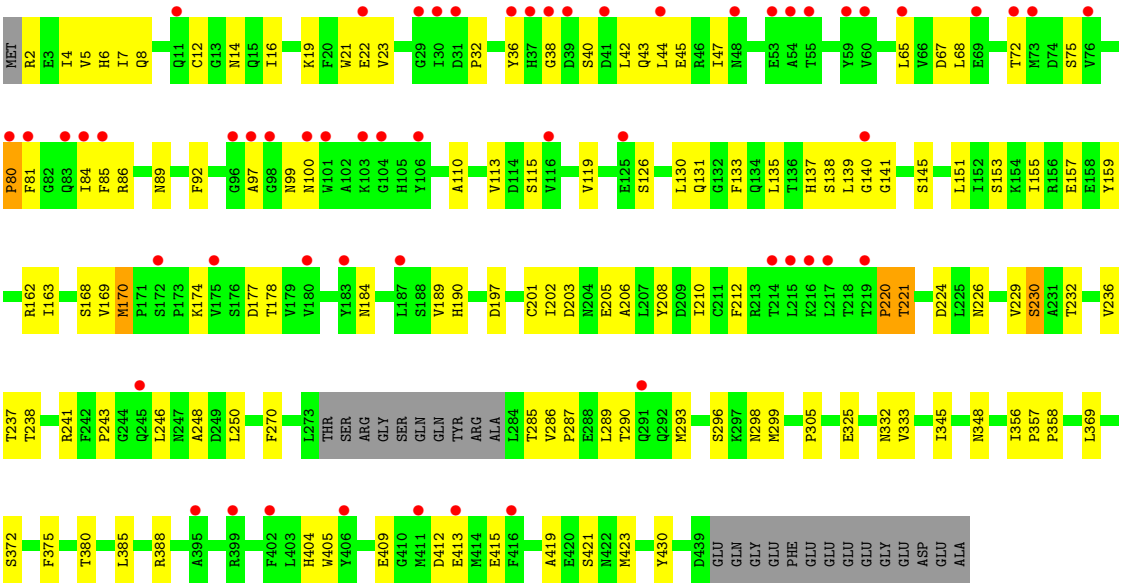
Chain B:





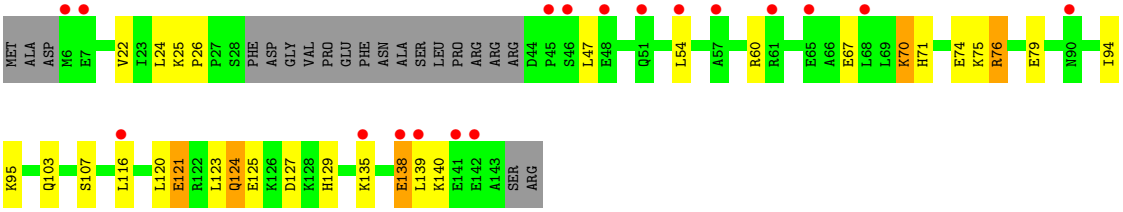
• Molecule 2: Tubulin beta-2B chain

Chain D:



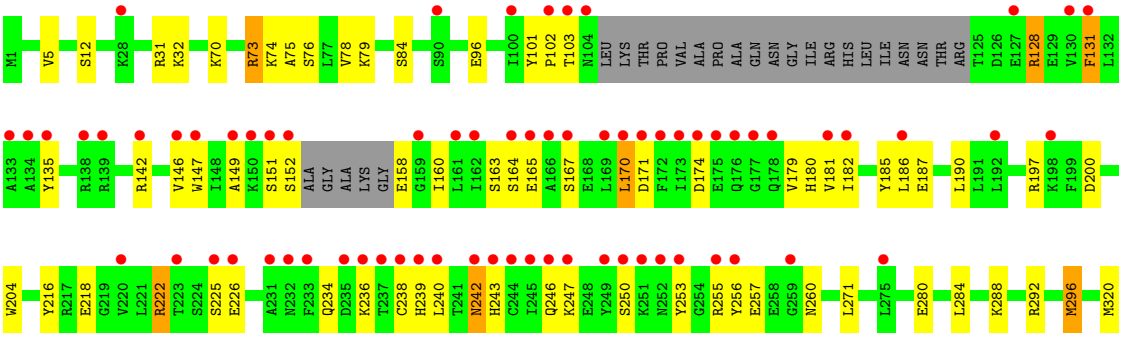
• Molecule 3: Stathmin-4

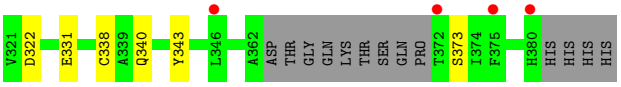
Chain E:



• Molecule 4: TTL

Chain F:




V321
D322
E331
C338
A339
Q340
Y343
L346
A362
ASP
THR
GLY
GLN
LYS
THR
SER
GLN
PRO
T372
S373
I374
F375
H380
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	105.33Å 158.21Å 182.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	91.24 – 2.39 119.54 – 2.39	Depositor EDS
% Data completeness (in resolution range)	99.7 (91.24-2.39) 95.6 (119.54-2.39)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.15 (at 2.40Å)	Xtriage
Refinement program	PHENIX 1.19_4092	Depositor
R, R_{free}	0.210 , 0.250 0.204 , 0.242	Depositor DCC
R_{free} test set	2000 reflections (1.65%)	wwPDB-VP
Wilson B-factor (Å^2)	52.2	Xtriage
Anisotropy	0.276	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 50.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	17851	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.25% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, MES, CL, CA, 7PB, GDP, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.46	1/3517 (0.0%)	0.63	0/4776
1	C	0.53	2/3570 (0.1%)	0.68	1/4847 (0.0%)
2	B	0.52	1/3447 (0.0%)	0.68	1/4667 (0.0%)
2	D	0.47	0/3364	0.68	1/4560 (0.0%)
3	E	0.51	0/1041	0.67	0/1382
4	F	0.39	0/2935	0.61	0/3966
All	All	0.48	4/17874 (0.0%)	0.66	3/24198 (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
4	F	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	281	TYR	CD2-CE2	-6.84	1.29	1.39
1	C	295	CYS	CB-SG	-5.71	1.72	1.81
1	A	20	CYS	CB-SG	-5.49	1.72	1.81
1	C	338	LYS	CD-CE	5.25	1.64	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	220	PRO	N-CA-C	6.12	128.03	112.10
1	C	338	LYS	CA-CB-CG	6.07	126.74	113.40
2	B	273	LEU	CA-CB-CG	-5.08	103.61	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	F	234	GLN	Peptide

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	3427	0	3340	34	0
1	C	3468	0	3388	38	0
2	B	3364	0	3249	41	0
2	D	3291	0	3155	86	0
3	E	1026	0	1042	26	0
4	F	2856	0	2837	50	0
5	A	32	0	12	2	0
5	C	32	0	12	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
7	A	1	0	0	0	0
7	C	1	0	0	0	0
8	A	1	0	0	0	0
8	D	1	0	0	0	0
9	B	28	0	12	1	0
9	D	28	0	12	1	0
10	B	24	0	26	4	0
11	B	28	0	0	1	0
11	D	28	0	0	2	0
12	A	55	0	0	1	0
12	B	51	0	0	0	0
12	C	82	0	0	2	0
12	D	4	0	0	1	0
12	E	5	0	0	0	0
12	F	15	0	0	0	0
All	All	17851	0	17085	265	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.

The worst 5 of 265 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:251:ARG:NH2	10:B:503:MES:O1S	2.02	0.92
2:D:99:ASN:HD22	2:D:178:THR:HG21	1.39	0.87
1:A:112:LYS:HD2	3:E:54:LEU:HB3	1.56	0.87
2:D:131:GLN:HB2	2:D:250:LEU:HD12	1.57	0.86
1:A:88:HIS:NE2	1:A:90:GLU:HG3	1.98	0.79

There are no symmetry-related clashes.

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	439/450 (98%)	427 (97%)	12 (3%)	0	100	100
1	C	446/450 (99%)	437 (98%)	9 (2%)	0	100	100
2	B	424/445 (95%)	412 (97%)	12 (3%)	0	100	100
2	D	416/445 (94%)	397 (95%)	19 (5%)	0	100	100
3	E	121/143 (85%)	119 (98%)	2 (2%)	0	100	100
4	F	343/384 (89%)	322 (94%)	21 (6%)	0	100	100
All	All	2189/2317 (94%)	2114 (97%)	75 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	371/378 (98%)	367 (99%)	4 (1%)	73 87
1	C	379/378 (100%)	367 (97%)	12 (3%)	39 59
2	B	370/383 (97%)	362 (98%)	8 (2%)	52 71
2	D	361/383 (94%)	341 (94%)	20 (6%)	21 35
3	E	112/127 (88%)	104 (93%)	8 (7%)	14 23
4	F	315/342 (92%)	299 (95%)	16 (5%)	24 39
All	All	1908/1991 (96%)	1840 (96%)	68 (4%)	38 54

5 of 68 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	F	142	ARG
4	F	170	LEU
4	F	296[A]	MET
2	D	75	SER
1	C	347[B]	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	332	ASN
2	D	99	ASN
3	E	103	GLN
1	A	356	ASN
1	A	88	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 15 ligands modelled in this entry, 7 are monoatomic - leaving 8 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	$\#\|Z\| > 2$
10	MES	B	503	2	12,12,12	1.05	1 (8%)	14,16,16	3.11	4 (28%)
9	GDP	B	501	6	24,30,30	0.94	1 (4%)	30,47,47	1.47	5 (16%)
11	7PB	B	505	-	31,31,31	2.46	11 (35%)	42,42,42	3.38	13 (30%)
9	GDP	D	501	-	24,30,30	0.90	1 (4%)	30,47,47	1.35	4 (13%)
5	GTP	A	501	6	26,34,34	1.07	2 (7%)	32,54,54	1.32	5 (15%)
5	GTP	C	501	6	26,34,34	1.14	2 (7%)	32,54,54	1.41	4 (12%)
11	7PB	D	502	-	31,31,31	3.22	17 (54%)	42,42,42	4.77	21 (50%)
10	MES	B	504	-	12,12,12	1.51	1 (8%)	14,16,16	2.80	8 (57%)

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
10	MES	B	503	2	-	3/6/14/14	0/1/1/1
9	GDP	B	501	6	-	3/12/32/32	0/3/3/3
11	7PB	B	505	-	-	1/18/20/20	0/4/4/4
9	GDP	D	501	-	-	4/12/32/32	0/3/3/3
5	GTP	A	501	6	-	6/18/38/38	0/3/3/3
5	GTP	C	501	6	-	7/18/38/38	0/3/3/3
11	7PB	D	502	-	-	0/18/20/20	0/4/4/4
10	MES	B	504	-	-	0/6/14/14	0/1/1/1

The worst 5 of 36 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	D	502	7PB	C08-N07	8.01	1.52	1.38
11	D	502	7PB	O27-C25	6.91	1.52	1.37
11	B	505	7PB	C08-N07	6.50	1.50	1.38
11	B	505	7PB	O27-C25	5.83	1.49	1.37
11	D	502	7PB	C21-N20	5.54	1.53	1.40

The worst 5 of 64 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	D	502	7PB	C13-C11-C10	-24.01	94.73	117.21
11	B	505	7PB	C12-C11-C10	-13.19	104.86	117.21
11	B	505	7PB	C13-C11-C10	-10.99	106.92	117.21
11	D	502	7PB	C12-C11-C10	-9.61	108.21	117.21
11	B	505	7PB	N17-C16-N15	-7.94	116.18	128.60

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
9	B	501	GDP	C5'-O5'-PA-O1A

There are no ring outliers.

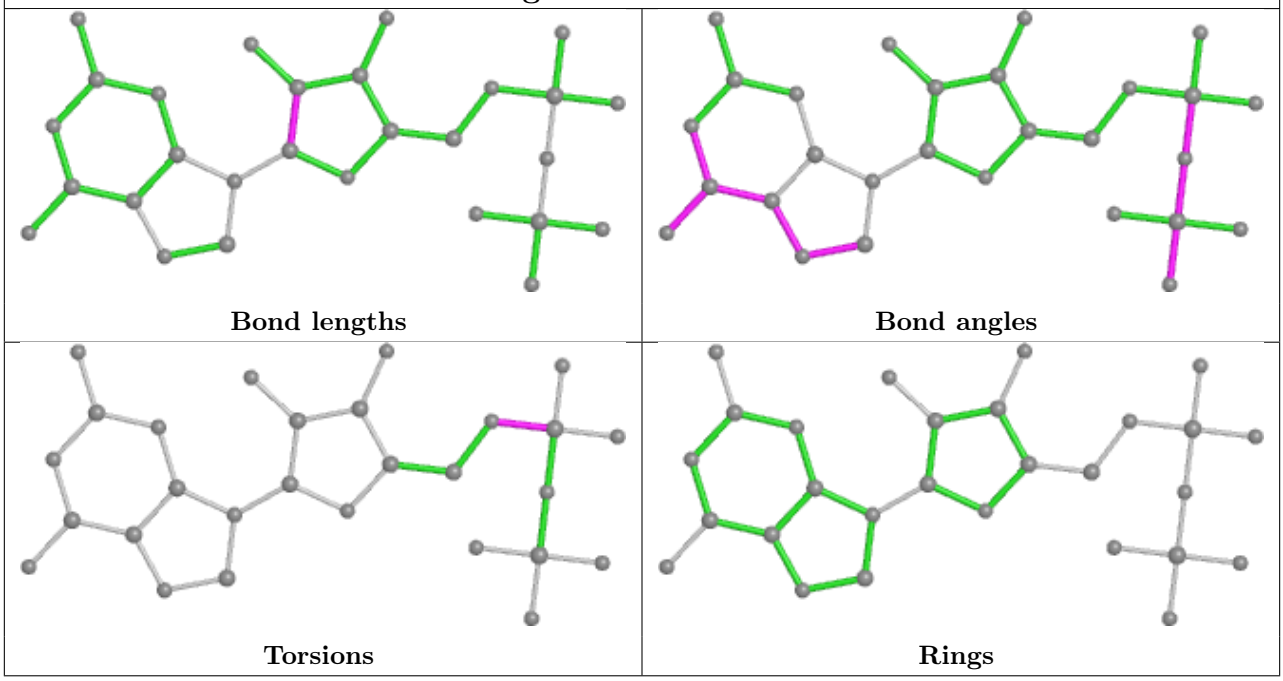
7 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	503	MES	3	0
9	B	501	GDP	1	0
11	B	505	7PB	1	0
9	D	501	GDP	1	0
5	A	501	GTP	2	0
11	D	502	7PB	2	0
10	B	504	MES	1	0

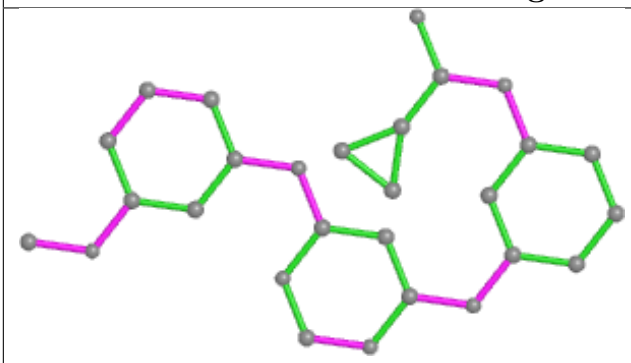
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

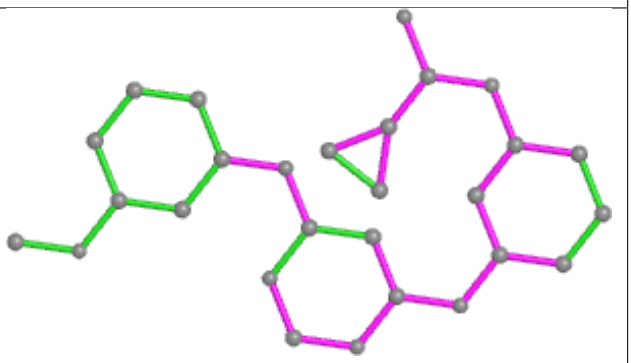
Ligand GDP B 501



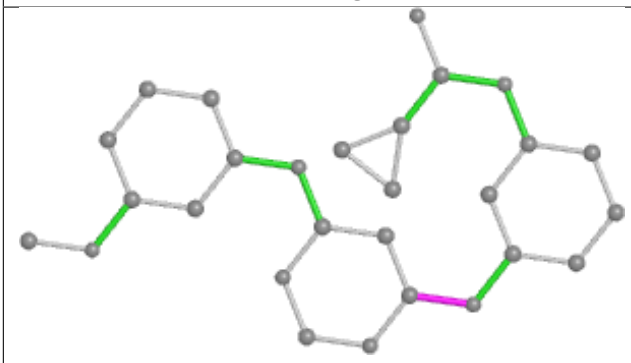
Ligand 7PB B 505



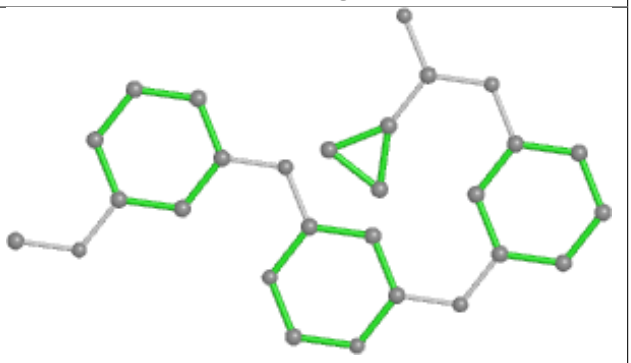
Bond lengths



Bond angles

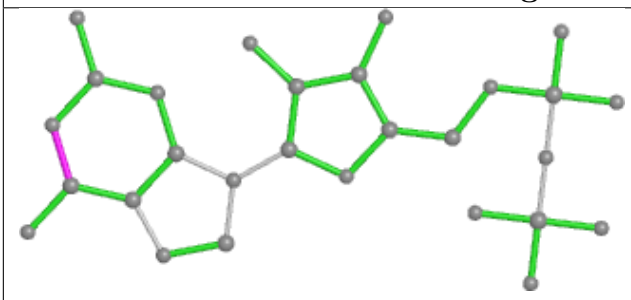


Torsions

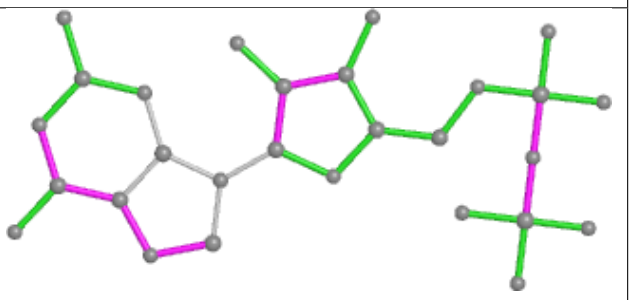


Rings

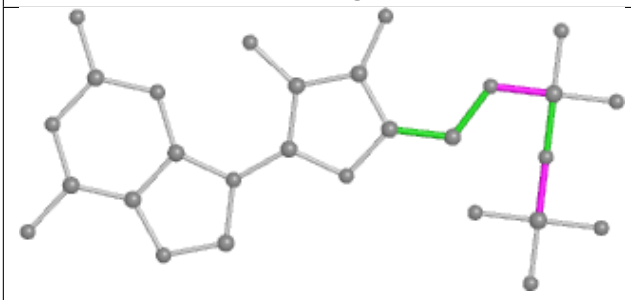
Ligand GDP D 501



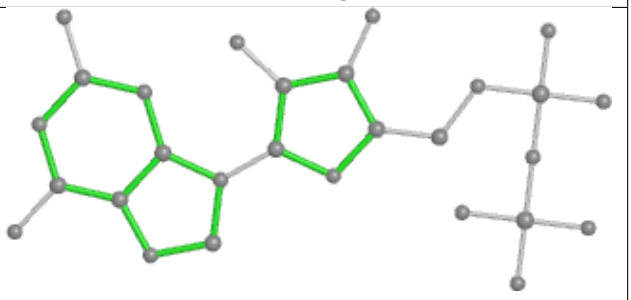
Bond lengths



Bond angles

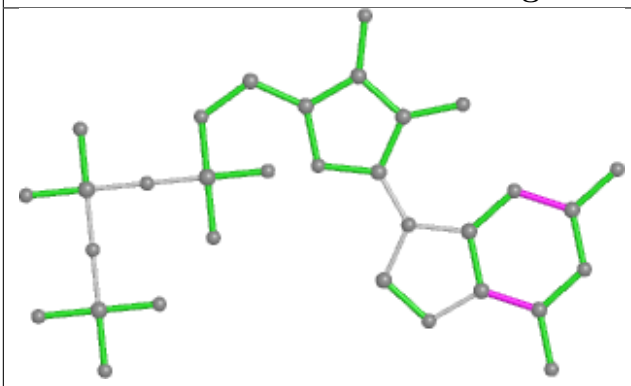


Torsions

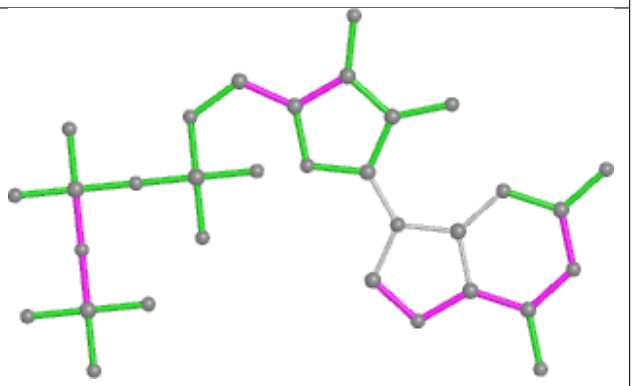


Rings

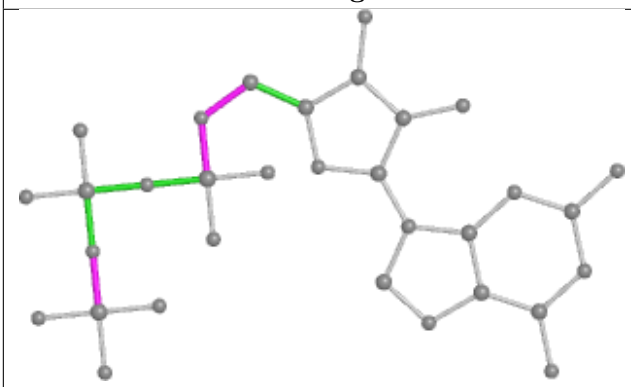
Ligand GTP A 501



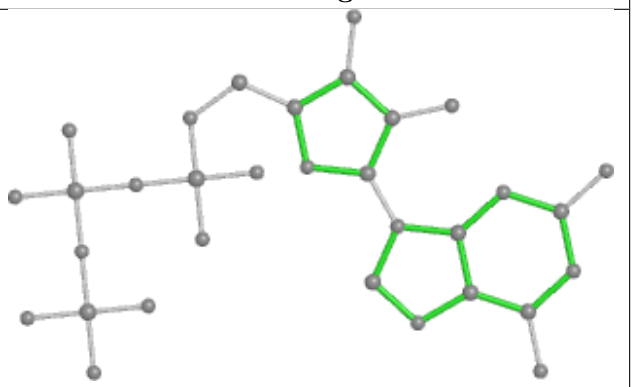
Bond lengths



Bond angles

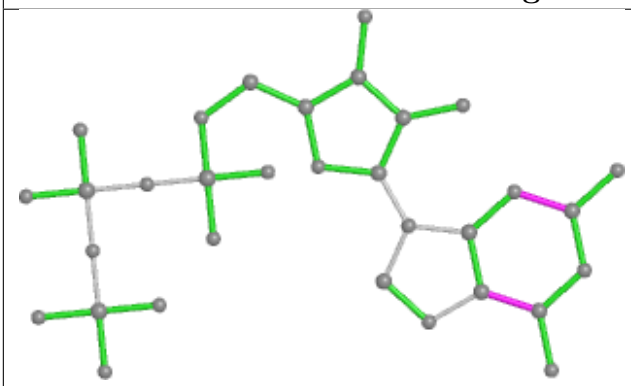


Torsions

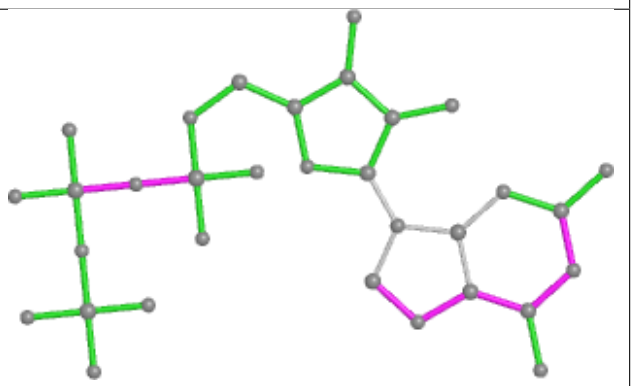


Rings

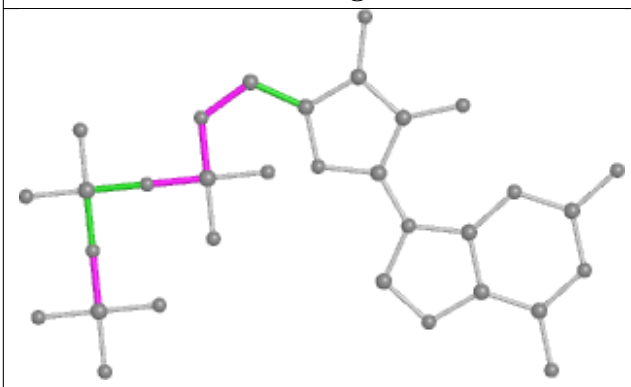
Ligand GTP C 501



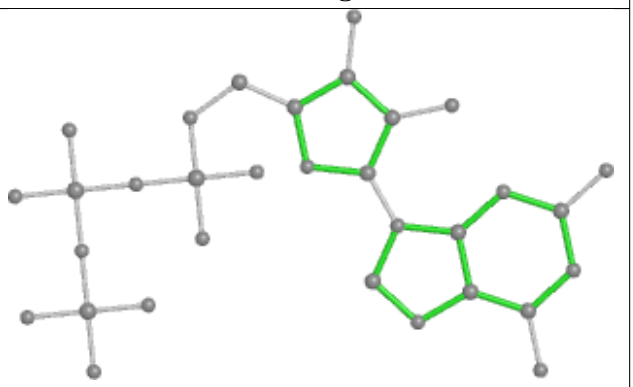
Bond lengths



Bond angles

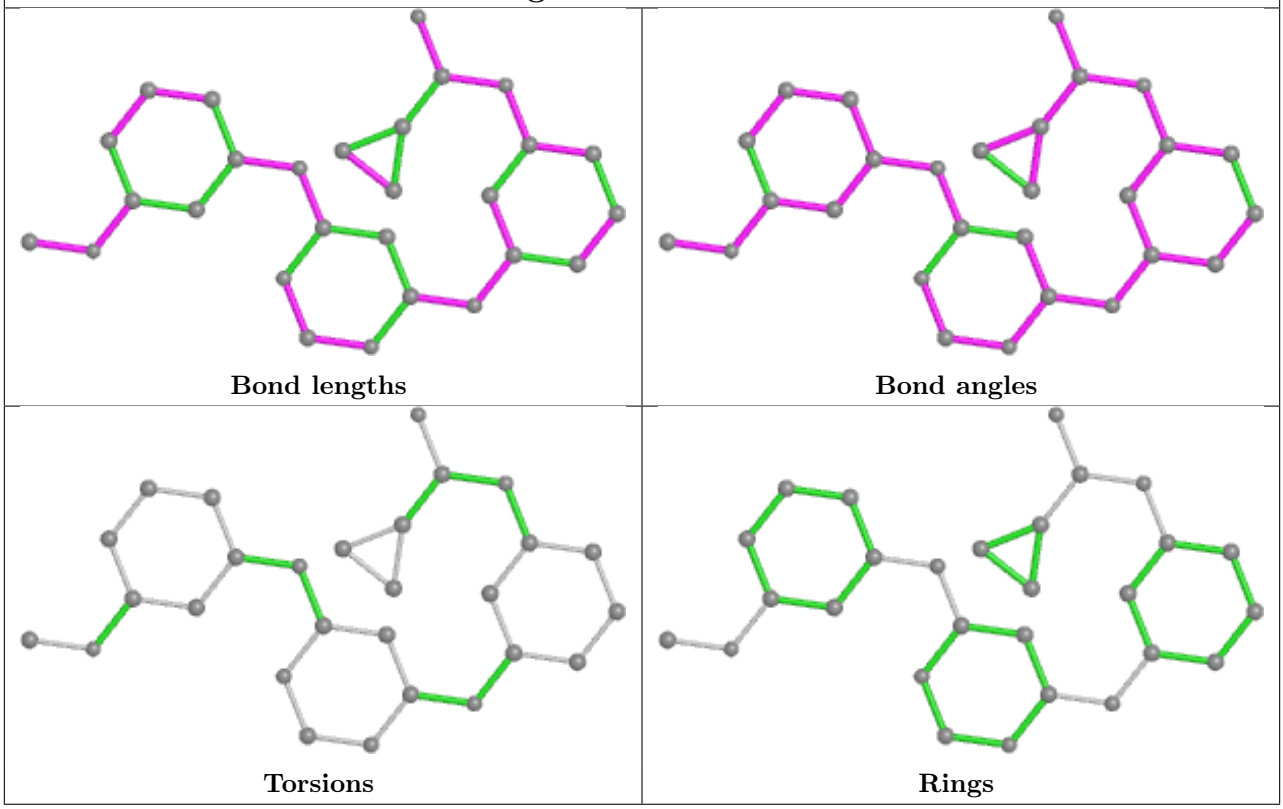


Torsions



Rings

Ligand 7PB D 502



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, 95^{th} 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	437/450 (97%)	0.56	8 (1%) 68 66	39, 53, 74, 89	0
1	C	440/450 (97%)	0.62	8 (1%) 68 66	32, 46, 68, 88	0
2	B	424/445 (95%)	0.62	11 (2%) 56 54	34, 51, 78, 116	3 (0%)
2	D	420/445 (94%)	1.05	57 (13%) 3 2	44, 75, 100, 126	2 (0%)
3	E	123/143 (86%)	1.02	18 (14%) 2 2	46, 74, 104, 130	0
4	F	346/384 (90%)	1.18	75 (21%) 0 0	46, 78, 142, 163	0
All	All	2190/2317 (94%)	0.80	177 (8%) 12 11	32, 59, 104, 163	5 (0%)

The worst 5 of 177 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	169	LEU	12.7
4	F	173	ILE	10.9
4	F	161	LEU	10.0
2	D	72	THR	7.1
2	D	73	MET	6.7

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

LIGAND-RSR INFOmissingINFO

6.5 Other polymers (i)

There are no such residues in this entry.