Full wwPDB X-ray Structure Validation Report ⓘ

Jan 4, 2024 – 06:46 am GMT

PDB ID	:	5LP6
Title	:	Crystal structure of Tubulin-Stathmin-TTL-Thiocolchicine Complex
Authors	:	Marangon, J.; Christodoulou, M.; Casagrande, F.; Tiana, G.; Dalla Via, L.; Aliverti, A.; Passarella, D.; Cappelletti, G.; Ricagno, S.
Deposited on	:	2016-08-11
Resolution	:	2.90 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:

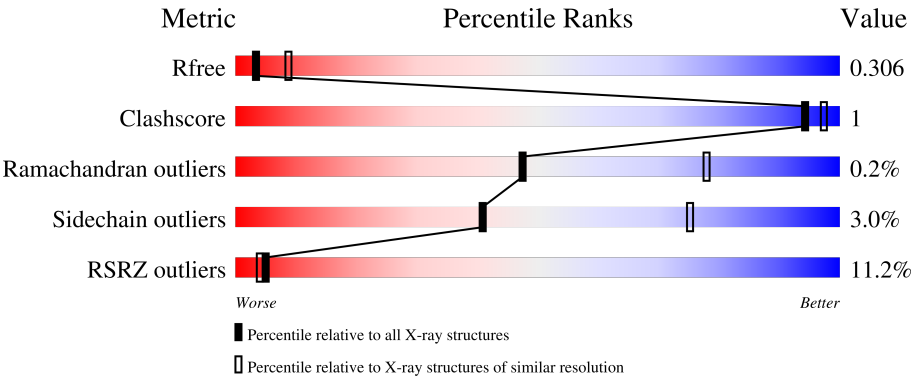
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	440	7% 94% 5%
1	C	440	2% 95% 5%
2	B	445	4% 92% • 5%
2	D	445	9% 91% • 5%
3	E	143	8% 80% • 15%

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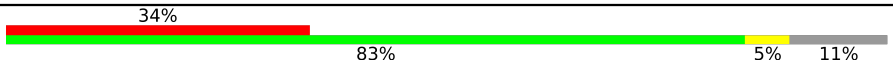
Mol	Chain	Length	Quality of chain
4	F	384	

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
10	71P	B	504	-	-	-	X
6	MG	A	506	-	-	-	X
6	MG	B	502	-	-	-	X
6	MG	B	506	-	-	-	X

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 17547 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	439	Total	C	N	O	S	0	0	0
			3430	2170	583	655	22			
1	C	440	Total	C	N	O	S	0	0	0
			3437	2175	584	656	22			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	422	Total	C	N	O	S	0	0	0
			3318	2085	566	640	27			
2	D	421	Total	C	N	O	S	0	0	0
			3308	2079	562	641	26			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	121	Total	C	N	O	S	0	0	0
			1000	617	181	197	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	ILE	conflict	UNP P63043
E	4	ALA	SER	conflict	UNP P63043

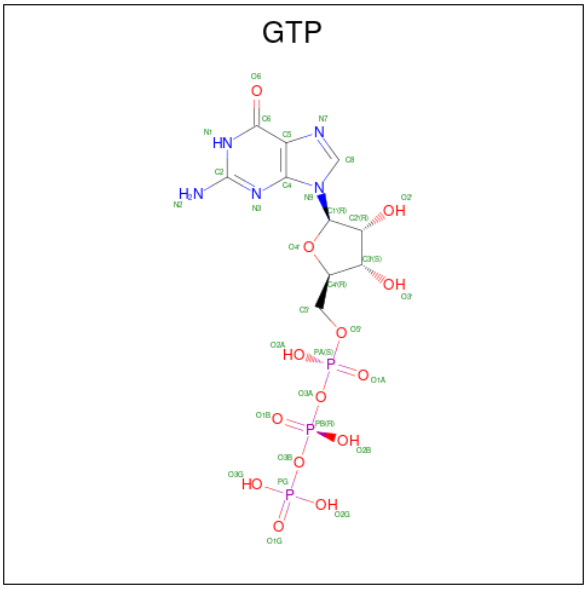
- Molecule 4 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	340	Total	C	N	O	S	0	0	0
			2794	1795	476	509	14			

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		

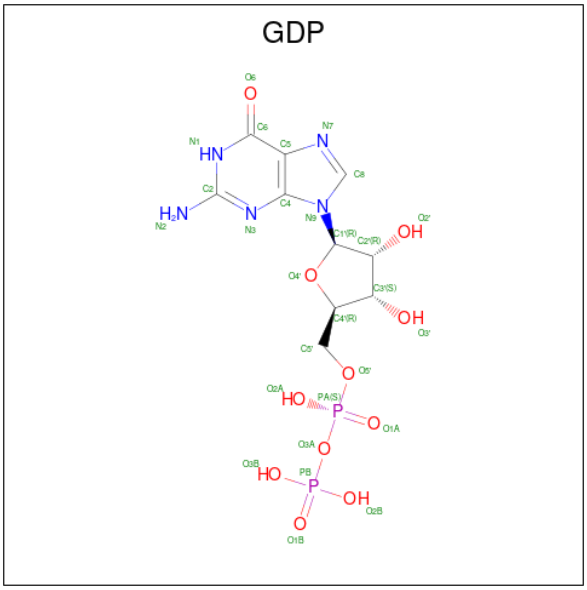
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	4	Total	Mg	0	0
			4	4		
6	B	3	Total	Mg	0	0
			3	3		
6	C	1	Total	Mg	0	0
			1	1		

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

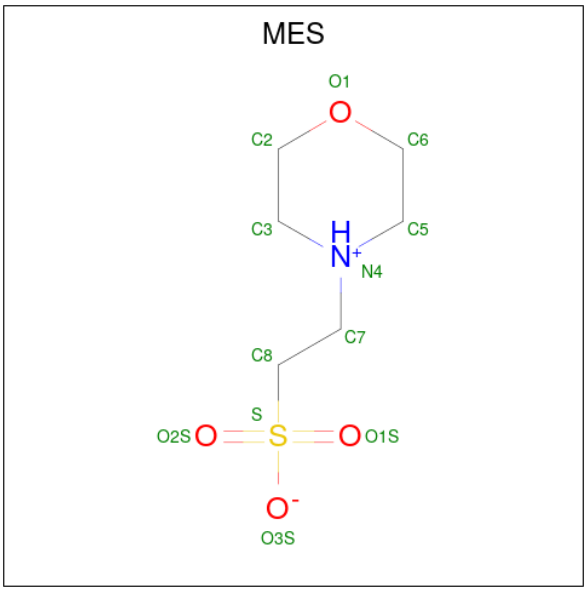
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Cl 1 1	0	0

- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



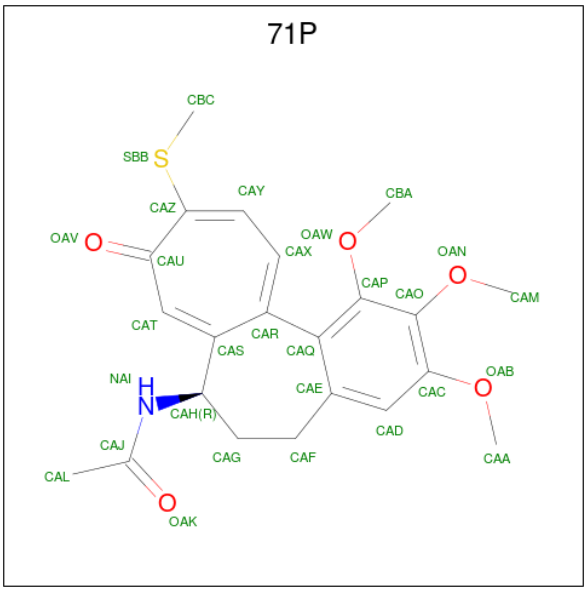
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total C N O P 28 10 5 11 2	0	0
8	D	1	Total C N O P 28 10 5 11 2	0	0

- Molecule 9 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



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

- Molecule 10 is {N}-[(7 {R})-1,2,3-trimethoxy-10-methylsulfanyl-9-oxidanylidene-6,7-dihydro-5 {H}-benzo[a]heptalen-7-yl]ethanamide (three-letter code: 71P) (formula: $C_{22}H_{25}NO_5S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	N	O	S	0	0
			29	22	1	5	1		

- Molecule 11 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	C	1	Total Ca 1 1	0	0

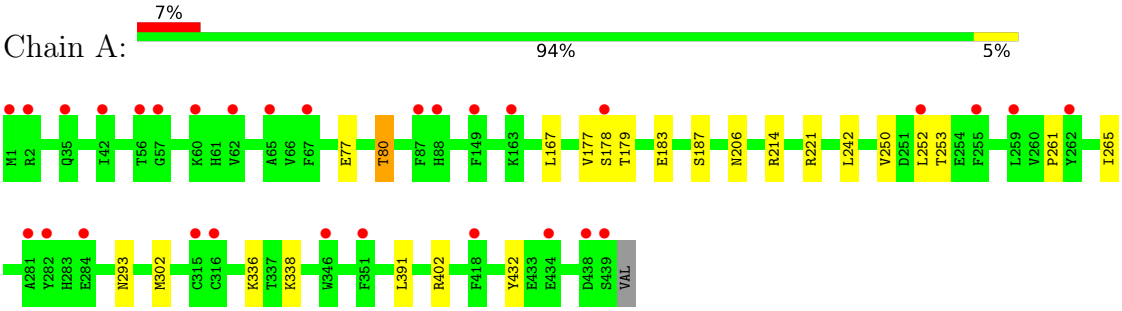
- Molecule 12 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	21	Total O 21 21	0	0
12	B	16	Total O 16 16	0	0
12	C	35	Total O 35 35	0	0
12	D	11	Total O 11 11	0	0
12	E	1	Total O 1 1	0	0
12	F	5	Total O 5 5	0	0

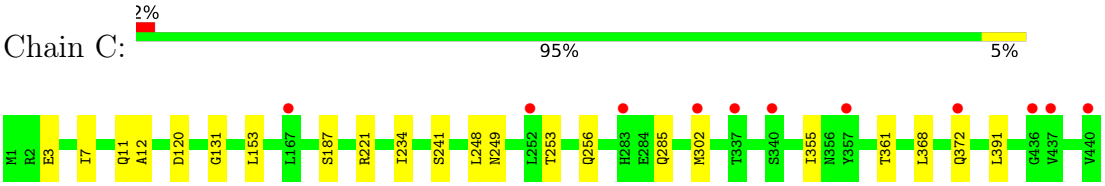
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

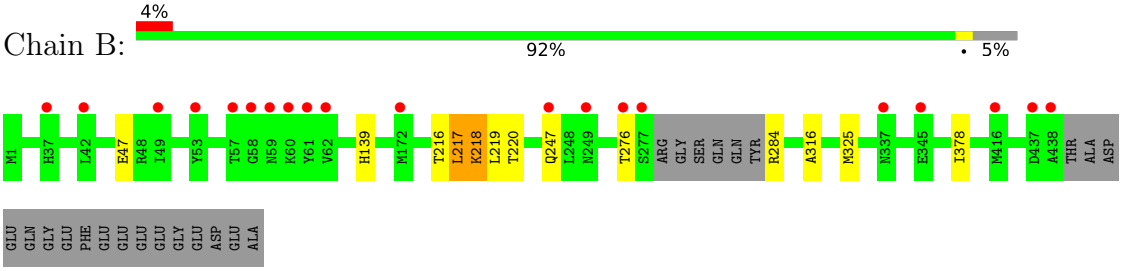
• Molecule 1: Tubulin alpha-1B chain



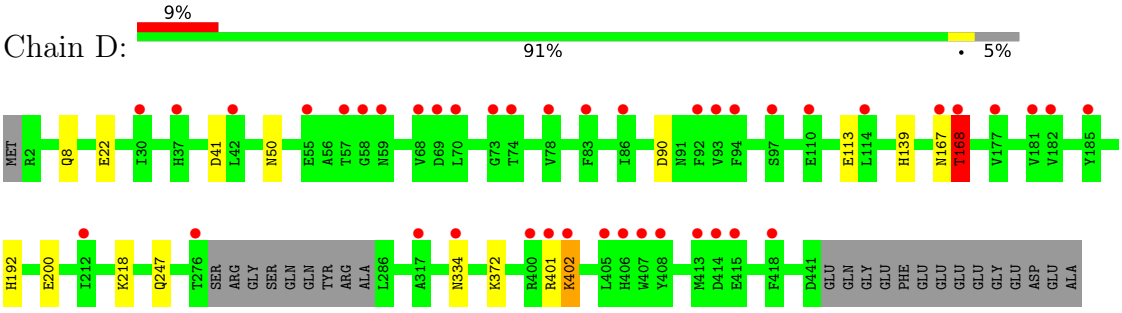
• Molecule 1: Tubulin alpha-1B chain



• Molecule 2: Tubulin beta-2B chain

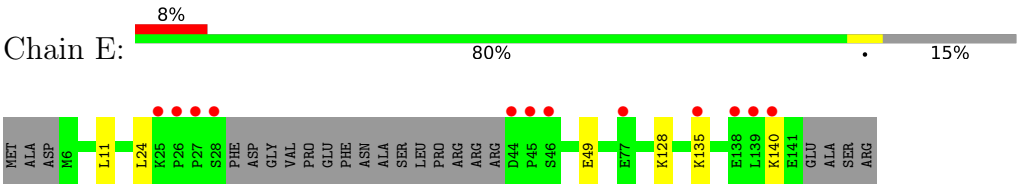


• Molecule 2: Tubulin beta-2B chain



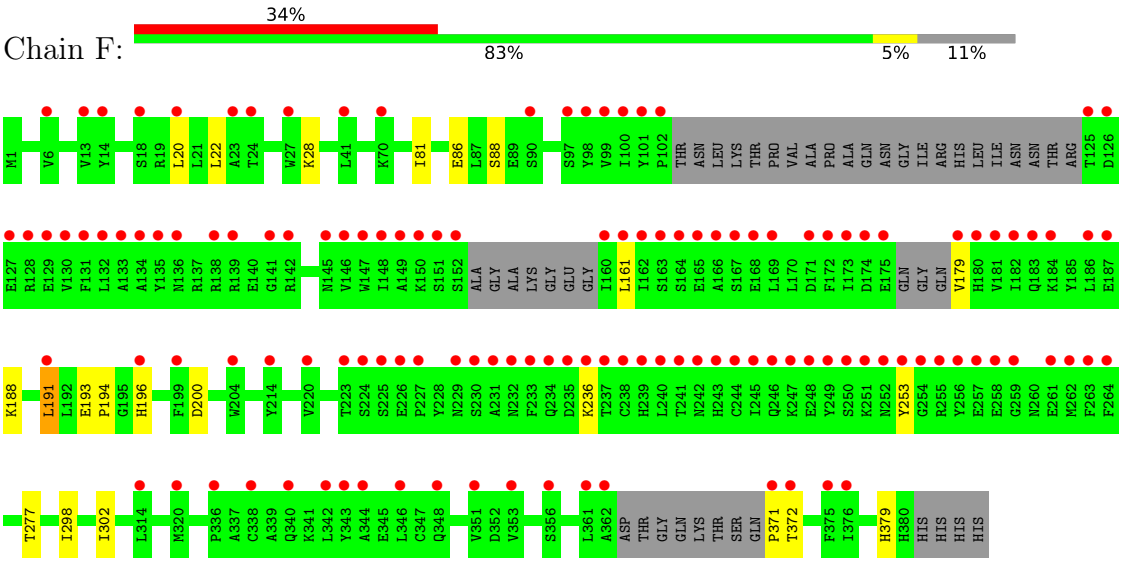
• Molecule 3: Stathmin-4

Chain E:



• Molecule 4: Uncharacterized protein

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	103.62Å 155.28Å 180.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	58.85 – 2.90 58.85 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (58.85-2.90) 99.8 (58.85-2.90)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.78 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.273 , 0.305 0.273 , 0.306	Depositor DCC
R_{free} test set	3307 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	83.2	Xtriage
Anisotropy	0.023	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 34.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	17547	wwPDB-VP
Average B, all atoms (Å^2)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.39% 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: 71P, MES, GDP, CA, GTP, MG, CL

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	0.38	0/3508	0.57	0/4762
1	C	0.35	0/3515	0.57	0/4772
2	B	0.36	0/3389	0.57	0/4586
2	D	0.37	0/3379	0.56	0/4575
3	E	0.35	0/1008	0.52	0/1337
4	F	0.39	0/2858	0.58	0/3860
All	All	0.37	0/17657	0.57	0/23892

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

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	3430	0	3340	14	0
1	C	3437	0	3348	10	0
2	B	3318	0	3201	9	0
2	D	3308	0	3182	3	0
3	E	1000	0	1018	0	0
4	F	2794	0	2765	8	0
5	A	32	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	32	0	12	0	0
6	A	4	0	0	0	0
6	B	3	0	0	0	0
6	C	1	0	0	0	0
7	A	1	0	0	0	0
8	B	28	0	12	0	0
8	D	28	0	12	0	0
9	B	12	0	13	0	0
10	B	29	0	0	2	0
11	C	1	0	0	0	0
12	A	21	0	0	0	0
12	B	16	0	0	0	0
12	C	35	0	0	1	0
12	D	11	0	0	0	0
12	E	1	0	0	0	0
12	F	5	0	0	0	0
All	All	17547	0	16915	44	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 1.

All (44) 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:216:THR:O	2:B:218:LYS:N	1.75	1.17
1:A:177:VAL:O	1:A:178:SER:OG	1.59	1.17
4:F:191:LEU:HG	4:F:196:HIS:CE1	2.13	0.82
1:A:177:VAL:C	1:A:178:SER:HG	1.83	0.77
1:A:177:VAL:O	1:A:178:SER:CB	2.42	0.68
1:A:177:VAL:HG21	1:A:206:ASN:HB3	1.82	0.61
2:B:218:LYS:C	2:B:219:LEU:HD23	2.21	0.61
1:A:179:THR:HB	1:A:183:GLU:CD	2.25	0.57
1:C:3:GLU:OE1	1:C:131:GLY:O	2.24	0.56
1:C:12:ALA:N	12:C:601:HOH:O	2.40	0.54
2:B:216:THR:O	2:B:218:LYS:CA	2.56	0.52
1:A:179:THR:HB	1:A:183:GLU:OE2	2.12	0.51
1:A:177:VAL:CG2	1:A:206:ASN:HB3	2.41	0.50
1:C:7:ILE:HG21	1:C:153:LEU:HD21	1.94	0.50
1:C:248:LEU:HD13	1:C:355:ILE:HD12	1.93	0.50
1:C:187:SER:HB3	1:C:391:LEU:HD21	1.94	0.49
2:B:216:THR:O	2:B:217:LEU:C	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:316:ALA:HB3	2:B:378:ILE:HB	1.95	0.49
10:B:504:71P:OAW	10:B:504:71P:CAX	2.60	0.49
1:A:177:VAL:HG21	1:A:206:ASN:CB	2.41	0.49
1:A:177:VAL:HG11	5:A:501:GTP:O2'	2.14	0.47
4:F:161:LEU:HA	4:F:236:LYS:HE2	1.97	0.47
4:F:191:LEU:HG	4:F:196:HIS:ND1	2.29	0.47
2:D:167:ASN:O	2:D:168:THR:HG22	2.15	0.47
2:D:401:ARG:C	2:D:402:LYS:HG2	2.36	0.46
2:B:219:LEU:HD23	2:B:219:LEU:N	2.30	0.46
1:A:242:LEU:HD11	1:A:252:LEU:HD21	1.97	0.46
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.99	0.45
1:C:234:ILE:HG21	1:C:302:MET:SD	2.57	0.45
2:B:216:THR:C	2:B:218:LYS:N	2.61	0.44
1:A:167:LEU:HD22	1:A:252:LEU:HD22	2.00	0.44
1:C:11:GLN:O	1:C:12:ALA:HB3	2.18	0.44
4:F:298:ILE:HD12	4:F:302:ILE:HD13	1.99	0.44
1:C:11:GLN:HE22	2:D:247:GLN:HE22	1.66	0.43
4:F:371:PRO:HA	4:F:372:THR:HB	1.99	0.43
2:B:216:THR:HG22	2:B:217:LEU:H	1.83	0.43
2:B:316:ALA:HB1	10:B:504:71P:CBA	2.49	0.43
1:C:241:SER:HA	1:C:249:ASN:HD21	1.83	0.43
4:F:81:ILE:O	4:F:88:SER:HB3	2.18	0.42
4:F:193:GLU:HA	4:F:194:PRO:C	2.39	0.42
4:F:191:LEU:HB3	4:F:196:HIS:HA	2.02	0.41
1:C:234:ILE:HD13	1:C:302:MET:HE3	2.02	0.41
1:A:77:GLU:HA	1:A:80:THR:HG22	2.02	0.41
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.56	0.41

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	437/440 (99%)	423 (97%)	13 (3%)	1 (0%)	47 78
1	C	438/440 (100%)	428 (98%)	10 (2%)	0	100 100
2	B	414/445 (93%)	400 (97%)	12 (3%)	2 (0%)	29 61
2	D	413/445 (93%)	400 (97%)	12 (3%)	1 (0%)	47 78
3	E	117/143 (82%)	114 (97%)	3 (3%)	0	100 100
4	F	330/384 (86%)	310 (94%)	20 (6%)	0	100 100
All	All	2149/2297 (94%)	2075 (97%)	70 (3%)	4 (0%)	47 78

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	217	LEU
2	B	218	LYS
2	D	168	THR
1	A	261	PRO

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	370/371 (100%)	360 (97%)	10 (3%)	44 77
1	C	371/371 (100%)	363 (98%)	8 (2%)	52 81
2	B	365/383 (95%)	358 (98%)	7 (2%)	57 84
2	D	364/383 (95%)	350 (96%)	14 (4%)	33 67
3	E	109/127 (86%)	103 (94%)	6 (6%)	21 53
4	F	308/342 (90%)	297 (96%)	11 (4%)	35 69
All	All	1887/1977 (95%)	1831 (97%)	56 (3%)	41 75

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	THR

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Mol	Chain	Res	Type
1	A	214	ARG
1	A	221	ARG
1	A	250	VAL
1	A	253	THR
1	A	293	ASN
1	A	302	MET
1	A	336	LYS
1	A	338	LYS
1	A	402	ARG
2	B	47	GLU
2	B	139	HIS
2	B	220	THR
2	B	247	GLN
2	B	276	THR
2	B	284	ARG
2	B	325	MET
1	C	120	ASP
1	C	221	ARG
1	C	253	THR
1	C	256	GLN
1	C	285	GLN
1	C	361	THR
1	C	368	LEU
1	C	372	GLN
2	D	8	GLN
2	D	22	GLU
2	D	41	ASP
2	D	50	ASN
2	D	90	ASP
2	D	113	GLU
2	D	139	HIS
2	D	168	THR
2	D	192	HIS
2	D	200	GLU
2	D	218	LYS
2	D	334	ASN
2	D	372	LYS
2	D	402	LYS
3	E	11	LEU
3	E	24	LEU
3	E	49	GLU
3	E	128	LYS

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Mol	Chain	Res	Type
3	E	135	LYS
3	E	140	LYS
4	F	20	LEU
4	F	22	LEU
4	F	28	LYS
4	F	86	GLU
4	F	179	VAL
4	F	188	LYS
4	F	191	LEU
4	F	200	ASP
4	F	253	TYR
4	F	277	THR
4	F	379	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	247	GLN
2	D	247	GLN
2	D	385	GLN
3	E	18	GLN

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 16 ligands modelled in this entry, 10 are monoatomic - leaving 6 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	$\#\|Z\| > 2$
8	GDP	D	600	-	24,30,30	0.91	0	30,47,47	1.15	3 (10%)
10	71P	B	504	-	31,31,31	2.48	9 (29%)	40,44,44	4.78	22 (55%)
5	GTP	A	501	6	26,34,34	0.91	1 (3%)	32,54,54	1.29	5 (15%)
5	GTP	C	501	6	26,34,34	0.90	0	32,54,54	1.22	4 (12%)
9	MES	B	503	-	12,12,12	2.31	1 (8%)	14,16,16	1.40	2 (14%)
8	GDP	B	501	6	24,30,30	0.93	0	30,47,47	1.15	3 (10%)

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
8	GDP	D	600	-	-	5/12/32/32	0/3/3/3
10	71P	B	504	-	-	3/12/25/25	1/3/3/3
5	GTP	A	501	6	-	4/18/38/38	0/3/3/3
5	GTP	C	501	6	-	7/18/38/38	0/3/3/3
9	MES	B	503	-	-	1/6/14/14	0/1/1/1
8	GDP	B	501	6	-	4/12/32/32	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	504	71P	CAZ-CAU	-8.11	1.38	1.47
9	B	503	MES	C8-S	-7.70	1.66	1.77
10	B	504	71P	CAH-CAS	-6.03	1.43	1.53
10	B	504	71P	CAF-CAE	-4.29	1.41	1.51
10	B	504	71P	CAG-CAF	-3.39	1.43	1.53
10	B	504	71P	CAX-CAR	3.12	1.41	1.37
10	B	504	71P	CAT-CAS	2.82	1.41	1.36
10	B	504	71P	CAQ-CAR	-2.68	1.46	1.50
10	B	504	71P	CAH-NAI	2.46	1.51	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	504	71P	CAQ-CAP	2.10	1.45	1.40
5	A	501	GTP	C6-N1	-2.07	1.34	1.37

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	B	504	71P	CAH-CAS-CAT	-18.20	99.90	117.12
10	B	504	71P	CAH-CAS-CAR	14.60	130.08	115.27
10	B	504	71P	CAQ-CAR-CAS	10.58	127.03	118.51
10	B	504	71P	CAF-CAE-CAQ	6.59	130.25	119.97
10	B	504	71P	CAF-CAE-CAD	-5.49	107.31	119.42
10	B	504	71P	CAG-CAH-NAI	5.14	119.39	110.11
10	B	504	71P	CAP-CAQ-CAE	-4.24	112.58	118.50
10	B	504	71P	CAX-CAR-CAS	-4.19	120.00	124.83
10	B	504	71P	CBA-OAW-CAP	-3.62	104.87	114.78
10	B	504	71P	CAA-OAB-CAC	-3.53	112.20	117.53
10	B	504	71P	OAW-CAP-CAO	-3.40	112.53	120.39
10	B	504	71P	CAE-CAQ-CAR	2.88	123.62	120.25
5	A	501	GTP	PB-O3B-PG	-2.85	123.06	132.83
8	D	600	GDP	PA-O3A-PB	-2.70	123.57	132.83
10	B	504	71P	CAP-CAQ-CAR	2.59	123.79	121.09
5	A	501	GTP	PA-O3A-PB	-2.57	124.01	132.83
8	B	501	GDP	C8-N7-C5	2.50	107.75	102.99
9	B	503	MES	O3S-S-C8	2.48	109.78	105.77
8	B	501	GDP	PA-O3A-PB	-2.47	124.36	132.83
10	B	504	71P	CAQ-CAR-CAX	-2.46	112.62	117.12
10	B	504	71P	CAT-CAS-CAR	2.45	130.03	127.62
8	D	600	GDP	C8-N7-C5	2.44	107.65	102.99
10	B	504	71P	OAV-CAU-CAZ	2.41	119.53	117.67
5	A	501	GTP	C8-N7-C5	2.39	107.54	102.99
5	C	501	GTP	C5-C6-N1	2.36	118.11	113.95
8	B	501	GDP	C5-C6-N1	2.35	118.11	113.95
10	B	504	71P	CAD-CAE-CAQ	2.35	122.30	119.47
10	B	504	71P	CAY-CAZ-SBB	-2.35	114.81	121.88
5	C	501	GTP	PB-O3B-PG	-2.35	124.78	132.83
10	B	504	71P	OAK-CAJ-NAI	2.33	126.23	121.95
5	C	501	GTP	C8-N7-C5	2.32	107.41	102.99
5	C	501	GTP	PA-O3A-PB	-2.32	124.88	132.83
8	D	600	GDP	C5-C6-N1	2.32	118.04	113.95
5	A	501	GTP	C3'-C2'-C1'	2.31	104.46	100.98
5	A	501	GTP	C5-C6-N1	2.29	118.00	113.95
10	B	504	71P	OAK-CAJ-CAL	-2.11	118.13	122.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	B	504	71P	CAM-OAN-CAO	2.03	120.35	114.78
9	B	503	MES	C5-N4-C3	2.02	113.39	108.83
10	B	504	71P	CAF-CAG-CAH	-2.01	109.63	112.21

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
8	B	501	GDP	C5'-O5'-PA-O1A
8	D	600	GDP	C5'-O5'-PA-O1A
10	B	504	71P	CAS-CAH-NAI-CAJ
10	B	504	71P	CAD-CAC-OAB-CAA
10	B	504	71P	CAO-CAC-OAB-CAA
5	A	501	GTP	C5'-O5'-PA-O3A
8	B	501	GDP	C5'-O5'-PA-O3A
8	D	600	GDP	C5'-O5'-PA-O3A
5	A	501	GTP	C5'-O5'-PA-O2A
8	B	501	GDP	C5'-O5'-PA-O2A
8	D	600	GDP	C5'-O5'-PA-O2A
5	C	501	GTP	C4'-C5'-O5'-PA
5	C	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	C5'-O5'-PA-O3A
5	A	501	GTP	PB-O3A-PA-O2A
5	C	501	GTP	PB-O3A-PA-O1A
5	C	501	GTP	PB-O3A-PA-O2A
8	B	501	GDP	PB-O3A-PA-O1A
8	D	600	GDP	PB-O3A-PA-O1A
8	D	600	GDP	PB-O3A-PA-O2A
9	B	503	MES	C8-C7-N4-C3

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	B	504	71P	CAE-CAF-CAG-CAH-CAQ-CAR-CAS

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	504	71P	2	0

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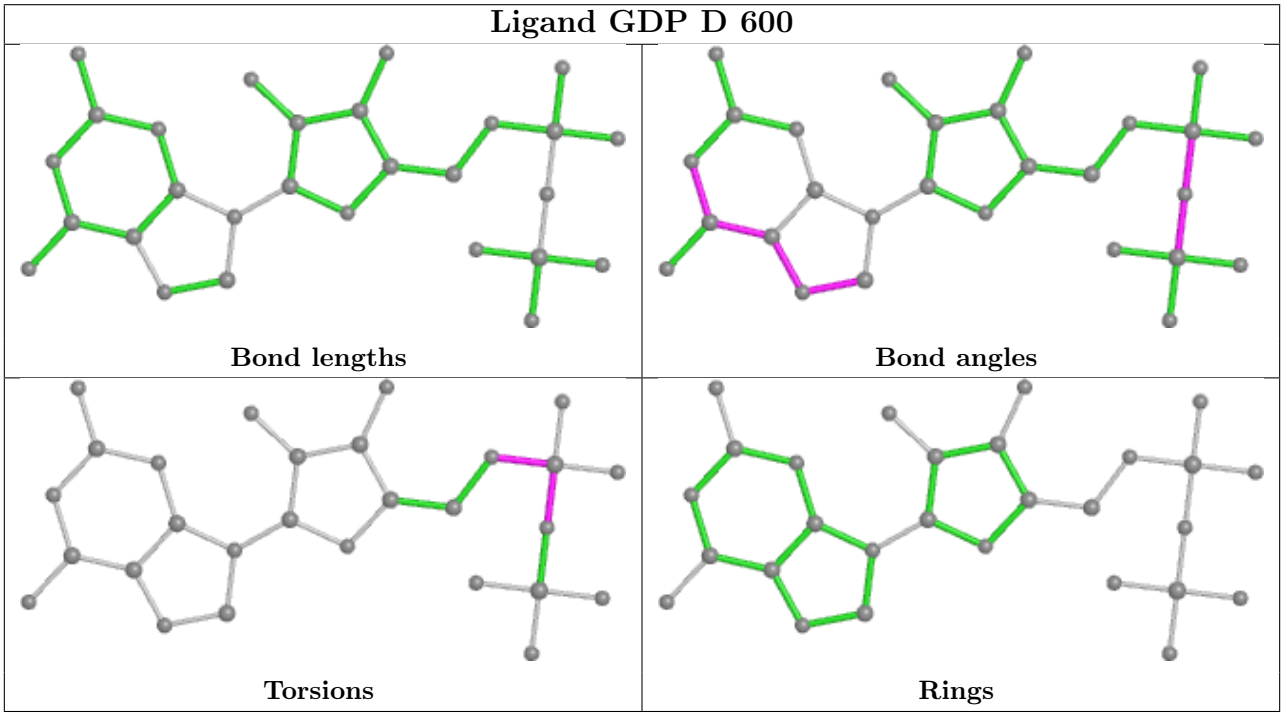
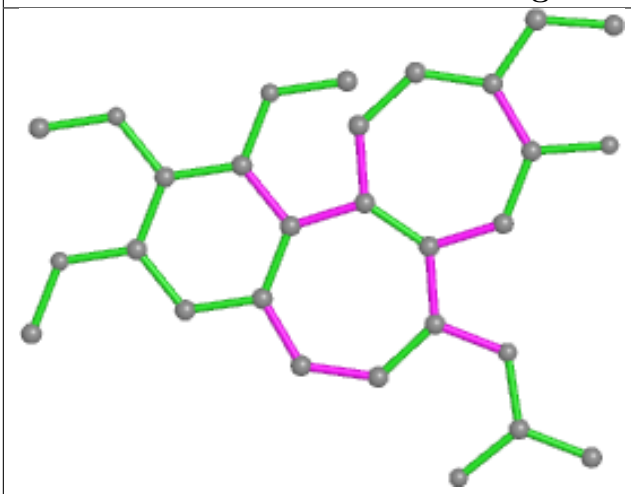
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	501	GTP	1	0

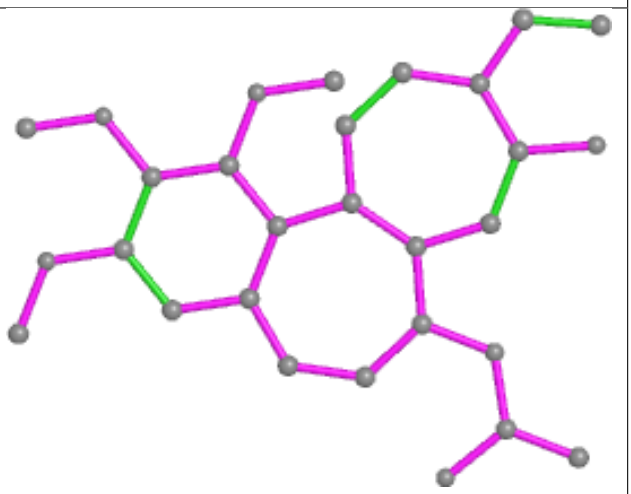
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



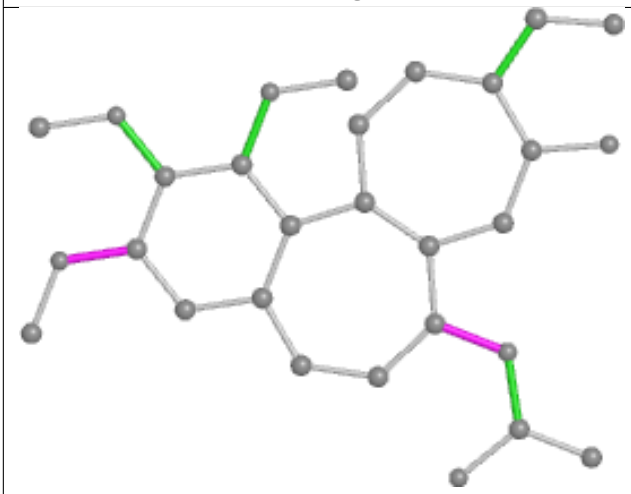
Ligand 71P B 504



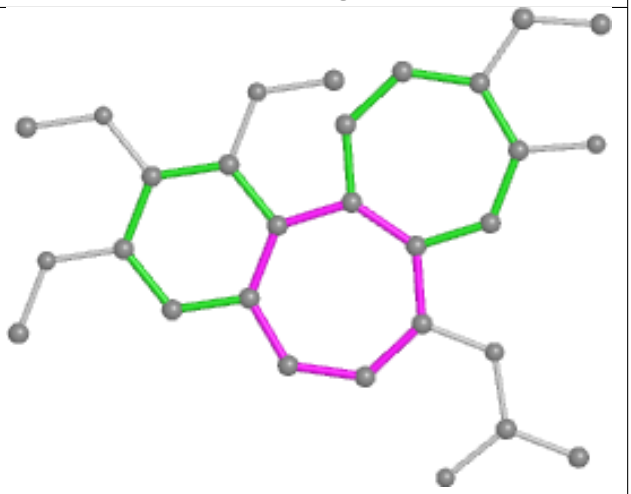
Bond lengths



Bond angles

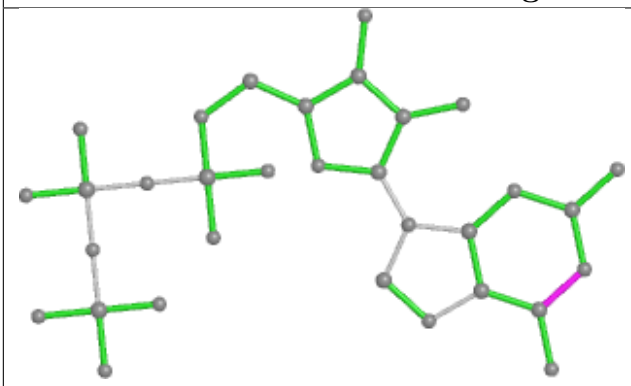


Torsions

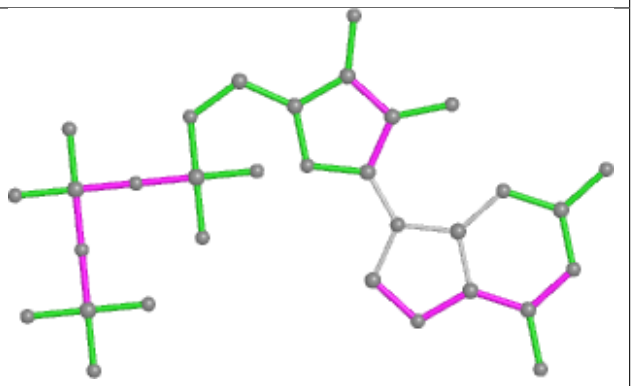


Rings

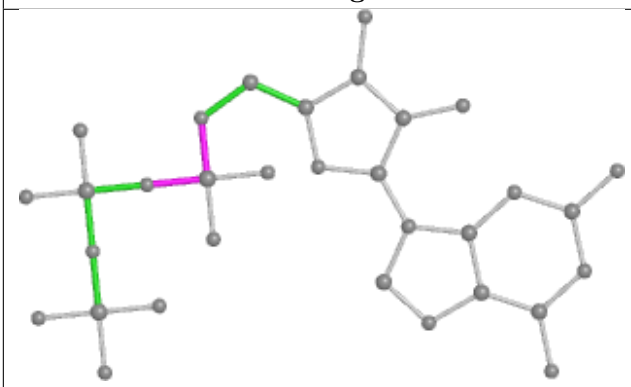
Ligand GTP A 501



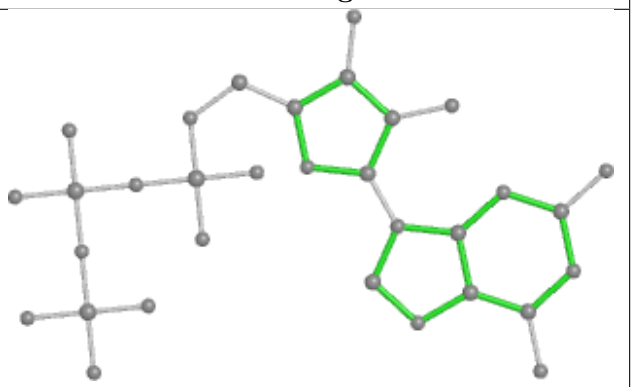
Bond lengths



Bond angles

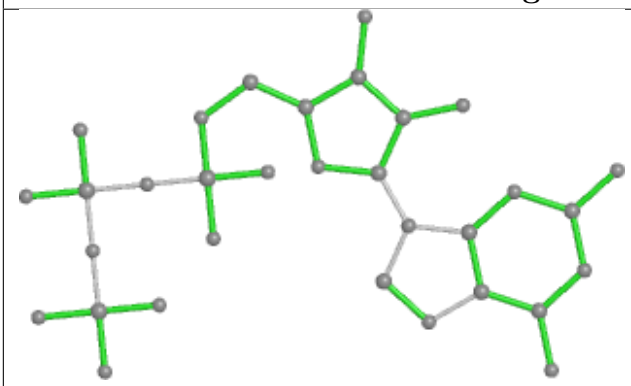


Torsions

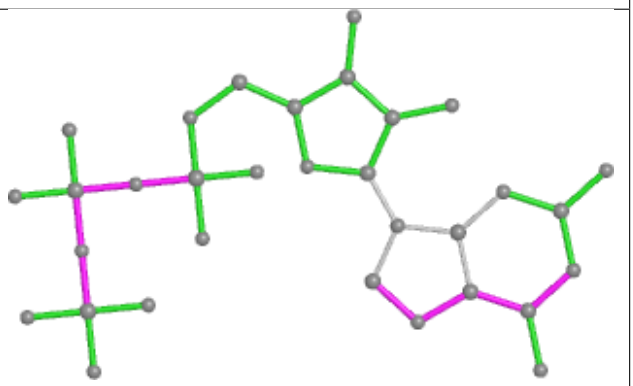


Rings

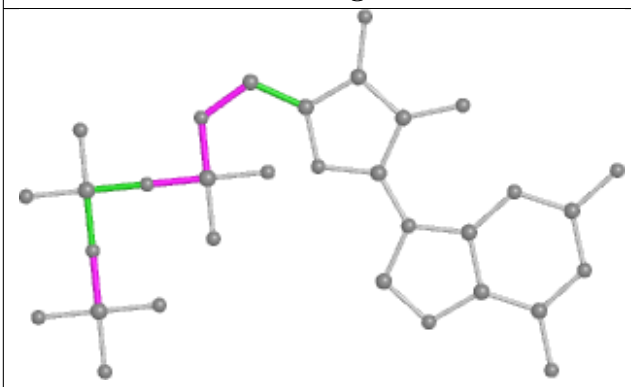
Ligand GTP C 501



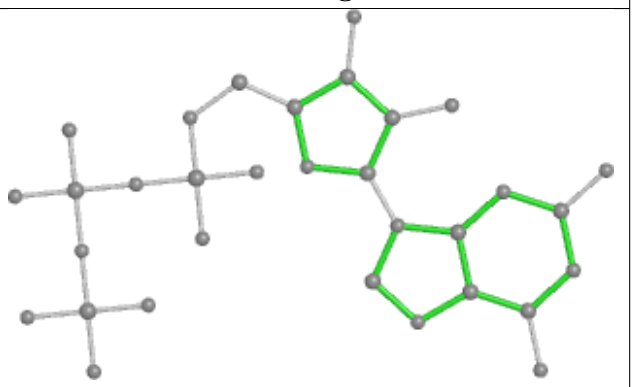
Bond lengths



Bond angles

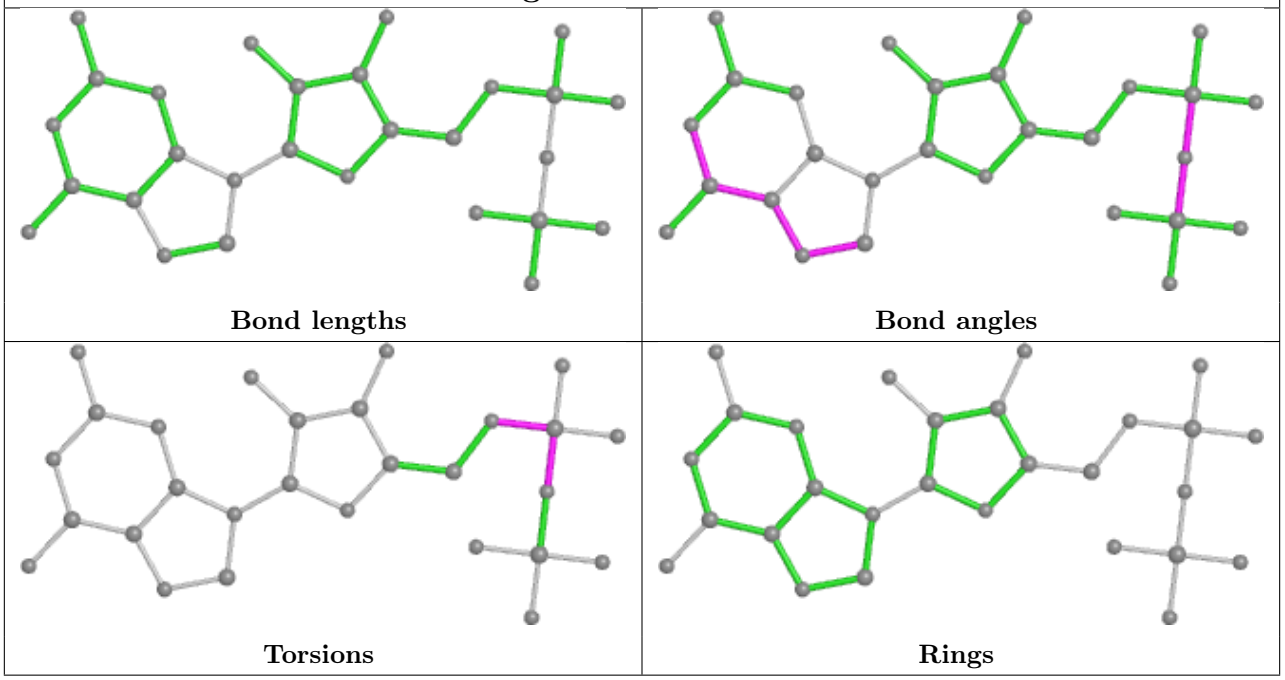


Torsions



Rings

Ligand GDP B 501



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	2
2	D	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	360:PRO	C	369:ARG	N	3.14
1	B	42:LEU	C	45:GLN	N	3.11
1	D	42:LEU	C	45:GLN	N	3.03
1	D	360:PRO	C	369:ARG	N	2.87

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	439/440 (99%)	0.78	30 (6%) 17 13	64, 76, 84, 94	0
1	C	440/440 (100%)	0.71	11 (2%) 57 55	64, 75, 83, 88	0
2	B	422/445 (94%)	0.80	20 (4%) 31 28	64, 76, 84, 92	1 (0%)
2	D	421/445 (94%)	0.84	42 (9%) 7 5	69, 77, 86, 93	5 (1%)
3	E	121/143 (84%)	0.91	12 (9%) 7 5	71, 80, 86, 91	0
4	F	340/384 (88%)	1.81	129 (37%) 0 0	72, 79, 91, 99	0
All	All	2183/2297 (95%)	0.95	244 (11%) 5 4	64, 77, 87, 99	6 (0%)

All (244) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	249	TYR	9.7
3	E	27	PRO	8.0
4	F	173	ILE	7.8
4	F	179	VAL	7.7
4	F	240	LEU	7.2
4	F	181	VAL	7.2
4	F	250	SER	6.9
4	F	100	ILE	6.7
4	F	130	VAL	6.5
4	F	131	PHE	6.4
4	F	231	ALA	6.1
1	A	439	SER	6.1
1	A	438	ASP	6.0
4	F	182	ILE	5.9
4	F	101	TYR	5.9
4	F	238	CYS	5.8
4	F	161	LEU	5.7
4	F	167	SER	5.7
4	F	248	GLU	5.6

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Mol	Chain	Res	Type	RSRZ
4	F	233	PHE	5.5
4	F	163	SER	5.5
4	F	134	ALA	5.5
4	F	251	LYS	5.4
4	F	256	TYR	5.3
4	F	232	ASN	5.2
4	F	253	TYR	5.0
4	F	239	HIS	5.0
4	F	224	SER	4.8
4	F	236	LYS	4.7
4	F	168	GLU	4.7
4	F	150	LYS	4.7
4	F	142	ARG	4.7
4	F	180	HIS	4.6
4	F	145	ASN	4.6
1	C	340	SER	4.6
4	F	149	ALA	4.5
4	F	225	SER	4.5
4	F	243	HIS	4.4
4	F	102	PRO	4.3
4	F	162	ILE	4.3
4	F	252	ASN	4.3
4	F	234	GLN	4.3
4	F	147	TRP	4.2
4	F	237	THR	4.2
4	F	244	CYS	4.1
4	F	196	HIS	4.1
4	F	139	ARG	4.1
4	F	128	ARG	4.0
2	D	401	ARG	4.0
2	B	61	TYR	4.0
4	F	174	ASP	4.0
1	A	1	MET	4.0
2	D	57	THR	3.9
1	A	346	TRP	3.9
4	F	230	SER	3.9
4	F	255	ARG	3.9
4	F	241	THR	3.9
4	F	136	ASN	3.9
4	F	254	GLY	3.9
4	F	169	LEU	3.9
4	F	245	ILE	3.8

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Mol	Chain	Res	Type	RSRZ
4	F	132	LEU	3.8
4	F	371	PRO	3.8
2	D	182	VAL	3.8
3	E	26	PRO	3.7
1	A	281	ALA	3.7
4	F	171	ASP	3.7
1	C	302	MET	3.7
4	F	138	ARG	3.7
4	F	165	GLU	3.7
4	F	166	ALA	3.7
3	E	28	SER	3.7
2	D	415	GLU	3.6
4	F	148	ILE	3.6
1	A	42	ILE	3.6
1	C	440	VAL	3.6
2	D	42	LEU	3.5
4	F	362	ALA	3.5
2	B	276	THR	3.5
2	D	414	ASP	3.5
4	F	372	THR	3.5
2	B	42	LEU	3.5
4	F	235	ASP	3.5
4	F	183	GLN	3.4
4	F	129	GLU	3.4
2	B	277	SER	3.4
2	B	57	THR	3.4
2	B	249	ASN	3.4
4	F	361	LEU	3.4
4	F	263	PHE	3.4
2	B	337	ASN	3.4
4	F	343	TYR	3.3
3	E	135	LYS	3.3
1	A	262	TYR	3.3
4	F	172	PHE	3.3
2	D	181	VAL	3.3
4	F	242	ASN	3.2
4	F	246	GLN	3.2
2	D	406	HIS	3.2
4	F	99	VAL	3.2
2	B	437	ASP	3.2
1	A	60	LYS	3.2
2	D	177	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
2	D	37	HIS	3.2
4	F	20	LEU	3.2
2	B	247	GLN	3.1
4	F	247	LYS	3.1
4	F	164	SER	3.1
4	F	229	ASN	3.1
2	D	73	GLY	3.1
4	F	344	ALA	3.0
4	F	199	PHE	3.0
2	B	59	ASN	3.0
4	F	141	GLY	3.0
4	F	133	ALA	3.0
2	D	74	THR	3.0
4	F	262	MET	2.9
3	E	77	GLU	2.9
4	F	151	SER	2.9
4	F	175	GLU	2.9
2	D	400	ARG	2.9
2	D	94	PHE	2.9
3	E	45	PRO	2.9
4	F	214	TYR	2.9
4	F	6	VAL	2.9
2	D	68	VAL	2.9
4	F	160	ILE	2.8
4	F	261	GLU	2.8
1	A	57	GLY	2.8
2	B	172	MET	2.8
2	B	37	HIS	2.8
4	F	127	GLU	2.8
3	E	46	SER	2.8
4	F	338	CYS	2.8
4	F	13	VAL	2.8
2	D	83	PHE	2.8
4	F	226	GLU	2.8
4	F	186	LEU	2.8
1	A	56	THR	2.8
4	F	258	GLU	2.7
4	F	126	ASP	2.7
4	F	351	VAL	2.7
2	D	405	LEU	2.7
1	A	434	GLU	2.7
4	F	27	TRP	2.7

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Mol	Chain	Res	Type	RSRZ
2	D	185	TYR	2.7
4	F	135	TYR	2.7
2	D	418	PHE	2.7
4	F	98	TYR	2.7
1	A	178	SER	2.6
2	D	30	ILE	2.6
4	F	340	GLN	2.6
2	D	276	THR	2.6
1	A	351	PHE	2.6
1	A	418	PHE	2.6
1	A	282	TYR	2.6
1	C	337	THR	2.6
2	B	438	ALA	2.6
4	F	348	GLN	2.5
1	A	255	PHE	2.5
2	B	60	LYS	2.5
2	D	408	TYR	2.5
4	F	14	TYR	2.5
2	D	78	VAL	2.5
4	F	257	GLU	2.5
4	F	223	THR	2.5
1	A	88	HIS	2.5
4	F	220	VAL	2.5
4	F	23	ALA	2.5
4	F	356	SER	2.4
1	A	316	CYS	2.4
1	C	437	VAL	2.4
4	F	146	VAL	2.4
4	F	90	SER	2.4
2	B	58	GLY	2.4
2	D	334	ASN	2.4
4	F	320	MET	2.4
1	A	315	CYS	2.4
3	E	140	LYS	2.4
4	F	187	GLU	2.4
4	F	353	VAL	2.4
4	F	18	SER	2.4
3	E	44	ASP	2.4
4	F	24	THR	2.4
4	F	97	SER	2.4
1	A	62	VAL	2.3
1	C	357	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
4	F	342	LEU	2.3
2	B	49	ILE	2.3
4	F	314	LEU	2.3
2	D	97	SER	2.3
4	F	184	LYS	2.3
1	A	284	GLU	2.3
4	F	204	TRP	2.3
3	E	138	GLU	2.3
2	D	212	ILE	2.3
1	A	163	LYS	2.3
3	E	139	LEU	2.3
4	F	346	LEU	2.3
4	F	375	PHE	2.3
2	D	59	ASN	2.3
2	D	110	GLU	2.3
2	B	416	MET	2.3
2	D	114	LEU	2.3
2	D	317	ALA	2.3
2	D	407	TRP	2.2
4	F	376	ILE	2.2
1	C	372	GLN	2.2
3	E	25	LYS	2.2
1	C	436	GLY	2.2
2	B	53	TYR	2.2
2	D	55	GLU	2.2
1	A	252	LEU	2.2
4	F	259	GLY	2.2
2	D	58	GLY	2.2
2	D	69	ASP	2.2
4	F	191	LEU	2.2
2	D	93	VAL	2.2
2	D	402	LYS	2.2
4	F	264	PHE	2.2
1	A	259	LEU	2.2
1	A	149	PHE	2.1
4	F	41	LEU	2.1
4	F	227	PRO	2.1
1	C	167	LEU	2.1
1	A	65	ALA	2.1
4	F	70	LYS	2.1
2	D	413	MET	2.1
1	A	87	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	167	ASN	2.1
4	F	125	THR	2.1
1	A	35	GLN	2.1
2	B	345	GLU	2.1
2	D	168	THR	2.1
4	F	152	SER	2.1
2	D	86	ILE	2.1
1	C	252	LEU	2.0
1	A	2	ARG	2.0
2	B	62	VAL	2.0
1	A	67	PHE	2.0
4	F	336	PRO	2.0
1	C	283	HIS	2.0
2	D	92	PHE	2.0
2	D	70	LEU	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 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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	MG	B	502	1/1	0.44	0.62	88,88,88,88	0
6	MG	B	506	1/1	0.52	0.57	87,87,87,87	0
6	MG	A	506	1/1	0.61	0.50	84,84,84,84	0
11	CA	C	503	1/1	0.65	0.27	123,123,123,123	0
10	71P	B	504	29/29	0.69	0.52	96,97,99,100	29
6	MG	A	505	1/1	0.77	0.31	79,79,79,79	0
6	MG	B	505	1/1	0.78	0.32	71,71,71,71	0
6	MG	A	504	1/1	0.80	0.19	95,95,95,95	0

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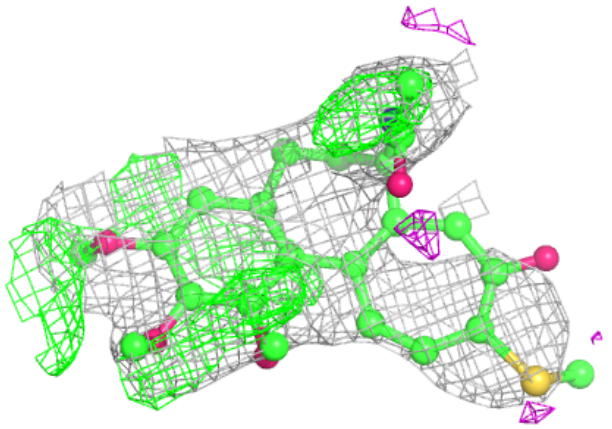
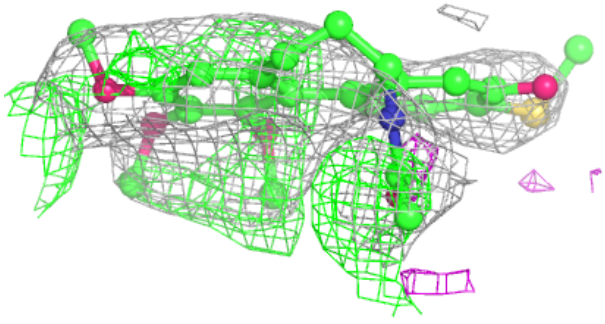
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	GDP	D	600	28/28	0.90	0.21	101,102,107,109	0
8	GDP	B	501	28/28	0.94	0.26	77,77,78,79	0
6	MG	C	502	1/1	0.94	0.48	55,55,55,55	0
9	MES	B	503	12/12	0.95	0.32	94,95,97,99	0
5	GTP	A	501	32/32	0.95	0.28	81,83,84,85	0
7	CL	A	503	1/1	0.95	0.08	98,98,98,98	0
5	GTP	C	501	32/32	0.96	0.30	77,79,80,81	0
6	MG	A	502	1/1	0.98	0.53	68,68,68,68	0

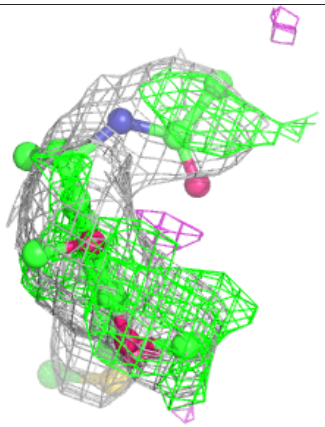
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 71P B 504:

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

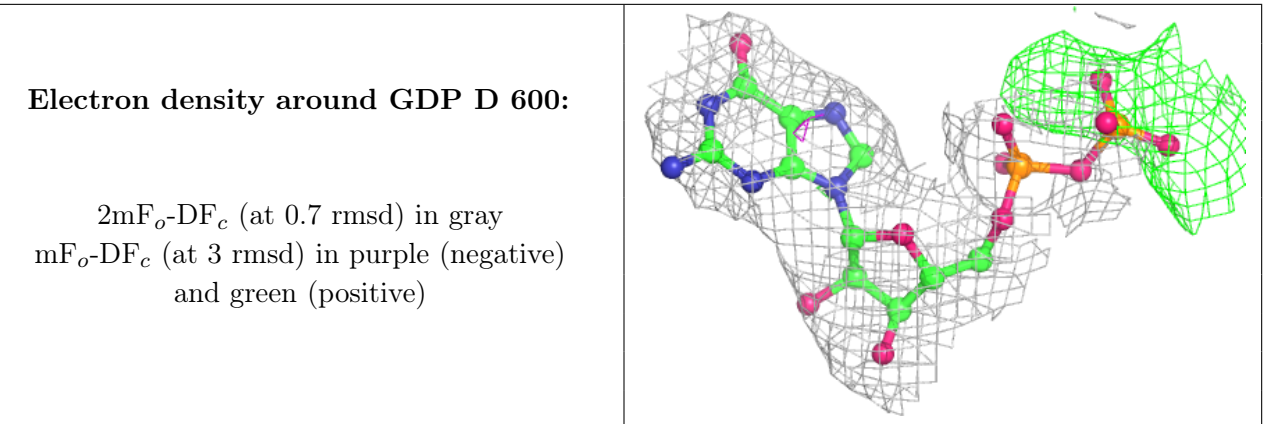


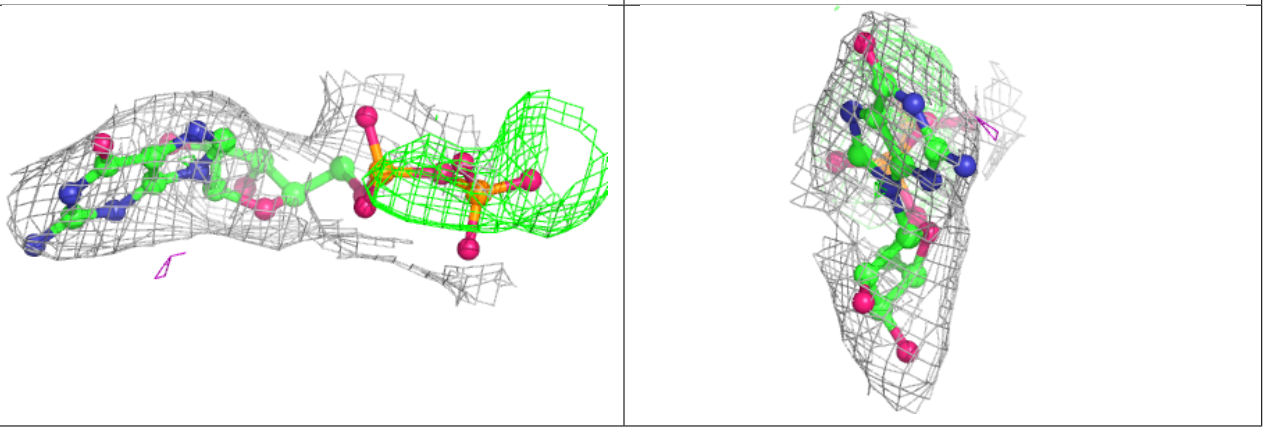




Electron density around GDP D 600:

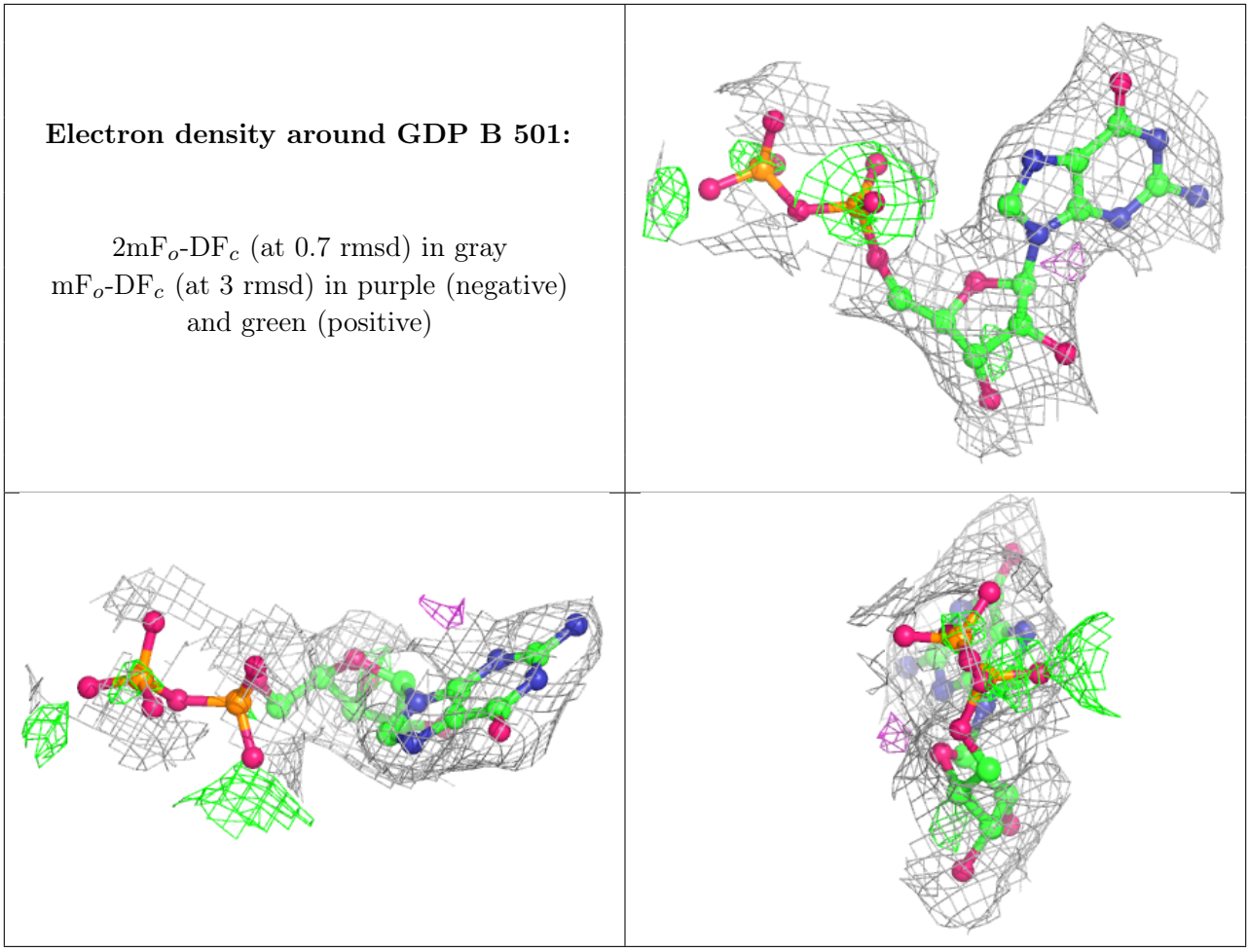
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





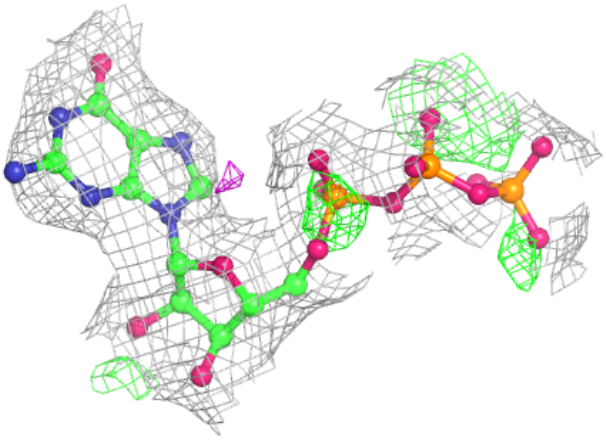
Electron density around GDP B 501:

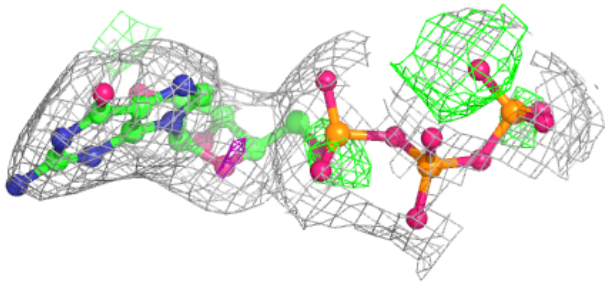
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

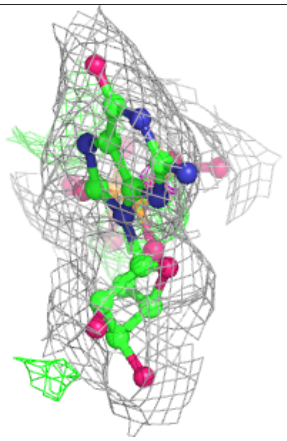


Electron density around GTP A 501:

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

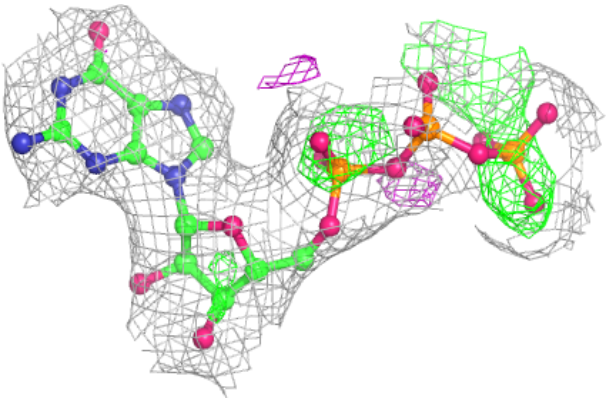


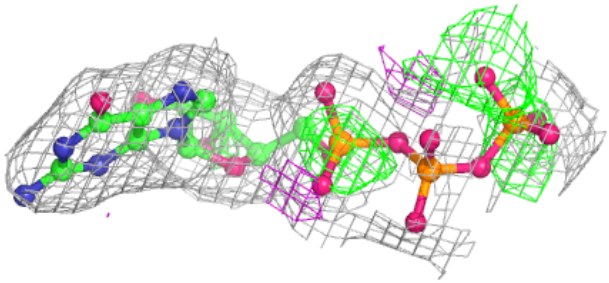


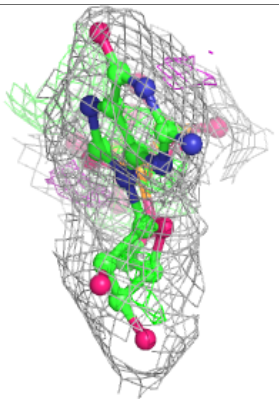


Electron density around GTP C 501:

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







6.5 Other polymers (i)

There are no such residues in this entry.