



wwPDB X-ray Structure Validation Summary Report ⓘ

May 26, 2020 – 09:06 am BST

PDB ID : 4IHJ
Title : Crystal structure of tubulin-stathmin-TTL-ADP complex
Authors : Prota, A.E.; Magiera, M.M.; Kuijpers, M.; Bargsten, K.; Frey, D.; Wieser, M.;
Jaussi, R.; Hoogenraad, C.C.; Kammerer, R.A.; Janke, C.; Steinmetz, M.O.
Deposited on : 2012-12-18
Resolution : 2.00 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

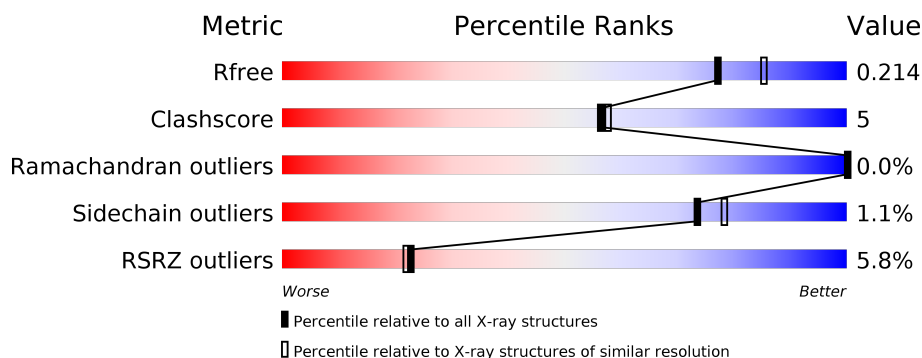
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 on 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	450	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 98%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> 88% 10% </div> </div>
1	C	450	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 98%, yellow 2%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> 85% 12% </div> </div>
2	B	445	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 98%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> 87% 8% 5% </div> </div>
2	D	445	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, orange 1%, yellow 1%, green 96%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> 83% 12% 5% </div> </div>
3	E	143	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 95%, yellow 5%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> 80% 5% 15% </div> </div>
4	F	384	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 28%, orange 1%, yellow 1%, green 70%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> 28% 76% 13% 10% </div> </div>

2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 36041 atoms, of which 17304 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	442	Total	C	H	N	O	S	0	8	0
			6927	2210	3432	594	666	25			
1	C	440	Total	C	H	N	O	S	0	10	0
			6898	2203	3419	586	664	26			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	422	Total	C	H	N	O	S	0	5	0
			6591	2103	3250	567	644	27			
2	D	422	Total	C	H	N	O	S	0	5	0
			6555	2093	3224	563	648	27			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	E	121	Total	C	H	N	O	S	0	3	0
			2062	629	1045	184	198	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	-	CLONING ARTIFACT	UNP P63043
E	4	ALA	-	CLONING ARTIFACT	UNP P63043

- Molecule 4 is a protein called TUBULIN TYROSINE LIGASE, TTL.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	F	344	Total	C	H	N	O	S	0	4	0
			5700	1837	2848	488	513	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	H	N	O	P	0	0
			42	10	10	5	14	3		
5	C	1	Total	C	H	N	O	P	0	0
			42	10	10	5	14	3		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Mg	0	0
			1	1		
6	A	1	Total	Mg	0	0
			1	1		
6	D	2	Total	Mg	0	0
			2	2		
6	C	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	2	Total	Mg	0	0
			2	2		

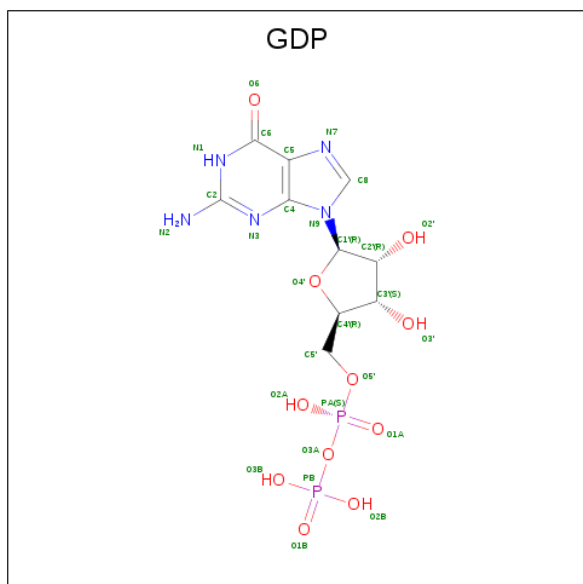
- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Ca	0	0
			1	1		
7	A	2	Total	Ca	0	0
			2	2		
7	C	1	Total	Ca	0	0
			1	1		

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

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

- Molecule 9 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



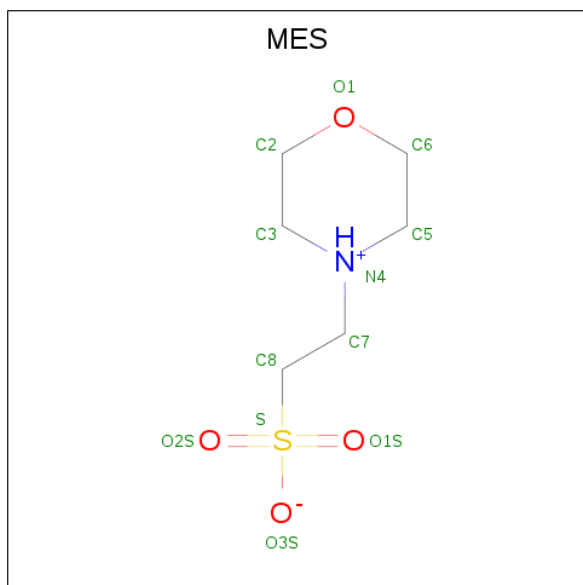
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	H	N	O	P	
			38	10	10	5	11	2	0

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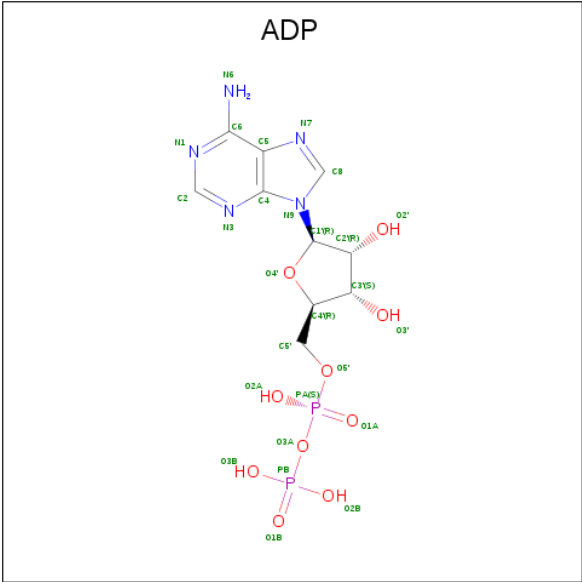
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	D	1	Total	C	H	N	O	P	
			38	10	10	5	11	2	
								0	0

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



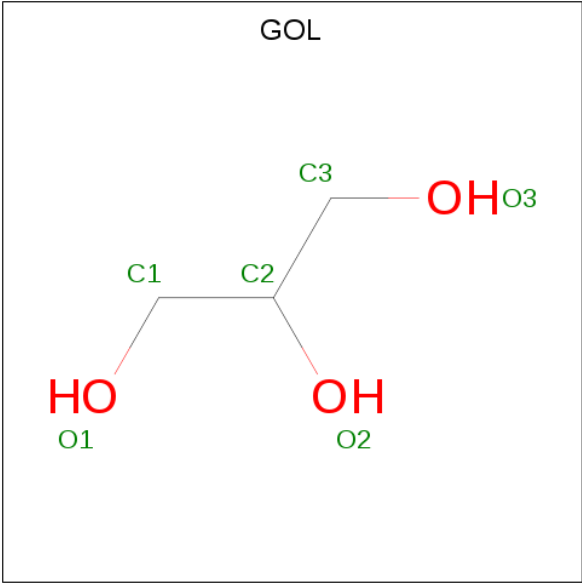
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	H	N	O	S	
			25	6	13	1	4	1	
10	B	1	Total	C	H	N	O	S	
			25	6	13	1	4	1	
								0	0

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
11	F	1	Total	C	H	N	O	P	0	0
			39	10	12	5	10	2		

- Molecule 12 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	F	1	Total	C	H	O	0	0
			14	3	8	3		

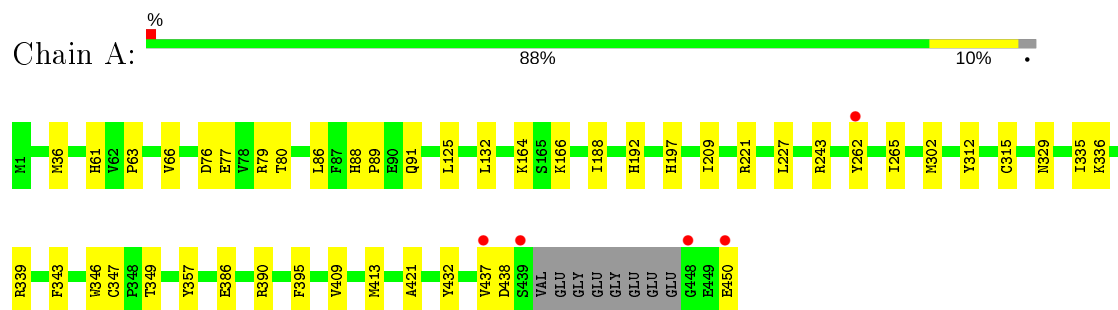
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	217	Total 217	O 217	0	0
13	B	189	Total 189	O 189	0	0
13	C	376	Total 376	O 376	0	0
13	D	117	Total 117	O 117	0	0
13	E	54	Total 54	O 54	0	0
13	F	80	Total 80	O 80	0	0

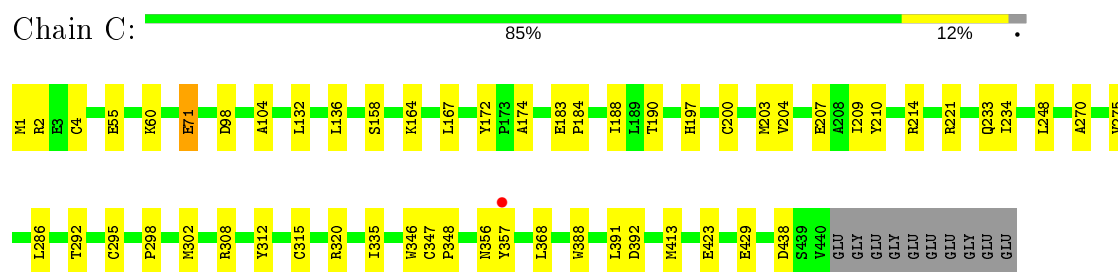
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

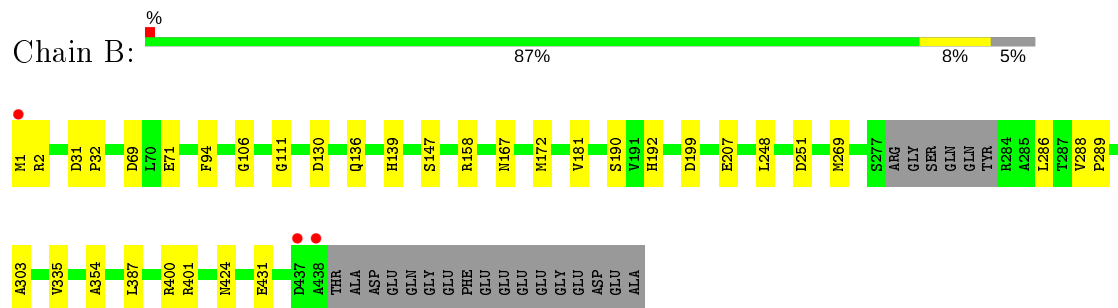
- Molecule 1: Tubulin alpha-1B chain



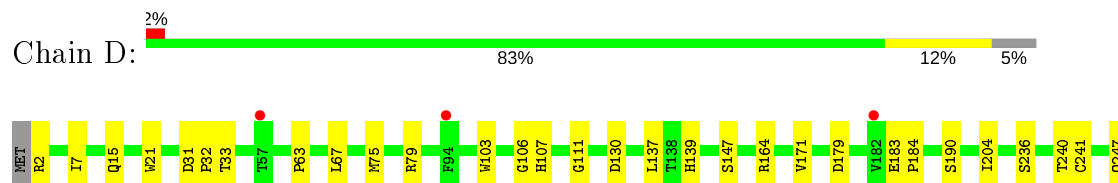
- Molecule 1: Tubulin alpha-1B chain

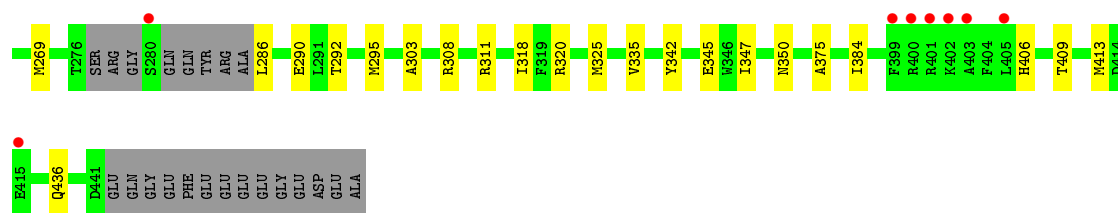


- Molecule 2: Tubulin beta-2B chain

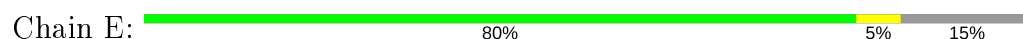


- Molecule 2: Tubulin beta-2B chain

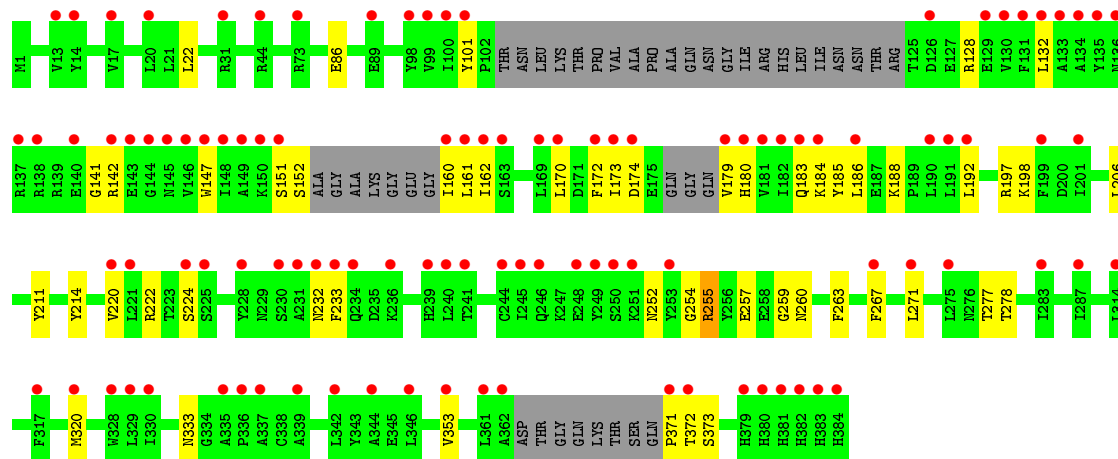
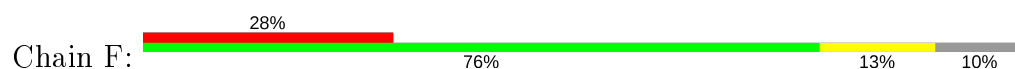




● Molecule 3: Stathmin-4



● Molecule 4: TUBULIN TYROSINE LIGASE, TTL



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	104.52Å 157.31Å 180.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	72.10 – 2.00 78.45 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.1 (72.10-2.00) 99.1 (78.45-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.41 (at 2.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.168 , 0.217 0.166 , 0.214	Depositor DCC
R_{free} test set	10033 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	36.2	Xtriage
Anisotropy	0.230	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 58.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	36041	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.52% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, GOL, MG, ADP, CL, CA, GTP, MES

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	0.42	0/3596	0.61	2/4875 (0.0%)
1	C	0.53	1/3587 (0.0%)	0.63	0/4871
2	B	0.46	0/3429	0.57	0/4644
2	D	0.39	0/3420	0.53	0/4632
3	E	0.42	0/1035	0.51	0/1373
4	F	0.34	0/2932	0.51	0/3962
All	All	0.44	1/17999 (0.0%)	0.57	2/24357 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	295	CYS	CB-SG	-5.25	1.73	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	243	ARG	NE-CZ-NH2	-6.43	117.08	120.30
1	A	243	ARG	NE-CZ-NH1	6.12	123.36	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3495	3432	3419	31	0
1	C	3479	3419	3406	39	0
2	B	3341	3250	3240	35	0
2	D	3331	3224	3212	33	0
3	E	1017	1045	1040	5	0
4	F	2852	2848	2833	37	0
5	A	32	10	12	0	0
5	C	32	10	12	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	2	0	0	0	0
6	F	2	0	0	0	0
7	A	2	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
8	A	1	0	0	0	0
9	B	28	10	12	0	0
9	D	28	10	12	0	0
10	B	24	26	26	6	0
11	F	27	12	12	0	0
12	F	6	8	8	0	0
13	A	217	0	0	3	0
13	B	189	0	0	5	0
13	C	376	0	0	5	0
13	D	117	0	0	3	0
13	E	54	0	0	0	0
13	F	80	0	0	1	0
All	All	18737	17304	17244	173	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 5.

The worst 5 of 173 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:192:HIS:ND1	13:B:770:HOH:O	1.98	0.96
1:C:234:ILE:HG21	1:C:302[B]:MET:SD	2.07	0.94
2:B:199:ASP:OD2	10:B:504:MES:H32	1.75	0.87
1:C:270:ALA:HB3	1:C:302[B]:MET:SD	2.16	0.84
2:D:241[B]:CYS:SG	13:D:772:HOH:O	2.35	0.84

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	446/450 (99%)	435 (98%)	11 (2%)	0	100	100
1	C	448/450 (100%)	432 (96%)	16 (4%)	0	100	100
2	B	423/445 (95%)	412 (97%)	11 (3%)	0	100	100
2	D	422/445 (95%)	414 (98%)	8 (2%)	0	100	100
3	E	120/143 (84%)	118 (98%)	2 (2%)	0	100	100
4	F	338/384 (88%)	318 (94%)	19 (6%)	1 (0%)	41	37
All	All	2197/2317 (95%)	2129 (97%)	67 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	F	232	ASN

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	380/378 (100%)	379 (100%)	1 (0%)	92	95
1	C	381/378 (101%)	379 (100%)	2 (0%)	88	92
2	B	370/383 (97%)	367 (99%)	3 (1%)	81	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	370/383 (97%)	366 (99%)	4 (1%)	73	78
3	E	112/127 (88%)	111 (99%)	1 (1%)	78	83
4	F	316/342 (92%)	307 (97%)	9 (3%)	43	44
All	All	1929/1991 (97%)	1909 (99%)	20 (1%)	73	81

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	345	GLU
3	E	135	LYS
4	F	211	TYR
2	D	139	HIS
2	D	179	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	301	GLN
1	A	309	HIS
2	B	192	HIS
2	B	229	HIS
1	C	197	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 20 ligands modelled in this entry, 12 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	505	-	12,12,12	2.21	1 (8%)	14,16,16	1.67	3 (21%)
5	GTP	A	501	6	26,34,34	0.79	1 (3%)	33,54,54	1.75	5 (15%)
9	GDP	B	501	6	24,30,30	1.23	3 (12%)	31,47,47	1.90	6 (19%)
5	GTP	C	501	6	26,34,34	0.99	2 (7%)	33,54,54	1.47	4 (12%)
11	ADP	F	703	6	24,29,29	1.03	1 (4%)	29,45,45	1.34	4 (13%)
10	MES	B	504	-	12,12,12	1.87	1 (8%)	14,16,16	2.03	2 (14%)
9	GDP	D	600	6	24,30,30	1.21	3 (12%)	31,47,47	1.83	7 (22%)
12	GOL	F	704	-	5,5,5	0.38	0	5,5,5	0.56	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
10	MES	B	505	-	-	5/6/14/14	0/1/1/1
5	GTP	A	501	6	-	5/18/38/38	0/3/3/3
9	GDP	B	501	6	-	5/12/32/32	0/3/3/3
5	GTP	C	501	6	-	6/18/38/38	0/3/3/3
11	ADP	F	703	6	-	2/12/32/32	0/3/3/3
10	MES	B	504	-	-	1/6/14/14	0/1/1/1
9	GDP	D	600	6	-	4/12/32/32	0/3/3/3
12	GOL	F	704	-	-	2/4/4/4	-

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	505	MES	C8-S	-7.31	1.67	1.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	504	MES	C8-S	-6.11	1.68	1.77
9	B	501	GDP	C6-C5	3.84	1.48	1.41
9	D	600	GDP	C6-C5	3.83	1.48	1.41
5	C	501	GTP	C6-N1	2.80	1.37	1.33

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	504	MES	O1S-S-C8	5.83	113.93	106.92
5	A	501	GTP	N3-C2-N1	-4.97	120.59	127.22
5	C	501	GTP	N3-C2-N1	-4.73	120.91	127.22
5	A	501	GTP	C5-C6-N1	-4.64	117.09	123.43
9	B	501	GDP	C6-N1-C2	4.60	123.24	115.93

There are no chirality outliers.

5 of 30 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
10	B	505	MES	C8-C7-N4-C3
10	B	505	MES	C7-C8-S-O1S

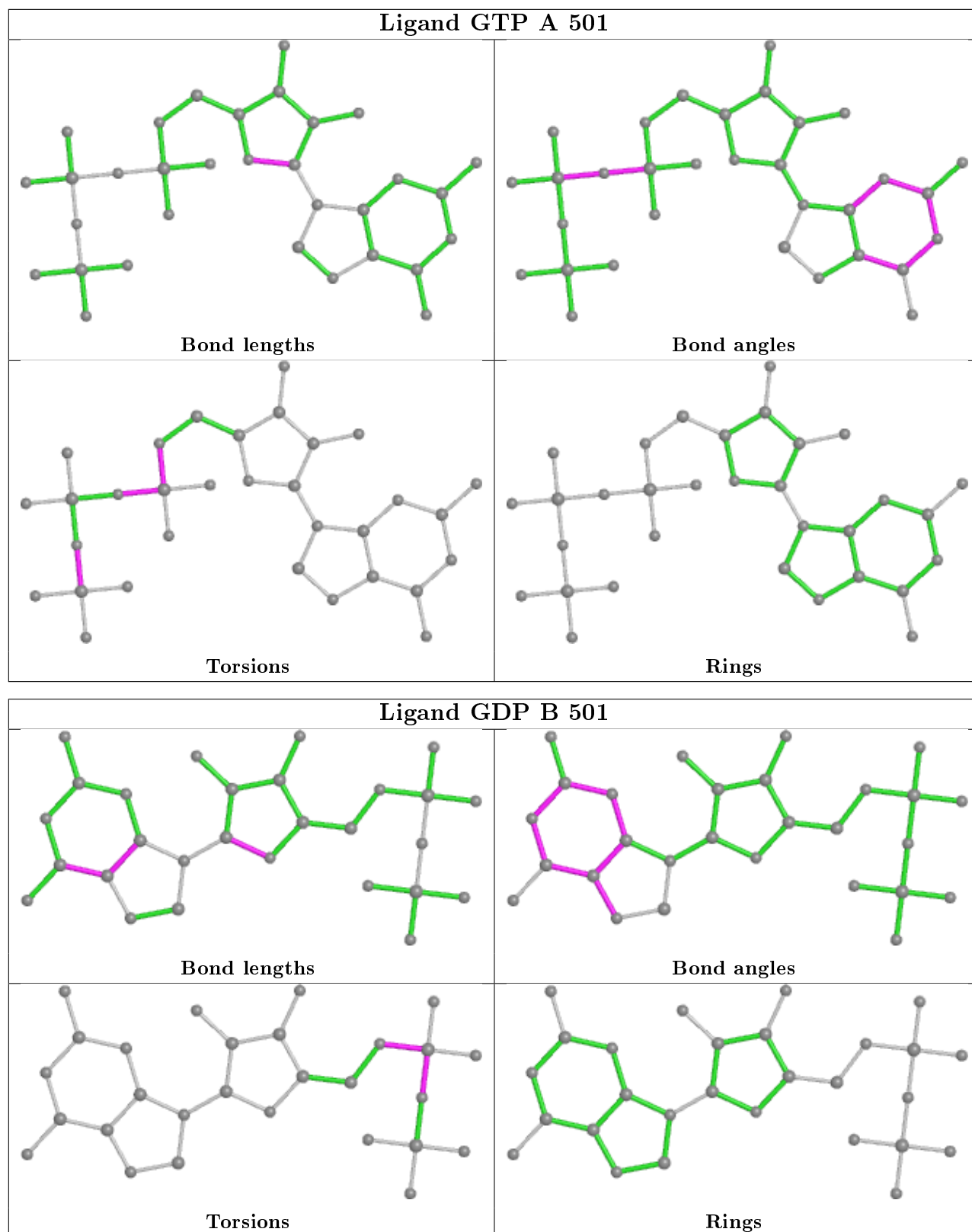
There are no ring outliers.

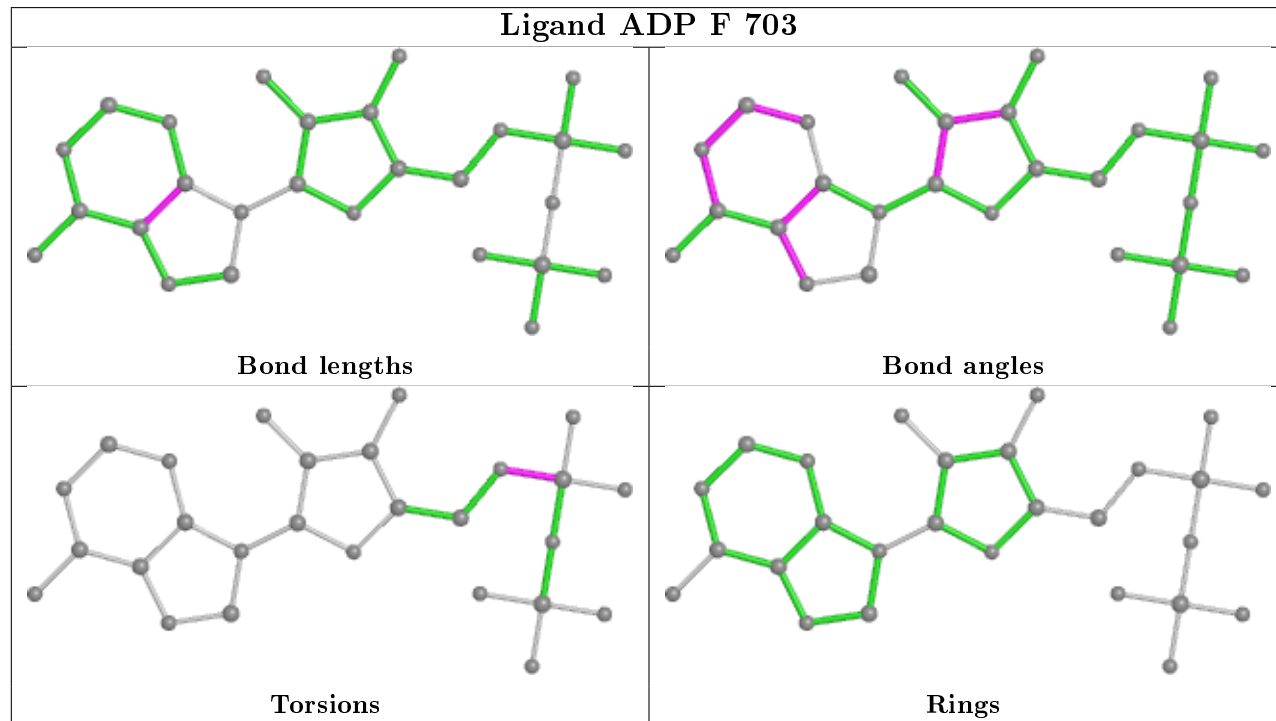
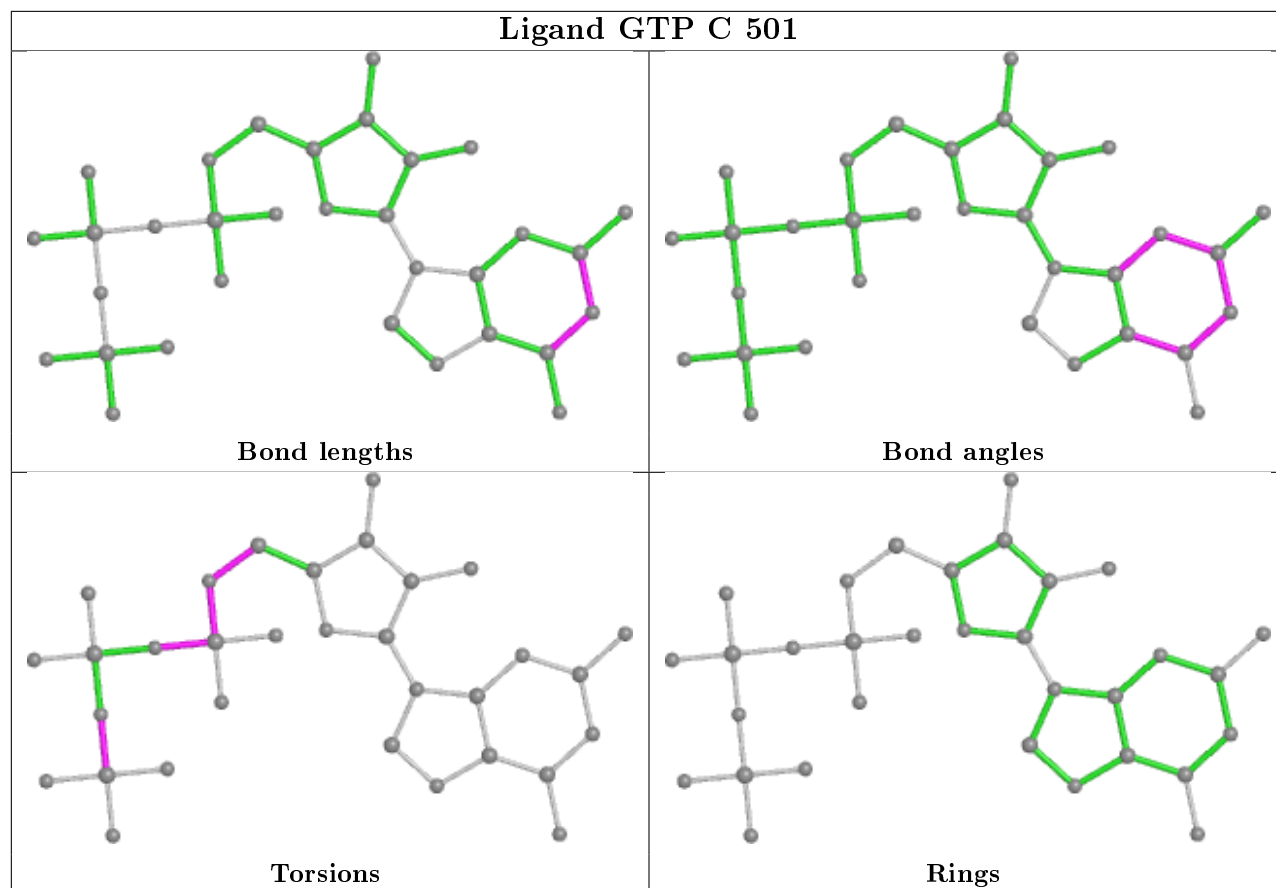
2 monomers are involved in 6 short contacts:

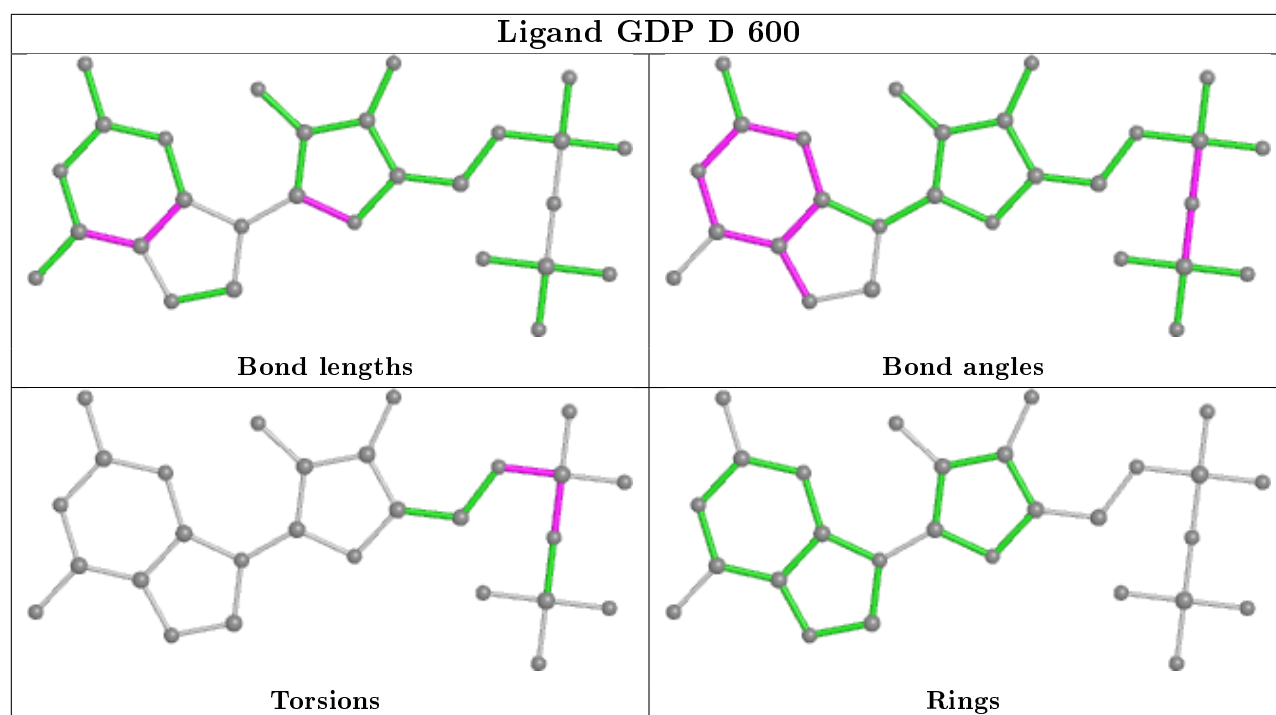
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	505	MES	1	0
10	B	504	MES	5	0

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

equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	442/450 (98%)	0.11	5 (1%) 80 79	24, 40, 78, 126	0
1	C	440/450 (97%)	0.20	1 (0%) 95 94	18, 31, 63, 95	0
2	B	422/445 (94%)	0.21	3 (0%) 87 87	21, 39, 80, 124	2 (0%)
2	D	422/445 (94%)	0.23	11 (2%) 56 54	25, 50, 89, 124	5 (1%)
3	E	121/143 (84%)	0.15	0 100 100	27, 56, 92, 108	0
4	F	344/384 (89%)	1.45	106 (30%) 0 0	33, 65, 125, 160	0
All	All	2191/2317 (94%)	0.38	126 (5%) 23 22	18, 44, 94, 160	7 (0%)

The worst 5 of 126 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	280	SER	9.3
4	F	182	ILE	8.9
2	D	401	ARG	8.5
4	F	173	ILE	7.8
4	F	186	LEU	7.8

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 carbohydrates in this entry.

6.4 Ligands ⓘ

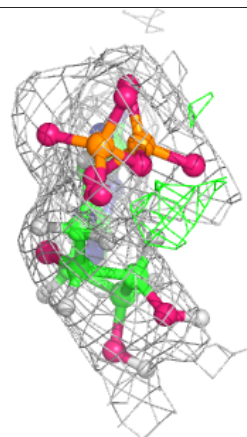
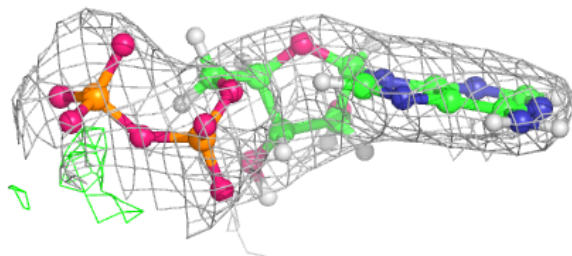
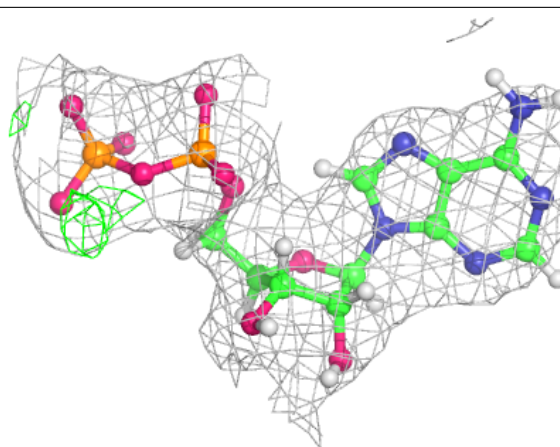
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
12	GOL	F	704	6/6	0.76	0.21	72,87,92,93	0
6	MG	D	602	1/1	0.86	0.17	100,100,100,100	0
6	MG	D	601	1/1	0.92	0.20	99,99,99,99	0
8	CL	A	504	1/1	0.94	0.21	72,72,72,72	0
7	CA	A	505	1/1	0.96	0.32	103,103,103,103	0
10	MES	B	505	12/12	0.96	0.12	73,77,89,90	0
7	CA	B	503	1/1	0.97	0.14	95,95,95,95	0
7	CA	A	503	1/1	0.97	0.15	59,59,59,59	0
10	MES	B	504	12/12	0.98	0.12	50,57,62,64	0
6	MG	F	702	1/1	0.98	0.07	66,66,66,66	0
11	ADP	F	703	27/27	0.98	0.14	70,75,87,88	0
9	GDP	D	600	28/28	0.98	0.13	50,54,67,69	0
6	MG	F	701	1/1	0.98	0.12	55,55,55,55	0
9	GDP	B	501	28/28	0.99	0.16	22,27,34,35	0
6	MG	C	502	1/1	0.99	0.19	27,27,27,27	0
7	CA	C	503	1/1	0.99	0.18	44,44,44,44	0
5	GTP	A	501	32/32	0.99	0.16	23,26,31,32	0
6	MG	B	502	1/1	0.99	0.20	27,27,27,27	0
6	MG	A	502	1/1	0.99	0.21	28,28,28,28	0
5	GTP	C	501	32/32	1.00	0.15	19,23,26,28	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.

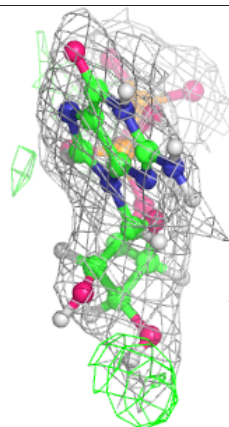
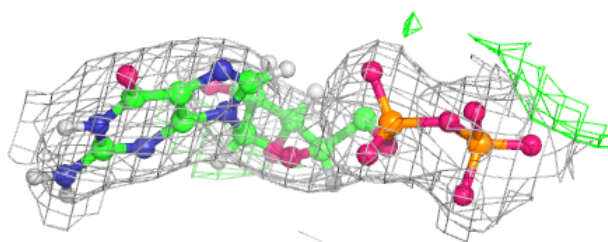
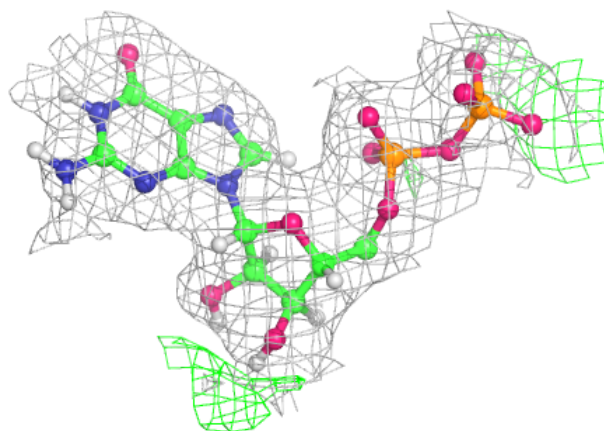
Electron density around ADP F 703:

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



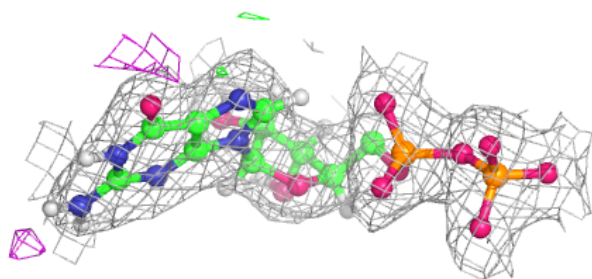
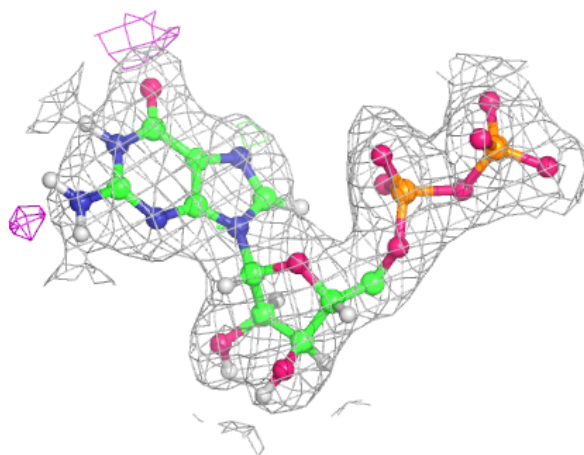
Electron density around GDP D 600:

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



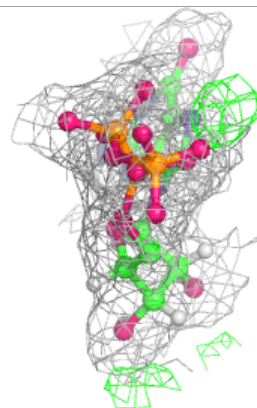
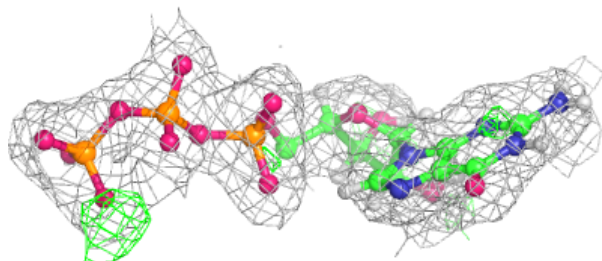
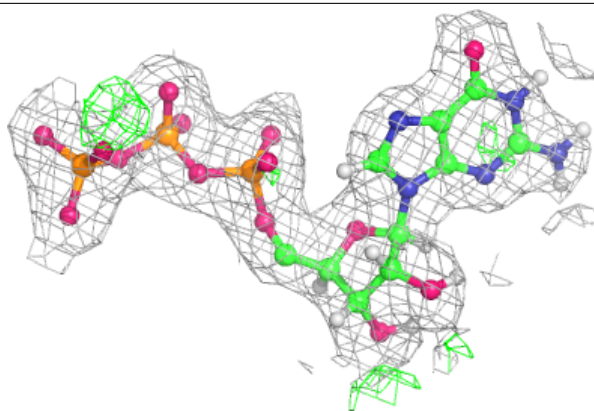
Electron density around GDP B 501:

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

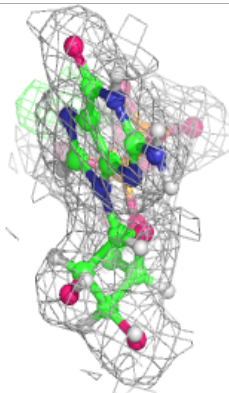
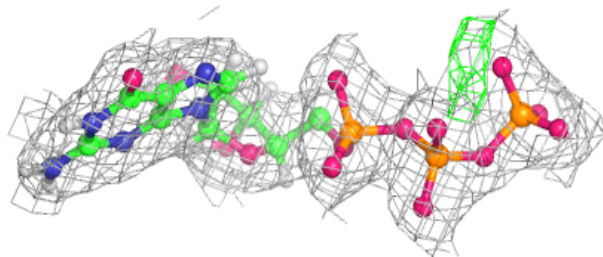
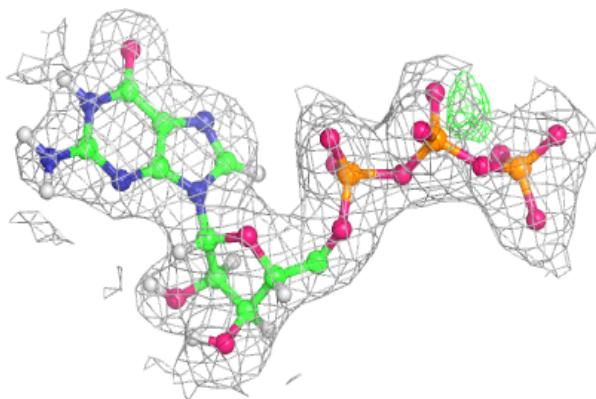


Electron density around GTP A 501:

$2mF_o-DF_c$ (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.