



wwPDB X-ray Structure Validation Summary Report ⓘ

May 14, 2020 – 06:01 am BST

PDB ID : 1SA0
Title : TUBULIN-COLCHICINE: STATHMIN-LIKE DOMAIN COMPLEX
Authors : Ravelli, R.B.; Gigant, B.; Curmi, P.A.; Jourdain, I.; Lachkar, S.; Sobel, A.; Knossow, M.
Deposited on : 2004-02-06
Resolution : 3.58 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

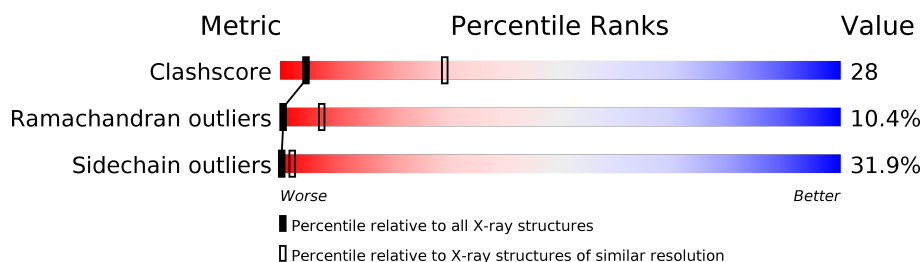
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.58 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))
Clashscore	141614	1181 (3.66-3.50)
Ramachandran outliers	138981	1143 (3.66-3.50)
Sidechain outliers	138945	1143 (3.66-3.50)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	451	<div> <div>43%</div> <div>34%</div> <div>14%</div> <div>• 5%</div> </div>
1	C	451	<div> <div>40%</div> <div>37%</div> <div>14%</div> <div>• 7%</div> </div>
2	B	445	<div> <div>36%</div> <div>37%</div> <div>18%</div> <div>• 6%</div> </div>
2	D	445	<div> <div>37%</div> <div>34%</div> <div>20%</div> <div>• 6%</div> </div>
3	E	142	<div> <div>49%</div> <div>27%</div> <div>11%</div> <div>13%</div> </div>

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
7	CN2	B	700	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 14074 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 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	427	Total	C	N	O	S	0	0	0
			3291	2091	555	624	21			
1	C	421	Total	C	N	O	S	0	0	0
			3220	2043	544	612	21			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	265	ILE	ALA	SEE REMARK 999	UNP P02550
C	265	ILE	ALA	SEE REMARK 999	UNP P02550

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	419	Total	C	N	O	S	0	0	0
			3236	2037	543	631	25			
2	D	419	Total	C	N	O	S	0	0	0
			3237	2037	544	631	25			

- Molecule 3 is a protein called Stathmin 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	124	Total	C	N	O	S	0	0	0
			907	549	170	183	5			

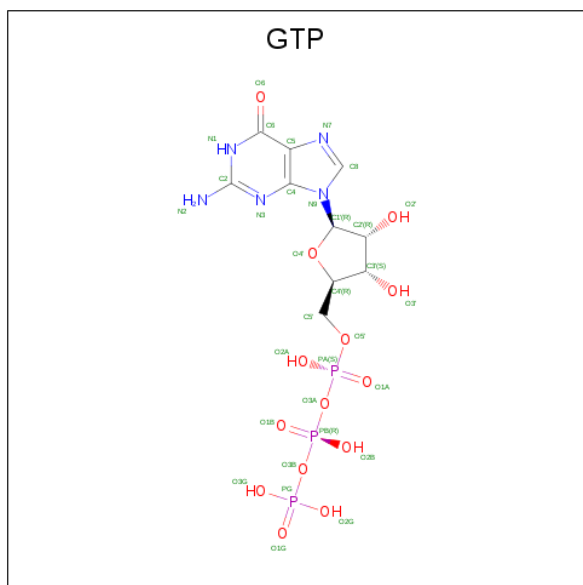
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	4	ALA	-	SEE REMARK 999	UNP P63043

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

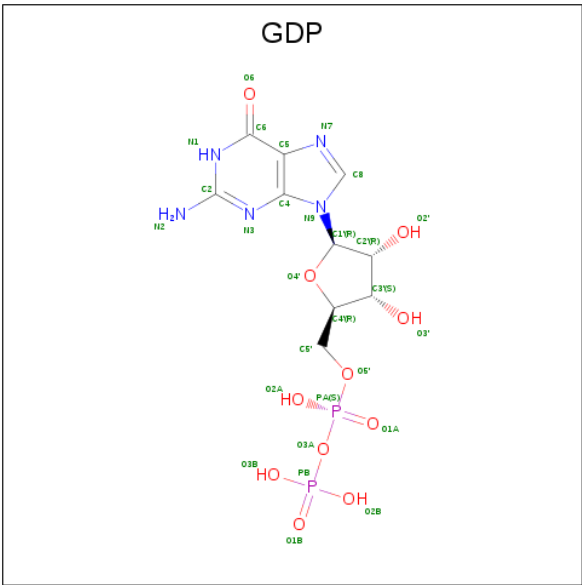
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Mg 1 1	0	0
4	A	1	Total Mg 1 1	0	0
4	C	1	Total Mg 1 1	0	0

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



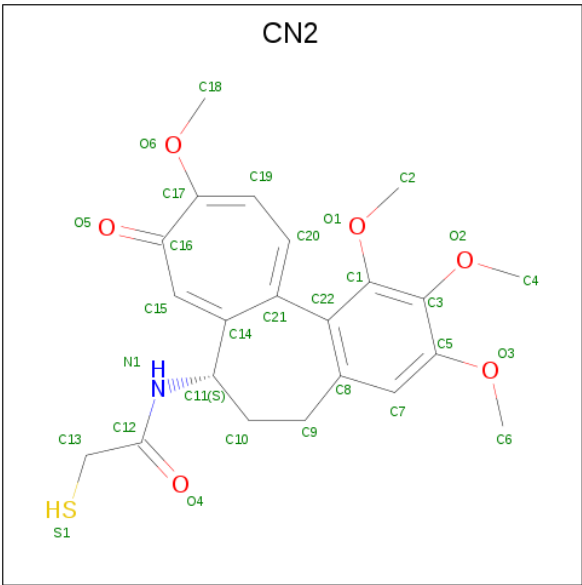
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O P 32 10 5 14 3	0	0
5	C	1	Total C N O P 32 10 5 14 3	0	0

- Molecule 6 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



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

- Molecule 7 is 2-MERCAPTO-N-[1,2,3,10-TETRAMETHOXY-9-OXO-5,6,7,9-TETRAHYDRO-BENZO[A]HEPTALEN-7-YL]ACETAMIDE (three-letter code: CN2) (formula: C₂₂H₂₅NO₆S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B	1	Total	C	N	O	S	0	0
			30	22	1	6	1		

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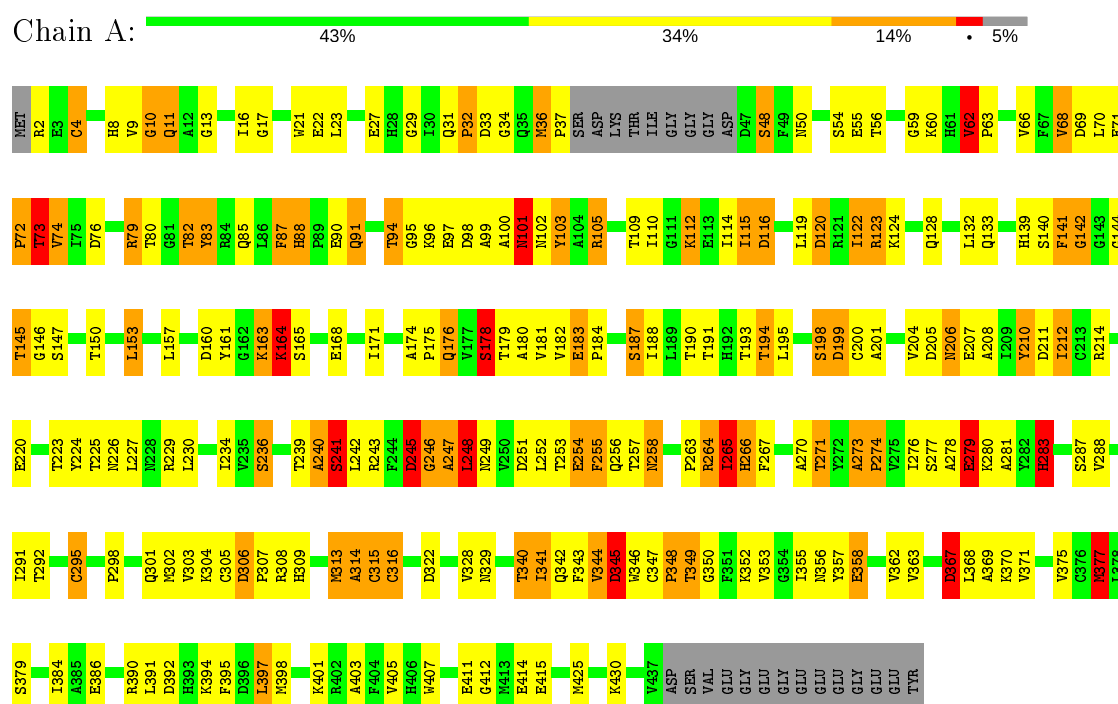
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	D	1	Total	C	N	O	S	0	0
			30	22	1	6	1		

3 Residue-property plots

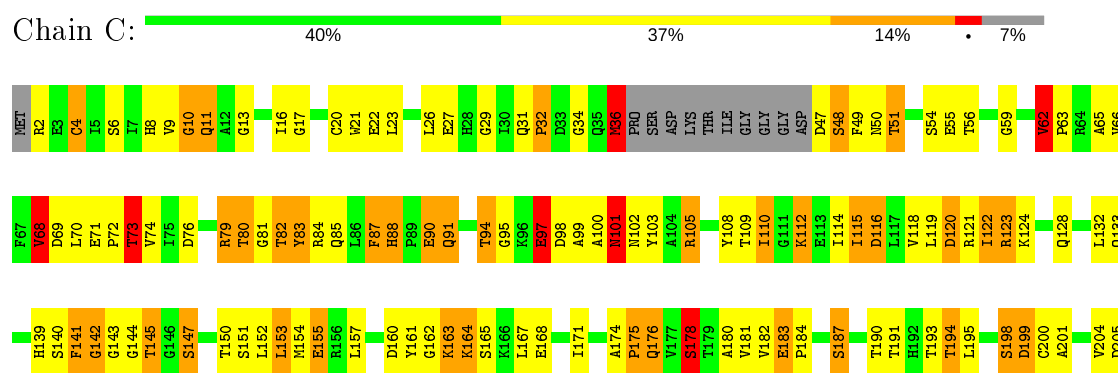
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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. 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.

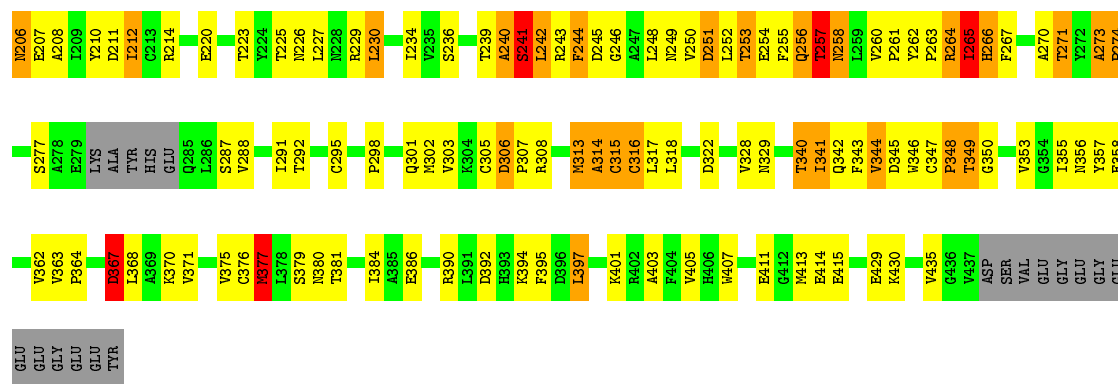
Note EDS was not executed.

• Molecule 1: Tubulin alpha chain



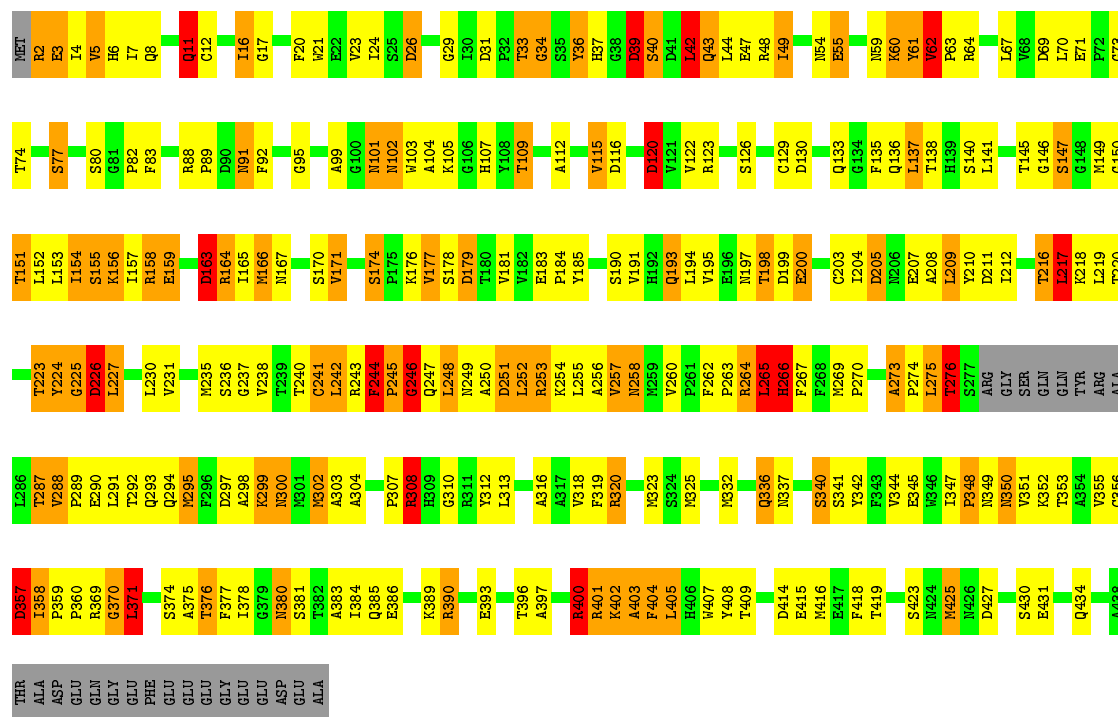
• Molecule 1: Tubulin alpha chain





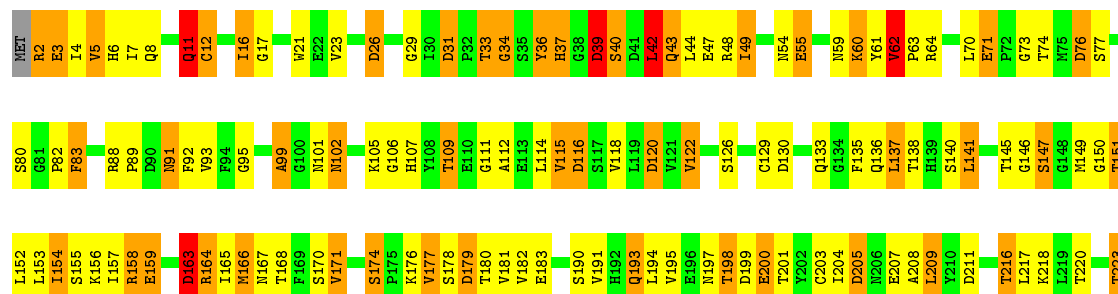
• Molecule 2: Tubulin beta chain

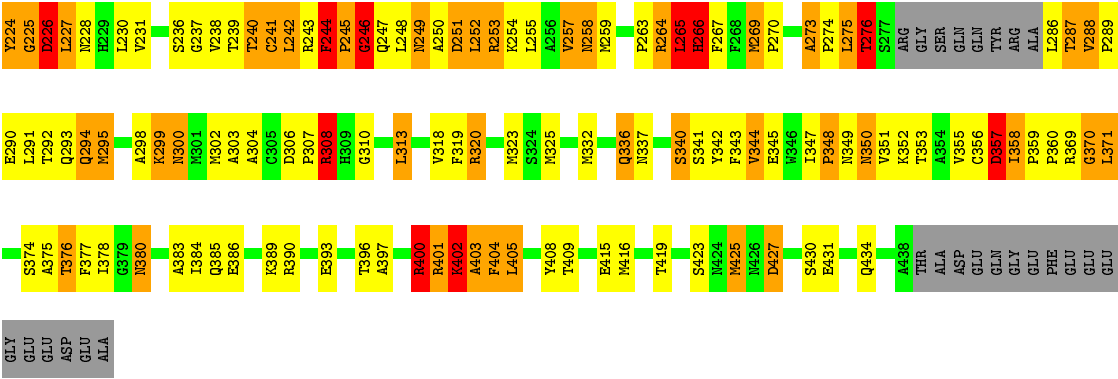
Chain B: 36% 37% 18% 6%



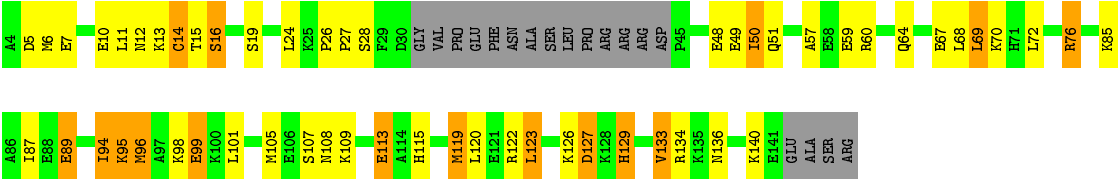
• Molecule 2: Tubulin beta chain

Chain D: 37% 34% 20% 6%





• Molecule 3: Stathmin 4



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	328.69Å 328.69Å 54.68Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.58	Depositor
% Data completeness (in resolution range)	98.8 (20.00-3.58)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.232 , 0.249	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	14074	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

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, GTP, MG, CN2

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	0.70	1/3368 (0.0%)	0.98	16/4581 (0.3%)
1	C	0.65	2/3292 (0.1%)	0.95	14/4479 (0.3%)
2	B	0.64	0/3308	1.01	20/4494 (0.4%)
2	D	0.61	0/3309	0.99	19/4494 (0.4%)
3	E	0.67	0/915	0.94	2/1230 (0.2%)
All	All	0.65	3/14192 (0.0%)	0.98	71/19278 (0.4%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	97	GLU	CD-OE1	-6.64	1.18	1.25
1	A	97	GLU	CD-OE1	-5.52	1.19	1.25
1	C	97	GLU	CD-OE2	-5.36	1.19	1.25

The worst 5 of 71 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	160	ASP	CB-CG-OD2	7.19	124.77	118.30
2	B	116	ASP	CB-CG-OD2	7.16	124.75	118.30
2	B	205	ASP	CB-CG-OD2	6.99	124.59	118.30
1	A	120	ASP	CB-CG-OD2	6.98	124.58	118.30
2	D	205	ASP	CB-CG-OD2	6.84	124.45	118.30

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	3291	0	3155	159	0
1	C	3220	0	3074	180	0
2	B	3236	0	3058	215	0
2	D	3237	0	3060	217	0
3	E	907	0	781	31	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
5	A	32	0	12	4	0
5	C	32	0	12	2	0
6	B	28	0	12	2	0
6	D	28	0	12	1	0
7	B	30	0	23	12	0
7	D	30	0	23	8	0
All	All	14074	0	13222	773	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 28.

The worst 5 of 773 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)
3:E:96:MET:SD	3:E:96:MET:CE	2.01	1.47
2:B:316:ALA:HB1	7:B:700:CN2:C2	1.55	1.36
2:B:316:ALA:CB	7:B:700:CN2:H21	1.70	1.20
1:A:99:ALA:HB2	1:A:145:THR:HG22	1.22	1.15
1:C:198:SER:CB	1:C:265:ILE:HD11	1.78	1.13

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	423/451 (94%)	327 (77%)	53 (12%)	43 (10%)	0	8
1	C	415/451 (92%)	316 (76%)	59 (14%)	40 (10%)	0	9
2	B	415/445 (93%)	310 (75%)	58 (14%)	47 (11%)	0	6
2	D	415/445 (93%)	311 (75%)	56 (14%)	48 (12%)	0	6
3	E	120/142 (84%)	91 (76%)	21 (18%)	8 (7%)	1	15
All	All	1788/1934 (92%)	1355 (76%)	247 (14%)	186 (10%)	0	7

5 of 186 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	62	VAL
1	A	73	THR
1	A	178	SER
1	A	240	ALA

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	346/378 (92%)	235 (68%)	111 (32%)	0	2
1	C	336/378 (89%)	229 (68%)	107 (32%)	0	2
2	B	348/381 (91%)	240 (69%)	108 (31%)	0	2
2	D	348/381 (91%)	241 (69%)	107 (31%)	0	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	E	78/126 (62%)	46 (59%)	32 (41%)	0	1
All	All	1456/1644 (89%)	991 (68%)	465 (32%)	0	2

5 of 465 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	401	ARG
1	C	155	GLU
2	D	419	THR
2	B	423	SER
1	C	85	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 54 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	339	ASN
1	C	101	ASN
2	D	339	ASN
2	B	350	ASN
2	B	385	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 3 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
6	GDP	D	603	-	24,30,30	1.06	1 (4%)	31,47,47	1.92	7 (22%)
7	CN2	B	700	-	28,32,32	3.11	7 (25%)	27,45,45	2.50	13 (48%)
6	GDP	B	602	4	24,30,30	1.10	3 (12%)	31,47,47	1.85	8 (25%)
5	GTP	A	600	4	26,34,34	0.97	2 (7%)	33,54,54	1.81	6 (18%)
5	GTP	C	601	4	26,34,34	1.18	3 (11%)	33,54,54	2.03	10 (30%)
7	CN2	D	701	-	28,32,32	2.94	7 (25%)	27,45,45	2.93	10 (37%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GDP	D	603	-	-	3/12/32/32	0/3/3/3
7	CN2	B	700	-	-	2/10/27/27	0/3/3/3
6	GDP	B	602	4	-	4/12/32/32	0/3/3/3
5	GTP	A	600	4	-	5/18/38/38	0/3/3/3
5	GTP	C	601	4	-	4/18/38/38	0/3/3/3
7	CN2	D	701	-	-	2/10/27/27	0/3/3/3

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	700	CN2	C19-C17	-8.89	1.23	1.39
7	D	701	CN2	C19-C17	-7.83	1.25	1.39
7	D	701	CN2	C15-C16	7.42	1.54	1.39
7	B	700	CN2	C20-C21	-7.05	1.23	1.40
7	B	700	CN2	C19-C20	-6.72	1.20	1.40

The worst 5 of 54 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	701	CN2	C10-C11-N1	-8.92	94.02	110.04
7	B	700	CN2	C20-C19-C17	6.39	145.16	129.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	603	GDP	N3-C2-N1	-5.85	119.42	127.22
5	C	601	GTP	N3-C2-N1	-5.83	119.45	127.22
6	B	602	GDP	N3-C2-N1	-5.58	119.78	127.22

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

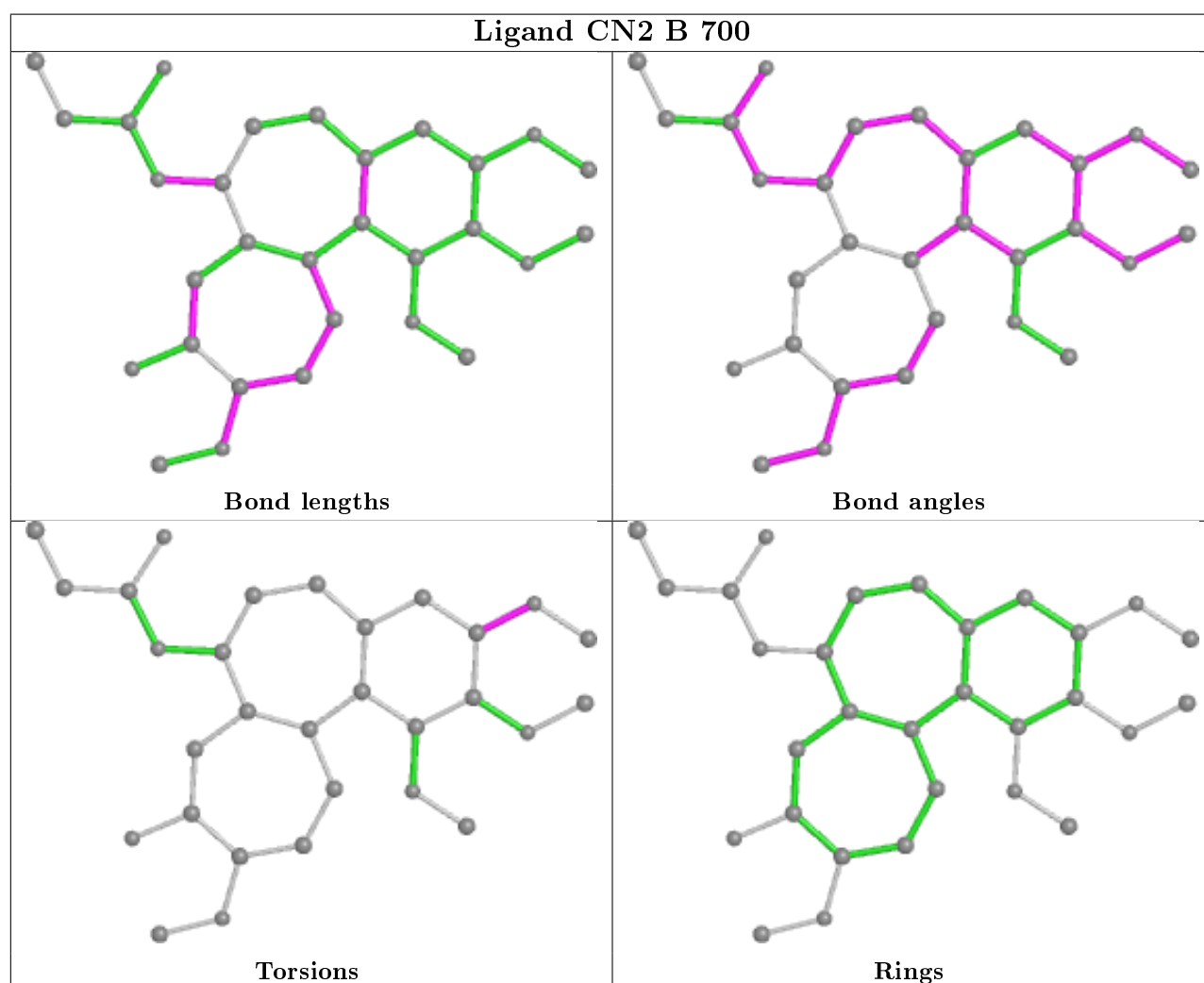
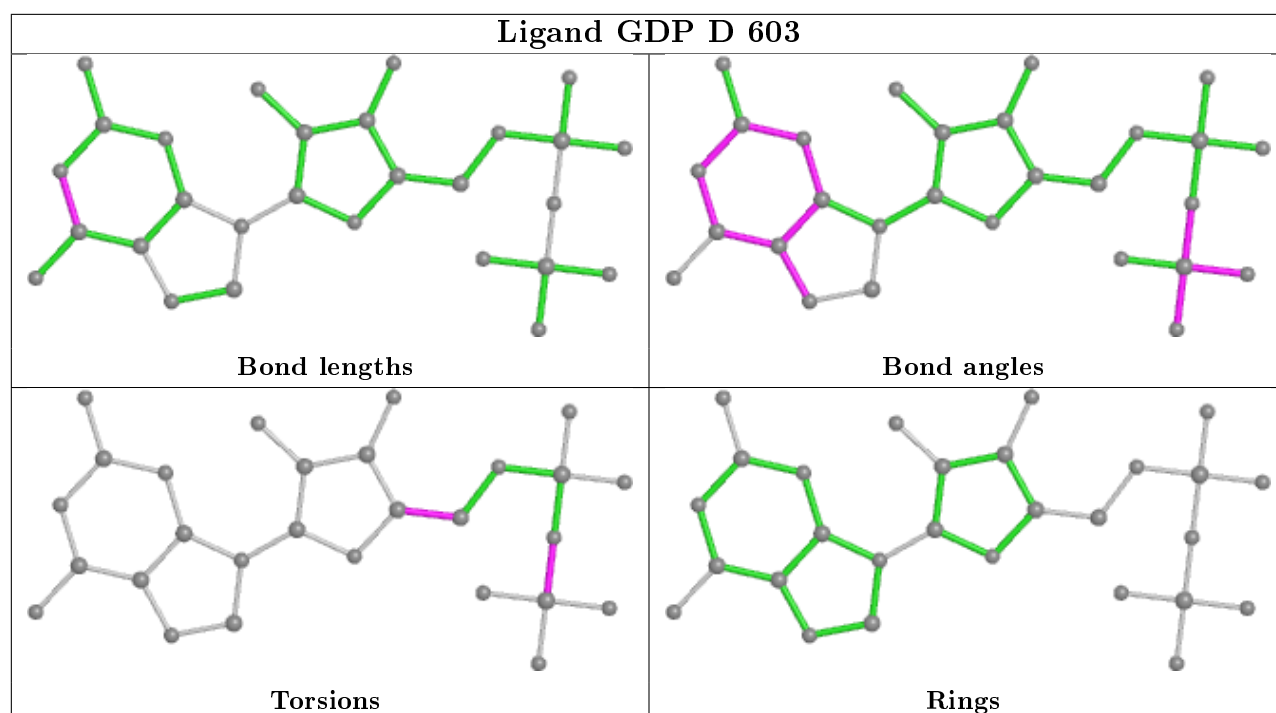
Mol	Chain	Res	Type	Atoms
6	B	602	GDP	PA-O3A-PB-O2B
6	B	602	GDP	O4'-C4'-C5'-O5'
6	B	602	GDP	C3'-C4'-C5'-O5'
5	A	600	GTP	C5'-O5'-PA-O1A
5	C	601	GTP	C5'-O5'-PA-O1A

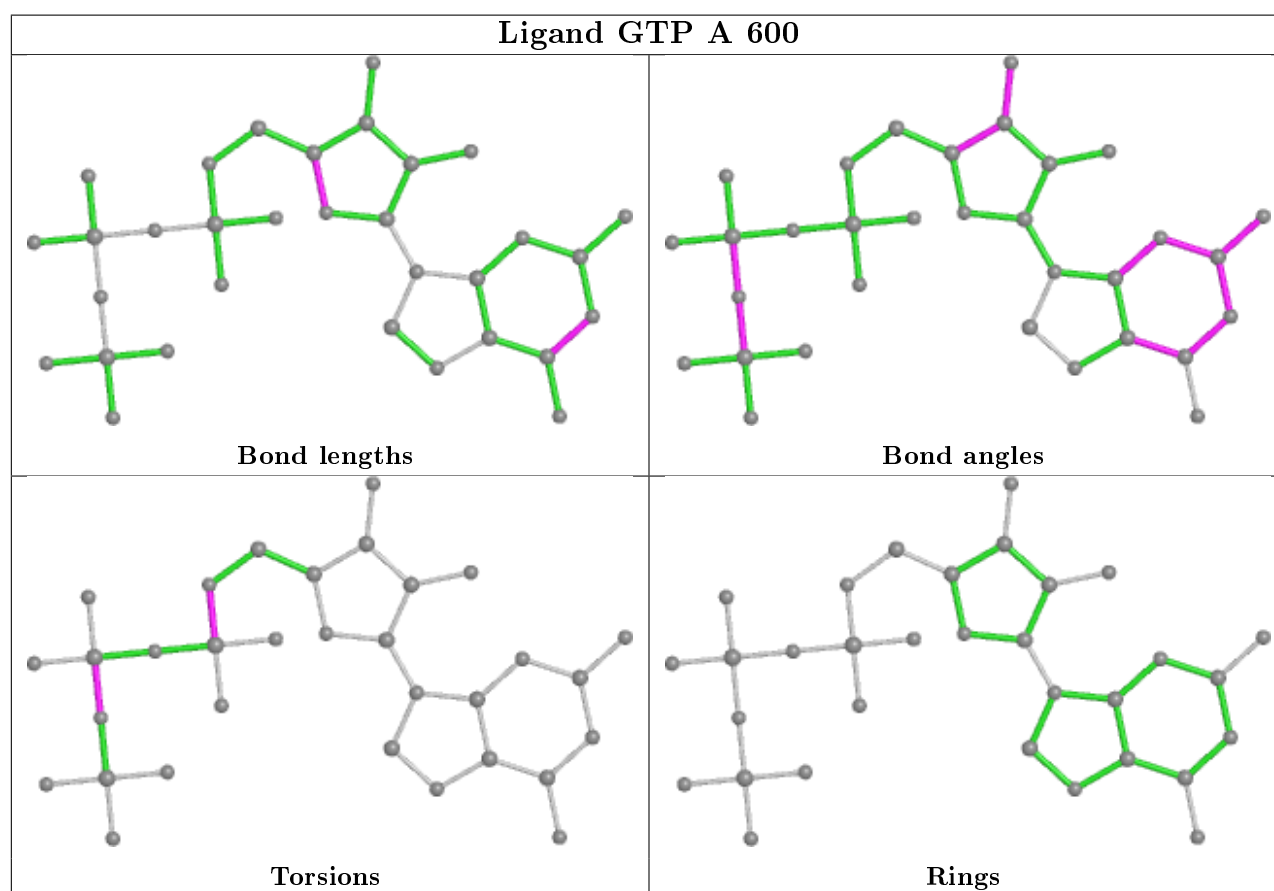
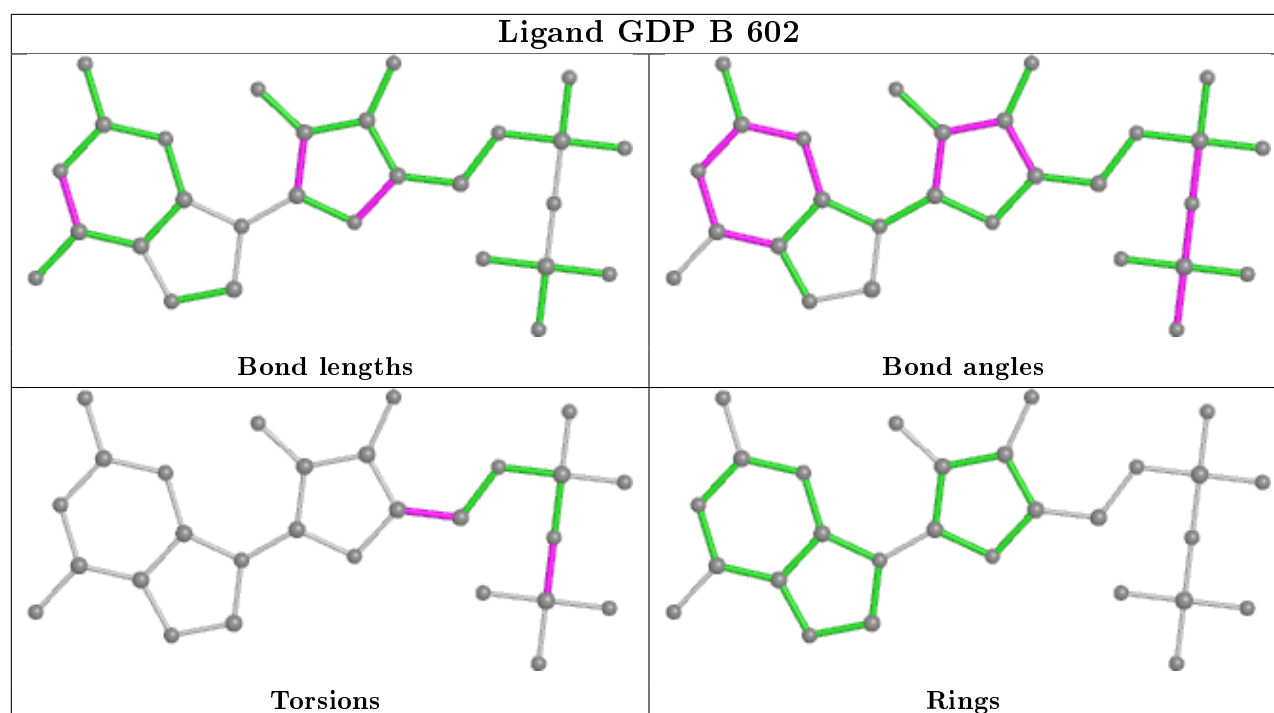
There are no ring outliers.

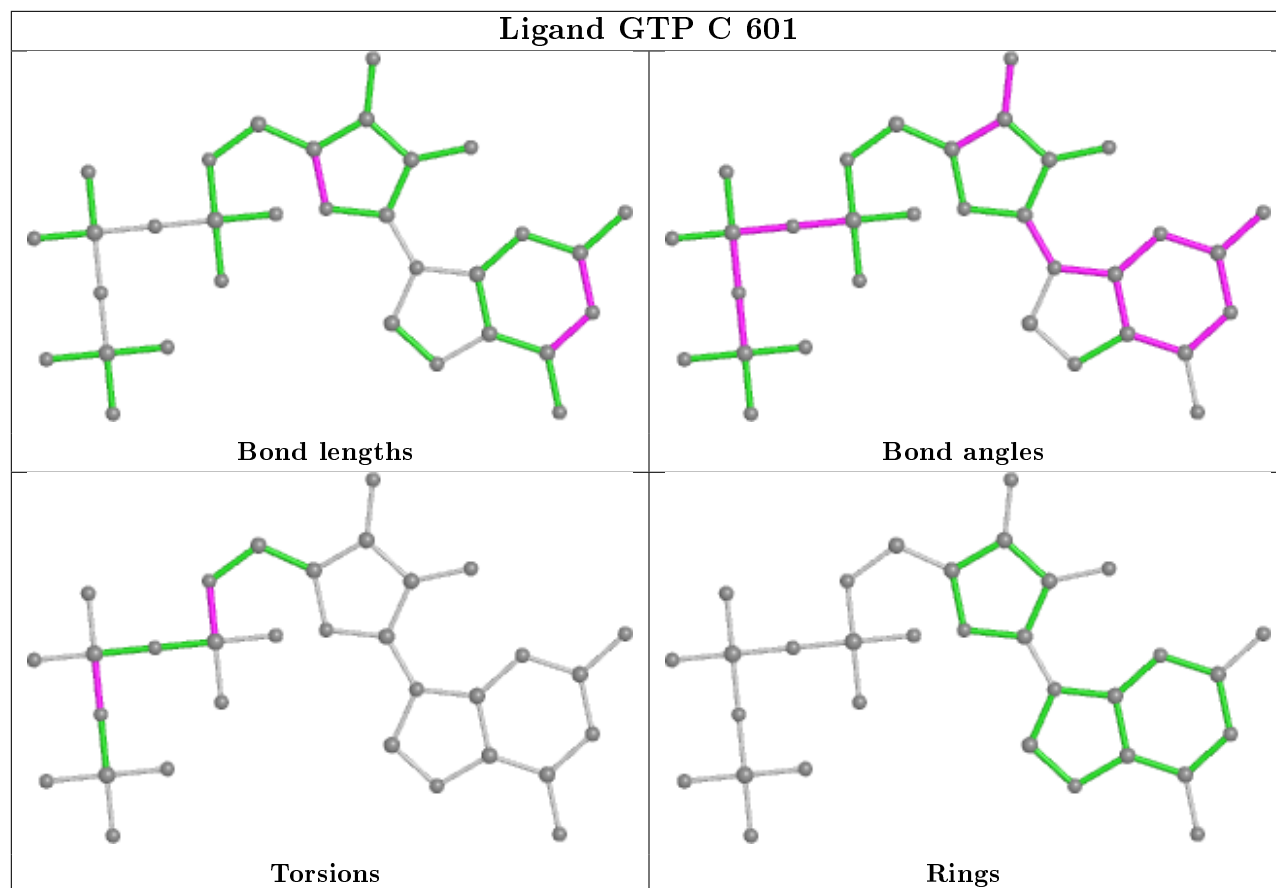
6 monomers are involved in 29 short contacts:

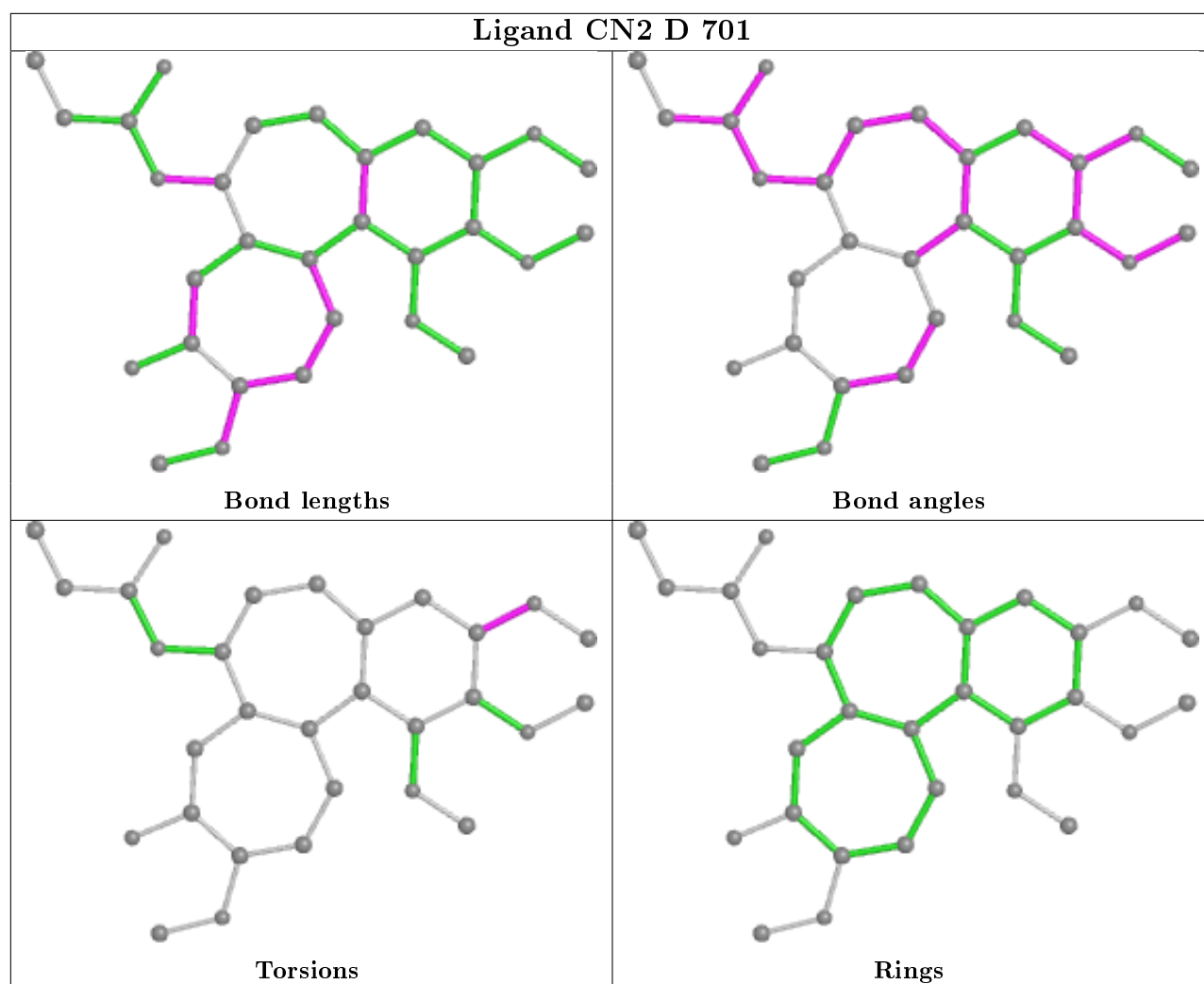
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	603	GDP	1	0
7	B	700	CN2	12	0
6	B	602	GDP	2	0
5	A	600	GTP	4	0
5	C	601	GTP	2	0
7	D	701	CN2	8	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.