W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

Feb 5, 2024 – 10:40 AM EST

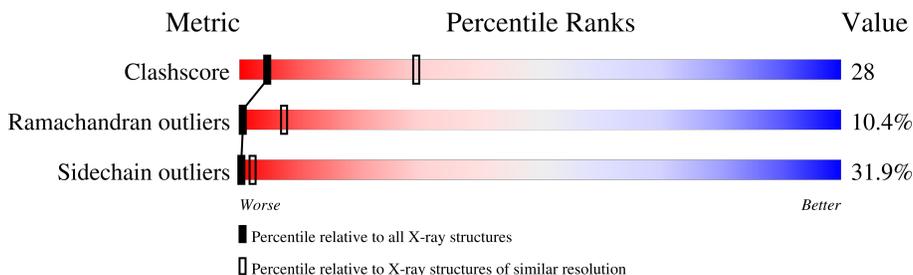|		
PDB ID	:	1SA0
Title	:	TUBULIN-COLCHICINE: STATHMIN-LIKE DOMAIN COMPLEX
Authors	:	Ravelli, R.B.; Gigant, B.; Curmi, P.A.; Jourdain, I.; Lachkar, S.; Sobel, A.; Knossow, M.
Deposited on	:	2004-02-06
Resolution	:	3.58 Å(reported)

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	Percentile Ranks	Value
Clashscore		28
Ramachandran outliers		10.4%
Sidechain outliers		31.9%

Worse .... *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

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 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%

Note EDS was not executed.

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

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 3291	C 2091	N 555	O 624	S 21	0	0	0
1	C	421	Total 3220	C 2043	N 544	O 612	S 21	0	0	0

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 3236	C 2037	N 543	O 631	S 25	0	0	0
2	D	419	Total 3237	C 2037	N 544	O 631	S 25	0	0	0

- Molecule 3 is a protein called Stathmin 4.

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

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	A	1	Total 1	Mg 1	0	0
4	B	1	Total 1	Mg 1	0	0
4	C	1	Total 1	Mg 1	0	0

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).
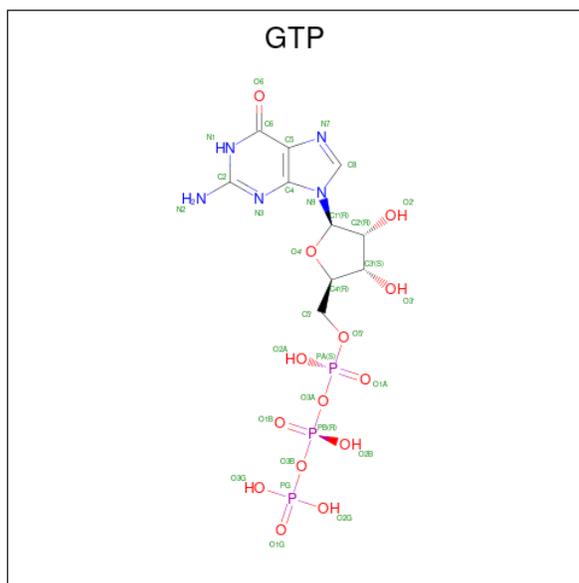
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 32	C 10	N 5	O 14	P 3	0	0
5	C	1	Total 32	C 10	N 5	O 14	P 3	0	0

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

GDP

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-TETRA HYDRO-BENZO[A]HEPTALEN-7-YL]ACETAMIDE (three-letter code: CN2) (formula: $C_{22}H_{25}NO_6S$).

CN2

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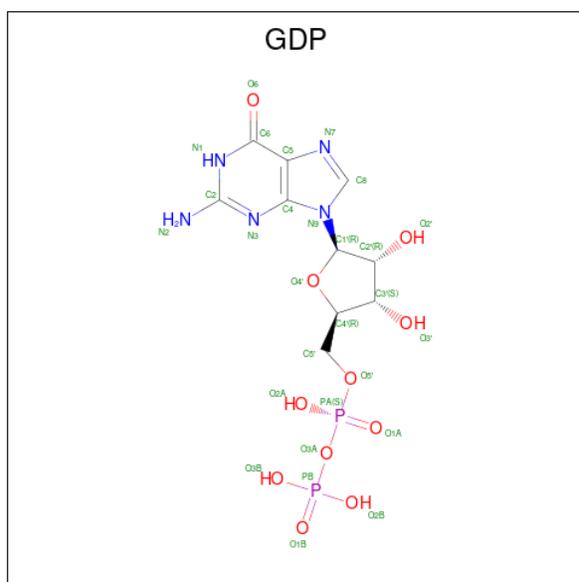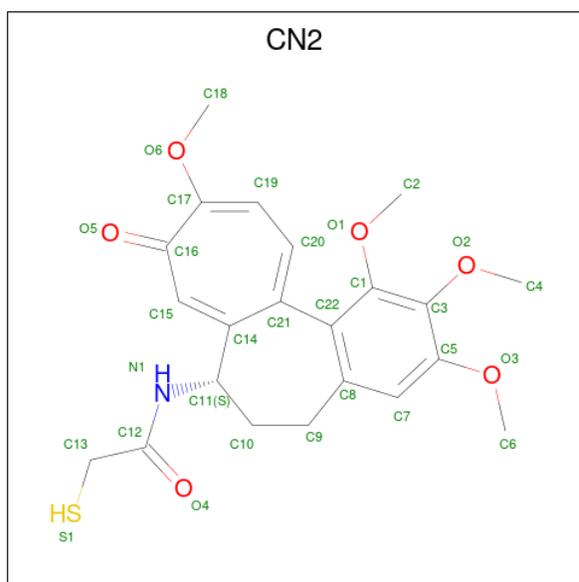
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
7	D	1	30	22	1	6	1	0	0

3 Residue-property plots ⓘ

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. 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

Chain A:

• Molecule 1: Tubulin alpha chain

Chain C:

N206 E207 A208 I209 Y210 D211 I212 C213 R214 E220 T223 Y224 T225 N226 L227 R229 L230 I234 V235 S236 T239 A240 S241 L242 R243 F244 D245 G246 A247 L248 N249 V250 D251 L252 T253 E254 F255 Q256 T257 N258 L259 V260 P261 Y262 P263 R264 I265 H266 F267 A270 T271 Y272 A273 P274

S277 A278 E279 LYS ALA TYR HIS GLU Q285 L286 S287 V288 I291 T292 C295 P298 Q301 M302 V303 K304 C305 D306 P307 R308 M313 A314 C315 C316 L317 L318 D322 V328 N329 T340 I341 Q342 F343 V344 D345 W346 C347 P348 T349 G350 V353 G354 I355 N356 Y357 E358

V362 V363 P364 D367 L368 A369 K370 V371 V375 C376 M377 L378 S379 N380 T381 I384 A385 E386 R390 L391 D392 H393 K394 F395 D396 L397 K401 R402 A403 F404 V405 H406 W407 E411 G412 M413 E414 E415 E429 K430 V435 G436 V437 ASP SER VAL GLU GLY GLU GLY GLU

GLU GLU GLY GLU TYR

• Molecule 2: Tubulin beta chain

Chain B:
36% 37% 18% • 6%

MET R2 E3 I4 V5 H6 I7 Q8 Q11 C12 I16 G17 F20 W21 E22 V23 I24 S25 D26 G29 I30 D31 P32 T33 G34 S35 Y36 H37 G38 D39 S40 D41 L42 Q43 L44 E47 R48 I49 N54 E55 N59 K60 Y61 V62 P63 R64 L67 V68 D69 L70 E71 P72 G73

T74 S77 S80 G81 P82 F83 R88 P89 D90 N91 F92 G95 A99 G100 N101 N102 W103 A104 K105 G106 H107 Y108 T109 A112 V115 D116 D120 V121 V122 R123 S126 C129 D130 Q133 G134 F135 Q136 L137 T138 H139 S140 L141 T145 G146 S147 G148 M149 G150
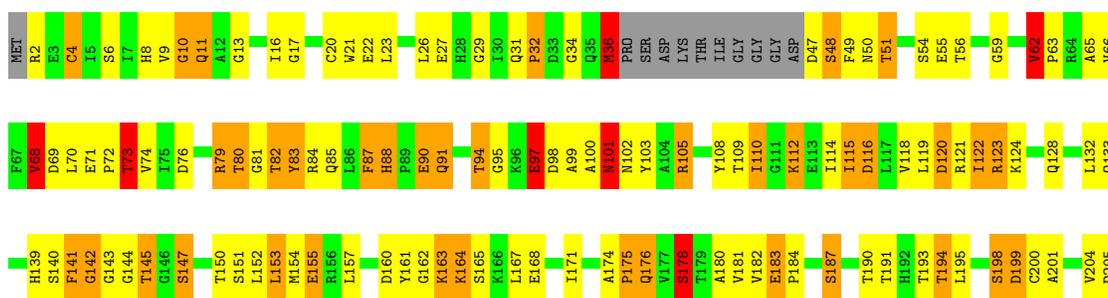
T151 L152 L153 I154 S155 K156 I157 R158 E159 D163 R164 I165 M166 N167 S170 V171 S174 P175 K176 V177 S178 D179 T180 V181 V182 E183 P184 Y185 S190 V191 H192 Q193 L194 V195 E196 N197 T198 D199 E200 C203 I204 D205 N206 E207 A208 L209 Y210 D211 I212 T216 L217 K218 L219 T220

T223 Y224 G225 D226 L227 L230 V231 M235 S236 G237 V238 T239 T240 C241 L242 R243 F244 P245 G296 Q247 L248 N249 A250 D251 L252 R253 K254 L255 A256 V257 N258 M259 V260 P261 F262 P263 R264 L265 H266 F267 F268 M269 P270 A273 P274 L275 T276 S277 ARG GLY SER GLN GLN TYR ARG ALA

L286 T287 V288 P289 E290 L291 T292 Q293 Q294 M295 F296 D297 A298 K299 N300 M301 M302 A303 A304 P307 H308 H309 G310 R311 Y312 L313 A316 A317 V318 F319 R320 M323 S324 M325 M332 Q336 N337 S340 S341 Y342 F343 V344 E345 W346 I347 P348 N349 N350 V351 K352 T353 A354 V355 C356

D357 I358 P359 P360 R369 G370 L371 S374 A375 T376 F377 I378 G379 N380 S381 T382 A383 I384 Q385 E386 K389 R390 E393 T396 A397 R400 R401 K402 A403 F404 L405 H406 W407 Y408 T409 D414 E415 M416 E417 F418 T419 S423 N424 M425 N426 D427 S430 E431 Q434 A438

THR ALA ASP GLU GLN GLY GLU PHE GLU GLU GLU GLY GLU GLU ASP GLU ALA

• Molecule 2: Tubulin beta chain

Chain D:
37% 34% 20% • 6%

MET R2 E3 I4 V5 H6 I7 Q8 Q11 C12 I16 G17 W21 E22 V23 D26 G29 I30 D31 P32 T33 G34 S35 Y36 H37 G38 D39 S40 D41 L42 Q43 L44 E47 R48 I49 N54 E55 N59 K60 Y61 V62 P63 R64 L70 E71 P72 G73 T74 M75 D76 S77

S80 G81 P82 F83 R88 P89 D90 N91 F92 V93 F94 G95 A99 G100 N101 N102 K105 G106 H107 Y108 T109 E110 G111 A112 E113 L114 V115 D116 S117 V118 L119 D120 V121 V122 S126 C129 D130 Q133 G134 F135 Q136 L137 T138 H139 S140 L141 T145 G146 S147 G148 M149 G150 T151

L152 L153 I154 S155 K156 I157 R158 E159 D163 R164 I165 M166 N167 T168 F169 S170 V171 S174 P175 K176 V177 S178 D179 T180 V181 V182 E183 S190 V191 H192 Q193 L194 V195 E196 N197 T198 D199 E200 T201 Y202 C203 I204 D205 N206 E207 A208 L209 Y210 D211 T216 L217 K218 L219 T220 T223

Y224 G225 D226 L227 N228 H229 L230 V231 S236 G237 V238 T239 T240 C241 L242 R243 F244 P245 G246 Q247 L248 N249 A250 D251 L252 R253 K254 L255 A256 V257 N258 M259 P263 R264 L265 H266 F267 F268 M269 P270 A273 P274 L275 T276 S277 ARG GLY SER GLN GLN TYR ARG ALA L286 T287 V288 P289

E290 L291 T292 Q293 Q294 M295 A298 K299 N300 M301 M302 A303 A304 C305 D306 P307 R308 H309 G310 L313 V318 F319 R320 M323 S324 M325 M332 Q336 N337 S340 S341 Y342 F343 V344 E345 W346 I347 P348 N349 N350 V351 K352 T353 A354 V355 C356 D357 I358 P359 P360 R369 G370 L371

S374 A375 T376 F377 I378 G379 N380 A383 I384 Q385 E386 K389 R390 E393 T396 A397 R400 R401 K402 A403 F404 L405 Y408 T409 E415 M416 T419 S423 N424 M425 N426 D427 S430 E431 Q434 A438 THR ALA ASP GLU GLN GLY GLU PHE GLU GLU GLU

GLY GLU GLU ASP GLU ALA

● Molecule 3: Stathmin 4

Chain E:

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                              49%                    27%         11%      13%
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A4 D5 M6 E7 E10 L11 N12 K13 C14 T15 S16 S19 L24 K25 P26 P27 S28 F29 D30 GLY VAL PRO GLU PHE ASN ALA SER LEU PRO ARG ARG ASP P45 E48 E49 I50 Q51 A57 E58 E59 R60 Q64 E67 L68 L69 K70 H71 L72 R76 K85

A86 I87 E88 E89 I94 K95 M96 A97 K98 E99 K100 L101 M105 E106 S107 N108 K109 E113 A114 H115 M119 L120 E121 R122 L123 K126 D127 K128 H129 V133 R134 K135 N136 K140 E141 GLU ALA SER ARG

4 Data and refinement statistics (i)

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

wwPDB X-ray Structure Validation Summary Report

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, MG, CN2, GTP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	A	0.70	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(^{o})	Ideal(^{o})
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:CE	3:E:96:MET:SD	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
1	C	73	THR
3	E	64	GLN
1	C	250	VAL
3	E	16	SER
2	D	286	LEU

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

Mol	Chain	Res	Type
1	C	88	HIS
1	C	206	ASN
2	D	339	ASN
1	C	91	GLN
1	C	133	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	B	602	4	24,30,30	1.28	3 (12%)	30,47,47	1.63	8 (26%)
5	GTP	A	600	4	26,34,34	1.15	2 (7%)	32,54,54	1.79	7 (21%)
5	GTP	C	601	4	26,34,34	1.22	2 (7%)	32,54,54	1.71	9 (28%)
7	CN2	B	700	-	27,32,32	3.60	7 (25%)	26,45,45	5.03	12 (46%)
7	CN2	D	701	-	27,32,32	3.27	7 (25%)	26,45,45	4.97	11 (42%)
6	GDP	D	603	-	24,30,30	1.22	2 (8%)	30,47,47	1.57	7 (23%)

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	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	B	700	-	-	2/10/27/27	0/3/3/3
7	CN2	D	701	-	-	2/10/27/27	0/3/3/3
6	GDP	D	603	-	-	3/12/32/32	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	C20-C19	-10.65	1.20	1.38
7	B	700	CN2	C19-C17	-8.89	1.23	1.39
7	D	701	CN2	C20-C19	-8.51	1.24	1.38
7	D	701	CN2	C19-C17	-7.83	1.25	1.39
7	B	700	CN2	C20-C21	-7.58	1.23	1.39

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	700	CN2	C19-C20-C21	22.70	148.34	129.68
7	D	701	CN2	C19-C20-C21	20.44	146.47	129.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
7	D	701	CN2	C20-C19-C17	5.34	142.63	129.69

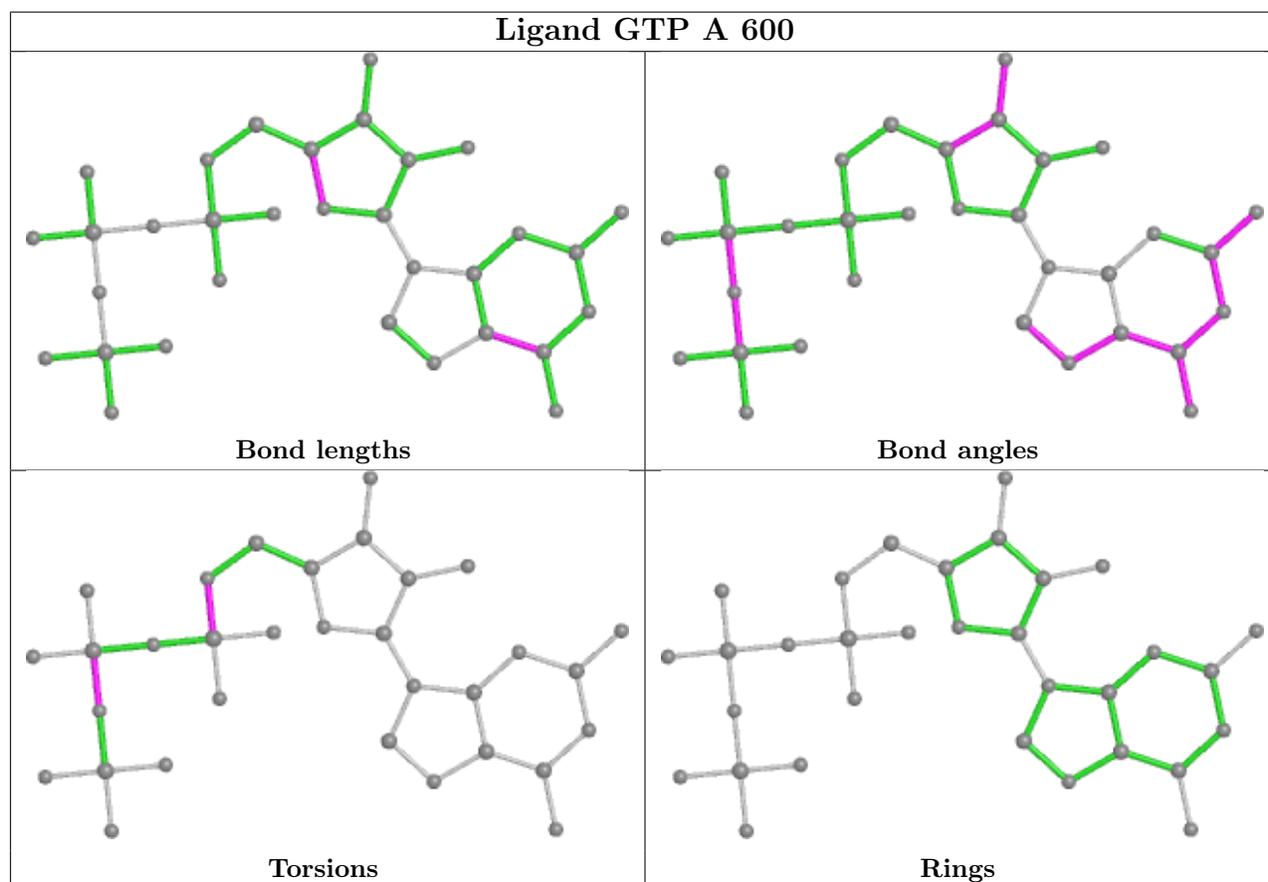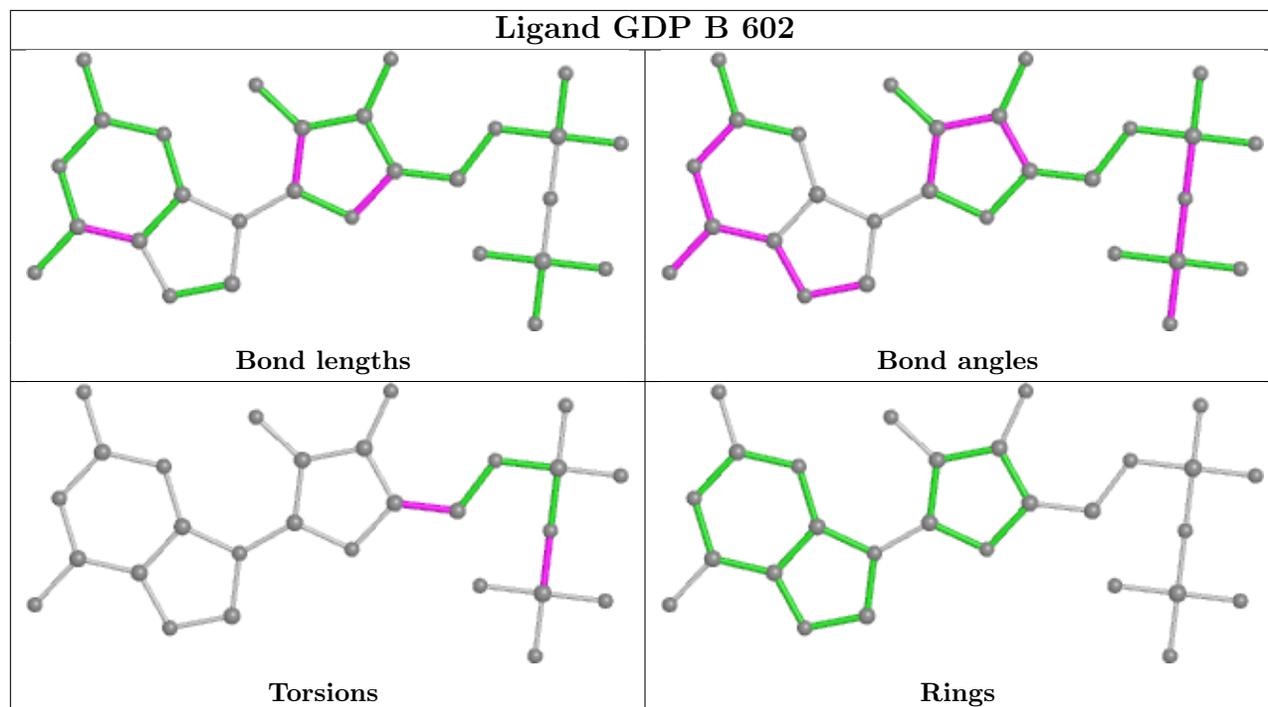There are no chirality outliers.

5 of 20 torsion outliers are listed below:

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

There are no ring outliers.

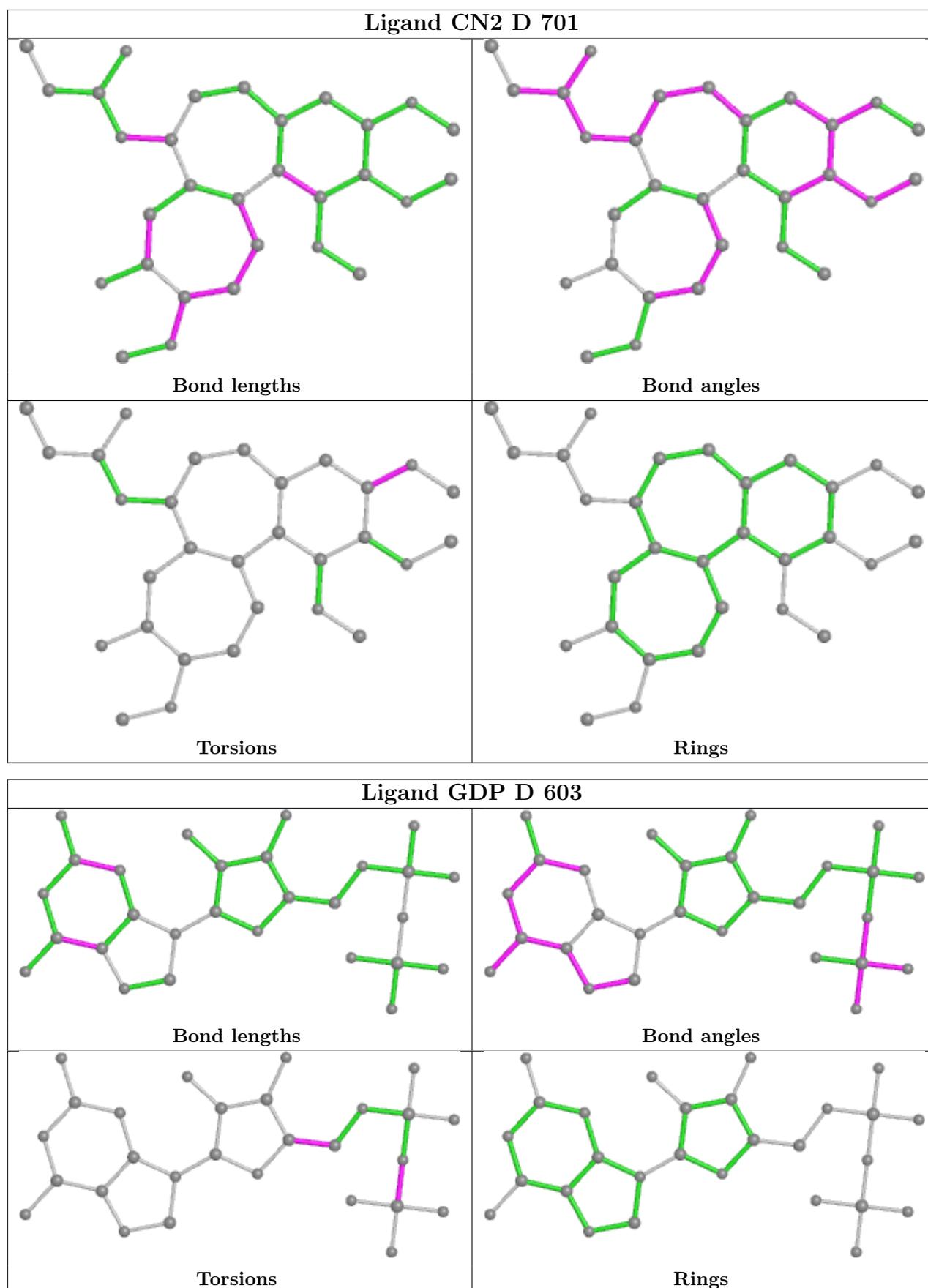6 monomers are involved in 29 short contacts:

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

Bond lengths

Bond angles

Torsions

Rings

Ligand GTP A 600

Bond lengths

Bond angles

Torsions

Rings

Ligand GTP C 601

Bond lengths

Bond angles

Torsions

Rings

Ligand CN2 B 700

Bond lengths

Bond angles

Torsions

Rings

Ligand CN2 D 701

Bond lengths

Bond angles

Torsions

Rings

Ligand GDP D 603

Bond lengths

Bond angles

Torsions

Rings
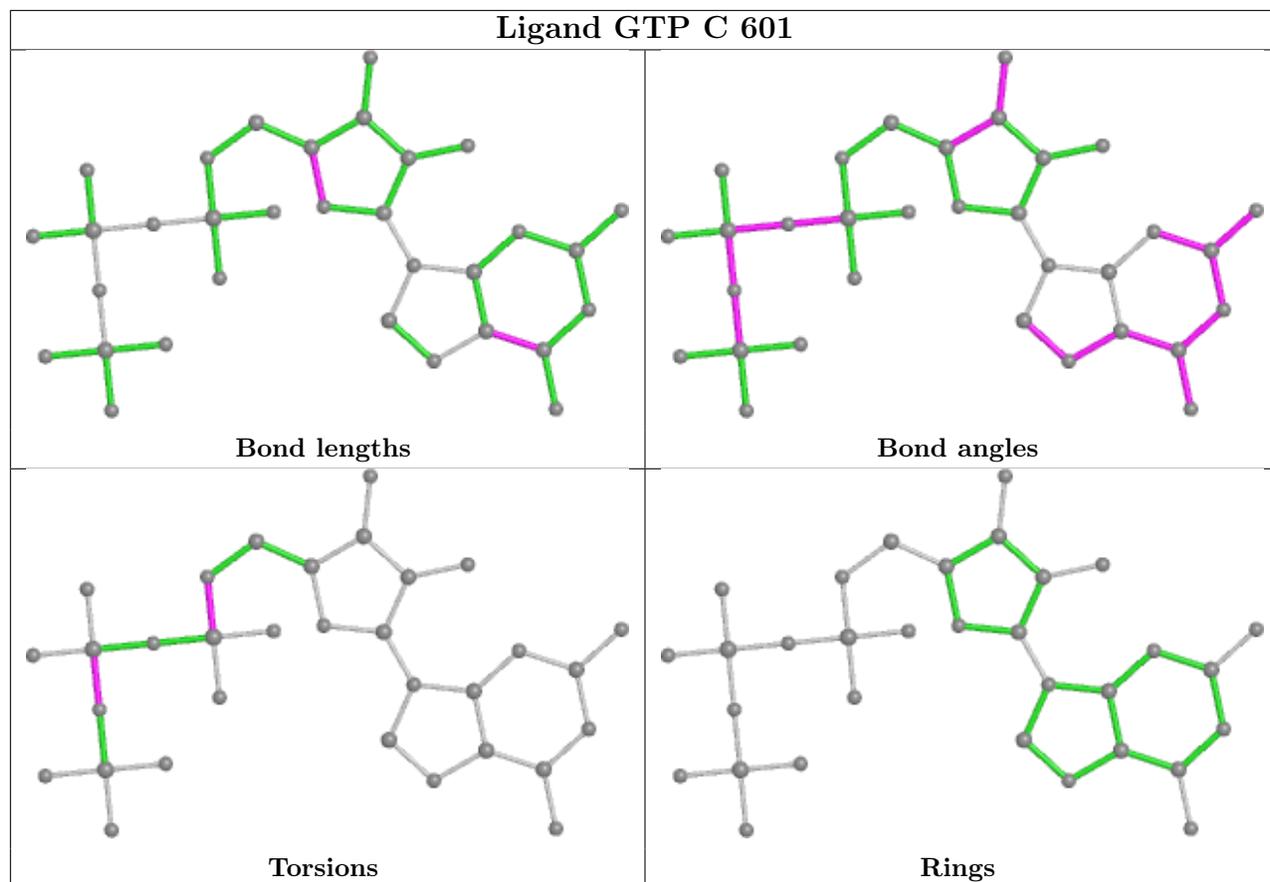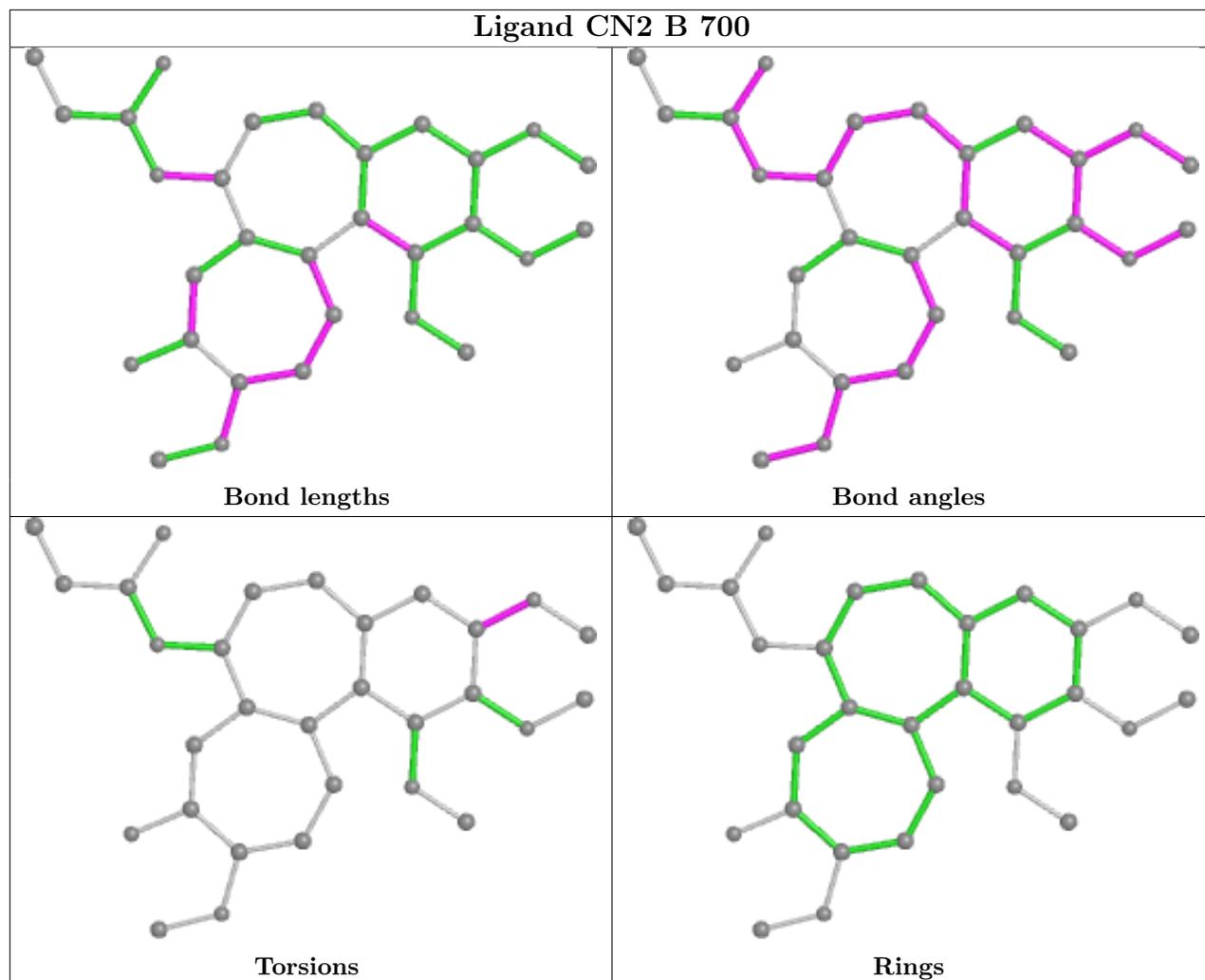
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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.