



# wwPDB X-ray Structure Validation Summary Report

Aug 14, 2023 – 11:02 PM EDT

PDB ID : 1SA1  
Title : Tubulin-podophyllotoxin: stathmin-like domain complex  
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Deposited on : 2004-02-06  
Resolution : 4.20 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](mailto: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>.

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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)  
Xtrriage (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) : 2.35

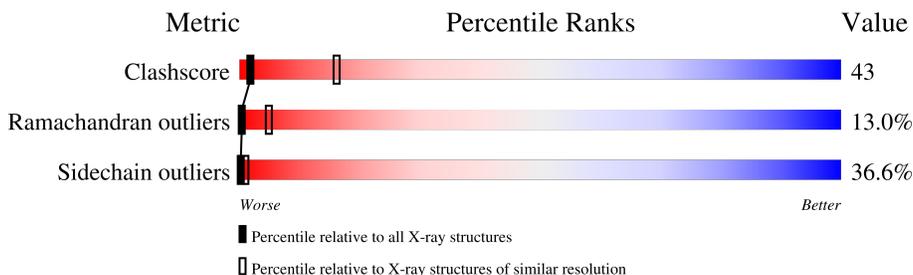
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.20 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	1044 (4.60-3.80)
Ramachandran outliers	138981	1000 (4.60-3.80)
Sidechain outliers	138945	1007 (4.62-3.78)

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  $\geq 3$ , 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	27% 42% 23% . .
1	C	451	31% 39% 23% . 5%
2	B	445	24% 44% 21% 6% 5%
2	D	445	26% 44% 20% 6% .
3	E	142	44% 34% 16% 6%

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	POD	B	700	X	-	-	-
7	POD	D	701	X	-	-	-

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 14180 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
			Total	C	N	O	S			
1	A	433	3299	2089	559	631	20	0	0	0
1	C	430	3275	2072	555	628	20	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
			Total	C	N	O	S			
2	B	422	3241	2040	545	631	25	0	0	0
2	D	426	3278	2059	556	638	25	0	0	0

- Molecule 3 is a protein called Stathmin 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	E	134	905	555	169	176	5	0	0	0

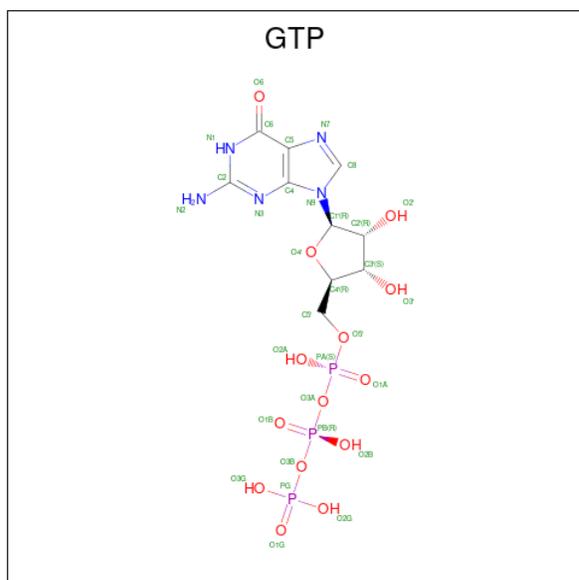
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	4	ALA	-	SEE REMARK 999	UNP P02554

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

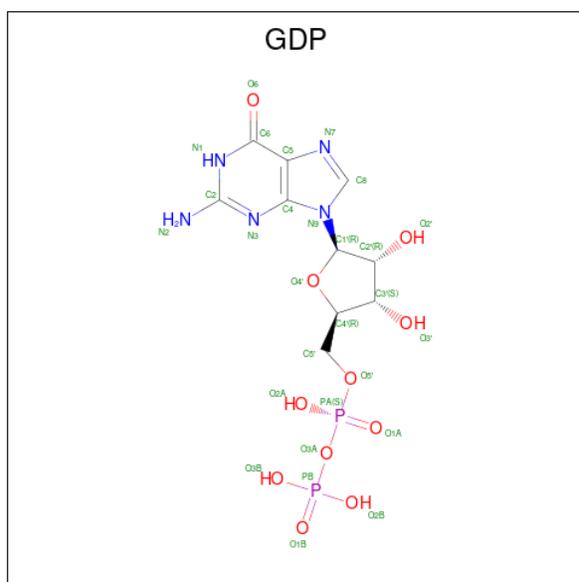
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mg 1 1	0	0
4	C	1	Total Mg 1 1	0	0

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



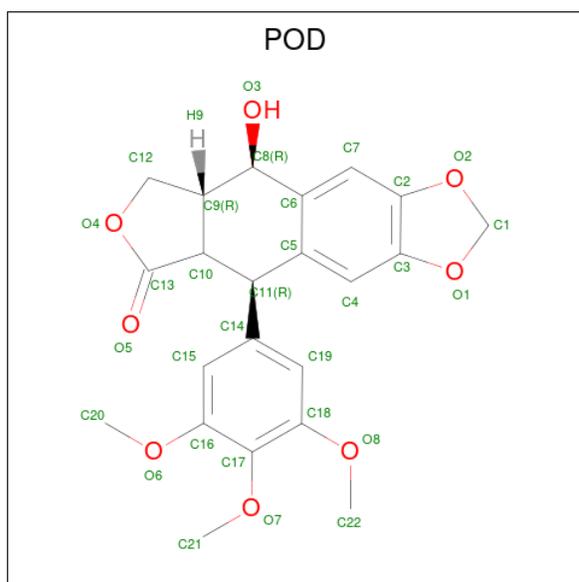
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O P 32 10 5 14 3	0	0
5	C	1	Total C N O P 32 10 5 14 3	0	0

- 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	
			Total	C	N	O			P
6	B	1	28	10	5	11	2	0	0
6	D	1	28	10	5	11	2	0	0

- Molecule 7 is 9-HYDROXY-5-(3,4,5-TRIMETHOXYPHENYL)-5,8,8A,9-TETRAHYDR OFURO[3',4':6,7]NAPHTHO[2,3-D][1,3]DIOXOL-6(5AH)-ONE (three-letter code: POD) (formula: C<sub>22</sub>H<sub>22</sub>O<sub>8</sub>).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	C O		
7	B	1	30	22 8	0	0

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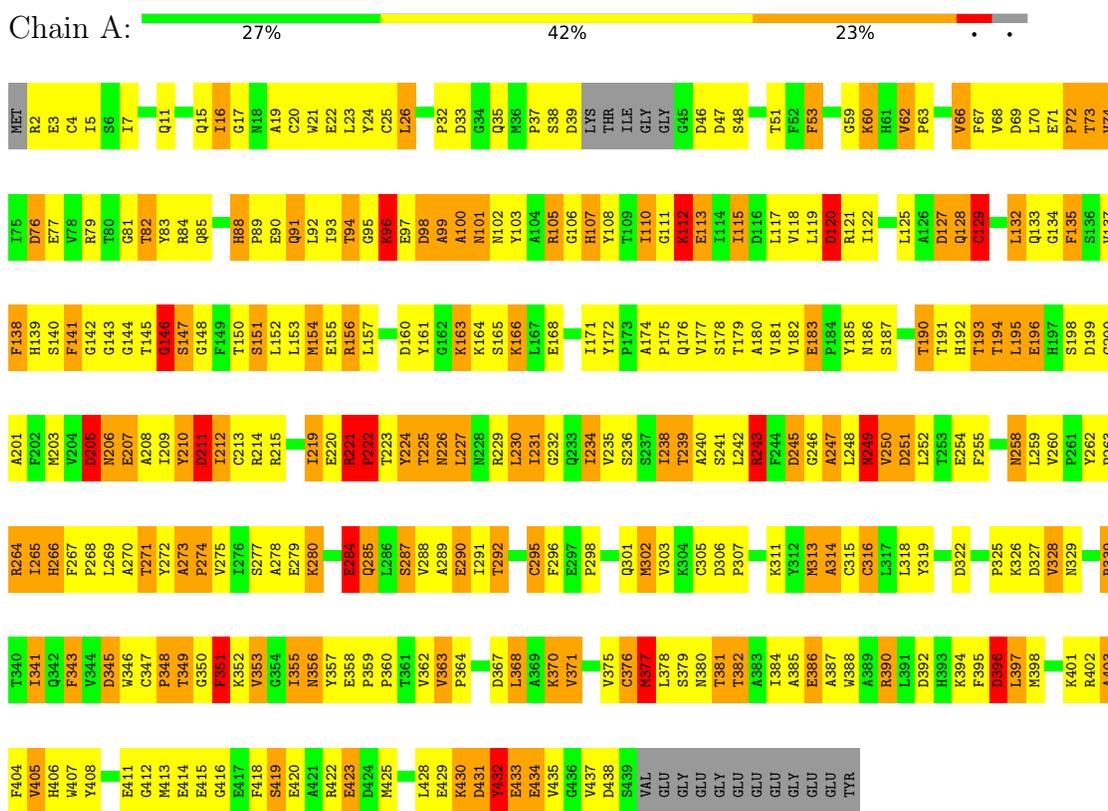
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
7	D	1	30	22	8	0	0

### 3 Residue-property plots

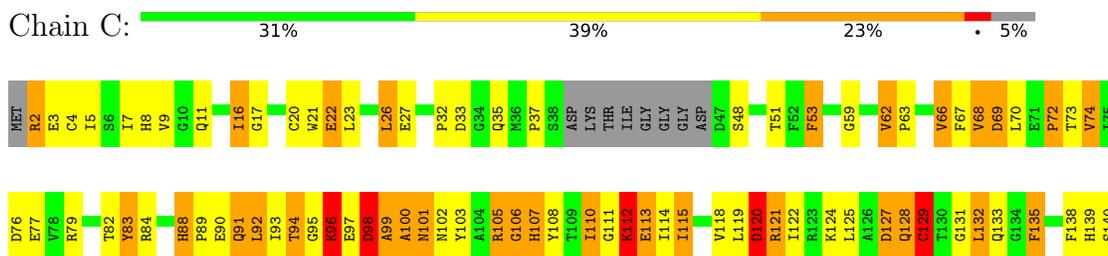
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



- Molecule 1: Tubulin alpha chain







## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	328.06Å 328.06Å 54.30Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 4.20	Depositor
% Data completeness (in resolution range)	98.3 (20.00-4.20)	Depositor
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.204 , 0.259	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	14180	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	116.0	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: GTP, MG, POD, GDP

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	0.89	1/3374 (0.0%)	1.09	19/4593 (0.4%)
1	C	0.74	0/3349	1.00	11/4561 (0.2%)
2	B	0.86	3/3314 (0.1%)	1.08	25/4506 (0.6%)
2	D	0.76	2/3352 (0.1%)	1.04	20/4556 (0.4%)
3	E	0.87	0/914	0.95	2/1238 (0.2%)
All	All	0.82	6/14303 (0.0%)	1.05	77/19454 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	C	0	3
2	B	0	3
2	D	0	2
3	E	0	3
All	All	0	15

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	44	LEU	C-N	11.14	1.59	1.34
2	B	44	LEU	C-N	9.19	1.55	1.34
2	B	360	PRO	C-N	8.02	1.52	1.34
2	D	360	PRO	C-N	6.55	1.49	1.34
2	B	2	ARG	NE-CZ	5.14	1.39	1.33

The worst 5 of 77 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	427	ASP	CB-CG-OD2	8.82	126.24	118.30
2	D	205	ASP	CB-CG-OD2	8.78	126.20	118.30
2	D	163	ASP	CB-CG-OD2	8.20	125.68	118.30
2	B	205	ASP	CB-CG-OD2	7.81	125.33	118.30
1	C	211	ASP	CB-CG-OD2	7.70	125.22	118.30

There are no chirality outliers.

5 of 15 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	146	GLY	Peptide
1	A	220	GLU	Peptide
1	A	221	ARG	Peptide
1	A	339	ARG	Peptide
2	B	49	ILE	Peptide

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3299	0	3129	275	0
1	C	3275	0	3104	271	0
2	B	3241	0	3033	321	0
2	D	3278	0	3074	297	0
3	E	905	0	730	59	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
5	A	32	0	12	3	0
5	C	32	0	12	2	0
6	B	28	0	12	1	0
6	D	28	0	12	2	0
7	B	30	0	19	5	0
7	D	30	0	19	4	0
All	All	14180	0	13156	1177	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 43.

The worst 5 of 1177 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:33:PRO:HB3	3:E:35:PHE:CZ	1.64	1.33
1:C:240:ALA:HB2	1:C:243:ARG:NH1	1.39	1.33
2:D:273:ALA:CB	2:D:274:PRO:HD3	1.74	1.18
2:B:191:VAL:HG11	2:B:425:MET:HE3	1.22	1.15
2:D:191:VAL:HG11	2:D:425:MET:HE3	1.22	1.14

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	429/451 (95%)	288 (67%)	88 (20%)	53 (12%)	0	5
1	C	426/451 (94%)	289 (68%)	90 (21%)	47 (11%)	0	8
2	B	418/445 (94%)	274 (66%)	87 (21%)	57 (14%)	0	4
2	D	424/445 (95%)	276 (65%)	87 (20%)	61 (14%)	0	4
3	E	130/142 (92%)	81 (62%)	29 (22%)	20 (15%)	0	3
All	All	1827/1934 (94%)	1208 (66%)	381 (21%)	238 (13%)	0	5

5 of 238 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	33	ASP
1	A	47	ASP
1	A	62	VAL
1	A	73	THR
1	A	96	LYS

### 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	342/378 (90%)	217 (64%)	125 (36%)	0	1
1	C	340/378 (90%)	219 (64%)	121 (36%)	0	1
2	B	343/381 (90%)	216 (63%)	127 (37%)	0	0
2	D	348/381 (91%)	214 (62%)	134 (38%)	0	0
3	E	65/126 (52%)	45 (69%)	20 (31%)	0	2
All	All	1438/1644 (88%)	911 (63%)	527 (37%)	0	1

5 of 527 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	281	GLN
2	D	331	GLN
2	D	280	SER
3	E	113	GLU
2	B	220	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 58 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	11	GLN
2	D	350	ASN
1	C	206	ASN
2	D	339	ASN
2	D	258	ASN

### 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 8 ligands modelled in this entry, 2 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	1.11	1 (4%)	30,47,47	1.74	10 (33%)
5	GTP	C	601	4	26,34,34	1.32	3 (11%)	32,54,54	1.67	8 (25%)
7	POD	D	701	-	34,34,34	3.27	12 (35%)	51,51,51	4.08	21 (41%)
6	GDP	B	602	-	24,30,30	1.12	1 (4%)	30,47,47	1.85	8 (26%)
5	GTP	A	600	4	26,34,34	1.31	2 (7%)	32,54,54	1.86	10 (31%)
7	POD	B	700	-	34,34,34	3.27	11 (32%)	51,51,51	4.32	25 (49%)

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	-	-	4/12/32/32	0/3/3/3
5	GTP	C	601	4	-	7/18/38/38	0/3/3/3
7	POD	D	701	-	1/1/5/5	6/10/45/45	0/5/5/5
6	GDP	B	602	-	-	4/12/32/32	0/3/3/3
5	GTP	A	600	4	-	8/18/38/38	0/3/3/3
7	POD	B	700	-	1/1/5/5	6/10/45/45	0/5/5/5

The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	701	POD	C7-C6	-10.83	1.21	1.39
7	B	700	POD	C7-C6	-9.64	1.23	1.39
7	D	701	POD	C7-C2	-9.57	1.21	1.38
7	B	700	POD	C7-C2	-9.09	1.22	1.38
7	B	700	POD	C10-C13	-6.41	1.42	1.51

The worst 5 of 82 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	700	POD	C2-C7-C6	13.71	149.06	119.42
7	D	701	POD	C2-C7-C6	13.16	147.85	119.42
7	D	701	POD	C7-C6-C5	-12.51	103.81	120.26
7	B	700	POD	C7-C6-C5	-12.19	104.22	120.26
7	B	700	POD	C7-C2-C3	-11.24	107.77	122.02

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	B	700	POD	C10
7	D	701	POD	C10

5 of 35 torsion outliers are listed below:

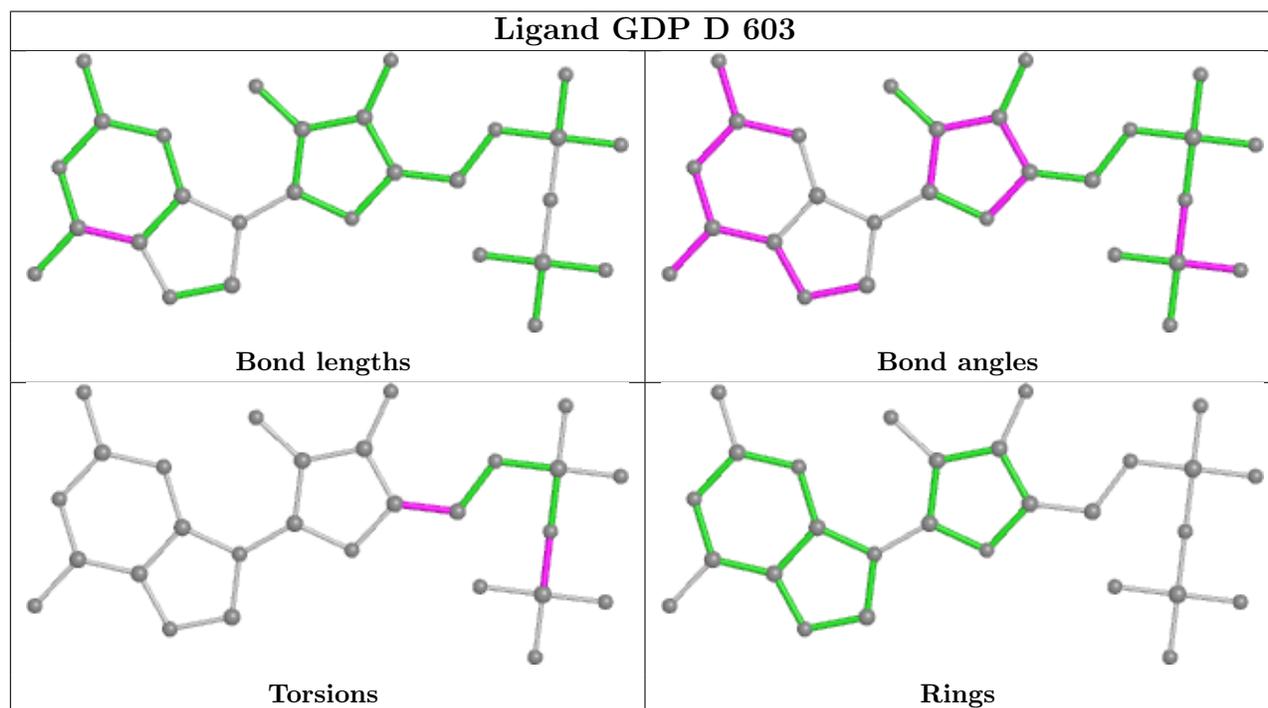
Mol	Chain	Res	Type	Atoms
5	A	600	GTP	C3'-C4'-C5'-O5'
5	C	601	GTP	C3'-C4'-C5'-O5'
6	B	602	GDP	PA-O3A-PB-O2B
6	B	602	GDP	PA-O3A-PB-O3B
6	B	602	GDP	O4'-C4'-C5'-O5'

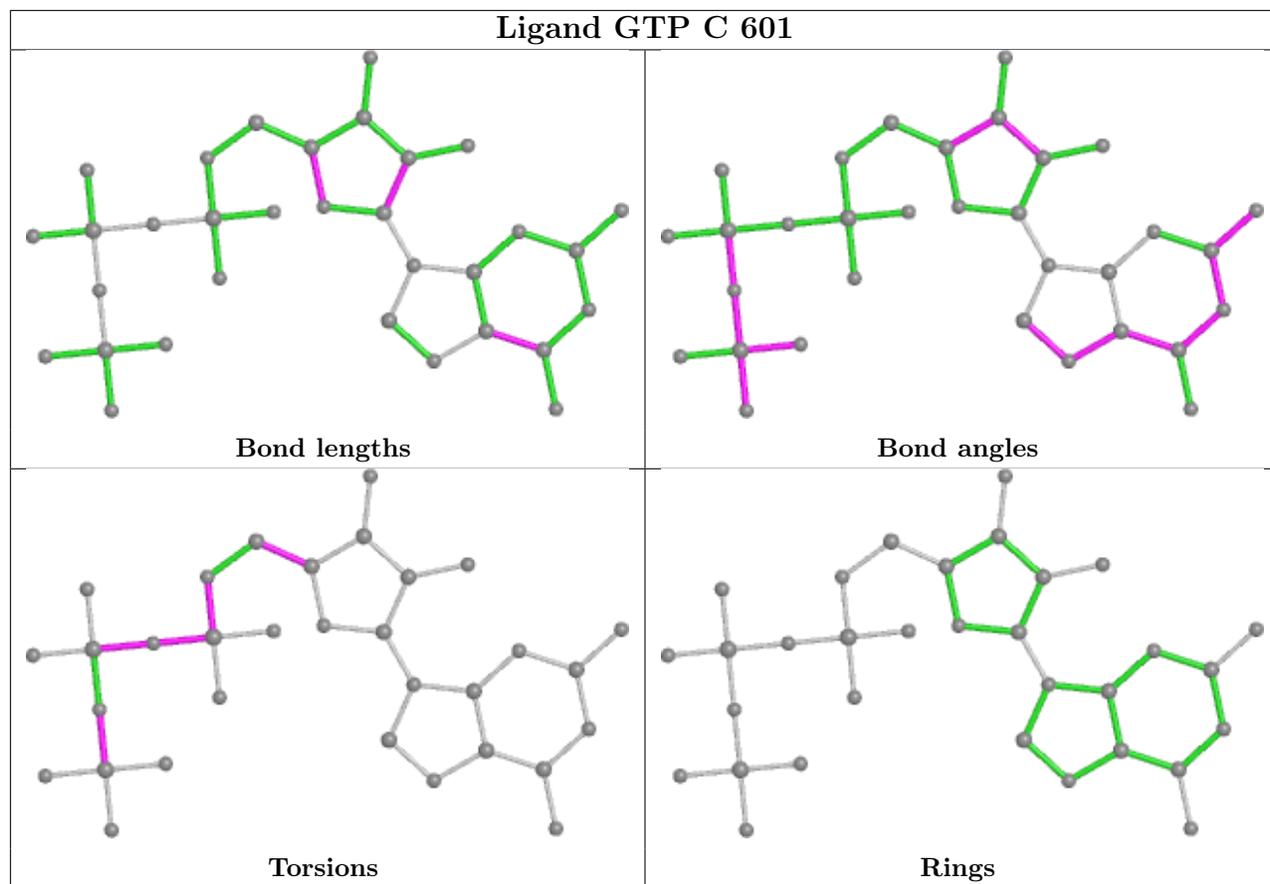
There are no ring outliers.

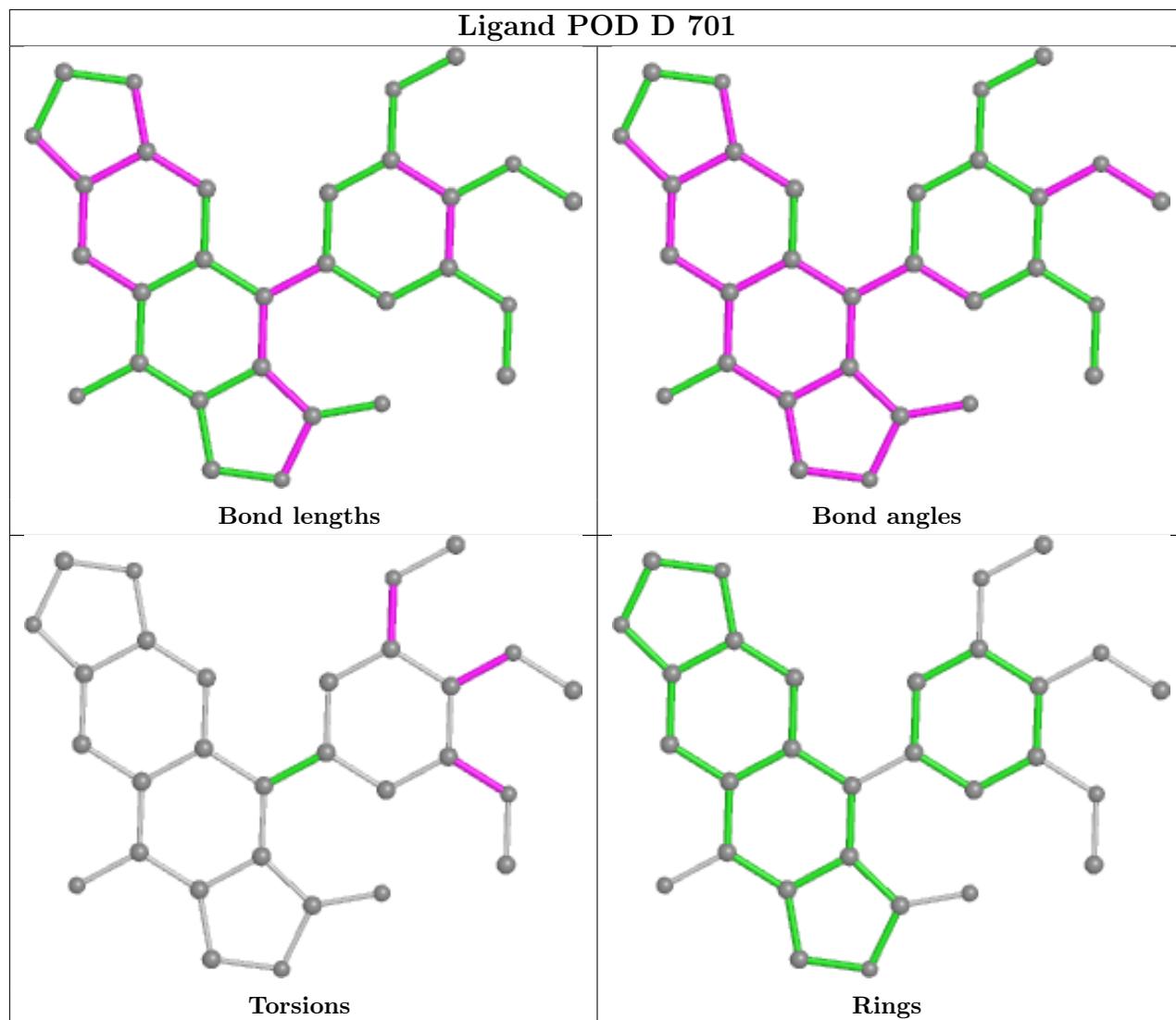
6 monomers are involved in 17 short contacts:

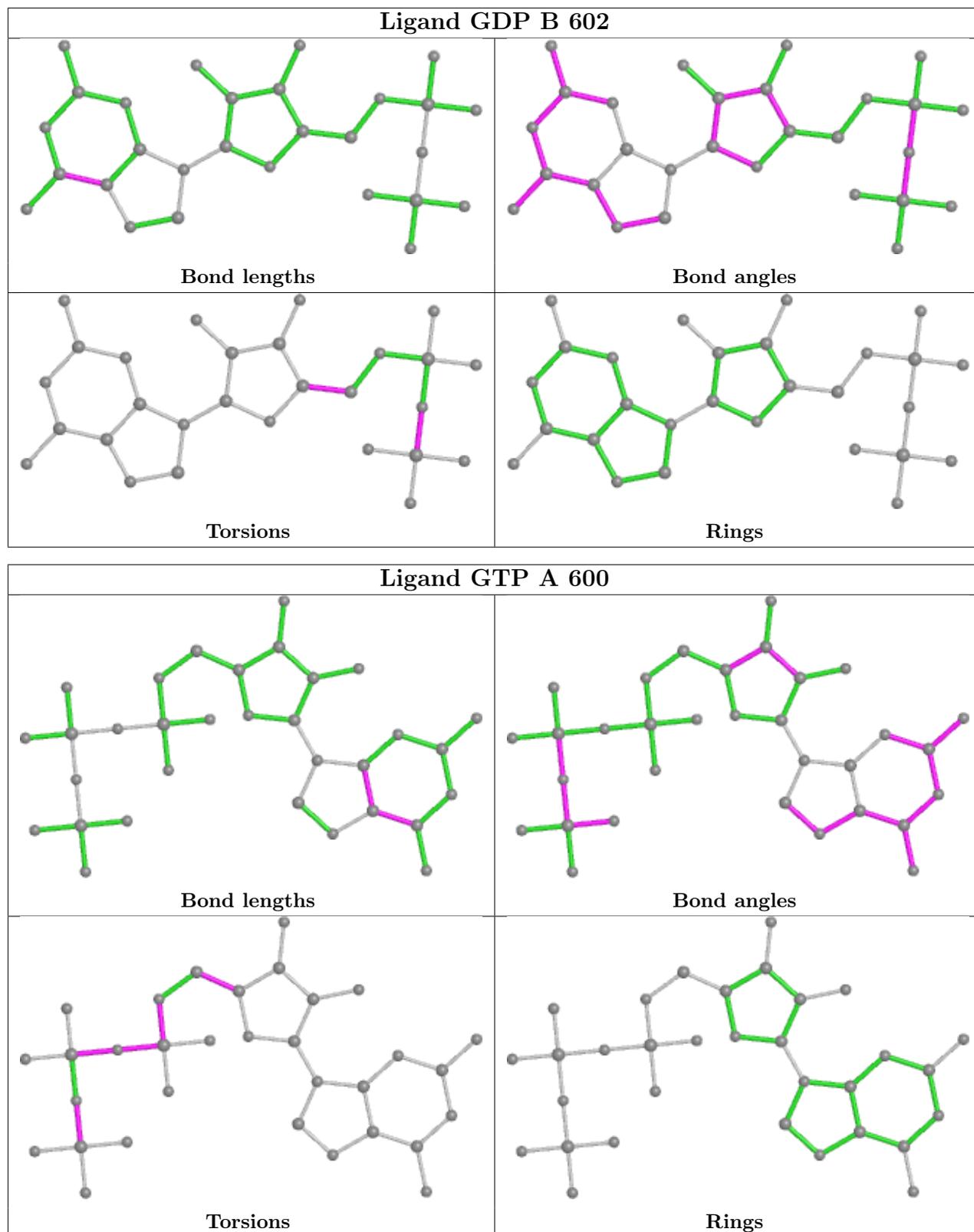
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	603	GDP	2	0
5	C	601	GTP	2	0
7	D	701	POD	4	0
6	B	602	GDP	1	0
5	A	600	GTP	3	0
7	B	700	POD	5	0

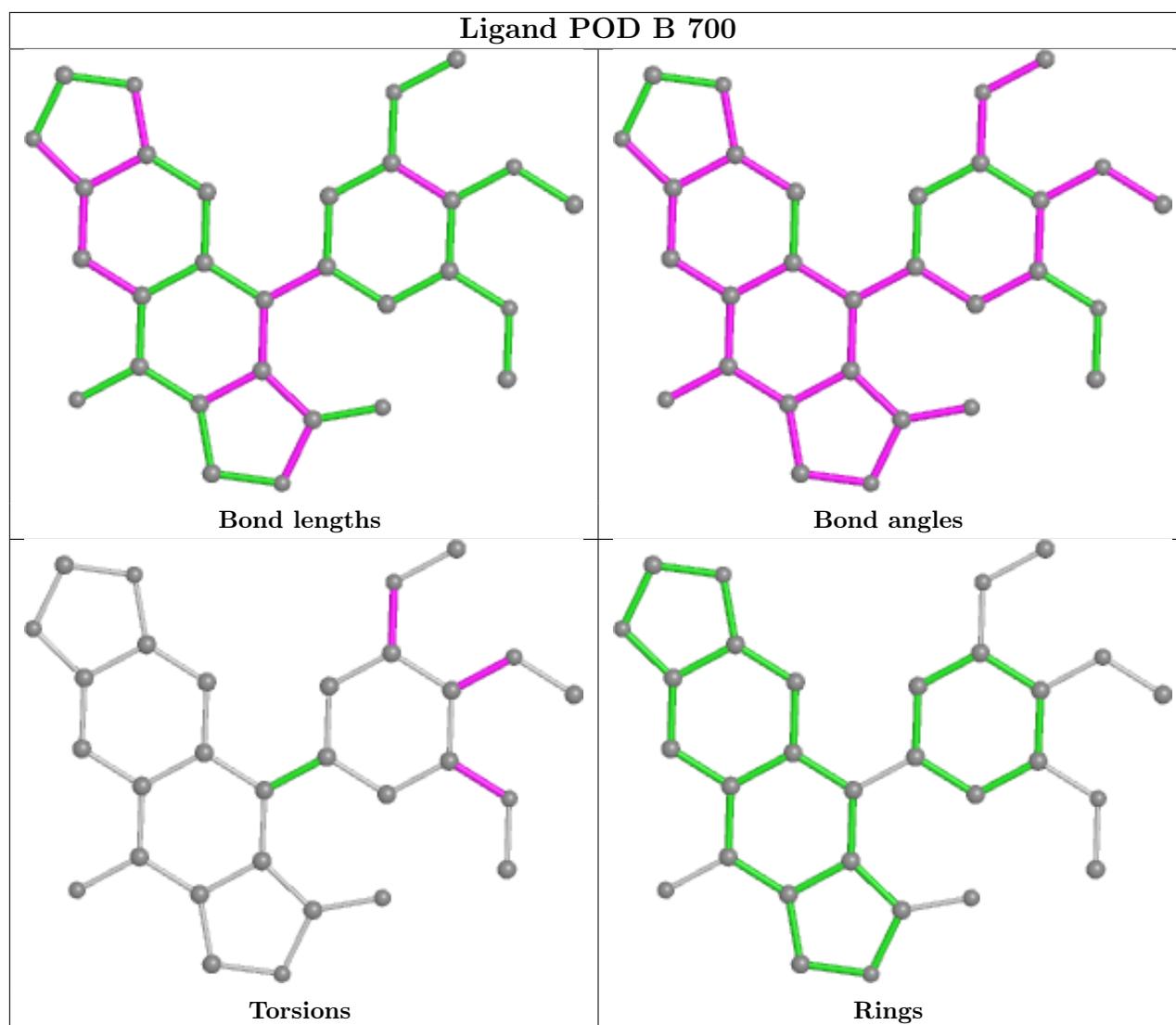
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

### 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.