



wwPDB EM Validation Summary Report ⓘ

Nov 17, 2022 – 01:59 AM EST

PDB ID : 7M2W
EMDB ID : EMD-23635
Title : Engineered disulfide cross-linked closed conformation of the Yeast gamma-TuRC(SS)
Authors : Brilot, A.F.; Lyon, A.S.; Zelter, A.; Viswanath, S.; Maxwell, A.; MacCoss, M.J.; Muller, E.G.; Sali, A.; Davis, T.N.; Agard, D.A.
Deposited on : 2021-03-17
Resolution : 3.00 Å(reported)

This is a wwPDB EM 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/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

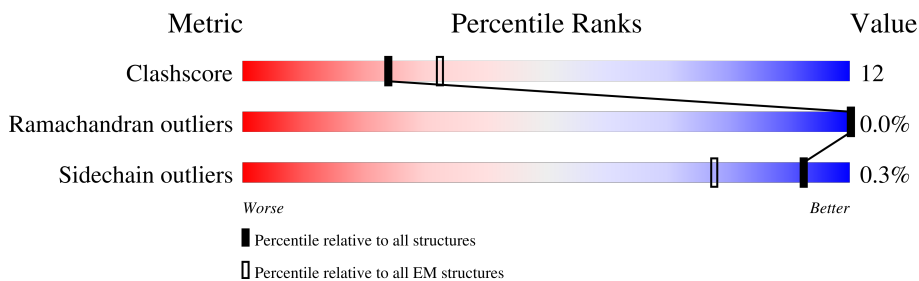
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 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)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	473	66% 30% .
1	B	473	64% 29% 7%
1	C	473	68% 26% 6%
1	D	473	62% 32% 5%
2	E	823	62% 24% 14%
2	G	823	64% 22% 13%
3	F	846	60% 20% 20%
3	H	846	58% 22% 20%
4	K	220	36% 7% 57%

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Mol	Chain	Length	Quality of chain
4	U	220	 17% 81%
4	X	220	 18% 81%
4	Y	220	 38% 5% 57%

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 39366 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 gamma chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	B	441	Total 3450	C 2159	N 585	O 688	S 18	0	0
1	A	453	Total 3547	C 2218	N 599	O 711	S 19	0	0
1	C	445	Total 3481	C 2176	N 589	O 698	S 18	0	0
1	D	447	Total 3500	C 2189	N 591	O 701	S 19	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	58	CYS	SER	engineered mutation	UNP P53378
B	288	CYS	GLY	engineered mutation	UNP P53378
A	58	CYS	SER	engineered mutation	UNP P53378
A	288	CYS	GLY	engineered mutation	UNP P53378
C	58	CYS	SER	engineered mutation	UNP P53378
C	288	CYS	GLY	engineered mutation	UNP P53378
D	58	CYS	SER	engineered mutation	UNP P53378
D	288	CYS	GLY	engineered mutation	UNP P53378

- Molecule 2 is a protein called Spindle pole body component SPC97.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	E	707	Total 5899	C 3796	N 991	O 1083	S 29	0	0
2	G	712	Total 5935	C 3819	N 997	O 1090	S 29	0	0

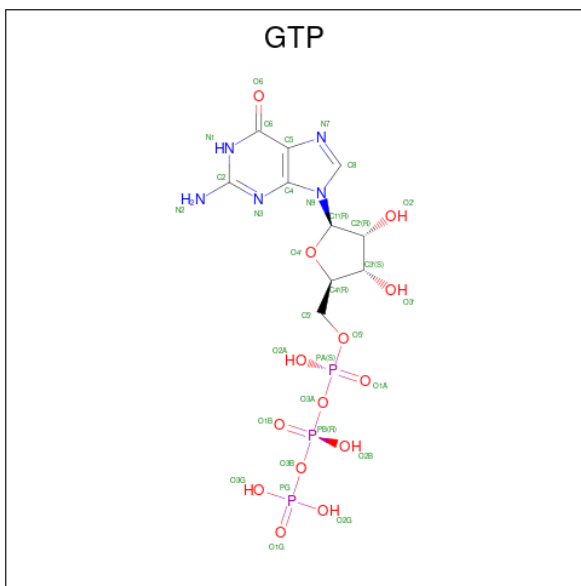
- Molecule 3 is a protein called Spindle pole body component SPC98.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	F	674	Total 5569	C 3601	N 920	O 1032	S 16	0	0
3	H	674	Total 5569	C 3601	N 920	O 1032	S 16	0	0

- Molecule 4 is a protein called Spindle pole body component 110.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	U	42	Total 352	C 215	N 61	O 76		0	0
4	K	95	Total 792	C 488	N 142	O 160	S 2	0	0
4	X	42	Total 352	C 215	N 61	O 76		0	0
4	Y	95	Total 792	C 488	N 142	O 160	S 2	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					AltConf
			Total	C	N	O	P	
5	B	1	Total 32	C 10	N 5	O 14	P 3	0
5	A	1	Total 32	C 10	N 5	O 14	P 3	0
5	C	1	Total 32	C 10	N 5	O 14	P 3	0

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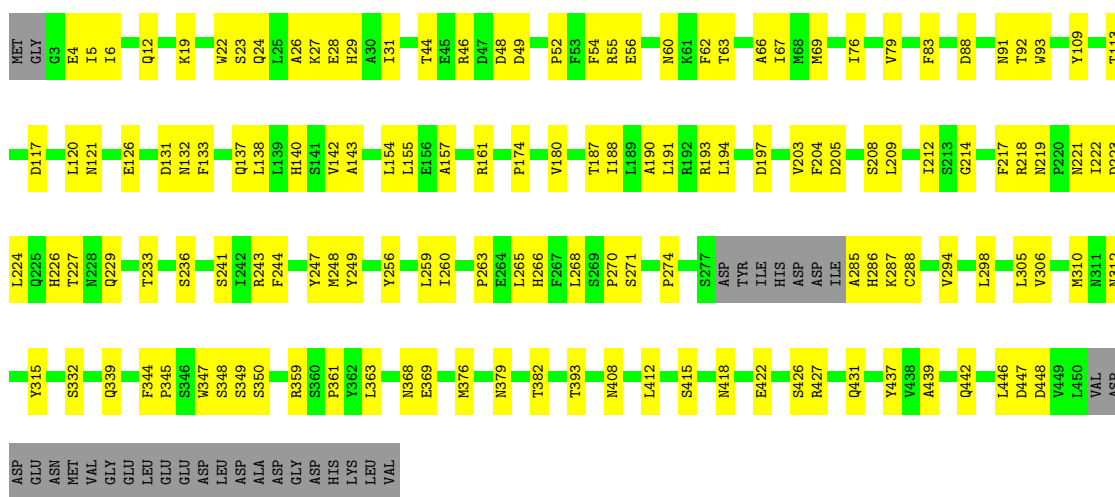
Mol	Chain	Residues	Atoms				AltConf	
			Total	C	N	O		P
5	D	1	32	10	5	14	3	0

3 Residue-property plots [i](#)

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

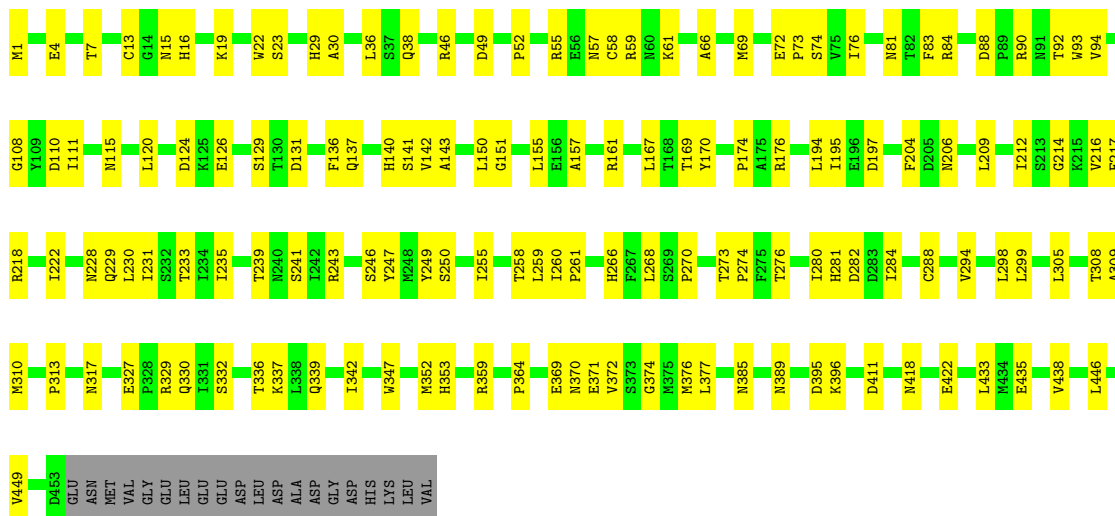
- Molecule 1: Tubulin gamma chain

Chain B: 

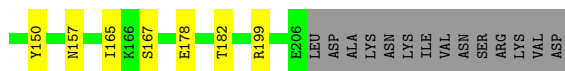


- Molecule 1: Tubulin gamma chain

Chain A: 



- Molecule 1: Tubulin gamma chain



4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=0°, rise=0.1 Å, axial sym=C1	Depositor
Number of segments used	148911	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; Final reconstruction in cis-TEM	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{Å}^2$)	72	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	47214	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

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

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	0.26	0/3622	0.43	0/4920
1	B	0.26	0/3522	0.43	0/4782
1	C	0.26	0/3553	0.43	0/4825
1	D	0.27	0/3573	0.45	0/4851
2	E	0.27	0/6015	0.42	1/8119 (0.0%)
2	G	0.27	0/6052	0.43	0/8170
3	F	0.28	0/5688	0.42	0/7688
3	H	0.28	0/5688	0.42	0/7688
4	K	0.73	0/800	0.71	0/1069
4	U	0.99	0/353	0.76	1/471 (0.2%)
4	X	0.60	0/353	0.85	1/471 (0.2%)
4	Y	0.66	0/800	0.95	4/1069 (0.4%)
All	All	0.32	0/40019	0.46	7/54123 (0.0%)

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	X	176	ARG	NE-CZ-NH1	7.71	124.15	120.30
4	U	176	ARG	NE-CZ-NH1	6.62	123.61	120.30
4	Y	125	ARG	NE-CZ-NH1	6.16	123.38	120.30
4	Y	146	ARG	NE-CZ-NH1	5.50	123.05	120.30
4	Y	136	ARG	NE-CZ-NH1	5.32	122.96	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	3547	0	3398	109	0
1	B	3450	0	3315	102	0
1	C	3481	0	3336	85	0
1	D	3500	0	3354	129	0
2	E	5899	0	5954	174	0
2	G	5935	0	5996	138	0
3	F	5569	0	5588	123	0
3	H	5569	0	5588	138	0
4	K	792	0	788	16	0
4	U	352	0	347	4	0
4	X	352	0	347	0	0
4	Y	792	0	788	40	0
5	A	32	0	11	4	0
5	B	32	0	12	2	0
5	C	32	0	12	1	0
5	D	32	0	11	5	0
All	All	39366	0	38845	937	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 12.

The worst 5 of 937 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:G:34:THR:HG21	4:K:178:GLU:OE2	1.12	1.30
2:E:226:LEU:HD11	4:Y:146:ARG:CZ	1.62	1.28
2:G:34:THR:CG2	4:K:178:GLU:OE2	2.03	1.06
2:E:226:LEU:CD1	4:Y:146:ARG:NH1	2.20	1.05
2:E:226:LEU:HG	4:Y:146:ARG:HG3	1.38	1.05

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 PDB entries followed by that with respect to all EM entries.

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	451/473 (95%)	429 (95%)	22 (5%)	0	100	100
1	B	437/473 (92%)	416 (95%)	21 (5%)	0	100	100
1	C	441/473 (93%)	414 (94%)	27 (6%)	0	100	100
1	D	443/473 (94%)	418 (94%)	24 (5%)	1 (0%)	47	82
2	E	695/823 (84%)	666 (96%)	29 (4%)	0	100	100
2	G	700/823 (85%)	675 (96%)	25 (4%)	0	100	100
3	F	670/846 (79%)	638 (95%)	32 (5%)	0	100	100
3	H	670/846 (79%)	642 (96%)	28 (4%)	0	100	100
4	K	93/220 (42%)	91 (98%)	2 (2%)	0	100	100
4	U	40/220 (18%)	40 (100%)	0	0	100	100
4	X	40/220 (18%)	40 (100%)	0	0	100	100
4	Y	93/220 (42%)	88 (95%)	5 (5%)	0	100	100
All	All	4773/6110 (78%)	4557 (96%)	215 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	288	CYS

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 PDB entries followed by that with respect to all EM entries.

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	404/421 (96%)	404 (100%)	0	100	100
1	B	393/421 (93%)	391 (100%)	2 (0%)	88	96
1	C	397/421 (94%)	397 (100%)	0	100	100
1	D	399/421 (95%)	398 (100%)	1 (0%)	92	97
2	E	663/766 (87%)	662 (100%)	1 (0%)	93	98
2	G	668/766 (87%)	667 (100%)	1 (0%)	93	98
3	F	628/787 (80%)	626 (100%)	2 (0%)	92	97
3	H	628/787 (80%)	627 (100%)	1 (0%)	93	98
4	K	89/206 (43%)	88 (99%)	1 (1%)	73	90
4	U	40/206 (19%)	39 (98%)	1 (2%)	47	79
4	X	40/206 (19%)	39 (98%)	1 (2%)	47	79
4	Y	89/206 (43%)	87 (98%)	2 (2%)	52	81
All	All	4438/5614 (79%)	4425 (100%)	13 (0%)	92	97

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	H	777	CYS
4	U	164	GLU
4	Y	165	ILE
4	X	164	GLU
4	Y	112	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 59 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	116	GLN
2	G	673	GLN
2	E	421	HIS
2	G	649	GLN
3	F	436	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](#)

4 ligands are modelled in this entry.

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
5	GTP	B	501	-	26,34,34	1.12	2 (7%)	32,54,54	1.62	7 (21%)
5	GTP	D	501	1	26,34,34	1.16	2 (7%)	32,54,54	1.52	7 (21%)
5	GTP	C	501	1	26,34,34	1.14	2 (7%)	32,54,54	1.60	7 (21%)
5	GTP	A	501	1	26,34,34	1.14	2 (7%)	32,54,54	1.52	6 (18%)

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
5	GTP	B	501	-	-	6/18/38/38	0/3/3/3
5	GTP	D	501	1	-	3/18/38/38	0/3/3/3
5	GTP	C	501	1	-	6/18/38/38	0/3/3/3
5	GTP	A	501	1	-	6/18/38/38	0/3/3/3

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	501	GTP	C5-C6	-4.17	1.38	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	501	GTP	C5-C6	-4.09	1.39	1.47
5	A	501	GTP	C5-C6	-4.08	1.39	1.47
5	B	501	GTP	C5-C6	-3.95	1.39	1.47
5	D	501	GTP	C2-N3	2.31	1.38	1.33

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	501	GTP	PA-O3A-PB	-4.14	118.62	132.83
5	C	501	GTP	PB-O3B-PG	-3.79	119.83	132.83
5	C	501	GTP	PA-O3A-PB	-3.59	120.52	132.83
5	B	501	GTP	PB-O3B-PG	-3.47	120.93	132.83
5	D	501	GTP	PA-O3A-PB	-3.43	121.05	132.83

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	501	GTP	C5'-O5'-PA-O2A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	O4'-C4'-C5'-O5'

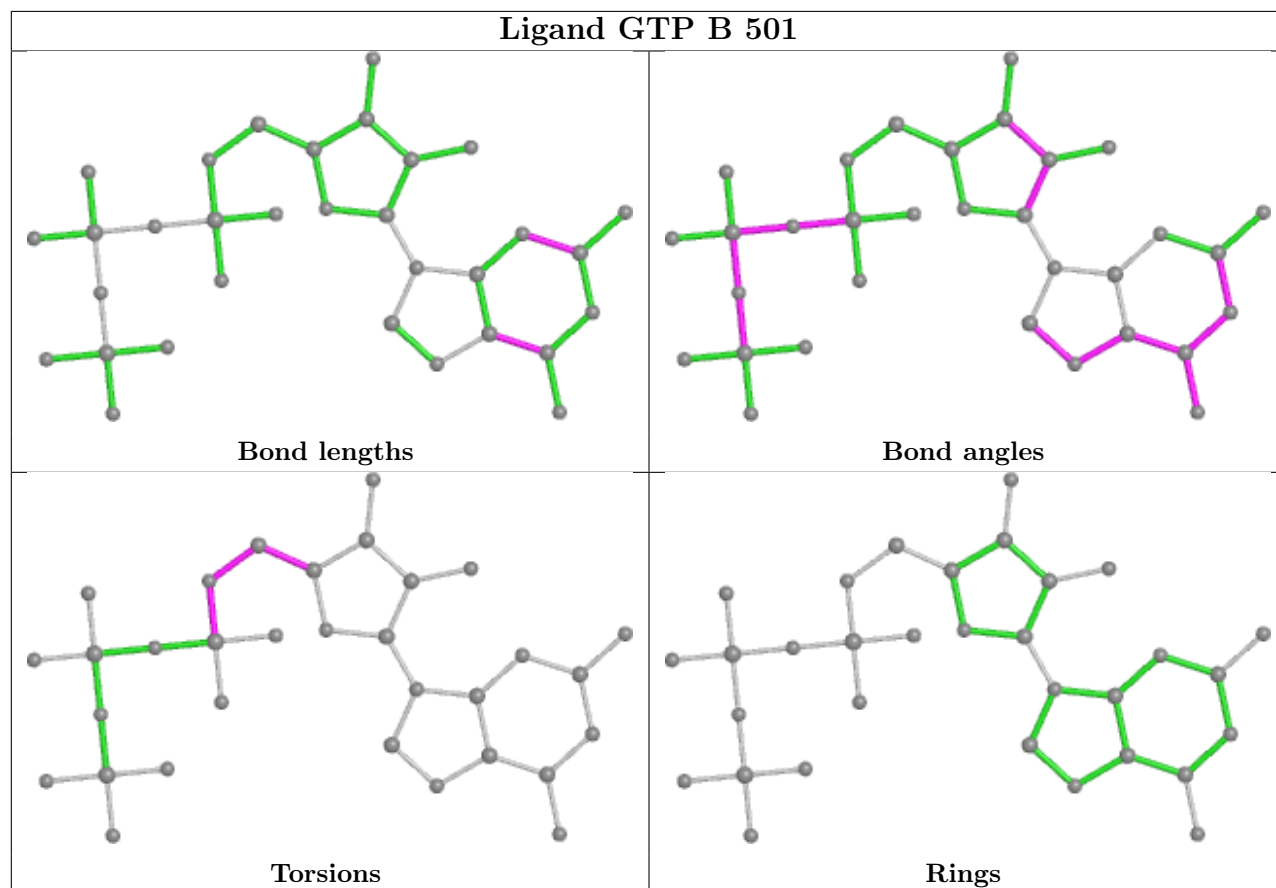
There are no ring outliers.

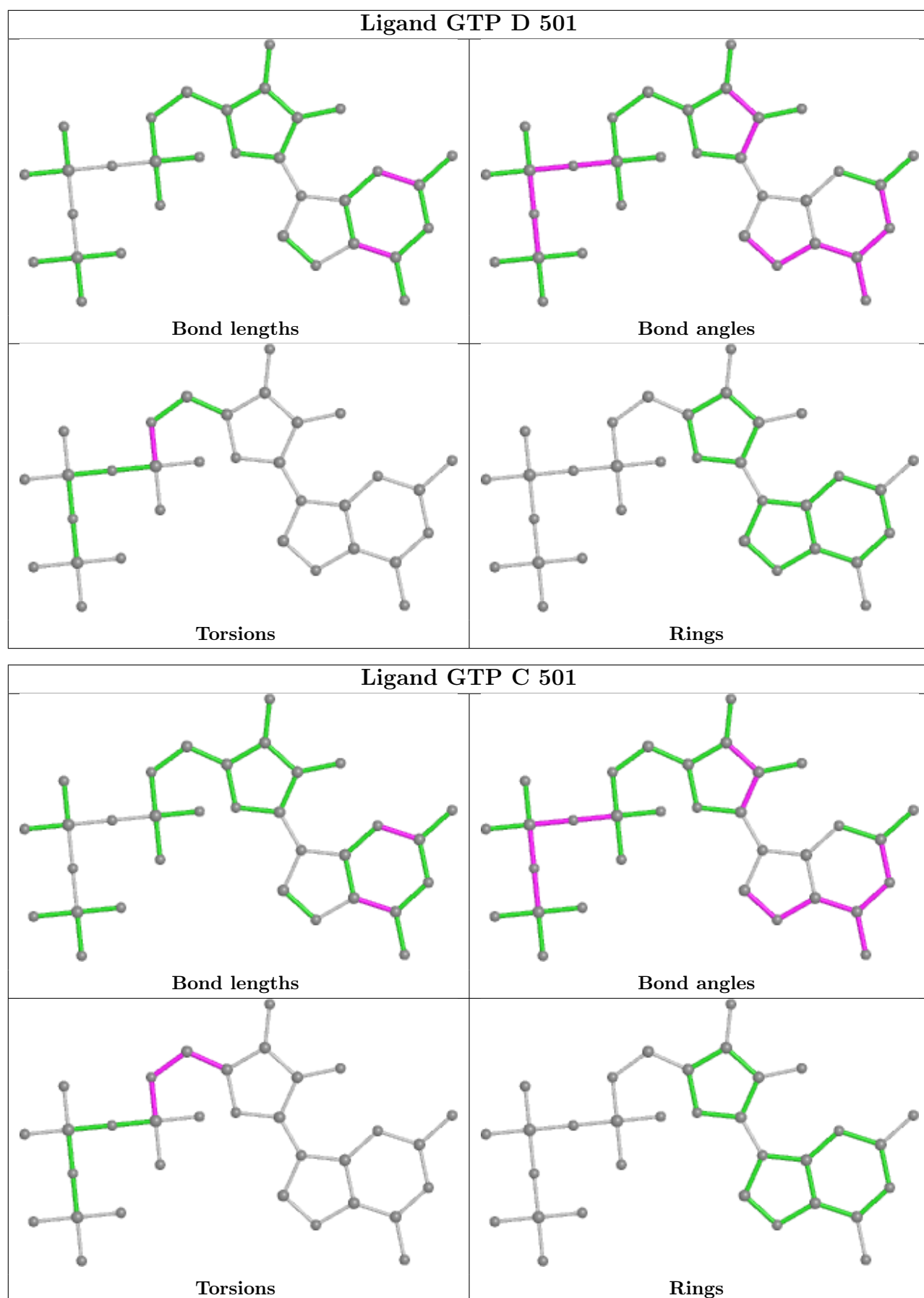
4 monomers are involved in 12 short contacts:

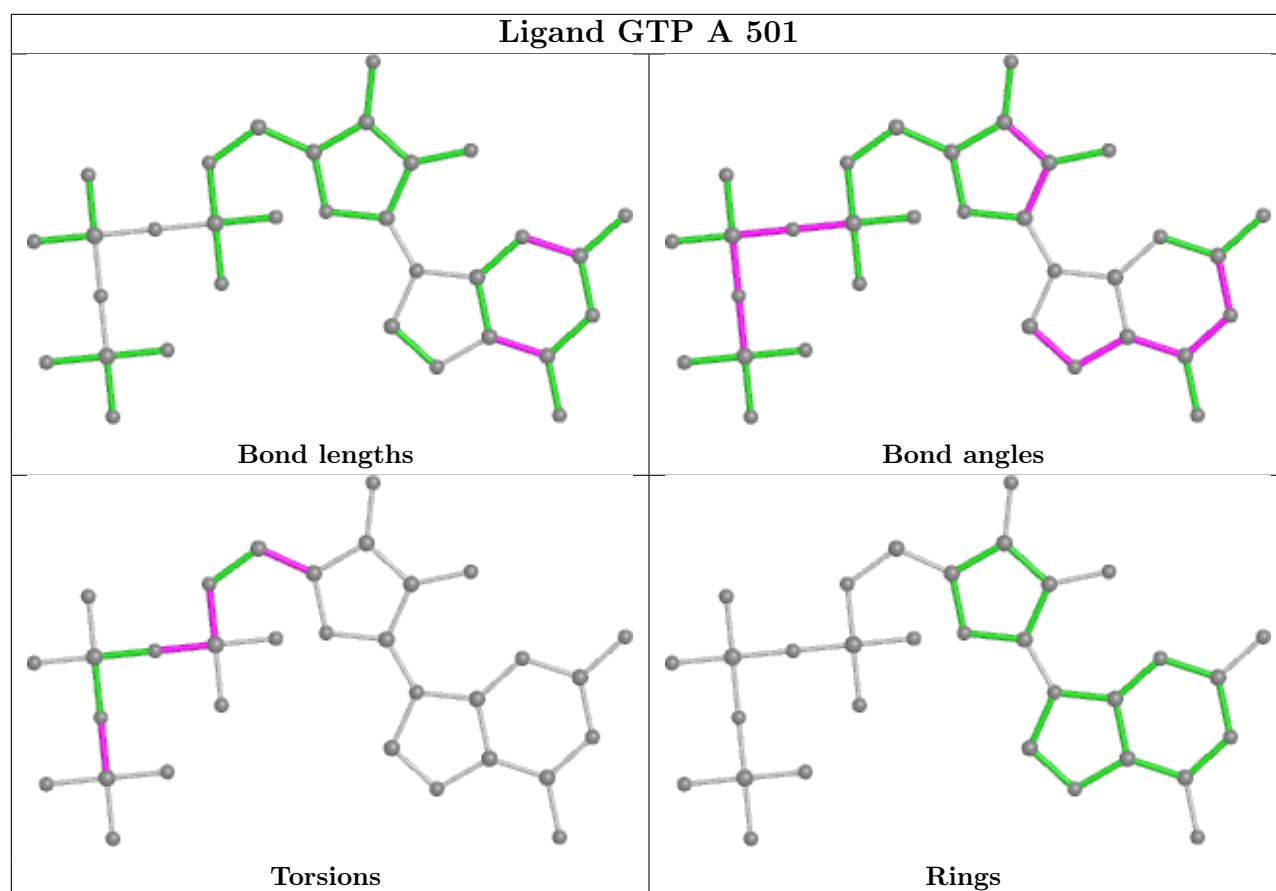
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	501	GTP	2	0
5	D	501	GTP	5	0
5	C	501	GTP	1	0
5	A	501	GTP	4	0

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 Map visualisation

This section contains visualisations of the EMDB entry EMD-23635. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal surface views

This section was not generated.

6.5 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution

This section was not generated.

7.2 Volume estimate versus contour level

This section was not generated.

7.3 Rotationally averaged power spectrum

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

This section was not generated.