



Full wwPDB EM Validation Report ⓘ

May 13, 2024 – 10:25 pm BST

PDB ID : 8QXJ
EMDB ID : EMD-18729
Title : Cryo-EM structure of tetrameric human SAMHD1 with dApNHpp
Authors : Acton, O.J.; Sheppard, D.; Rosenthal, P.B.; Taylor, I.A.
Deposited on : 2023-10-24
Resolution : 2.65 Å (reported)

This is a Full wwPDB EM Validation 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.dev92
Mogul : 1.8.4, 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) : 2.36.2

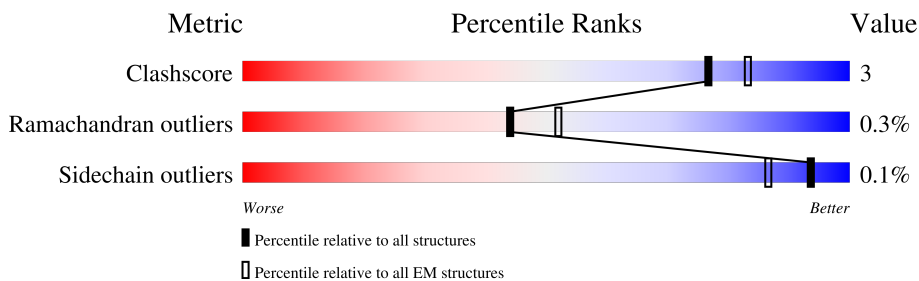
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.65 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	626	
1	B	626	
1	C	626	
1	D	626	

2 Entry composition [i](#)

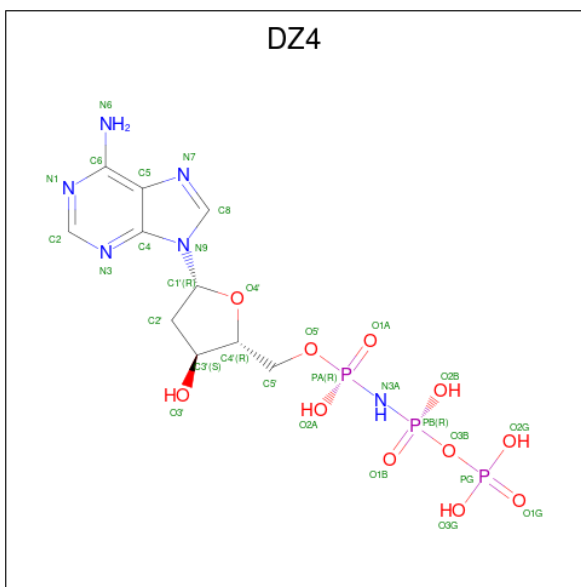
There are 6 unique types of molecules in this entry. The entry contains 15953 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Deoxynucleoside triphosphate triphosphohydrolase SAMHD1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	477	Total 3895	C 2491	N 677	O 707	S 20	2	0
1	B	477	Total 3856	C 2469	N 669	O 698	S 20	2	0
1	C	477	Total 3804	C 2434	N 660	O 690	S 20	1	0
1	D	477	Total 3800	C 2431	N 659	O 690	S 20	0	0

- Molecule 2 is 2'-deoxy-5'-O-[(R)-hydroxy{[(R)-hydroxy(phosphonoxy)phosphoryl]amino}phosphoryl]adenosine (three-letter code: DZ4) (formula: C₁₀H₁₇N₆O₁₁P₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf	
			Total	C	N	O		P
2	A	1	Total 30	C 10	N 6	O 11	P 3	0
2	A	1	Total 30	C 10	N 6	O 11	P 3	0

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Mol	Chain	Residues	Atoms					AltConf
2	B	1	Total	C	N	O	P	0
			30	10	6	11	3	
2	B	1	Total	C	N	O	P	0
			30	10	6	11	3	
2	C	1	Total	C	N	O	P	0
			30	10	6	11	3	
2	C	1	Total	C	N	O	P	0
			30	10	6	11	3	
2	D	1	Total	C	N	O	P	0
			30	10	6	11	3	
2	D	1	Total	C	N	O	P	0
			30	10	6	11	3	

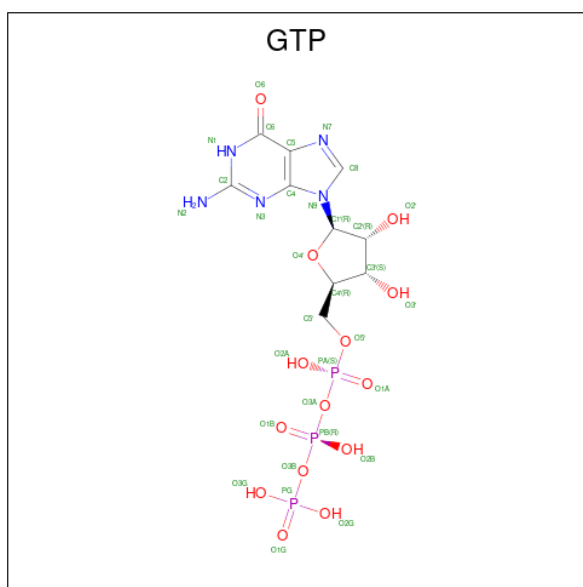
- Molecule 3 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Fe	0
			1	1	
3	B	1	Total	Fe	0
			1	1	
3	C	1	Total	Fe	0
			1	1	
3	D	1	Total	Fe	0
			1	1	

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

Mol	Chain	Residues	Atoms		AltConf
4	A	3	Total	Mg	0
			3	3	
4	B	3	Total	Mg	0
			3	3	
4	C	3	Total	Mg	0
			3	3	
4	D	3	Total	Mg	0
			3	3	

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



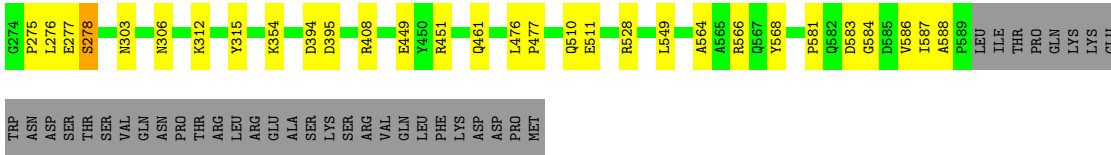
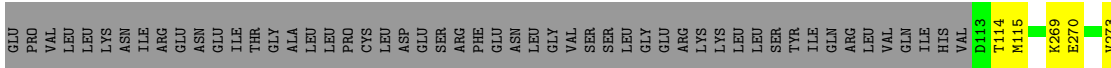
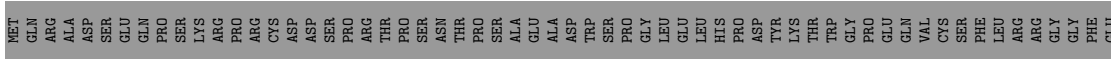
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
5	A	1	Total	C	N	O	P	0
			32	10	5	14	3	
5	B	1	Total	C	N	O	P	0
			32	10	5	14	3	
5	C	1	Total	C	N	O	P	0
			32	10	5	14	3	
5	D	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		AltConf
			Total	O	
6	A	56	Total	O	0
			56	56	
6	B	53	Total	O	0
			53	53	
6	C	55	Total	O	0
			55	55	
6	D	50	Total	O	0
			50	50	



• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	139594	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	48.6	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	130000	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: DZ4, GTP, FE, MG

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	0.25	0/3990	0.50	0/5389
1	B	0.25	0/3954	0.49	0/5346
1	C	0.25	0/3899	0.49	0/5281
1	D	0.25	0/3892	0.49	0/5273
All	All	0.25	0/15735	0.49	0/21289

There are no bond length outliers.

There are no bond angle outliers.

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	3895	0	3873	30	0
1	B	3856	0	3809	21	0
1	C	3804	0	3700	21	0
1	D	3800	0	3694	25	0
2	A	60	0	26	2	0
2	B	60	0	26	2	0
2	C	60	0	26	0	0
2	D	60	0	26	1	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	3	0	0	0	0
4	B	3	0	0	0	0
4	C	3	0	0	0	0
4	D	3	0	0	0	0
5	A	32	0	12	2	0
5	B	32	0	12	0	0
5	C	32	0	12	2	0
5	D	32	0	12	1	0
6	A	56	0	0	3	0
6	B	53	0	0	2	0
6	C	55	0	0	1	0
6	D	50	0	0	1	0
All	All	15953	0	15228	93	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 3.

All (93) 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)
1:B:395:ASP:OD1	1:B:408:ARG:NH1	2.05	0.90
1:A:395:ASP:OD1	1:A:408:ARG:NH1	2.10	0.84
1:A:303:ASN:ND2	1:A:306:ASN:OD1	2.12	0.82
1:D:303:ASN:ND2	1:D:306:ASN:OD1	2.13	0.81
1:C:303:ASN:ND2	1:C:306:ASN:OD1	2.12	0.81
1:D:449:GLU:OE1	6:D:801:HOH:O	2.04	0.75
1:B:449:GLU:OE1	6:B:801:HOH:O	2.05	0.74
1:C:449:GLU:OE2	6:C:801:HOH:O	2.05	0.73
1:A:449:GLU:OE1	6:A:801:HOH:O	2.06	0.72
1:A:462:PRO:O	6:A:802:HOH:O	2.10	0.68
1:D:395:ASP:OD1	1:D:408:ARG:NH1	2.28	0.66
1:A:487:VAL:O	6:A:803:HOH:O	2.14	0.65
1:B:528:ARG:HH22	1:D:586:VAL:HG22	1.61	0.64
1:A:276:LEU:HD23	1:A:277:GLU:N	2.14	0.62
1:B:470:ARG:NE	6:B:802:HOH:O	2.31	0.62
1:C:394:ASP:OD2	1:C:408:ARG:NH2	2.33	0.61
1:B:303:ASN:ND2	1:B:306:ASN:OD1	2.35	0.60
1:A:557:VAL:HG12	1:A:557:VAL:O	2.00	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:276:LEU:HD23	1:D:277:GLU:N	2.18	0.59
1:A:510:GLN:O	1:A:511:GLU:HG3	2.04	0.57
1:D:510:GLN:O	1:D:511:GLU:HG3	2.04	0.57
1:B:510:GLN:O	1:B:511:GLU:HG3	2.05	0.56
1:D:583:ASP:OD2	1:D:587:ILE:HD12	2.05	0.55
1:C:510:GLN:O	1:C:511:GLU:HG3	2.08	0.54
1:A:466:ILE:HG22	1:A:466:ILE:O	2.08	0.54
1:D:394:ASP:O	1:D:395:ASP:HB2	2.09	0.53
1:C:394:ASP:O	1:C:395:ASP:HB2	2.09	0.53
1:A:352:ARG:NH2	2:A:707:DZ4:O2G	2.41	0.53
1:B:342:GLU:OE2	1:B:345:ASN:N	2.43	0.52
1:A:342:GLU:OE2	1:A:345:ASN:N	2.41	0.52
1:B:352:ARG:NH1	2:B:707:DZ4:O3G	2.41	0.52
1:B:276:LEU:HD23	1:B:277:GLU:N	2.26	0.51
1:C:276:LEU:HD23	1:C:277:GLU:N	2.26	0.50
1:A:352:ARG:NH1	2:A:707:DZ4:O3G	2.40	0.50
1:D:277:GLU:O	1:D:278:SER:OG	2.28	0.49
1:C:566:ARG:HE	1:C:588:ALA:HB2	1.77	0.49
1:D:312:LYS:HA	1:D:315:TYR:CE2	2.48	0.48
1:B:352:ARG:NH2	2:B:707:DZ4:O2G	2.45	0.48
1:D:395:ASP:OD1	1:D:408:ARG:NH2	2.46	0.48
1:D:564:ALA:O	1:D:568:TYR:HD1	1.97	0.48
1:C:564:ALA:O	1:C:568:TYR:HD1	1.97	0.48
1:B:564:ALA:O	1:B:568:TYR:HD1	1.97	0.47
1:D:354:LYS:NZ	2:D:701:DZ4:O2A	2.46	0.47
1:A:451:ARG:NH2	5:A:706:GTP:H5'	2.29	0.47
1:B:586:VAL:HG22	1:D:528:ARG:HH22	1.80	0.47
1:B:522:CYS:SG	1:D:586:VAL:HG11	2.55	0.46
1:C:276:LEU:HD23	1:C:277:GLU:HG2	1.98	0.46
1:C:566:ARG:CD	1:C:587:ILE:HG22	2.46	0.46
1:C:583:ASP:OD2	1:C:587:ILE:HD12	2.16	0.46
1:D:581:PRO:O	1:D:584:GLY:N	2.49	0.46
1:A:312:LYS:HA	1:A:315:TYR:CE2	2.52	0.45
1:C:451:ARG:NH2	5:C:707:GTP:H5'	2.31	0.45
1:C:312:LYS:HA	1:C:315:TYR:CE2	2.52	0.45
1:B:276:LEU:HD23	1:B:277:GLU:HG2	1.98	0.45
1:B:312:LYS:HA	1:B:315:TYR:CE2	2.52	0.45
1:B:394:ASP:O	1:B:395:ASP:HB2	2.17	0.45
1:D:566:ARG:CD	1:D:587:ILE:HG22	2.48	0.44
1:D:114:THR:HG22	1:D:115:MET:N	2.33	0.44
1:A:564:ALA:O	1:A:568:TYR:HD1	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:451:ARG:NH2	5:D:702:GTP:H5'	2.33	0.44
1:A:482:SER:O	1:A:482:SER:OG	2.30	0.44
1:A:483:ALA:O	1:A:485:PRO:HD3	2.18	0.44
1:B:572:TRP:O	1:B:575:ASP:OD1	2.36	0.44
1:C:269:LYS:O	1:C:273:VAL:HG22	2.18	0.43
1:D:566:ARG:HE	1:D:588:ALA:HB2	1.83	0.43
1:A:114:THR:HG22	1:A:115:MET:N	2.32	0.43
1:C:476:LEU:N	1:C:477:PRO:HD2	2.34	0.43
1:B:114:THR:HG22	1:B:115:MET:N	2.33	0.43
1:B:270:GLU:O	1:B:273:VAL:O	2.37	0.43
1:A:566:ARG:CD	1:A:587:ILE:HG22	2.48	0.42
1:A:269:LYS:O	1:A:273:VAL:HG22	2.19	0.42
1:C:270:GLU:O	1:C:273:VAL:O	2.37	0.42
1:D:270:GLU:O	1:D:273:VAL:O	2.38	0.42
1:A:394:ASP:O	1:A:395:ASP:HB2	2.19	0.42
1:D:269:LYS:O	1:D:273:VAL:HG22	2.19	0.42
1:A:194:ARG:CZ	1:A:260:ILE:HD13	2.50	0.42
1:B:269:LYS:O	1:B:273:VAL:HG22	2.19	0.42
1:D:275:PRO:O	1:D:276:LEU:HB3	2.19	0.42
1:A:270:GLU:O	1:A:273:VAL:O	2.38	0.42
1:A:528:ARG:HH22	1:C:586:VAL:HG22	1.84	0.42
1:D:461:GLN:HG2	1:D:549:LEU:HD23	2.02	0.42
1:A:277:GLU:HG2	1:A:277:GLU:O	2.20	0.42
1:A:451:ARG:NH2	5:A:706:GTP:O1A	2.42	0.42
1:D:476:LEU:N	1:D:477:PRO:HD2	2.35	0.41
1:B:378:VAL:O	1:B:381:ILE:HG22	2.20	0.41
1:C:114:THR:HG22	1:C:115:MET:N	2.34	0.41
1:A:275:PRO:O	1:A:276:LEU:HB3	2.21	0.41
1:A:575:ASP:OD1	1:A:575:ASP:C	2.59	0.41
1:C:451:ARG:NH2	5:C:707:GTP:O1A	2.43	0.41
1:A:566:ARG:HE	1:A:588:ALA:HB2	1.86	0.41
1:C:262:GLU:HG2	1:C:263:GLU:N	2.36	0.41
1:A:466:ILE:O	1:A:467:LYS:C	2.58	0.40
1:C:275:PRO:O	1:C:276:LEU:HB3	2.22	0.40

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	477/626 (76%)	458 (96%)	18 (4%)	1 (0%)	47	64
1	B	477/626 (76%)	460 (96%)	15 (3%)	2 (0%)	34	48
1	C	476/626 (76%)	459 (96%)	16 (3%)	1 (0%)	47	64
1	D	475/626 (76%)	455 (96%)	19 (4%)	1 (0%)	47	64
All	All	1905/2504 (76%)	1832 (96%)	68 (4%)	5 (0%)	44	56

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	579	THR
1	A	278	SER
1	B	278	SER
1	C	278	SER
1	D	278	SER

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	423/560 (76%)	423 (100%)	0	100	100
1	B	414/560 (74%)	412 (100%)	2 (0%)	88	94
1	C	401/560 (72%)	401 (100%)	0	100	100
1	D	401/560 (72%)	401 (100%)	0	100	100
All	All	1639/2240 (73%)	1637 (100%)	2 (0%)	93	97

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	492[A]	LYS
1	B	492[B]	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 28 ligands modelled in this entry, 16 are monoatomic - leaving 12 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
2	DZ4	D	703	4,3	29,32,32	3.18	14 (48%)	33,50,50	2.10	5 (15%)
5	GTP	D	702	4	26,34,34	1.14	2 (7%)	32,54,54	1.50	7 (21%)
2	DZ4	B	707	4	29,32,32	3.13	14 (48%)	33,50,50	2.08	4 (12%)
2	DZ4	C	702	4,3	29,32,32	3.18	14 (48%)	33,50,50	2.10	4 (12%)
5	GTP	B	701	4	26,34,34	1.13	2 (7%)	32,54,54	1.50	7 (21%)
2	DZ4	B	702	4,3	29,32,32	3.18	14 (48%)	33,50,50	2.10	5 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	DZ4	C	701	4	29,32,32	3.14	14 (48%)	33,50,50	2.08	4 (12%)
5	GTP	A	706	4	26,34,34	1.14	2 (7%)	32,54,54	1.50	7 (21%)
2	DZ4	A	707	4	29,32,32	3.12	14 (48%)	33,50,50	2.09	4 (12%)
2	DZ4	A	701	4,3	29,32,32	3.18	14 (48%)	33,50,50	2.09	5 (15%)
5	GTP	C	707	4	26,34,34	1.14	2 (7%)	32,54,54	1.51	7 (21%)
2	DZ4	D	701	4	29,32,32	3.13	14 (48%)	33,50,50	2.14	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
2	DZ4	D	703	4,3	-	10/15/34/34	0/3/3/3
5	GTP	D	702	4	-	5/18/38/38	0/3/3/3
2	DZ4	B	707	4	-	6/15/34/34	0/3/3/3
2	DZ4	C	702	4,3	-	10/15/34/34	0/3/3/3
5	GTP	B	701	4	-	1/18/38/38	0/3/3/3
2	DZ4	B	702	4,3	-	10/15/34/34	0/3/3/3
2	DZ4	C	701	4	-	6/15/34/34	0/3/3/3
5	GTP	A	706	4	-	5/18/38/38	0/3/3/3
2	DZ4	A	707	4	-	6/15/34/34	0/3/3/3
2	DZ4	A	701	4,3	-	10/15/34/34	0/3/3/3
5	GTP	C	707	4	-	5/18/38/38	0/3/3/3
2	DZ4	D	701	4	-	7/15/34/34	0/3/3/3

All (120) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	701	DZ4	O4'-C1'	7.94	1.60	1.42
2	D	701	DZ4	O4'-C1'	7.92	1.60	1.42
2	B	707	DZ4	O4'-C1'	7.92	1.60	1.42
2	A	701	DZ4	O4'-C1'	7.88	1.60	1.42
2	A	707	DZ4	O4'-C1'	7.88	1.60	1.42
2	C	702	DZ4	O4'-C1'	7.85	1.60	1.42
2	B	702	DZ4	O4'-C1'	7.84	1.59	1.42
2	D	703	DZ4	O4'-C1'	7.81	1.59	1.42
2	A	701	DZ4	C2'-C1'	-7.36	1.31	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	702	DZ4	C2'-C1'	-7.35	1.31	1.52
2	C	702	DZ4	C2'-C1'	-7.34	1.31	1.52
2	D	703	DZ4	C2'-C1'	-7.32	1.31	1.52
2	D	701	DZ4	C2'-C1'	-7.17	1.32	1.52
2	B	707	DZ4	C2'-C1'	-7.13	1.32	1.52
2	C	701	DZ4	C2'-C1'	-7.11	1.32	1.52
2	A	707	DZ4	C2'-C1'	-7.11	1.32	1.52
2	B	707	DZ4	C3'-C4'	-6.03	1.36	1.53
2	D	703	DZ4	C3'-C4'	-6.02	1.36	1.53
2	A	701	DZ4	C3'-C4'	-6.02	1.36	1.53
2	A	707	DZ4	C3'-C4'	-6.00	1.36	1.53
2	C	701	DZ4	C3'-C4'	-6.00	1.36	1.53
2	C	702	DZ4	C3'-C4'	-6.00	1.36	1.53
2	B	702	DZ4	C3'-C4'	-5.99	1.36	1.53
2	D	701	DZ4	C3'-C4'	-5.95	1.36	1.53
2	A	701	DZ4	PB-O3B	5.67	1.66	1.59
2	C	702	DZ4	PB-O3B	5.66	1.66	1.59
2	B	702	DZ4	PB-O3B	5.66	1.66	1.59
2	D	703	DZ4	PB-O3B	5.65	1.66	1.59
2	C	701	DZ4	PB-O3B	5.54	1.66	1.59
2	D	701	DZ4	PB-O3B	5.49	1.66	1.59
2	B	707	DZ4	PB-O3B	5.45	1.65	1.59
2	A	707	DZ4	PB-O3B	5.41	1.65	1.59
5	B	701	GTP	C5-C6	-4.11	1.39	1.47
5	D	702	GTP	C5-C6	-4.11	1.39	1.47
5	A	706	GTP	C5-C6	-4.09	1.39	1.47
5	C	707	GTP	C5-C6	-4.07	1.39	1.47
2	B	702	DZ4	PA-O1A	3.76	1.52	1.46
2	D	703	DZ4	PA-O1A	3.73	1.52	1.46
2	C	702	DZ4	PA-O1A	3.73	1.52	1.46
2	D	701	DZ4	C2'-C3'	3.68	1.62	1.52
2	A	701	DZ4	PA-O1A	3.66	1.52	1.46
2	C	701	DZ4	C2'-C3'	3.61	1.62	1.52
2	D	703	DZ4	C2'-C3'	3.61	1.62	1.52
2	A	701	DZ4	C2'-C3'	3.60	1.62	1.52
2	A	707	DZ4	C2'-C3'	3.60	1.62	1.52
2	C	702	DZ4	C2'-C3'	3.59	1.62	1.52
2	C	702	DZ4	PA-N3A	3.58	1.72	1.63
2	B	702	DZ4	C2'-C3'	3.58	1.62	1.52
2	B	707	DZ4	C2'-C3'	3.58	1.62	1.52
2	D	703	DZ4	PA-N3A	3.58	1.72	1.63
2	B	702	DZ4	PA-N3A	3.57	1.72	1.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	DZ4	PA-N3A	3.56	1.72	1.63
2	C	701	DZ4	PA-O1A	3.42	1.51	1.46
2	C	701	DZ4	PA-N3A	3.40	1.72	1.63
2	A	707	DZ4	PA-O1A	3.39	1.51	1.46
2	B	707	DZ4	PA-N3A	3.38	1.72	1.63
2	A	707	DZ4	PA-N3A	3.36	1.72	1.63
2	B	707	DZ4	PA-O1A	3.30	1.51	1.46
2	C	702	DZ4	O4'-C4'	3.30	1.52	1.45
2	B	702	DZ4	O4'-C4'	3.29	1.52	1.45
2	D	701	DZ4	PA-O1A	3.29	1.51	1.46
2	A	701	DZ4	O4'-C4'	3.28	1.52	1.45
2	D	701	DZ4	O4'-C4'	3.28	1.52	1.45
2	D	701	DZ4	PA-N3A	3.26	1.71	1.63
2	C	701	DZ4	O4'-C4'	3.26	1.52	1.45
2	D	703	DZ4	O4'-C4'	3.26	1.52	1.45
2	A	707	DZ4	O4'-C4'	3.25	1.52	1.45
2	B	707	DZ4	O4'-C4'	3.24	1.52	1.45
2	B	707	DZ4	PB-O1B	3.08	1.51	1.46
2	A	701	DZ4	PB-O1B	3.06	1.51	1.46
2	B	702	DZ4	PB-O1B	3.05	1.51	1.46
2	C	702	DZ4	PB-O1B	3.05	1.51	1.46
2	A	707	DZ4	PB-O1B	3.02	1.50	1.46
2	D	703	DZ4	PB-O1B	3.02	1.50	1.46
2	C	701	DZ4	PB-O1B	2.99	1.50	1.46
2	D	701	DZ4	PB-O1B	2.93	1.50	1.46
2	D	703	DZ4	C5-C4	-2.73	1.33	1.40
2	C	702	DZ4	C5-C4	-2.72	1.33	1.40
2	B	702	DZ4	C5-C4	-2.70	1.33	1.40
2	A	701	DZ4	C5-C4	-2.70	1.33	1.40
2	A	707	DZ4	C5-C4	-2.66	1.33	1.40
2	C	701	DZ4	C5-C4	-2.65	1.33	1.40
2	B	707	DZ4	C5-C4	-2.65	1.33	1.40
2	D	701	DZ4	C5-C4	-2.63	1.34	1.40
2	D	703	DZ4	C2-N3	2.58	1.36	1.32
2	C	701	DZ4	C2-N3	2.58	1.36	1.32
2	C	702	DZ4	C2-N3	2.57	1.36	1.32
2	B	707	DZ4	C2-N3	2.56	1.36	1.32
2	B	702	DZ4	C2-N3	2.53	1.36	1.32
2	A	701	DZ4	C2-N3	2.53	1.36	1.32
2	A	707	DZ4	C2-N3	2.52	1.36	1.32
2	D	701	DZ4	C2-N3	2.51	1.36	1.32
2	D	701	DZ4	PA-O5'	2.37	1.66	1.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	DZ4	PA-O5'	2.31	1.66	1.57
2	D	703	DZ4	PA-O5'	2.30	1.66	1.57
2	B	702	DZ4	PA-O5'	2.30	1.66	1.57
2	B	707	DZ4	PA-O5'	2.29	1.66	1.57
2	A	707	DZ4	PA-O5'	2.29	1.66	1.57
2	A	701	DZ4	PB-N3A	2.27	1.69	1.63
2	C	702	DZ4	PA-O5'	2.26	1.66	1.57
2	C	701	DZ4	PA-O5'	2.26	1.66	1.57
2	C	702	DZ4	PB-N3A	2.23	1.69	1.63
2	D	703	DZ4	PB-N3A	2.23	1.69	1.63
2	B	702	DZ4	PB-N3A	2.22	1.69	1.63
2	D	701	DZ4	PB-O2B	-2.16	1.50	1.56
2	B	707	DZ4	PB-N3A	2.16	1.69	1.63
2	B	707	DZ4	PB-O2B	-2.15	1.51	1.56
2	C	701	DZ4	PB-N3A	2.14	1.69	1.63
2	A	707	DZ4	PB-N3A	2.13	1.68	1.63
2	A	707	DZ4	PB-O2B	-2.13	1.51	1.56
2	B	702	DZ4	PB-O2B	-2.13	1.51	1.56
2	C	701	DZ4	PB-O2B	-2.12	1.51	1.56
2	D	703	DZ4	PB-O2B	-2.12	1.51	1.56
2	C	702	DZ4	PB-O2B	-2.10	1.51	1.56
5	C	707	GTP	C2-N3	2.10	1.38	1.33
5	A	706	GTP	C2-N3	2.10	1.38	1.33
2	A	701	DZ4	PB-O2B	-2.09	1.51	1.56
5	D	702	GTP	C2-N3	2.09	1.38	1.33
2	D	701	DZ4	PB-N3A	2.07	1.68	1.63
5	B	701	GTP	C2-N3	2.02	1.38	1.33

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	707	DZ4	C5-C6-N6	7.60	131.90	120.35
2	D	701	DZ4	C5-C6-N6	7.58	131.87	120.35
2	C	701	DZ4	C5-C6-N6	7.56	131.85	120.35
2	B	707	DZ4	C5-C6-N6	7.54	131.81	120.35
2	C	702	DZ4	C5-C6-N6	7.48	131.72	120.35
2	B	702	DZ4	C5-C6-N6	7.48	131.71	120.35
2	D	703	DZ4	C5-C6-N6	7.46	131.69	120.35
2	A	701	DZ4	C5-C6-N6	7.45	131.67	120.35
2	C	702	DZ4	N3-C2-N1	-5.60	119.92	128.68
2	D	703	DZ4	N3-C2-N1	-5.59	119.95	128.68
2	A	701	DZ4	N3-C2-N1	-5.58	119.95	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	702	DZ4	N3-C2-N1	-5.57	119.97	128.68
2	B	707	DZ4	N3-C2-N1	-5.56	119.99	128.68
2	C	701	DZ4	N3-C2-N1	-5.55	120.01	128.68
2	A	707	DZ4	N3-C2-N1	-5.53	120.03	128.68
2	D	701	DZ4	N3-C2-N1	-5.51	120.06	128.68
2	B	707	DZ4	N6-C6-N1	-5.12	107.94	118.57
2	A	707	DZ4	N6-C6-N1	-5.12	107.95	118.57
2	C	701	DZ4	N6-C6-N1	-5.10	107.98	118.57
2	D	701	DZ4	N6-C6-N1	-5.10	108.00	118.57
2	D	703	DZ4	N6-C6-N1	-5.08	108.03	118.57
2	B	702	DZ4	N6-C6-N1	-5.07	108.05	118.57
2	C	702	DZ4	N6-C6-N1	-5.05	108.08	118.57
2	A	701	DZ4	N6-C6-N1	-5.04	108.10	118.57
5	B	701	GTP	C5-C6-N1	3.29	119.77	113.95
5	C	707	GTP	C5-C6-N1	3.26	119.71	113.95
5	D	702	GTP	C5-C6-N1	3.26	119.70	113.95
5	A	706	GTP	C5-C6-N1	3.22	119.64	113.95
5	B	701	GTP	PB-O3B-PG	-3.08	122.25	132.83
5	C	707	GTP	C8-N7-C5	3.07	108.84	102.99
5	A	706	GTP	C8-N7-C5	3.07	108.84	102.99
5	D	702	GTP	C8-N7-C5	3.06	108.81	102.99
5	D	702	GTP	PB-O3B-PG	-3.04	122.40	132.83
5	A	706	GTP	PB-O3B-PG	-3.03	122.41	132.83
5	B	701	GTP	C8-N7-C5	3.03	108.76	102.99
5	C	707	GTP	PB-O3B-PG	-3.02	122.47	132.83
5	B	701	GTP	C2-N1-C6	-2.96	119.66	125.10
5	C	707	GTP	C2-N1-C6	-2.94	119.69	125.10
5	B	701	GTP	PA-O3A-PB	-2.91	122.85	132.83
5	A	706	GTP	C2-N1-C6	-2.90	119.75	125.10
5	D	702	GTP	C2-N1-C6	-2.90	119.76	125.10
5	A	706	GTP	PA-O3A-PB	-2.89	122.91	132.83
5	C	707	GTP	PA-O3A-PB	-2.89	122.92	132.83
5	D	702	GTP	PA-O3A-PB	-2.88	122.93	132.83
5	B	701	GTP	C3'-C2'-C1'	2.77	105.15	100.98
5	A	706	GTP	C3'-C2'-C1'	2.70	105.04	100.98
5	C	707	GTP	C3'-C2'-C1'	2.69	105.03	100.98
5	D	702	GTP	C3'-C2'-C1'	2.68	105.01	100.98
2	A	707	DZ4	PB-O3B-PG	-2.59	123.51	132.62
2	B	707	DZ4	PB-O3B-PG	-2.58	123.52	132.62
2	D	701	DZ4	PB-O3B-PG	-2.55	123.62	132.62
2	C	701	DZ4	PB-O3B-PG	-2.55	123.65	132.62
2	D	701	DZ4	O1B-PB-N3A	-2.29	108.40	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	702	DZ4	PB-O3B-PG	-2.19	124.89	132.62
2	B	702	DZ4	PB-O3B-PG	-2.19	124.90	132.62
2	D	703	DZ4	PB-O3B-PG	-2.19	124.91	132.62
2	D	703	DZ4	C2'-C3'-C4'	2.18	107.31	102.76
2	A	701	DZ4	PB-O3B-PG	-2.18	124.94	132.62
5	B	701	GTP	O6-C6-C5	-2.14	120.19	124.37
5	D	702	GTP	O6-C6-C5	-2.13	120.20	124.37
5	C	707	GTP	O6-C6-C5	-2.13	120.21	124.37
5	A	706	GTP	O6-C6-C5	-2.12	120.24	124.37
2	B	702	DZ4	C2'-C3'-C4'	2.05	107.04	102.76
2	D	701	DZ4	O1A-PA-N3A	-2.03	108.78	111.77
2	A	701	DZ4	C2'-C3'-C4'	2.01	106.94	102.76

There are no chirality outliers.

All (81) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	DZ4	PB-N3A-PA-O5'
2	A	701	DZ4	C5'-O5'-PA-O2A
2	A	701	DZ4	PA-N3A-PB-O1B
2	A	701	DZ4	PA-N3A-PB-O3B
2	A	701	DZ4	PG-O3B-PB-O1B
2	A	701	DZ4	PG-O3B-PB-O2B
2	A	701	DZ4	PB-O3B-PG-O3G
2	A	707	DZ4	PA-N3A-PB-O1B
2	A	707	DZ4	PG-O3B-PB-O1B
2	A	707	DZ4	PG-O3B-PB-O2B
2	B	702	DZ4	PB-N3A-PA-O1A
2	B	702	DZ4	C5'-O5'-PA-O2A
2	B	702	DZ4	PA-N3A-PB-O1B
2	B	702	DZ4	PA-N3A-PB-O3B
2	B	702	DZ4	PG-O3B-PB-O1B
2	B	702	DZ4	PG-O3B-PB-O2B
2	B	702	DZ4	PB-O3B-PG-O3G
2	B	707	DZ4	PA-N3A-PB-O1B
2	B	707	DZ4	PG-O3B-PB-O1B
2	B	707	DZ4	PG-O3B-PB-O2B
2	C	701	DZ4	PA-N3A-PB-O1B
2	C	701	DZ4	PG-O3B-PB-O1B
2	C	701	DZ4	PG-O3B-PB-O2B
2	C	702	DZ4	PB-N3A-PA-O5'
2	C	702	DZ4	C5'-O5'-PA-O2A

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Mol	Chain	Res	Type	Atoms
2	C	702	DZ4	PA-N3A-PB-O1B
2	C	702	DZ4	PA-N3A-PB-O3B
2	C	702	DZ4	PG-O3B-PB-O1B
2	C	702	DZ4	PG-O3B-PB-O2B
2	C	702	DZ4	PB-O3B-PG-O3G
2	D	701	DZ4	PB-N3A-PA-O1A
2	D	701	DZ4	C5'-O5'-PA-O1A
2	D	701	DZ4	C5'-O5'-PA-O2A
2	D	703	DZ4	PB-N3A-PA-O1A
2	D	703	DZ4	PB-N3A-PA-O5'
2	D	703	DZ4	C5'-O5'-PA-O2A
2	D	703	DZ4	PA-N3A-PB-O1B
2	D	703	DZ4	PA-N3A-PB-O3B
2	D	703	DZ4	PG-O3B-PB-O1B
2	D	703	DZ4	PG-O3B-PB-O2B
2	D	703	DZ4	PB-O3B-PG-O3G
5	A	706	GTP	O4'-C4'-C5'-O5'
5	C	707	GTP	O4'-C4'-C5'-O5'
5	D	702	GTP	O4'-C4'-C5'-O5'
5	A	706	GTP	C3'-C4'-C5'-O5'
5	C	707	GTP	C3'-C4'-C5'-O5'
5	D	702	GTP	C3'-C4'-C5'-O5'
2	A	701	DZ4	C5'-O5'-PA-N3A
2	B	702	DZ4	C5'-O5'-PA-N3A
2	C	702	DZ4	C5'-O5'-PA-N3A
2	D	701	DZ4	C5'-O5'-PA-N3A
2	D	703	DZ4	C5'-O5'-PA-N3A
5	A	706	GTP	PB-O3B-PG-O2G
5	A	706	GTP	PB-O3B-PG-O3G
5	C	707	GTP	PB-O3B-PG-O3G
5	D	702	GTP	PB-O3B-PG-O3G
5	B	701	GTP	PB-O3A-PA-O2A
2	A	707	DZ4	C5'-O5'-PA-O1A
2	B	707	DZ4	C5'-O5'-PA-O1A
2	C	701	DZ4	C5'-O5'-PA-O1A
2	B	702	DZ4	PB-N3A-PA-O5'
2	A	707	DZ4	C5'-O5'-PA-N3A
2	B	707	DZ4	C5'-O5'-PA-N3A
2	C	701	DZ4	C5'-O5'-PA-N3A
2	D	701	DZ4	PB-O3B-PG-O1G
2	A	701	DZ4	PB-N3A-PA-O1A
2	C	702	DZ4	PB-N3A-PA-O1A

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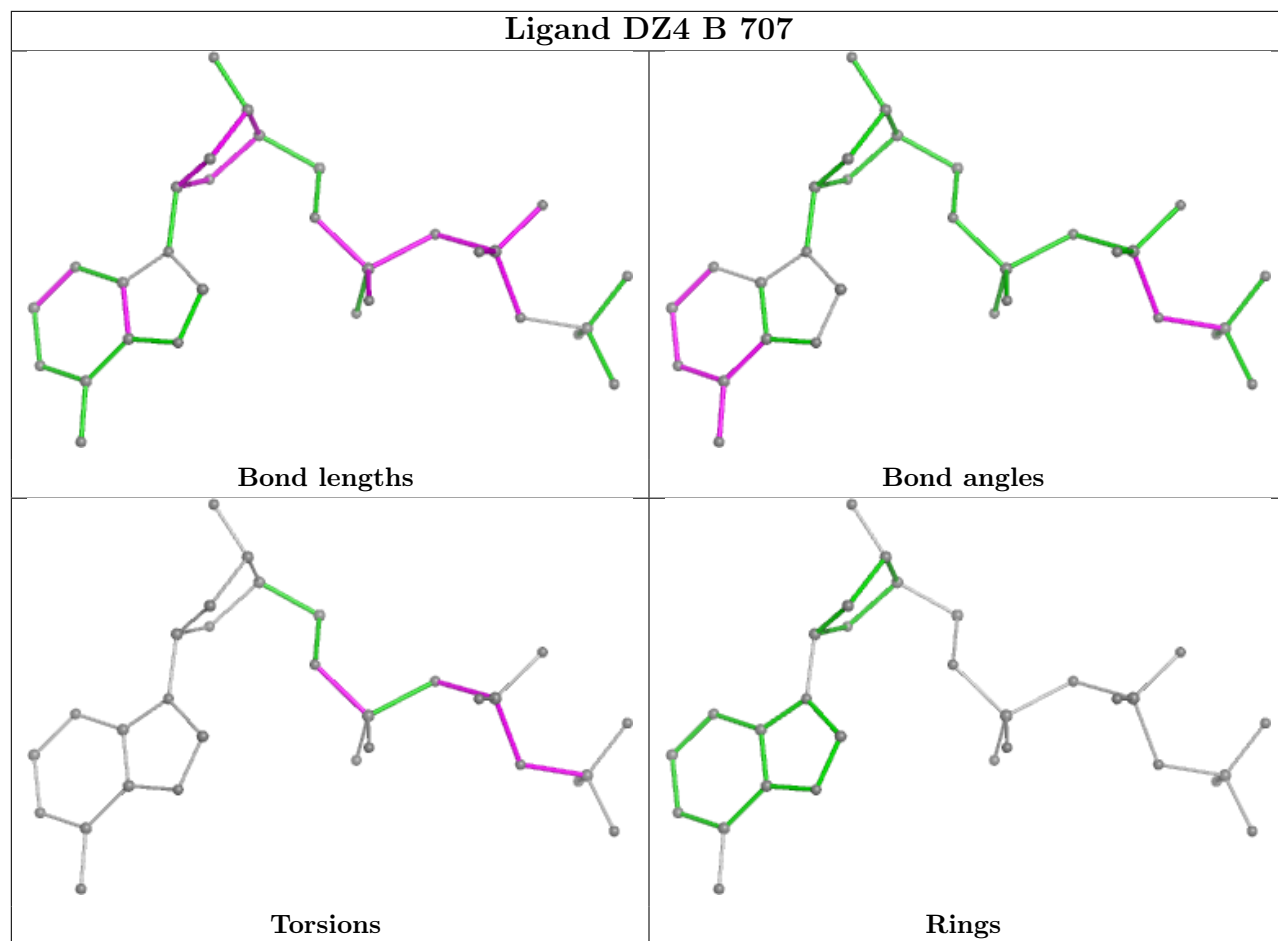
Mol	Chain	Res	Type	Atoms
2	A	707	DZ4	PB-O3B-PG-O2G
2	B	707	DZ4	PB-O3B-PG-O2G
2	C	701	DZ4	PB-O3B-PG-O2G
2	D	701	DZ4	PB-O3B-PG-O2G
2	D	701	DZ4	PB-O3B-PG-O3G
5	C	707	GTP	PB-O3B-PG-O2G
5	D	702	GTP	PB-O3B-PG-O2G
5	A	706	GTP	PG-O3B-PB-O2B
5	C	707	GTP	PG-O3B-PB-O2B
5	D	702	GTP	PG-O3B-PB-O2B
2	A	701	DZ4	C5'-O5'-PA-O1A
2	B	702	DZ4	C5'-O5'-PA-O1A
2	C	702	DZ4	C5'-O5'-PA-O1A
2	D	703	DZ4	C5'-O5'-PA-O1A

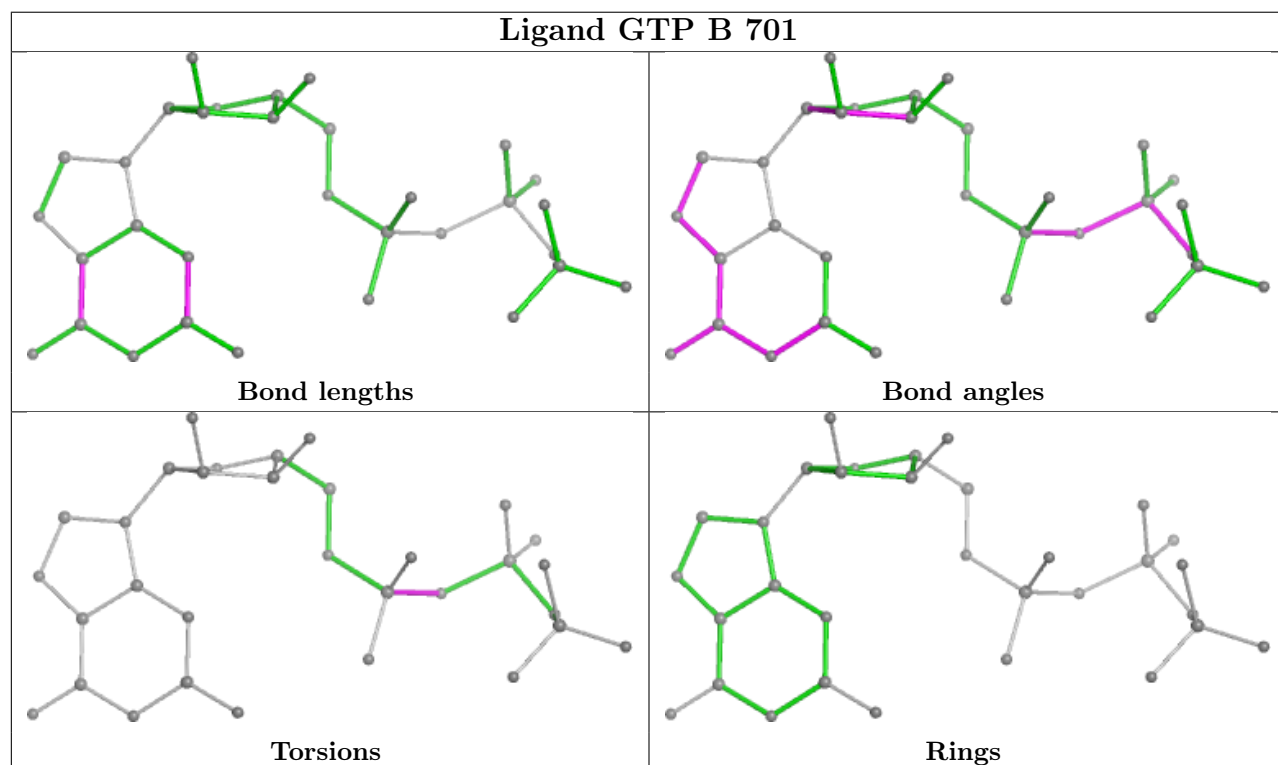
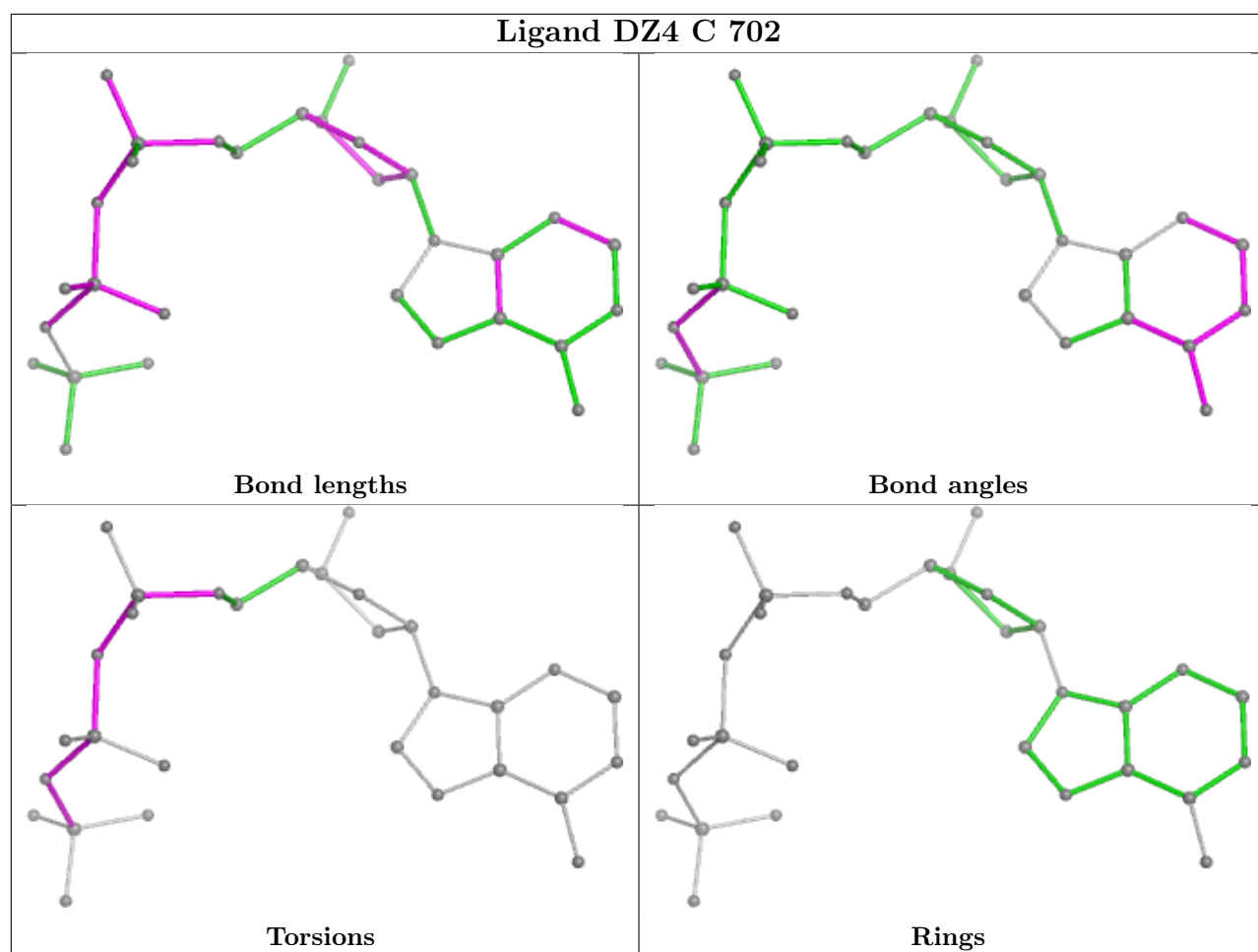
There are no ring outliers.

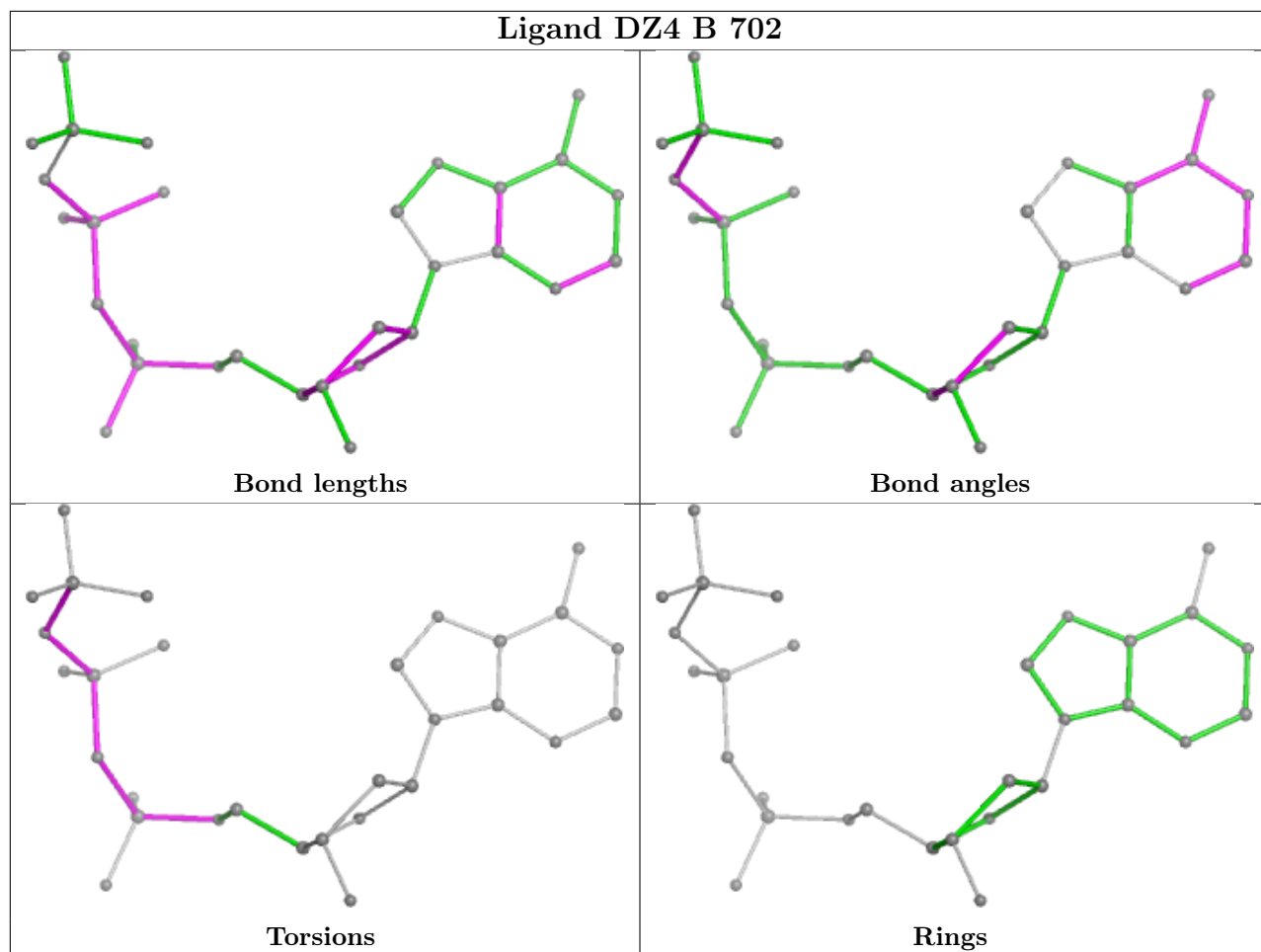
6 monomers are involved in 10 short contacts:

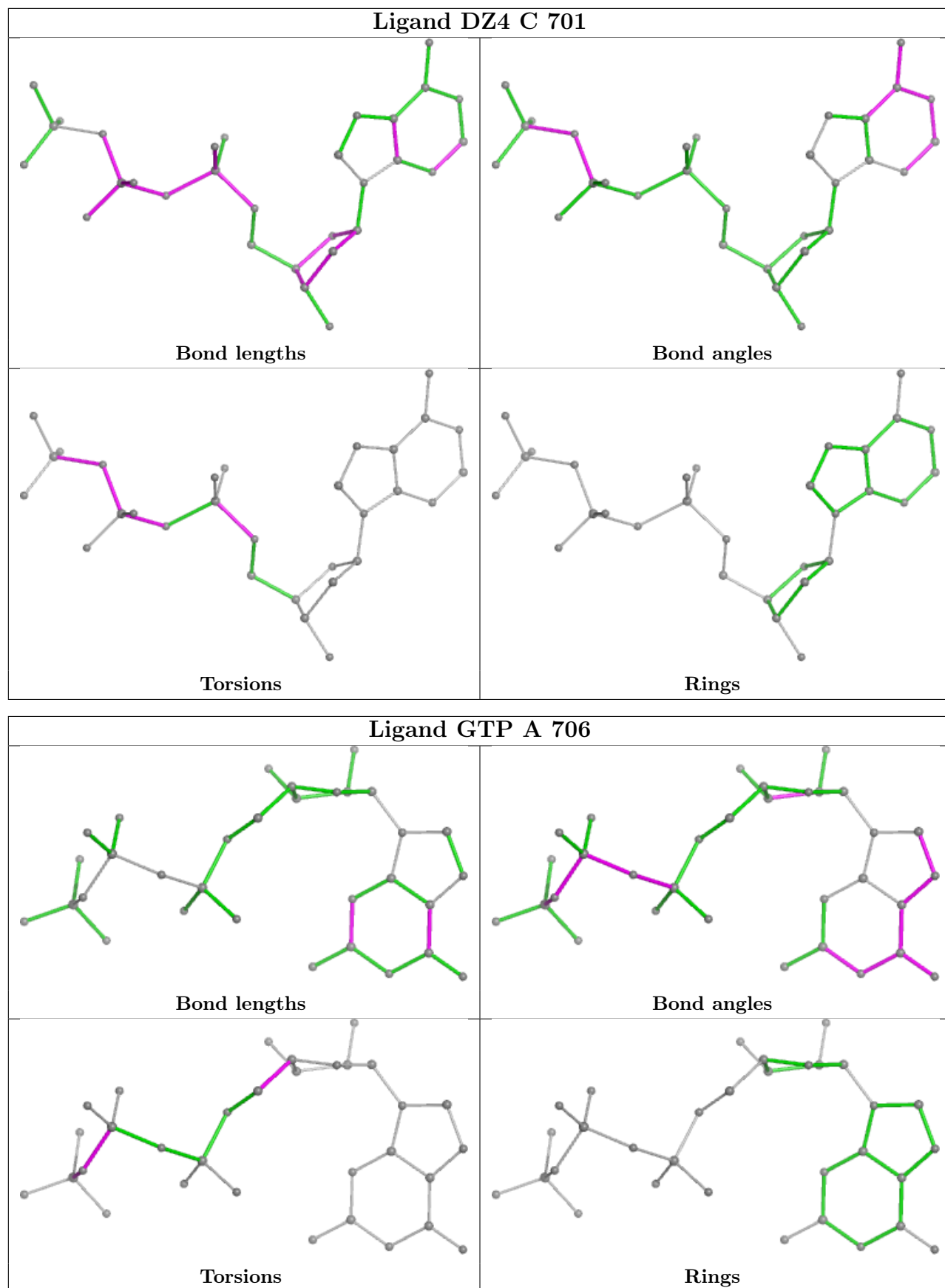
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	702	GTP	1	0
2	B	707	DZ4	2	0
5	A	706	GTP	2	0
2	A	707	DZ4	2	0
5	C	707	GTP	2	0
2	D	701	DZ4	1	0

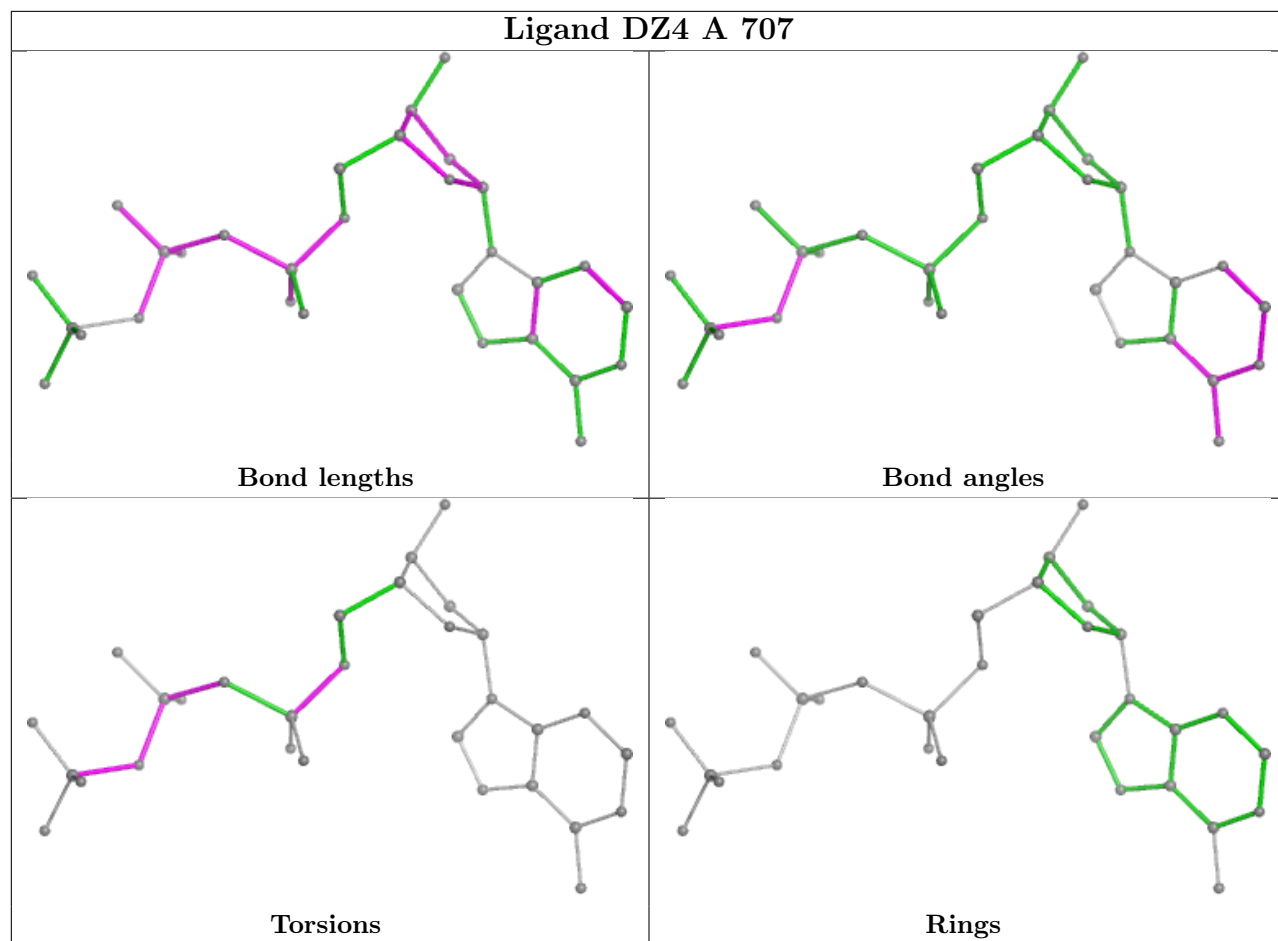
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

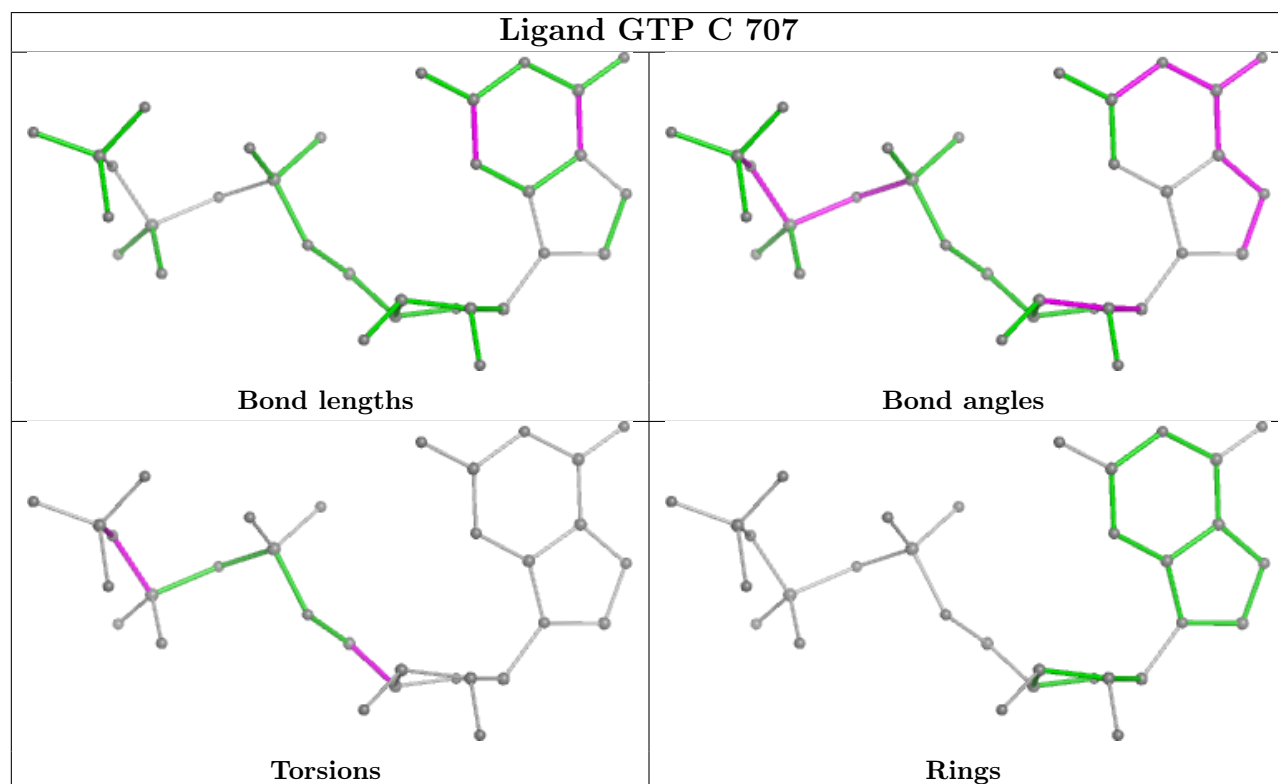
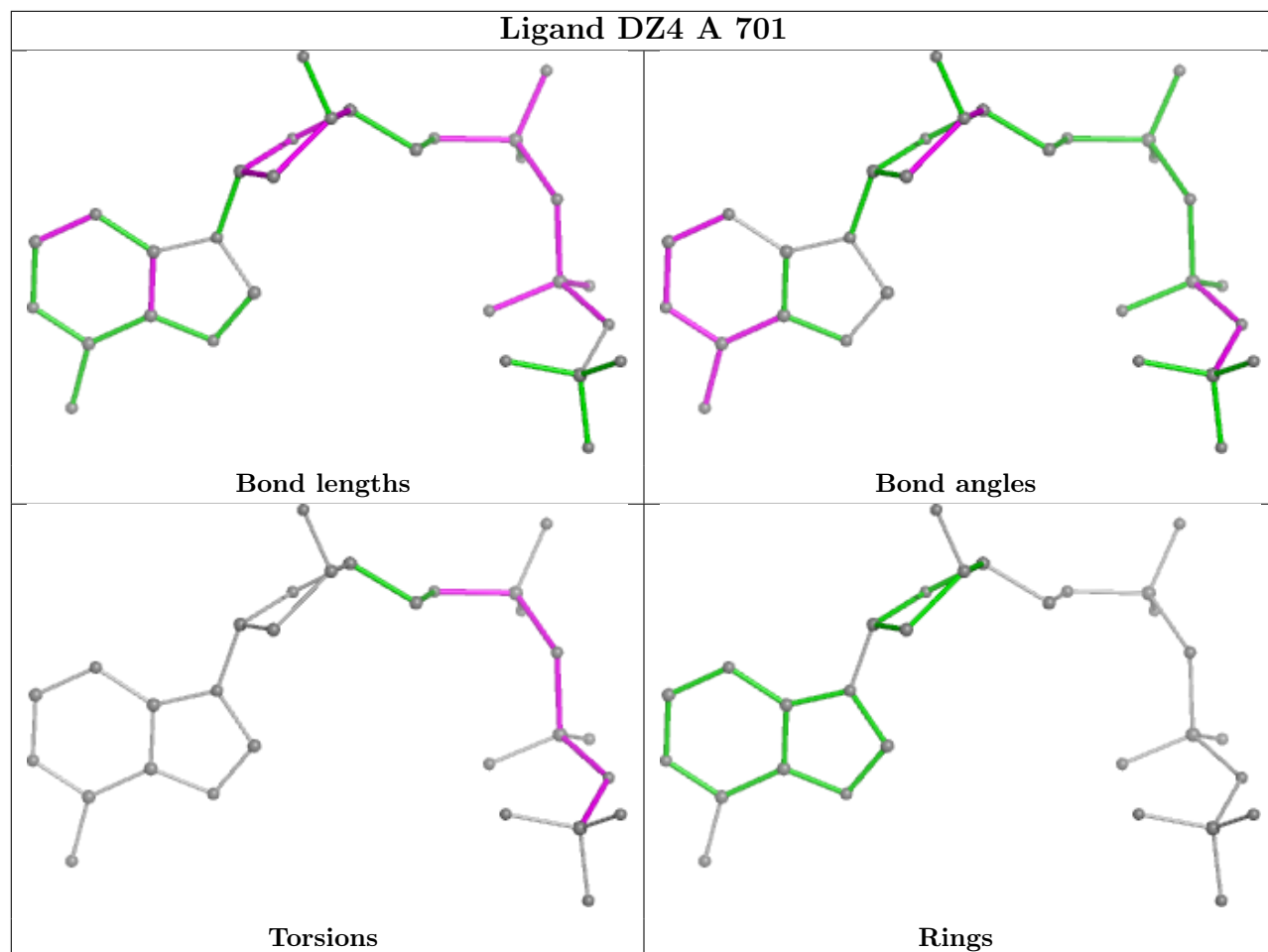


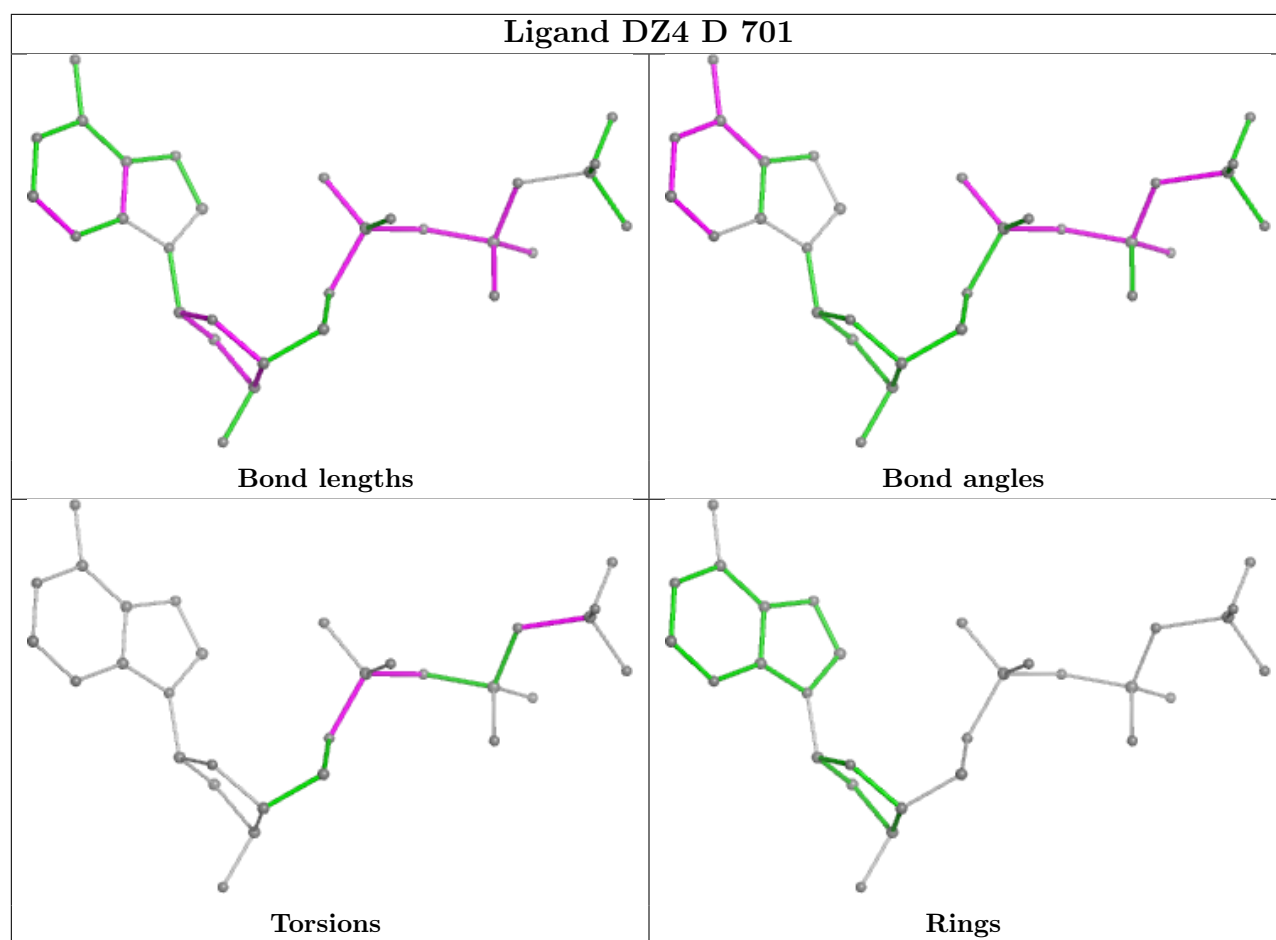












5.7 Other polymers [i](#)

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-18729. 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 standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 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.