



Full wwPDB EM Validation Report ⓘ

Apr 1, 2025 – 07:52 pm BST

PDB ID : 7ADB / pdb_00007adb
EMDB ID : EMD-11722
Title : Transcription termination intermediate complex 1 delta NusG
Authors : Said, N.; Hilal, T.; Loll, B.; Wahl, C.M.
Deposited on : 2020-09-14
Resolution : 4.40 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.dev117
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

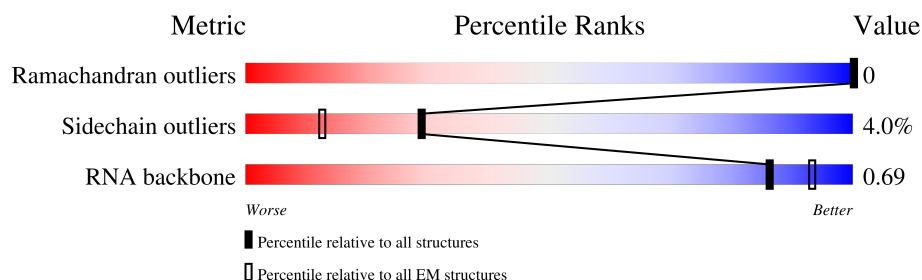
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.40 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)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	419	
1	b	419	
1	c	419	
1	d	419	
1	e	419	
1	f	419	
2	A	497	
3	U	329	
3	V	329	

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Mol	Chain	Length	Quality of chain
4	W	91	<div><div></div><div>87%13%</div></div>
5	X	1342	<div><div></div><div>100%</div></div>
6	Y	1416	<div><div></div><div>96%. </div></div>
7	K	50	<div><div></div><div>48%52%</div></div>
8	L	50	<div><div></div><div>68%32%</div></div>
9	R	99	<div><div></div><div>16%. 83%</div></div>

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 51330 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 Transcription termination factor Rho.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	417	Total	C	N	O	S	0	0
			3280	2065	581	617	17		
1	b	417	Total	C	N	O	S	0	0
			3280	2065	581	617	17		
1	c	417	Total	C	N	O	S	0	0
			3280	2065	581	617	17		
1	d	417	Total	C	N	O	S	0	0
			3280	2065	581	617	17		
1	e	417	Total	C	N	O	S	0	0
			3280	2065	581	617	17		
1	f	417	Total	C	N	O	S	0	0
			3280	2065	581	617	17		

- Molecule 2 is a protein called Transcription termination/antitermination protein NusA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	495	Total	C	N	O	S	0	0
			3852	2396	669	774	13		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP C3SSN7
A	0	ALA	-	expression tag	UNP C3SSN7

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	U	322	Total	C	N	O	S	0	0
			2510	1569	442	491	8		
3	V	235	Total	C	N	O	S	0	0
			1828	1137	326	359	6		

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	W	79	Total	C	N	O	S	0	0
			627	382	118	126	1		

- Molecule 5 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	X	1340	Total	C	N	O	S	0	0
			10567	6631	1841	2052	43		

- Molecule 6 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	Y	1358	Total	C	N	O	S	0	0
			10545	6620	1883	1992	50		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	1408	LEU	-	expression tag	UNP C3SIA2
Y	1409	GLU	-	expression tag	UNP C3SIA2
Y	1410	VAL	-	expression tag	UNP C3SIA2
Y	1411	HIS	-	expression tag	UNP C3SIA2
Y	1412	HIS	-	expression tag	UNP C3SIA2
Y	1413	HIS	-	expression tag	UNP C3SIA2
Y	1414	HIS	-	expression tag	UNP C3SIA2
Y	1415	HIS	-	expression tag	UNP C3SIA2
Y	1416	HIS	-	expression tag	UNP C3SIA2

- Molecule 7 is a DNA chain called ntDNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	K	24	Total	C	N	O	P	0	0
			497	235	95	143	24		

- Molecule 8 is a DNA chain called tDNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	L	34	Total	C	N	O	P	0	0
			682	325	122	202	33		

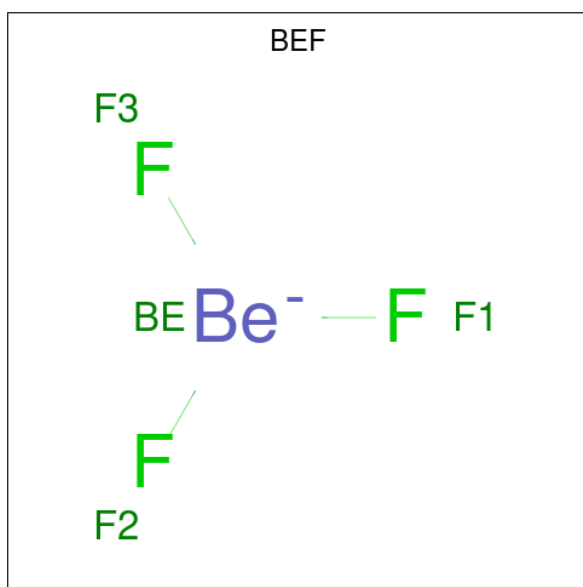
- Molecule 9 is a RNA chain called rut RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	R	17	Total 364	C 162	N 65	O 120	P 17	0	0

There are 27 discrepancies between the modelled and reference sequences:

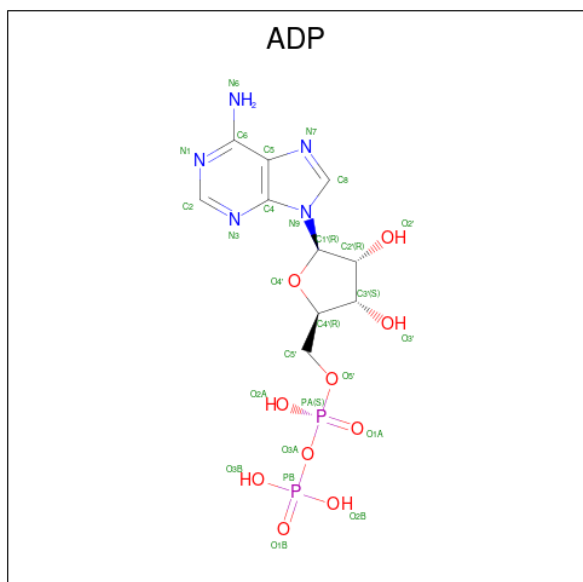
Chain	Residue	Modelled	Actual	Comment	Reference
R	1	G	-	expression tag	GB 1227111474
R	2	G	-	expression tag	GB 1227111474
R	3	G	-	expression tag	GB 1227111474
R	72	U	-	insertion	GB 1227111474
R	77	U	-	expression tag	GB 1227111474
R	78	U	-	expression tag	GB 1227111474
R	79	A	-	expression tag	GB 1227111474
R	80	A	-	expression tag	GB 1227111474
R	81	A	-	expression tag	GB 1227111474
R	82	C	-	expression tag	GB 1227111474
R	83	C	-	expression tag	GB 1227111474
R	84	A	-	expression tag	GB 1227111474
R	85	C	-	expression tag	GB 1227111474
R	86	A	-	expression tag	GB 1227111474
R	87	C	-	expression tag	GB 1227111474
R	88	C	-	expression tag	GB 1227111474
R	89	U	-	expression tag	GB 1227111474
R	90	G	-	expression tag	GB 1227111474
R	91	G	-	expression tag	GB 1227111474
R	92	C	-	expression tag	GB 1227111474
R	93	G	-	expression tag	GB 1227111474
R	94	U	-	expression tag	GB 1227111474
R	95	G	-	expression tag	GB 1227111474
R	96	U	-	expression tag	GB 1227111474
R	97	G	-	expression tag	GB 1227111474
R	98	G	-	expression tag	GB 1227111474
R	99	C	-	expression tag	GB 1227111474

- Molecule 10 is BERYLLIUM TRIFLUORIDE ION (CCD ID: BEF) (formula: BeF₃).



Mol	Chain	Residues	Atoms			AltConf
10	b	1	Total	Be	F	0
			4	1	3	
10	c	1	Total	Be	F	0
			4	1	3	
10	d	1	Total	Be	F	0
			4	1	3	
10	e	1	Total	Be	F	0
			4	1	3	
10	f	1	Total	Be	F	0
			4	1	3	

- Molecule 11 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms					AltConf
11	b	1	Total	C	N	O	P	0
			27	10	5	10	2	
11	c	1	Total	C	N	O	P	0
			27	10	5	10	2	
11	d	1	Total	C	N	O	P	0
			27	10	5	10	2	
11	e	1	Total	C	N	O	P	0
			27	10	5	10	2	
11	f	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 12 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
12	b	1	Total	Mg	0
			1	1	
12	c	1	Total	Mg	0
			1	1	
12	d	1	Total	Mg	0
			1	1	
12	e	1	Total	Mg	0
			1	1	
12	f	1	Total	Mg	0
			1	1	
12	Y	1	Total	Mg	0
			1	1	

- Molecule 13 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
13	Y	2	Total	Zn	0
			2	2	

- Molecule 14 is water.

Mol	Chain	Residues	Atoms		AltConf
14	b	3	Total	O	0
			3	3	
14	c	3	Total	O	0
			3	3	
14	d	3	Total	O	0
			3	3	

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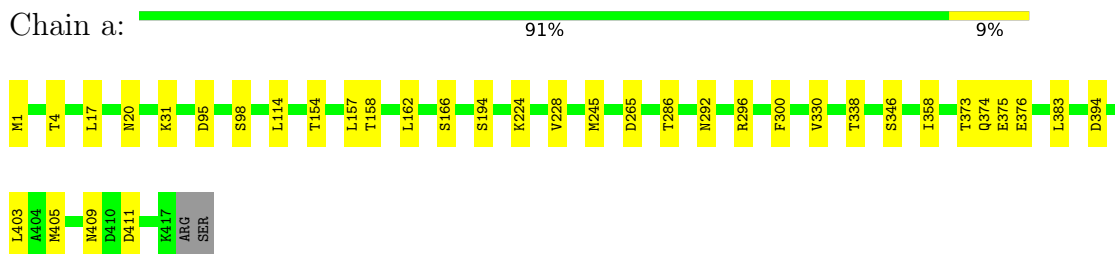
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Mol	Chain	Residues	Atoms		AltConf
14	e	3	Total	O	0
			3	3	
14	f	3	Total	O	0
			3	3	

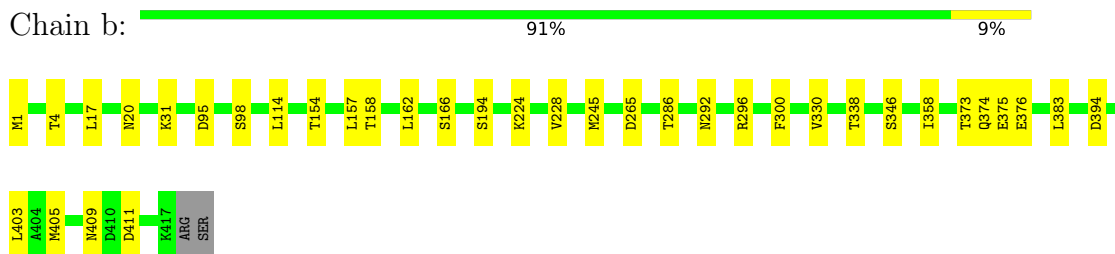
3 Residue-property plots [i](#)

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.

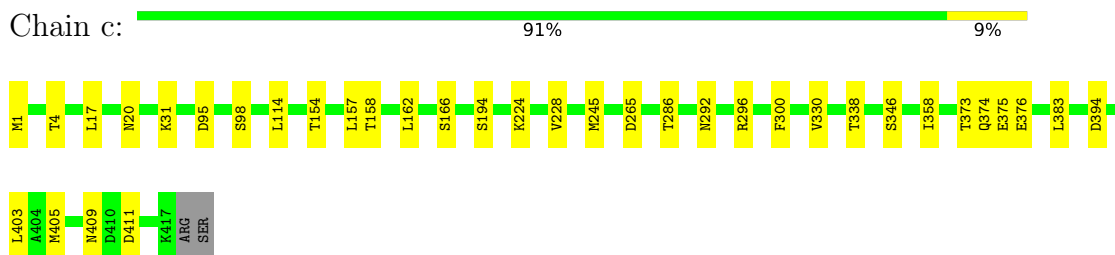
- Molecule 1: Transcription termination factor Rho



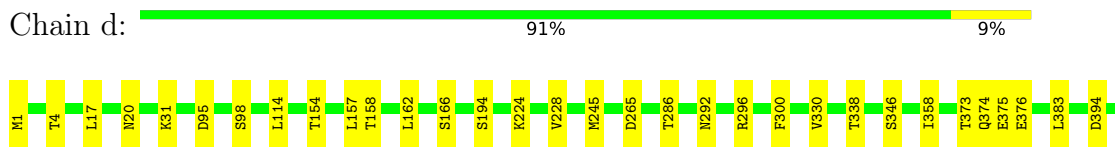
- Molecule 1: Transcription termination factor Rho

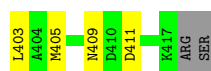


- Molecule 1: Transcription termination factor Rho



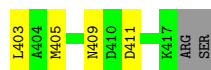
- Molecule 1: Transcription termination factor Rho





- Molecule 1: Transcription termination factor Rho

Chain e: 91% 9%



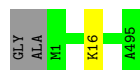
- Molecule 1: Transcription termination factor Rho

Chain f: 91% 9%



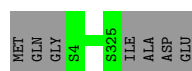
- Molecule 2: Transcription termination/antitermination protein NusA

Chain A: 99%



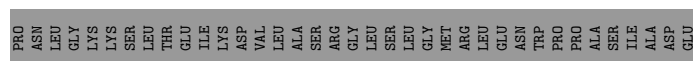
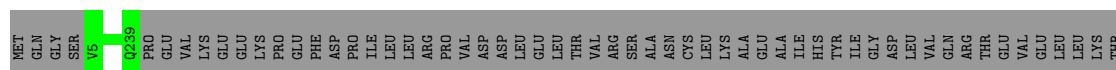
- Molecule 3: DNA-directed RNA polymerase subunit alpha

Chain U: 98%



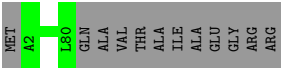
- Molecule 3: DNA-directed RNA polymerase subunit alpha

Chain V: 71% 29%



- Molecule 4: DNA-directed RNA polymerase subunit omega

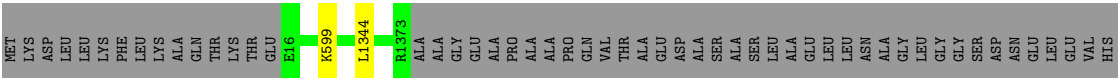
Chain W: 87% 13%



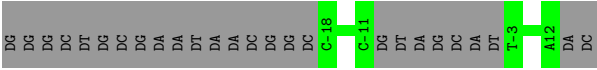
- Molecule 5: DNA-directed RNA polymerase subunit beta



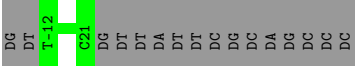
- Molecule 6: DNA-directed RNA polymerase subunit beta'



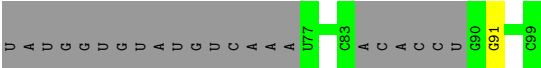
- Molecule 7: ntDNA



- Molecule 8: tDNA



- Molecule 9: rut RNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	27226	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	8000	Depositor
Maximum defocus (nm)	25000	Depositor
Magnification	31000	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: BEF, ADP, ZN, 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	0.28	0/3329	0.48	0/4483
1	b	0.28	0/3329	0.48	0/4483
1	c	0.28	0/3329	0.48	0/4483
1	d	0.28	0/3329	0.48	0/4483
1	e	0.28	0/3329	0.48	0/4483
1	f	0.28	0/3329	0.48	0/4483
2	A	0.25	0/3897	0.44	0/5273
3	U	0.23	0/2544	0.44	0/3449
3	V	0.24	0/1850	0.45	0/2507
4	W	0.23	0/629	0.43	0/847
5	X	0.25	0/10736	0.42	0/14487
6	Y	0.24	0/10706	0.42	1/14456 (0.0%)
7	K	0.55	0/557	0.94	0/856
8	L	0.53	0/762	0.88	0/1171
9	R	0.20	0/405	0.83	0/627
All	All	0.27	0/52060	0.47	1/70571 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	Y	1344	LEU	CA-CB-CG	5.13	127.10	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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 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	415/419 (99%)	397 (96%)	18 (4%)	0	100	100
1	b	415/419 (99%)	397 (96%)	18 (4%)	0	100	100
1	c	415/419 (99%)	397 (96%)	18 (4%)	0	100	100
1	d	415/419 (99%)	397 (96%)	18 (4%)	0	100	100
1	e	415/419 (99%)	397 (96%)	18 (4%)	0	100	100
1	f	415/419 (99%)	397 (96%)	18 (4%)	0	100	100
2	A	493/497 (99%)	453 (92%)	40 (8%)	0	100	100
3	U	320/329 (97%)	292 (91%)	28 (9%)	0	100	100
3	V	233/329 (71%)	218 (94%)	15 (6%)	0	100	100
4	W	77/91 (85%)	72 (94%)	5 (6%)	0	100	100
5	X	1338/1342 (100%)	1251 (94%)	87 (6%)	0	100	100
6	Y	1356/1416 (96%)	1302 (96%)	54 (4%)	0	100	100
All	All	6307/6518 (97%)	5970 (95%)	337 (5%)	0	100	100

There are no Ramachandran outliers to report.

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 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	357/359 (99%)	321 (90%)	36 (10%)	6	21
1	b	357/359 (99%)	321 (90%)	36 (10%)	6	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	c	357/359 (99%)	321 (90%)	36 (10%)	6	21
1	d	357/359 (99%)	321 (90%)	36 (10%)	6	21
1	e	357/359 (99%)	321 (90%)	36 (10%)	6	21
1	f	357/359 (99%)	321 (90%)	36 (10%)	6	21
2	A	409/409 (100%)	408 (100%)	1 (0%)	92	94
3	U	281/286 (98%)	281 (100%)	0	100	100
3	V	203/286 (71%)	203 (100%)	0	100	100
4	W	67/75 (89%)	67 (100%)	0	100	100
5	X	1155/1157 (100%)	1155 (100%)	0	100	100
6	Y	1134/1177 (96%)	1133 (100%)	1 (0%)	92	95
All	All	5391/5544 (97%)	5173 (96%)	218 (4%)	29	48

All (218) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	1	MET
1	a	4	THR
1	a	17	LEU
1	a	20	ASN
1	a	31	LYS
1	a	95	ASP
1	a	98	SER
1	a	114	LEU
1	a	154	THR
1	a	157	LEU
1	a	158	THR
1	a	162	LEU
1	a	166	SER
1	a	194	SER
1	a	224	LYS
1	a	228	VAL
1	a	245	MET
1	a	265	ASP
1	a	286	THR
1	a	292	ASN
1	a	296	ARG
1	a	300	PHE
1	a	330	VAL

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Mol	Chain	Res	Type
1	a	338	THR
1	a	346	SER
1	a	358	ILE
1	a	373	THR
1	a	374	GLN
1	a	375	GLU
1	a	376	GLU
1	a	383	LEU
1	a	394	ASP
1	a	403	LEU
1	a	405	MET
1	a	409	ASN
1	a	411	ASP
1	b	1	MET
1	b	4	THR
1	b	17	LEU
1	b	20	ASN
1	b	31	LYS
1	b	95	ASP
1	b	98	SER
1	b	114	LEU
1	b	154	THR
1	b	157	LEU
1	b	158	THR
1	b	162	LEU
1	b	166	SER
1	b	194	SER
1	b	224	LYS
1	b	228	VAL
1	b	245	MET
1	b	265	ASP
1	b	286	THR
1	b	292	ASN
1	b	296	ARG
1	b	300	PHE
1	b	330	VAL
1	b	338	THR
1	b	346	SER
1	b	358	ILE
1	b	373	THR
1	b	374	GLN
1	b	375	GLU

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Mol	Chain	Res	Type
1	b	376	GLU
1	b	383	LEU
1	b	394	ASP
1	b	403	LEU
1	b	405	MET
1	b	409	ASN
1	b	411	ASP
1	c	1	MET
1	c	4	THR
1	c	17	LEU
1	c	20	ASN
1	c	31	LYS
1	c	95	ASP
1	c	98	SER
1	c	114	LEU
1	c	154	THR
1	c	157	LEU
1	c	158	THR
1	c	162	LEU
1	c	166	SER
1	c	194	SER
1	c	224	LYS
1	c	228	VAL
1	c	245	MET
1	c	265	ASP
1	c	286	THR
1	c	292	ASN
1	c	296	ARG
1	c	300	PHE
1	c	330	VAL
1	c	338	THR
1	c	346	SER
1	c	358	ILE
1	c	373	THR
1	c	374	GLN
1	c	375	GLU
1	c	376	GLU
1	c	383	LEU
1	c	394	ASP
1	c	403	LEU
1	c	405	MET
1	c	409	ASN

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Mol	Chain	Res	Type
1	c	411	ASP
1	d	1	MET
1	d	4	THR
1	d	17	LEU
1	d	20	ASN
1	d	31	LYS
1	d	95	ASP
1	d	98	SER
1	d	114	LEU
1	d	154	THR
1	d	157	LEU
1	d	158	THR
1	d	162	LEU
1	d	166	SER
1	d	194	SER
1	d	224	LYS
1	d	228	VAL
1	d	245	MET
1	d	265	ASP
1	d	286	THR
1	d	292	ASN
1	d	296	ARG
1	d	300	PHE
1	d	330	VAL
1	d	338	THR
1	d	346	SER
1	d	358	ILE
1	d	373	THR
1	d	374	GLN
1	d	375	GLU
1	d	376	GLU
1	d	383	LEU
1	d	394	ASP
1	d	403	LEU
1	d	405	MET
1	d	409	ASN
1	d	411	ASP
1	e	1	MET
1	e	4	THR
1	e	17	LEU
1	e	20	ASN
1	e	31	LYS

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Mol	Chain	Res	Type
1	e	95	ASP
1	e	98	SER
1	e	114	LEU
1	e	154	THR
1	e	157	LEU
1	e	158	THR
1	e	162	LEU
1	e	166	SER
1	e	194	SER
1	e	224	LYS
1	e	228	VAL
1	e	245	MET
1	e	265	ASP
1	e	286	THR
1	e	292	ASN
1	e	296	ARG
1	e	300	PHE
1	e	330	VAL
1	e	338	THR
1	e	346	SER
1	e	358	ILE
1	e	373	THR
1	e	374	GLN
1	e	375	GLU
1	e	376	GLU
1	e	383	LEU
1	e	394	ASP
1	e	403	LEU
1	e	405	MET
1	e	409	ASN
1	e	411	ASP
1	f	1	MET
1	f	4	THR
1	f	17	LEU
1	f	20	ASN
1	f	31	LYS
1	f	95	ASP
1	f	98	SER
1	f	114	LEU
1	f	154	THR
1	f	157	LEU
1	f	158	THR

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Mol	Chain	Res	Type
1	f	162	LEU
1	f	166	SER
1	f	194	SER
1	f	224	LYS
1	f	228	VAL
1	f	245	MET
1	f	265	ASP
1	f	286	THR
1	f	292	ASN
1	f	296	ARG
1	f	300	PHE
1	f	330	VAL
1	f	338	THR
1	f	346	SER
1	f	358	ILE
1	f	373	THR
1	f	374	GLN
1	f	375	GLU
1	f	376	GLU
1	f	383	LEU
1	f	394	ASP
1	f	403	LEU
1	f	405	MET
1	f	409	ASN
1	f	411	ASP
2	A	16	LYS
6	Y	599	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	a	32	GLN
1	a	295	HIS
1	a	388	HIS
1	b	32	GLN
1	b	295	HIS
1	b	388	HIS
1	c	32	GLN
1	c	198	ASN
1	c	295	HIS
1	d	32	GLN
1	d	90	ASN

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Mol	Chain	Res	Type
1	e	32	GLN
1	e	140	HIS
1	e	295	HIS
1	e	388	HIS
1	f	32	GLN
1	f	295	HIS
2	A	48	GLN
2	A	96	GLN
2	A	129	GLN
2	A	157	ASN
2	A	260	GLN
2	A	303	HIS
2	A	321	ASN
2	A	324	ASN
2	A	412	ASN
3	U	227	GLN
4	W	29	GLN
5	X	139	ASN
5	X	193	ASN
5	X	513	GLN
5	X	684	ASN
5	X	688	GLN
5	X	798	GLN
5	X	799	ASN
5	X	932	GLN
5	X	1116	HIS
6	Y	365	GLN
6	Y	488	ASN
6	Y	739	GLN
6	Y	1049	GLN
6	Y	1295	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
9	R	15/99 (15%)	1 (6%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
9	R	91	G

There are no RNA pucker outliers to report.

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 8 are monoatomic - leaving 10 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	$\# Z > 2$
10	BEF	b	501	-	0,3,3	-	-	-		
11	ADP	b	502	1,12	24,29,29	0.97	1 (4%)	29,45,45	1.45	4 (13%)
11	ADP	d	1000	1,12	24,29,29	0.96	1 (4%)	29,45,45	1.49	4 (13%)
11	ADP	c	1000	1,12	24,29,29	0.95	1 (4%)	29,45,45	1.50	4 (13%)
11	ADP	f	1000	1	24,29,29	0.97	1 (4%)	29,45,45	1.42	4 (13%)
11	ADP	e	1000	12	24,29,29	0.95	1 (4%)	29,45,45	1.47	4 (13%)
10	BEF	e	1002	-	0,3,3	-	-	-		
10	BEF	f	1002	-	0,3,3	-	-	-		
10	BEF	c	1002	-	0,3,3	-	-	-		
10	BEF	d	1002	-	0,3,3	-	-	-		

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
11	ADP	d	1000	1,12	-	1/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	ADP	b	502	1,12	-	6/12/32/32	0/3/3/3
11	ADP	f	1000	1	-	2/12/32/32	0/3/3/3
11	ADP	c	1000	1,12	-	1/12/32/32	0/3/3/3
11	ADP	e	1000	12	-	1/12/32/32	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	b	502	ADP	C5-C4	2.56	1.47	1.40
11	f	1000	ADP	C5-C4	2.53	1.47	1.40
11	d	1000	ADP	C5-C4	2.51	1.47	1.40
11	e	1000	ADP	C5-C4	2.50	1.47	1.40
11	c	1000	ADP	C5-C4	2.48	1.47	1.40

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	e	1000	ADP	C3'-C2'-C1'	3.66	106.50	100.98
11	c	1000	ADP	C3'-C2'-C1'	3.60	106.40	100.98
11	d	1000	ADP	C3'-C2'-C1'	3.55	106.32	100.98
11	b	502	ADP	C3'-C2'-C1'	3.51	106.27	100.98
11	f	1000	ADP	C3'-C2'-C1'	3.46	106.19	100.98
11	d	1000	ADP	PA-O3A-PB	-3.36	121.29	132.83
11	c	1000	ADP	PA-O3A-PB	-3.26	121.63	132.83
11	c	1000	ADP	N3-C2-N1	-3.18	123.71	128.68
11	d	1000	ADP	N3-C2-N1	-3.17	123.73	128.68
11	e	1000	ADP	PA-O3A-PB	-3.17	121.96	132.83
11	f	1000	ADP	N3-C2-N1	-3.15	123.75	128.68
11	e	1000	ADP	N3-C2-N1	-3.13	123.78	128.68
11	b	502	ADP	N3-C2-N1	-3.08	123.86	128.68
11	b	502	ADP	PA-O3A-PB	-3.04	122.39	132.83
11	f	1000	ADP	PA-O3A-PB	-3.03	122.42	132.83
11	d	1000	ADP	C4-C5-N7	-2.65	106.64	109.40
11	c	1000	ADP	C4-C5-N7	-2.64	106.65	109.40
11	f	1000	ADP	C4-C5-N7	-2.63	106.66	109.40
11	e	1000	ADP	C4-C5-N7	-2.62	106.67	109.40
11	b	502	ADP	C4-C5-N7	-2.55	106.74	109.40

There are no chirality outliers.

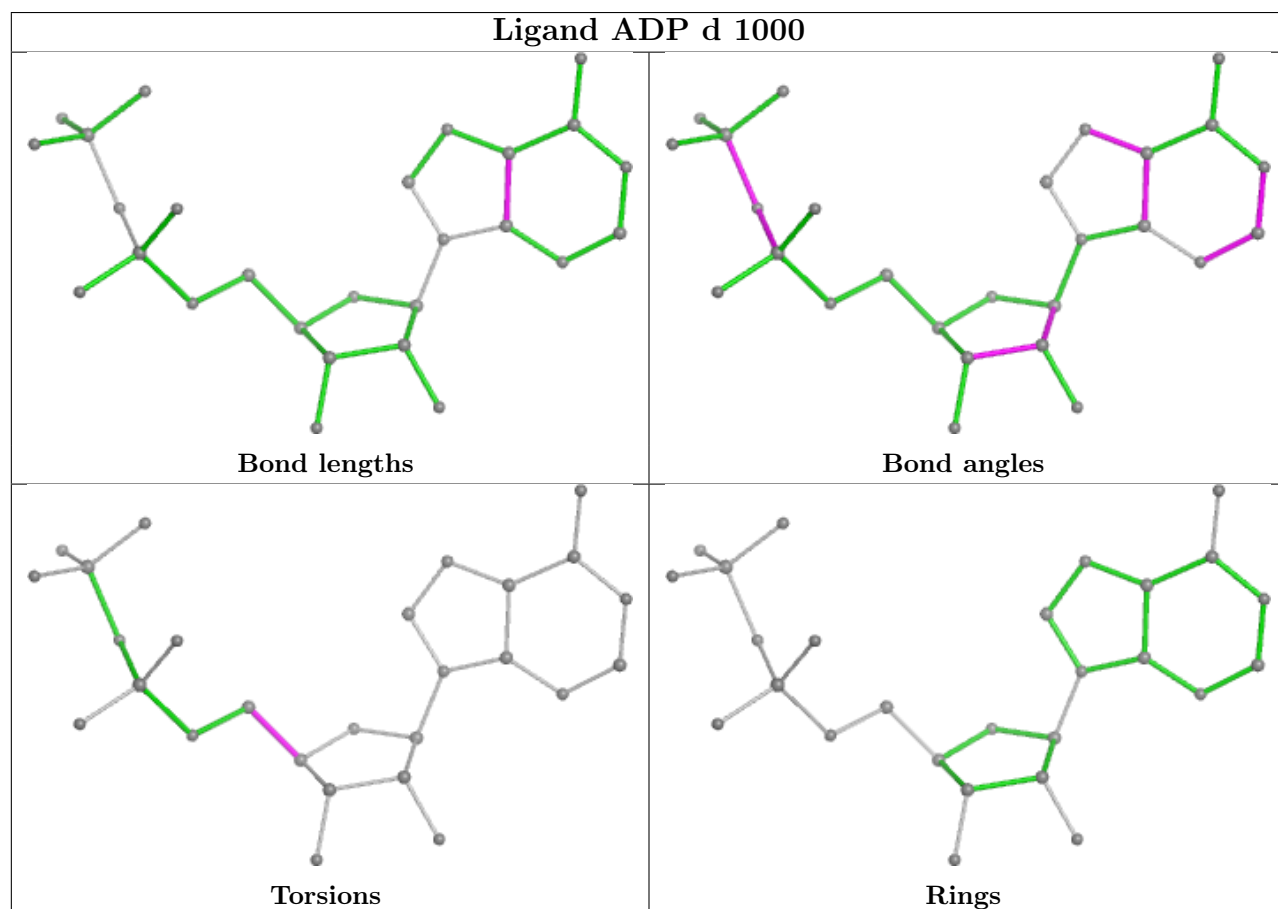
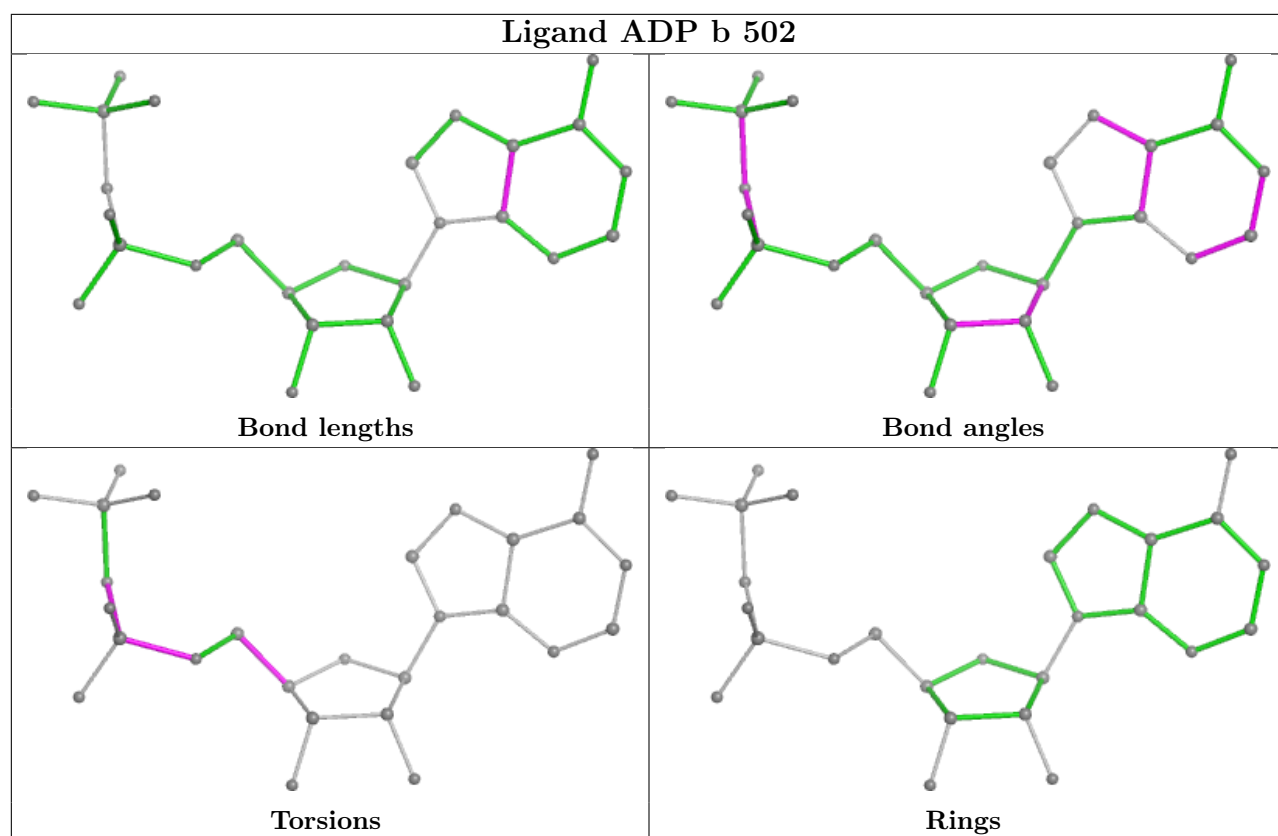
All (11) torsion outliers are listed below:

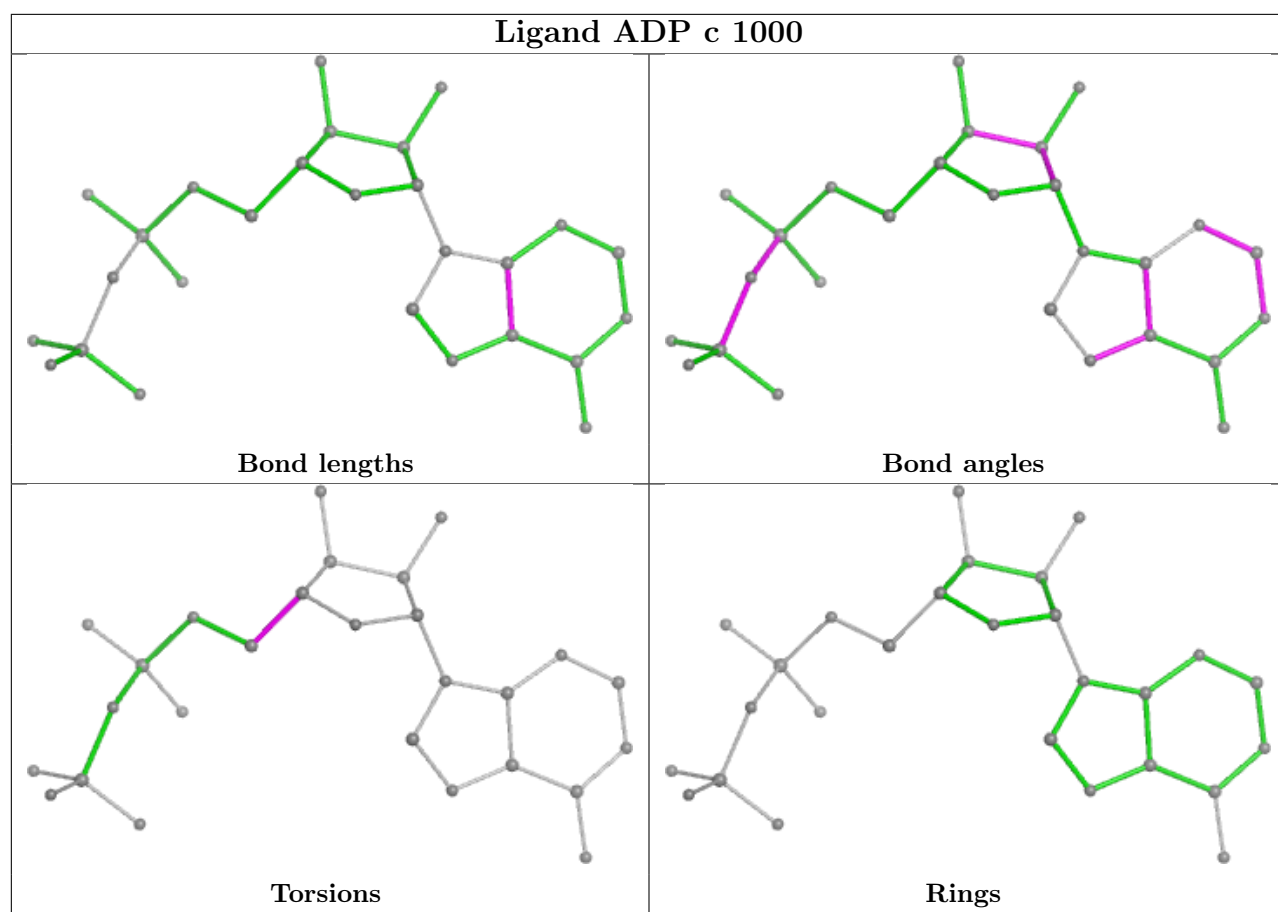
Mol	Chain	Res	Type	Atoms
11	b	502	ADP	C5'-O5'-PA-O2A
11	b	502	ADP	C5'-O5'-PA-O3A
11	f	1000	ADP	O4'-C4'-C5'-O5'
11	b	502	ADP	PB-O3A-PA-O1A
11	b	502	ADP	O4'-C4'-C5'-O5'
11	f	1000	ADP	PB-O3A-PA-O2A
11	b	502	ADP	C5'-O5'-PA-O1A
11	b	502	ADP	PB-O3A-PA-O2A
11	d	1000	ADP	O4'-C4'-C5'-O5'
11	e	1000	ADP	O4'-C4'-C5'-O5'
11	c	1000	ADP	O4'-C4'-C5'-O5'

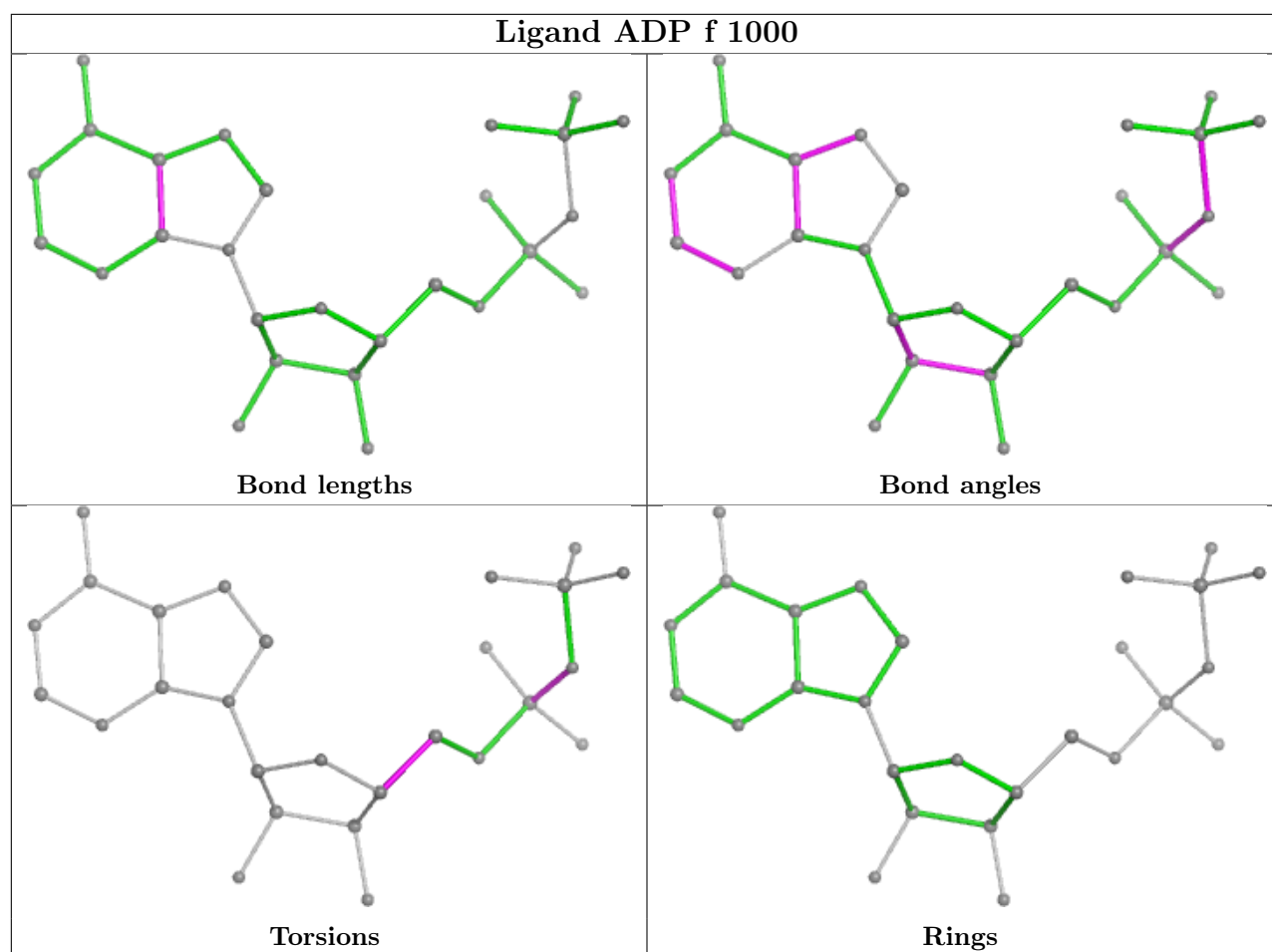
There are no ring outliers.

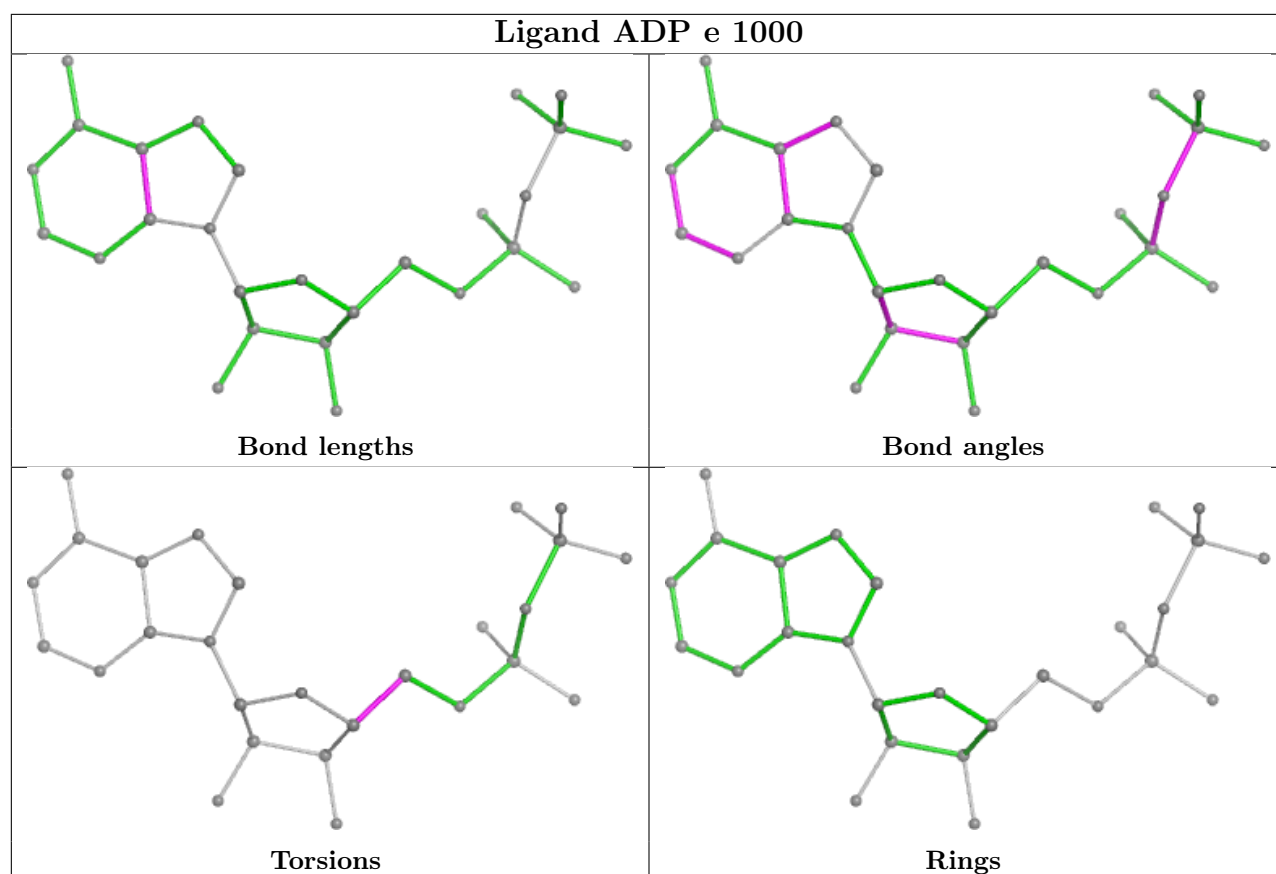
No monomer is involved in short contacts.

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-11722. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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.