



Full wwPDB EM Validation Report ⓘ

Apr 2, 2025 – 01:53 am BST

PDB ID : 6Z9T / pdb_00006z9t
EMDB ID : EMD-11091
Title : Transcription termination intermediate complex 5
Authors : Said, N.; Hilal, T.; Loll, B.; Wahl, M.C.
Deposited on : 2020-06-04
Resolution : 4.10 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

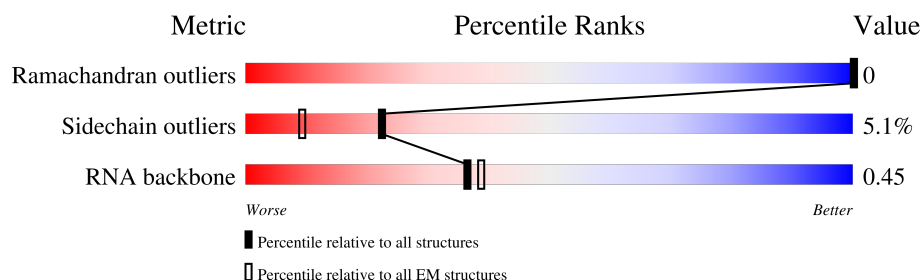
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.10 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	89% 11%
1	b	419	89% 11%
1	c	419	89% 10%
1	d	419	89% 11%
1	e	419	89% 11%
1	f	419	89% 11%
2	A	497	99%
3	U	329	71% 29%
3	V	329	98% .

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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>95%5%</div></div>
7	L	53	<div><div></div><div>64%32%</div></div>
8	K	50	<div><div></div><div>42%58%</div></div>
9	R	99	<div><div></div><div>19%8%72%</div></div>

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 51415 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	f	417	Total	C	N	O	S	0	0
			3280	2065	581	617	17		
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		

- 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
			3850	2395	669	773	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	235	Total	C	N	O	S	0	0
			1825	1135	325	359	6		
3	V	321	Total	C	N	O	S	0	0
			2504	1566	441	489	8		

- 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	1343	Total	C	N	O	S	0	0
			10433	6550	1862	1971	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 template strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	L	36	Total	C	N	O	P	0	0
			724	345	129	215	35		

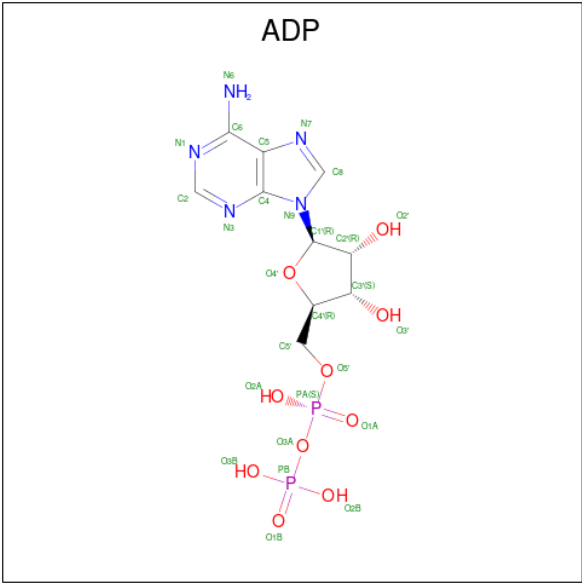
- Molecule 8 is a DNA chain called non template strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	K	21	Total	C	N	O	P	0	0
			437	205	86	125	21		

- Molecule 9 is a RNA chain called rut RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	R	28	Total	C	N	O	P	0	0
			590	264	103	195	28		

- Molecule 10 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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

- Molecule 11 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

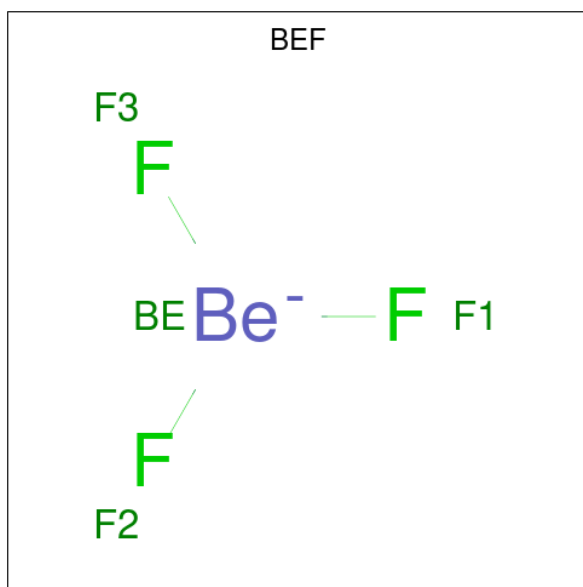
Mol	Chain	Residues	Atoms		AltConf
11	a	1	Total	Mg	0
			1	1	
11	b	1	Total	Mg	0
			1	1	
11	c	1	Total	Mg	0
			1	1	
11	d	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
11	e	1	Total	Mg	0
			1	1	
11	Y	1	Total	Mg	0
			1	1	

- Molecule 12 is BERYLLIUM TRIFLUORIDE ION (CCD ID: BEF) (formula: BeF₃).



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

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

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

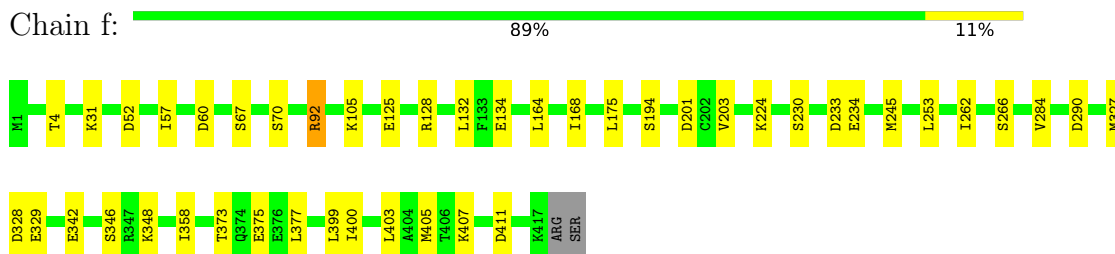
- Molecule 14 is water.

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

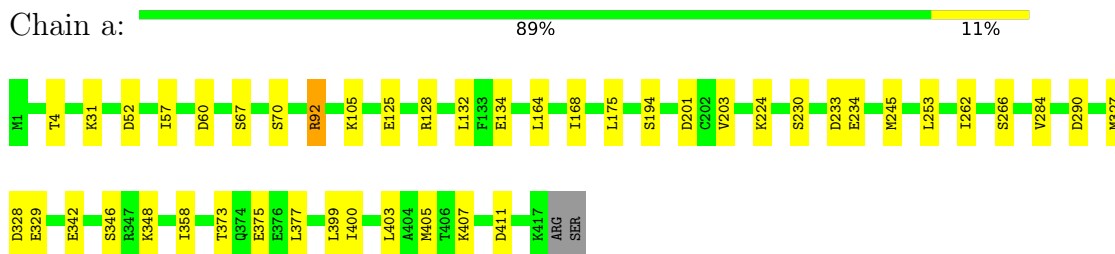
3 Residue-property plots

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.

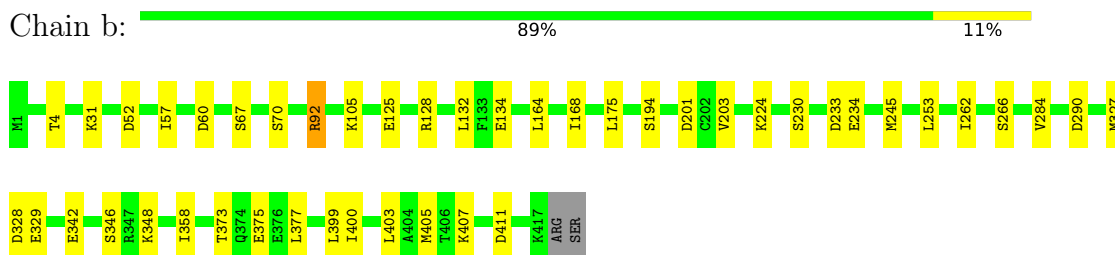
- Molecule 1: Transcription termination factor Rho



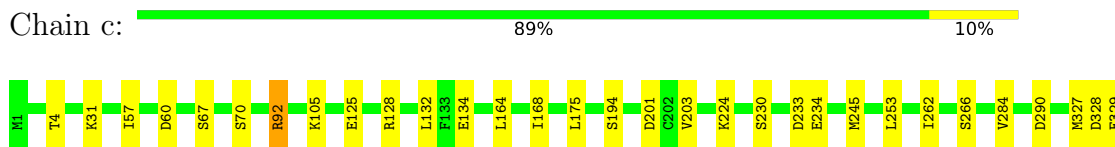
- Molecule 1: Transcription termination factor Rho



- Molecule 1: Transcription termination factor Rho



- Molecule 1: Transcription termination factor Rho





- Molecule 1: Transcription termination factor Rho

Chain d: 89% 11%



- Molecule 1: Transcription termination factor Rho

Chain e: 89% 11%



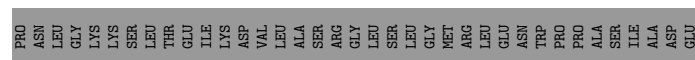
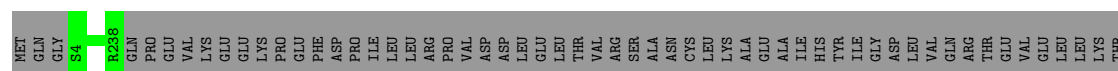
- Molecule 2: Transcription termination/antitermination protein NusA

Chain A: 99%



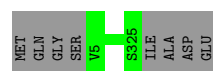
- Molecule 3: DNA-directed RNA polymerase subunit alpha

Chain U: 71% 29%



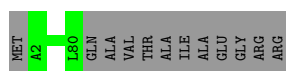
- Molecule 3: DNA-directed RNA polymerase subunit alpha

Chain V: 98%



- Molecule 4: DNA-directed RNA polymerase subunit omega

Chain W: 87% 13%



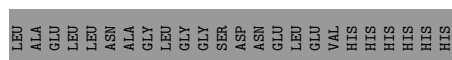
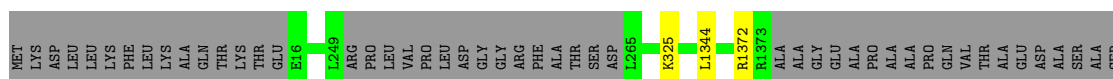
- Molecule 5: DNA-directed RNA polymerase subunit beta

Chain X: 100%



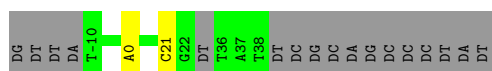
- Molecule 6: DNA-directed RNA polymerase subunit beta'

Chain Y: 95%



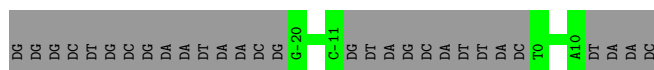
- Molecule 7: template strand

Chain L: 64%



- Molecule 8: non template strand

Chain K: 42%



- Molecule 9: rut RNA

Chain R: 19%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	38054	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)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
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, MG, ZN, ADP

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	0.27	0/3329	0.49	1/4483 (0.0%)
1	b	0.27	0/3329	0.49	1/4483 (0.0%)
1	c	0.27	0/3329	0.49	1/4483 (0.0%)
1	d	0.27	0/3329	0.49	1/4483 (0.0%)
1	e	0.27	0/3329	0.49	1/4483 (0.0%)
1	f	0.27	0/3329	0.49	1/4483 (0.0%)
2	A	0.24	0/3895	0.45	0/5270
3	U	0.23	0/1847	0.42	0/2503
3	V	0.23	0/2538	0.46	0/3441
4	W	0.22	0/629	0.39	0/847
5	X	0.25	0/10736	0.42	0/14487
6	Y	0.24	0/10590	0.43	1/14296 (0.0%)
7	L	0.66	1/807 (0.1%)	0.95	1/1236 (0.1%)
8	K	0.46	0/490	0.81	0/753
9	R	0.25	0/656	1.03	3/1016 (0.3%)
All	All	0.27	1/52162 (0.0%)	0.49	11/70747 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	L	21	DC	O3'-P	12.04	1.75	1.61

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	L	0	DA	O4'-C1'-N9	7.73	113.41	108.00
1	e	92	ARG	NE-CZ-NH2	6.93	123.77	120.30
1	b	92	ARG	NE-CZ-NH2	6.91	123.76	120.30
1	c	92	ARG	NE-CZ-NH2	6.89	123.75	120.30
1	a	92	ARG	NE-CZ-NH2	6.88	123.74	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	d	92	ARG	NE-CZ-NH2	6.88	123.74	120.30
1	f	92	ARG	NE-CZ-NH2	6.83	123.72	120.30
9	R	88	C	C2-N1-C1'	6.66	126.12	118.80
9	R	88	C	N1-C2-O2	6.54	122.82	118.90
9	R	88	C	N3-C2-O2	-5.38	118.13	121.90
6	Y	1344	LEU	CA-CB-CG	5.06	126.94	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 [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	415/419 (99%)	402 (97%)	13 (3%)	0	100	100
1	b	415/419 (99%)	402 (97%)	13 (3%)	0	100	100
1	c	415/419 (99%)	402 (97%)	13 (3%)	0	100	100
1	d	415/419 (99%)	401 (97%)	14 (3%)	0	100	100
1	e	415/419 (99%)	402 (97%)	13 (3%)	0	100	100
1	f	415/419 (99%)	402 (97%)	13 (3%)	0	100	100
2	A	493/497 (99%)	448 (91%)	45 (9%)	0	100	100
3	U	233/329 (71%)	224 (96%)	9 (4%)	0	100	100
3	V	319/329 (97%)	295 (92%)	24 (8%)	0	100	100
4	W	77/91 (85%)	75 (97%)	2 (3%)	0	100	100
5	X	1338/1342 (100%)	1255 (94%)	83 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	Y	1339/1416 (95%)	1257 (94%)	82 (6%)	0	100	100
All	All	6289/6518 (96%)	5965 (95%)	324 (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%)	312 (87%)	45 (13%)	3	17
1	b	357/359 (99%)	312 (87%)	45 (13%)	3	17
1	c	357/359 (99%)	313 (88%)	44 (12%)	4	18
1	d	357/359 (99%)	312 (87%)	45 (13%)	3	17
1	e	357/359 (99%)	312 (87%)	45 (13%)	3	17
1	f	357/359 (99%)	312 (87%)	45 (13%)	3	17
2	A	408/409 (100%)	407 (100%)	1 (0%)	92	94
3	U	203/286 (71%)	203 (100%)	0	100	100
3	V	280/286 (98%)	280 (100%)	0	100	100
4	W	67/75 (89%)	67 (100%)	0	100	100
5	X	1155/1157 (100%)	1151 (100%)	4 (0%)	91	92
6	Y	1122/1177 (95%)	1120 (100%)	2 (0%)	92	94
All	All	5377/5544 (97%)	5101 (95%)	276 (5%)	22	43

All (276) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	f	4	THR
1	f	31	LYS
1	f	52	ASP
1	f	57	ILE
1	f	60	ASP

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Mol	Chain	Res	Type
1	f	67	SER
1	f	70	SER
1	f	92	ARG
1	f	105	LYS
1	f	125	GLU
1	f	128	ARG
1	f	132	LEU
1	f	134	GLU
1	f	164	LEU
1	f	168	ILE
1	f	175	LEU
1	f	194	SER
1	f	201	ASP
1	f	203	VAL
1	f	224	LYS
1	f	230	SER
1	f	233	ASP
1	f	234	GLU
1	f	245	MET
1	f	253	LEU
1	f	262	ILE
1	f	266	SER
1	f	284	VAL
1	f	290	ASP
1	f	327	MET
1	f	328	ASP
1	f	329	GLU
1	f	342	GLU
1	f	346	SER
1	f	348	LYS
1	f	358	ILE
1	f	373	THR
1	f	375	GLU
1	f	377	LEU
1	f	399	LEU
1	f	400	ILE
1	f	403	LEU
1	f	405	MET
1	f	407	LYS
1	f	411	ASP
1	a	4	THR
1	a	31	LYS

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Mol	Chain	Res	Type
1	a	52	ASP
1	a	57	ILE
1	a	60	ASP
1	a	67	SER
1	a	70	SER
1	a	92	ARG
1	a	105	LYS
1	a	125	GLU
1	a	128	ARG
1	a	132	LEU
1	a	134	GLU
1	a	164	LEU
1	a	168	ILE
1	a	175	LEU
1	a	194	SER
1	a	201	ASP
1	a	203	VAL
1	a	224	LYS
1	a	230	SER
1	a	233	ASP
1	a	234	GLU
1	a	245	MET
1	a	253	LEU
1	a	262	ILE
1	a	266	SER
1	a	284	VAL
1	a	290	ASP
1	a	327	MET
1	a	328	ASP
1	a	329	GLU
1	a	342	GLU
1	a	346	SER
1	a	348	LYS
1	a	358	ILE
1	a	373	THR
1	a	375	GLU
1	a	377	LEU
1	a	399	LEU
1	a	400	ILE
1	a	403	LEU
1	a	405	MET
1	a	407	LYS

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Mol	Chain	Res	Type
1	a	411	ASP
1	b	4	THR
1	b	31	LYS
1	b	52	ASP
1	b	57	ILE
1	b	60	ASP
1	b	67	SER
1	b	70	SER
1	b	92	ARG
1	b	105	LYS
1	b	125	GLU
1	b	128	ARG
1	b	132	LEU
1	b	134	GLU
1	b	164	LEU
1	b	168	ILE
1	b	175	LEU
1	b	194	SER
1	b	201	ASP
1	b	203	VAL
1	b	224	LYS
1	b	230	SER
1	b	233	ASP
1	b	234	GLU
1	b	245	MET
1	b	253	LEU
1	b	262	ILE
1	b	266	SER
1	b	284	VAL
1	b	290	ASP
1	b	327	MET
1	b	328	ASP
1	b	329	GLU
1	b	342	GLU
1	b	346	SER
1	b	348	LYS
1	b	358	ILE
1	b	373	THR
1	b	375	GLU
1	b	377	LEU
1	b	399	LEU
1	b	400	ILE

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Mol	Chain	Res	Type
1	b	403	LEU
1	b	405	MET
1	b	407	LYS
1	b	411	ASP
1	c	4	THR
1	c	31	LYS
1	c	57	ILE
1	c	60	ASP
1	c	67	SER
1	c	70	SER
1	c	92	ARG
1	c	105	LYS
1	c	125	GLU
1	c	128	ARG
1	c	132	LEU
1	c	134	GLU
1	c	164	LEU
1	c	168	ILE
1	c	175	LEU
1	c	194	SER
1	c	201	ASP
1	c	203	VAL
1	c	224	LYS
1	c	230	SER
1	c	233	ASP
1	c	234	GLU
1	c	245	MET
1	c	253	LEU
1	c	262	ILE
1	c	266	SER
1	c	284	VAL
1	c	290	ASP
1	c	327	MET
1	c	328	ASP
1	c	329	GLU
1	c	342	GLU
1	c	346	SER
1	c	348	LYS
1	c	358	ILE
1	c	373	THR
1	c	375	GLU
1	c	377	LEU

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Mol	Chain	Res	Type
1	c	399	LEU
1	c	400	ILE
1	c	403	LEU
1	c	405	MET
1	c	407	LYS
1	c	411	ASP
1	d	4	THR
1	d	31	LYS
1	d	52	ASP
1	d	57	ILE
1	d	60	ASP
1	d	67	SER
1	d	70	SER
1	d	92	ARG
1	d	105	LYS
1	d	125	GLU
1	d	128	ARG
1	d	132	LEU
1	d	134	GLU
1	d	164	LEU
1	d	168	ILE
1	d	175	LEU
1	d	194	SER
1	d	201	ASP
1	d	203	VAL
1	d	224	LYS
1	d	230	SER
1	d	233	ASP
1	d	234	GLU
1	d	245	MET
1	d	253	LEU
1	d	262	ILE
1	d	266	SER
1	d	284	VAL
1	d	290	ASP
1	d	327	MET
1	d	328	ASP
1	d	329	GLU
1	d	342	GLU
1	d	346	SER
1	d	348	LYS
1	d	358	ILE

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Mol	Chain	Res	Type
1	d	373	THR
1	d	375	GLU
1	d	377	LEU
1	d	399	LEU
1	d	400	ILE
1	d	403	LEU
1	d	405	MET
1	d	407	LYS
1	d	411	ASP
1	e	4	THR
1	e	31	LYS
1	e	52	ASP
1	e	57	ILE
1	e	60	ASP
1	e	67	SER
1	e	70	SER
1	e	92	ARG
1	e	105	LYS
1	e	125	GLU
1	e	128	ARG
1	e	132	LEU
1	e	134	GLU
1	e	164	LEU
1	e	168	ILE
1	e	175	LEU
1	e	194	SER
1	e	201	ASP
1	e	203	VAL
1	e	224	LYS
1	e	230	SER
1	e	233	ASP
1	e	234	GLU
1	e	245	MET
1	e	253	LEU
1	e	262	ILE
1	e	266	SER
1	e	284	VAL
1	e	290	ASP
1	e	327	MET
1	e	328	ASP
1	e	329	GLU
1	e	342	GLU

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Mol	Chain	Res	Type
1	e	346	SER
1	e	348	LYS
1	e	358	ILE
1	e	373	THR
1	e	375	GLU
1	e	377	LEU
1	e	399	LEU
1	e	400	ILE
1	e	403	LEU
1	e	405	MET
1	e	407	LYS
1	e	411	ASP
2	A	16	LYS
5	X	202	ARG
5	X	265	LYS
5	X	919	ARG
5	X	1156	ARG
6	Y	325	LYS
6	Y	1372	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (71) such sidechains are listed below:

Mol	Chain	Res	Type
1	f	117	ASN
1	f	275	ASN
1	f	292	ASN
1	f	401	ASN
1	a	25	ASN
1	a	117	ASN
1	a	275	ASN
1	a	292	ASN
1	a	401	ASN
1	b	117	ASN
1	b	275	ASN
1	b	292	ASN
1	b	401	ASN
1	c	117	ASN
1	c	275	ASN
1	c	292	ASN
1	c	401	ASN
1	d	117	ASN
1	d	275	ASN

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Mol	Chain	Res	Type
1	d	292	ASN
1	d	401	ASN
1	e	117	ASN
1	e	275	ASN
1	e	292	ASN
1	e	401	ASN
2	A	14	ASN
2	A	48	GLN
2	A	70	GLN
2	A	129	GLN
2	A	157	ASN
2	A	323	GLN
2	A	330	GLN
2	A	349	GLN
2	A	353	HIS
2	A	421	GLN
3	U	132	HIS
3	U	147	GLN
3	V	93	GLN
4	W	43	ASN
4	W	70	GLN
5	X	41	GLN
5	X	46	GLN
5	X	214	ASN
5	X	276	GLN
5	X	314	ASN
5	X	343	HIS
5	X	604	HIS
5	X	618	GLN
5	X	659	GLN
5	X	737	ASN
5	X	760	ASN
5	X	932	GLN
5	X	1008	GLN
5	X	1010	GLN
5	X	1013	GLN
5	X	1061	GLN
5	X	1209	GLN
5	X	1324	ASN
6	Y	113	HIS
6	Y	232	ASN
6	Y	266	ASN

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Mol	Chain	Res	Type
6	Y	340	GLN
6	Y	365	GLN
6	Y	435	GLN
6	Y	545	HIS
6	Y	665	GLN
6	Y	669	GLN
6	Y	861	ASN
6	Y	910	ASN
6	Y	1108	GLN
6	Y	1367	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
9	R	26/99 (26%)	9 (34%)	2 (7%)

All (9) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
9	R	23	U
9	R	24	U
9	R	25	C
9	R	26	C
9	R	84	A
9	R	86	A
9	R	88	C
9	R	90	G
9	R	91	G

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
9	R	23	U
9	R	90	G

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [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	$\# Z > 2$
12	BEF	e	1002	-	0,3,3	-	-	-		
10	ADP	e	1000	11	24,29,29	0.95	1 (4%)	29,45,45	1.52	4 (13%)
10	ADP	d	1000	11	24,29,29	0.97	1 (4%)	29,45,45	1.49	4 (13%)
12	BEF	a	1002	-	0,3,3	-	-	-		
10	ADP	a	1000	11	24,29,29	0.96	1 (4%)	29,45,45	1.47	4 (13%)
10	ADP	b	1000	11	24,29,29	0.96	1 (4%)	29,45,45	1.53	4 (13%)
12	BEF	c	1002	-	0,3,3	-	-	-		
12	BEF	d	1002	-	0,3,3	-	-	-		
10	ADP	c	1000	11	24,29,29	0.99	1 (4%)	29,45,45	1.58	5 (17%)
12	BEF	b	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
10	ADP	e	1000	11	-	2/12/32/32	0/3/3/3
10	ADP	d	1000	11	-	2/12/32/32	0/3/3/3
10	ADP	a	1000	11	-	2/12/32/32	0/3/3/3
10	ADP	b	1000	11	-	2/12/32/32	0/3/3/3
10	ADP	c	1000	11	-	2/12/32/32	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	c	1000	ADP	C5-C4	2.55	1.47	1.40
10	d	1000	ADP	C5-C4	2.52	1.47	1.40
10	a	1000	ADP	C5-C4	2.50	1.47	1.40
10	e	1000	ADP	C5-C4	2.50	1.47	1.40
10	b	1000	ADP	C5-C4	2.48	1.47	1.40

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	b	1000	ADP	PA-O3A-PB	-4.03	118.99	132.83
10	c	1000	ADP	C3'-C2'-C1'	3.93	106.89	100.98
10	e	1000	ADP	PA-O3A-PB	-3.91	119.42	132.83
10	c	1000	ADP	PA-O3A-PB	-3.78	119.84	132.83
10	a	1000	ADP	C3'-C2'-C1'	3.66	106.49	100.98
10	e	1000	ADP	C3'-C2'-C1'	3.54	106.31	100.98
10	d	1000	ADP	C3'-C2'-C1'	3.52	106.28	100.98
10	d	1000	ADP	PA-O3A-PB	-3.52	120.75	132.83
10	d	1000	ADP	N3-C2-N1	-3.23	123.63	128.68
10	e	1000	ADP	N3-C2-N1	-3.22	123.64	128.68
10	b	1000	ADP	N3-C2-N1	-3.22	123.65	128.68
10	b	1000	ADP	C3'-C2'-C1'	3.21	105.82	100.98
10	a	1000	ADP	N3-C2-N1	-3.07	123.89	128.68
10	a	1000	ADP	PA-O3A-PB	-3.03	122.42	132.83
10	c	1000	ADP	N3-C2-N1	-2.98	124.01	128.68
10	a	1000	ADP	C4-C5-N7	-2.78	106.50	109.40
10	b	1000	ADP	C4-C5-N7	-2.63	106.66	109.40
10	d	1000	ADP	C4-C5-N7	-2.61	106.67	109.40
10	e	1000	ADP	C4-C5-N7	-2.59	106.70	109.40
10	c	1000	ADP	C4-C5-N7	-2.58	106.71	109.40
10	c	1000	ADP	O5'-C5'-C4'	2.29	116.88	108.99

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	b	1000	ADP	O4'-C4'-C5'-O5'
10	c	1000	ADP	O4'-C4'-C5'-O5'
10	c	1000	ADP	C3'-C4'-C5'-O5'
10	b	1000	ADP	C3'-C4'-C5'-O5'
10	d	1000	ADP	O4'-C4'-C5'-O5'
10	a	1000	ADP	O4'-C4'-C5'-O5'
10	d	1000	ADP	C3'-C4'-C5'-O5'

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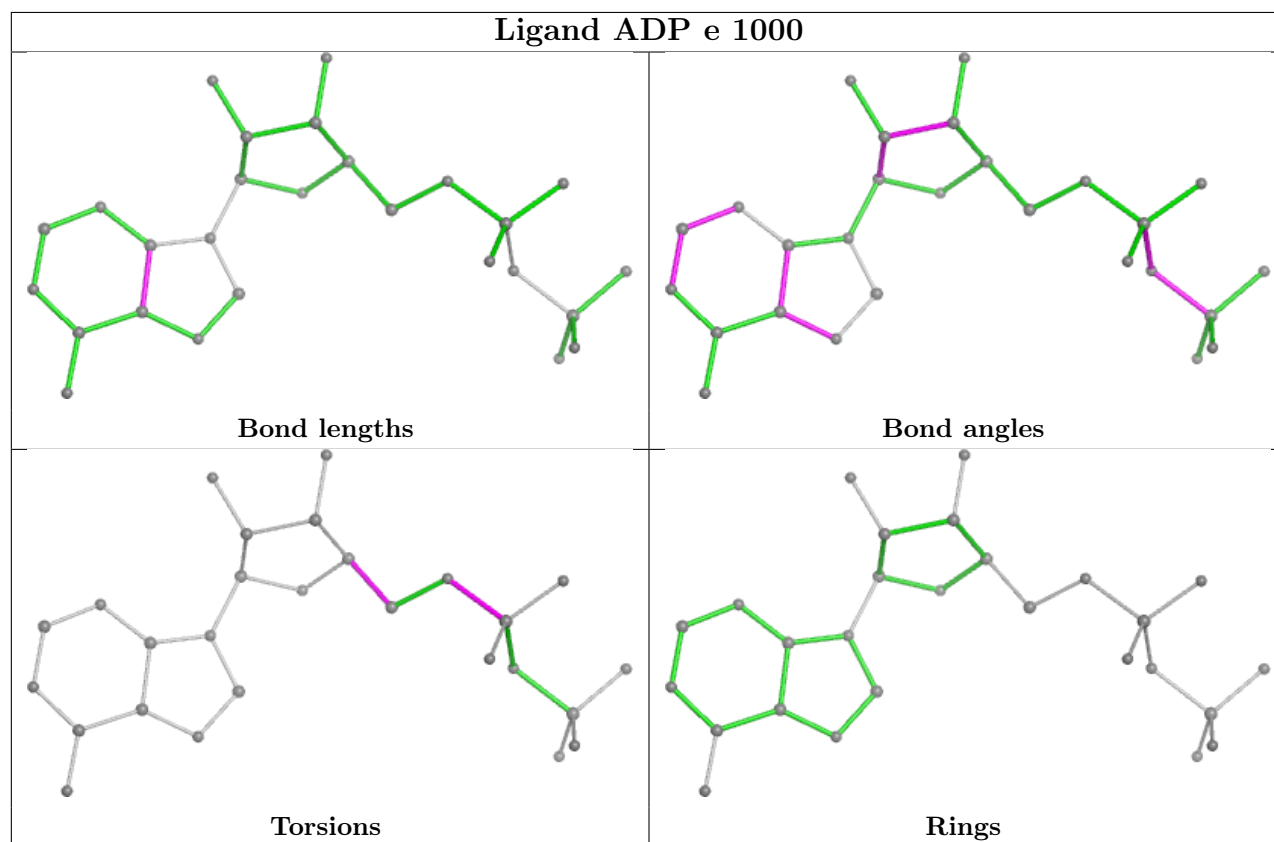
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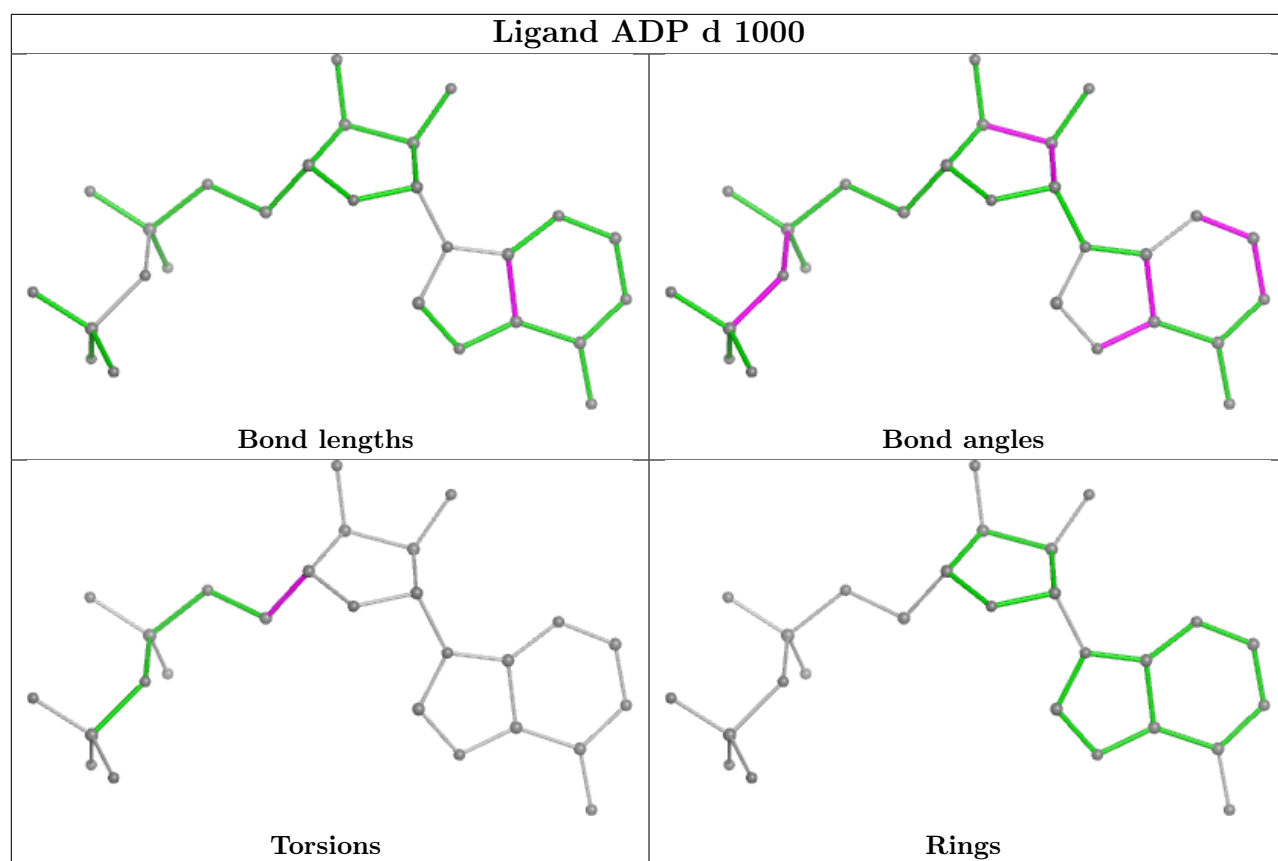
Mol	Chain	Res	Type	Atoms
10	a	1000	ADP	C3'-C4'-C5'-O5'
10	e	1000	ADP	O4'-C4'-C5'-O5'
10	e	1000	ADP	C5'-O5'-PA-O1A

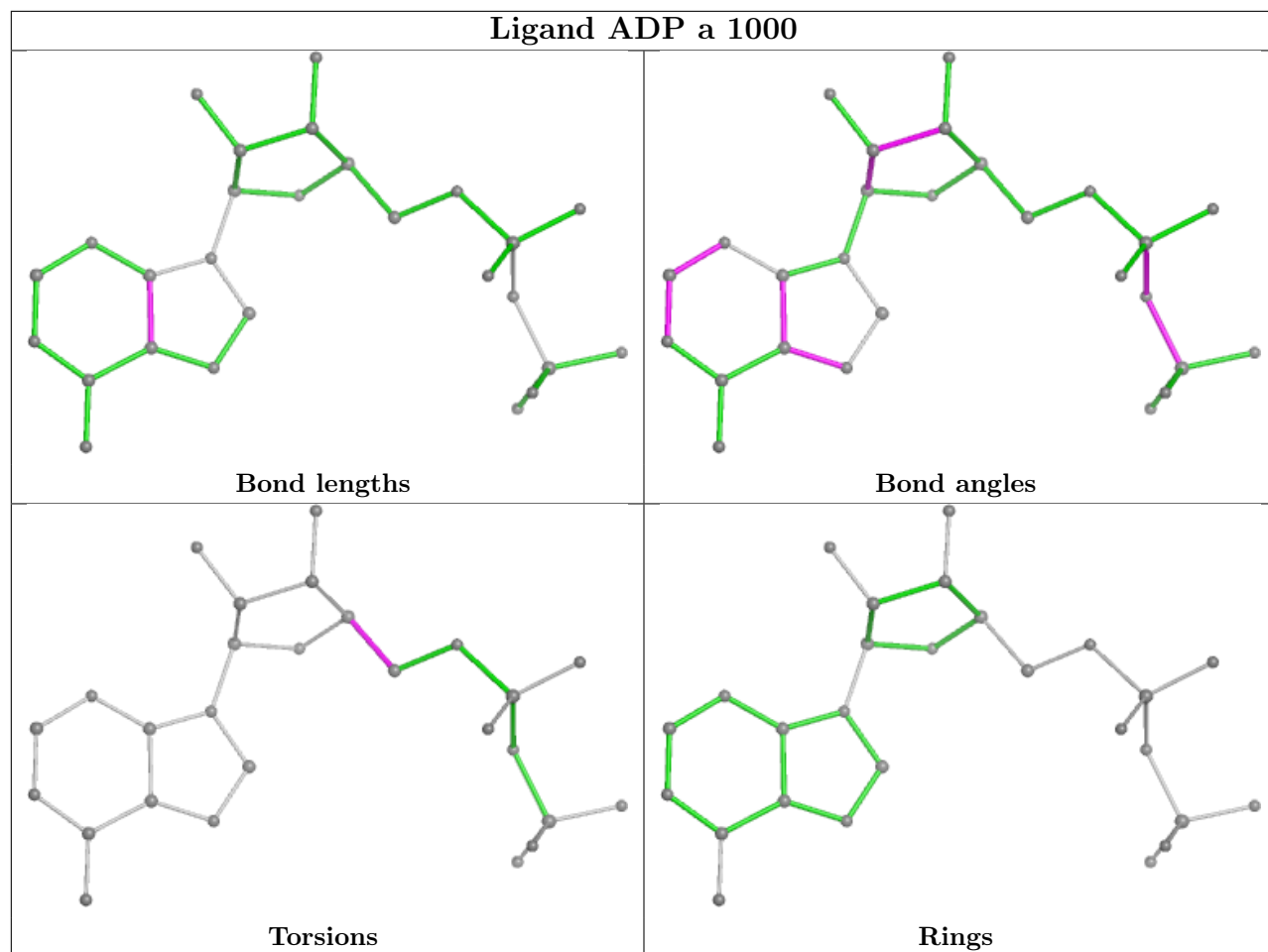
There are no ring outliers.

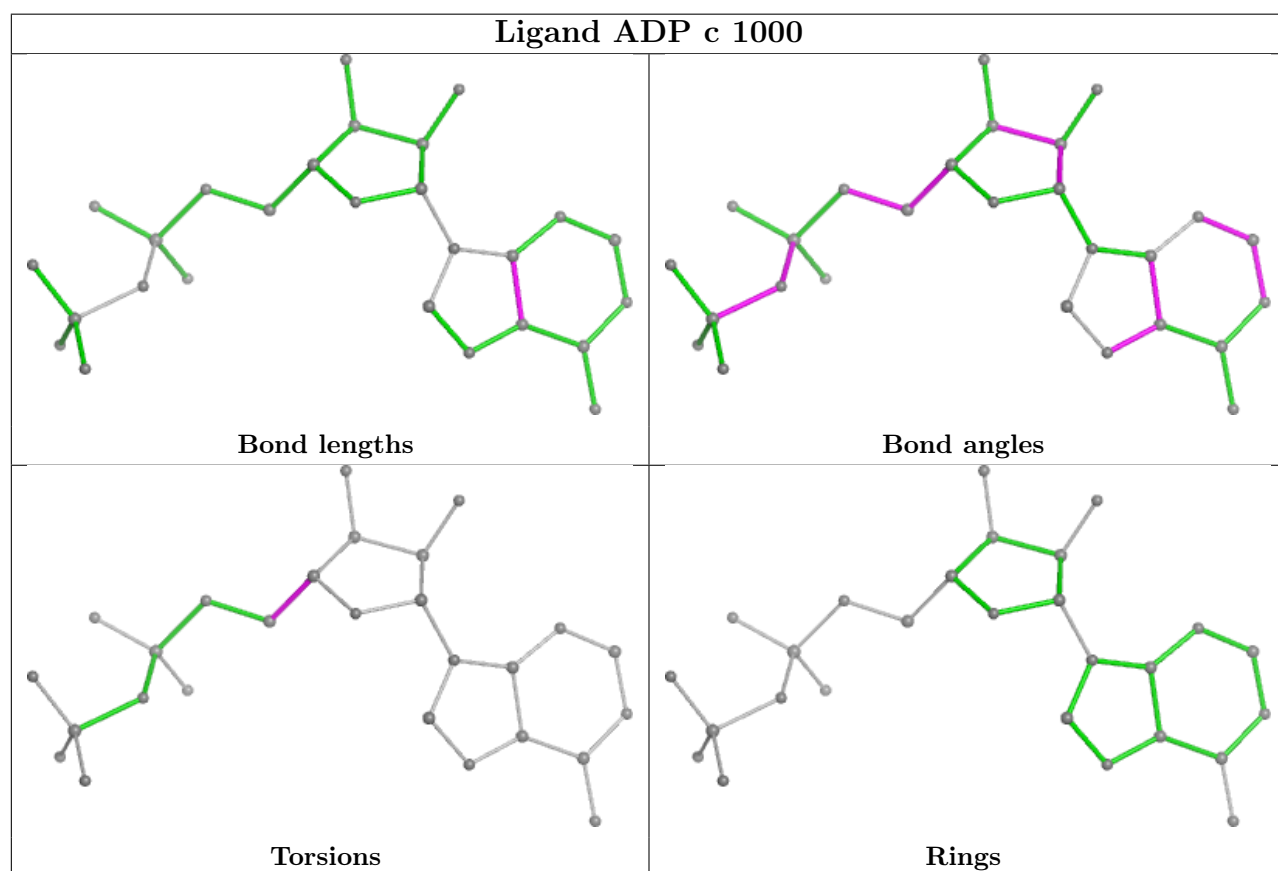
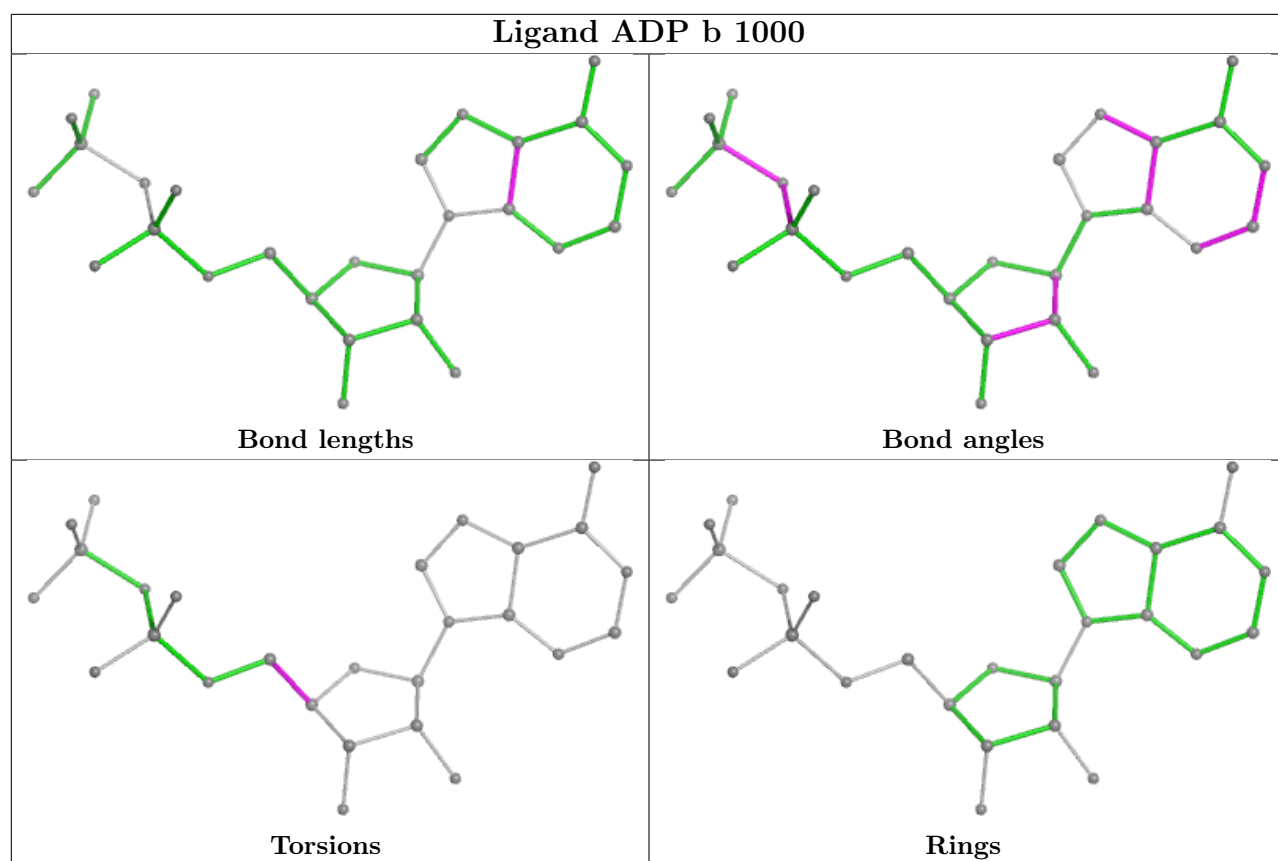
No monomer is involved in short contacts.

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
7	L	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	L	37:DA	O3'	38:DT	P	15.03
1	L	21:DC	O3'	22:DG	P	1.75

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-11091. 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.