



Full wwPDB EM Validation Report ⓘ

Jul 24, 2025 – 10:10 PM JST

PDB ID : 9KUF / pdb_00009kuf
EMDB ID : EMD-62577
Title : Cryo-EM structure of HsClpP bound to CLPP-2068
Authors : Zhao, H.; Yuan, Q.; Yin, W.
Deposited on : 2024-12-03
Resolution : 2.45 Å(reported)
Based on initial model : 7UVM

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 : **FAILED**
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0rc1
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) : 2.44

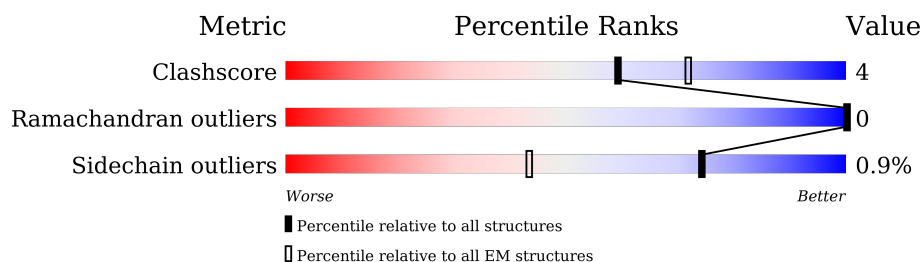
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.45 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	219	72% 7% 21%
1	B	219	74% 5% 21%
1	C	219	65% 15% 21%
1	D	219	71% 7% 21%
1	E	219	66% 13% 21%
1	F	219	74% 6% 21%
1	G	219	70% 10% 21%
1	H	219	67% 12% 21%
1	I	219	68% 11% 21%

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Mol	Chain	Length	Quality of chain
1	J	219	 69% 10% 21%
1	K	219	 70% 10% 21%
1	L	219	 66% 14% 21%
1	M	219	 70% 9% 21%
1	N	219	 72% 8% 21%

2 Entry composition [i](#)

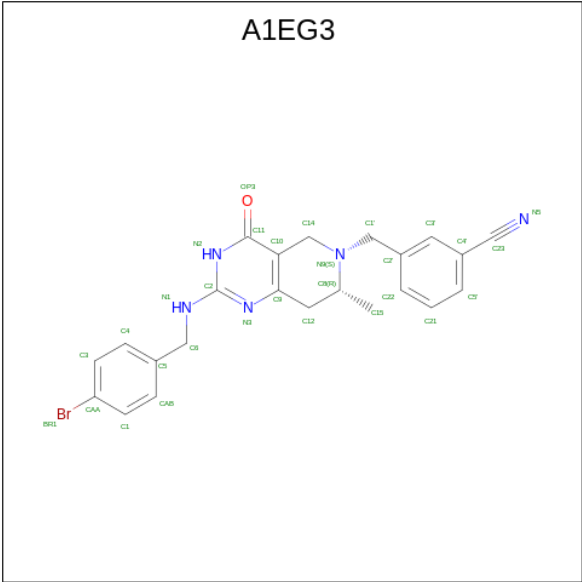
There are 2 unique types of molecules in this entry. The entry contains 19404 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ATP-dependent Clp protease proteolytic subunit, mitochondrial.

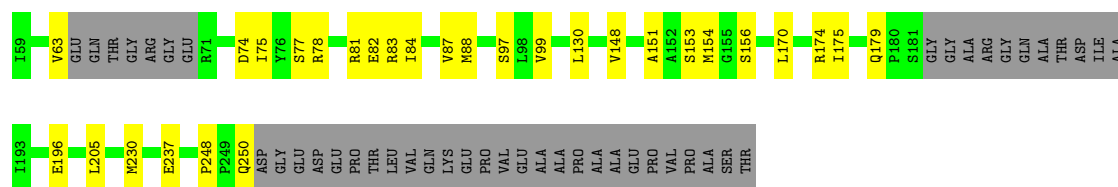
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	174	Total	C	N	O	S	0	0
			1356	867	233	243	13		
1	B	174	Total	C	N	O	S	0	0
			1356	867	233	243	13		
1	C	174	Total	C	N	O	S	0	0
			1356	867	233	243	13		
1	D	174	Total	C	N	O	S	0	0
			1356	867	233	243	13		
1	E	174	Total	C	N	O	S	0	0
			1356	867	233	243	13		
1	F	174	Total	C	N	O	S	0	0
			1356	867	233	243	13		
1	G	174	Total	C	N	O	S	0	0
			1356	867	233	243	13		
1	H	174	Total	C	N	O	S	0	0
			1356	867	233	243	13		
1	I	174	Total	C	N	O	S	0	0
			1356	867	233	243	13		
1	J	174	Total	C	N	O	S	0	0
			1356	867	233	243	13		
1	K	174	Total	C	N	O	S	0	0
			1356	867	233	243	13		
1	L	174	Total	C	N	O	S	0	0
			1356	867	233	243	13		
1	M	174	Total	C	N	O	S	0	0
			1356	867	233	243	13		
1	N	174	Total	C	N	O	S	0	0
			1356	867	233	243	13		

- Molecule 2 is 3-[[[7 {R}]-2-[(4-bromophenyl)methylamino]-7-methyl-4-oxidanylidene-3,5,7,8-tetrahydropyrido[4,3-d]pyrimidin-6-yl]methyl]benzenecarbonitrile (CCD ID: A1EG3) (formula: C₂₃H₂₂BrN₅O).



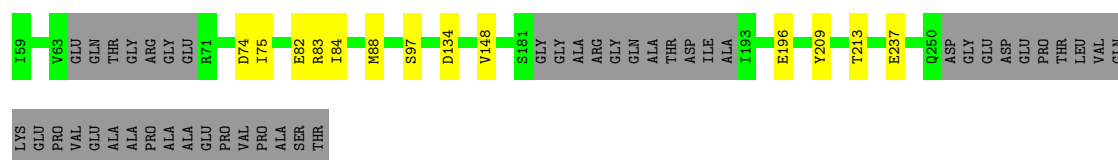
Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	Br	C	N	O	0
			30	1	23	5	1	
2	B	1	Total	Br	C	N	O	0
			30	1	23	5	1	
2	C	1	Total	Br	C	N	O	0
			30	1	23	5	1	
2	D	1	Total	Br	C	N	O	0
			30	1	23	5	1	
2	E	1	Total	Br	C	N	O	0
			30	1	23	5	1	
2	F	1	Total	Br	C	N	O	0
			30	1	23	5	1	
2	G	1	Total	Br	C	N	O	0
			30	1	23	5	1	
2	H	1	Total	Br	C	N	O	0
			30	1	23	5	1	
2	I	1	Total	Br	C	N	O	0
			30	1	23	5	1	
2	J	1	Total	Br	C	N	O	0
			30	1	23	5	1	
2	K	1	Total	Br	C	N	O	0
			30	1	23	5	1	
2	L	1	Total	Br	C	N	O	0
			30	1	23	5	1	
2	M	1	Total	Br	C	N	O	0
			30	1	23	5	1	
2	N	1	Total	Br	C	N	O	0
			30	1	23	5	1	

Chain E:  66% 13% 21%



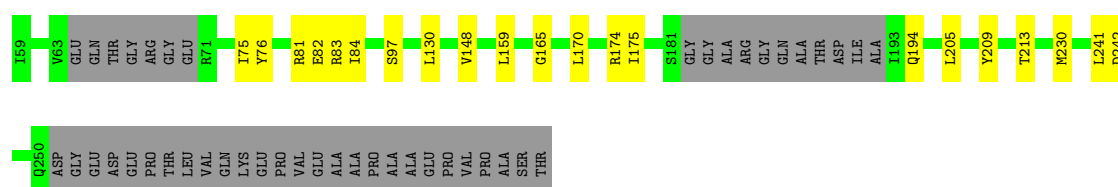
- Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial

Chain F:  74% 6% 21%



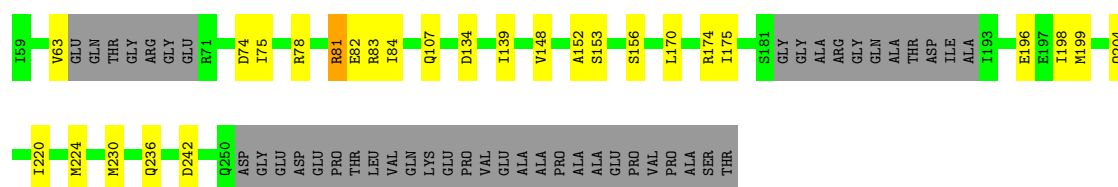
- Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial

Chain G:  70% 10% 21%



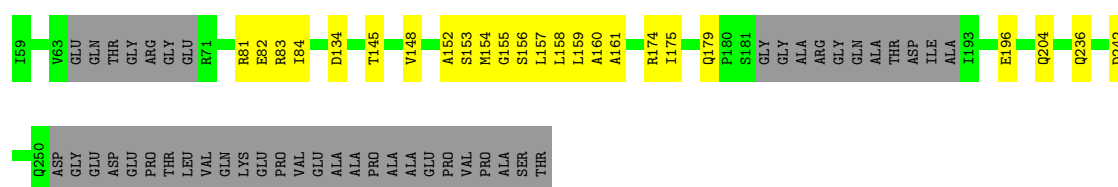
- Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial

Chain H:  67% 12% 21%



- Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial

Chain I:  68% 11% 21%



- Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1480526	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50.0	Depositor
Minimum defocus (nm)	8000	Depositor
Maximum defocus (nm)	18000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (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: A1EG3

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	0.23	1/1381 (0.1%)	0.32	0/1868
1	B	0.24	1/1381 (0.1%)	0.30	0/1868
1	C	0.23	1/1381 (0.1%)	0.35	0/1868
1	D	0.24	1/1381 (0.1%)	0.32	0/1868
1	E	0.24	1/1381 (0.1%)	0.33	0/1868
1	F	0.23	1/1381 (0.1%)	0.32	0/1868
1	G	0.24	1/1381 (0.1%)	0.36	0/1868
1	H	0.23	1/1381 (0.1%)	0.38	0/1868
1	I	0.22	0/1381	0.37	2/1868 (0.1%)
1	J	0.23	1/1381 (0.1%)	0.35	0/1868
1	K	0.23	1/1381 (0.1%)	0.31	0/1868
1	L	0.23	1/1381 (0.1%)	0.33	0/1868
1	M	0.23	1/1381 (0.1%)	0.35	0/1868
1	N	0.38	3/1381 (0.2%)	0.37	1/1868 (0.1%)
All	All	0.25	15/19334 (0.1%)	0.34	3/26152 (0.0%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	84	ILE	N-CA	-6.30	1.38	1.46
1	N	84	ILE	CA-C	-6.03	1.45	1.52
1	D	83	ARG	CA-C	-5.84	1.45	1.53
1	G	83	ARG	CA-C	-5.84	1.45	1.53
1	E	83	ARG	CA-C	-5.74	1.45	1.53
1	A	83	ARG	CA-C	-5.71	1.45	1.53
1	K	83	ARG	CA-C	-5.69	1.45	1.53
1	F	83	ARG	CA-C	-5.63	1.45	1.53
1	B	83	ARG	CA-C	-5.61	1.46	1.53
1	J	83	ARG	CA-C	-5.54	1.46	1.53
1	N	83	ARG	CA-C	-5.18	1.45	1.53
1	H	83	ARG	CA-C	-5.15	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	83	ARG	CA-C	-5.10	1.45	1.53
1	M	83	ARG	CA-C	-5.07	1.45	1.53
1	L	83	ARG	CA-C	-5.05	1.46	1.53

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	82	GLU	N-CA-C	-5.69	104.75	112.26
1	I	83	ARG	CA-C-N	-5.10	116.18	123.11
1	I	83	ARG	C-N-CA	-5.10	116.18	123.11

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	1356	0	1398	10	0
1	B	1356	0	1398	7	0
1	C	1356	0	1398	21	0
1	D	1356	0	1398	13	0
1	E	1356	0	1398	18	0
1	F	1356	0	1398	8	0
1	G	1356	0	1398	13	0
1	H	1356	0	1398	20	0
1	I	1356	0	1398	16	0
1	J	1356	0	1398	14	0
1	K	1356	0	1398	13	0
1	L	1356	0	1398	16	0
1	M	1356	0	1398	12	0
1	N	1356	0	1398	7	0
2	A	30	0	0	1	0
2	B	30	0	0	1	0
2	C	30	0	0	2	0
2	D	30	0	0	2	0
2	E	30	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	30	0	0	1	0
2	G	30	0	0	1	0
2	H	30	0	0	1	0
2	I	30	0	0	1	0
2	J	30	0	0	3	0
2	K	30	0	0	1	0
2	L	30	0	0	1	0
2	M	30	0	0	1	0
2	N	30	0	0	1	0
All	All	19404	0	19572	173	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 4.

All (173) 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:I:153:SER:O	1:I:156:SER:OG	2.02	0.74
1:H:74:ASP:OD1	1:H:75:ILE:N	2.20	0.74
1:E:153:SER:O	1:E:156:SER:OG	2.04	0.74
1:F:74:ASP:OD1	1:F:75:ILE:N	2.22	0.72
1:B:148:VAL:HG21	2:B:301:A1EG3:C23	2.27	0.64
1:N:63:VAL:O	1:N:78:ARG:NH2	2.31	0.63
1:A:209:TYR:O	1:A:213:THR:OG1	2.14	0.63
1:D:157:LEU:CD1	1:D:205:LEU:HD22	2.29	0.63
1:A:88:MET:SD	1:B:97:SER:OG	2.56	0.62
1:L:148:VAL:HG21	2:L:301:A1EG3:C23	2.30	0.62
1:H:153:SER:O	1:H:156:SER:OG	2.15	0.61
1:F:209:TYR:O	1:F:213:THR:OG1	2.16	0.61
1:H:63:VAL:O	1:H:78:ARG:NH2	2.34	0.61
1:L:153:SER:O	1:L:156:SER:OG	2.15	0.60
1:M:74:ASP:OD1	1:M:75:ILE:N	2.34	0.60
1:A:148:VAL:HG21	2:A:301:A1EG3:C23	2.32	0.59
1:E:248:PRO:O	1:E:250:GLN:NE2	2.36	0.59
1:N:148:VAL:HG21	2:N:301:A1EG3:C23	2.32	0.59
1:B:236:GLN:NE2	1:B:242:ASP:O	2.34	0.59
1:D:209:TYR:O	1:D:213:THR:OG1	2.13	0.59
1:C:153:SER:O	1:C:156:SER:OG	2.17	0.59
1:H:78:ARG:HG3	1:H:81:ARG:HH21	1.67	0.59
1:A:63:VAL:O	1:A:78:ARG:NH2	2.36	0.58
1:F:148:VAL:HG21	2:F:301:A1EG3:C23	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:ASP:N	1:B:77:SER:OG	2.37	0.58
1:A:152:ALA:O	1:A:156:SER:N	2.34	0.57
1:D:74:ASP:OD1	1:D:75:ILE:N	2.37	0.57
1:C:209:TYR:O	1:C:213:THR:OG1	2.15	0.57
1:D:157:LEU:HD13	1:D:205:LEU:HD22	1.86	0.57
1:A:78:ARG:HG3	1:A:81:ARG:HH21	1.68	0.57
1:E:63:VAL:O	1:E:78:ARG:NH2	2.38	0.57
1:H:82:GLU:O	1:H:84:ILE:HG13	2.05	0.57
1:I:82:GLU:O	1:I:84:ILE:HG13	2.04	0.57
1:L:209:TYR:O	1:L:213:THR:OG1	2.14	0.56
1:M:153:SER:O	1:M:156:SER:OG	2.18	0.56
1:H:236:GLN:NE2	1:H:242:ASP:O	2.38	0.56
1:M:82:GLU:O	1:M:84:ILE:HG13	2.05	0.56
1:L:152:ALA:O	1:L:156:SER:N	2.34	0.55
1:J:220:ILE:HG23	1:J:224:MET:HE3	1.89	0.55
1:I:236:GLN:NE2	1:I:242:ASP:O	2.40	0.55
1:I:148:VAL:HG21	2:I:301:A1EG3:C23	2.37	0.54
1:A:236:GLN:NE2	1:A:242:ASP:O	2.39	0.54
1:C:82:GLU:O	1:C:84:ILE:HG13	2.07	0.54
1:E:74:ASP:OD1	1:E:75:ILE:N	2.41	0.54
1:G:209:TYR:O	1:G:213:THR:OG1	2.22	0.53
1:D:236:GLN:NE2	1:D:242:ASP:O	2.41	0.53
1:M:107:GLN:NE2	1:M:139:ILE:HG22	2.24	0.53
1:H:220:ILE:CG2	1:H:224:MET:HE3	2.38	0.53
1:L:79:LEU:HD11	1:L:84:ILE:HG21	1.91	0.53
1:B:157:LEU:HD13	1:B:205:LEU:HD22	1.91	0.53
1:M:152:ALA:O	1:M:156:SER:N	2.39	0.53
1:G:148:VAL:HG21	2:G:301:A1EG3:C23	2.39	0.52
1:J:82:GLU:O	1:J:84:ILE:HG13	2.10	0.52
1:L:175:ILE:O	1:L:230:MET:N	2.41	0.52
1:J:74:ASP:OD1	1:J:75:ILE:N	2.44	0.51
1:L:74:ASP:OD1	1:L:75:ILE:N	2.44	0.51
1:A:154:MET:HE3	1:A:154:MET:HA	1.91	0.51
1:I:196:GLU:OE1	1:I:196:GLU:N	2.41	0.51
1:I:155:GLY:O	1:I:159:LEU:N	2.43	0.51
1:H:148:VAL:HG21	2:H:301:A1EG3:C23	2.40	0.51
1:E:82:GLU:O	1:E:84:ILE:HG13	2.11	0.51
1:C:63:VAL:O	1:C:78:ARG:NH2	2.44	0.50
1:F:196:GLU:OE1	1:F:196:GLU:N	2.43	0.50
1:E:148:VAL:HG21	2:E:301:A1EG3:C23	2.40	0.50
1:D:75:ILE:HD11	2:D:301:A1EG3:BR1	2.67	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:88:MET:SD	1:F:97:SER:OG	2.62	0.50
1:C:175:ILE:O	1:C:230:MET:N	2.40	0.50
1:D:148:VAL:HG21	2:D:301:A1EG3:C23	2.43	0.49
1:A:82:GLU:O	1:A:84:ILE:HG13	2.12	0.49
1:C:74:ASP:OD1	1:C:75:ILE:N	2.45	0.49
1:M:148:VAL:HG21	2:M:301:A1EG3:C23	2.42	0.49
1:K:148:VAL:HG21	2:K:301:A1EG3:C23	2.44	0.48
1:G:175:ILE:O	1:G:230:MET:N	2.41	0.48
1:B:62:VAL:HG12	1:C:80:LEU:HD23	1.94	0.48
1:I:152:ALA:O	1:I:156:SER:N	2.38	0.48
1:N:107:GLN:NE2	1:N:139:ILE:HG22	2.28	0.48
1:K:236:GLN:NE2	1:K:242:ASP:O	2.44	0.48
1:G:175:ILE:HD12	1:G:175:ILE:N	2.29	0.47
1:L:63:VAL:O	1:L:78:ARG:NH2	2.47	0.47
1:C:107:GLN:NE2	1:C:139:ILE:HG22	2.29	0.47
1:H:107:GLN:NE2	1:H:139:ILE:HG22	2.30	0.47
1:C:145:THR:HG21	1:C:158:LEU:O	2.15	0.47
1:F:88:MET:SD	1:G:97:SER:OG	2.63	0.47
1:H:170:LEU:HD13	1:I:134:ASP:HB3	1.96	0.47
1:H:220:ILE:HG22	1:H:224:MET:HE3	1.97	0.47
1:E:97:SER:HG	1:K:88:MET:CE	2.27	0.47
1:K:249:PRO:O	1:K:250:GLN:NE2	2.48	0.47
1:E:196:GLU:OE1	1:E:196:GLU:N	2.44	0.47
1:J:196:GLU:OE1	1:J:196:GLU:N	2.44	0.47
1:H:152:ALA:O	1:H:156:SER:N	2.39	0.47
1:C:175:ILE:HD12	1:C:175:ILE:N	2.31	0.46
1:C:152:ALA:O	1:C:156:SER:N	2.40	0.46
1:D:82:GLU:O	1:D:84:ILE:HG13	2.16	0.46
1:J:209:TYR:CD2	1:J:224:MET:HE1	2.50	0.46
1:C:196:GLU:OE1	1:C:196:GLU:N	2.44	0.46
1:G:159:LEU:HD21	1:G:241:LEU:HD21	1.97	0.46
1:M:175:ILE:O	1:M:230:MET:N	2.40	0.46
1:B:82:GLU:O	1:B:84:ILE:HG13	2.15	0.46
1:F:82:GLU:O	1:F:84:ILE:HG13	2.15	0.46
1:L:107:GLN:NE2	1:L:139:ILE:HG22	2.31	0.45
1:I:156:SER:O	1:I:160:ALA:N	2.46	0.45
1:L:145:THR:HG21	1:L:158:LEU:O	2.16	0.45
1:E:151:ALA:N	1:E:174:ARG:O	2.46	0.45
1:G:194:GLN:N	1:G:194:GLN:OE1	2.50	0.45
1:C:148:VAL:HG21	2:C:301:A1EG3:C23	2.46	0.45
1:E:97:SER:OG	1:K:88:MET:SD	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:175:ILE:HD12	1:J:175:ILE:N	2.32	0.45
1:G:130:LEU:HD21	1:G:205:LEU:CD2	2.47	0.45
1:K:82:GLU:O	1:K:84:ILE:HG13	2.17	0.44
1:K:209:TYR:O	1:K:213:THR:OG1	2.20	0.44
1:C:165:GLY:N	1:C:242:ASP:OD2	2.50	0.44
1:E:154:MET:SD	1:E:179:GLN:NE2	2.88	0.44
1:N:144:CYS:SG	1:N:166:MET:HE2	2.58	0.44
1:I:145:THR:HG21	1:I:158:LEU:O	2.18	0.44
1:G:170:LEU:HD13	1:H:134:ASP:HB3	2.00	0.44
1:E:175:ILE:HD12	1:E:175:ILE:N	2.32	0.44
1:M:157:LEU:O	1:M:161:ALA:N	2.49	0.43
1:L:82:GLU:O	1:L:84:ILE:HG13	2.18	0.43
1:J:148:VAL:HG21	2:J:301:A1EG3:C23	2.47	0.43
1:L:157:LEU:O	1:L:161:ALA:N	2.49	0.43
1:N:165:GLY:N	1:N:242:ASP:OD2	2.50	0.43
1:K:120:ASN:ND2	1:K:148:VAL:O	2.51	0.43
1:C:75:ILE:HG23	1:C:76:TYR:N	2.33	0.43
1:D:179:GLN:O	1:D:181:SER:N	2.51	0.43
1:I:175:ILE:HD12	1:I:175:ILE:N	2.34	0.43
1:L:167:ARG:NH1	1:L:239:GLY:O	2.51	0.43
1:H:175:ILE:N	1:H:175:ILE:HD12	2.34	0.43
1:I:154:MET:SD	1:I:179:GLN:NE2	2.86	0.43
1:N:75:ILE:HG23	1:N:76:TYR:N	2.33	0.43
1:J:107:GLN:NE2	1:J:139:ILE:HG22	2.34	0.42
1:N:159:LEU:HD21	1:N:241:LEU:HD21	1.99	0.42
1:G:174:ARG:NH1	1:H:204:GLN:OE1	2.52	0.42
1:C:195:ALA:HB2	1:H:198:ILE:HD12	2.01	0.42
1:G:82:GLU:O	1:G:84:ILE:HG13	2.19	0.42
1:M:237:GLU:OE1	1:M:238:PHE:N	2.52	0.42
1:C:144:CYS:SG	1:C:166:MET:HE2	2.60	0.42
1:J:159:LEU:HD21	1:J:241:LEU:HD21	2.02	0.42
1:D:175:ILE:N	1:D:175:ILE:HD12	2.34	0.42
1:D:201:LEU:O	1:D:205:LEU:HG	2.19	0.42
1:E:170:LEU:HD13	1:F:134:ASP:HB3	2.02	0.42
1:J:165:GLY:N	1:J:242:ASP:OD2	2.52	0.41
1:H:196:GLU:OE1	1:H:196:GLU:N	2.45	0.41
1:I:157:LEU:O	1:I:161:ALA:N	2.51	0.41
1:J:74:ASP:N	1:J:77:SER:OG	2.53	0.41
1:J:148:VAL:HG21	2:J:301:A1EG3:N5	2.36	0.41
1:K:196:GLU:OE1	1:K:196:GLU:N	2.47	0.41
1:L:154:MET:HE3	1:L:154:MET:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:92:ASP:OD1	1:M:92:ASP:N	2.52	0.41
1:M:175:ILE:HD12	1:M:175:ILE:N	2.35	0.41
1:C:199:MET:HG3	1:H:199:MET:HG3	2.01	0.41
1:I:174:ARG:NH1	1:J:204:GLN:OE1	2.54	0.41
1:G:75:ILE:HG23	1:G:76:TYR:N	2.36	0.41
1:H:174:ARG:NH1	1:I:204:GLN:OE1	2.54	0.41
1:E:175:ILE:O	1:E:230:MET:N	2.44	0.41
1:G:165:GLY:N	1:G:242:ASP:OD2	2.52	0.41
1:C:96:ALA:HB2	1:C:128:ALA:HB1	2.03	0.41
1:E:130:LEU:HD21	1:E:205:LEU:CD2	2.51	0.41
1:H:175:ILE:O	1:H:230:MET:N	2.42	0.41
2:J:301:A1EG3:OP3	1:K:104:LEU:HD22	2.21	0.41
1:K:87:VAL:HG22	1:K:99:VAL:HG21	2.03	0.41
1:D:81:ARG:HE	1:D:81:ARG:HB3	1.78	0.40
1:C:136:MET:HE3	1:C:143:ILE:HG21	2.03	0.40
1:K:159:LEU:HD21	1:K:241:LEU:HD21	2.03	0.40
1:E:74:ASP:N	1:E:77:SER:OG	2.55	0.40
1:E:87:VAL:HG22	1:E:99:VAL:HG21	2.03	0.40
1:J:87:VAL:HG22	1:J:99:VAL:HG21	2.03	0.40
1:L:105:PHE:O	1:L:108:SER:OG	2.30	0.40
1:L:170:LEU:HD13	1:M:134:ASP:HB3	2.03	0.40
1:D:120:ASN:ND2	1:D:148:VAL:O	2.54	0.40
1:A:79:LEU:HD23	1:A:84:ILE:O	2.22	0.40
1:C:148:VAL:HG21	2:C:301:A1EG3:N5	2.36	0.40
1:I:153:SER:OG	1:I:179:GLN:N	2.48	0.40
1:K:75:ILE:HG23	1:K:76:TYR:N	2.36	0.40

There are no symmetry-related clashes.

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	168/219 (77%)	165 (98%)	3 (2%)	0	100	100
1	B	168/219 (77%)	167 (99%)	1 (1%)	0	100	100
1	C	168/219 (77%)	163 (97%)	5 (3%)	0	100	100
1	D	168/219 (77%)	163 (97%)	5 (3%)	0	100	100
1	E	168/219 (77%)	164 (98%)	4 (2%)	0	100	100
1	F	168/219 (77%)	164 (98%)	4 (2%)	0	100	100
1	G	168/219 (77%)	165 (98%)	3 (2%)	0	100	100
1	H	168/219 (77%)	166 (99%)	2 (1%)	0	100	100
1	I	168/219 (77%)	163 (97%)	5 (3%)	0	100	100
1	J	168/219 (77%)	164 (98%)	4 (2%)	0	100	100
1	K	168/219 (77%)	163 (97%)	5 (3%)	0	100	100
1	L	168/219 (77%)	164 (98%)	4 (2%)	0	100	100
1	M	168/219 (77%)	164 (98%)	4 (2%)	0	100	100
1	N	168/219 (77%)	165 (98%)	3 (2%)	0	100	100
All	All	2352/3066 (77%)	2300 (98%)	52 (2%)	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	151/183 (82%)	150 (99%)	1 (1%)	81	89
1	B	151/183 (82%)	149 (99%)	2 (1%)	65	78
1	C	151/183 (82%)	151 (100%)	0	100	100
1	D	151/183 (82%)	149 (99%)	2 (1%)	65	78
1	E	151/183 (82%)	149 (99%)	2 (1%)	65	78
1	F	151/183 (82%)	150 (99%)	1 (1%)	81	89
1	G	151/183 (82%)	150 (99%)	1 (1%)	81	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	151/183 (82%)	150 (99%)	1 (1%)	81	89
1	I	151/183 (82%)	150 (99%)	1 (1%)	81	89
1	J	151/183 (82%)	150 (99%)	1 (1%)	81	89
1	K	151/183 (82%)	150 (99%)	1 (1%)	81	89
1	L	151/183 (82%)	149 (99%)	2 (1%)	65	78
1	M	151/183 (82%)	149 (99%)	2 (1%)	65	78
1	N	151/183 (82%)	150 (99%)	1 (1%)	81	89
All	All	2114/2562 (82%)	2096 (99%)	18 (1%)	74	86

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	81	ARG
1	B	62	VAL
1	B	81	ARG
1	D	81	ARG
1	D	83	ARG
1	E	81	ARG
1	E	237	GLU
1	F	237	GLU
1	G	81	ARG
1	H	81	ARG
1	I	81	ARG
1	J	81	ARG
1	K	81	ARG
1	L	81	ARG
1	L	237	GLU
1	M	224	MET
1	M	237	GLU
1	N	81	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	102	GLN
1	C	107	GLN
1	H	102	GLN
1	H	107	GLN

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Mol	Chain	Res	Type
1	I	107	GLN
1	J	107	GLN
1	K	194	GLN
1	L	107	GLN
1	M	102	GLN
1	N	102	GLN
1	N	107	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

14 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	$\# Z > 2$
2	A1EG3	F	301	-	33,33,33	4.64	21 (63%)	36,46,46	1.69	4 (11%)
2	A1EG3	C	301	-	33,33,33	4.67	21 (63%)	36,46,46	1.58	4 (11%)
2	A1EG3	A	301	-	33,33,33	4.64	21 (63%)	36,46,46	1.74	5 (13%)
2	A1EG3	L	301	-	33,33,33	4.65	21 (63%)	36,46,46	1.56	4 (11%)
2	A1EG3	D	301	-	33,33,33	4.65	21 (63%)	36,46,46	1.63	4 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	A1EG3	H	301	-	33,33,33	4.67	21 (63%)	36,46,46	1.53	4 (11%)
2	A1EG3	I	301	-	33,33,33	4.73	22 (66%)	36,46,46	1.83	6 (16%)
2	A1EG3	J	301	-	33,33,33	4.66	22 (66%)	36,46,46	1.50	4 (11%)
2	A1EG3	M	301	-	33,33,33	4.67	21 (63%)	36,46,46	1.53	4 (11%)
2	A1EG3	B	301	-	33,33,33	4.65	21 (63%)	36,46,46	1.69	5 (13%)
2	A1EG3	N	301	-	33,33,33	4.66	21 (63%)	36,46,46	1.59	4 (11%)
2	A1EG3	E	301	-	33,33,33	4.63	21 (63%)	36,46,46	1.60	4 (11%)
2	A1EG3	G	301	-	33,33,33	4.71	21 (63%)	36,46,46	1.63	4 (11%)
2	A1EG3	K	301	-	33,33,33	4.64	21 (63%)	36,46,46	1.69	5 (13%)

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	A1EG3	F	301	-	-	2/11/23/23	0/4/4/4
2	A1EG3	C	301	-	-	2/11/23/23	0/4/4/4
2	A1EG3	A	301	-	-	2/11/23/23	0/4/4/4
2	A1EG3	L	301	-	-	2/11/23/23	0/4/4/4
2	A1EG3	D	301	-	-	2/11/23/23	0/4/4/4
2	A1EG3	H	301	-	-	2/11/23/23	0/4/4/4
2	A1EG3	I	301	-	-	2/11/23/23	0/4/4/4
2	A1EG3	J	301	-	-	2/11/23/23	0/4/4/4
2	A1EG3	M	301	-	-	2/11/23/23	0/4/4/4
2	A1EG3	B	301	-	-	3/11/23/23	0/4/4/4
2	A1EG3	N	301	-	-	2/11/23/23	0/4/4/4
2	A1EG3	E	301	-	-	2/11/23/23	0/4/4/4
2	A1EG3	G	301	-	-	2/11/23/23	0/4/4/4
2	A1EG3	K	301	-	-	2/11/23/23	0/4/4/4

All (296) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	301	A1EG3	C1'-N9	-11.54	1.27	1.47
2	G	301	A1EG3	C1'-N9	-11.15	1.28	1.47
2	H	301	A1EG3	C1'-N9	-10.70	1.29	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	A1EG3	C1'-N9	-10.64	1.29	1.47
2	C	301	A1EG3	C1'-N9	-10.63	1.29	1.47
2	N	301	A1EG3	C1'-N9	-10.59	1.29	1.47
2	F	301	A1EG3	C1'-N9	-10.58	1.29	1.47
2	J	301	A1EG3	C1'-N9	-10.54	1.29	1.47
2	M	301	A1EG3	C1'-N9	-10.54	1.29	1.47
2	B	301	A1EG3	C1'-N9	-10.54	1.29	1.47
2	K	301	A1EG3	C1'-N9	-10.49	1.29	1.47
2	E	301	A1EG3	C1'-N9	-10.48	1.29	1.47
2	L	301	A1EG3	C1'-N9	-10.46	1.29	1.47
2	D	301	A1EG3	C1'-N9	-10.45	1.29	1.47
2	M	301	A1EG3	OP3-C11	7.99	1.38	1.23
2	B	301	A1EG3	OP3-C11	7.97	1.38	1.23
2	H	301	A1EG3	OP3-C11	7.97	1.38	1.23
2	G	301	A1EG3	OP3-C11	7.95	1.38	1.23
2	L	301	A1EG3	OP3-C11	7.94	1.38	1.23
2	D	301	A1EG3	OP3-C11	7.92	1.38	1.23
2	N	301	A1EG3	OP3-C11	7.89	1.38	1.23
2	G	301	A1EG3	C3'-C4'	7.86	1.53	1.39
2	I	301	A1EG3	OP3-C11	7.86	1.38	1.23
2	A	301	A1EG3	OP3-C11	7.84	1.38	1.23
2	C	301	A1EG3	OP3-C11	7.84	1.38	1.23
2	F	301	A1EG3	OP3-C11	7.84	1.38	1.23
2	E	301	A1EG3	OP3-C11	7.83	1.38	1.23
2	M	301	A1EG3	C3'-C4'	7.83	1.53	1.39
2	I	301	A1EG3	C3'-C4'	7.82	1.53	1.39
2	K	301	A1EG3	OP3-C11	7.81	1.38	1.23
2	N	301	A1EG3	C14-N9	-7.81	1.28	1.47
2	K	301	A1EG3	C14-N9	-7.80	1.28	1.47
2	J	301	A1EG3	C14-N9	-7.79	1.28	1.47
2	M	301	A1EG3	C14-N9	-7.78	1.28	1.47
2	J	301	A1EG3	OP3-C11	7.78	1.38	1.23
2	C	301	A1EG3	C14-N9	-7.77	1.28	1.47
2	L	301	A1EG3	C14-N9	-7.76	1.29	1.47
2	F	301	A1EG3	C14-N9	-7.74	1.29	1.47
2	J	301	A1EG3	C3'-C4'	7.74	1.52	1.39
2	H	301	A1EG3	C14-N9	-7.73	1.29	1.47
2	I	301	A1EG3	C14-N9	-7.72	1.29	1.47
2	B	301	A1EG3	C14-N9	-7.71	1.29	1.47
2	E	301	A1EG3	C14-N9	-7.70	1.29	1.47
2	D	301	A1EG3	C14-N9	-7.69	1.29	1.47
2	A	301	A1EG3	C14-N9	-7.69	1.29	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	301	A1EG3	C14-N9	-7.67	1.29	1.47
2	H	301	A1EG3	C3'-C4'	7.62	1.52	1.39
2	C	301	A1EG3	C3'-C4'	7.61	1.52	1.39
2	G	301	A1EG3	C3-C4	7.52	1.52	1.38
2	L	301	A1EG3	C3'-C4'	7.52	1.52	1.39
2	M	301	A1EG3	C3-C4	7.51	1.52	1.38
2	N	301	A1EG3	C3'-C4'	7.51	1.52	1.39
2	C	301	A1EG3	C3-C4	7.43	1.52	1.38
2	B	301	A1EG3	C3-C4	7.43	1.52	1.38
2	H	301	A1EG3	C3-C4	7.41	1.52	1.38
2	J	301	A1EG3	C3-C4	7.39	1.52	1.38
2	D	301	A1EG3	C3'-C4'	7.38	1.52	1.39
2	E	301	A1EG3	C3'-C4'	7.38	1.52	1.39
2	L	301	A1EG3	C3-C4	7.37	1.52	1.38
2	F	301	A1EG3	C3-C4	7.35	1.52	1.38
2	E	301	A1EG3	C3-C4	7.34	1.52	1.38
2	D	301	A1EG3	C3-C4	7.34	1.52	1.38
2	I	301	A1EG3	C3-C4	7.33	1.52	1.38
2	A	301	A1EG3	C3-C4	7.33	1.52	1.38
2	N	301	A1EG3	C3-C4	7.33	1.52	1.38
2	K	301	A1EG3	C3'-C4'	7.32	1.52	1.39
2	K	301	A1EG3	C3-C4	7.30	1.52	1.38
2	F	301	A1EG3	C3'-C4'	7.26	1.52	1.39
2	A	301	A1EG3	C3'-C4'	7.21	1.52	1.39
2	B	301	A1EG3	C3'-C4'	7.12	1.51	1.39
2	M	301	A1EG3	C1-CAA	6.93	1.52	1.38
2	F	301	A1EG3	C1-CAA	6.93	1.52	1.38
2	C	301	A1EG3	C1-CAA	6.90	1.52	1.38
2	J	301	A1EG3	C1-CAA	6.89	1.52	1.38
2	D	301	A1EG3	C1-CAA	6.87	1.52	1.38
2	K	301	A1EG3	C1-CAA	6.87	1.52	1.38
2	F	301	A1EG3	CAB-C5	6.85	1.53	1.38
2	L	301	A1EG3	CAB-C5	6.85	1.53	1.38
2	C	301	A1EG3	CAB-C5	6.85	1.53	1.38
2	N	301	A1EG3	C1-CAA	6.84	1.52	1.38
2	A	301	A1EG3	C1-CAA	6.84	1.52	1.38
2	L	301	A1EG3	C1-CAA	6.84	1.52	1.38
2	E	301	A1EG3	C1-CAA	6.83	1.52	1.38
2	J	301	A1EG3	CAB-C5	6.83	1.53	1.38
2	G	301	A1EG3	C1-CAA	6.82	1.52	1.38
2	E	301	A1EG3	CAB-C5	6.82	1.53	1.38
2	N	301	A1EG3	CAB-C5	6.82	1.53	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	301	A1EG3	C1-CAA	6.81	1.52	1.38
2	K	301	A1EG3	CAB-C5	6.81	1.53	1.38
2	H	301	A1EG3	C1-CAA	6.81	1.52	1.38
2	I	301	A1EG3	CAB-C5	6.80	1.53	1.38
2	B	301	A1EG3	CAB-C5	6.79	1.53	1.38
2	H	301	A1EG3	CAB-C5	6.79	1.53	1.38
2	A	301	A1EG3	CAB-C5	6.78	1.53	1.38
2	M	301	A1EG3	CAB-C5	6.78	1.53	1.38
2	D	301	A1EG3	CAB-C5	6.78	1.53	1.38
2	B	301	A1EG3	C1-CAA	6.76	1.52	1.38
2	G	301	A1EG3	CAB-C5	6.76	1.53	1.38
2	D	301	A1EG3	C21-C5'	6.47	1.52	1.38
2	E	301	A1EG3	C21-C5'	6.45	1.52	1.38
2	K	301	A1EG3	C21-C5'	6.42	1.52	1.38
2	B	301	A1EG3	C21-C5'	6.36	1.52	1.38
2	N	301	A1EG3	C21-C5'	6.35	1.52	1.38
2	H	301	A1EG3	C22-C2'	6.33	1.52	1.38
2	E	301	A1EG3	C22-C2'	6.33	1.52	1.38
2	F	301	A1EG3	C21-C5'	6.32	1.52	1.38
2	A	301	A1EG3	C21-C5'	6.32	1.52	1.38
2	K	301	A1EG3	C22-C2'	6.31	1.52	1.38
2	J	301	A1EG3	C21-C5'	6.30	1.52	1.38
2	A	301	A1EG3	C22-C2'	6.29	1.52	1.38
2	D	301	A1EG3	C22-C2'	6.29	1.52	1.38
2	H	301	A1EG3	C21-C5'	6.29	1.52	1.38
2	I	301	A1EG3	C22-C2'	6.28	1.52	1.38
2	C	301	A1EG3	C21-C5'	6.28	1.52	1.38
2	L	301	A1EG3	C21-C5'	6.28	1.52	1.38
2	C	301	A1EG3	C22-C2'	6.27	1.52	1.38
2	N	301	A1EG3	C22-C2'	6.25	1.52	1.38
2	L	301	A1EG3	C22-C2'	6.25	1.52	1.38
2	M	301	A1EG3	C22-C2'	6.25	1.52	1.38
2	B	301	A1EG3	C22-C2'	6.24	1.52	1.38
2	J	301	A1EG3	C22-C2'	6.24	1.52	1.38
2	M	301	A1EG3	C21-C5'	6.22	1.52	1.38
2	G	301	A1EG3	C22-C2'	6.22	1.52	1.38
2	F	301	A1EG3	C22-C2'	6.21	1.52	1.38
2	I	301	A1EG3	C21-C5'	6.11	1.51	1.38
2	G	301	A1EG3	C21-C5'	6.10	1.51	1.38
2	B	301	A1EG3	C3'-C2'	-5.56	1.29	1.39
2	A	301	A1EG3	C3'-C2'	-5.49	1.29	1.39
2	F	301	A1EG3	C3'-C2'	-5.42	1.30	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	301	A1EG3	C3'-C2'	-5.33	1.30	1.39
2	K	301	A1EG3	C3'-C2'	-5.30	1.30	1.39
2	N	301	A1EG3	C3'-C2'	-5.22	1.30	1.39
2	L	301	A1EG3	C3'-C2'	-5.21	1.30	1.39
2	E	301	A1EG3	C3'-C2'	-5.19	1.30	1.39
2	C	301	A1EG3	C3'-C2'	-5.15	1.30	1.39
2	H	301	A1EG3	C3'-C2'	-5.03	1.30	1.39
2	J	301	A1EG3	C3'-C2'	-5.03	1.30	1.39
2	G	301	A1EG3	C3'-C2'	-4.97	1.30	1.39
2	I	301	A1EG3	C3'-C2'	-4.96	1.30	1.39
2	M	301	A1EG3	C3'-C2'	-4.92	1.30	1.39
2	G	301	A1EG3	C2-N1	4.91	1.44	1.34
2	I	301	A1EG3	C2-N1	4.86	1.44	1.34
2	H	301	A1EG3	C2-N1	4.85	1.44	1.34
2	J	301	A1EG3	C2-N1	4.85	1.44	1.34
2	K	301	A1EG3	C2-N1	4.82	1.44	1.34
2	B	301	A1EG3	C2-N1	4.82	1.44	1.34
2	D	301	A1EG3	C2-N1	4.82	1.44	1.34
2	M	301	A1EG3	C2-N1	4.80	1.44	1.34
2	C	301	A1EG3	C2-N1	4.80	1.44	1.34
2	N	301	A1EG3	C2-N1	4.78	1.44	1.34
2	A	301	A1EG3	C2-N1	4.78	1.44	1.34
2	E	301	A1EG3	C2-N1	4.73	1.44	1.34
2	L	301	A1EG3	C2-N1	4.73	1.44	1.34
2	F	301	A1EG3	C2-N1	4.67	1.44	1.34
2	G	301	A1EG3	C1-CAB	-4.36	1.30	1.38
2	B	301	A1EG3	C1-CAB	-4.35	1.30	1.38
2	N	301	A1EG3	C1-CAB	-4.32	1.30	1.38
2	H	301	A1EG3	C1-CAB	-4.31	1.30	1.38
2	C	301	A1EG3	C1-CAB	-4.30	1.30	1.38
2	J	301	A1EG3	C1-CAB	-4.28	1.31	1.38
2	A	301	A1EG3	C1-CAB	-4.24	1.31	1.38
2	L	301	A1EG3	C1-CAB	-4.23	1.31	1.38
2	I	301	A1EG3	C1-CAB	-4.22	1.31	1.38
2	E	301	A1EG3	C1-CAB	-4.19	1.31	1.38
2	M	301	A1EG3	C1-CAB	-4.19	1.31	1.38
2	M	301	A1EG3	C11-C10	4.19	1.51	1.44
2	G	301	A1EG3	C11-C10	4.15	1.51	1.44
2	F	301	A1EG3	C1-CAB	-4.14	1.31	1.38
2	B	301	A1EG3	C11-C10	4.11	1.51	1.44
2	D	301	A1EG3	C1-CAB	-4.11	1.31	1.38
2	D	301	A1EG3	C11-C10	4.11	1.51	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	301	A1EG3	C1-CAB	-4.07	1.31	1.38
2	H	301	A1EG3	C11-C10	4.07	1.51	1.44
2	L	301	A1EG3	C11-C10	4.01	1.50	1.44
2	C	301	A1EG3	C11-C10	3.97	1.50	1.44
2	E	301	A1EG3	C11-C10	3.95	1.50	1.44
2	I	301	A1EG3	C8-N9	-3.93	1.35	1.48
2	N	301	A1EG3	C11-C10	3.92	1.50	1.44
2	A	301	A1EG3	C11-C10	3.92	1.50	1.44
2	M	301	A1EG3	C8-N9	-3.91	1.35	1.48
2	J	301	A1EG3	C11-C10	3.91	1.50	1.44
2	I	301	A1EG3	C11-C10	3.90	1.50	1.44
2	K	301	A1EG3	C11-C10	3.89	1.50	1.44
2	F	301	A1EG3	C11-C10	3.88	1.50	1.44
2	G	301	A1EG3	C5'-C4'	-3.88	1.31	1.39
2	K	301	A1EG3	C8-N9	-3.88	1.35	1.48
2	A	301	A1EG3	C8-N9	-3.87	1.35	1.48
2	D	301	A1EG3	C8-N9	-3.87	1.35	1.48
2	I	301	A1EG3	C5'-C4'	-3.87	1.31	1.39
2	B	301	A1EG3	C8-N9	-3.87	1.35	1.48
2	N	301	A1EG3	C5'-C4'	-3.86	1.31	1.39
2	C	301	A1EG3	C5'-C4'	-3.86	1.31	1.39
2	M	301	A1EG3	C5'-C4'	-3.86	1.31	1.39
2	D	301	A1EG3	C5'-C4'	-3.85	1.31	1.39
2	G	301	A1EG3	C8-N9	-3.85	1.35	1.48
2	H	301	A1EG3	C5'-C4'	-3.84	1.31	1.39
2	H	301	A1EG3	C8-N9	-3.84	1.35	1.48
2	N	301	A1EG3	C8-N9	-3.84	1.35	1.48
2	E	301	A1EG3	C8-N9	-3.83	1.35	1.48
2	F	301	A1EG3	C5'-C4'	-3.83	1.31	1.39
2	C	301	A1EG3	C8-N9	-3.83	1.35	1.48
2	J	301	A1EG3	C5'-C4'	-3.83	1.31	1.39
2	J	301	A1EG3	C8-N9	-3.82	1.35	1.48
2	K	301	A1EG3	C5'-C4'	-3.82	1.31	1.39
2	L	301	A1EG3	C5'-C4'	-3.81	1.31	1.39
2	F	301	A1EG3	C8-N9	-3.81	1.36	1.48
2	A	301	A1EG3	C5'-C4'	-3.81	1.31	1.39
2	E	301	A1EG3	C5'-C4'	-3.80	1.31	1.39
2	L	301	A1EG3	C8-N9	-3.79	1.36	1.48
2	K	301	A1EG3	C2-N2	3.75	1.42	1.36
2	B	301	A1EG3	C5'-C4'	-3.75	1.31	1.39
2	E	301	A1EG3	C2-N2	3.74	1.42	1.36
2	A	301	A1EG3	C2-N2	3.73	1.42	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	A1EG3	C2-N2	3.73	1.42	1.36
2	N	301	A1EG3	C2-N2	3.73	1.42	1.36
2	I	301	A1EG3	C2-N2	3.69	1.42	1.36
2	K	301	A1EG3	C4-C5	-3.69	1.30	1.38
2	H	301	A1EG3	C2-N2	3.67	1.42	1.36
2	F	301	A1EG3	C4-C5	-3.66	1.30	1.38
2	F	301	A1EG3	C2-N2	3.65	1.42	1.36
2	J	301	A1EG3	C2-N2	3.65	1.42	1.36
2	D	301	A1EG3	C2-N2	3.65	1.42	1.36
2	L	301	A1EG3	C4-C5	-3.65	1.31	1.38
2	N	301	A1EG3	C4-C5	-3.63	1.31	1.38
2	C	301	A1EG3	C2-N2	3.61	1.42	1.36
2	L	301	A1EG3	C2-N2	3.61	1.42	1.36
2	I	301	A1EG3	C4-C5	-3.60	1.31	1.38
2	C	301	A1EG3	C4-C5	-3.60	1.31	1.38
2	A	301	A1EG3	C4-C5	-3.59	1.31	1.38
2	J	301	A1EG3	C4-C5	-3.58	1.31	1.38
2	E	301	A1EG3	C4-C5	-3.58	1.31	1.38
2	M	301	A1EG3	C2-N2	3.57	1.42	1.36
2	D	301	A1EG3	C4-C5	-3.55	1.31	1.38
2	B	301	A1EG3	C4-C5	-3.55	1.31	1.38
2	G	301	A1EG3	C2-N2	3.55	1.42	1.36
2	H	301	A1EG3	C4-C5	-3.51	1.31	1.38
2	M	301	A1EG3	C4-C5	-3.49	1.31	1.38
2	G	301	A1EG3	C4-C5	-3.45	1.31	1.38
2	I	301	A1EG3	C21-C22	-3.37	1.31	1.38
2	A	301	A1EG3	C3-CAA	-3.35	1.31	1.38
2	G	301	A1EG3	C21-C22	-3.34	1.31	1.38
2	F	301	A1EG3	C3-CAA	-3.32	1.31	1.38
2	K	301	A1EG3	C3-CAA	-3.31	1.31	1.38
2	L	301	A1EG3	C3-CAA	-3.31	1.31	1.38
2	N	301	A1EG3	C3-CAA	-3.29	1.31	1.38
2	J	301	A1EG3	C21-C22	-3.29	1.32	1.38
2	J	301	A1EG3	C4'-C23	3.29	1.51	1.44
2	M	301	A1EG3	C21-C22	-3.28	1.32	1.38
2	H	301	A1EG3	C21-C22	-3.27	1.32	1.38
2	B	301	A1EG3	C3-CAA	-3.27	1.31	1.38
2	I	301	A1EG3	C3-CAA	-3.26	1.31	1.38
2	N	301	A1EG3	C21-C22	-3.26	1.32	1.38
2	C	301	A1EG3	C3-CAA	-3.25	1.31	1.38
2	L	301	A1EG3	C21-C22	-3.25	1.32	1.38
2	D	301	A1EG3	C3-CAA	-3.25	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	A1EG3	C21-C22	-3.24	1.32	1.38
2	E	301	A1EG3	C3-CAA	-3.24	1.31	1.38
2	H	301	A1EG3	C3-CAA	-3.23	1.31	1.38
2	J	301	A1EG3	C3-CAA	-3.23	1.31	1.38
2	H	301	A1EG3	C4'-C23	3.22	1.51	1.44
2	E	301	A1EG3	C4'-C23	3.22	1.51	1.44
2	N	301	A1EG3	C4'-C23	3.22	1.51	1.44
2	K	301	A1EG3	C4'-C23	3.21	1.51	1.44
2	D	301	A1EG3	C4'-C23	3.20	1.51	1.44
2	C	301	A1EG3	C4'-C23	3.19	1.51	1.44
2	M	301	A1EG3	C3-CAA	-3.18	1.31	1.38
2	D	301	A1EG3	C21-C22	-3.18	1.32	1.38
2	E	301	A1EG3	C21-C22	-3.17	1.32	1.38
2	F	301	A1EG3	C21-C22	-3.17	1.32	1.38
2	B	301	A1EG3	C21-C22	-3.17	1.32	1.38
2	B	301	A1EG3	C4'-C23	3.17	1.51	1.44
2	G	301	A1EG3	C4'-C23	3.17	1.51	1.44
2	M	301	A1EG3	C4'-C23	3.17	1.51	1.44
2	A	301	A1EG3	C21-C22	-3.16	1.32	1.38
2	F	301	A1EG3	C4'-C23	3.16	1.51	1.44
2	L	301	A1EG3	C4'-C23	3.16	1.51	1.44
2	I	301	A1EG3	C4'-C23	3.16	1.51	1.44
2	K	301	A1EG3	C21-C22	-3.14	1.32	1.38
2	G	301	A1EG3	C3-CAA	-3.12	1.31	1.38
2	A	301	A1EG3	C4'-C23	3.11	1.51	1.44
2	G	301	A1EG3	C12-C9	2.95	1.53	1.50
2	I	301	A1EG3	C12-C9	2.93	1.53	1.50
2	D	301	A1EG3	C12-C9	2.71	1.53	1.50
2	M	301	A1EG3	C12-C9	2.69	1.53	1.50
2	J	301	A1EG3	C12-C9	2.69	1.53	1.50
2	N	301	A1EG3	C12-C9	2.69	1.53	1.50
2	H	301	A1EG3	C12-C9	2.69	1.53	1.50
2	L	301	A1EG3	C12-C9	2.68	1.53	1.50
2	C	301	A1EG3	C12-C9	2.68	1.53	1.50
2	E	301	A1EG3	C12-C9	2.67	1.53	1.50
2	F	301	A1EG3	C12-C9	2.65	1.53	1.50
2	K	301	A1EG3	C12-C9	2.63	1.53	1.50
2	B	301	A1EG3	C12-C9	2.63	1.53	1.50
2	A	301	A1EG3	C12-C9	2.53	1.53	1.50
2	I	301	A1EG3	C12-C8	2.03	1.58	1.52
2	J	301	A1EG3	C12-C8	2.03	1.58	1.52

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	301	A1EG3	C10-C14-N9	5.53	118.55	110.70
2	G	301	A1EG3	C10-C14-N9	5.48	118.48	110.70
2	A	301	A1EG3	C10-C14-N9	5.47	118.47	110.70
2	B	301	A1EG3	C10-C14-N9	5.22	118.12	110.70
2	F	301	A1EG3	C10-C14-N9	5.12	117.97	110.70
2	I	301	A1EG3	C2-N2-C11	-4.92	118.82	124.48
2	K	301	A1EG3	C10-C14-N9	4.88	117.62	110.70
2	K	301	A1EG3	C2-N2-C11	-4.85	118.90	124.48
2	D	301	A1EG3	C10-C14-N9	4.84	117.58	110.70
2	E	301	A1EG3	C10-C14-N9	4.79	117.50	110.70
2	F	301	A1EG3	C2-N2-C11	-4.78	118.98	124.48
2	C	301	A1EG3	C2-N2-C11	-4.76	119.00	124.48
2	E	301	A1EG3	C2-N2-C11	-4.76	119.00	124.48
2	A	301	A1EG3	C2-N2-C11	-4.75	119.02	124.48
2	C	301	A1EG3	C10-C14-N9	4.75	117.44	110.70
2	M	301	A1EG3	C2-N2-C11	-4.73	119.04	124.48
2	D	301	A1EG3	C2-N2-C11	-4.72	119.05	124.48
2	N	301	A1EG3	C2-N2-C11	-4.70	119.07	124.48
2	J	301	A1EG3	C2-N2-C11	-4.64	119.14	124.48
2	N	301	A1EG3	C10-C14-N9	4.63	117.27	110.70
2	M	301	A1EG3	C10-C14-N9	4.62	117.25	110.70
2	L	301	A1EG3	C10-C14-N9	4.61	117.24	110.70
2	L	301	A1EG3	C2-N2-C11	-4.54	119.26	124.48
2	H	301	A1EG3	C10-C14-N9	4.54	117.14	110.70
2	B	301	A1EG3	C2-N2-C11	-4.53	119.26	124.48
2	H	301	A1EG3	C2-N2-C11	-4.50	119.31	124.48
2	G	301	A1EG3	C2-N2-C11	-4.37	119.45	124.48
2	J	301	A1EG3	C10-C14-N9	3.91	116.25	110.70
2	B	301	A1EG3	C10-C11-N2	-3.65	112.96	115.69
2	L	301	A1EG3	C10-C11-N2	-3.58	113.01	115.69
2	N	301	A1EG3	C10-C11-N2	-3.50	113.07	115.69
2	H	301	A1EG3	C10-C11-N2	-3.45	113.11	115.69
2	F	301	A1EG3	C10-C11-N2	-3.44	113.12	115.69
2	A	301	A1EG3	C10-C11-N2	-3.42	113.13	115.69
2	J	301	A1EG3	C10-C11-N2	-3.38	113.16	115.69
2	G	301	A1EG3	C10-C11-N2	-3.35	113.18	115.69
2	C	301	A1EG3	C10-C11-N2	-3.35	113.19	115.69
2	E	301	A1EG3	C10-C11-N2	-3.32	113.20	115.69
2	K	301	A1EG3	C10-C11-N2	-3.28	113.23	115.69
2	D	301	A1EG3	C10-C11-N2	-3.27	113.24	115.69
2	I	301	A1EG3	C12-C9-N3	3.14	121.63	114.98
2	M	301	A1EG3	C10-C11-N2	-3.12	113.36	115.69
2	I	301	A1EG3	C10-C11-N2	-3.10	113.37	115.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	301	A1EG3	C1'-N9-C8	3.06	119.46	113.07
2	K	301	A1EG3	C12-C9-N3	3.05	121.44	114.98
2	D	301	A1EG3	C12-C9-N3	2.92	121.17	114.98
2	A	301	A1EG3	C12-C9-N3	2.89	121.11	114.98
2	N	301	A1EG3	C12-C9-N3	2.89	121.10	114.98
2	G	301	A1EG3	C12-C9-N3	2.89	121.10	114.98
2	E	301	A1EG3	C12-C9-N3	2.88	121.08	114.98
2	J	301	A1EG3	C12-C9-N3	2.87	121.07	114.98
2	F	301	A1EG3	C12-C9-N3	2.82	120.97	114.98
2	B	301	A1EG3	C12-C9-N3	2.81	120.94	114.98
2	C	301	A1EG3	C12-C9-N3	2.79	120.89	114.98
2	L	301	A1EG3	C12-C9-N3	2.67	120.64	114.98
2	H	301	A1EG3	C12-C9-N3	2.65	120.61	114.98
2	M	301	A1EG3	C12-C9-N3	2.60	120.50	114.98
2	I	301	A1EG3	C2'-C1'-N9	2.55	116.93	112.75
2	B	301	A1EG3	C1'-N9-C14	-2.08	107.80	111.52
2	A	301	A1EG3	C1'-N9-C14	-2.06	107.85	111.52
2	K	301	A1EG3	OP3-C11-N2	2.04	124.04	120.12

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	A1EG3	N3-C2-N1-C6
2	A	301	A1EG3	N2-C2-N1-C6
2	B	301	A1EG3	N3-C2-N1-C6
2	B	301	A1EG3	N2-C2-N1-C6
2	C	301	A1EG3	N3-C2-N1-C6
2	C	301	A1EG3	N2-C2-N1-C6
2	D	301	A1EG3	N3-C2-N1-C6
2	D	301	A1EG3	N2-C2-N1-C6
2	E	301	A1EG3	N3-C2-N1-C6
2	E	301	A1EG3	N2-C2-N1-C6
2	F	301	A1EG3	N3-C2-N1-C6
2	F	301	A1EG3	N2-C2-N1-C6
2	G	301	A1EG3	N3-C2-N1-C6
2	H	301	A1EG3	N3-C2-N1-C6
2	I	301	A1EG3	N3-C2-N1-C6
2	J	301	A1EG3	N3-C2-N1-C6
2	K	301	A1EG3	N3-C2-N1-C6
2	K	301	A1EG3	N2-C2-N1-C6
2	L	301	A1EG3	N3-C2-N1-C6

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Mol	Chain	Res	Type	Atoms
2	L	301	A1EG3	N2-C2-N1-C6
2	M	301	A1EG3	N3-C2-N1-C6
2	N	301	A1EG3	N3-C2-N1-C6
2	G	301	A1EG3	N2-C2-N1-C6
2	H	301	A1EG3	N2-C2-N1-C6
2	I	301	A1EG3	N2-C2-N1-C6
2	J	301	A1EG3	N2-C2-N1-C6
2	M	301	A1EG3	N2-C2-N1-C6
2	N	301	A1EG3	N2-C2-N1-C6
2	B	301	A1EG3	N5-C23-C4'-C3'

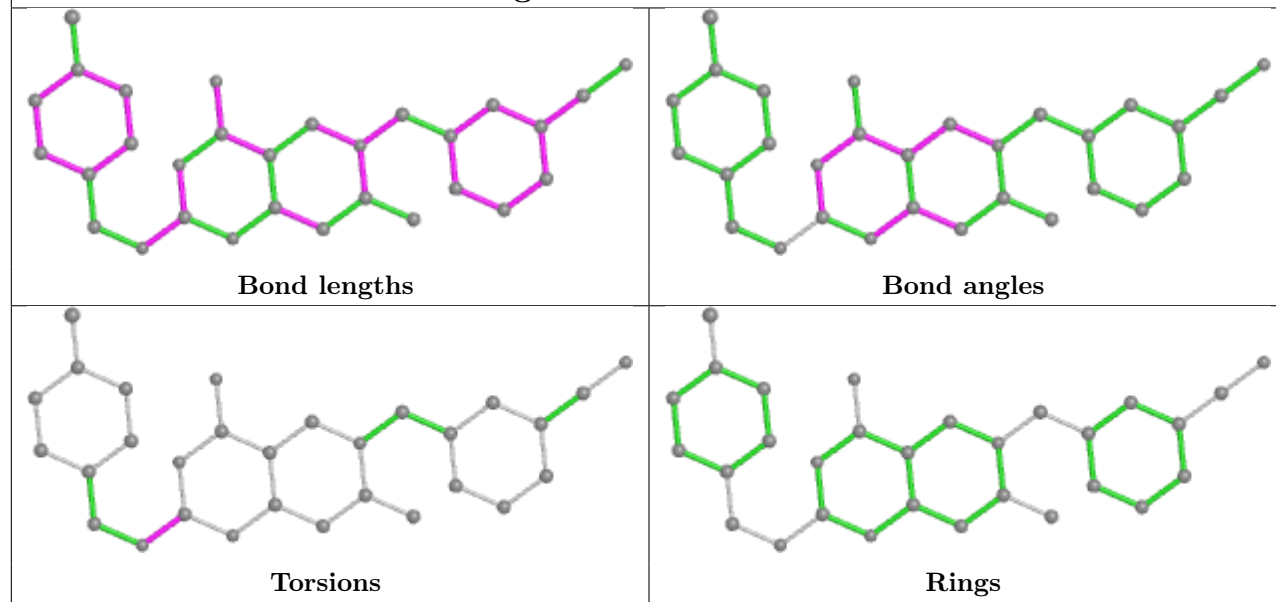
There are no ring outliers.

14 monomers are involved in 18 short contacts:

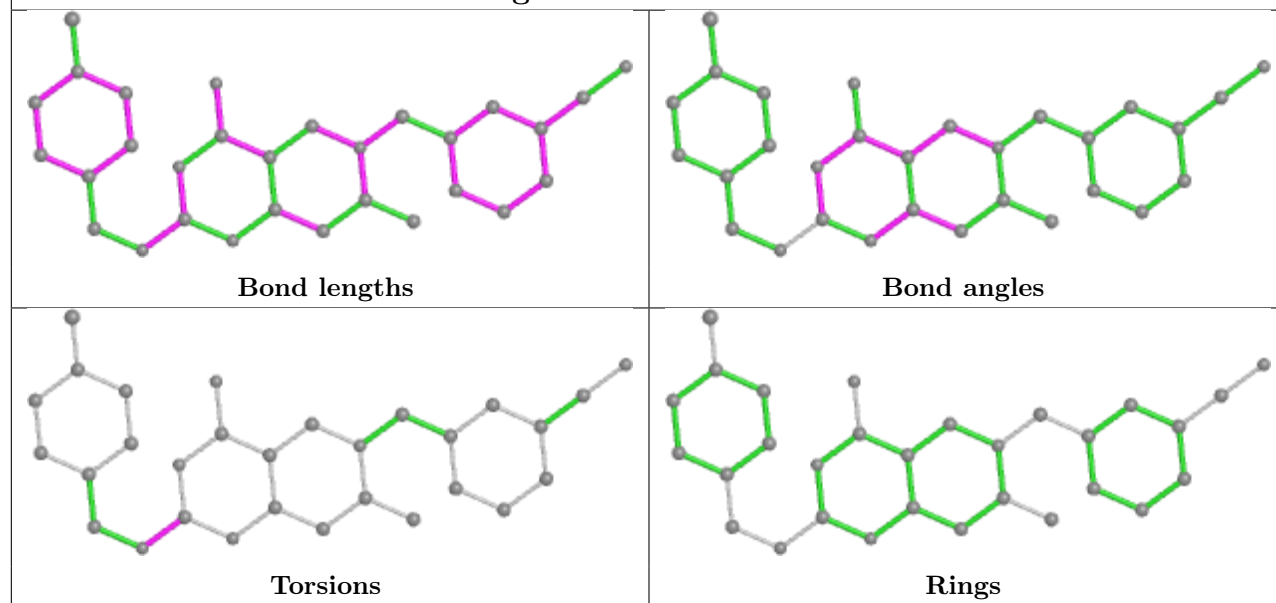
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	301	A1EG3	1	0
2	C	301	A1EG3	2	0
2	A	301	A1EG3	1	0
2	L	301	A1EG3	1	0
2	D	301	A1EG3	2	0
2	H	301	A1EG3	1	0
2	I	301	A1EG3	1	0
2	J	301	A1EG3	3	0
2	M	301	A1EG3	1	0
2	B	301	A1EG3	1	0
2	N	301	A1EG3	1	0
2	E	301	A1EG3	1	0
2	G	301	A1EG3	1	0
2	K	301	A1EG3	1	0

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.

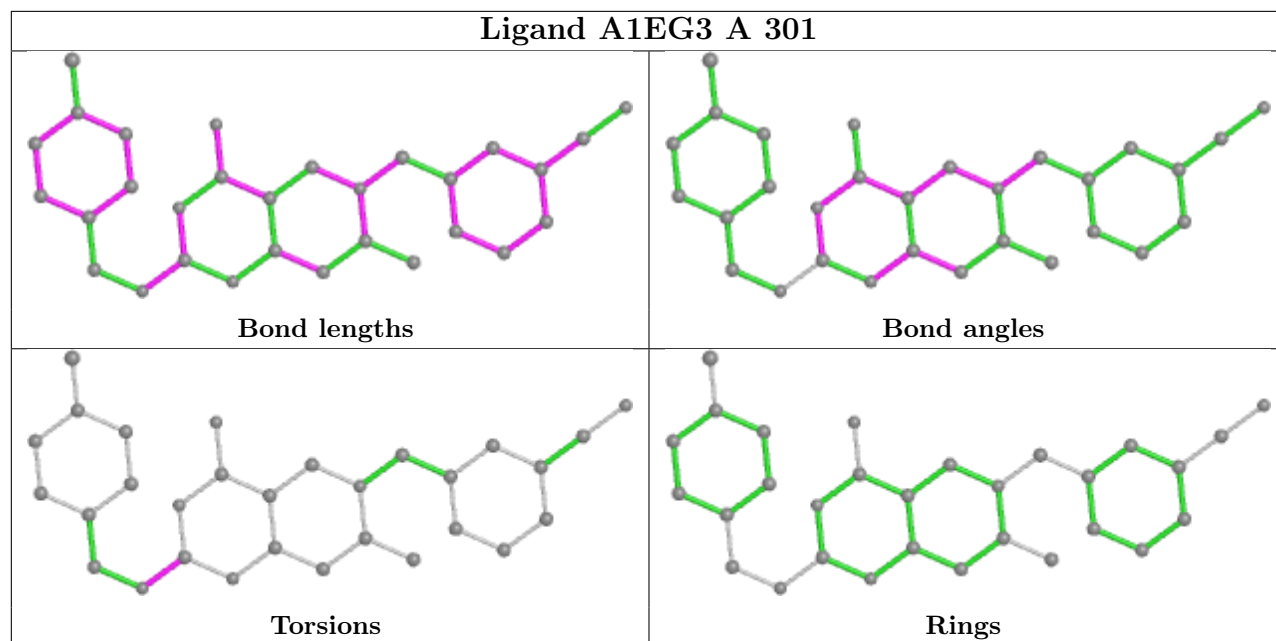
Ligand A1EG3 F 301



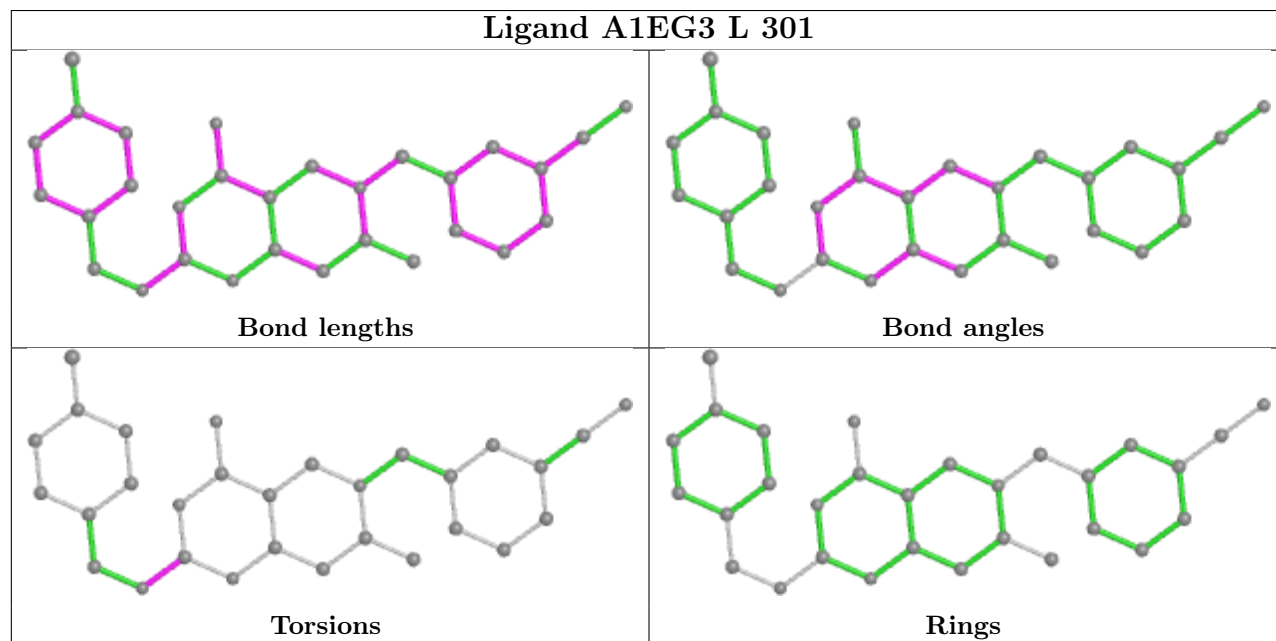
Ligand A1EG3 C 301



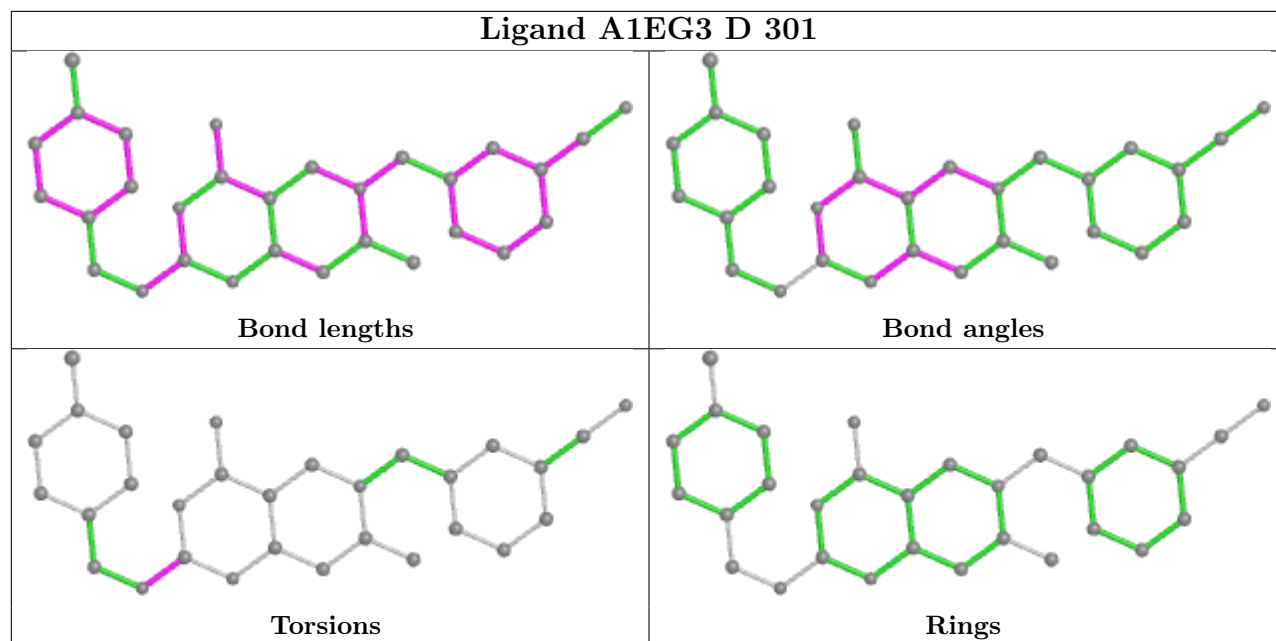
Ligand A1EG3 A 301



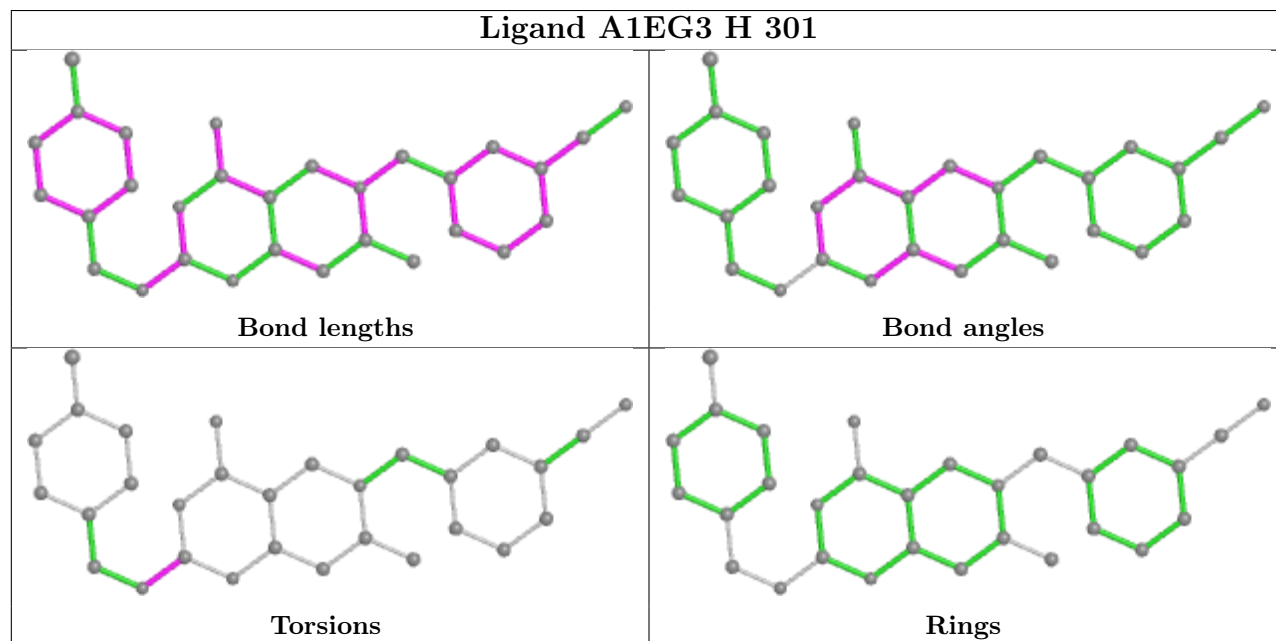
Ligand A1EG3 L 301



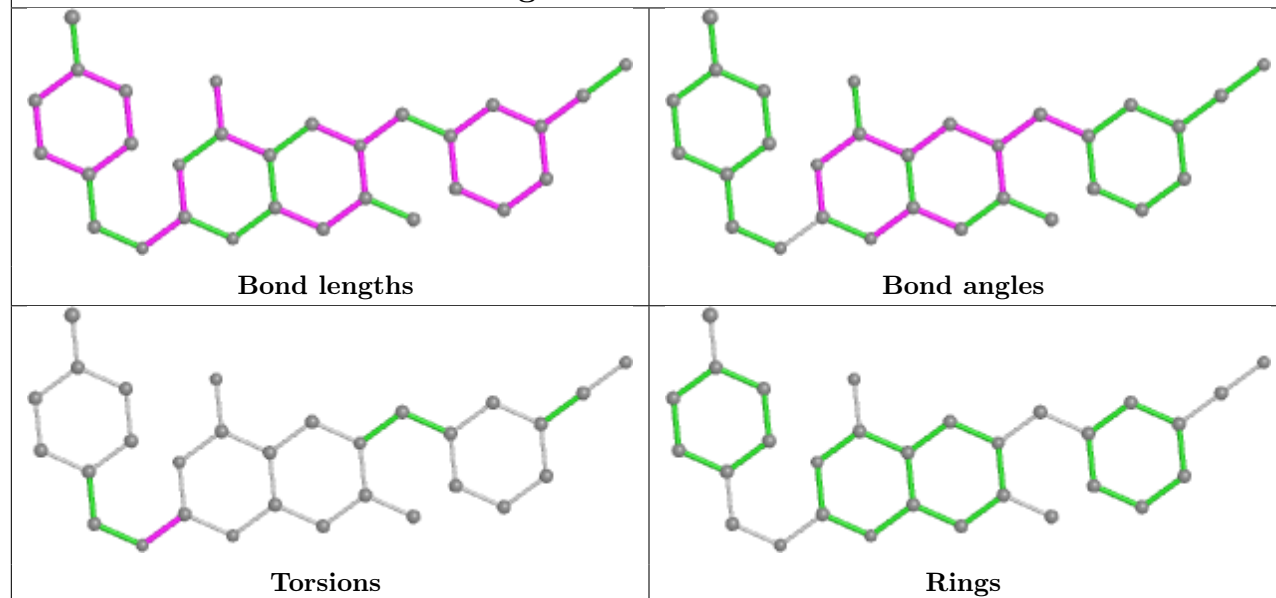
Ligand A1EG3 D 301



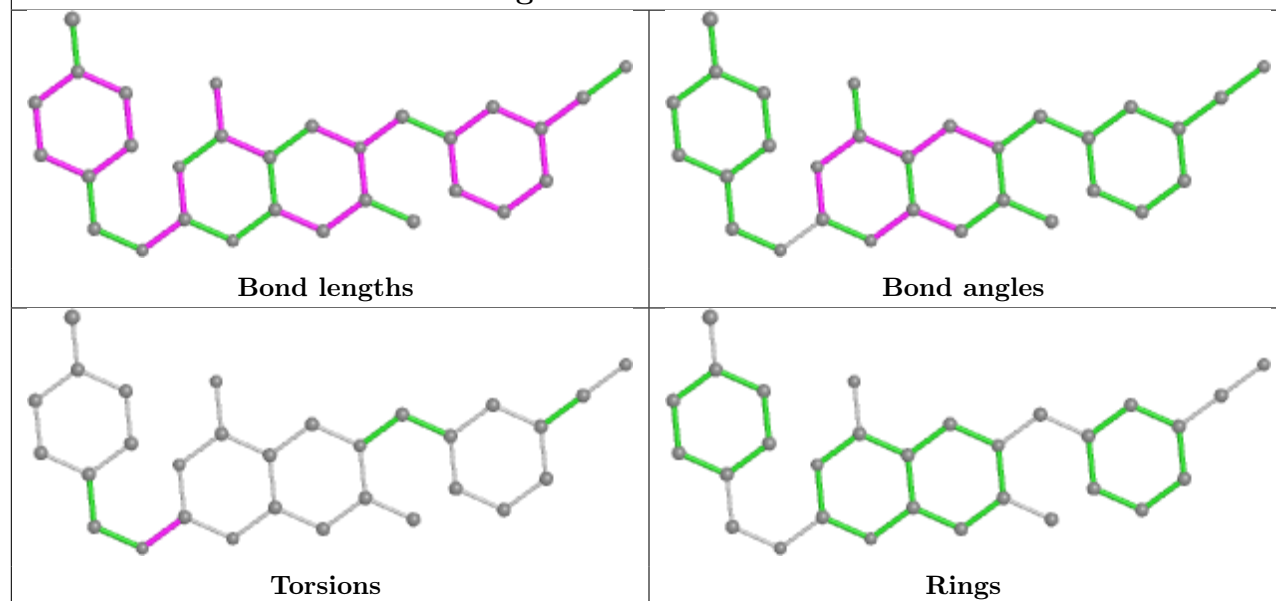
Ligand A1EG3 H 301



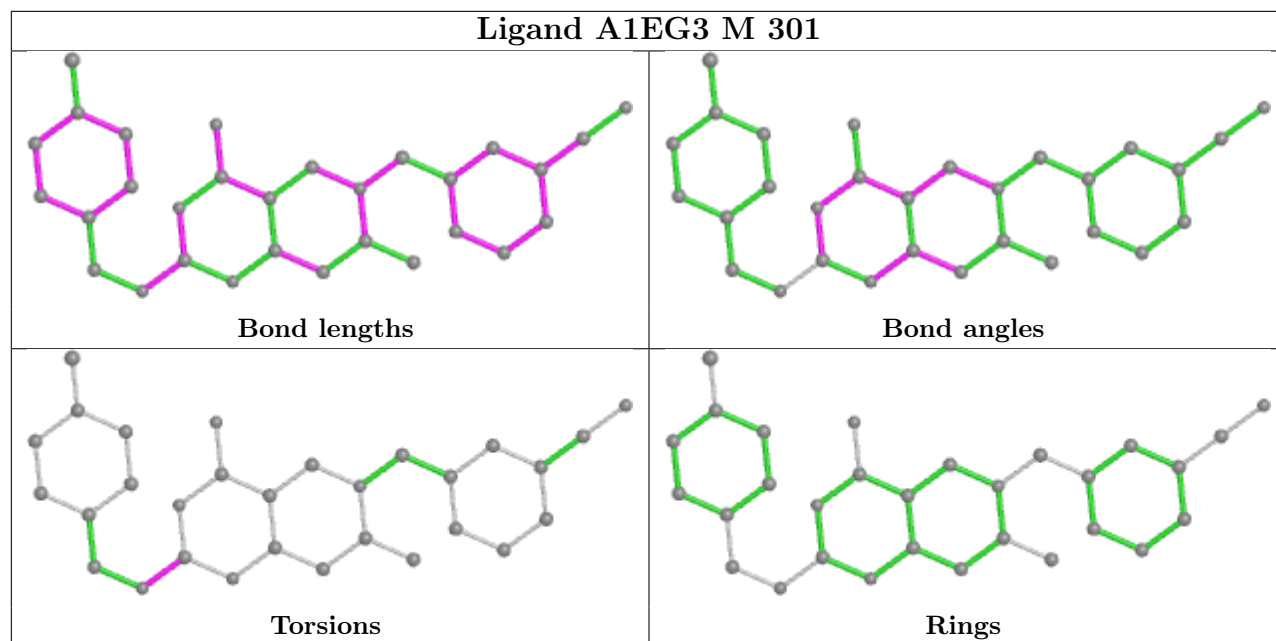
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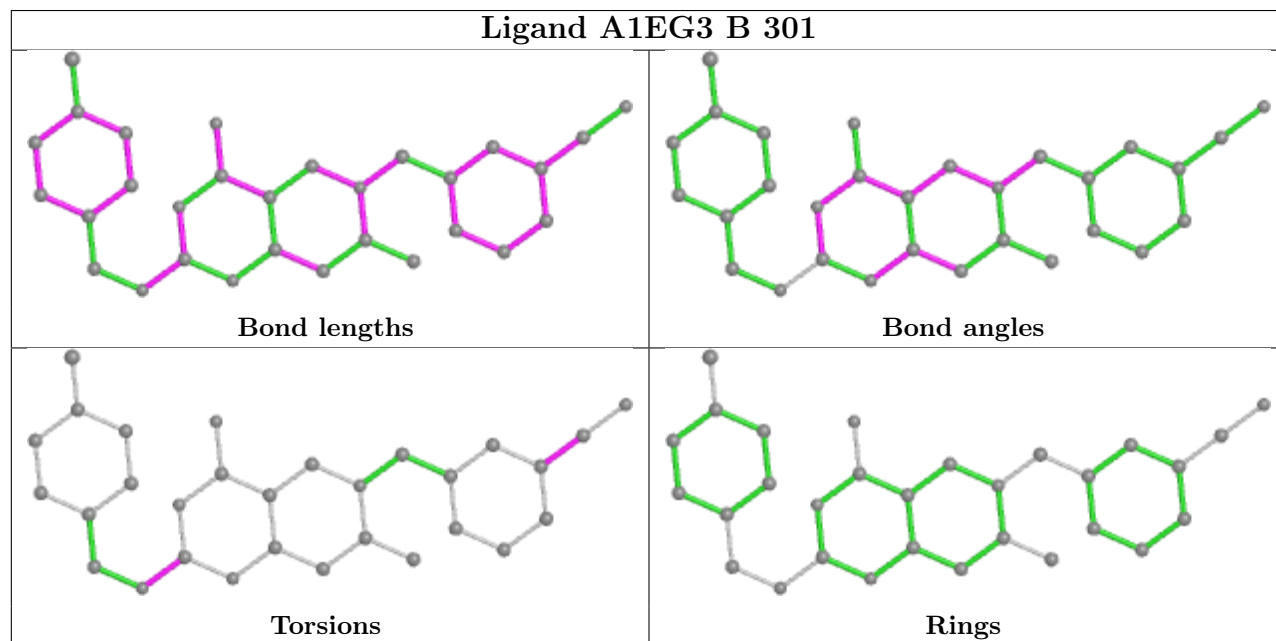
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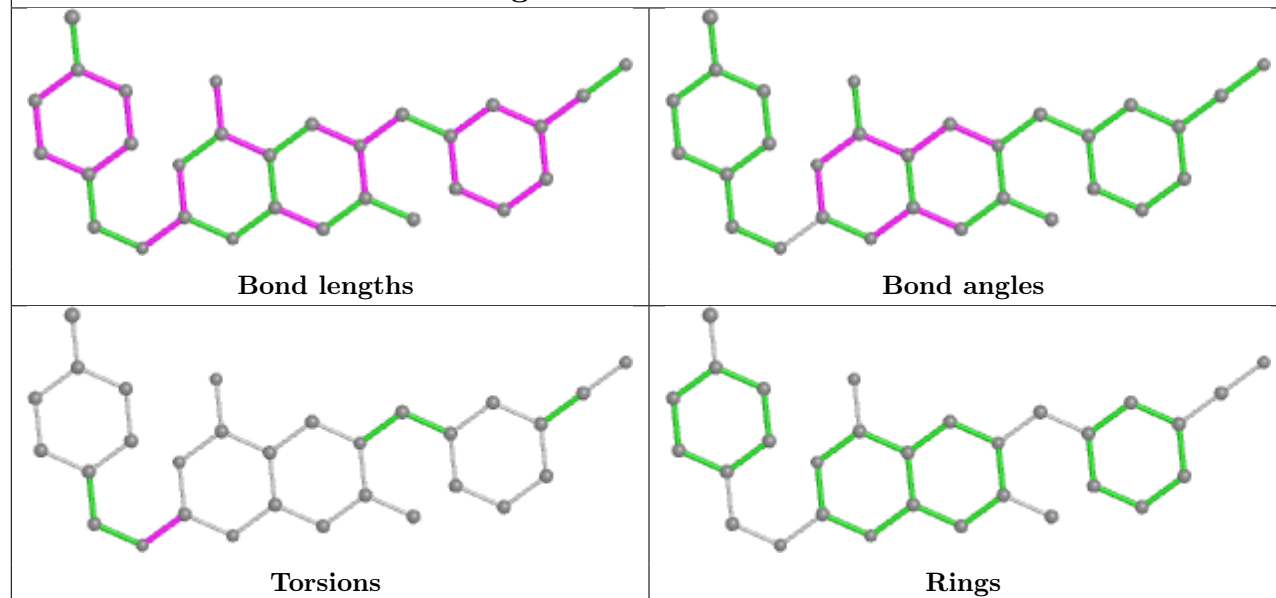
Ligand A1EG3 M 301



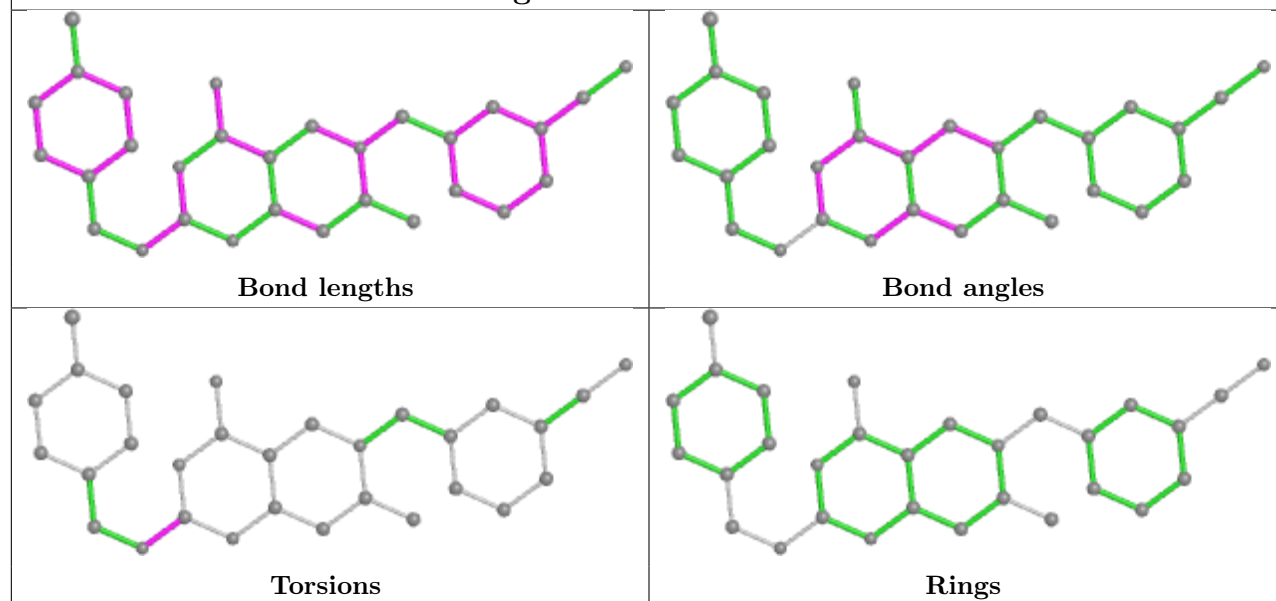
Ligand A1EG3 B 301

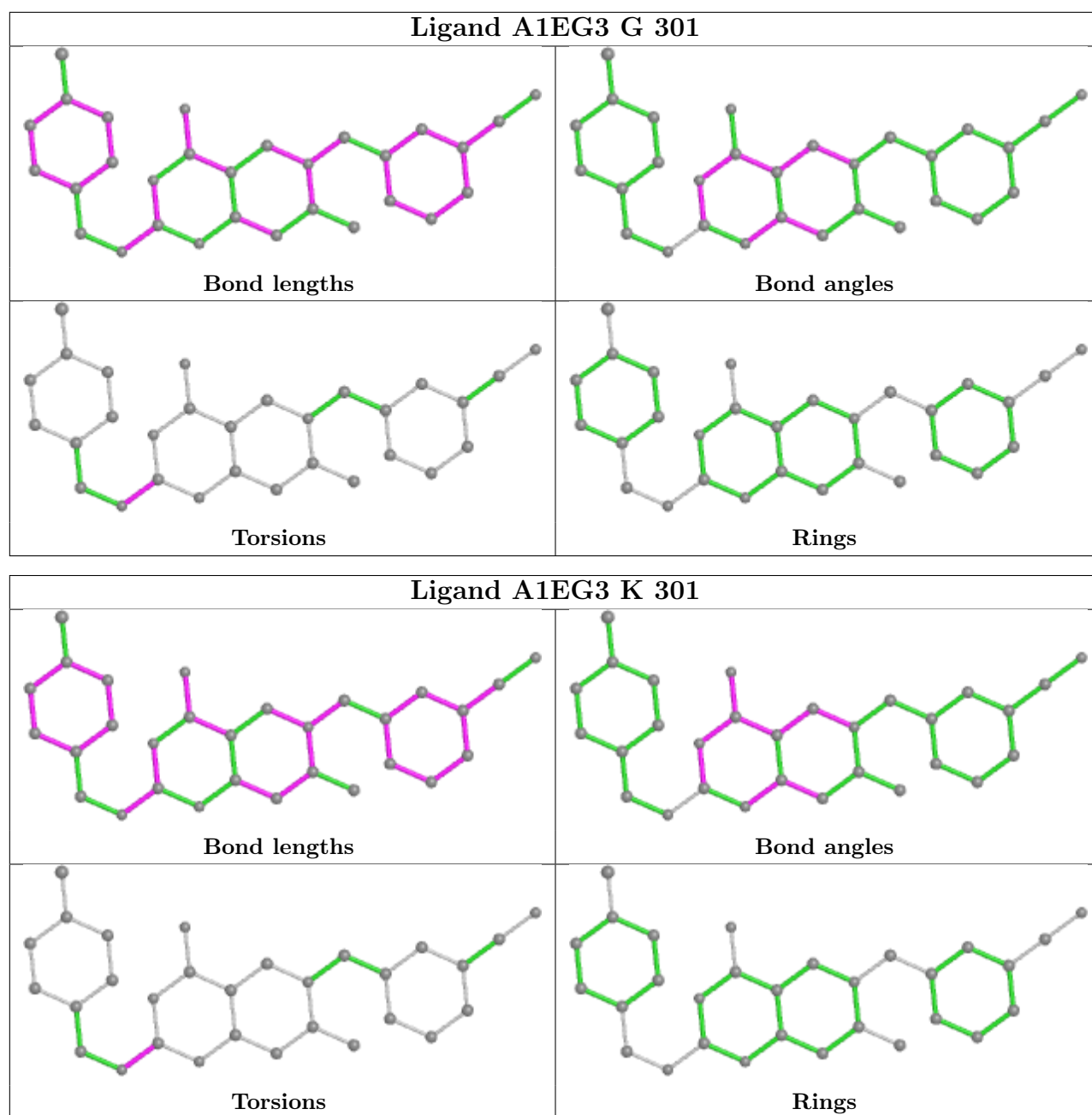


Ligand A1EG3 N 301



Ligand A1EG3 E 301





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.