



Full wwPDB EM Validation Report ⓘ

Mar 30, 2026 – 12:47 AM UTC

PDB ID : 7X0S / pdb_00007x0s
EMDB ID : EMD-32923
Title : Human TRiC-tubulin-S3
Authors : Cong, Y.; Liu, C.X.
Deposited on : 2022-02-22
Resolution : 3.10 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:

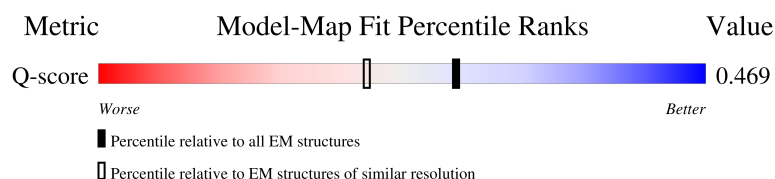
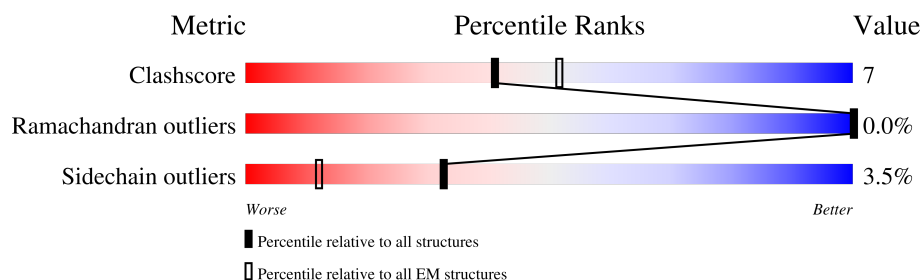
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 3.10 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14724 (2.60 - 3.60)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	K	531	82% 16% ..
1	z	531	85% 13% .
2	J	548	81% 14% . .
2	P	548	81% 14% . .

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Mol	Chain	Length	Quality of chain
3	H	543	
3	O	543	
4	G	545	
4	N	545	
5	E	539	
5	e	539	
6	I	539	
6	M	539	
7	B	535	
7	L	535	
8	A	556	
8	a	556	
9	R	444	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	ADP	A	601	-	-	X	-
10	ADP	G	601	-	-	X	-
10	ADP	H	601	-	-	X	-
10	ADP	I	601	-	-	X	-
10	ADP	J	601	-	-	X	-
10	ADP	K	601	-	-	X	-
10	ADP	M	601	-	-	X	-
10	ADP	N	601	-	-	X	-
10	ADP	O	603	-	-	X	-
10	ADP	P	601	-	-	X	-
10	ADP	z	601	-	-	X	-
11	MG	K	602	-	-	X	-
11	MG	z	602	-	-	X	-
12	AF3	A	603	-	-	X	-
12	AF3	B	603	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	AF3	E	603	-	-	X	-
12	AF3	G	603	-	-	X	-
12	AF3	H	603	-	-	X	-
12	AF3	J	603	-	-	X	-
12	AF3	K	603	-	-	X	-
12	AF3	L	603	-	-	X	-
12	AF3	N	603	-	-	X	-
12	AF3	O	602	-	-	X	-
12	AF3	P	603	-	-	X	-
12	AF3	a	603	-	-	X	-
12	AF3	e	603	-	-	X	-
12	AF3	z	603	-	-	X	-

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 68346 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 T-complex protein 1 subunit zeta.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	K	525	Total	C	N	O	S	0	0
			4022	2528	704	769	21		
1	z	525	Total	C	N	O	S	0	0
			4022	2528	704	769	21		

- Molecule 2 is a protein called T-complex protein 1 subunit theta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	J	527	Total	C	N	O	S	0	0
			4008	2529	682	770	27		
2	P	527	Total	C	N	O	S	0	0
			4008	2529	682	770	27		

- Molecule 3 is a protein called T-complex protein 1 subunit eta.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	526	Total	C	N	O	S	0	0
			4037	2549	697	766	25		
3	O	526	Total	C	N	O	S	0	0
			4037	2549	697	766	25		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	290	SER	LEU	engineered mutation	UNP Q99832
O	290	SER	LEU	engineered mutation	UNP Q99832

- Molecule 4 is a protein called T-complex protein 1 subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	526	Total	C	N	O	S	0	0
			4094	2552	727	785	30		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	N	526	Total	C	N	O	S	0	0
			4094	2552	727	785	30		

- Molecule 5 is a protein called T-complex protein 1 subunit epsilon.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	535	Total	C	N	O	S	0	0
			4126	2583	718	795	30		
5	e	535	Total	C	N	O	S	0	0
			4126	2583	718	795	30		

- Molecule 6 is a protein called T-complex protein 1 subunit delta.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	I	521	Total	C	N	O	S	0	0
			3935	2459	687	766	23		
6	M	521	Total	C	N	O	S	0	0
			3935	2459	687	766	23		

- Molecule 7 is a protein called T-complex protein 1 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	B	523	Total	C	N	O	S	0	0
			3937	2463	696	759	19		
7	L	523	Total	C	N	O	S	0	0
			3937	2463	696	759	19		

- Molecule 8 is a protein called T-complex protein 1 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	A	537	Total	C	N	O	S	0	0
			4077	2553	713	788	23		
8	a	537	Total	C	N	O	S	0	0
			4077	2553	713	788	23		

- Molecule 9 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	R	426	Total	C	N	O	S	0	0
			3346	2106	573	642	25		

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

The diagram illustrates the chemical structure of Adenosine Diphosphate (ADP). It consists of an adenine base (a purine ring system) attached to a ribose sugar, which is in turn linked to two phosphate groups. The adenine base is shown with atoms N1, N3, N6, N7, C2, C4, C5, C6, C8, and N9. The ribose sugar is shown with atoms C1', C2', C3', C4', and C5'. The two phosphate groups are shown with atoms O1A, O1B, O2A, O2B, O3A, O3B, O4A, O4B, O5A, O5B, O6A, O6B, O7A, O7B, O8A, O8B, O9A, O9B, O10A, O10B, O11A, O11B, O12A, O12B, O13A, O13B, O14A, O14B, O15A, O15B, O16A, O16B, O17A, O17B, O18A, O18B, O19A, O19B, O20A, O20B, O21A, O21B, O22A, O22B, O23A, O23B, O24A, O24B, O25A, O25B, O26A, O26B, O27A, O27B, O28A, O28B, O29A, O29B, O30A, O30B, O31A, O31B, O32A, O32B, O33A, O33B, O34A, O34B, O35A, O35B, O36A, O36B, O37A, O37B, O38A, O38B, O39A, O39B, O40A, O40B, O41A, O41B, O42A, O42B, O43A, O43B, O44A, O44B, O45A, O45B, O46A, O46B, O47A, O47B, O48A, O48B, O49A, O49B, O50A, O50B, O51A, O51B, O52A, O52B, O53A, O53B, O54A, O54B, O55A, O55B, O56A, O56B, O57A, O57B, O58A, O58B, O59A, O59B, O60A, O60B, O61A, O61B, O62A, O62B, O63A, O63B, O64A, O64B, O65A, O65B, O66A, O66B, O67A, O67B, O68A, O68B, O69A, O69B, O70A, O70B, O71A, O71B, O72A, O72B, O73A, O73B, O74A, O74B, O75A, O75B, O76A, O76B, O77A, O77B, O78A, O78B, O79A, O79B, O80A, O80B, O81A, O81B, O82A, O82B, O83A, O83B, O84A, O84B, O85A, O85B, O86A, O86B, O87A, O87B, O88A, O88B, O89A, O89B, O90A, O90B, O91A, O91B, O92A, O92B, O93A, O93B, O94A, O94B, O95A, O95B, O96A, O96B, O97A, O97B, O98A, O98B, O99A, O99B, O100A, O100B, O101A, O101B, O102A, O102B, O103A, O103B, O104A, O104B, O105A, O105B, O106A, O106B, O107A, O107B, O108A, O108B, O109A, O109B, O110A, O110B, O111A, O111B, O112A, O112B, O113A, O113B, O114A, O114B, O115A, O115B, O116A, O116B, O117A, O117B, O118A, O118B, O119A, O119B, O120A, O120B, O121A, O121B, O122A, O122B, O123A, O123B, O124A, O124B, O125A, O125B, O126A, O126B, O127A, O127B, O128A, O128B, O129A, O129B, O130A, O130B, O131A, O131B, O132A, O132B, O133A, O133B, O134A, O134B, O135A, O135B, O136A, O136B, O137A, O137B, O138A, O138B, O139A, O139B, O140A, O140B, O141A, O141B, O142A, O142B, O143A, O143B, O144A, O144B, O145A, O145B, O146A, O146B, O147A, O147B, O148A, O148B, O149A, O149B, O150A, O150B, O151A, O151B, O152A, O152B, O153A, O153B, O154A, O154B, O155A, O155B, O156A, O156B, O157A, O157B, O158A, O158B, O159A, O159B, O160A, O160B, O161A, O161B, O162A, O162B, O163A, O163B, O164A, O164B, O165A, O165B, O166A, O166B, O167A, O167B, O168A, O168B, O169A, O169B, O170A, O170B, O171A, O171B, O172A, O172B, O173A, O173B, O174A, O174B, O175A, O175B, O176A, O176B, O177A, O177B, O178A, O178B, O179A, O179B, O180A, O180B, O181A, O181B, O182A, O182B, O183A, O183B, O184A, O184B, O185A, O185B, O186A, O186B, O187A, O187B, O188A, O188B, O189A, O189B, O190A, O190B, O191A, O191B, O192A, O192B, O193A, O193B, O194A, O194B, O195A, O195B, O196A, O196B, O197A, O197B, O198A, O198B, O199A, O199B, O200A, O200B, O201A, O201B, O202A, O202B, O203A, O203B, O204A, O204B, O205A, O205B, O206A, O206B, O207A, O207B, O208A, O208B, O209A, O209B, O210A, O210B, O211A, O211B, O212A, O212B, O213A, O213B, O214A, O214B, O215A, O215B, O216A, O216B, O217A, O217B, O218A, O218B, O219A, O219B, O220A, O220B, O221A, O221B, O222A, O222B, O223A, O223B, O224A, O224B, O225A, O225B, O226A, O226B, O227A, O227B, O228A, O228B, O229A, O229B, O230A, O230B, O231A, O231B, O232A, O232B, O233A, O233B, O234A, O234B, O235A, O235B, O236A, O236B, O237A, O237B, O238A, O238B, O239A, O239B, O240A, O240B, O241A, O241B, O242A, O242B, O243A, O243B, O244A, O244B, O245A, O245B, O246A, O246B, O247A, O247B, O248A, O248B, O249A, O249B, O250A, O250B, O251A, O251B, O252A, O252B, O253A, O253B, O254A, O254B, O255A, O255B, O256A, O256B, O257A, O257B, O258A, O258B, O259A, O259B, O260A, O260B, O261A, O261B, O262A, O262B, O263A, O263B, O264A, O264B, O265A, O265B, O266A, O266B, O267A, O267B, O268A, O268B, O269A, O269B, O270A, O270B, O271A, O271B, O272A, O272B, O273A, O273B, O274A, O274B, O275A, O275B, O276A, O276B, O277A, O277B, O278A, O278B, O279A, O279B, O280A, O280B, O281A, O281B, O282A, O282B, O283A, O283B, O284A, O284B, O285A, O285B, O286A, O286B, O287A, O287B, O288A, O288B, O289A, O289B, O290A, O290B, O291A, O291B, O292A, O292B, O293A, O293B, O294A, O294B, O295A, O295B, O296A, O296B, O297A, O297B, O298A, O298B, O299A, O299B, O300A, O300B, O301A, O301B, O302A, O302B, O303A, O303B, O304A, O304B, O305A, O305B, O306A, O306B, O307A, O307B, O308A, O308B, O309A, O309B, O310A, O310B, O311A, O311B, O312A, O312B, O313A, O313B, O314A, O314B, O315A, O315B, O316A, O316B, O317A, O317B, O318A, O318B, O319A, O319B, O320A, O320B, O321A, O321B, O322A, O322B, O323A, O323B, O324A, O324B, O325A, O325B, O326A, O326B, O327A, O327B, O328A, O328B, O329A, O329B, O330A, O330B, O331A, O331B, O332A, O332B, O333A, O333B, O334A, O334B, O335A, O335B, O336A, O336B, O337A, O337B, O338A, O338B, O339A, O339B, O340A, O340B, O341A, O341B, O342A, O342B, O343A, O343B, O344A, O344B, O345A, O345B, O346A, O346B, O347A,

Mol	Chain	Residues	Atoms					AltConf
10	K	1	Total 27	C 10	N 5	O 10	P 2	0
10	J	1	Total 27	C 10	N 5	O 10	P 2	0
10	H	1	Total 27	C 10	N 5	O 10	P 2	0
10	G	1	Total 27	C 10	N 5	O 10	P 2	0
10	E	1	Total 27	C 10	N 5	O 10	P 2	0
10	I	1	Total 27	C 10	N 5	O 10	P 2	0
10	B	1	Total 27	C 10	N 5	O 10	P 2	0
10	A	1	Total 27	C 10	N 5	O 10	P 2	0
10	z	1	Total 27	C 10	N 5	O 10	P 2	0
10	P	1	Total 27	C 10	N 5	O 10	P 2	0
10	O	1	Total 27	C 10	N 5	O 10	P 2	0
10	N	1	Total 27	C 10	N 5	O 10	P 2	0
10	e	1	Total 27	C 10	N 5	O 10	P 2	0

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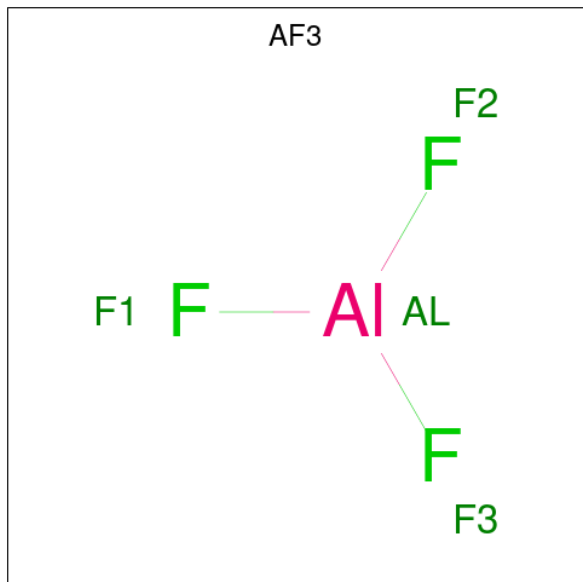
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Mol	Chain	Residues	Atoms					AltConf
10	a	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	M	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	L	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 11 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
11	K	1	Total	Mg	0
			1	1	
11	J	1	Total	Mg	0
			1	1	
11	H	1	Total	Mg	0
			1	1	
11	G	1	Total	Mg	0
			1	1	
11	E	1	Total	Mg	0
			1	1	
11	I	1	Total	Mg	0
			1	1	
11	B	1	Total	Mg	0
			1	1	
11	A	1	Total	Mg	0
			1	1	
11	z	1	Total	Mg	0
			1	1	
11	P	1	Total	Mg	0
			1	1	
11	O	1	Total	Mg	0
			1	1	
11	N	1	Total	Mg	0
			1	1	
11	e	1	Total	Mg	0
			1	1	
11	a	1	Total	Mg	0
			1	1	
11	M	1	Total	Mg	0
			1	1	
11	L	1	Total	Mg	0
			1	1	

- Molecule 12 is ALUMINUM FLUORIDE (CCD ID: AF3) (formula: AlF_3) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
12	K	1	Total	Al	F	0
			4	1	3	
12	J	1	Total	Al	F	0
			4	1	3	
12	H	1	Total	Al	F	0
			4	1	3	
12	G	1	Total	Al	F	0
			4	1	3	
12	E	1	Total	Al	F	0
			4	1	3	
12	I	1	Total	Al	F	0
			4	1	3	
12	B	1	Total	Al	F	0
			4	1	3	
12	A	1	Total	Al	F	0
			4	1	3	
12	z	1	Total	Al	F	0
			4	1	3	
12	P	1	Total	Al	F	0
			4	1	3	
12	O	1	Total	Al	F	0
			4	1	3	
12	N	1	Total	Al	F	0
			4	1	3	

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Mol	Chain	Residues	Atoms			AltConf
12	e	1	Total 4	Al 1	F 3	0
12	a	1	Total 4	Al 1	F 3	0
12	M	1	Total 4	Al 1	F 3	0
12	L	1	Total 4	Al 1	F 3	0

- Molecule 13 is water.

Mol	Chain	Residues	Atoms		AltConf
13	K	1	Total 1	O 1	0
13	J	1	Total 1	O 1	0
13	H	1	Total 1	O 1	0
13	G	1	Total 1	O 1	0
13	E	1	Total 1	O 1	0
13	I	1	Total 1	O 1	0
13	B	1	Total 1	O 1	0
13	A	1	Total 1	O 1	0
13	z	1	Total 1	O 1	0
13	P	1	Total 1	O 1	0
13	O	1	Total 1	O 1	0
13	N	1	Total 1	O 1	0
13	e	1	Total 1	O 1	0
13	a	1	Total 1	O 1	0
13	M	1	Total 1	O 1	0

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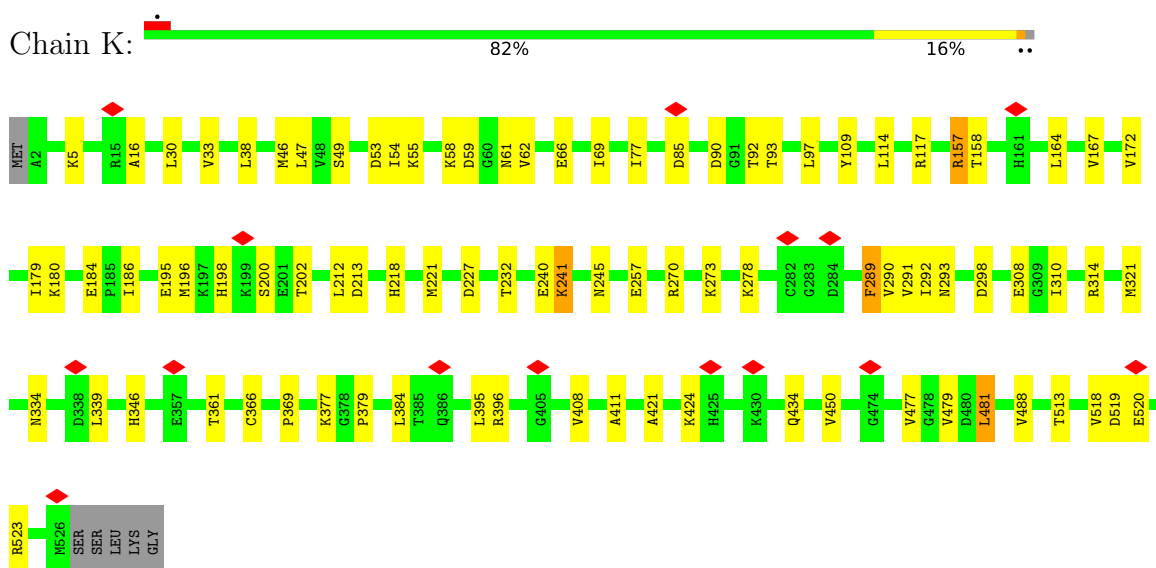
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Mol	Chain	Residues	Atoms		AltConf
13	L	1	Total	O	0
			1	1	

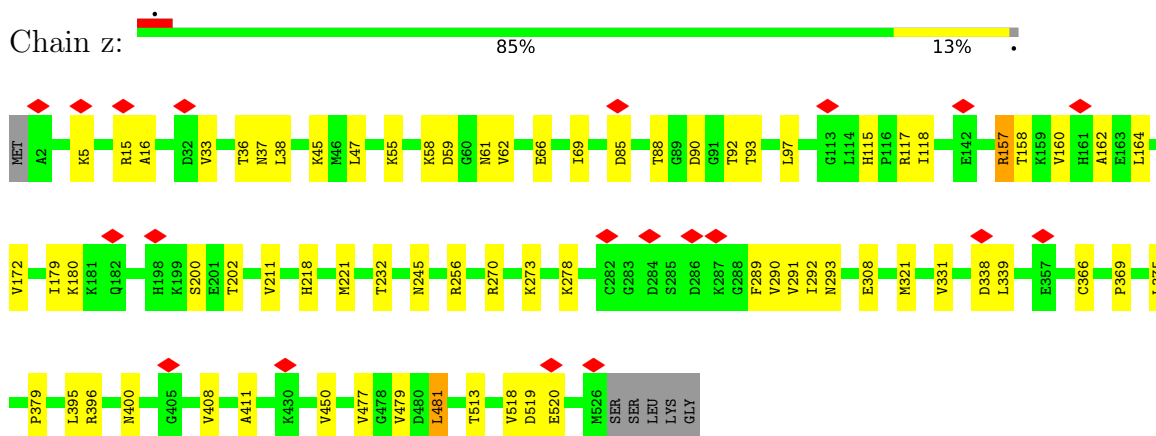
3 Residue-property plots

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 and atom inclusion in map density. 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. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

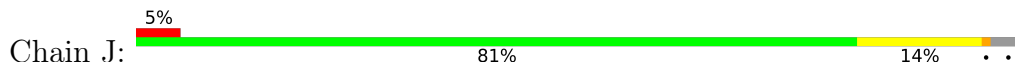
- Molecule 1: T-complex protein 1 subunit zeta

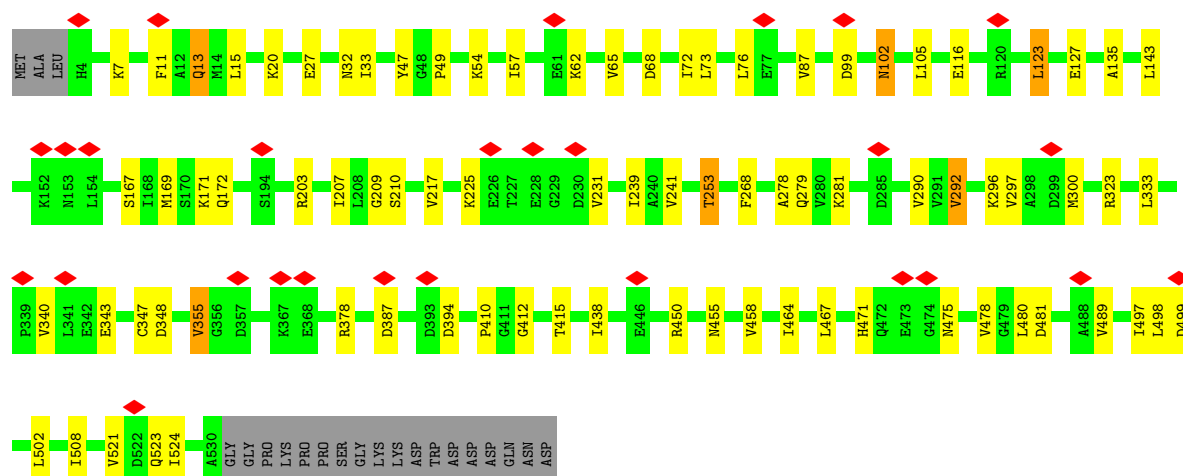


- Molecule 1: T-complex protein 1 subunit zeta

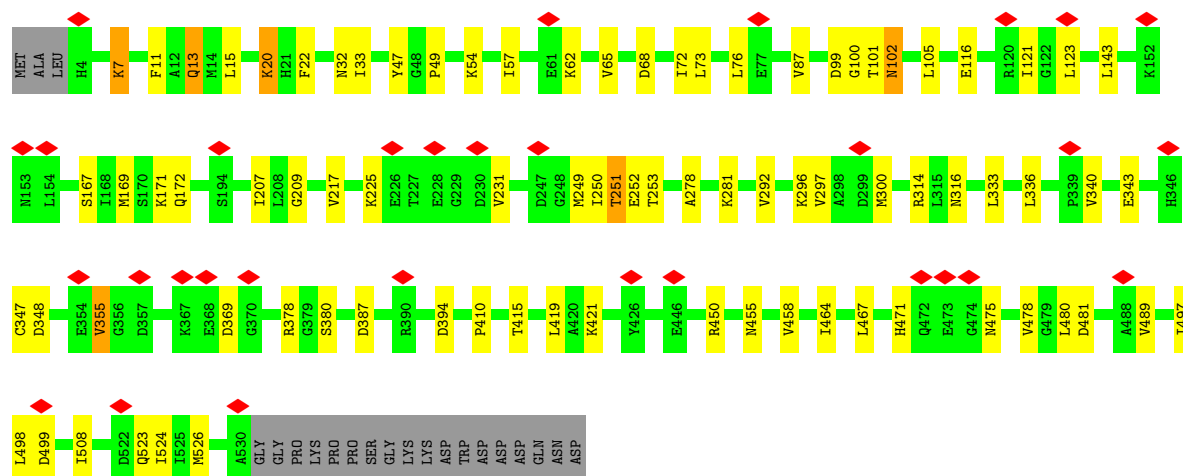
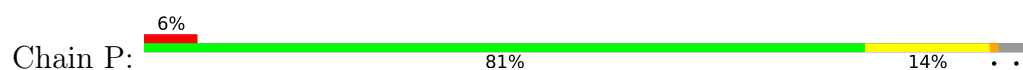


- Molecule 2: T-complex protein 1 subunit theta

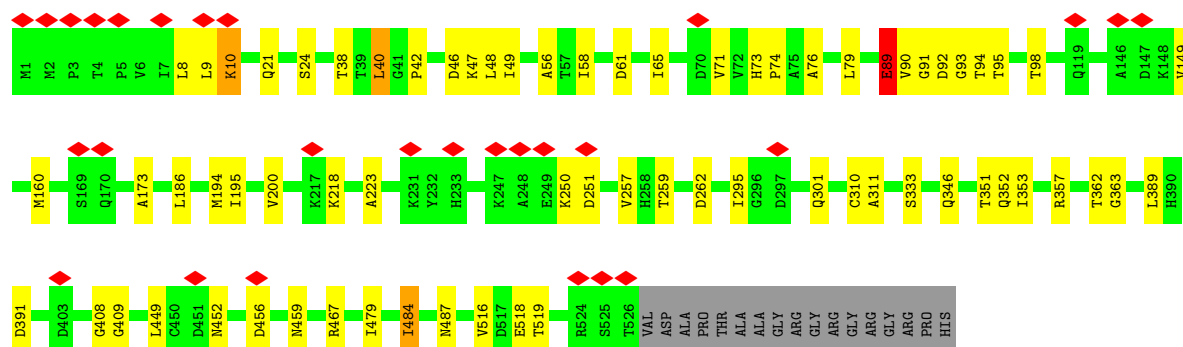
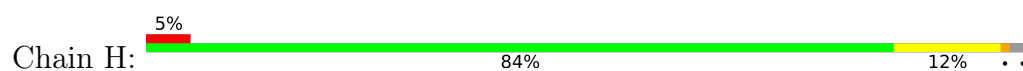




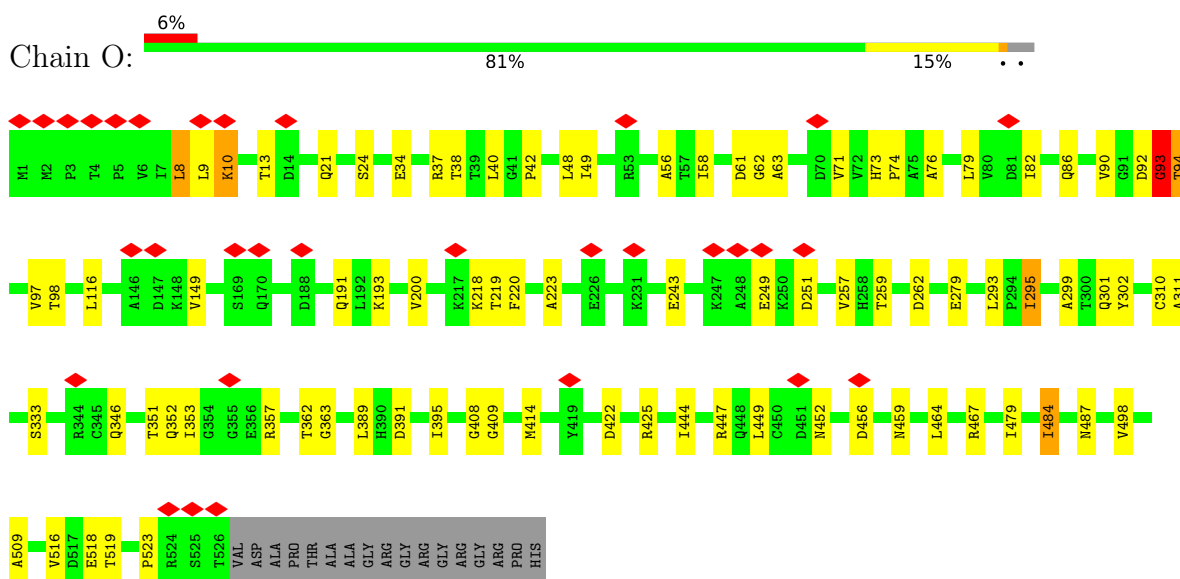
• Molecule 2: T-complex protein 1 subunit theta



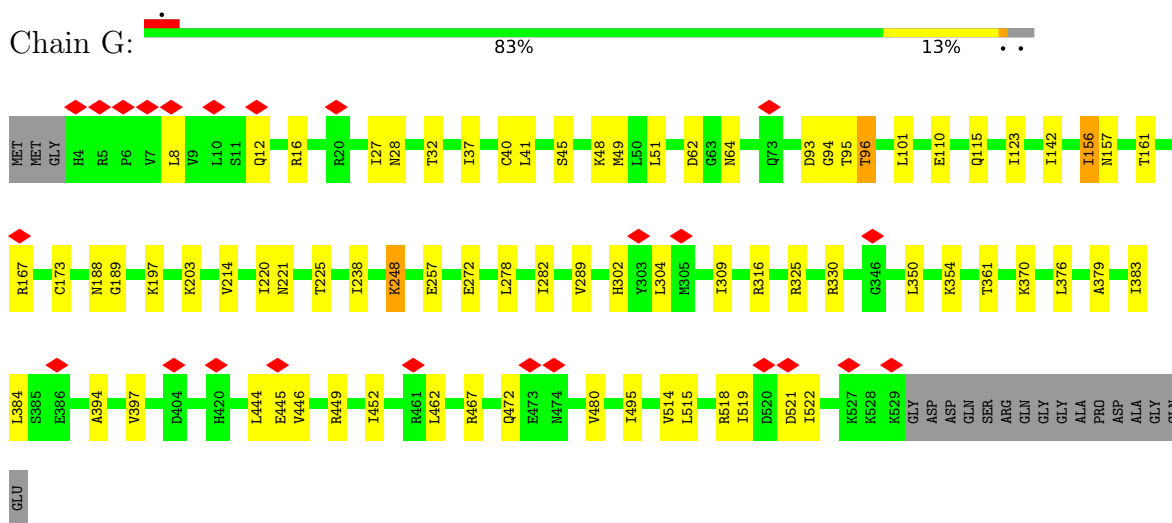
• Molecule 3: T-complex protein 1 subunit eta



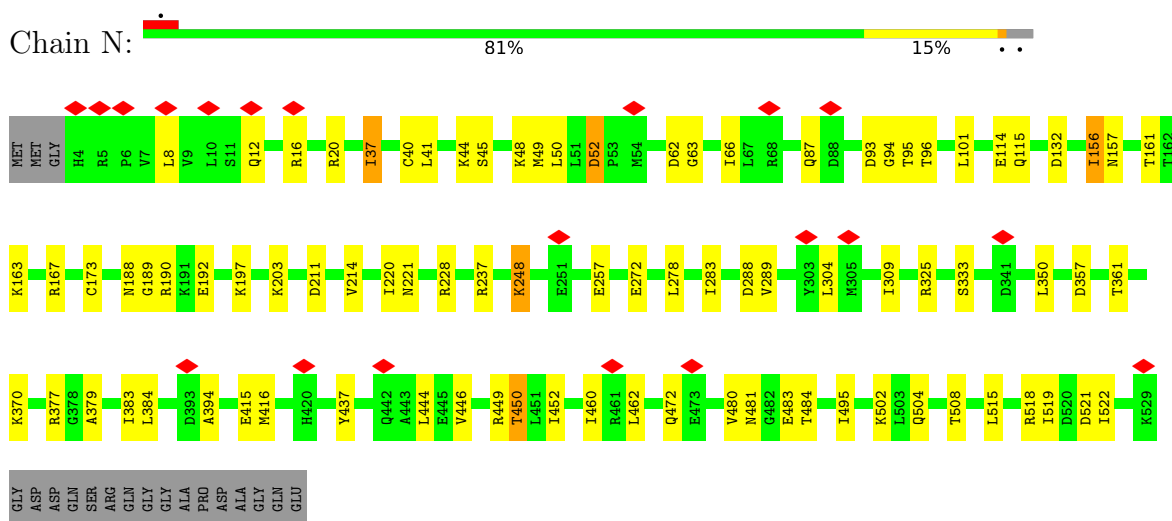
• Molecule 3: T-complex protein 1 subunit eta



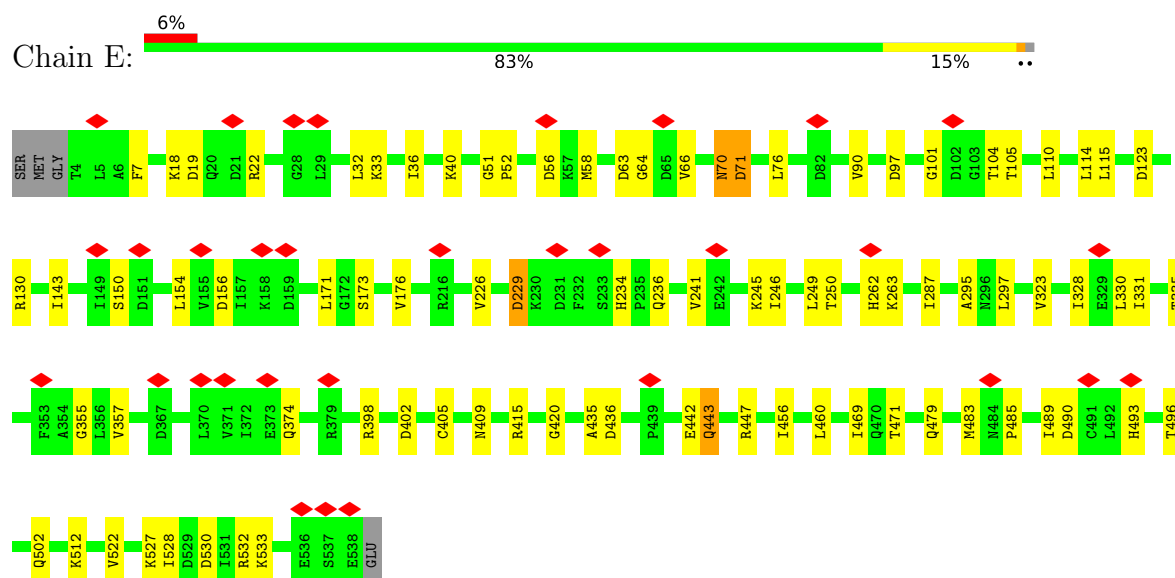
• Molecule 4: T-complex protein 1 subunit gamma



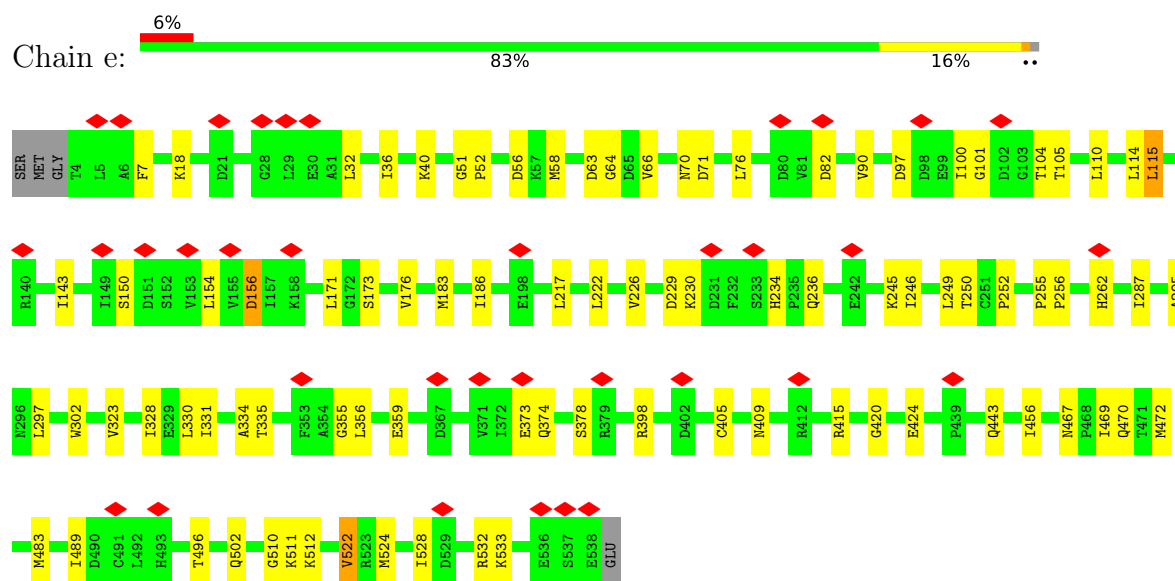
• Molecule 4: T-complex protein 1 subunit gamma



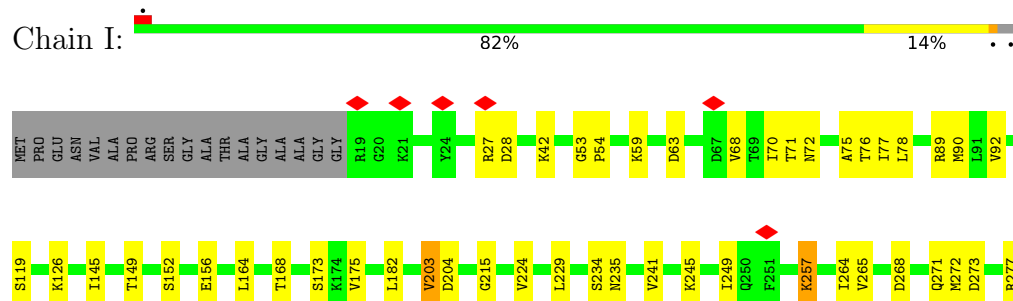
- Molecule 5: T-complex protein 1 subunit epsilon



- Molecule 5: T-complex protein 1 subunit epsilon

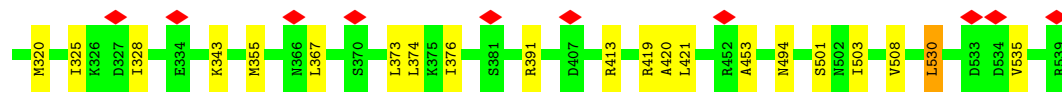
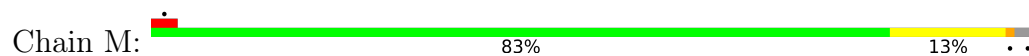


- Molecule 6: T-complex protein 1 subunit delta

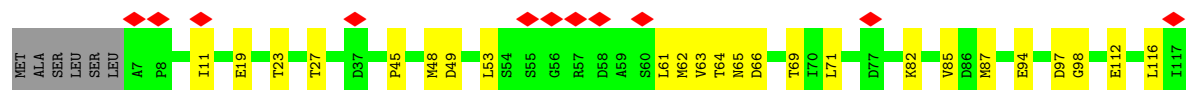
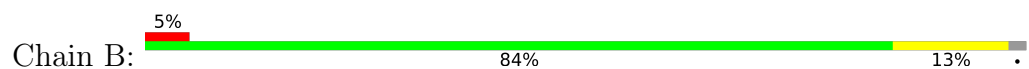




• Molecule 6: T-complex protein 1 subunit delta

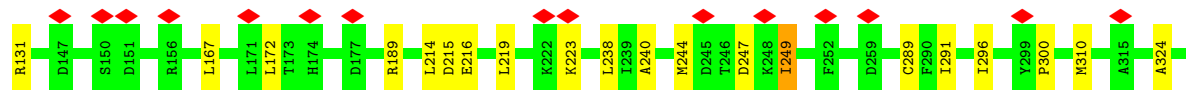
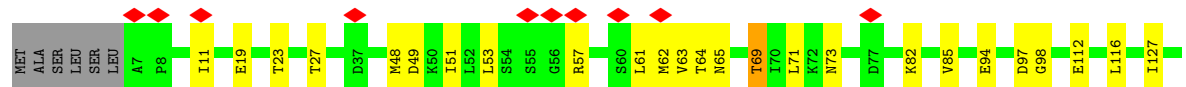
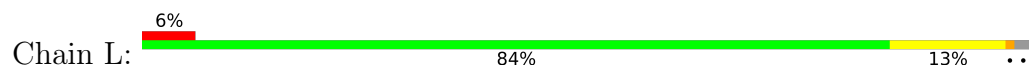


• Molecule 7: T-complex protein 1 subunit beta

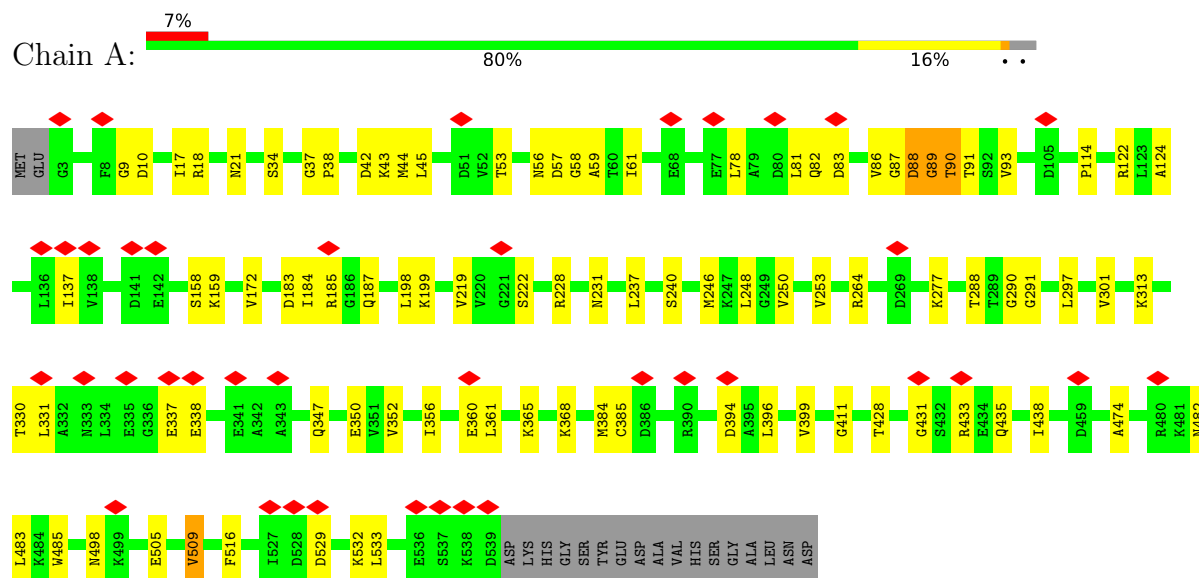


PRO
CYS

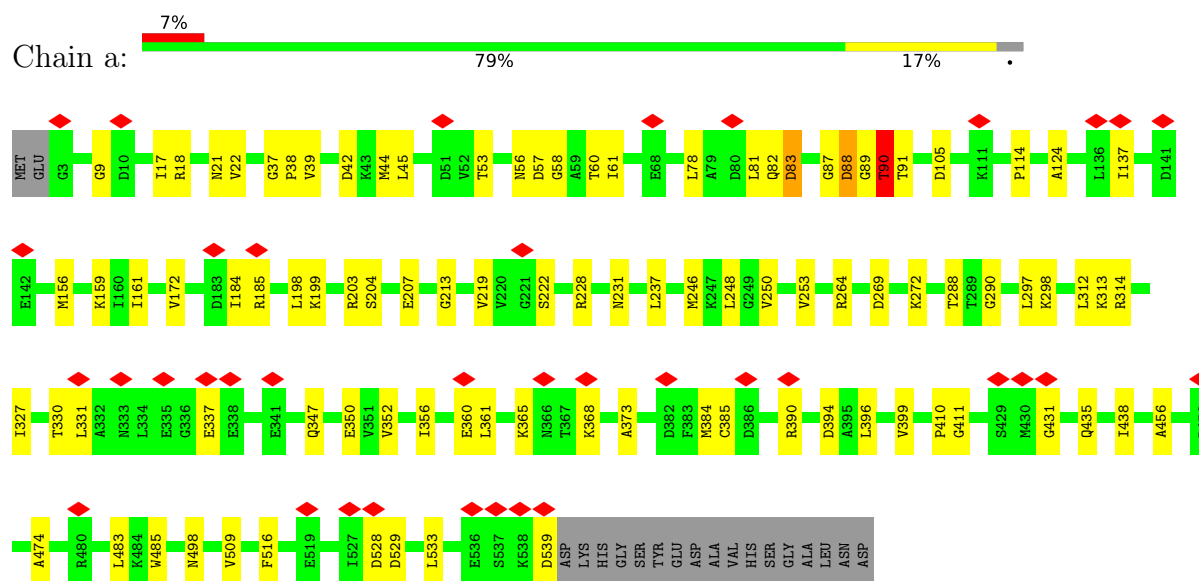
• Molecule 7: T-complex protein 1 subunit beta



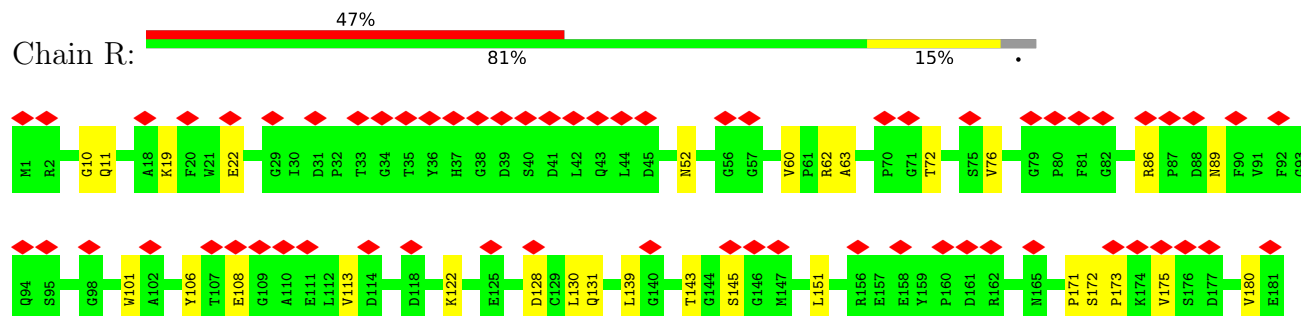
- Molecule 8: T-complex protein 1 subunit alpha

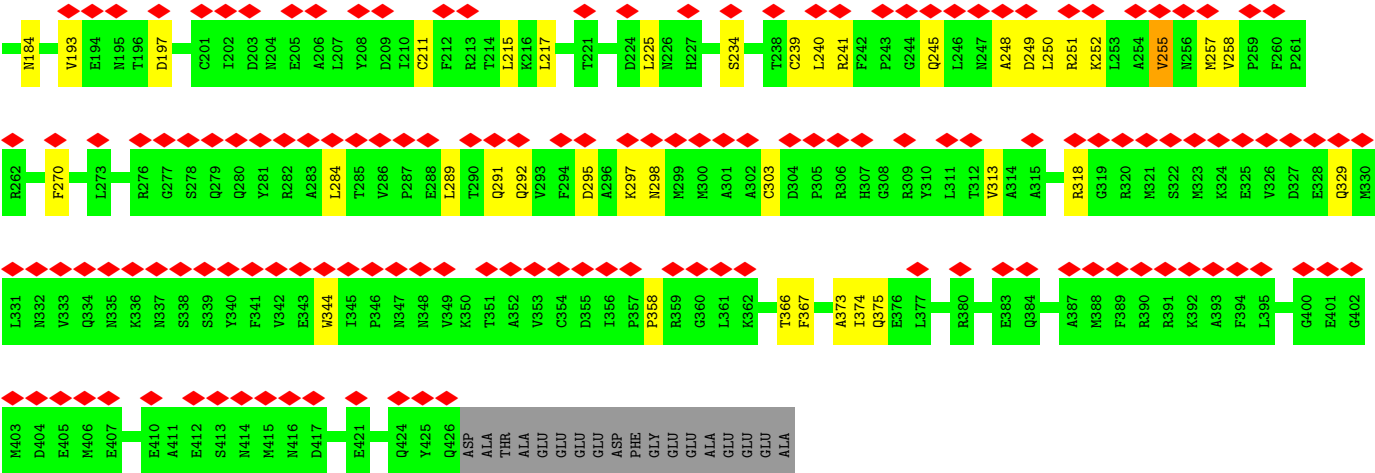


- Molecule 8: T-complex protein 1 subunit alpha



- Molecule 9: Tubulin beta chain





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	103406	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	38	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	3.603	Depositor
Minimum map value	-1.789	Depositor
Average map value	0.014	Depositor
Map value standard deviation	0.165	Depositor
Recommended contour level	0.761	Depositor
Map size ($\text{\AA}$)	337.408, 337.408, 337.408	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.318, 1.318, 1.318	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: ADP, AF3, 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	K	0.31	4/4069 (0.1%)	0.34	1/5486 (0.0%)
1	z	0.23	2/4069 (0.0%)	0.33	0/5486
2	J	0.11	0/4066	0.33	0/5498
2	P	0.28	2/4066 (0.0%)	0.35	1/5498 (0.0%)
3	H	0.35	5/4094 (0.1%)	0.38	3/5526 (0.1%)
3	O	0.36	6/4094 (0.1%)	0.36	2/5526 (0.0%)
4	G	0.11	0/4141	0.31	0/5585
4	N	0.11	0/4141	0.31	0/5585
5	E	0.25	3/4176 (0.1%)	0.38	4/5626 (0.1%)
5	e	0.12	0/4176	0.33	0/5626
6	I	0.30	3/3967 (0.1%)	0.35	2/5352 (0.0%)
6	M	0.34	3/3967 (0.1%)	0.38	2/5352 (0.0%)
7	B	0.12	0/3980	0.34	0/5365
7	L	0.12	0/3980	0.35	0/5365
8	A	0.32	4/4117 (0.1%)	0.41	4/5558 (0.1%)
8	a	0.30	4/4117 (0.1%)	0.38	0/5558
9	R	0.11	0/3421	0.30	0/4637
All	All	0.25	36/68641 (0.1%)	0.35	19/92629 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	P	0	1
3	O	0	1
6	M	0	2
8	A	0	1
8	a	0	1
All	All	0	6

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	M	106	THR	CA-C	-12.25	1.36	1.52
6	I	106	THR	CA-C	-11.78	1.38	1.52
3	O	94	THR	CA-C	-11.71	1.37	1.52
2	P	102	ASN	CA-C	-11.38	1.38	1.52
3	H	90	VAL	C-O	-10.99	1.12	1.23
6	M	106	THR	C-O	-10.93	1.10	1.24
8	A	88	ASP	CB-CG	10.46	1.78	1.52
8	A	88	ASP	CA-C	-10.32	1.41	1.53
3	O	94	THR	C-O	-10.27	1.11	1.24
1	K	157	ARG	C-O	-10.22	1.10	1.24
8	a	88	ASP	C-O	-9.75	1.11	1.23
5	E	71	ASP	C-O	-9.64	1.12	1.23
1	K	157	ARG	CA-C	-9.46	1.39	1.52
3	H	89	GLU	CA-C	-9.35	1.40	1.52
3	O	94	THR	N-CA	-8.79	1.34	1.46
8	A	88	ASP	C-O	-8.05	1.14	1.23
3	H	89	GLU	N-CA	-8.00	1.36	1.46
8	a	87	GLY	C-O	-7.98	1.13	1.24
6	M	106	THR	N-CA	-7.85	1.36	1.46
6	I	106	THR	C-O	-7.76	1.11	1.23
3	H	90	VAL	CA-C	-7.55	1.45	1.52
1	z	157	ARG	C-O	-7.43	1.14	1.24
2	P	102	ASN	C-O	-7.33	1.14	1.23
6	I	106	THR	N-CA	-7.23	1.36	1.46
1	K	157	ARG	CA-CB	-7.12	1.41	1.53
3	H	89	GLU	C-O	-7.12	1.15	1.24
3	O	94	THR	CA-CB	-6.99	1.41	1.53
5	E	71	ASP	CB-CG	6.79	1.69	1.52
1	K	157	ARG	N-CA	-6.76	1.37	1.46
8	A	88	ASP	N-CA	6.22	1.54	1.46
1	z	157	ARG	N-CA	-6.17	1.38	1.46
3	O	94	THR	C-N	-5.85	1.25	1.34
8	a	88	ASP	CB-CG	-5.72	1.37	1.52
8	a	88	ASP	CA-CB	-5.67	1.43	1.53
3	O	94	THR	CB-CG2	-5.30	1.35	1.52
5	E	71	ASP	CA-C	-5.17	1.46	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	87	GLY	O-C-N	-9.10	114.21	122.77
6	M	105	GLY	CA-C-N	-8.59	105.13	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	M	105	GLY	C-N-CA	-8.59	105.13	121.54
3	O	93	GLY	CA-C-N	-6.96	108.26	121.54
3	O	93	GLY	C-N-CA	-6.96	108.26	121.54
2	P	102	ASN	N-CA-C	-6.43	105.74	113.97
5	E	70	ASN	CA-C-N	6.21	129.57	120.82
5	E	70	ASN	C-N-CA	6.21	129.57	120.82
6	I	105	GLY	CA-C-N	-6.13	109.88	122.58
6	I	105	GLY	C-N-CA	-6.13	109.88	122.58
3	H	91	GLY	N-CA-C	6.11	127.67	113.18
3	H	90	VAL	CG1-CB-CG2	-5.86	97.90	110.80
8	A	88	ASP	OD1-CG-OD2	-5.68	109.26	122.90
3	H	90	VAL	CA-C-O	-5.59	115.04	120.30
5	E	71	ASP	CA-CB-CG	5.46	118.06	112.60
5	E	71	ASP	OD1-CG-OD2	-5.42	109.88	122.90
8	A	88	ASP	CB-CG-OD1	5.35	130.71	118.40
8	A	88	ASP	CA-CB-CG	5.29	117.89	112.60
1	K	157	ARG	CA-CB-CG	-5.19	103.72	114.10

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	A	90	THR	Peptide
6	M	105	GLY	Mainchain
6	M	29	LYS	Peptide
3	O	93	GLY	Mainchain
2	P	101	THR	Mainchain
8	a	90	THR	Peptide

5.2 Too-close contacts ⓘ

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	K	4022	0	4161	60	0
1	z	4022	0	4161	60	0
2	J	4008	0	4067	68	0
2	P	4008	0	4068	61	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	4037	0	4140	51	0
3	O	4037	0	4141	80	0
4	G	4094	0	4233	74	0
4	N	4094	0	4234	81	0
5	E	4126	0	4236	50	0
5	e	4126	0	4236	51	0
6	I	3935	0	4144	61	0
6	M	3935	0	4144	61	0
7	B	3937	0	4055	45	0
7	L	3937	0	4055	43	0
8	A	4077	0	4235	77	0
8	a	4077	0	4235	71	0
9	R	3346	0	3239	32	0
10	A	27	0	12	18	0
10	B	27	0	11	7	0
10	E	27	0	12	7	0
10	G	27	0	12	30	0
10	H	27	0	12	14	0
10	I	27	0	12	15	0
10	J	27	0	12	18	0
10	K	27	0	12	11	0
10	L	27	0	11	7	0
10	M	27	0	12	13	0
10	N	27	0	12	28	0
10	O	27	0	12	17	0
10	P	27	0	12	13	0
10	a	27	0	12	7	0
10	e	27	0	12	6	0
10	z	27	0	12	16	0
11	A	1	0	0	0	0
11	B	1	0	0	0	0
11	E	1	0	0	0	0
11	G	1	0	0	0	0
11	H	1	0	0	0	0
11	I	1	0	0	0	0
11	J	1	0	0	0	0
11	K	1	0	0	3	0
11	L	1	0	0	0	0
11	M	1	0	0	0	0
11	N	1	0	0	0	0
11	O	1	0	0	0	0
11	P	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	a	1	0	0	0	0
11	e	1	0	0	0	0
11	z	1	0	0	3	0
12	A	4	0	0	2	0
12	B	4	0	0	4	0
12	E	4	0	0	2	0
12	G	4	0	0	2	0
12	H	4	0	0	2	0
12	I	4	0	0	1	0
12	J	4	0	0	6	0
12	K	4	0	0	5	0
12	L	4	0	0	3	0
12	M	4	0	0	1	0
12	N	4	0	0	4	0
12	O	4	0	0	6	0
12	P	4	0	0	5	0
12	a	4	0	0	4	0
12	e	4	0	0	3	0
12	z	4	0	0	5	0
13	A	1	0	0	2	0
13	B	1	0	0	4	0
13	E	1	0	0	0	0
13	G	1	0	0	0	0
13	H	1	0	0	3	0
13	I	1	0	0	0	0
13	J	1	0	0	3	0
13	K	1	0	0	0	0
13	L	1	0	0	3	0
13	M	1	0	0	0	0
13	N	1	0	0	0	0
13	O	1	0	0	2	0
13	P	1	0	0	2	0
13	a	1	0	0	4	0
13	e	1	0	0	0	0
13	z	1	0	0	0	0
All	All	68346	0	69974	954	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 7.

All (954) 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)
8:A:88:ASP:CB	8:A:88:ASP:CG	1.78	1.55
2:J:102:ASN:ND2	10:J:601:ADP:O1A	1.58	1.35
8:A:89:GLY:CA	10:A:601:ADP:O3B	1.76	1.32
8:A:90:THR:N	10:A:601:ADP:O3B	1.63	1.30
6:I:105:GLY:HA2	10:I:601:ADP:O3B	1.30	1.30
6:M:98:GLN:CG	6:M:105:GLY:O	1.81	1.28
4:G:94:GLY:CA	10:G:601:ADP:O3B	1.82	1.28
3:H:93:GLY:CA	10:H:601:ADP:O3B	1.80	1.27
6:I:98:GLN:CG	6:I:105:GLY:O	1.83	1.26
3:O:93:GLY:HA2	10:O:603:ADP:O3B	1.29	1.25
4:N:94:GLY:CA	10:N:601:ADP:O3B	1.85	1.24
3:H:93:GLY:HA2	10:H:601:ADP:O3B	1.08	1.22
8:A:394:ASP:OD2	13:A:701:HOH:O	1.56	1.22
3:O:86:GLN:HG2	3:O:93:GLY:O	1.09	1.22
6:I:98:GLN:HG2	6:I:105:GLY:C	1.66	1.21
8:A:89:GLY:C	10:A:601:ADP:O3B	1.81	1.21
3:O:86:GLN:HG2	3:O:93:GLY:C	1.66	1.20
6:M:105:GLY:HA2	10:M:601:ADP:O3B	1.37	1.19
2:J:394:ASP:OD1	13:J:701:HOH:O	1.54	1.19
4:N:93:ASP:OD1	10:N:601:ADP:O1B	1.62	1.18
8:A:90:THR:H	10:A:601:ADP:PB	1.65	1.18
3:O:94:THR:HB	12:O:602:AF3:F3	1.32	1.16
6:M:98:GLN:HG2	6:M:105:GLY:C	1.70	1.15
6:M:106:THR:H	10:M:601:ADP:PB	1.68	1.15
2:J:102:ASN:CG	10:J:601:ADP:O1B	1.89	1.15
3:O:92:ASP:O	10:O:603:ADP:O1B	1.61	1.15
6:I:105:GLY:CA	10:I:601:ADP:O3B	1.95	1.14
1:z:90:ASP:CG	11:z:602:MG:MG	1.16	1.13
1:z:157:ARG:NE	1:z:162:ALA:HB2	1.64	1.13
1:K:90:ASP:OD1	12:K:603:AF3:F1	1.56	1.13
4:N:94:GLY:HA2	10:N:601:ADP:O3B	1.41	1.12
4:G:495:ILE:HD13	10:G:601:ADP:C6	1.82	1.12
6:M:106:THR:N	10:M:601:ADP:O3B	1.83	1.11
4:G:495:ILE:CD1	10:G:601:ADP:C6	2.32	1.11
6:M:105:GLY:CA	10:M:601:ADP:O3B	2.00	1.10
1:K:90:ASP:CG	11:K:602:MG:MG	1.19	1.09
6:I:106:THR:H	10:I:601:ADP:PB	1.75	1.09
3:O:86:GLN:CG	3:O:93:GLY:O	2.01	1.09
3:O:93:GLY:CA	10:O:603:ADP:O3B	2.00	1.08
3:H:94:THR:H	10:H:601:ADP:PB	1.77	1.08
4:N:495:ILE:HD13	10:N:601:ADP:C6	1.89	1.07
6:I:98:GLN:HG2	6:I:105:GLY:O	0.88	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:93:ASP:OD2	4:G:397:VAL:HG11	1.56	1.06
8:A:91:THR:N	10:A:601:ADP:O1B	1.88	1.05
4:G:94:GLY:HA2	10:G:601:ADP:O3B	1.45	1.04
4:G:95:THR:H	10:G:601:ADP:PB	1.79	1.04
2:P:394:ASP:OD1	13:P:701:HOH:O	1.76	1.03
6:M:98:GLN:HG2	6:M:105:GLY:O	0.86	1.03
3:O:61:ASP:OD2	13:O:701:HOH:O	1.74	1.03
4:G:495:ILE:HD11	10:G:601:ADP:N6	1.73	1.01
8:a:91:THR:N	10:a:601:ADP:O2B	1.93	1.01
1:z:157:ARG:CZ	1:z:162:ALA:HB2	1.89	1.01
2:J:171:LYS:NZ	12:J:603:AF3:F2	1.84	1.01
3:H:94:THR:N	10:H:601:ADP:O3B	1.92	1.01
4:N:495:ILE:CD1	10:N:601:ADP:C6	2.43	1.01
2:P:171:LYS:NZ	12:P:603:AF3:F2	1.85	1.00
3:O:92:ASP:O	10:O:603:ADP:PB	2.20	1.00
1:z:90:ASP:OD1	11:z:602:MG:MG	1.04	0.97
1:z:90:ASP:OD1	12:z:603:AF3:F1	1.73	0.97
8:A:89:GLY:HA2	10:A:601:ADP:O3B	1.59	0.97
6:I:106:THR:N	10:I:601:ADP:O3B	1.97	0.96
1:z:59:ASP:OD1	12:z:603:AF3:F2	1.74	0.96
4:G:95:THR:N	10:G:601:ADP:O3B	1.99	0.95
7:B:97:ASP:OD1	10:B:601:ADP:O2B	1.85	0.94
8:a:394:ASP:OD2	13:a:701:HOH:O	1.85	0.94
3:O:94:THR:H	10:O:603:ADP:PB	1.91	0.93
3:H:391:ASP:OD1	13:H:701:HOH:O	1.87	0.93
4:G:93:ASP:O	10:G:601:ADP:PB	2.27	0.92
7:L:97:ASP:OD1	10:L:601:ADP:O1B	1.87	0.91
1:K:59:ASP:OD1	12:K:603:AF3:F2	1.78	0.91
2:J:394:ASP:CG	13:J:701:HOH:O	2.03	0.91
4:G:93:ASP:C	10:G:601:ADP:O3B	2.14	0.91
3:H:93:GLY:C	10:H:601:ADP:O3B	2.14	0.91
4:G:93:ASP:OD2	4:G:397:VAL:CG1	2.18	0.90
6:I:98:GLN:HE21	6:I:105:GLY:HA3	1.33	0.90
6:I:104:ASP:OD2	6:I:411:VAL:HG23	1.72	0.90
7:B:98:GLY:N	10:B:601:ADP:O2B	2.04	0.90
3:O:94:THR:N	10:O:603:ADP:O3B	2.04	0.89
8:a:82:GLN:HB3	8:a:90:THR:HG22	1.53	0.89
3:H:61:ASP:OD2	13:H:701:HOH:O	1.91	0.89
7:L:98:GLY:N	10:L:601:ADP:O1B	2.05	0.88
4:N:93:ASP:O	10:N:601:ADP:PB	2.32	0.88
4:G:93:ASP:C	10:G:601:ADP:PB	2.58	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:392:ASP:OD1	13:L:701:HOH:O	1.92	0.87
5:e:71:ASP:OD1	12:e:603:AF3:F3	1.81	0.87
4:N:93:ASP:C	10:N:601:ADP:O3B	2.18	0.86
5:e:489:ILE:O	10:e:601:ADP:H2	1.58	0.85
4:G:93:ASP:O	10:G:601:ADP:O3B	1.94	0.85
4:N:495:ILE:HD11	10:N:601:ADP:N6	1.93	0.84
4:N:94:GLY:N	10:N:601:ADP:O3B	2.11	0.83
4:G:94:GLY:N	10:G:601:ADP:O3B	2.09	0.83
2:J:497:ILE:HD13	10:J:601:ADP:C6	2.14	0.83
4:N:93:ASP:C	10:N:601:ADP:PB	2.62	0.83
4:G:93:ASP:C	10:G:601:ADP:O2B	2.22	0.82
7:B:392:ASP:OD1	13:B:701:HOH:O	1.95	0.82
2:P:497:ILE:HD13	10:P:601:ADP:C6	2.14	0.82
8:A:89:GLY:N	10:A:601:ADP:O3B	2.13	0.82
8:a:83:ASP:OD1	8:a:90:THR:HG21	1.79	0.82
1:z:411:ALA:HA	10:z:601:ADP:O2'	1.79	0.82
4:G:94:GLY:C	10:G:601:ADP:O3B	2.23	0.81
4:G:95:THR:OG1	10:G:601:ADP:O1B	1.99	0.81
8:A:82:GLN:HG2	8:A:89:GLY:O	1.81	0.81
6:I:105:GLY:C	10:I:601:ADP:O3B	2.24	0.80
6:I:98:GLN:NE2	6:I:105:GLY:HA3	1.95	0.80
4:N:93:ASP:C	10:N:601:ADP:O1B	2.24	0.80
1:K:38:LEU:HD12	10:K:601:ADP:H5'1	1.62	0.79
4:G:495:ILE:HD11	10:G:601:ADP:C6	2.09	0.79
1:K:90:ASP:OD2	11:K:602:MG:MG	1.26	0.79
6:M:98:GLN:HE21	6:M:105:GLY:HA3	1.48	0.79
6:M:105:GLY:C	10:M:601:ADP:O3B	2.25	0.79
1:K:90:ASP:OD1	11:K:602:MG:MG	1.23	0.79
8:a:394:ASP:CG	13:a:701:HOH:O	2.20	0.79
4:N:95:THR:N	10:N:601:ADP:O3B	2.16	0.79
3:H:409:GLY:HA2	10:H:601:ADP:O2'	1.83	0.78
8:A:89:GLY:O	8:A:93:VAL:HG23	1.83	0.78
3:O:62:GLY:HA3	3:O:94:THR:HG22	1.63	0.78
3:O:449:LEU:HD21	10:O:603:ADP:H1'	1.64	0.78
7:B:392:ASP:CG	13:B:701:HOH:O	2.25	0.78
8:A:394:ASP:CG	13:A:701:HOH:O	2.11	0.78
3:O:61:ASP:CG	12:O:602:AF3:F2	2.17	0.78
3:O:391:ASP:OD1	13:O:701:HOH:O	2.00	0.78
4:N:93:ASP:O	10:N:601:ADP:O3B	2.02	0.78
8:a:82:GLN:HB3	8:a:90:THR:CG2	2.14	0.78
12:O:602:AF3:F3	10:O:603:ADP:O2B	1.92	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:495:ILE:CD1	10:N:601:ADP:N1	2.46	0.77
2:P:49:PRO:HG3	10:P:601:ADP:C8	2.20	0.77
3:O:86:GLN:CG	3:O:93:GLY:C	2.54	0.77
3:H:94:THR:N	10:H:601:ADP:PB	2.56	0.77
6:I:107:THR:N	10:I:601:ADP:O1B	2.14	0.77
4:G:495:ILE:CD1	10:G:601:ADP:N1	2.47	0.76
4:N:495:ILE:HD11	10:N:601:ADP:C6	2.20	0.76
5:E:489:ILE:O	10:E:601:ADP:H2	1.68	0.76
3:O:409:GLY:HA2	10:O:603:ADP:O2'	1.84	0.76
8:a:58:GLY:HA3	8:a:90:THR:O	1.86	0.76
1:K:38:LEU:CD1	10:K:601:ADP:H5'1	2.16	0.76
8:A:58:GLY:HA3	8:A:90:THR:O	1.85	0.75
3:O:92:ASP:C	10:O:603:ADP:O1B	2.28	0.75
6:M:105:GLY:C	6:M:106:THR:CG2	2.56	0.75
1:K:411:ALA:HA	10:K:601:ADP:O2'	1.86	0.74
3:O:86:GLN:HG2	3:O:93:GLY:CA	2.17	0.74
3:H:449:LEU:HD21	10:H:601:ADP:H1'	1.69	0.74
7:L:392:ASP:CG	13:L:701:HOH:O	2.30	0.74
6:I:104:ASP:CG	6:I:411:VAL:HG23	2.13	0.73
5:e:105:THR:N	10:e:601:ADP:O2B	2.15	0.73
3:H:61:ASP:OD1	12:H:603:AF3:F3	1.97	0.73
1:z:38:LEU:CD1	10:z:601:ADP:H5'1	2.19	0.72
8:a:90:THR:O	12:a:603:AF3:F3	1.98	0.72
8:A:59:ALA:HB2	8:A:90:THR:HG21	1.70	0.72
7:L:493:ILE:HD13	10:L:601:ADP:N1	2.04	0.72
8:a:90:THR:C	10:a:601:ADP:O2B	2.31	0.72
2:P:171:LYS:HE3	12:P:603:AF3:F1	1.79	0.72
2:J:171:LYS:HE3	12:J:603:AF3:F1	1.79	0.71
6:I:98:GLN:CG	6:I:105:GLY:C	2.48	0.71
4:G:495:ILE:CD1	10:G:601:ADP:N6	2.44	0.71
4:G:93:ASP:CA	10:G:601:ADP:O2B	2.38	0.70
8:a:37:GLY:HA2	10:a:601:ADP:O4'	1.90	0.70
2:J:102:ASN:OD1	10:J:601:ADP:O1B	2.09	0.70
4:N:495:ILE:HD13	10:N:601:ADP:N1	2.07	0.70
8:a:57:ASP:OD1	12:a:603:AF3:F2	1.99	0.70
5:E:420:GLY:HA2	10:E:601:ADP:N3	2.06	0.70
4:G:95:THR:N	10:G:601:ADP:PB	2.61	0.70
8:A:37:GLY:HA2	10:A:601:ADP:O4'	1.91	0.70
7:B:493:ILE:HD13	10:B:601:ADP:N1	2.06	0.69
2:P:102:ASN:O	2:P:102:ASN:ND2	2.22	0.69
6:M:107:THR:N	10:M:601:ADP:O2B	2.18	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:102:ASN:N	10:J:601:ADP:O1B	2.21	0.69
4:N:87:GLN:HB3	4:N:95:THR:HG22	1.74	0.69
6:M:106:THR:N	10:M:601:ADP:PB	2.52	0.69
2:J:49:PRO:HG3	10:J:601:ADP:C8	2.27	0.69
7:B:392:ASP:OD2	13:B:701:HOH:O	2.10	0.69
1:z:157:ARG:NE	1:z:162:ALA:CB	2.49	0.68
1:z:157:ARG:NH1	1:z:160:VAL:O	2.26	0.68
4:N:94:GLY:C	10:N:601:ADP:O3B	2.36	0.68
6:I:106:THR:N	10:I:601:ADP:PB	2.57	0.68
4:G:480:VAL:O	10:G:601:ADP:H2	1.76	0.67
6:M:98:GLN:NE2	6:M:105:GLY:HA3	2.09	0.67
4:G:64:ASN:HB2	4:G:95:THR:HG21	1.77	0.67
4:N:93:ASP:CA	10:N:601:ADP:O1B	2.43	0.66
3:H:93:GLY:HA2	10:H:601:ADP:PB	2.32	0.65
1:z:38:LEU:HD12	10:z:601:ADP:H5'1	1.78	0.65
1:z:157:ARG:NH1	1:z:157:ARG:O	2.30	0.65
3:O:86:GLN:NE2	3:O:93:GLY:HA3	2.13	0.64
8:a:394:ASP:OD1	13:a:701:HOH:O	2.12	0.64
2:J:102:ASN:ND2	10:J:601:ADP:O1B	2.30	0.64
8:A:91:THR:H	10:A:601:ADP:PB	2.20	0.64
2:P:171:LYS:CE	12:P:603:AF3:F1	2.36	0.64
2:J:394:ASP:OD2	13:J:701:HOH:O	2.10	0.64
8:A:82:GLN:HG2	8:A:89:GLY:C	2.23	0.64
5:E:71:ASP:OD2	5:E:402:ASP:OD2	2.17	0.63
1:z:481:LEU:CD2	10:z:601:ADP:N1	2.61	0.63
3:H:409:GLY:CA	10:H:601:ADP:O2'	2.46	0.63
7:L:244:MET:HG3	7:L:296:ILE:HG12	1.80	0.63
3:O:86:GLN:CG	3:O:93:GLY:CA	2.76	0.63
6:I:53:GLY:HA2	10:I:601:ADP:O4'	1.98	0.63
8:A:88:ASP:OD1	10:A:601:ADP:O2B	2.17	0.63
3:O:93:GLY:C	10:O:603:ADP:O3B	2.42	0.63
1:z:157:ARG:HE	1:z:162:ALA:HB2	1.60	0.62
3:O:409:GLY:CA	10:O:603:ADP:O2'	2.47	0.62
8:a:58:GLY:CA	8:a:90:THR:O	2.48	0.62
1:K:93:THR:HB	10:K:601:ADP:O1B	1.99	0.62
5:E:105:THR:N	10:E:601:ADP:O1B	2.23	0.62
8:a:288:THR:HG22	8:a:290:GLY:H	1.65	0.62
4:N:95:THR:H	10:N:601:ADP:PB	2.22	0.62
4:G:495:ILE:HD11	10:G:601:ADP:HN62	1.61	0.61
5:e:355:GLY:HA3	5:e:374:GLN:HB2	1.81	0.61
5:e:489:ILE:O	10:e:601:ADP:C2	2.51	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:41:LEU:O	10:N:601:ADP:H5'2	2.00	0.61
6:M:105:GLY:C	6:M:106:THR:HG22	2.24	0.61
1:z:481:LEU:HD23	10:z:601:ADP:C2	2.35	0.61
6:M:53:GLY:HA2	10:M:601:ADP:O4'	2.01	0.61
6:M:98:GLN:HB3	6:M:106:THR:HG22	1.82	0.61
4:G:495:ILE:HD13	10:G:601:ADP:N1	2.14	0.61
5:E:226:VAL:HG11	5:E:331:ILE:HG12	1.83	0.61
8:A:88:ASP:O	8:A:509:VAL:CG2	2.48	0.61
8:A:90:THR:O	8:A:90:THR:HG22	2.00	0.61
3:O:62:GLY:CA	3:O:94:THR:HG22	2.31	0.61
4:G:93:ASP:HA	10:G:601:ADP:O2B	2.01	0.61
4:N:480:VAL:O	10:N:601:ADP:H2	1.83	0.61
5:e:226:VAL:HG11	5:e:331:ILE:HG12	1.82	0.60
2:P:49:PRO:HD3	10:P:601:ADP:O4'	2.01	0.60
3:O:86:GLN:HE21	3:O:93:GLY:HA3	1.65	0.60
3:O:92:ASP:O	10:O:603:ADP:O3B	2.19	0.60
6:I:104:ASP:OD2	6:I:411:VAL:CG2	2.45	0.60
1:z:90:ASP:OD2	11:z:602:MG:MG	1.43	0.60
3:O:391:ASP:OD2	12:O:602:AF3:F2	2.10	0.60
2:J:209:GLY:HA3	2:J:378:ARG:HH21	1.66	0.60
6:M:98:GLN:CG	6:M:105:GLY:C	2.50	0.59
4:N:62:ASP:OD1	12:N:603:AF3:F2	2.10	0.59
2:J:475:ASN:HD21	2:J:478:VAL:H	1.50	0.59
6:I:104:ASP:OD1	6:I:407:ASP:O	2.21	0.59
7:B:410:GLY:HA2	10:B:601:ADP:N3	2.16	0.59
3:O:61:ASP:OD1	12:O:602:AF3:F2	2.11	0.59
3:O:94:THR:N	10:O:603:ADP:PB	2.70	0.59
6:I:54:PRO:HG3	10:I:601:ADP:C5	2.38	0.58
7:B:244:MET:HG3	7:B:296:ILE:HG12	1.83	0.58
2:J:171:LYS:CE	12:J:603:AF3:F1	2.41	0.58
3:H:49:ILE:HA	5:E:532:ARG:HB2	1.85	0.58
4:N:495:ILE:CD1	10:N:601:ADP:N6	2.59	0.58
5:e:420:GLY:HA2	10:e:601:ADP:N3	2.18	0.58
5:E:355:GLY:HA3	5:E:374:GLN:HB2	1.86	0.58
1:z:411:ALA:HB2	10:z:601:ADP:N3	2.19	0.58
3:O:86:GLN:CG	3:O:93:GLY:HA3	2.33	0.58
8:a:529:ASP:HB2	6:M:59:LYS:HG2	1.86	0.58
4:G:495:ILE:HD13	10:G:601:ADP:C5	2.36	0.58
3:H:89:GLU:HG3	3:H:89:GLU:O	2.01	0.58
7:B:214:LEU:HD11	7:B:371:CYS:HB3	1.86	0.58
1:z:90:ASP:OD1	10:z:601:ADP:O3A	2.22	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:209:GLY:HA3	2:P:378:ARG:HH21	1.69	0.58
6:M:98:GLN:CG	6:M:106:THR:HG22	2.34	0.58
7:B:244:MET:HB3	7:B:300:PRO:HG3	1.86	0.57
3:O:49:ILE:HA	5:e:532:ARG:HB2	1.86	0.57
8:a:219:VAL:HG12	8:a:360:GLU:HB2	1.86	0.57
1:K:245:ASN:HD22	9:R:255:VAL:HG23	1.69	0.57
2:P:99:ASP:OD1	10:P:601:ADP:O1B	2.22	0.57
8:A:89:GLY:O	8:A:93:VAL:CG2	2.52	0.57
1:K:334:ASN:HB2	4:G:302:HIS:HB2	1.87	0.57
8:a:56:ASN:HD21	8:a:159:LYS:HA	1.69	0.57
4:G:96:THR:N	10:G:601:ADP:O1B	2.34	0.57
8:A:288:THR:HG22	8:A:290:GLY:H	1.69	0.57
2:P:475:ASN:HD21	2:P:478:VAL:H	1.52	0.57
1:z:38:LEU:HD11	10:z:601:ADP:H5'1	1.87	0.57
2:J:68:ASP:OD1	12:J:603:AF3:F3	2.13	0.56
6:I:59:LYS:HD3	6:I:77:ILE:HD13	1.86	0.56
5:e:234:HIS:HD2	5:e:236:GLN:H	1.54	0.56
6:I:98:GLN:HG2	6:I:105:GLY:CA	2.35	0.56
2:J:49:PRO:HD3	10:J:601:ADP:O4'	2.05	0.56
1:z:38:LEU:HD11	10:z:601:ADP:C5'	2.35	0.56
1:z:481:LEU:HD23	10:z:601:ADP:N1	2.20	0.56
3:O:61:ASP:OD2	12:O:602:AF3:F2	2.13	0.56
1:K:33:VAL:HG13	2:J:523:GLN:HE22	1.71	0.56
1:K:38:LEU:HD11	10:K:601:ADP:C5'	2.35	0.56
1:K:179:ILE:HG22	1:K:180:LYS:HG2	1.86	0.56
4:N:519:ILE:HD13	8:a:44:MET:HE3	1.86	0.56
8:A:219:VAL:HG12	8:A:360:GLU:HB2	1.88	0.55
7:L:49:ASP:OD1	7:L:65:ASN:ND2	2.39	0.55
2:J:412:GLY:HA2	10:J:601:ADP:O2'	2.07	0.55
1:z:37:ASN:HB3	1:z:45:LYS:HZ3	1.71	0.55
7:B:49:ASP:OD1	7:B:65:ASN:ND2	2.40	0.55
8:A:56:ASN:HD21	8:A:159:LYS:HA	1.70	0.55
6:I:72:ASN:ND2	6:I:173:SER:O	2.40	0.55
3:H:21:GLN:O	3:H:24:SER:OG	2.23	0.55
6:I:104:ASP:O	10:I:601:ADP:O2B	2.24	0.55
2:J:481:ASP:H	2:J:489:VAL:HG12	1.71	0.55
8:A:411:GLY:O	8:A:498:ASN:ND2	2.40	0.54
2:P:169:MET:SD	10:P:601:ADP:N6	2.68	0.54
3:O:79:LEU:HB3	3:O:98:THR:HG23	1.89	0.54
7:L:214:LEU:HD11	7:L:371:CYS:HB3	1.89	0.54
1:K:90:ASP:OD2	10:K:601:ADP:O2A	2.25	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:21:GLN:NE2	3:H:519:THR:OG1	2.40	0.54
4:G:189:GLY:O	8:A:228:ARG:NH1	2.40	0.54
6:I:98:GLN:CG	6:I:105:GLY:CA	2.85	0.54
9:R:240:LEU:HD21	9:R:250:LEU:HB2	1.89	0.54
4:N:52:ASP:OD1	4:N:52:ASP:N	2.40	0.54
2:J:203:ARG:HD2	2:J:323:ARG:HD3	1.89	0.54
8:a:411:GLY:O	8:a:498:ASN:ND2	2.41	0.54
2:J:76:LEU:HD13	3:H:10:LYS:HE2	1.89	0.54
8:A:474:ALA:HB2	8:A:483:LEU:HB2	1.89	0.54
4:N:189:GLY:O	8:a:228:ARG:NH1	2.41	0.54
7:L:410:GLY:HA2	10:L:601:ADP:N3	2.22	0.54
5:e:97:ASP:OD2	5:e:398:ARG:NH2	2.40	0.54
5:E:496:THR:O	5:E:502:GLN:NE2	2.41	0.54
4:N:95:THR:OG1	12:N:603:AF3:F3	2.15	0.54
8:a:390:ARG:NH2	13:a:701:HOH:O	2.40	0.54
1:z:157:ARG:NH2	1:z:162:ALA:HB2	2.22	0.54
2:P:47:TYR:O	2:P:455:ASN:ND2	2.41	0.54
2:J:497:ILE:HD13	10:J:601:ADP:N1	2.23	0.53
6:I:119:SER:HB2	6:I:453:ALA:HB1	1.90	0.53
6:M:72:ASN:ND2	6:M:173:SER:O	2.41	0.53
6:M:367:LEU:HD13	6:M:391:ARG:HH12	1.72	0.53
5:E:97:ASP:OD2	5:E:398:ARG:NH2	2.41	0.53
2:P:54:LYS:HG2	3:O:518:GLU:HB2	1.91	0.53
6:M:105:GLY:O	6:M:106:THR:HG22	2.08	0.53
3:O:40:LEU:O	3:O:452:ASN:ND2	2.42	0.53
2:J:102:ASN:ND2	12:J:603:AF3:F1	2.18	0.53
2:J:450:ARG:NH1	4:N:115:GLN:OE1	2.41	0.53
5:E:405:CYS:O	5:E:409:ASN:ND2	2.42	0.53
7:L:244:MET:HB3	7:L:300:PRO:HG3	1.90	0.53
1:K:16:ALA:HA	1:K:519:ASP:HB2	1.90	0.53
6:I:54:PRO:CG	10:I:601:ADP:C5	2.92	0.53
1:z:117:ARG:NH2	4:N:45:SER:O	2.40	0.53
2:P:481:ASP:H	2:P:489:VAL:HG12	1.74	0.53
5:e:405:CYS:O	5:e:409:ASN:ND2	2.41	0.53
6:M:59:LYS:HD3	6:M:77:ILE:HD13	1.89	0.53
5:E:234:HIS:HD2	5:E:236:GLN:H	1.56	0.53
8:A:183:ASP:HB3	8:A:187:GLN:HB2	1.90	0.53
4:N:93:ASP:HA	10:N:601:ADP:O1B	2.08	0.53
8:a:89:GLY:O	8:a:91:THR:N	2.42	0.53
4:N:495:ILE:HD11	10:N:601:ADP:HN62	1.74	0.53
1:K:245:ASN:OD1	1:K:245:ASN:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:97:ASP:HA	5:E:101:GLY:HA2	1.91	0.52
5:e:51:GLY:HA2	10:e:601:ADP:O4'	2.09	0.52
4:N:93:ASP:O	10:N:601:ADP:O1B	2.24	0.52
6:M:152:SER:HB2	6:M:420:ALA:HB1	1.91	0.52
1:K:117:ARG:NH2	4:G:45:SER:O	2.41	0.52
1:K:518:VAL:HG11	4:G:49:MET:HE3	1.91	0.52
4:N:93:ASP:CG	10:N:601:ADP:O1B	2.46	0.52
4:G:115:GLN:OE1	2:P:450:ARG:NH1	2.42	0.52
7:B:348:LEU:HB2	7:B:363:SER:HB3	1.91	0.52
1:z:90:ASP:OD2	10:z:601:ADP:O1A	2.27	0.52
8:a:42:ASP:HA	8:a:56:ASN:HB3	1.92	0.52
4:G:93:ASP:O	10:G:601:ADP:O2B	2.25	0.52
1:z:93:THR:HB	10:z:601:ADP:O3B	2.08	0.52
2:P:497:ILE:HD13	10:P:601:ADP:N6	2.24	0.52
8:A:18:ARG:HH22	8:A:114:PRO:HG2	1.75	0.52
1:z:85:ASP:O	1:z:396:ARG:NH1	2.42	0.52
2:P:394:ASP:CG	13:P:701:HOH:O	2.40	0.52
5:e:496:THR:O	5:e:502:GLN:NE2	2.43	0.52
10:B:601:ADP:O2A	12:B:603:AF3:F1	2.18	0.52
4:N:16:ARG:NH2	4:N:521:ASP:OD1	2.43	0.52
3:H:40:LEU:O	3:H:452:ASN:ND2	2.43	0.52
5:E:36:ILE:HG12	5:E:115:LEU:HG	1.92	0.52
1:K:366:CYS:HB2	1:K:369:PRO:HG3	1.92	0.52
5:E:63:ASP:OD1	7:B:526:ARG:NH1	2.43	0.52
4:G:16:ARG:NH2	4:G:521:ASP:OD1	2.43	0.51
3:H:79:LEU:HB3	3:H:98:THR:HG23	1.91	0.51
10:L:601:ADP:O1A	12:L:603:AF3:F1	2.18	0.51
9:R:131:GLN:HE21	9:R:251:ARG:HG3	1.76	0.51
6:I:152:SER:HB2	6:I:420:ALA:HB1	1.91	0.51
8:a:18:ARG:HH22	8:a:114:PRO:HG2	1.75	0.51
5:E:76:LEU:HB3	5:E:90:VAL:HG22	1.93	0.51
5:E:246:ILE:HG12	5:E:297:LEU:HD23	1.93	0.51
7:B:116:LEU:O	6:M:27:ARG:NH2	2.43	0.51
3:O:21:GLN:O	3:O:24:SER:OG	2.23	0.51
8:a:222:SER:HB2	8:a:297:LEU:HD13	1.92	0.51
4:G:64:ASN:HB2	4:G:95:THR:CG2	2.40	0.51
5:E:143:ILE:HD12	5:E:512:LYS:HG3	1.93	0.51
3:O:21:GLN:NE2	3:O:519:THR:OG1	2.43	0.51
3:O:456:ASP:OD2	3:O:459:ASN:ND2	2.43	0.51
3:H:94:THR:OG1	10:H:601:ADP:O1B	2.29	0.51
8:A:42:ASP:HA	8:A:56:ASN:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:90:THR:N	10:A:601:ADP:PB	2.48	0.51
2:P:340:VAL:HG13	2:P:343:GLU:HG2	1.92	0.51
6:M:104:ASP:O	10:M:601:ADP:O1B	2.29	0.51
2:J:102:ASN:ND2	10:J:601:ADP:PA	2.77	0.51
4:G:188:ASN:ND2	8:A:228:ARG:O	2.43	0.51
3:O:48:LEU:HD11	3:O:56:ALA:HB1	1.92	0.51
2:J:467:LEU:HD11	2:J:480:LEU:HD21	1.93	0.51
7:B:289:CYS:HA	7:B:310:MET:HB2	1.93	0.51
8:a:474:ALA:HB2	8:a:483:LEU:HB2	1.92	0.51
4:G:325:ARG:HB3	4:G:370:LYS:HB2	1.93	0.51
3:O:63:ALA:H	3:O:94:THR:HG21	1.76	0.51
1:K:38:LEU:CD1	10:K:601:ADP:C5'	2.85	0.50
6:I:104:ASP:CG	6:I:411:VAL:CG2	2.84	0.50
1:z:33:VAL:HG13	2:P:523:GLN:HE22	1.76	0.50
5:e:63:ASP:OD1	7:L:526:ARG:NH1	2.43	0.50
1:K:186:ILE:O	4:G:354:LYS:NZ	2.40	0.50
4:G:220:ILE:HG13	4:G:361:THR:HB	1.92	0.50
7:B:45:PRO:HG2	7:B:480:MET:HG3	1.93	0.50
8:a:45:LEU:HB2	8:a:53:THR:HB	1.93	0.50
4:G:445:GLU:OE2	4:G:467:ARG:NH2	2.43	0.50
9:R:291:GLN:OE1	9:R:329:GLN:NE2	2.43	0.50
1:z:518:VAL:HG11	4:N:49:MET:HE3	1.94	0.50
2:P:251:THR:OG1	2:P:252:GLU:N	2.44	0.50
1:K:278:LYS:NZ	1:K:308:GLU:O	2.44	0.50
2:J:172:GLN:NE2	2:J:387:ASP:OD2	2.45	0.50
5:e:56:ASP:OD1	5:e:70:ASN:ND2	2.44	0.50
6:M:98:GLN:CB	6:M:106:THR:HG22	2.41	0.50
7:L:392:ASP:OD2	13:L:701:HOH:O	2.19	0.50
3:H:456:ASP:OD2	3:H:459:ASN:ND2	2.44	0.50
6:M:265:VAL:O	6:M:271:GLN:NE2	2.45	0.50
4:G:515:LEU:HD22	8:A:384:MET:HG3	1.92	0.50
8:A:172:VAL:HG13	8:A:396:LEU:HD23	1.94	0.50
4:N:20:ARG:NH2	4:N:114:GLU:OE1	2.44	0.50
4:N:197:LYS:NZ	8:a:360:GLU:OE2	2.45	0.50
1:K:213:ASP:OD2	9:R:122:LYS:NZ	2.45	0.50
1:K:257:GLU:OE2	2:J:279:GLN:NE2	2.45	0.50
10:a:601:ADP:O2B	12:a:603:AF3:F3	2.20	0.50
1:K:92:THR:HB	12:K:603:AF3:F3	2.02	0.50
10:H:601:ADP:O1B	12:H:603:AF3:F3	2.20	0.50
7:B:131:ARG:NH2	7:B:512:GLU:OE2	2.43	0.50
10:P:601:ADP:O2B	12:P:603:AF3:F3	2.20	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:347:CYS:SG	2:J:348:ASP:N	2.83	0.50
9:R:234:SER:OG	9:R:241:ARG:NH2	2.45	0.50
5:e:143:ILE:HD12	5:e:512:LYS:HG3	1.94	0.50
5:e:246:ILE:HG12	5:e:297:LEU:HD23	1.94	0.50
1:K:291:VAL:HG12	1:K:293:ASN:HB2	1.94	0.49
3:H:47:LYS:NZ	5:E:530:ASP:OD2	2.45	0.49
8:a:78:LEU:HD11	8:a:516:PHE:HB3	1.94	0.49
10:A:601:ADP:O1B	12:A:603:AF3:F3	2.20	0.49
10:e:601:ADP:O2B	12:e:603:AF3:F3	2.20	0.49
10:M:601:ADP:O2B	12:M:603:AF3:F3	2.20	0.49
10:K:601:ADP:O2B	12:K:603:AF3:F3	2.20	0.49
2:J:102:ASN:OD1	2:J:102:ASN:N	2.45	0.49
10:E:601:ADP:O1B	12:E:603:AF3:F3	2.20	0.49
6:I:89:ARG:HD2	7:B:61:LEU:HD11	1.95	0.49
7:B:48:MET:SD	7:B:48:MET:N	2.85	0.49
1:z:38:LEU:CD1	10:z:601:ADP:O3B	2.60	0.49
8:a:38:PRO:HG3	10:a:601:ADP:C5	2.47	0.49
1:K:85:ASP:O	1:K:396:ARG:NH1	2.45	0.49
5:e:36:ILE:HA	5:e:115:LEU:HD23	1.94	0.49
8:a:350:GLU:HB3	8:a:365:LYS:HD2	1.94	0.49
6:M:98:GLN:CG	6:M:105:GLY:CA	2.91	0.49
1:K:411:ALA:HB2	10:K:601:ADP:N3	2.27	0.49
5:E:246:ILE:HD12	5:E:335:THR:HG21	1.93	0.49
6:I:90:MET:HG2	7:B:381:GLN:HG3	1.94	0.49
10:N:601:ADP:O2B	12:N:603:AF3:F3	2.20	0.49
5:e:58:MET:HE3	7:L:517:VAL:HG21	1.94	0.49
6:M:78:LEU:HB3	6:M:92:VAL:HG22	1.94	0.49
2:J:33:ILE:HG21	2:J:116:GLU:HB2	1.95	0.49
2:J:210:SER:HB3	3:H:89:GLU:OE2	2.13	0.49
5:E:483:MET:SD	5:E:483:MET:N	2.86	0.49
8:A:78:LEU:HD11	8:A:516:PHE:HB3	1.94	0.49
8:A:431:GLY:HA3	8:A:435:GLN:HB3	1.95	0.49
2:P:171:LYS:NZ	2:P:394:ASP:OD2	2.45	0.49
4:N:452:ILE:HD13	4:N:462:LEU:HD22	1.95	0.49
5:e:110:LEU:HB2	5:e:456:ILE:HD11	1.95	0.49
5:e:246:ILE:HD12	5:e:335:THR:HG21	1.94	0.49
8:a:356:ILE:HG12	8:a:361:LEU:HD22	1.94	0.49
1:K:270:ARG:NH2	4:G:272:GLU:OE2	2.46	0.49
2:J:73:LEU:HD11	2:J:105:LEU:HD11	1.93	0.49
2:P:467:LEU:HD11	2:P:480:LEU:HD21	1.93	0.49
4:G:197:LYS:NZ	8:A:360:GLU:OE2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:51:GLY:HA2	10:E:601:ADP:O4'	2.13	0.49
5:E:64:GLY:O	7:B:82:LYS:NZ	2.44	0.49
8:A:330:THR:OG1	8:A:331:LEU:N	2.46	0.49
10:z:601:ADP:O2B	12:z:603:AF3:F3	2.20	0.49
4:N:87:GLN:HG2	4:N:95:THR:HA	1.94	0.49
4:N:481:ASN:ND2	4:N:484:THR:OG1	2.46	0.49
8:a:410:PRO:HG3	8:a:485:TRP:HD1	1.77	0.49
3:H:48:LEU:HD11	3:H:56:ALA:HB1	1.94	0.49
9:R:19:LYS:HD3	9:R:22:GLU:HG3	1.95	0.49
2:P:497:ILE:HD13	10:P:601:ADP:N1	2.28	0.49
5:e:97:ASP:HA	5:e:101:GLY:HA2	1.94	0.49
10:G:601:ADP:O1B	12:G:603:AF3:F3	2.20	0.49
8:A:88:ASP:CG	10:A:601:ADP:O2B	2.56	0.49
2:J:57:ILE:HD11	3:H:74:PRO:HG3	1.95	0.48
10:J:601:ADP:O1B	12:J:603:AF3:F3	2.20	0.48
10:I:601:ADP:O1B	12:I:603:AF3:F3	2.20	0.48
8:a:172:VAL:HG13	8:a:396:LEU:HD23	1.94	0.48
6:I:265:VAL:O	6:I:271:GLN:NE2	2.45	0.48
7:B:189:ARG:HH12	7:B:216:GLU:HA	1.78	0.48
7:B:449:ILE:O	7:B:453:ASN:ND2	2.44	0.48
2:P:467:LEU:O	2:P:471:HIS:ND1	2.46	0.48
3:O:9:LEU:HG	3:O:10:LYS:HG2	1.95	0.48
4:N:87:GLN:HE21	4:N:94:GLY:HA3	1.77	0.48
3:H:200:VAL:HG11	3:H:353:ILE:HG22	1.96	0.48
3:O:249:GLU:HG2	3:O:251:ASP:H	1.79	0.48
7:L:289:CYS:HA	7:L:310:MET:HB2	1.93	0.48
6:I:156:GLU:OE1	6:I:419:ARG:NH1	2.47	0.48
6:I:367:LEU:HD13	6:I:391:ARG:HH12	1.78	0.48
3:O:218:LYS:HD2	3:O:357:ARG:HB2	1.95	0.48
5:e:52:PRO:HA	5:e:173:SER:HA	1.96	0.48
8:a:57:ASP:OD1	12:a:603:AF3:F3	2.21	0.48
6:M:89:ARG:HD2	7:L:61:LEU:HD11	1.95	0.48
6:M:268:ASP:HB3	6:M:271:GLN:HB2	1.96	0.48
7:L:167:LEU:HD22	7:L:172:LEU:HD12	1.95	0.48
9:R:248:ALA:HA	9:R:252:LYS:HD3	1.95	0.48
8:a:231:ASN:OD1	8:a:368:LYS:NZ	2.46	0.48
2:J:143:LEU:HD11	2:J:508:ILE:HD12	1.95	0.48
3:H:346:GLN:HB2	3:H:363:GLY:HA3	1.94	0.48
9:R:292:GLN:O	9:R:298:ASN:ND2	2.47	0.48
4:N:188:ASN:ND2	8:a:228:ARG:O	2.47	0.48
3:H:47:LYS:HD3	3:H:65:ILE:HD13	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:62:ASP:OD1	12:G:603:AF3:F2	2.21	0.48
6:I:268:ASP:HB3	6:I:271:GLN:HB2	1.94	0.48
1:K:523:ARG:HB2	4:G:51:LEU:HD12	1.95	0.48
4:G:221:ASN:OD1	4:G:221:ASN:N	2.45	0.48
6:I:75:ALA:HB2	6:I:106:THR:HG21	1.95	0.48
4:N:101:LEU:HD11	4:N:444:LEU:HD23	1.96	0.48
10:L:601:ADP:O2B	12:L:603:AF3:F3	2.22	0.48
2:J:73:LEU:HD13	2:J:87:VAL:HG22	1.96	0.48
5:E:52:PRO:HA	5:E:173:SER:HA	1.94	0.48
5:E:56:ASP:OD1	5:E:70:ASN:ND2	2.45	0.48
7:B:167:LEU:HD22	7:B:172:LEU:HD12	1.96	0.48
8:a:199:LYS:HB3	8:a:385:CYS:HB3	1.95	0.48
6:M:130:PRO:HB3	6:M:530:LEU:HB2	1.96	0.48
2:P:172:GLN:NE2	2:P:387:ASP:OD2	2.46	0.48
5:e:230:LYS:HD3	5:e:359:GLU:HB3	1.96	0.48
8:a:58:GLY:N	8:a:90:THR:O	2.47	0.48
6:M:229:LEU:HB2	6:M:374:LEU:HD12	1.95	0.48
7:L:19:GLU:O	7:L:519:ASN:ND2	2.47	0.48
6:I:257:LYS:HD2	6:I:306:ARG:HD3	1.96	0.47
5:e:483:MET:SD	5:e:483:MET:N	2.87	0.47
3:H:391:ASP:CG	13:H:701:HOH:O	2.47	0.47
5:E:110:LEU:HB2	5:E:456:ILE:HD11	1.95	0.47
10:B:601:ADP:O1B	12:B:603:AF3:F3	2.22	0.47
8:A:248:LEU:HB3	9:R:344:TRP:HE1	1.80	0.47
1:z:366:CYS:HB2	1:z:369:PRO:HG3	1.96	0.47
3:O:259:THR:HG23	3:O:262:ASP:H	1.79	0.47
8:a:431:GLY:HA3	8:a:435:GLN:HB3	1.95	0.47
6:M:156:GLU:OE1	6:M:419:ARG:NH1	2.47	0.47
3:H:93:GLY:CA	10:H:601:ADP:PB	2.97	0.47
2:P:102:ASN:N	10:P:601:ADP:O2B	2.47	0.47
3:O:479:ILE:CG1	10:O:603:ADP:C2	2.97	0.47
6:M:98:GLN:HG2	6:M:105:GLY:CA	2.41	0.47
6:I:27:ARG:NH2	7:L:116:LEU:O	2.47	0.47
8:a:312:LEU:HD13	8:a:314:ARG:HE	1.79	0.47
8:a:539:ASP:OD2	7:L:57:ARG:NH1	2.47	0.47
2:J:47:TYR:O	2:J:455:ASN:ND2	2.47	0.47
2:J:300:MET:HE1	3:H:333:SER:HB2	1.96	0.47
3:H:218:LYS:HD2	3:H:357:ARG:HB2	1.95	0.47
1:z:291:VAL:HG12	1:z:293:ASN:HB2	1.96	0.47
3:O:346:GLN:HB2	3:O:363:GLY:HA3	1.95	0.47
1:K:314:ARG:HH12	9:R:128:ASP:HA	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:R:284:LEU:HD22	9:R:289:LEU:HD21	1.97	0.47
2:P:22:PHE:HB2	2:P:524:ILE:HB	1.96	0.47
3:H:42:PRO:HG2	3:H:479:ILE:HG13	1.97	0.47
4:G:93:ASP:OD2	4:G:397:VAL:HG13	2.08	0.47
4:G:156:ILE:HD11	4:G:394:ALA:HB1	1.97	0.47
4:G:330:ARG:NH2	8:A:301:VAL:O	2.48	0.47
5:E:236:GLN:HE21	7:B:324:ALA:HB1	1.80	0.47
6:I:325:ILE:HG12	6:I:374:LEU:HD11	1.95	0.47
1:z:36:THR:OG1	1:z:45:LYS:NZ	2.47	0.47
2:P:13:GLN:HE21	2:P:13:GLN:HB2	1.57	0.47
2:P:49:PRO:CG	10:P:601:ADP:C8	2.96	0.47
2:P:249:MET:HB2	2:P:336:LEU:HD22	1.95	0.47
3:O:223:ALA:O	3:O:301:GLN:NE2	2.47	0.47
6:M:119:SER:HB2	6:M:453:ALA:HB1	1.96	0.47
6:M:325:ILE:HG12	6:M:374:LEU:HD11	1.96	0.47
7:L:48:MET:SD	7:L:48:MET:N	2.88	0.47
2:J:464:ILE:HD12	2:J:467:LEU:HD12	1.95	0.47
3:H:9:LEU:HG	3:H:10:LYS:HG2	1.97	0.47
3:H:351:THR:OG1	3:H:352:GLN:N	2.45	0.47
4:G:519:ILE:HD13	8:A:44:MET:HE3	1.97	0.47
5:e:236:GLN:HE21	7:L:324:ALA:HB1	1.78	0.47
6:I:215:GLY:HA2	8:A:81:LEU:HD11	1.97	0.47
6:I:264:ILE:HB	8:A:250:VAL:HA	1.96	0.47
3:O:92:ASP:C	10:O:603:ADP:PB	2.94	0.47
4:N:157:ASN:O	4:N:161:THR:OG1	2.32	0.47
6:M:54:PRO:HG3	10:M:601:ADP:C5	2.49	0.47
2:P:73:LEU:HD13	2:P:87:VAL:HG22	1.96	0.47
2:P:100:GLY:N	10:P:601:ADP:O1B	2.39	0.47
5:e:71:ASP:OD1	12:e:603:AF3:F2	2.23	0.47
1:K:109:TYR:HB3	1:K:114:LEU:HD12	1.98	0.46
2:J:32:ASN:HD21	2:J:524:ILE:HD11	1.80	0.46
4:G:316:ARG:NH1	9:R:106:TYR:OH	2.48	0.46
6:I:98:GLN:CB	6:I:105:GLY:O	2.60	0.46
6:I:503:ILE:HG23	6:I:508:VAL:HB	1.97	0.46
2:P:300:MET:HE1	3:O:333:SER:HB2	1.97	0.46
3:O:414:MET:HG2	3:O:464:LEU:HB3	1.97	0.46
3:O:479:ILE:HG12	10:O:603:ADP:C2	2.50	0.46
4:N:515:LEU:HD22	8:a:384:MET:HG3	1.96	0.46
6:M:203:VAL:HG13	6:M:413:ARG:HG3	1.97	0.46
7:L:127:ILE:HD12	7:L:512:GLU:HG3	1.97	0.46
1:K:49:SER:OG	1:K:53:ASP:OD1	2.32	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:69:ILE:HG22	2:J:15:LEU:HB2	1.97	0.46
5:E:114:LEU:HB2	5:E:522:VAL:HG21	1.98	0.46
8:a:250:VAL:HA	6:M:264:ILE:HB	1.98	0.46
8:A:45:LEU:HB2	8:A:53:THR:HB	1.97	0.46
9:R:211:CYS:HA	9:R:215:LEU:HB2	1.96	0.46
2:P:54:LYS:HD2	2:P:72:ILE:HD13	1.98	0.46
4:N:248:LYS:O	8:a:264:ARG:NH2	2.44	0.46
5:e:226:VAL:HG23	5:e:330:LEU:HD23	1.98	0.46
6:M:54:PRO:CG	10:M:601:ADP:C5	2.98	0.46
6:M:105:GLY:C	6:M:106:THR:HG23	2.36	0.46
4:G:101:LEU:HD11	4:G:444:LEU:HD23	1.98	0.46
7:B:403:ASP:OD2	7:B:498:GLN:NE2	2.48	0.46
8:A:433:ARG:NH1	3:O:459:ASN:OD1	2.48	0.46
3:O:200:VAL:HG11	3:O:353:ILE:HG22	1.96	0.46
4:N:325:ARG:HB3	4:N:370:LYS:HB2	1.96	0.46
7:L:69:THR:O	7:L:73:ASN:ND2	2.45	0.46
7:L:223:LYS:HA	7:L:360:ILE:HD11	1.96	0.46
1:K:195:GLU:HB3	1:K:384:LEU:HD13	1.96	0.46
2:J:99:ASP:OD1	10:J:601:ADP:O2B	2.34	0.46
6:I:229:LEU:HB2	6:I:374:LEU:HD12	1.98	0.46
9:R:197:ASP:OD1	9:R:197:ASP:N	2.49	0.46
1:z:270:ARG:NH2	4:N:272:GLU:OE2	2.49	0.46
2:P:464:ILE:HD12	2:P:467:LEU:HD12	1.97	0.46
3:H:95:THR:N	10:H:601:ADP:O1B	2.47	0.46
4:G:157:ASN:O	4:G:161:THR:OG1	2.34	0.46
1:z:69:ILE:HG22	2:P:15:LEU:HB2	1.97	0.46
1:z:200:SER:HA	1:z:379:PRO:HG3	1.97	0.46
2:P:68:ASP:OD1	12:P:603:AF3:F3	2.24	0.46
3:O:408:GLY:O	3:O:487:ASN:ND2	2.46	0.46
1:K:30:LEU:HD12	1:K:77:ILE:HD12	1.98	0.46
6:I:126:LYS:HB3	5:e:469:ILE:HB	1.98	0.46
6:I:245:LYS:HB2	6:I:295:CYS:HA	1.97	0.46
7:B:223:LYS:HA	7:B:360:ILE:HD11	1.96	0.46
3:O:63:ALA:N	3:O:94:THR:HG21	2.30	0.46
2:J:49:PRO:HG2	10:J:601:ADP:C5	2.51	0.46
9:R:101:TRP:HD1	9:R:145:SER:HB2	1.81	0.46
9:R:295:ASP:OD2	9:R:297:LYS:NZ	2.48	0.46
3:O:42:PRO:HG2	3:O:479:ILE:HG13	1.98	0.46
3:O:219:THR:OG1	3:O:220:PHE:N	2.49	0.46
1:K:164:LEU:HD13	1:K:202:THR:HA	1.98	0.46
5:E:150:SER:HB2	5:E:415:ARG:HB3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:203:VAL:HG13	6:I:413:ARG:HG3	1.98	0.46
9:R:63:ALA:O	9:R:89:ASN:ND2	2.48	0.46
2:P:347:CYS:SG	2:P:348:ASP:N	2.88	0.46
4:N:156:ILE:HD11	4:N:394:ALA:HB1	1.97	0.46
1:K:513:THR:HG21	4:G:167:ARG:HH12	1.81	0.46
3:H:310:CYS:SG	3:H:311:ALA:N	2.89	0.46
3:H:408:GLY:O	3:H:487:ASN:ND2	2.48	0.46
6:I:104:ASP:C	10:I:601:ADP:O2B	2.59	0.46
1:z:179:ILE:HG22	1:z:180:LYS:HG2	1.97	0.46
3:H:61:ASP:OD1	3:H:94:THR:OG1	2.34	0.45
4:G:452:ILE:HD13	4:G:462:LEU:HD22	1.98	0.45
9:R:211:CYS:HB3	9:R:217:LEU:HD12	1.98	0.45
2:P:76:LEU:HD13	3:O:10:LYS:HE2	1.98	0.45
4:N:304:LEU:HB3	4:N:309:ILE:HB	1.97	0.45
8:a:330:THR:OG1	8:a:331:LEU:N	2.46	0.45
7:L:71:LEU:HB3	7:L:85:VAL:HG22	1.98	0.45
7:L:94:GLU:O	7:L:399:GLN:NE2	2.44	0.45
7:L:131:ARG:NH2	7:L:512:GLU:OE2	2.46	0.45
1:K:241:LYS:HZ3	2:J:253:THR:HA	1.80	0.45
10:K:601:ADP:O2B	12:K:603:AF3:F1	2.24	0.45
5:E:58:MET:HE3	7:B:517:VAL:HG21	1.97	0.45
7:B:247:ASP:HB3	7:B:249:ILE:HG23	1.97	0.45
9:R:139:LEU:HB2	9:R:171:PRO:HD3	1.97	0.45
2:P:333:LEU:HD21	2:P:343:GLU:HG3	1.98	0.45
3:O:86:GLN:CB	3:O:93:GLY:O	2.62	0.45
9:R:313:VAL:HG13	9:R:367:PHE:HE1	1.82	0.45
3:O:310:CYS:SG	3:O:311:ALA:N	2.90	0.45
4:N:211:ASP:O	4:N:377:ARG:NH2	2.49	0.45
4:N:220:ILE:HG13	4:N:361:THR:HB	1.99	0.45
1:K:289:PHE:HB3	1:K:310:ILE:HG23	1.99	0.45
4:G:28:ASN:O	4:G:32:THR:OG1	2.29	0.45
6:I:291:LYS:HD3	6:I:320:MET:HB3	1.98	0.45
9:R:52:ASN:HD22	9:R:62:ARG:HG2	1.81	0.45
1:z:211:VAL:HG21	1:z:375:LEU:HD13	1.99	0.45
4:N:446:VAL:O	4:N:450:THR:OG1	2.34	0.45
7:L:247:ASP:HB3	7:L:249:ILE:HG23	1.98	0.45
5:E:436:ASP:OD1	5:E:447:ARG:NH2	2.50	0.45
7:B:94:GLU:O	7:B:399:GLN:NE2	2.43	0.45
7:B:480:MET:SD	7:B:480:MET:N	2.87	0.45
1:z:278:LYS:NZ	1:z:308:GLU:O	2.47	0.45
4:N:156:ILE:HD12	4:N:173:CYS:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:415:GLU:OE2	4:N:502:LYS:NZ	2.48	0.45
2:J:239:ILE:HG13	2:J:290:VAL:HB	1.99	0.45
10:z:601:ADP:O2B	12:z:603:AF3:F1	2.24	0.45
4:G:248:LYS:O	8:A:264:ARG:NH2	2.44	0.45
1:z:513:THR:HG21	4:N:167:ARG:HH12	1.80	0.45
8:a:9:GLY:HA3	8:a:533:LEU:HA	1.99	0.45
8:a:45:LEU:HD11	8:a:61:ILE:HA	1.99	0.45
8:a:81:LEU:HD11	6:M:215:GLY:HA2	1.99	0.45
6:M:494:ASN:HD22	6:M:501:SER:HB3	1.82	0.45
3:H:467:ARG:HG3	3:H:484:ILE:HD13	1.98	0.45
4:G:304:LEU:HB3	4:G:309:ILE:HB	1.99	0.45
3:O:243:GLU:HG3	3:O:293:LEU:HD13	1.99	0.45
1:z:157:ARG:HA	1:z:157:ARG:HD2	1.42	0.45
7:L:189:ARG:HH12	7:L:216:GLU:HA	1.82	0.45
8:A:356:ILE:HG12	8:A:361:LEU:HD22	1.99	0.45
9:R:10:GLY:HA2	9:R:143:THR:HB	1.98	0.45
5:e:183:MET:HE1	5:e:217:LEU:HD12	1.98	0.45
7:L:403:ASP:OD2	7:L:498:GLN:NE2	2.50	0.45
2:J:54:LYS:HG2	3:H:518:GLU:HB2	1.99	0.44
7:B:71:LEU:HB3	7:B:85:VAL:HG22	1.98	0.44
2:P:20:LYS:HE2	2:P:20:LYS:HB3	1.89	0.44
2:P:143:LEU:HD11	2:P:508:ILE:HD12	1.98	0.44
3:O:34:GLU:OE1	3:O:37:ARG:NE	2.46	0.44
5:e:356:LEU:HB2	5:e:373:GLU:HB3	1.98	0.44
6:M:196:ASP:O	6:M:199:THR:OG1	2.35	0.44
1:K:200:SER:HA	1:K:379:PRO:HG3	1.99	0.44
2:J:54:LYS:HD2	2:J:72:ILE:HD13	2.00	0.44
6:I:78:LEU:HB3	6:I:92:VAL:HG22	1.99	0.44
6:I:164:LEU:O	6:I:168:THR:OG1	2.33	0.44
2:P:73:LEU:HD11	2:P:105:LEU:HD11	1.99	0.44
2:P:278:ALA:HA	2:P:281:LYS:HE2	1.99	0.44
8:A:199:LYS:HB3	8:A:385:CYS:HB3	1.99	0.44
3:O:467:ARG:HG3	3:O:484:ILE:HD13	1.99	0.44
5:E:469:ILE:HG13	6:M:126:LYS:HB3	1.99	0.44
7:B:19:GLU:O	7:B:519:ASN:ND2	2.50	0.44
4:N:190:ARG:NH2	4:N:192:GLU:OE1	2.50	0.44
8:a:269:ASP:HA	8:a:272:LYS:HG2	1.99	0.44
6:M:90:MET:HG2	7:L:381:GLN:HG3	1.99	0.44
1:K:47:LEU:HD23	1:K:66:GLU:HB2	2.00	0.44
1:K:172:VAL:HG13	1:K:395:LEU:HD23	1.98	0.44
1:K:227:ASP:OD1	1:K:346:HIS:NE2	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:49:ILE:HD11	3:H:65:ILE:HG23	2.00	0.44
4:G:518:ARG:HH21	8:A:56:ASN:HD22	1.65	0.44
6:I:272:MET:HE3	8:A:246:MET:HE2	1.99	0.44
7:B:484:THR:OG1	7:B:485:ILE:N	2.51	0.44
8:A:38:PRO:CG	10:A:601:ADP:C5	3.00	0.44
1:z:97:LEU:HD13	1:z:450:VAL:HG21	2.00	0.44
3:O:191:GLN:HG2	3:O:193:LYS:H	1.82	0.44
8:a:88:ASP:OD2	8:a:88:ASP:N	2.48	0.44
1:K:218:HIS:HB3	1:K:221:MET:HG3	2.00	0.44
2:J:123:LEU:HD23	4:N:460:ILE:HG13	2.00	0.44
2:J:207:ILE:HG21	2:J:355:VAL:HG22	1.98	0.44
4:G:379:ALA:H	4:G:383:ILE:HD11	1.83	0.44
10:B:601:ADP:O2B	12:B:603:AF3:F1	2.26	0.44
2:J:102:ASN:CB	10:J:601:ADP:O1B	2.61	0.44
8:A:90:THR:C	10:A:601:ADP:O1B	2.59	0.44
9:R:60:VAL:HG11	9:R:86:ARG:HG3	2.00	0.44
2:P:22:PHE:HE1	2:P:526:MET:HE2	1.83	0.44
4:N:163:LYS:NZ	12:N:603:AF3:F2	2.38	0.44
4:N:333:SER:H	8:a:298:LYS:HD2	1.83	0.44
8:a:533:LEU:HD12	6:M:63:ASP:HA	1.99	0.44
1:K:180:LYS:HB3	1:K:184:GLU:HB3	2.00	0.44
4:G:95:THR:N	10:G:601:ADP:O1B	2.46	0.44
2:P:33:ILE:HG21	2:P:116:GLU:HB2	1.99	0.44
4:N:495:ILE:HD13	10:N:601:ADP:C5	2.49	0.44
2:J:169:MET:SD	10:J:601:ADP:N6	2.75	0.44
4:G:41:LEU:O	10:G:601:ADP:H5'2	2.17	0.44
8:A:231:ASN:OD1	8:A:368:LYS:NZ	2.51	0.44
5:e:64:GLY:O	7:L:82:LYS:NZ	2.46	0.44
1:K:481:LEU:HD23	10:K:601:ADP:C2	2.53	0.43
6:I:494:ASN:HD22	6:I:501:SER:HB3	1.82	0.43
8:A:56:ASN:ND2	8:A:158:SER:O	2.51	0.43
8:A:198:LEU:HD22	8:A:361:LEU:HD21	2.00	0.43
8:A:482:ASN:HB3	8:A:485:TRP:HZ3	1.82	0.43
8:A:505:GLU:OE2	10:A:601:ADP:H2'	2.18	0.43
2:P:143:LEU:HD21	2:P:419:LEU:HD11	2.00	0.43
7:L:112:GLU:HB3	7:L:438:SER:HB3	2.00	0.43
1:K:97:LEU:HD13	1:K:450:VAL:HG21	2.01	0.43
4:G:40:CYS:SG	4:G:48:LYS:NZ	2.77	0.43
9:R:270:PHE:HA	9:R:366:THR:HA	1.99	0.43
3:H:186:LEU:HD22	3:H:194:MET:HE3	2.00	0.43
8:A:124:ALA:HB2	8:A:438:ILE:HG23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:314:ARG:HH11	2:P:316:ASN:HD21	1.66	0.43
5:e:150:SER:HB2	5:e:415:ARG:HB3	2.00	0.43
5:e:334:ALA:O	5:e:378:SER:OG	2.36	0.43
10:L:601:ADP:O1B	12:L:603:AF3:F1	2.26	0.43
2:J:467:LEU:O	2:J:471:HIS:ND1	2.51	0.43
4:G:203:LYS:HB2	4:G:384:LEU:HD13	2.00	0.43
5:E:229:ASP:OD1	5:E:229:ASP:N	2.49	0.43
8:A:17:ILE:HG22	8:A:21:ASN:HD21	1.83	0.43
3:O:13:THR:HG22	3:O:523:PRO:HD3	2.01	0.43
4:N:518:ARG:O	8:a:42:ASP:N	2.51	0.43
8:a:42:ASP:OD1	8:a:56:ASN:ND2	2.51	0.43
6:M:503:ILE:HG23	6:M:508:VAL:HB	1.98	0.43
7:L:423:GLN:O	7:L:427:ARG:NH1	2.52	0.43
1:K:421:ALA:HA	1:K:424:LYS:HE2	2.00	0.43
2:J:13:GLN:HE21	2:J:13:GLN:HB2	1.54	0.43
6:I:204:ASP:OD2	7:B:358:LYS:NZ	2.49	0.43
8:A:38:PRO:HG3	10:A:601:ADP:N7	2.34	0.43
1:z:61:ASN:HB2	1:z:92:THR:HG21	2.00	0.43
1:z:273:LYS:HB3	1:z:339:LEU:HD12	2.01	0.43
4:N:248:LYS:HE2	4:N:248:LYS:HB3	1.90	0.43
3:H:259:THR:HG23	3:H:262:ASP:H	1.83	0.43
4:G:289:VAL:HG21	4:G:350:LEU:HD13	2.00	0.43
5:e:114:LEU:HB2	5:e:522:VAL:HG21	2.01	0.43
2:J:49:PRO:CG	10:J:601:ADP:C8	2.99	0.43
2:J:123:LEU:H	2:J:123:LEU:HG	1.62	0.43
2:J:340:VAL:HG13	2:J:343:GLU:HG2	2.00	0.43
1:z:92:THR:HB	12:z:603:AF3:F3	2.08	0.43
8:a:17:ILE:HG22	8:a:21:ASN:HD21	1.83	0.43
8:a:124:ALA:HB2	8:a:438:ILE:HG23	2.01	0.43
8:a:347:GLN:HB3	8:a:368:LYS:HD2	2.00	0.43
6:M:164:LEU:O	6:M:168:THR:OG1	2.32	0.43
7:L:62:MET:HE3	7:L:62:MET:HB3	1.85	0.43
7:L:484:THR:OG1	7:L:485:ILE:N	2.51	0.43
2:J:410:PRO:O	2:J:415:THR:OG1	2.34	0.43
1:z:396:ARG:NH2	4:N:357:ASP:OD2	2.52	0.43
2:P:32:ASN:HD21	2:P:524:ILE:HD11	1.84	0.43
3:O:279:GLU:OE2	3:O:302:TYR:OH	2.36	0.43
3:O:295:ILE:HG13	3:O:299:ALA:HB3	2.00	0.43
9:R:11:GLN:HG3	9:R:72:THR:HG21	2.00	0.43
3:O:90:VAL:HG11	3:O:498:VAL:HG13	2.01	0.43
8:a:184:ILE:HG23	8:a:185:ARG:HG3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:171:LEU:HD22	5:E:176:VAL:HG21	2.00	0.43
6:I:234:SER:HA	6:I:235:ASN:HA	1.78	0.43
1:z:172:VAL:HG13	1:z:395:LEU:HD23	1.99	0.43
4:N:132:ASP:OD2	4:N:437:TYR:OH	2.34	0.43
4:N:446:VAL:HA	4:N:449:ARG:HD2	2.00	0.43
5:e:82:ASP:OD1	5:e:82:ASP:N	2.46	0.43
6:M:98:GLN:CB	6:M:105:GLY:O	2.60	0.43
6:M:343:LYS:HD2	6:M:355:MET:HG2	2.01	0.43
8:A:10:ASP:N	8:A:532:LYS:O	2.50	0.42
5:e:36:ILE:HG22	5:e:40:LYS:HE2	2.00	0.42
8:a:91:THR:H	10:a:601:ADP:PB	2.41	0.42
1:K:298:ASP:OD1	1:K:298:ASP:N	2.52	0.42
3:H:46:ASP:OD1	5:E:527:LYS:NZ	2.46	0.42
7:B:219:LEU:HB2	7:B:372:THR:HG21	2.01	0.42
8:A:45:LEU:HD11	8:A:61:ILE:HA	2.01	0.42
3:O:82:ILE:HD12	3:O:97:VAL:HG12	2.01	0.42
4:N:203:LYS:HB2	4:N:384:LEU:HD13	2.00	0.42
1:K:46:MET:HG3	1:K:54:ILE:HG23	2.02	0.42
4:G:123:ILE:HG23	4:G:514:VAL:HG22	2.01	0.42
8:A:122:ARG:HD3	8:A:122:ARG:HA	1.88	0.42
1:z:164:LEU:HD13	1:z:202:THR:HA	2.00	0.42
5:e:156:ASP:OD1	5:e:156:ASP:N	2.52	0.42
8:a:198:LEU:HD22	8:a:361:LEU:HD21	2.02	0.42
1:K:58:LYS:NZ	1:K:158:THR:O	2.41	0.42
2:J:135:ALA:HB2	2:J:438:ILE:HG23	1.99	0.42
5:E:226:VAL:HG23	5:E:330:LEU:HD23	2.02	0.42
5:E:71:ASP:OD2	12:E:603:AF3:F2	2.27	0.42
5:E:489:ILE:O	10:E:601:ADP:C2	2.60	0.42
7:B:197:GLU:O	7:B:322:ARG:NE	2.45	0.42
8:A:222:SER:HB2	8:A:297:LEU:HD13	2.01	0.42
4:N:50:LEU:HD11	4:N:66:ILE:HA	2.00	0.42
5:e:56:ASP:N	7:L:516:ARG:O	2.52	0.42
1:K:196:MET:HB2	1:K:377:LYS:HG2	2.02	0.42
3:H:73:HIS:HB3	3:H:76:ALA:HB3	2.02	0.42
6:I:63:ASP:HA	8:A:533:LEU:HD12	2.01	0.42
6:I:343:LYS:HD2	6:I:355:MET:HG2	2.01	0.42
3:O:422:ASP:OD1	3:O:425:ARG:NH2	2.47	0.42
5:e:36:ILE:HG12	5:e:115:LEU:HG	2.01	0.42
5:e:524:MET:HE3	5:e:524:MET:HB2	1.94	0.42
5:E:241:VAL:HB	5:E:357:VAL:HB	2.02	0.42
6:I:104:ASP:O	10:I:601:ADP:PB	2.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:63:GLY:HA3	4:N:96:THR:OG1	2.19	0.42
5:e:467:ASN:HB3	5:e:470:GLN:HB2	2.01	0.42
8:a:18:ARG:HH21	8:a:528:ASP:HB2	1.85	0.42
6:M:104:ASP:C	10:M:601:ADP:O1B	2.63	0.42
7:L:215:ASP:OD1	7:L:361:HIS:NE2	2.52	0.42
5:E:479:GLN:HG2	5:E:485:PRO:HD2	2.02	0.42
2:P:380:SER:HB2	3:O:82:ILE:HG22	2.02	0.42
3:O:395:ILE:HD13	3:O:395:ILE:HA	1.94	0.42
6:M:291:LYS:HD3	6:M:320:MET:HB3	2.02	0.42
3:H:160:MET:HE2	3:H:173:ALA:HA	2.01	0.42
2:P:410:PRO:O	2:P:415:THR:OG1	2.36	0.42
4:N:518:ARG:HH21	8:a:56:ASN:HD22	1.67	0.42
6:M:234:SER:HA	6:M:235:ASN:HA	1.78	0.42
7:B:62:MET:HE3	7:B:62:MET:HB3	1.87	0.42
8:A:199:LYS:HE2	8:A:199:LYS:HB2	1.95	0.42
1:z:16:ALA:HA	1:z:519:ASP:HB2	2.01	0.42
3:O:116:LEU:HD12	3:O:116:LEU:HA	1.93	0.42
4:G:27:ILE:HG21	4:G:110:GLU:HB2	2.02	0.41
5:E:130:ARG:NH1	5:E:442:GLU:OE2	2.46	0.41
2:P:57:ILE:HD11	3:O:74:PRO:HG3	2.01	0.41
3:O:73:HIS:HB3	3:O:76:ALA:HB3	2.01	0.41
5:e:255:PRO:HA	5:e:256:PRO:HD3	1.89	0.41
8:a:213:GLY:H	8:a:373:ALA:HA	1.85	0.41
2:J:268:PHE:HE2	3:H:250:LYS:HG3	1.85	0.41
3:H:251:ASP:OD2	9:R:245:GLN:NE2	2.51	0.41
4:G:156:ILE:HD12	4:G:173:CYS:HA	2.02	0.41
4:G:376:LEU:HB3	4:G:384:LEU:HD22	2.02	0.41
5:E:104:THR:N	10:E:601:ADP:PB	2.89	0.41
4:N:40:CYS:SG	4:N:48:LYS:NZ	2.78	0.41
5:e:71:ASP:OD1	5:e:104:THR:OG1	2.38	0.41
5:e:186:ILE:HG23	5:e:222:LEU:HB2	2.01	0.41
2:J:123:LEU:HD13	2:J:127:GLU:HB2	2.01	0.41
2:J:241:VAL:HA	2:J:292:VAL:HG13	2.02	0.41
5:E:263:LYS:HD3	7:B:255:ARG:HH22	1.85	0.41
8:A:277:LYS:HD2	8:A:338:GLU:HB3	2.03	0.41
1:z:256:ARG:HD3	2:P:250:ILE:HD12	2.02	0.41
2:P:49:PRO:HG2	10:P:601:ADP:C5	2.55	0.41
2:P:167:SER:OG	2:P:499:ASP:OD2	2.37	0.41
1:K:46:MET:HE2	2:J:521:VAL:HG11	2.02	0.41
3:H:223:ALA:O	3:H:301:GLN:NE2	2.53	0.41
4:G:446:VAL:HA	4:G:449:ARG:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:245:LYS:HB2	5:E:295:ALA:HA	2.02	0.41
5:E:460:LEU:HB2	5:E:489:ILE:HD11	2.02	0.41
6:I:98:GLN:CG	6:I:105:GLY:HA3	2.50	0.41
8:A:347:GLN:HB3	8:A:368:LYS:HD2	2.02	0.41
8:A:34:SER:OG	8:A:43:LYS:NZ	2.53	0.41
8:A:86:VAL:HG11	8:A:509:VAL:HG23	2.02	0.41
1:z:58:LYS:NZ	1:z:158:THR:O	2.41	0.41
1:z:88:THR:OG1	1:z:400:ASN:ND2	2.54	0.41
1:z:338:ASP:N	1:z:338:ASP:OD1	2.53	0.41
5:e:245:LYS:HB2	5:e:295:ALA:HA	2.02	0.41
7:L:219:LEU:HB3	7:L:359:LEU:HD23	2.02	0.41
9:R:303:CYS:HB2	9:R:373:ALA:HB1	2.03	0.41
3:O:351:THR:OG1	3:O:352:GLN:N	2.53	0.41
4:N:221:ASN:OD1	4:N:221:ASN:N	2.48	0.41
4:N:237:ARG:H	4:N:288:ASP:HB2	1.85	0.41
4:N:289:VAL:HG21	4:N:350:LEU:HD13	2.01	0.41
7:B:66:ASP:CG	13:B:701:HOH:O	2.64	0.41
7:B:97:ASP:OD1	12:B:603:AF3:F1	2.29	0.41
3:O:82:ILE:HG21	3:O:509:ALA:HB2	2.02	0.41
3:O:444:ILE:HA	3:O:447:ARG:HB2	2.03	0.41
8:a:22:VAL:HG21	8:a:105:ASP:HB2	2.02	0.41
1:K:212:LEU:HB2	1:K:361:THR:HB	2.02	0.41
2:J:497:ILE:HD13	10:J:601:ADP:N6	2.34	0.41
5:E:33:LYS:NZ	5:E:123:ASP:OD1	2.44	0.41
9:R:131:GLN:HE22	9:R:249:ASP:HB2	1.86	0.41
9:R:318:ARG:HB3	9:R:358:PRO:HD3	2.02	0.41
7:L:348:LEU:HB2	7:L:363:SER:HB3	2.02	0.41
1:K:164:LEU:HD12	1:K:167:VAL:HB	2.02	0.41
2:J:27:GLU:OE2	1:z:15:ARG:NH1	2.49	0.41
4:G:282:ILE:HD11	4:G:304:LEU:HD21	2.02	0.41
6:I:54:PRO:CG	10:I:601:ADP:C4	3.03	0.41
6:I:145:ILE:O	6:I:149:THR:OG1	2.36	0.41
8:A:9:GLY:HA3	8:A:533:LEU:HA	2.02	0.41
8:A:350:GLU:HB3	8:A:365:LYS:HD2	2.03	0.41
1:z:218:HIS:HB3	1:z:221:MET:HG3	2.03	0.41
2:P:497:ILE:CD1	10:P:601:ADP:N6	2.84	0.41
5:e:171:LEU:HD22	5:e:176:VAL:HG21	2.03	0.41
8:a:88:ASP:HB2	10:a:601:ADP:O1B	2.21	0.41
8:a:246:MET:HE2	6:M:272:MET:HE3	2.02	0.41
6:M:227:LEU:HB3	6:M:376:ILE:HD13	2.03	0.41
6:M:257:LYS:HD2	6:M:306:ARG:HD3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:167:SER:OG	2:J:499:ASP:OD2	2.38	0.41
2:J:278:ALA:HA	2:J:281:LYS:HE2	2.03	0.41
5:E:63:ASP:OD1	5:E:63:ASP:N	2.54	0.41
7:B:87:MET:HE2	7:B:87:MET:HB3	1.88	0.41
7:B:112:GLU:HB3	7:B:438:SER:HB3	2.03	0.41
7:B:238:LEU:HB2	7:B:343:LEU:HD22	2.03	0.41
1:z:331:VAL:HA	4:N:228:ARG:HH21	1.86	0.41
1:z:481:LEU:HD21	10:z:601:ADP:N1	2.33	0.41
2:P:7:LYS:HB3	2:P:7:LYS:HE3	1.85	0.41
8:a:204:SER:OG	8:a:207:GLU:OE1	2.35	0.41
6:M:190:ALA:HB2	6:M:223:LEU:HD11	2.03	0.41
7:L:238:LEU:HB2	7:L:343:LEU:HD22	2.03	0.41
7:B:127:ILE:HD12	7:B:512:GLU:HG3	2.03	0.40
3:O:62:GLY:CA	3:O:94:THR:CG2	2.98	0.40
4:N:504:GLN:HE22	8:a:203:ARG:HA	1.86	0.40
7:L:240:ALA:N	7:L:291:ILE:O	2.53	0.40
4:G:238:ILE:HG12	4:G:289:VAL:HB	2.03	0.40
5:E:36:ILE:HG22	5:E:40:LYS:HE2	2.02	0.40
8:A:57:ASP:OD1	12:A:603:AF3:F2	2.29	0.40
8:A:89:GLY:N	10:A:601:ADP:PB	2.94	0.40
1:z:115:HIS:HB3	1:z:118:ILE:HG12	2.03	0.40
3:O:8:LEU:H	3:O:8:LEU:HG	1.53	0.40
4:N:37:ILE:H	4:N:37:ILE:HG13	1.70	0.40
8:a:39:VAL:HG21	8:a:456:ALA:HB2	2.04	0.40
7:L:480:MET:SD	7:L:480:MET:N	2.90	0.40
1:K:61:ASN:HB2	1:K:92:THR:HG21	2.03	0.40
2:J:333:LEU:HD21	2:J:343:GLU:HG3	2.03	0.40
1:z:245:ASN:OD1	1:z:245:ASN:N	2.44	0.40
2:P:207:ILE:HG21	2:P:355:VAL:HG22	2.03	0.40
2:P:369:ASP:OD1	2:P:369:ASP:N	2.52	0.40
4:N:446:VAL:HA	4:N:449:ARG:HB2	2.04	0.40
5:e:76:LEU:HB3	5:e:90:VAL:HG22	2.03	0.40
5:e:100:ILE:HG21	5:e:510:GLY:HA2	2.02	0.40
5:e:424:GLU:OE2	5:e:511:LYS:NZ	2.47	0.40
1:K:273:LYS:HB3	1:K:339:LEU:HD12	2.03	0.40
5:E:435:ALA:O	5:E:443:GLN:NE2	2.54	0.40
6:I:273:ASP:OD1	6:I:277:ARG:NE	2.52	0.40
8:A:240:SER:HA	8:A:291:GLY:H	1.87	0.40
9:R:172:SER:HA	9:R:173:PRO:HD3	1.98	0.40
9:R:180:VAL:O	9:R:184:ASN:ND2	2.44	0.40
1:z:47:LEU:HD23	1:z:66:GLU:HB2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:421:LYS:NZ	2:P:471:HIS:O	2.50	0.40
5:e:252:PRO:HB3	5:e:302:TRP:HB2	2.03	0.40
1:K:434:GLN:HE21	1:K:434:GLN:HB2	1.64	0.40
5:E:19:ASP:OD2	5:E:22:ARG:NH2	2.46	0.40
5:E:490:ASP:HB3	5:E:493:HIS:HA	2.03	0.40
8:A:184:ILE:HG23	8:A:185:ARG:HG3	2.03	0.40
4:N:44:LYS:HE2	4:N:483:GLU:HA	2.03	0.40
4:N:379:ALA:H	4:N:383:ILE:HD11	1.85	0.40
8:a:156:MET:HB3	8:a:161:ILE:HG13	2.04	0.40
6:M:503:ILE:HD13	6:M:503:ILE:HA	1.96	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	K	523/531 (98%)	496 (95%)	27 (5%)	0	100	100
1	z	523/531 (98%)	493 (94%)	30 (6%)	0	100	100
2	J	525/548 (96%)	486 (93%)	39 (7%)	0	100	100
2	P	525/548 (96%)	490 (93%)	35 (7%)	0	100	100
3	H	524/543 (96%)	498 (95%)	26 (5%)	0	100	100
3	O	524/543 (96%)	500 (95%)	24 (5%)	0	100	100
4	G	524/545 (96%)	504 (96%)	20 (4%)	0	100	100
4	N	524/545 (96%)	501 (96%)	23 (4%)	0	100	100
5	E	533/539 (99%)	506 (95%)	27 (5%)	0	100	100
5	e	533/539 (99%)	508 (95%)	25 (5%)	0	100	100
6	I	519/539 (96%)	503 (97%)	16 (3%)	0	100	100
6	M	519/539 (96%)	503 (97%)	16 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	B	521/535 (97%)	493 (95%)	28 (5%)	0	100	100
7	L	521/535 (97%)	496 (95%)	25 (5%)	0	100	100
8	A	535/556 (96%)	509 (95%)	25 (5%)	1 (0%)	43	73
8	a	535/556 (96%)	511 (96%)	23 (4%)	1 (0%)	43	73
9	R	424/444 (96%)	413 (97%)	11 (3%)	0	100	100
All	All	8832/9116 (97%)	8410 (95%)	420 (5%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	a	90	THR
8	A	89	GLY

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	K	437/442 (99%)	419 (96%)	18 (4%)	27	59
1	z	437/442 (99%)	424 (97%)	13 (3%)	36	65
2	J	433/452 (96%)	414 (96%)	19 (4%)	25	56
2	P	433/452 (96%)	414 (96%)	19 (4%)	25	56
3	H	433/443 (98%)	417 (96%)	16 (4%)	30	61
3	O	433/443 (98%)	421 (97%)	12 (3%)	38	66
4	G	457/469 (97%)	444 (97%)	13 (3%)	38	66
4	N	457/469 (97%)	442 (97%)	15 (3%)	33	63
5	E	452/455 (99%)	435 (96%)	17 (4%)	29	60
5	e	452/455 (99%)	433 (96%)	19 (4%)	26	58
6	I	443/452 (98%)	423 (96%)	20 (4%)	24	56
6	M	443/452 (98%)	425 (96%)	18 (4%)	27	59
7	B	416/427 (97%)	404 (97%)	12 (3%)	37	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	L	416/427 (97%)	404 (97%)	12 (3%)	37	66
8	A	448/463 (97%)	437 (98%)	11 (2%)	42	69
8	a	448/463 (97%)	436 (97%)	12 (3%)	39	67
9	R	366/379 (97%)	352 (96%)	14 (4%)	29	60
All	All	7404/7585 (98%)	7144 (96%)	260 (4%)	32	62

All (260) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	5	LYS
1	K	55	LYS
1	K	62	VAL
1	K	157	ARG
1	K	198	HIS
1	K	232	THR
1	K	240	GLU
1	K	241	LYS
1	K	289	PHE
1	K	290	VAL
1	K	292	ILE
1	K	321	MET
1	K	408	VAL
1	K	477	VAL
1	K	479	VAL
1	K	481	LEU
1	K	488	VAL
1	K	520	GLU
2	J	7	LYS
2	J	11	PHE
2	J	13	GLN
2	J	20	LYS
2	J	62	LYS
2	J	65	VAL
2	J	102	ASN
2	J	123	LEU
2	J	217	VAL
2	J	225	LYS
2	J	231	VAL
2	J	253	THR
2	J	292	VAL
2	J	296	LYS

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Mol	Chain	Res	Type
2	J	297	VAL
2	J	355	VAL
2	J	458	VAL
2	J	498	LEU
2	J	502	LEU
3	H	8	LEU
3	H	10	LYS
3	H	38	THR
3	H	40	LEU
3	H	58	ILE
3	H	71	VAL
3	H	89	GLU
3	H	92	ASP
3	H	149	VAL
3	H	195	ILE
3	H	257	VAL
3	H	295	ILE
3	H	362	THR
3	H	389	LEU
3	H	484	ILE
3	H	516	VAL
4	G	8	LEU
4	G	12	GLN
4	G	37	ILE
4	G	96	THR
4	G	142	ILE
4	G	156	ILE
4	G	214	VAL
4	G	225	THR
4	G	248	LYS
4	G	257	GLU
4	G	278	LEU
4	G	472	GLN
4	G	522	ILE
5	E	7	PHE
5	E	18	LYS
5	E	32	LEU
5	E	66	VAL
5	E	154	LEU
5	E	156	ASP
5	E	229	ASP
5	E	249	LEU

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Mol	Chain	Res	Type
5	E	250	THR
5	E	262	HIS
5	E	287	ILE
5	E	323	VAL
5	E	328	ILE
5	E	443	GLN
5	E	471	THR
5	E	528	ILE
5	E	533	LYS
6	I	28	ASP
6	I	42	LYS
6	I	68	VAL
6	I	70	ILE
6	I	71	THR
6	I	76	THR
6	I	106	THR
6	I	175	VAL
6	I	182	LEU
6	I	203	VAL
6	I	224	VAL
6	I	241	VAL
6	I	249	ILE
6	I	257	LYS
6	I	314	LEU
6	I	328	ILE
6	I	373	LEU
6	I	421	LEU
6	I	530	LEU
6	I	535	VAL
7	B	11	ILE
7	B	23	THR
7	B	27	THR
7	B	53	LEU
7	B	63	VAL
7	B	64	THR
7	B	69	THR
7	B	147	ASP
7	B	249	ILE
7	B	349	ILE
7	B	452	ASP
7	B	519	ASN
8	A	83	ASP

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Mol	Chain	Res	Type
8	A	137	ILE
8	A	237	LEU
8	A	253	VAL
8	A	313	LYS
8	A	337	GLU
8	A	352	VAL
8	A	399	VAL
8	A	428	THR
8	A	509	VAL
8	A	529	ASP
9	R	76	VAL
9	R	108	GLU
9	R	113	VAL
9	R	130	LEU
9	R	151	LEU
9	R	175	VAL
9	R	193	VAL
9	R	225	LEU
9	R	239	CYS
9	R	255	VAL
9	R	257	MET
9	R	258	VAL
9	R	374	ILE
9	R	375	GLN
1	z	5	LYS
1	z	55	LYS
1	z	62	VAL
1	z	232	THR
1	z	289	PHE
1	z	290	VAL
1	z	292	ILE
1	z	321	MET
1	z	408	VAL
1	z	477	VAL
1	z	479	VAL
1	z	481	LEU
1	z	520	GLU
2	P	7	LYS
2	P	11	PHE
2	P	13	GLN
2	P	20	LYS
2	P	62	LYS

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Mol	Chain	Res	Type
2	P	65	VAL
2	P	121	ILE
2	P	123	LEU
2	P	217	VAL
2	P	225	LYS
2	P	231	VAL
2	P	251	THR
2	P	253	THR
2	P	292	VAL
2	P	296	LYS
2	P	297	VAL
2	P	355	VAL
2	P	458	VAL
2	P	498	LEU
3	O	8	LEU
3	O	10	LYS
3	O	38	THR
3	O	58	ILE
3	O	71	VAL
3	O	149	VAL
3	O	257	VAL
3	O	295	ILE
3	O	362	THR
3	O	389	LEU
3	O	484	ILE
3	O	516	VAL
4	N	8	LEU
4	N	12	GLN
4	N	37	ILE
4	N	52	ASP
4	N	156	ILE
4	N	214	VAL
4	N	248	LYS
4	N	257	GLU
4	N	278	LEU
4	N	283	ILE
4	N	416	MET
4	N	450	THR
4	N	472	GLN
4	N	508	THR
4	N	522	ILE
5	e	7	PHE

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Mol	Chain	Res	Type
5	e	18	LYS
5	e	32	LEU
5	e	66	VAL
5	e	115	LEU
5	e	154	LEU
5	e	156	ASP
5	e	229	ASP
5	e	249	LEU
5	e	250	THR
5	e	262	HIS
5	e	287	ILE
5	e	323	VAL
5	e	328	ILE
5	e	443	GLN
5	e	472	MET
5	e	522	VAL
5	e	528	ILE
5	e	533	LYS
8	a	60	THR
8	a	83	ASP
8	a	137	ILE
8	a	237	LEU
8	a	248	LEU
8	a	253	VAL
8	a	313	LYS
8	a	327	ILE
8	a	337	GLU
8	a	352	VAL
8	a	399	VAL
8	a	509	VAL
6	M	28	ASP
6	M	42	LYS
6	M	68	VAL
6	M	70	ILE
6	M	71	THR
6	M	76	THR
6	M	175	VAL
6	M	182	LEU
6	M	203	VAL
6	M	224	VAL
6	M	241	VAL
6	M	257	LYS

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Mol	Chain	Res	Type
6	M	314	LEU
6	M	328	ILE
6	M	373	LEU
6	M	421	LEU
6	M	530	LEU
6	M	535	VAL
7	L	11	ILE
7	L	23	THR
7	L	27	THR
7	L	51	ILE
7	L	53	LEU
7	L	63	VAL
7	L	64	THR
7	L	69	THR
7	L	249	ILE
7	L	349	ILE
7	L	452	ASP
7	L	519	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (110) such sidechains are listed below:

Mol	Chain	Res	Type
1	K	61	ASN
1	K	161	HIS
1	K	234	ASN
1	K	334	ASN
1	K	400	ASN
1	K	434	GLN
2	J	13	GLN
2	J	80	HIS
2	J	219	HIS
2	J	279	GLN
2	J	289	ASN
2	J	303	HIS
2	J	383	ASN
2	J	461	ASN
2	J	475	ASN
2	J	523	GLN
3	H	21	GLN
3	H	170	GLN
3	H	331	GLN
3	H	335	ASN

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Mol	Chain	Res	Type
3	H	448	GLN
3	H	452	ASN
4	G	12	GLN
4	G	64	ASN
4	G	174	ASN
4	G	390	ASN
4	G	396	GLN
4	G	472	GLN
4	G	481	ASN
4	G	526	HIS
5	E	177	ASN
5	E	234	HIS
5	E	409	ASN
5	E	479	GLN
5	E	502	GLN
6	I	32	GLN
6	I	82	GLN
6	I	98	GLN
6	I	178	GLN
6	I	262	ASN
6	I	486	GLN
6	I	494	ASN
7	B	65	ASN
7	B	419	HIS
7	B	464	GLN
7	B	502	GLN
8	A	20	GLN
8	A	21	ASN
8	A	56	ASN
8	A	69	HIS
8	A	251	GLN
8	A	333	ASN
8	A	498	ASN
9	R	43	GLN
9	R	52	ASN
9	R	100	ASN
9	R	131	GLN
9	R	137	HIS
9	R	291	GLN
9	R	292	GLN
9	R	298	ASN
9	R	329	GLN

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Mol	Chain	Res	Type
9	R	334	GLN
9	R	423	GLN
1	z	31	GLN
1	z	37	ASN
1	z	234	ASN
1	z	293	ASN
1	z	294	GLN
1	z	334	ASN
1	z	400	ASN
1	z	434	GLN
2	P	13	GLN
2	P	79	GLN
2	P	140	HIS
2	P	289	ASN
2	P	303	HIS
2	P	316	ASN
2	P	435	GLN
2	P	523	GLN
3	O	21	GLN
3	O	234	ASN
3	O	331	GLN
3	O	452	ASN
4	N	12	GLN
4	N	64	ASN
4	N	111	HIS
4	N	253	GLN
4	N	302	HIS
4	N	390	ASN
4	N	396	GLN
4	N	472	GLN
4	N	481	ASN
5	e	20	GLN
5	e	234	HIS
8	a	21	ASN
8	a	56	ASN
8	a	69	HIS
8	a	139	ASN
8	a	242	GLN
8	a	251	GLN
8	a	333	ASN
8	a	498	ASN
6	M	98	GLN

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Mol	Chain	Res	Type
6	M	262	ASN
6	M	315	HIS
6	M	486	GLN
6	M	494	ASN
7	L	419	HIS
7	L	502	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 48 ligands modelled in this entry, 16 are monoatomic - leaving 32 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	AF3	E	603	-	0,3,3	-	-	-		
12	AF3	I	603	-	0,3,3	-	-	-		
10	ADP	H	601	11	28,29,29	1.38	4 (14%)	43,45,45	1.87	11 (25%)
10	ADP	I	601	11	28,29,29	1.37	4 (14%)	43,45,45	1.86	11 (25%)
10	ADP	G	601	11	28,29,29	1.38	4 (14%)	43,45,45	1.88	11 (25%)
12	AF3	H	603	-	0,3,3	-	-	-		
10	ADP	O	603	11	28,29,29	1.38	4 (14%)	43,45,45	1.87	11 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	AF3	N	603	-	0,3,3	-	-	-		
12	AF3	e	603	-	0,3,3	-	-	-		
12	AF3	P	603	-	0,3,3	-	-	-		
10	ADP	P	601	11	28,29,29	1.37	4 (14%)	43,45,45	1.87	11 (25%)
12	AF3	G	603	-	0,3,3	-	-	-		
12	AF3	B	603	-	0,3,3	-	-	-		
12	AF3	K	603	-	0,3,3	-	-	-		
10	ADP	K	601	11	28,29,29	1.40	4 (14%)	43,45,45	1.88	11 (25%)
12	AF3	L	603	-	0,3,3	-	-	-		
10	ADP	E	601	11	28,29,29	1.36	4 (14%)	43,45,45	1.87	11 (25%)
10	ADP	M	601	11	28,29,29	1.38	4 (14%)	43,45,45	1.87	11 (25%)
12	AF3	J	603	-	0,3,3	-	-	-		
10	ADP	J	601	11	28,29,29	1.38	4 (14%)	43,45,45	1.87	11 (25%)
10	ADP	z	601	11	28,29,29	1.40	4 (14%)	43,45,45	1.87	11 (25%)
10	ADP	A	601	11	28,29,29	1.39	4 (14%)	43,45,45	1.88	11 (25%)
10	ADP	N	601	11	28,29,29	1.37	4 (14%)	43,45,45	1.87	11 (25%)
10	ADP	e	601	11	28,29,29	1.38	4 (14%)	43,45,45	1.87	11 (25%)
10	ADP	a	601	11	28,29,29	1.38	4 (14%)	43,45,45	1.87	11 (25%)
12	AF3	a	603	-	0,3,3	-	-	-		
12	AF3	M	603	-	0,3,3	-	-	-		
12	AF3	z	603	-	0,3,3	-	-	-		
10	ADP	B	601	11	28,29,29	1.39	4 (14%)	43,45,45	1.88	11 (25%)
12	AF3	A	603	-	0,3,3	-	-	-		
12	AF3	O	602	-	0,3,3	-	-	-		
10	ADP	L	601	11	28,29,29	1.39	4 (14%)	43,45,45	1.87	11 (25%)

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	B	601	11	-	2/16/32/32	0/3/3/3
10	ADP	O	603	11	-	1/16/32/32	0/3/3/3
10	ADP	E	601	11	-	2/16/32/32	0/3/3/3
10	ADP	M	601	11	-	1/16/32/32	0/3/3/3
10	ADP	J	601	11	-	2/16/32/32	0/3/3/3
10	ADP	z	601	11	-	2/16/32/32	0/3/3/3
10	ADP	P	601	11	-	1/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	ADP	H	601	11	-	2/16/32/32	0/3/3/3
10	ADP	I	601	11	-	2/16/32/32	0/3/3/3
10	ADP	K	601	11	-	1/16/32/32	0/3/3/3
10	ADP	A	601	11	-	2/16/32/32	0/3/3/3
10	ADP	N	601	11	-	1/16/32/32	0/3/3/3
10	ADP	e	601	11	-	1/16/32/32	0/3/3/3
10	ADP	L	601	11	-	1/16/32/32	0/3/3/3
10	ADP	a	601	11	-	1/16/32/32	0/3/3/3
10	ADP	G	601	11	-	2/16/32/32	0/3/3/3

All (64) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	K	601	ADP	C5-C4	4.54	1.47	1.39
10	A	601	ADP	C5-C4	4.53	1.47	1.39
10	L	601	ADP	C5-C4	4.51	1.47	1.39
10	G	601	ADP	C5-C4	4.51	1.47	1.39
10	B	601	ADP	C5-C4	4.51	1.47	1.39
10	H	601	ADP	C5-C4	4.51	1.47	1.39
10	O	603	ADP	C5-C4	4.50	1.47	1.39
10	z	601	ADP	C5-C4	4.49	1.47	1.39
10	e	601	ADP	C5-C4	4.49	1.47	1.39
10	J	601	ADP	C5-C4	4.48	1.47	1.39
10	a	601	ADP	C5-C4	4.48	1.47	1.39
10	P	601	ADP	C5-C4	4.47	1.47	1.39
10	N	601	ADP	C5-C4	4.46	1.47	1.39
10	E	601	ADP	C5-C4	4.45	1.47	1.39
10	M	601	ADP	C5-C4	4.43	1.47	1.39
10	I	601	ADP	C5-C4	4.39	1.46	1.39
10	e	601	ADP	C5-C6	2.69	1.48	1.41
10	K	601	ADP	C5-C6	2.68	1.48	1.41
10	O	603	ADP	C5-C6	2.68	1.48	1.41
10	z	601	ADP	C5-C6	2.67	1.48	1.41
10	P	601	ADP	C5-C6	2.67	1.48	1.41
10	B	601	ADP	C5-C6	2.67	1.48	1.41
10	L	601	ADP	C5-C6	2.67	1.48	1.41
10	M	601	ADP	C5-C6	2.67	1.48	1.41
10	a	601	ADP	C5-C6	2.67	1.48	1.41
10	I	601	ADP	C5-C6	2.65	1.48	1.41
10	A	601	ADP	C5-C6	2.65	1.48	1.41
10	N	601	ADP	C5-C6	2.65	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	E	601	ADP	C5-C6	2.65	1.48	1.41
10	G	601	ADP	C5-C6	2.65	1.48	1.41
10	H	601	ADP	C5-C6	2.65	1.48	1.41
10	J	601	ADP	C5-C6	2.62	1.48	1.41
10	J	601	ADP	C8-N7	2.43	1.36	1.31
10	M	601	ADP	C8-N7	2.41	1.36	1.31
10	e	601	ADP	C8-N7	2.39	1.36	1.31
10	A	601	ADP	C8-N7	2.38	1.36	1.31
10	O	603	ADP	C8-N7	2.38	1.36	1.31
10	M	601	ADP	C5-N7	-2.38	1.34	1.39
10	I	601	ADP	C8-N7	2.37	1.36	1.31
10	H	601	ADP	C8-N7	2.37	1.36	1.31
10	N	601	ADP	C8-N7	2.36	1.36	1.31
10	z	601	ADP	C8-N7	2.35	1.36	1.31
10	K	601	ADP	C8-N7	2.35	1.36	1.31
10	a	601	ADP	C8-N7	2.35	1.36	1.31
10	a	601	ADP	C5-N7	-2.35	1.34	1.39
10	H	601	ADP	C5-N7	-2.35	1.34	1.39
10	e	601	ADP	C5-N7	-2.35	1.34	1.39
10	P	601	ADP	C8-N7	2.33	1.36	1.31
10	B	601	ADP	C5-N7	-2.33	1.34	1.39
10	G	601	ADP	C8-N7	2.33	1.36	1.31
10	E	601	ADP	C8-N7	2.32	1.36	1.31
10	z	601	ADP	C5-N7	-2.32	1.34	1.39
10	P	601	ADP	C5-N7	-2.32	1.34	1.39
10	L	601	ADP	C5-N7	-2.31	1.34	1.39
10	A	601	ADP	C5-N7	-2.31	1.34	1.39
10	L	601	ADP	C8-N7	2.30	1.36	1.31
10	I	601	ADP	C5-N7	-2.30	1.34	1.39
10	K	601	ADP	C5-N7	-2.30	1.34	1.39
10	O	603	ADP	C5-N7	-2.30	1.34	1.39
10	J	601	ADP	C5-N7	-2.29	1.34	1.39
10	N	601	ADP	C5-N7	-2.29	1.34	1.39
10	G	601	ADP	C5-N7	-2.29	1.34	1.39
10	B	601	ADP	C8-N7	2.27	1.36	1.31
10	E	601	ADP	C5-N7	-2.27	1.34	1.39

All (176) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	K	601	ADP	C5-C4-N3	-5.89	118.61	126.72
10	A	601	ADP	C5-C4-N3	-5.88	118.62	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	G	601	ADP	C5-C4-N3	-5.85	118.66	126.72
10	J	601	ADP	C5-C4-N3	-5.82	118.70	126.72
10	z	601	ADP	C5-C4-N3	-5.81	118.71	126.72
10	I	601	ADP	C5-C4-N3	-5.81	118.72	126.72
10	O	603	ADP	C5-C4-N3	-5.81	118.72	126.72
10	E	601	ADP	C5-C4-N3	-5.80	118.73	126.72
10	a	601	ADP	C5-C4-N3	-5.80	118.73	126.72
10	M	601	ADP	C5-C4-N3	-5.79	118.74	126.72
10	H	601	ADP	C5-C4-N3	-5.79	118.75	126.72
10	P	601	ADP	C5-C4-N3	-5.79	118.75	126.72
10	N	601	ADP	C5-C4-N3	-5.79	118.75	126.72
10	B	601	ADP	C5-C4-N3	-5.77	118.78	126.72
10	e	601	ADP	C5-C4-N3	-5.75	118.80	126.72
10	L	601	ADP	C5-C4-N3	-5.73	118.83	126.72
10	K	601	ADP	N3-C4-N9	4.64	135.06	127.17
10	z	601	ADP	N3-C4-N9	4.61	135.00	127.17
10	B	601	ADP	N3-C4-N9	4.60	134.99	127.17
10	L	601	ADP	N3-C4-N9	4.60	134.98	127.17
10	A	601	ADP	N3-C4-N9	4.58	134.95	127.17
10	G	601	ADP	N3-C4-N9	4.57	134.94	127.17
10	O	603	ADP	N3-C4-N9	4.55	134.90	127.17
10	E	601	ADP	N3-C4-N9	4.54	134.90	127.17
10	P	601	ADP	N3-C4-N9	4.54	134.88	127.17
10	e	601	ADP	N3-C4-N9	4.54	134.88	127.17
10	a	601	ADP	N3-C4-N9	4.53	134.88	127.17
10	J	601	ADP	N3-C4-N9	4.53	134.87	127.17
10	H	601	ADP	N3-C4-N9	4.52	134.86	127.17
10	M	601	ADP	N3-C4-N9	4.52	134.86	127.17
10	N	601	ADP	N3-C4-N9	4.52	134.86	127.17
10	I	601	ADP	N3-C4-N9	4.50	134.83	127.17
10	K	601	ADP	C2-N3-C4	3.88	121.31	111.83
10	G	601	ADP	C2-N3-C4	3.88	121.30	111.83
10	M	601	ADP	C2-N3-C4	3.88	121.30	111.83
10	A	601	ADP	C2-N3-C4	3.87	121.28	111.83
10	B	601	ADP	C2-N3-C4	3.86	121.26	111.83
10	z	601	ADP	C2-N3-C4	3.86	121.25	111.83
10	E	601	ADP	C2-N3-C4	3.86	121.25	111.83
10	a	601	ADP	C2-N3-C4	3.85	121.24	111.83
10	H	601	ADP	C2-N3-C4	3.85	121.23	111.83
10	O	603	ADP	C2-N3-C4	3.85	121.22	111.83
10	J	601	ADP	C2-N3-C4	3.84	121.22	111.83
10	N	601	ADP	C2-N3-C4	3.84	121.22	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	P	601	ADP	C2-N3-C4	3.84	121.21	111.83
10	e	601	ADP	C2-N3-C4	3.84	121.21	111.83
10	I	601	ADP	C2-N3-C4	3.84	121.20	111.83
10	L	601	ADP	C2-N3-C4	3.83	121.19	111.83
10	M	601	ADP	N3-C2-N1	-3.73	122.93	128.58
10	B	601	ADP	N3-C2-N1	-3.72	122.95	128.58
10	L	601	ADP	N3-C2-N1	-3.70	122.97	128.58
10	e	601	ADP	N3-C2-N1	-3.70	122.97	128.58
10	E	601	ADP	N3-C2-N1	-3.70	122.98	128.58
10	a	601	ADP	N3-C2-N1	-3.69	122.99	128.58
10	A	601	ADP	N3-C2-N1	-3.68	123.01	128.58
10	N	601	ADP	N3-C2-N1	-3.68	123.01	128.58
10	H	601	ADP	N3-C2-N1	-3.68	123.01	128.58
10	K	601	ADP	N3-C2-N1	-3.68	123.02	128.58
10	J	601	ADP	N3-C2-N1	-3.68	123.02	128.58
10	O	603	ADP	N3-C2-N1	-3.67	123.02	128.58
10	z	601	ADP	N3-C2-N1	-3.67	123.02	128.58
10	G	601	ADP	N3-C2-N1	-3.67	123.03	128.58
10	I	601	ADP	N3-C2-N1	-3.67	123.03	128.58
10	P	601	ADP	N3-C2-N1	-3.66	123.04	128.58
10	G	601	ADP	C4-C5-N7	-3.63	106.43	110.58
10	A	601	ADP	C4-C5-N7	-3.60	106.47	110.58
10	J	601	ADP	C4-C5-N7	-3.58	106.49	110.58
10	K	601	ADP	C4-C5-N7	-3.57	106.50	110.58
10	H	601	ADP	C4-C5-N7	-3.57	106.50	110.58
10	N	601	ADP	C4-C5-N7	-3.56	106.51	110.58
10	E	601	ADP	C4-C5-N7	-3.56	106.51	110.58
10	O	603	ADP	C4-C5-N7	-3.56	106.51	110.58
10	a	601	ADP	C4-C5-N7	-3.55	106.52	110.58
10	P	601	ADP	C4-C5-N7	-3.54	106.54	110.58
10	I	601	ADP	C4-C5-N7	-3.53	106.54	110.58
10	e	601	ADP	C4-C5-N7	-3.52	106.56	110.58
10	z	601	ADP	C4-C5-N7	-3.51	106.57	110.58
10	M	601	ADP	C4-C5-N7	-3.51	106.57	110.58
10	B	601	ADP	C4-C5-N7	-3.50	106.58	110.58
10	L	601	ADP	C4-C5-N7	-3.44	106.65	110.58
10	L	601	ADP	C4-N9-C8	2.89	108.78	105.74
10	z	601	ADP	C4-N9-C8	2.89	108.77	105.74
10	B	601	ADP	C4-N9-C8	2.88	108.76	105.74
10	K	601	ADP	C4-N9-C8	2.86	108.74	105.74
10	G	601	ADP	C4-N9-C8	2.84	108.72	105.74
10	G	601	ADP	C5-N7-C8	2.83	107.89	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	e	601	ADP	C4-N9-C8	2.82	108.70	105.74
10	E	601	ADP	C4-N9-C8	2.80	108.68	105.74
10	O	603	ADP	C4-N9-C8	2.79	108.67	105.74
10	J	601	ADP	C4-N9-C8	2.78	108.66	105.74
10	A	601	ADP	C4-N9-C8	2.78	108.66	105.74
10	a	601	ADP	C4-N9-C8	2.78	108.65	105.74
10	N	601	ADP	C4-N9-C8	2.77	108.65	105.74
10	H	601	ADP	C5-N7-C8	2.77	107.81	103.45
10	H	601	ADP	C4-N9-C8	2.77	108.65	105.74
10	P	601	ADP	C5-N7-C8	2.76	107.79	103.45
10	N	601	ADP	C5-N7-C8	2.76	107.79	103.45
10	a	601	ADP	C5-N7-C8	2.76	107.78	103.45
10	P	601	ADP	C4-N9-C8	2.76	108.63	105.74
10	K	601	ADP	C5-N7-C8	2.76	107.78	103.45
10	O	603	ADP	C5-N7-C8	2.75	107.78	103.45
10	J	601	ADP	C5-N7-C8	2.75	107.77	103.45
10	E	601	ADP	C5-N7-C8	2.75	107.77	103.45
10	M	601	ADP	C4-N9-C8	2.74	108.62	105.74
10	M	601	ADP	C5-N7-C8	2.74	107.76	103.45
10	e	601	ADP	C5-N7-C8	2.74	107.75	103.45
10	z	601	ADP	C5-N7-C8	2.73	107.75	103.45
10	I	601	ADP	C4-N9-C8	2.73	108.61	105.74
10	A	601	ADP	C5-N7-C8	2.73	107.73	103.45
10	I	601	ADP	C5-N7-C8	2.72	107.72	103.45
10	B	601	ADP	C5-N7-C8	2.71	107.71	103.45
10	L	601	ADP	C5-N7-C8	2.70	107.69	103.45
10	G	601	ADP	N9-C8-N7	-2.38	110.56	113.94
10	z	601	ADP	N9-C8-N7	-2.33	110.63	113.94
10	K	601	ADP	N9-C8-N7	-2.32	110.64	113.94
10	J	601	ADP	N9-C8-N7	-2.32	110.64	113.94
10	H	601	ADP	N9-C8-N7	-2.32	110.65	113.94
10	a	601	ADP	N9-C8-N7	-2.31	110.65	113.94
10	M	601	ADP	N9-C8-N7	-2.31	110.66	113.94
10	O	603	ADP	N9-C8-N7	-2.31	110.66	113.94
10	N	601	ADP	N9-C8-N7	-2.31	110.66	113.94
10	e	601	ADP	N9-C8-N7	-2.31	110.66	113.94
10	E	601	ADP	N9-C8-N7	-2.30	110.67	113.94
10	P	601	ADP	N9-C8-N7	-2.30	110.67	113.94
10	I	601	ADP	N9-C8-N7	-2.30	110.68	113.94
10	L	601	ADP	N9-C8-N7	-2.29	110.69	113.94
10	B	601	ADP	N9-C8-N7	-2.27	110.71	113.94
10	A	601	ADP	N9-C8-N7	-2.27	110.71	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	G	601	ADP	C3'-C2'-C1'	2.25	105.73	101.46
10	a	601	ADP	C3'-C2'-C1'	2.25	105.72	101.46
10	e	601	ADP	C3'-C2'-C1'	2.23	105.69	101.46
10	P	601	ADP	C3'-C2'-C1'	2.23	105.69	101.46
10	E	601	ADP	C3'-C2'-C1'	2.23	105.68	101.46
10	N	601	ADP	C3'-C2'-C1'	2.23	105.68	101.46
10	J	601	ADP	C3'-C2'-C1'	2.23	105.67	101.46
10	M	601	ADP	C3'-C2'-C1'	2.23	105.67	101.46
10	I	601	ADP	C3'-C2'-C1'	2.22	105.67	101.46
10	O	603	ADP	C3'-C2'-C1'	2.22	105.67	101.46
10	B	601	ADP	C3'-C2'-C1'	2.22	105.67	101.46
10	H	601	ADP	C3'-C2'-C1'	2.22	105.66	101.46
10	L	601	ADP	C3'-C2'-C1'	2.21	105.64	101.46
10	G	601	ADP	C6-C5-N7	2.21	136.34	132.09
10	A	601	ADP	C3'-C2'-C1'	2.20	105.62	101.46
10	a	601	ADP	C6-C5-N7	2.19	136.32	132.09
10	N	601	ADP	C6-C5-N7	2.19	136.31	132.09
10	e	601	ADP	C6-C5-N7	2.19	136.31	132.09
10	O	603	ADP	C6-C5-N7	2.19	136.31	132.09
10	H	601	ADP	C6-C5-N7	2.18	136.29	132.09
10	E	601	ADP	C6-C5-N7	2.18	136.29	132.09
10	A	601	ADP	C6-C5-N7	2.18	136.29	132.09
10	B	601	ADP	C6-C5-N7	2.17	136.28	132.09
10	J	601	ADP	C6-C5-N7	2.17	136.27	132.09
10	P	601	ADP	C6-C5-N7	2.17	136.27	132.09
10	z	601	ADP	C6-C5-N7	2.16	136.25	132.09
10	L	601	ADP	C6-C5-N7	2.16	136.25	132.09
10	M	601	ADP	C6-C5-N7	2.15	136.24	132.09
10	K	601	ADP	C6-C5-N7	2.15	136.23	132.09
10	I	601	ADP	C6-C5-N7	2.13	136.20	132.09
10	L	601	ADP	C2-N1-C6	2.10	122.18	118.73
10	B	601	ADP	C2-N1-C6	2.10	122.18	118.73
10	K	601	ADP	C3'-C2'-C1'	2.10	105.43	101.46
10	E	601	ADP	C2-N1-C6	2.09	122.16	118.73
10	a	601	ADP	C2-N1-C6	2.08	122.15	118.73
10	J	601	ADP	C2-N1-C6	2.08	122.15	118.73
10	O	603	ADP	C2-N1-C6	2.08	122.14	118.73
10	e	601	ADP	C2-N1-C6	2.08	122.14	118.73
10	M	601	ADP	C2-N1-C6	2.07	122.14	118.73
10	z	601	ADP	C3'-C2'-C1'	2.07	105.38	101.46
10	A	601	ADP	C2-N1-C6	2.06	122.12	118.73
10	H	601	ADP	C2-N1-C6	2.06	122.11	118.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	I	601	ADP	C2-N1-C6	2.05	122.10	118.73
10	P	601	ADP	C2-N1-C6	2.05	122.10	118.73
10	N	601	ADP	C2-N1-C6	2.04	122.08	118.73
10	K	601	ADP	C2-N1-C6	2.04	122.07	118.73
10	G	601	ADP	C2-N1-C6	2.03	122.06	118.73
10	z	601	ADP	C2-N1-C6	2.01	122.03	118.73

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	J	601	ADP	C5'-O5'-PA-O1A
10	H	601	ADP	C5'-O5'-PA-O1A
10	G	601	ADP	C5'-O5'-PA-O1A
10	E	601	ADP	C5'-O5'-PA-O1A
10	I	601	ADP	C5'-O5'-PA-O1A
10	B	601	ADP	C5'-O5'-PA-O1A
10	A	601	ADP	C5'-O5'-PA-O1A
10	z	601	ADP	PB-O3A-PA-O1A
10	z	601	ADP	PB-O3A-PA-O2A
10	N	601	ADP	O4'-C4'-C5'-O5'
10	J	601	ADP	O4'-C4'-C5'-O5'
10	H	601	ADP	O4'-C4'-C5'-O5'
10	G	601	ADP	O4'-C4'-C5'-O5'
10	E	601	ADP	O4'-C4'-C5'-O5'
10	I	601	ADP	O4'-C4'-C5'-O5'
10	A	601	ADP	O4'-C4'-C5'-O5'
10	P	601	ADP	O4'-C4'-C5'-O5'
10	O	603	ADP	O4'-C4'-C5'-O5'
10	e	601	ADP	O4'-C4'-C5'-O5'
10	a	601	ADP	O4'-C4'-C5'-O5'
10	M	601	ADP	O4'-C4'-C5'-O5'
10	B	601	ADP	O4'-C4'-C5'-O5'
10	L	601	ADP	O4'-C4'-C5'-O5'
10	K	601	ADP	PB-O3A-PA-O2A

There are no ring outliers.

32 monomers are involved in 260 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	E	603	AF3	2	0

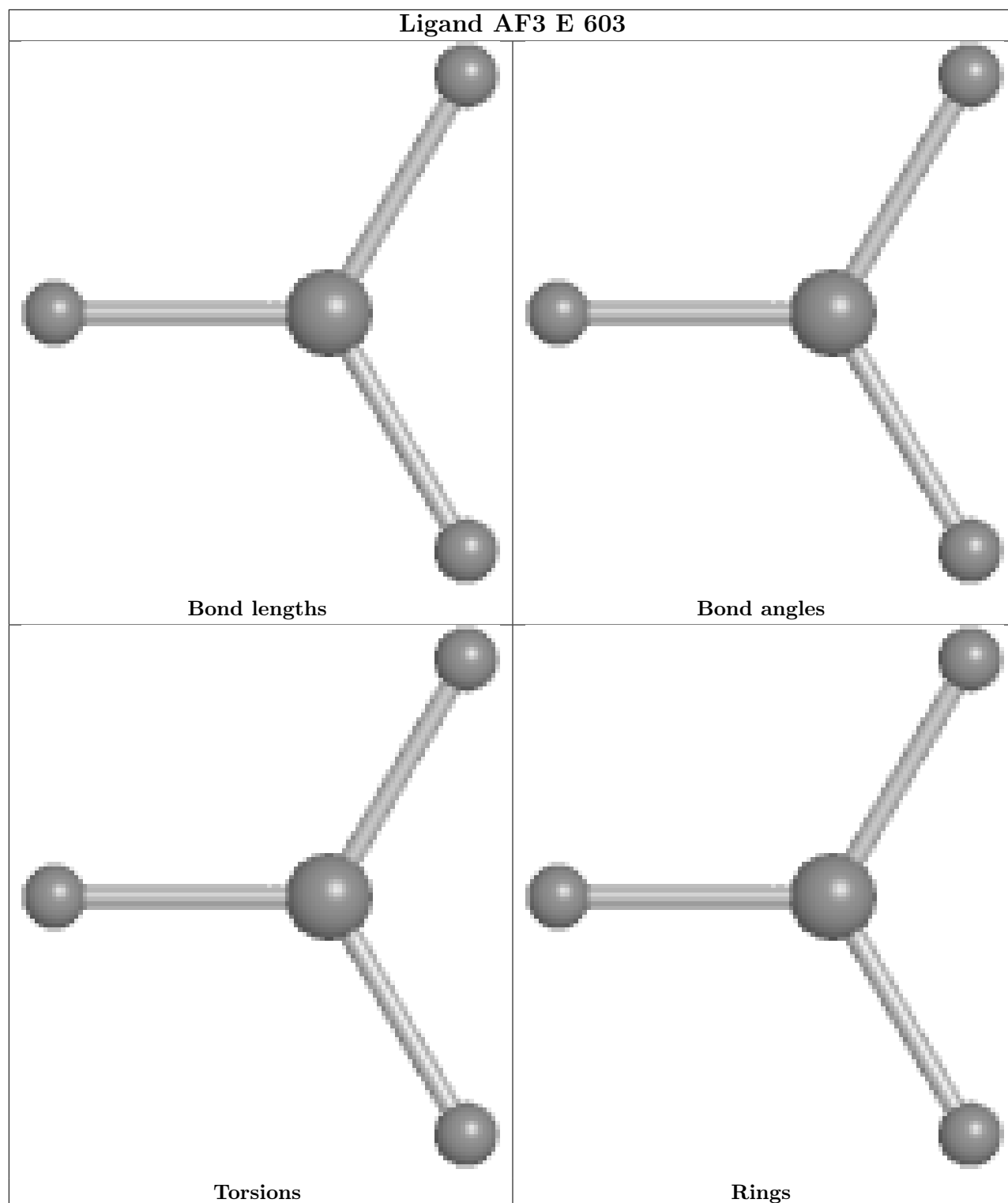
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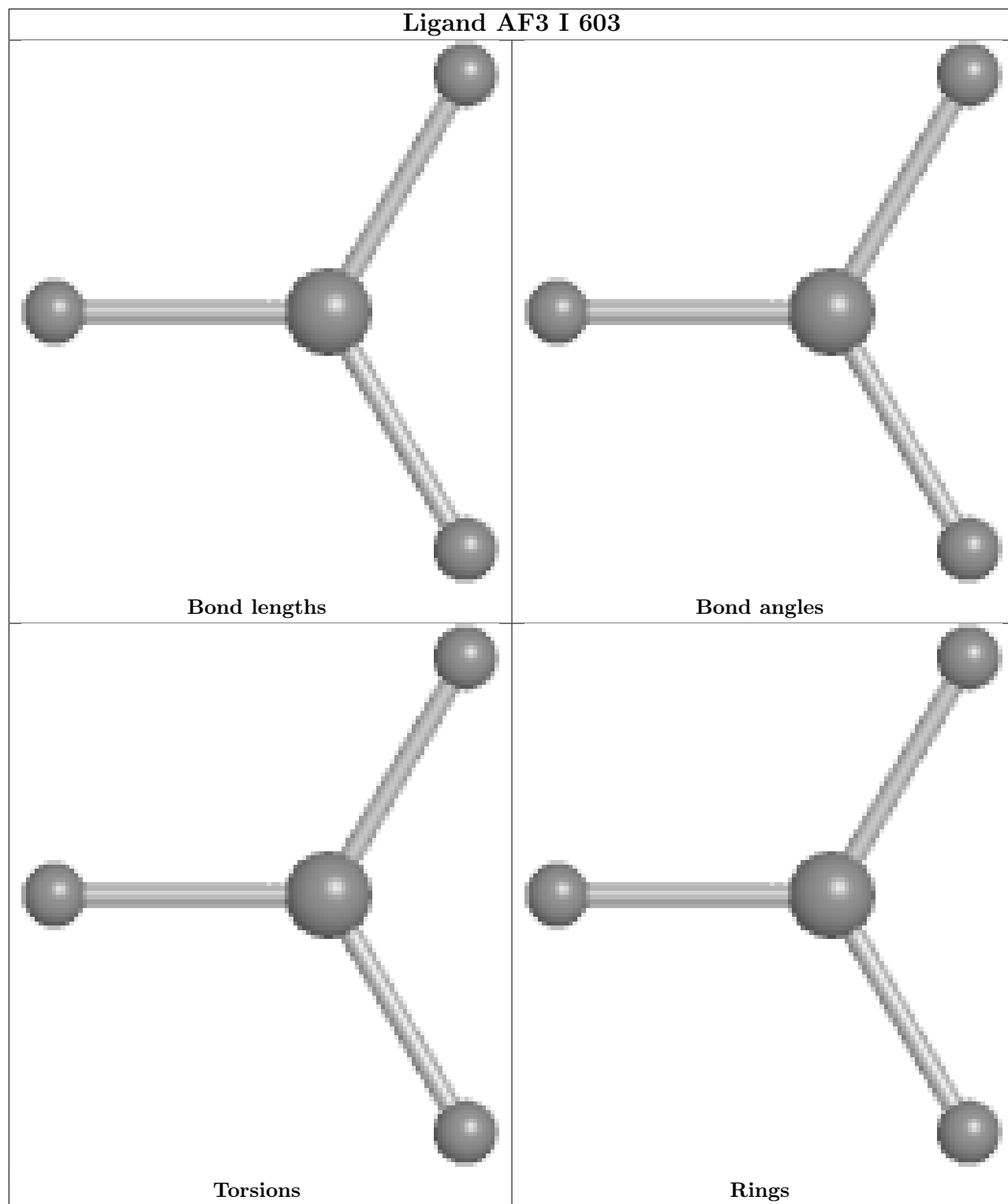
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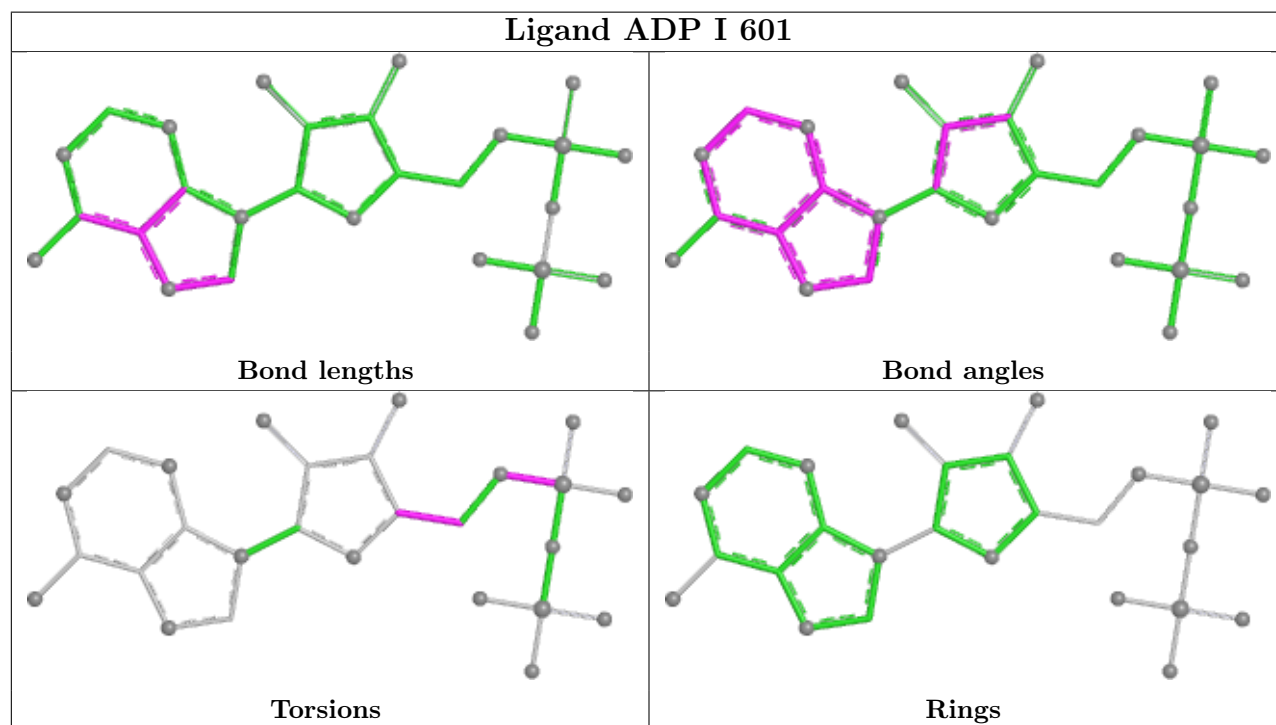
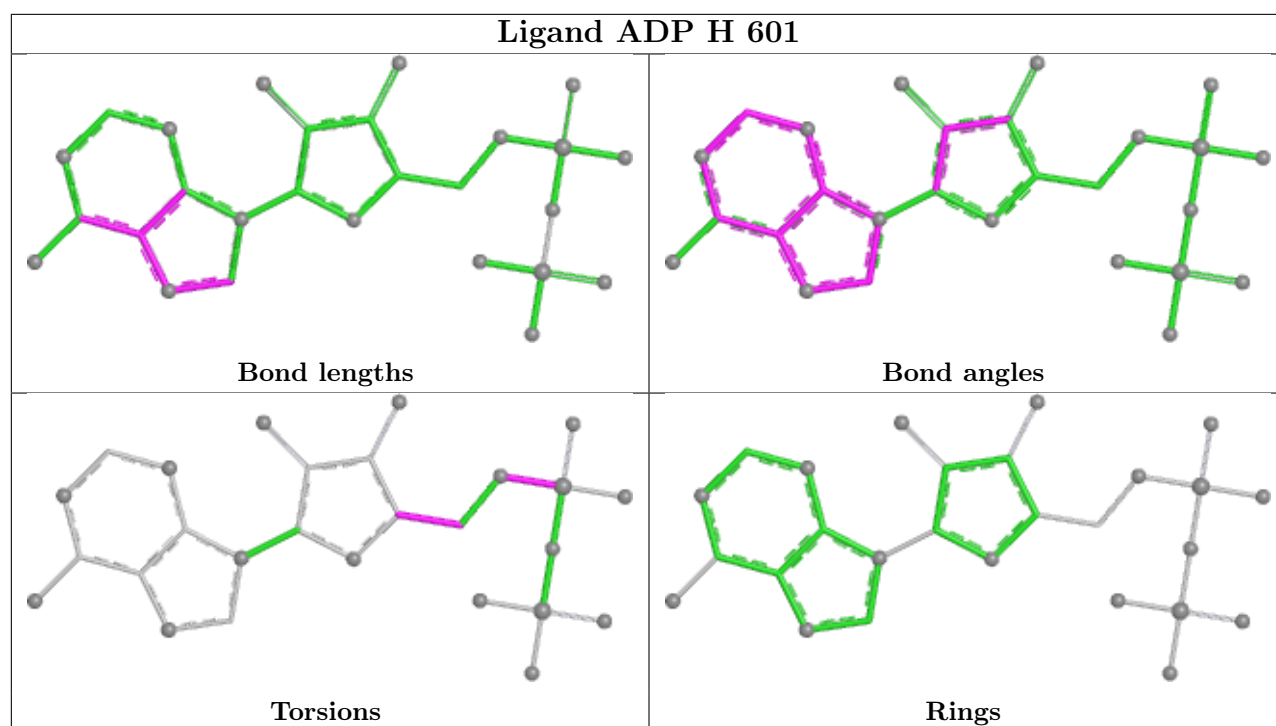
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	I	603	AF3	1	0
10	H	601	ADP	14	0
10	I	601	ADP	15	0
10	G	601	ADP	30	0
12	H	603	AF3	2	0
10	O	603	ADP	17	0
12	N	603	AF3	4	0
12	e	603	AF3	3	0
12	P	603	AF3	5	0
10	P	601	ADP	13	0
12	G	603	AF3	2	0
12	B	603	AF3	4	0
12	K	603	AF3	5	0
10	K	601	ADP	11	0
12	L	603	AF3	3	0
10	E	601	ADP	7	0
10	M	601	ADP	13	0
12	J	603	AF3	6	0
10	J	601	ADP	18	0
10	z	601	ADP	16	0
10	A	601	ADP	18	0
10	N	601	ADP	28	0
10	e	601	ADP	6	0
10	a	601	ADP	7	0
12	a	603	AF3	4	0
12	M	603	AF3	1	0
12	z	603	AF3	5	0
10	B	601	ADP	7	0
12	A	603	AF3	2	0
12	O	602	AF3	6	0
10	L	601	ADP	7	0

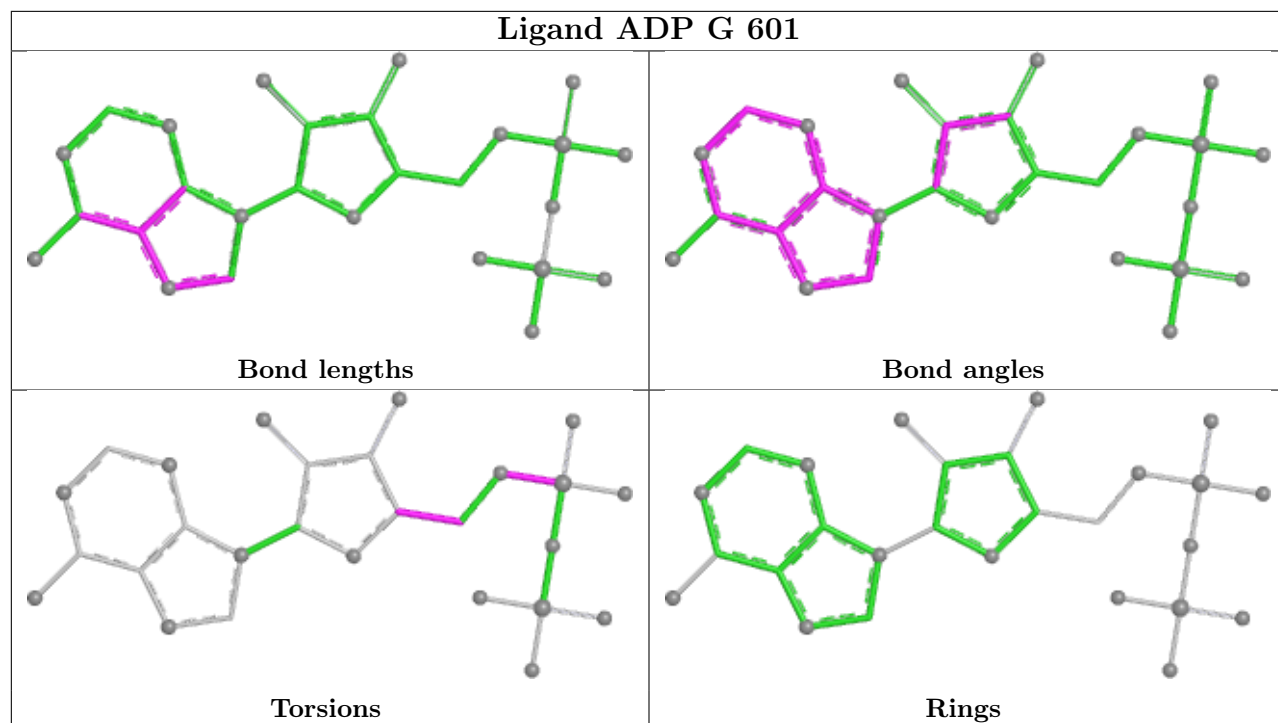
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient

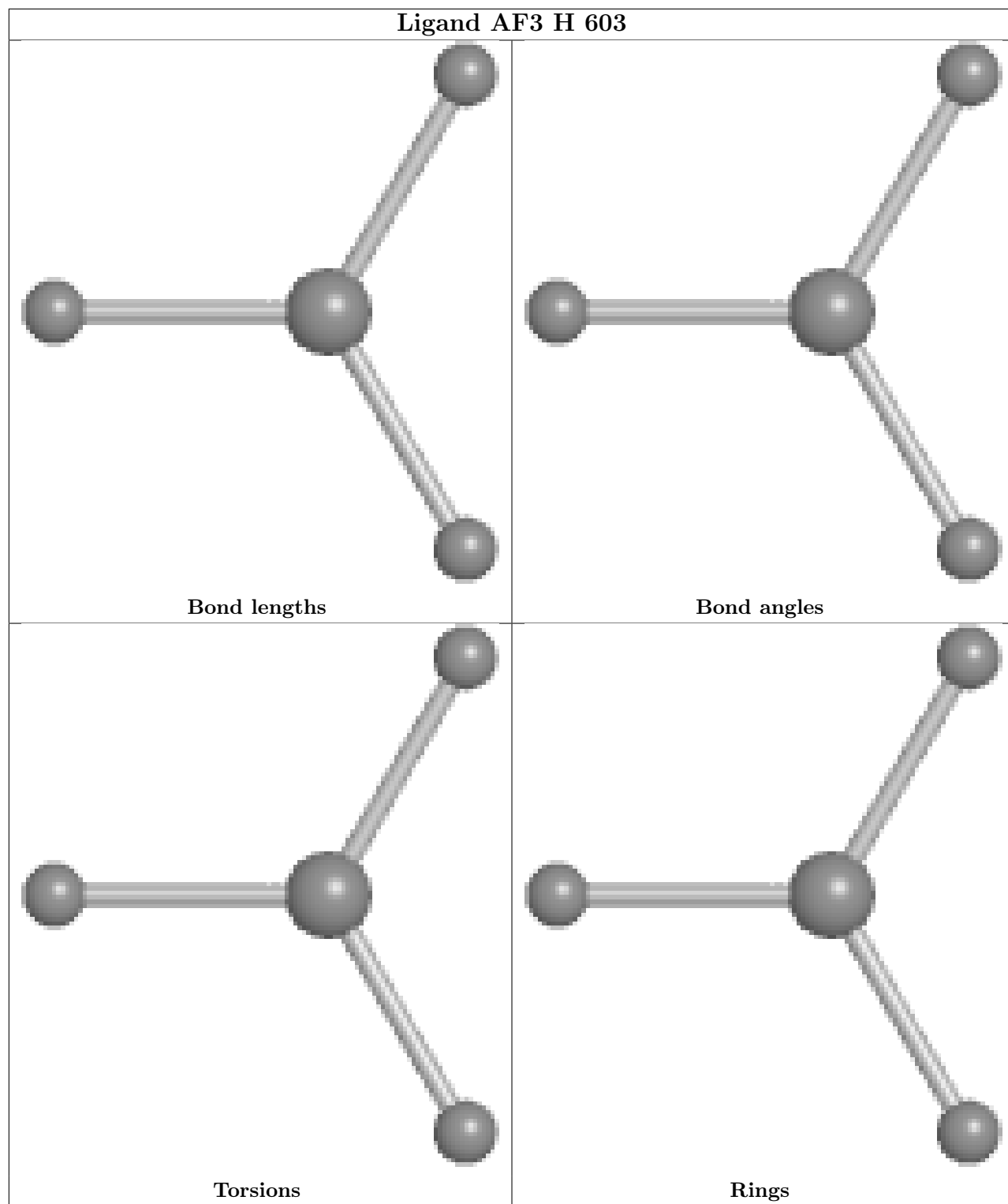
equivalents in the CSD to analyse the geometry.

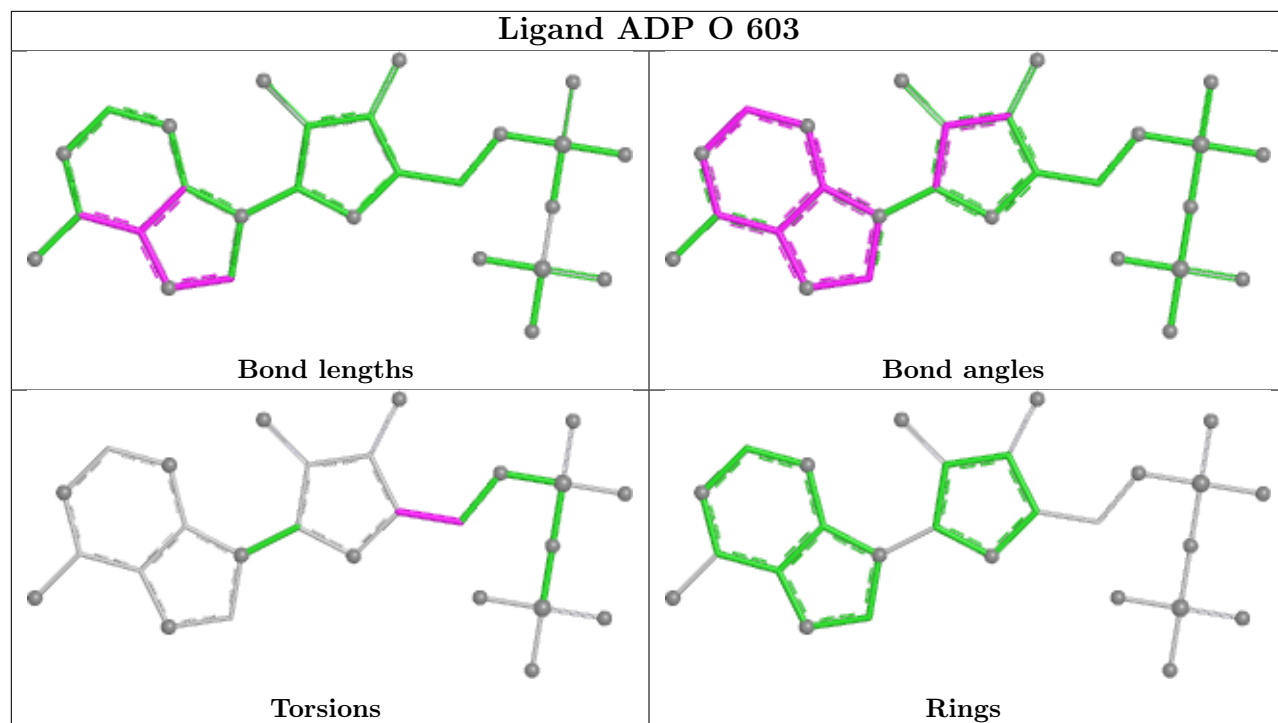


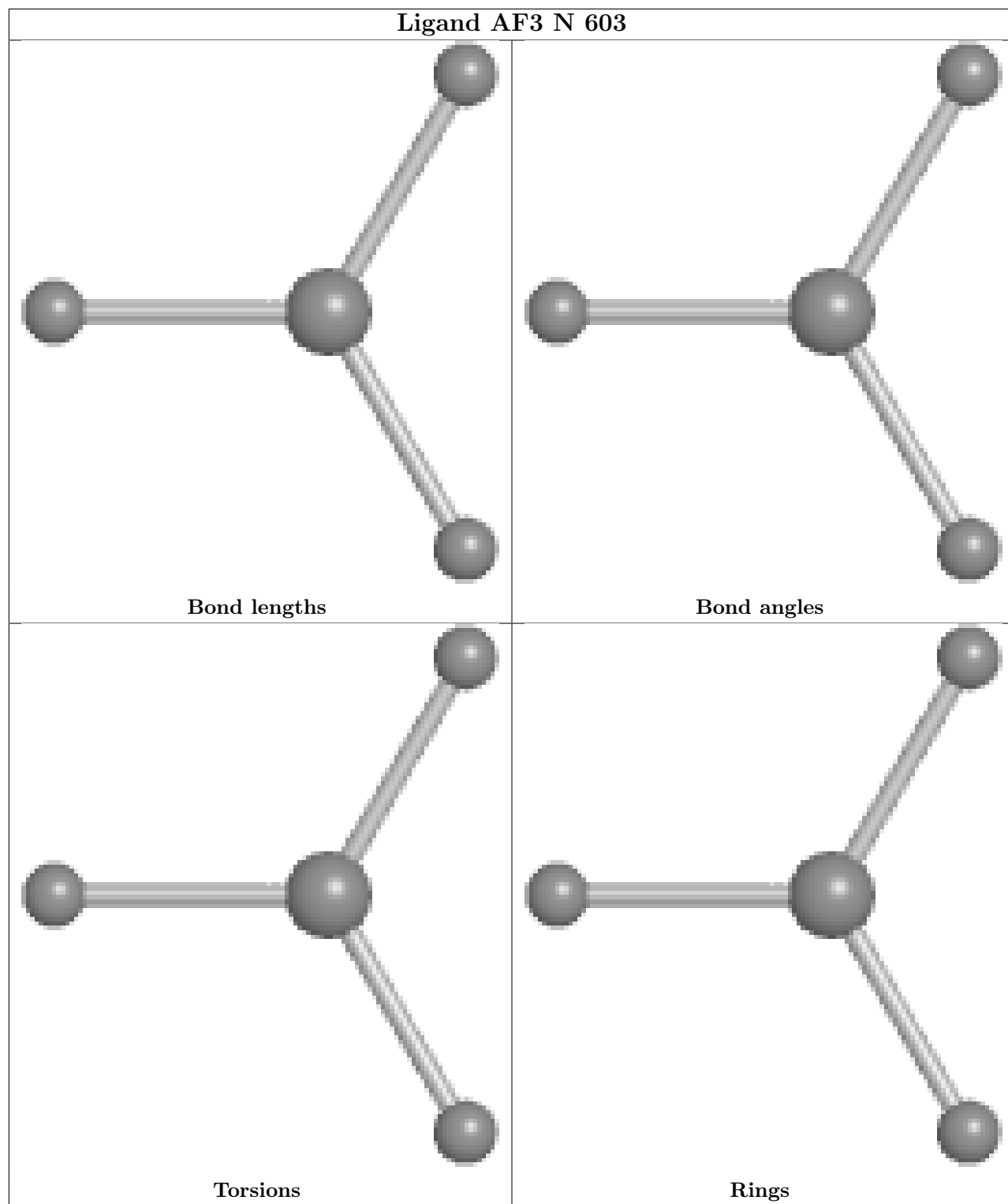


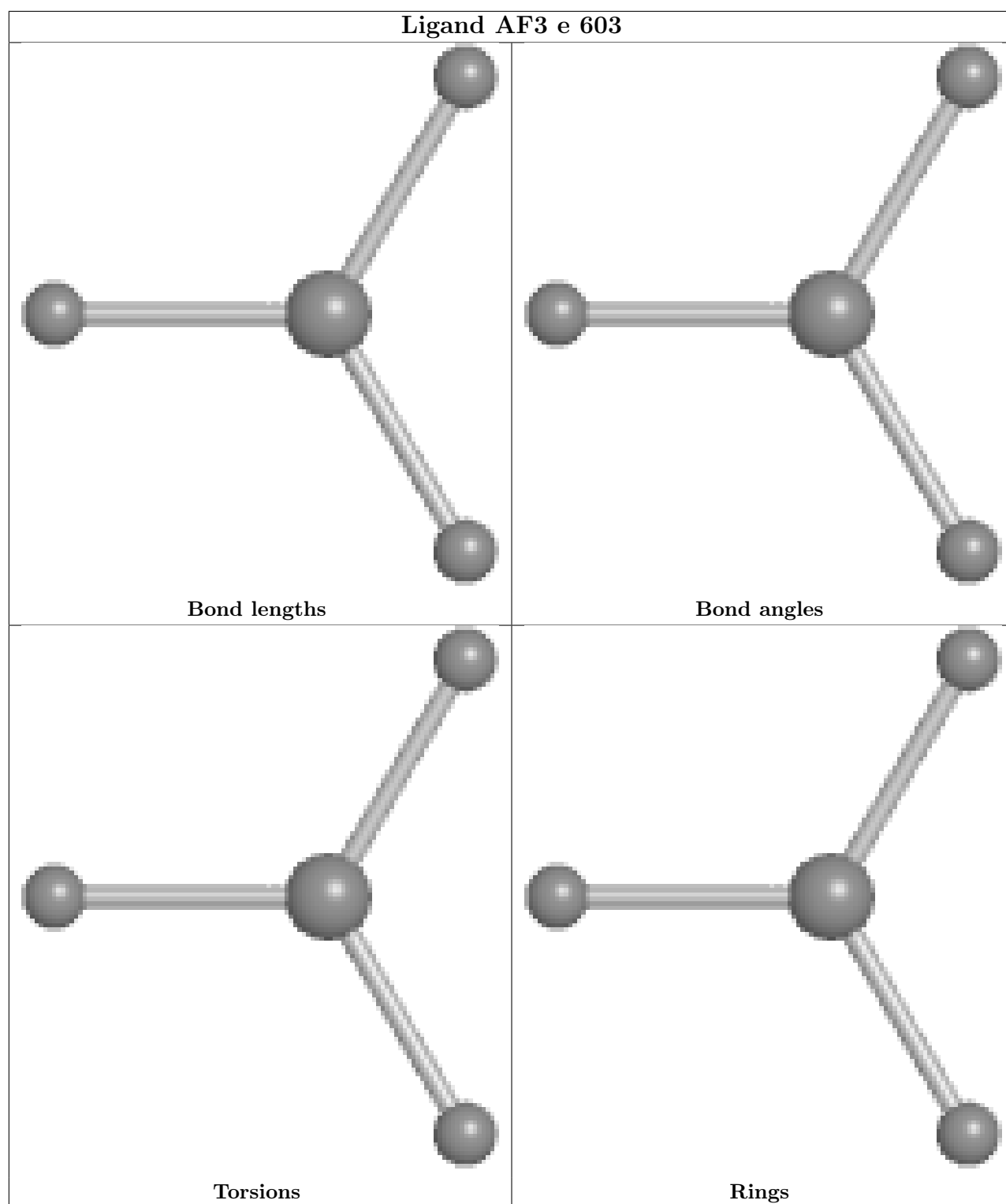


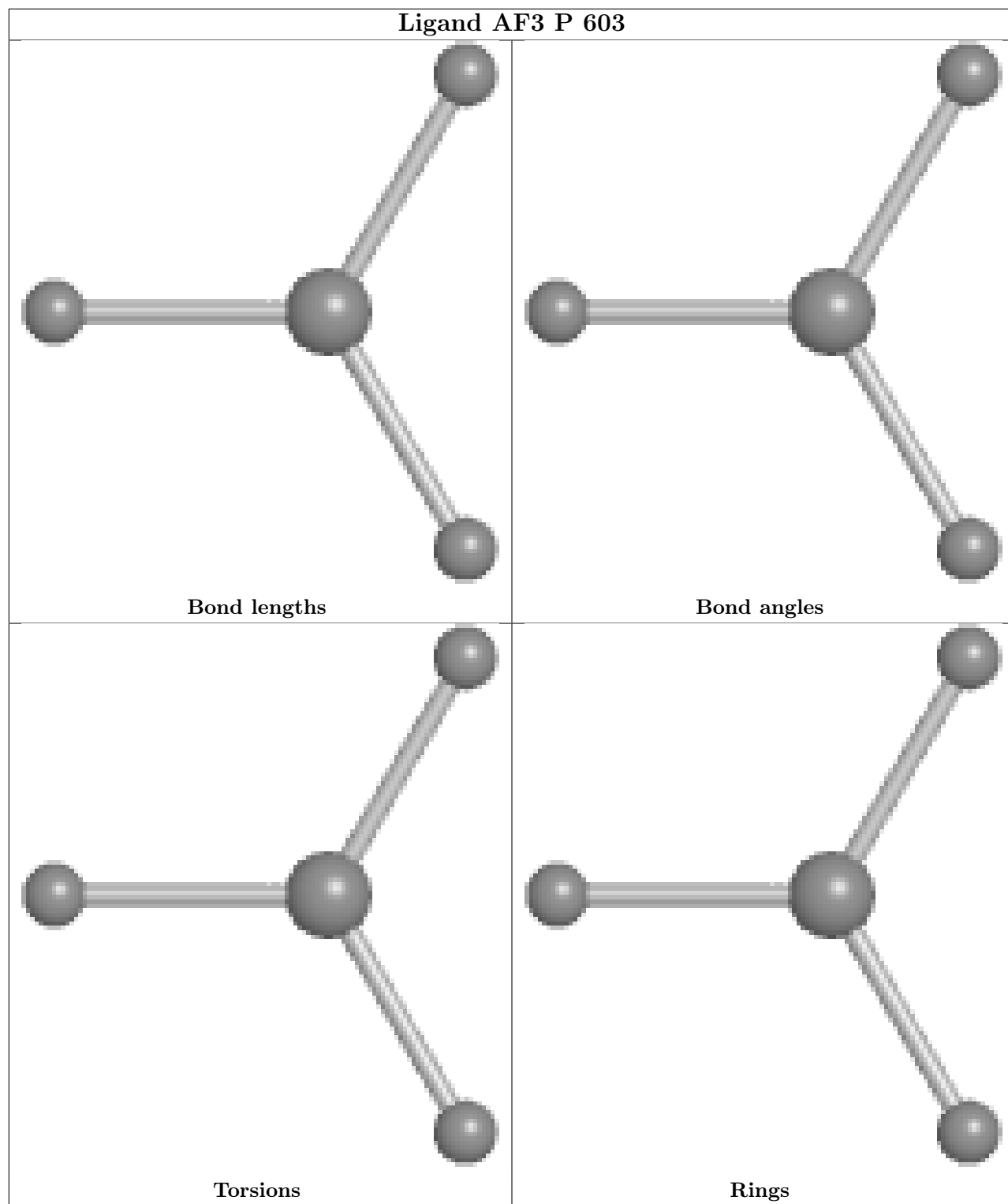


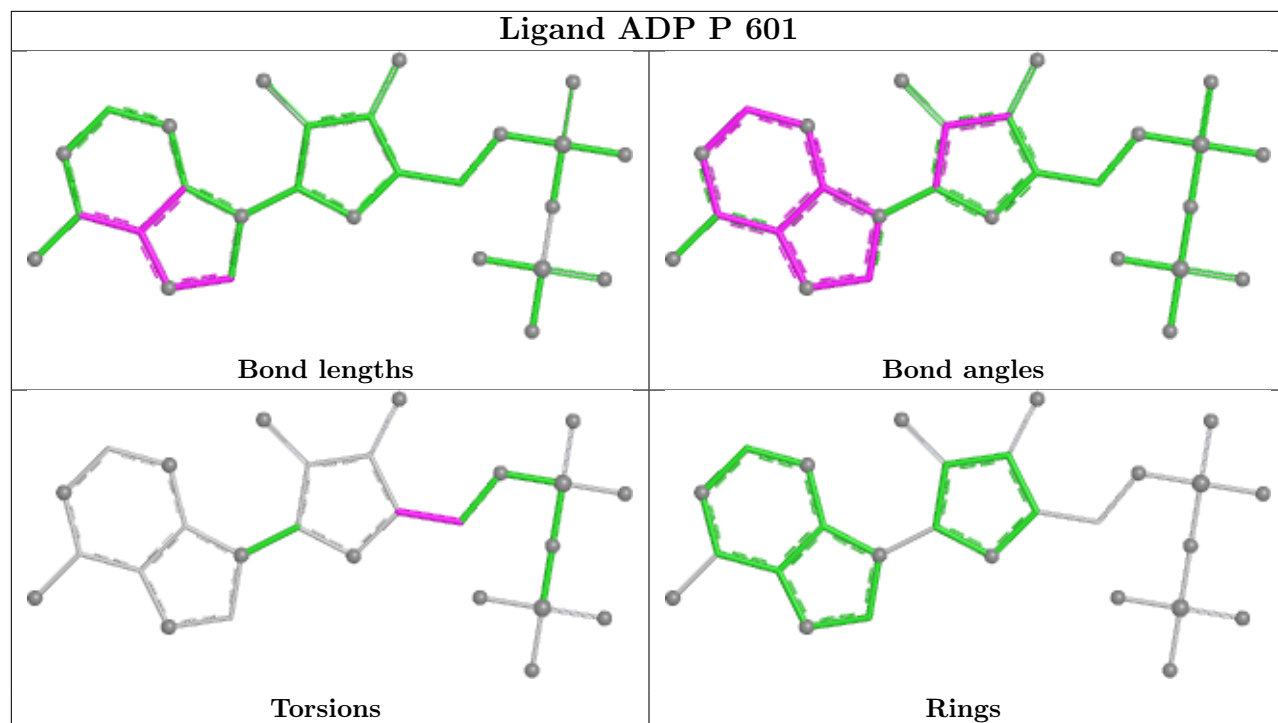


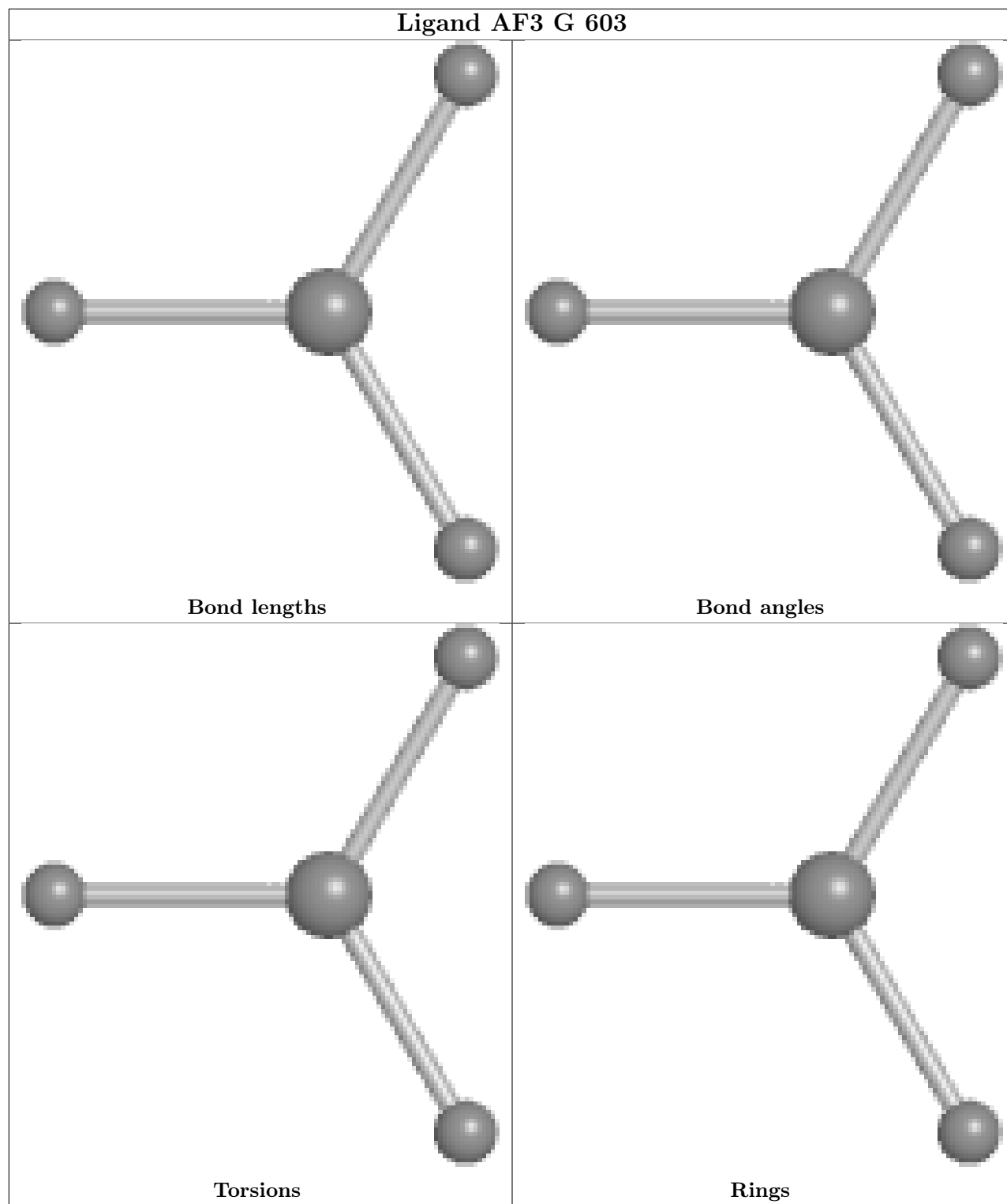


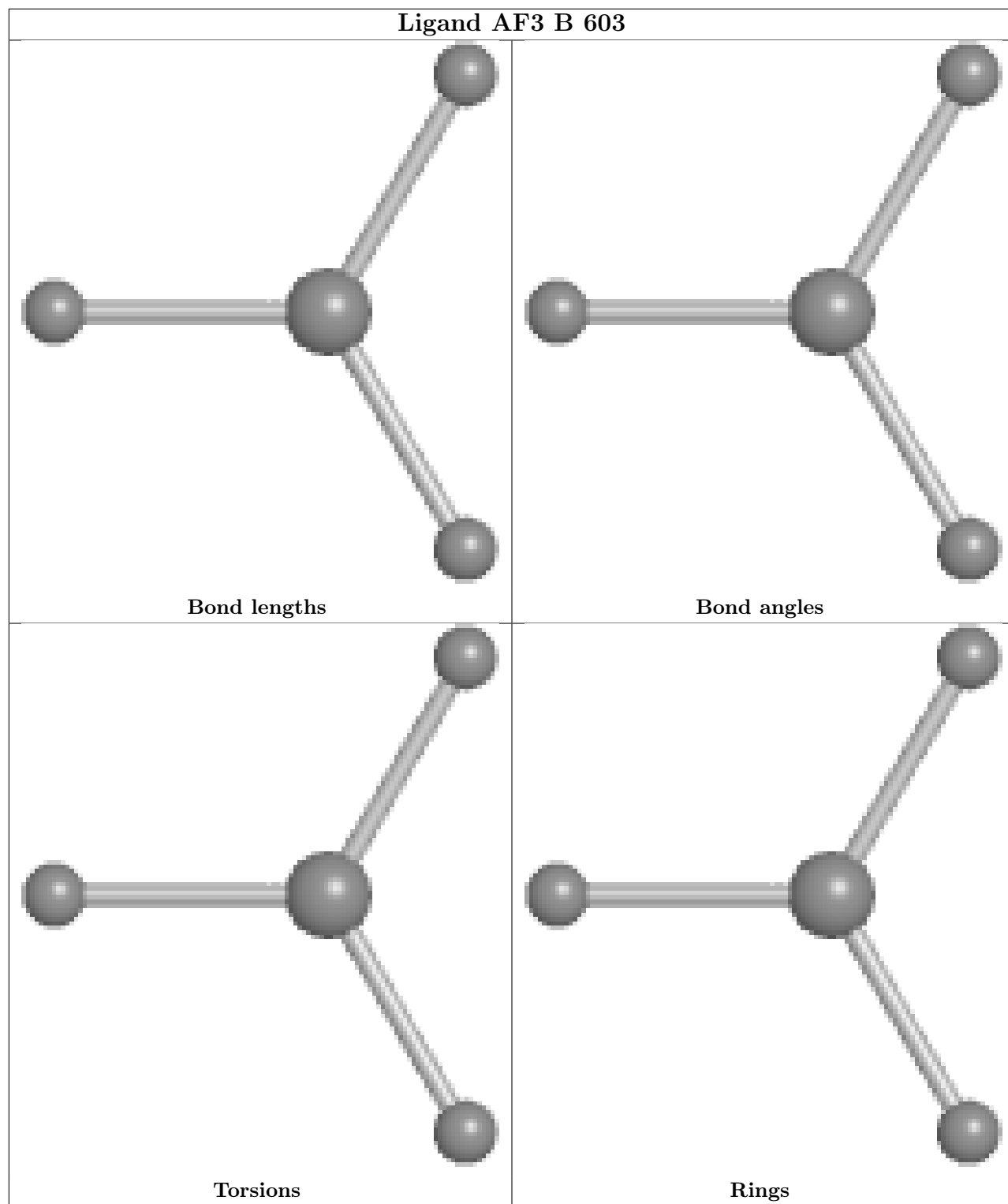


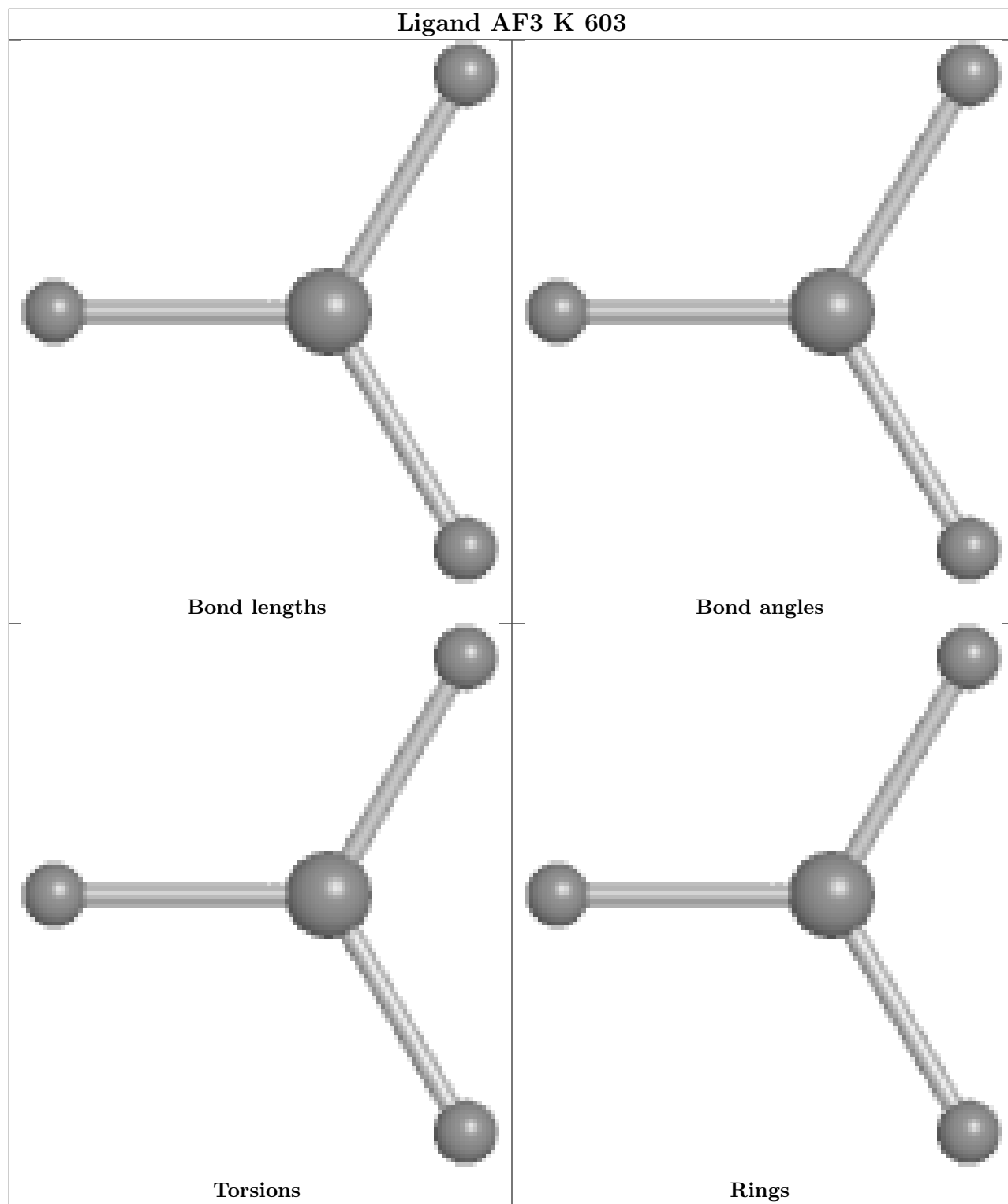


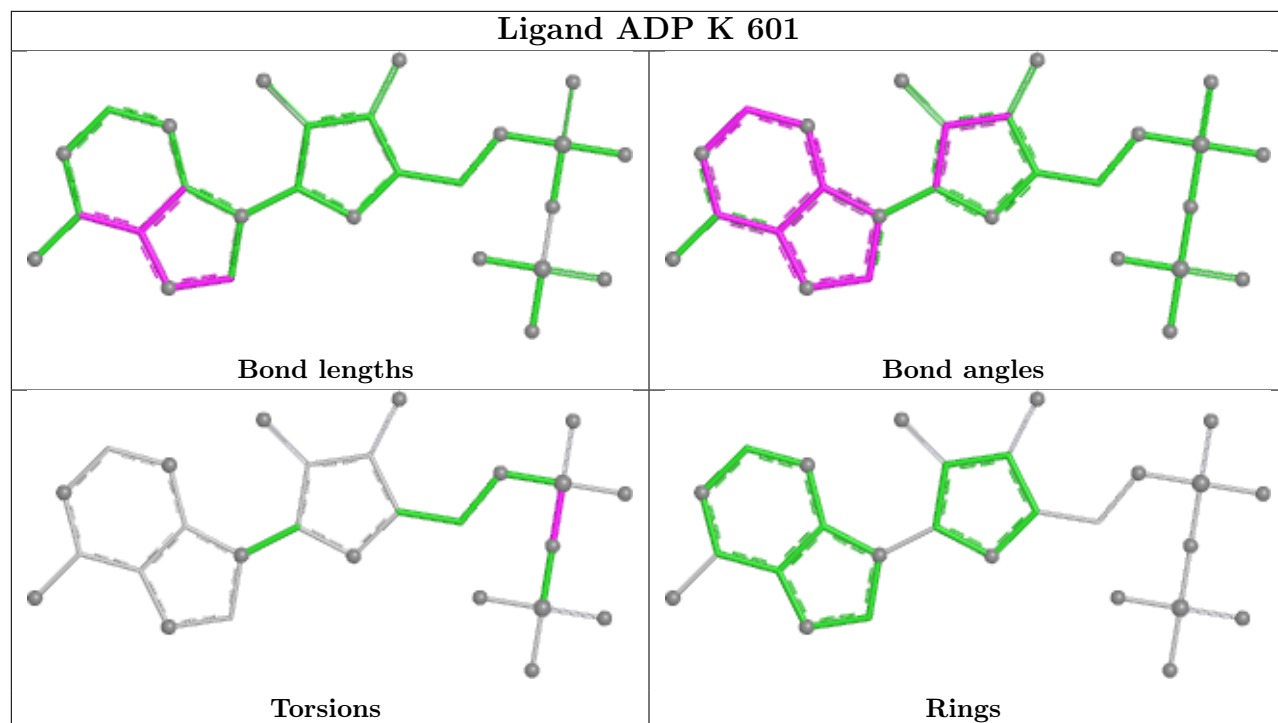


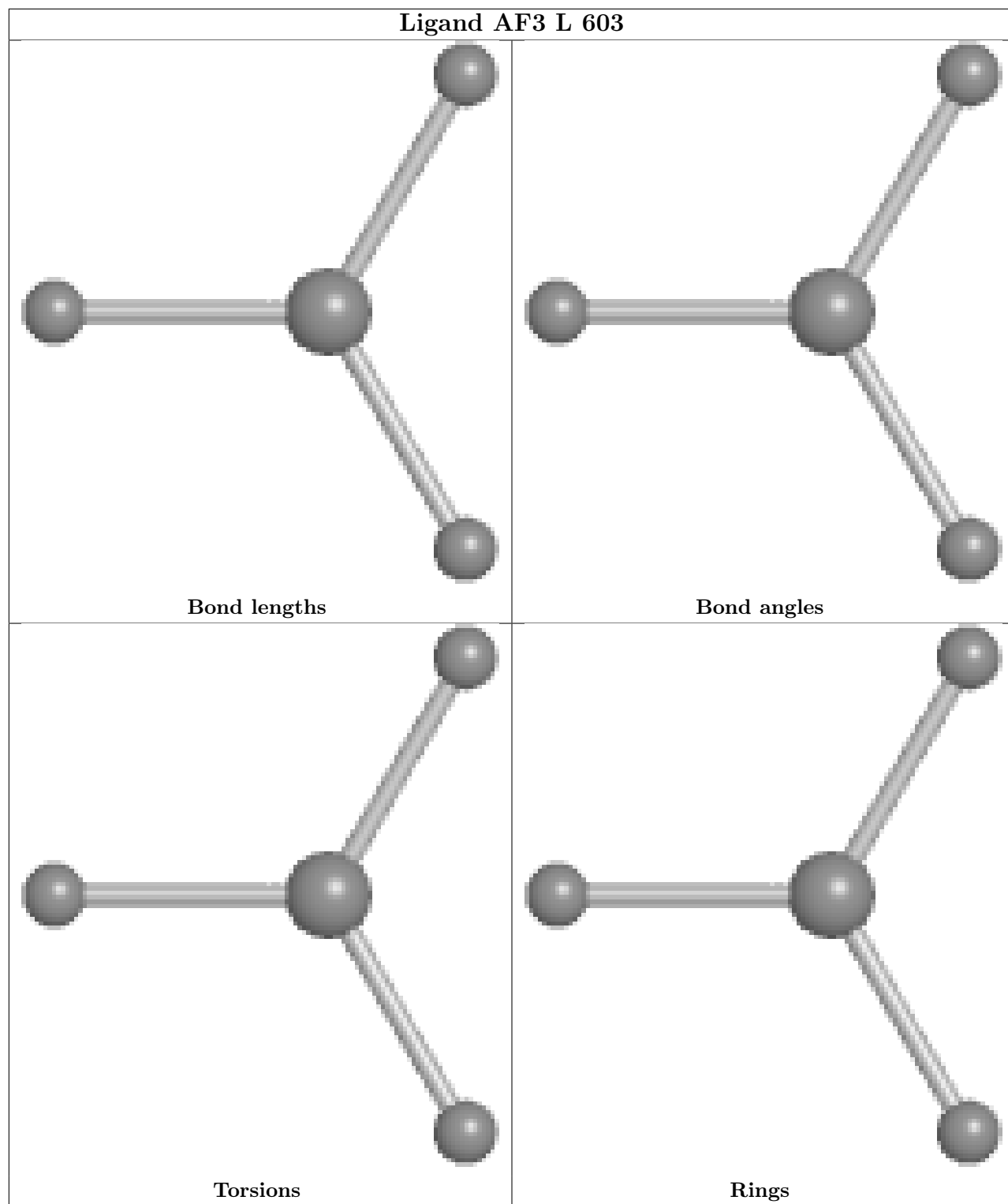


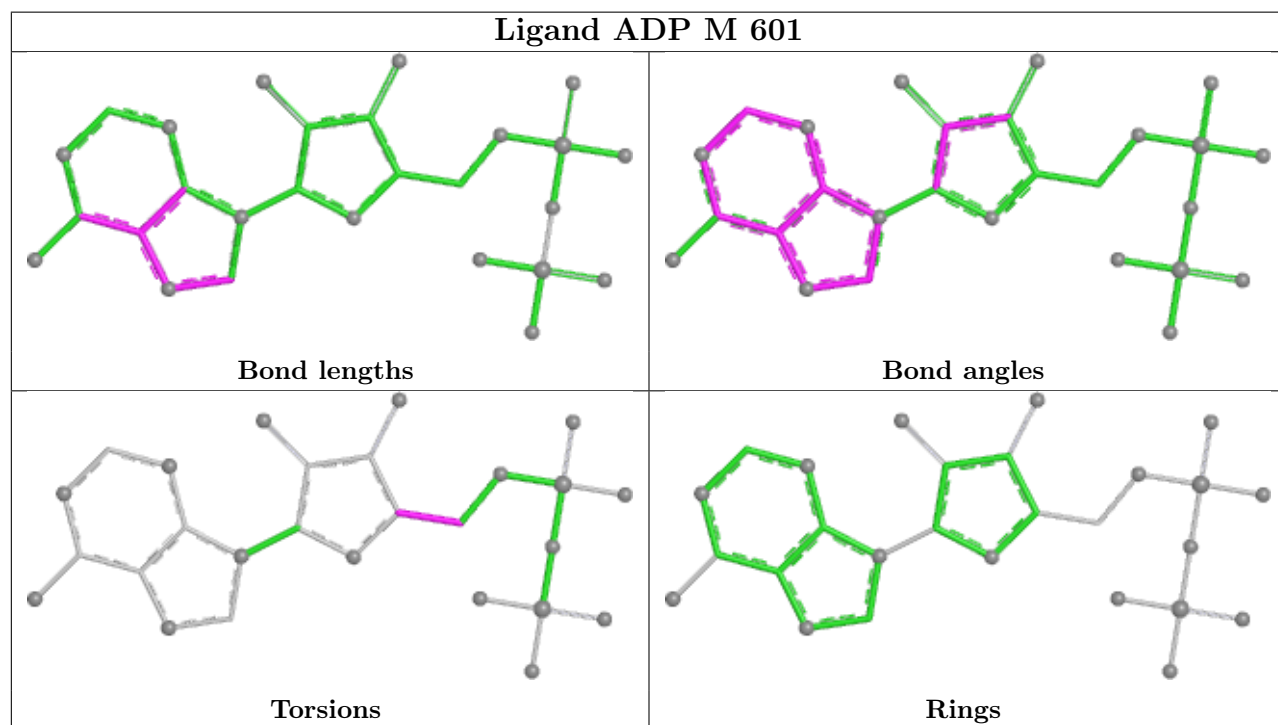
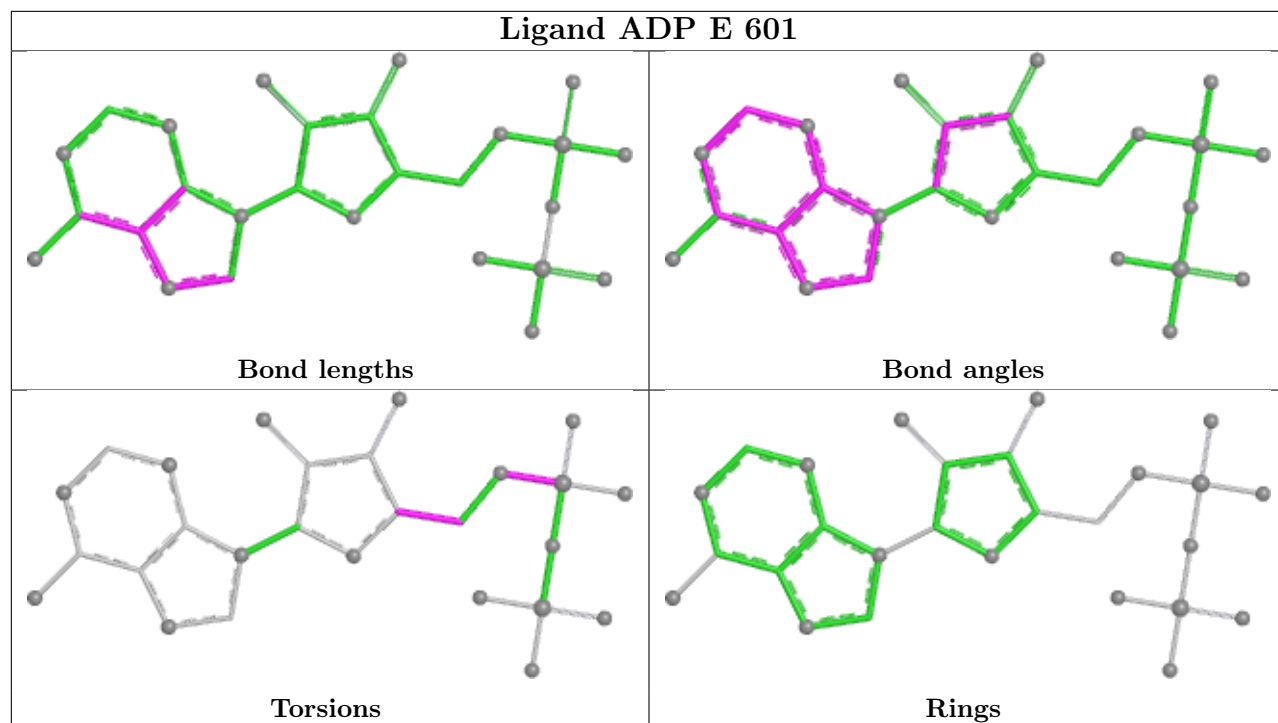


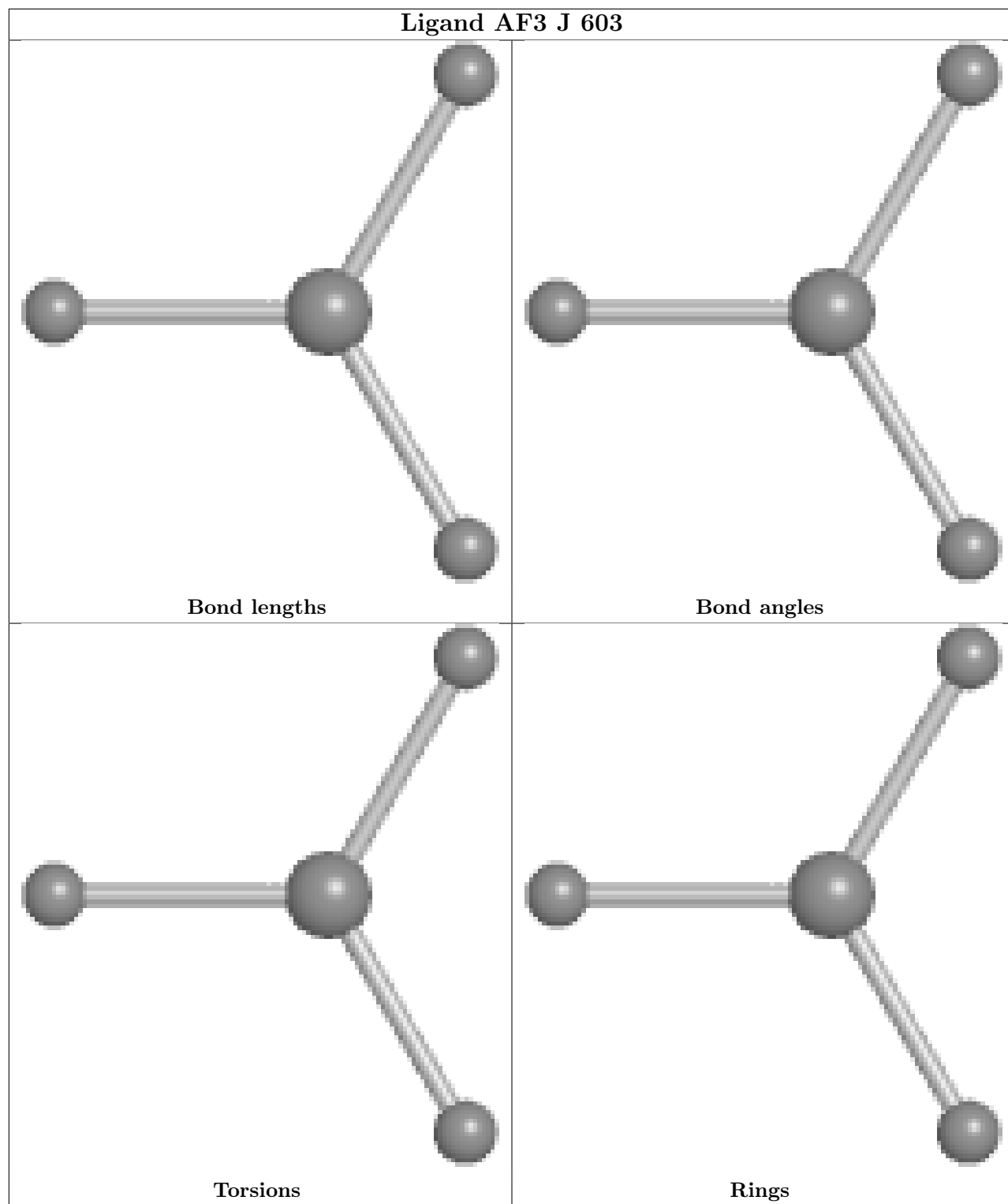


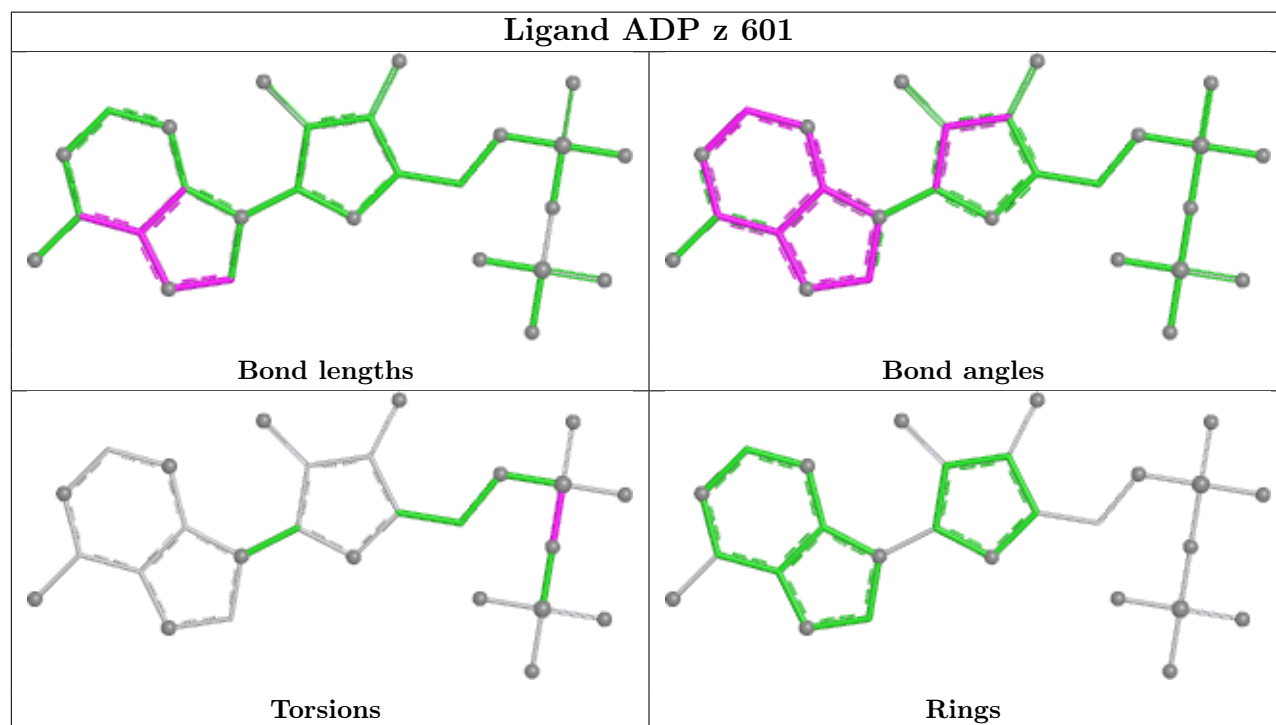
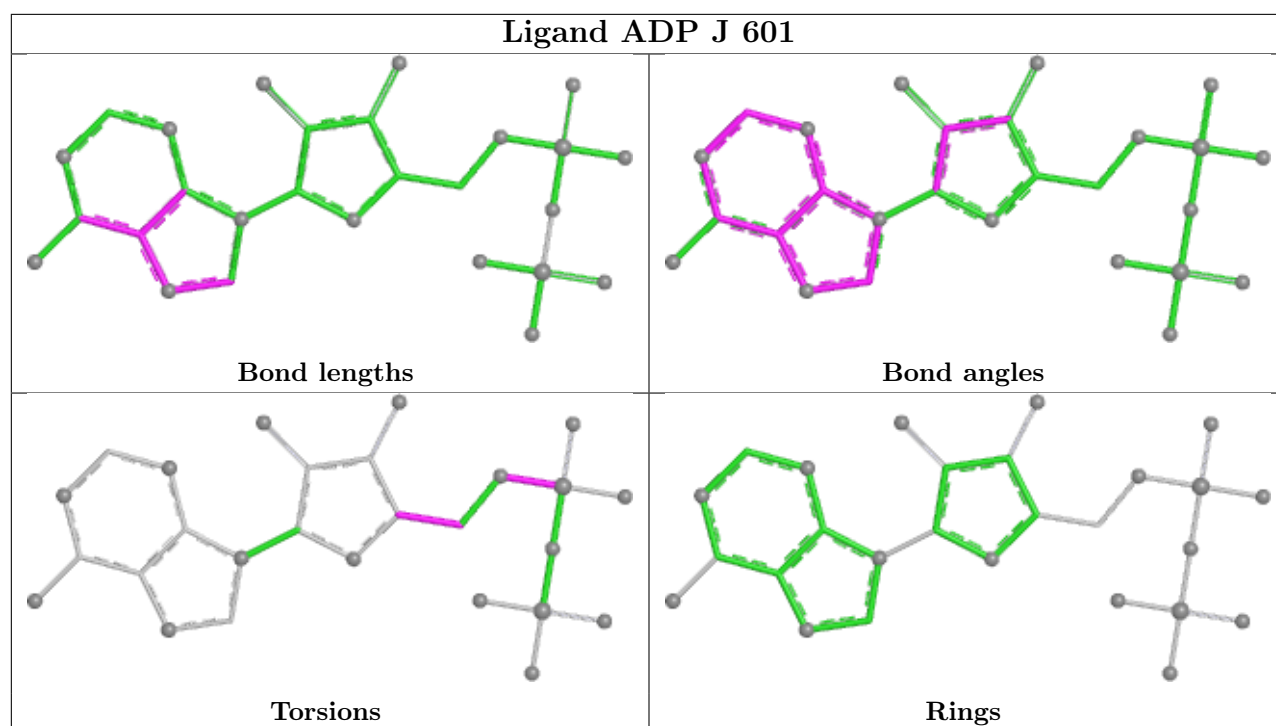


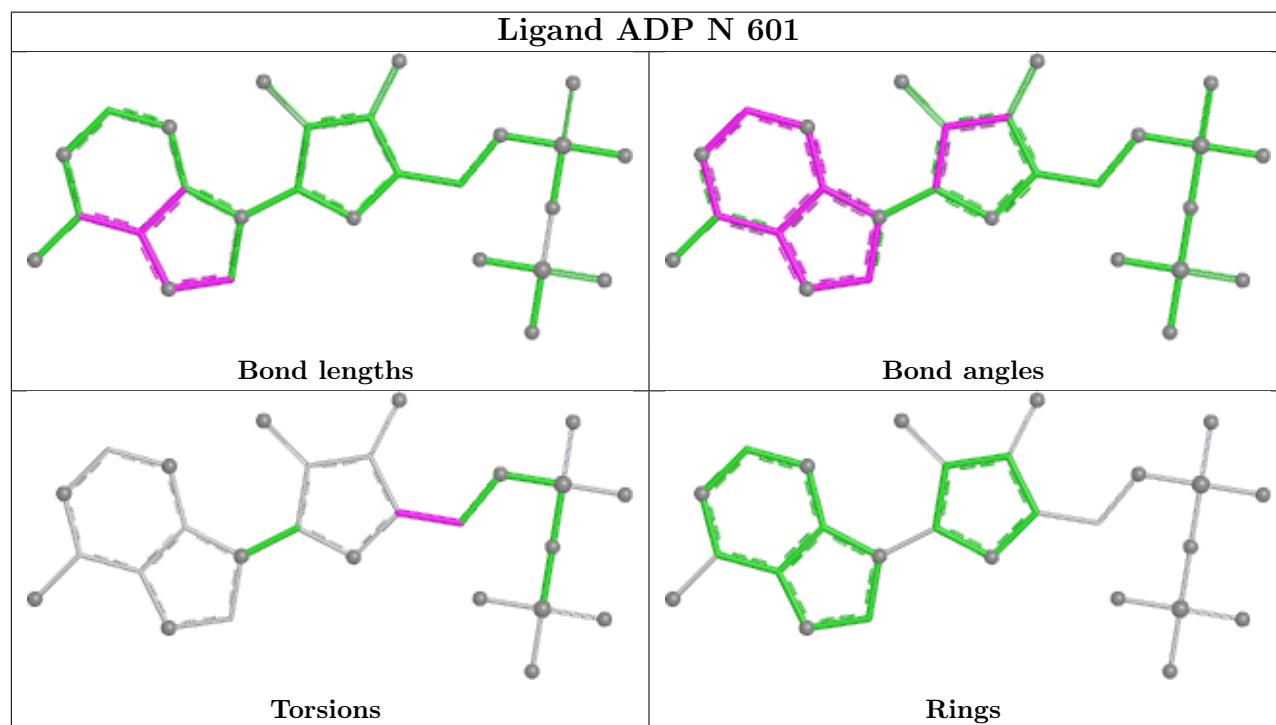
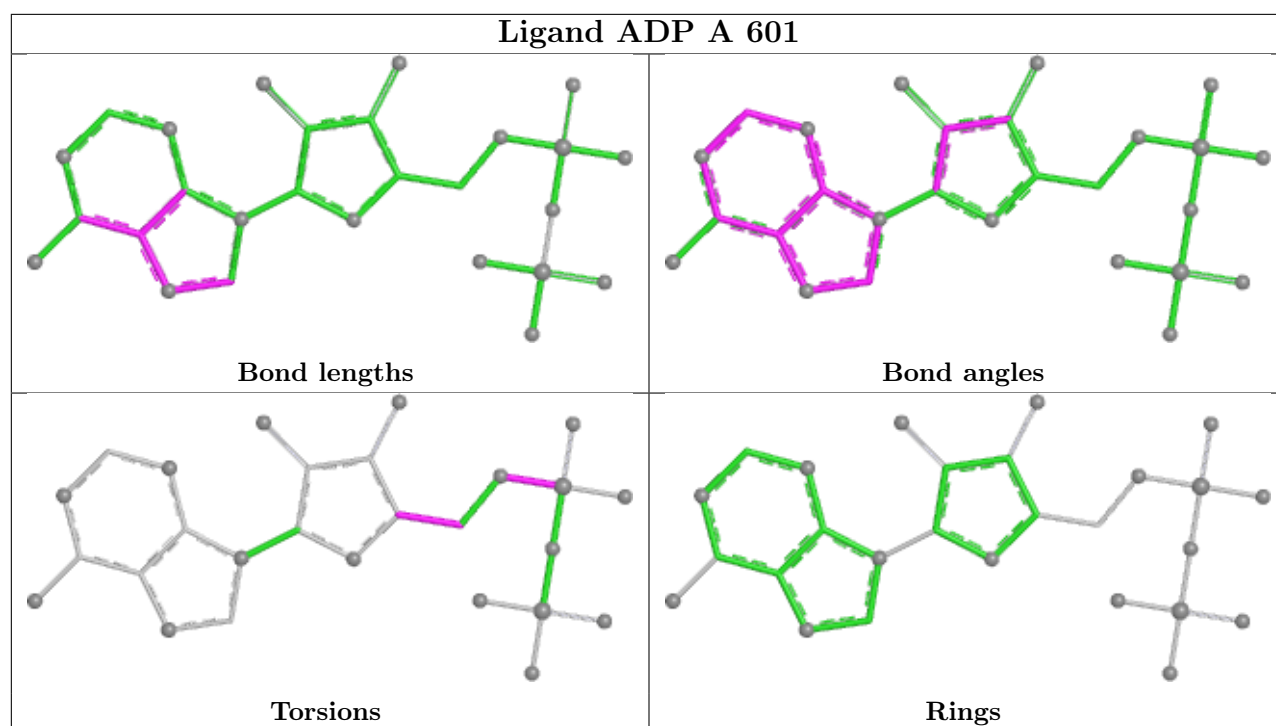


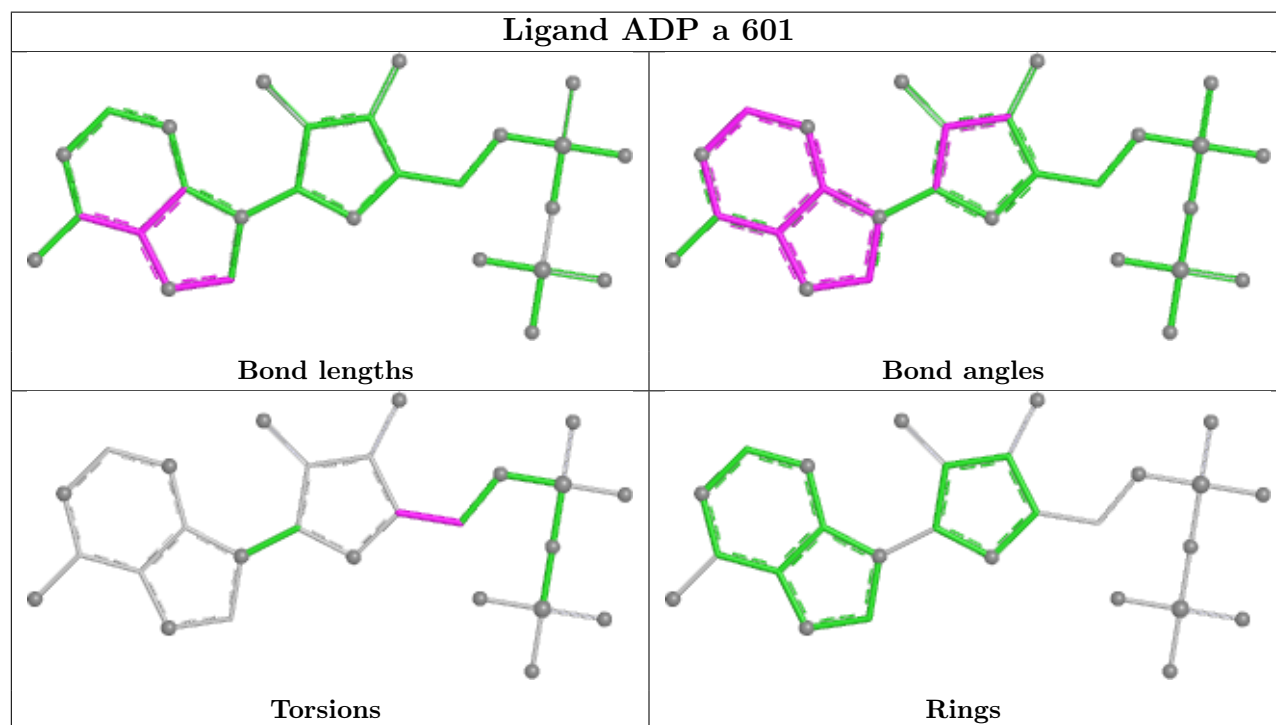
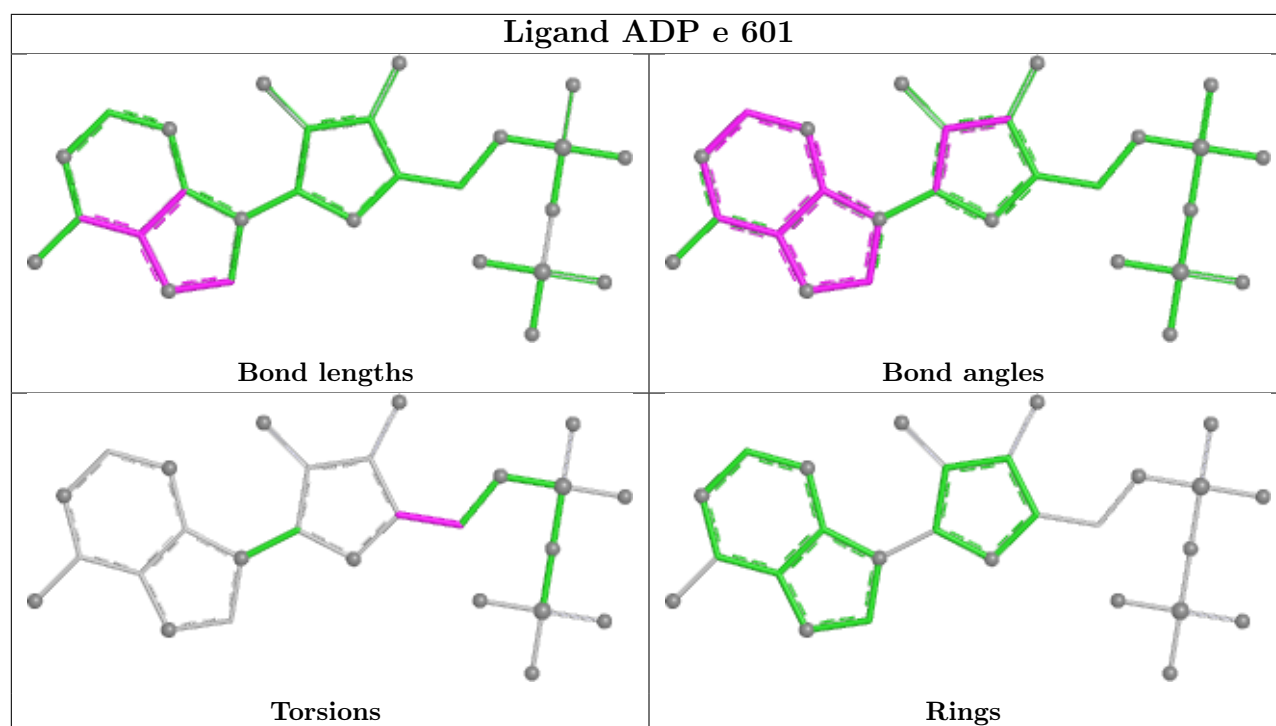


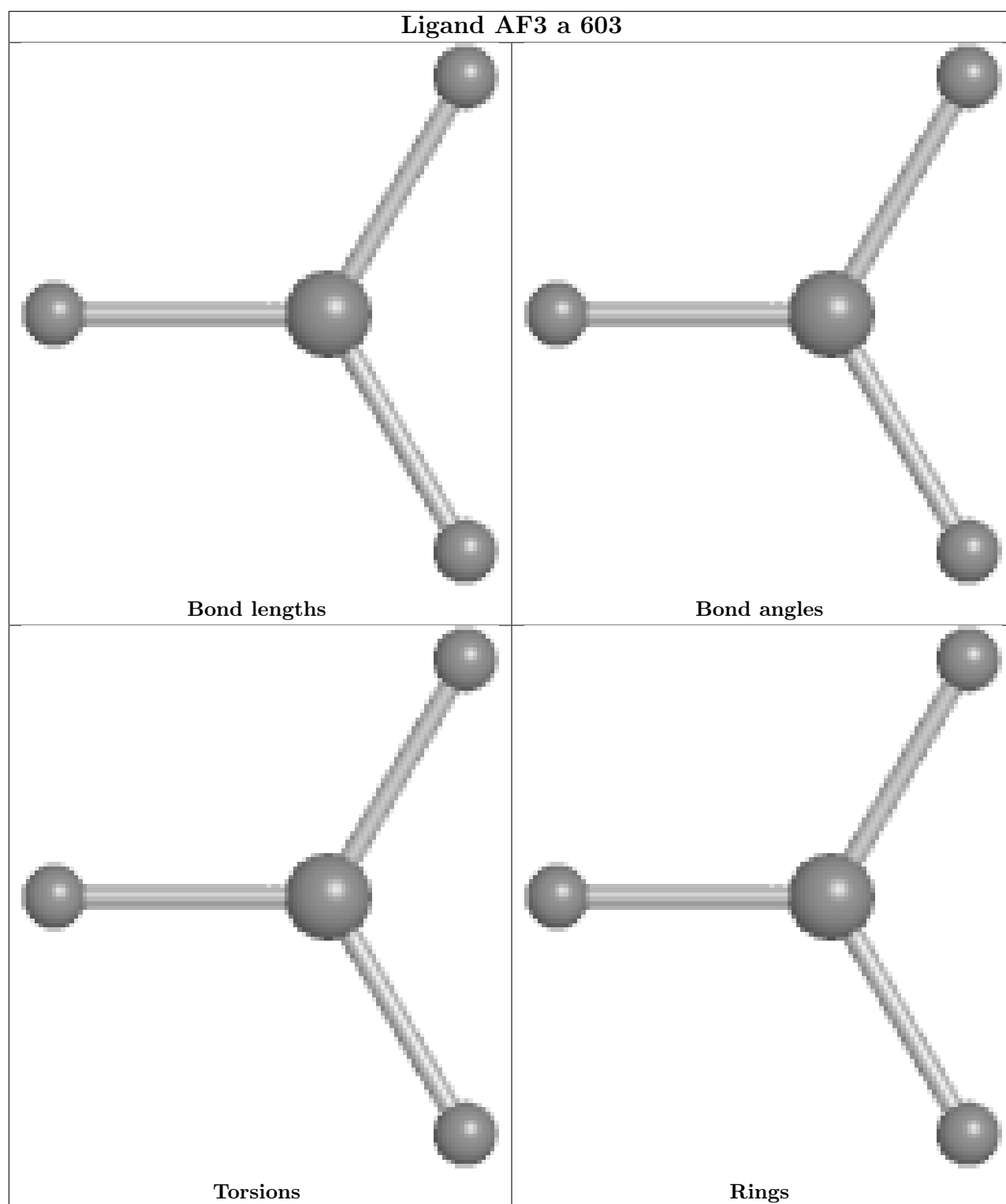


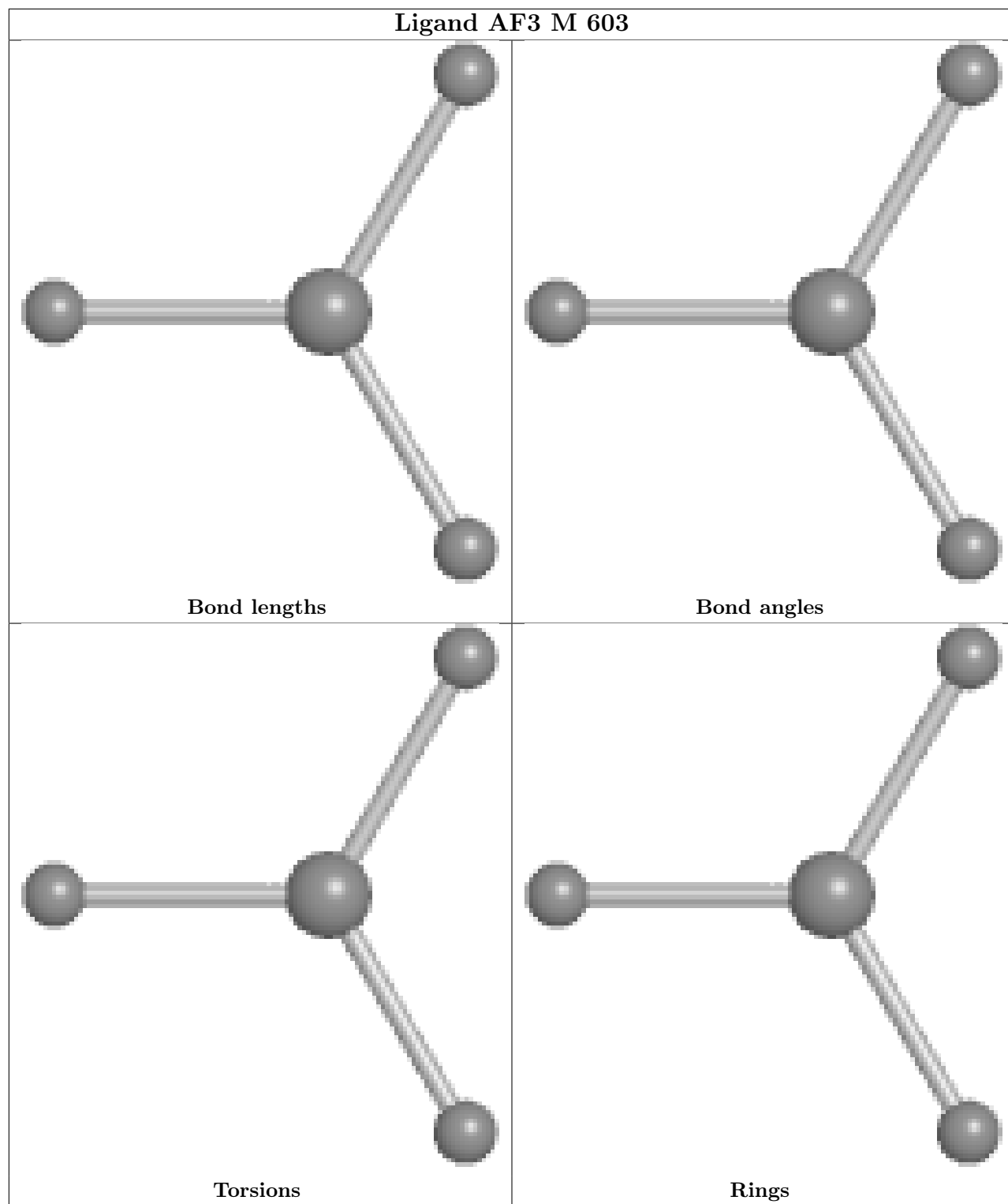


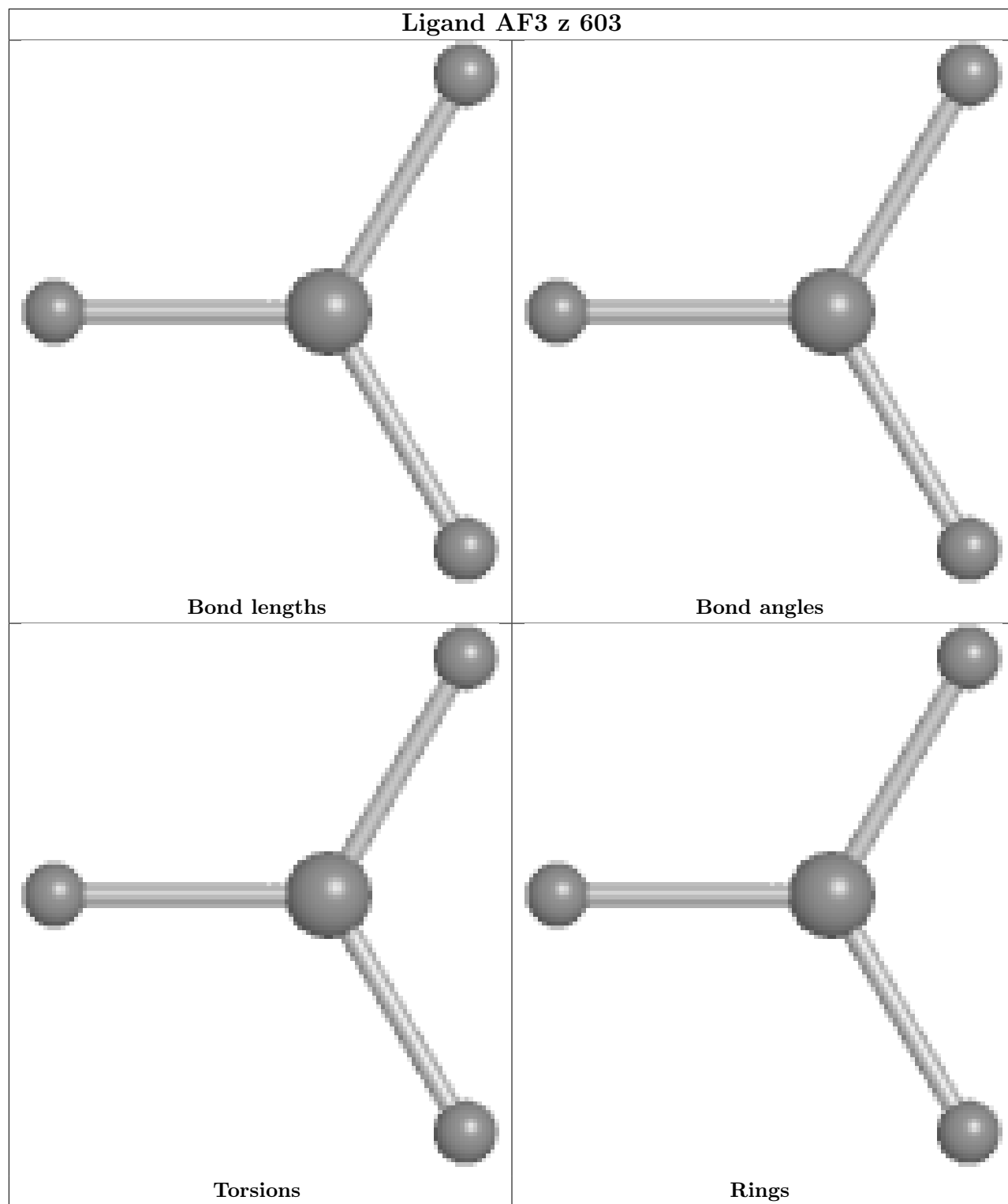


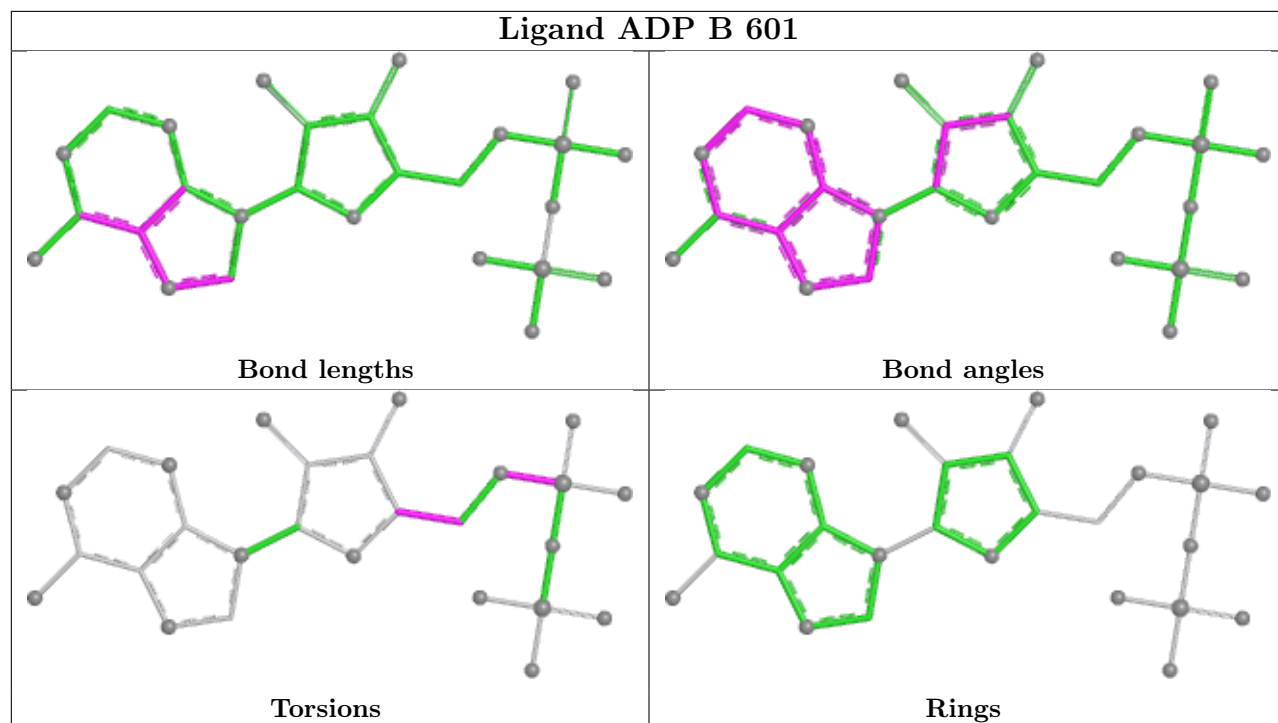


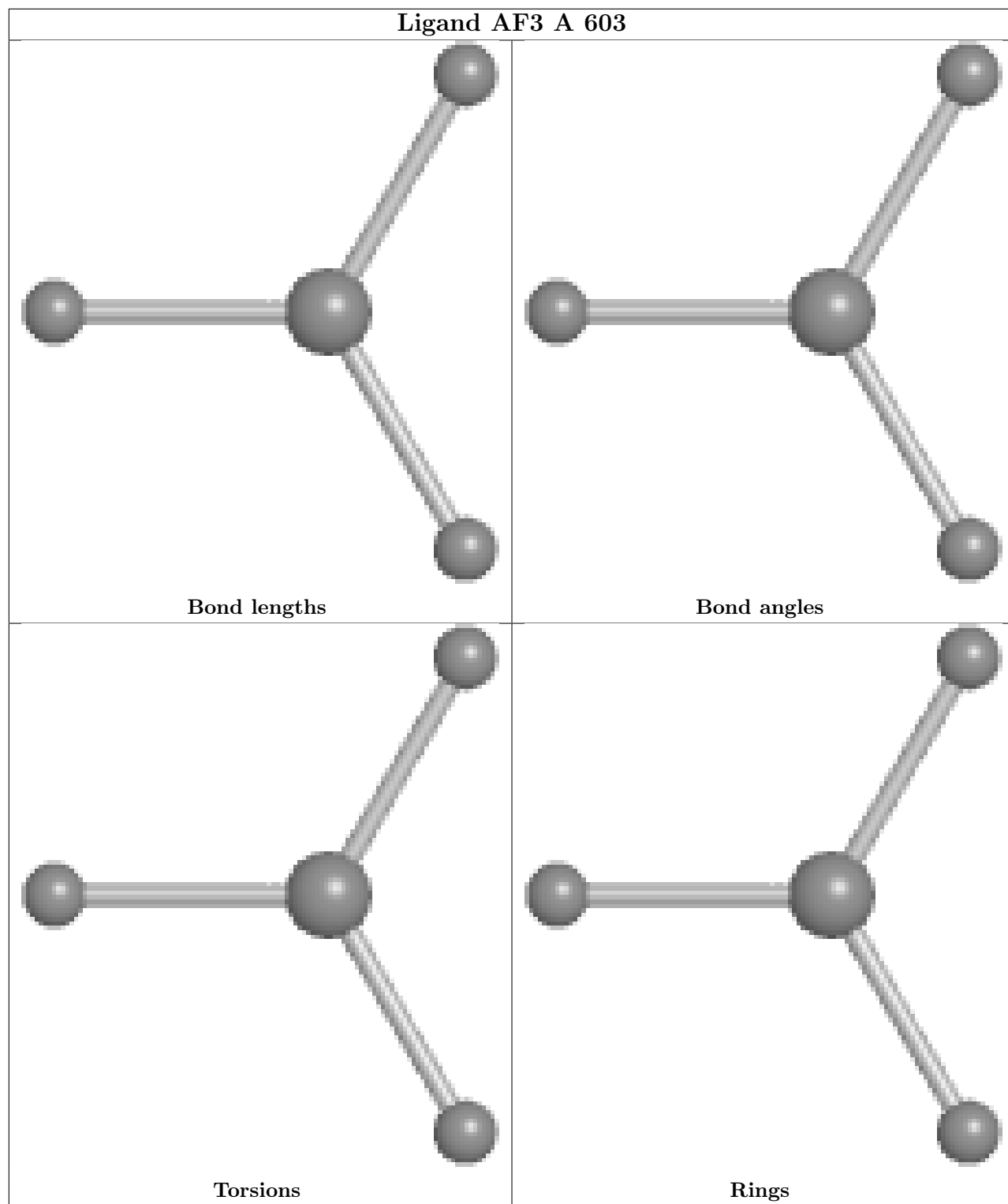


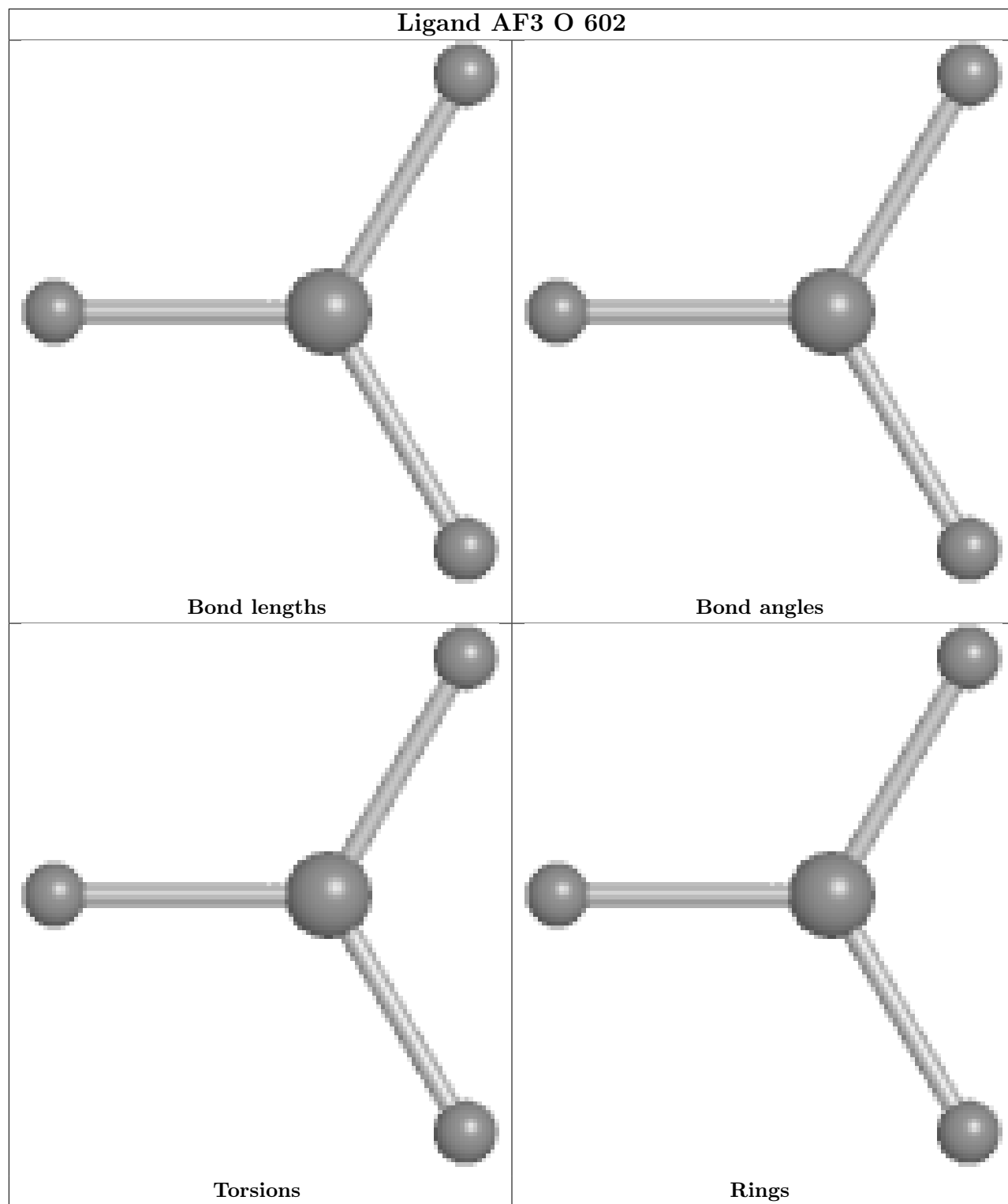


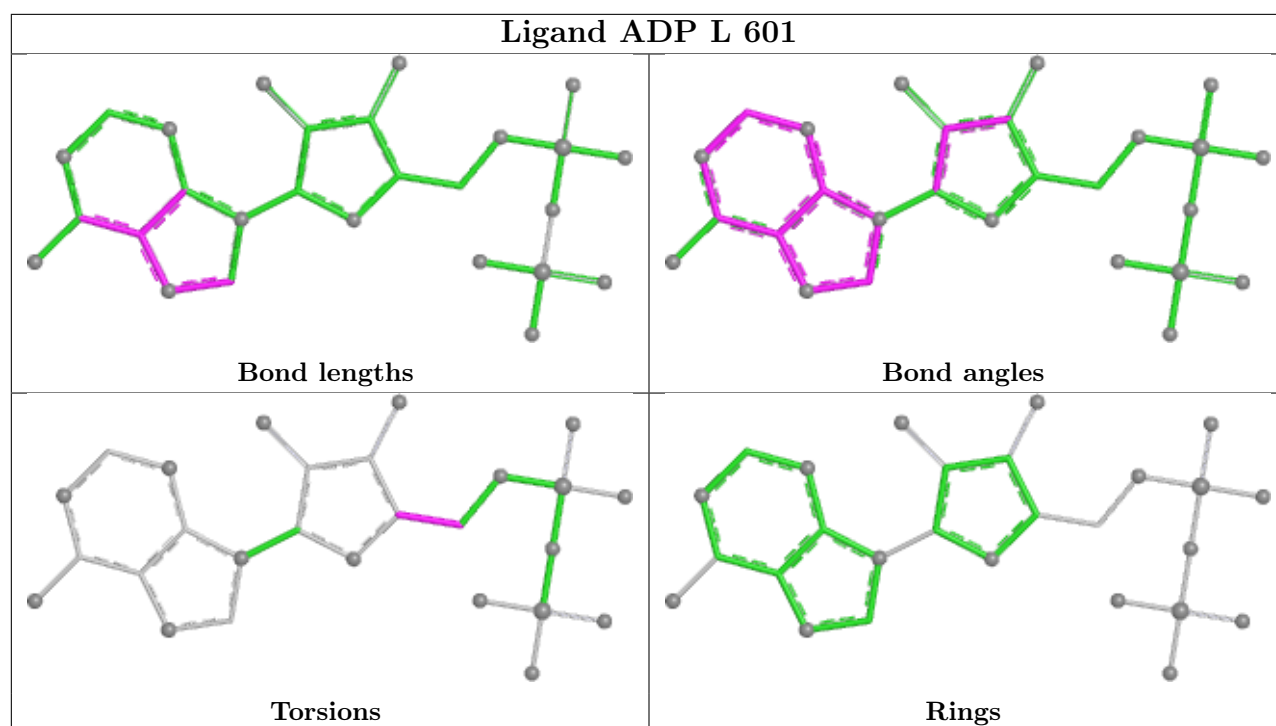












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

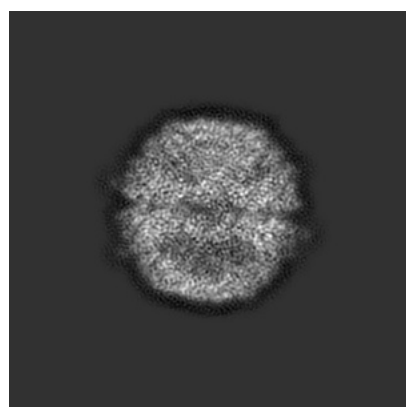
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32923. These allow visual inspection of the internal detail of the map and identification of artifacts.

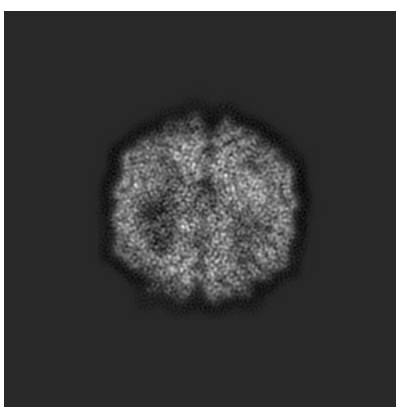
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

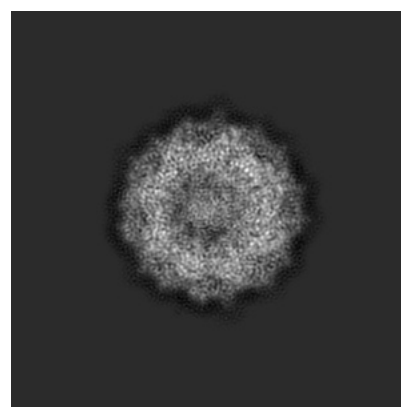
6.1.1 Primary map



X



Y

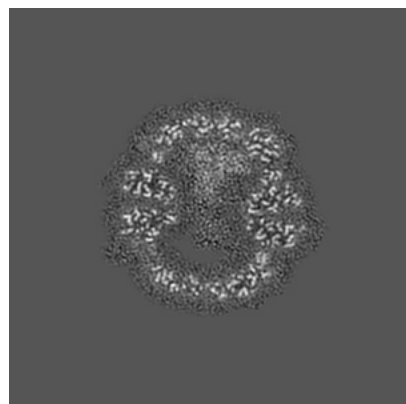


Z

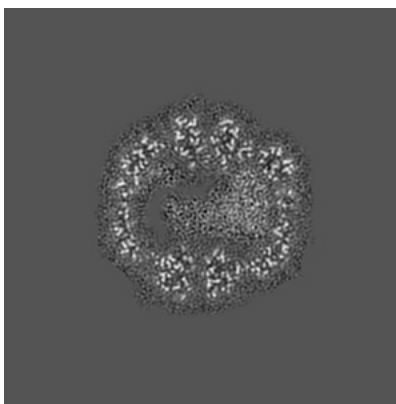
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

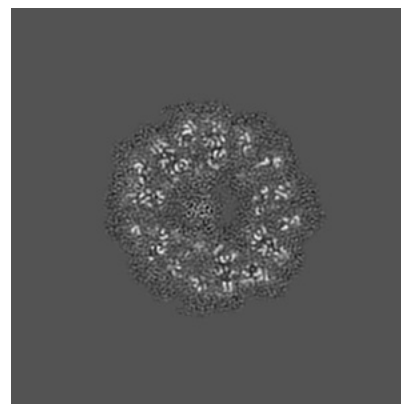
6.2.1 Primary map



X Index: 128



Y Index: 128

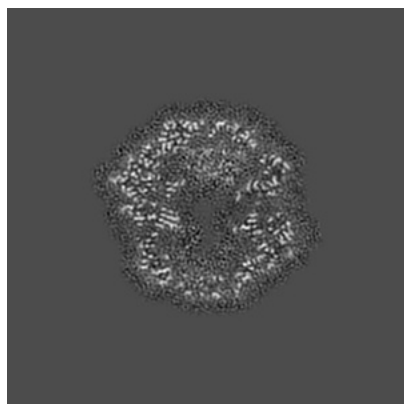


Z Index: 128

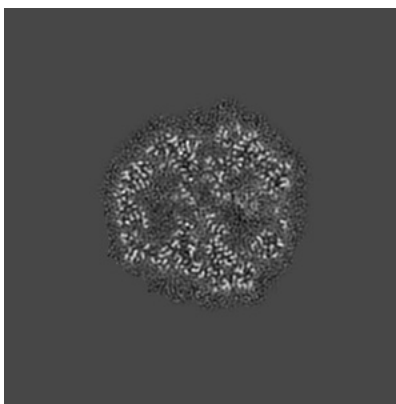
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

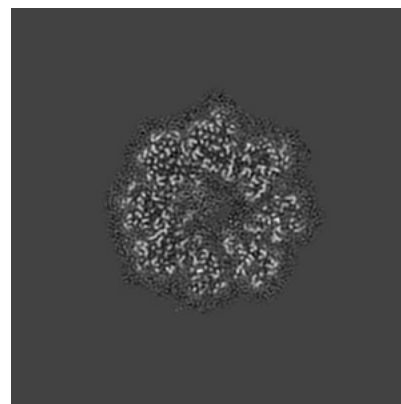
6.3.1 Primary map



X Index: 140



Y Index: 149

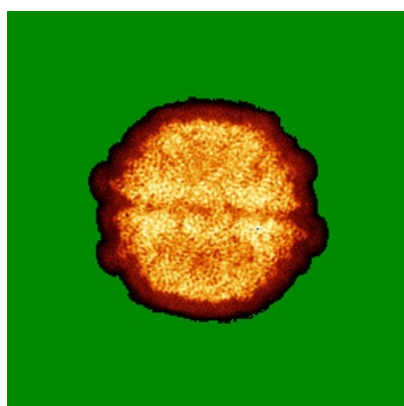


Z Index: 115

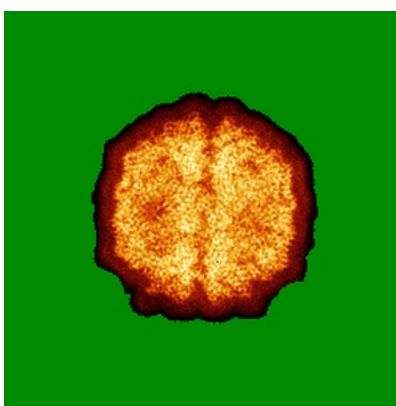
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

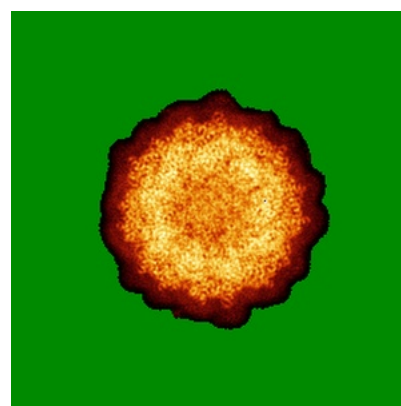
6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

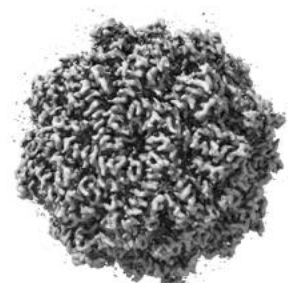
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.761. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

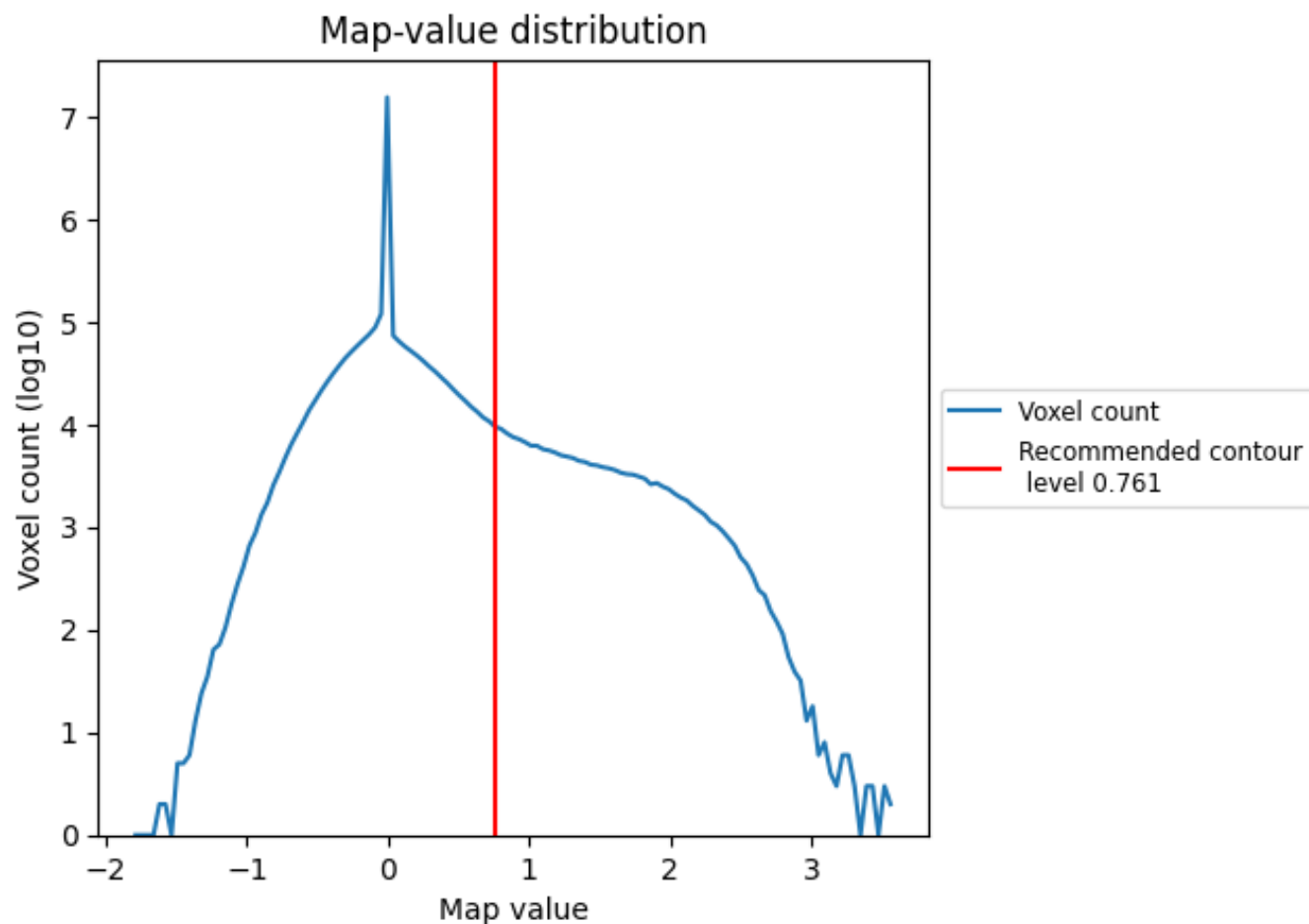
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

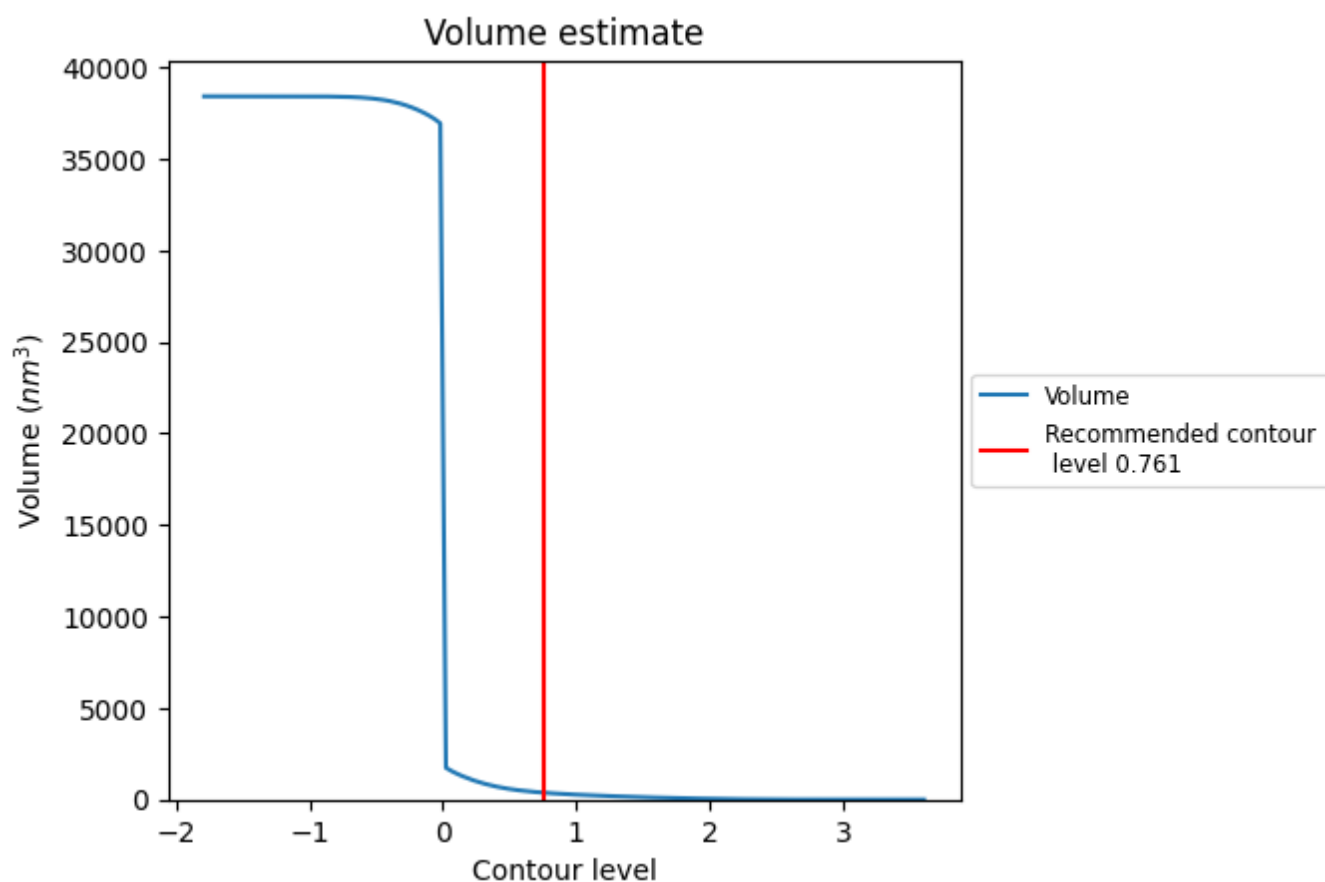
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

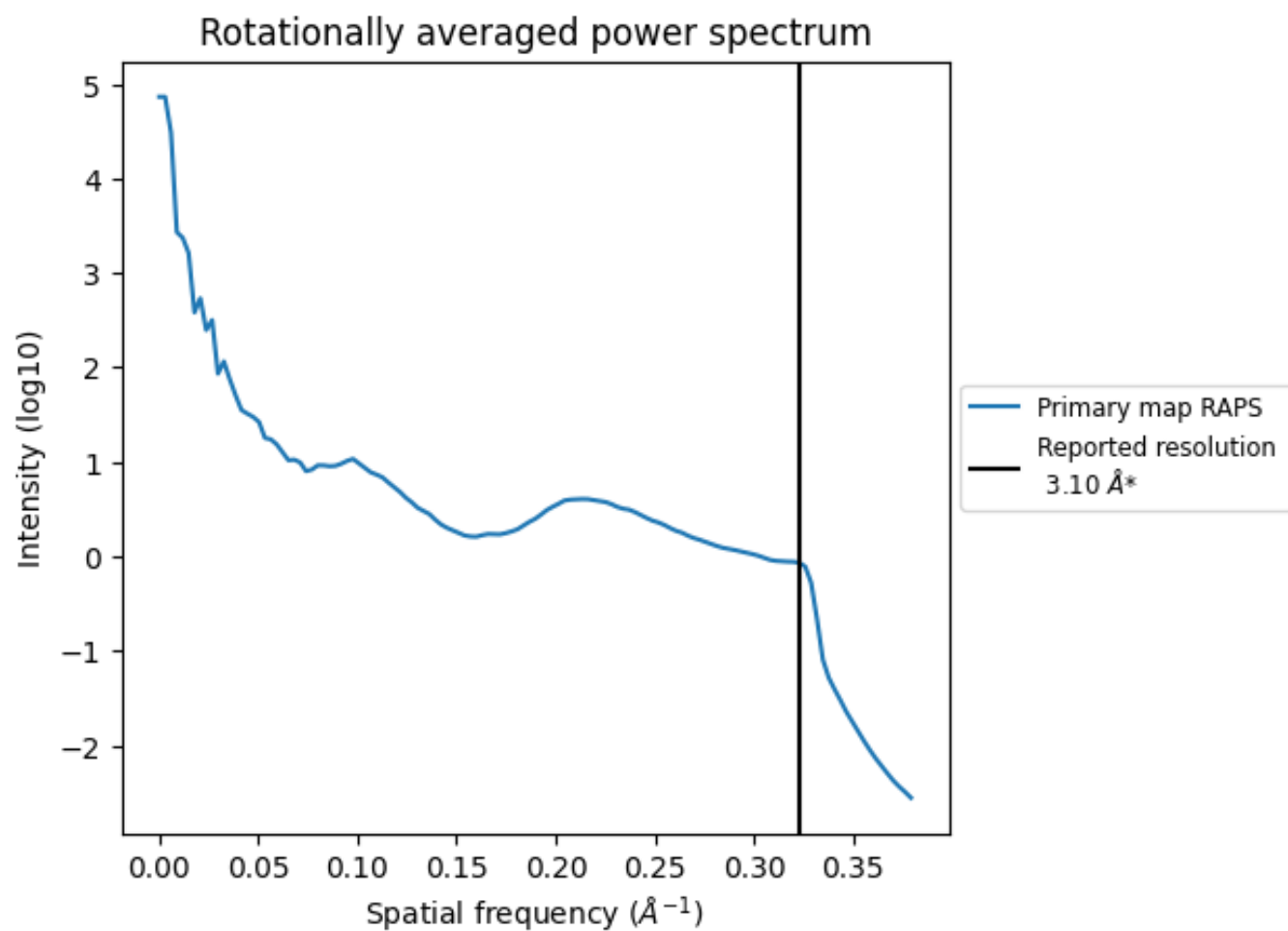
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 372 nm³; this corresponds to an approximate mass of 336 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

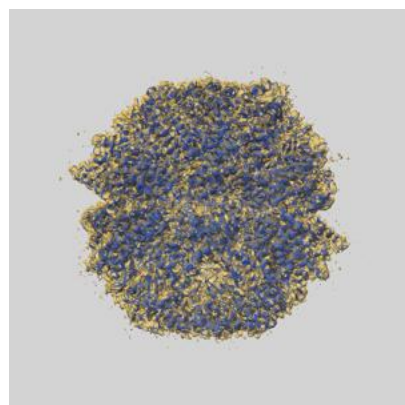
8 Fourier-Shell correlation

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

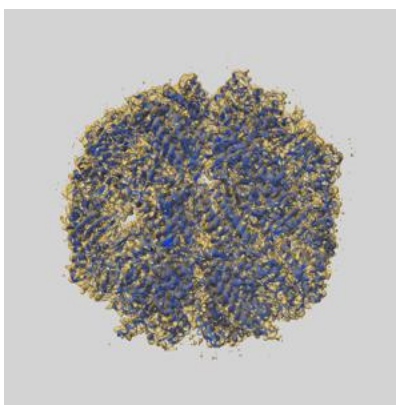
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-32923 and PDB model 7X0S. Per-residue inclusion information can be found in section [3](#) on page [12](#).

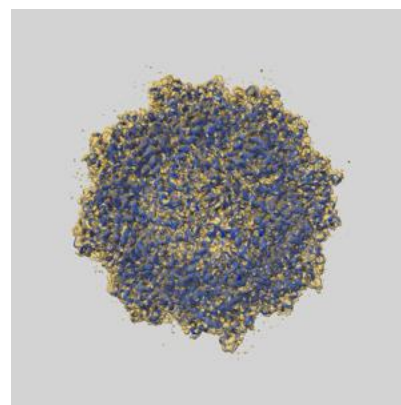
9.1 Map-model overlay [i](#)



X



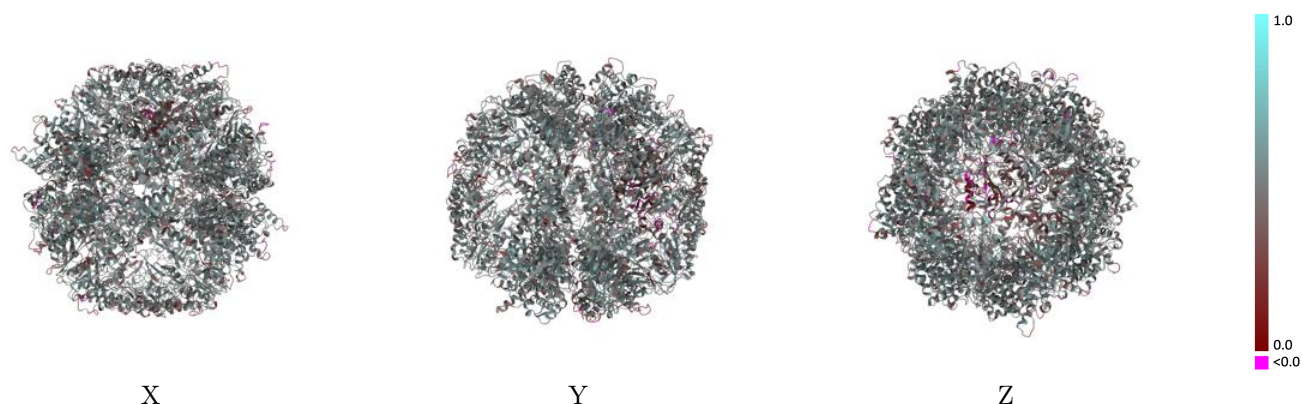
Y



Z

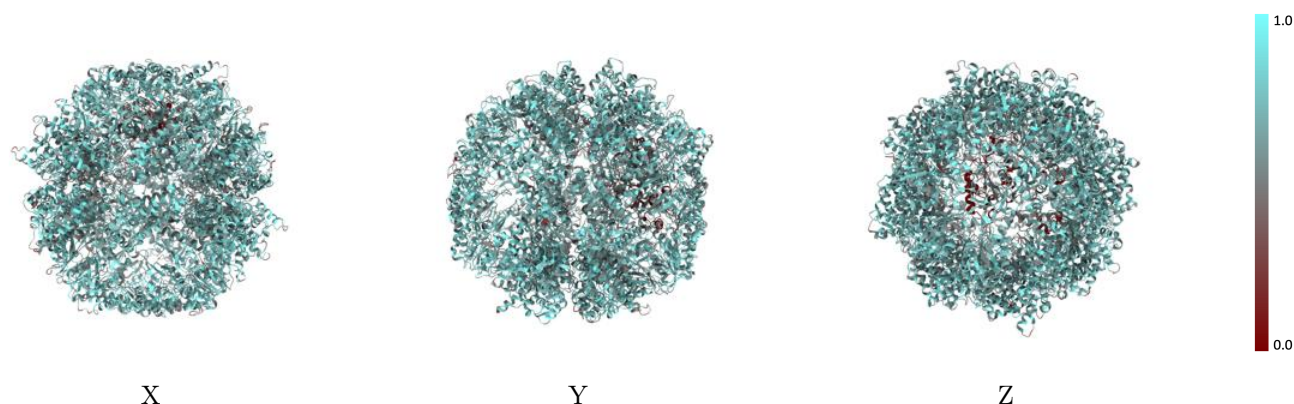
The images above show the 3D surface view of the map at the recommended contour level 0.761 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



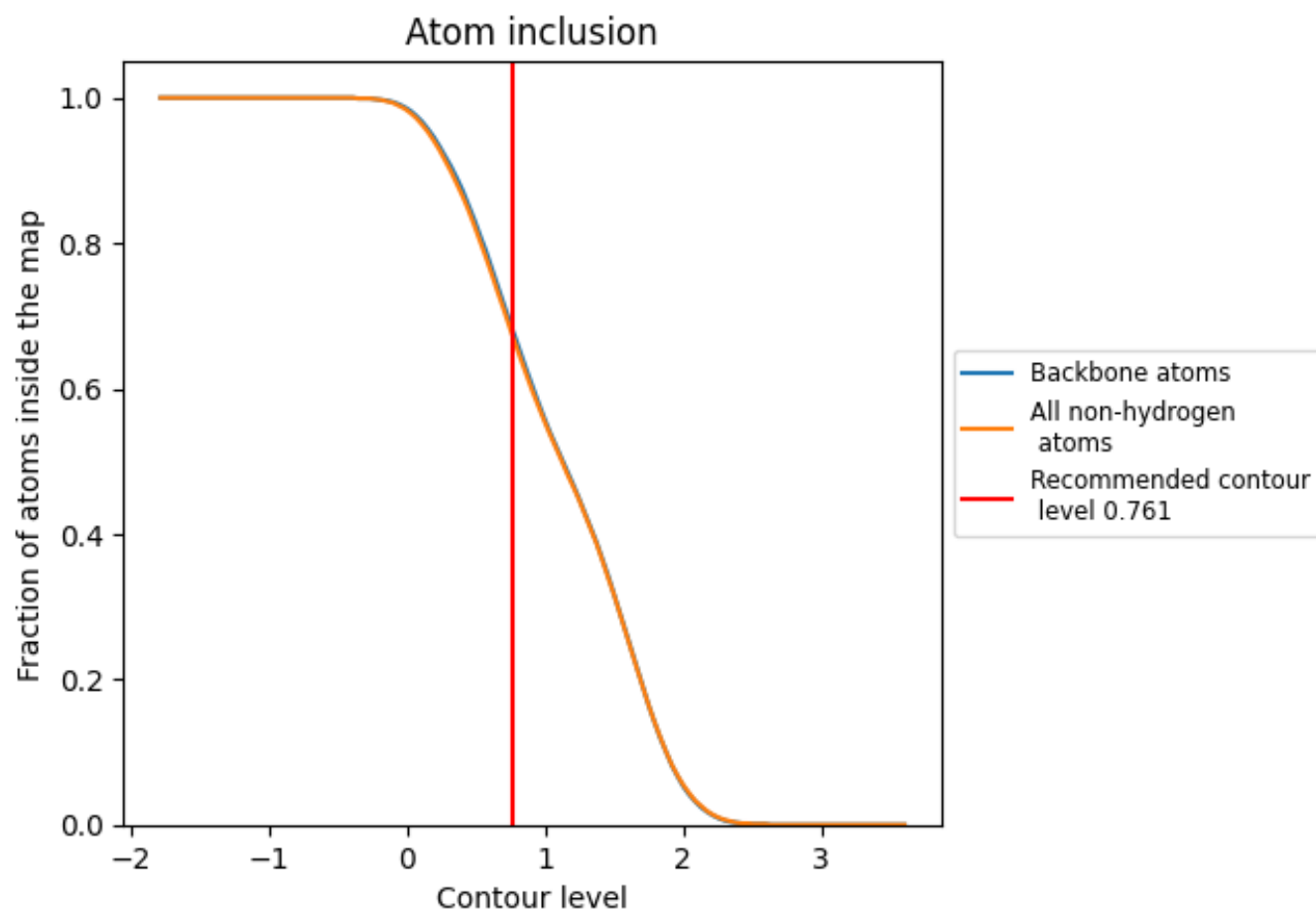
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.761).

9.4 Atom inclusion [i](#)



At the recommended contour level, 68% of all backbone atoms, 67% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.761) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6730	0.4690
A	0.6840	0.4790
B	0.6930	0.4840
E	0.6840	0.4700
G	0.7050	0.4930
H	0.6860	0.4710
I	0.6980	0.4900
J	0.6980	0.4720
K	0.7070	0.4820
L	0.6990	0.4790
M	0.6970	0.4820
N	0.7050	0.4860
O	0.6830	0.4660
P	0.7010	0.4710
R	0.4080	0.3000
a	0.6890	0.4720
e	0.6830	0.4690
z	0.7090	0.4750

1.0

0.0

<0.0