



## Full wwPDB EM Validation Report ⓘ

Dec 22, 2022 – 04:28 AM EST

PDB ID : 7TTN  
EMDB ID : EMD-26120  
Title : The beta-tubulin folding intermediate II  
Authors : Zhao, Y.; Frydman, J.; Chiu, W.  
Deposited on : 2022-02-01  
Resolution : 3.30 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

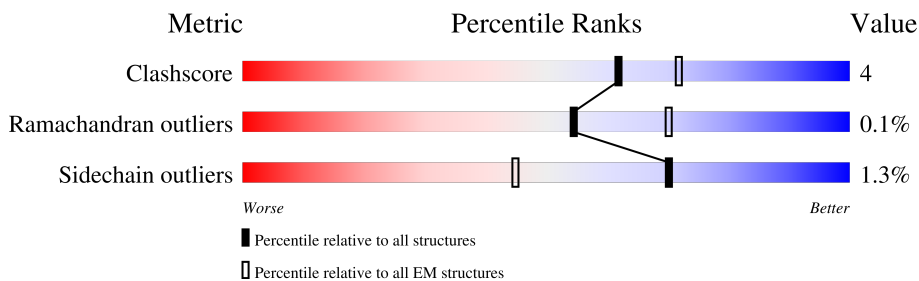
EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	A	444	
2	B	547	
3	C	553	
4	D	541	
5	E	535	
6	F	539	
7	G	556	
8	H	545	

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Mol	Chain	Length	Quality of chain
9	I	531	 A horizontal bar chart representing the quality of chain. The bar is primarily green, indicating a 90% quality score. A small yellow segment at the end indicates a 9% quality score. The bar is flanked by small red and grey segments.

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	AF3	I	603	-	-	X	-

## 2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 34563 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 Tubulin beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	269	2119	1328	352	426	13	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	529	4029	2543	685	774	27	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	521	4003	2530	692	758	23	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	472	GLY	-	insertion	UNP Q99832
C	473	SER	-	insertion	UNP Q99832
C	474	HIS	-	insertion	UNP Q99832
C	475	HIS	-	insertion	UNP Q99832
C	476	HIS	-	insertion	UNP Q99832
C	477	HIS	-	insertion	UNP Q99832
C	478	HIS	-	insertion	UNP Q99832
C	479	HIS	-	insertion	UNP Q99832
C	480	GLY	-	insertion	UNP Q99832
C	481	SER	-	insertion	UNP Q99832

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	528	4072	2549	711	782	30	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	528	3974	2487	701	767	19	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	520	3924	2453	683	765	23	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	535	4063	2545	710	785	23	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	523	4064	2534	718	782	30	0	0

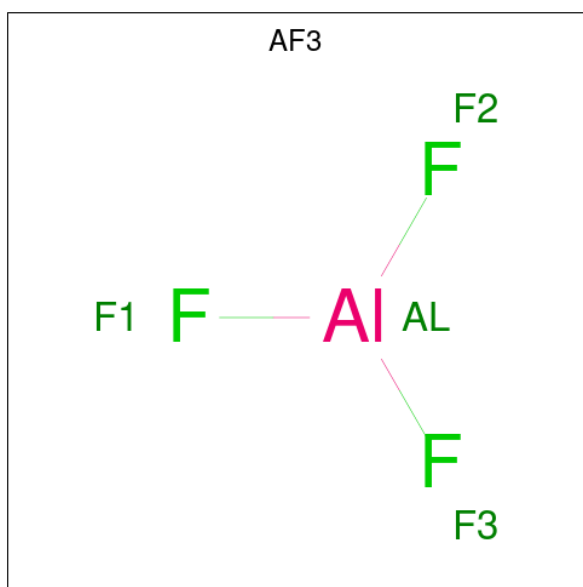
- Molecule 9 is a protein called T-complex protein 1 subunit zeta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	528	4051	2549	708	773	21	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	528	PHE	SER	conflict	UNP P40227

- Molecule 10 is ALUMINUM FLUORIDE (three-letter code: AF3) (formula:  $AlF_3$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	Al	F	
10	B	1	4	1	3	0
10	C	1	4	1	3	0
10	D	1	4	1	3	0
10	E	1	4	1	3	0
10	F	1	4	1	3	0
10	G	1	4	1	3	0
10	H	1	4	1	3	0
10	I	1	4	1	3	0

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

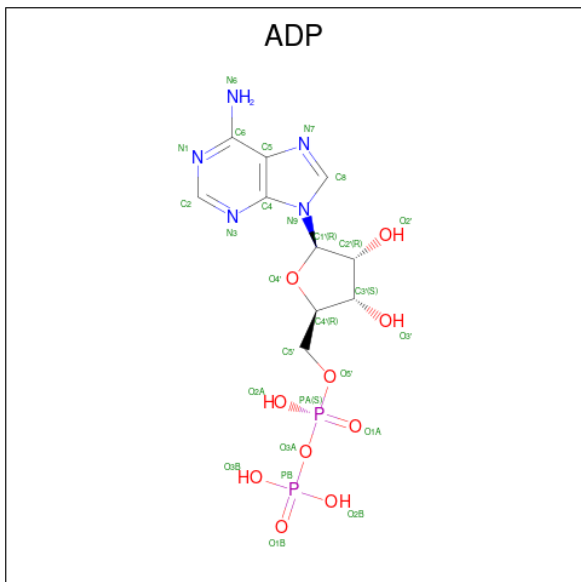
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
11	B	1	1	1	0
11	C	1	1	1	0
11	D	1	1	1	0

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Mol	Chain	Residues	Atoms		AltConf
11	E	1	Total	Mg	0
			1	1	
11	F	1	Total	Mg	0
			1	1	
11	G	1	Total	Mg	0
			1	1	
11	H	1	Total	Mg	0
			1	1	
11	I	1	Total	Mg	0
			1	1	

- Molecule 12 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
12	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
12	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
12	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
12	E	1	Total	C	N	O	P	0
			27	10	5	10	2	
12	F	1	Total	C	N	O	P	0
			27	10	5	10	2	
12	G	1	Total	C	N	O	P	0
			27	10	5	10	2	

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
12	H	1	27	10	5	10	2	0
12	I	1	27	10	5	10	2	0

- Molecule 13 is water.

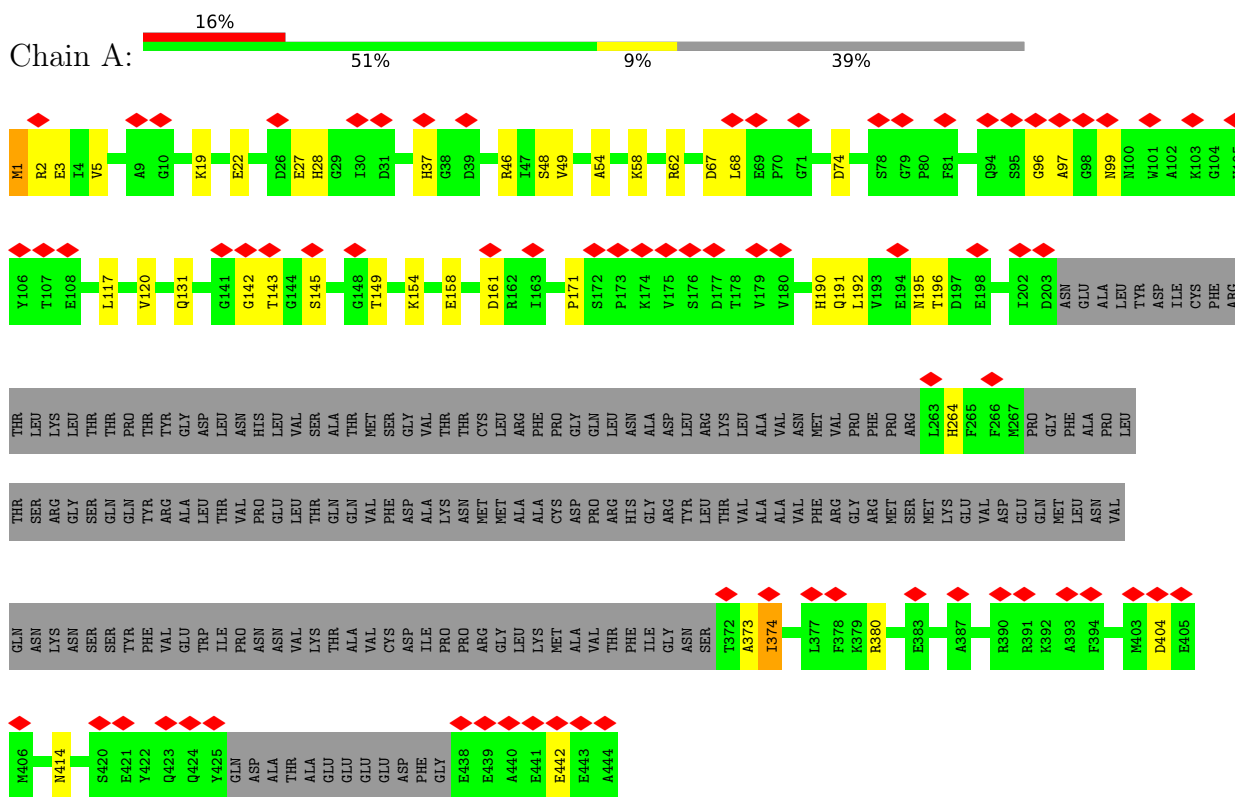
Mol	Chain	Residues	Atoms		AltConf
13	B	1	Total 1	O 1	0
13	C	1	Total 1	O 1	0
13	D	1	Total 1	O 1	0
13	E	1	Total 1	O 1	0
13	F	1	Total 1	O 1	0
13	G	1	Total 1	O 1	0
13	H	1	Total 1	O 1	0
13	I	1	Total 1	O 1	0



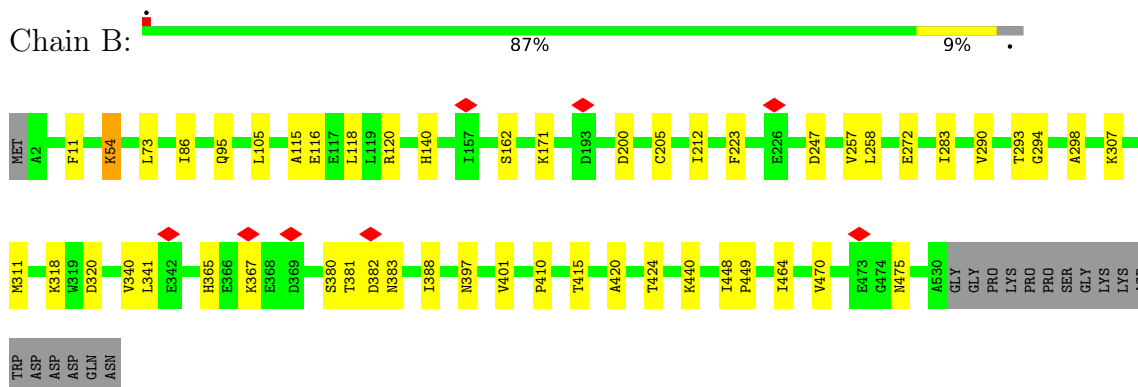
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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.

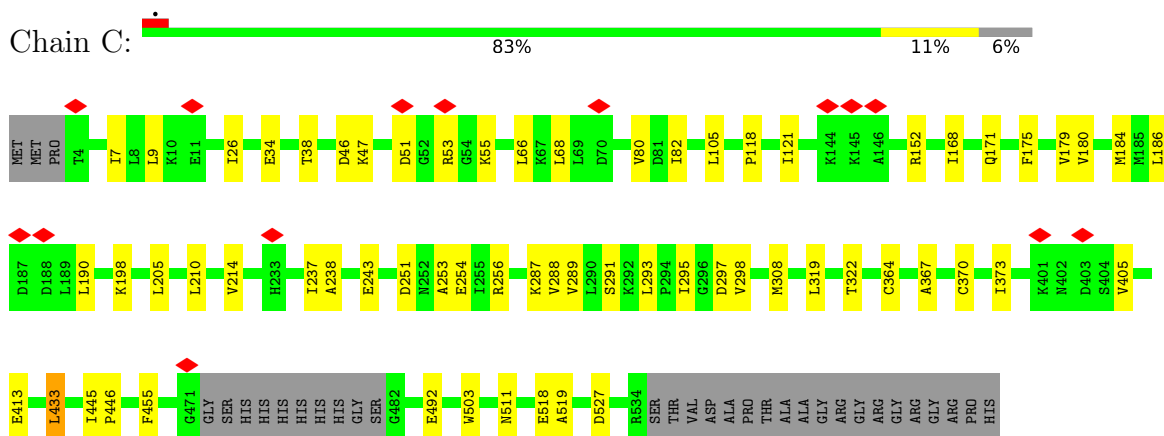
#### • Molecule 1: Tubulin beta chain



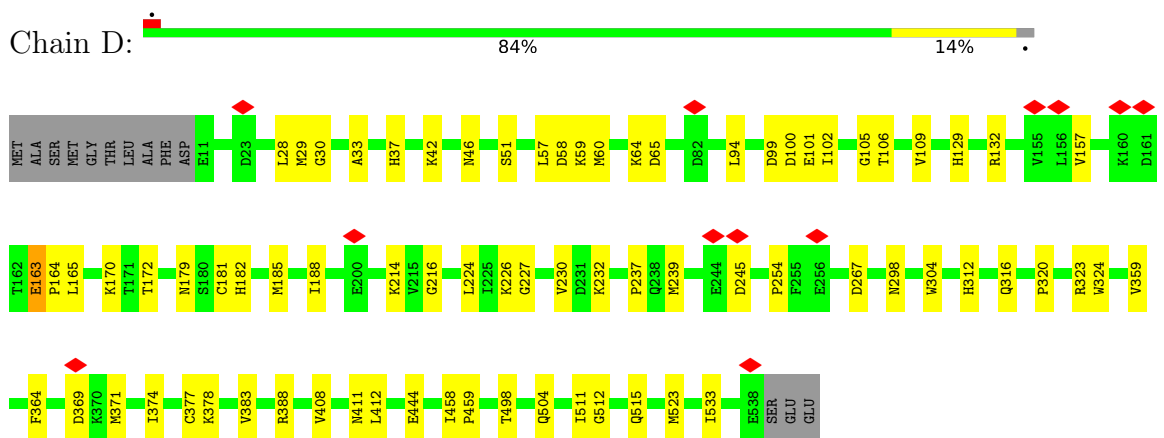
#### • Molecule 2: T-complex protein 1 subunit theta



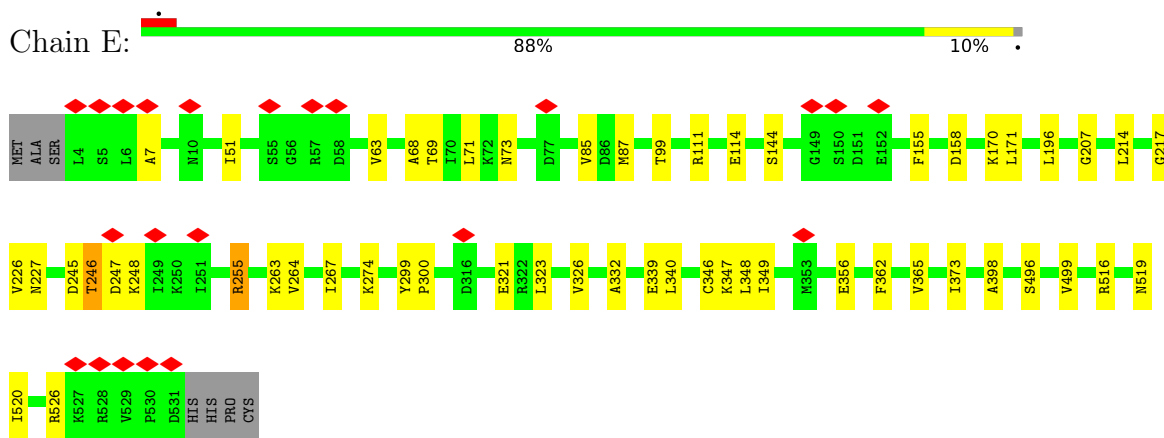
• Molecule 3: T-complex protein 1 subunit eta



• Molecule 4: T-complex protein 1 subunit epsilon

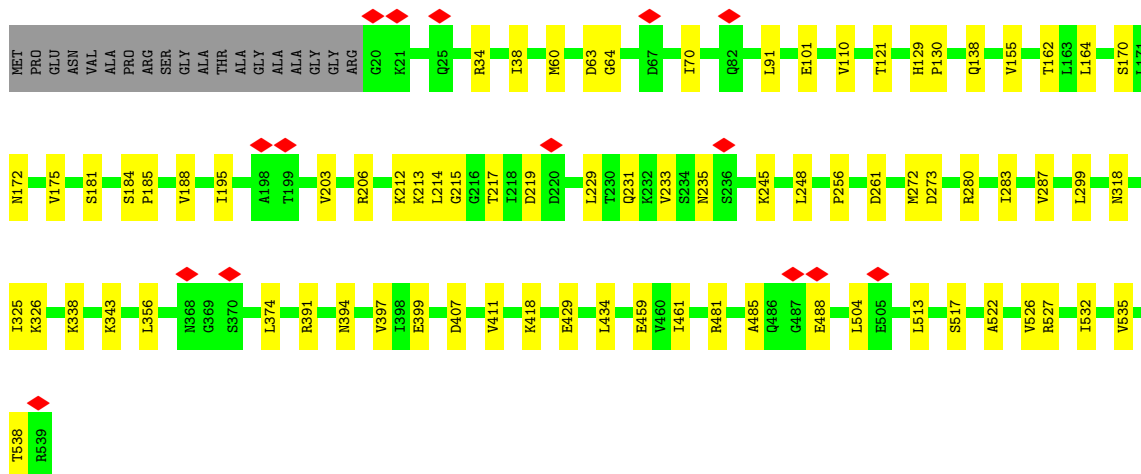


• Molecule 5: T-complex protein 1 subunit beta

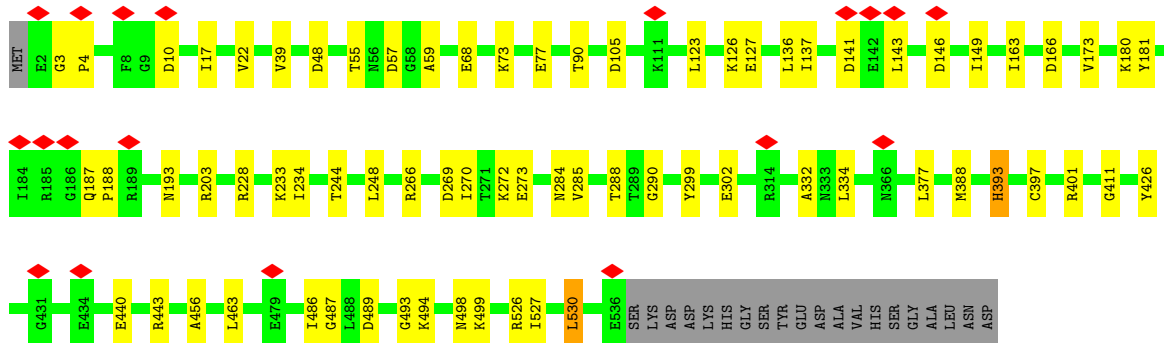
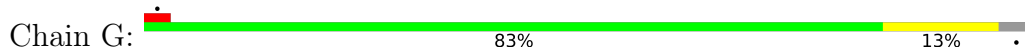


• Molecule 6: T-complex protein 1 subunit delta

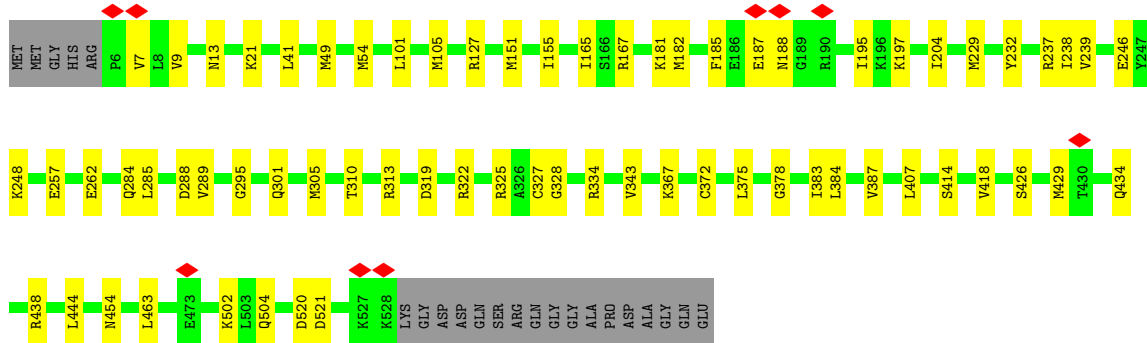
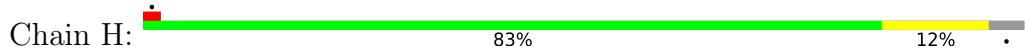




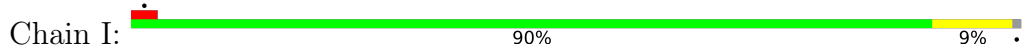
• Molecule 7: T-complex protein 1 subunit alpha

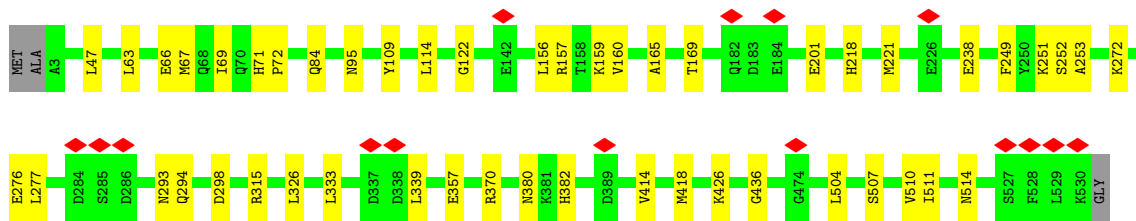


• Molecule 8: T-complex protein 1 subunit gamma



• Molecule 9: T-complex protein 1 subunit zeta





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	42804	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	1.21	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	18.672	Depositor
Minimum map value	-7.632	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	4.0	Depositor
Map size ( $\text{\AA}$ )	352.0, 352.0, 352.0	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.1, 1.1, 1.1	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AF3, ADP, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.26	0/2163	0.48	0/2923
2	B	0.26	0/4087	0.46	0/5525
3	C	0.28	0/4058	0.47	0/5476
4	D	0.28	0/4121	0.50	0/5551
5	E	0.28	0/4018	0.49	0/5418
6	F	0.30	0/3956	0.49	0/5338
7	G	0.29	0/4103	0.50	0/5540
8	H	0.25	0/4110	0.51	0/5544
9	I	0.28	0/4099	0.50	0/5525
All	All	0.28	0/34715	0.49	0/46840

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2119	0	1986	28	0
2	B	4029	0	4099	25	0
3	C	4003	0	4106	34	0
4	D	4072	0	4189	45	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	3974	0	4093	38	0
6	F	3924	0	4131	49	0
7	G	4063	0	4219	51	0
8	H	4064	0	4202	43	0
9	I	4051	0	4194	32	0
10	B	4	0	0	0	0
10	C	4	0	0	0	0
10	D	4	0	0	0	0
10	E	4	0	0	0	0
10	F	4	0	0	1	0
10	G	4	0	0	0	0
10	H	4	0	0	0	0
10	I	4	0	0	3	0
11	B	1	0	0	0	0
11	C	1	0	0	0	0
11	D	1	0	0	0	0
11	E	1	0	0	0	0
11	F	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
12	B	27	0	12	0	0
12	C	27	0	12	0	0
12	D	27	0	12	0	0
12	E	27	0	12	0	0
12	F	27	0	12	2	0
12	G	27	0	12	0	0
12	H	27	0	12	0	0
12	I	27	0	12	0	0
13	B	1	0	0	0	0
13	C	1	0	0	0	0
13	D	1	0	0	0	0
13	E	1	0	0	0	0
13	F	1	0	0	0	0
13	G	1	0	0	0	0
13	H	1	0	0	0	0
13	I	1	0	0	0	0
All	All	34563	0	35315	312	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (312) 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)
3:C:214:VAL:HG11	3:C:322:THR:HG22	1.63	0.80
4:D:37:HIS:HE1	4:D:533:ILE:HD11	1.47	0.80
7:G:68:GLU:N	7:G:68:GLU:OE1	2.19	0.75
5:E:227:ASN:OD1	6:F:343:LYS:NZ	2.21	0.73
3:C:243:GLU:HG3	3:C:293:LEU:HB3	1.70	0.72
7:G:59:ALA:HB2	7:G:90:THR:HG21	1.72	0.71
7:G:163:ILE:HB	8:H:127:ARG:HH11	1.53	0.71
6:F:138:GLN:OE1	6:F:527:ARG:NH1	2.23	0.71
2:B:272:GLU:HG2	9:I:253:ALA:HB2	1.73	0.71
4:D:179:ASN:HA	4:D:182:HIS:HB3	1.73	0.70
6:F:434:LEU:HD21	6:F:485:ALA:HB2	1.74	0.70
2:B:73:LEU:HD11	2:B:105:LEU:HD11	1.73	0.69
5:E:339:GLU:HG2	5:E:340:LEU:HD12	1.74	0.69
1:A:158:GLU:N	1:A:158:GLU:OE1	2.26	0.68
4:D:267:ASP:OD1	5:E:255:ARG:NH1	2.27	0.67
9:I:71:HIS:CD2	9:I:72:PRO:HD2	2.29	0.67
3:C:413:GLU:N	3:C:413:GLU:OE1	2.28	0.67
6:F:214:LEU:HD12	6:F:215:GLY:H	1.63	0.64
9:I:414:VAL:HG12	9:I:418:MET:HE1	1.79	0.63
9:I:218:HIS:HB3	9:I:221:MET:HG3	1.80	0.63
1:A:54:ALA:HB3	1:A:58:LYS:HB2	1.81	0.63
4:D:359:VAL:HG22	4:D:374:ILE:HG12	1.80	0.63
8:H:238:ILE:HG22	8:H:289:VAL:HB	1.79	0.63
4:D:37:HIS:CE1	4:D:533:ILE:HD11	2.33	0.62
4:D:101:GLU:HG3	4:D:102:ILE:HG13	1.81	0.62
8:H:165:ILE:HD11	8:H:387:VAL:HG13	1.80	0.62
4:D:42:LYS:O	4:D:46:ASN:ND2	2.32	0.62
4:D:172:THR:HG21	4:D:408:VAL:HG21	1.82	0.62
4:D:99:ASP:OD2	4:D:100:ASP:N	2.33	0.62
9:I:159:LYS:CE	10:I:603:AF3:F1	2.37	0.61
2:B:464:ILE:HD12	2:B:464:ILE:H	1.64	0.60
5:E:326:VAL:HG12	5:E:365:VAL:HG11	1.81	0.60
4:D:364:PHE:HE2	4:D:371:MET:HG3	1.66	0.60
3:C:26:ILE:HG23	3:C:105:LEU:HB3	1.83	0.60
6:F:60:MET:SD	7:G:530:LEU:HD13	2.42	0.60
6:F:63:ASP:OD1	6:F:64:GLY:N	2.33	0.59
6:F:155:VAL:HG21	6:F:162:THR:HG21	1.84	0.59
1:A:67:ASP:OD2	1:A:68:LEU:N	2.35	0.59
4:D:59:LYS:HG3	5:E:519:ASN:HB3	1.83	0.59
1:A:1:MET:SD	1:A:1:MET:N	2.68	0.58
9:I:159:LYS:HE2	10:I:603:AF3:F1	1.92	0.58
7:G:166:ASP:N	7:G:166:ASP:OD1	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:65:ASP:OD1	5:E:526:ARG:NE	2.35	0.58
3:C:168:ILE:HG22	3:C:205:LEU:HD21	1.85	0.57
7:G:136:LEU:O	7:G:137:ILE:HD13	2.05	0.57
6:F:418:LYS:HD3	6:F:513:LEU:HD13	1.87	0.57
8:H:21:LYS:HD3	8:H:21:LYS:N	2.19	0.57
6:F:213:LYS:HB3	6:F:391:ARG:HH11	1.70	0.57
6:F:101:GLU:OE1	6:F:517:SER:OG	2.23	0.56
6:F:245:LYS:HB3	6:F:356:LEU:HD23	1.87	0.56
7:G:187:GLN:OE1	7:G:187:GLN:N	2.38	0.56
5:E:246:THR:OG1	5:E:247:ASP:N	2.39	0.56
7:G:10:ASP:OD1	7:G:10:ASP:N	2.38	0.56
9:I:201:GLU:OE2	9:I:201:GLU:N	2.38	0.56
5:E:207:GLY:N	6:F:101:GLU:OE2	2.39	0.56
7:G:137:ILE:HG13	7:G:499:LYS:HE2	1.88	0.56
7:G:486:ILE:HG13	7:G:487:GLY:H	1.71	0.56
3:C:364:CYS:HB2	3:C:367:ALA:HB2	1.88	0.56
2:B:257:VAL:HG22	3:C:253:ALA:HA	1.88	0.56
5:E:73:ASN:O	6:F:538:THR:OG1	2.22	0.56
7:G:39:VAL:HG21	7:G:456:ALA:HB2	1.88	0.56
3:C:405:VAL:HG21	3:C:503:TRP:HB3	1.88	0.55
1:A:3:GLU:OE1	1:A:62:ARG:NH2	2.39	0.55
2:B:258:LEU:HD11	3:C:256:ARG:HD2	1.88	0.55
3:C:210:LEU:HD11	3:C:370:CYS:HB2	1.87	0.55
7:G:244:THR:HG21	7:G:270:ILE:HD12	1.88	0.55
9:I:238:GLU:OE1	9:I:315:ARG:NH2	2.40	0.55
4:D:102:ILE:HD13	4:D:512:GLY:HA2	1.88	0.55
4:D:498:THR:O	4:D:504:GLN:NE2	2.39	0.55
6:F:217:THR:OG1	6:F:219:ASP:OD2	2.20	0.55
7:G:55:THR:OG1	7:G:57:ASP:OD1	2.23	0.55
1:A:191:GLN:O	1:A:195:ASN:ND2	2.38	0.54
5:E:71:LEU:HB3	5:E:85:VAL:HG13	1.89	0.54
9:I:277:LEU:HD22	9:I:339:LEU:HG	1.88	0.54
3:C:38:THR:HG1	3:C:47:LYS:HZ1	1.54	0.54
6:F:212:LYS:NZ	6:F:399:GLU:OE2	2.30	0.54
3:C:455:PHE:CE2	3:C:492:GLU:HG3	2.42	0.54
6:F:429:GLU:HG2	6:F:461:ILE:HD12	1.90	0.54
4:D:58:ASP:OD2	5:E:516:ARG:NH1	2.40	0.54
8:H:284:GLN:HG2	8:H:285:LEU:HD22	1.90	0.54
2:B:340:VAL:HG23	2:B:341:LEU:H	1.72	0.54
7:G:411:GLY:O	7:G:498:ASN:ND2	2.41	0.54
9:I:272:LYS:O	9:I:276:GLU:HG2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:69:THR:O	5:E:73:ASN:ND2	2.42	0.53
9:I:238:GLU:HA	9:I:298:ASP:OD1	2.09	0.53
9:I:510:VAL:O	9:I:514:ASN:ND2	2.37	0.53
2:B:420:ALA:O	2:B:424:THR:OG1	2.20	0.53
4:D:312:HIS:CE1	5:E:332:ALA:HA	2.43	0.53
1:A:404:ASP:N	1:A:404:ASP:OD1	2.40	0.53
1:A:145:SER:O	1:A:149:THR:OG1	2.21	0.53
2:B:116:GLU:OE2	2:B:120:ARG:NH2	2.40	0.53
9:I:326:LEU:HB3	9:I:370:ARG:HB2	1.90	0.53
3:C:319:LEU:O	3:C:322:THR:OG1	2.21	0.52
5:E:196:LEU:HD21	5:E:398:ALA:HB2	1.91	0.52
9:I:63:LEU:O	9:I:67:MET:HG2	2.09	0.52
4:D:411:ASN:HB3	4:D:511:ILE:HD11	1.89	0.52
9:I:201:GLU:H	9:I:201:GLU:CD	2.13	0.52
7:G:377:LEU:HD22	7:G:388:MET:HE2	1.89	0.52
9:I:122:GLY:HA3	9:I:436:GLY:HA3	1.91	0.52
4:D:29:MET:HG2	4:D:30:GLY:H	1.75	0.52
4:D:99:ASP:HB3	4:D:106:THR:HG21	1.91	0.52
8:H:246:GLU:OE2	8:H:248:LYS:NZ	2.42	0.52
5:E:245:ASP:O	5:E:247:ASP:N	2.43	0.52
9:I:84:GLN:OE1	9:I:95:ASN:ND2	2.40	0.52
1:A:442:GLU:HB2	7:G:181:TYR:HE2	1.74	0.52
7:G:299:TYR:OH	8:H:334:ARG:NH2	2.28	0.51
1:A:161:ASP:OD1	1:A:161:ASP:N	2.43	0.51
2:B:118:LEU:HD11	2:B:440:LYS:HG3	1.92	0.51
6:F:91:LEU:HD12	6:F:110:VAL:HG13	1.92	0.51
8:H:262:GLU:OE2	8:H:262:GLU:N	2.43	0.51
5:E:247:ASP:N	5:E:247:ASP:OD1	2.44	0.51
8:H:295:GLY:HA2	8:H:313:ARG:HG3	1.93	0.51
5:E:144:SER:O	5:E:144:SER:OG	2.29	0.51
6:F:219:ASP:OD2	6:F:219:ASP:N	2.43	0.51
7:G:440:GLU:OE2	7:G:443:ARG:NH2	2.44	0.51
1:A:68:LEU:HB3	1:A:96:GLY:HA2	1.92	0.50
5:E:51:ILE:HG12	5:E:63:VAL:HG22	1.94	0.50
2:B:223:PHE:HE1	2:B:320:ASP:OD2	1.95	0.50
1:A:192:LEU:O	1:A:196:THR:OG1	2.25	0.50
4:D:323:ARG:HG2	4:D:324:TRP:CD1	2.47	0.50
5:E:68:ALA:HB2	5:E:99:THR:HG21	1.93	0.50
2:B:381:THR:HG22	2:B:383:ASN:H	1.76	0.50
3:C:251:ASP:N	3:C:251:ASP:OD1	2.45	0.49
3:C:238:ALA:HB3	3:C:289:VAL:HG12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:MET:SD	1:A:48:SER:OG	2.70	0.49
7:G:233:LYS:H	7:G:284:ASN:HB2	1.77	0.49
7:G:143:LEU:HB3	7:G:146:ASP:HB2	1.94	0.49
6:F:261:ASP:OD2	6:F:261:ASP:N	2.44	0.49
7:G:299:TYR:HH	8:H:334:ARG:HH21	1.54	0.49
8:H:195:ILE:HD11	8:H:197:LYS:HE3	1.94	0.49
3:C:66:LEU:HB3	3:C:80:VAL:HG13	1.94	0.49
7:G:68:GLU:OE2	8:H:9:VAL:HG23	2.13	0.49
7:G:73:LYS:O	7:G:77:GLU:HG2	2.12	0.49
9:I:507:SER:O	9:I:511:ILE:HG22	2.13	0.49
4:D:188:ILE:HG23	4:D:224:LEU:HB2	1.95	0.48
4:D:237:PRO:HG3	5:E:321:GLU:OE2	2.12	0.48
3:C:186:LEU:HB2	3:C:190:LEU:HD23	1.94	0.48
4:D:312:HIS:HD2	4:D:316:GLN:HB2	1.78	0.48
5:E:51:ILE:HD11	6:F:532:ILE:HD13	1.94	0.48
4:D:157:VAL:HG22	4:D:165:LEU:HD21	1.95	0.48
7:G:248:LEU:HD23	7:G:248:LEU:H	1.77	0.48
9:I:414:VAL:HG12	9:I:418:MET:CE	2.44	0.48
1:A:2:ARG:HE	1:A:131:GLN:HB3	1.79	0.48
1:A:154:LYS:HB3	1:A:154:LYS:HE2	1.72	0.48
8:H:257:GLU:HG3	9:I:249:PHE:CD1	2.49	0.48
5:E:248:LYS:HB2	5:E:274:LYS:NZ	2.29	0.47
4:D:226:LYS:HA	4:D:383:VAL:HG12	1.96	0.47
3:C:82:ILE:HG21	3:C:519:ALA:HB2	1.96	0.47
4:D:129:HIS:HB3	4:D:132:ARG:HG2	1.95	0.47
6:F:70:ILE:HD13	7:G:527:ILE:HD11	1.96	0.47
7:G:149:ILE:HD13	7:G:173:VAL:HG21	1.97	0.47
3:C:51:ASP:OD1	3:C:55:LYS:N	2.44	0.47
8:H:185:PHE:CE2	8:H:187:GLU:HB2	2.49	0.47
2:B:410:PRO:O	2:B:415:THR:OG1	2.30	0.47
4:D:163:GLU:HB3	4:D:164:PRO:HD3	1.97	0.47
5:E:111:ARG:O	5:E:114:GLU:HG2	2.15	0.47
5:E:226:VAL:O	5:E:227:ASN:ND2	2.47	0.47
1:A:99:ASN:HA	1:A:142:GLY:H	1.80	0.47
7:G:393:HIS:HE1	7:G:397:CYS:SG	2.38	0.47
9:I:156:LEU:O	9:I:160:VAL:HG22	2.15	0.47
2:B:290:VAL:HG22	2:B:311:MET:HB3	1.96	0.46
4:D:377:CYS:SG	4:D:378:LYS:N	2.88	0.46
4:D:458:ILE:HB	4:D:459:PRO:HD3	1.97	0.46
8:H:367:LYS:HE3	8:H:367:LYS:HB2	1.56	0.46
8:H:182:MET:SD	8:H:372:CYS:HB3	2.55	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:ALA:N	1:A:58:LYS:O	2.47	0.46
1:A:74:ASP:OD1	1:A:74:ASP:N	2.45	0.46
4:D:60:MET:HB3	5:E:520:ILE:HA	1.96	0.46
3:C:46:ASP:OD2	3:C:46:ASP:N	2.47	0.46
8:H:237:ARG:H	8:H:288:ASP:HB2	1.81	0.46
1:A:171:PRO:O	1:A:380:ARG:NH2	2.48	0.46
4:D:254:PRO:HB3	4:D:304:TRP:HB2	1.97	0.46
8:H:521:ASP:N	8:H:521:ASP:OD1	2.49	0.46
4:D:64:LYS:HE3	5:E:526:ARG:HB2	1.97	0.46
8:H:13:ASN:O	8:H:13:ASN:ND2	2.49	0.46
6:F:459:GLU:OE2	6:F:481:ARG:NH2	2.49	0.45
7:G:489:ASP:HB3	7:G:494:LYS:O	2.16	0.45
6:F:170:SER:OG	6:F:411:VAL:HG21	2.16	0.45
6:F:394:ASN:HB2	6:F:397:VAL:HG23	1.98	0.45
7:G:397:CYS:O	7:G:401:ARG:HG2	2.17	0.45
9:I:159:LYS:HE3	10:I:603:AF3:F1	2.03	0.45
4:D:239:MET:SD	4:D:320:PRO:HA	2.56	0.45
6:F:172:ASN:HD21	12:F:602:ADP:HN61	1.65	0.45
8:H:301:GLN:O	8:H:305:MET:HG3	2.17	0.45
5:E:217:GLY:HA3	5:E:362:PHE:O	2.16	0.45
6:F:233:VAL:HG12	6:F:325:ILE:HG12	1.97	0.45
5:E:51:ILE:HB	6:F:535:VAL:HG22	1.98	0.45
9:I:165:ALA:O	9:I:169:THR:OG1	2.26	0.45
9:I:47:LEU:HD13	9:I:66:GLU:HG2	1.99	0.45
1:A:28:HIS:N	1:A:28:HIS:CD2	2.85	0.45
2:B:115:ALA:HA	2:B:118:LEU:HD12	1.99	0.45
6:F:248:LEU:HD12	6:F:299:LEU:HB2	1.98	0.45
7:G:234:ILE:HD13	7:G:285:VAL:HB	1.98	0.45
7:G:486:ILE:HG13	7:G:487:GLY:N	2.32	0.45
7:G:180:LYS:HE3	7:G:188:PRO:HB3	1.99	0.44
8:H:238:ILE:HD11	8:H:327:CYS:SG	2.57	0.44
3:C:433:LEU:HD12	3:C:433:LEU:H	1.82	0.44
6:F:229:LEU:HB2	6:F:374:LEU:HB3	1.99	0.44
8:H:155:ILE:HD11	8:H:407:LEU:HD11	2.00	0.44
9:I:380:ASN:HD22	9:I:382:HIS:CE1	2.35	0.44
7:G:272:LYS:HD3	8:H:334:ARG:NH2	2.32	0.44
3:C:445:ILE:HB	3:C:446:PRO:HD3	2.00	0.44
4:D:245:ASP:O	4:D:298:ASN:ND2	2.50	0.44
8:H:414:SER:O	8:H:418:VAL:HG22	2.18	0.44
2:B:54:LYS:HE2	2:B:54:LYS:HB2	1.73	0.44
3:C:7:ILE:HD12	3:C:9:LEU:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:198:LYS:HB2	3:C:373:ILE:HD13	2.00	0.44
6:F:273:ASP:OD1	7:G:266:ARG:NH2	2.50	0.44
4:D:51:SER:OG	4:D:57:LEU:O	2.26	0.44
6:F:164:LEU:HD23	6:F:188:VAL:HG21	2.00	0.44
8:H:378:GLY:HA3	8:H:384:LEU:HD21	2.00	0.44
12:F:602:ADP:O1B	10:F:603:AF3:F3	2.26	0.43
7:G:123:LEU:O	7:G:127:GLU:HG2	2.17	0.43
3:C:175:PHE:O	3:C:179:VAL:HG23	2.18	0.43
7:G:48:ASP:OD1	7:G:48:ASP:N	2.51	0.43
8:H:187:GLU:OE2	8:H:188:ASN:HB2	2.17	0.43
6:F:280:ARG:HD2	7:G:332:ALA:HB2	2.00	0.43
6:F:407:ASP:O	6:F:411:VAL:HG23	2.17	0.43
6:F:38:ILE:HG21	6:F:121:THR:OG1	2.19	0.43
7:G:126:LYS:HE2	7:G:126:LYS:HB3	1.86	0.43
5:E:496:SER:HB3	5:E:499:VAL:HG23	2.00	0.43
6:F:129:HIS:CG	6:F:130:PRO:HD2	2.53	0.43
9:I:426:LYS:HE2	9:I:426:LYS:HB3	1.69	0.43
3:C:291:SER:HB3	3:C:295:ILE:HD11	1.99	0.43
7:G:3:GLY:HA3	7:G:4:PRO:HD3	1.91	0.43
8:H:204:ILE:HD12	8:H:375:LEU:HD11	2.01	0.43
1:A:117:LEU:HA	1:A:120:VAL:HG22	2.01	0.43
5:E:264:VAL:HG12	6:F:256:PRO:HB2	2.00	0.43
8:H:41:LEU:O	8:H:454:ASN:ND2	2.40	0.43
6:F:195:ILE:HG21	6:F:203:VAL:HG22	1.99	0.43
6:F:504:LEU:HD23	6:F:504:LEU:HA	1.89	0.43
8:H:101:LEU:O	8:H:105:MET:HG3	2.18	0.43
6:F:34:ARG:O	6:F:38:ILE:HG12	2.18	0.43
8:H:101:LEU:HD11	8:H:444:LEU:HD23	2.01	0.43
3:C:237:ILE:HD13	3:C:288:VAL:HB	2.01	0.43
4:D:101:GLU:HG2	4:D:515:GLN:NE2	2.34	0.43
8:H:319:ASP:OD1	8:H:322:ARG:NH2	2.51	0.43
4:D:412:LEU:HD23	4:D:412:LEU:HA	1.89	0.42
6:F:175:VAL:HG23	7:G:526:ARG:HD3	2.00	0.42
5:E:356:GLU:O	6:F:206:ARG:NH1	2.52	0.42
6:F:184:SER:OG	6:F:185:PRO:HD3	2.19	0.42
8:H:434:GLN:OE1	8:H:438:ARG:NH2	2.47	0.42
2:B:11:PHE:CE1	9:I:69:ILE:HD11	2.54	0.42
4:D:181:CYS:O	4:D:185:MET:HG2	2.19	0.42
7:G:288:THR:HG22	7:G:290:GLY:H	1.85	0.42
1:A:5:VAL:HG12	1:A:62:ARG:HD3	2.01	0.42
7:G:203:ARG:HG2	8:H:504:GLN:HE22	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:86:ILE:H	2:B:86:ILE:HG12	1.66	0.42
3:C:171:GLN:OE1	3:C:171:GLN:N	2.53	0.42
6:F:272:MET:HE3	6:F:272:MET:HB3	1.95	0.42
6:F:374:LEU:HD12	6:F:374:LEU:HA	1.91	0.42
7:G:272:LYS:HD3	8:H:334:ARG:HH22	1.85	0.42
8:H:327:CYS:SG	8:H:328:GLY:N	2.92	0.42
8:H:463:LEU:HD23	8:H:463:LEU:HA	1.88	0.42
2:B:448:ILE:HB	2:B:449:PRO:HD3	2.02	0.42
4:D:94:LEU:HD13	4:D:523:MET:HG2	2.01	0.42
8:H:229:MET:SD	8:H:310:THR:HA	2.60	0.42
9:I:293:ASN:OD1	9:I:294:GLN:N	2.53	0.42
4:D:28:LEU:HB3	4:D:33:ALA:HB2	2.01	0.42
7:G:393:HIS:CE1	7:G:397:CYS:SG	3.13	0.42
1:A:190:HIS:HB2	1:A:414:ASN:ND2	2.34	0.42
2:B:470:VAL:HG12	2:B:475:ASN:HB2	2.00	0.42
4:D:216:GLY:O	4:D:388:ARG:NH2	2.48	0.42
7:G:17:ILE:HD12	7:G:17:ILE:HA	1.90	0.42
8:H:325:ARG:HE	8:H:325:ARG:HB3	1.56	0.41
1:A:27:GLU:HG2	1:A:28:HIS:HD2	1.85	0.41
2:B:397:ASN:O	2:B:401:VAL:HG23	2.19	0.41
3:C:152:ARG:NH2	3:C:184:MET:HG3	2.35	0.41
6:F:231:GLN:NE2	6:F:326:LYS:O	2.53	0.41
2:B:293:THR:OG1	2:B:294:GLY:N	2.54	0.41
5:E:323:LEU:HD23	5:E:323:LEU:HA	1.88	0.41
9:I:109:TYR:O	9:I:114:LEU:HB3	2.21	0.41
2:B:380:SER:OG	3:C:518:GLU:OE1	2.31	0.41
6:F:283:ILE:O	6:F:287:VAL:HG23	2.19	0.41
8:H:426:SER:O	8:H:429:MET:HG2	2.21	0.41
8:H:502:LYS:HA	8:H:502:LYS:HD2	1.88	0.41
9:I:357:GLU:OE1	9:I:357:GLU:N	2.53	0.41
2:B:247:ASP:HB3	2:B:298:ALA:HB2	2.02	0.41
2:B:283:ILE:H	2:B:283:ILE:HG13	1.72	0.41
4:D:227:GLY:HA3	4:D:374:ILE:O	2.20	0.41
5:E:171:LEU:O	5:E:171:LEU:HD12	2.20	0.41
5:E:214:LEU:HD12	5:E:373:ILE:HG12	2.01	0.41
7:G:22:VAL:HG21	7:G:105:ASP:OD2	2.21	0.41
6:F:338:LYS:HE3	6:F:338:LYS:HB3	1.96	0.41
8:H:7:VAL:HG13	8:H:7:VAL:O	2.20	0.41
2:B:212:ILE:HD12	2:B:388:ILE:HD12	2.02	0.41
3:C:180:VAL:O	3:C:184:MET:HG2	2.21	0.41
3:C:118:PRO:HA	3:C:121:ILE:HD12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:297:ASP:OD1	3:C:298:VAL:N	2.54	0.41
4:D:105:GLY:O	4:D:109:VAL:HG23	2.21	0.41
5:E:346:CYS:SG	5:E:347:LYS:N	2.93	0.41
5:E:348:LEU:HD12	5:E:349:ILE:N	2.35	0.41
7:G:302:GLU:OE1	7:G:302:GLU:N	2.51	0.41
8:H:383:ILE:HD13	8:H:383:ILE:HA	1.87	0.41
9:I:251:LYS:HB3	9:I:252:SER:H	1.75	0.41
1:A:373:ALA:O	1:A:374:ILE:HG22	2.20	0.41
7:G:334:LEU:HD23	7:G:334:LEU:HA	1.83	0.40
7:G:463:LEU:HD21	7:G:493:GLY:O	2.21	0.40
1:A:19:LYS:O	1:A:22:GLU:HB2	2.21	0.40
6:F:522:ALA:O	6:F:526:VAL:HG23	2.21	0.40
7:G:269:ASP:O	7:G:273:GLU:HG3	2.21	0.40
1:A:46:ARG:O	1:A:49:VAL:HG12	2.22	0.40
1:A:97:ALA:HB3	1:A:143:THR:HA	2.02	0.40
6:F:235:ASN:HD21	6:F:318:ASN:HA	1.85	0.40
8:H:239:VAL:HG12	8:H:343:VAL:HG22	2.02	0.40
9:I:109:TYR:HB3	9:I:114:LEU:HD23	2.03	0.40
3:C:287:LYS:HA	3:C:308:MET:HG2	2.04	0.40
4:D:214:LYS:NZ	4:D:369:ASP:OD1	2.39	0.40
5:E:263:LYS:O	5:E:267:ILE:HG12	2.21	0.40
5:E:299:TYR:HB3	5:E:300:PRO:HD3	2.03	0.40
4:D:364:PHE:CE2	4:D:371:MET:HG3	2.52	0.40
7:G:127:GLU:HG3	7:G:426:TYR:CE2	2.57	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [\(i\)](#)

### 5.3.1 Protein backbone [\(i\)](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	261/444 (59%)	256 (98%)	4 (2%)	1 (0%)	34 66

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	527/547 (96%)	508 (96%)	18 (3%)	1 (0%)	47	77
3	C	517/553 (94%)	507 (98%)	10 (2%)	0	100	100
4	D	526/541 (97%)	501 (95%)	24 (5%)	1 (0%)	47	77
5	E	526/535 (98%)	507 (96%)	17 (3%)	2 (0%)	34	66
6	F	518/539 (96%)	505 (98%)	13 (2%)	0	100	100
7	G	533/556 (96%)	510 (96%)	23 (4%)	0	100	100
8	H	521/545 (96%)	509 (98%)	12 (2%)	0	100	100
9	I	526/531 (99%)	507 (96%)	19 (4%)	0	100	100
All	All	4455/4791 (93%)	4310 (97%)	140 (3%)	5 (0%)	54	81

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	163	GLU
1	A	374	ILE
5	E	246	THR
2	B	318	LYS
5	E	7	ALA

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	229/379 (60%)	226 (99%)	3 (1%)	69	82
2	B	436/451 (97%)	425 (98%)	11 (2%)	47	72
3	C	428/451 (95%)	421 (98%)	7 (2%)	62	79
4	D	446/456 (98%)	442 (99%)	4 (1%)	78	87
5	E	421/427 (99%)	416 (99%)	5 (1%)	71	83
6	F	442/452 (98%)	440 (100%)	2 (0%)	88	93
7	G	446/463 (96%)	441 (99%)	5 (1%)	73	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	H	454/469 (97%)	447 (98%)	7 (2%)	65	81
9	I	441/442 (100%)	438 (99%)	3 (1%)	84	90
All	All	3743/3990 (94%)	3696 (99%)	47 (1%)	70	82

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	37	HIS
1	A	264	HIS
2	B	54	LYS
2	B	95	GLN
2	B	140	HIS
2	B	162	SER
2	B	171	LYS
2	B	200	ASP
2	B	205	CYS
2	B	307	LYS
2	B	365	HIS
2	B	367	LYS
2	B	382	ASP
3	C	34	GLU
3	C	53	ARG
3	C	68	LEU
3	C	254	GLU
3	C	433	LEU
3	C	511	ASN
3	C	527	ASP
4	D	170	LYS
4	D	230	VAL
4	D	232	LYS
4	D	444	GLU
5	E	87	MET
5	E	155	PHE
5	E	158	ASP
5	E	170	LYS
5	E	255	ARG
6	F	181	SER
6	F	488	GLU
7	G	141	ASP
7	G	193	ASN

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Mol	Chain	Res	Type
7	G	228	ARG
7	G	393	HIS
7	G	530	LEU
8	H	49	MET
8	H	54	MET
8	H	151	MET
8	H	167	ARG
8	H	181	LYS
8	H	232	TYR
8	H	520	ASP
9	I	157	ARG
9	I	333	LEU
9	I	504	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
4	D	37	HIS
7	G	393	HIS
9	I	71	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 8 are monoatomic - leaving 16 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	ADP	C	602	11	24,29,29	0.92	1 (4%)	29,45,45	1.49	4 (13%)
10	AF3	C	603	-	0,3,3	-	-	-	-	-
10	AF3	B	601	-	0,3,3	-	-	-	-	-
12	ADP	G	602	11	24,29,29	0.95	1 (4%)	29,45,45	1.39	4 (13%)
12	ADP	H	602	11	24,29,29	0.95	1 (4%)	29,45,45	1.35	4 (13%)
10	AF3	G	603	-	0,3,3	-	-	-	-	-
12	ADP	D	602	11	24,29,29	0.94	1 (4%)	29,45,45	1.38	4 (13%)
12	ADP	F	602	11	24,29,29	0.93	1 (4%)	29,45,45	1.38	4 (13%)
10	AF3	F	603	-	0,3,3	-	-	-	-	-
12	ADP	E	602	11	24,29,29	0.95	1 (4%)	29,45,45	1.37	4 (13%)
12	ADP	B	603	-	24,29,29	0.94	1 (4%)	29,45,45	1.34	4 (13%)
10	AF3	D	603	-	0,3,3	-	-	-	-	-
10	AF3	H	603	-	0,3,3	-	-	-	-	-
12	ADP	I	602	11	24,29,29	0.94	1 (4%)	29,45,45	1.35	4 (13%)
10	AF3	E	603	-	0,3,3	-	-	-	-	-
10	AF3	I	603	-	0,3,3	-	-	-	-	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	ADP	C	602	11	-	5/12/32/32	0/3/3/3
12	ADP	G	602	11	-	1/12/32/32	0/3/3/3
12	ADP	H	602	11	-	5/12/32/32	0/3/3/3
12	ADP	D	602	11	-	1/12/32/32	0/3/3/3
12	ADP	F	602	11	-	4/12/32/32	0/3/3/3
12	ADP	E	602	11	-	4/12/32/32	0/3/3/3
12	ADP	B	603	-	-	1/12/32/32	0/3/3/3
12	ADP	I	602	11	-	0/12/32/32	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	G	602	ADP	C5-C4	2.38	1.47	1.40
12	C	602	ADP	C5-C4	2.36	1.47	1.40
12	D	602	ADP	C5-C4	2.36	1.47	1.40
12	E	602	ADP	C5-C4	2.35	1.47	1.40
12	H	602	ADP	C5-C4	2.35	1.47	1.40
12	I	602	ADP	C5-C4	2.33	1.47	1.40
12	F	602	ADP	C5-C4	2.32	1.47	1.40
12	B	603	ADP	C5-C4	2.31	1.47	1.40

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	C	602	ADP	PA-O3A-PB	-3.73	120.04	132.83
12	G	602	ADP	N3-C2-N1	-3.33	123.47	128.68
12	F	602	ADP	N3-C2-N1	-3.28	123.55	128.68
12	C	602	ADP	N3-C2-N1	-3.27	123.57	128.68
12	E	602	ADP	N3-C2-N1	-3.25	123.59	128.68
12	H	602	ADP	N3-C2-N1	-3.24	123.61	128.68
12	D	602	ADP	N3-C2-N1	-3.23	123.63	128.68
12	B	603	ADP	N3-C2-N1	-3.20	123.68	128.68
12	I	602	ADP	N3-C2-N1	-3.19	123.69	128.68
12	C	602	ADP	C3'-C2'-C1'	3.17	105.75	100.98
12	G	602	ADP	PA-O3A-PB	-3.11	122.16	132.83
12	F	602	ADP	PA-O3A-PB	-3.02	122.46	132.83
12	D	602	ADP	PA-O3A-PB	-3.00	122.53	132.83
12	I	602	ADP	C3'-C2'-C1'	2.87	105.30	100.98
12	E	602	ADP	PA-O3A-PB	-2.86	123.02	132.83
12	B	603	ADP	C4-C5-N7	-2.85	106.43	109.40
12	F	602	ADP	C4-C5-N7	-2.80	106.48	109.40
12	E	602	ADP	C3'-C2'-C1'	2.79	105.17	100.98
12	E	602	ADP	C4-C5-N7	-2.78	106.50	109.40
12	H	602	ADP	C4-C5-N7	-2.76	106.52	109.40
12	I	602	ADP	C4-C5-N7	-2.70	106.59	109.40
12	F	602	ADP	C3'-C2'-C1'	2.70	105.04	100.98
12	B	603	ADP	C3'-C2'-C1'	2.68	105.02	100.98
12	D	602	ADP	C4-C5-N7	-2.67	106.61	109.40
12	C	602	ADP	C4-C5-N7	-2.65	106.64	109.40
12	G	602	ADP	C3'-C2'-C1'	2.64	104.95	100.98
12	I	602	ADP	PA-O3A-PB	-2.60	123.90	132.83
12	G	602	ADP	C4-C5-N7	-2.57	106.72	109.40
12	H	602	ADP	PA-O3A-PB	-2.51	124.20	132.83
12	D	602	ADP	C3'-C2'-C1'	2.46	104.68	100.98
12	B	603	ADP	PA-O3A-PB	-2.39	124.63	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	H	602	ADP	C3'-C2'-C1'	2.23	104.33	100.98

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	C	602	ADP	C5'-O5'-PA-O2A
12	C	602	ADP	C5'-O5'-PA-O3A
12	F	602	ADP	C5'-O5'-PA-O2A
12	H	602	ADP	PA-O3A-PB-O2B
12	H	602	ADP	C5'-O5'-PA-O2A
12	H	602	ADP	C5'-O5'-PA-O3A
12	C	602	ADP	O4'-C4'-C5'-O5'
12	C	602	ADP	C3'-C4'-C5'-O5'
12	D	602	ADP	PB-O3A-PA-O5'
12	E	602	ADP	PB-O3A-PA-O5'
12	F	602	ADP	PB-O3A-PA-O5'
12	G	602	ADP	PB-O3A-PA-O5'
12	E	602	ADP	C5'-O5'-PA-O3A
12	F	602	ADP	C5'-O5'-PA-O3A
12	C	602	ADP	C5'-O5'-PA-O1A
12	F	602	ADP	C5'-O5'-PA-O1A
12	H	602	ADP	C5'-O5'-PA-O1A
12	B	603	ADP	PA-O3A-PB-O1B
12	H	602	ADP	PA-O3A-PB-O3B
12	E	602	ADP	C5'-O5'-PA-O1A
12	E	602	ADP	C5'-O5'-PA-O2A

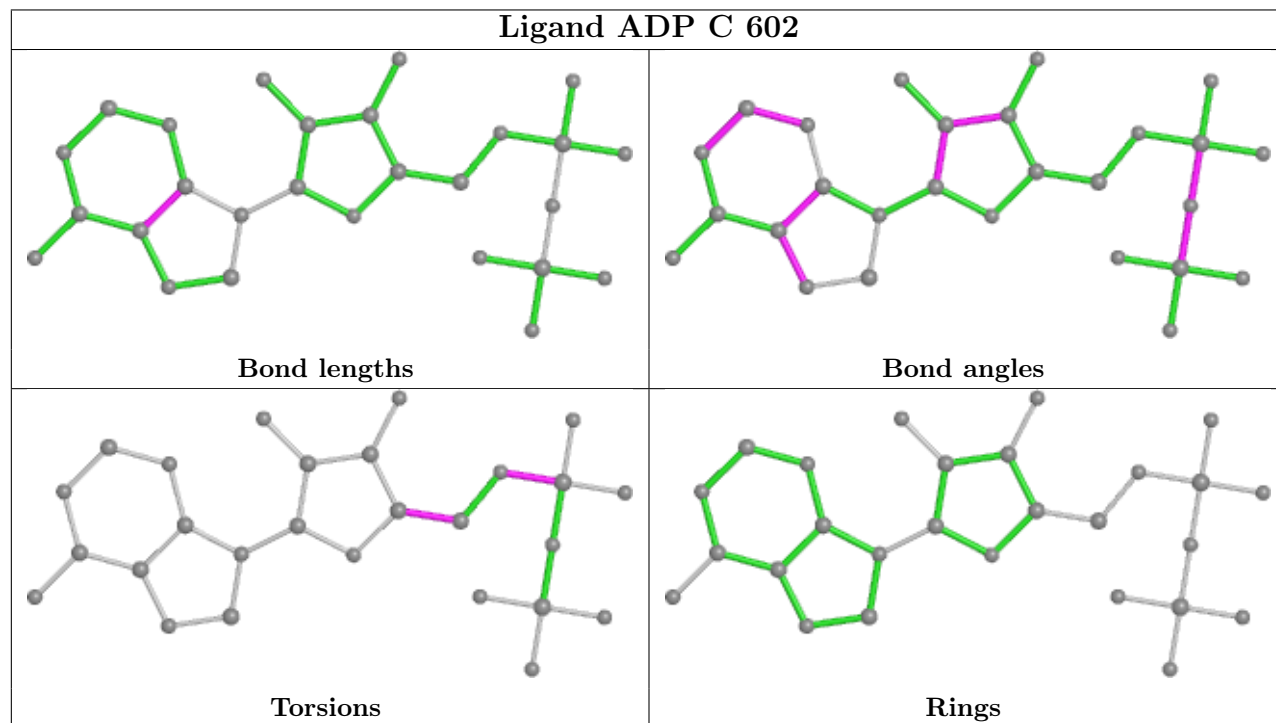
There are no ring outliers.

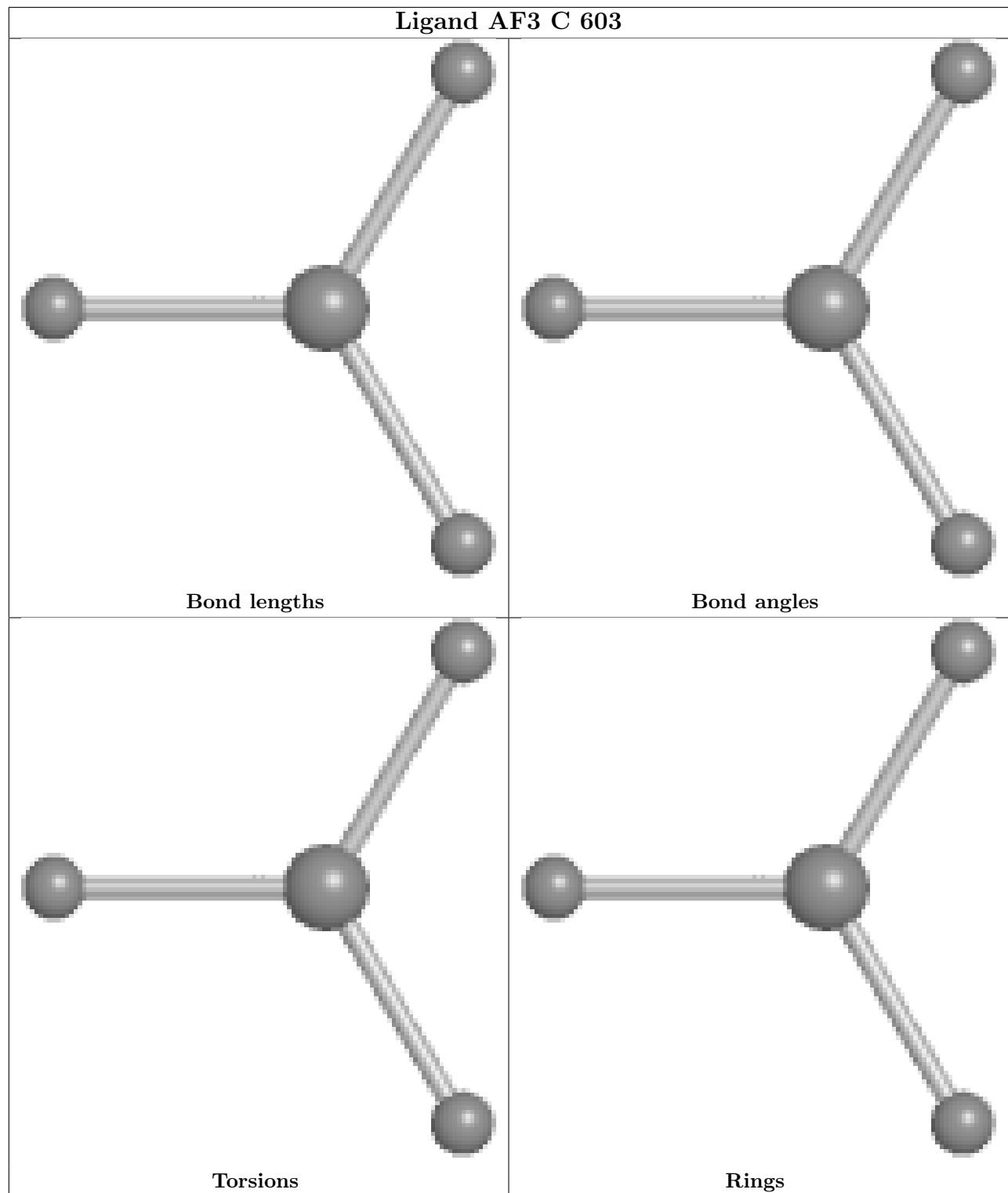
3 monomers are involved in 5 short contacts:

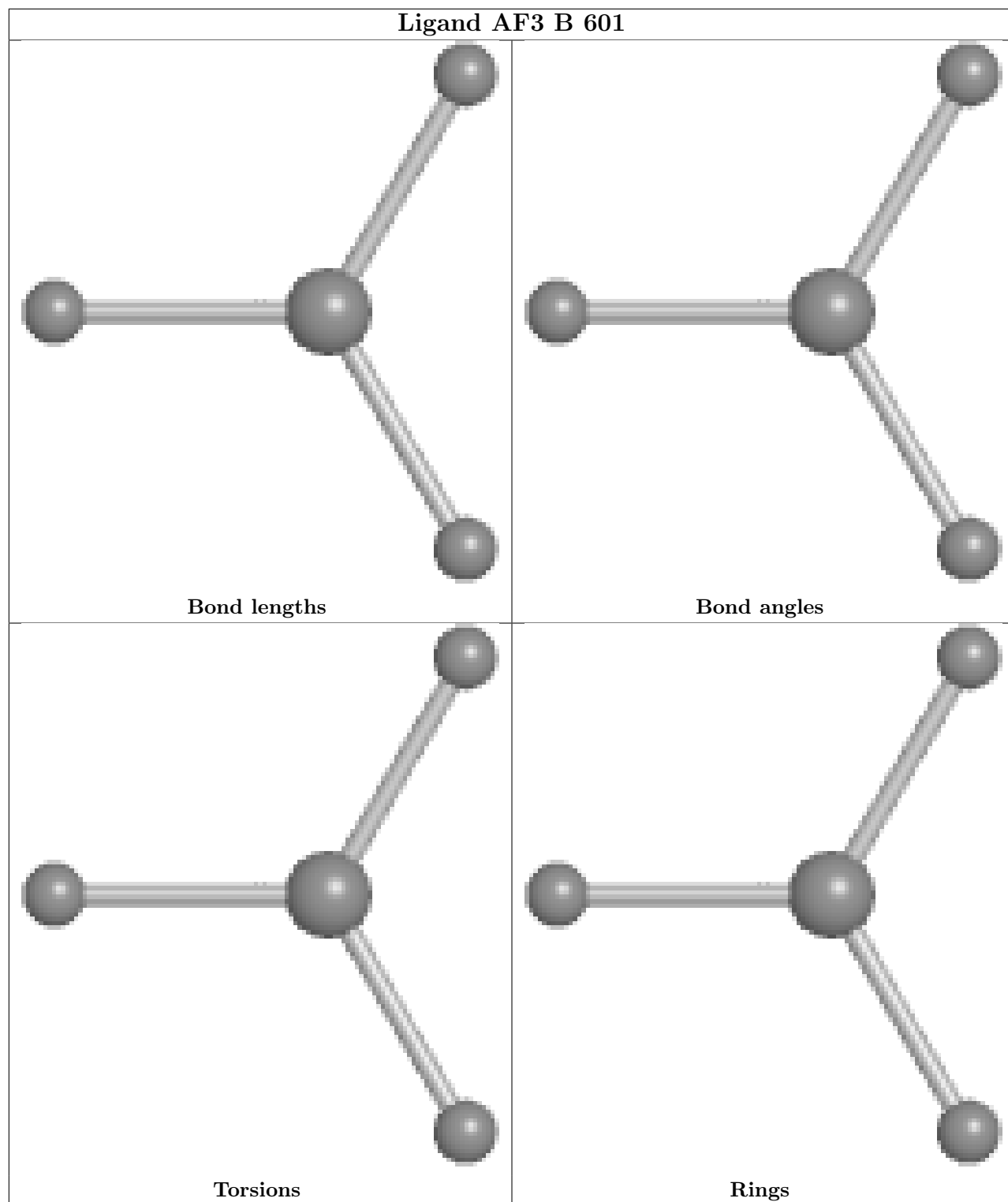
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	F	602	ADP	2	0
10	F	603	AF3	1	0
10	I	603	AF3	3	0

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

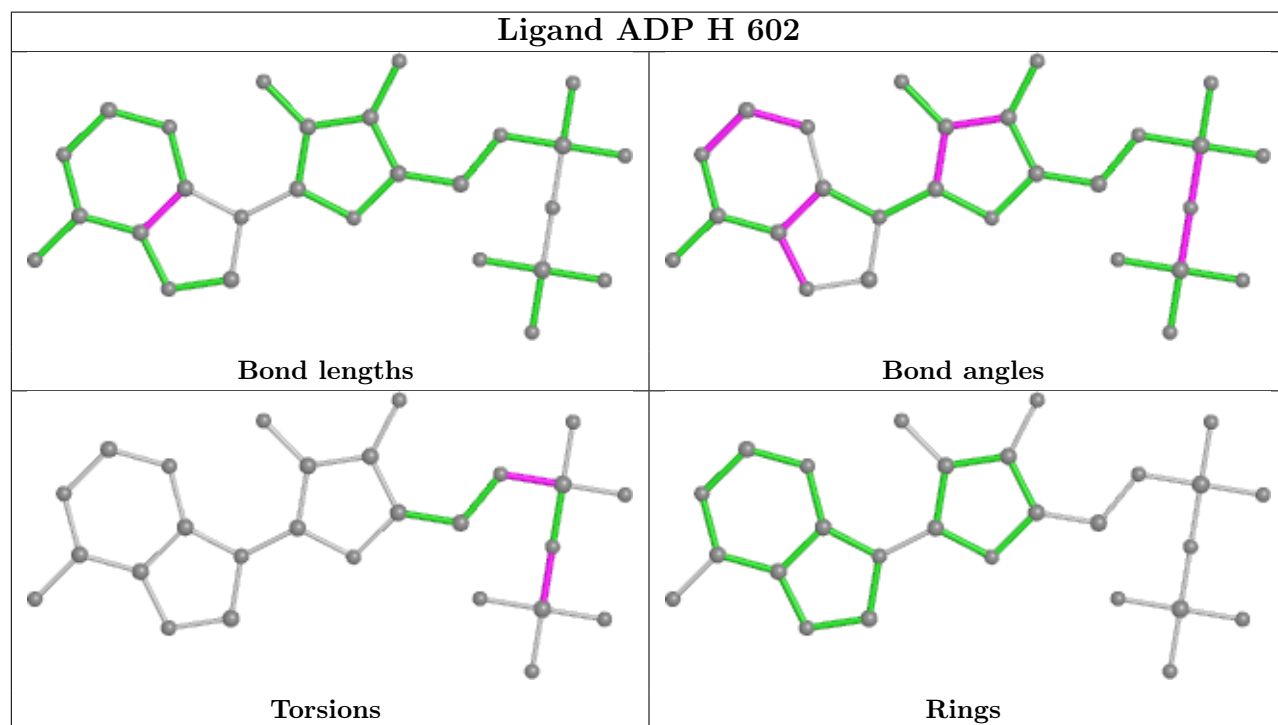
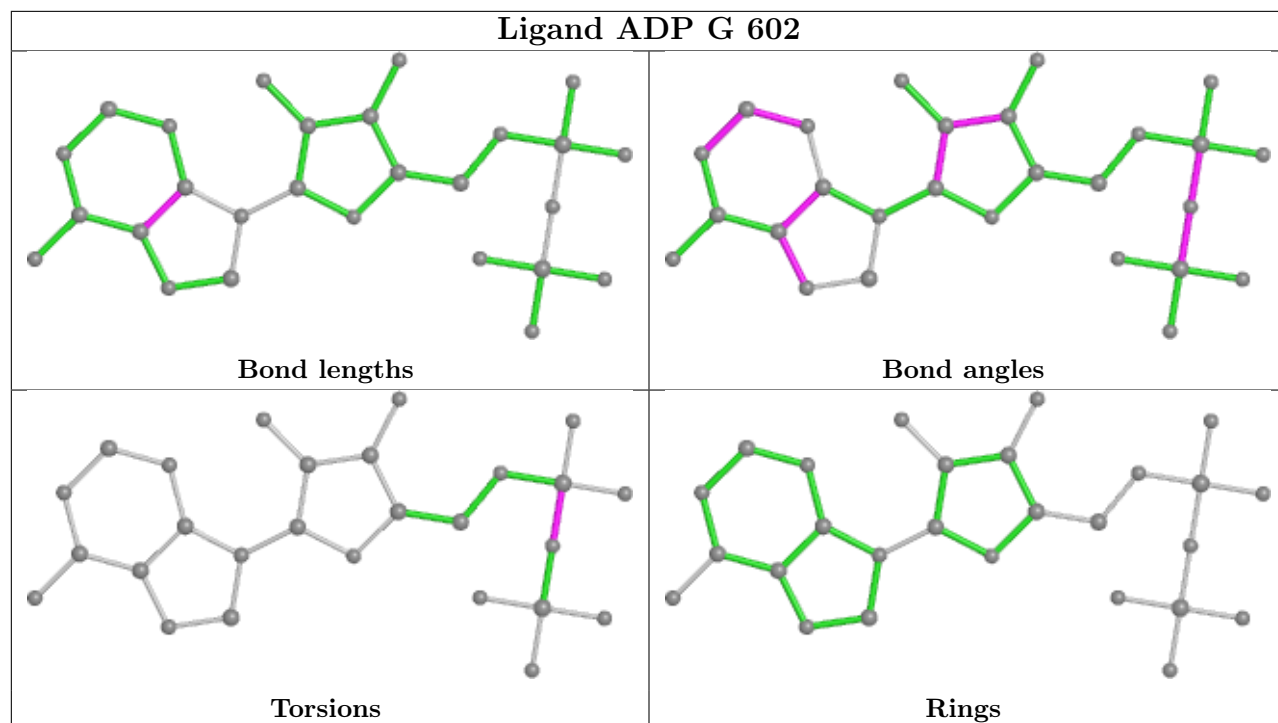
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.

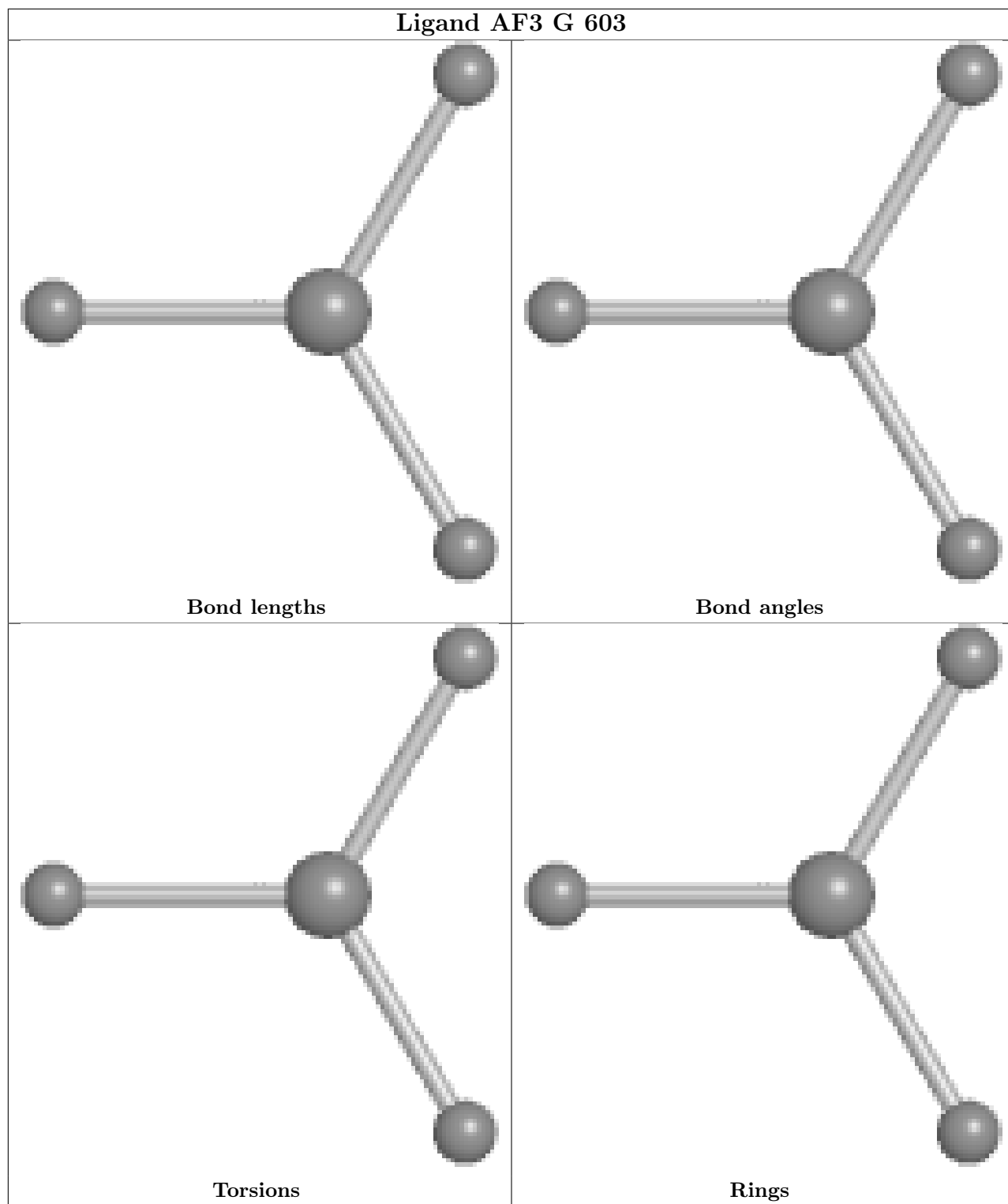


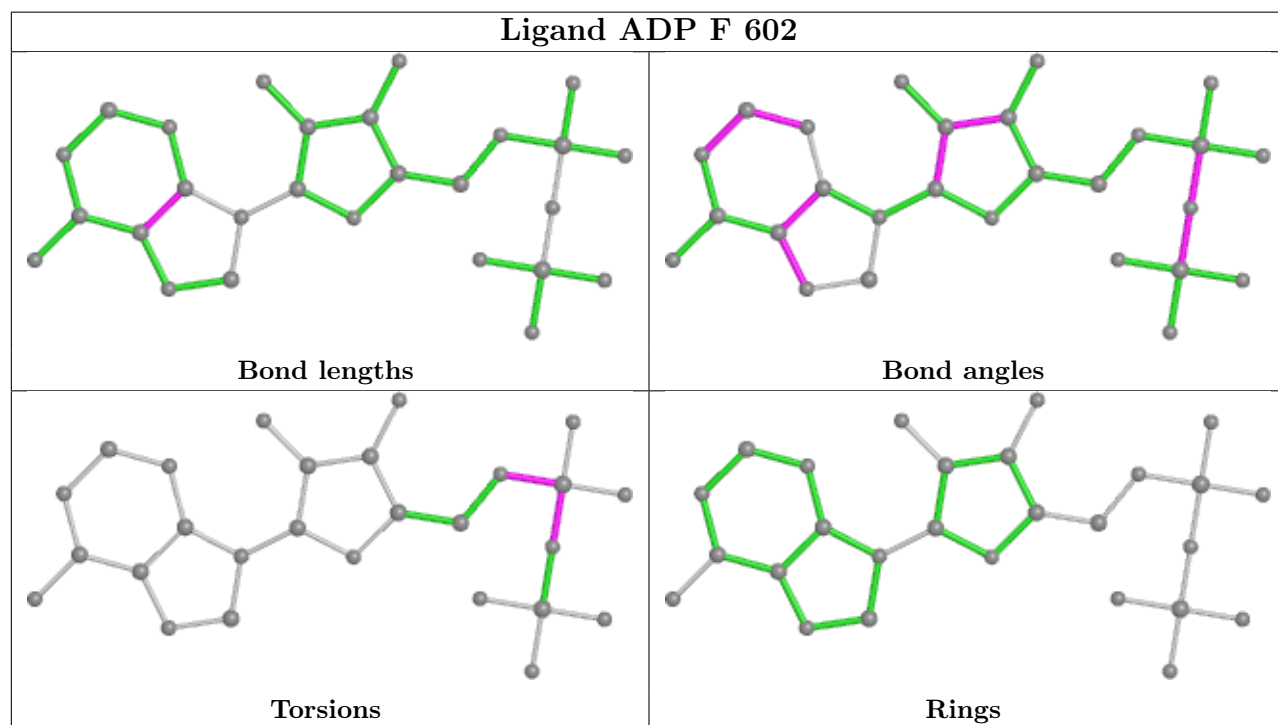
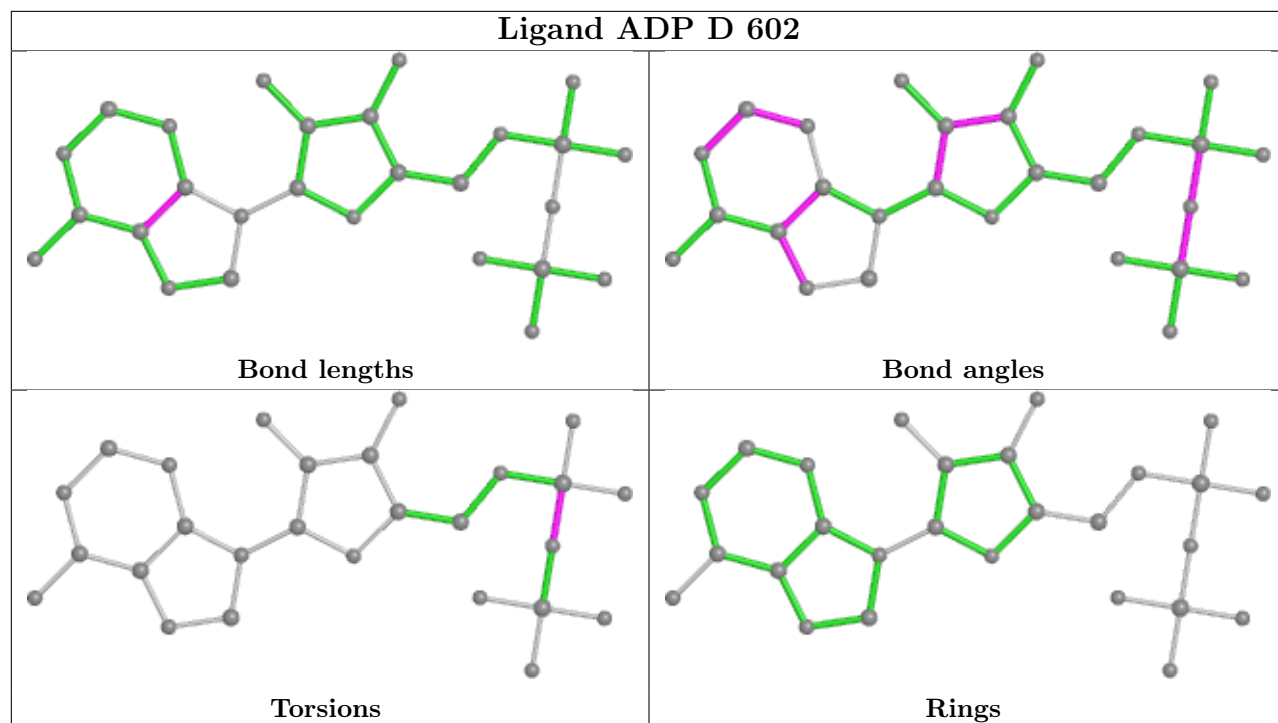


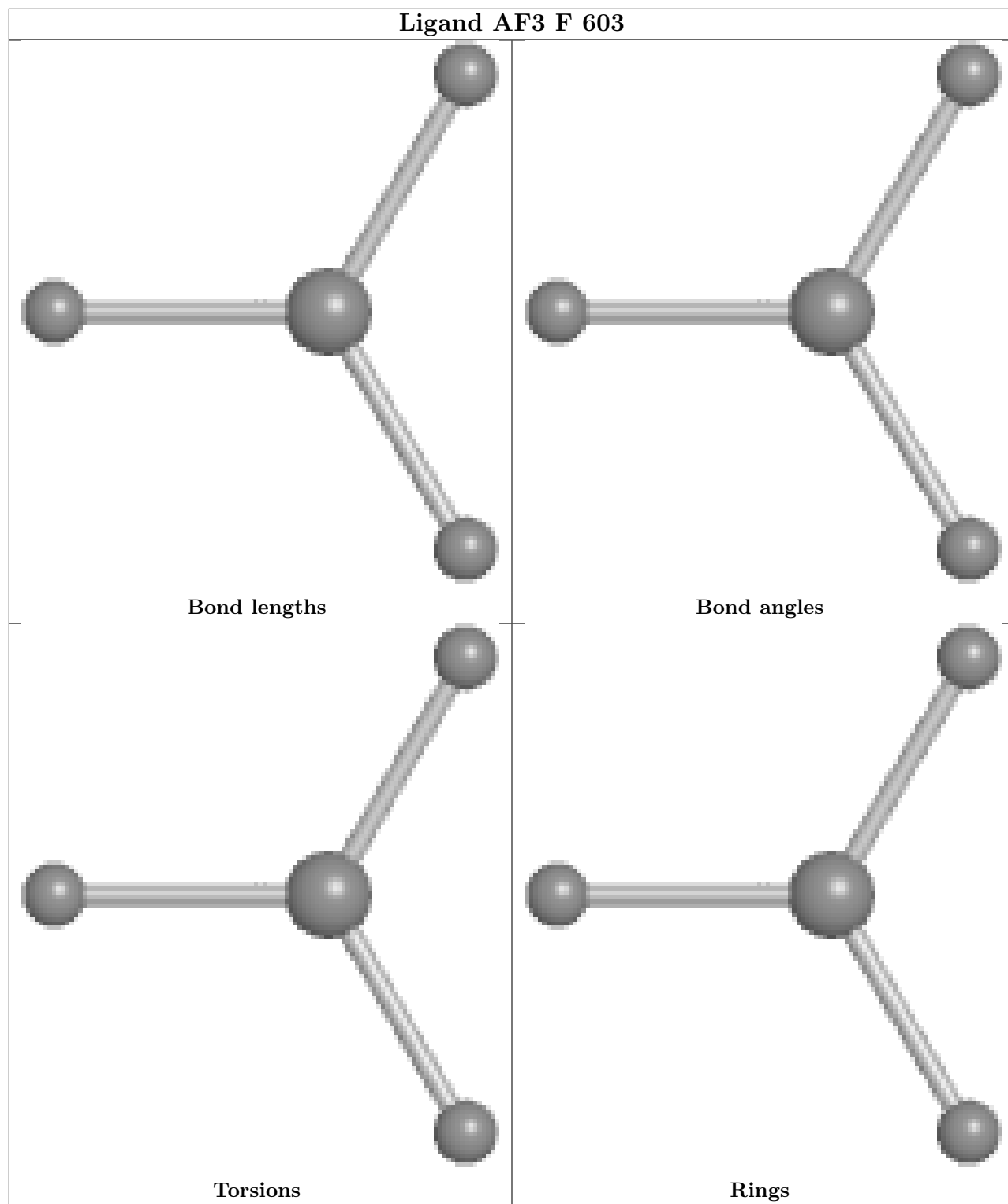


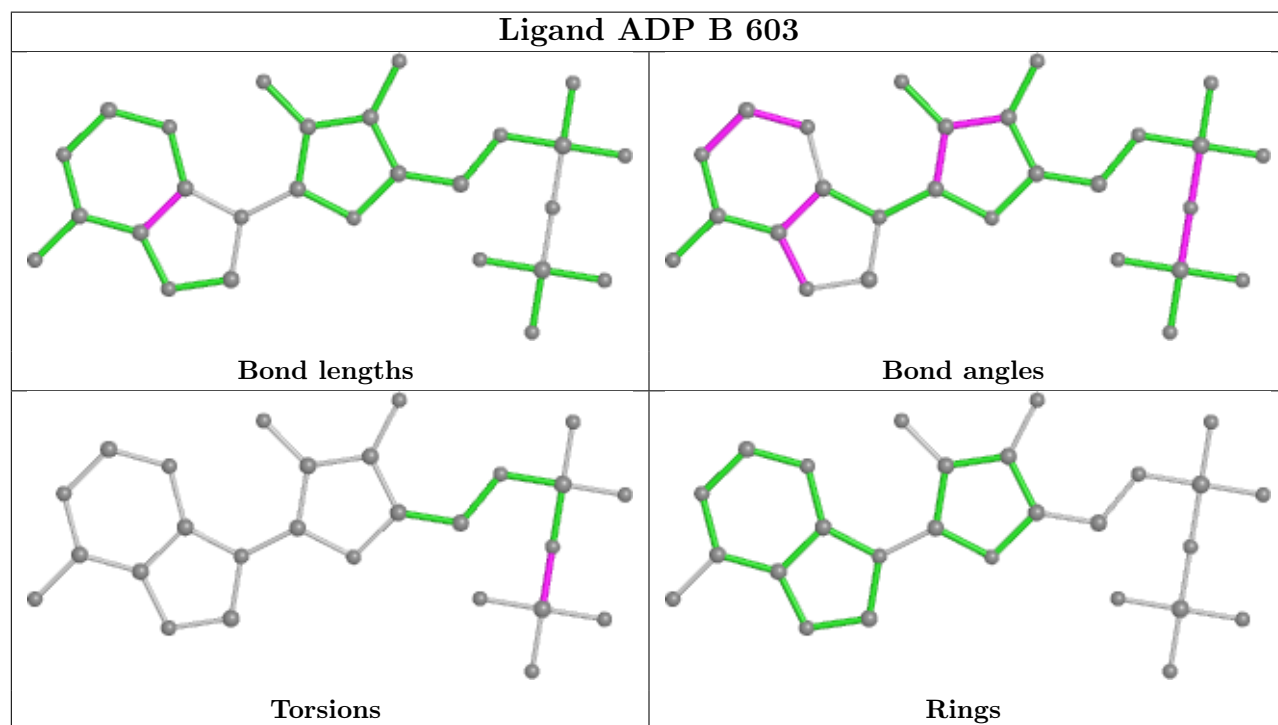
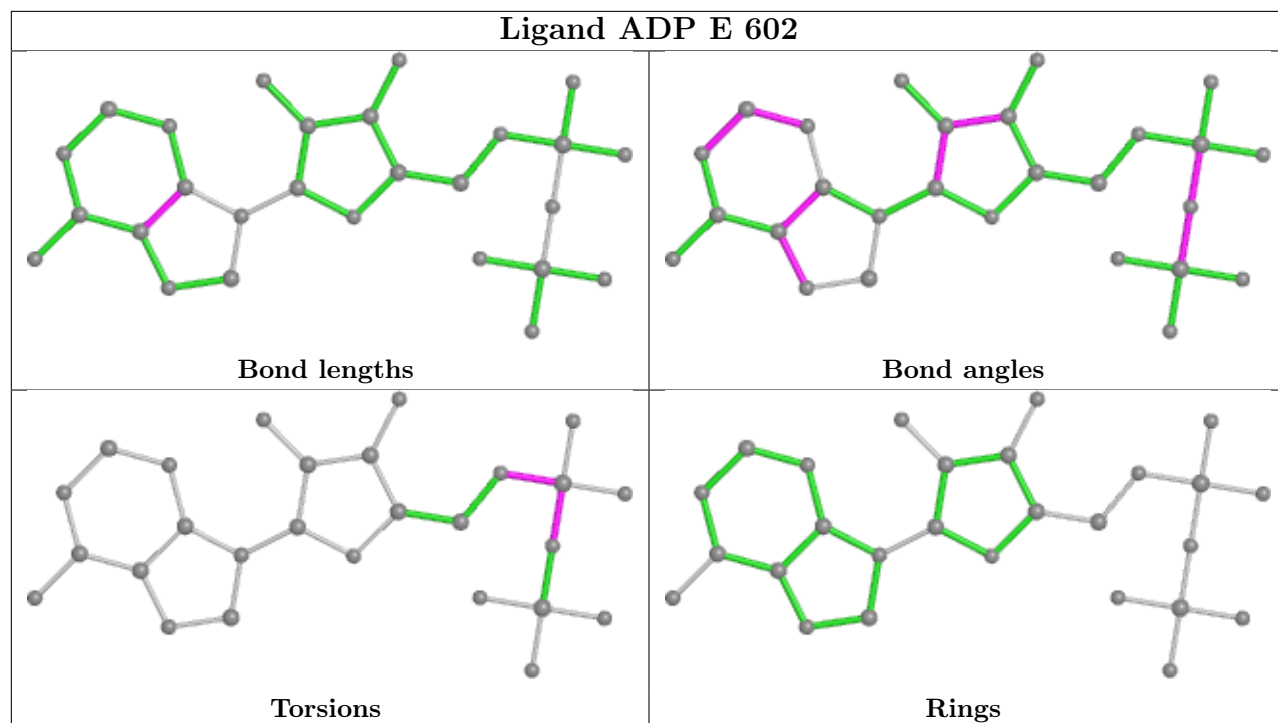


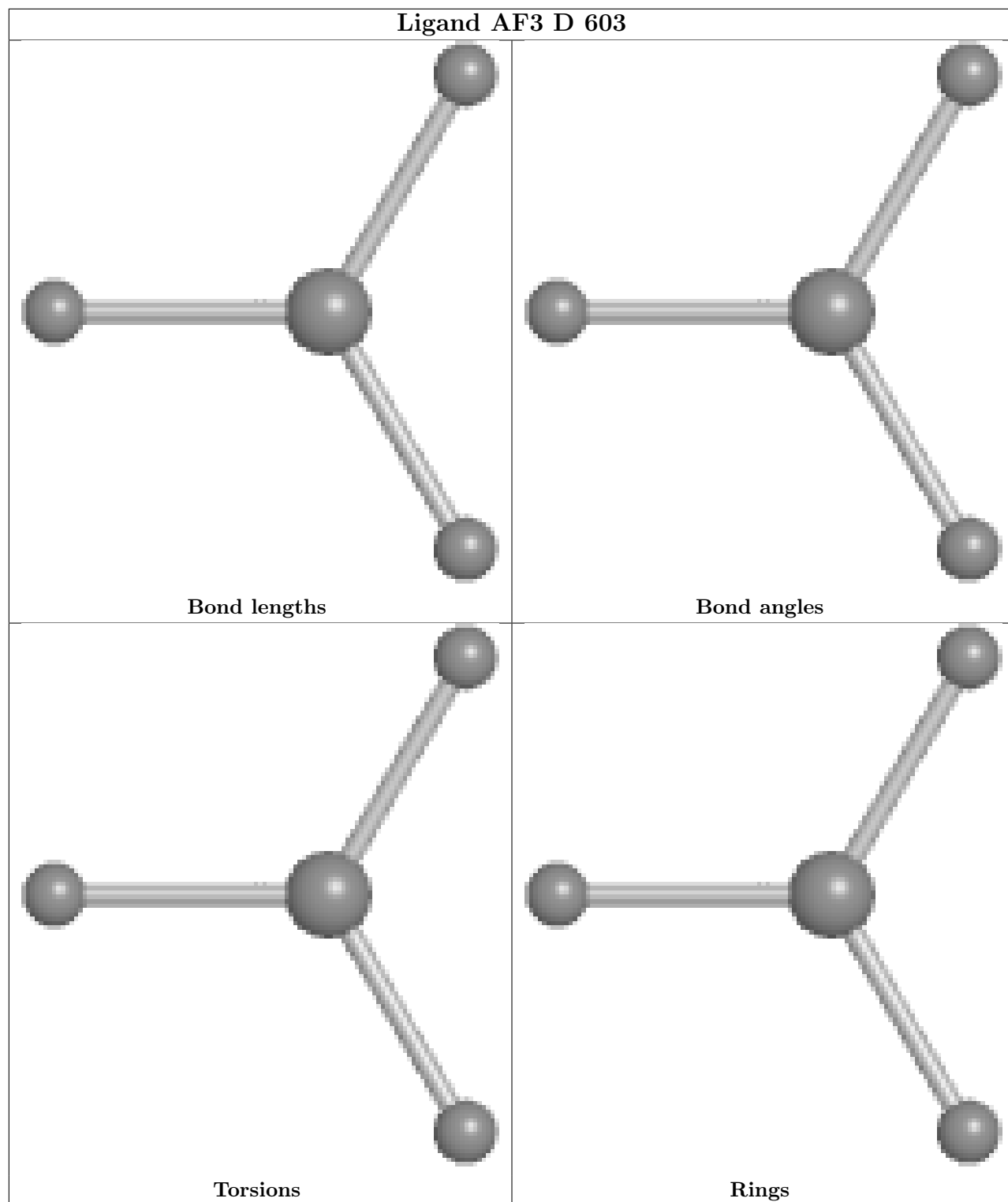


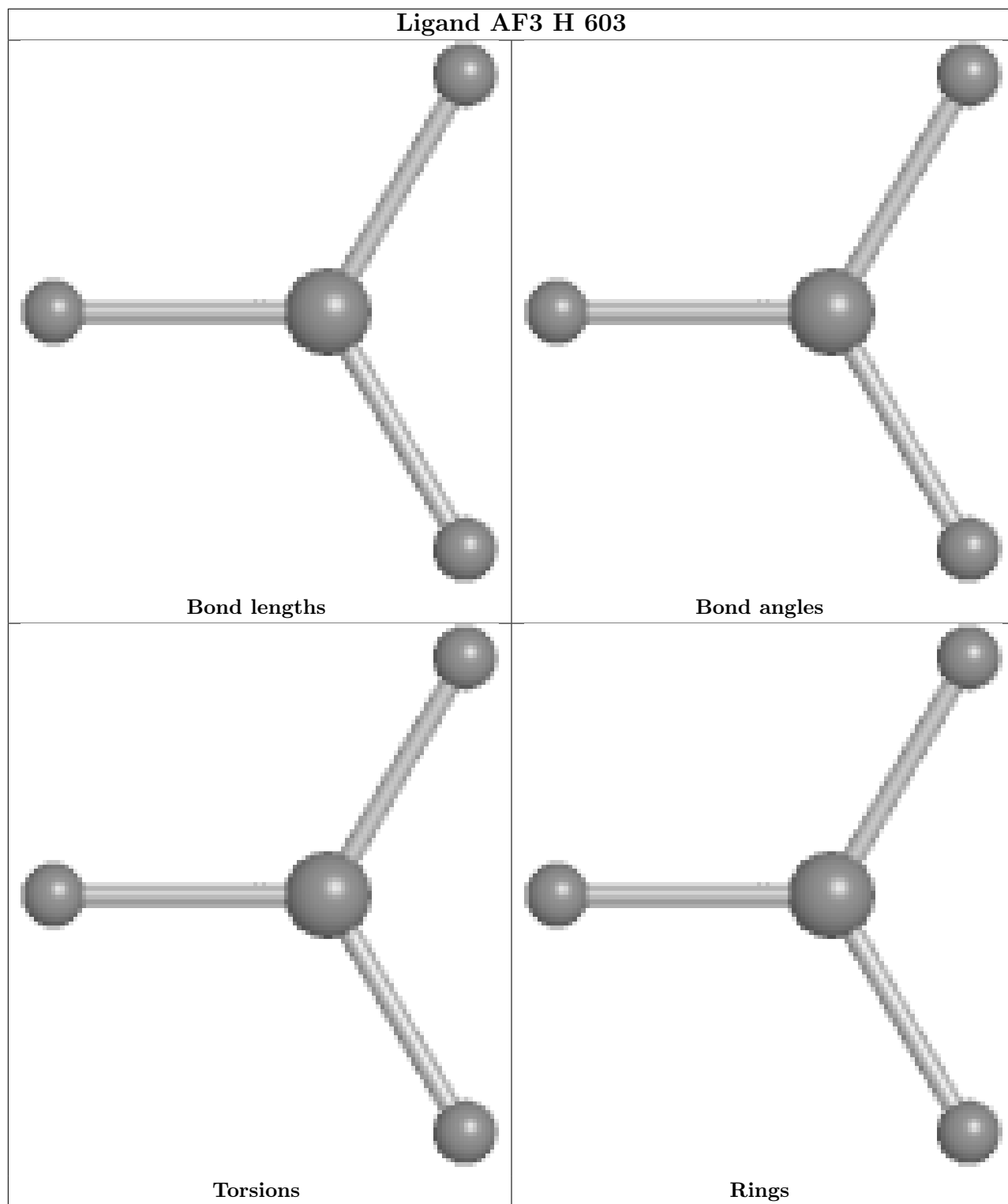


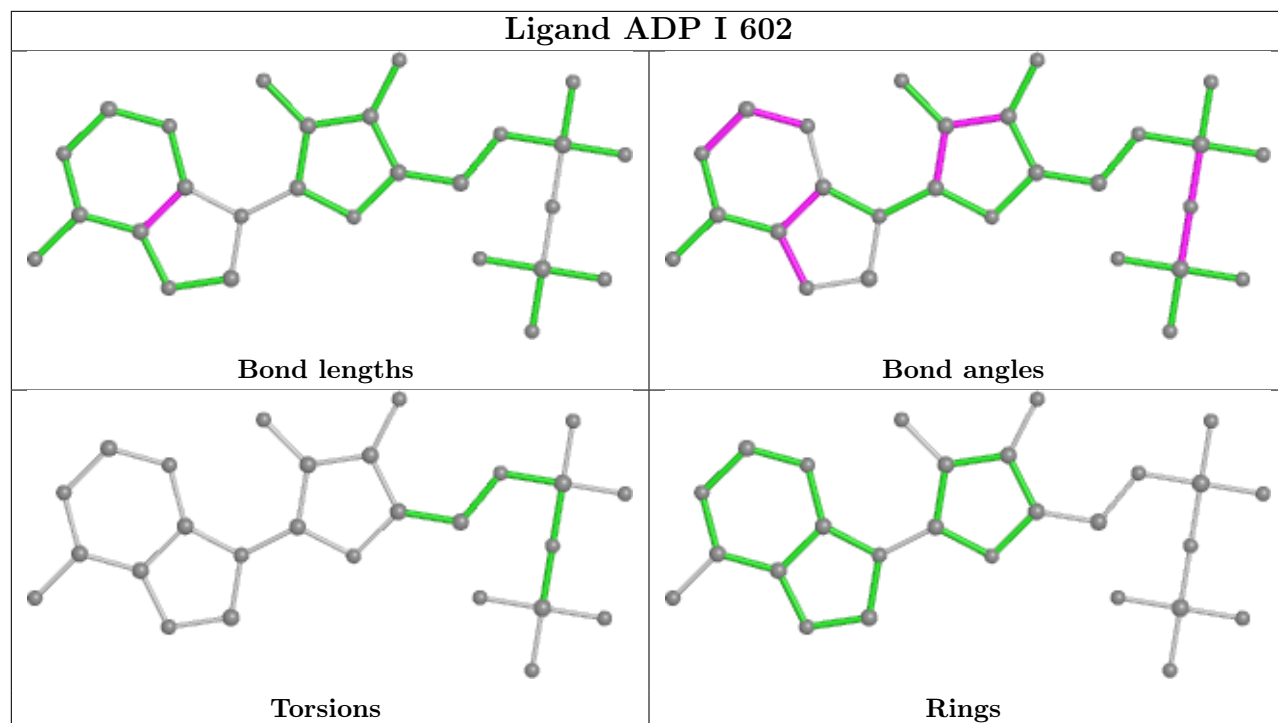




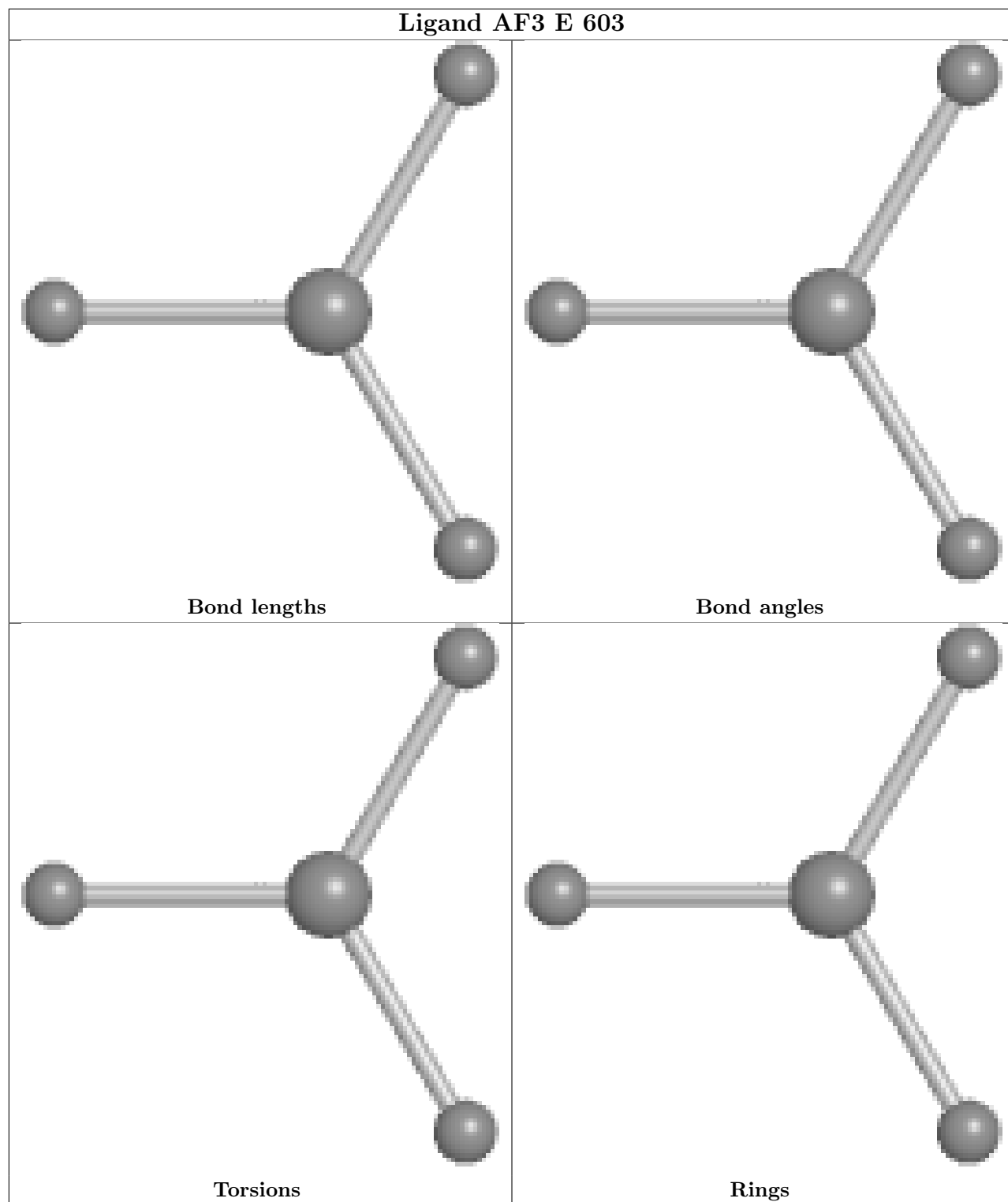


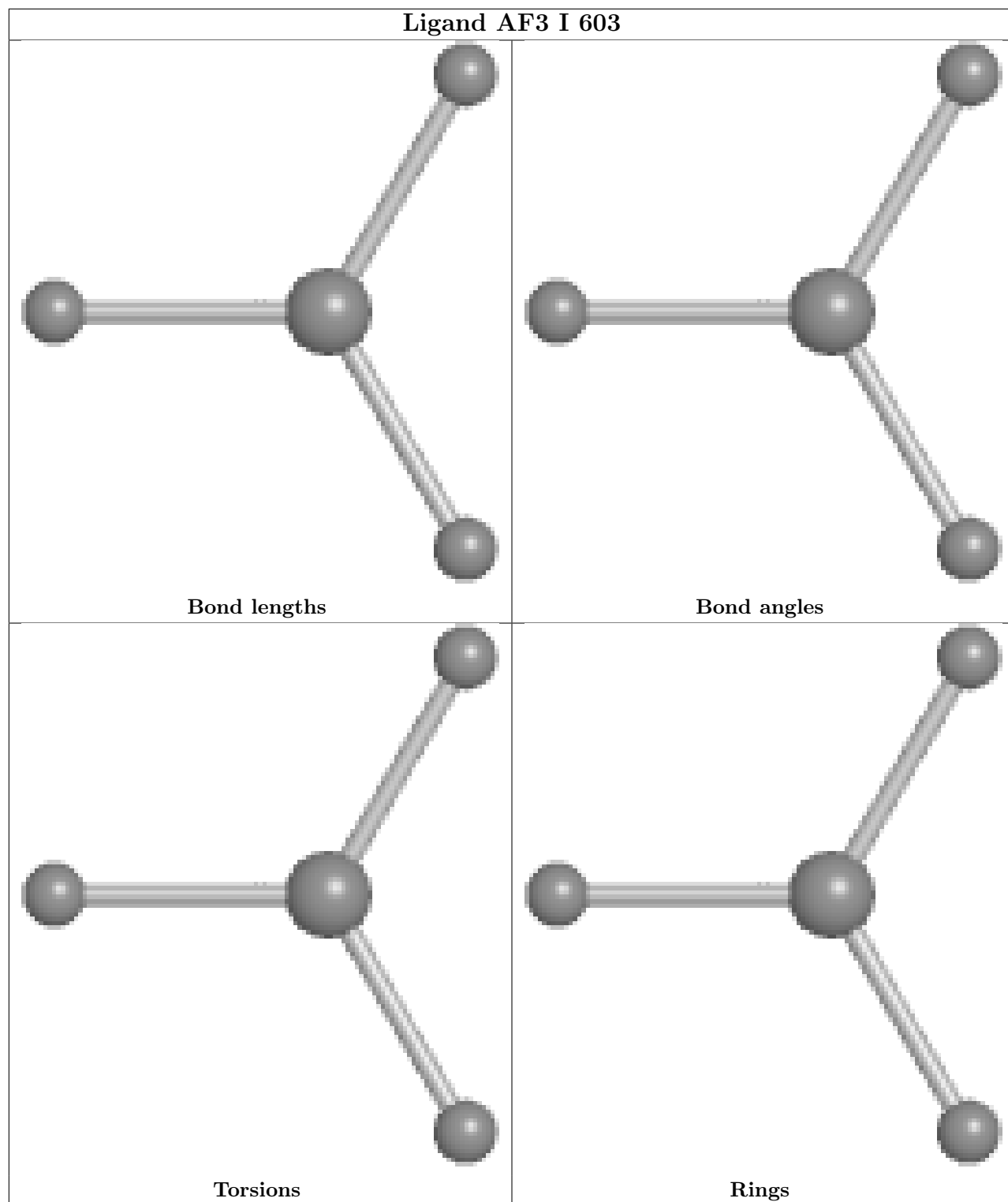












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

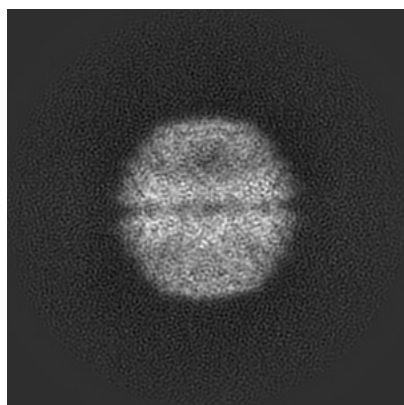
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26120. These allow visual inspection of the internal detail of the map and identification of artifacts.

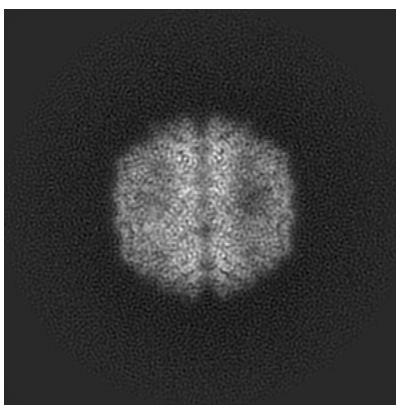
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

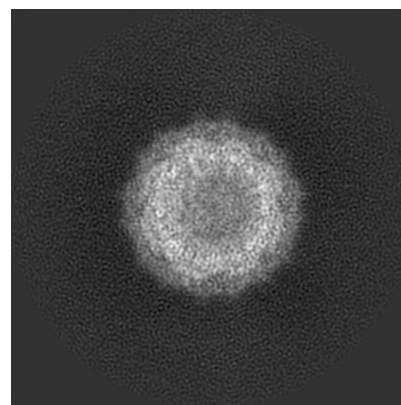
#### 6.1.1 Primary map



X



Y

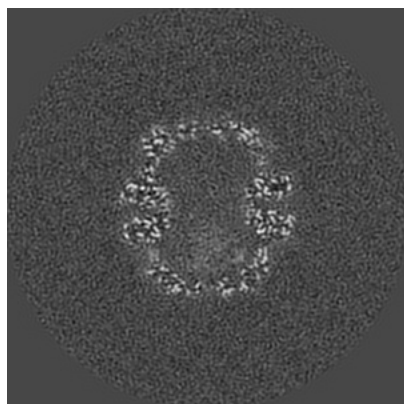


Z

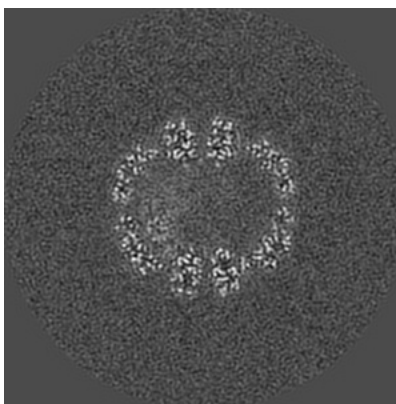
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

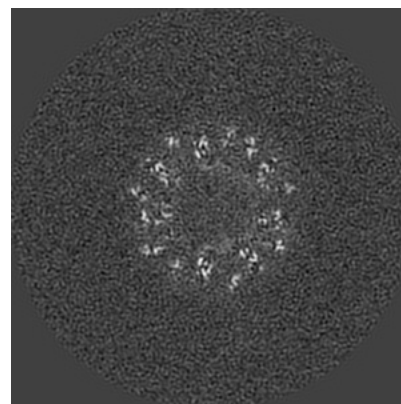
#### 6.2.1 Primary map



X Index: 160



Y Index: 160

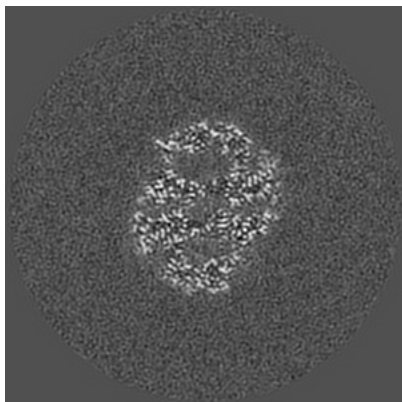


Z Index: 160

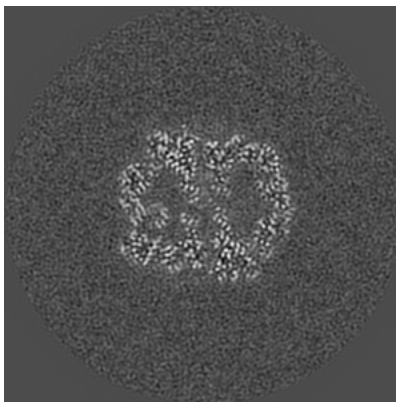
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

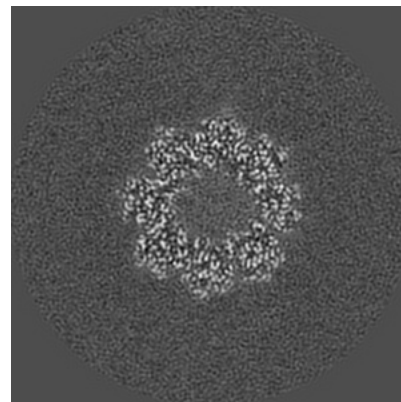
### 6.3.1 Primary map



X Index: 198



Y Index: 188



Z Index: 148

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

## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 4.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

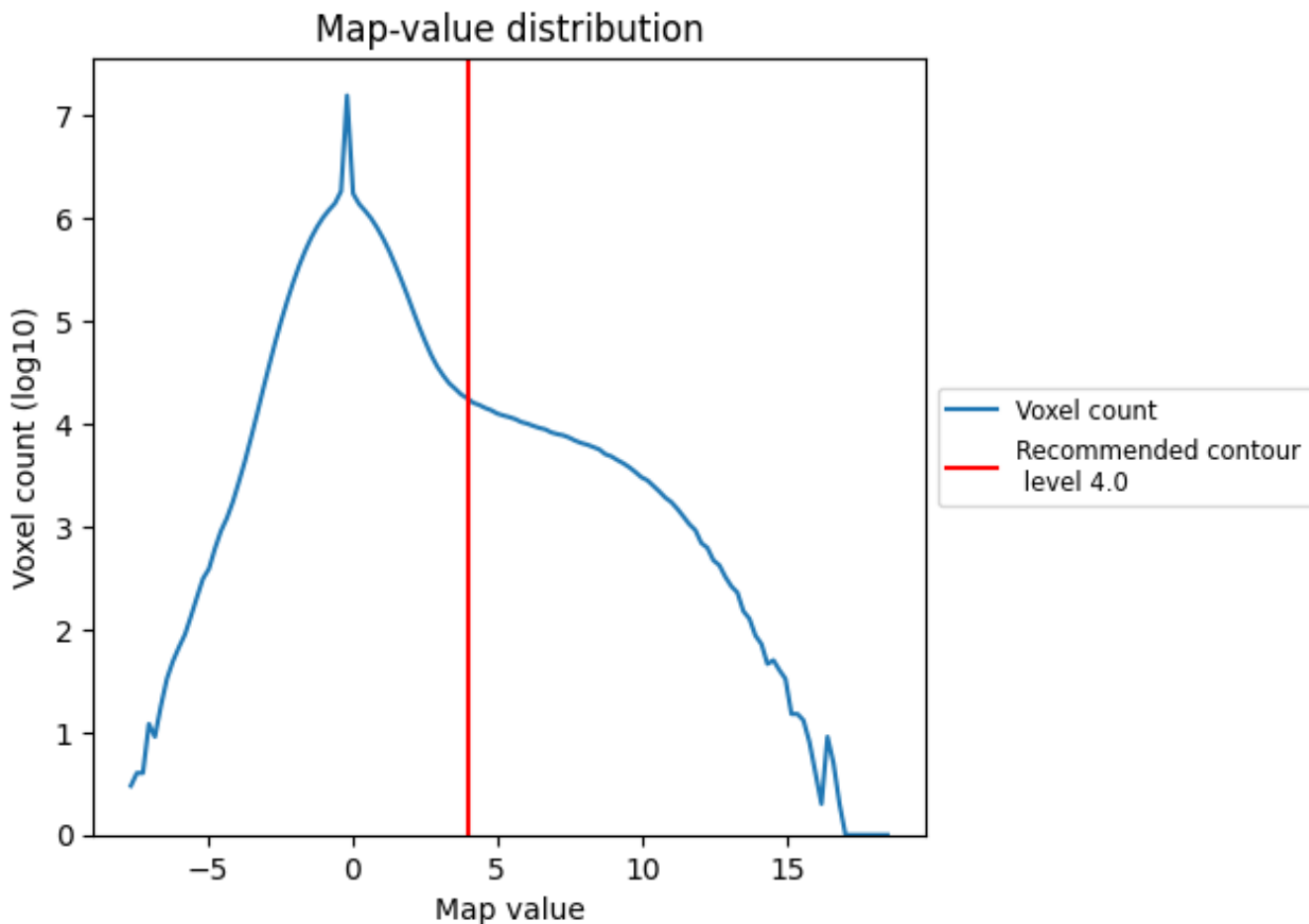
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

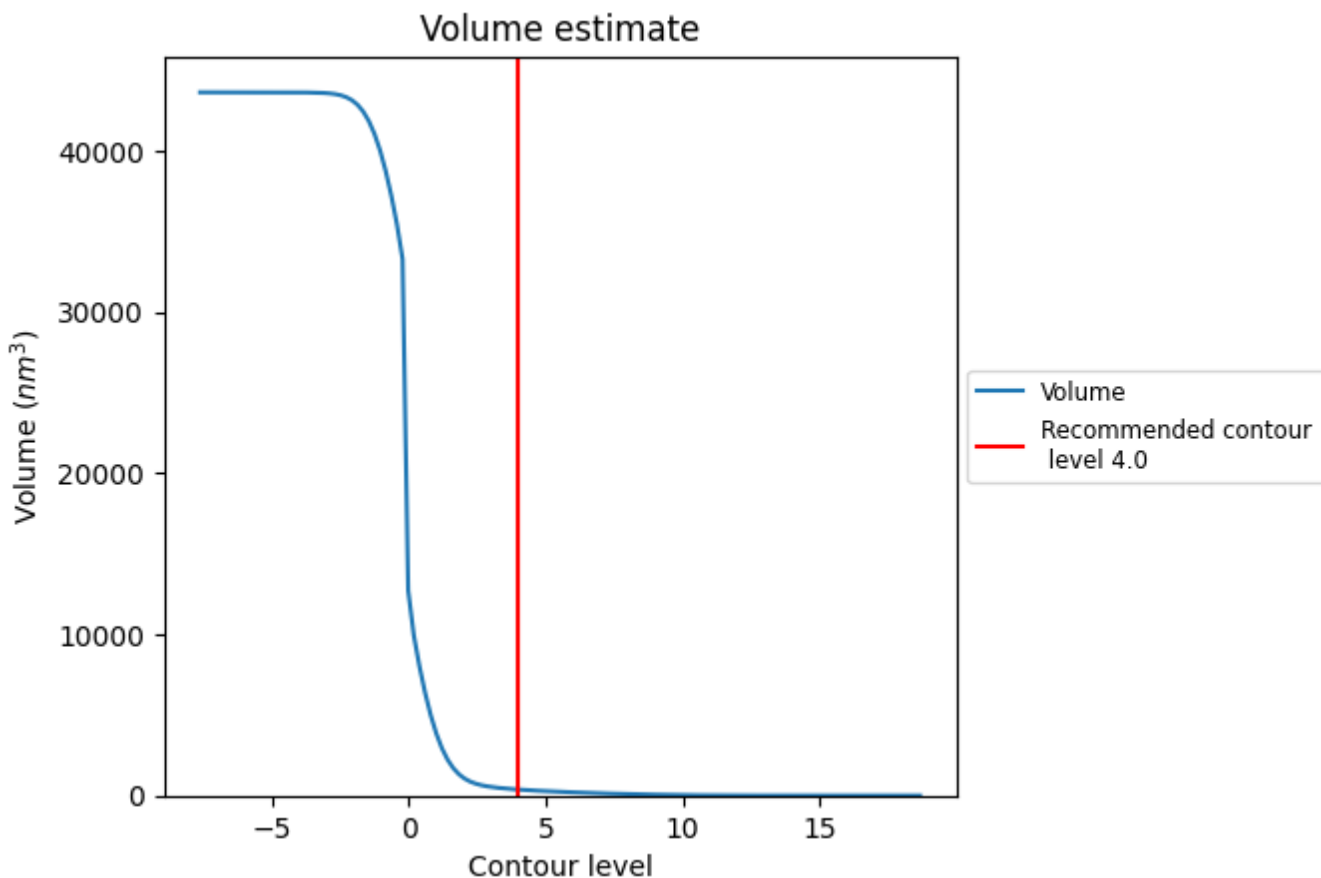
This section contains the results of statistical analysis of the map.

### 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](#)

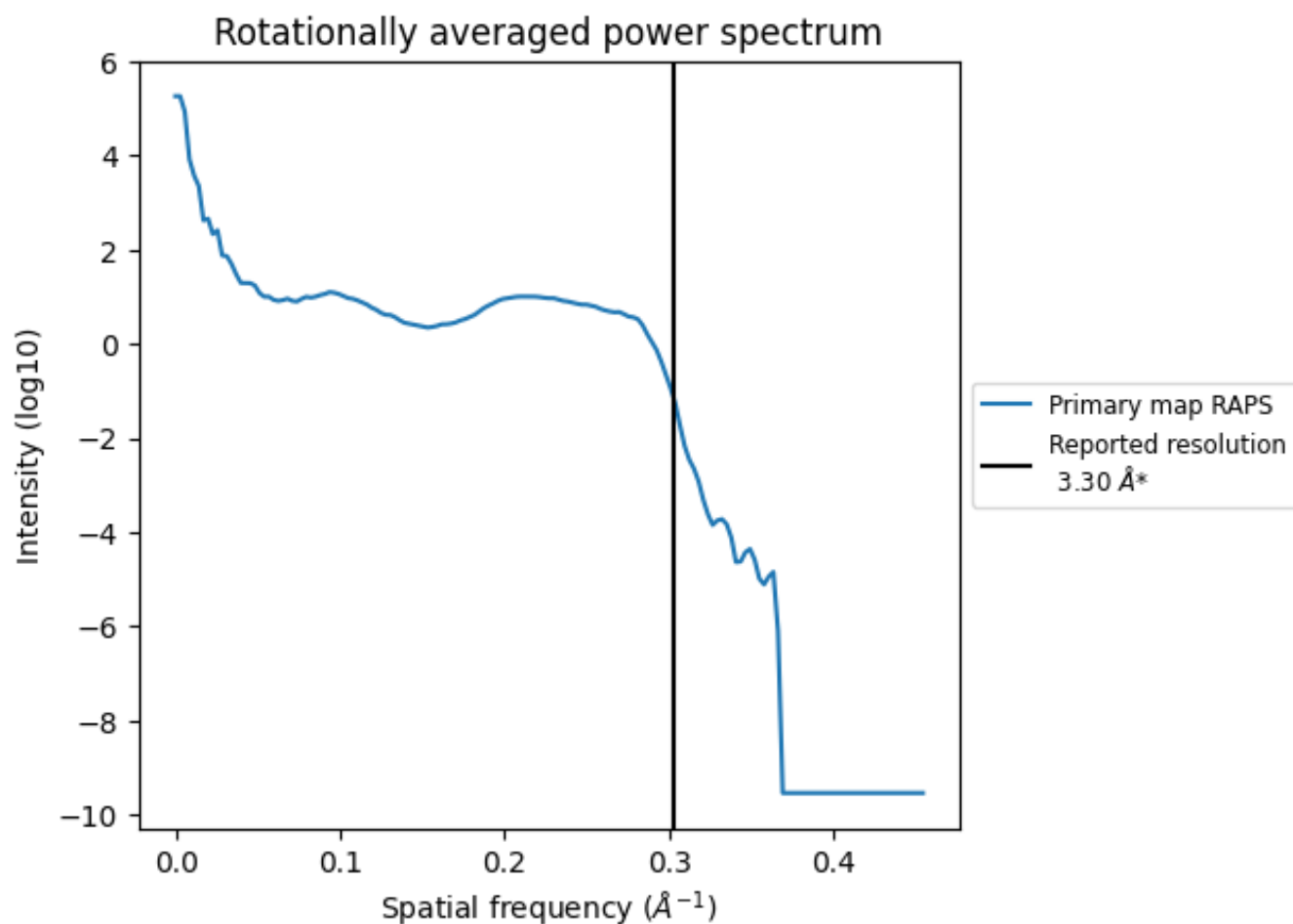


The volume at the recommended contour level is 372  $\text{nm}^3$ ; this corresponds to an approximate mass of 336 kDa.

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 [\(i\)](#)



\*Reported resolution corresponds to spatial frequency of 0.303 Å<sup>-1</sup>

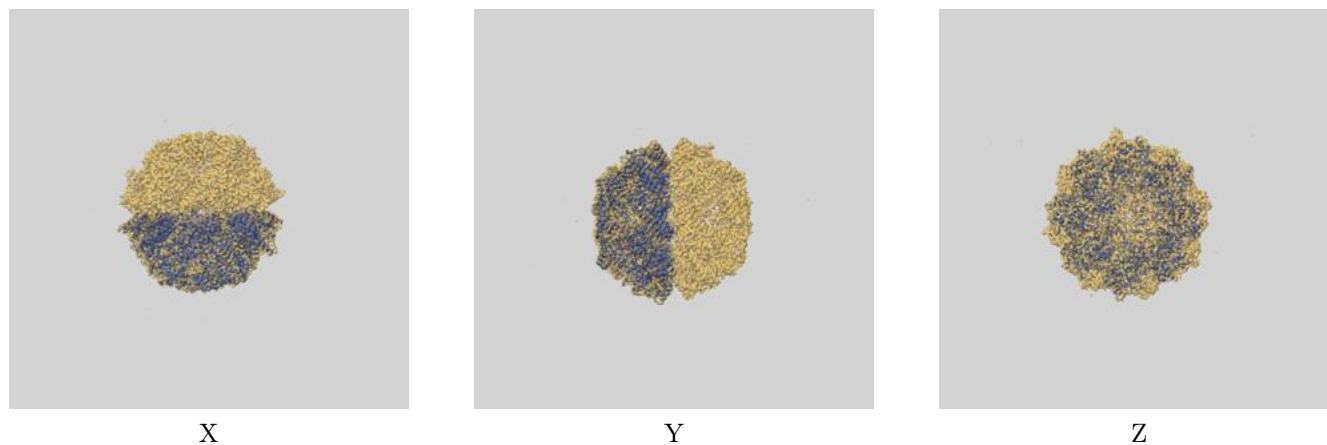
## 8 Fourier-Shell correlation

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

## 9 Map-model fit [i](#)

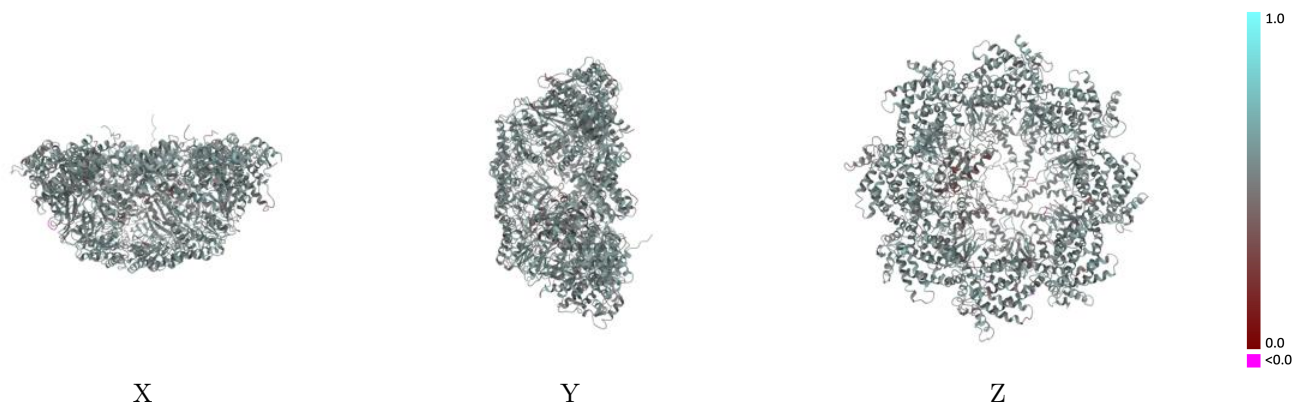
This section contains information regarding the fit between EMDB map EMD-26120 and PDB model 7TTN. Per-residue inclusion information can be found in section 3 on page 9.

### 9.1 Map-model overlay [i](#)



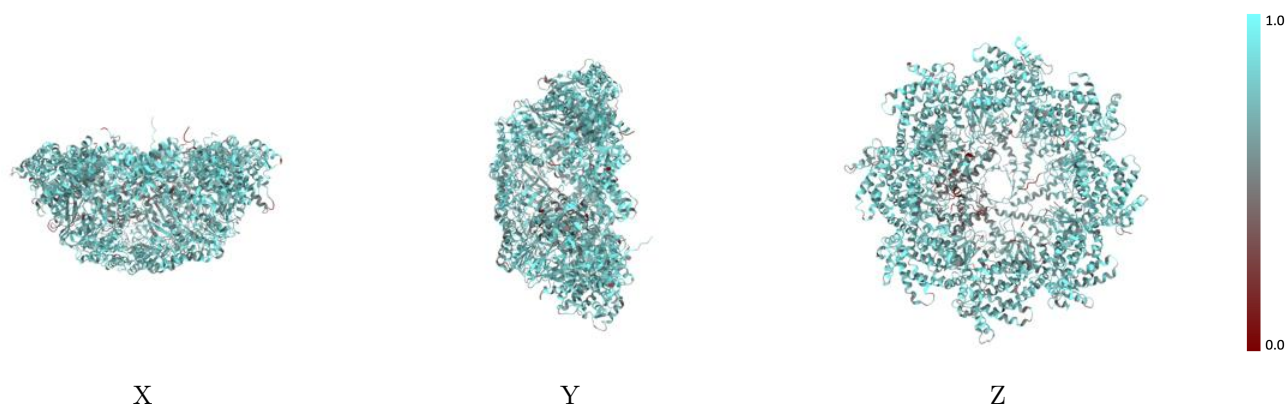
The images above show the 3D surface view of the map at the recommended contour level 4.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



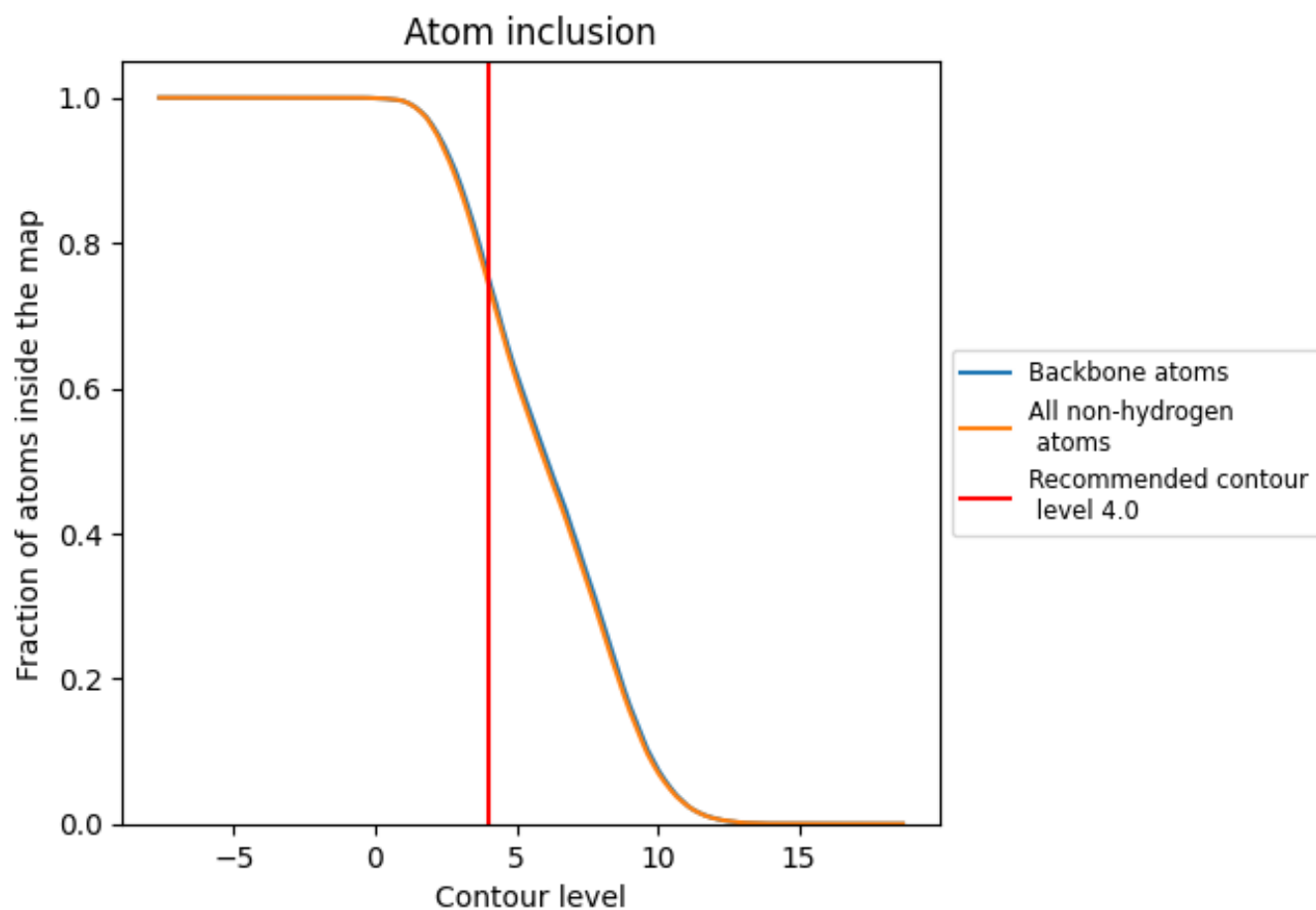
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (4.0).





















## 9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 74% 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 (4.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7436	 0.5260
A	 0.5554	 0.4510
B	 0.7691	 0.5380
C	 0.7794	 0.5350
D	 0.7659	 0.5310
E	 0.7565	 0.5240
F	 0.7449	 0.5280
G	 0.7540	 0.5250
H	 0.7682	 0.5310
I	 0.7590	 0.5320

