



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 05:43 PM UTC

PDB ID : 7TRG / pdb_00007trg
EMDB ID : EMD-26089
Title : The beta-tubulin folding intermediate I
Authors : Zhao, Y.; Frydman, J.; Chiu, W.
Deposited on : 2022-01-28
Resolution : 3.00 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:

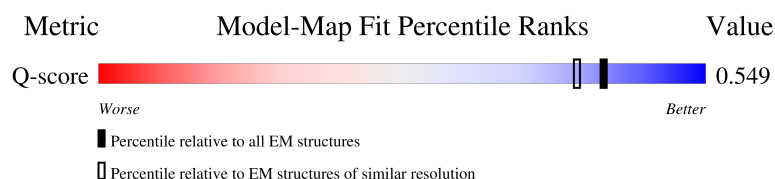
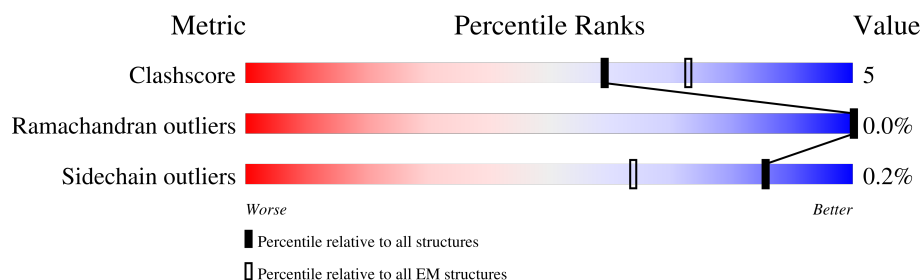
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.00 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	14081 (2.50 - 3.50)

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	A	444	
2	B	547	
3	C	553	
4	D	541	

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Mol	Chain	Length	Quality of chain
5	E	535	
6	F	539	
7	G	556	
8	H	545	
9	I	531	

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
12	AF3	B	603	-	-	X	-
12	AF3	E	603	-	-	X	-
12	AF3	F	603	-	-	X	-

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 33714 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
1	A	170	Total	C	N	O	S	0	0
			1316	822	223	264	7		

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

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

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

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

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	473	GLY	-	insertion	UNP Q99832
C	474	SER	-	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	HIS	-	insertion	UNP Q99832
C	481	GLY	-	insertion	UNP Q99832
C	482	SER	-	insertion	UNP Q99832
C	535	ARG	-	insertion	UNP Q99832

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	527	Total	C	N	O	S	0	0
			4063	2544	710	779	30		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	526	Total	C	N	O	S	0	0
			3960	2478	699	764	19		

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	526	Total	C	N	O	S	0	0
			4028	2531	705	771	21		

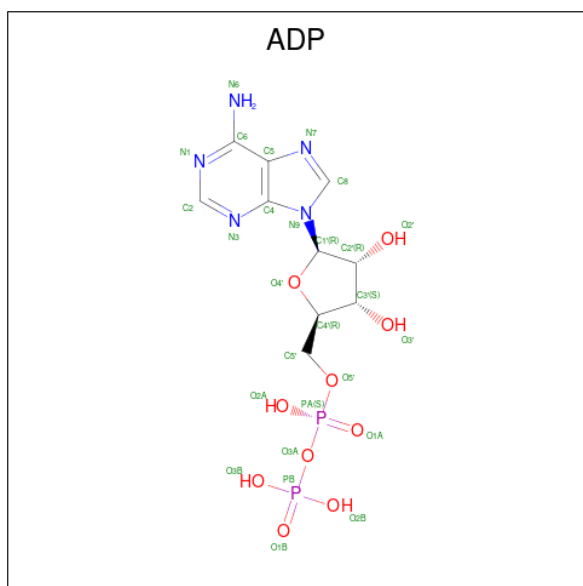
There is a discrepancy between the modelled and reference sequences:

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

- Molecule 10 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 11 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



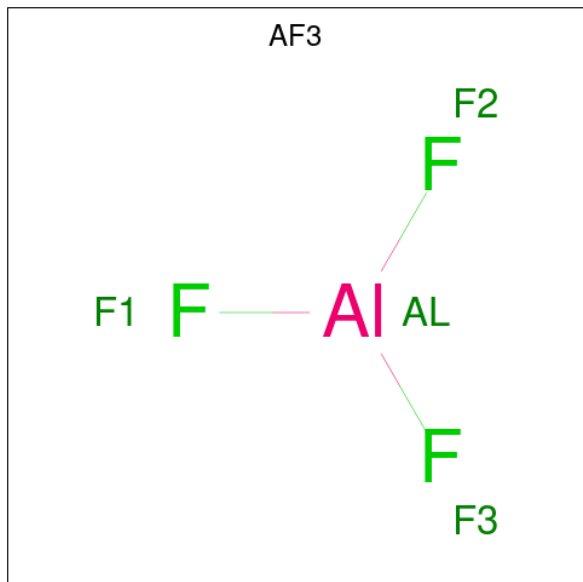
Mol	Chain	Residues	Atoms					AltConf
11	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
11	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
11	D	1	Total	C	N	O	P	0
			27	10	5	10	2	

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Mol	Chain	Residues	Atoms					AltConf
11	E	1	Total	C	N	O	P	0
			27	10	5	10	2	
11	F	1	Total	C	N	O	P	0
			27	10	5	10	2	
11	G	1	Total	C	N	O	P	0
			27	10	5	10	2	
11	H	1	Total	C	N	O	P	0
			27	10	5	10	2	
11	I	1	Total	C	N	O	P	0
			27	10	5	10	2	

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



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

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Mol	Chain	Residues	Atoms			AltConf
12	H	1	Total	Al	F	0
			4	1	3	
12	I	1	Total	Al	F	0
			4	1	3	

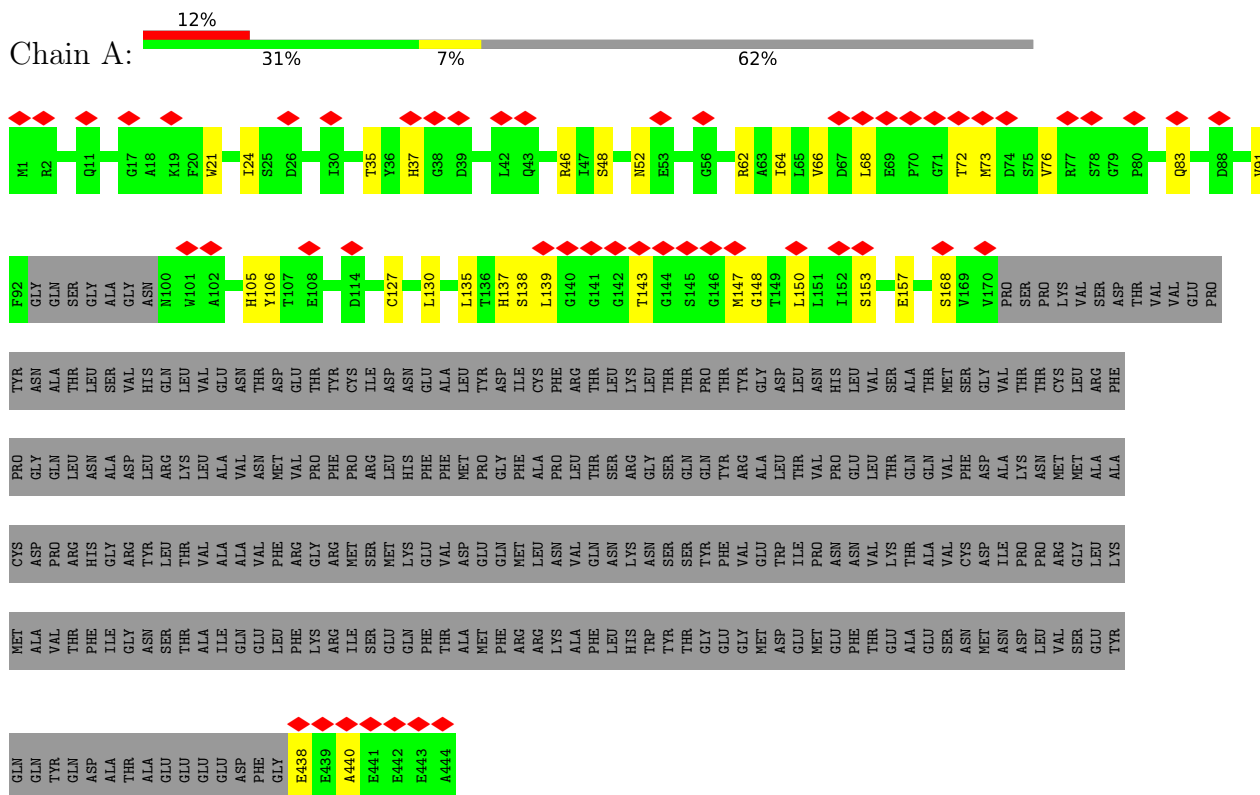
- Molecule 13 is water.

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

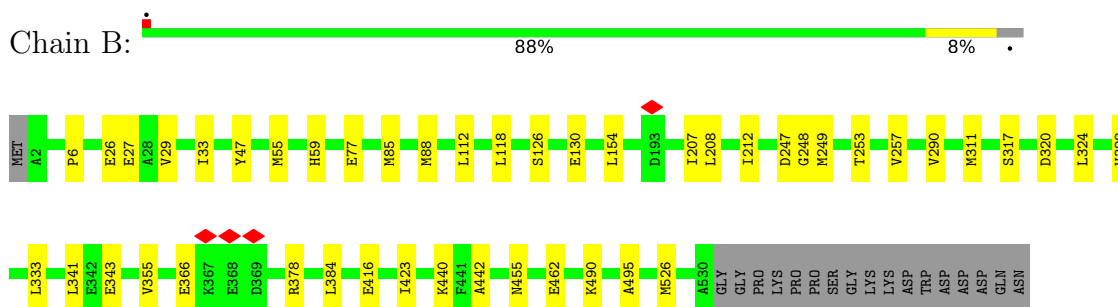
3 Residue-property plots

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.

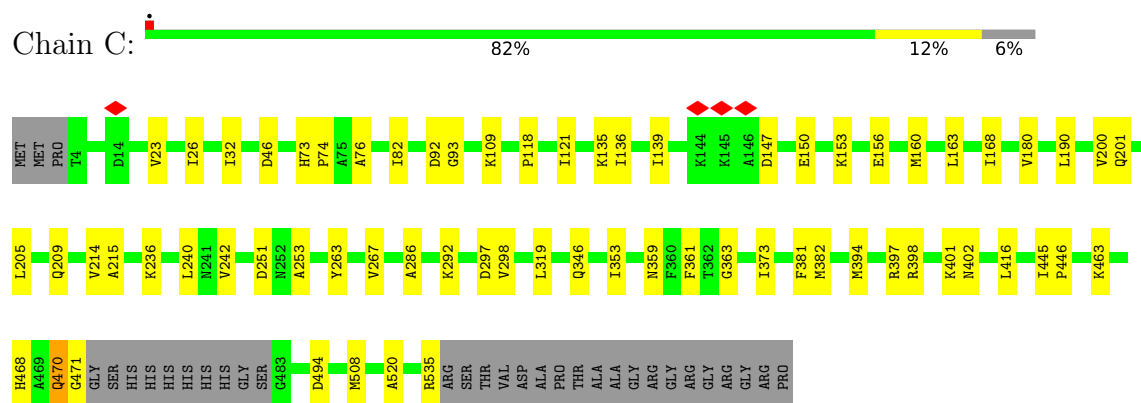
- Molecule 1: Tubulin beta chain



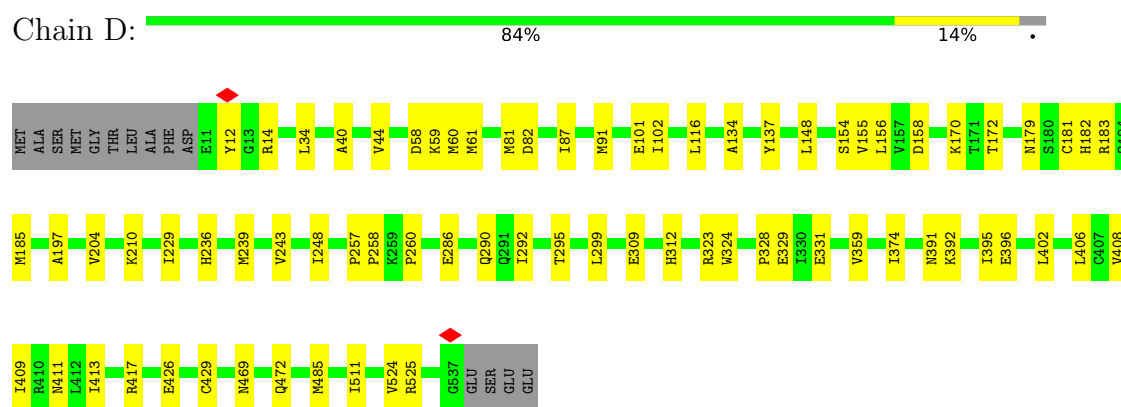
- Molecule 2: T-complex protein 1 subunit theta



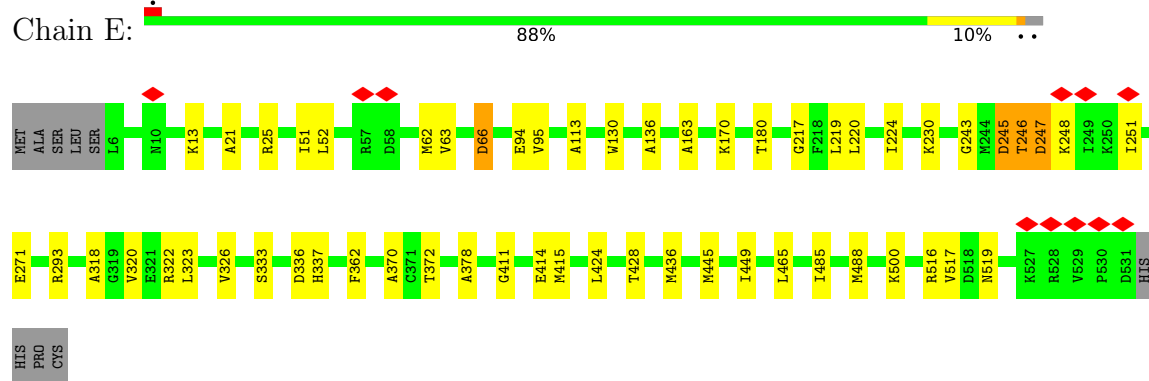
- Molecule 3: T-complex protein 1 subunit eta



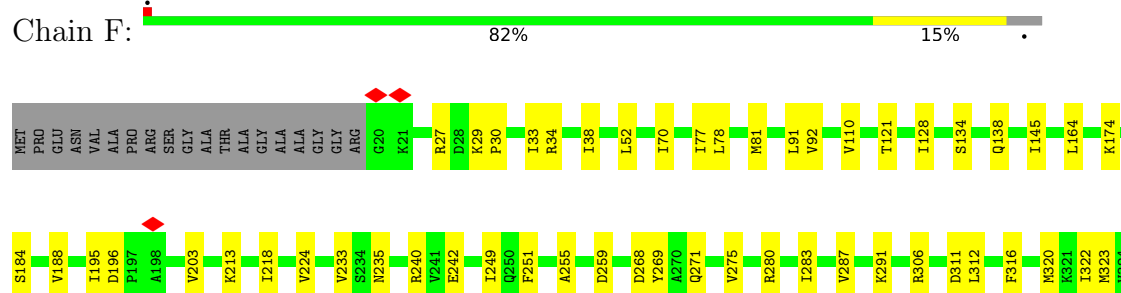
• Molecule 4: T-complex protein 1 subunit epsilon



• Molecule 5: T-complex protein 1 subunit beta

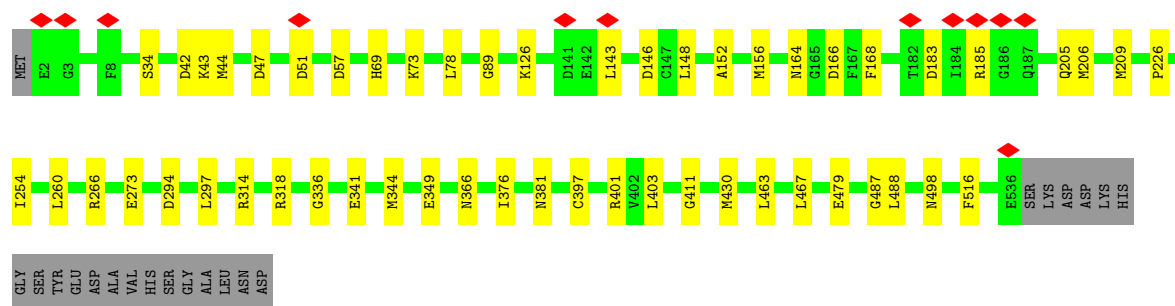
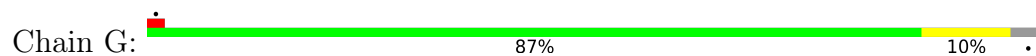


• Molecule 6: T-complex protein 1 subunit delta

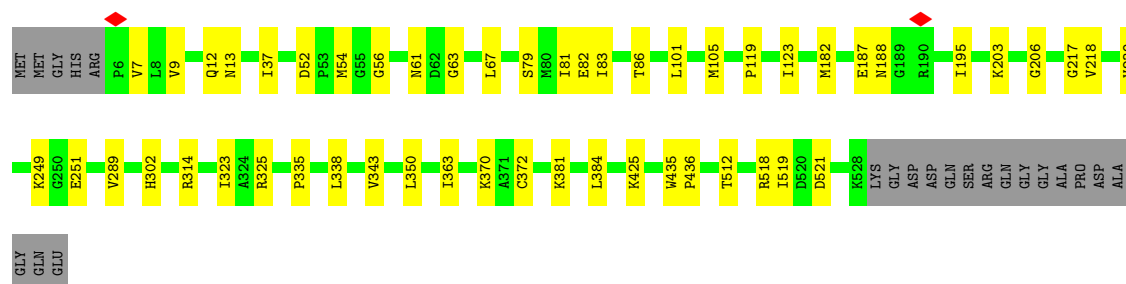
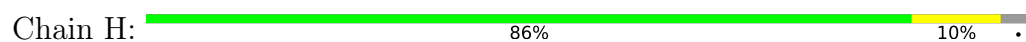




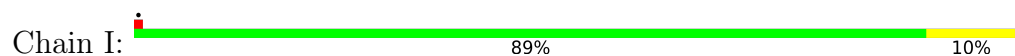
• Molecule 7: T-complex protein 1 subunit alpha



• 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	110984	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	21.237	Depositor
Minimum map value	-7.940	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	3.46	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 [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.17	0/1341	0.39	0/1811
2	B	0.14	0/4087	0.34	0/5525
3	C	0.20	0/4058	0.36	1/5476 (0.0%)
4	D	0.15	0/4112	0.36	0/5539
5	E	0.27	3/4004 (0.1%)	0.43	6/5399 (0.1%)
6	F	0.14	0/3956	0.32	0/5338
7	G	0.17	0/4103	0.39	2/5540 (0.0%)
8	H	0.17	0/4110	0.36	0/5544
9	I	0.14	0/4075	0.36	0/5494
All	All	0.18	3/33846 (0.0%)	0.37	9/45666 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	66	ASP	C-O	-7.43	1.14	1.23
5	E	66	ASP	C-N	-5.70	1.26	1.33
5	E	243	GLY	C-O	-5.24	1.16	1.23

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	66	ASP	CA-CB-CG	8.05	120.65	112.60
5	E	245	ASP	CA-CB-CG	7.10	119.70	112.60
7	G	57	ASP	CA-C-N	6.31	126.99	119.98
7	G	57	ASP	C-N-CA	6.31	126.99	119.98
5	E	246	THR	N-CA-C	-6.14	103.80	111.90
5	E	66	ASP	CB-CA-C	5.66	119.95	109.54
5	E	66	ASP	CA-C-N	5.64	126.21	120.00
5	E	66	ASP	C-N-CA	5.64	126.21	120.00
3	C	468	HIS	O-C-N	-5.26	115.20	122.46

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	1316	0	1246	20	0
2	B	4029	0	4099	31	0
3	C	4003	0	4106	48	0
4	D	4063	0	4183	50	0
5	E	3960	0	4077	37	0
6	F	3924	0	4131	52	0
7	G	4063	0	4219	34	0
8	H	4064	0	4202	33	0
9	I	4028	0	4166	30	0
10	B	1	0	0	0	0
10	C	1	0	0	0	0
10	D	1	0	0	0	0
10	E	1	0	0	0	0
10	F	1	0	0	0	0
10	G	1	0	0	0	0
10	H	1	0	0	0	0
10	I	1	0	0	0	0
11	B	27	0	12	2	0
11	C	27	0	12	0	0
11	D	27	0	12	0	0
11	E	27	0	12	0	0
11	F	27	0	12	0	0
11	G	27	0	12	1	0
11	H	27	0	12	0	0
11	I	27	0	12	1	0
12	B	4	0	0	2	0
12	C	4	0	0	0	0
12	D	4	0	0	0	0
12	E	4	0	0	2	0
12	F	4	0	0	3	0
12	G	4	0	0	0	0
12	H	4	0	0	0	0
12	I	4	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	33714	0	34525	311	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 5.

All (311) 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)
9:I:198:HIS:HD1	9:I:199:LYS:HG3	1.47	0.79
3:C:201:GLN:HA	3:C:382:MET:HE1	1.67	0.77
1:A:83:GLN:OE1	1:A:83:GLN:N	2.20	0.71
4:D:426:GLU:N	4:D:426:GLU:OE2	2.23	0.71
4:D:485:MET:HE3	4:D:485:MET:HA	1.73	0.70
3:C:147:ASP:HB3	3:C:150:GLU:H	1.57	0.69
7:G:479:GLU:OE2	7:G:479:GLU:N	2.23	0.69
3:C:402:ASN:HB2	3:C:508:MET:HE1	1.72	0.68
5:E:465:LEU:HD13	5:E:485:ILE:HD12	1.75	0.68
6:F:138:GLN:OE1	6:F:527:ARG:NH1	2.26	0.67
3:C:150:GLU:HA	3:C:153:LYS:HE2	1.76	0.66
6:F:476:THR:HG23	6:F:500:ILE:HD11	1.78	0.66
5:E:248:LYS:HE3	6:F:259:ASP:HB2	1.77	0.66
3:C:190:LEU:O	3:C:397:ARG:NH1	2.29	0.65
9:I:118:ILE:HG21	9:I:432:ARG:HB2	1.77	0.65
4:D:309:GLU:OE1	4:D:309:GLU:N	2.29	0.65
6:F:224:VAL:HB	6:F:387:THR:HG23	1.77	0.65
5:E:220:LEU:HD11	5:E:323:LEU:HD11	1.77	0.64
2:B:26:GLU:HG2	2:B:27:GLU:HG3	1.79	0.64
8:H:12:GLN:OE1	8:H:13:ASN:N	2.30	0.64
1:A:143:THR:HA	1:A:147:MET:HB3	1.80	0.63
6:F:416:VAL:O	6:F:419:ARG:NH1	2.32	0.63
5:E:224:ILE:HD11	5:E:230:LYS:HD3	1.80	0.62
4:D:286:GLU:O	4:D:290:GLN:HG2	2.00	0.62
7:G:209:MET:HE3	7:G:376:ILE:HD12	1.80	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:445:MET:O	5:E:449:ILE:HG12	2.00	0.61
2:B:257:VAL:HG23	3:C:253:ALA:HA	1.82	0.60
7:G:266:ARG:NH1	7:G:273:GLU:OE2	2.33	0.60
7:G:411:GLY:O	7:G:498:ASN:ND2	2.32	0.60
7:G:467:LEU:HD11	7:G:488:LEU:HD13	1.83	0.60
2:B:341:LEU:HD12	2:B:341:LEU:H	1.66	0.60
4:D:155:VAL:HG23	4:D:156:LEU:H	1.66	0.60
3:C:118:PRO:HA	3:C:121:ILE:HD12	1.84	0.60
7:G:143:LEU:HB3	7:G:146:ASP:OD1	2.02	0.59
7:G:146:ASP:OD1	7:G:146:ASP:N	2.34	0.59
8:H:251:GLU:N	8:H:251:GLU:OE1	2.35	0.59
6:F:235:ASN:ND2	6:F:322:ILE:O	2.35	0.59
2:B:247:ASP:OD1	2:B:248:GLY:N	2.36	0.59
2:B:366:GLU:N	2:B:366:GLU:OE1	2.36	0.59
6:F:195:ILE:HG21	6:F:203:VAL:HG22	1.85	0.59
1:A:438:GLU:HG3	1:A:440:ALA:H	1.67	0.59
5:E:414:GLU:OE2	5:E:500:LYS:NZ	2.34	0.58
1:A:157:GLU:OE2	8:H:314:ARG:NE	2.34	0.58
5:E:94:GLU:HG3	5:E:95:VAL:HG13	1.84	0.58
8:H:187:GLU:CD	8:H:188:ASN:H	2.12	0.58
2:B:59:HIS:HB2	3:C:535:ARG:HH12	1.69	0.57
6:F:255:ALA:O	6:F:306:ARG:NH2	2.37	0.57
6:F:91:LEU:HD12	6:F:110:VAL:HG13	1.86	0.56
7:G:42:ASP:OD1	8:H:518:ARG:NH2	2.38	0.56
3:C:32:ILE:HG13	3:C:76:ALA:HB1	1.87	0.56
2:B:462:GLU:N	2:B:462:GLU:OE1	2.38	0.56
4:D:179:ASN:HA	4:D:182:HIS:HB3	1.85	0.56
6:F:164:LEU:HD23	6:F:188:VAL:HG21	1.86	0.56
8:H:206:GLY:HA3	9:I:87:ILE:HG13	1.86	0.56
8:H:217:GLY:HA3	8:H:363:ILE:O	2.06	0.56
3:C:46:ASP:OD2	3:C:46:ASP:N	2.37	0.56
3:C:267:VAL:HG22	4:D:260:PRO:HD3	1.88	0.56
4:D:172:THR:HG21	4:D:408:VAL:HG21	1.87	0.55
1:A:139:LEU:HD22	1:A:168:SER:HB2	1.88	0.55
1:A:150:LEU:HB3	1:A:153:SER:HB3	1.88	0.55
4:D:170:LYS:HD3	4:D:183:ARG:HA	1.87	0.55
6:F:235:ASN:HD22	6:F:323:MET:HA	1.71	0.55
9:I:135:GLU:OE1	9:I:498:TYR:OH	2.24	0.55
5:E:245:ASP:O	5:E:246:THR:C	2.50	0.55
2:B:29:VAL:O	2:B:33:ILE:HG12	2.07	0.55
9:I:80:VAL:HG21	9:I:511:ILE:HG13	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:317:SER:HG	2:B:320:ASP:H	1.52	0.54
9:I:236:SER:O	9:I:270:ARG:NH1	2.40	0.54
1:A:68:LEU:HD23	1:A:68:LEU:H	1.73	0.54
4:D:87:ILE:O	4:D:91:MET:HG2	2.07	0.54
1:A:127:CYS:SG	1:A:130:LEU:HB3	2.48	0.54
6:F:480:LEU:HD13	6:F:500:ILE:HD12	1.90	0.54
9:I:24:ILE:HD13	9:I:103:LEU:HB3	1.90	0.54
5:E:248:LYS:HD3	5:E:271:GLU:HG2	1.89	0.54
7:G:44:MET:HE3	8:H:519:ILE:HG21	1.89	0.54
7:G:78:LEU:HD11	7:G:516:PHE:HB3	1.90	0.54
9:I:127:LYS:HD3	9:I:509:THR:HG21	1.90	0.54
3:C:82:ILE:HG21	3:C:520:ALA:HB2	1.90	0.54
3:C:92:ASP:OD2	3:C:93:GLY:N	2.41	0.53
2:B:126:SER:O	2:B:130:GLU:HG3	2.09	0.53
3:C:136:ILE:HD11	3:C:416:LEU:HD11	1.91	0.53
8:H:218:VAL:HG21	8:H:323:ILE:HG12	1.90	0.53
9:I:34:LEU:HD12	9:I:96:VAL:HG11	1.90	0.53
5:E:170:LYS:NZ	12:E:603:AF3:F3	2.27	0.53
6:F:27:ARG:HA	6:F:27:ARG:NE	2.24	0.53
9:I:277:LEU:HD22	9:I:339:LEU:HG	1.91	0.52
4:D:236:HIS:HB3	4:D:239:MET:HG3	1.91	0.52
6:F:268:ASP:OD2	6:F:269:TYR:N	2.41	0.52
6:F:233:VAL:HG12	6:F:325:ILE:HG12	1.91	0.52
6:F:394:ASN:O	6:F:398:ILE:HG13	2.09	0.52
4:D:257:PRO:HD2	5:E:251:ILE:HD11	1.90	0.52
8:H:82:GLU:O	8:H:86:THR:HG23	2.09	0.52
7:G:152:ALA:O	7:G:156:MET:HG3	2.10	0.52
4:D:58:ASP:OD2	5:E:516:ARG:NH1	2.44	0.51
2:B:33:ILE:HD12	2:B:112:LEU:HB3	1.92	0.51
6:F:394:ASN:HB3	6:F:397:VAL:HG23	1.93	0.51
3:C:535:ARG:HH11	3:C:535:ARG:HG2	1.75	0.51
8:H:249:LYS:HG3	9:I:243:GLU:HG3	1.92	0.51
9:I:218:HIS:HB3	9:I:221:MET:HG3	1.93	0.51
3:C:402:ASN:HB2	3:C:508:MET:CE	2.41	0.51
9:I:272:LYS:O	9:I:276:GLU:HG2	2.11	0.50
4:D:154:SER:HA	4:D:417:ARG:HA	1.93	0.50
9:I:195:GLU:HB2	9:I:384:LEU:HD13	1.94	0.50
2:B:207:ILE:HG21	2:B:355:VAL:HG23	1.94	0.50
3:C:209:GLN:HG2	3:C:373:ILE:HB	1.93	0.50
6:F:52:LEU:O	6:F:468:ASN:ND2	2.42	0.50
6:F:421:LEU:HD21	6:F:509:VAL:HG21	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:166:ASP:N	7:G:166:ASP:OD1	2.44	0.50
1:A:48:SER:O	1:A:62:ARG:NH1	2.43	0.50
8:H:101:LEU:O	8:H:105:MET:HG3	2.12	0.50
2:B:212:ILE:HD11	2:B:384:LEU:HD21	1.92	0.50
8:H:203:LYS:HD2	8:H:384:LEU:HB3	1.93	0.50
2:B:85:MET:HA	2:B:88:MET:HE3	1.94	0.50
6:F:213:LYS:HB3	6:F:391:ARG:HH11	1.76	0.50
2:B:253:THR:OG1	9:I:239:TYR:OH	2.30	0.49
4:D:12:TYR:O	4:D:14:ARG:HG3	2.12	0.49
6:F:70:ILE:HD12	6:F:396:LEU:HD13	1.93	0.49
7:G:89:GLY:HA2	11:G:602:ADP:O3B	2.11	0.49
6:F:174:LYS:CE	12:F:603:AF3:F3	2.51	0.49
2:B:47:TYR:O	2:B:455:ASN:ND2	2.41	0.49
3:C:168:ILE:HG22	3:C:205:LEU:HD21	1.95	0.49
5:E:66:ASP:HA	12:E:603:AF3:F3	2.02	0.49
6:F:174:LYS:NZ	12:F:603:AF3:F3	2.36	0.49
8:H:37:ILE:HD11	8:H:63:GLY:HA2	1.94	0.49
8:H:289:VAL:HG21	8:H:350:LEU:HD13	1.93	0.49
3:C:251:ASP:N	3:C:251:ASP:OD1	2.43	0.49
6:F:399:GLU:N	6:F:399:GLU:OE2	2.45	0.49
6:F:29:LYS:O	6:F:33:ILE:HG12	2.12	0.49
8:H:182:MET:SD	8:H:372:CYS:HB3	2.53	0.49
3:C:200:VAL:HG11	3:C:353:ILE:HG22	1.95	0.49
4:D:134:ALA:HB1	4:D:525:ARG:HG3	1.95	0.48
7:G:34:SER:OG	7:G:43:LYS:NZ	2.43	0.48
8:H:325:ARG:HG2	8:H:370:LYS:HB2	1.95	0.48
7:G:226:PRO:HB3	8:H:188:ASN:HD22	1.77	0.48
6:F:271:GLN:O	6:F:275:VAL:HG23	2.13	0.48
9:I:37:ASN:HD21	9:I:63:LEU:HD22	1.77	0.48
4:D:392:LYS:O	4:D:396:GLU:HG2	2.14	0.48
9:I:59:ASP:OD2	9:I:60:GLY:N	2.47	0.48
5:E:411:GLY:O	5:E:415:MET:HG2	2.14	0.48
7:G:397:CYS:O	7:G:401:ARG:HG2	2.14	0.48
5:E:217:GLY:HA3	5:E:362:PHE:O	2.14	0.47
6:F:34:ARG:O	6:F:38:ILE:HG12	2.13	0.47
5:E:21:ALA:HB1	5:E:25:ARG:HH21	1.78	0.47
5:E:428:THR:HG21	5:E:436:MET:HE3	1.96	0.47
3:C:136:ILE:HG13	3:C:416:LEU:HD21	1.95	0.47
7:G:183:ASP:C	7:G:185:ARG:H	2.23	0.47
7:G:381:ASN:OD1	7:G:381:ASN:N	2.45	0.47
4:D:312:HIS:CE1	5:E:333:SER:H	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:302:HIS:HB2	9:I:334:ASN:HB2	1.95	0.47
4:D:312:HIS:ND1	5:E:333:SER:O	2.47	0.47
7:G:349:GLU:HB3	7:G:366:ASN:HB2	1.95	0.47
7:G:126:LYS:HE2	7:G:126:LYS:HB3	1.62	0.47
1:A:35:THR:HG23	1:A:37:HIS:CE1	2.50	0.47
1:A:46:ARG:HE	1:A:46:ARG:HA	1.78	0.47
2:B:324:LEU:O	2:B:328:VAL:HG22	2.14	0.47
3:C:346:GLN:HB3	3:C:363:GLY:HA3	1.95	0.47
6:F:30:PRO:HB3	6:F:533:ASP:HB2	1.97	0.47
4:D:210:LYS:NZ	4:D:229:ILE:O	2.48	0.47
3:C:463:LYS:NZ	3:C:494:ASP:OD1	2.34	0.46
4:D:391:ASN:O	4:D:395:ILE:HG12	2.15	0.46
6:F:145:ILE:HD12	6:F:516:VAL:HG13	1.97	0.46
6:F:128:ILE:HD12	6:F:446:MET:HB3	1.96	0.46
4:D:59:LYS:HG3	5:E:519:ASN:HB3	1.96	0.46
4:D:148:LEU:HD13	4:D:429:CYS:SG	2.54	0.46
6:F:412:ILE:O	6:F:416:VAL:HG23	2.14	0.46
2:B:59:HIS:HB2	3:C:535:ARG:NH1	2.29	0.46
3:C:163:LEU:HD22	3:C:168:ILE:HD11	1.97	0.46
8:H:79:SER:O	8:H:83:ILE:HG23	2.16	0.46
8:H:435:TRP:HB2	8:H:436:PRO:HD3	1.97	0.46
1:A:66:VAL:HG22	1:A:91:VAL:HB	1.98	0.46
3:C:23:VAL:HG13	3:C:109:LYS:HE3	1.97	0.46
8:H:52:ASP:OD1	8:H:56:GLY:N	2.49	0.45
7:G:294:ASP:HA	7:G:297:LEU:HD12	1.98	0.45
5:E:326:VAL:HG23	5:E:370:ALA:HB3	1.97	0.45
8:H:61:ASN:OD1	8:H:61:ASN:O	2.34	0.45
5:E:488:MET:HE2	5:E:488:MET:HA	1.97	0.45
8:H:119:PRO:O	8:H:123:ILE:HG12	2.17	0.45
3:C:508:MET:SD	3:C:508:MET:N	2.89	0.45
9:I:189:PHE:HB3	9:I:319:ARG:HD3	1.98	0.45
11:I:602:ADP:O3B	12:I:603:AF3:F3	2.23	0.45
2:B:416:GLU:OE1	2:B:416:GLU:N	2.47	0.45
3:C:73:HIS:HB3	3:C:76:ALA:HB3	1.98	0.45
6:F:78:LEU:HB3	6:F:92:VAL:HG12	1.99	0.45
4:D:116:LEU:HD23	4:D:524:VAL:HG21	1.98	0.45
5:E:318:ALA:O	5:E:322:ARG:HG3	2.17	0.45
2:B:55:MET:HE2	2:B:55:MET:HB2	1.80	0.45
6:F:280:ARG:NE	7:G:336:GLY:O	2.49	0.45
7:G:164:ASN:OD1	7:G:205:GLN:NE2	2.48	0.45
6:F:77:ILE:HG22	6:F:81:MET:HE3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:283:ILE:O	6:F:287:VAL:HG23	2.18	0.44
7:G:487:GLY:HA3	7:G:498:ASN:ND2	2.30	0.44
1:A:21:TRP:HA	1:A:24:ILE:HG22	2.00	0.44
6:F:184:SER:O	6:F:188:VAL:HG23	2.17	0.44
9:I:196:MET:HE3	9:I:355:LEU:HD11	1.97	0.44
3:C:240:LEU:HB3	3:C:242:VAL:HG12	1.97	0.44
3:C:401:LYS:HD2	3:C:401:LYS:HA	1.69	0.44
4:D:328:PRO:HA	4:D:331:GLU:HG2	1.99	0.44
5:E:163:ALA:HB3	5:E:180:THR:HG23	2.00	0.44
4:D:248:ILE:HD12	4:D:299:LEU:HD22	1.98	0.44
8:H:239:VAL:HG12	8:H:343:VAL:HG22	1.98	0.44
4:D:60:MET:HE2	5:E:517:VAL:HG21	1.99	0.44
4:D:243:VAL:HG23	4:D:359:VAL:HB	2.00	0.44
2:B:490:LYS:HE3	2:B:495:ALA:HB2	1.97	0.44
3:C:156:GLU:O	3:C:160:MET:HG3	2.17	0.44
4:D:359:VAL:HG22	4:D:374:ILE:HG12	1.98	0.44
5:E:51:ILE:HG12	5:E:63:VAL:HG22	2.00	0.44
2:B:208:LEU:O	2:B:378:ARG:NH1	2.51	0.44
4:D:155:VAL:HG23	4:D:156:LEU:N	2.31	0.44
5:E:136:ALA:HB2	5:E:424:LEU:HD22	2.00	0.44
4:D:101:GLU:HG3	4:D:102:ILE:HG12	2.00	0.44
5:E:113:ALA:HB2	5:E:130:TRP:CH2	2.53	0.44
6:F:336:ILE:O	6:F:340:ILE:HG12	2.17	0.44
4:D:61:MET:HE1	4:D:81:MET:HG3	2.00	0.43
6:F:174:LYS:HE2	12:F:603:AF3:F3	2.07	0.43
3:C:214:VAL:HG12	3:C:361:PHE:HB2	2.00	0.43
3:C:263:TYR:O	3:C:267:VAL:HG23	2.19	0.43
6:F:218:ILE:HD11	6:F:397:VAL:HG12	2.00	0.43
9:I:98:ILE:HD12	9:I:504:LEU:HD21	2.00	0.43
4:D:156:LEU:HD13	4:D:158:ASP:OD1	2.18	0.43
6:F:432:LEU:HD23	6:F:432:LEU:HA	1.82	0.43
9:I:426:LYS:N	9:I:427:PRO:HD2	2.34	0.43
4:D:172:THR:HG21	4:D:408:VAL:HG11	2.00	0.43
6:F:291:LYS:HD3	6:F:320:MET:HB3	1.99	0.43
7:G:314:ARG:O	7:G:318:ARG:HG3	2.19	0.43
8:H:381:LYS:HE3	8:H:381:LYS:HB3	1.79	0.43
3:C:445:ILE:HB	3:C:446:PRO:HD3	1.99	0.43
3:C:470:GLN:HG3	3:C:471:GLY:N	2.33	0.43
4:D:116:LEU:HG	4:D:137:TYR:CE2	2.54	0.43
6:F:407:ASP:O	6:F:411:VAL:HG23	2.19	0.43
7:G:156:MET:HE1	7:G:168:PHE:CB	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:336:ASP:O	5:E:337:HIS:ND1	2.52	0.43
9:I:86:ASP:OD2	9:I:86:ASP:C	2.62	0.43
9:I:194:MET:HE3	9:I:194:MET:HB3	1.94	0.43
2:B:423:ILE:HG22	2:B:442:ALA:HB2	2.01	0.43
3:C:236:LYS:HB2	3:C:286:ALA:HA	2.01	0.43
1:A:135:LEU:HG	1:A:137:HIS:HD2	1.83	0.42
11:B:602:ADP:O3B	12:B:603:AF3:F3	2.27	0.42
3:C:267:VAL:HG11	4:D:258:PRO:HB2	2.01	0.42
3:C:297:ASP:OD1	3:C:298:VAL:N	2.52	0.42
4:D:292:ILE:O	4:D:295:THR:HG22	2.19	0.42
6:F:311:ASP:OD1	6:F:312:LEU:N	2.52	0.42
7:G:164:ASN:ND2	7:G:206:MET:SD	2.92	0.42
1:A:148:GLY:O	1:A:150:LEU:N	2.52	0.42
4:D:469:ASN:OD1	4:D:472:GLN:HG3	2.19	0.42
9:I:4:VAL:HG21	9:I:522:MET:HE2	2.01	0.42
3:C:135:LYS:O	3:C:139:ILE:HG12	2.20	0.42
4:D:82:ASP:HB2	5:E:13:LYS:HE2	2.01	0.42
4:D:323:ARG:HG2	4:D:324:TRP:CD1	2.55	0.42
8:H:335:PRO:O	8:H:338:LEU:HB2	2.19	0.42
9:I:182:GLN:H	9:I:182:GLN:CD	2.27	0.42
1:A:73:MET:HE2	1:A:73:MET:HB2	1.95	0.42
2:B:118:LEU:HD11	2:B:440:LYS:HG3	2.00	0.42
3:C:205:LEU:HD13	3:C:381:PHE:HE1	1.84	0.42
6:F:249:ILE:HG22	6:F:251:PHE:H	1.83	0.42
3:C:292:LYS:HG3	3:C:319:LEU:HD22	2.02	0.42
4:D:181:CYS:O	4:D:185:MET:HG2	2.19	0.42
4:D:329:GLU:OE2	4:D:329:GLU:N	2.53	0.42
5:E:219:LEU:HB2	5:E:372:THR:HG21	2.02	0.42
8:H:54:MET:HB2	8:H:54:MET:HE2	1.80	0.42
4:D:34:LEU:HD12	4:D:34:LEU:HA	1.85	0.42
5:E:293:ARG:HB3	5:E:320:VAL:HG21	2.01	0.42
6:F:196:ASP:OD1	6:F:196:ASP:N	2.43	0.42
7:G:463:LEU:HD23	7:G:463:LEU:HA	1.90	0.42
5:E:246:THR:O	5:E:248:LYS:N	2.52	0.42
7:G:254:ILE:HG13	7:G:260:LEU:HD13	2.02	0.42
2:B:59:HIS:O	3:C:535:ARG:NH1	2.53	0.41
3:C:394:MET:O	3:C:398:ARG:HG2	2.20	0.41
9:I:414:VAL:O	9:I:418:MET:HG3	2.20	0.41
4:D:411:ASN:HB3	4:D:511:ILE:HD11	2.01	0.41
5:E:245:ASP:C	5:E:247:ASP:N	2.72	0.41
8:H:67:LEU:HB3	8:H:81:ILE:HD13	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:154:LEU:HD23	2:B:154:LEU:HA	1.89	0.41
1:A:137:HIS:ND1	1:A:138:SER:O	2.52	0.41
2:B:290:VAL:HG23	2:B:311:MET:HG2	2.03	0.41
11:B:602:ADP:O3B	12:B:603:AF3:F1	2.27	0.41
3:C:215:ALA:HA	3:C:359:ASN:O	2.21	0.41
3:C:394:MET:HE3	3:C:394:MET:HB3	1.80	0.41
4:D:40:ALA:O	4:D:44:VAL:HG23	2.21	0.41
6:F:38:ILE:HG21	6:F:121:THR:OG1	2.21	0.41
6:F:287:VAL:HG11	6:F:316:PHE:HB3	2.02	0.41
8:H:521:ASP:OD2	8:H:521:ASP:C	2.63	0.41
9:I:208:ARG:HA	9:I:372:VAL:HG12	2.02	0.41
5:E:248:LYS:CE	6:F:259:ASP:HB2	2.49	0.41
3:C:32:ILE:HD13	3:C:32:ILE:HA	1.95	0.41
4:D:409:ILE:O	4:D:413:ILE:HG12	2.20	0.41
5:E:52:LEU:HD12	5:E:62:MET:HG3	2.02	0.41
1:A:52:ASN:OD1	1:A:62:ARG:NH2	2.54	0.41
2:B:526:MET:HG2	9:I:48:VAL:HB	2.01	0.41
4:D:61:MET:HE3	4:D:61:MET:HB3	1.84	0.41
6:F:240:ARG:NE	6:F:242:GLU:OE2	2.50	0.41
8:H:7:VAL:HG12	8:H:9:VAL:HG13	2.03	0.41
8:H:83:ILE:HD13	8:H:512:THR:HG21	2.03	0.41
2:B:249:MET:H	2:B:249:MET:HG2	1.67	0.41
6:F:366:ASN:OD1	6:F:366:ASN:N	2.46	0.41
7:G:69:HIS:O	7:G:73:LYS:HG3	2.21	0.41
8:H:425:LYS:HB2	8:H:425:LYS:HE2	1.84	0.41
9:I:279:ARG:NH2	9:I:308:GLU:OE2	2.53	0.41
2:B:55:MET:SD	3:C:74:PRO:HB2	2.61	0.40
2:B:333:LEU:HD21	2:B:343:GLU:HG2	2.03	0.40
7:G:148:LEU:HD11	7:G:403:LEU:HD21	2.03	0.40
7:G:430:MET:HE3	7:G:430:MET:HB3	1.91	0.40
1:A:72:THR:O	1:A:76:VAL:HG23	2.21	0.40
4:D:197:ALA:HA	4:D:204:VAL:HG12	2.03	0.40
5:E:378:ALA:HB2	6:F:521:LEU:HD22	2.03	0.40
7:G:341:GLU:H	7:G:344:MET:HE2	1.87	0.40
1:A:105:HIS:O	1:A:106:TYR:HB3	2.21	0.40
3:C:156:GLU:HG2	3:C:180:VAL:HG21	2.04	0.40
4:D:402:LEU:O	4:D:406:LEU:HG	2.22	0.40
7:G:47:ASP:OD1	7:G:51:ASP:N	2.53	0.40
4:D:91:MET:HE3	4:D:91:MET:HB3	1.88	0.40
6:F:134:SER:HB3	6:F:527:ARG:HE	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	164/444 (37%)	152 (93%)	12 (7%)	0	100	100
2	B	527/547 (96%)	516 (98%)	10 (2%)	1 (0%)	43	76
3	C	517/553 (94%)	498 (96%)	19 (4%)	0	100	100
4	D	525/541 (97%)	505 (96%)	20 (4%)	0	100	100
5	E	524/535 (98%)	501 (96%)	22 (4%)	1 (0%)	43	76
6	F	518/539 (96%)	509 (98%)	9 (2%)	0	100	100
7	G	533/556 (96%)	506 (95%)	27 (5%)	0	100	100
8	H	521/545 (96%)	498 (96%)	23 (4%)	0	100	100
9	I	524/531 (99%)	502 (96%)	22 (4%)	0	100	100
All	All	4353/4791 (91%)	4187 (96%)	164 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	247	ASP
2	B	6	PRO

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	71/379 (19%)	70 (99%)	1 (1%)	59	80
2	B	416/451 (92%)	415 (100%)	1 (0%)	87	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	386/451 (86%)	384 (100%)	2 (0%)	81	89
4	D	445/456 (98%)	445 (100%)	0	100	100
5	E	419/427 (98%)	419 (100%)	0	100	100
6	F	429/452 (95%)	429 (100%)	0	100	100
7	G	446/463 (96%)	446 (100%)	0	100	100
8	H	454/469 (97%)	453 (100%)	1 (0%)	87	92
9	I	438/442 (99%)	437 (100%)	1 (0%)	87	92
All	All	3504/3990 (88%)	3498 (100%)	6 (0%)	85	92

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	ILE
2	B	77	GLU
3	C	26	ILE
3	C	470	GLN
8	H	195	ILE
9	I	333	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
2	B	59	HIS
2	B	365	HIS
3	C	60	ASN
3	C	241	ASN
3	C	331	GLN
3	C	431	GLN
3	C	432	GLN
3	C	533	ASN
4	D	139	GLN
4	D	167	GLN
4	D	316	GLN
4	D	317	ASN
4	D	376	GLN
4	D	403	HIS
5	E	157	GLN

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Mol	Chain	Res	Type
5	E	175	HIS
5	E	269	HIS
5	E	294	GLN
5	E	502	GLN
6	F	25	GLN
6	F	62	GLN
6	F	235	ASN
6	F	296	ASN
6	F	406	HIS
7	G	20	GLN
7	G	472	ASN
8	H	474	ASN
8	H	504	GLN
9	I	68	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	AF3	E	603	-	0,3,3	-	-	-		
12	AF3	G	603	-	0,3,3	-	-	-		
11	ADP	B	602	10	28,29,29	1.40	4 (14%)	43,45,45	1.90	10 (23%)
12	AF3	F	603	-	0,3,3	-	-	-		
11	ADP	G	602	10	28,29,29	1.00	3 (10%)	43,45,45	0.68	0
11	ADP	I	602	10	28,29,29	1.39	4 (14%)	43,45,45	1.87	10 (23%)
12	AF3	D	603	-	0,3,3	-	-	-		
12	AF3	I	603	-	0,3,3	-	-	-		
12	AF3	H	603	-	0,3,3	-	-	-		
12	AF3	C	603	-	0,3,3	-	-	-		
11	ADP	D	602	10	28,29,29	1.40	4 (14%)	43,45,45	1.86	11 (25%)
11	ADP	F	602	10	28,29,29	0.99	2 (7%)	43,45,45	0.70	0
11	ADP	H	602	10	28,29,29	1.39	4 (14%)	43,45,45	1.86	10 (23%)
12	AF3	B	603	-	0,3,3	-	-	-		
11	ADP	C	602	10	28,29,29	1.41	5 (17%)	43,45,45	1.84	8 (18%)
11	ADP	E	602	10	28,29,29	1.03	2 (7%)	43,45,45	0.78	1 (2%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	ADP	B	602	10	-	5/16/32/32	0/3/3/3
11	ADP	G	602	10	-	4/16/32/32	0/3/3/3
11	ADP	I	602	10	-	1/16/32/32	0/3/3/3
11	ADP	D	602	10	-	1/16/32/32	0/3/3/3
11	ADP	F	602	10	-	5/16/32/32	0/3/3/3
11	ADP	H	602	10	-	1/16/32/32	0/3/3/3
11	ADP	C	602	10	-	4/16/32/32	0/3/3/3
11	ADP	E	602	10	-	4/16/32/32	0/3/3/3

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	C	602	ADP	C5-C4	4.51	1.47	1.39
11	I	602	ADP	C5-C4	4.50	1.47	1.39
11	D	602	ADP	C5-C4	4.47	1.47	1.39
11	H	602	ADP	C5-C4	4.46	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	602	ADP	C5-C4	4.44	1.47	1.39
11	E	602	ADP	PB-O2B	-3.20	1.42	1.54
11	F	602	ADP	PA-O3A	-3.12	1.56	1.59
11	G	602	ADP	PB-O2B	-3.05	1.43	1.54
11	E	602	ADP	PB-O3B	-2.93	1.43	1.54
11	B	602	ADP	C5-C6	2.73	1.48	1.41
11	C	602	ADP	C5-C6	2.67	1.48	1.41
11	I	602	ADP	C5-C6	2.67	1.48	1.41
11	H	602	ADP	C5-C6	2.65	1.48	1.41
11	D	602	ADP	C5-C6	2.63	1.48	1.41
11	F	602	ADP	PB-O2B	-2.51	1.45	1.54
11	B	602	ADP	C8-N7	2.39	1.36	1.31
11	G	602	ADP	PA-O3A	-2.39	1.56	1.59
11	D	602	ADP	C5-N7	-2.37	1.34	1.39
11	H	602	ADP	C5-N7	-2.34	1.34	1.39
11	D	602	ADP	C8-N7	2.34	1.36	1.31
11	I	602	ADP	C5-N7	-2.33	1.34	1.39
11	B	602	ADP	C5-N7	-2.33	1.34	1.39
11	G	602	ADP	PB-O3B	-2.33	1.46	1.54
11	I	602	ADP	C8-N7	2.32	1.36	1.31
11	C	602	ADP	C5-N7	-2.31	1.34	1.39
11	H	602	ADP	C8-N7	2.30	1.36	1.31
11	C	602	ADP	C8-N7	2.29	1.36	1.31
11	C	602	ADP	PA-O3A	2.12	1.61	1.59

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	C	602	ADP	C5-C4-N3	-5.93	118.56	126.72
11	B	602	ADP	C5-C4-N3	-5.84	118.68	126.72
11	H	602	ADP	C5-C4-N3	-5.83	118.69	126.72
11	I	602	ADP	C5-C4-N3	-5.81	118.72	126.72
11	D	602	ADP	C5-C4-N3	-5.79	118.74	126.72
11	C	602	ADP	N3-C4-N9	4.65	135.08	127.17
11	H	602	ADP	N3-C4-N9	4.53	134.87	127.17
11	D	602	ADP	N3-C4-N9	4.51	134.83	127.17
11	B	602	ADP	N3-C4-N9	4.46	134.76	127.17
11	I	602	ADP	N3-C4-N9	4.45	134.73	127.17
11	B	602	ADP	C2-N3-C4	3.81	121.12	111.83
11	H	602	ADP	C2-N3-C4	3.76	121.01	111.83
11	C	602	ADP	C2-N3-C4	3.75	120.99	111.83
11	D	602	ADP	C2-N3-C4	3.72	120.92	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	I	602	ADP	C2-N3-C4	3.71	120.89	111.83
11	I	602	ADP	C4-C5-N7	-3.65	106.41	110.58
11	B	602	ADP	C4-C5-N7	-3.62	106.44	110.58
11	D	602	ADP	C4-C5-N7	-3.56	106.51	110.58
11	H	602	ADP	C4-C5-N7	-3.56	106.52	110.58
11	C	602	ADP	C4-C5-N7	-3.50	106.58	110.58
11	H	602	ADP	N3-C2-N1	-3.36	123.50	128.58
11	B	602	ADP	N3-C2-N1	-3.35	123.51	128.58
11	D	602	ADP	N3-C2-N1	-3.31	123.56	128.58
11	I	602	ADP	N3-C2-N1	-3.25	123.66	128.58
11	C	602	ADP	N3-C2-N1	-3.24	123.67	128.58
11	B	602	ADP	O4'-C1'-N9	3.08	114.00	108.09
11	D	602	ADP	C4-N9-C8	2.67	108.55	105.74
11	B	602	ADP	C5-N7-C8	2.66	107.63	103.45
11	D	602	ADP	C5-N7-C8	2.63	107.59	103.45
11	I	602	ADP	C5-N7-C8	2.62	107.57	103.45
11	H	602	ADP	C5-N7-C8	2.61	107.56	103.45
11	H	602	ADP	C4-N9-C8	2.61	108.48	105.74
11	B	602	ADP	C4-N9-C8	2.61	108.48	105.74
11	C	602	ADP	C4-N9-C8	2.58	108.45	105.74
11	C	602	ADP	C5-N7-C8	2.56	107.47	103.45
11	E	602	ADP	O2A-PA-O3A	2.56	114.19	107.27
11	I	602	ADP	C4-N9-C8	2.53	108.40	105.74
11	I	602	ADP	O4'-C1'-N9	2.47	112.84	108.09
11	D	602	ADP	O4'-C1'-N9	2.33	112.57	108.09
11	B	602	ADP	C6-C5-N7	2.28	136.49	132.09
11	I	602	ADP	C6-C5-N7	2.19	136.32	132.09
11	H	602	ADP	C6-C5-N7	2.17	136.27	132.09
11	D	602	ADP	C6-C5-N7	2.17	136.27	132.09
11	B	602	ADP	N9-C8-N7	-2.15	110.89	113.94
11	D	602	ADP	N9-C8-N7	-2.12	110.93	113.94
11	H	602	ADP	O4'-C1'-N9	2.12	112.15	108.09
11	C	602	ADP	C6-C5-N7	2.09	136.12	132.09
11	H	602	ADP	N9-C8-N7	-2.07	111.01	113.94
11	D	602	ADP	C3'-C2'-C1'	2.06	105.36	101.46
11	I	602	ADP	N9-C8-N7	-2.03	111.06	113.94

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	B	602	ADP	PB-O3A-PA-O5'

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

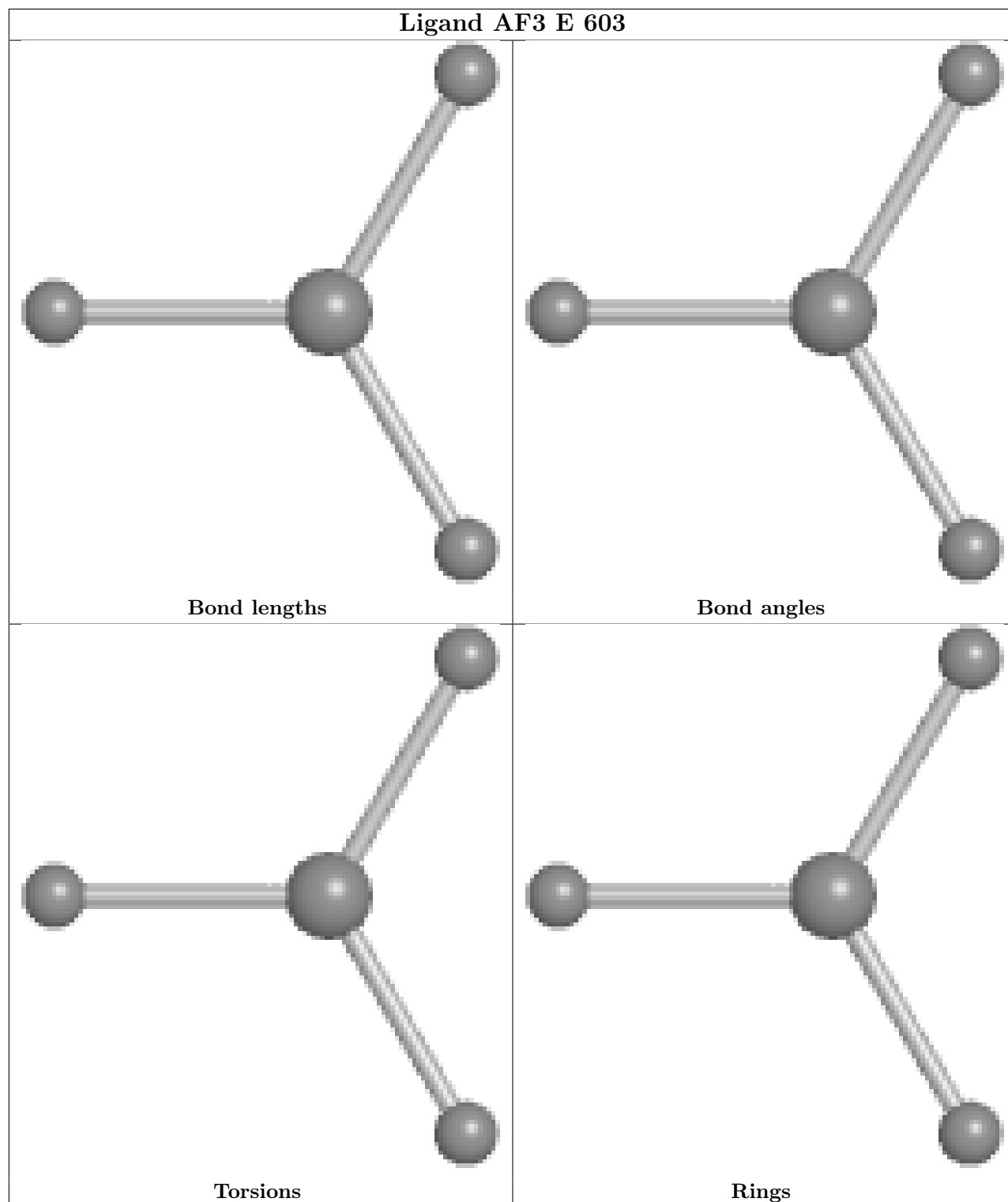
There are no ring outliers.

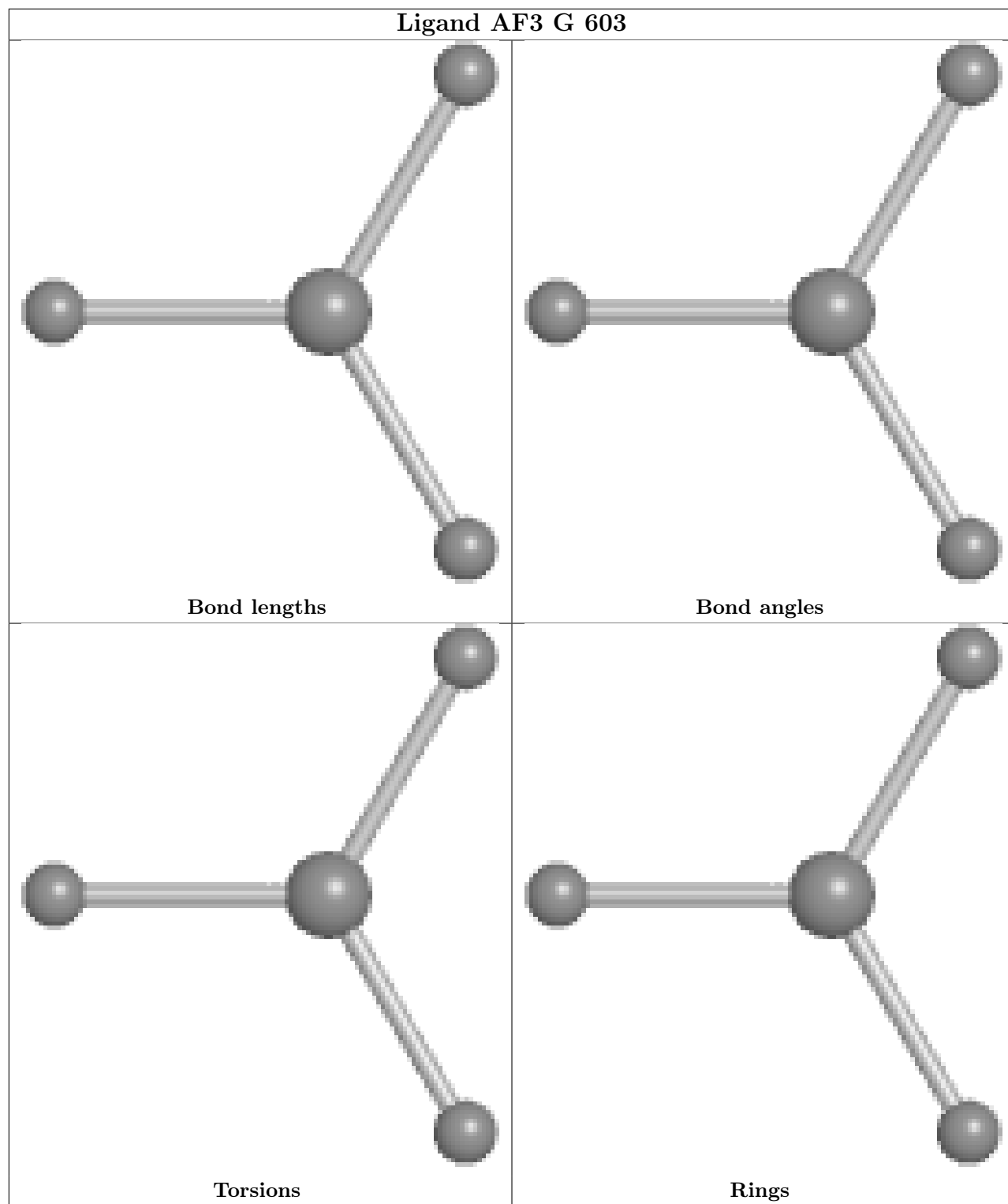
7 monomers are involved in 9 short contacts:

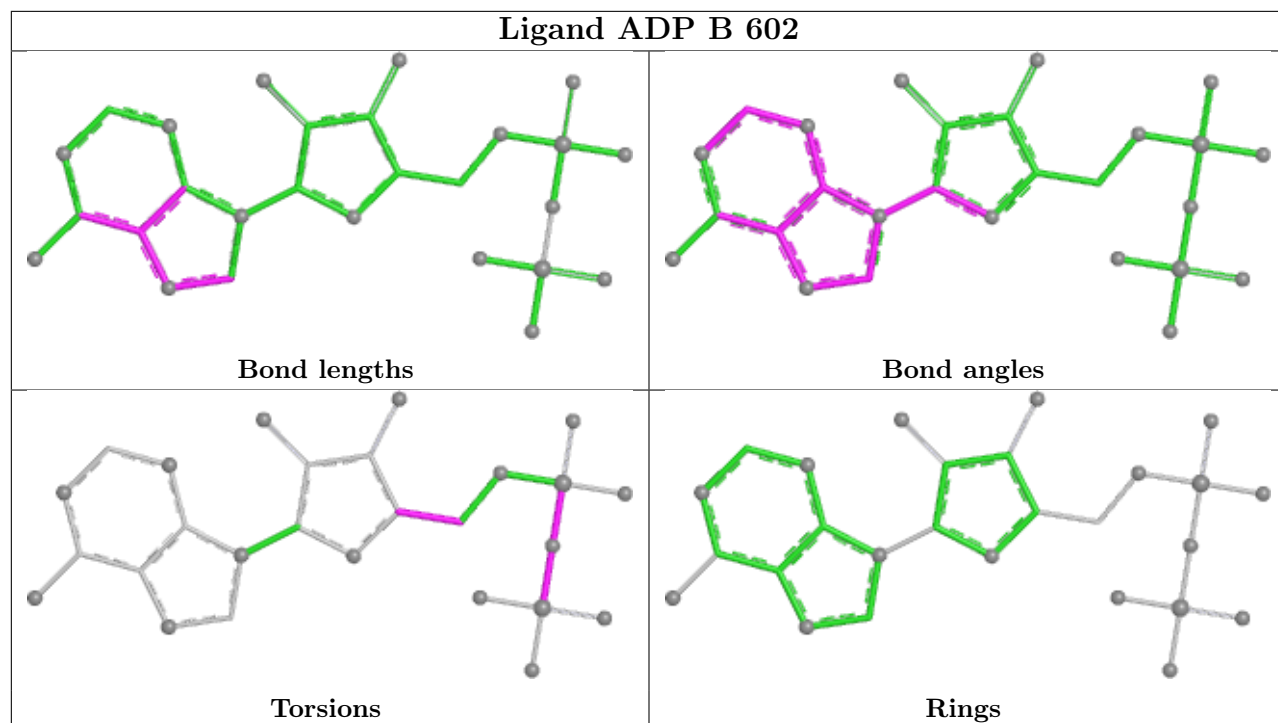
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	E	603	AF3	2	0
11	B	602	ADP	2	0
12	F	603	AF3	3	0
11	G	602	ADP	1	0
11	I	602	ADP	1	0
12	I	603	AF3	1	0
12	B	603	AF3	2	0

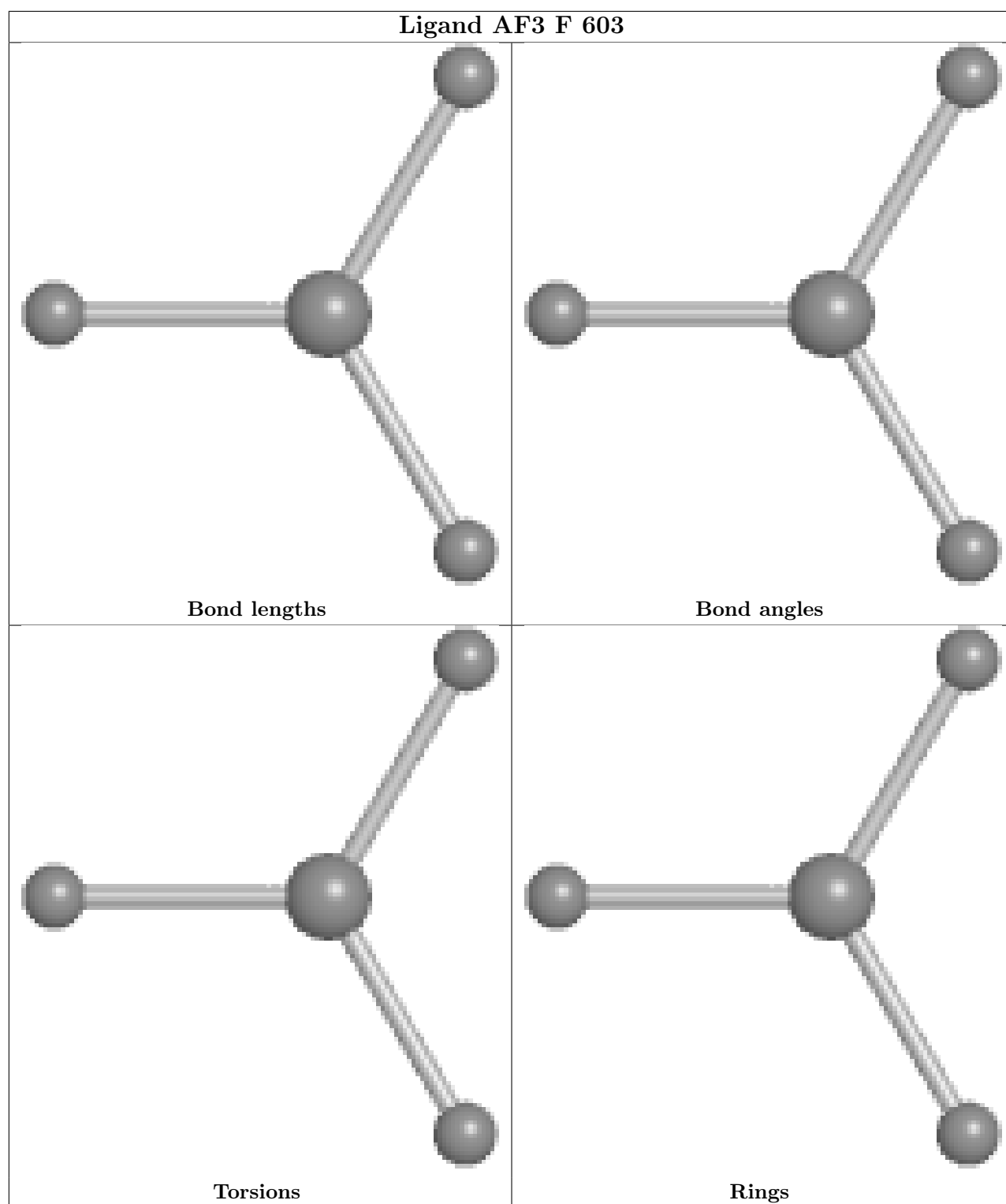
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

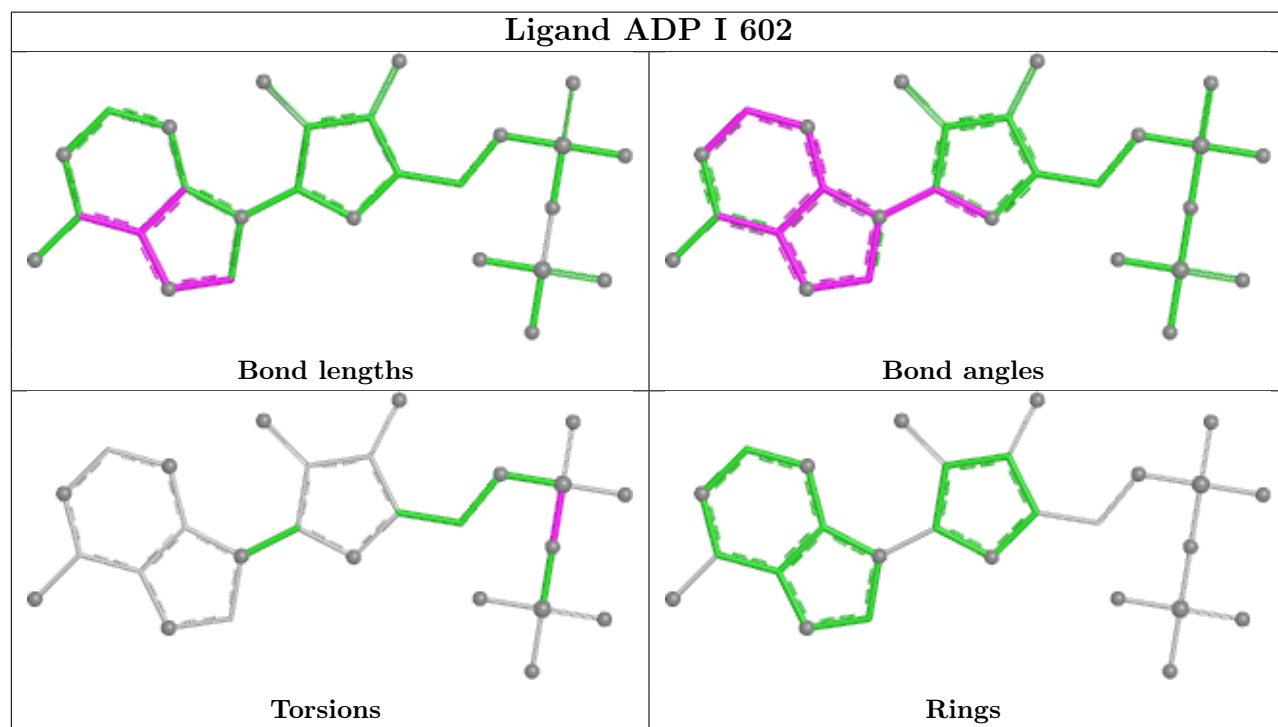
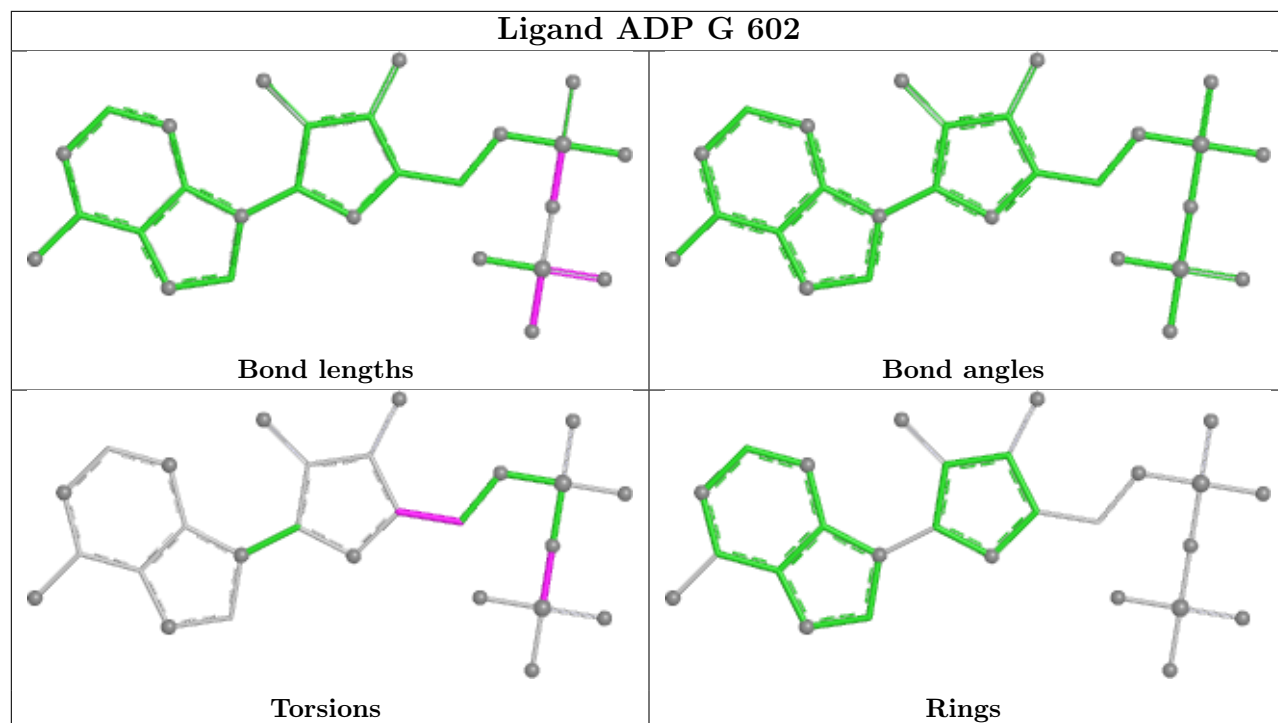
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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.

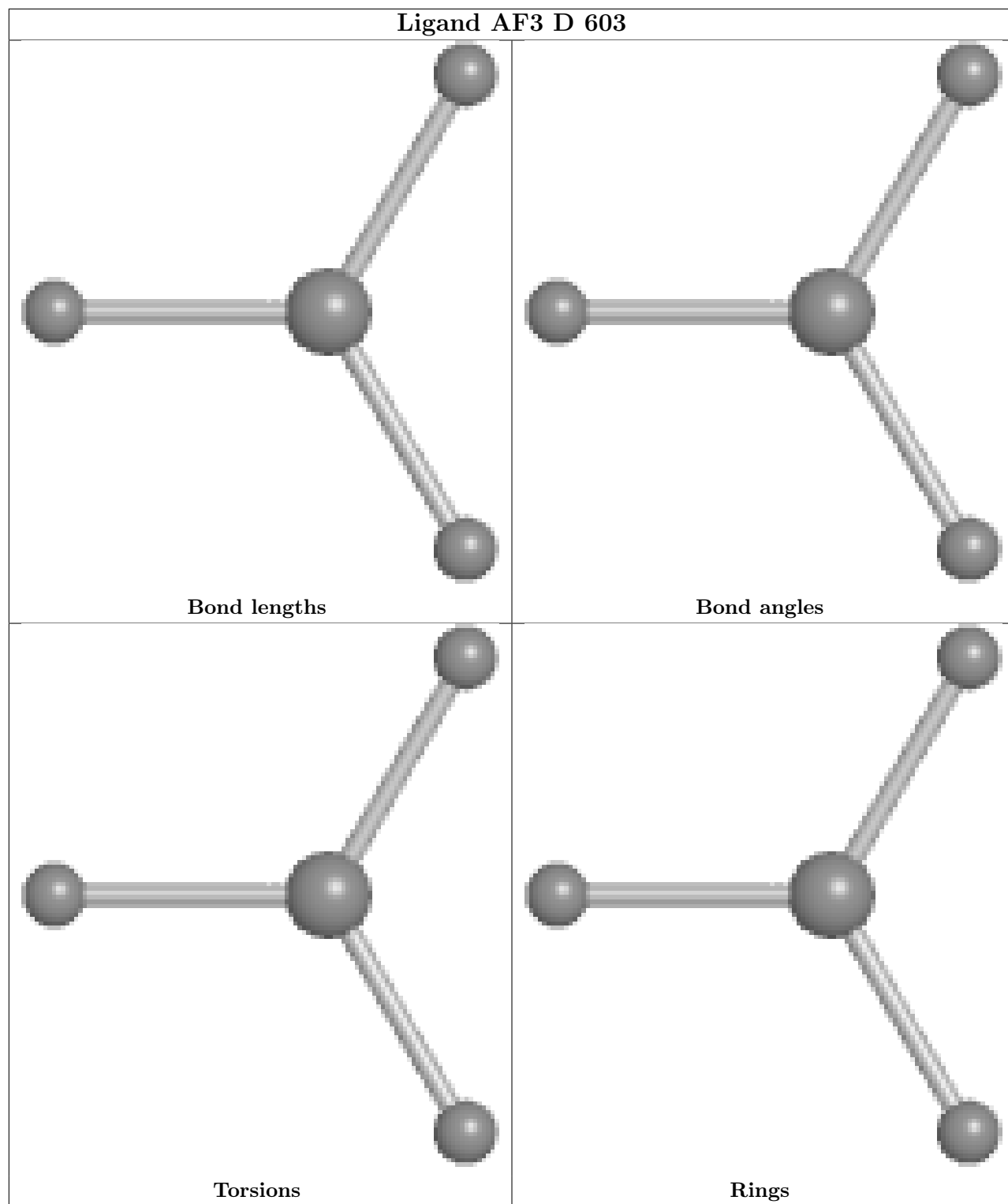


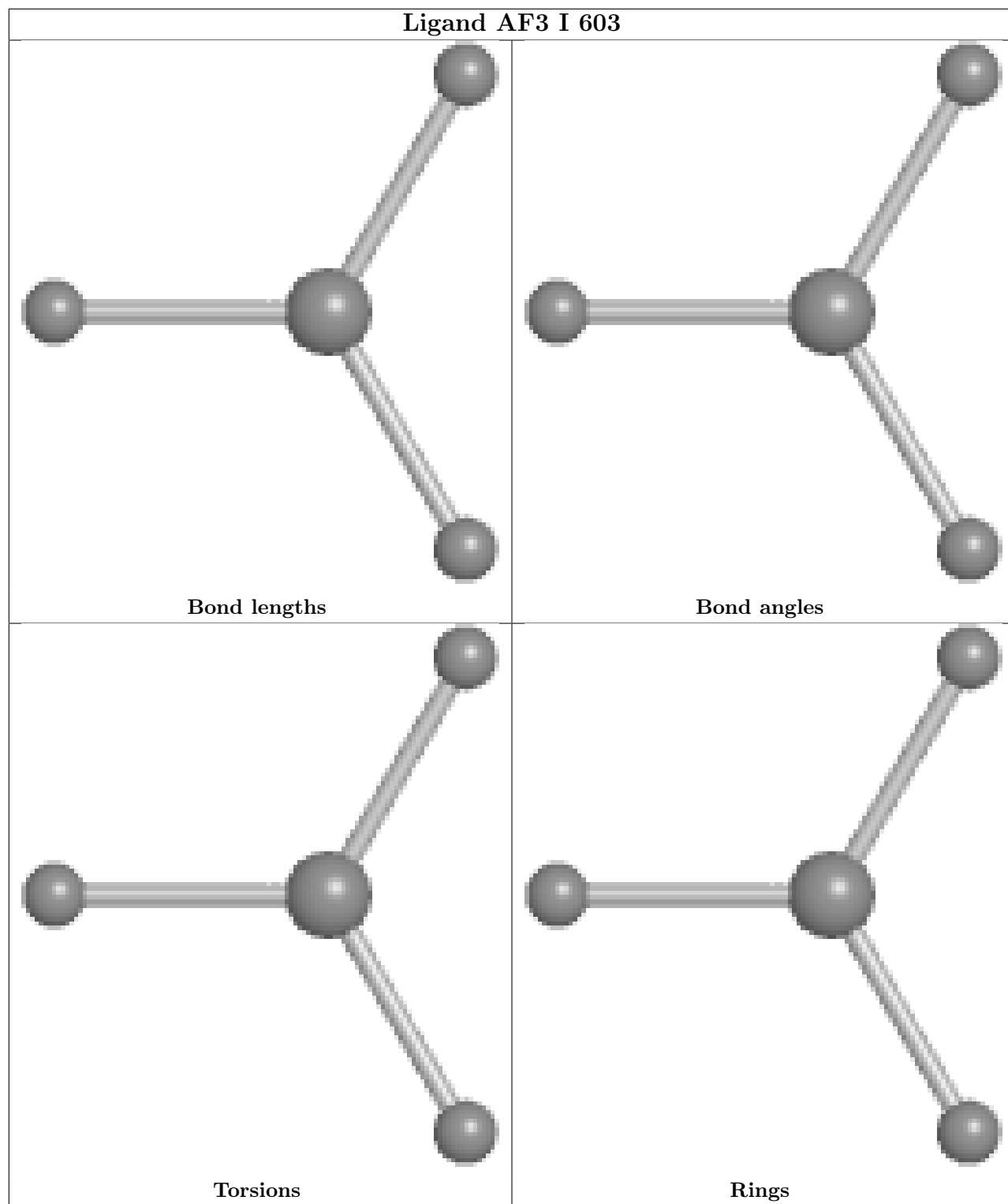


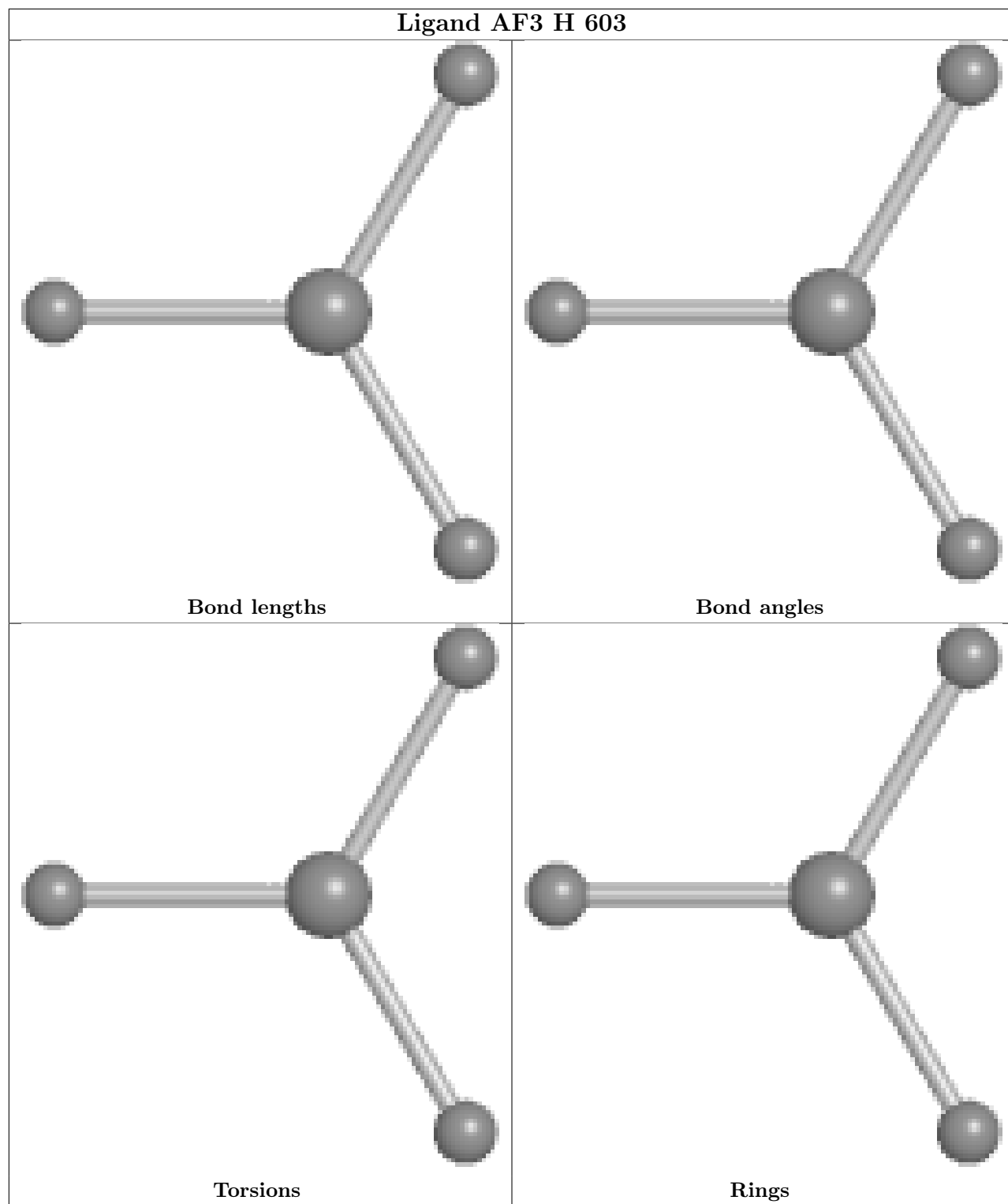


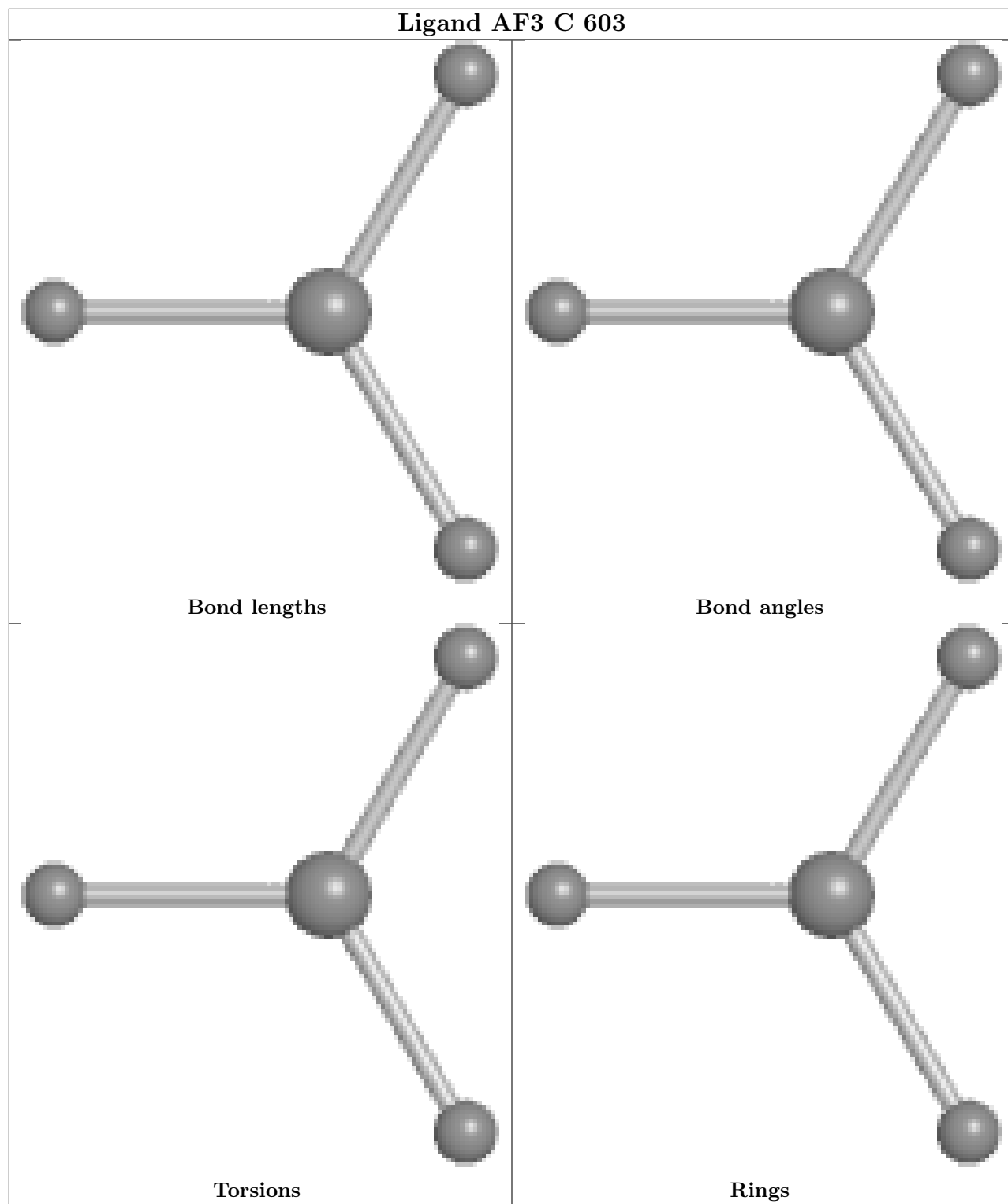


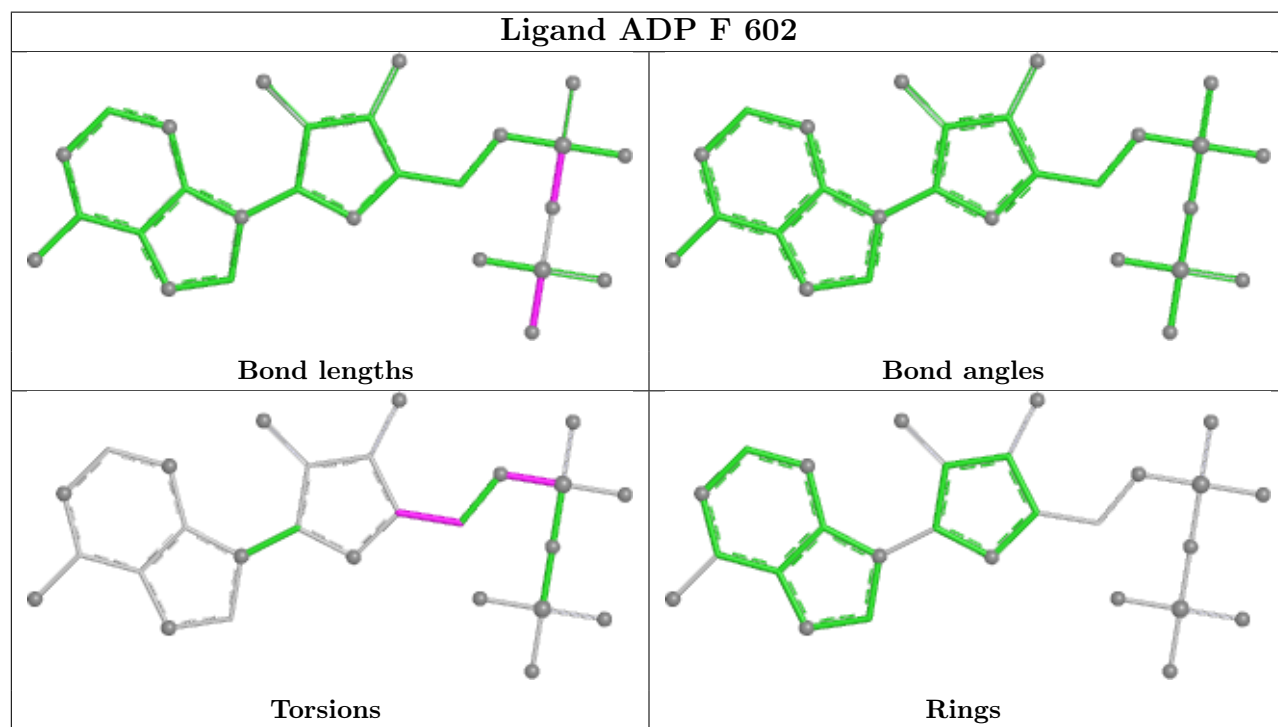
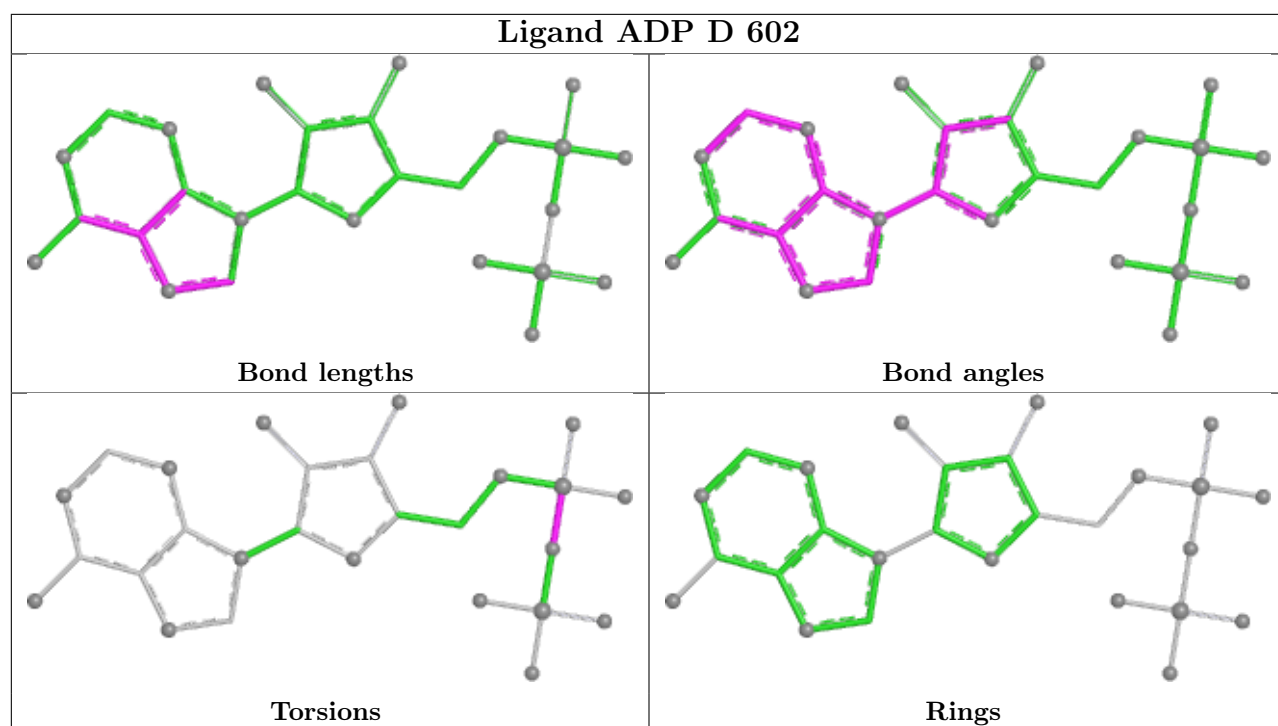


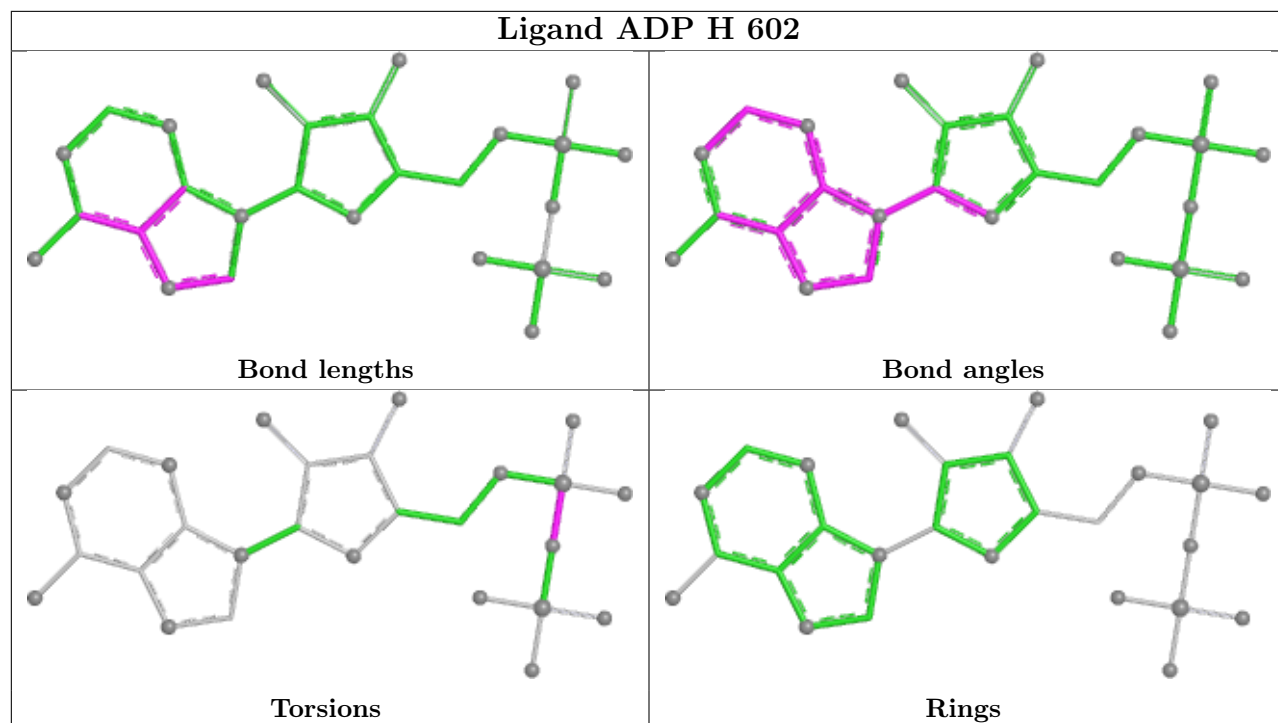


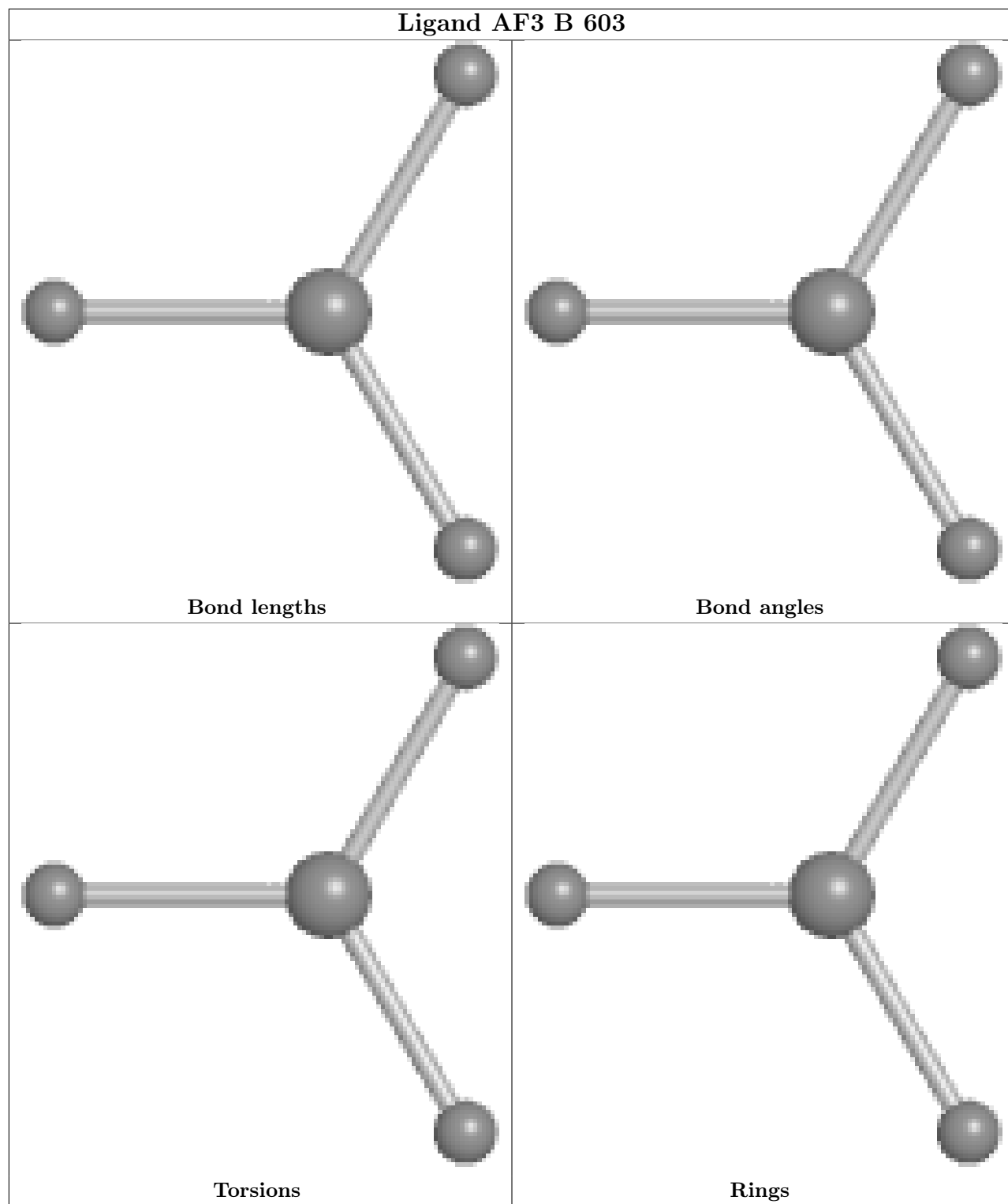


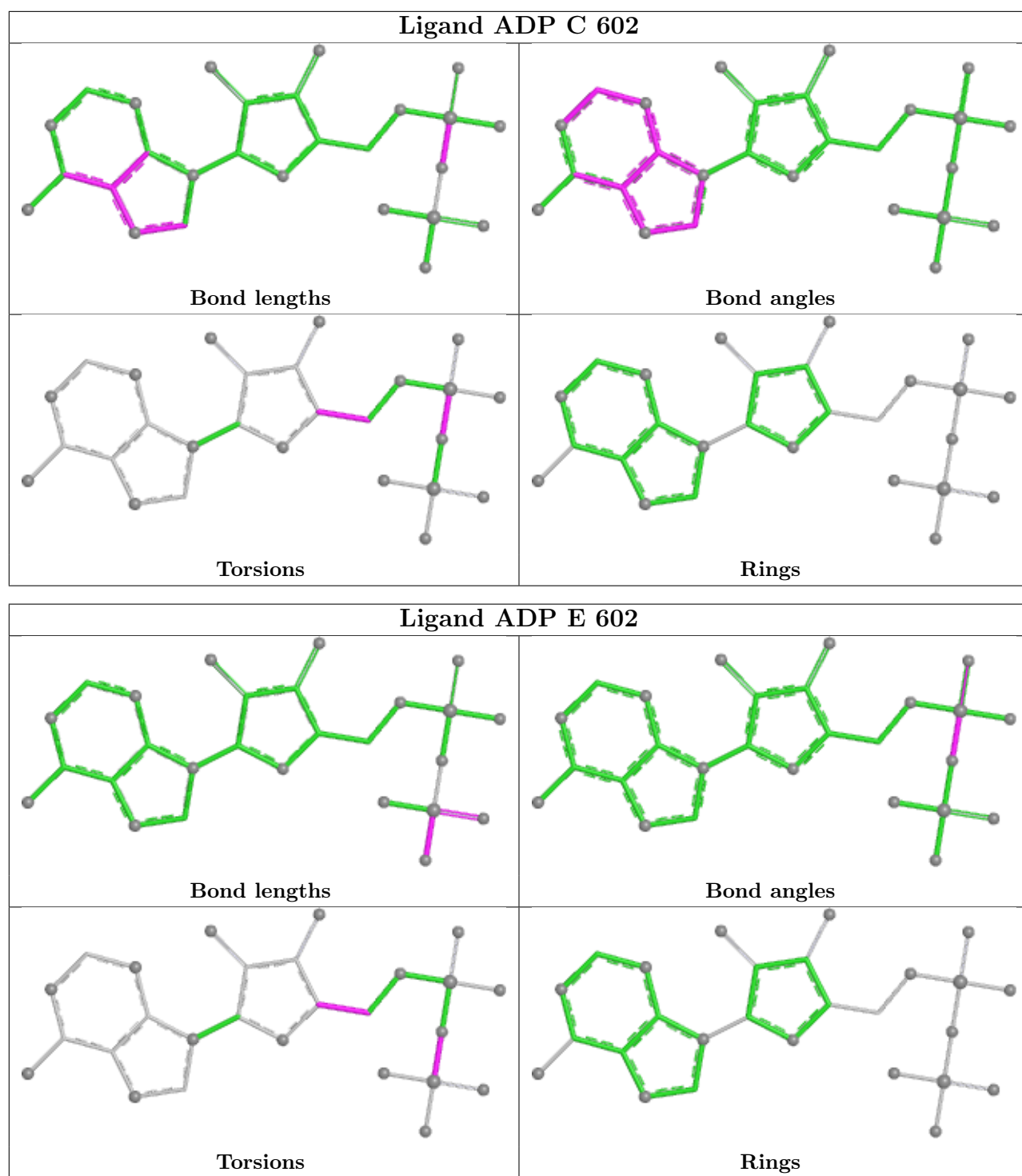












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

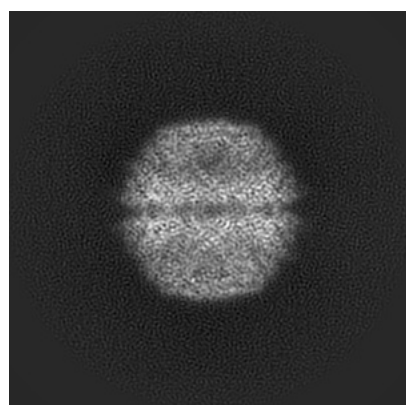
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26089. These allow visual inspection of the internal detail of the map and identification of artifacts.

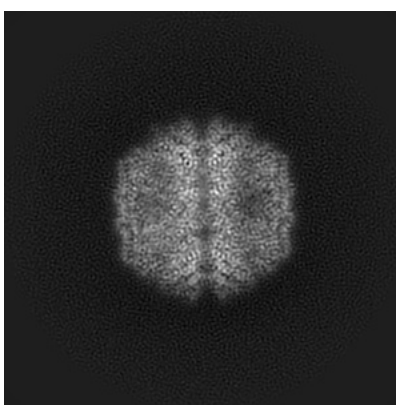
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

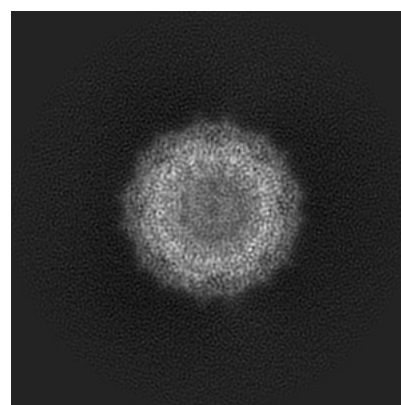
6.1.1 Primary map



X



Y

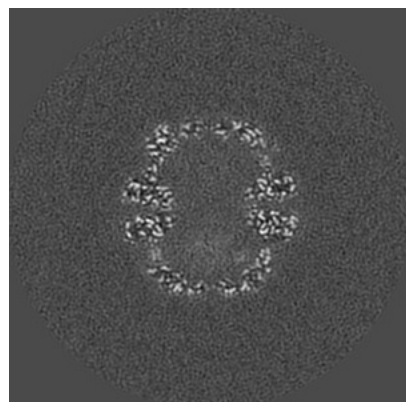


Z

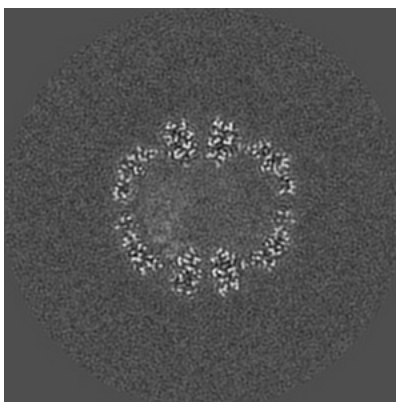
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

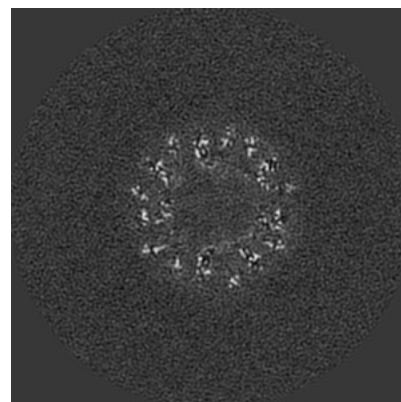
6.2.1 Primary map



X Index: 160



Y Index: 160

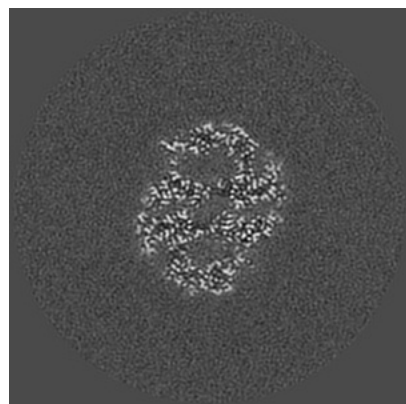


Z Index: 160

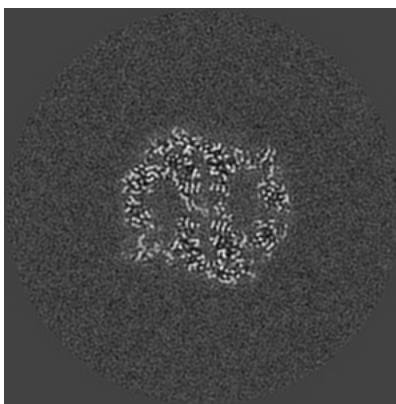
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

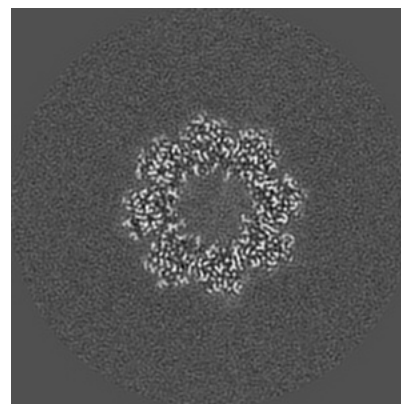
6.3.1 Primary map



X Index: 198



Y Index: 193

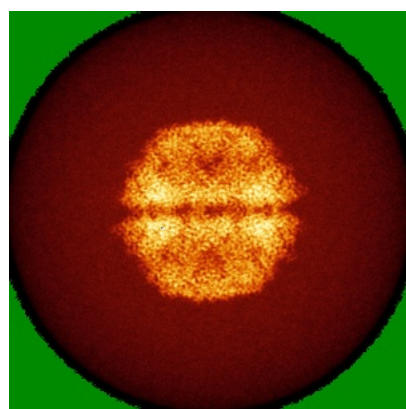


Z Index: 172

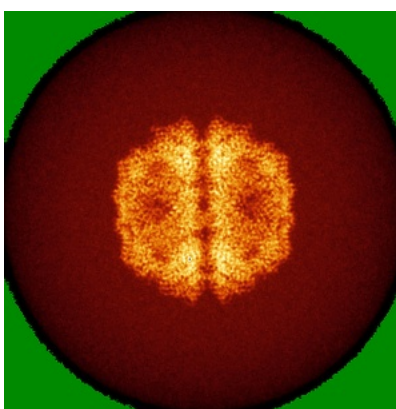
The images above show the largest variance slices of the map in three orthogonal directions.

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

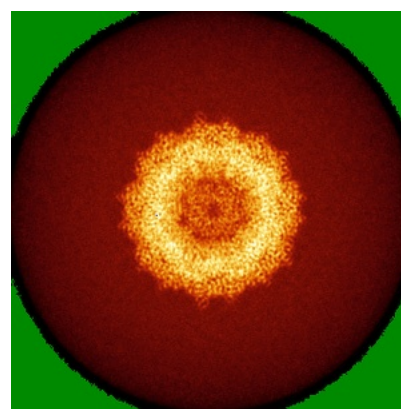
6.4.1 Primary map



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 3.46. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

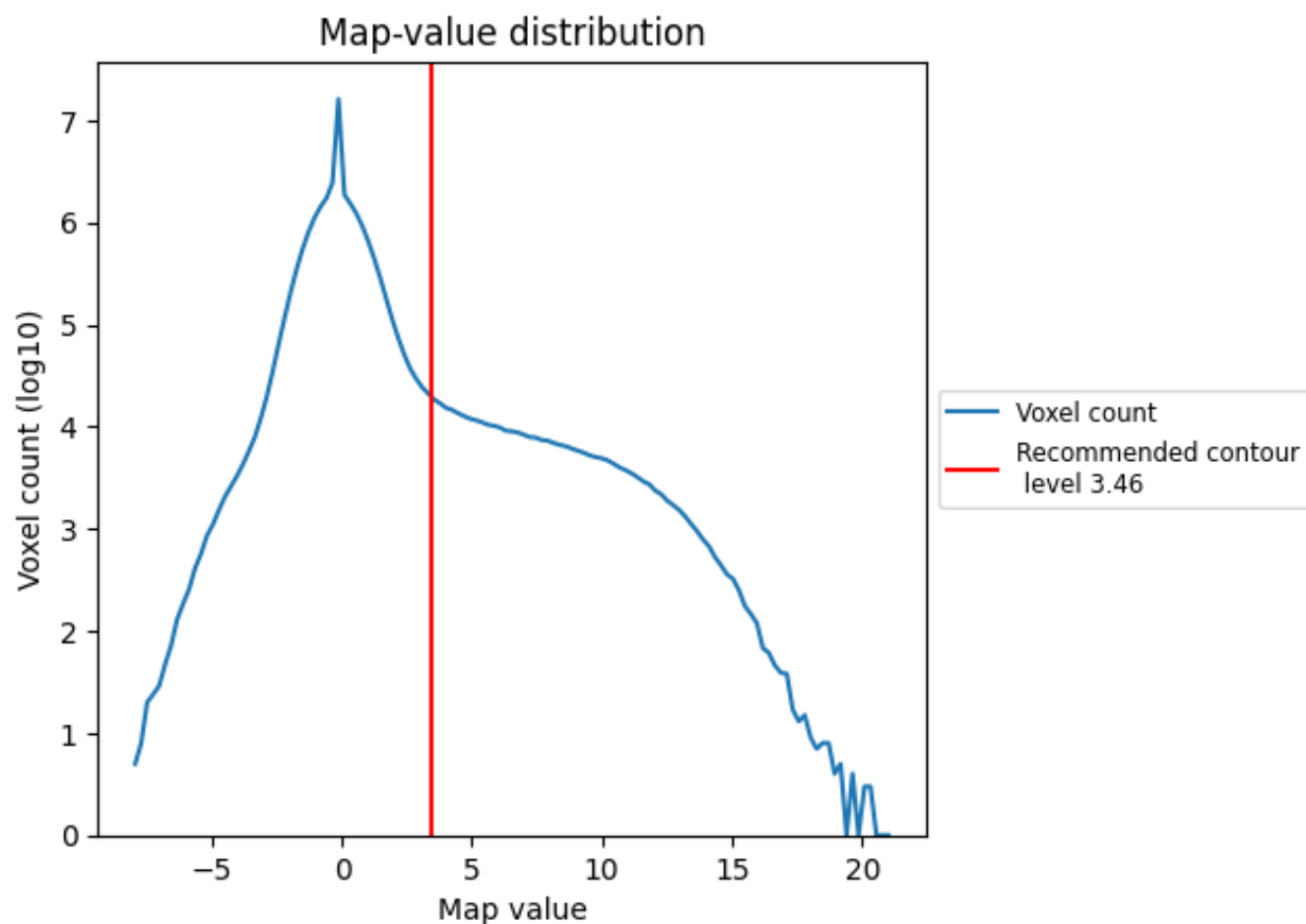
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

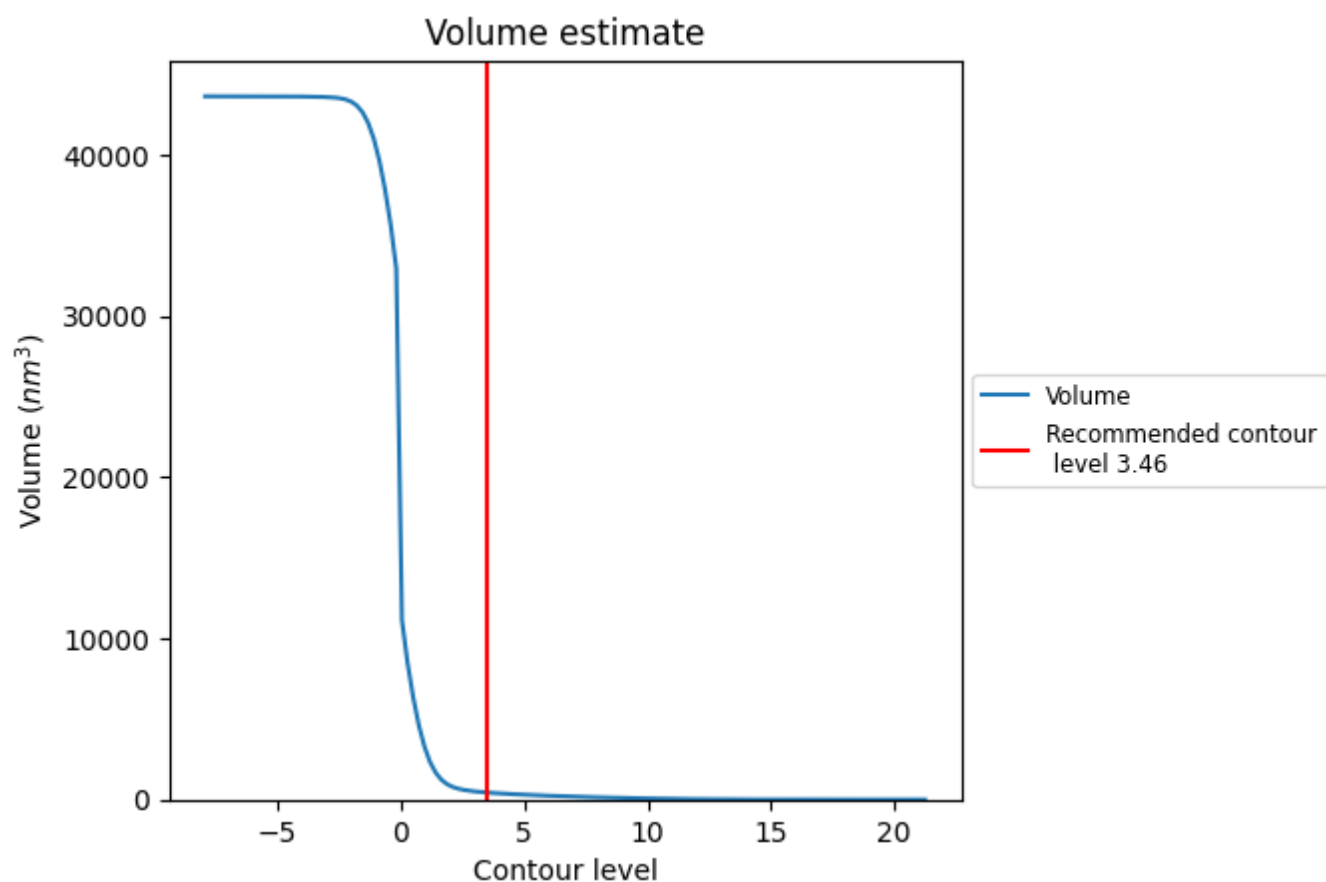
This section contains the results of statistical analysis of the map.

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.

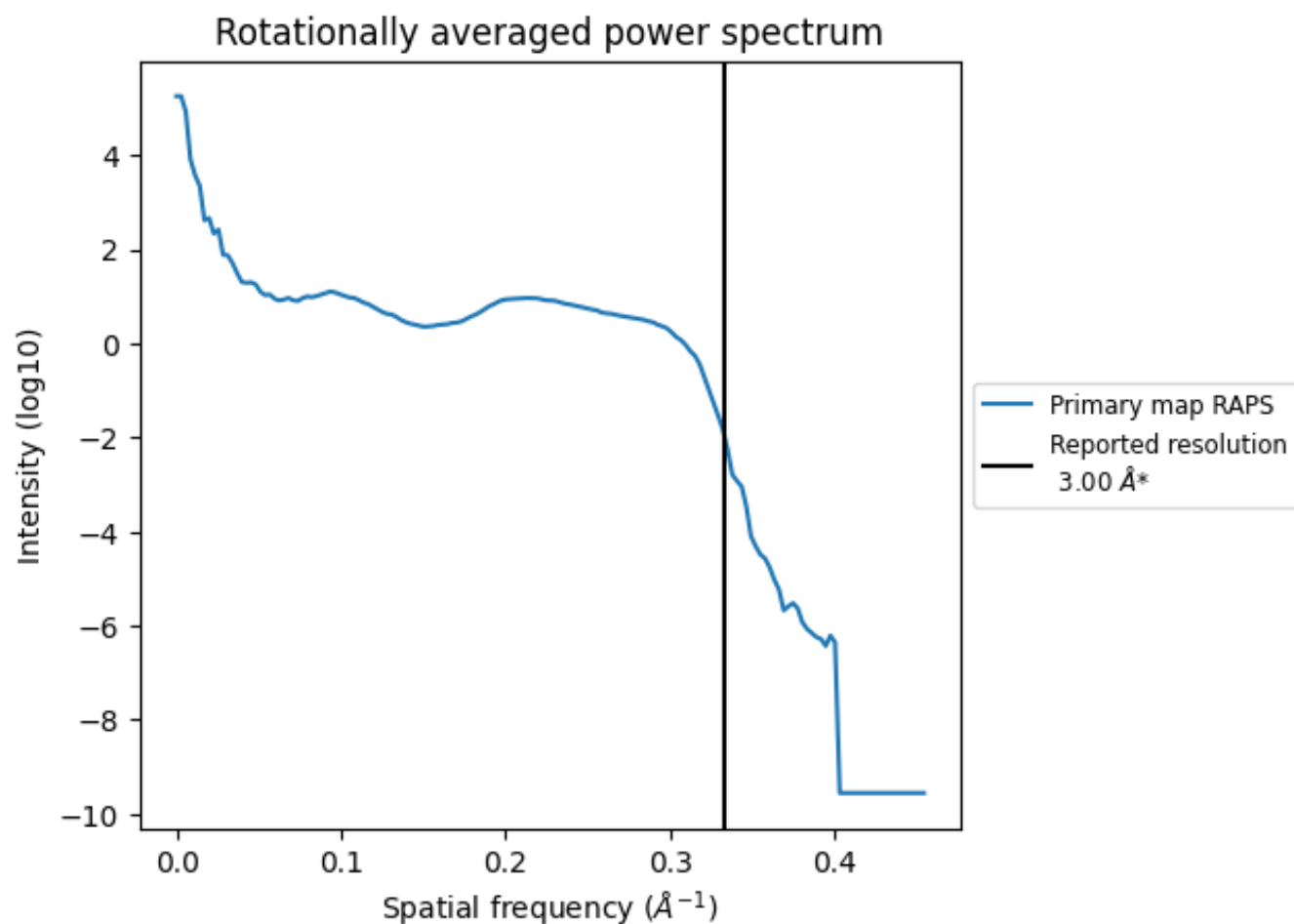
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 438 nm³; this corresponds to an approximate mass of 395 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 0.333 Å⁻¹

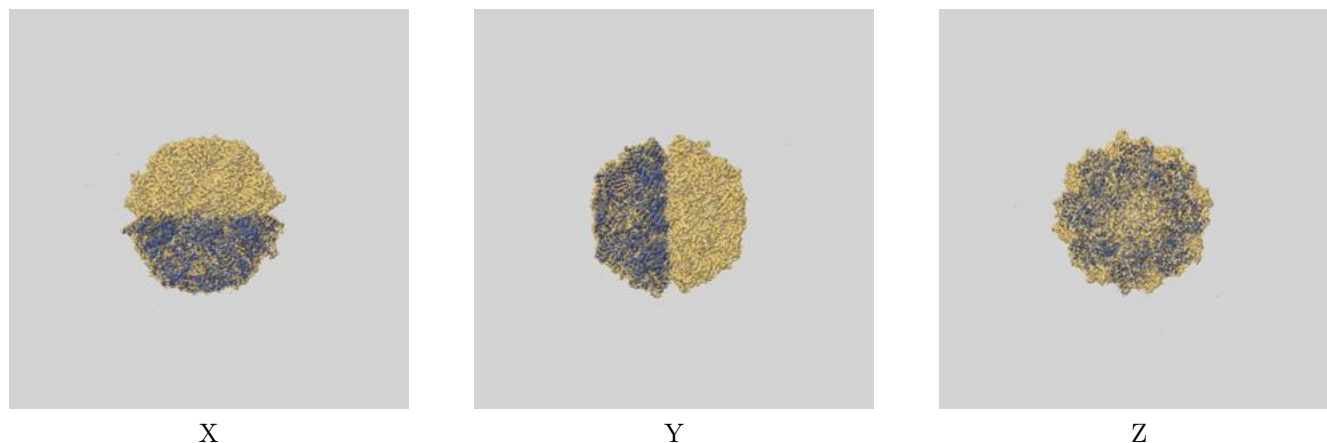
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

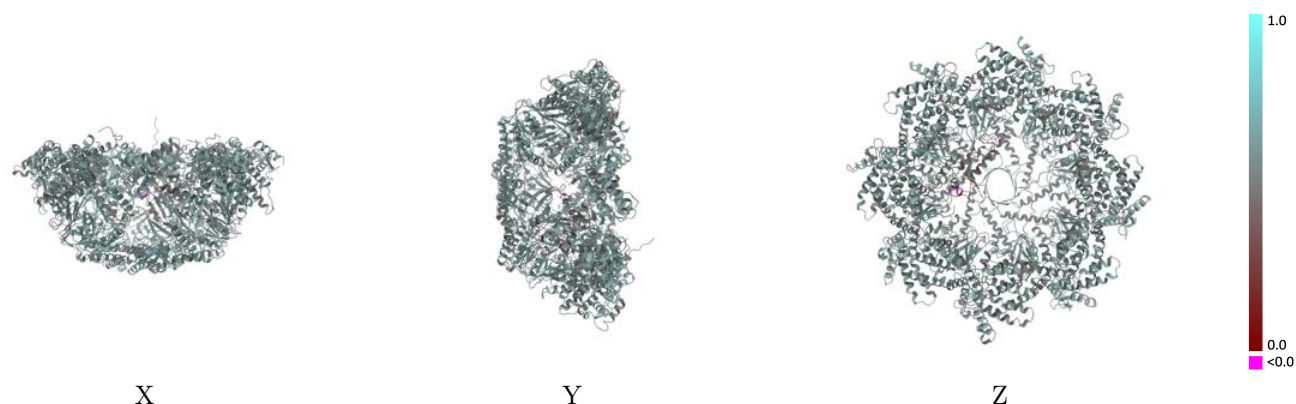
This section contains information regarding the fit between EMDB map EMD-26089 and PDB model 7TRG. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

9.1 Map-model overlay [i](#)



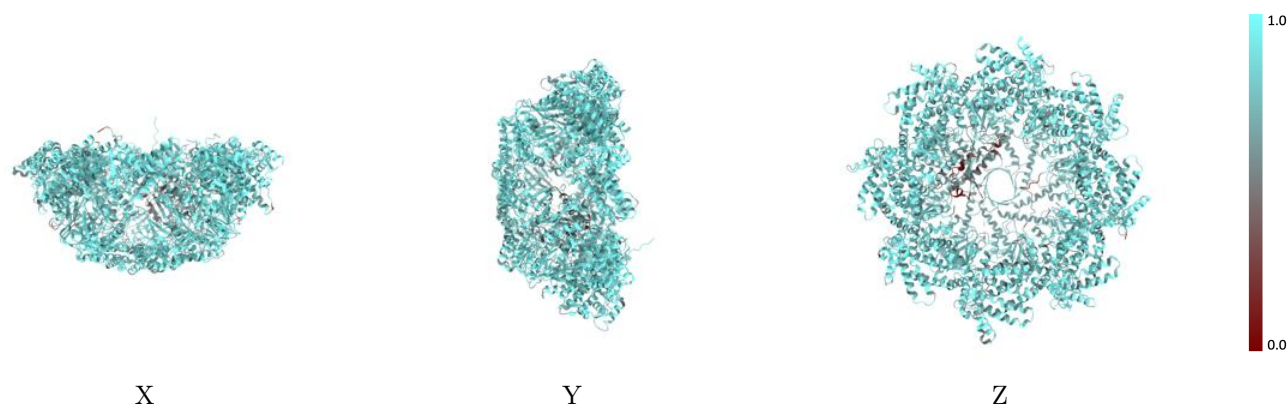
The images above show the 3D surface view of the map at the recommended contour level 3.46 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



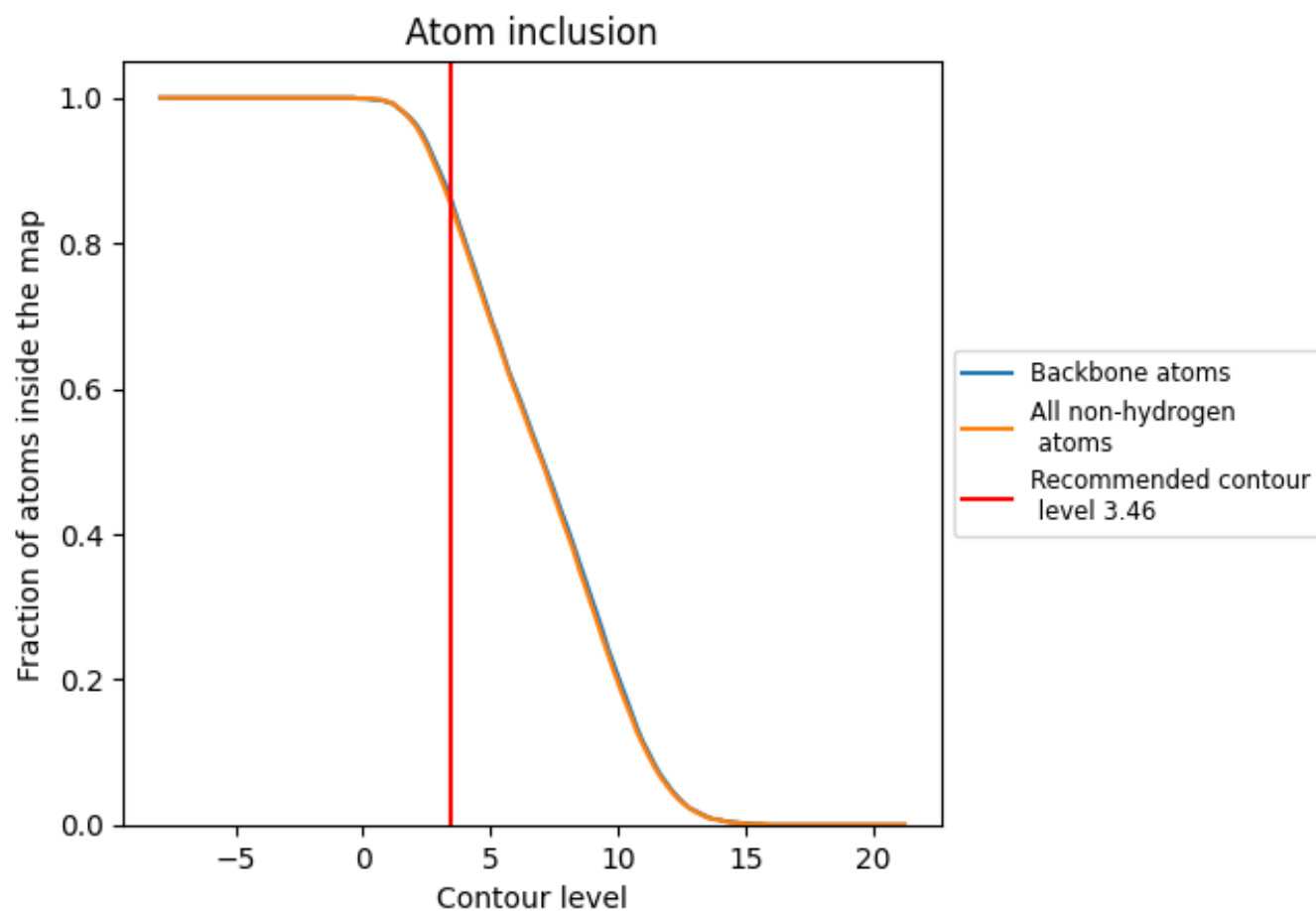
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3.46).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 85% 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 (3.46) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8520	0.5490
A	0.5320	0.4450
B	0.8750	0.5540
C	0.8860	0.5610
D	0.8750	0.5550
E	0.8650	0.5500
F	0.8600	0.5520
G	0.8560	0.5480
H	0.8650	0.5560
I	0.8640	0.5510

1.0

0.0

<0.0