



Full wwPDB EM Validation Report ⓘ

Aug 6, 2026 – 04:27 PM JST

PDB ID : 7YLW / pdb_00007ylw
EMDB ID : EMD-33919
Title : yeast TRiC-plp2-tubulin complex at S3 closed TRiC state
Authors : Han, W.Y.
Deposited on : 2022-07-27
Resolution : 3.39 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:

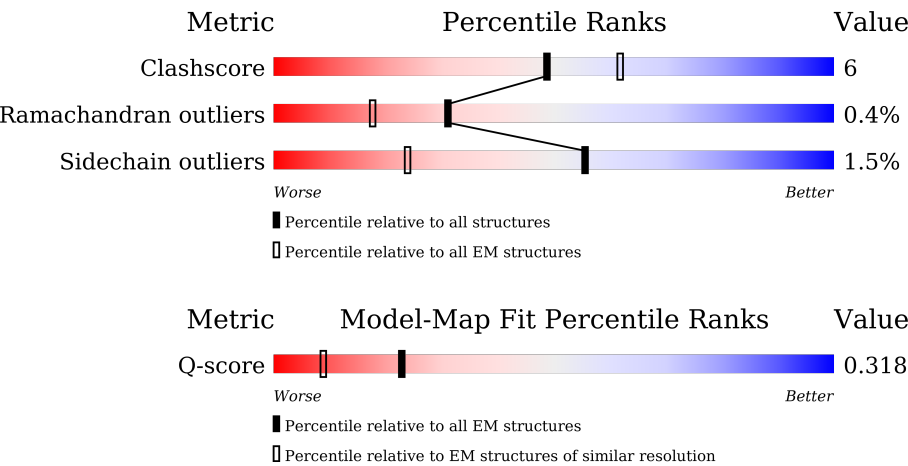
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using 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) : 2.50

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.39 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	14220 (2.89 - 3.89)

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	559	
1	a	559	
2	B	527	
2	b	527	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	D	528	
3	d	528	
4	E	562	
4	e	562	
5	G	594	
5	g	594	
6	H	550	
6	h	550	
7	Q	568	
7	q	568	
8	T	457	
9	Z	546	
9	z	546	
10	p	286	

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
13	AF3	B	603	-	-	X	-
13	AF3	D	603	-	-	X	-
13	AF3	E	603	-	-	X	-
13	AF3	G	603	-	-	X	-
13	AF3	d	603	-	-	X	-
13	AF3	e	603	-	-	X	-

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 70338 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	550	Total	C	N	O	S	0	0
			4158	2599	725	813	21		
1	a	546	Total	C	N	O	S	0	0
			4129	2582	721	806	20		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	518	Total	C	N	O	S	0	0
			3937	2461	680	782	14		
2	b	518	Total	C	N	O	S	0	0
			3937	2461	680	782	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	523	Total	C	N	O	S	0	0
			3998	2492	711	778	17		
3	d	524	Total	C	N	O	S	0	0
			4005	2497	712	779	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	536	Total	C	N	O	S	0	0
			4133	2595	710	806	22		
4	e	535	Total	C	N	O	S	0	0
			4124	2590	709	803	22		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	520	Total 4004	C 2510	N 703	O 764	S 27	0	0
5	g	520	Total 4003	C 2511	N 703	O 762	S 27	0	0

There are 122 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	375	LEU	-	see sequence details	UNP P39077
G	376	GLU	-	see sequence details	UNP P39077
G	377	GLY	-	see sequence details	UNP P39077
G	378	SER	-	see sequence details	UNP P39077
G	379	GLY	-	see sequence details	UNP P39077
G	380	SER	-	see sequence details	UNP P39077
G	381	GLY	-	see sequence details	UNP P39077
G	382	TRP	-	see sequence details	UNP P39077
G	383	SER	-	see sequence details	UNP P39077
G	384	HIS	-	see sequence details	UNP P39077
G	385	PRO	-	see sequence details	UNP P39077
G	386	GLN	-	see sequence details	UNP P39077
G	387	PHE	-	see sequence details	UNP P39077
G	388	GLU	-	see sequence details	UNP P39077
G	389	LYS	-	see sequence details	UNP P39077
G	390	GLY	-	see sequence details	UNP P39077
G	391	SER	-	see sequence details	UNP P39077
G	392	GLY	-	see sequence details	UNP P39077
G	393	LYS	-	see sequence details	UNP P39077
G	394	ARG	-	see sequence details	UNP P39077
G	395	ARG	-	see sequence details	UNP P39077
G	396	TRP	-	see sequence details	UNP P39077
G	397	LYS	-	see sequence details	UNP P39077
G	398	LYS	-	see sequence details	UNP P39077
G	399	ASN	-	see sequence details	UNP P39077
G	400	PHE	-	see sequence details	UNP P39077
G	401	ILE	-	see sequence details	UNP P39077
G	402	ALA	-	see sequence details	UNP P39077
G	403	VAL	-	see sequence details	UNP P39077
G	404	SER	-	see sequence details	UNP P39077
G	405	ALA	-	see sequence details	UNP P39077
G	406	ALA	-	see sequence details	UNP P39077
G	407	ASN	-	see sequence details	UNP P39077
G	408	ARG	-	see sequence details	UNP P39077
G	409	PHE	-	see sequence details	UNP P39077

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	410	LYS	-	see sequence details	UNP P39077
G	411	LYS	-	see sequence details	UNP P39077
G	412	ILE	-	see sequence details	UNP P39077
G	413	SER	-	see sequence details	UNP P39077
G	414	SER	-	see sequence details	UNP P39077
G	415	SER	-	see sequence details	UNP P39077
G	416	GLY	-	see sequence details	UNP P39077
G	417	ALA	-	see sequence details	UNP P39077
G	418	LEU	-	see sequence details	UNP P39077
G	419	GLY	-	see sequence details	UNP P39077
G	420	SER	-	see sequence details	UNP P39077
G	421	GLY	-	see sequence details	UNP P39077
G	422	HIS	-	see sequence details	UNP P39077
G	423	HIS	-	see sequence details	UNP P39077
G	424	HIS	-	see sequence details	UNP P39077
G	425	HIS	-	see sequence details	UNP P39077
G	426	HIS	-	see sequence details	UNP P39077
G	427	HIS	-	see sequence details	UNP P39077
G	428	HIS	-	see sequence details	UNP P39077
G	429	HIS	-	see sequence details	UNP P39077
G	430	GLY	-	see sequence details	UNP P39077
G	431	SER	-	see sequence details	UNP P39077
G	432	GLY	-	see sequence details	UNP P39077
G	433	LEU	-	see sequence details	UNP P39077
G	434	GLN	-	see sequence details	UNP P39077
G	435	LYS	-	see sequence details	UNP P39077
g	375	LEU	-	see sequence details	UNP P39077
g	376	GLU	-	see sequence details	UNP P39077
g	377	GLY	-	see sequence details	UNP P39077
g	378	SER	-	see sequence details	UNP P39077
g	379	GLY	-	see sequence details	UNP P39077
g	380	SER	-	see sequence details	UNP P39077
g	381	GLY	-	see sequence details	UNP P39077
g	382	TRP	-	see sequence details	UNP P39077
g	383	SER	-	see sequence details	UNP P39077
g	384	HIS	-	see sequence details	UNP P39077
g	385	PRO	-	see sequence details	UNP P39077
g	386	GLN	-	see sequence details	UNP P39077
g	387	PHE	-	see sequence details	UNP P39077
g	388	GLU	-	see sequence details	UNP P39077
g	389	LYS	-	see sequence details	UNP P39077
g	390	GLY	-	see sequence details	UNP P39077

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
g	391	SER	-	see sequence details	UNP P39077
g	392	GLY	-	see sequence details	UNP P39077
g	393	LYS	-	see sequence details	UNP P39077
g	394	ARG	-	see sequence details	UNP P39077
g	395	ARG	-	see sequence details	UNP P39077
g	396	TRP	-	see sequence details	UNP P39077
g	397	LYS	-	see sequence details	UNP P39077
g	398	LYS	-	see sequence details	UNP P39077
g	399	ASN	-	see sequence details	UNP P39077
g	400	PHE	-	see sequence details	UNP P39077
g	401	ILE	-	see sequence details	UNP P39077
g	402	ALA	-	see sequence details	UNP P39077
g	403	VAL	-	see sequence details	UNP P39077
g	404	SER	-	see sequence details	UNP P39077
g	405	ALA	-	see sequence details	UNP P39077
g	406	ALA	-	see sequence details	UNP P39077
g	407	ASN	-	see sequence details	UNP P39077
g	408	ARG	-	see sequence details	UNP P39077
g	409	PHE	-	see sequence details	UNP P39077
g	410	LYS	-	see sequence details	UNP P39077
g	411	LYS	-	see sequence details	UNP P39077
g	412	ILE	-	see sequence details	UNP P39077
g	413	SER	-	see sequence details	UNP P39077
g	414	SER	-	see sequence details	UNP P39077
g	415	SER	-	see sequence details	UNP P39077
g	416	GLY	-	see sequence details	UNP P39077
g	417	ALA	-	see sequence details	UNP P39077
g	418	LEU	-	see sequence details	UNP P39077
g	419	GLY	-	see sequence details	UNP P39077
g	420	SER	-	see sequence details	UNP P39077
g	421	GLY	-	see sequence details	UNP P39077
g	422	HIS	-	see sequence details	UNP P39077
g	423	HIS	-	see sequence details	UNP P39077
g	424	HIS	-	see sequence details	UNP P39077
g	425	HIS	-	see sequence details	UNP P39077
g	426	HIS	-	see sequence details	UNP P39077
g	427	HIS	-	see sequence details	UNP P39077
g	428	HIS	-	see sequence details	UNP P39077
g	429	HIS	-	see sequence details	UNP P39077
g	430	GLY	-	see sequence details	UNP P39077
g	431	SER	-	see sequence details	UNP P39077
g	432	GLY	-	see sequence details	UNP P39077

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
g	433	LEU	-	see sequence details	UNP P39077
g	434	GLN	-	see sequence details	UNP P39077
g	435	LYS	-	see sequence details	UNP P39077

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	520	Total	C	N	O	S	0	0
			3980	2510	678	773	19		
6	h	527	Total	C	N	O	S	0	0
			4032	2540	688	784	20		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	Q	548	Total	C	N	O	S	0	0
			4163	2622	711	804	26		
7	q	541	Total	C	N	O	S	0	0
			4115	2592	703	794	26		

- Molecule 8 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	T	412	Total	C	N	O	S	0	0
			3221	2017	551	632	21		

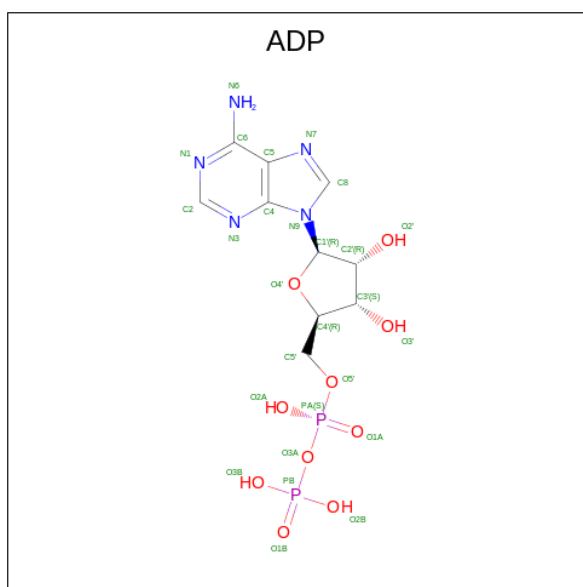
- Molecule 9 is a protein called T-complex protein 1 subunit zeta.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	Z	538	Total	C	N	O	S	0	0
			4139	2599	717	806	17		
9	z	538	Total	C	N	O	S	0	0
			4139	2599	717	806	17		

- Molecule 10 is a protein called Phosducin-like protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	p	191	Total	C	N	O	S	0	0
			1571	983	272	310	6		

- Molecule 11 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
11	A	1	Total 27	C 10	N 5	O 10	P 2	0
11	B	1	Total 27	C 10	N 5	O 10	P 2	0
11	D	1	Total 27	C 10	N 5	O 10	P 2	0
11	E	1	Total 27	C 10	N 5	O 10	P 2	0
11	G	1	Total 27	C 10	N 5	O 10	P 2	0
11	H	1	Total 27	C 10	N 5	O 10	P 2	0
11	Q	1	Total 27	C 10	N 5	O 10	P 2	0
11	Z	1	Total 27	C 10	N 5	O 10	P 2	0
11	a	1	Total 27	C 10	N 5	O 10	P 2	0
11	b	1	Total 27	C 10	N 5	O 10	P 2	0
11	d	1	Total 27	C 10	N 5	O 10	P 2	0
11	e	1	Total 27	C 10	N 5	O 10	P 2	0
11	g	1	Total 27	C 10	N 5	O 10	P 2	0
11	h	1	Total 27	C 10	N 5	O 10	P 2	0

Continued on next page...

Continued from previous page...

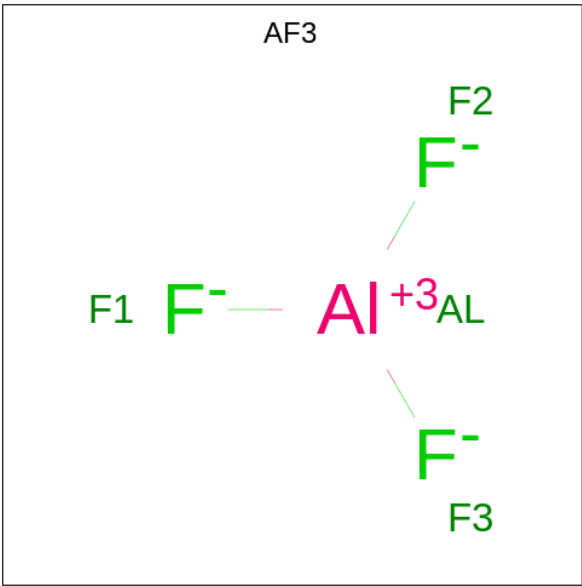
Mol	Chain	Residues	Atoms					AltConf
11	q	1	Total	C	N	O	P	0
			27	10	5	10	2	
11	z	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 12 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
12	A	1	Total	Mg	0
			1	1	
12	B	1	Total	Mg	0
			1	1	
12	D	1	Total	Mg	0
			1	1	
12	E	1	Total	Mg	0
			1	1	
12	G	1	Total	Mg	0
			1	1	
12	H	1	Total	Mg	0
			1	1	
12	Q	1	Total	Mg	0
			1	1	
12	Z	1	Total	Mg	0
			1	1	
12	a	1	Total	Mg	0
			1	1	
12	b	1	Total	Mg	0
			1	1	
12	d	1	Total	Mg	0
			1	1	
12	e	1	Total	Mg	0
			1	1	
12	g	1	Total	Mg	0
			1	1	
12	h	1	Total	Mg	0
			1	1	
12	q	1	Total	Mg	0
			1	1	
12	z	1	Total	Mg	0
			1	1	

- Molecule 13 is ALUMINUM FLUORIDE (CCD ID: AF3) (formula: AlF₃) (labeled as "Lig-

and of Interest" by depositor).



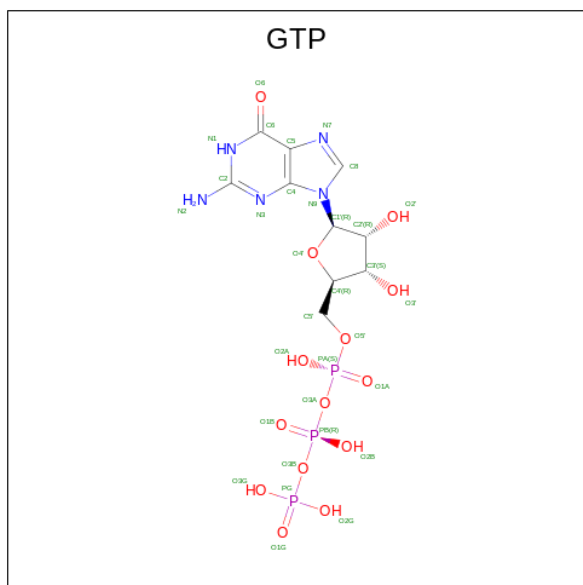
Mol	Chain	Residues	Atoms			AltConf
13	A	1	Total	Al	F	0
			4	1	3	
13	B	1	Total	Al	F	0
			4	1	3	
13	D	1	Total	Al	F	0
			4	1	3	
13	E	1	Total	Al	F	0
			4	1	3	
13	G	1	Total	Al	F	0
			4	1	3	
13	H	1	Total	Al	F	0
			4	1	3	
13	Z	1	Total	Al	F	0
			4	1	3	
13	a	1	Total	Al	F	0
			4	1	3	
13	b	1	Total	Al	F	0
			4	1	3	
13	d	1	Total	Al	F	0
			4	1	3	
13	e	1	Total	Al	F	0
			4	1	3	
13	g	1	Total	Al	F	0
			4	1	3	
13	h	1	Total	Al	F	0
			4	1	3	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
13	z	1	Total	Al	F	0
			4	1	3	

- Molecule 14 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
14	T	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 15 is water.

Mol	Chain	Residues	Atoms		AltConf
15	A	1	Total	O	0
			1	1	
15	B	1	Total	O	0
			1	1	
15	D	1	Total	O	0
			1	1	
15	E	1	Total	O	0
			1	1	
15	G	1	Total	O	0
			1	1	
15	H	1	Total	O	0
			1	1	
15	Z	1	Total	O	0
			1	1	

Continued on next page...

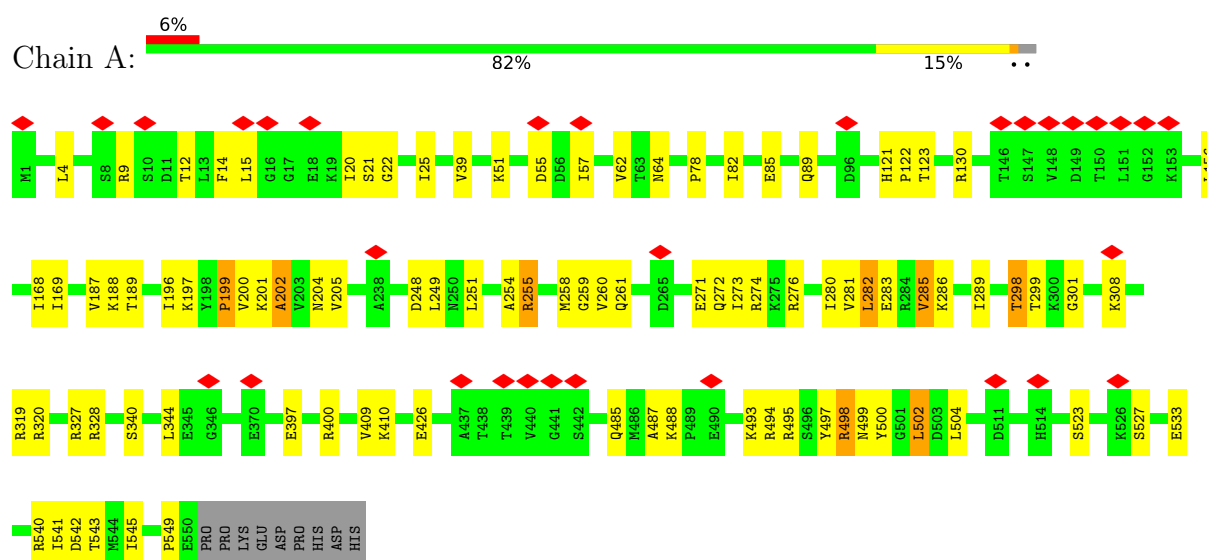
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
15	a	1	Total 1	O 1	0
15	b	1	Total 1	O 1	0
15	d	1	Total 1	O 1	0
15	e	1	Total 1	O 1	0
15	g	1	Total 1	O 1	0
15	h	1	Total 1	O 1	0
15	z	1	Total 1	O 1	0

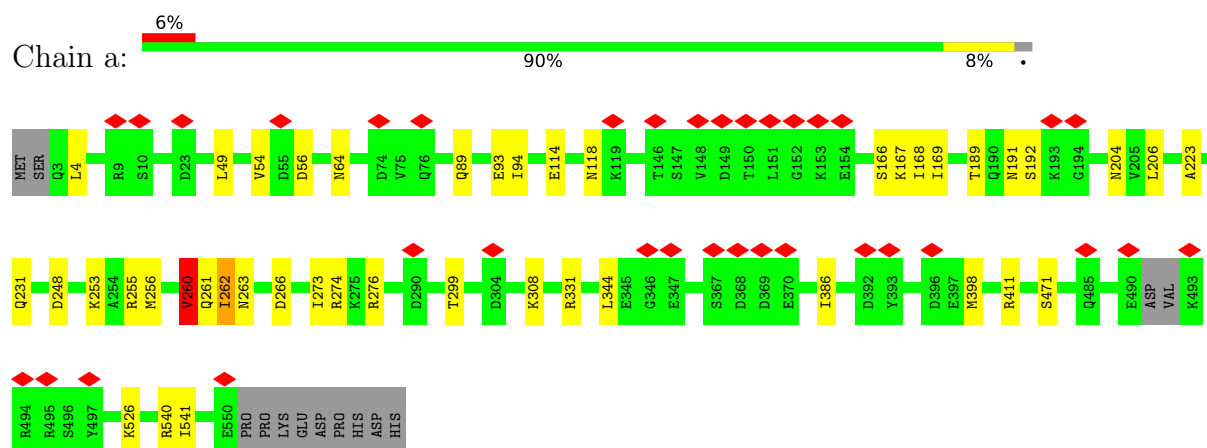
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: T-complex protein 1 subunit alpha

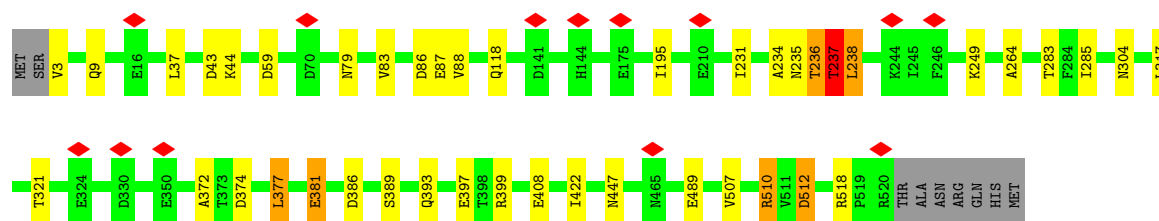


- Molecule 1: T-complex protein 1 subunit alpha

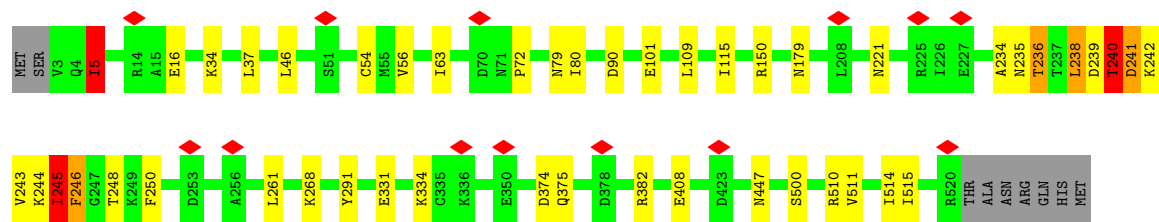
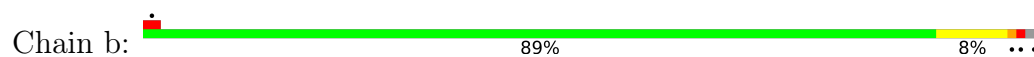


- Molecule 2: T-complex protein 1 subunit beta

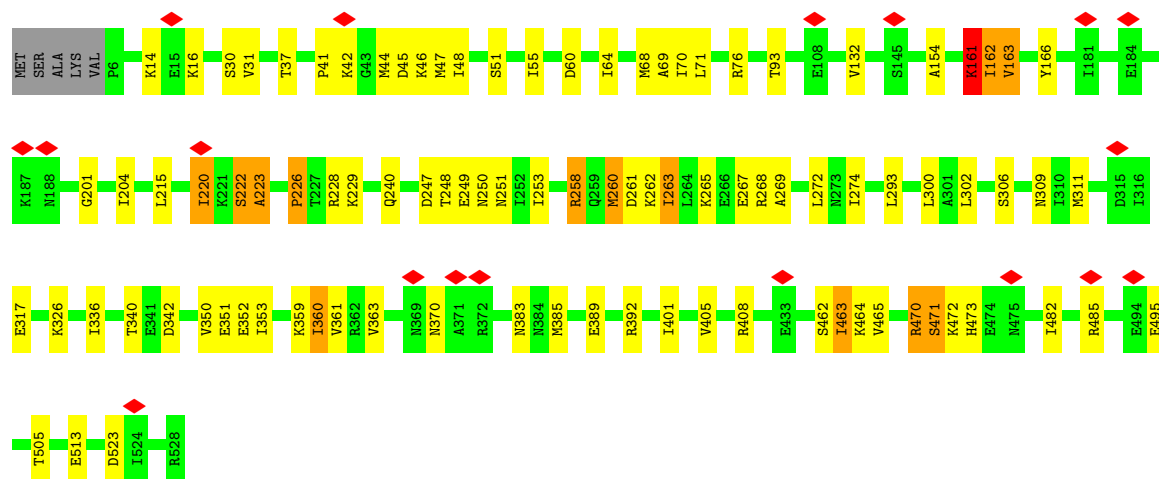
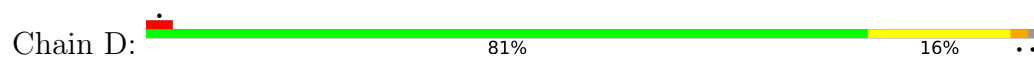




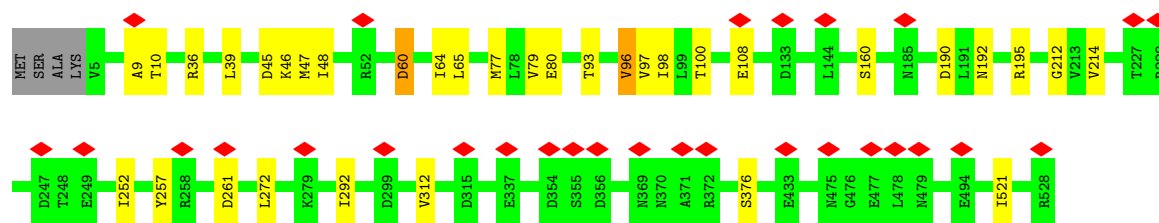
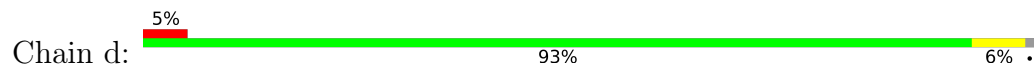
• Molecule 2: T-complex protein 1 subunit beta



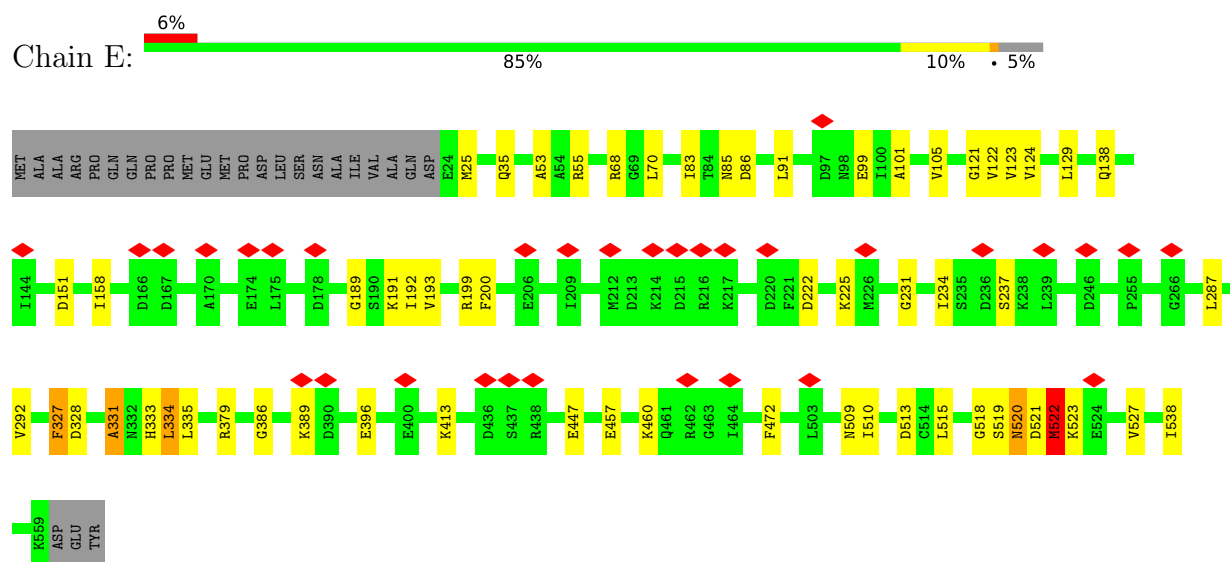
• Molecule 3: T-complex protein 1 subunit delta



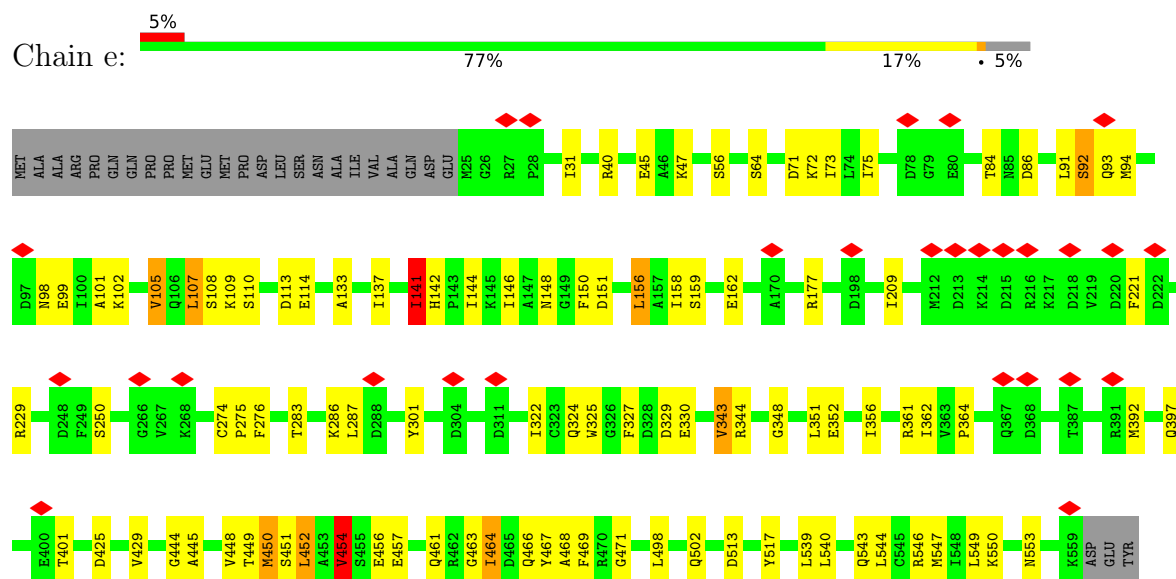
• Molecule 3: T-complex protein 1 subunit delta



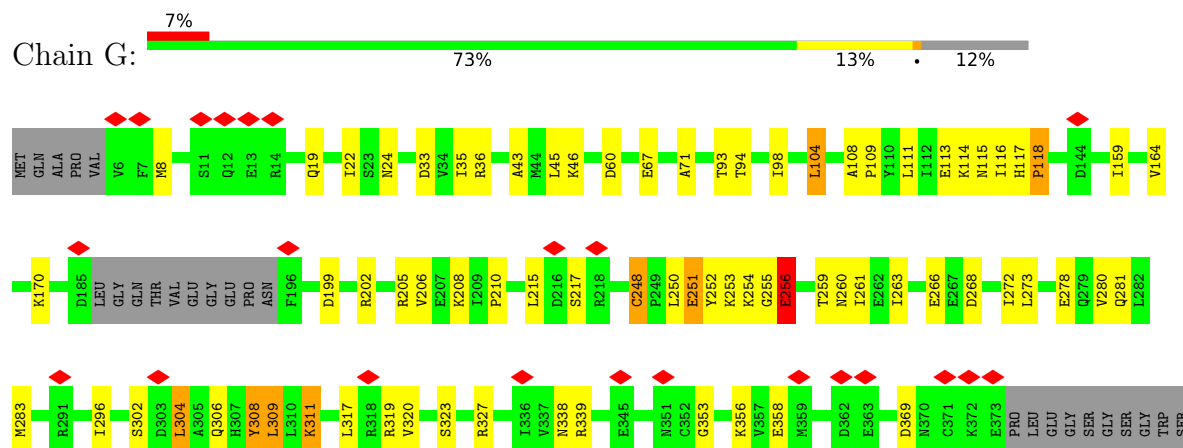
• Molecule 4: T-complex protein 1 subunit epsilon

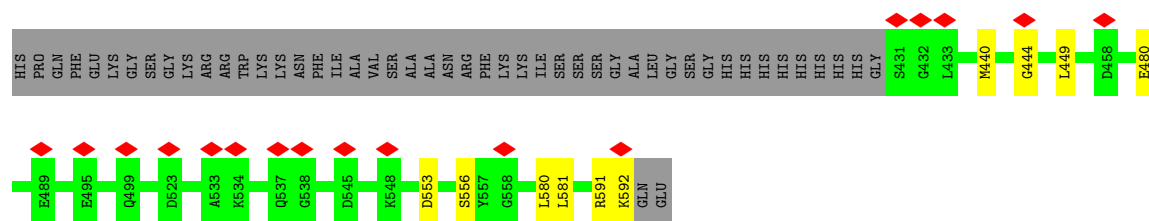


• Molecule 4: T-complex protein 1 subunit epsilon

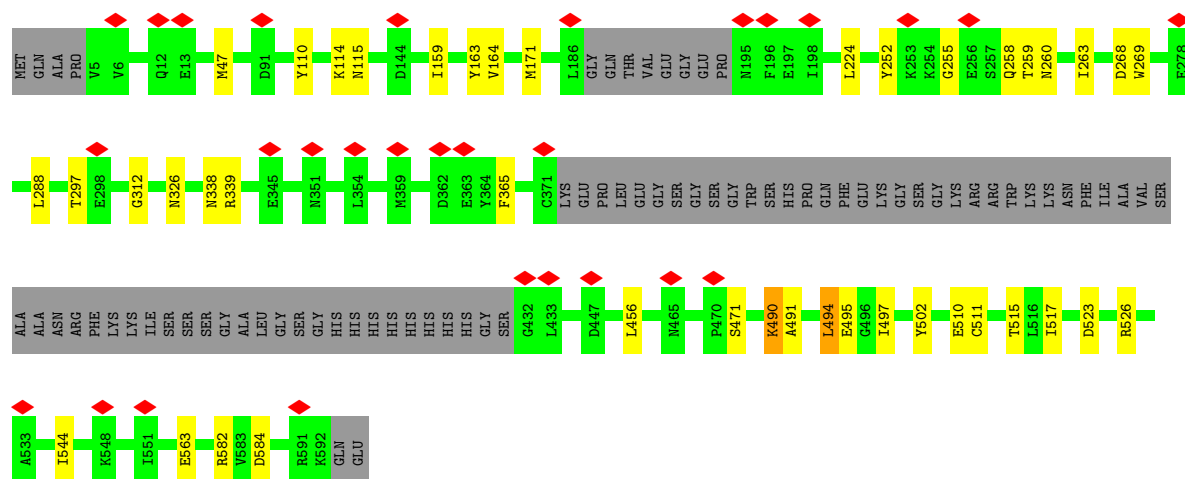
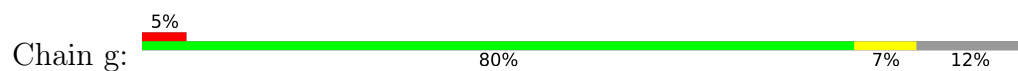


• Molecule 5: T-complex protein 1 subunit gamma

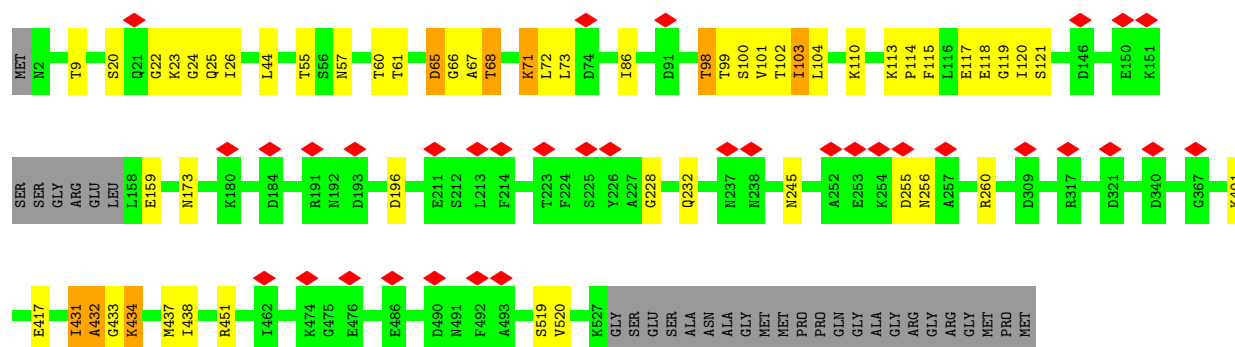
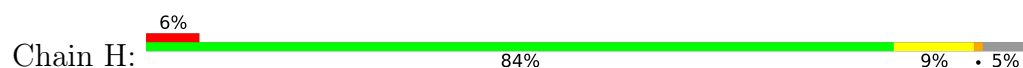




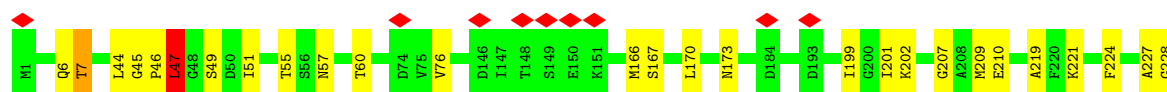
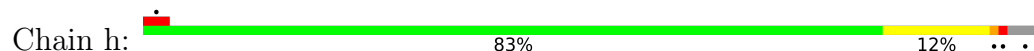
• Molecule 5: T-complex protein 1 subunit gamma

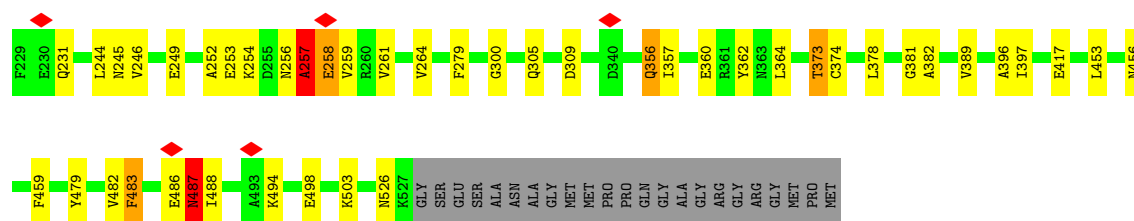


• Molecule 6: T-complex protein 1 subunit eta

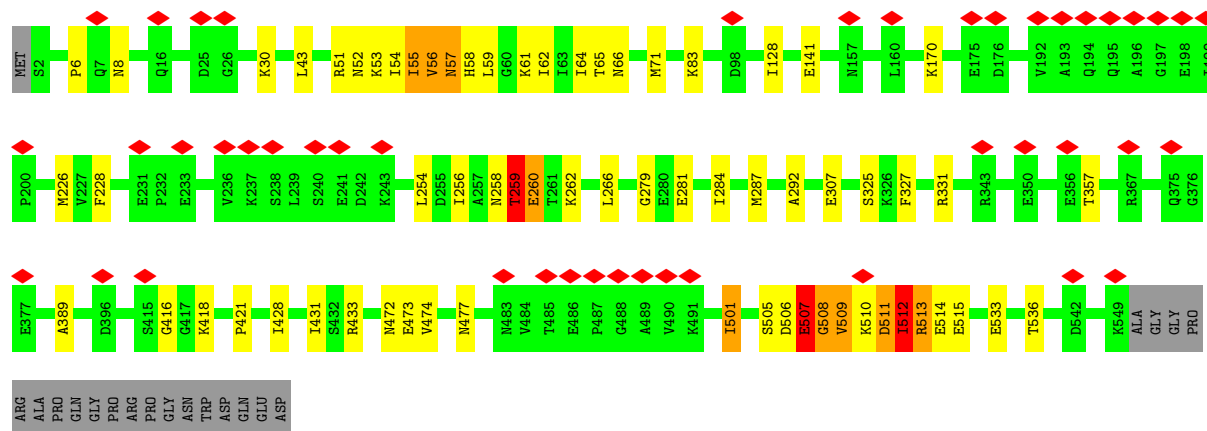
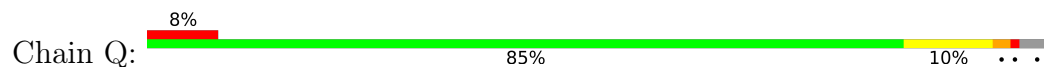


• Molecule 6: T-complex protein 1 subunit eta

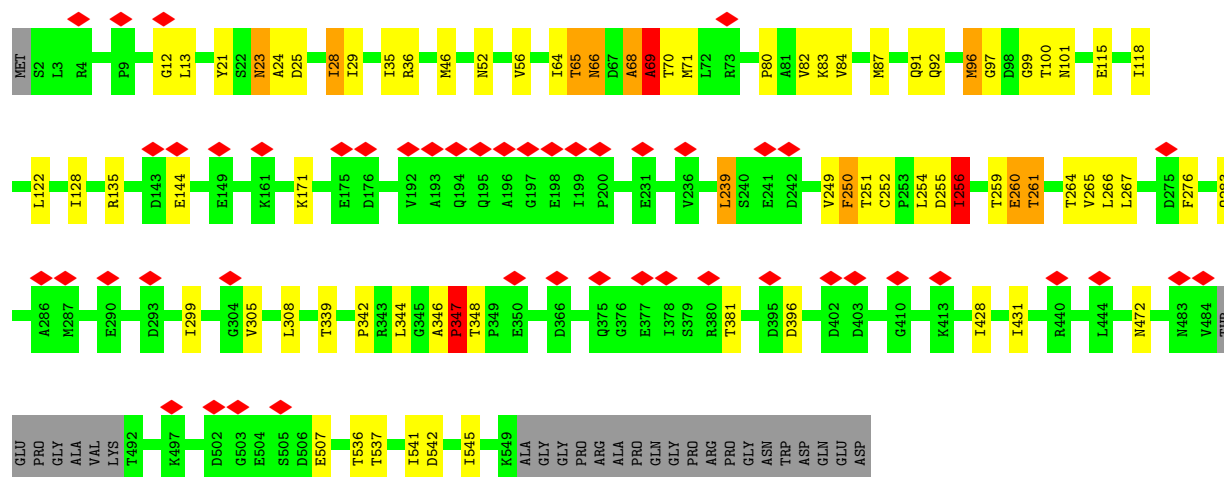
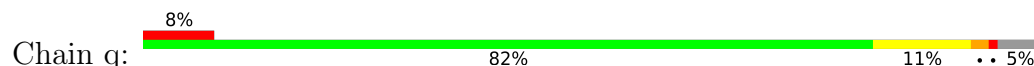




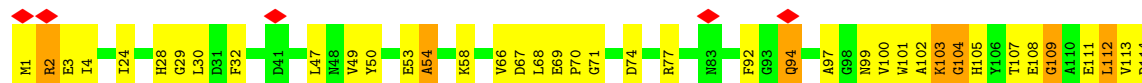
• Molecule 7: T-complex protein 1 subunit theta

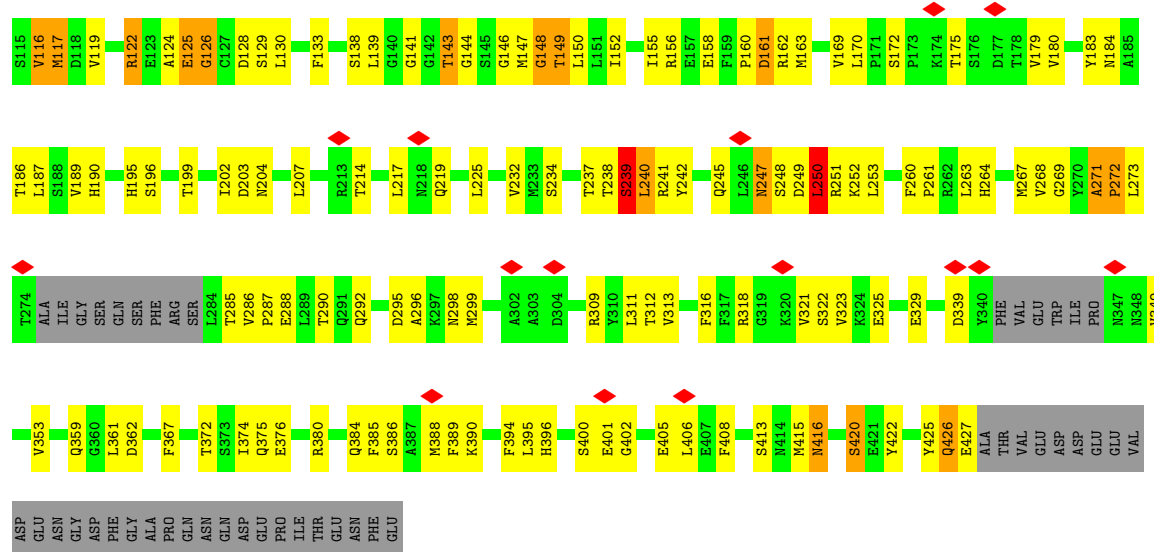


• Molecule 7: T-complex protein 1 subunit theta

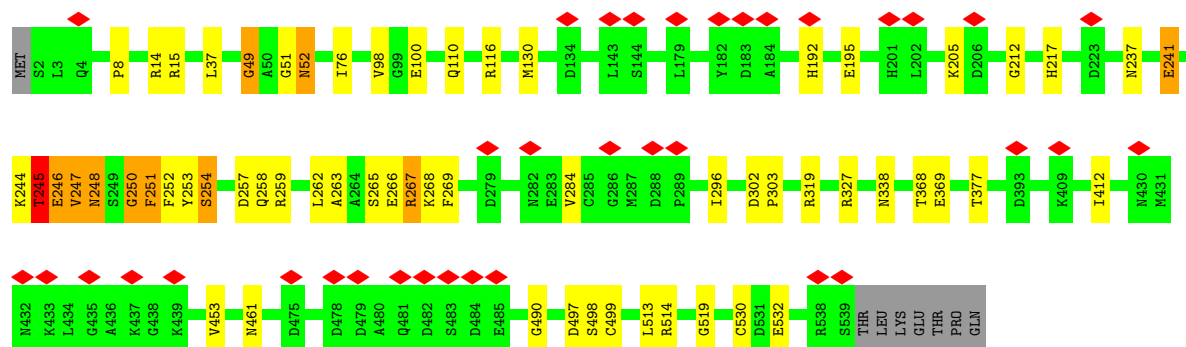
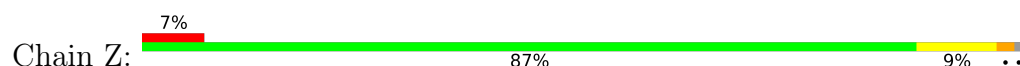


• Molecule 8: Tubulin beta chain

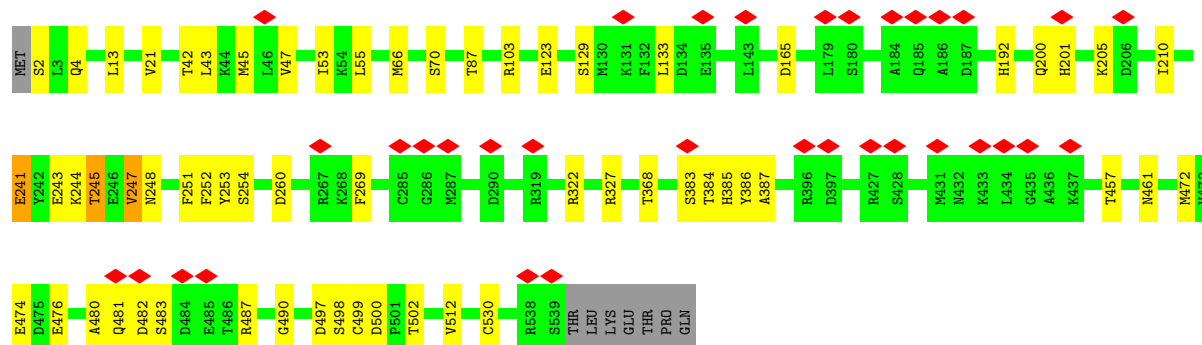
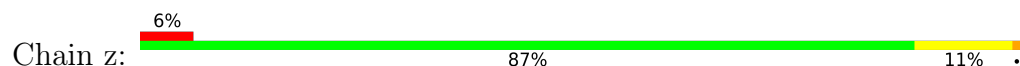




• Molecule 9: T-complex protein 1 subunit zeta

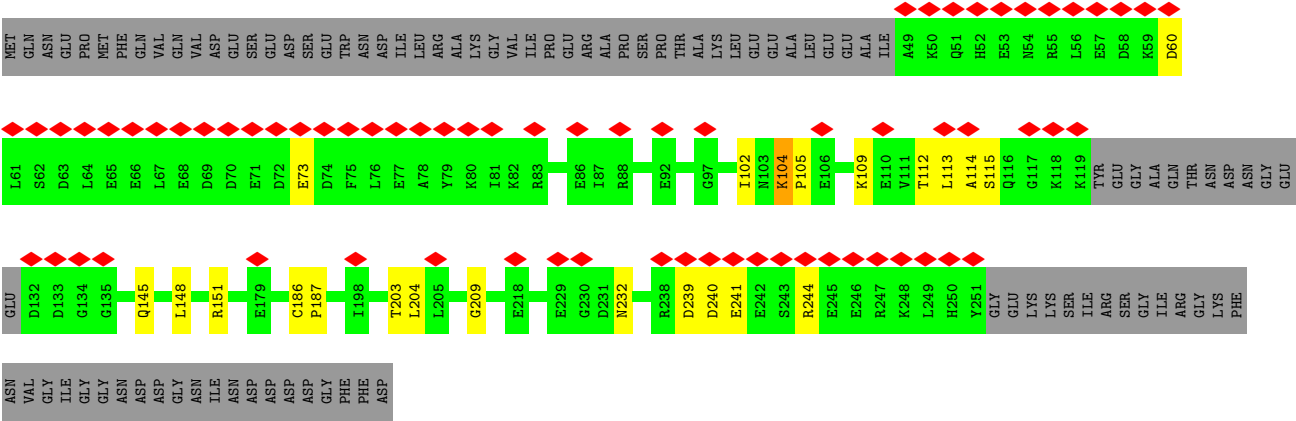


• Molecule 9: T-complex protein 1 subunit zeta



• Molecule 10: Phosducin-like protein 2





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	28063	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	38	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.961	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.056	Depositor
Recommended contour level	0.1	Depositor
Map size ($\text{\AA}$)	337.408, 337.408, 337.408	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.318, 1.318, 1.318	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.58	6/4196 (0.1%)	0.76	21/5661 (0.4%)
1	a	0.38	2/4166 (0.0%)	0.50	4/5619 (0.1%)
2	B	0.44	5/3976 (0.1%)	0.52	5/5358 (0.1%)
2	b	0.40	3/3976 (0.1%)	0.56	10/5358 (0.2%)
3	D	0.64	6/4036 (0.1%)	0.72	20/5440 (0.4%)
3	d	0.38	2/4043 (0.0%)	0.47	3/5451 (0.1%)
4	E	0.55	6/4184 (0.1%)	0.63	11/5629 (0.2%)
4	e	0.75	9/4175 (0.2%)	0.72	18/5617 (0.3%)
5	G	0.52	2/4048 (0.0%)	0.69	13/5459 (0.2%)
5	g	0.40	0/4047	0.55	4/5460 (0.1%)
6	H	0.59	7/4030 (0.2%)	0.67	9/5440 (0.2%)
6	h	0.54	5/4083 (0.1%)	0.65	8/5511 (0.1%)
7	Q	0.60	9/4214 (0.2%)	0.68	11/5689 (0.2%)
7	q	0.55	6/4164 (0.1%)	0.71	17/5619 (0.3%)
8	T	1.00	9/3287 (0.3%)	1.16	41/4448 (0.9%)
9	Z	0.51	5/4191 (0.1%)	0.65	13/5663 (0.2%)
9	z	0.44	3/4191 (0.1%)	0.55	6/5663 (0.1%)
10	p	0.49	0/1594	0.64	4/2134 (0.2%)
All	All	0.56	85/70601 (0.1%)	0.67	218/95219 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
8	T	0	2

All (85) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	T	143	THR	CA-C	-8.24	1.42	1.52
9	Z	267	ARG	C-O	-8.00	1.14	1.24
4	e	114	GLU	C-N	-7.70	1.24	1.33
8	T	143	THR	C-O	-7.52	1.15	1.24
3	D	249	GLU	CA-C	-7.23	1.43	1.52
6	h	356	GLN	CA-C	-7.07	1.43	1.52
3	D	462	SER	CA-C	-7.00	1.43	1.52
7	Q	511	ASP	CA-C	-6.91	1.43	1.52
4	E	122	VAL	N-CA	-6.86	1.38	1.46
8	T	325	GLU	C-O	6.83	1.31	1.24
9	Z	263	ALA	C-O	6.67	1.32	1.24
4	e	445	ALA	CA-C	-6.67	1.44	1.52
1	A	498	ARG	CA-C	-6.65	1.43	1.52
5	G	248	CYS	CA-C	-6.64	1.44	1.53
8	T	247	ASN	CA-C	-6.63	1.43	1.52
7	q	23	ASN	CA-C	-6.62	1.43	1.53
7	Q	509	VAL	CA-C	-6.58	1.44	1.52
9	z	247	VAL	CA-C	-6.57	1.45	1.52
6	h	357	ILE	N-CA	-6.45	1.39	1.46
7	Q	55	ILE	CA-C	-6.43	1.46	1.52
1	A	283	GLU	CA-C	-6.42	1.44	1.52
4	E	333	HIS	CA-C	-6.32	1.44	1.52
6	h	382	ALA	CA-C	-6.24	1.44	1.52
7	q	69	ALA	CA-C	-6.09	1.44	1.52
9	Z	253	TYR	CA-C	-6.08	1.45	1.52
9	z	243	GLU	CA-C	-6.08	1.45	1.52
1	A	255	ARG	CA-C	-6.04	1.45	1.52
4	e	114	GLU	CA-C	-5.96	1.45	1.52
1	a	263	ASN	CA-C	-5.87	1.45	1.52
2	b	240	THR	CA-C	-5.87	1.45	1.52
7	q	100	THR	CA-C	-5.85	1.44	1.52
3	D	228	ARG	CA-C	-5.81	1.45	1.52
7	q	68	ALA	CA-C	-5.80	1.45	1.52
2	B	381	GLU	CA-C	-5.79	1.45	1.52
8	T	103	LYS	CA-C	-5.79	1.45	1.52
2	B	512	ASP	CA-C	-5.77	1.45	1.53
4	e	456	GLU	C-O	5.76	1.30	1.24
9	Z	254	SER	CA-C	-5.73	1.47	1.53
1	a	255	ARG	CA-C	-5.69	1.45	1.53
7	Q	281	GLU	CA-C	-5.67	1.45	1.52
5	G	252	TYR	CA-C	-5.66	1.45	1.52
3	D	222	SER	CA-C	-5.62	1.45	1.52
6	H	98	THR	C-O	5.62	1.30	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	e	454	VAL	C-O	-5.57	1.17	1.24
7	Q	512	ILE	N-CA	-5.56	1.38	1.46
1	A	273	ILE	C-O	5.55	1.30	1.24
3	D	260	MET	CA-C	-5.54	1.45	1.52
6	H	121	SER	CA-C	-5.54	1.45	1.53
9	z	245	THR	CA-C	-5.54	1.45	1.52
8	T	148	GLY	CA-C	-5.54	1.46	1.52
4	e	450	MET	N-CA	-5.53	1.39	1.46
8	T	111	GLU	C-O	5.50	1.31	1.24
3	d	96	VAL	CA-C	-5.49	1.45	1.52
4	e	107	LEU	CA-C	-5.46	1.45	1.52
4	E	521	ASP	CA-C	-5.46	1.45	1.52
6	H	67	ALA	CA-C	-5.44	1.46	1.52
6	H	100	SER	N-CA	-5.43	1.39	1.46
2	b	246	PHE	CA-C	-5.39	1.46	1.52
4	e	449	THR	CA-C	-5.38	1.46	1.52
4	E	513	ASP	CA-C	-5.37	1.46	1.53
2	b	5	ILE	N-CA	-5.36	1.41	1.46
6	H	99	THR	CA-C	-5.34	1.45	1.52
2	B	237	THR	CA-C	-5.32	1.45	1.52
7	q	346	ALA	N-CA	-5.32	1.41	1.46
3	D	223	ALA	CA-C	-5.30	1.45	1.52
8	T	149	THR	N-CA	-5.30	1.40	1.46
8	T	420	SER	N-CA	-5.29	1.40	1.46
1	A	488	LYS	CA-C	-5.26	1.47	1.53
2	B	510	ARG	C-O	-5.26	1.17	1.24
2	B	235	ASN	CA-C	-5.25	1.45	1.52
7	Q	511	ASP	N-CA	-5.25	1.39	1.46
7	Q	254	LEU	CA-C	-5.24	1.46	1.53
9	Z	258	GLN	N-CA	-5.22	1.39	1.46
7	Q	57	ASN	CA-C	-5.21	1.48	1.53
4	e	467	TYR	N-CA	-5.21	1.40	1.46
6	H	434	LYS	CA-C	-5.21	1.46	1.52
3	d	100	THR	CA-C	-5.21	1.46	1.52
4	E	331	ALA	CA-C	-5.14	1.45	1.52
7	Q	55	ILE	N-CA	-5.11	1.39	1.46
1	A	274	ARG	N-CA	-5.08	1.40	1.46
6	h	257	ALA	C-O	-5.08	1.17	1.24
6	H	65	ASP	C-N	-5.07	1.27	1.33
6	h	483	PHE	N-CA	-5.04	1.40	1.46
4	E	122	VAL	CA-C	-5.03	1.46	1.52
7	q	68	ALA	N-CA	-5.03	1.40	1.46

All (218) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	q	346	ALA	N-CA-C	-16.92	93.01	108.07
7	Q	512	ILE	N-CA-C	-14.47	98.69	112.29
6	h	245	ASN	N-CA-C	-14.09	96.15	113.20
1	A	202	ALA	N-CA-C	-14.04	96.64	114.04
5	G	256	GLU	N-CA-C	13.69	126.28	111.36
1	A	201	LYS	N-CA-C	-12.28	96.49	113.56
5	G	309	LEU	N-CA-C	-11.44	98.82	111.28
2	b	235	ASN	N-CA-C	-11.12	101.18	112.97
6	H	431	ILE	N-CA-C	10.55	123.67	108.48
8	T	247	ASN	N-CA-C	-10.12	98.77	112.03
5	G	260	ASN	N-CA-C	9.26	122.59	111.02
5	g	495	GLU	N-CA-C	9.25	122.58	111.02
2	b	238	LEU	N-CA-C	-9.18	101.63	112.92
8	T	109	GLY	N-CA-C	-8.91	101.36	112.77
7	Q	65	THR	N-CA-C	8.84	122.31	108.79
9	Z	250	GLY	N-CA-C	8.77	123.47	111.54
2	B	374	ASP	N-CA-C	-8.74	101.68	111.82
9	Z	52	ASN	CA-C-N	-8.73	111.84	123.10
9	Z	52	ASN	C-N-CA	-8.73	111.84	123.10
5	G	304	LEU	N-CA-C	8.72	122.41	111.69
3	D	471	SER	N-CA-C	8.37	120.48	111.36
9	z	241	GLU	N-CA-C	8.35	122.38	109.60
7	q	252	CYS	CA-C-N	-8.34	112.05	120.98
7	q	252	CYS	C-N-CA	-8.34	112.05	120.98
7	Q	292	ALA	N-CA-C	8.33	121.48	111.82
7	q	256	ILE	N-CA-C	-8.31	98.14	109.37
1	A	500	TYR	N-CA-C	8.29	121.62	109.69
6	H	23	LYS	N-CA-C	-8.28	102.63	112.89
1	A	272	GLN	N-CA-C	8.27	120.29	111.28
3	D	472	LYS	N-CA-C	-8.19	102.39	112.38
6	H	118	GLU	N-CA-C	-8.16	96.96	109.85
8	T	152	ILE	N-CA-C	-8.00	102.46	110.62
7	q	259	THR	N-CA-C	8.00	121.09	110.53
9	Z	258	GLN	N-CA-C	-8.00	102.62	112.38
1	A	271	GLU	N-CA-C	-7.95	102.55	111.14
8	T	97	ALA	N-CA-C	-7.86	102.71	111.82
6	h	254	LYS	N-CA-C	-7.83	97.39	109.52
6	H	101	VAL	CB-CA-C	-7.74	102.07	111.97
6	H	22	GLY	N-CA-C	7.64	121.71	110.63
3	D	462	SER	N-CA-C	7.62	119.58	111.28
9	z	474	GLU	N-CA-C	-7.52	103.08	111.28
8	T	416	ASN	N-CA-C	-7.51	103.10	111.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	235	ASN	N-CA-C	-7.49	100.58	111.30
4	e	101	ALA	N-CA-C	-7.44	103.19	111.82
1	A	301	GLY	N-CA-C	7.40	122.01	112.54
9	Z	267	ARG	CA-C-O	-7.37	113.26	121.00
10	p	104	LYS	N-CA-C	7.37	122.77	112.75
3	D	163	VAL	CA-C-N	-7.34	110.72	122.24
3	D	163	VAL	C-N-CA	-7.34	110.72	122.24
7	Q	56	VAL	N-CA-C	-7.32	102.07	110.05
7	q	66	ASN	N-CA-C	-7.26	103.52	112.88
6	H	432	ALA	N-CA-C	7.22	126.19	110.80
4	e	110	SER	CA-C-N	-7.21	110.62	120.28
4	e	110	SER	C-N-CA	-7.21	110.62	120.28
4	e	105	VAL	CB-CA-C	-7.17	102.45	112.14
8	T	161	ASP	N-CA-C	7.17	119.09	111.28
6	h	47	LEU	CA-C-N	7.16	130.32	122.16
6	h	47	LEU	C-N-CA	7.16	130.32	122.16
7	q	96	MET	N-CA-C	7.13	119.06	111.28
9	Z	245	THR	N-CA-C	7.11	125.95	110.80
6	h	256	ASN	N-CA-C	-7.11	98.97	110.20
1	A	280	ILE	CA-C-N	-7.07	110.78	120.46
1	A	280	ILE	C-N-CA	-7.07	110.78	120.46
5	G	259	THR	N-CA-C	7.01	122.29	111.56
9	Z	266	GLU	CA-C-N	-6.96	111.46	120.65
9	Z	266	GLU	C-N-CA	-6.96	111.46	120.65
6	H	20	SER	N-CA-C	6.92	122.86	108.53
3	D	250	ASN	CA-C-N	-6.86	113.64	122.77
3	D	250	ASN	C-N-CA	-6.86	113.64	122.77
5	G	248	CYS	N-CA-C	6.85	120.06	110.20
3	D	260	MET	CA-C-N	-6.81	111.16	120.28
3	D	260	MET	C-N-CA	-6.81	111.16	120.28
2	b	236	THR	N-CA-C	6.74	119.22	110.53
8	T	271	ALA	CA-C-N	6.73	128.25	119.84
8	T	271	ALA	C-N-CA	6.73	128.25	119.84
8	T	117	MET	N-CA-C	-6.72	103.95	111.28
7	Q	279	GLY	N-CA-C	-6.70	104.69	112.73
7	q	249	VAL	O-C-N	6.67	130.28	123.20
8	T	172	SER	CA-C-N	-6.66	112.04	118.97
8	T	172	SER	C-N-CA	-6.66	112.04	118.97
4	E	122	VAL	N-CA-C	-6.64	103.85	110.62
1	a	260	VAL	N-CA-C	6.62	117.58	108.84
9	Z	267	ARG	CA-C-N	6.56	134.08	121.54
9	Z	267	ARG	C-N-CA	6.56	134.08	121.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	351	GLU	N-CA-C	6.56	119.85	108.76
2	b	241	ASP	N-CA-C	6.53	119.22	111.71
4	E	522	MET	CA-C-N	-6.53	110.41	122.09
4	E	522	MET	C-N-CA	-6.53	110.41	122.09
7	q	239	LEU	N-CA-CB	-6.50	106.76	114.17
6	h	357	ILE	N-CA-C	-6.46	98.22	107.98
4	E	333	HIS	CA-C-N	-6.44	110.30	120.60
4	E	333	HIS	C-N-CA	-6.44	110.30	120.60
8	T	126	GLY	N-CA-C	6.43	121.53	114.40
4	e	343	VAL	N-CA-C	-6.41	99.15	108.89
8	T	242	TYR	CB-CA-C	6.40	118.48	108.88
8	T	219	GLN	CA-C-N	-6.40	113.36	119.76
8	T	219	GLN	C-N-CA	-6.40	113.36	119.76
5	g	497	ILE	CA-C-N	-6.35	109.25	121.94
5	g	497	ILE	C-N-CA	-6.35	109.25	121.94
3	D	247	ASP	N-CA-C	6.34	118.19	111.28
9	Z	246	GLU	N-CA-C	6.32	124.25	110.80
9	Z	267	ARG	N-CA-C	6.30	117.84	110.97
1	A	248	ASP	N-CA-C	-6.30	103.93	113.89
4	e	141	ILE	N-CA-C	6.30	118.18	109.80
8	T	148	GLY	N-CA-C	-6.29	104.89	112.49
3	D	260	MET	N-CA-C	-6.28	104.35	111.07
4	e	445	ALA	N-CA-C	-6.28	104.35	111.14
1	a	253	LYS	O-C-N	6.26	130.63	122.93
8	T	240	LEU	N-CA-C	6.25	121.03	112.04
4	E	123	VAL	N-CA-C	6.21	116.95	110.62
8	T	104	GLY	N-CA-C	-6.21	105.30	112.50
1	A	498	ARG	CA-C-N	-6.20	111.20	121.92
1	A	498	ARG	C-N-CA	-6.20	111.20	121.92
8	T	325	GLU	N-CA-C	-6.18	104.45	111.07
8	T	58	LYS	N-CA-C	-6.17	97.82	108.56
1	a	266	ASP	CA-C-N	6.15	125.85	119.82
1	a	266	ASP	C-N-CA	6.15	125.85	119.82
8	T	3	GLU	N-CA-C	6.14	119.04	109.52
8	T	239	SER	N-CA-C	-6.13	103.90	111.75
4	E	518	GLY	N-CA-C	-6.13	101.10	112.37
4	e	92	SER	O-C-N	-6.12	115.42	122.89
2	B	236	THR	N-CA-C	6.12	119.21	109.24
4	E	189	GLY	N-CA-C	-6.02	103.94	112.37
8	T	156	ARG	N-CA-C	-5.95	104.80	111.28
3	D	229	LYS	CA-C-N	-5.95	111.60	120.94
3	D	229	LYS	C-N-CA	-5.95	111.60	120.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	115	ASN	N-CA-C	5.89	119.55	111.54
8	T	143	THR	N-CA-CB	5.89	118.55	110.01
8	T	2	ARG	N-CA-C	5.88	117.69	111.28
1	A	255	ARG	N-CA-C	-5.88	99.07	109.06
1	A	502	LEU	N-CA-C	5.86	118.72	110.23
3	D	220	ILE	O-C-N	5.85	129.50	121.90
10	p	112	THR	CA-C-N	-5.84	112.45	120.28
10	p	112	THR	C-N-CA	-5.84	112.45	120.28
8	T	114	ASP	CA-C-N	-5.83	111.89	120.28
8	T	114	ASP	C-N-CA	-5.83	111.89	120.28
8	T	250	LEU	N-CA-C	5.82	123.19	110.80
3	d	9	ALA	N-CA-CB	-5.80	107.55	114.17
4	E	327	PHE	N-CA-C	5.79	123.12	110.80
4	E	523	LYS	N-CA-C	-5.76	106.38	113.41
4	E	520	ASN	N-CA-C	-5.74	106.12	113.01
5	G	113	GLU	CA-C-N	-5.72	112.72	122.56
5	G	113	GLU	C-N-CA	-5.72	112.72	122.56
8	T	362	ASP	N-CA-C	5.72	117.60	111.36
7	Q	507	GLU	N-CA-C	5.68	122.90	110.80
8	T	359	GLN	N-CA-C	-5.67	101.66	110.10
7	Q	281	GLU	N-CA-C	-5.66	105.01	111.07
6	h	224	PHE	N-CA-C	5.64	117.43	111.28
9	z	502	THR	N-CA-C	5.63	117.22	111.14
7	q	13	LEU	CA-C-N	5.63	129.09	120.82
7	q	13	LEU	C-N-CA	5.63	129.09	120.82
2	b	240	THR	N-CA-C	-5.58	99.69	108.63
8	T	122	ARG	N-CA-C	5.55	117.33	111.28
1	A	280	ILE	N-CA-C	-5.54	105.10	110.42
2	b	245	ILE	N-CA-C	-5.52	97.85	109.34
1	A	283	GLU	N-CA-C	-5.51	105.28	111.28
3	D	258	ARG	N-CA-C	-5.48	105.40	111.71
2	b	242	LYS	CA-C-N	-5.48	116.00	122.36
2	b	242	LYS	C-N-CA	-5.48	116.00	122.36
5	G	118	PRO	CA-C-N	5.46	128.79	122.35
5	G	118	PRO	C-N-CA	5.46	128.79	122.35
6	H	102	THR	N-CA-C	5.45	117.22	111.28
7	q	347	PRO	N-CA-C	5.43	123.67	112.47
1	A	202	ALA	CA-C-N	-5.43	112.60	122.43
1	A	202	ALA	C-N-CA	-5.43	112.60	122.43
7	q	65	THR	N-CA-C	5.42	117.50	108.99
6	h	487	ASN	N-CA-C	-5.42	99.26	110.80
3	D	161	LYS	CB-CA-C	-5.40	102.72	114.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	e	444	GLY	O-C-N	5.39	129.09	122.46
10	p	102	ILE	CB-CA-C	-5.38	102.47	111.29
5	g	494	LEU	N-CA-C	5.36	122.22	110.80
4	e	150	PHE	N-CA-C	-5.34	105.46	111.28
8	T	103	LYS	CB-CA-C	-5.34	102.50	110.88
5	G	113	GLU	N-CA-C	5.34	119.55	112.72
4	e	114	GLU	CA-C-N	5.33	129.54	121.65
4	e	114	GLU	C-N-CA	5.33	129.54	121.65
1	A	487	ALA	N-CA-C	5.32	122.13	110.80
7	Q	258	ASN	N-CA-C	-5.29	101.13	109.50
6	H	67	ALA	N-CA-C	5.29	116.73	111.07
4	e	449	THR	CB-CA-C	-5.29	102.58	110.88
1	A	254	ALA	N-CA-C	5.26	117.92	110.50
8	T	155	ILE	CB-CA-C	-5.26	104.97	112.22
8	T	107	THR	CA-C-N	-5.25	112.29	122.06
8	T	107	THR	C-N-CA	-5.25	112.29	122.06
4	e	109	LYS	N-CA-C	-5.25	105.67	111.71
2	b	5	ILE	CB-CA-C	5.23	116.27	110.62
7	Q	501	ILE	N-CA-C	-5.23	106.59	111.45
1	A	204	ASN	N-CA-C	5.20	117.78	110.14
3	D	161	LYS	N-CA-C	5.19	114.89	108.19
8	T	71	GLY	N-CA-C	5.18	118.95	112.73
8	T	54	ALA	N-CA-C	-5.18	102.53	110.14
4	e	451	SER	CA-C-N	-5.17	112.46	120.31
4	e	451	SER	C-N-CA	-5.17	112.46	120.31
8	T	116	VAL	N-CA-C	5.15	115.92	110.72
1	A	298	THR	O-C-N	-5.14	117.39	123.25
4	e	113	ASP	CA-C-N	-5.12	112.15	120.71
4	e	113	ASP	C-N-CA	-5.12	112.15	120.71
8	T	184	ASN	N-CA-C	-5.12	105.87	112.68
2	b	246	PHE	N-CA-C	-5.12	102.81	110.23
3	D	262	LYS	N-CA-C	5.11	116.93	111.36
3	d	96	VAL	CA-C-N	-5.10	113.47	120.46
3	d	96	VAL	C-N-CA	-5.10	113.47	120.46
7	q	97	GLY	N-CA-C	5.09	122.35	115.32
8	T	103	LYS	N-CA-C	5.09	116.52	111.07
8	T	92	PHE	N-CA-C	5.09	116.70	108.26
3	D	464	LYS	N-CA-C	-5.08	105.64	111.07
9	Z	251	PHE	N-CA-C	-5.07	102.02	109.62
5	G	98	ILE	O-C-N	-5.06	116.08	121.80
7	Q	57	ASN	CB-CA-C	-5.06	101.76	114.11
7	Q	508	GLY	N-CA-C	-5.06	101.19	113.18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	422	ILE	CA-C-N	5.04	128.00	120.90
2	B	422	ILE	C-N-CA	5.04	128.00	120.90
9	z	500	ASP	CA-C-N	-5.03	113.46	119.05
9	z	500	ASP	C-N-CA	-5.03	113.46	119.05
9	z	245	THR	N-CA-C	-5.03	102.93	110.23
7	q	250	PHE	N-CA-CB	-5.00	102.27	110.43
7	q	339	THR	CA-C-N	-5.00	114.76	119.76
7	q	339	THR	C-N-CA	-5.00	114.76	119.76

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	T	271	ALA	Peptide
8	T	94	GLN	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4158	0	4322	95	0
1	a	4129	0	4291	35	0
2	B	3937	0	4043	38	0
2	b	3937	0	4043	31	0
3	D	3998	0	4170	110	0
3	d	4005	0	4178	29	0
4	E	4133	0	4236	46	0
4	e	4124	0	4231	92	0
5	G	4004	0	4152	61	0
5	g	4003	0	4154	31	0
6	H	3980	0	4060	33	0
6	h	4032	0	4116	77	0
7	Q	4163	0	4300	53	0
7	q	4115	0	4249	72	0
8	T	3221	0	3090	142	0
9	Z	4139	0	4233	45	0
9	z	4139	0	4233	65	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	p	1571	0	1537	15	0
11	A	27	0	12	1	0
11	B	27	0	12	1	0
11	D	27	0	12	3	0
11	E	27	0	12	0	0
11	G	27	0	12	1	0
11	H	27	0	12	0	0
11	Q	27	0	12	1	0
11	Z	27	0	12	1	0
11	a	27	0	12	1	0
11	b	27	0	12	0	0
11	d	27	0	12	1	0
11	e	27	0	12	1	0
11	g	27	0	12	0	0
11	h	27	0	12	1	0
11	q	27	0	12	2	0
11	z	27	0	12	1	0
12	A	1	0	0	0	0
12	B	1	0	0	0	0
12	D	1	0	0	0	0
12	E	1	0	0	0	0
12	G	1	0	0	0	0
12	H	1	0	0	0	0
12	Q	1	0	0	0	0
12	Z	1	0	0	0	0
12	a	1	0	0	0	0
12	b	1	0	0	0	0
12	d	1	0	0	0	0
12	e	1	0	0	0	0
12	g	1	0	0	0	0
12	h	1	0	0	0	0
12	q	1	0	0	0	0
12	z	1	0	0	0	0
13	A	4	0	0	1	0
13	B	4	0	0	3	0
13	D	4	0	0	3	0
13	E	4	0	0	2	0
13	G	4	0	0	2	0
13	H	4	0	0	1	0
13	Z	4	0	0	1	0
13	a	4	0	0	1	0
13	b	4	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	d	4	0	0	6	0
13	e	4	0	0	2	0
13	g	4	0	0	0	0
13	h	4	0	0	1	0
13	z	4	0	0	1	0
14	T	32	0	12	6	0
15	A	1	0	0	0	0
15	B	1	0	0	0	0
15	D	1	0	0	0	0
15	E	1	0	0	0	0
15	G	1	0	0	0	0
15	H	1	0	0	0	0
15	Z	1	0	0	0	0
15	a	1	0	0	0	0
15	b	1	0	0	0	0
15	d	1	0	0	0	0
15	e	1	0	0	0	0
15	g	1	0	0	0	0
15	h	1	0	0	0	0
15	z	1	0	0	0	0
All	All	70338	0	71842	818	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 6.

All (818) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:T:141:GLY:HA3	14:T:502:GTP:O2A	1.44	1.15
4:e:539:LEU:HD22	6:h:210:GLU:OE2	1.47	1.14
4:e:91:LEU:HD13	4:e:105:VAL:HA	1.32	1.08
7:q:84:VAL:HG13	9:z:386:TYR:OH	1.64	0.97
1:A:542:ASP:OD2	3:D:37:THR:HG21	1.63	0.96
3:d:93:THR:OG1	13:d:603:AF3:F3	1.72	0.96
8:T:125:GLU:HG2	9:Z:217:HIS:CE1	2.01	0.95
9:Z:241:GLU:HA	9:Z:302:ASP:HB2	1.52	0.91
1:A:545:ILE:HD13	3:D:68:MET:SD	2.09	0.91
3:d:60:ASP:OD1	13:d:603:AF3:F2	1.77	0.91
1:A:200:VAL:HB	1:A:410:LYS:HZ1	1.36	0.90
3:D:353:ILE:HG13	3:D:360:ILE:HG23	1.53	0.90
6:H:71:LYS:C	6:H:73:LEU:H	1.70	0.90

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:266:GLU:HB2	9:Z:265:SER:HB2	1.53	0.88
2:b:240:THR:H	2:b:291:TYR:HE2	1.18	0.86
2:B:234:ALA:HB1	2:B:236:THR:HG22	1.54	0.86
4:e:352:GLU:HB2	6:h:227:ALA:HB1	1.56	0.85
4:e:543:GLN:NE2	6:h:209:MET:SD	2.51	0.83
4:e:352:GLU:HG2	6:h:228:GLY:H	1.43	0.83
5:G:250:LEU:HD23	5:G:283:MET:HE2	1.60	0.82
3:D:465:VAL:HG11	3:D:482:ILE:HD11	1.60	0.81
7:Q:477:ASN:HD21	7:Q:506:ASP:HB3	1.45	0.81
7:q:542:ASP:OD2	9:z:42:THR:HG22	1.81	0.80
2:b:240:THR:N	2:b:291:TYR:HE2	1.80	0.80
6:H:71:LYS:C	6:H:73:LEU:N	2.37	0.80
4:e:448:VAL:HG21	4:e:498:LEU:HB3	1.62	0.79
8:T:186:THR:HG23	8:T:415:MET:HE3	1.65	0.79
8:T:311:LEU:HD23	8:T:312:THR:HG23	1.65	0.79
8:T:100:VAL:CG2	8:T:103:LYS:HB3	2.14	0.78
3:D:162:ILE:HG23	3:D:163:VAL:HG23	1.64	0.78
8:T:313:VAL:HG23	8:T:367:PHE:HE1	1.49	0.78
6:h:244:LEU:HB3	6:h:246:VAL:HB	1.66	0.76
4:e:352:GLU:OE2	6:h:228:GLY:HA2	1.85	0.76
4:e:352:GLU:CD	6:h:228:GLY:N	2.43	0.76
7:Q:511:ASP:HB3	7:Q:513:ARG:H	1.49	0.76
6:H:110:LYS:O	6:H:114:PRO:HD2	1.85	0.75
1:A:545:ILE:HG21	3:D:68:MET:HG2	1.67	0.75
6:H:98:THR:OG1	13:H:603:AF3:F3	1.94	0.75
8:T:109:GLY:HA3	8:T:150:LEU:CD2	2.17	0.75
8:T:267:MET:HG3	8:T:374:ILE:HD11	1.67	0.75
8:T:237:THR:HG23	8:T:241:ARG:HH21	1.51	0.75
3:D:267:GLU:C	3:D:269:ALA:H	1.91	0.75
8:T:141:GLY:CA	14:T:502:GTP:O2A	2.30	0.74
1:A:14:PHE:HD1	3:D:70:ILE:HG23	1.52	0.74
8:T:204:ASN:ND2	14:T:502:GTP:O2'	2.20	0.74
8:T:299:MET:HE1	8:T:367:PHE:HE2	1.51	0.73
4:e:356:ILE:HG12	6:h:231:GLN:CG	2.18	0.73
8:T:238:THR:HG21	8:T:318:ARG:HH21	1.53	0.73
9:z:480:ALA:HA	9:z:487:ARG:HH21	1.52	0.73
6:h:244:LEU:C	6:h:246:VAL:H	1.96	0.72
4:e:352:GLU:CD	6:h:228:GLY:CA	2.62	0.72
5:G:254:LYS:HD2	8:T:261:PRO:HB3	1.71	0.72
5:G:319:ARG:NH2	8:T:195:HIS:HE1	1.86	0.72
8:T:204:ASN:OD1	14:T:502:GTP:N2	2.21	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:e:31:ILE:O	6:h:76:VAL:N	2.20	0.72
1:A:14:PHE:CD1	3:D:70:ILE:HG23	2.25	0.72
8:T:179:VAL:HG11	8:T:394:PHE:CE2	2.24	0.71
6:h:360:GLU:HB3	6:h:362:TYR:HE2	1.56	0.71
4:e:352:GLU:CD	6:h:228:GLY:HA2	2.15	0.70
2:B:236:THR:HG23	2:B:238:LEU:HB2	1.73	0.70
1:a:540:ARG:NH2	3:d:160:SER:O	2.24	0.70
1:a:276:ARG:NH2	3:d:261:ASP:OD2	2.23	0.70
8:T:234:SER:O	8:T:238:THR:HG23	1.92	0.70
1:A:121:HIS:NE2	3:D:42:LYS:HB3	2.06	0.70
1:A:540:ARG:O	3:D:45:ASP:N	2.24	0.70
1:A:123:THR:HG21	3:D:41:PRO:O	1.92	0.70
1:A:200:VAL:CB	1:A:410:LYS:HZ1	2.04	0.70
1:A:121:HIS:CG	3:D:42:LYS:HD2	2.27	0.69
8:T:239:SER:HB2	8:T:316:PHE:CE2	2.26	0.69
1:A:12:THR:OG1	3:D:30:SER:HB3	1.92	0.69
8:T:100:VAL:HG21	8:T:103:LYS:HB3	1.73	0.69
7:Q:510:LYS:O	7:Q:511:ASP:HB2	1.92	0.69
8:T:239:SER:HB2	8:T:316:PHE:HE2	1.58	0.69
7:q:52:ASN:HD22	7:q:66:ASN:N	1.91	0.68
4:e:452:LEU:HD21	4:e:502:GLN:HB3	1.75	0.68
7:q:46:MET:SD	7:q:101:ASN:ND2	2.66	0.68
8:T:125:GLU:HB2	9:Z:319:ARG:HB3	1.75	0.68
1:A:121:HIS:CE1	3:D:42:LYS:HA	2.29	0.68
2:B:79:ASN:OD1	4:E:413:LYS:N	2.25	0.68
7:q:99:GLY:HA2	11:q:601:ADP:O2B	1.94	0.67
8:T:105:HIS:HB2	8:T:146:GLY:HA3	1.76	0.67
4:e:322:ILE:HG22	4:e:343:VAL:HB	1.76	0.67
8:T:68:LEU:HD23	8:T:112:LEU:HD22	1.77	0.67
1:a:308:LYS:HE2	5:g:339:ARG:HG3	1.77	0.67
3:D:389:GLU:OE1	3:D:392:ARG:NH2	2.28	0.66
3:D:293:LEU:CD1	8:T:339:ASP:OD1	2.43	0.66
4:e:356:ILE:CG1	6:h:231:GLN:HG3	2.25	0.66
1:A:121:HIS:CE1	3:D:42:LYS:CA	2.79	0.66
7:Q:51:ARG:O	7:Q:53:LYS:NZ	2.29	0.66
1:a:93:GLU:O	1:a:411:ARG:NH2	2.28	0.66
5:g:171:MET:HE1	5:g:456:LEU:HD22	1.78	0.66
4:e:356:ILE:HG12	6:h:231:GLN:HG2	1.77	0.66
1:A:15:LEU:N	3:D:69:ALA:O	2.28	0.65
8:T:163:MET:HE2	8:T:163:MET:HA	1.77	0.65
2:B:83:VAL:HG13	4:E:231:GLY:HA2	1.78	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:192:ILE:HG23	4:E:193:VAL:HG23	1.77	0.65
8:T:269:GLY:O	8:T:367:PHE:N	2.30	0.65
9:Z:195:GLU:OE1	9:Z:327:ARG:NH1	2.29	0.65
7:Q:59:LEU:HD23	7:Q:61:LYS:HB2	1.78	0.65
3:D:226:PRO:O	3:D:311:MET:HG2	1.96	0.65
3:D:485:ARG:NH2	3:D:495:GLU:OE1	2.30	0.65
7:Q:533:GLU:OE2	9:Z:205:LYS:NZ	2.30	0.65
8:T:128:ASP:HB2	9:Z:303:PRO:HD3	1.78	0.65
1:a:308:LYS:HD3	5:g:338:ASN:HB3	1.77	0.65
1:A:497:TYR:C	1:A:499:ASN:N	2.52	0.64
1:A:497:TYR:C	1:A:499:ASN:H	2.05	0.64
9:Z:37:LEU:O	9:Z:461:ASN:ND2	2.30	0.64
8:T:187:LEU:HD11	8:T:408:PHE:HE1	1.63	0.64
1:a:64:ASN:ND2	1:a:166:SER:O	2.31	0.64
3:d:60:ASP:OD1	13:d:603:AF3:AL	1.23	0.64
7:Q:170:LYS:NZ	11:Q:602:ADP:O2B	2.29	0.64
4:e:352:GLU:CG	6:h:228:GLY:H	2.10	0.64
4:e:546:ARG:CD	6:h:170:LEU:HA	2.27	0.64
1:A:255:ARG:HG2	5:G:256:GLU:HB2	1.79	0.64
8:T:100:VAL:HG23	8:T:103:LYS:HB3	1.79	0.64
4:e:64:SER:OG	4:e:72:LYS:NZ	2.31	0.64
3:d:195:ARG:NH2	3:d:214:VAL:O	2.31	0.64
6:H:61:THR:HG21	6:H:72:LEU:HG	1.81	0.63
6:h:244:LEU:C	6:h:246:VAL:N	2.49	0.63
3:D:162:ILE:HG12	3:D:163:VAL:H	1.63	0.63
2:b:5:ILE:HG13	4:e:56:SER:OG	1.99	0.63
4:e:352:GLU:HB2	6:h:227:ALA:CB	2.29	0.63
7:q:256:ILE:HD11	7:q:308:LEU:HD12	1.81	0.63
4:E:509:ASN:O	4:E:522:MET:HB2	1.98	0.62
1:a:167:LYS:O	5:g:582:ARG:NH1	2.32	0.62
3:d:36:ARG:HA	3:d:98:ILE:HD11	1.80	0.62
2:B:389:SER:O	2:B:393:GLN:NE2	2.32	0.62
4:e:356:ILE:HG12	6:h:231:GLN:HG3	1.81	0.62
3:D:293:LEU:HD11	8:T:339:ASP:HA	1.80	0.62
7:q:283:GLN:NE2	9:z:260:ASP:CG	2.56	0.62
3:D:226:PRO:HG2	3:D:309:ASN:HA	1.81	0.62
3:d:39:LEU:HD13	3:d:98:ILE:HD12	1.80	0.62
4:e:452:LEU:HD11	4:e:502:GLN:HG3	1.81	0.62
1:A:78:PRO:HB2	3:D:47:MET:HE3	1.80	0.62
3:D:352:GLU:HA	3:D:360:ILE:O	1.99	0.62
8:T:245:GLN:HA	8:T:248:SER:HB2	1.82	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:326:LYS:O	3:D:370:ASN:ND2	2.32	0.62
8:T:292:GLN:O	8:T:298:ASN:ND2	2.32	0.62
6:h:44:LEU:O	6:h:456:ASN:ND2	2.32	0.62
8:T:238:THR:HG21	8:T:318:ARG:NH2	2.15	0.62
4:e:546:ARG:HD2	6:h:170:LEU:HA	1.82	0.62
1:A:55:ASP:O	5:G:592:LYS:HA	2.00	0.61
4:e:543:GLN:HE21	6:h:209:MET:CE	2.13	0.61
2:B:9:GLN:OE1	2:B:518:ARG:NH1	2.32	0.61
6:H:196:ASP:OD1	6:H:401:LYS:NZ	2.34	0.61
8:T:269:GLY:N	8:T:367:PHE:O	2.32	0.61
9:z:457:THR:O	9:z:461:ASN:ND2	2.34	0.61
4:e:543:GLN:HE21	6:h:209:MET:HE3	1.65	0.61
6:h:257:ALA:O	6:h:259:VAL:HG23	2.00	0.61
5:G:33:ASP:OD1	5:G:36:ARG:NH2	2.33	0.61
2:b:239:ASP:HB2	2:b:291:TYR:CE2	2.36	0.61
9:z:480:ALA:HB2	9:z:487:ARG:HE	1.65	0.61
8:T:108:GLU:O	8:T:112:LEU:N	2.34	0.61
2:b:54:CYS:SG	2:b:375:GLN:NE2	2.73	0.61
1:A:200:VAL:HB	1:A:410:LYS:NZ	2.15	0.61
6:H:24:GLY:O	6:H:26:ILE:N	2.31	0.60
2:b:240:THR:N	2:b:291:TYR:CE2	2.66	0.60
4:e:91:LEU:HB3	4:e:105:VAL:HG22	1.84	0.60
1:A:64:ASN:ND2	1:A:397:GLU:OE2	2.34	0.60
7:q:264:THR:HG22	9:z:252:PHE:CD1	2.37	0.60
6:H:245:ASN:ND2	7:Q:307:GLU:OE2	2.34	0.60
10:p:60:ASP:OD2	10:p:232:ASN:ND2	2.34	0.60
8:T:143:THR:HG22	14:T:502:GTP:O1B	2.02	0.60
1:A:82:ILE:HG12	3:D:385:MET:SD	2.42	0.60
8:T:69:GLU:O	8:T:70:PRO:C	2.44	0.60
5:G:170:LYS:NZ	5:G:215:LEU:O	2.35	0.60
6:H:115:PHE:CZ	6:H:437:MET:HG2	2.36	0.59
8:T:196:SER:HG	8:T:264:HIS:HD1	1.48	0.59
4:e:539:LEU:CD2	6:h:210:GLU:OE2	2.37	0.59
7:Q:66:ASN:HD21	7:Q:170:LYS:HA	1.66	0.59
8:T:109:GLY:HA3	8:T:150:LEU:HD23	1.83	0.59
8:T:29:GLY:C	8:T:30:LEU:HD12	2.27	0.59
2:b:37:LEU:O	2:b:447:ASN:ND2	2.35	0.59
8:T:169:VAL:HG11	14:T:502:GTP:HN22	1.68	0.58
4:E:35:GLN:NE2	1:a:4:LEU:O	2.36	0.58
7:q:83:LYS:HB2	9:z:53:ILE:CD1	2.34	0.58
7:Q:477:ASN:ND2	7:Q:506:ASP:HB3	2.17	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:g:164:VAL:HG21	5:g:171:MET:HE2	1.84	0.58
5:g:517:ILE:HG12	5:g:544:ILE:HG21	1.84	0.58
8:T:415:MET:O	8:T:416:ASN:C	2.40	0.58
7:q:92:GLN:OE1	7:q:96:MET:HB2	2.03	0.58
1:A:533:GLU:OE2	3:D:204:ILE:HG13	2.03	0.58
6:H:255:ASP:OD1	6:H:256:ASN:ND2	2.36	0.58
8:T:28:HIS:CE1	8:T:47:LEU:HD13	2.38	0.58
10:p:73:GLU:OE1	9:z:322:ARG:HB3	2.03	0.58
1:A:121:HIS:CE1	3:D:42:LYS:HB3	2.37	0.58
3:D:223:ALA:HB2	3:D:302:LEU:HB3	1.85	0.58
4:E:222:ASP:O	4:E:225:LYS:NZ	2.35	0.58
9:Z:192:HIS:O	9:Z:327:ARG:NE	2.36	0.58
3:d:60:ASP:OD1	13:d:603:AF3:F1	2.11	0.58
1:a:274:ARG:HH12	5:g:255:GLY:N	2.01	0.58
4:e:148:ASN:HA	6:h:173:ASN:HD21	1.69	0.58
7:q:80:PRO:HB2	9:z:45:MET:CE	2.34	0.58
7:q:256:ILE:HD11	7:q:308:LEU:CD1	2.33	0.58
7:q:283:GLN:HE22	9:z:260:ASP:CG	2.12	0.58
1:A:541:ILE:HD13	3:D:45:ASP:HB2	1.86	0.58
5:G:24:ASN:HB3	5:G:580:LEU:HD21	1.86	0.58
2:b:239:ASP:HA	2:b:291:TYR:CD2	2.39	0.58
5:g:523:ASP:OD2	5:g:526:ARG:NH1	2.37	0.58
2:B:512:ASP:HB3	4:E:70:LEU:CD1	2.34	0.57
10:p:73:GLU:CD	9:z:322:ARG:HB2	2.29	0.57
2:B:37:LEU:O	2:B:447:ASN:ND2	2.37	0.57
3:D:223:ALA:CB	3:D:302:LEU:HB3	2.34	0.57
5:G:319:ARG:NH2	8:T:195:HIS:CE1	2.70	0.57
1:A:9:ARG:HH12	4:e:45:GLU:HB3	1.68	0.57
8:T:311:LEU:CD2	8:T:312:THR:HG23	2.34	0.57
4:e:286:LYS:NZ	6:h:258:GLU:OE2	2.38	0.57
4:E:86:ASP:OD1	13:E:603:AF3:F2	2.13	0.57
8:T:70:PRO:HG2	8:T:94:GLN:HE21	1.69	0.57
9:Z:490:GLY:N	9:Z:499:CYS:O	2.37	0.57
1:A:4:LEU:HB2	4:e:40:ARG:HD2	1.87	0.57
1:A:340:SER:OG	3:D:300:LEU:HD12	2.05	0.57
2:B:249:LYS:N	4:E:287:LEU:O	2.36	0.57
7:q:91:GLN:OE1	9:z:383:SER:HA	2.05	0.57
7:q:99:GLY:HA2	11:q:601:ADP:PB	2.44	0.57
8:T:24:ILE:HD11	8:T:237:THR:HG21	1.87	0.57
7:q:91:GLN:NE2	9:z:201:HIS:O	2.38	0.57
4:E:85:ASN:HD21	4:E:191:LYS:HG3	1.70	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Q:511:ASP:HB3	7:Q:513:ARG:HB2	1.87	0.57
1:a:206:LEU:HD12	1:a:386:ILE:HG12	1.87	0.57
6:h:202:LYS:HD3	6:h:362:TYR:HE1	1.69	0.57
1:A:78:PRO:HB3	3:D:55:ILE:CD1	2.35	0.56
1:a:344:LEU:O	3:d:272:LEU:HD21	2.04	0.56
5:G:304:LEU:HG	5:G:308:TYR:OH	2.04	0.56
1:A:4:LEU:O	4:e:40:ARG:HG2	2.05	0.56
4:e:352:GLU:CG	6:h:228:GLY:N	2.67	0.56
3:d:212:GLY:O	3:d:376:SER:OG	2.24	0.56
4:e:92:SER:O	4:e:94:MET:N	2.39	0.56
1:A:82:ILE:HG23	3:D:383:ASN:HD21	1.70	0.56
9:Z:267:ARG:O	9:Z:269:PHE:N	2.38	0.56
4:e:550:LYS:O	6:h:49:SER:HB2	2.05	0.56
6:h:498:GLU:OE1	6:h:503:LYS:NZ	2.38	0.56
7:q:545:ILE:HG21	9:z:66:MET:SD	2.46	0.56
3:D:267:GLU:C	3:D:269:ALA:N	2.58	0.56
8:T:405:GLU:HA	8:T:408:PHE:HD2	1.71	0.56
9:Z:76:ILE:HD12	9:Z:98:VAL:HG21	1.88	0.56
10:p:73:GLU:OE1	9:z:322:ARG:CB	2.54	0.56
1:A:549:PRO:HA	3:D:51:SER:HB2	1.88	0.56
4:e:352:GLU:OE2	6:h:228:GLY:CA	2.52	0.56
4:e:547:MET:HB2	6:h:170:LEU:HD21	1.88	0.56
5:g:471:SER:OG	5:g:563:GLU:OE1	2.20	0.56
7:q:250:PHE:CD2	7:q:299:ILE:HG23	2.41	0.56
6:H:65:ASP:O	6:H:66:GLY:C	2.43	0.56
4:E:193:VAL:HG13	4:E:234:ILE:HG21	1.87	0.55
8:T:186:THR:HG23	8:T:415:MET:CE	2.34	0.55
2:B:234:ALA:CB	2:B:236:THR:HG22	2.32	0.55
6:H:119:GLY:O	6:H:120:ILE:C	2.50	0.55
1:a:168:ILE:HG23	1:a:169:ILE:HG23	1.88	0.55
5:g:288:LEU:HD11	5:g:312:GLY:HA3	1.89	0.55
6:H:228:GLY:O	6:H:232:GLN:NE2	2.40	0.55
7:Q:30:LYS:HZ1	9:z:2:SER:N	2.05	0.55
10:p:104:LYS:O	10:p:105:PRO:C	2.47	0.55
9:z:165:ASP:OD2	9:z:205:LYS:NZ	2.38	0.55
6:H:44:LEU:HD13	6:H:103:ILE:HD11	1.88	0.55
3:D:220:ILE:HG22	3:D:222:SER:H	1.72	0.55
5:G:111:LEU:HD11	5:G:581:LEU:CD2	2.37	0.55
7:q:254:LEU:HD21	7:q:299:ILE:HG21	1.89	0.55
8:T:380:ARG:O	8:T:384:GLN:OE1	2.25	0.55
4:e:364:PRO:HG2	6:h:279:PHE:HZ	1.72	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:e:553:ASN:HB2	6:h:51:ILE:HG23	1.87	0.55
1:a:541:ILE:HD13	3:d:47:MET:HE2	1.89	0.54
7:q:91:GLN:OE1	9:z:383:SER:CA	2.55	0.54
1:A:89:GLN:HG3	3:D:201:GLY:HA2	1.89	0.54
1:A:261:GLN:O	3:D:253:ILE:HD13	2.08	0.54
4:e:141:ILE:HB	4:e:146:ILE:HD11	1.89	0.54
5:G:263:ILE:HG23	5:G:268:ASP:HB2	1.89	0.54
7:Q:507:GLU:O	7:Q:508:GLY:C	2.49	0.54
2:b:234:ALA:C	2:b:236:THR:H	2.14	0.54
7:q:171:LYS:NZ	7:q:396:ASP:OD2	2.39	0.54
5:G:255:GLY:O	8:T:261:PRO:HG3	2.08	0.54
8:T:116:VAL:HA	8:T:119:VAL:HG22	1.89	0.54
2:b:56:VAL:O	2:b:382:ARG:NH2	2.40	0.54
4:e:356:ILE:CG1	6:h:231:GLN:CG	2.83	0.54
9:z:192:HIS:O	9:z:327:ARG:NH2	2.39	0.54
7:q:28:ILE:HD12	7:q:118:ILE:HG21	1.90	0.54
6:h:219:ALA:HB2	6:h:364:LEU:HD23	1.89	0.54
5:G:199:ASP:OD1	5:G:199:ASP:N	2.40	0.54
9:Z:15:ARG:NH2	7:q:24:ALA:HB3	2.23	0.54
4:e:513:ASP:OD2	4:e:517:TYR:N	2.41	0.54
2:B:285:ILE:HD13	2:B:317:LEU:HD21	1.90	0.53
4:e:324:GLN:HG3	4:e:351:LEU:HD22	1.90	0.53
1:A:545:ILE:CD1	3:D:68:MET:SD	2.90	0.53
5:G:114:LYS:HD3	7:q:472:ASN:HD21	1.72	0.53
6:H:55:THR:OG1	6:H:57:ASN:OD1	2.27	0.53
1:A:188:LYS:HE3	1:A:196:ILE:HG21	1.90	0.53
7:q:23:ASN:C	7:q:25:ASP:H	2.16	0.53
7:q:266:LEU:O	9:z:254:SER:HA	2.08	0.53
3:D:352:GLU:HG2	3:D:359:LYS:HD2	1.91	0.53
4:e:91:LEU:HD22	4:e:105:VAL:HG22	1.90	0.53
6:h:360:GLU:HB3	6:h:362:TYR:CE2	2.41	0.53
1:A:121:HIS:CE1	3:D:42:LYS:O	2.61	0.53
6:h:55:THR:OG1	6:h:57:ASN:OD1	2.26	0.53
8:T:238:THR:C	8:T:240:LEU:N	2.63	0.53
4:e:540:LEU:HD22	6:h:381:GLY:HA2	1.91	0.53
8:T:207:LEU:HD23	8:T:225:LEU:HB3	1.91	0.53
1:a:231:GLN:HB2	5:g:326:ASN:ND2	2.24	0.53
1:A:14:PHE:CZ	3:D:31:VAL:HG23	2.43	0.52
3:D:267:GLU:O	3:D:269:ALA:N	2.42	0.52
7:q:254:LEU:HB2	7:q:305:VAL:HG13	1.92	0.52
2:B:512:ASP:CG	4:E:70:LEU:HB2	2.35	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:T:66:VAL:HG22	8:T:147:MET:HE1	1.92	0.52
8:T:313:VAL:HG23	8:T:367:PHE:CE1	2.37	0.52
7:q:542:ASP:HB2	9:z:42:THR:HB	1.91	0.52
7:Q:428:ILE:HD12	7:Q:431:ILE:HD12	1.92	0.52
6:h:378:LEU:HD13	6:h:389:VAL:HG12	1.91	0.52
7:Q:58:HIS:HB2	8:T:32:PHE:HZ	1.73	0.52
8:T:286:VAL:O	8:T:290:THR:HG23	2.10	0.52
6:h:373:THR:OG1	6:h:374:CYS:N	2.43	0.52
2:B:507:VAL:HG13	4:E:83:ILE:HD13	1.90	0.52
7:Q:56:VAL:HG22	7:Q:62:ILE:HG12	1.89	0.52
4:e:276:PHE:HB2	4:e:327:PHE:HB3	1.90	0.52
5:G:35:ILE:HD12	5:G:94:THR:HG23	1.92	0.52
8:T:124:ALA:C	8:T:126:GLY:N	2.57	0.52
2:B:512:ASP:HB3	4:E:70:LEU:HD12	1.92	0.52
7:Q:8:ASN:HA	9:z:13:LEU:HD21	1.92	0.52
9:Z:251:PHE:HB3	9:Z:262:LEU:HD13	1.92	0.52
6:h:7:THR:HG22	7:q:21:TYR:CZ	2.45	0.52
4:E:379:ARG:NH2	4:E:396:GLU:OE1	2.43	0.52
8:T:1:MET:HB3	8:T:129:SER:HB3	1.92	0.51
7:q:69:ALA:C	7:q:71:MET:N	2.68	0.51
1:A:200:VAL:N	1:A:410:LYS:HZ1	2.08	0.51
5:G:356:LYS:NZ	5:G:358:GLU:OE2	2.43	0.51
5:g:47:MET:HE3	9:z:530:CYS:CB	2.39	0.51
1:A:200:VAL:C	1:A:202:ALA:N	2.64	0.51
2:B:236:THR:O	2:B:237:THR:C	2.54	0.51
3:D:293:LEU:HD11	8:T:339:ASP:OD1	2.09	0.51
3:D:353:ILE:N	3:D:360:ILE:O	2.39	0.51
10:p:145:GLN:O	10:p:151:ARG:NH1	2.44	0.51
4:e:352:GLU:HG2	6:h:228:GLY:N	2.20	0.51
1:A:545:ILE:HB	3:D:48:ILE:HG12	1.93	0.51
8:T:130:LEU:HD21	8:T:133:PHE:CZ	2.46	0.51
3:d:39:LEU:CD1	3:d:98:ILE:HD12	2.41	0.51
4:e:156:LEU:HD11	4:e:457:GLU:HG3	1.92	0.51
9:Z:237:ASN:HB3	9:Z:338:ASN:CG	2.36	0.51
10:p:239:ASP:O	10:p:244:ARG:NH1	2.43	0.51
7:Q:513:ARG:C	7:Q:515:GLU:N	2.68	0.51
8:T:272:PRO:HG2	8:T:361:LEU:HD13	1.91	0.51
3:D:70:ILE:O	3:D:76:ARG:NH1	2.44	0.51
3:D:471:SER:C	3:D:473:HIS:N	2.64	0.51
9:Z:14:ARG:NH2	9:Z:532:GLU:OE2	2.43	0.51
2:B:88:VAL:O	2:B:389:SER:OG	2.26	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:71:LYS:O	6:H:73:LEU:N	2.44	0.50
6:H:120:ILE:HD11	1:a:471:SER:HB3	1.91	0.50
9:Z:412:ILE:HG21	9:Z:513:LEU:HD12	1.93	0.50
1:A:122:PRO:HG2	3:D:44:MET:HE1	1.93	0.50
6:H:9:THR:N	9:z:4:GLN:OE1	2.43	0.50
8:T:105:HIS:HB2	8:T:146:GLY:CA	2.41	0.50
4:e:91:LEU:CD1	4:e:105:VAL:HA	2.24	0.50
4:e:221:PHE:HB3	6:h:356:GLN:HE22	1.76	0.50
7:q:80:PRO:CG	9:z:47:VAL:HG21	2.42	0.50
1:A:523:SER:O	1:A:527:SER:OG	2.22	0.50
8:T:161:ASP:O	8:T:162:ARG:C	2.51	0.50
6:h:47:LEU:O	6:h:456:ASN:HB3	2.12	0.50
1:A:258:MET:C	1:A:260:VAL:H	2.18	0.50
7:Q:226:MET:HE1	7:Q:331:ARG:HG3	1.94	0.50
6:h:482:VAL:HG22	6:h:488:ILE:HA	1.94	0.50
2:B:510:ARG:O	4:E:70:LEU:HB3	2.12	0.50
1:A:202:ALA:HA	1:A:328:ARG:CD	2.42	0.50
7:Q:83:LYS:NZ	9:Z:51:GLY:HA3	2.26	0.50
8:T:128:ASP:HB2	9:Z:303:PRO:HG3	1.93	0.50
8:T:426:GLN:O	8:T:427:GLU:C	2.53	0.50
1:a:308:LYS:HE2	5:g:339:ARG:CG	2.42	0.50
4:e:361:ARG:HD3	6:h:309:ASP:CG	2.36	0.50
2:B:86:ASP:HB2	4:E:389:LYS:HE2	1.93	0.50
2:b:510:ARG:O	4:e:71:ASP:N	2.42	0.50
3:d:60:ASP:CG	13:d:603:AF3:F2	2.45	0.50
6:h:459:PHE:CZ	6:h:486:GLU:HB3	2.46	0.50
7:Q:266:LEU:CD2	9:Z:252:PHE:HB3	2.42	0.50
1:a:260:VAL:HA	3:d:252:ILE:O	2.12	0.50
7:q:144:GLU:OE1	7:q:144:GLU:N	2.44	0.50
5:G:108:ALA:O	5:G:109:PRO:C	2.52	0.49
11:G:601:ADP:O3B	13:G:603:AF3:F3	2.20	0.49
9:Z:130:MET:SD	9:Z:514:ARG:NH1	2.85	0.49
2:b:109:LEU:HD12	2:b:115:ILE:HD12	1.93	0.49
3:d:65:LEU:HB3	3:d:79:VAL:HG22	1.93	0.49
3:D:16:LYS:NZ	3:D:523:ASP:OD1	2.44	0.49
3:D:162:ILE:HG12	3:D:163:VAL:N	2.26	0.49
11:D:601:ADP:O3B	13:D:603:AF3:F3	2.20	0.49
1:A:130:ARG:NH1	3:D:166:TYR:HE2	2.11	0.49
7:q:80:PRO:HB2	9:z:45:MET:HE2	1.94	0.49
7:q:260:GLU:O	7:q:261:THR:C	2.55	0.49
5:G:67:GLU:OE2	8:T:396:HIS:NE2	2.45	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:h:6:GLN:N	6:h:6:GLN:OE1	2.45	0.49
2:B:86:ASP:CB	4:E:389:LYS:HE2	2.42	0.49
9:Z:245:THR:O	9:Z:248:ASN:HB3	2.12	0.49
6:h:244:LEU:HB3	6:h:246:VAL:CB	2.37	0.49
1:A:121:HIS:CE1	3:D:42:LYS:CB	2.95	0.49
5:G:43:ALA:O	9:Z:116:ARG:NH2	2.43	0.49
8:T:128:ASP:HB2	9:Z:303:PRO:CD	2.42	0.49
6:h:7:THR:HG22	7:q:21:TYR:CE1	2.48	0.49
7:q:91:GLN:OE1	9:z:383:SER:HB2	2.13	0.49
1:A:542:ASP:HB2	3:D:44:MET:CB	2.43	0.49
4:E:447:GLU:N	4:E:447:GLU:OE1	2.46	0.49
3:D:220:ILE:HG22	3:D:222:SER:CB	2.43	0.49
5:G:553:ASP:OD1	5:G:556:SER:OG	2.25	0.49
7:Q:226:MET:HE2	7:Q:228:PHE:CE2	2.48	0.49
4:e:468:ALA:O	4:e:471:GLY:N	2.45	0.49
8:T:183:TYR:OH	8:T:395:LEU:HD13	2.13	0.49
8:T:299:MET:HE1	8:T:367:PHE:CE2	2.40	0.49
11:d:601:ADP:O1B	13:d:603:AF3:F1	2.21	0.49
4:e:47:LYS:NZ	4:e:549:LEU:O	2.41	0.49
7:q:52:ASN:ND2	7:q:66:ASN:N	2.58	0.49
1:A:187:VAL:HG23	1:A:199:PRO:HD2	1.93	0.49
3:D:226:PRO:HG2	3:D:309:ASN:CA	2.42	0.49
3:D:226:PRO:CG	3:D:309:ASN:HA	2.43	0.49
3:D:352:GLU:HA	3:D:361:VAL:HA	1.93	0.49
4:E:457:GLU:OE1	4:E:460:LYS:NZ	2.43	0.49
5:G:280:VAL:HG23	5:G:308:TYR:OH	2.13	0.49
6:H:24:GLY:C	6:H:26:ILE:N	2.71	0.49
1:a:94:ILE:HD11	1:a:526:LYS:HG3	1.94	0.49
6:h:166:MET:HE3	6:h:396:ALA:HB2	1.95	0.49
6:h:257:ALA:O	6:h:259:VAL:N	2.46	0.49
4:E:86:ASP:OD1	13:E:603:AF3:F3	2.21	0.48
5:G:71:ALA:HB3	9:Z:8:PRO:HD3	1.94	0.48
6:h:417:GLU:N	6:h:417:GLU:OE1	2.45	0.48
6:H:519:SER:O	7:Q:52:ASN:N	2.45	0.48
1:a:114:GLU:OE1	1:a:114:GLU:N	2.45	0.48
4:e:99:GLU:O	4:e:102:LYS:HB2	2.13	0.48
7:q:69:ALA:O	7:q:71:MET:N	2.46	0.48
1:A:200:VAL:N	1:A:410:LYS:NZ	2.61	0.48
5:G:319:ARG:HH22	8:T:195:HIS:HE1	1.60	0.48
8:T:425:TYR:O	8:T:426:GLN:C	2.56	0.48
5:g:47:MET:HE3	9:z:530:CYS:HB2	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:541:ILE:HA	3:D:45:ASP:O	2.12	0.48
8:T:103:LYS:CA	8:T:401:GLU:HG3	2.44	0.48
4:e:156:LEU:HD21	4:e:457:GLU:HG3	1.95	0.48
7:q:23:ASN:C	7:q:25:ASP:N	2.71	0.48
8:T:143:THR:O	8:T:144:GLY:C	2.55	0.48
1:A:78:PRO:HB3	3:D:55:ILE:HD11	1.95	0.48
2:B:408:GLU:N	2:B:408:GLU:OE1	2.46	0.48
7:Q:505:SER:O	7:Q:506:ASP:HB2	2.14	0.48
4:e:142:HIS:O	4:e:146:ILE:HG12	2.13	0.48
2:B:397:GLU:OE2	2:B:399:ARG:NH2	2.47	0.48
6:H:451:ARG:NH2	1:a:118:ASN:OD1	2.45	0.48
8:T:247:ASN:O	8:T:248:SER:C	2.54	0.48
4:E:121:GLY:HA2	4:E:124:VAL:HG12	1.95	0.48
4:e:463:GLY:O	4:e:466:GLN:HG2	2.14	0.48
9:z:497:ASP:OD1	9:z:498:SER:N	2.46	0.48
3:D:352:GLU:HG3	3:D:361:VAL:HG22	1.95	0.48
5:G:202:ARG:O	5:G:327:ARG:NH2	2.46	0.48
10:p:187:PRO:HD2	10:p:203:THR:HG22	1.95	0.48
1:A:261:GLN:OE1	3:D:251:ASN:ND2	2.34	0.48
4:E:522:MET:HG3	4:E:527:VAL:CG1	2.44	0.48
5:G:114:LYS:HG3	5:G:116:ILE:HG13	1.94	0.48
2:b:243:VAL:HG13	2:b:245:ILE:HG13	1.96	0.48
6:h:199:ILE:HD13	6:h:397:ILE:HG21	1.95	0.48
5:G:480:GLU:N	5:G:480:GLU:OE1	2.47	0.47
11:e:601:ADP:O2B	13:e:603:AF3:F1	2.22	0.47
6:H:115:PHE:HE2	6:H:438:ILE:HA	1.77	0.47
7:Q:55:ILE:CD1	7:Q:71:MET:HB2	2.44	0.47
7:q:84:VAL:CG1	9:z:386:TYR:OH	2.50	0.47
2:B:283:THR:HG22	2:B:304:ASN:HB2	1.96	0.47
1:a:169:ILE:HG21	1:a:398:MET:HE3	1.96	0.47
1:A:39:VAL:O	1:A:51:LYS:NZ	2.43	0.47
6:H:417:GLU:N	6:H:417:GLU:OE1	2.47	0.47
4:e:86:ASP:OD1	13:e:603:AF3:F3	2.23	0.47
7:q:135:ARG:HH22	9:z:205:LYS:CD	2.27	0.47
3:D:274:ILE:HD12	3:D:336:ILE:HG13	1.95	0.47
5:G:60:ASP:OD1	5:G:93:THR:OG1	2.33	0.47
7:q:91:GLN:CD	9:z:383:SER:HA	2.39	0.47
1:A:82:ILE:CG1	3:D:385:MET:SD	3.03	0.47
2:B:3:VAL:HG11	4:E:53:ALA:HB2	1.96	0.47
7:Q:513:ARG:O	7:Q:515:GLU:N	2.47	0.47
8:T:321:VAL:HG23	8:T:353:VAL:HG13	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:408:GLU:N	2:b:408:GLU:OE1	2.47	0.47
1:A:485:GLN:HA	1:A:498:ARG:NH2	2.29	0.47
4:E:91:LEU:HB3	4:E:105:VAL:HG22	1.97	0.47
5:G:309:LEU:HD23	5:G:309:LEU:HA	1.68	0.47
6:H:260:ARG:HH11	7:Q:266:LEU:HD13	1.79	0.47
7:Q:141:GLU:OE1	7:Q:433:ARG:NH1	2.48	0.47
8:T:67:ASP:OD1	8:T:143:THR:HG21	2.15	0.47
8:T:103:LYS:HB2	8:T:401:GLU:CD	2.40	0.47
1:A:82:ILE:HG23	3:D:383:ASN:ND2	2.30	0.47
3:D:220:ILE:C	3:D:222:SER:N	2.71	0.47
9:Z:257:ASP:C	9:Z:259:ARG:N	2.67	0.47
7:q:250:PHE:HD2	7:q:299:ILE:HG23	1.78	0.47
8:T:74:ASP:HB3	9:Z:49:GLY:HA3	1.95	0.47
11:Z:601:ADP:O2B	13:Z:603:AF3:F1	2.23	0.47
4:e:461:GLN:O	4:e:466:GLN:HB3	2.15	0.47
4:e:546:ARG:HD2	6:h:170:LEU:HG	1.97	0.47
5:g:491:ALA:HB2	5:g:502:TYR:HD2	1.80	0.47
7:q:12:GLY:O	9:z:70:SER:HB2	2.15	0.47
1:A:14:PHE:HA	3:D:70:ILE:HA	1.97	0.47
2:B:372:ALA:HB2	3:D:513:GLU:OE1	2.15	0.47
11:B:601:ADP:O1B	13:B:603:AF3:F1	2.23	0.46
3:D:220:ILE:C	3:D:222:SER:H	2.22	0.46
7:Q:6:PRO:HG2	9:z:21:VAL:HG13	1.97	0.46
8:T:267:MET:CG	8:T:374:ILE:HD11	2.41	0.46
2:b:374:ASP:N	3:d:80:GLU:OE1	2.46	0.46
4:e:91:LEU:HB3	4:e:105:VAL:HG13	1.97	0.46
4:e:275:PRO:HG3	4:e:325:TRP:HB2	1.98	0.46
7:q:23:ASN:O	7:q:24:ALA:HB3	2.16	0.46
1:A:308:LYS:HE2	5:G:339:ARG:HB2	1.97	0.46
7:Q:327:PHE:HE2	8:T:54:ALA:C	2.24	0.46
2:b:34:LYS:NZ	2:b:101:GLU:OE2	2.45	0.46
5:G:8:MET:SD	5:G:8:MET:N	2.88	0.46
6:H:159:GLU:OE1	6:H:159:GLU:N	2.47	0.46
8:T:99:ASN:OD1	8:T:99:ASN:O	2.33	0.46
8:T:295:ASP:OD1	8:T:296:ALA:N	2.48	0.46
4:e:301:TYR:HB2	6:h:264:VAL:HG11	1.96	0.46
4:e:362:ILE:HB	6:h:305:GLN:HG2	1.96	0.46
1:A:21:SER:OG	1:A:22:GLY:N	2.49	0.46
2:B:86:ASP:HB3	4:E:389:LYS:CE	2.46	0.46
6:H:434:LYS:HB2	6:H:434:LYS:HE2	1.55	0.46
9:Z:368:THR:OG1	9:Z:369:GLU:N	2.49	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:g:263:ILE:HG23	5:g:268:ASP:HB2	1.96	0.46
1:A:122:PRO:HG2	3:D:44:MET:CE	2.46	0.46
7:Q:506:ASP:O	7:Q:507:GLU:HB3	2.16	0.46
8:T:128:ASP:HB2	9:Z:303:PRO:CG	2.46	0.46
3:d:45:ASP:OD1	3:d:46:LYS:N	2.48	0.46
3:d:48:ILE:HD11	3:d:64:ILE:HG23	1.97	0.46
6:h:46:PRO:HB3	6:h:167:SER:HB2	1.96	0.46
7:Q:58:HIS:HB2	8:T:32:PHE:CZ	2.51	0.46
4:e:107:LEU:HD13	4:e:544:LEU:HD22	1.97	0.46
1:A:543:THR:OG1	3:D:46:LYS:CE	2.64	0.46
8:T:139:LEU:HD21	8:T:189:VAL:HG13	1.98	0.46
3:d:36:ARG:HA	3:d:98:ILE:CD1	2.43	0.46
7:q:267:LEU:HD23	9:z:254:SER:O	2.16	0.46
9:z:247:VAL:O	9:z:248:ASN:C	2.59	0.46
1:A:121:HIS:ND1	3:D:42:LYS:HD2	2.31	0.46
8:T:68:LEU:HD22	8:T:108:GLU:HG2	1.98	0.46
1:a:261:GLN:N	3:d:252:ILE:O	2.45	0.46
3:d:77:MET:HE1	3:d:521:ILE:HD11	1.97	0.46
5:g:110:TYR:O	5:g:115:ASN:N	2.48	0.46
6:h:257:ALA:HA	7:q:265:VAL:HB	1.98	0.46
3:D:223:ALA:HB3	3:D:306:SER:OG	2.16	0.46
8:T:162:ARG:HA	8:T:162:ARG:HD3	1.66	0.46
2:b:46:LEU:HD11	2:b:63:ILE:HA	1.97	0.46
4:e:540:LEU:HD21	6:h:207:GLY:C	2.41	0.46
7:q:80:PRO:HB2	9:z:45:MET:HE1	1.98	0.46
5:G:60:ASP:OD1	13:G:603:AF3:F3	2.24	0.46
1:a:54:VAL:HG12	1:a:56:ASP:H	1.81	0.45
2:b:331:GLU:OE1	2:b:334:LYS:NZ	2.49	0.45
6:h:487:ASN:C	6:h:488:ILE:HG23	2.41	0.45
4:E:158:ILE:HG13	4:E:538:ILE:HD11	1.97	0.45
8:T:287:PRO:O	8:T:290:THR:OG1	2.25	0.45
8:T:386:SER:O	8:T:390:LYS:N	2.49	0.45
5:G:353:GLY:N	5:G:369:ASP:O	2.47	0.45
8:T:148:GLY:O	8:T:149:THR:C	2.56	0.45
2:b:515:ILE:HG12	4:e:94:MET:HE2	1.98	0.45
4:e:133:ALA:O	4:e:137:ILE:HG12	2.16	0.45
1:A:494:ARG:HA	1:A:497:TYR:HD2	1.81	0.45
8:T:238:THR:O	8:T:239:SER:C	2.57	0.45
8:T:321:VAL:CG2	8:T:353:VAL:HG13	2.47	0.45
1:A:276:ARG:HD2	1:A:276:ARG:HA	1.48	0.45
3:D:220:ILE:HG22	3:D:222:SER:HB3	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Q:327:PHE:HE2	8:T:54:ALA:CA	2.30	0.45
8:T:372:THR:HA	8:T:422:TYR:HD1	1.80	0.45
2:b:514:ILE:HD13	4:e:73:ILE:HD13	1.99	0.45
6:h:45:GLY:C	6:h:47:LEU:H	2.24	0.45
10:p:204:LEU:O	10:p:209:GLY:N	2.49	0.45
5:G:208:LYS:NZ	8:T:400:SER:O	2.43	0.45
7:Q:55:ILE:HD12	7:Q:71:MET:HB2	1.98	0.45
1:a:189:THR:OG1	1:a:331:ARG:NH2	2.50	0.45
5:g:224:LEU:HD11	5:g:365:PHE:HB3	1.99	0.45
1:A:426:GLU:N	1:A:426:GLU:OE1	2.49	0.45
5:G:210:PRO:HA	5:G:449:LEU:HD11	1.99	0.45
8:T:372:THR:O	8:T:375:GLN:HG2	2.17	0.45
8:T:385:PHE:O	8:T:389:PHE:HB2	2.17	0.45
2:b:511:VAL:CG1	4:e:73:ILE:HD11	2.46	0.45
4:e:364:PRO:HG2	6:h:279:PHE:CZ	2.50	0.45
1:A:55:ASP:HA	5:G:591:ARG:O	2.16	0.45
7:Q:473:GLU:OE1	7:Q:473:GLU:N	2.50	0.45
8:T:103:LYS:HA	8:T:401:GLU:HG3	1.98	0.45
8:T:125:GLU:HG3	8:T:126:GLY:N	2.26	0.45
9:z:384:THR:HG23	9:z:387:ALA:H	1.81	0.45
1:A:282:LEU:O	1:A:286:LYS:HG2	2.17	0.45
7:q:537:THR:HG23	9:z:55:LEU:HD11	1.97	0.45
1:A:319:ARG:HH22	8:T:413:SER:HB2	1.82	0.45
7:Q:128:ILE:HD12	7:Q:536:THR:HG23	1.99	0.45
1:a:262:ILE:HG21	1:a:273:ILE:HD12	1.99	0.45
2:b:90:ASP:OD1	13:b:603:AF3:F1	2.24	0.45
4:e:159:SER:O	4:e:162:GLU:N	2.50	0.45
4:e:450:MET:O	4:e:454:VAL:HG22	2.17	0.45
7:q:36:ARG:NH2	7:q:115:GLU:OE1	2.50	0.45
7:q:256:ILE:H	7:q:256:ILE:HG12	1.36	0.45
8:T:67:ASP:OD1	8:T:68:LEU:N	2.49	0.44
8:T:101:TRP:O	8:T:102:ALA:C	2.59	0.44
8:T:130:LEU:HD23	8:T:162:ARG:HG3	1.99	0.44
8:T:186:THR:HA	8:T:415:MET:CE	2.46	0.44
1:a:49:LEU:HD22	5:g:584:ASP:HB3	2.00	0.44
7:q:507:GLU:OE1	7:q:507:GLU:N	2.49	0.44
11:z:601:ADP:O3B	13:z:603:AF3:F1	2.25	0.44
2:B:195:ILE:HG21	2:B:381:GLU:HG3	2.00	0.44
5:G:296:ILE:HG12	5:G:317:LEU:HD12	1.98	0.44
3:D:340:THR:OG1	3:D:342:ASP:OD1	2.33	0.44
1:a:262:ILE:H	1:a:262:ILE:HG12	1.41	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:q:91:GLN:OE1	9:z:383:SER:CB	2.66	0.44
3:D:350:VAL:HG13	3:D:363:VAL:HG22	1.98	0.44
5:G:205:ARG:NH2	8:T:402:GLY:O	2.47	0.44
8:T:103:LYS:O	8:T:104:GLY:C	2.58	0.44
7:q:541:ILE:HG22	9:z:43:LEU:HB2	1.99	0.44
9:z:129:SER:O	9:z:133:LEU:N	2.50	0.44
1:A:199:PRO:HA	1:A:410:LYS:HE2	1.99	0.44
1:A:533:GLU:CD	3:D:204:ILE:HG13	2.43	0.44
5:G:272:ILE:HG22	9:Z:245:THR:CG2	2.48	0.44
8:T:313:VAL:HG13	8:T:349:VAL:HA	1.99	0.44
7:q:28:ILE:H	7:q:28:ILE:HG12	1.41	0.44
7:q:87:MET:HE2	9:z:384:THR:OG1	2.17	0.44
9:z:481:GLN:C	9:z:483:SER:H	2.25	0.44
11:D:601:ADP:O1B	13:D:603:AF3:F1	2.26	0.44
5:G:323:SER:HA	8:T:406:LEU:HD23	1.99	0.44
1:a:262:ILE:O	5:g:259:THR:HG23	2.16	0.44
1:a:276:ARG:HH11	3:d:257:TYR:HD2	1.65	0.44
7:q:83:LYS:HB2	9:z:53:ILE:HD11	2.00	0.44
4:E:55:ARG:NH1	3:d:108:GLU:OE2	2.51	0.44
7:Q:262:LYS:HZ3	8:T:252:LYS:HE3	1.82	0.44
8:T:50:TYR:CD2	8:T:241:ARG:HD3	2.53	0.44
8:T:117:MET:HE2	8:T:117:MET:HA	1.99	0.44
8:T:232:VAL:HG11	8:T:268:VAL:HB	2.00	0.44
5:g:159:ILE:HG23	5:g:164:VAL:HG23	2.00	0.44
7:q:537:THR:CG2	9:z:55:LEU:HD11	2.47	0.44
3:D:260:MET:O	3:D:261:ASP:C	2.59	0.44
4:E:193:VAL:HG11	4:E:200:PHE:CE1	2.53	0.44
5:G:208:LYS:HB3	5:G:449:LEU:HD13	1.98	0.44
7:Q:259:THR:HB	7:Q:260:GLU:H	1.45	0.44
4:e:177:ARG:HD3	4:e:209:ILE:HD11	2.00	0.44
1:a:191:ASN:OD1	1:a:192:SER:N	2.51	0.44
2:b:80:ILE:HD11	2:b:500:SER:HB3	2.00	0.44
5:g:47:MET:HE3	9:z:530:CYS:SG	2.58	0.44
7:q:83:LYS:CB	9:z:53:ILE:CD1	2.96	0.44
1:A:57:ILE:HG21	5:G:592:LYS:HE3	1.99	0.43
3:D:161:LYS:HE2	3:D:161:LYS:HB3	1.42	0.43
7:Q:472:ASN:ND2	5:g:114:LYS:O	2.51	0.43
4:e:98:ASN:O	4:e:102:LYS:HG3	2.17	0.43
7:q:35:ILE:HG22	7:q:82:VAL:HG22	2.00	0.43
1:A:199:PRO:CA	1:A:410:LYS:HE2	2.48	0.43
5:G:281:GLN:NE2	5:G:308:TYR:CE1	2.85	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:a:601:ADP:O3B	13:a:603:AF3:F3	2.26	0.43
3:d:292:ILE:HD11	10:p:148:LEU:HD21	2.00	0.43
3:D:132:VAL:HG22	3:D:505:THR:HG23	2.01	0.43
6:H:520:VAL:HG11	7:Q:54:ILE:HG13	1.99	0.43
8:T:250:LEU:HA	8:T:253:LEU:HD12	2.00	0.43
1:a:204:ASN:ND2	1:a:223:ALA:O	2.49	0.43
3:D:215:LEU:HB2	3:D:361:VAL:HB	2.00	0.43
5:G:19:GLN:HA	5:G:22:ILE:HD12	1.99	0.43
7:Q:509:VAL:C	7:Q:511:ASP:H	2.25	0.43
8:T:322:SER:OG	8:T:323:VAL:N	2.51	0.43
11:h:601:ADP:O2B	13:h:603:AF3:F3	2.26	0.43
9:z:490:GLY:N	9:z:499:CYS:O	2.50	0.43
3:D:60:ASP:OD1	13:D:603:AF3:F2	2.26	0.43
3:D:258:ARG:H	3:D:258:ARG:HG2	1.55	0.43
5:G:248:CYS:HB3	5:G:338:ASN:OD1	2.19	0.43
8:T:105:HIS:CD2	8:T:150:LEU:HB2	2.54	0.43
6:h:482:VAL:HG11	6:h:494:LYS:HG3	2.00	0.43
7:q:68:ALA:O	7:q:71:MET:HB2	2.18	0.43
1:A:494:ARG:HA	1:A:494:ARG:HD3	1.85	0.43
2:B:87:GLU:O	4:E:386:GLY:HA2	2.19	0.43
5:G:273:LEU:HD23	9:Z:245:THR:HG23	2.01	0.43
8:T:196:SER:OG	8:T:264:HIS:ND1	2.45	0.43
1:a:308:LYS:HD3	5:g:338:ASN:CB	2.45	0.43
1:A:121:HIS:CE1	3:D:42:LYS:C	2.97	0.43
1:A:258:MET:O	1:A:260:VAL:N	2.52	0.43
2:B:489:GLU:N	2:B:489:GLU:OE1	2.52	0.43
4:E:334:LEU:HA	4:E:334:LEU:HD12	1.69	0.43
3:D:260:MET:HE2	3:D:260:MET:HB3	1.72	0.43
8:T:180:VAL:HG22	8:T:180:VAL:O	2.19	0.43
8:T:203:ASP:O	8:T:207:LEU:HD13	2.19	0.43
4:e:546:ARG:HD3	6:h:170:LEU:HA	1.99	0.43
2:B:118:GLN:HB3	4:E:68:ARG:HH11	1.83	0.43
3:D:154:ALA:HB2	3:D:401:ILE:HD11	2.00	0.43
4:e:329:ASP:O	4:e:330:GLU:C	2.60	0.43
7:q:276:PHE:HE1	9:z:253:TYR:HE1	1.67	0.43
2:B:43:ASP:OD1	2:B:44:LYS:N	2.51	0.42
3:D:93:THR:N	11:D:601:ADP:O3B	2.52	0.42
3:D:293:LEU:CD1	8:T:339:ASP:HA	2.47	0.42
8:T:260:PHE:HB2	8:T:261:PRO:CD	2.49	0.42
1:a:248:ASP:OD1	1:a:299:THR:OG1	2.35	0.42
3:d:93:THR:O	3:d:96:VAL:HG12	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:q:239:LEU:O	7:q:239:LEU:HD23	2.19	0.42
3:D:470:ARG:O	3:D:473:HIS:HB2	2.19	0.42
5:G:251:GLU:HB3	5:G:302:SER:HB3	2.01	0.42
5:G:444:GLY:HA3	9:Z:519:GLY:HA2	2.01	0.42
1:A:156:LEU:HD12	1:A:409:VAL:HG13	2.00	0.42
1:A:542:ASP:OD2	3:D:37:THR:CG2	2.51	0.42
8:T:285:THR:O	8:T:288:GLU:N	2.52	0.42
4:e:107:LEU:HD22	4:e:544:LEU:HD22	2.01	0.42
4:e:464:ILE:H	4:e:464:ILE:HG12	1.65	0.42
4:e:546:ARG:HD2	6:h:170:LEU:CA	2.49	0.42
1:A:20:ILE:HG23	1:A:25:ILE:HD11	2.02	0.42
3:D:265:LYS:O	3:D:268:ARG:HG3	2.20	0.42
5:G:104:LEU:HD13	5:G:104:LEU:HA	1.90	0.42
7:Q:327:PHE:CE2	8:T:54:ALA:C	2.98	0.42
1:a:274:ARG:NH2	5:g:252:TYR:OH	2.53	0.42
2:b:243:VAL:O	2:b:244:LYS:HB2	2.19	0.42
10:p:114:ALA:O	10:p:115:SER:C	2.62	0.42
7:q:52:ASN:ND2	7:q:66:ASN:HB3	2.34	0.42
3:D:463:ILE:HD13	3:D:463:ILE:HA	1.67	0.42
4:E:510:ILE:HG23	4:E:520:ASN:C	2.45	0.42
5:G:217:SER:OG	5:G:440:MET:O	2.38	0.42
7:Q:284:ILE:HA	7:Q:287:MET:HE2	2.02	0.42
4:e:229:ARG:NH1	4:e:392:MET:SD	2.91	0.42
6:h:249:GLU:HA	6:h:300:GLY:HA3	2.00	0.42
1:A:168:ILE:HG23	1:A:169:ILE:HG23	2.01	0.42
1:A:344:LEU:HA	3:D:272:LEU:HD11	2.02	0.42
4:e:287:LEU:HD13	6:h:261:VAL:HG23	2.01	0.42
5:g:163:TYR:OH	9:z:123:GLU:OE2	2.35	0.42
1:A:327:ARG:HH22	3:D:222:SER:HA	1.85	0.42
1:A:497:TYR:O	1:A:499:ASN:N	2.52	0.42
5:G:159:ILE:HG23	5:G:164:VAL:HG23	2.00	0.42
6:H:68:THR:HG22	6:H:72:LEU:HD23	2.02	0.42
8:T:124:ALA:O	8:T:125:GLU:C	2.62	0.42
8:T:309:ARG:HG2	8:T:309:ARG:HH11	1.85	0.42
2:b:245:ILE:HG13	2:b:245:ILE:H	1.50	0.42
4:e:425:ASP:O	4:e:429:VAL:HG23	2.19	0.42
1:A:251:LEU:HD23	1:A:251:LEU:HA	1.89	0.42
1:A:261:GLN:O	3:D:253:ILE:CD1	2.68	0.42
2:B:512:ASP:HB3	4:E:70:LEU:HD13	2.01	0.42
5:G:45:LEU:O	9:Z:530:CYS:HA	2.19	0.42
5:G:254:LYS:HG3	9:Z:247:VAL:CG2	2.50	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:T:68:LEU:HD11	8:T:108:GLU:HB2	2.02	0.42
8:T:199:THR:HG22	8:T:264:HIS:CB	2.50	0.42
9:Z:110:GLN:OE1	9:z:103:ARG:NH1	2.53	0.42
9:Z:497:ASP:OD1	9:Z:498:SER:N	2.48	0.42
6:h:257:ALA:O	6:h:258:GLU:C	2.60	0.42
6:h:453:LEU:HB3	6:h:483:PHE:HZ	1.85	0.42
10:p:73:GLU:CD	9:z:322:ARG:CB	2.92	0.42
9:z:210:ILE:HG23	9:z:368:THR:HG22	2.01	0.42
4:E:138:GLN:OE1	3:d:36:ARG:NH1	2.53	0.42
8:T:388:MET:CE	8:T:389:PHE:CE2	3.03	0.42
4:e:348:GLY:O	6:h:227:ALA:HB2	2.19	0.42
10:p:240:ASP:OD1	10:p:241:GLU:N	2.53	0.42
1:A:89:GLN:CG	3:D:201:GLY:HA2	2.49	0.42
1:A:542:ASP:HB2	3:D:44:MET:HB2	2.00	0.42
2:B:386:ASP:OD2	13:B:603:AF3:F2	2.28	0.42
3:D:260:MET:O	3:D:263:ILE:HG12	2.20	0.42
4:e:452:LEU:HD11	4:e:502:GLN:CG	2.49	0.42
6:h:252:ALA:O	6:h:253:GLU:C	2.62	0.42
7:q:128:ILE:HG23	7:q:536:THR:HG23	2.02	0.42
1:A:285:VAL:HG13	1:A:289:ILE:HD12	2.02	0.41
1:A:320:ARG:HH21	8:T:420:SER:HB2	1.84	0.41
2:B:231:ILE:HB	2:B:321:THR:HG21	2.01	0.41
3:D:405:VAL:O	3:D:408:ARG:NH1	2.51	0.41
5:G:170:LYS:NZ	5:G:217:SER:O	2.37	0.41
7:Q:474:VAL:HG13	7:Q:507:GLU:CD	2.45	0.41
8:T:170:LEU:N	8:T:202:ILE:O	2.48	0.41
8:T:405:GLU:HA	8:T:408:PHE:CD2	2.54	0.41
9:Z:247:VAL:O	9:Z:248:ASN:C	2.60	0.41
9:z:244:LYS:H	9:z:244:LYS:HG2	1.60	0.41
2:B:86:ASP:CB	4:E:389:LYS:CE	2.98	0.41
3:D:161:LYS:HB2	3:D:162:ILE:H	1.47	0.41
3:D:353:ILE:HD11	3:D:360:ILE:HD13	2.02	0.41
5:G:46:LYS:HE3	9:Z:532:GLU:HB3	2.01	0.41
1:a:231:GLN:HB2	5:g:326:ASN:CG	2.45	0.41
4:e:397:GLN:HG3	4:e:401:THR:HG21	2.02	0.41
6:H:113:LYS:O	6:H:117:GLU:HG3	2.20	0.41
7:Q:262:LYS:HB3	9:Z:250:GLY:HA2	2.03	0.41
8:T:2:ARG:O	8:T:49:VAL:HG22	2.19	0.41
8:T:273:LEU:HD12	8:T:273:LEU:HA	1.88	0.41
4:e:148:ASN:HA	6:h:173:ASN:ND2	2.35	0.41
4:e:250:SER:HA	4:e:344:ARG:HD2	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:g:269:TRP:HZ3	9:z:269:PHE:CB	2.34	0.41
5:g:511:CYS:O	5:g:515:THR:N	2.47	0.41
4:E:331:ALA:O	4:E:335:LEU:HG	2.21	0.41
5:G:296:ILE:HG23	5:G:320:VAL:HG21	2.02	0.41
5:G:311:LYS:HE2	5:G:311:LYS:HB3	1.81	0.41
7:Q:266:LEU:HD23	9:Z:252:PHE:HB3	2.03	0.41
2:b:72:PRO:HB3	4:e:75:ILE:HD11	2.02	0.41
2:b:241:ASP:HB2	2:b:268:LYS:NZ	2.35	0.41
2:b:245:ILE:O	2:b:246:PHE:C	2.64	0.41
5:g:490:LYS:HB2	5:g:490:LYS:HE2	1.85	0.41
6:H:86:ILE:HG22	7:Q:389:ALA:HB1	2.03	0.41
7:q:255:ASP:O	7:q:256:ILE:C	2.61	0.41
1:A:15:LEU:HD13	3:D:71:LEU:HD21	2.01	0.41
1:A:340:SER:HB2	3:D:300:LEU:HD13	2.03	0.41
7:Q:325:SER:HB2	8:T:53:GLU:CD	2.45	0.41
8:T:388:MET:SD	8:T:388:MET:O	2.79	0.41
3:d:190:ASP:OD2	3:d:192:ASN:ND2	2.54	0.41
7:q:251:THR:H	7:q:342:PRO:HA	1.86	0.41
9:z:384:THR:OG1	9:z:385:HIS:N	2.53	0.41
2:B:264:ALA:HB2	4:E:292:VAL:HG23	2.02	0.41
4:E:101:ALA:O	4:E:105:VAL:HG23	2.21	0.41
2:b:150:ARG:NH2	2:b:179:ASN:OD1	2.54	0.41
7:q:347:PRO:HB2	7:q:348:THR:H	1.71	0.41
2:B:377:LEU:HD13	2:B:377:LEU:HA	1.67	0.41
2:B:512:ASP:OD2	4:E:70:LEU:HB2	2.21	0.41
3:D:14:LYS:NZ	2:b:16:GLU:OE2	2.30	0.41
4:E:129:LEU:HD11	4:E:472:PHE:HD1	1.86	0.41
5:G:266:GLU:OE1	5:G:266:GLU:N	2.52	0.41
7:Q:266:LEU:O	9:Z:254:SER:HA	2.21	0.41
4:e:158:ILE:HD13	4:e:158:ILE:HA	1.96	0.41
10:p:73:GLU:OE2	9:z:322:ARG:HB2	2.21	0.41
7:q:276:PHE:CE1	9:z:253:TYR:HE1	2.39	0.41
9:z:472:MET:O	9:z:476:GLU:N	2.49	0.41
2:B:59:ASP:OD1	13:B:603:AF3:F2	2.29	0.41
8:T:109:GLY:CA	8:T:150:LEU:HD23	2.48	0.41
8:T:376:GLU:OE1	8:T:376:GLU:HA	2.21	0.41
3:d:96:VAL:O	3:d:97:VAL:C	2.62	0.41
5:g:263:ILE:HB	9:z:251:PHE:HD1	1.86	0.41
1:A:14:PHE:HZ	3:D:31:VAL:HG23	1.85	0.40
11:A:601:ADP:O1B	13:A:603:AF3:F1	2.29	0.40
7:Q:421:PRO:HB3	7:Q:512:ILE:HD12	2.02	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:h:526:ASN:ND2	7:q:56:VAL:O	2.39	0.40
10:p:109:LYS:HB3	10:p:113:LEU:HD12	2.02	0.40
4:E:151:ASP:OD2	6:H:173:ASN:ND2	2.54	0.40
7:Q:416:GLY:O	7:Q:418:LYS:NZ	2.54	0.40
8:T:77:ARG:HH22	9:Z:52:ASN:CG	2.29	0.40
8:T:189:VAL:O	8:T:190:HIS:C	2.64	0.40
7:q:87:MET:SD	9:z:384:THR:OG1	2.79	0.40
9:z:200:GLN:N	9:z:200:GLN:OE1	2.54	0.40
7:q:428:ILE:HA	7:q:431:ILE:HD12	2.04	0.40
4:E:99:GLU:OE1	6:H:60:THR:OG1	2.33	0.40
4:E:327:PHE:HB2	4:E:328:ASP:H	1.31	0.40
5:G:111:LEU:HD11	5:G:581:LEU:HD22	2.03	0.40
5:G:117:HIS:HA	5:G:118:PRO:HD3	1.97	0.40
6:H:72:LEU:HD13	6:H:72:LEU:HA	1.93	0.40
7:Q:266:LEU:HD22	9:Z:252:PHE:HB3	2.03	0.40
9:Z:100:GLU:CD	9:Z:453:VAL:HG21	2.46	0.40
9:Z:212:GLY:O	9:Z:377:THR:HG22	2.21	0.40
9:z:87:THR:HG21	9:z:512:VAL:HG22	2.04	0.40
1:A:62:VAL:O	1:A:400:ARG:NH2	2.50	0.40
1:A:85:GLU:OE1	3:D:383:ASN:HB2	2.21	0.40
3:D:64:ILE:HG22	3:D:68:MET:HE2	2.03	0.40
4:E:25:MET:SD	4:E:25:MET:N	2.94	0.40
4:E:199:ARG:NH1	4:E:237:SER:O	2.55	0.40
7:Q:52:ASN:HB3	7:Q:64:ILE:HG22	2.03	0.40
8:T:260:PHE:CZ	8:T:263:LEU:HD12	2.55	0.40
2:b:250:PHE:CD1	2:b:261:LEU:HD21	2.56	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	548/559 (98%)	522 (95%)	24 (4%)	2 (0%)	30	59
1	a	542/559 (97%)	518 (96%)	24 (4%)	0	100	100
2	B	516/527 (98%)	495 (96%)	21 (4%)	0	100	100
2	b	516/527 (98%)	501 (97%)	15 (3%)	0	100	100
3	D	521/528 (99%)	504 (97%)	17 (3%)	0	100	100
3	d	522/528 (99%)	508 (97%)	14 (3%)	0	100	100
4	E	534/562 (95%)	511 (96%)	22 (4%)	1 (0%)	43	71
4	e	533/562 (95%)	513 (96%)	19 (4%)	1 (0%)	43	71
5	G	514/594 (86%)	487 (95%)	26 (5%)	1 (0%)	43	71
5	g	514/594 (86%)	492 (96%)	21 (4%)	1 (0%)	43	71
6	H	516/550 (94%)	493 (96%)	20 (4%)	3 (1%)	21	50
6	h	525/550 (96%)	505 (96%)	16 (3%)	4 (1%)	16	44
7	Q	546/568 (96%)	514 (94%)	28 (5%)	4 (1%)	18	47
7	q	537/568 (94%)	501 (93%)	31 (6%)	5 (1%)	14	42
8	T	406/457 (89%)	370 (91%)	31 (8%)	5 (1%)	10	35
9	Z	536/546 (98%)	514 (96%)	17 (3%)	5 (1%)	14	42
9	z	536/546 (98%)	518 (97%)	17 (3%)	1 (0%)	43	71
10	p	187/286 (65%)	177 (95%)	10 (5%)	0	100	100
All	All	9049/9611 (94%)	8643 (96%)	373 (4%)	33 (0%)	31	59

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	H	25	GLN
6	H	432	ALA
7	Q	513	ARG
7	Q	514	GLU
9	Z	247	VAL
9	Z	268	LYS
7	q	70	THR
7	q	347	PRO
9	z	482	ASP
1	A	259	GLY
8	T	250	LEU
8	T	272	PRO
8	T	426	GLN
9	Z	49	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	Z	245	THR
6	h	257	ALA
6	h	258	GLU
7	q	260	GLU
1	A	199	PRO
5	G	311	LYS
7	Q	259	THR
8	T	249	ASP
4	e	469	PHE
5	g	258	GLN
7	Q	260	GLU
6	h	221	LYS
7	q	69	ALA
7	q	261	THR
6	H	433	GLY
4	E	519	SER
8	T	160	PRO
9	Z	246	GLU
6	h	487	ASN

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	462/471 (98%)	449 (97%)	13 (3%)	38	60
1	a	458/471 (97%)	454 (99%)	4 (1%)	70	76
2	B	433/441 (98%)	430 (99%)	3 (1%)	76	78
2	b	433/441 (98%)	426 (98%)	7 (2%)	55	68
3	D	449/453 (99%)	439 (98%)	10 (2%)	45	63
3	d	450/453 (99%)	447 (99%)	3 (1%)	76	78
4	E	461/483 (95%)	458 (99%)	3 (1%)	76	78
4	e	460/483 (95%)	448 (97%)	12 (3%)	40	61
5	G	443/501 (88%)	434 (98%)	9 (2%)	48	65

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	g	443/501 (88%)	438 (99%)	5 (1%)	65	74
6	H	434/454 (96%)	429 (99%)	5 (1%)	63	72
6	h	440/454 (97%)	434 (99%)	6 (1%)	59	70
7	Q	458/473 (97%)	450 (98%)	8 (2%)	53	67
7	q	453/473 (96%)	445 (98%)	8 (2%)	51	67
8	T	353/392 (90%)	340 (96%)	13 (4%)	30	55
9	Z	455/463 (98%)	449 (99%)	6 (1%)	61	71
9	z	455/463 (98%)	453 (100%)	2 (0%)	84	83
10	p	173/251 (69%)	172 (99%)	1 (1%)	78	80
All	All	7713/8121 (95%)	7595 (98%)	118 (2%)	55	69

All (118) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	189	THR
1	A	197	LYS
1	A	205	VAL
1	A	249	LEU
1	A	281	VAL
1	A	282	LEU
1	A	285	VAL
1	A	298	THR
1	A	299	THR
1	A	493	LYS
1	A	495	ARG
1	A	502	LEU
1	A	504	LEU
2	B	237	THR
2	B	238	LEU
2	B	377	LEU
3	D	161	LYS
3	D	162	ILE
3	D	226	PRO
3	D	240	GLN
3	D	248	THR
3	D	263	ILE
3	D	317	GLU
3	D	360	ILE
3	D	463	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	D	470	ARG
4	E	334	LEU
4	E	515	LEU
4	E	522	MET
5	G	104	LEU
5	G	206	VAL
5	G	251	GLU
5	G	253	LYS
5	G	256	GLU
5	G	261	ILE
5	G	278	GLU
5	G	306	GLN
5	G	308	TYR
6	H	68	THR
6	H	71	LYS
6	H	103	ILE
6	H	104	LEU
6	H	431	ILE
7	Q	43	LEU
7	Q	57	ASN
7	Q	256	ILE
7	Q	259	THR
7	Q	357	THR
7	Q	501	ILE
7	Q	507	GLU
7	Q	512	ILE
8	T	4	ILE
8	T	112	LEU
8	T	113	VAL
8	T	122	ARG
8	T	125	GLU
8	T	138	SER
8	T	158	GLU
8	T	175	THR
8	T	214	THR
8	T	217	LEU
8	T	239	SER
8	T	251	ARG
8	T	329	GLU
9	Z	241	GLU
9	Z	244	LYS
9	Z	245	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	Z	248	ASN
9	Z	284	VAL
9	Z	296	ILE
1	a	89	GLN
1	a	256	MET
1	a	260	VAL
1	a	262	ILE
2	b	5	ILE
2	b	79	ASN
2	b	221	ASN
2	b	238	LEU
2	b	240	THR
2	b	245	ILE
2	b	248	THR
3	d	10	THR
3	d	60	ASP
3	d	312	VAL
4	e	84	THR
4	e	93	GLN
4	e	108	SER
4	e	141	ILE
4	e	144	ILE
4	e	151	ASP
4	e	156	LEU
4	e	274	CYS
4	e	283	THR
4	e	452	LEU
4	e	454	VAL
4	e	464	ILE
5	g	260	ASN
5	g	297	THR
5	g	490	LYS
5	g	494	LEU
5	g	510	GLU
6	h	7	THR
6	h	47	LEU
6	h	60	THR
6	h	201	ILE
6	h	373	THR
6	h	479	TYR
10	p	186	CYS
7	q	28	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	q	29	ILE
7	q	64	ILE
7	q	65	THR
7	q	122	LEU
7	q	256	ILE
7	q	344	LEU
7	q	381	THR
9	z	241	GLU
9	z	245	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (63) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	481	HIS
1	A	485	GLN
2	B	235	ASN
2	B	282	ASN
3	D	125	GLN
3	D	240	GLN
3	D	255	ASN
3	D	303	HIS
4	E	35	GLN
4	E	42	HIS
4	E	85	ASN
4	E	253	GLN
4	E	299	GLN
5	G	106	GLN
5	G	231	HIS
5	G	258	GLN
5	G	260	ASN
5	G	279	GLN
5	G	281	GLN
5	G	450	ASN
6	H	231	GLN
6	H	245	ASN
6	H	256	ASN
6	H	305	GLN
6	H	515	ASN
7	Q	23	ASN
7	Q	40	GLN
7	Q	52	ASN
7	Q	58	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	Q	477	ASN
8	T	28	HIS
8	T	94	GLN
8	T	131	GLN
8	T	134	GLN
8	T	195	HIS
8	T	256	ASN
8	T	334	GLN
8	T	423	GLN
9	Z	67	GLN
9	Z	217	HIS
9	Z	248	ASN
2	b	375	GLN
2	b	439	GLN
3	d	192	ASN
3	d	284	ASN
4	e	93	GLN
4	e	138	GLN
4	e	142	HIS
4	e	296	GLN
4	e	299	GLN
4	e	543	GLN
5	g	260	ASN
5	g	326	ASN
5	g	568	GLN
6	h	173	ASN
6	h	174	ASN
6	h	245	ASN
10	p	91	GLN
7	q	52	ASN
7	q	79	HIS
7	q	219	ASN
7	q	245	HIS
7	q	472	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 47 ligands modelled in this entry, 16 are monoatomic - leaving 31 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	$\# Z > 2$
13	AF3	Z	603	11	0,3,3	-	-	-		
11	ADP	A	601	13,12	27,29,29	1.35	4 (14%)	42,45,45	1.98	11 (26%)
13	AF3	h	603	-	0,3,3	-	-	-		
13	AF3	D	603	11	0,3,3	-	-	-		
11	ADP	Q	602	12	27,29,29	1.35	4 (14%)	42,45,45	2.00	11 (26%)
11	ADP	B	601	12	27,29,29	1.35	4 (14%)	42,45,45	2.05	11 (26%)
13	AF3	H	603	11	0,3,3	-	-	-		
11	ADP	g	601	12	27,29,29	1.34	4 (14%)	42,45,45	2.03	11 (26%)
11	ADP	a	601	12	27,29,29	1.34	4 (14%)	42,45,45	2.03	11 (26%)
13	AF3	z	603	-	0,3,3	-	-	-		
11	ADP	h	601	12	27,29,29	1.37	6 (22%)	42,45,45	2.14	11 (26%)
13	AF3	e	603	11	0,3,3	-	-	-		
13	AF3	a	603	-	0,3,3	-	-	-		
11	ADP	d	601	13,12	27,29,29	1.35	4 (14%)	42,45,45	2.00	11 (26%)
13	AF3	E	603	11,4	0,3,3	-	-	-		
11	ADP	Z	601	13,12	27,29,29	1.35	4 (14%)	42,45,45	1.99	11 (26%)
11	ADP	G	601	13,12	27,29,29	1.35	4 (14%)	42,45,45	1.96	11 (26%)
13	AF3	A	603	11	0,3,3	-	-	-		
11	ADP	z	601	12	27,29,29	1.35	4 (14%)	42,45,45	2.02	11 (26%)
13	AF3	b	603	11	0,3,3	-	-	-		
13	AF3	d	603	11	0,3,3	-	-	-		
13	AF3	g	603	5	0,3,3	-	-	-		
11	ADP	D	601	13,12	27,29,29	1.35	4 (14%)	42,45,45	2.03	11 (26%)
14	GTP	T	502	-	30,34,34	1.18	4 (13%)	46,54,54	1.83	8 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	AF3	G	603	11	0,3,3	-	-	-		
11	ADP	H	601	13,12	27,29,29	1.35	4 (14%)	42,45,45	1.95	11 (26%)
11	ADP	b	601	13,12	27,29,29	1.34	4 (14%)	42,45,45	2.04	11 (26%)
11	ADP	e	601	13,12	27,29,29	1.35	4 (14%)	42,45,45	2.06	11 (26%)
11	ADP	q	601	12	27,29,29	1.35	4 (14%)	42,45,45	2.02	11 (26%)
13	AF3	B	603	2	0,3,3	-	-	-		
11	ADP	E	601	13,12	27,29,29	1.34	4 (14%)	42,45,45	1.98	11 (26%)

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	h	601	12	-	4/16/32/32	0/3/3/3
11	ADP	H	601	13,12	-	0/16/32/32	0/3/3/3
11	ADP	A	601	13,12	-	1/16/32/32	0/3/3/3
11	ADP	d	601	13,12	-	0/16/32/32	0/3/3/3
11	ADP	Z	601	13,12	-	5/16/32/32	0/3/3/3
11	ADP	G	601	13,12	-	2/16/32/32	0/3/3/3
11	ADP	D	601	13,12	-	1/16/32/32	0/3/3/3
11	ADP	Q	602	12	-	4/16/32/32	0/3/3/3
11	ADP	b	601	13,12	-	0/16/32/32	0/3/3/3
11	ADP	e	601	13,12	-	4/16/32/32	0/3/3/3
11	ADP	q	601	12	-	3/16/32/32	0/3/3/3
11	ADP	B	601	12	-	3/16/32/32	0/3/3/3
11	ADP	g	601	12	-	5/16/32/32	0/3/3/3
11	ADP	z	601	12	-	2/16/32/32	0/3/3/3
14	GTP	T	502	-	-	6/22/38/38	0/3/3/3
11	ADP	a	601	12	-	5/16/32/32	0/3/3/3
11	ADP	E	601	13,12	-	3/16/32/32	0/3/3/3

All (70) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	601	ADP	C5-C4	4.50	1.47	1.39
11	e	601	ADP	C5-C4	4.49	1.47	1.39
11	D	601	ADP	C5-C4	4.48	1.47	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	z	601	ADP	C5-C4	4.46	1.47	1.39
11	g	601	ADP	C5-C4	4.46	1.47	1.39
11	a	601	ADP	C5-C4	4.45	1.47	1.39
11	Q	602	ADP	C5-C4	4.45	1.47	1.39
11	G	601	ADP	C5-C4	4.45	1.47	1.39
11	A	601	ADP	C5-C4	4.44	1.47	1.39
11	q	601	ADP	C5-C4	4.44	1.47	1.39
11	Z	601	ADP	C5-C4	4.42	1.47	1.39
11	b	601	ADP	C5-C4	4.42	1.47	1.39
11	d	601	ADP	C5-C4	4.42	1.47	1.39
11	E	601	ADP	C5-C4	4.41	1.47	1.39
11	H	601	ADP	C5-C4	4.39	1.47	1.39
11	h	601	ADP	C5-C4	3.50	1.45	1.39
14	T	502	GTP	C6-N1	-2.81	1.33	1.38
11	Q	602	ADP	C5-C6	2.73	1.48	1.41
11	q	601	ADP	C5-C6	2.72	1.48	1.41
11	d	601	ADP	C5-C6	2.72	1.48	1.41
11	H	601	ADP	C5-C6	2.72	1.48	1.41
11	G	601	ADP	C5-C6	2.70	1.48	1.41
11	E	601	ADP	C5-C6	2.70	1.48	1.41
11	a	601	ADP	C5-C6	2.70	1.48	1.41
11	z	601	ADP	C5-C6	2.68	1.48	1.41
11	A	601	ADP	C5-C6	2.68	1.48	1.41
11	Z	601	ADP	C5-C6	2.68	1.48	1.41
11	b	601	ADP	C5-C6	2.68	1.48	1.41
11	e	601	ADP	C5-C6	2.67	1.48	1.41
11	g	601	ADP	C5-C6	2.66	1.48	1.41
11	B	601	ADP	C5-C6	2.65	1.48	1.41
11	D	601	ADP	C5-C6	2.65	1.48	1.41
11	h	601	ADP	C5-N7	-2.65	1.34	1.39
11	E	601	ADP	C8-N7	2.51	1.36	1.31
11	d	601	ADP	C8-N7	2.51	1.36	1.31
14	T	502	GTP	C5-N7	-2.49	1.34	1.39
11	q	601	ADP	C8-N7	2.47	1.36	1.31
14	T	502	GTP	C5-C4	2.47	1.45	1.38
11	H	601	ADP	C8-N7	2.47	1.36	1.31
11	z	601	ADP	C8-N7	2.47	1.36	1.31
11	a	601	ADP	C8-N7	2.46	1.36	1.31
11	A	601	ADP	C8-N7	2.46	1.36	1.31
11	b	601	ADP	C8-N7	2.46	1.36	1.31
11	B	601	ADP	C8-N7	2.45	1.36	1.31
11	Z	601	ADP	C8-N7	2.45	1.36	1.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	g	601	ADP	C8-N7	2.44	1.36	1.31
11	G	601	ADP	C8-N7	2.44	1.36	1.31
11	Q	602	ADP	C8-N7	2.41	1.36	1.31
11	e	601	ADP	C8-N7	2.39	1.36	1.31
11	D	601	ADP	C8-N7	2.38	1.36	1.31
11	h	601	ADP	C4-N9	-2.32	1.32	1.37
14	T	502	GTP	C4-N9	-2.31	1.32	1.38
11	D	601	ADP	C5-N7	-2.22	1.34	1.39
11	G	601	ADP	C5-N7	-2.21	1.34	1.39
11	h	601	ADP	C5-C6	2.21	1.47	1.41
11	e	601	ADP	C5-N7	-2.21	1.34	1.39
11	Q	602	ADP	C5-N7	-2.20	1.34	1.39
11	h	601	ADP	C8-N9	-2.17	1.33	1.37
11	B	601	ADP	C5-N7	-2.17	1.34	1.39
11	d	601	ADP	C5-N7	-2.17	1.34	1.39
11	g	601	ADP	C5-N7	-2.17	1.34	1.39
11	Z	601	ADP	C5-N7	-2.16	1.34	1.39
11	E	601	ADP	C5-N7	-2.16	1.34	1.39
11	q	601	ADP	C5-N7	-2.14	1.35	1.39
11	H	601	ADP	C5-N7	-2.14	1.35	1.39
11	b	601	ADP	C5-N7	-2.13	1.35	1.39
11	z	601	ADP	C5-N7	-2.12	1.35	1.39
11	A	601	ADP	C5-N7	-2.11	1.35	1.39
11	a	601	ADP	C5-N7	-2.07	1.35	1.39
11	h	601	ADP	C8-N7	2.04	1.35	1.31

All (184) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	e	601	ADP	C5-C4-N3	-6.31	118.52	126.75
11	D	601	ADP	C5-C4-N3	-6.30	118.53	126.75
11	A	601	ADP	C5-C4-N3	-6.28	118.55	126.75
11	b	601	ADP	C5-C4-N3	-6.27	118.57	126.75
11	a	601	ADP	C5-C4-N3	-6.27	118.57	126.75
11	q	601	ADP	C5-C4-N3	-6.25	118.59	126.75
11	G	601	ADP	C5-C4-N3	-6.23	118.62	126.75
11	B	601	ADP	C5-C4-N3	-6.22	118.63	126.75
11	Q	602	ADP	C5-C4-N3	-6.22	118.64	126.75
11	g	601	ADP	C5-C4-N3	-6.21	118.65	126.75
11	z	601	ADP	C5-C4-N3	-6.18	118.68	126.75
11	H	601	ADP	C5-C4-N3	-6.17	118.70	126.75
11	h	601	ADP	C5-C4-N3	-6.16	118.72	126.75

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	d	601	ADP	C5-C4-N3	-6.15	118.72	126.75
11	Z	601	ADP	C5-C4-N3	-6.12	118.77	126.75
11	E	601	ADP	C5-C4-N3	-6.10	118.79	126.75
14	T	502	GTP	C5-C4-N3	-5.41	119.69	128.46
11	h	601	ADP	PA-O3A-PB	-4.97	115.77	132.83
11	e	601	ADP	N3-C4-N9	4.95	135.24	127.08
11	g	601	ADP	N3-C4-N9	4.90	135.16	127.08
11	A	601	ADP	N3-C4-N9	4.90	135.15	127.08
11	a	601	ADP	N3-C4-N9	4.89	135.13	127.08
11	B	601	ADP	N3-C4-N9	4.88	135.12	127.08
11	b	601	ADP	N3-C4-N9	4.85	135.07	127.08
11	Q	602	ADP	N3-C4-N9	4.84	135.06	127.08
11	G	601	ADP	N3-C4-N9	4.82	135.02	127.08
11	q	601	ADP	N3-C4-N9	4.81	135.01	127.08
11	Z	601	ADP	N3-C4-N9	4.80	135.00	127.08
11	D	601	ADP	N3-C4-N9	4.80	134.99	127.08
11	z	601	ADP	N3-C4-N9	4.79	134.97	127.08
11	H	601	ADP	N3-C4-N9	4.78	134.97	127.08
11	d	601	ADP	N3-C4-N9	4.71	134.84	127.08
11	E	601	ADP	N3-C4-N9	4.70	134.83	127.08
11	h	601	ADP	N3-C4-N9	4.58	134.63	127.08
14	T	502	GTP	C2-N3-C4	4.55	120.41	112.30
11	D	601	ADP	PA-O3A-PB	-4.28	118.15	132.83
14	T	502	GTP	PB-O3B-PG	-4.18	118.50	132.83
14	T	502	GTP	N9-C4-N3	4.11	134.19	125.94
11	G	601	ADP	C2-N3-C4	4.10	121.44	111.75
11	A	601	ADP	C2-N3-C4	4.09	121.41	111.75
11	b	601	ADP	C2-N3-C4	4.09	121.41	111.75
11	e	601	ADP	PA-O3A-PB	-4.08	118.83	132.83
11	a	601	ADP	C2-N3-C4	4.07	121.37	111.75
11	e	601	ADP	C2-N3-C4	4.06	121.35	111.75
11	Q	602	ADP	C2-N3-C4	4.06	121.35	111.75
11	q	601	ADP	C2-N3-C4	4.06	121.35	111.75
11	H	601	ADP	C2-N3-C4	4.05	121.32	111.75
11	d	601	ADP	C2-N3-C4	4.05	121.31	111.75
11	z	601	ADP	C2-N3-C4	4.04	121.31	111.75
11	g	601	ADP	C2-N3-C4	4.04	121.29	111.75
11	B	601	ADP	C2-N3-C4	4.03	121.26	111.75
11	E	601	ADP	C2-N3-C4	4.02	121.24	111.75
11	Z	601	ADP	C2-N3-C4	4.00	121.21	111.75
11	D	601	ADP	C2-N3-C4	4.00	121.19	111.75
11	B	601	ADP	PA-O3A-PB	-3.91	119.43	132.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	d	601	ADP	PA-O3A-PB	-3.83	119.68	132.83
11	h	601	ADP	C2-N3-C4	3.81	120.75	111.75
11	G	601	ADP	N3-C2-N1	-3.66	122.88	128.60
11	H	601	ADP	N3-C2-N1	-3.64	122.91	128.60
11	A	601	ADP	N3-C2-N1	-3.64	122.91	128.60
11	b	601	ADP	N3-C2-N1	-3.63	122.92	128.60
11	z	601	ADP	N3-C2-N1	-3.61	122.95	128.60
11	Q	602	ADP	N3-C2-N1	-3.61	122.95	128.60
11	Z	601	ADP	N3-C2-N1	-3.60	122.96	128.60
11	d	601	ADP	N3-C2-N1	-3.60	122.98	128.60
11	q	601	ADP	N3-C2-N1	-3.59	122.98	128.60
11	a	601	ADP	N3-C2-N1	-3.59	122.99	128.60
11	E	601	ADP	N3-C2-N1	-3.57	123.02	128.60
11	e	601	ADP	N3-C2-N1	-3.56	123.03	128.60
11	b	601	ADP	PA-O3A-PB	-3.55	120.64	132.83
11	g	601	ADP	N3-C2-N1	-3.55	123.06	128.60
11	B	601	ADP	N3-C2-N1	-3.54	123.07	128.60
11	z	601	ADP	PA-O3A-PB	-3.52	120.74	132.83
11	Q	602	ADP	PA-O3A-PB	-3.51	120.77	132.83
11	h	601	ADP	C4-C5-N7	-3.50	106.36	110.62
11	a	601	ADP	PA-O3A-PB	-3.47	120.92	132.83
11	b	601	ADP	C4-C5-N7	-3.43	106.44	110.62
11	D	601	ADP	N3-C2-N1	-3.43	123.23	128.60
11	z	601	ADP	C4-C5-N7	-3.43	106.44	110.62
11	A	601	ADP	C4-C5-N7	-3.41	106.46	110.62
11	q	601	ADP	C4-C5-N7	-3.41	106.47	110.62
11	g	601	ADP	PA-O3A-PB	-3.40	121.16	132.83
11	a	601	ADP	C4-C5-N7	-3.39	106.49	110.62
11	H	601	ADP	C4-C5-N7	-3.38	106.50	110.62
11	Z	601	ADP	PA-O3A-PB	-3.36	121.29	132.83
11	B	601	ADP	C4-C5-N7	-3.36	106.53	110.62
11	d	601	ADP	C4-C5-N7	-3.36	106.53	110.62
11	G	601	ADP	C4-C5-N7	-3.35	106.54	110.62
11	Z	601	ADP	C4-C5-N7	-3.35	106.54	110.62
11	E	601	ADP	C4-C5-N7	-3.34	106.55	110.62
11	g	601	ADP	C4-C5-N7	-3.32	106.58	110.62
14	T	502	GTP	PA-O3A-PB	-3.31	121.48	132.83
11	D	601	ADP	C4-C5-N7	-3.30	106.59	110.62
11	e	601	ADP	C4-C5-N7	-3.30	106.60	110.62
11	Q	602	ADP	C4-C5-N7	-3.28	106.62	110.62
11	E	601	ADP	PA-O3A-PB	-3.24	121.71	132.83
11	q	601	ADP	PA-O3A-PB	-3.24	121.72	132.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	T	502	GTP	C6-C5-N7	3.23	136.25	130.25
11	h	601	ADP	C3'-C2'-C1'	3.10	107.31	101.43
11	b	601	ADP	C5-N7-C8	3.05	107.85	103.51
11	A	601	ADP	C5-N7-C8	3.05	107.84	103.51
11	z	601	ADP	C5-N7-C8	3.02	107.80	103.51
11	Z	601	ADP	C5-N7-C8	3.01	107.79	103.51
11	G	601	ADP	C5-N7-C8	3.01	107.78	103.51
11	H	601	ADP	C5-N7-C8	3.00	107.78	103.51
11	q	601	ADP	C5-N7-C8	3.00	107.78	103.51
11	a	601	ADP	C5-N7-C8	3.00	107.77	103.51
11	g	601	ADP	C5-N7-C8	3.00	107.77	103.51
11	B	601	ADP	C5-N7-C8	2.99	107.76	103.51
11	E	601	ADP	C5-N7-C8	2.98	107.75	103.51
11	e	601	ADP	C5-N7-C8	2.97	107.72	103.51
11	Q	602	ADP	C5-N7-C8	2.96	107.72	103.51
11	d	601	ADP	C5-N7-C8	2.96	107.71	103.51
11	D	601	ADP	C5-N7-C8	2.89	107.62	103.51
11	h	601	ADP	C5-N7-C8	2.88	107.61	103.51
11	h	601	ADP	N3-C2-N1	-2.88	124.10	128.60
11	Z	601	ADP	C4-N9-C8	2.82	108.78	105.73
11	g	601	ADP	C4-N9-C8	2.82	108.78	105.73
11	A	601	ADP	C4-N9-C8	2.81	108.78	105.73
11	B	601	ADP	C4-N9-C8	2.80	108.76	105.73
11	z	601	ADP	C4-N9-C8	2.79	108.75	105.73
11	a	601	ADP	C4-N9-C8	2.77	108.72	105.73
11	H	601	ADP	C4-N9-C8	2.75	108.71	105.73
11	h	601	ADP	C4-N9-C8	2.75	108.71	105.73
11	b	601	ADP	C4-N9-C8	2.75	108.70	105.73
11	E	601	ADP	C4-N9-C8	2.71	108.66	105.73
11	e	601	ADP	C4-N9-C8	2.67	108.63	105.73
11	q	601	ADP	C4-N9-C8	2.67	108.62	105.73
11	G	601	ADP	C4-N9-C8	2.63	108.58	105.73
11	d	601	ADP	C4-N9-C8	2.59	108.53	105.73
11	Q	602	ADP	C4-N9-C8	2.58	108.53	105.73
11	B	601	ADP	C3'-C2'-C1'	2.48	106.13	101.43
11	e	601	ADP	C3'-C2'-C1'	2.43	106.04	101.43
11	A	601	ADP	N9-C8-N7	-2.41	110.62	113.91
11	g	601	ADP	C3'-C2'-C1'	2.41	106.00	101.43
11	Z	601	ADP	N9-C8-N7	-2.39	110.65	113.91
11	b	601	ADP	N9-C8-N7	-2.38	110.65	113.91
11	E	601	ADP	N9-C8-N7	-2.38	110.66	113.91
11	z	601	ADP	N9-C8-N7	-2.38	110.66	113.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	H	601	ADP	N9-C8-N7	-2.37	110.67	113.91
11	h	601	ADP	N9-C8-N7	-2.37	110.67	113.91
11	g	601	ADP	N9-C8-N7	-2.36	110.68	113.91
11	z	601	ADP	C6-C5-N7	2.36	136.42	132.02
11	D	601	ADP	C3'-C2'-C1'	2.35	105.89	101.43
11	B	601	ADP	N9-C8-N7	-2.35	110.70	113.91
11	G	601	ADP	PA-O3A-PB	-2.35	124.78	132.83
11	G	601	ADP	C3'-C2'-C1'	2.34	105.88	101.43
11	a	601	ADP	N9-C8-N7	-2.34	110.72	113.91
11	z	601	ADP	C3'-C2'-C1'	2.33	105.86	101.43
11	H	601	ADP	C6-C5-N7	2.33	136.37	132.02
11	d	601	ADP	C6-C5-N7	2.33	136.36	132.02
14	T	502	GTP	C4-C5-N7	-2.33	107.04	110.72
11	D	601	ADP	C4-N9-C8	2.33	108.25	105.73
11	q	601	ADP	N9-C8-N7	-2.32	110.73	113.91
11	G	601	ADP	N9-C8-N7	-2.32	110.74	113.91
11	q	601	ADP	C6-C5-N7	2.32	136.34	132.02
11	Z	601	ADP	C6-C5-N7	2.32	136.34	132.02
11	E	601	ADP	C6-C5-N7	2.32	136.34	132.02
11	G	601	ADP	C6-C5-N7	2.31	136.33	132.02
11	b	601	ADP	C6-C5-N7	2.30	136.30	132.02
11	a	601	ADP	C6-C5-N7	2.29	136.29	132.02
11	d	601	ADP	N9-C8-N7	-2.29	110.79	113.91
11	A	601	ADP	C3'-C2'-C1'	2.28	105.76	101.43
11	B	601	ADP	C6-C5-N7	2.27	136.26	132.02
11	e	601	ADP	N9-C8-N7	-2.27	110.81	113.91
11	A	601	ADP	C6-C5-N7	2.26	136.24	132.02
11	Q	602	ADP	N9-C8-N7	-2.25	110.83	113.91
11	g	601	ADP	C6-C5-N7	2.24	136.20	132.02
11	Q	602	ADP	C6-C5-N7	2.24	136.19	132.02
11	a	601	ADP	C3'-C2'-C1'	2.21	105.62	101.43
11	h	601	ADP	C6-C5-N7	2.20	136.13	132.02
11	Q	602	ADP	C3'-C2'-C1'	2.20	105.61	101.43
11	e	601	ADP	C6-C5-N7	2.20	136.11	132.02
11	A	601	ADP	PA-O3A-PB	-2.18	125.34	132.83
11	D	601	ADP	C6-C5-N7	2.15	136.03	132.02
14	T	502	GTP	O6-C6-C5	-2.14	120.92	126.60
11	b	601	ADP	C3'-C2'-C1'	2.14	105.49	101.43
11	d	601	ADP	C3'-C2'-C1'	2.12	105.46	101.43
11	H	601	ADP	C3'-C2'-C1'	2.12	105.45	101.43
11	q	601	ADP	C3'-C2'-C1'	2.10	105.41	101.43
11	D	601	ADP	N9-C8-N7	-2.09	111.05	113.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	E	601	ADP	C3'-C2'-C1'	2.09	105.40	101.43
11	H	601	ADP	C2-N1-C6	2.01	122.22	118.77
11	Z	601	ADP	C3'-C2'-C1'	2.01	105.25	101.43

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	E	601	ADP	C5'-O5'-PA-O1A
11	E	601	ADP	C5'-O5'-PA-O2A
11	Q	602	ADP	C5'-O5'-PA-O1A
11	Q	602	ADP	C5'-O5'-PA-O2A
11	Z	601	ADP	C5'-O5'-PA-O3A
11	a	601	ADP	C5'-O5'-PA-O2A
11	g	601	ADP	PB-O3A-PA-O5'
11	g	601	ADP	C5'-O5'-PA-O1A
11	h	601	ADP	C5'-O5'-PA-O1A
11	h	601	ADP	C5'-O5'-PA-O2A
11	q	601	ADP	C5'-O5'-PA-O3A
14	T	502	GTP	C5'-O5'-PA-O1A
14	T	502	GTP	C5'-O5'-PA-O2A
14	T	502	GTP	C3'-C4'-C5'-O5'
14	T	502	GTP	O4'-C4'-C5'-O5'
11	a	601	ADP	O4'-C4'-C5'-O5'
11	a	601	ADP	C3'-C4'-C5'-O5'
11	Z	601	ADP	PB-O3A-PA-O1A
11	Q	602	ADP	O4'-C4'-C5'-O5'
14	T	502	GTP	C4'-C5'-O5'-PA
11	g	601	ADP	O4'-C4'-C5'-O5'
11	E	601	ADP	C5'-O5'-PA-O3A
11	g	601	ADP	C5'-O5'-PA-O3A
14	T	502	GTP	C5'-O5'-PA-O3A
11	e	601	ADP	O4'-C4'-C5'-O5'
11	A	601	ADP	PB-O3A-PA-O2A
11	G	601	ADP	PB-O3A-PA-O2A
11	z	601	ADP	PB-O3A-PA-O2A
11	Z	601	ADP	C5'-O5'-PA-O1A
11	Z	601	ADP	C5'-O5'-PA-O2A
11	e	601	ADP	C5'-O5'-PA-O2A
11	g	601	ADP	C5'-O5'-PA-O2A
11	q	601	ADP	C5'-O5'-PA-O1A
11	h	601	ADP	O4'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	e	601	ADP	PB-O3A-PA-O1A
11	B	601	ADP	O4'-C4'-C5'-O5'
11	B	601	ADP	C5'-O5'-PA-O3A
11	Q	602	ADP	C5'-O5'-PA-O3A
11	a	601	ADP	C5'-O5'-PA-O3A
11	e	601	ADP	C5'-O5'-PA-O3A
11	h	601	ADP	C5'-O5'-PA-O3A
11	D	601	ADP	O4'-C4'-C5'-O5'
11	G	601	ADP	PB-O3A-PA-O1A
11	Z	601	ADP	PB-O3A-PA-O2A
11	z	601	ADP	PB-O3A-PA-O1A
11	B	601	ADP	C5'-O5'-PA-O2A
11	a	601	ADP	C5'-O5'-PA-O1A
11	q	601	ADP	O4'-C4'-C5'-O5'

There are no ring outliers.

26 monomers are involved in 35 short contacts:

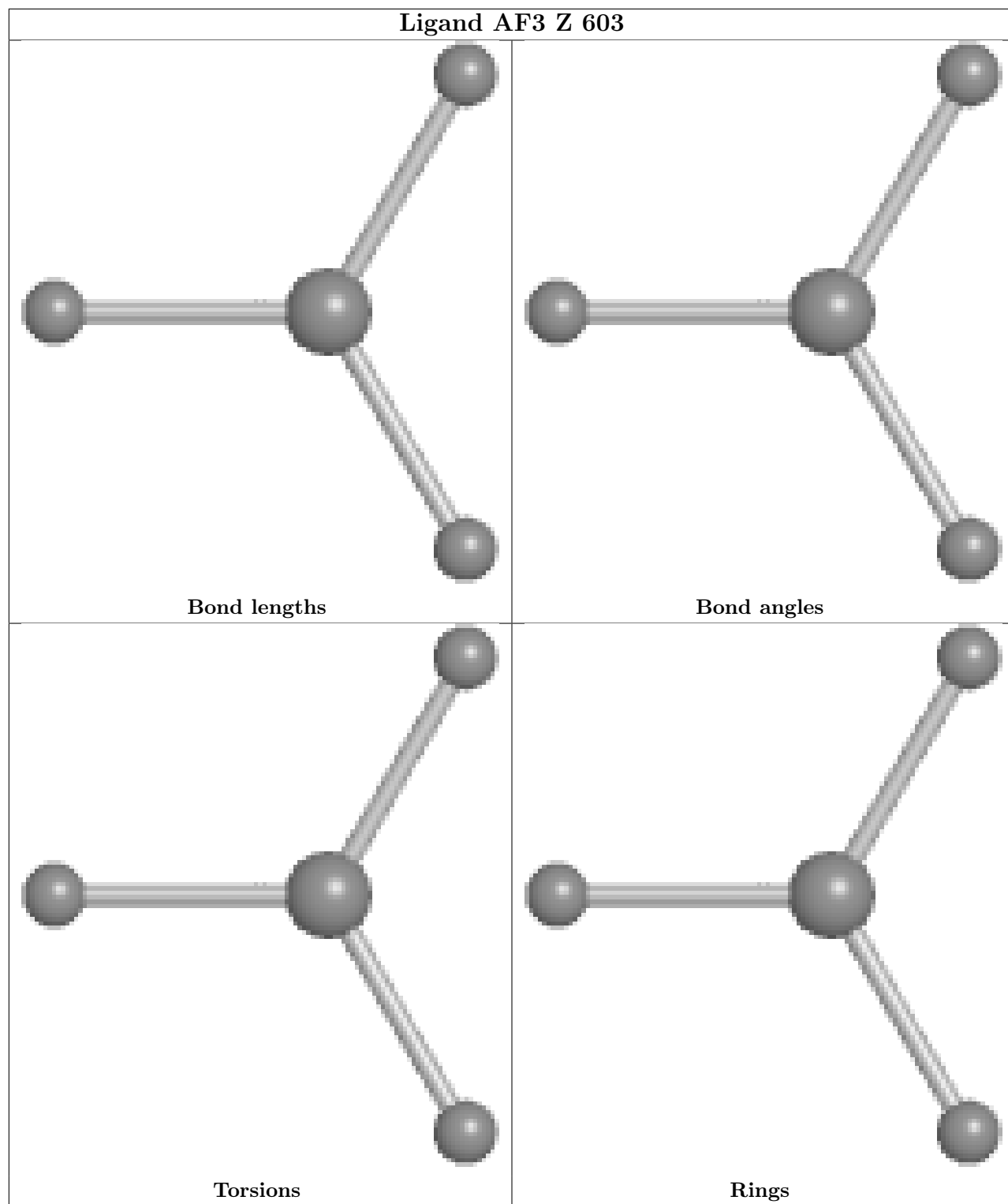
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	Z	603	AF3	1	0
11	A	601	ADP	1	0
13	h	603	AF3	1	0
13	D	603	AF3	3	0
11	Q	602	ADP	1	0
11	B	601	ADP	1	0
13	H	603	AF3	1	0
11	a	601	ADP	1	0
13	z	603	AF3	1	0
11	h	601	ADP	1	0
13	e	603	AF3	2	0
13	a	603	AF3	1	0
11	d	601	ADP	1	0
13	E	603	AF3	2	0
11	Z	601	ADP	1	0
11	G	601	ADP	1	0
13	A	603	AF3	1	0
11	z	601	ADP	1	0
13	b	603	AF3	1	0
13	d	603	AF3	6	0
11	D	601	ADP	3	0
14	T	502	GTP	6	0
13	G	603	AF3	2	0

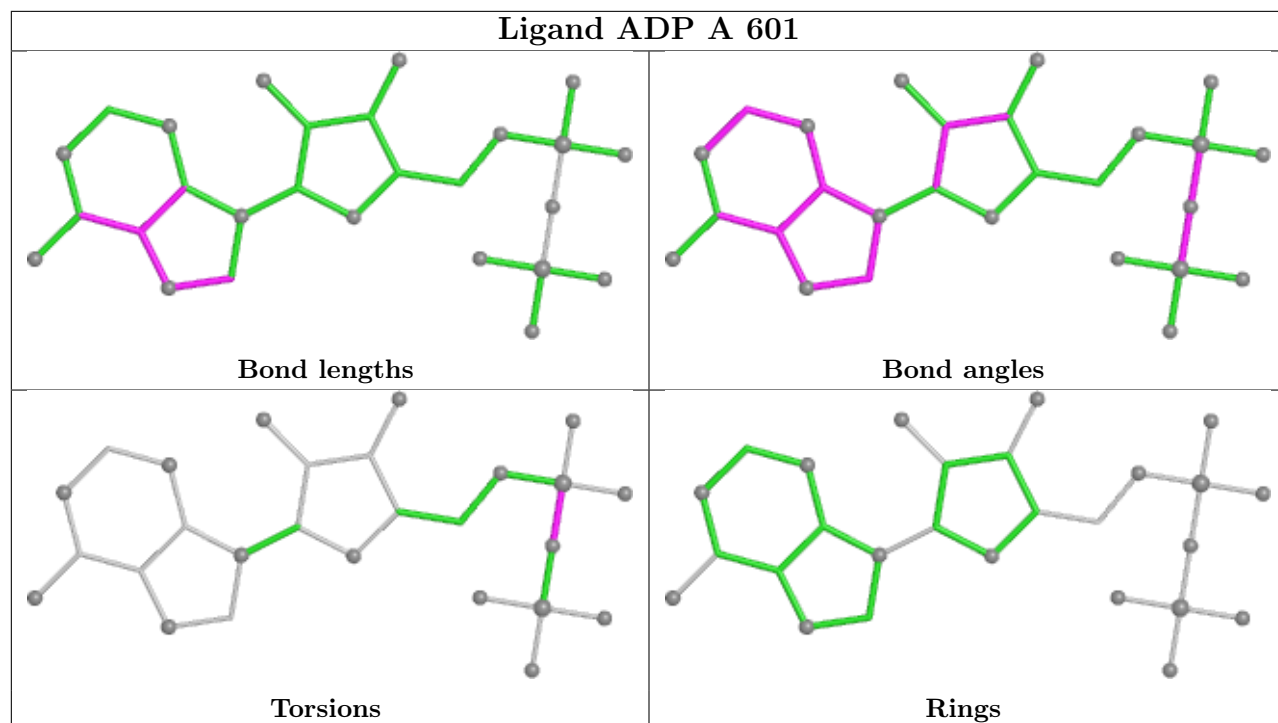
Continued on next page...

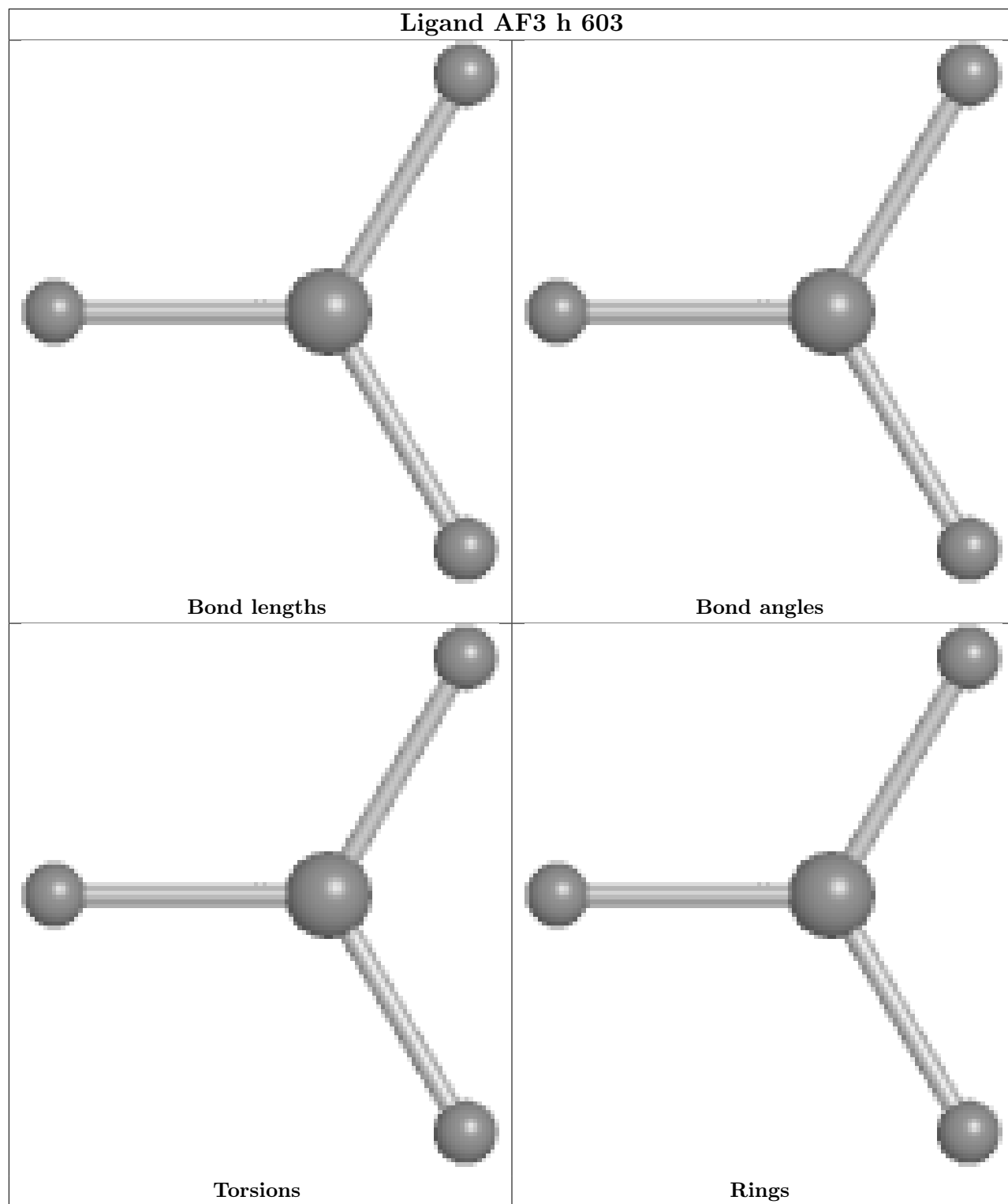
Continued from previous page...

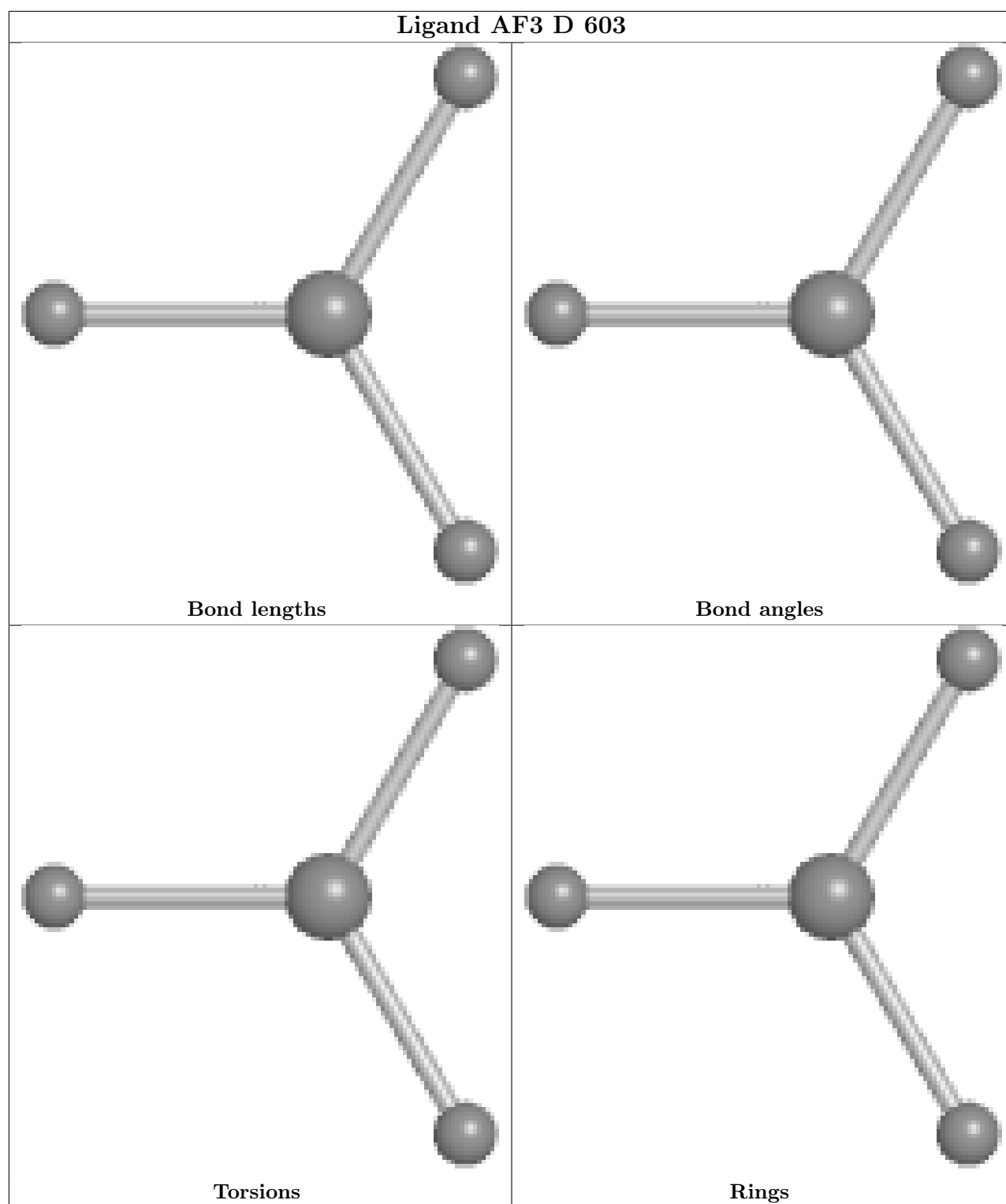
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	e	601	ADP	1	0
11	q	601	ADP	2	0
13	B	603	AF3	3	0

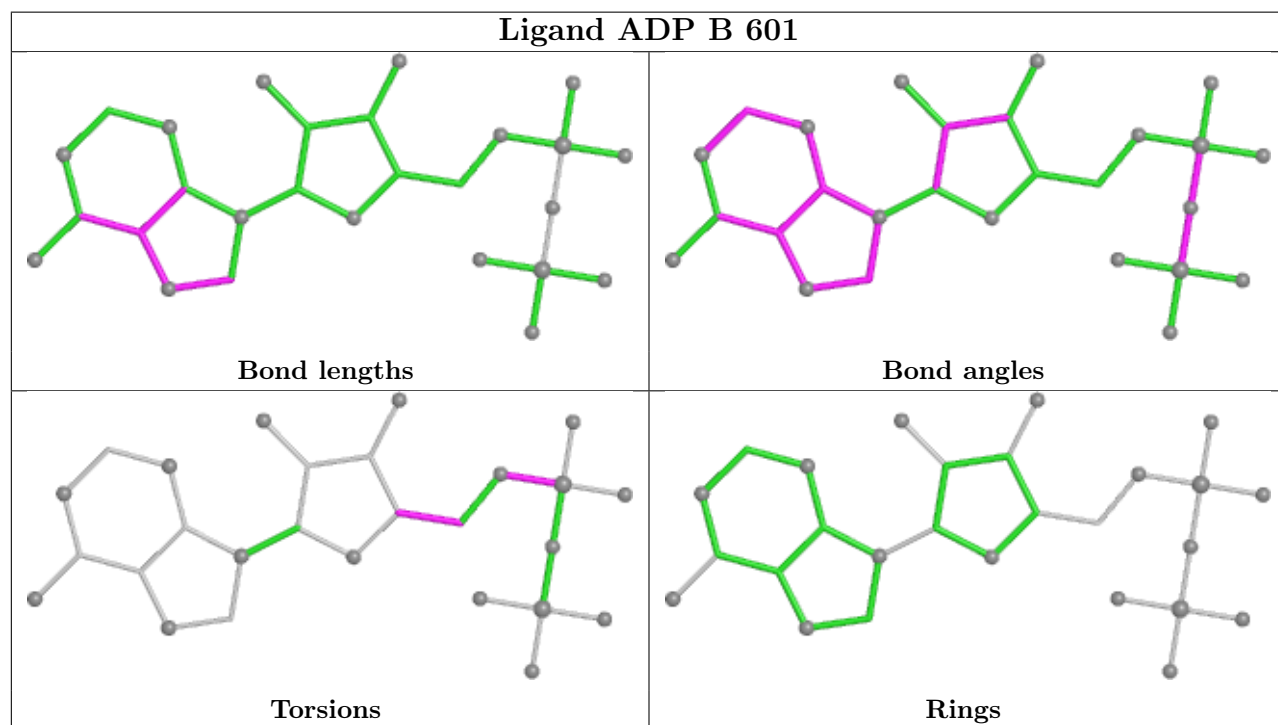
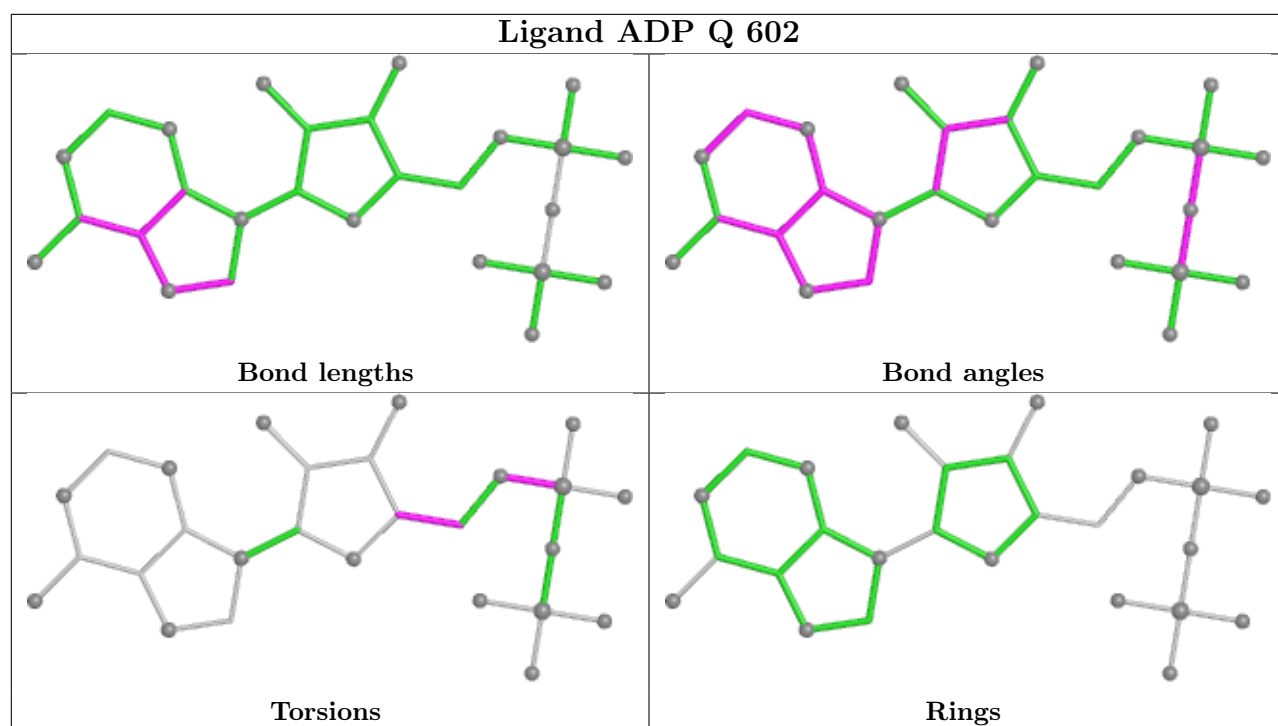
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

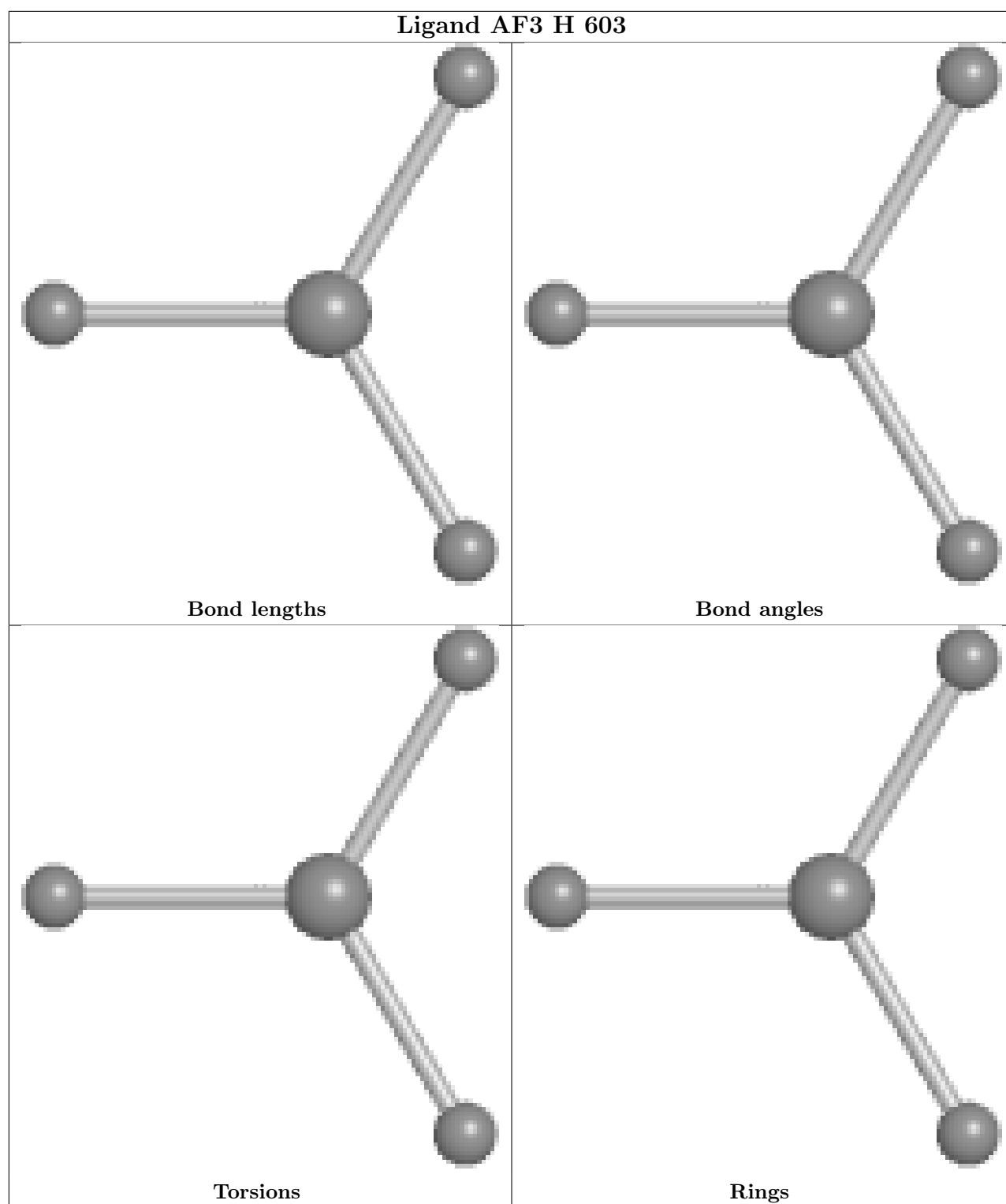


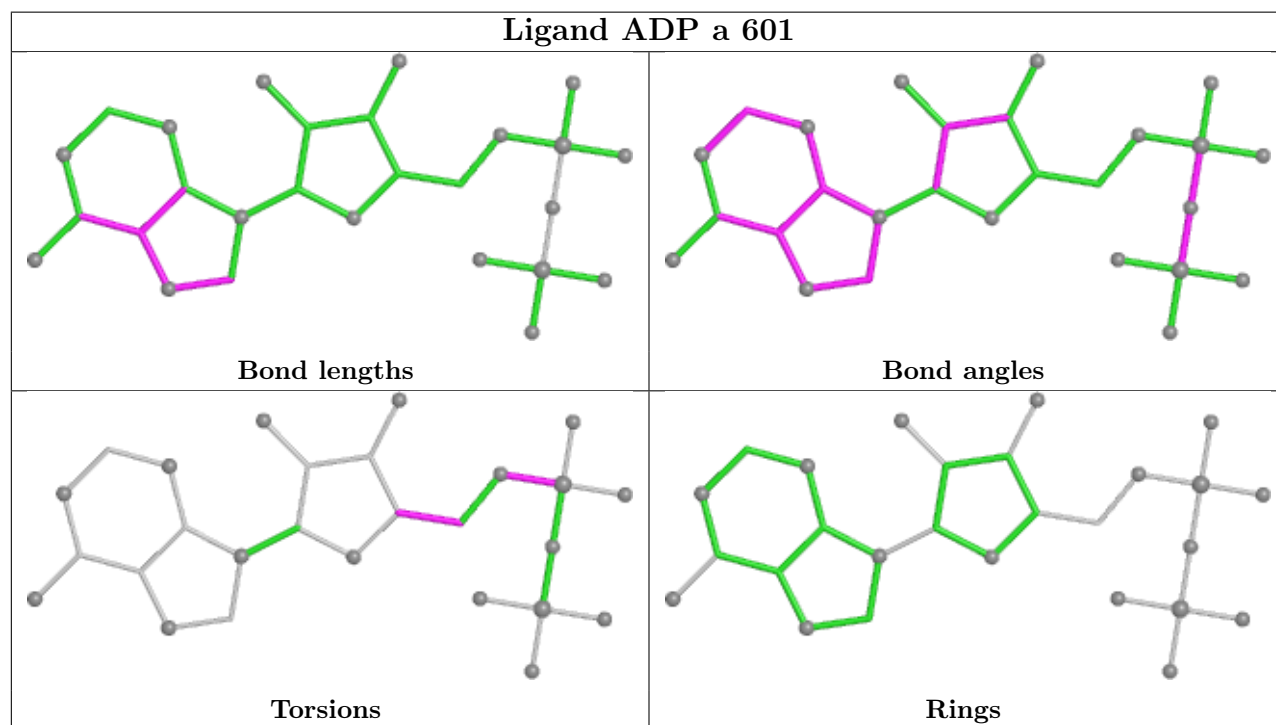
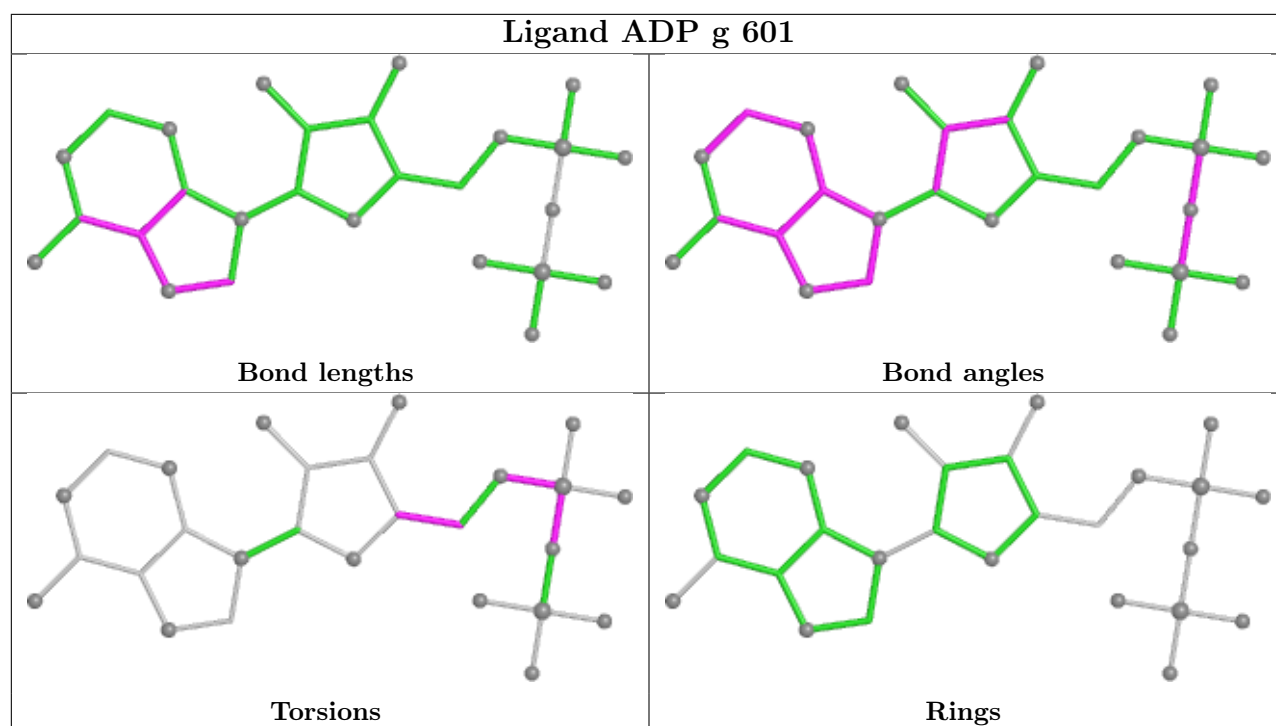


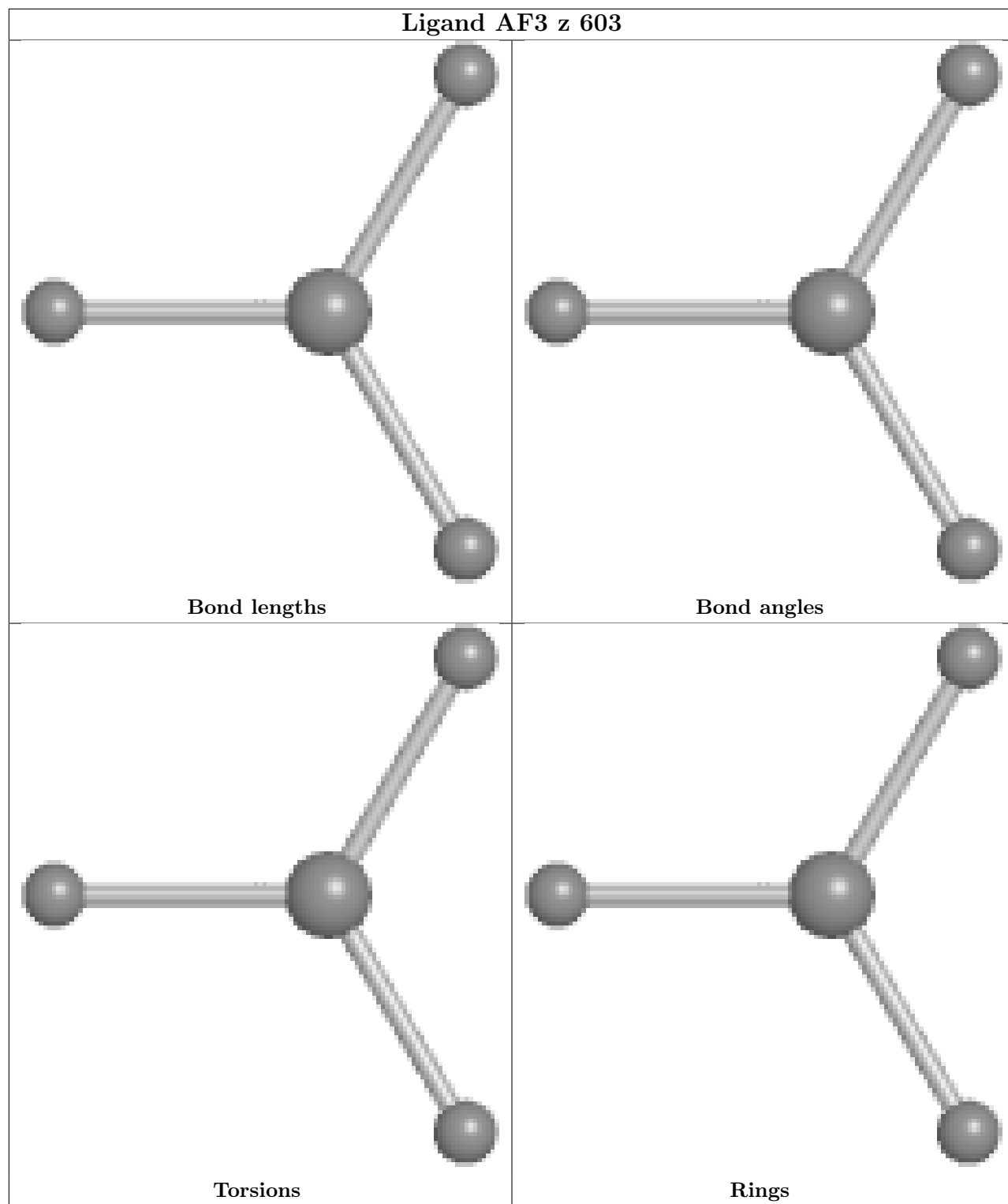


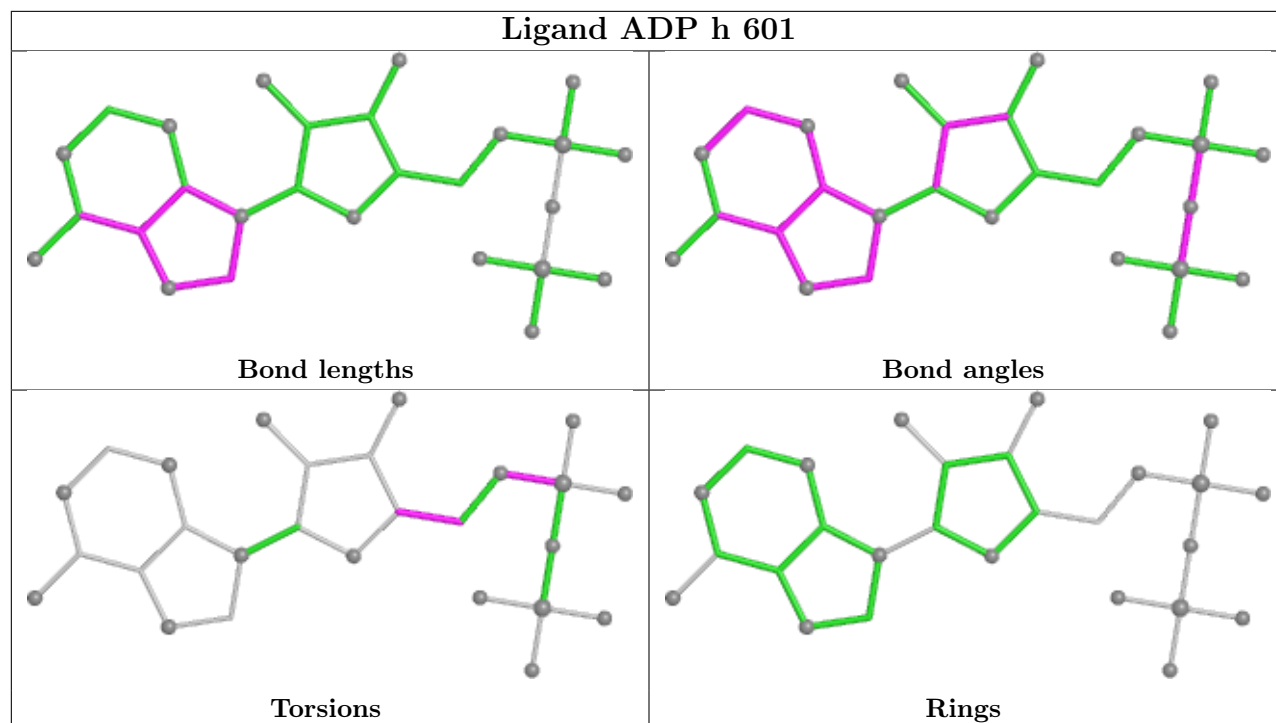


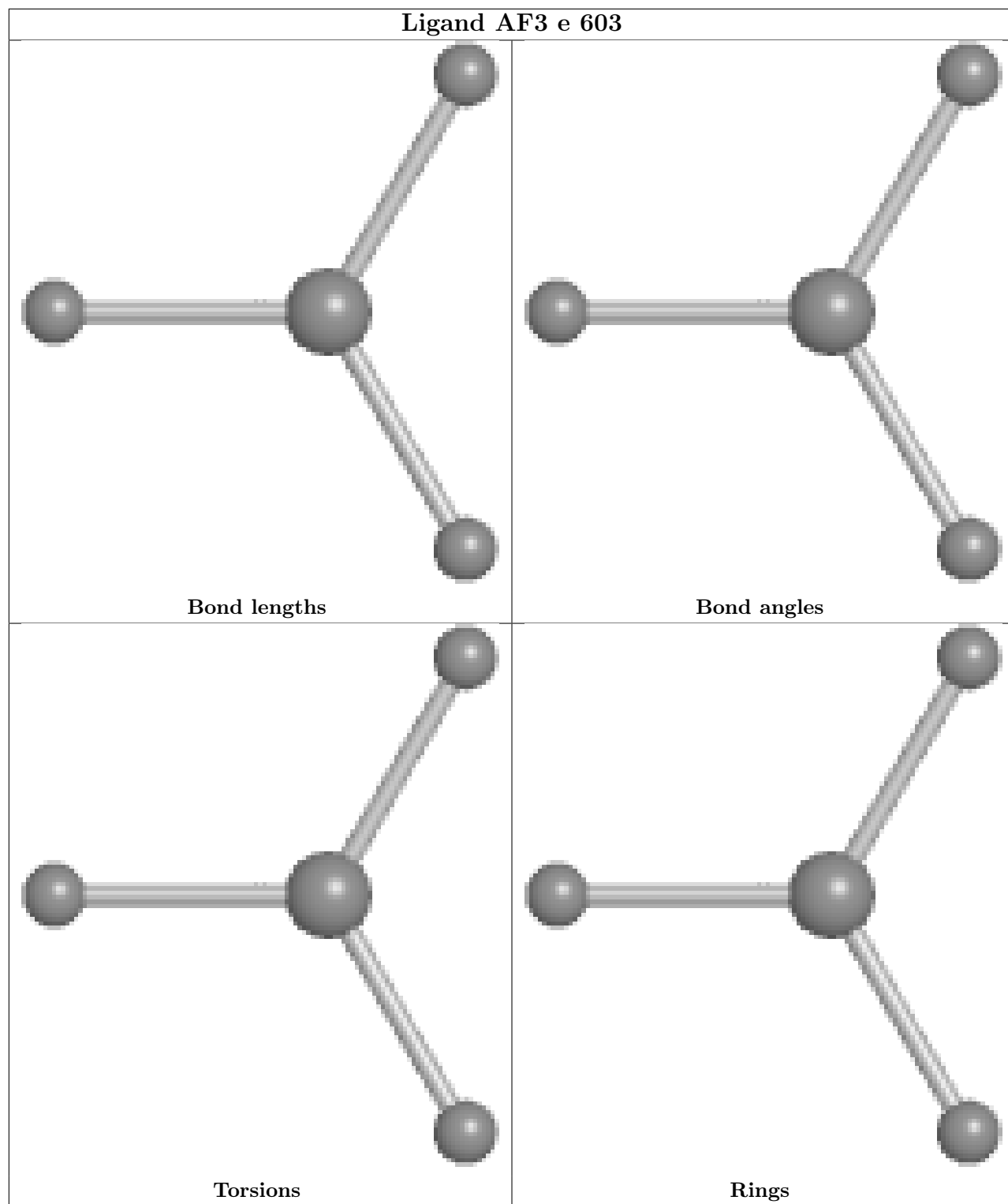


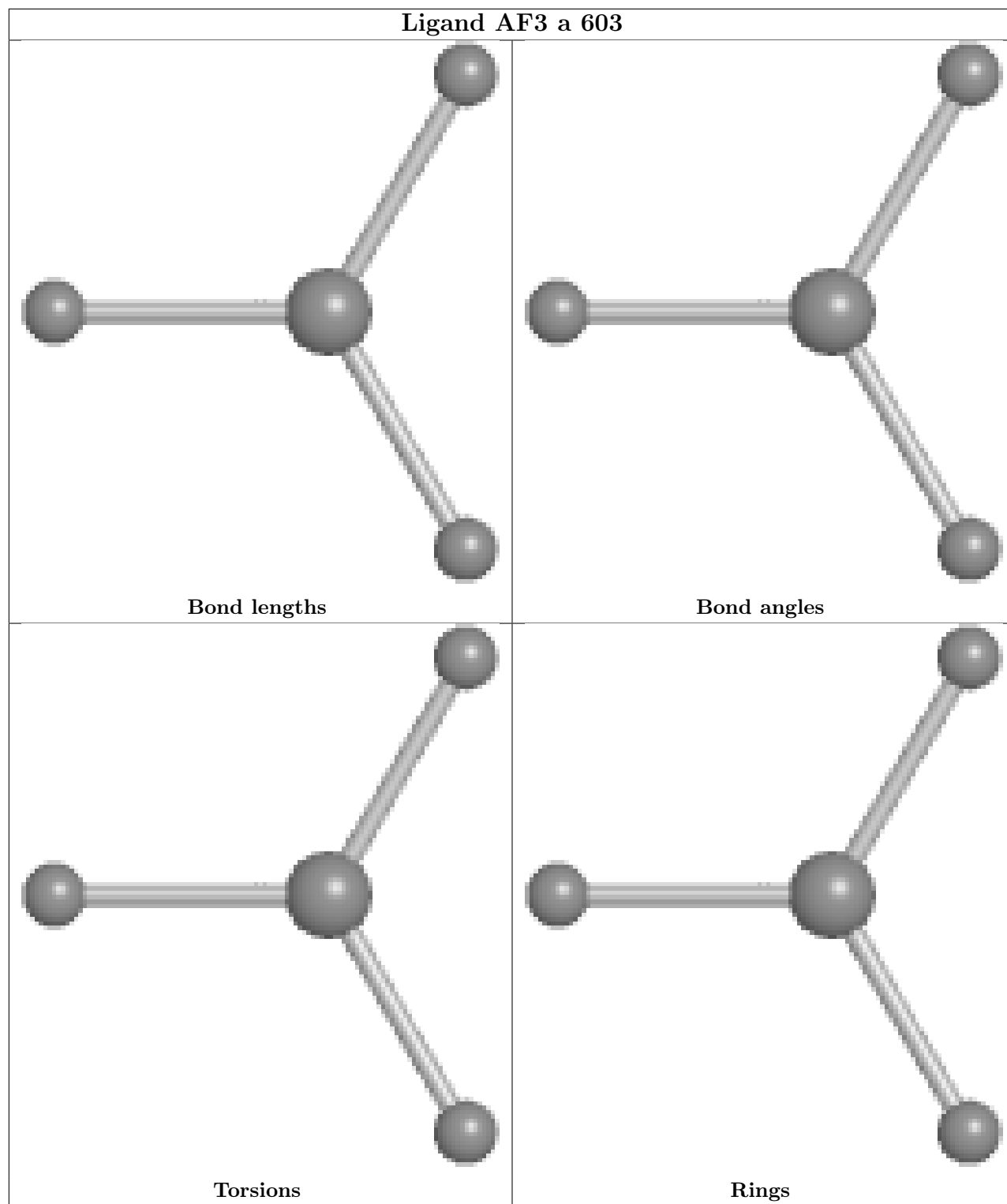


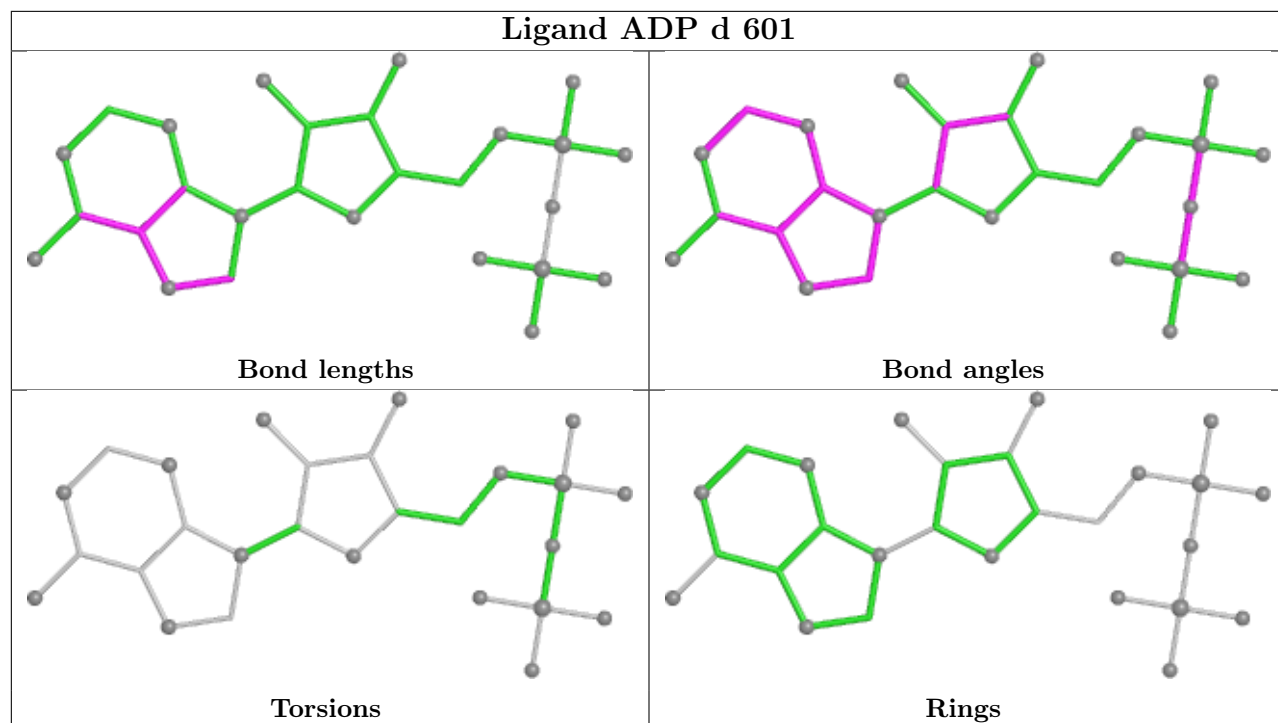


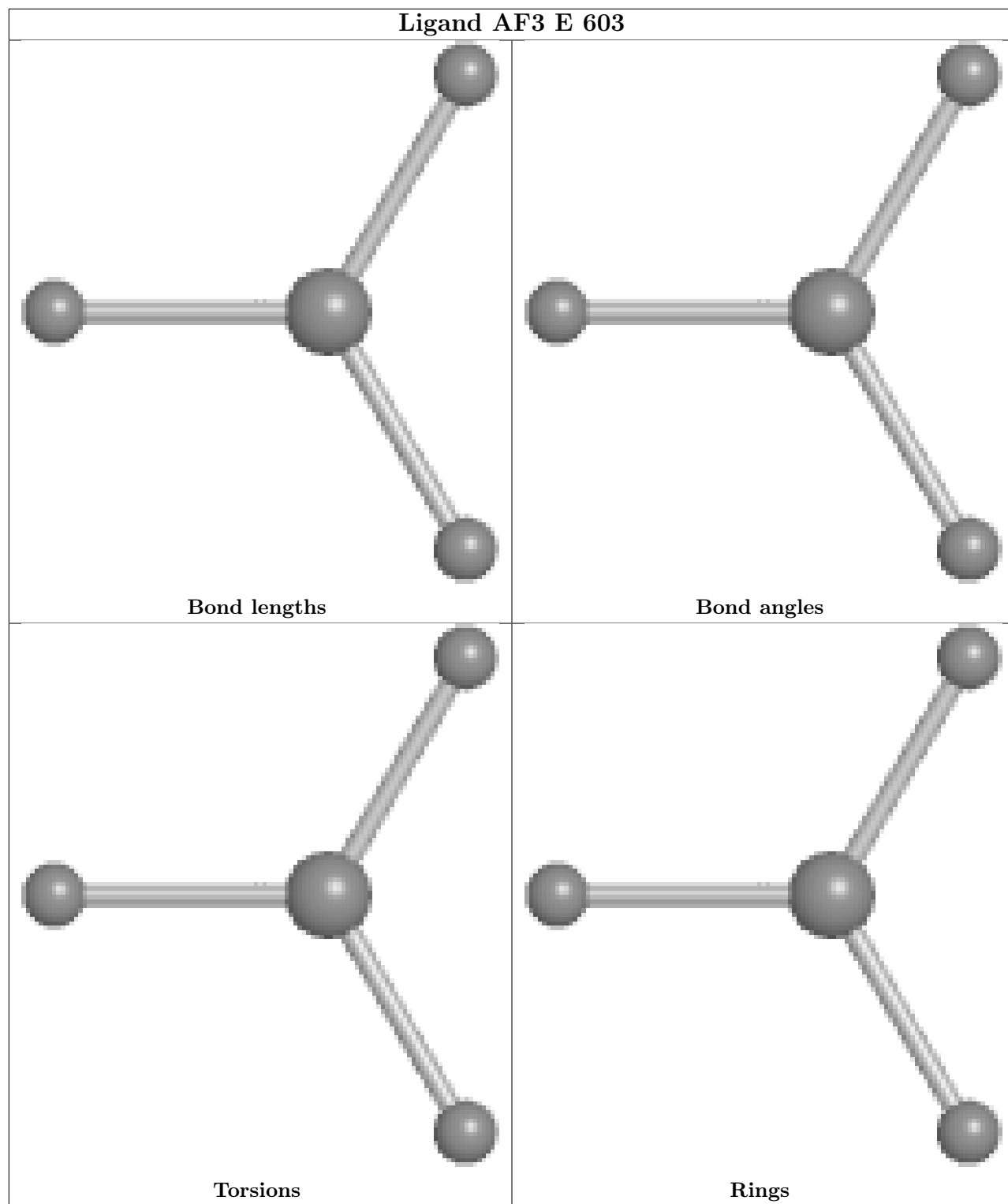


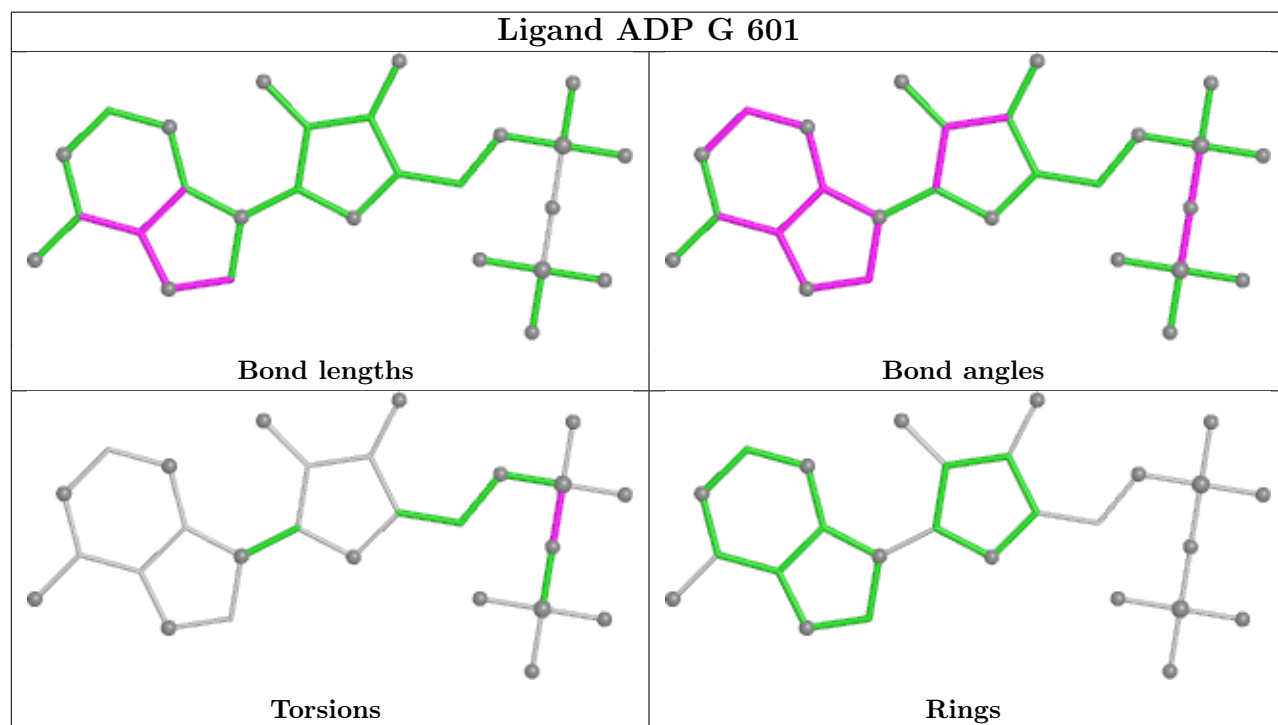
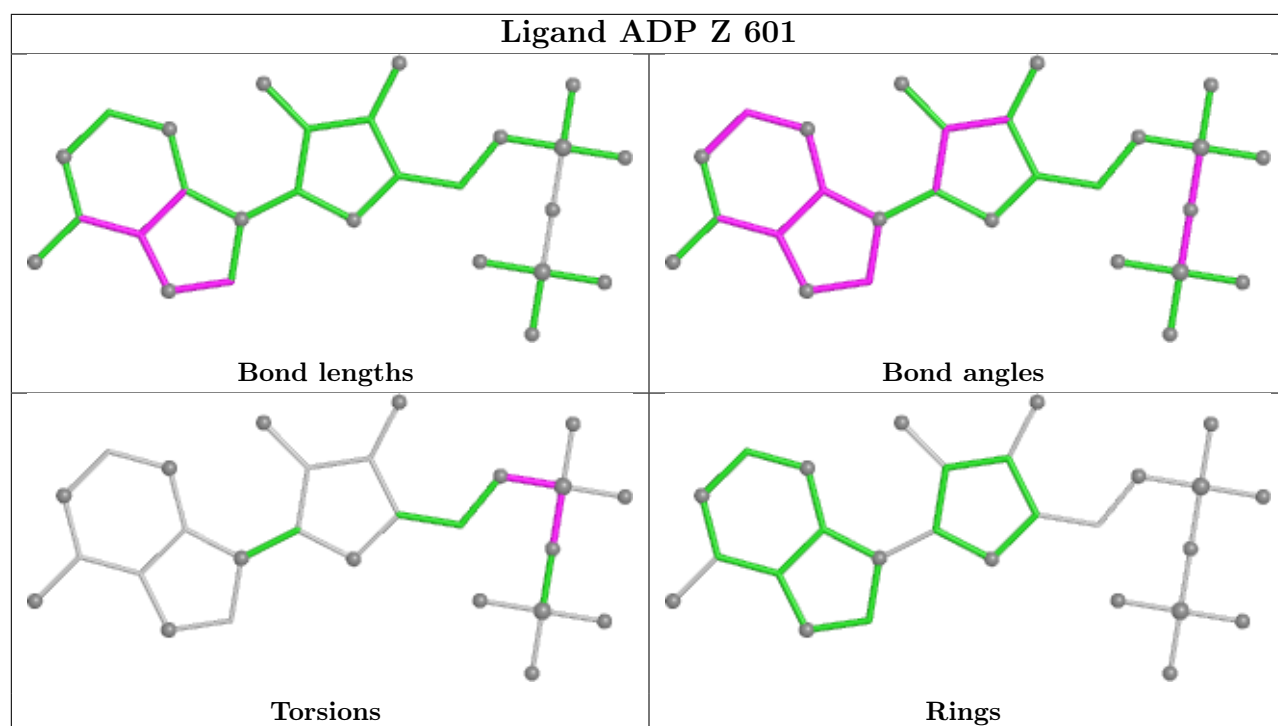


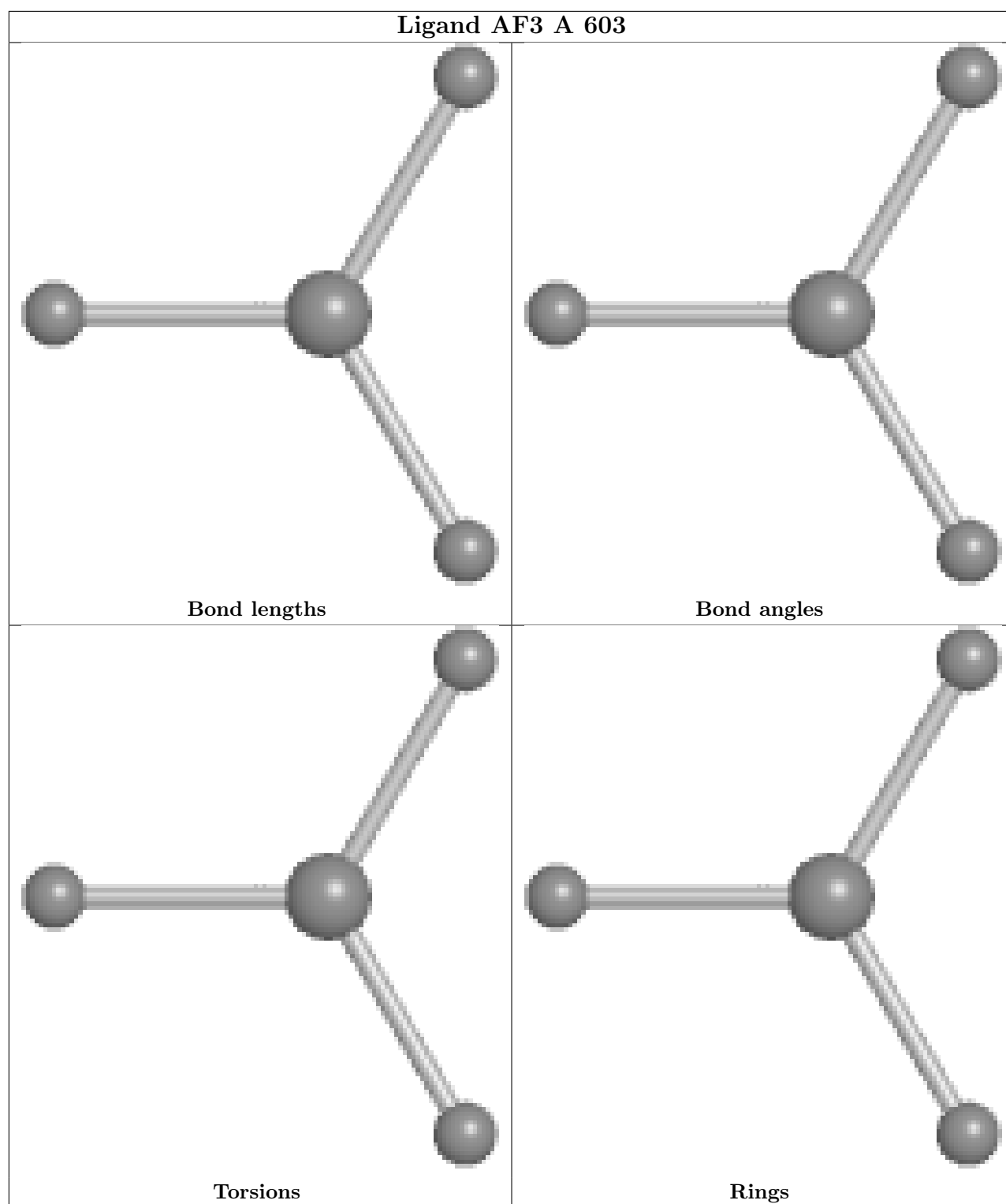


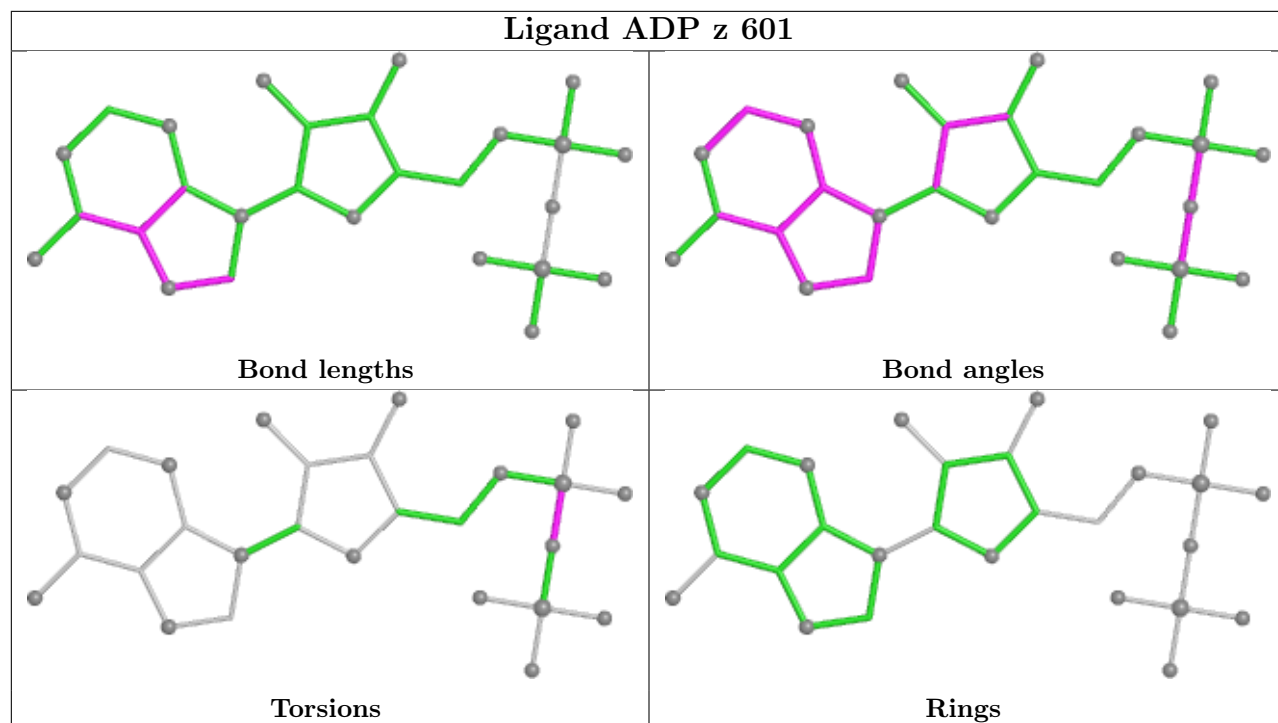


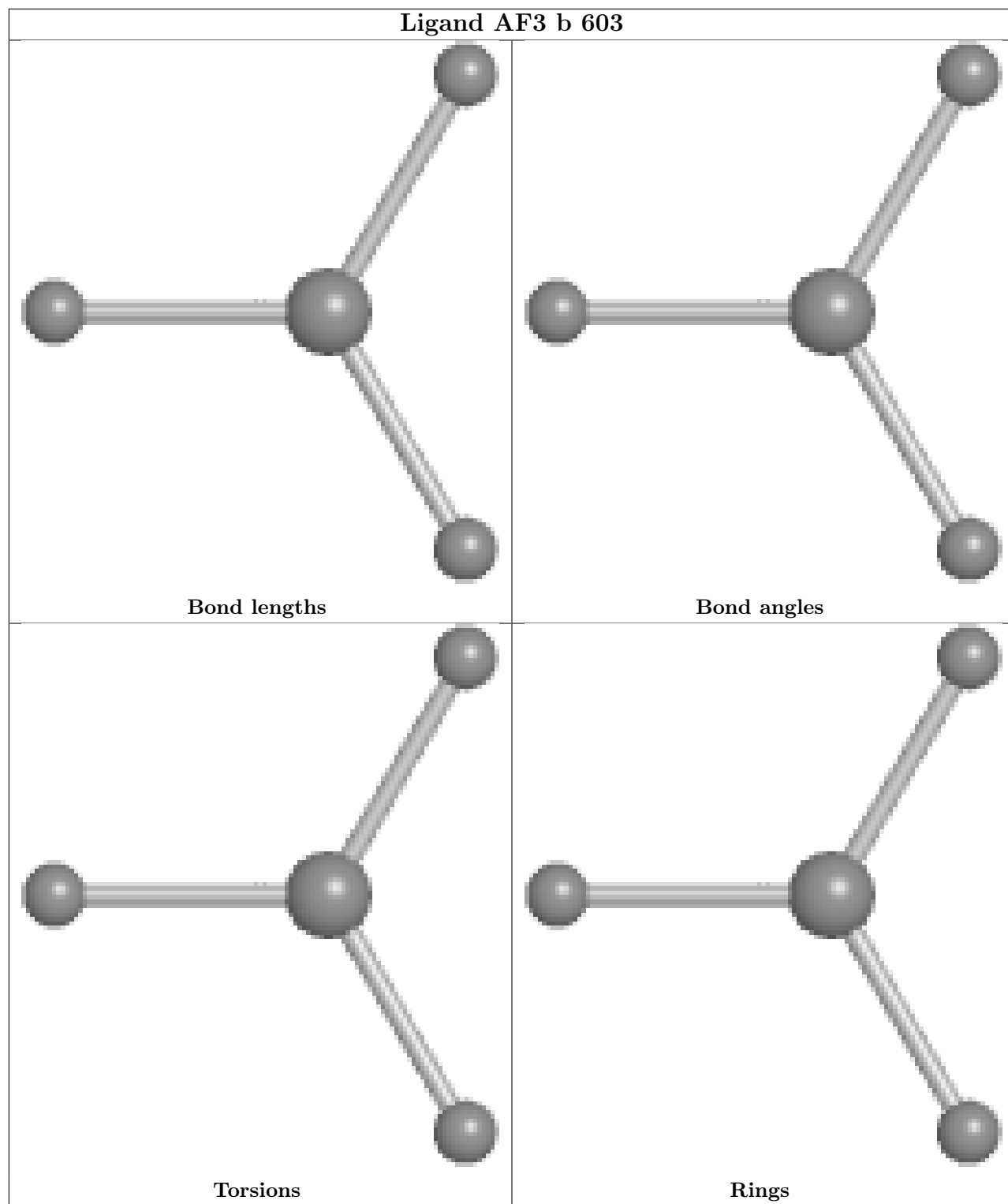


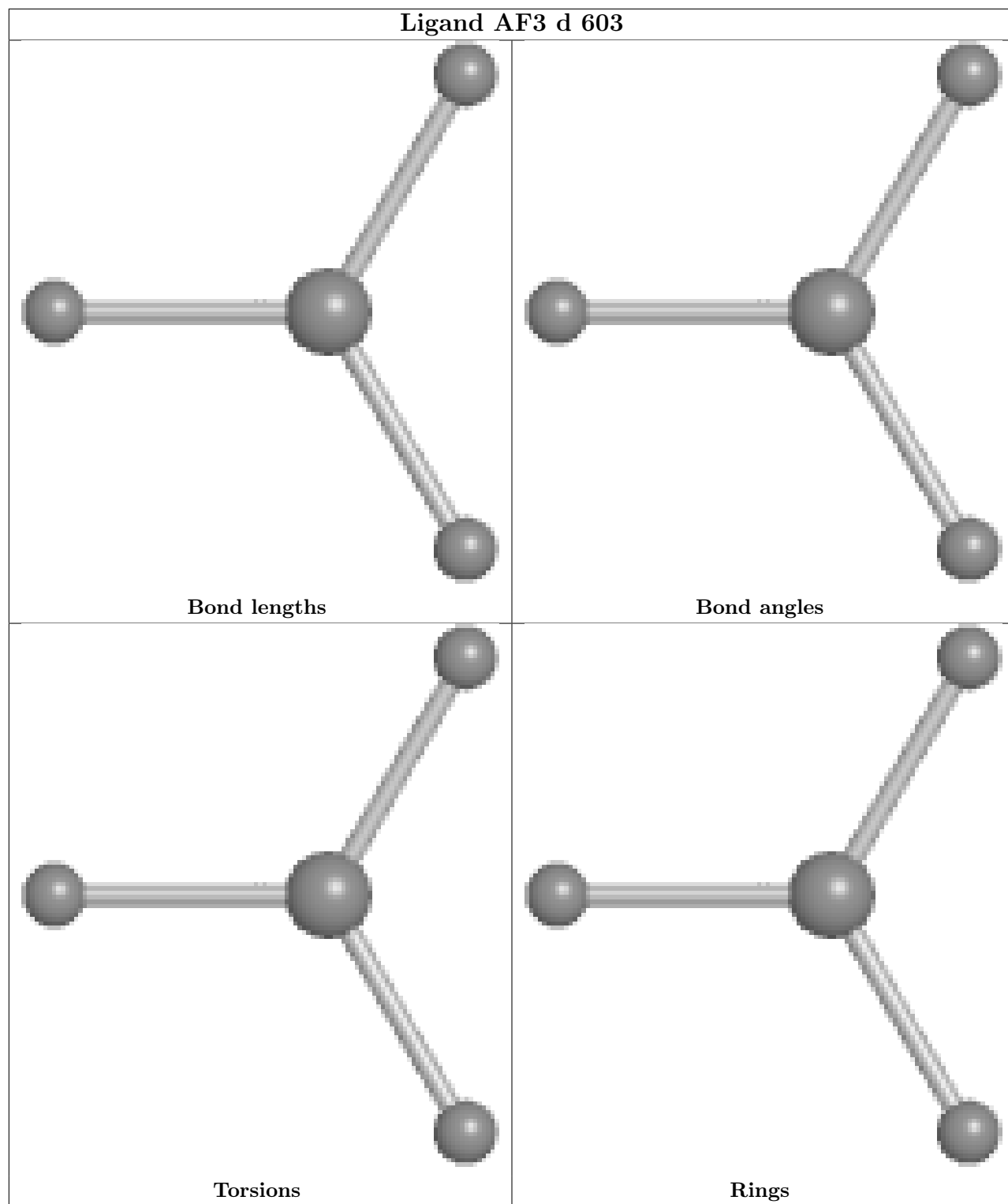


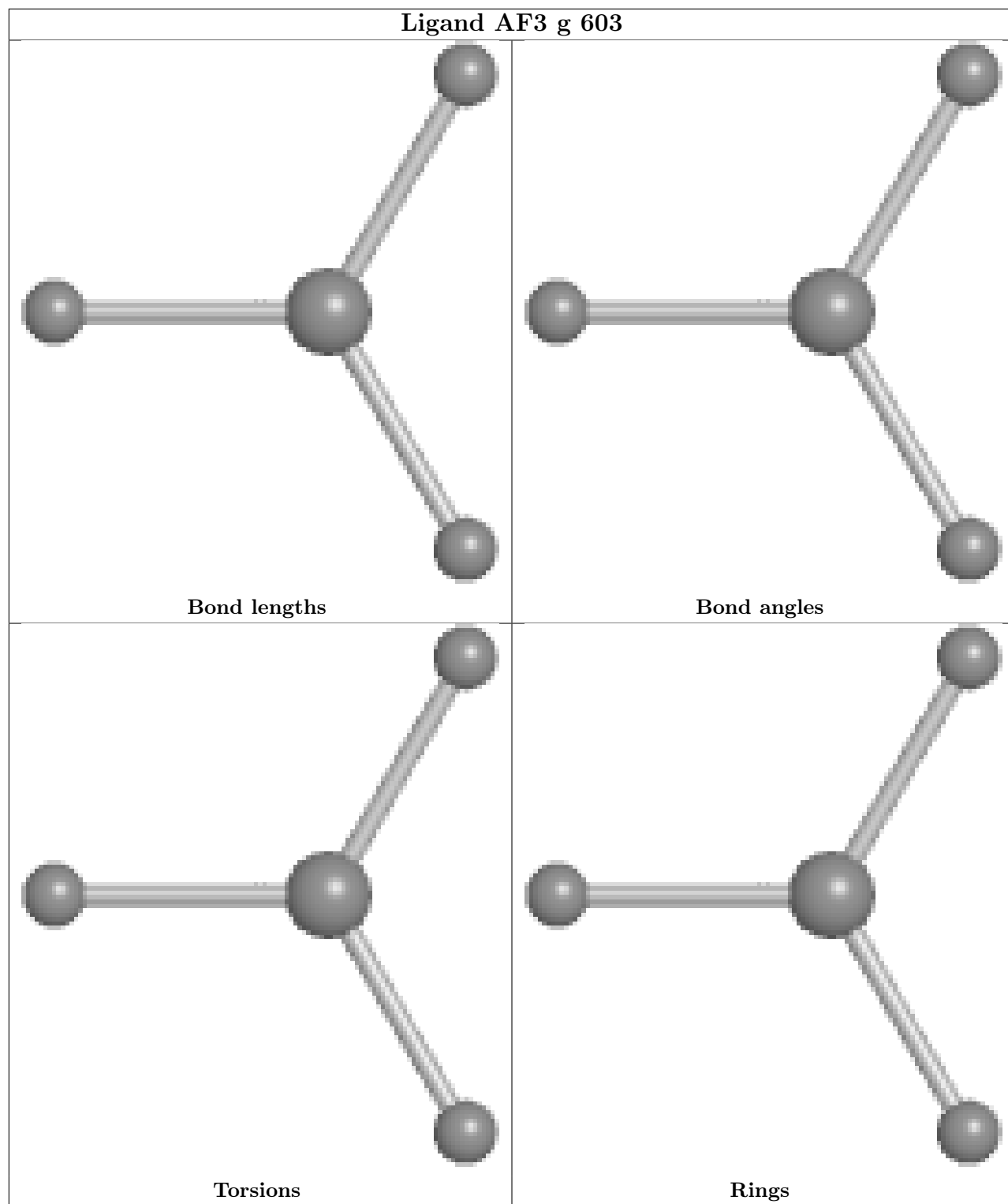


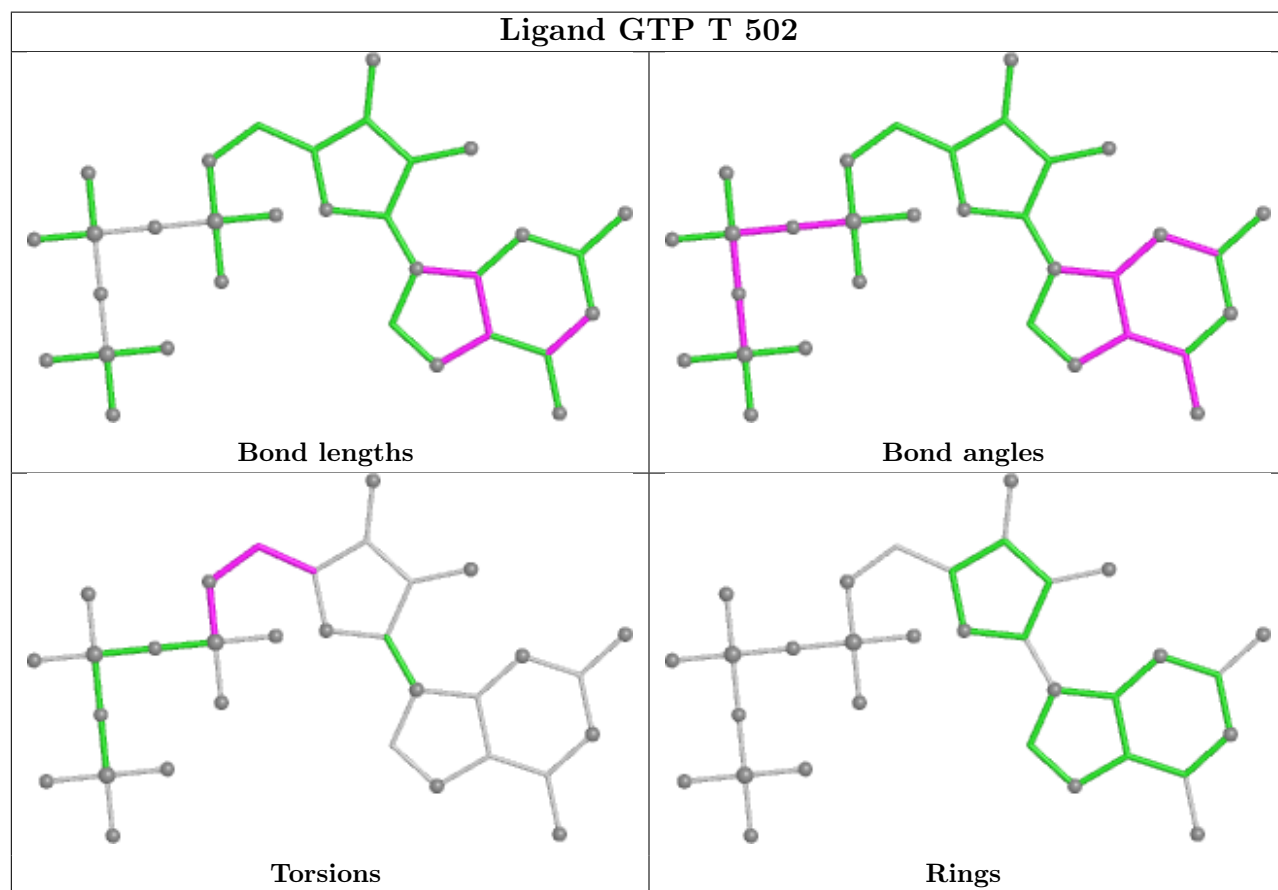
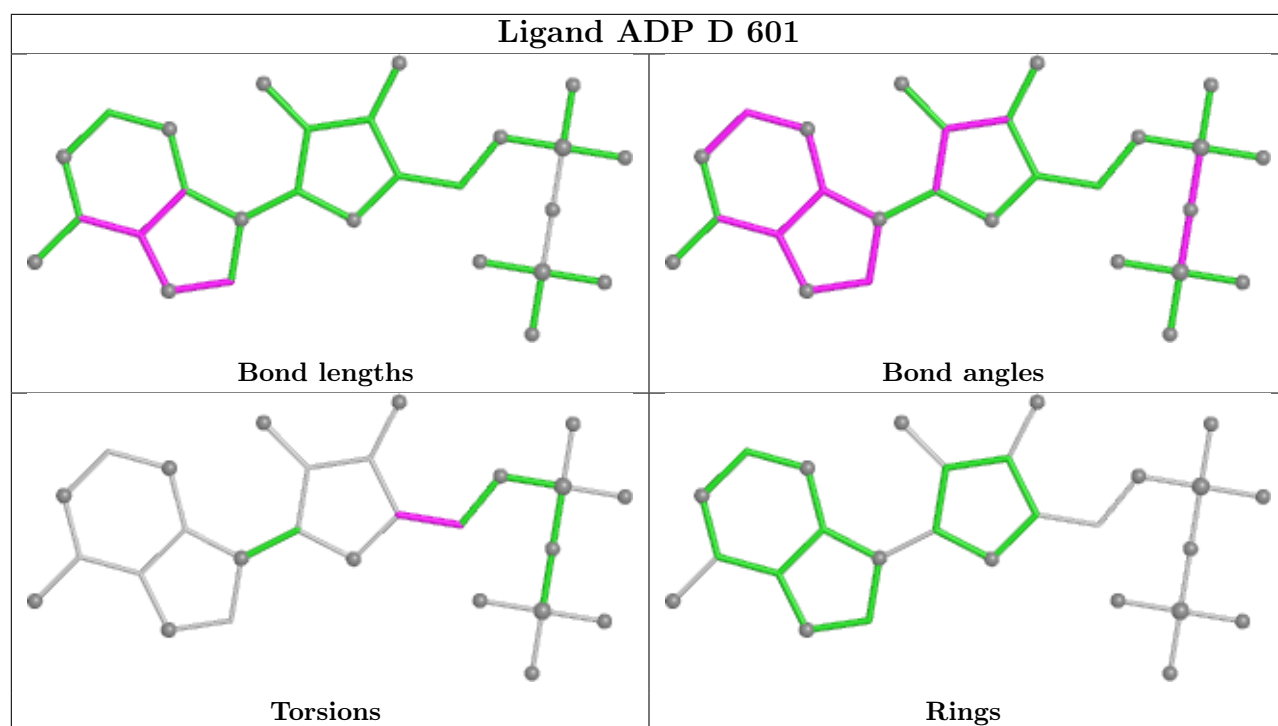


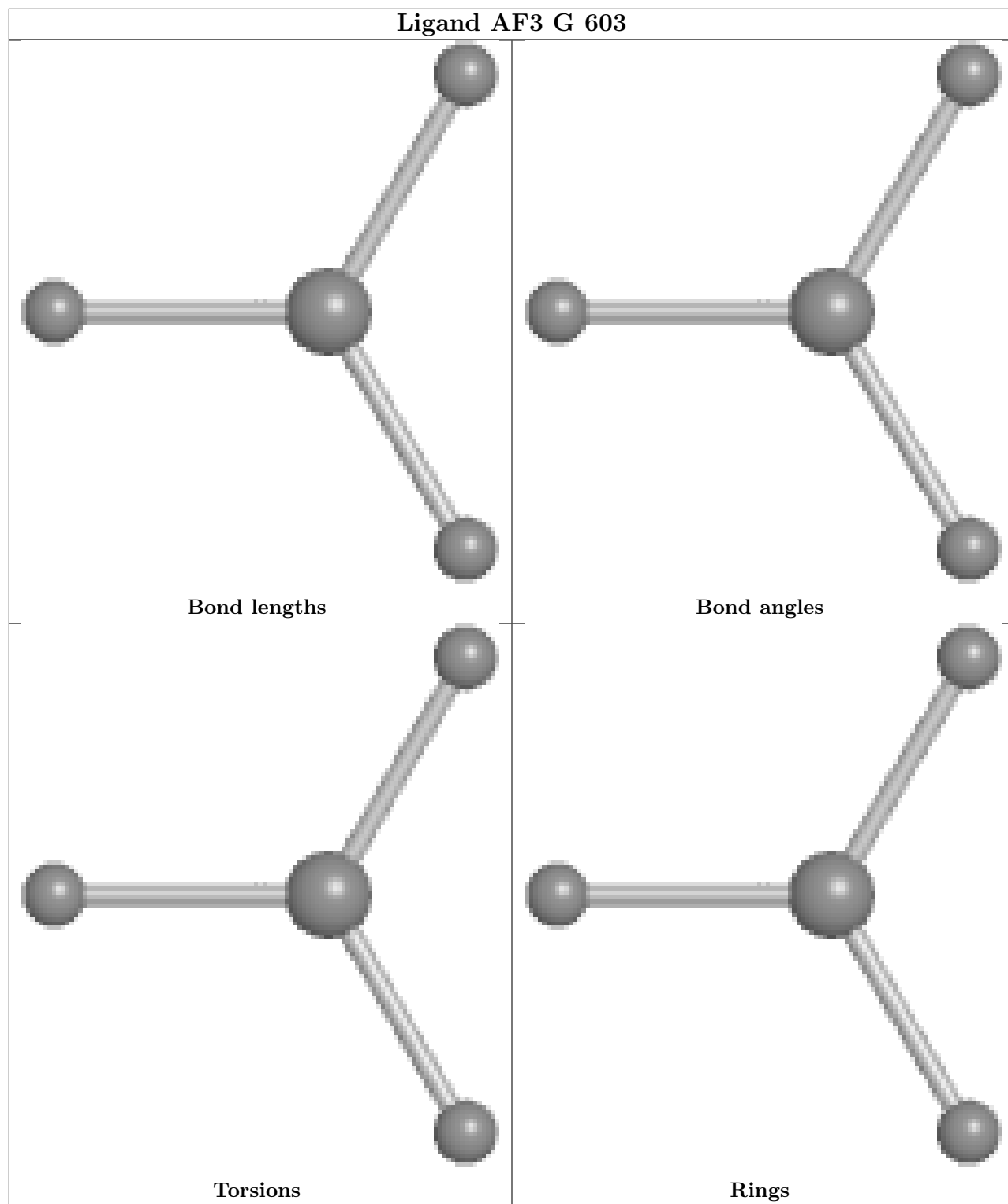


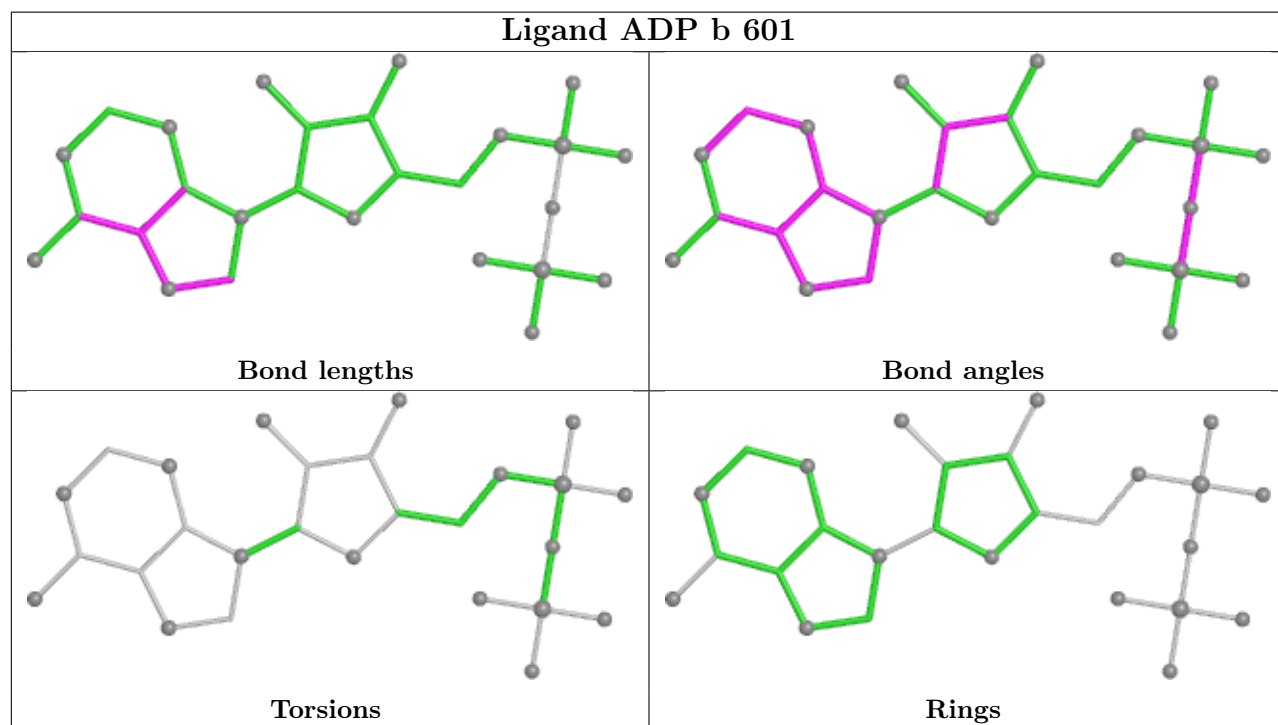
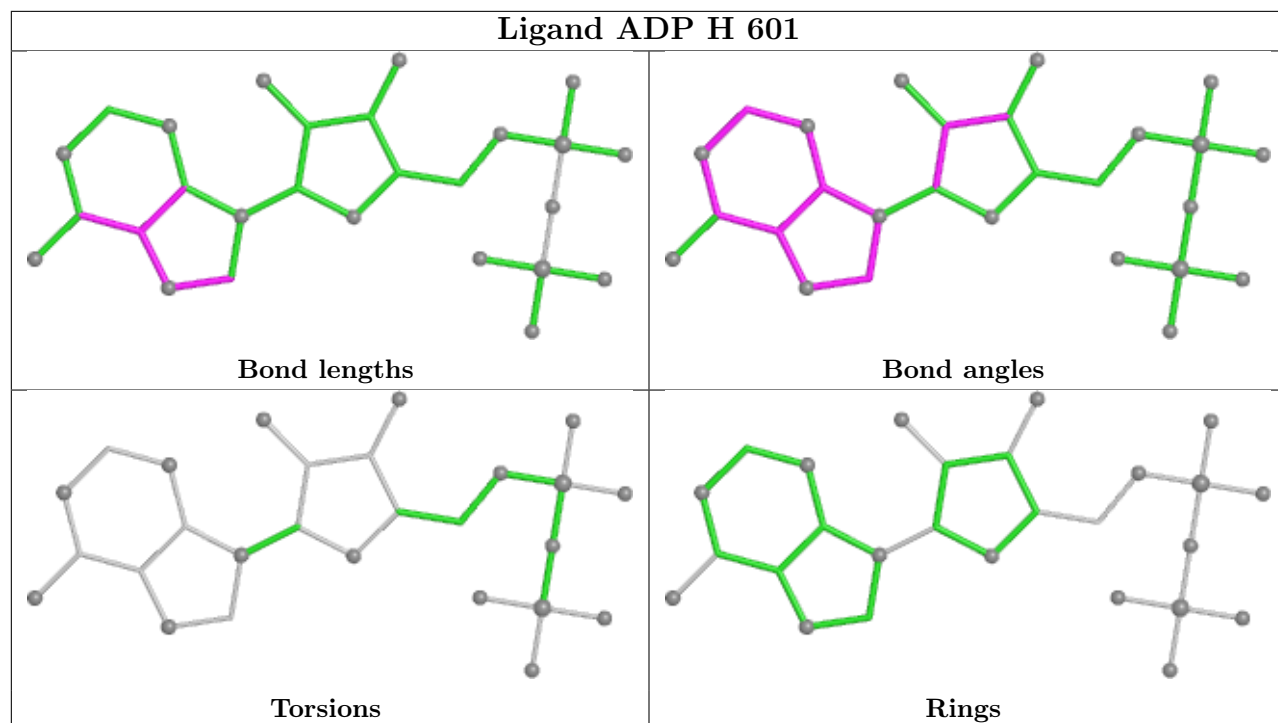


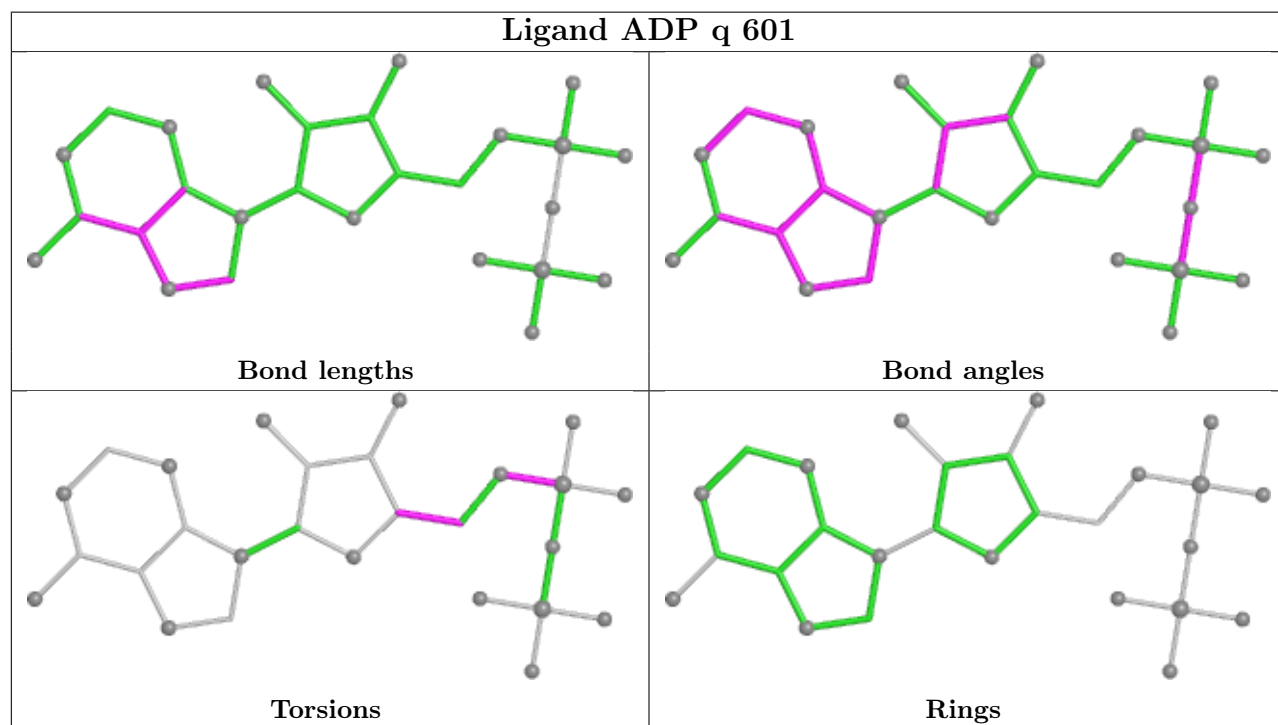
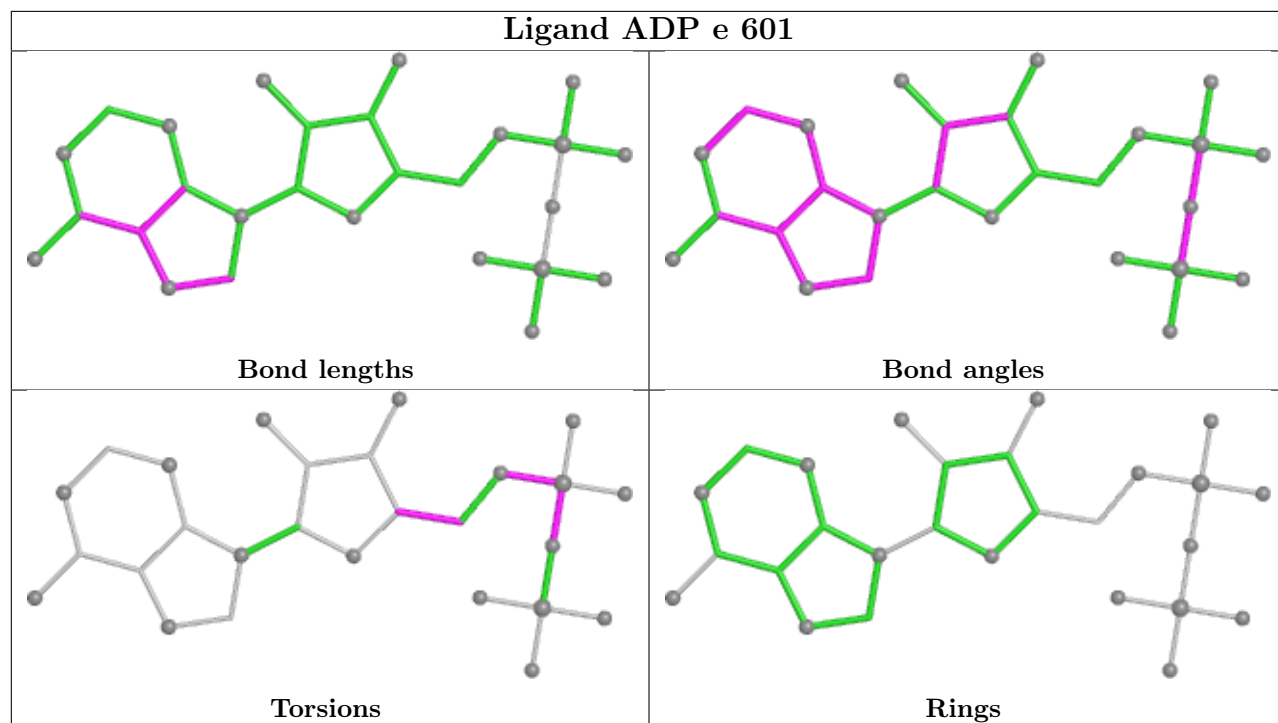


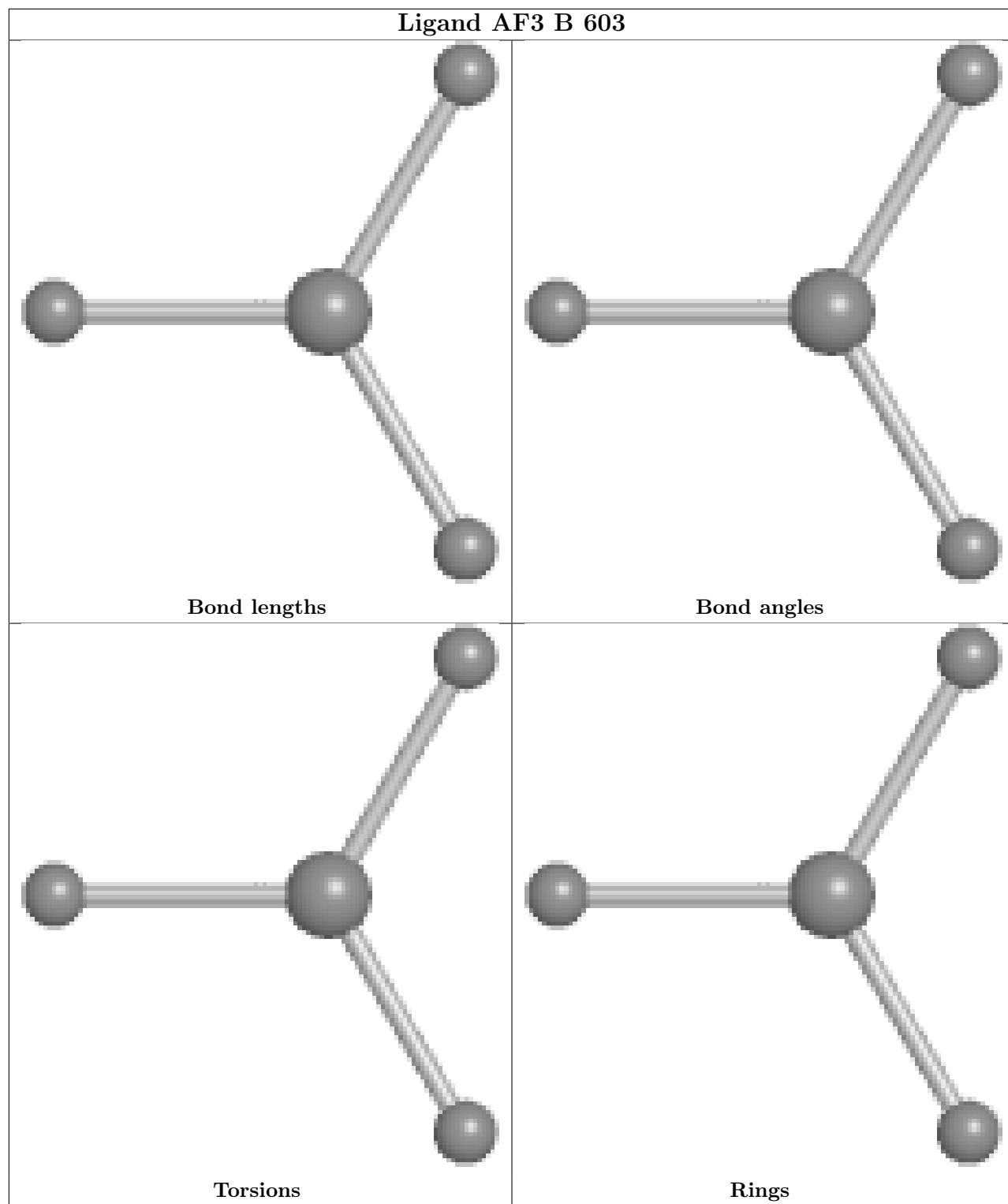


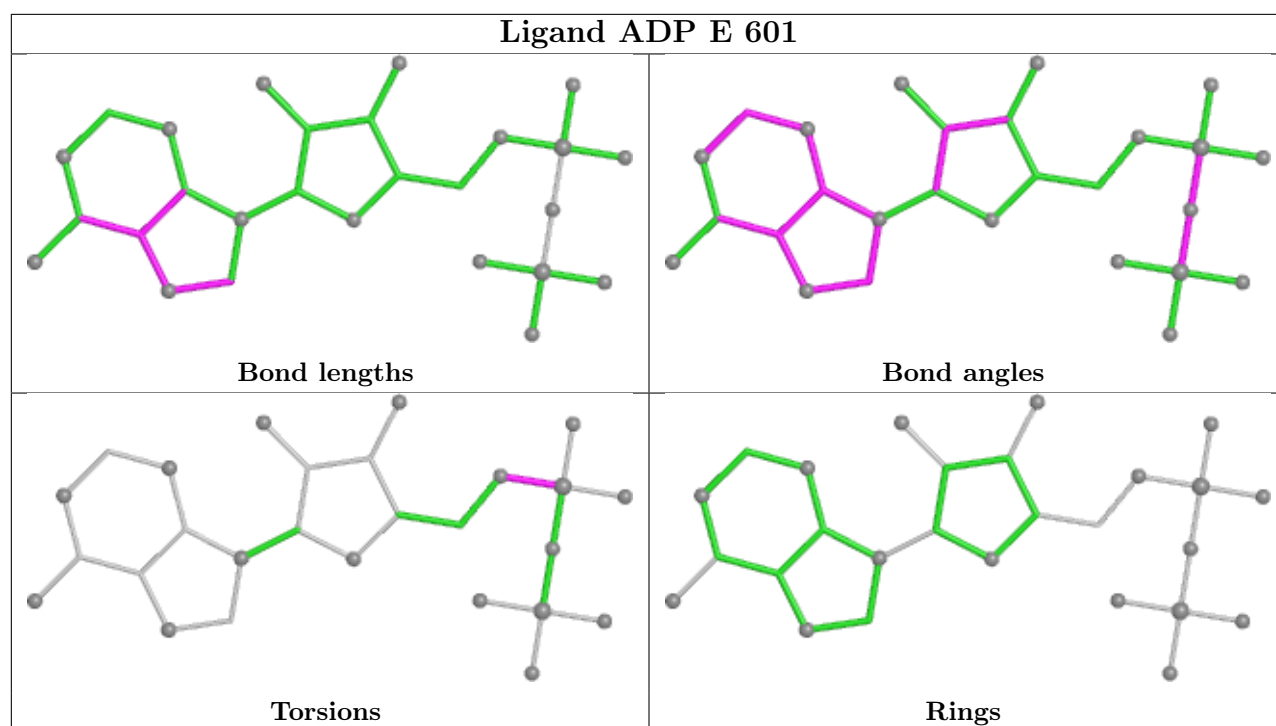












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

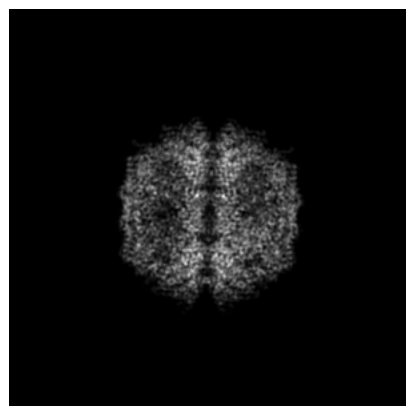
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33919. These allow visual inspection of the internal detail of the map and identification of artifacts.

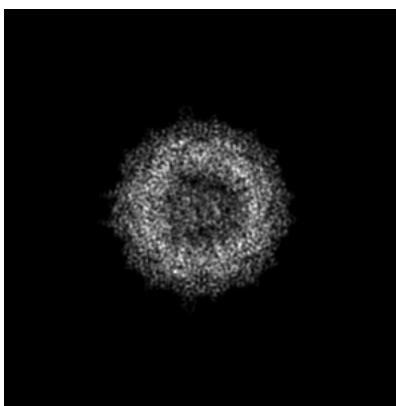
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

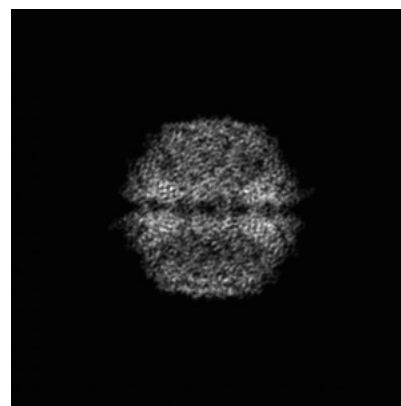
6.1.1 Primary map



X

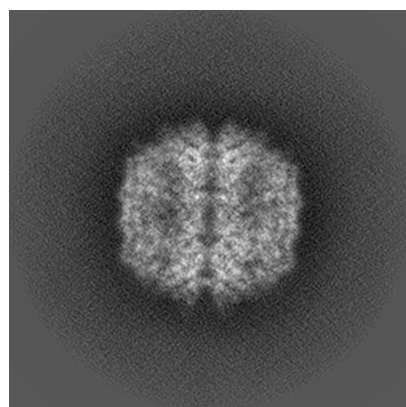


Y

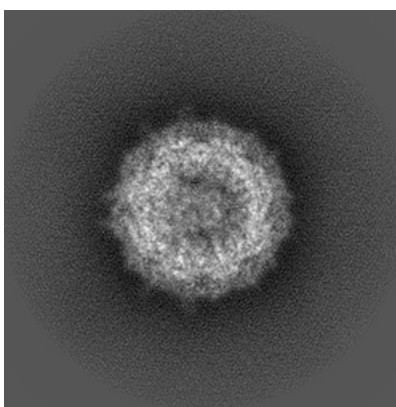


Z

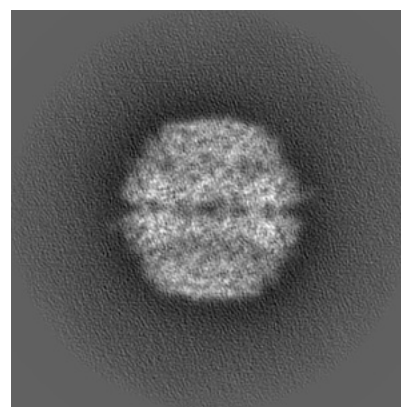
6.1.2 Raw map



X



Y

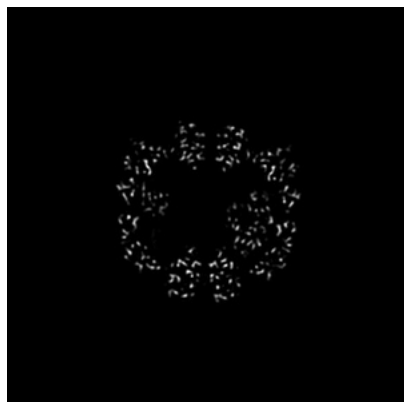


Z

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

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 128

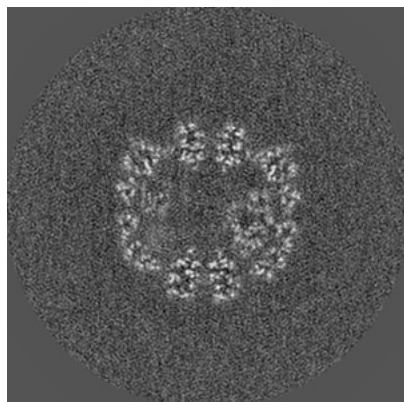


Y Index: 128

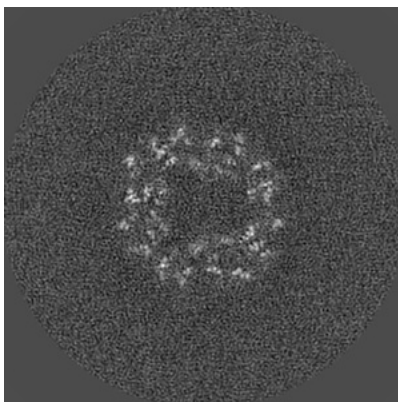


Z Index: 128

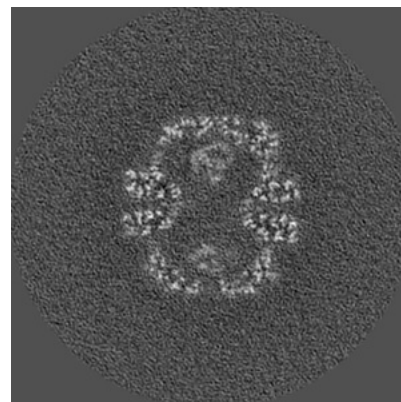
6.2.2 Raw map



X Index: 128



Y Index: 128

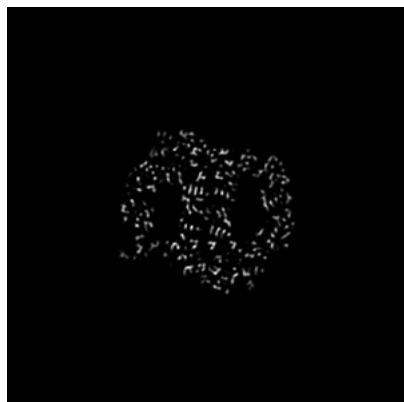


Z Index: 128

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

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 154

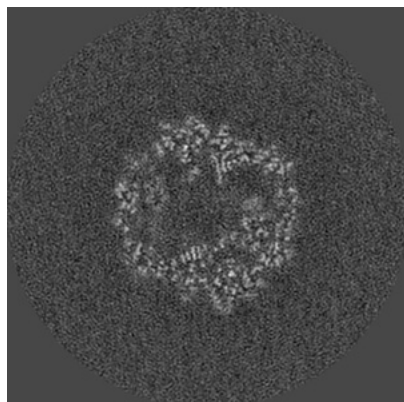


Y Index: 118

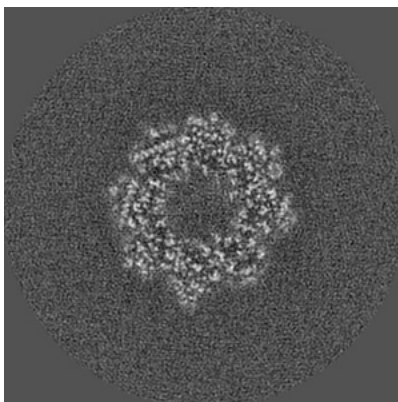


Z Index: 101

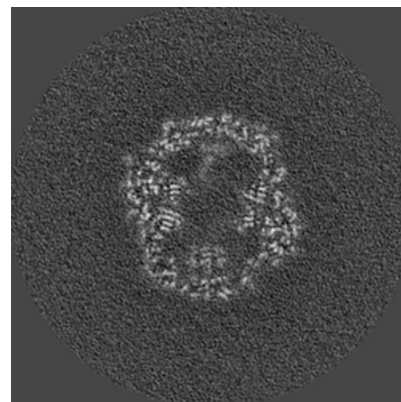
6.3.2 Raw map



X Index: 118



Y Index: 118

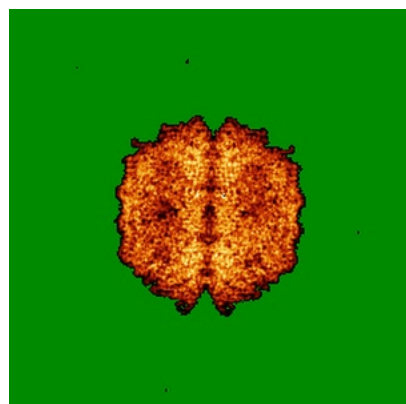


Z Index: 137

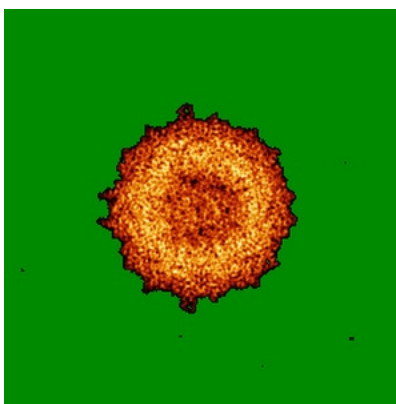
The images above show the largest variance slices of the map in three orthogonal directions.

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

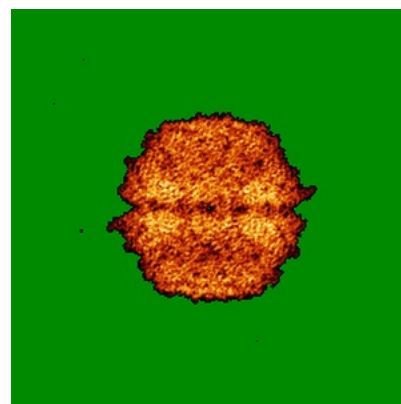
6.4.1 Primary map



X

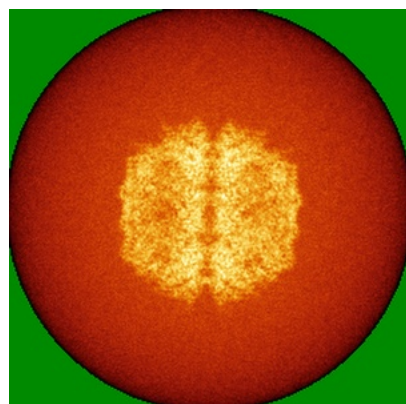


Y

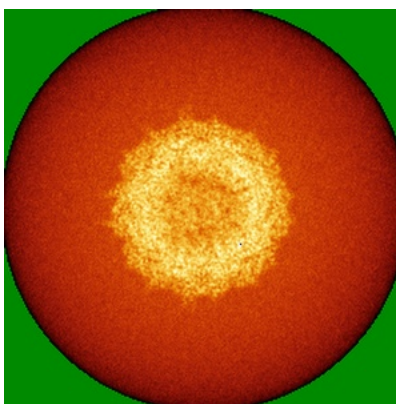


Z

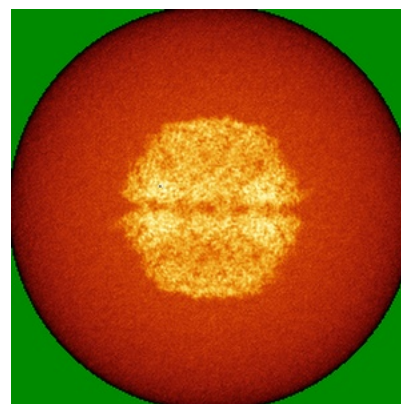
6.4.2 Raw map



X



Y

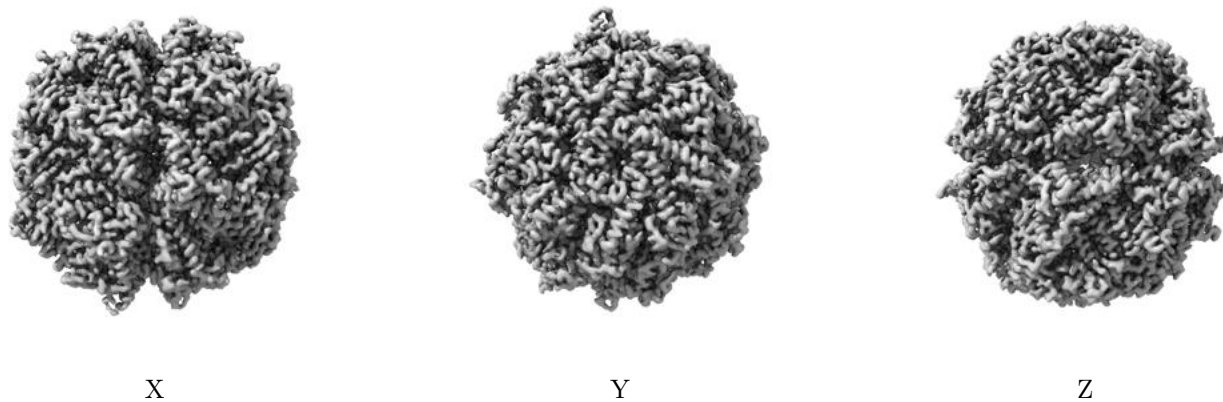


Z

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.

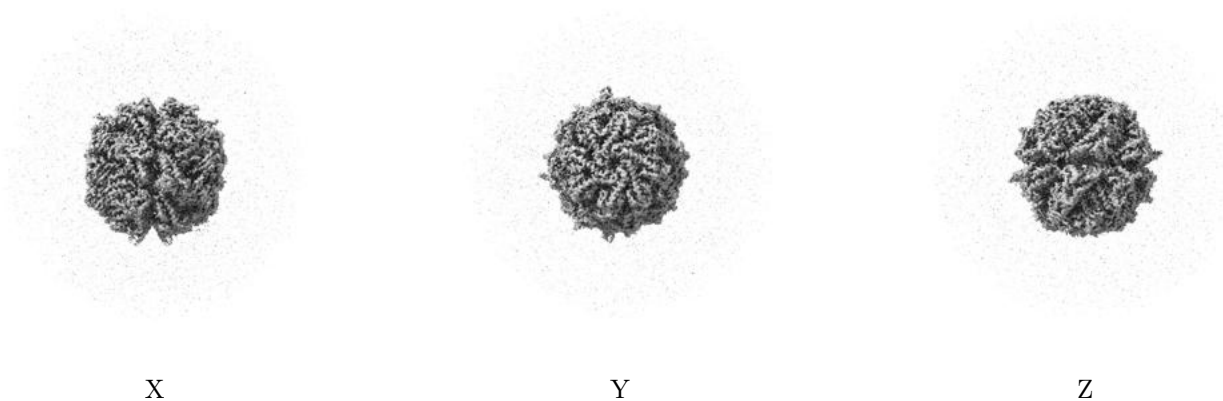
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

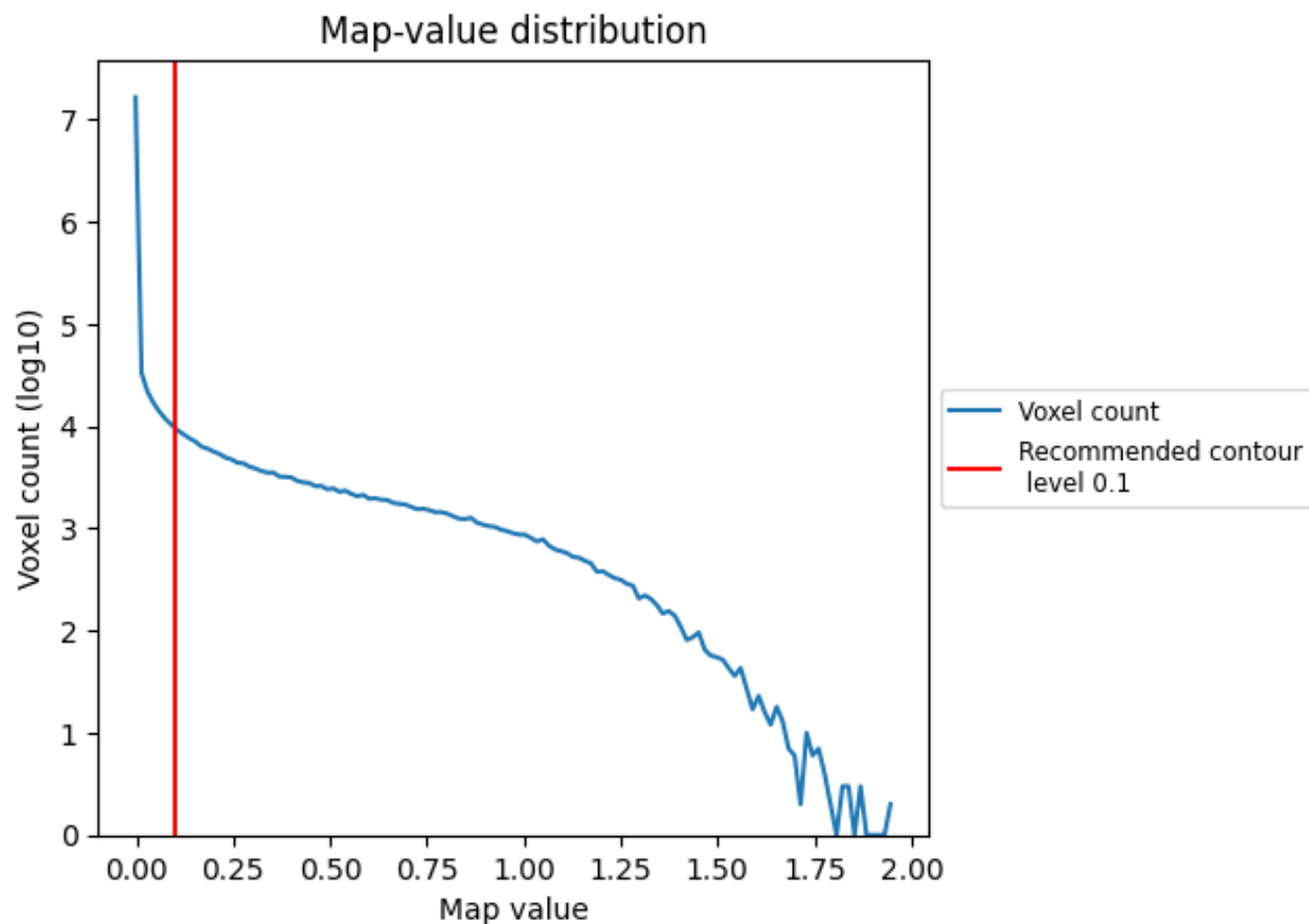
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

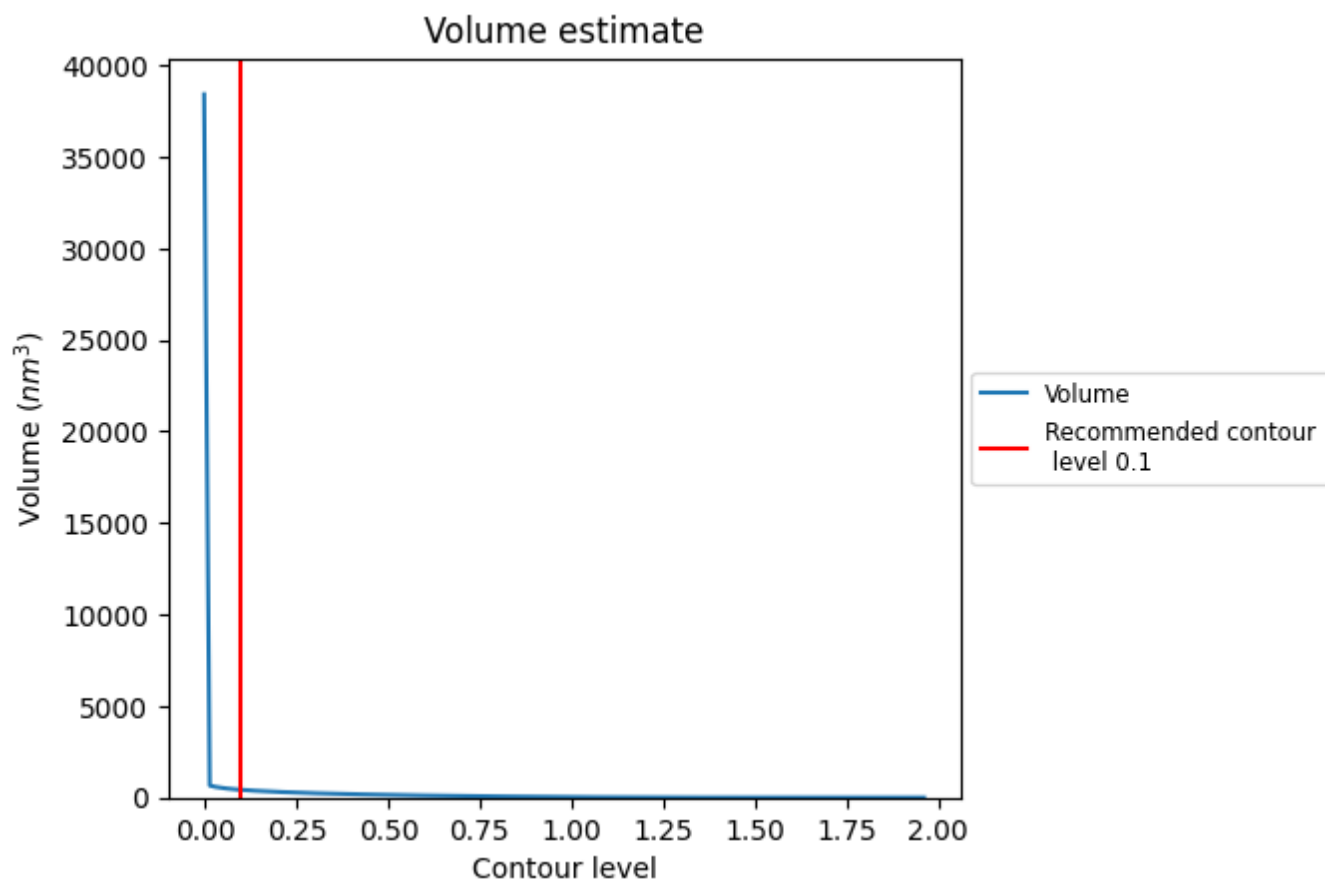
This section contains the results of statistical analysis of the map.

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.

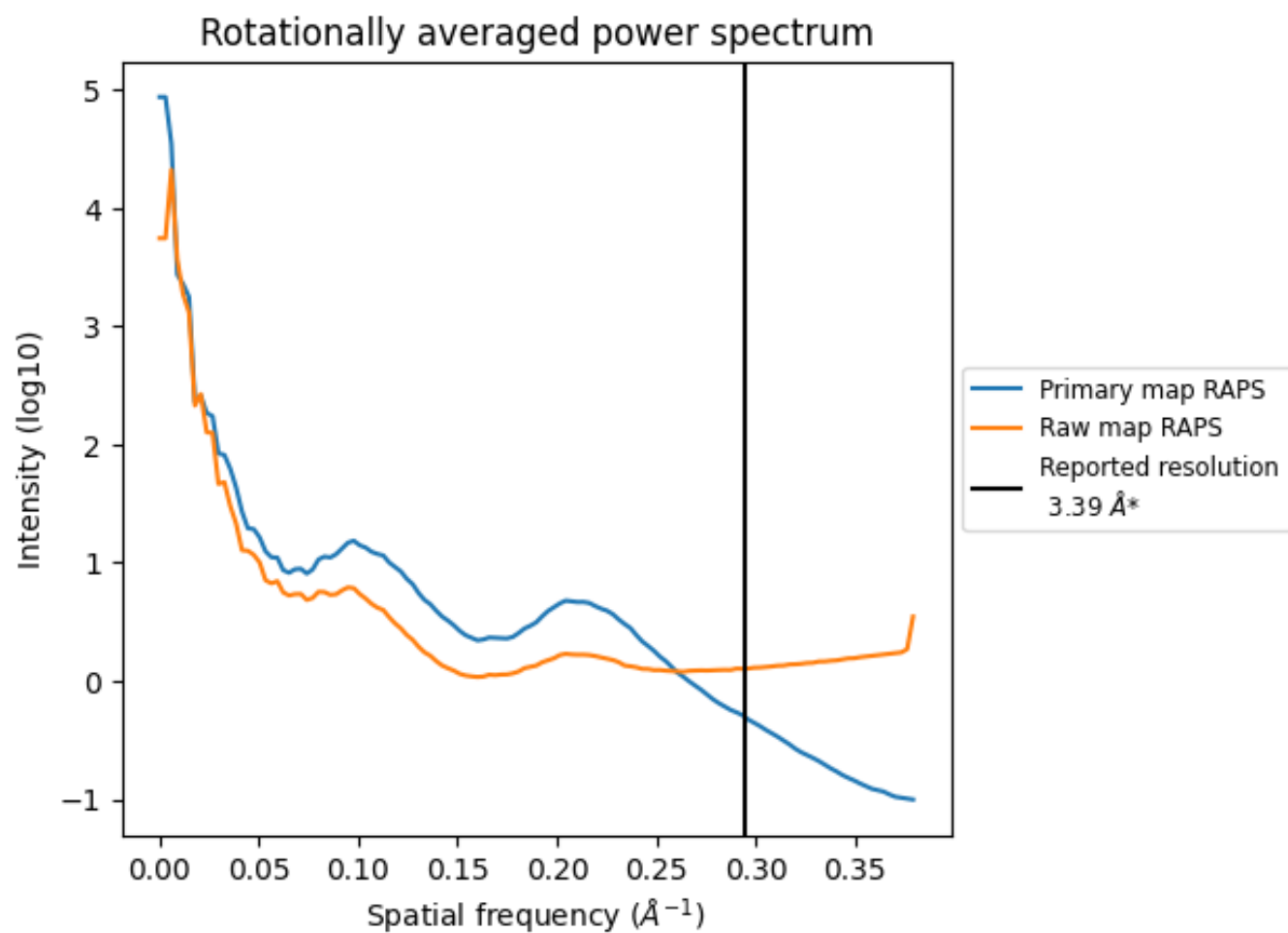
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 422 nm^3 ; this corresponds to an approximate mass of 381 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 ⓘ

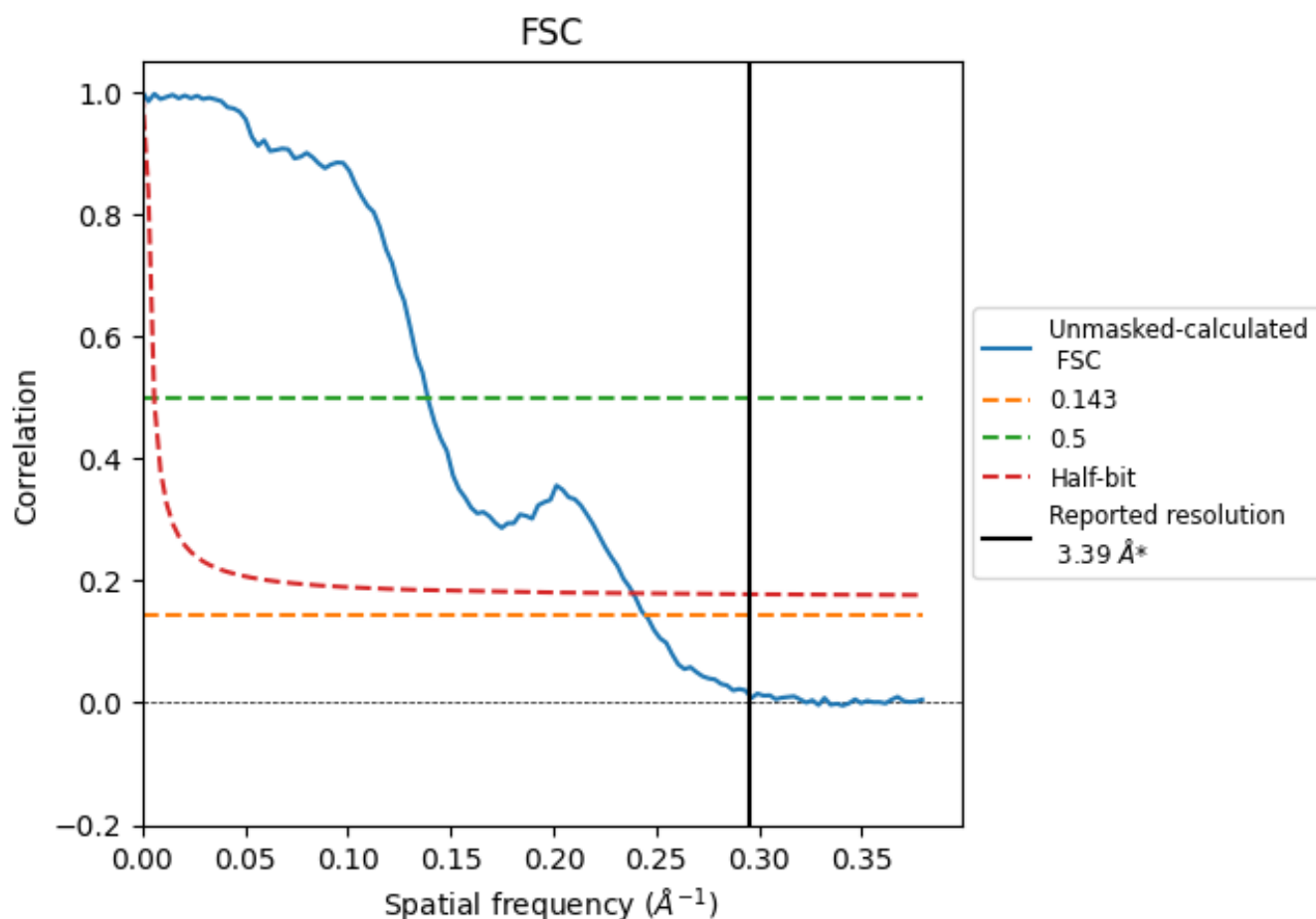


*Reported resolution corresponds to spatial frequency of 0.295 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.295 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

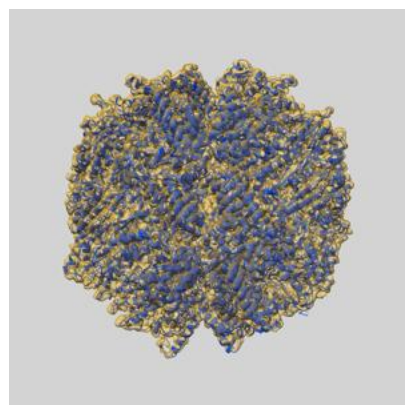
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.39	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.09	7.20	4.19

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.09 differs from the reported value 3.39 by more than 10 %

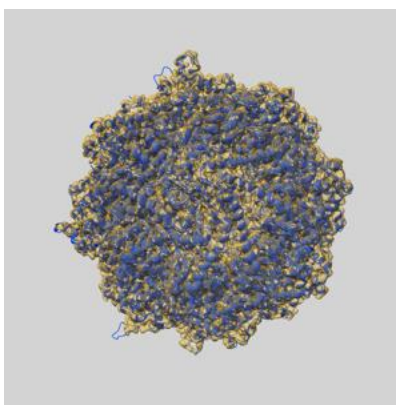
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-33919 and PDB model 7YLW. Per-residue inclusion information can be found in section [3](#) on page [14](#).

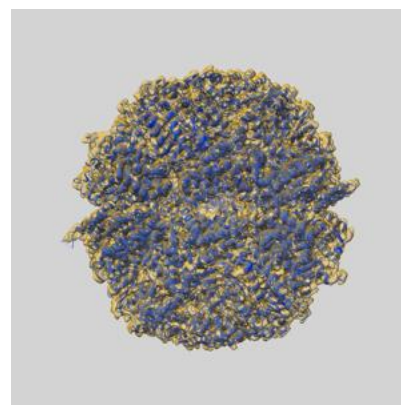
9.1 Map-model overlay [i](#)



X



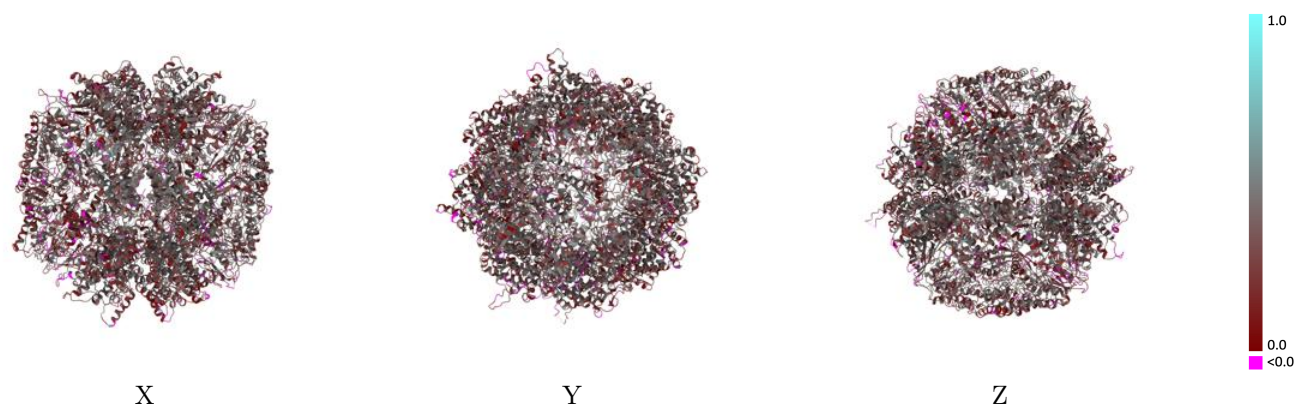
Y



Z

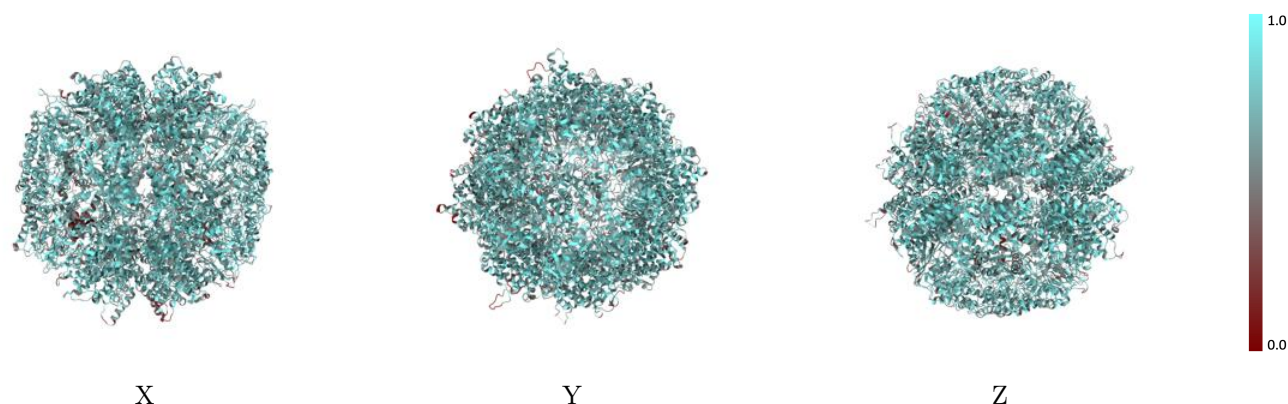
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



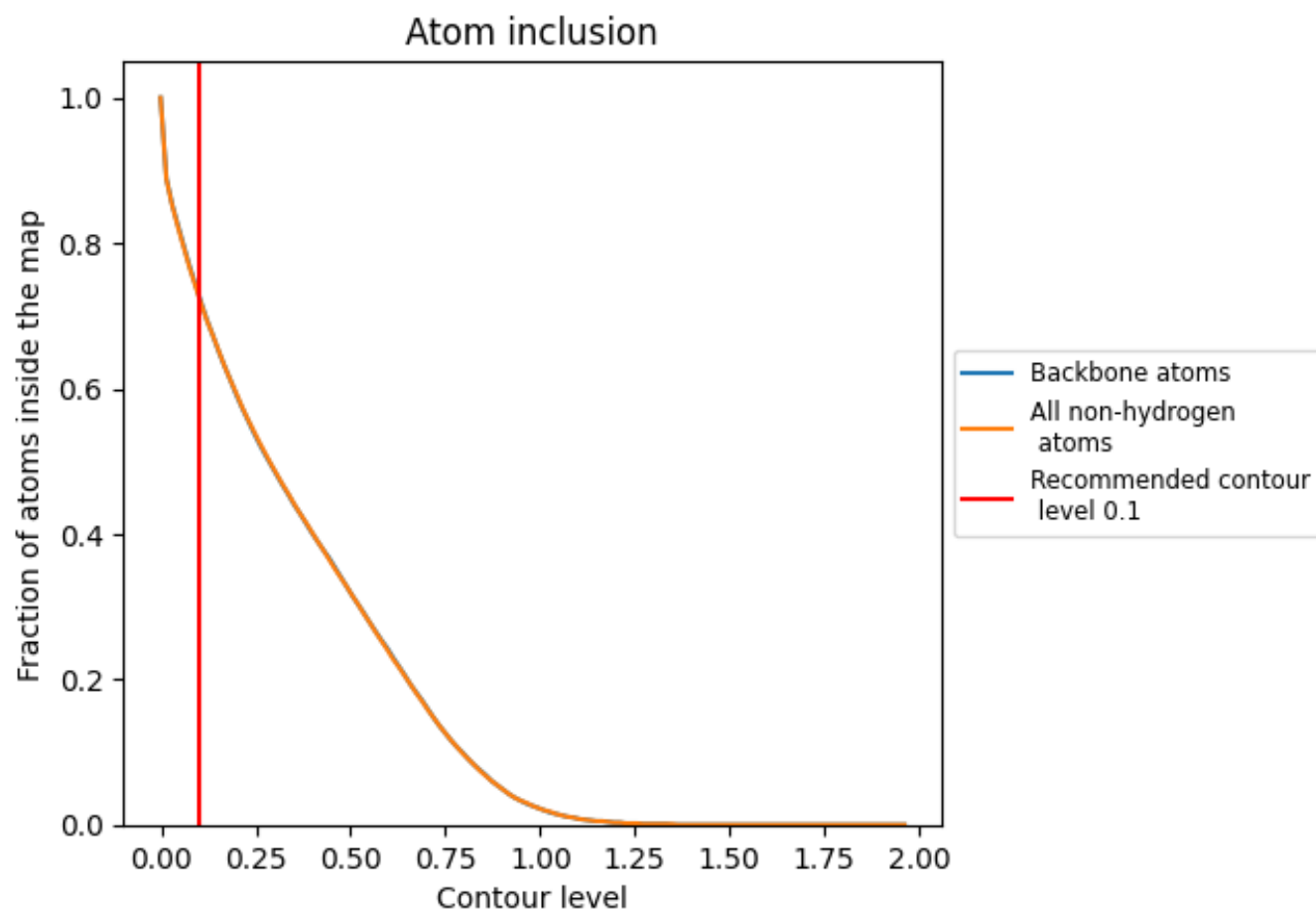
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 73% of all backbone atoms, 72% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7250	 0.3180
A	 0.7420	 0.3260
B	 0.7600	 0.3490
D	 0.7330	 0.3090
E	 0.7310	 0.3080
G	 0.7200	 0.3020
H	 0.7470	 0.3250
Q	 0.7270	 0.3210
T	 0.7380	 0.3590
Z	 0.7320	 0.3190
a	 0.7310	 0.3210
b	 0.7610	 0.3370
d	 0.7440	 0.3210
e	 0.7340	 0.3030
g	 0.7380	 0.3000
h	 0.7670	 0.3460
p	 0.4640	 0.2140
q	 0.7030	 0.2730
z	 0.7440	 0.3330

