



wwPDB EM Validation Summary Report ⓘ

Sep 14, 2026 – 02:33 PM EDT

PDB ID : 12AH / pdb_000012ah
EMDB ID : EMD-76263
Title : Cryo-EM structure of Nitrogenase MoFe protein from Methanosarcina acetivorans bound to the NifI inhibitor complex in C3 symmetry
Authors : Kashyap, R.; Antony, E.
Deposited on : 2026-03-23
Resolution : 2.97 Å(reported)
Based on initial model : 9P1X

This is a wwPDB EM Validation Summary 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:

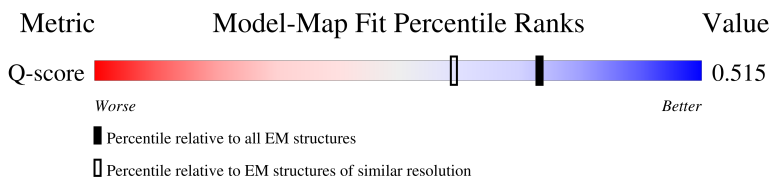
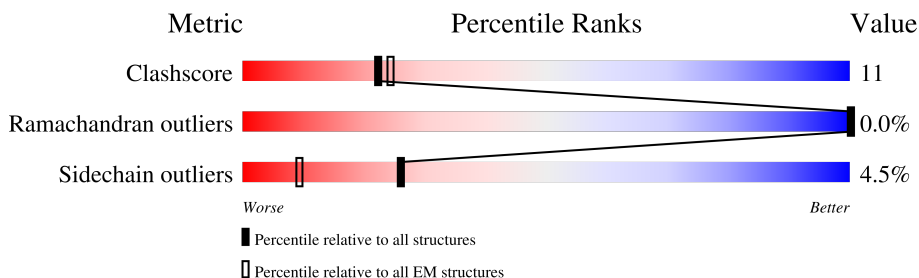
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance

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

The reported resolution of this entry is 2.97 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.



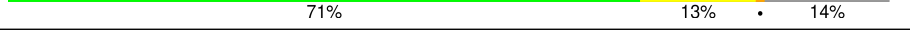
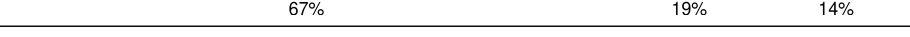
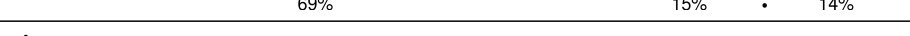
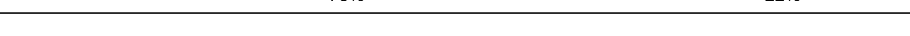
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13205 (2.47 - 3.47)

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	B	456	 77% 22% .
1	D	456	 76% 23% .
1	M	456	 77% 22% .
1	N	456	 74% 25% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	W	456	
1	X	456	
2	e	559	
2	f	559	
2	k	559	
2	l	559	
2	p	559	
2	q	559	
3	F	105	
3	H	105	
3	P	105	
3	T	105	
3	Z	105	
3	b	105	
3	i	105	
3	j	105	
3	n	105	
3	o	105	
3	s	105	
3	t	105	
4	Q	125	
4	a	125	
4	g	125	
4	h	125	
4	m	125	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	r	125	

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
5	CLF	N	501	-	-	X	-
5	CLF	W	601	-	-	X	-
5	CLF	e	601	-	-	X	-
5	CLF	f	601	-	-	X	-
5	CLF	q	601	-	-	X	-
6	ICS	e	602	-	-	X	-
6	ICS	f	602	-	-	X	-
6	ICS	k	602	-	-	X	-
6	ICS	l	601	-	-	X	-
6	ICS	p	602	-	-	X	-
6	ICS	q	603	-	-	X	-
7	HCA	l	602	-	-	X	-
8	ADP	a	200	-	-	X	-
8	ADP	j	201	-	-	X	-
8	ADP	m	201	-	-	X	-
8	ADP	n	201	-	-	X	-
8	ADP	s	201	-	-	X	-
8	ADP	t	201	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 60855 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 Nitrogenase molybdenum-iron protein beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	456	Total	C	N	O	S	1	0
			3474	2202	585	665	22		
1	D	456	Total	C	N	O	S	0	0
			3467	2197	583	665	22		
1	M	456	Total	C	N	O	S	0	0
			3467	2197	583	665	22		
1	N	456	Total	C	N	O	S	0	0
			3467	2197	583	665	22		
1	W	456	Total	C	N	O	S	0	0
			3467	2197	583	665	22		
1	X	456	Total	C	N	O	S	1	0
			3477	2203	586	666	22		

- Molecule 2 is a protein called Nitrogenase protein alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	e	525	Total	C	N	O	S	0	0
			4181	2655	720	785	21		
2	q	527	Total	C	N	O	S	0	0
			4190	2660	722	787	21		
2	f	524	Total	C	N	O	S	0	0
			4171	2648	718	784	21		
2	k	525	Total	C	N	O	S	0	0
			4181	2655	720	785	21		
2	l	520	Total	C	N	O	S	0	0
			4141	2629	714	777	21		
2	p	521	Total	C	N	O	S	0	0
			4145	2631	714	780	20		

There are 186 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
e	-30	MET	-	initiating methionine	UNP Q8TJ90
e	-29	TRP	-	expression tag	UNP Q8TJ90

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
e	-28	SER	-	expression tag	UNP Q8TJ90
e	-27	HIS	-	expression tag	UNP Q8TJ90
e	-26	PRO	-	expression tag	UNP Q8TJ90
e	-25	GLN	-	expression tag	UNP Q8TJ90
e	-24	PHE	-	expression tag	UNP Q8TJ90
e	-23	GLU	-	expression tag	UNP Q8TJ90
e	-22	LYS	-	expression tag	UNP Q8TJ90
e	-21	GLY	-	expression tag	UNP Q8TJ90
e	-20	GLY	-	expression tag	UNP Q8TJ90
e	-19	GLY	-	expression tag	UNP Q8TJ90
e	-18	SER	-	expression tag	UNP Q8TJ90
e	-17	GLY	-	expression tag	UNP Q8TJ90
e	-16	GLY	-	expression tag	UNP Q8TJ90
e	-15	GLY	-	expression tag	UNP Q8TJ90
e	-14	SER	-	expression tag	UNP Q8TJ90
e	-13	GLY	-	expression tag	UNP Q8TJ90
e	-12	GLY	-	expression tag	UNP Q8TJ90
e	-11	GLY	-	expression tag	UNP Q8TJ90
e	-10	SER	-	expression tag	UNP Q8TJ90
e	-9	TRP	-	expression tag	UNP Q8TJ90
e	-8	SER	-	expression tag	UNP Q8TJ90
e	-7	HIS	-	expression tag	UNP Q8TJ90
e	-6	PRO	-	expression tag	UNP Q8TJ90
e	-5	GLN	-	expression tag	UNP Q8TJ90
e	-4	PHE	-	expression tag	UNP Q8TJ90
e	-3	GLU	-	expression tag	UNP Q8TJ90
e	-2	LYS	-	expression tag	UNP Q8TJ90
e	-1	SER	-	expression tag	UNP Q8TJ90
e	0	GLY	-	expression tag	UNP Q8TJ90
q	-30	MET	-	initiating methionine	UNP Q8TJ90
q	-29	TRP	-	expression tag	UNP Q8TJ90
q	-28	SER	-	expression tag	UNP Q8TJ90
q	-27	HIS	-	expression tag	UNP Q8TJ90
q	-26	PRO	-	expression tag	UNP Q8TJ90
q	-25	GLN	-	expression tag	UNP Q8TJ90
q	-24	PHE	-	expression tag	UNP Q8TJ90
q	-23	GLU	-	expression tag	UNP Q8TJ90
q	-22	LYS	-	expression tag	UNP Q8TJ90
q	-21	GLY	-	expression tag	UNP Q8TJ90
q	-20	GLY	-	expression tag	UNP Q8TJ90
q	-19	GLY	-	expression tag	UNP Q8TJ90
q	-18	SER	-	expression tag	UNP Q8TJ90

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
q	-17	GLY	-	expression tag	UNP Q8TJ90
q	-16	GLY	-	expression tag	UNP Q8TJ90
q	-15	GLY	-	expression tag	UNP Q8TJ90
q	-14	SER	-	expression tag	UNP Q8TJ90
q	-13	GLY	-	expression tag	UNP Q8TJ90
q	-12	GLY	-	expression tag	UNP Q8TJ90
q	-11	GLY	-	expression tag	UNP Q8TJ90
q	-10	SER	-	expression tag	UNP Q8TJ90
q	-9	TRP	-	expression tag	UNP Q8TJ90
q	-8	SER	-	expression tag	UNP Q8TJ90
q	-7	HIS	-	expression tag	UNP Q8TJ90
q	-6	PRO	-	expression tag	UNP Q8TJ90
q	-5	GLN	-	expression tag	UNP Q8TJ90
q	-4	PHE	-	expression tag	UNP Q8TJ90
q	-3	GLU	-	expression tag	UNP Q8TJ90
q	-2	LYS	-	expression tag	UNP Q8TJ90
q	-1	SER	-	expression tag	UNP Q8TJ90
q	0	GLY	-	expression tag	UNP Q8TJ90
f	-30	MET	-	initiating methionine	UNP Q8TJ90
f	-29	TRP	-	expression tag	UNP Q8TJ90
f	-28	SER	-	expression tag	UNP Q8TJ90
f	-27	HIS	-	expression tag	UNP Q8TJ90
f	-26	PRO	-	expression tag	UNP Q8TJ90
f	-25	GLN	-	expression tag	UNP Q8TJ90
f	-24	PHE	-	expression tag	UNP Q8TJ90
f	-23	GLU	-	expression tag	UNP Q8TJ90
f	-22	LYS	-	expression tag	UNP Q8TJ90
f	-21	GLY	-	expression tag	UNP Q8TJ90
f	-20	GLY	-	expression tag	UNP Q8TJ90
f	-19	GLY	-	expression tag	UNP Q8TJ90
f	-18	SER	-	expression tag	UNP Q8TJ90
f	-17	GLY	-	expression tag	UNP Q8TJ90
f	-16	GLY	-	expression tag	UNP Q8TJ90
f	-15	GLY	-	expression tag	UNP Q8TJ90
f	-14	SER	-	expression tag	UNP Q8TJ90
f	-13	GLY	-	expression tag	UNP Q8TJ90
f	-12	GLY	-	expression tag	UNP Q8TJ90
f	-11	GLY	-	expression tag	UNP Q8TJ90
f	-10	SER	-	expression tag	UNP Q8TJ90
f	-9	TRP	-	expression tag	UNP Q8TJ90
f	-8	SER	-	expression tag	UNP Q8TJ90
f	-7	HIS	-	expression tag	UNP Q8TJ90

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
f	-6	PRO	-	expression tag	UNP Q8TJ90
f	-5	GLN	-	expression tag	UNP Q8TJ90
f	-4	PHE	-	expression tag	UNP Q8TJ90
f	-3	GLU	-	expression tag	UNP Q8TJ90
f	-2	LYS	-	expression tag	UNP Q8TJ90
f	-1	SER	-	expression tag	UNP Q8TJ90
f	0	GLY	-	expression tag	UNP Q8TJ90
k	-30	MET	-	initiating methionine	UNP Q8TJ90
k	-29	TRP	-	expression tag	UNP Q8TJ90
k	-28	SER	-	expression tag	UNP Q8TJ90
k	-27	HIS	-	expression tag	UNP Q8TJ90
k	-26	PRO	-	expression tag	UNP Q8TJ90
k	-25	GLN	-	expression tag	UNP Q8TJ90
k	-24	PHE	-	expression tag	UNP Q8TJ90
k	-23	GLU	-	expression tag	UNP Q8TJ90
k	-22	LYS	-	expression tag	UNP Q8TJ90
k	-21	GLY	-	expression tag	UNP Q8TJ90
k	-20	GLY	-	expression tag	UNP Q8TJ90
k	-19	GLY	-	expression tag	UNP Q8TJ90
k	-18	SER	-	expression tag	UNP Q8TJ90
k	-17	GLY	-	expression tag	UNP Q8TJ90
k	-16	GLY	-	expression tag	UNP Q8TJ90
k	-15	GLY	-	expression tag	UNP Q8TJ90
k	-14	SER	-	expression tag	UNP Q8TJ90
k	-13	GLY	-	expression tag	UNP Q8TJ90
k	-12	GLY	-	expression tag	UNP Q8TJ90
k	-11	GLY	-	expression tag	UNP Q8TJ90
k	-10	SER	-	expression tag	UNP Q8TJ90
k	-9	TRP	-	expression tag	UNP Q8TJ90
k	-8	SER	-	expression tag	UNP Q8TJ90
k	-7	HIS	-	expression tag	UNP Q8TJ90
k	-6	PRO	-	expression tag	UNP Q8TJ90
k	-5	GLN	-	expression tag	UNP Q8TJ90
k	-4	PHE	-	expression tag	UNP Q8TJ90
k	-3	GLU	-	expression tag	UNP Q8TJ90
k	-2	LYS	-	expression tag	UNP Q8TJ90
k	-1	SER	-	expression tag	UNP Q8TJ90
k	0	GLY	-	expression tag	UNP Q8TJ90
l	-30	MET	-	initiating methionine	UNP Q8TJ90
l	-29	TRP	-	expression tag	UNP Q8TJ90
l	-28	SER	-	expression tag	UNP Q8TJ90
l	-27	HIS	-	expression tag	UNP Q8TJ90

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
l	-26	PRO	-	expression tag	UNP Q8TJ90
l	-25	GLN	-	expression tag	UNP Q8TJ90
l	-24	PHE	-	expression tag	UNP Q8TJ90
l	-23	GLU	-	expression tag	UNP Q8TJ90
l	-22	LYS	-	expression tag	UNP Q8TJ90
l	-21	GLY	-	expression tag	UNP Q8TJ90
l	-20	GLY	-	expression tag	UNP Q8TJ90
l	-19	GLY	-	expression tag	UNP Q8TJ90
l	-18	SER	-	expression tag	UNP Q8TJ90
l	-17	GLY	-	expression tag	UNP Q8TJ90
l	-16	GLY	-	expression tag	UNP Q8TJ90
l	-15	GLY	-	expression tag	UNP Q8TJ90
l	-14	SER	-	expression tag	UNP Q8TJ90
l	-13	GLY	-	expression tag	UNP Q8TJ90
l	-12	GLY	-	expression tag	UNP Q8TJ90
l	-11	GLY	-	expression tag	UNP Q8TJ90
l	-10	SER	-	expression tag	UNP Q8TJ90
l	-9	TRP	-	expression tag	UNP Q8TJ90
l	-8	SER	-	expression tag	UNP Q8TJ90
l	-7	HIS	-	expression tag	UNP Q8TJ90
l	-6	PRO	-	expression tag	UNP Q8TJ90
l	-5	GLN	-	expression tag	UNP Q8TJ90
l	-4	PHE	-	expression tag	UNP Q8TJ90
l	-3	GLU	-	expression tag	UNP Q8TJ90
l	-2	LYS	-	expression tag	UNP Q8TJ90
l	-1	SER	-	expression tag	UNP Q8TJ90
l	0	GLY	-	expression tag	UNP Q8TJ90
p	-30	MET	-	initiating methionine	UNP Q8TJ90
p	-29	TRP	-	expression tag	UNP Q8TJ90
p	-28	SER	-	expression tag	UNP Q8TJ90
p	-27	HIS	-	expression tag	UNP Q8TJ90
p	-26	PRO	-	expression tag	UNP Q8TJ90
p	-25	GLN	-	expression tag	UNP Q8TJ90
p	-24	PHE	-	expression tag	UNP Q8TJ90
p	-23	GLU	-	expression tag	UNP Q8TJ90
p	-22	LYS	-	expression tag	UNP Q8TJ90
p	-21	GLY	-	expression tag	UNP Q8TJ90
p	-20	GLY	-	expression tag	UNP Q8TJ90
p	-19	GLY	-	expression tag	UNP Q8TJ90
p	-18	SER	-	expression tag	UNP Q8TJ90
p	-17	GLY	-	expression tag	UNP Q8TJ90
p	-16	GLY	-	expression tag	UNP Q8TJ90

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
p	-15	GLY	-	expression tag	UNP Q8TJ90
p	-14	SER	-	expression tag	UNP Q8TJ90
p	-13	GLY	-	expression tag	UNP Q8TJ90
p	-12	GLY	-	expression tag	UNP Q8TJ90
p	-11	GLY	-	expression tag	UNP Q8TJ90
p	-10	SER	-	expression tag	UNP Q8TJ90
p	-9	TRP	-	expression tag	UNP Q8TJ90
p	-8	SER	-	expression tag	UNP Q8TJ90
p	-7	HIS	-	expression tag	UNP Q8TJ90
p	-6	PRO	-	expression tag	UNP Q8TJ90
p	-5	GLN	-	expression tag	UNP Q8TJ90
p	-4	PHE	-	expression tag	UNP Q8TJ90
p	-3	GLU	-	expression tag	UNP Q8TJ90
p	-2	LYS	-	expression tag	UNP Q8TJ90
p	-1	SER	-	expression tag	UNP Q8TJ90
p	0	GLY	-	expression tag	UNP Q8TJ90

- Molecule 3 is a protein called P-II family nitrogen regulatory protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	90	Total	C	N	O	S	0	0
			704	443	122	130	9		
3	H	90	Total	C	N	O	S	0	0
			704	443	122	130	9		
3	P	90	Total	C	N	O	S	0	0
			704	443	122	130	9		
3	T	90	Total	C	N	O	S	0	0
			704	443	122	130	9		
3	Z	90	Total	C	N	O	S	0	0
			704	443	122	130	9		
3	b	90	Total	C	N	O	S	0	0
			704	443	122	130	9		
3	i	103	Total	C	N	O	S	0	0
			813	511	142	151	9		
3	j	97	Total	C	N	O	S	0	0
			764	481	132	142	9		
3	n	101	Total	C	N	O	S	0	0
			787	494	138	146	9		
3	o	100	Total	C	N	O	S	0	0
			790	496	137	148	9		
3	s	103	Total	C	N	O	S	0	0
			813	511	142	151	9		

Continued on next page...

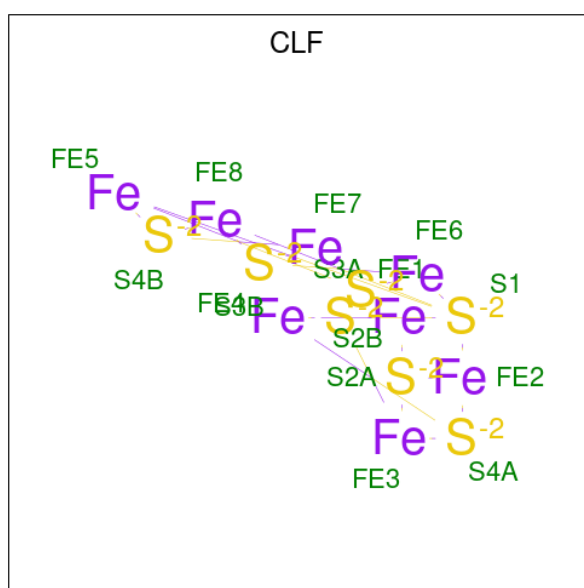
Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
3	t	101	Total	C	N	O	S	0	0
			795	499	138	149	9		

- Molecule 4 is a protein called P-II family nitrogen regulatory protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	Q	118	Total	C	N	O	S	0	0
			922	580	166	170	6		
4	a	116	Total	C	N	O	S	0	0
			905	570	163	166	6		
4	g	116	Total	C	N	O	S	1	0
			914	577	163	167	7		
4	h	120	Total	C	N	O	S	0	0
			936	588	168	174	6		
4	m	116	Total	C	N	O	S	1	0
			914	577	163	167	7		
4	r	115	Total	C	N	O	S	1	0
			905	572	162	165	6		

- Molecule 5 is FE(8)-S(7) CLUSTER (CCD ID: CLF) (formula: Fe_8S_7) (labeled as "Ligand of Interest" by depositor).



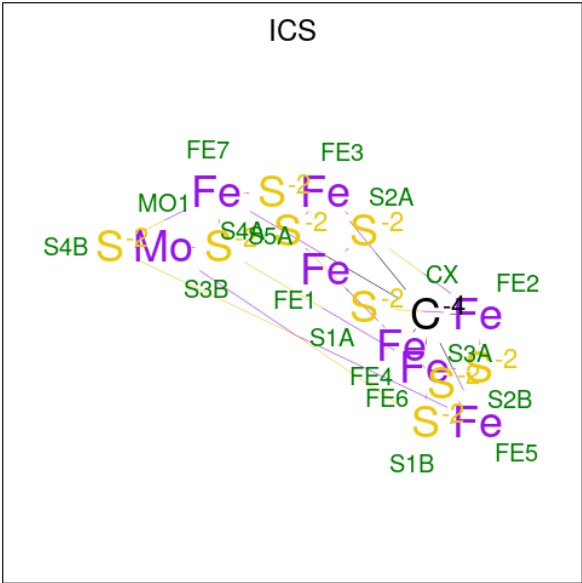
Mol	Chain	Residues	Atoms			AltConf
5	M	1	Total	Fe	S	0
			15	8	7	
5	N	1	Total	Fe	S	0
			15	8	7	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
5	W	1	Total	Fe	S	0
			15	8	7	
5	e	1	Total	Fe	S	0
			15	8	7	
5	q	1	Total	Fe	S	0
			15	8	7	
5	f	1	Total	Fe	S	0
			15	8	7	

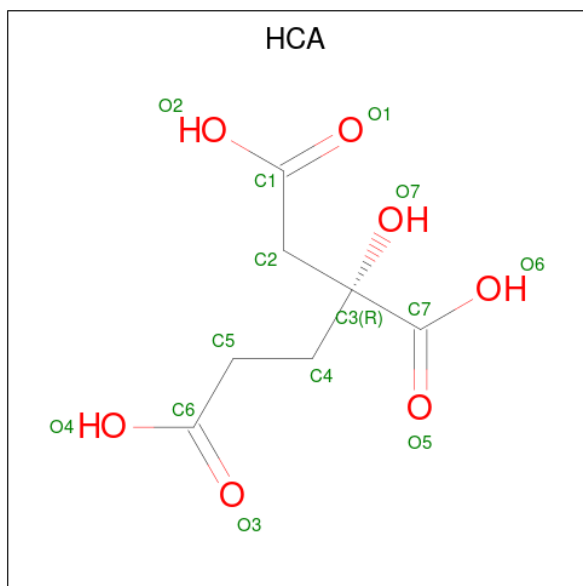
- Molecule 6 is iron-sulfur-molybdenum cluster with interstitial carbon (CCD ID: ICS) (formula: CFe₇MoS₉) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
6	e	1	Total	C	Fe	Mo	S	0
			18	1	7	1	9	
6	q	1	Total	C	Fe	Mo	S	0
			18	1	7	1	9	
6	f	1	Total	C	Fe	Mo	S	0
			18	1	7	1	9	
6	k	1	Total	C	Fe	Mo	S	0
			18	1	7	1	9	
6	l	1	Total	C	Fe	Mo	S	0
			18	1	7	1	9	
6	p	1	Total	C	Fe	Mo	S	0
			18	1	7	1	9	

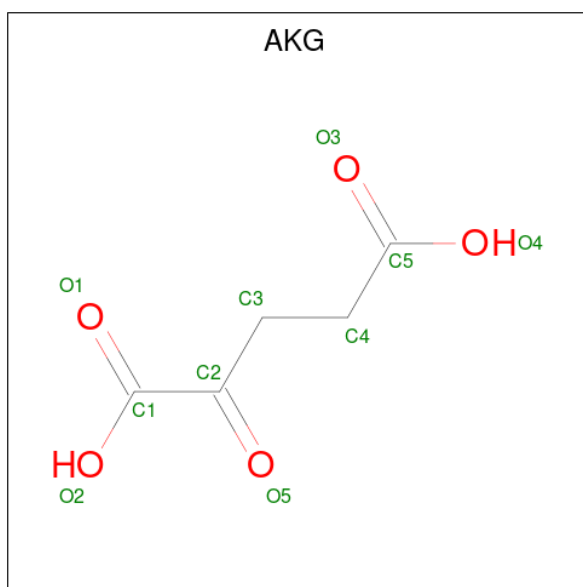
- Molecule 7 is 3-HYDROXY-3-CARBOXY-ADIPIC ACID (CCD ID: HCA) (formula:

C₇H₁₀O₇) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
7	e	1	Total	C	O	0
			14	7	7	
7	q	1	Total	C	O	0
			14	7	7	
7	f	1	Total	C	O	0
			14	7	7	
7	k	1	Total	C	O	0
			14	7	7	
7	l	1	Total	C	O	0
			14	7	7	
7	p	1	Total	C	O	0
			14	7	7	

- Molecule 8 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).

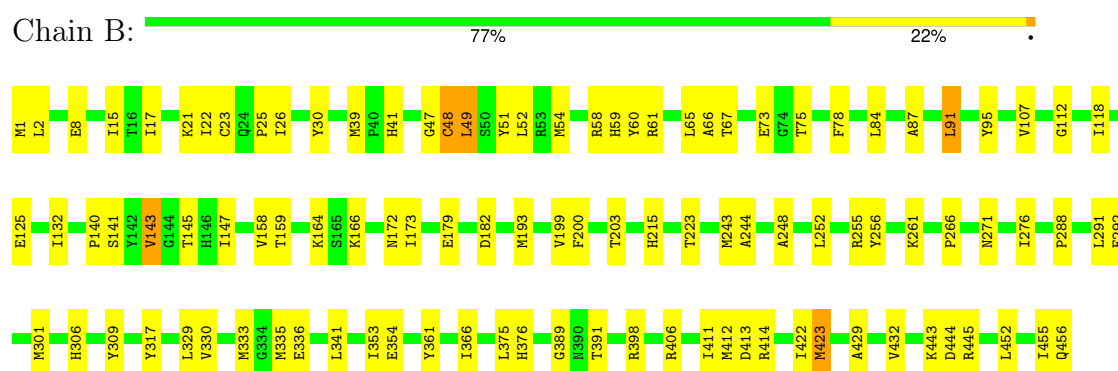


Mol	Chain	Residues	Atoms			AltConf
9	h	1	Total	C	O	0
			10	5	5	
9	r	1	Total	C	O	0
			10	5	5	

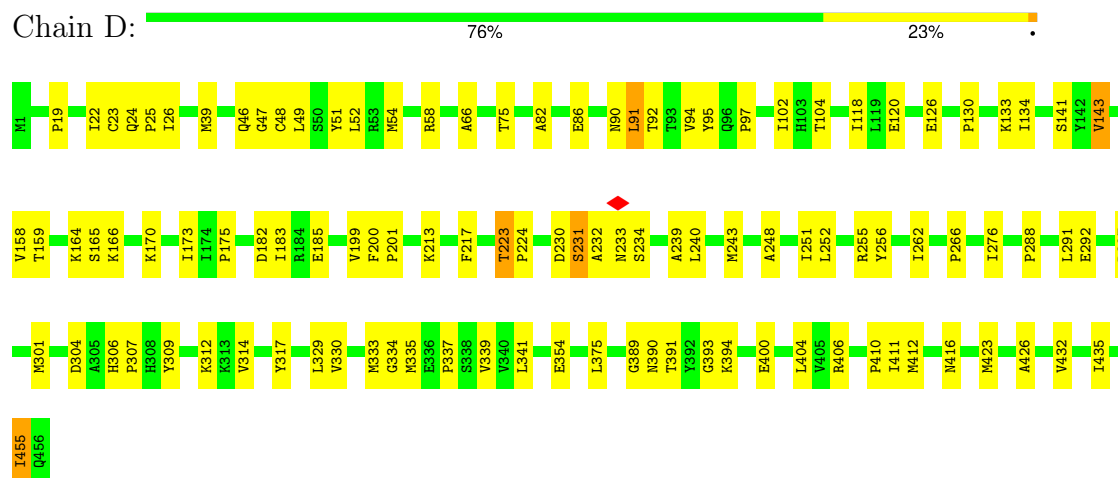
3 Residue-property plots [i](#)

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

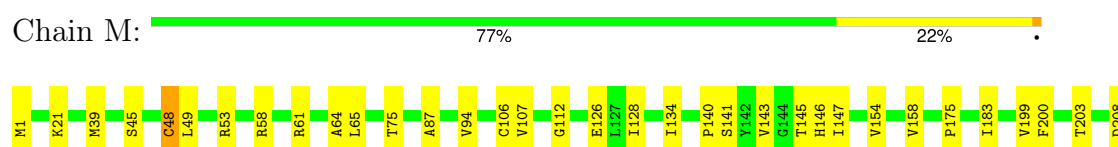
- Molecule 1: Nitrogenase molybdenum-iron protein beta chain

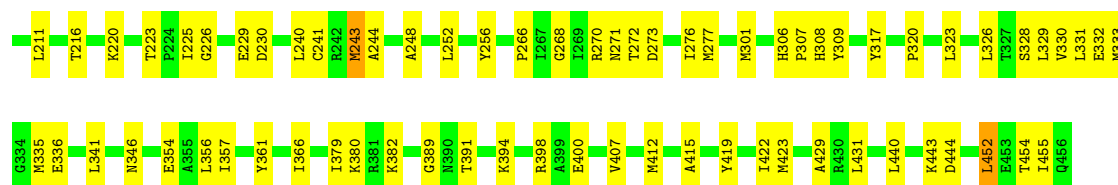


- Molecule 1: Nitrogenase molybdenum-iron protein beta chain

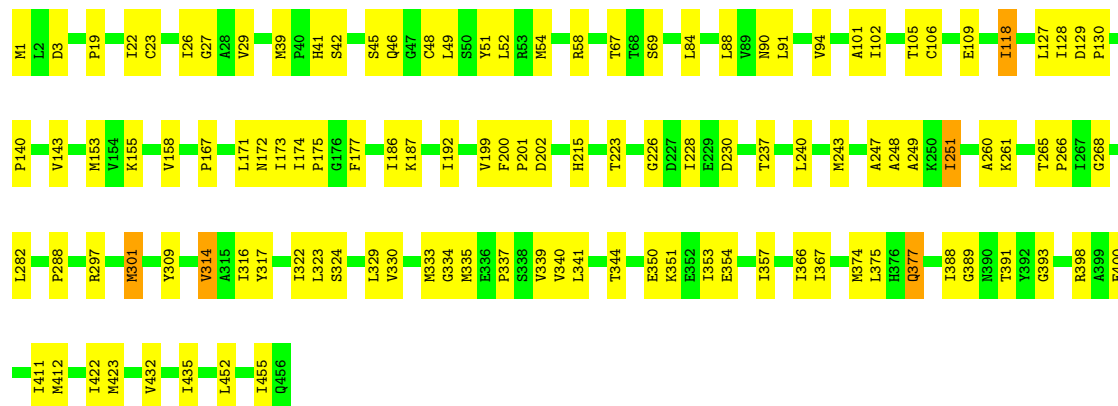


- Molecule 1: Nitrogenase molybdenum-iron protein beta chain

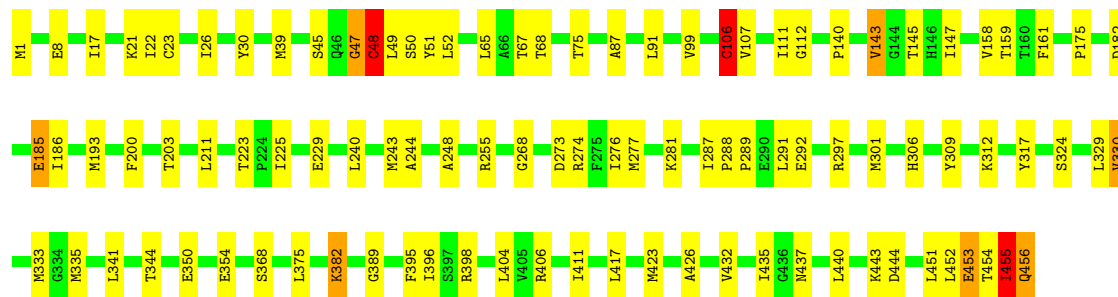
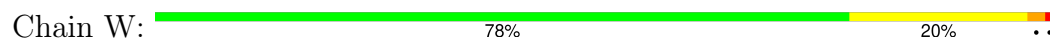




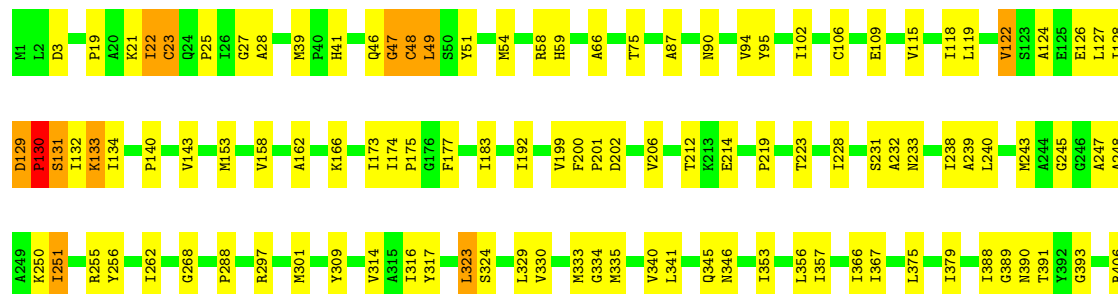
- Molecule 1: Nitrogenase molybdenum-iron protein beta chain

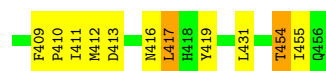


- Molecule 1: Nitrogenase molybdenum-iron protein beta chain



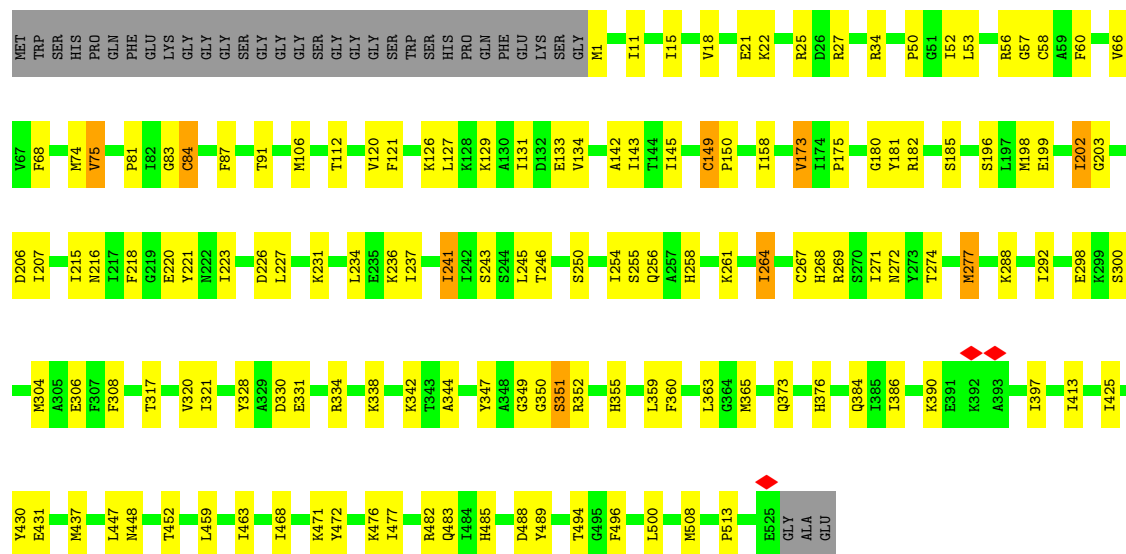
- Molecule 1: Nitrogenase molybdenum-iron protein beta chain





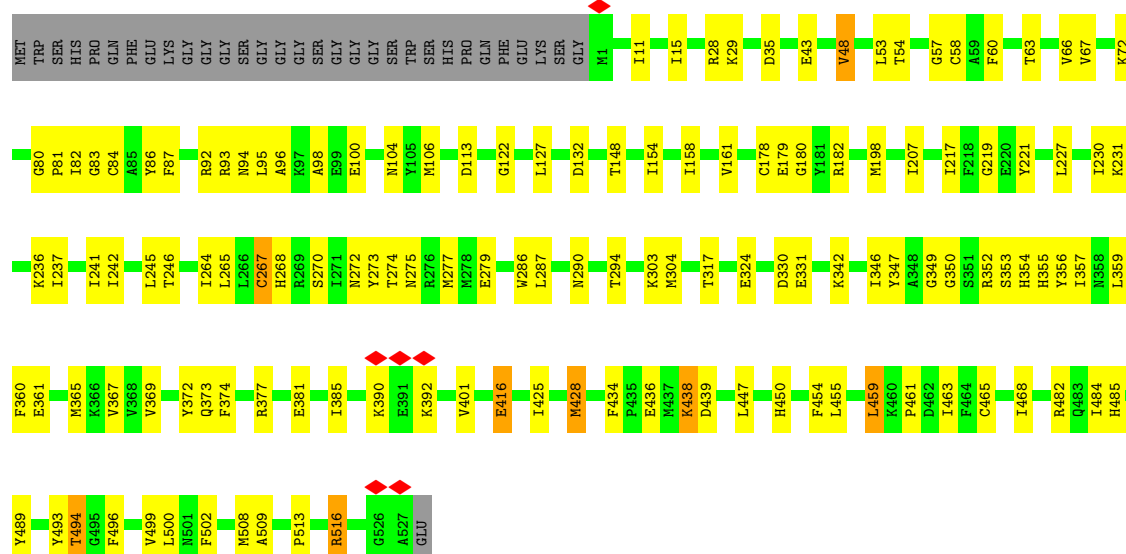
• Molecule 2: Nitrogenase protein alpha chain

Chain e: 69% 24% 6%



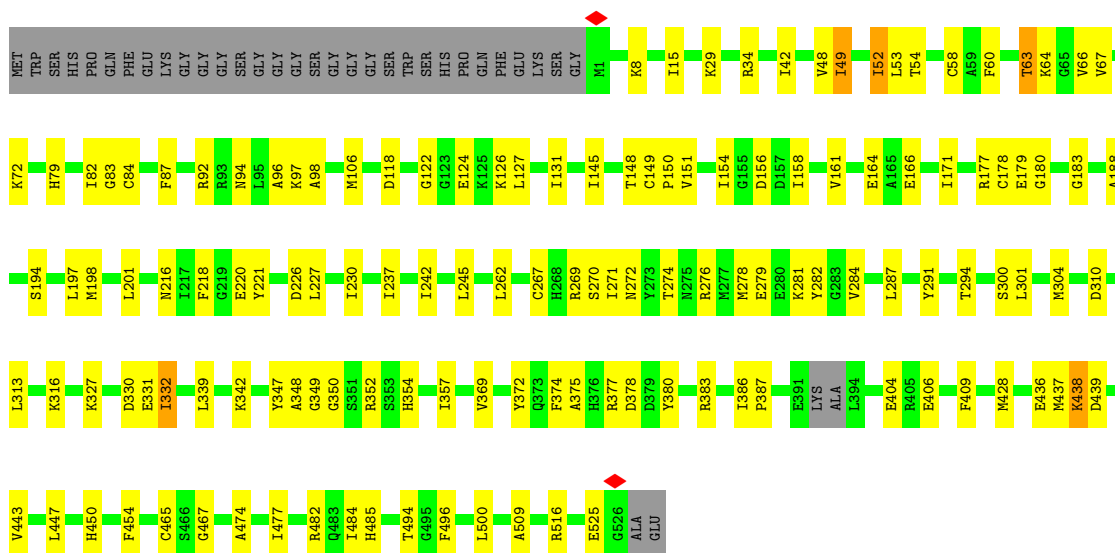
• Molecule 2: Nitrogenase protein alpha chain

Chain q: 70% 23% 6%

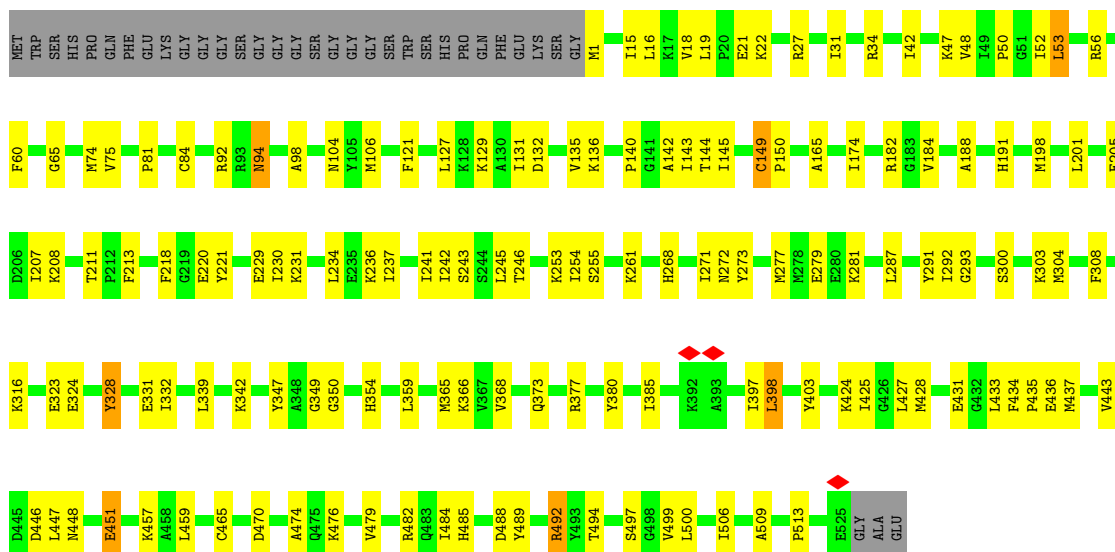


• Molecule 2: Nitrogenase protein alpha chain

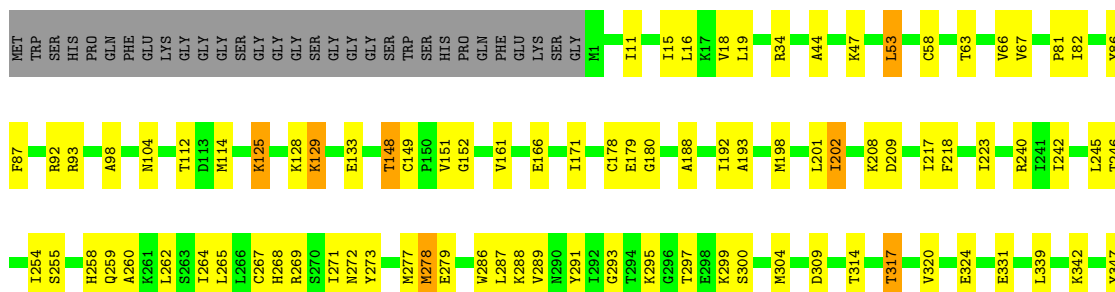
Chain f: 69% 23% 6%

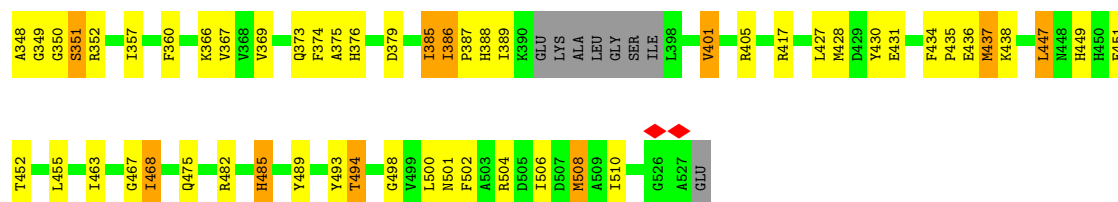


- Molecule 2: Nitrogenase protein alpha chain

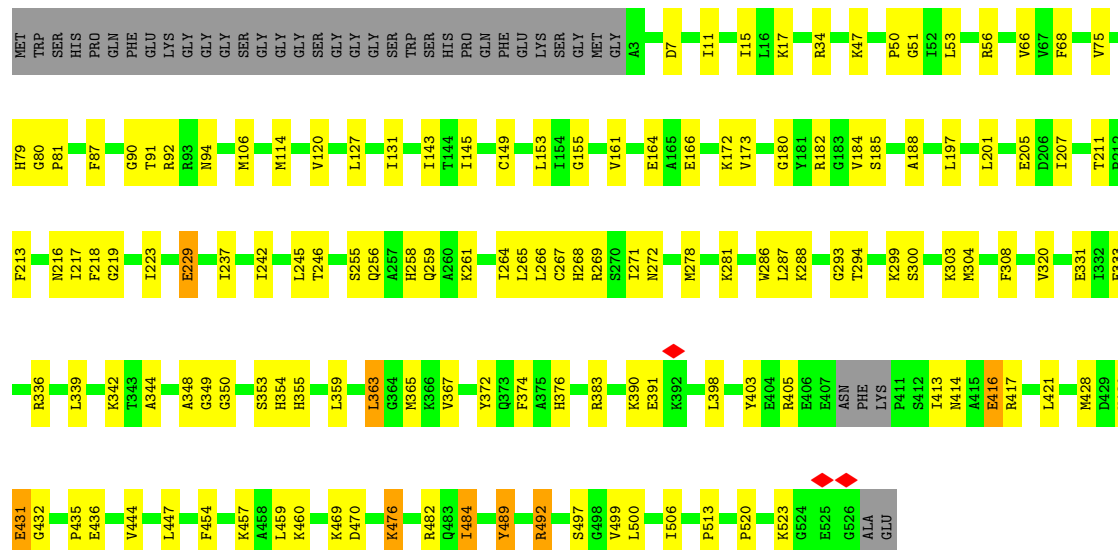


- Molecule 2: Nitrogenase protein alpha chain

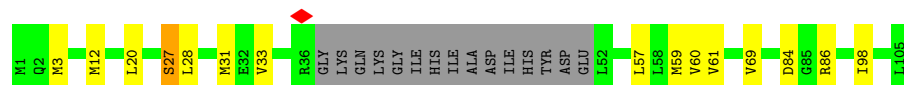




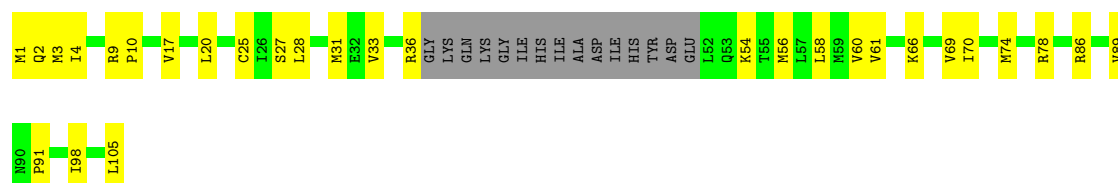
• Molecule 2: Nitrogenase protein alpha chain



• Molecule 3: P-II family nitrogen regulatory protein

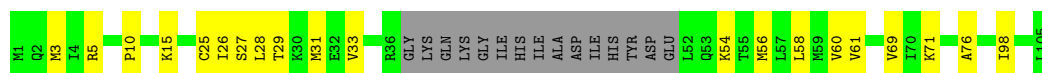


• Molecule 3: P-II family nitrogen regulatory protein

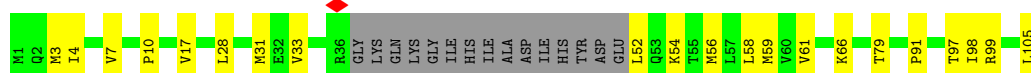


• Molecule 3: P-II family nitrogen regulatory protein

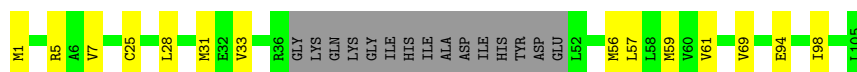




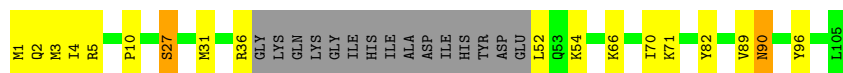
- Molecule 3: P-II family nitrogen regulatory protein



- Molecule 3: P-II family nitrogen regulatory protein



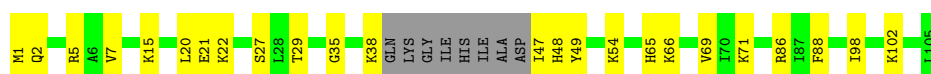
- Molecule 3: P-II family nitrogen regulatory protein



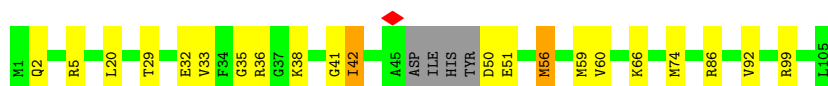
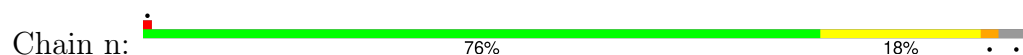
- Molecule 3: P-II family nitrogen regulatory protein



- Molecule 3: P-II family nitrogen regulatory protein

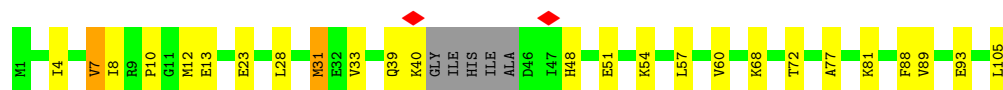


- Molecule 3: P-II family nitrogen regulatory protein

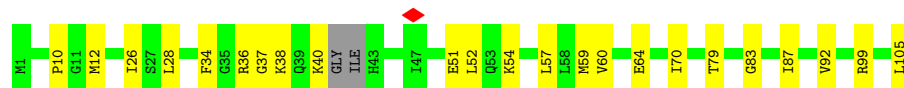
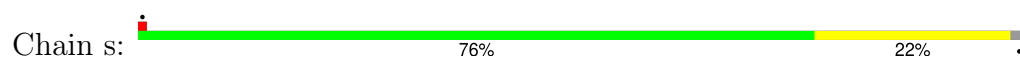


- Molecule 3: P-II family nitrogen regulatory protein





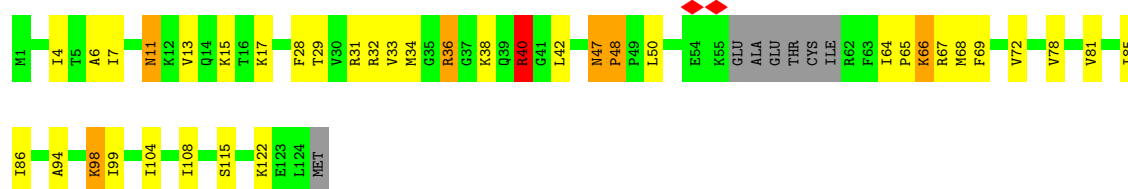
- Molecule 3: P-II family nitrogen regulatory protein



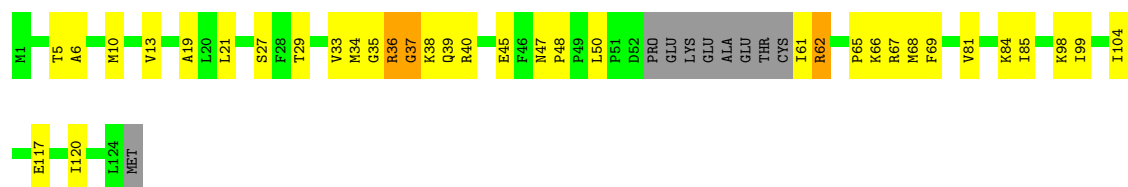
- Molecule 3: P-II family nitrogen regulatory protein



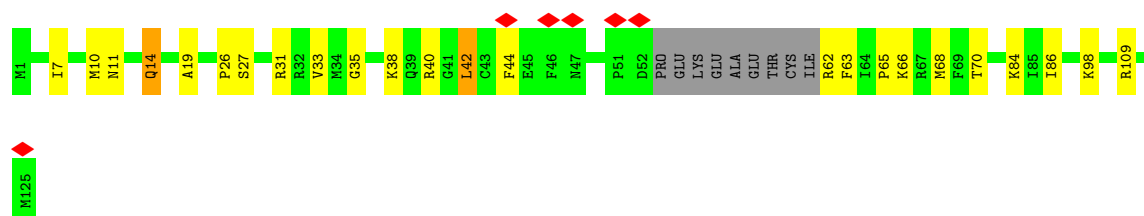
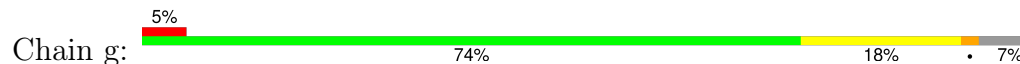
- Molecule 4: P-II family nitrogen regulatory protein



- Molecule 4: P-II family nitrogen regulatory protein

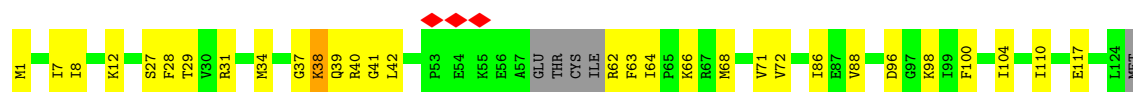


- Molecule 4: P-II family nitrogen regulatory protein



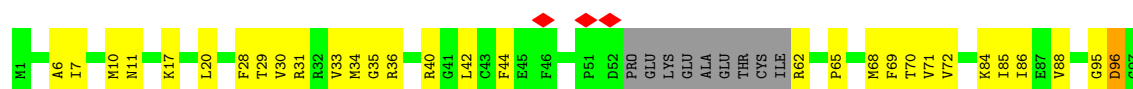
- Molecule 4: P-II family nitrogen regulatory protein

Chain h:  72% 23%



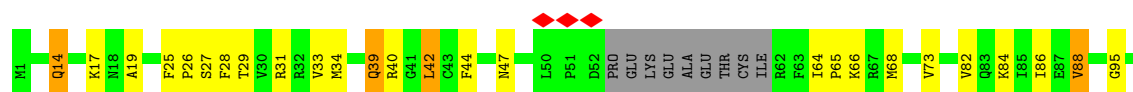
- Molecule 4: P-II family nitrogen regulatory protein

Chain m:  66% 26% 7%



- Molecule 4: P-II family nitrogen regulatory protein

Chain r:  68% 21% 8%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	70378	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	52	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	150000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	2.413	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.038	Depositor
Recommended contour level	0.0141	Depositor
Map size ($\text{\AA}$)	371.19998, 371.19998, 371.19998	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.928, 0.928, 0.928	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, HCA, ICS, CLF, AKG

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	B	0.20	0/3548	0.35	1/4819 (0.0%)
1	D	0.21	0/3537	0.40	0/4804
1	M	0.19	0/3537	0.37	1/4804 (0.0%)
1	N	0.18	0/3537	0.36	0/4804
1	W	0.25	0/3537	0.53	8/4804 (0.2%)
1	X	0.32	0/3548	0.65	16/4819 (0.3%)
2	e	0.20	0/4273	0.38	2/5760 (0.0%)
2	f	0.18	0/4262	0.34	0/5744
2	k	0.18	0/4273	0.38	2/5760 (0.0%)
2	l	0.19	0/4232	0.41	5/5704 (0.1%)
2	p	0.19	0/4235	0.33	0/5708
2	q	0.18	0/4282	0.38	2/5772 (0.0%)
3	F	0.25	1/709 (0.1%)	0.36	0/942
3	H	0.13	0/709	0.23	0/942
3	P	0.21	0/709	0.37	1/942 (0.1%)
3	T	0.13	0/709	0.23	0/942
3	Z	0.12	0/709	0.22	0/942
3	b	0.13	0/709	0.23	0/942
3	i	0.15	0/821	0.31	0/1092
3	j	0.26	0/771	0.48	3/1025 (0.3%)
3	n	0.12	0/793	0.22	0/1053
3	o	0.12	0/797	0.27	0/1059
3	s	0.12	0/821	0.21	0/1092
3	t	0.21	0/802	0.48	3/1066 (0.3%)
4	Q	0.36	0/933	0.80	4/1250 (0.3%)
4	a	0.20	0/915	0.39	0/1226
4	g	0.13	0/928	0.29	0/1241
4	h	0.15	0/947	0.30	0/1269
4	m	0.13	0/928	0.27	0/1241
4	r	0.14	0/919	0.29	0/1231
All	All	0.20	1/61430 (0.0%)	0.40	48/82799 (0.1%)

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
1	D	0	1
1	W	0	1
3	t	0	1
4	Q	0	2
4	a	0	1
All	All	0	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	27	SER	CA-CB	-5.29	1.45	1.53

The worst 5 of 48 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	W	48	CYS	CB-CA-C	-18.13	83.04	110.96
1	X	23	CYS	CB-CA-C	-16.74	75.50	113.33
2	k	149	CYS	CB-CA-C	-13.71	92.04	113.57
1	M	48	CYS	CB-CA-C	-12.35	91.80	110.95
4	Q	48	PRO	N-CA-C	-11.79	96.31	110.70

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	234	SER	Peptide
4	Q	36	ARG	Sidechain
4	Q	40	ARG	Sidechain
1	W	453	GLU	Mainchain
4	a	36	ARG	Sidechain

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	B	3474	0	3490	77	0
1	D	3467	0	3480	80	0
1	M	3467	0	3481	64	0
1	N	3467	0	3481	84	0
1	W	3467	0	3481	66	0
1	X	3477	0	3486	91	0
2	e	4181	0	4131	106	0
2	f	4171	0	4115	104	0
2	k	4181	0	4130	102	0
2	l	4141	0	4084	112	0
2	p	4145	0	4090	98	0
2	q	4190	0	4139	108	0
3	F	704	0	745	17	0
3	H	704	0	745	17	0
3	P	704	0	745	16	0
3	T	704	0	745	15	0
3	Z	704	0	745	8	0
3	b	704	0	745	15	0
3	i	813	0	846	25	0
3	j	764	0	798	35	0
3	n	787	0	829	19	0
3	o	790	0	823	17	0
3	s	813	0	846	22	0
3	t	795	0	828	27	0
4	Q	922	0	960	30	0
4	a	905	0	945	38	0
4	g	914	0	952	28	0
4	h	936	0	971	27	0
4	m	914	0	952	38	0
4	r	905	0	943	29	0
5	M	15	0	0	3	0
5	N	15	0	0	13	0
5	W	15	0	0	6	0
5	e	15	0	0	13	0
5	f	15	0	0	7	0
5	q	15	0	0	8	0
6	e	18	0	0	6	0
6	f	18	0	0	16	0
6	k	18	0	0	4	0
6	l	18	0	0	17	0
6	p	18	0	0	11	0
6	q	18	0	0	13	0
7	e	14	0	6	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	f	14	0	6	0	0
7	k	14	0	6	1	0
7	l	14	0	7	7	0
7	p	14	0	6	0	0
7	q	14	0	7	1	0
8	a	27	0	12	14	0
8	g	27	0	12	8	0
8	i	27	0	12	7	0
8	j	27	0	12	23	0
8	m	27	0	12	19	0
8	n	27	0	12	9	0
8	o	27	0	12	7	0
8	s	27	0	12	16	0
8	t	27	0	12	26	0
9	h	10	0	4	2	0
9	r	10	0	4	1	0
All	All	60855	0	60905	1389	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 11.

The worst 5 of 1389 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)
4:g:27:SER:HB3	8:j:201:ADP:C8	1.57	1.36
4:g:27:SER:CB	8:j:201:ADP:N7	1.88	1.35
4:m:95:GLY:N	8:m:201:ADP:O2B	1.61	1.31
2:l:374:PHE:CZ	6:l:601:ICS:S1A	2.25	1.29
4:m:95:GLY:CA	8:m:201:ADP:O2B	1.81	1.27

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	455/456 (100%)	437 (96%)	18 (4%)	0	100	100
1	D	454/456 (100%)	420 (92%)	34 (8%)	0	100	100
1	M	454/456 (100%)	442 (97%)	12 (3%)	0	100	100
1	N	454/456 (100%)	427 (94%)	27 (6%)	0	100	100
1	W	454/456 (100%)	439 (97%)	15 (3%)	0	100	100
1	X	455/456 (100%)	426 (94%)	28 (6%)	1 (0%)	43	73
2	e	523/559 (94%)	488 (93%)	34 (6%)	1 (0%)	43	73
2	f	520/559 (93%)	497 (96%)	23 (4%)	0	100	100
2	k	523/559 (94%)	489 (94%)	34 (6%)	0	100	100
2	l	516/559 (92%)	492 (95%)	24 (5%)	0	100	100
2	p	517/559 (92%)	482 (93%)	35 (7%)	0	100	100
2	q	525/559 (94%)	500 (95%)	25 (5%)	0	100	100
3	F	86/105 (82%)	84 (98%)	2 (2%)	0	100	100
3	H	86/105 (82%)	86 (100%)	0	0	100	100
3	P	86/105 (82%)	83 (96%)	3 (4%)	0	100	100
3	T	86/105 (82%)	86 (100%)	0	0	100	100
3	Z	86/105 (82%)	85 (99%)	1 (1%)	0	100	100
3	b	86/105 (82%)	86 (100%)	0	0	100	100
3	i	99/105 (94%)	96 (97%)	3 (3%)	0	100	100
3	j	93/105 (89%)	92 (99%)	1 (1%)	0	100	100
3	n	97/105 (92%)	94 (97%)	3 (3%)	0	100	100
3	o	96/105 (91%)	93 (97%)	3 (3%)	0	100	100
3	s	99/105 (94%)	96 (97%)	3 (3%)	0	100	100
3	t	97/105 (92%)	96 (99%)	1 (1%)	0	100	100
4	Q	114/125 (91%)	105 (92%)	9 (8%)	0	100	100
4	a	112/125 (90%)	101 (90%)	10 (9%)	1 (1%)	14	45
4	g	113/125 (90%)	106 (94%)	7 (6%)	0	100	100
4	h	116/125 (93%)	105 (90%)	11 (10%)	0	100	100
4	m	113/125 (90%)	109 (96%)	4 (4%)	0	100	100
4	r	112/125 (90%)	109 (97%)	3 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	7627/8100 (94%)	7251 (95%)	373 (5%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	X	130	PRO
2	e	351	SER
4	a	37	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	379/378 (100%)	365 (96%)	14 (4%)	30	62
1	D	378/378 (100%)	363 (96%)	15 (4%)	28	60
1	M	378/378 (100%)	366 (97%)	12 (3%)	34	65
1	N	378/378 (100%)	367 (97%)	11 (3%)	37	68
1	W	378/378 (100%)	360 (95%)	18 (5%)	23	55
1	X	379/378 (100%)	362 (96%)	17 (4%)	24	57
2	e	445/467 (95%)	425 (96%)	20 (4%)	24	57
2	f	444/467 (95%)	425 (96%)	19 (4%)	26	58
2	k	445/467 (95%)	429 (96%)	16 (4%)	31	63
2	l	440/467 (94%)	410 (93%)	30 (7%)	14	43
2	p	441/467 (94%)	421 (96%)	20 (4%)	24	57
2	q	445/467 (95%)	426 (96%)	19 (4%)	26	58
3	F	77/89 (86%)	77 (100%)	0	100	100
3	H	77/89 (86%)	71 (92%)	6 (8%)	11	37
3	P	77/89 (86%)	76 (99%)	1 (1%)	61	81
3	T	77/89 (86%)	73 (95%)	4 (5%)	21	53
3	Z	77/89 (86%)	75 (97%)	2 (3%)	40	70

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	b	77/89 (86%)	73 (95%)	4 (5%)	21	53
3	i	88/89 (99%)	82 (93%)	6 (7%)	14	43
3	j	83/89 (93%)	78 (94%)	5 (6%)	17	48
3	n	85/89 (96%)	82 (96%)	3 (4%)	32	63
3	o	86/89 (97%)	81 (94%)	5 (6%)	18	49
3	s	88/89 (99%)	81 (92%)	7 (8%)	11	36
3	t	86/89 (97%)	81 (94%)	5 (6%)	18	49
4	Q	103/109 (94%)	96 (93%)	7 (7%)	14	43
4	a	101/109 (93%)	94 (93%)	7 (7%)	14	42
4	g	102/109 (94%)	100 (98%)	2 (2%)	48	75
4	h	104/109 (95%)	99 (95%)	5 (5%)	23	55
4	m	102/109 (94%)	97 (95%)	5 (5%)	22	54
4	r	101/109 (93%)	96 (95%)	5 (5%)	22	54
All	All	6521/6792 (96%)	6231 (96%)	290 (4%)	26	58

5 of 290 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	l	437	MET
3	t	38	LYS
2	l	494	THR
2	p	363	LEU
2	e	264	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 54 such sidechains are listed below:

Mol	Chain	Res	Type
2	f	40	GLN
2	k	30	HIS
3	o	48	HIS
2	f	290	ASN
4	h	47	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

29 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	AKG	r	201	-	9,9,9	5.24	2 (22%)	11,11,11	1.59	1 (9%)
8	ADP	t	201	-	28,29,29	0.41	0	43,45,45	0.51	0
5	CLF	f	601	1,2	0,24,24	-	-	-		
6	ICS	l	601	7,2	6,30,30	1.78	2 (33%)	-		
7	HCA	l	602	6	13,13,13	1.16	0	15,18,18	1.23	2 (13%)
5	CLF	W	601	1,2	0,24,24	-	-	-		
8	ADP	n	201	-	28,29,29	0.51	0	43,45,45	0.54	0
5	CLF	M	601	1,2	0,24,24	-	-	-		
5	CLF	q	601	1,2	0,24,24	-	-	-		
8	ADP	a	200	-	28,29,29	0.46	0	43,45,45	0.45	0
7	HCA	f	603	6	13,13,13	1.13	0	15,18,18	1.22	2 (13%)
8	ADP	i	201	-	28,29,29	0.47	0	43,45,45	0.63	0
8	ADP	s	201	-	28,29,29	0.46	0	43,45,45	0.46	0
6	ICS	k	602	7,2	6,30,30	2.19	2 (33%)	-		
5	CLF	e	601	2	0,24,24	-	-	-		
9	AKG	h	201	-	9,9,9	5.27	2 (22%)	11,11,11	1.85	3 (27%)
8	ADP	j	201	-	28,29,29	0.44	0	43,45,45	0.45	0
6	ICS	q	603	7,2	6,30,30	2.20	2 (33%)	-		
5	CLF	N	501	1,2	0,24,24	-	-	-		
6	ICS	e	602	7,2	6,30,30	2.11	2 (33%)	-		
8	ADP	o	201	-	28,29,29	0.51	0	43,45,45	0.68	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	HCA	k	601	6	13,13,13	1.14	1 (7%)	15,18,18	1.31	2 (13%)
8	ADP	m	201	-	28,29,29	0.48	0	43,45,45	0.48	0
6	ICS	f	602	7,2	6,30,30	1.96	2 (33%)	-		
6	ICS	p	602	7,2	6,30,30	1.81	2 (33%)	-		
7	HCA	q	602	6	13,13,13	1.14	0	15,18,18	1.26	2 (13%)
7	HCA	p	601	6	13,13,13	1.14	0	15,18,18	1.15	2 (13%)
7	HCA	e	603	6	13,13,13	1.08	0	15,18,18	1.20	2 (13%)
8	ADP	g	201	-	28,29,29	0.52	0	43,45,45	0.53	0

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
9	AKG	r	201	-	-	3/9/9/9	-
5	CLF	f	601	1,2	-	-	0/12/10/10
7	HCA	l	602	6	-	11/17/17/17	-
5	CLF	W	601	1,2	-	-	0/12/10/10
8	ADP	n	201	-	-	8/16/32/32	0/3/3/3
5	CLF	M	601	1,2	-	-	0/12/10/10
7	HCA	e	603	6	-	12/17/17/17	-
5	CLF	q	601	1,2	-	-	0/12/10/10
8	ADP	a	200	-	-	4/16/32/32	0/3/3/3
7	HCA	f	603	6	-	4/17/17/17	-
8	ADP	i	201	-	-	6/16/32/32	0/3/3/3
8	ADP	s	201	-	-	3/16/32/32	0/3/3/3
5	CLF	e	601	2	-	-	0/12/10/10
9	AKG	h	201	-	-	6/9/9/9	-
8	ADP	j	201	-	-	5/16/32/32	0/3/3/3
5	CLF	N	501	1,2	-	-	0/12/10/10
8	ADP	o	201	-	-	3/16/32/32	0/3/3/3
7	HCA	k	601	6	-	5/17/17/17	-
8	ADP	m	201	-	-	3/16/32/32	0/3/3/3
7	HCA	q	602	6	-	12/17/17/17	-
7	HCA	p	601	6	-	10/17/17/17	-
8	ADP	t	201	-	-	6/16/32/32	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	ADP	g	201	-	-	5/16/32/32	0/3/3/3

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	h	201	AKG	C2-C1	-15.41	1.30	1.53
9	r	201	AKG	C2-C1	-15.32	1.30	1.53
6	q	603	ICS	S2B-FE6	-4.46	2.14	2.24
6	k	602	ICS	S2B-FE6	-4.09	2.15	2.24
6	e	602	ICS	S2B-FE6	-3.76	2.16	2.24

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	h	201	AKG	C3-C2-C1	4.28	123.13	115.86
9	r	201	AKG	C3-C2-C1	3.94	122.56	115.86
9	h	201	AKG	O1-C1-C2	-2.73	118.41	121.81
7	q	602	HCA	O5-C7-C3	-2.56	117.12	122.09
7	k	601	HCA	O5-C7-C3	-2.48	117.29	122.09

There are no chirality outliers.

5 of 106 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	e	603	HCA	C2-C3-C4-C5
7	e	603	HCA	C7-C3-C4-C5
7	e	603	HCA	O7-C3-C4-C5
7	e	603	HCA	C2-C3-C7-O5
7	e	603	HCA	C2-C3-C7-O6

There are no ring outliers.

26 monomers are involved in 257 short contacts:

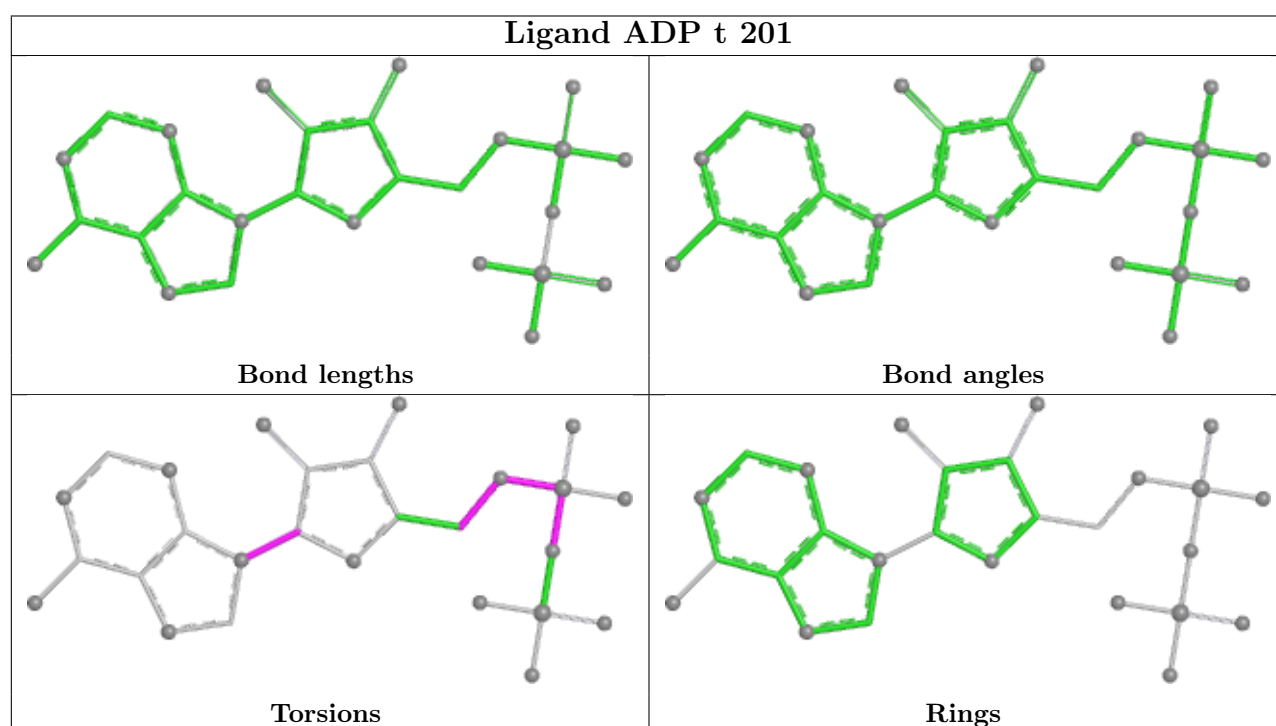
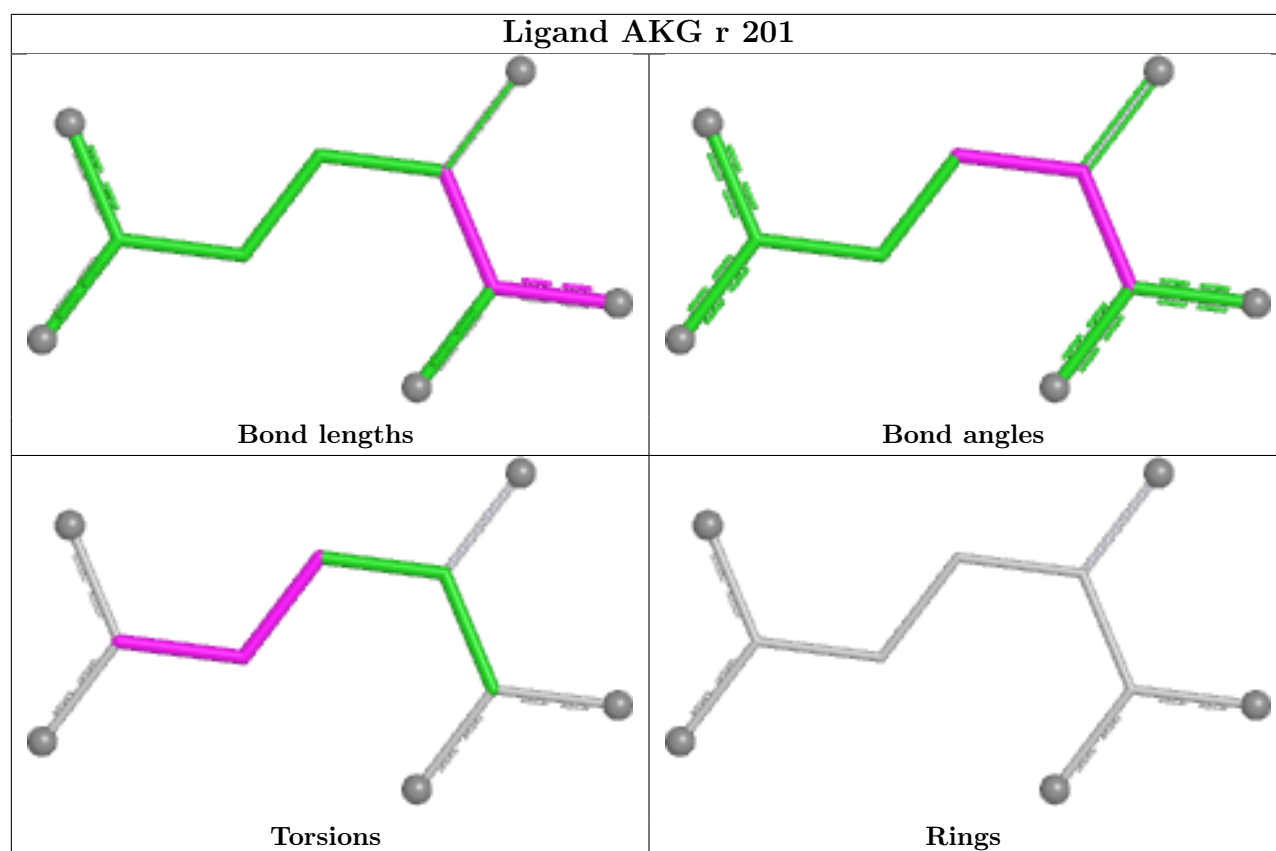
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	r	201	AKG	1	0
8	t	201	ADP	26	0
5	f	601	CLF	7	0
6	l	601	ICS	17	0
7	l	602	HCA	7	0
5	W	601	CLF	6	0
8	n	201	ADP	9	0

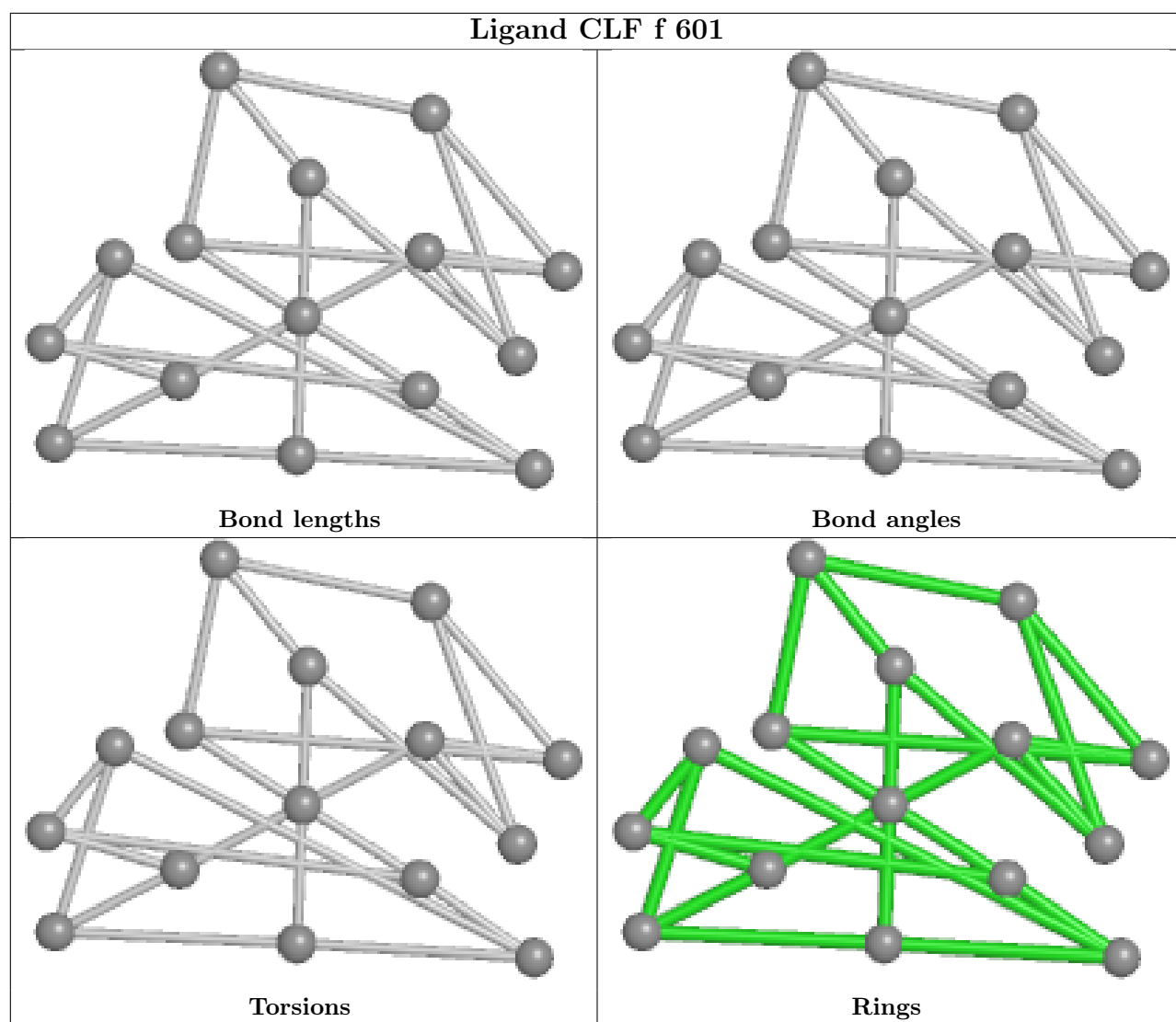
Continued on next page...

Continued from previous page...

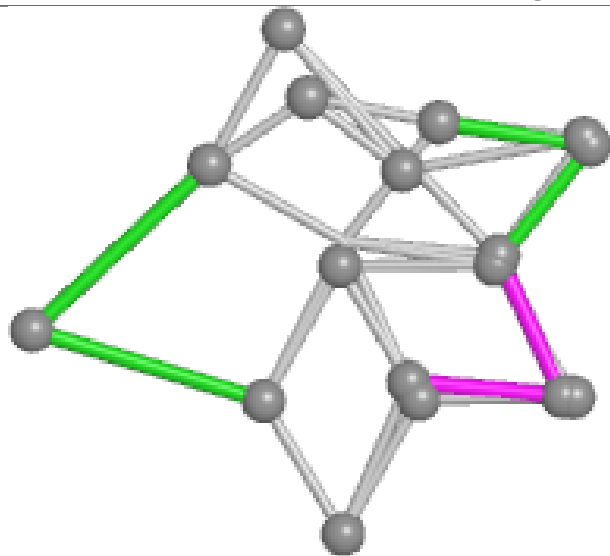
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	M	601	CLF	3	0
5	q	601	CLF	8	0
8	a	200	ADP	14	0
8	i	201	ADP	7	0
8	s	201	ADP	16	0
6	k	602	ICS	4	0
5	e	601	CLF	13	0
9	h	201	AKG	2	0
8	j	201	ADP	23	0
6	q	603	ICS	13	0
5	N	501	CLF	13	0
6	e	602	ICS	6	0
8	o	201	ADP	7	0
7	k	601	HCA	1	0
8	m	201	ADP	19	0
6	f	602	ICS	16	0
6	p	602	ICS	11	0
7	q	602	HCA	1	0
8	g	201	ADP	8	0

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

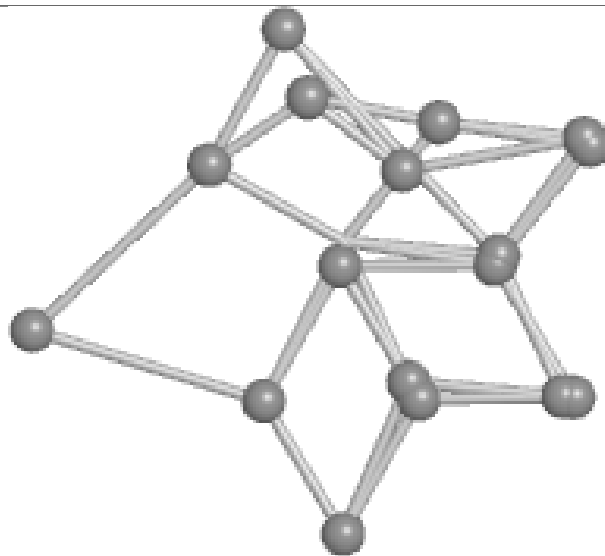




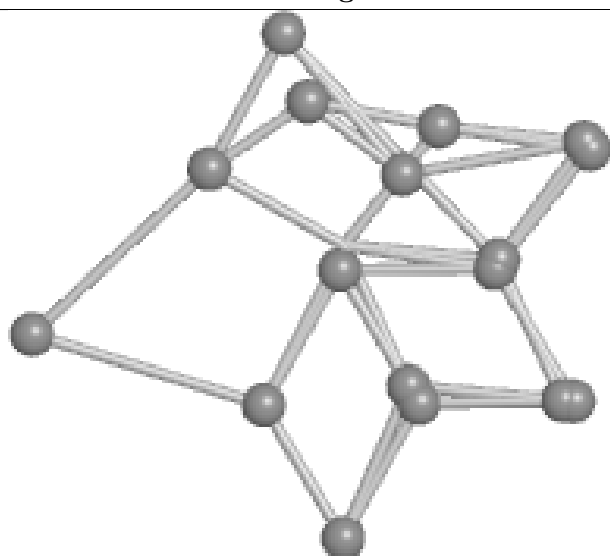
Ligand ICS 1 601



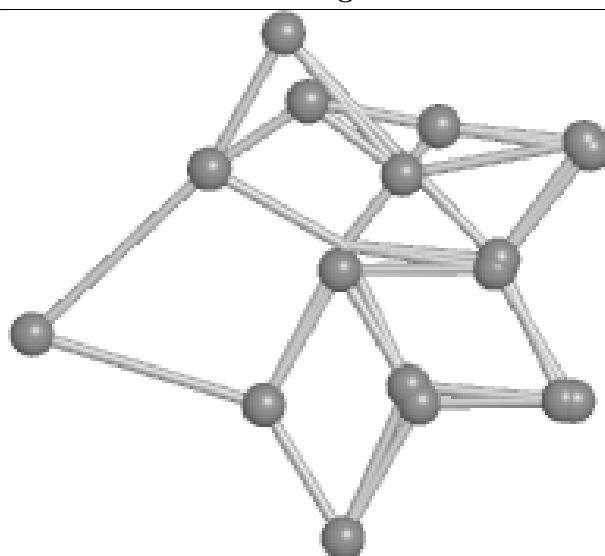
Bond lengths



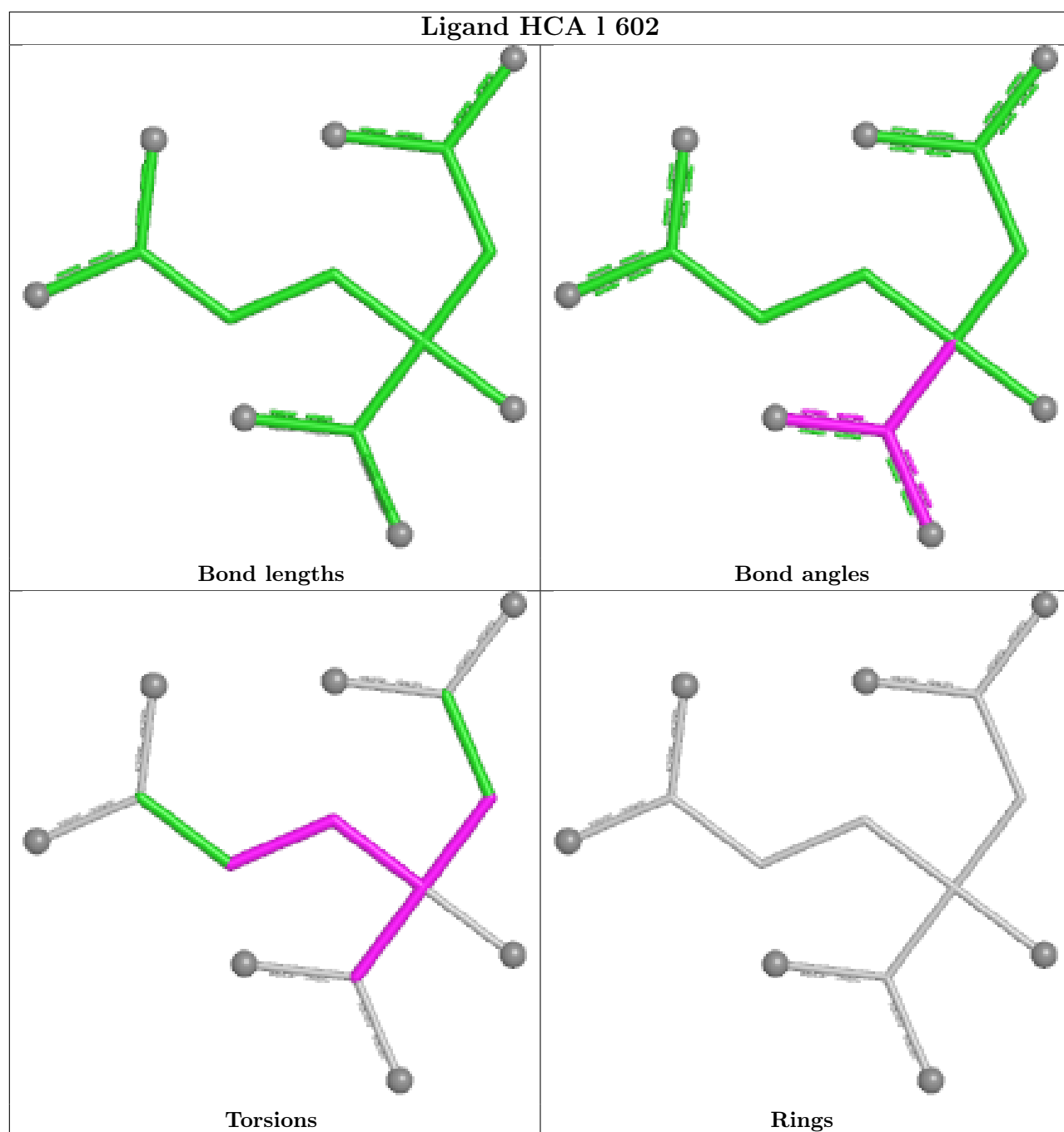
Bond angles

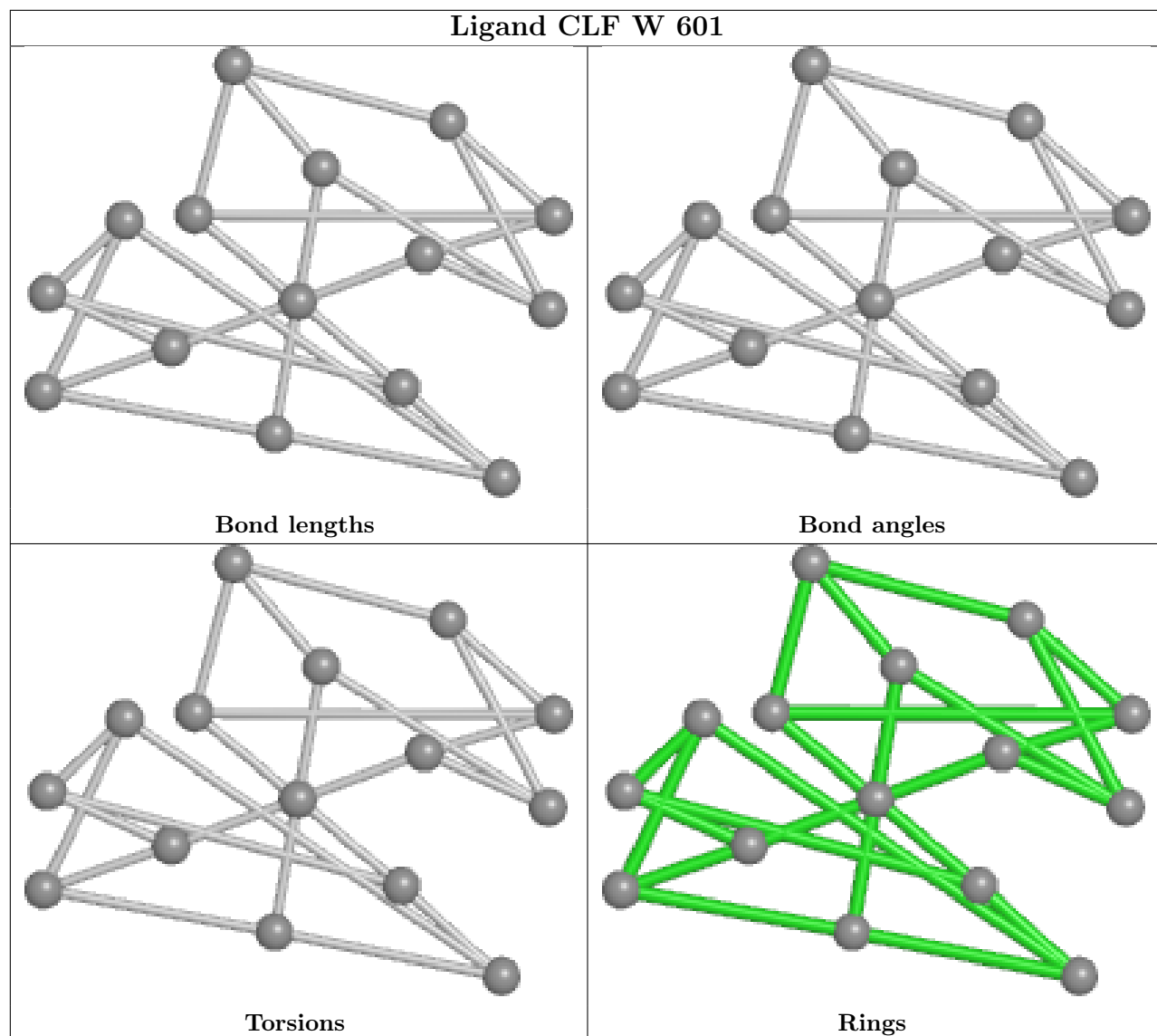


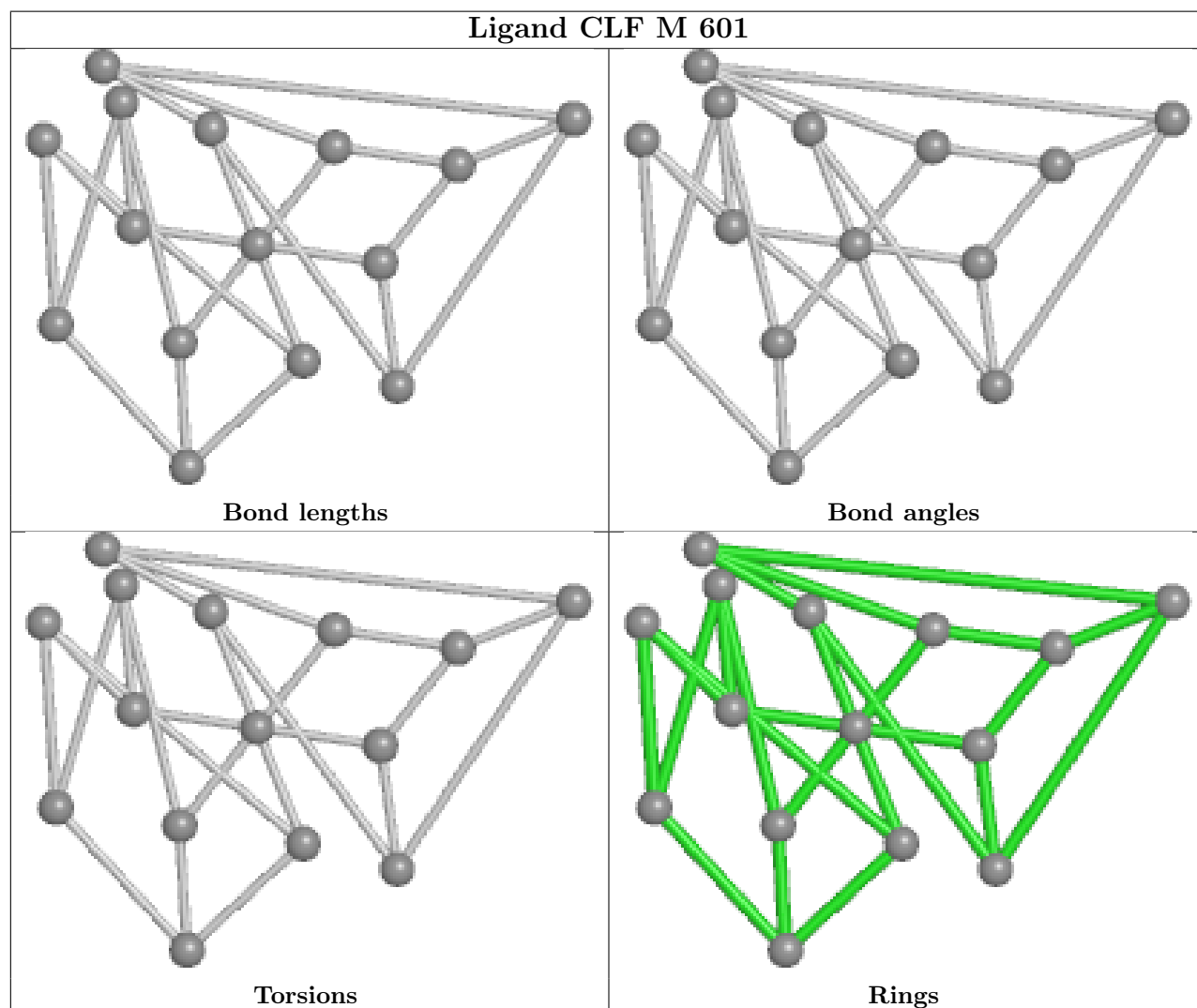
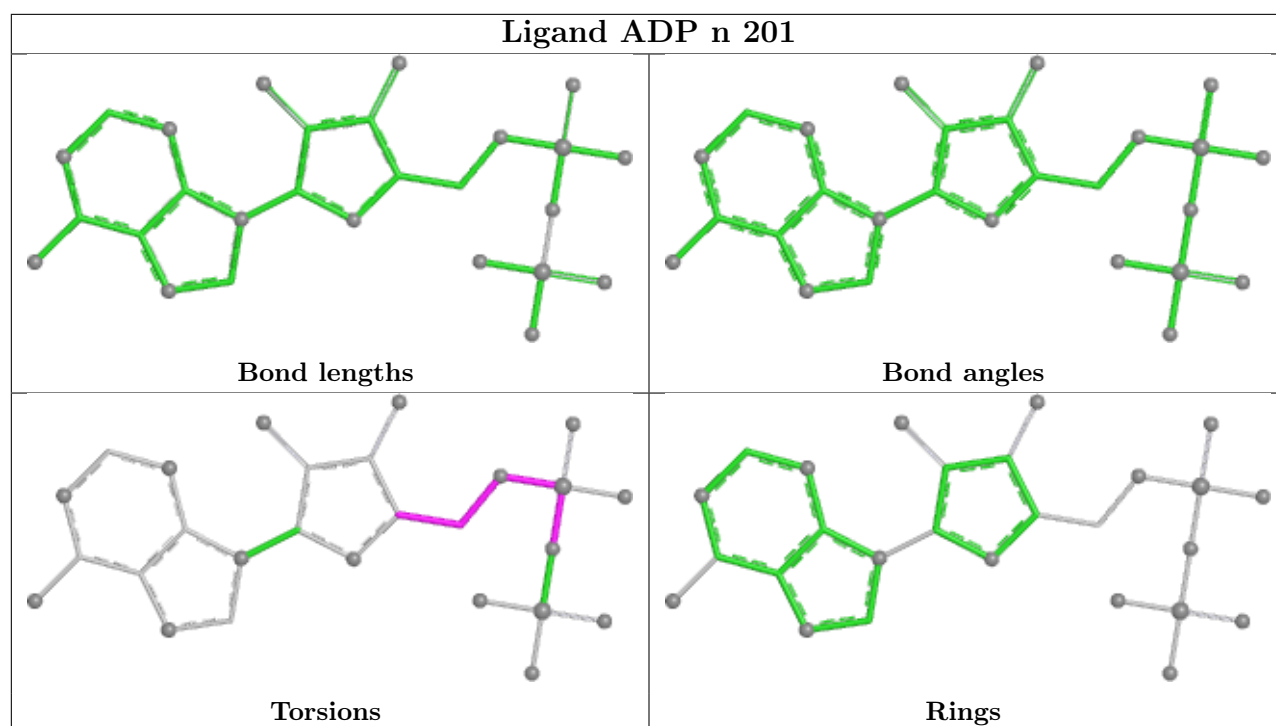
Torsions

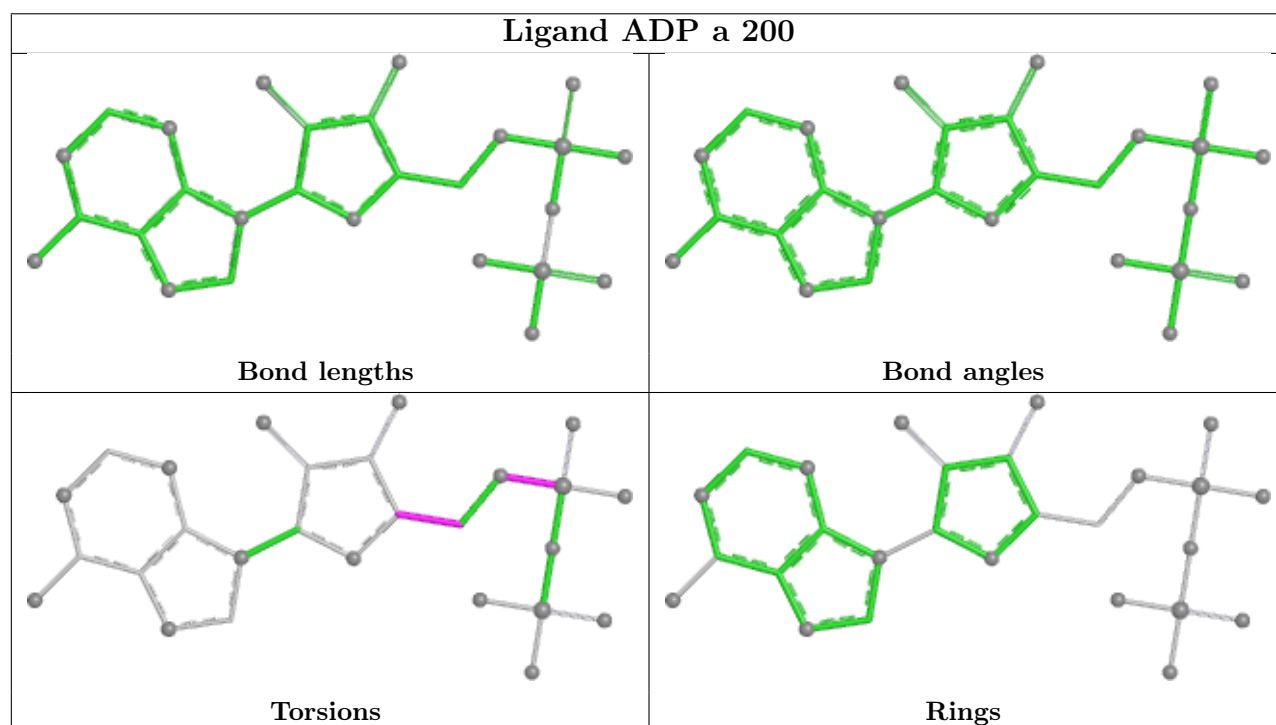
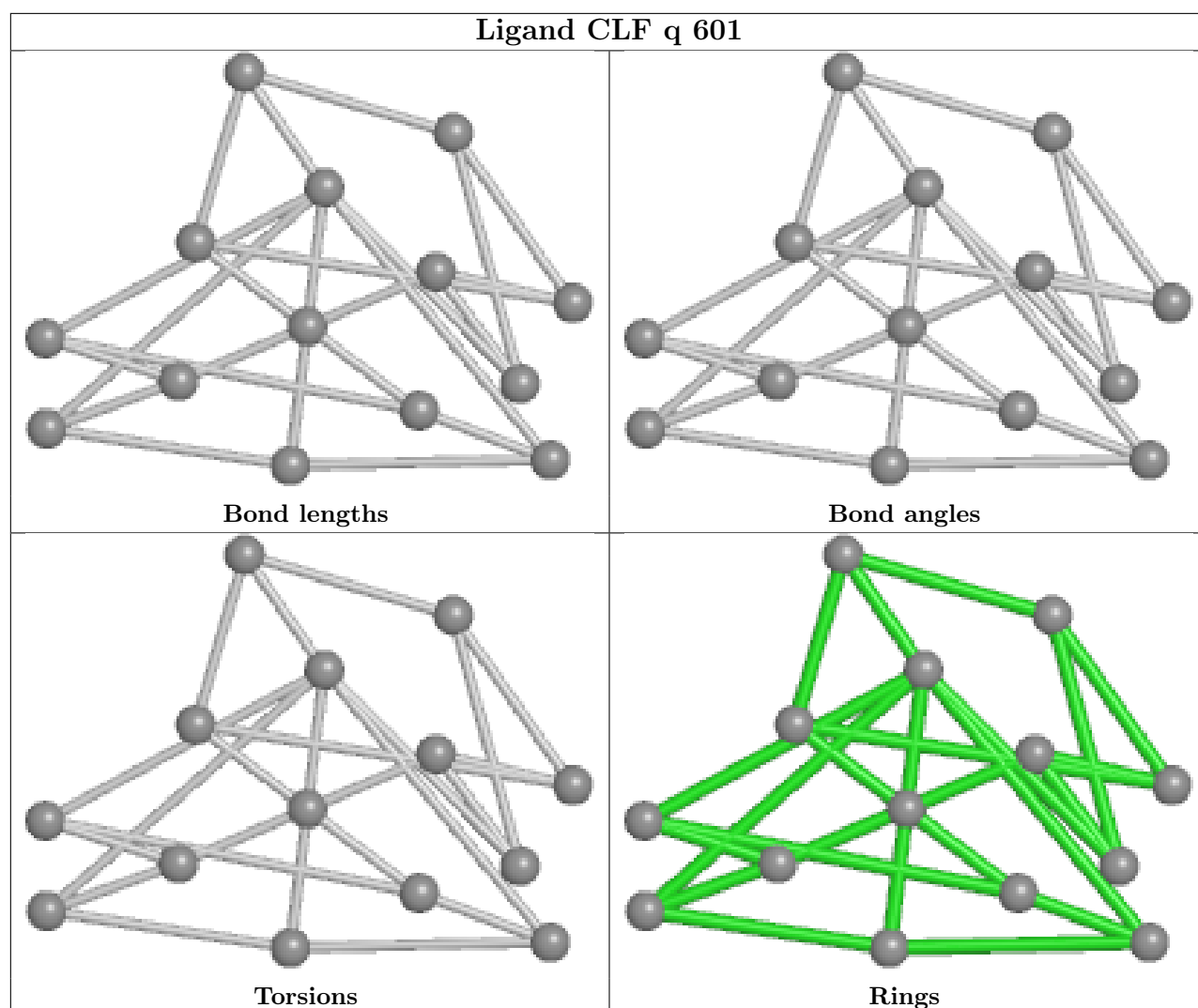


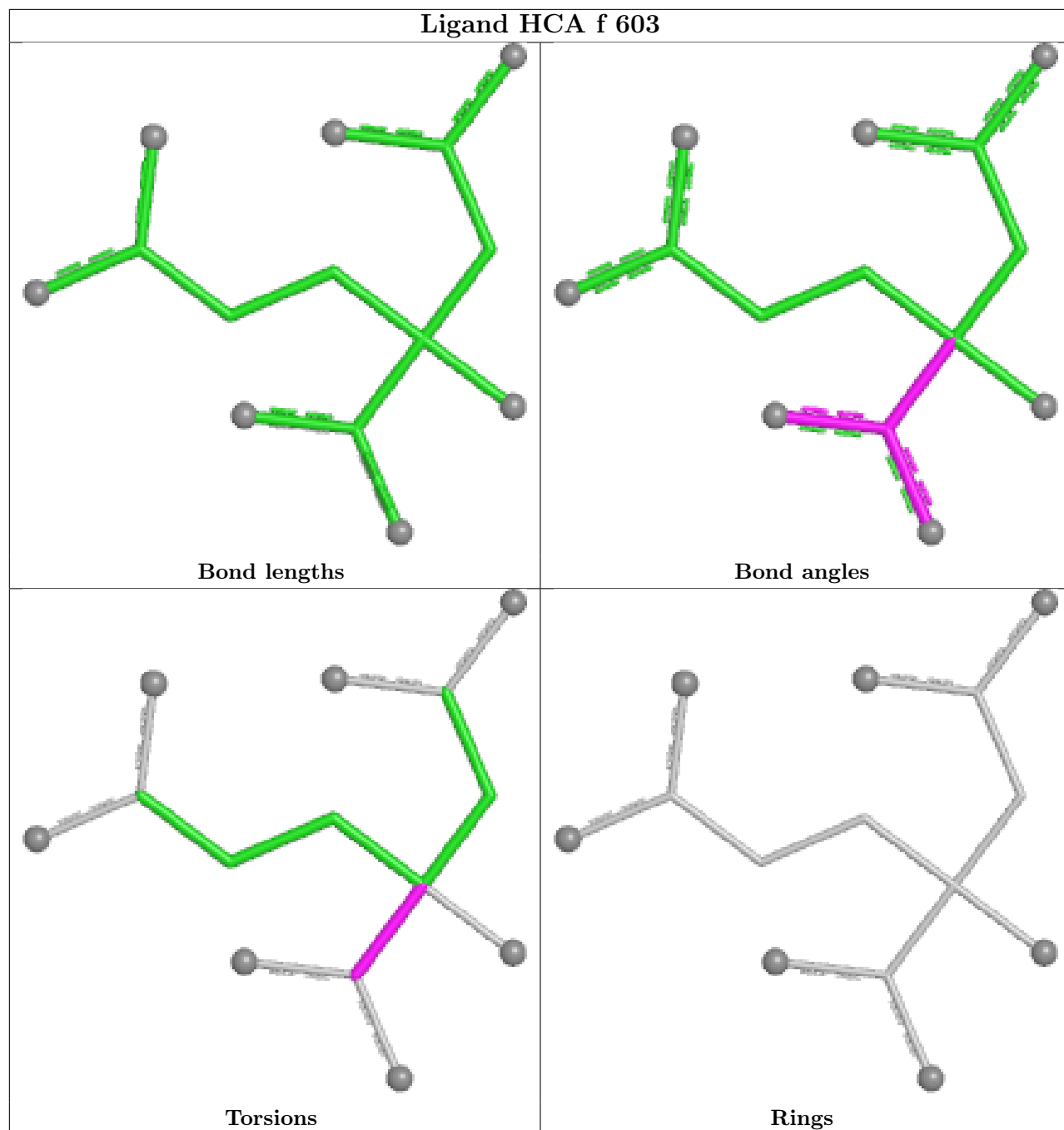
Rings

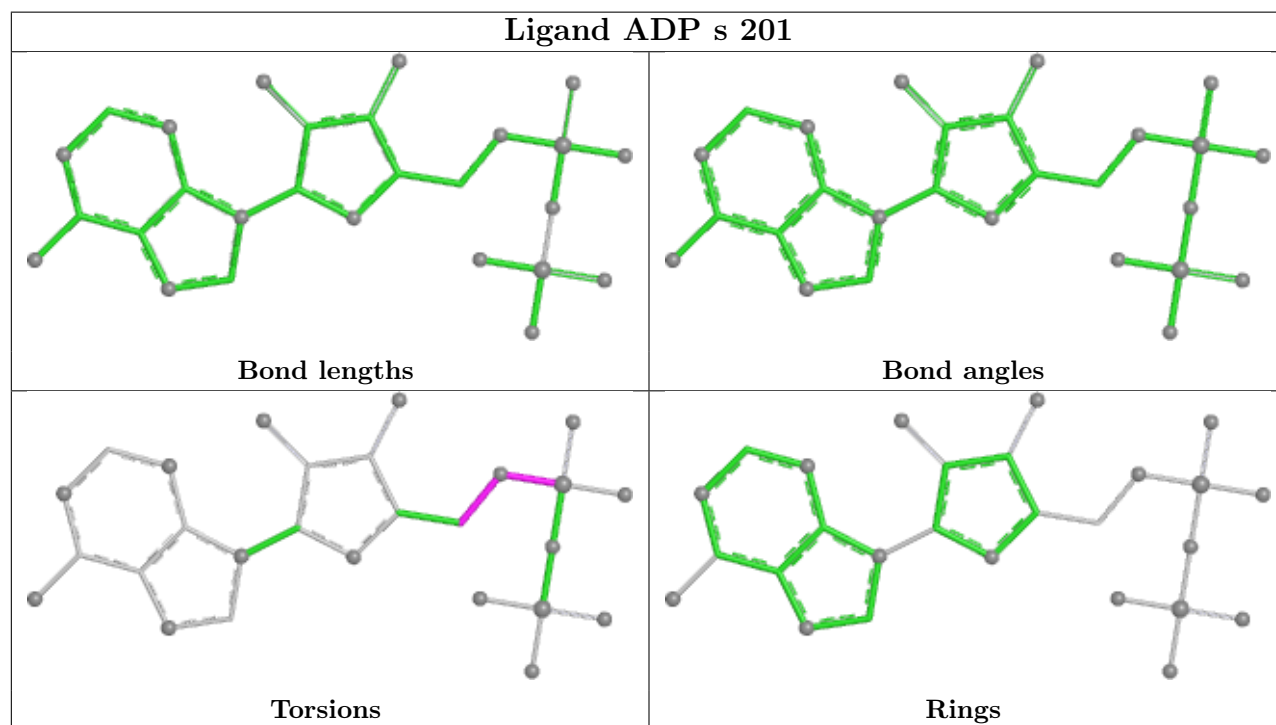
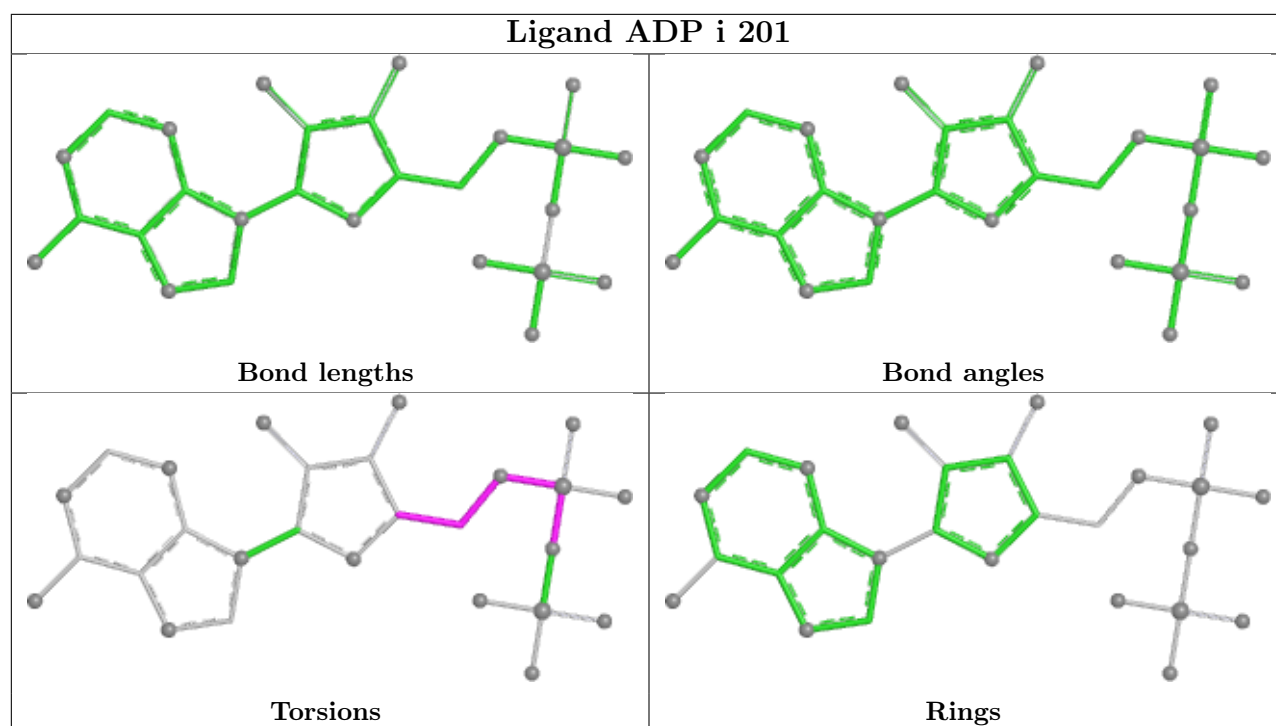


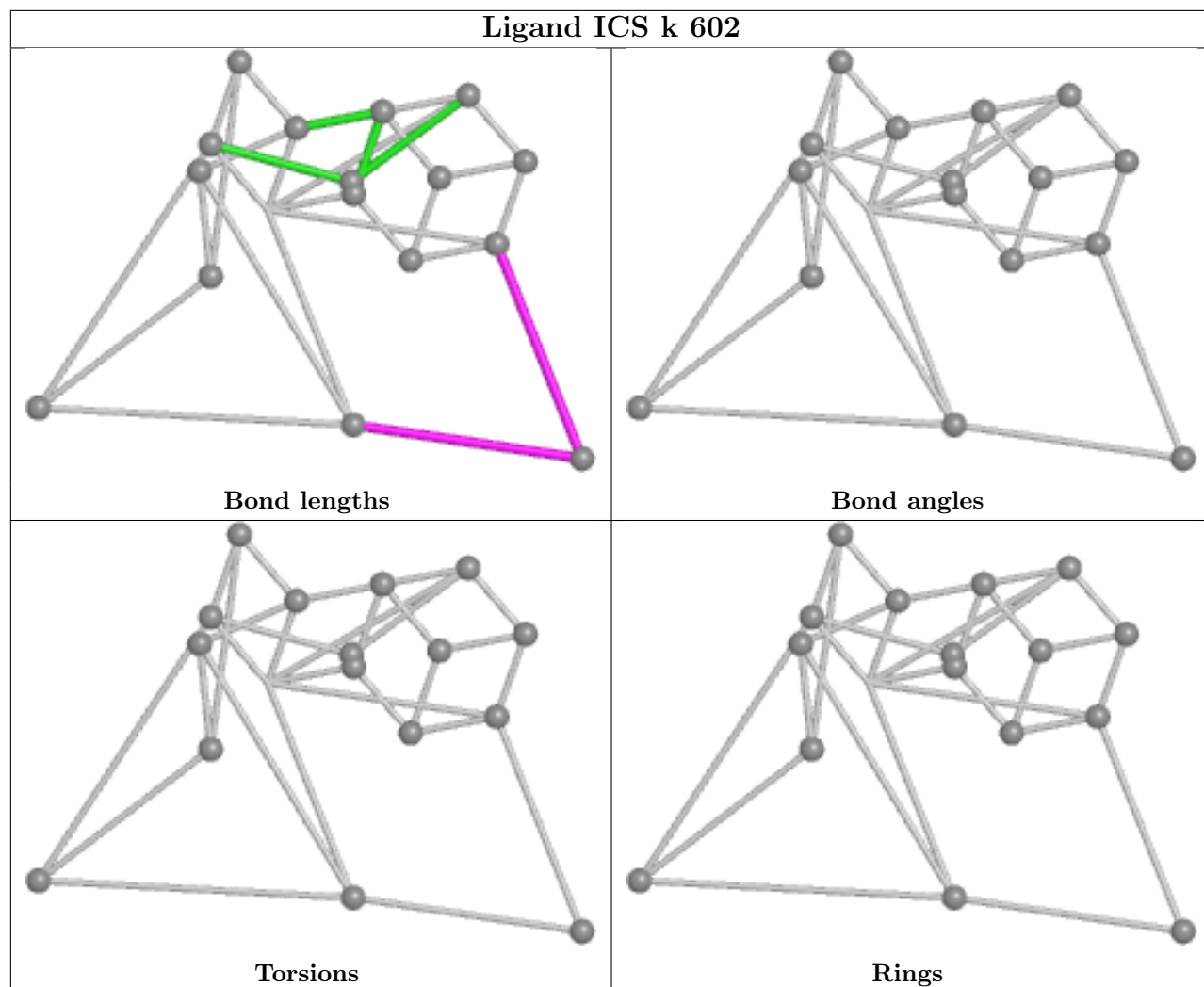


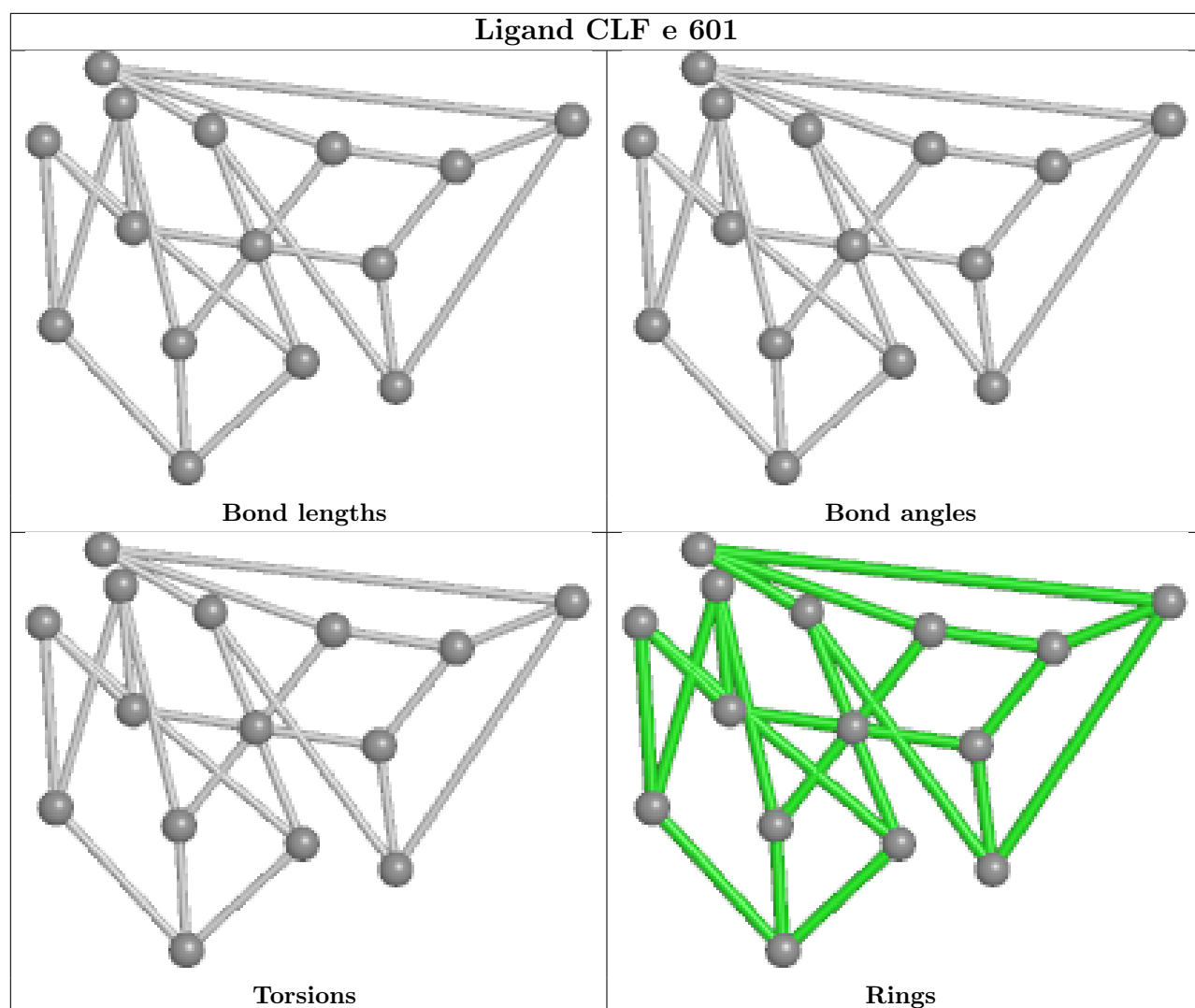


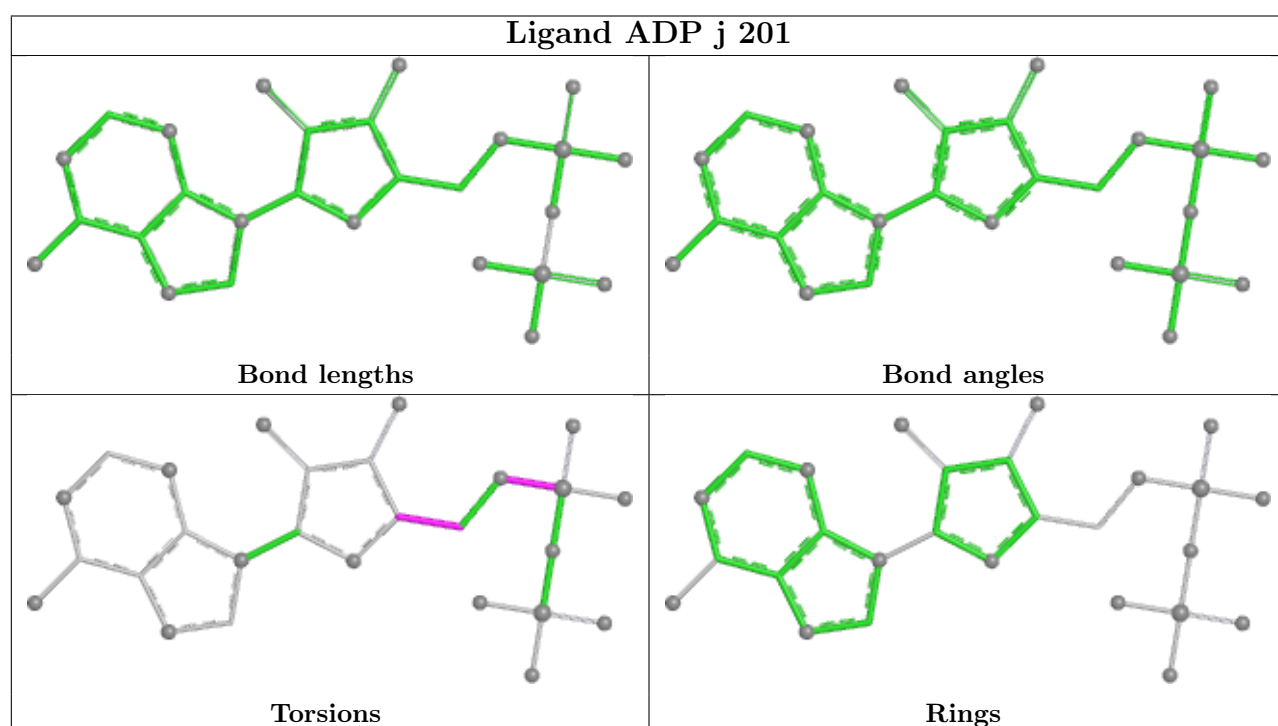
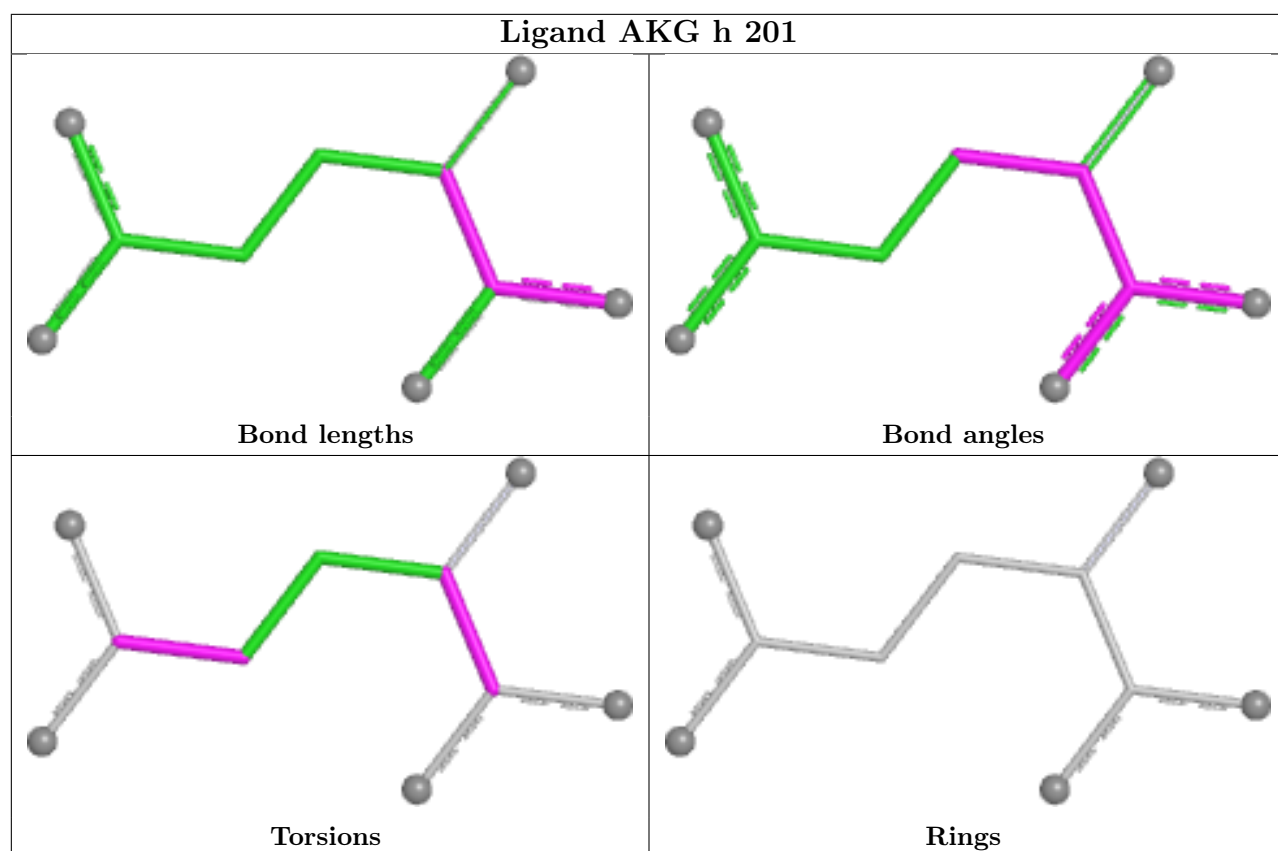


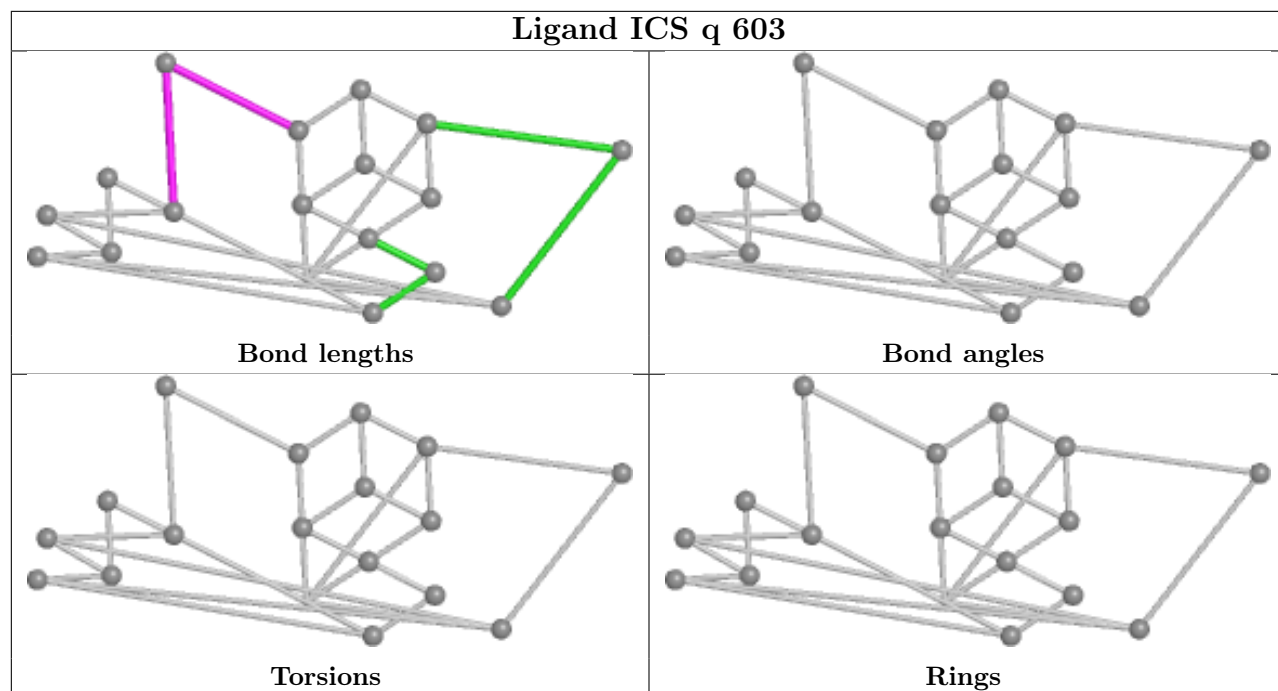


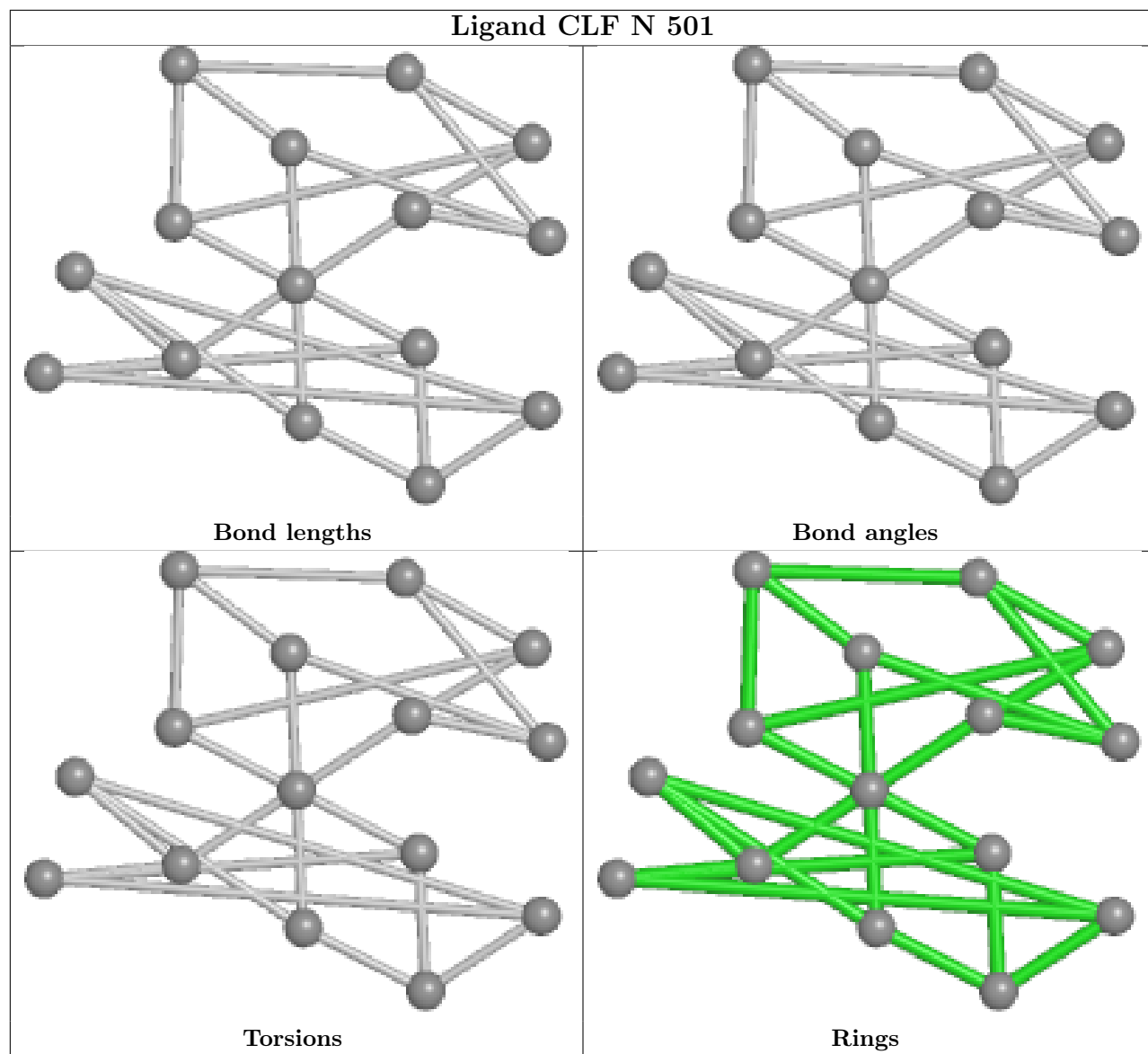




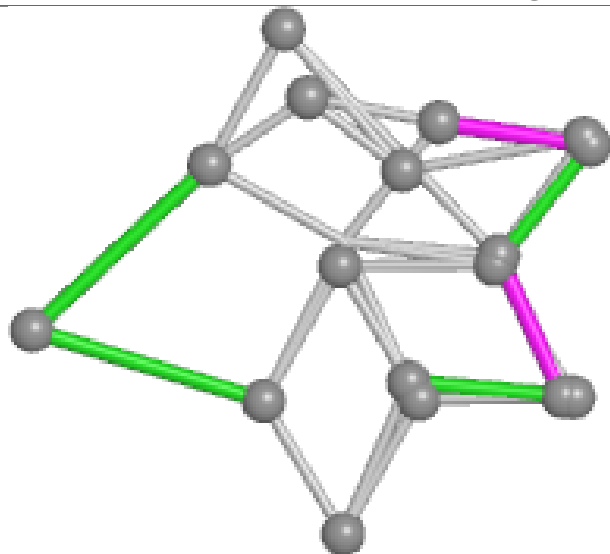




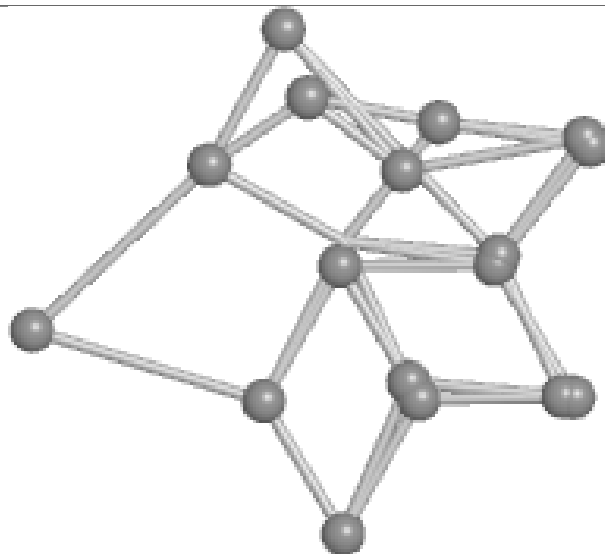




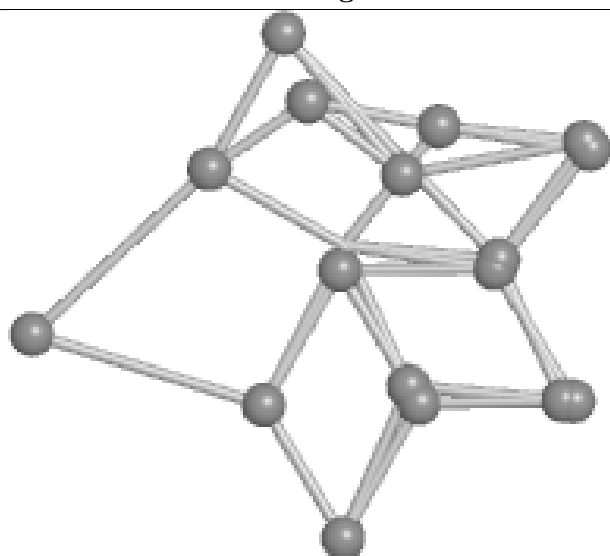
Ligand ICS e 602



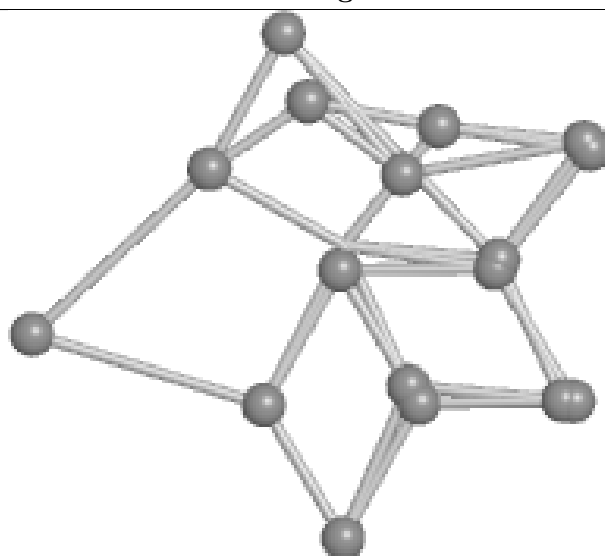
Bond lengths



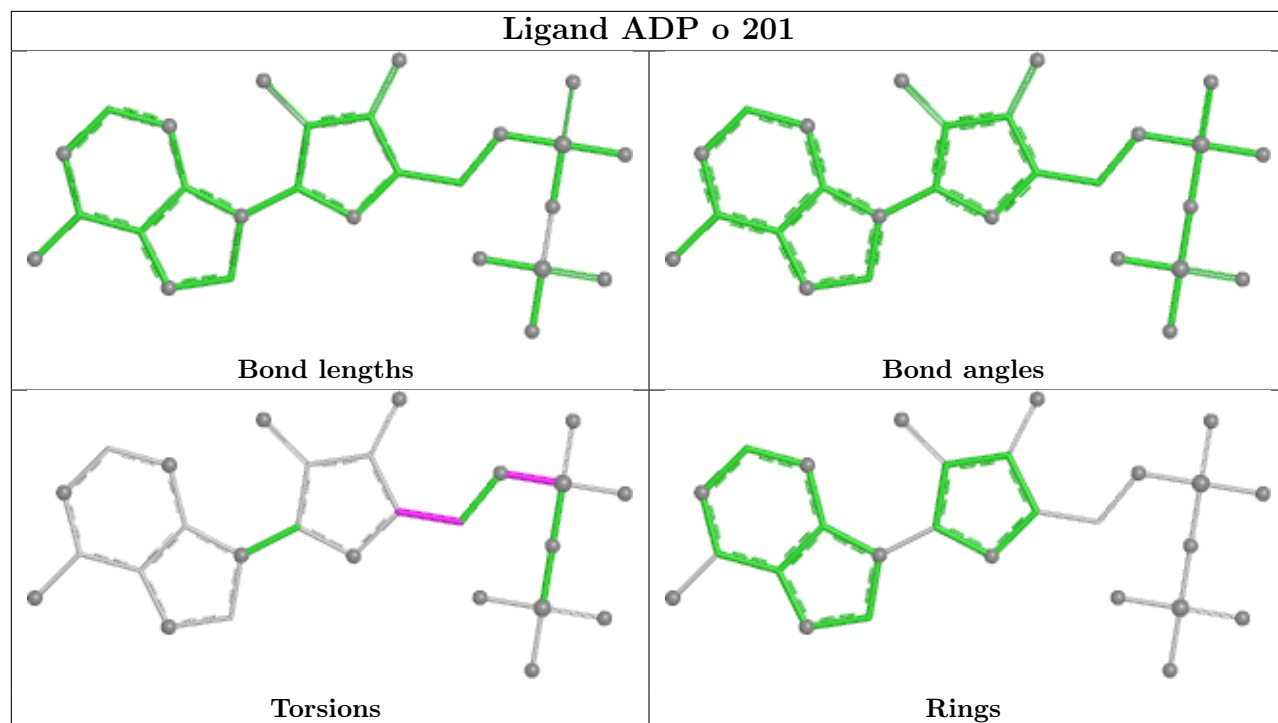
Bond angles

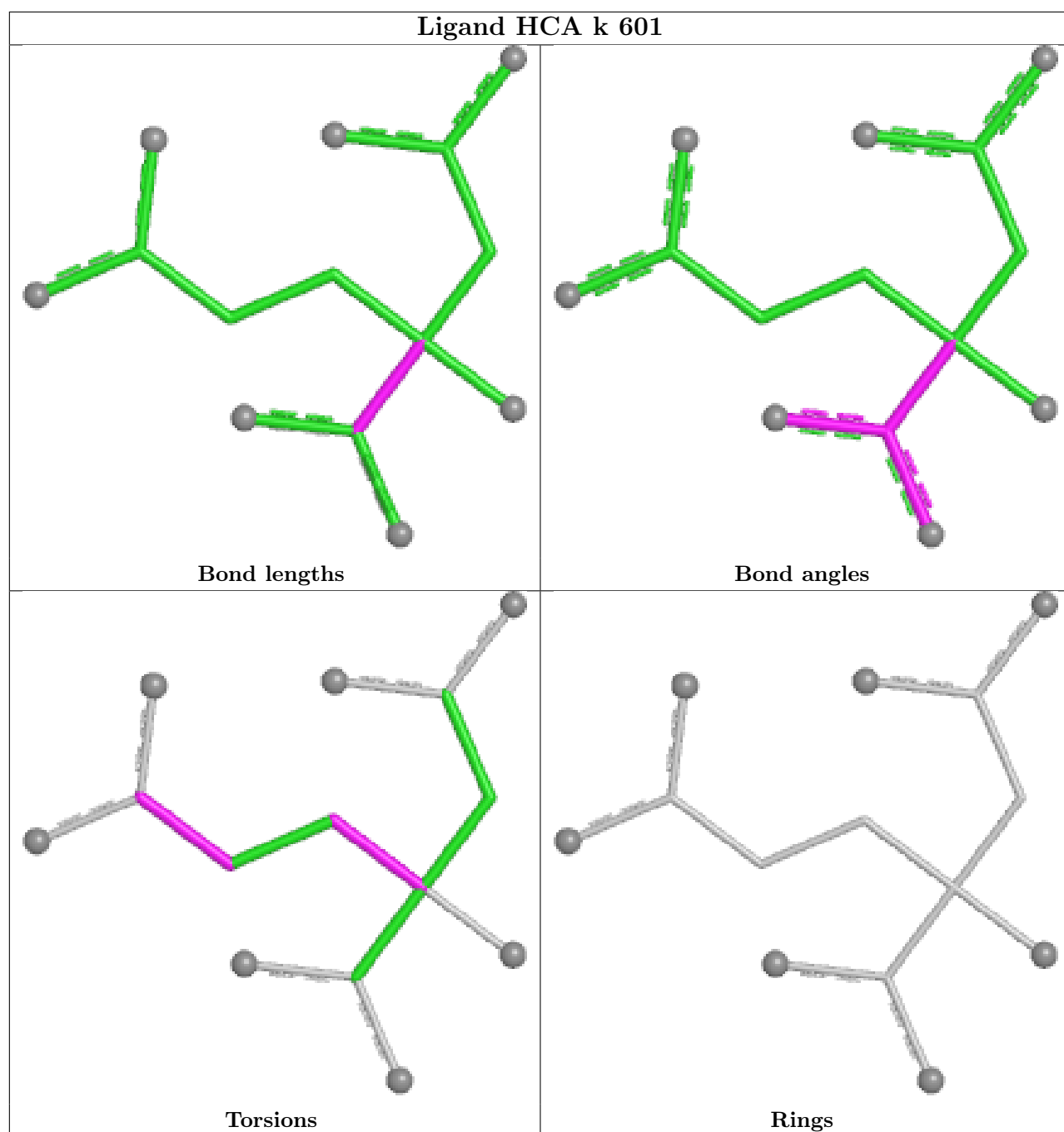


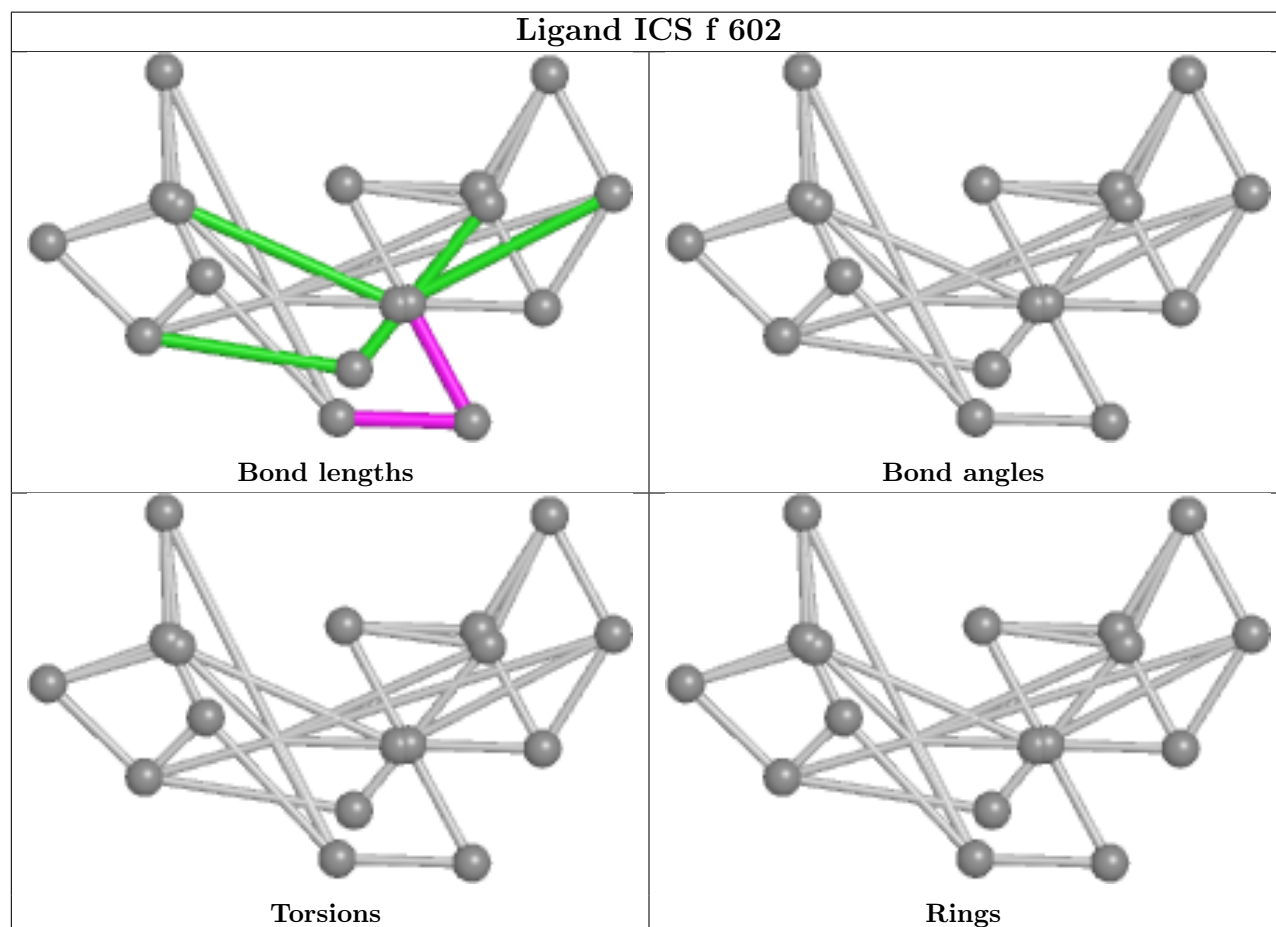
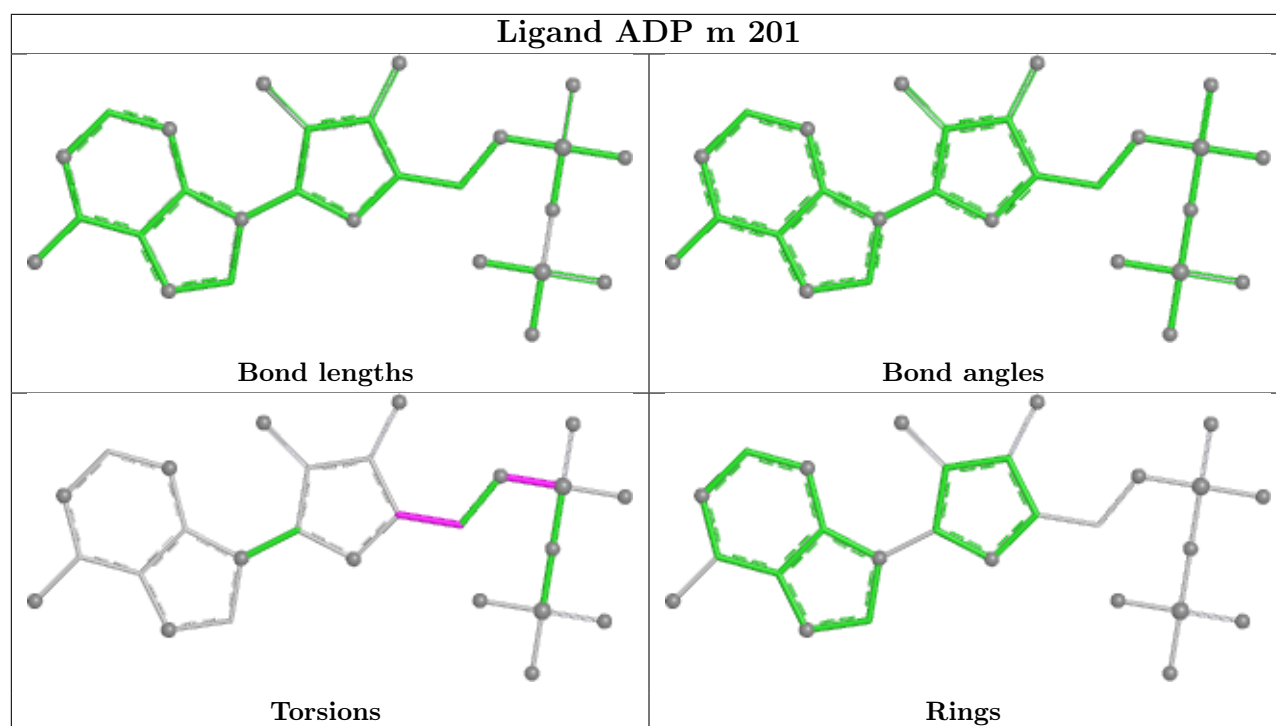
Torsions

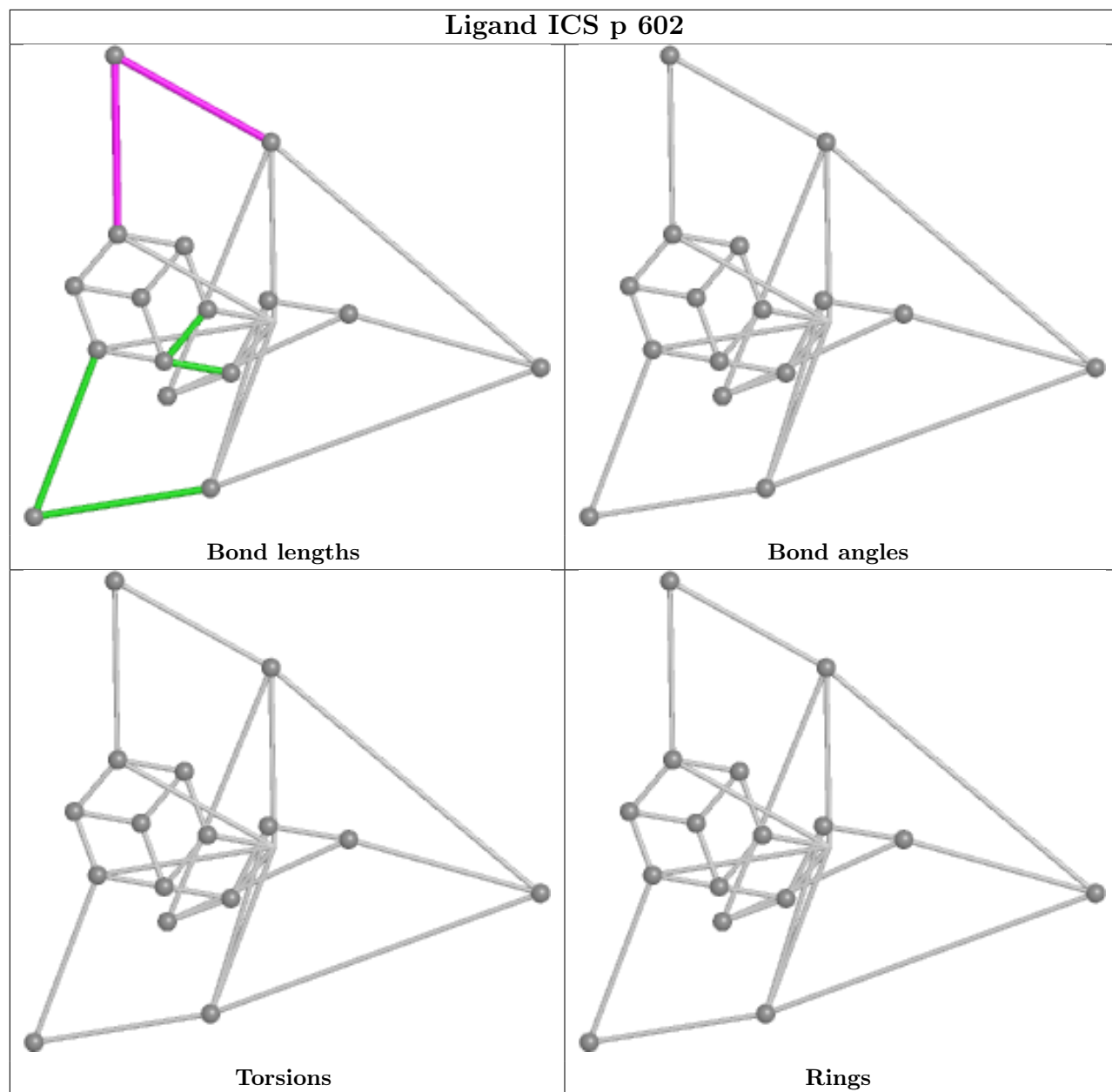


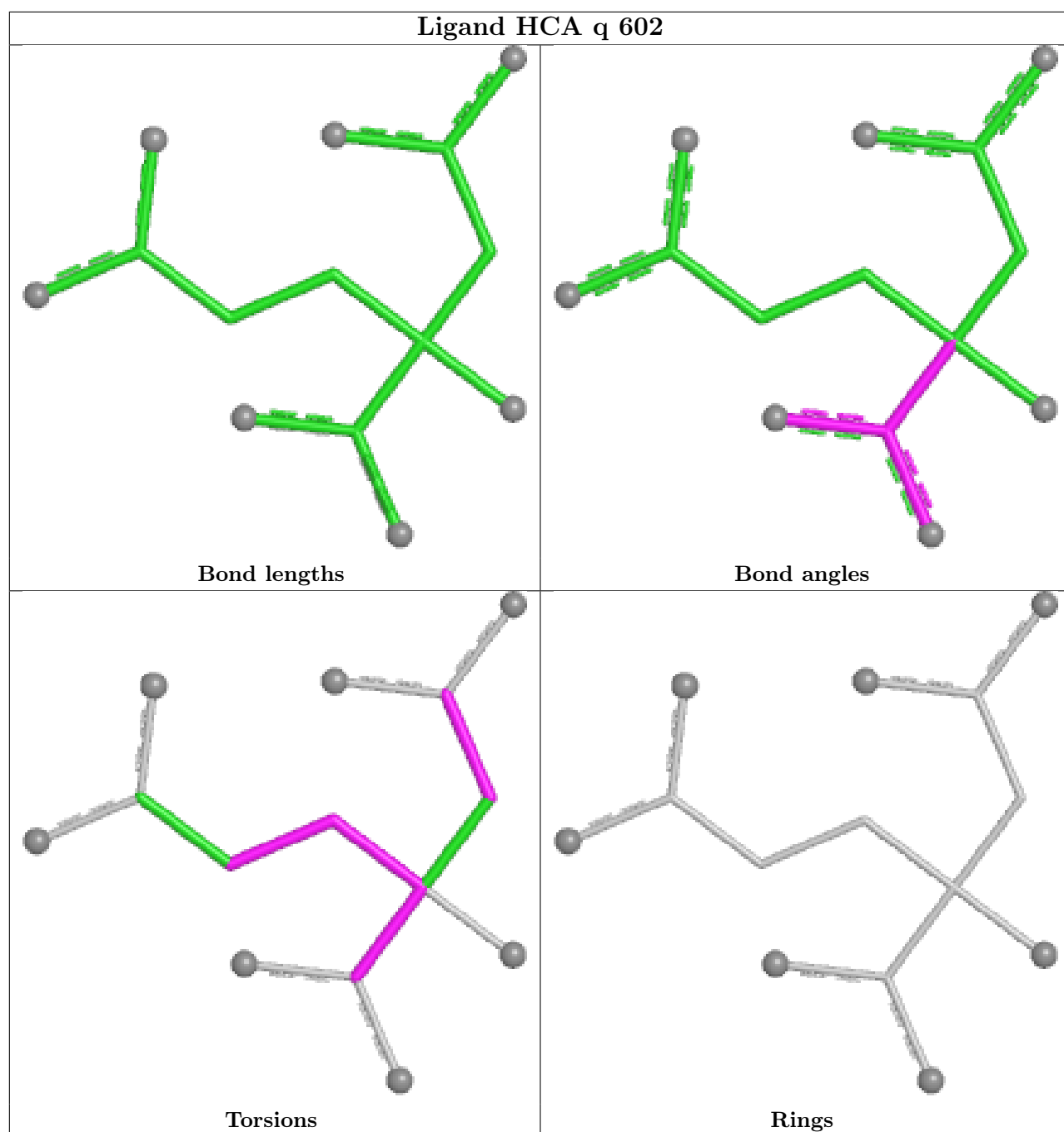
Rings

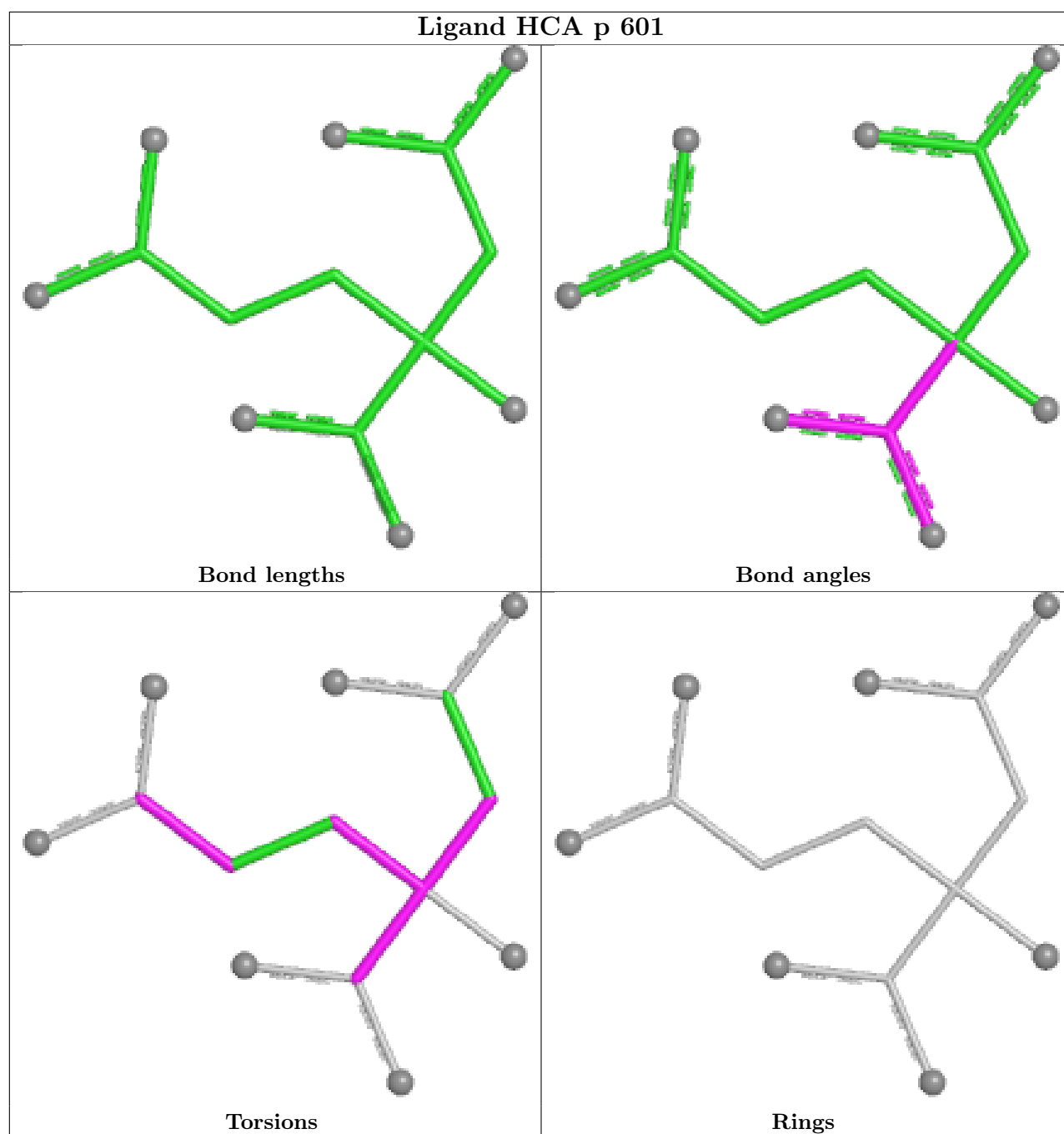


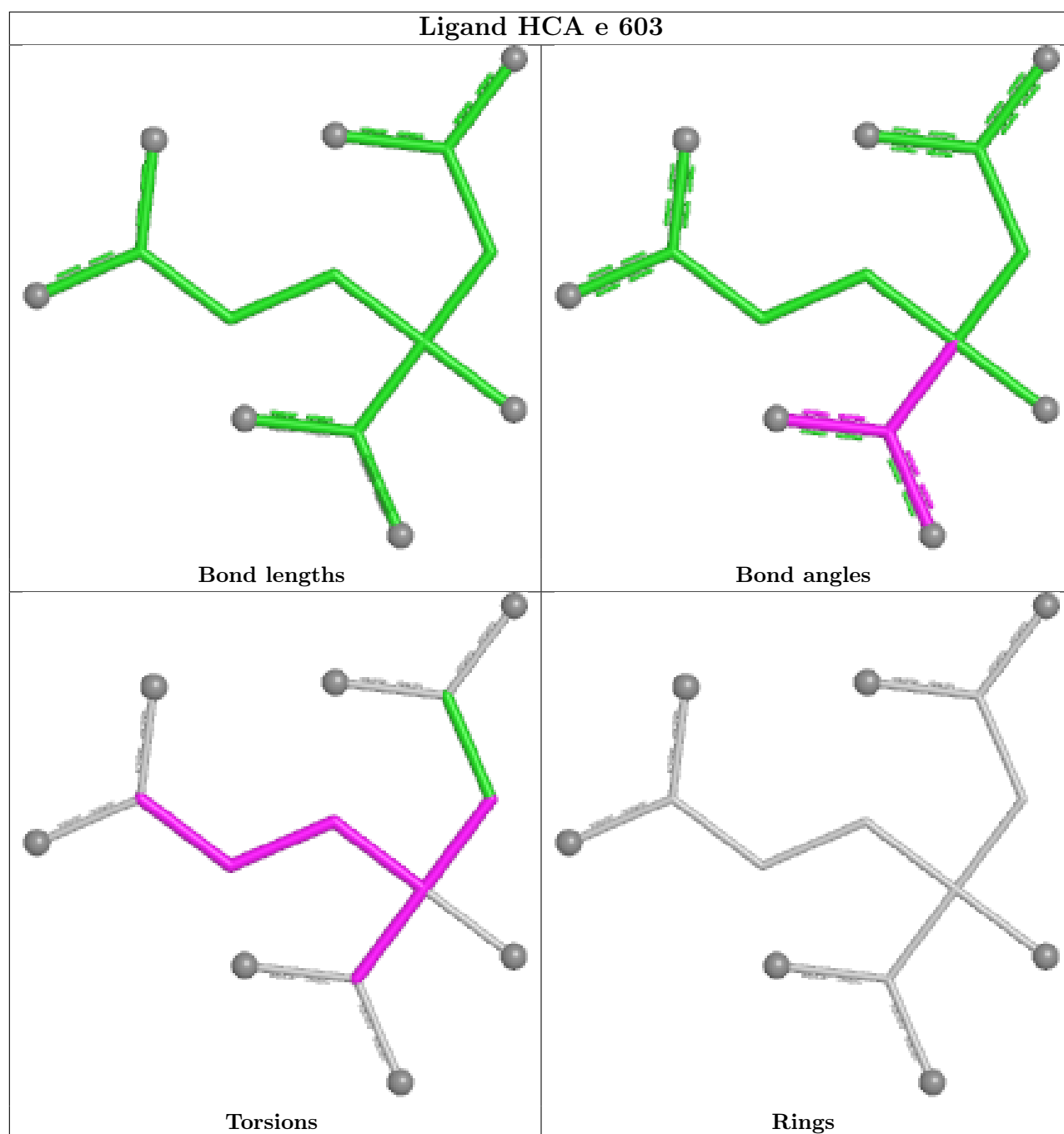


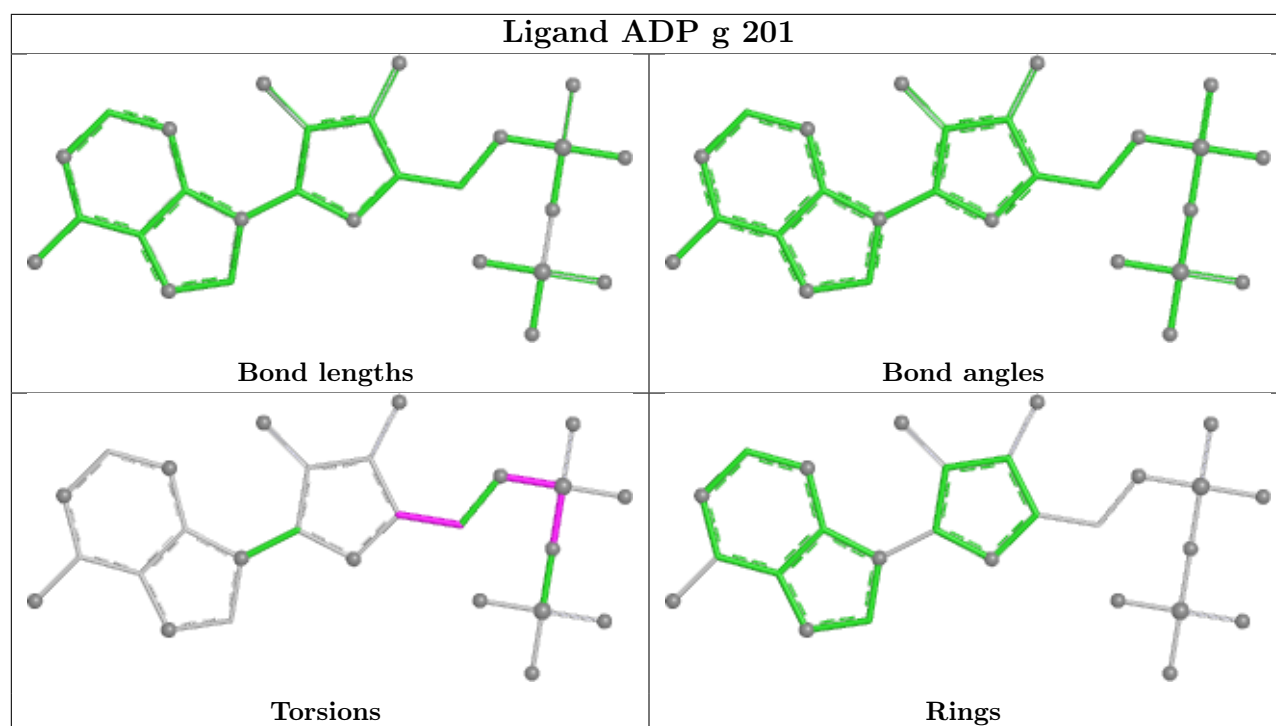












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

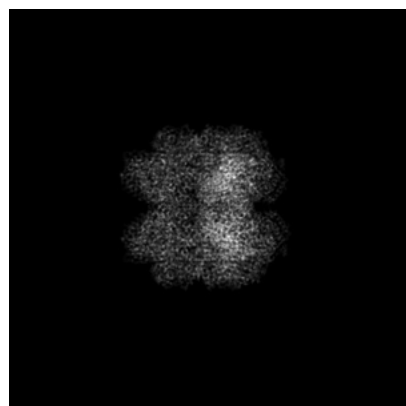
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-76263. These allow visual inspection of the internal detail of the map and identification of artifacts.

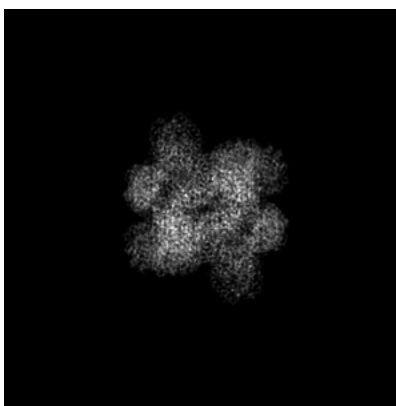
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

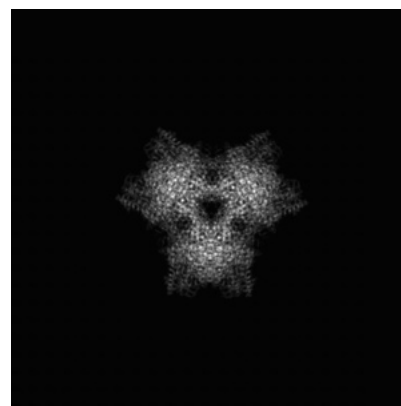
6.1.1 Primary map



X

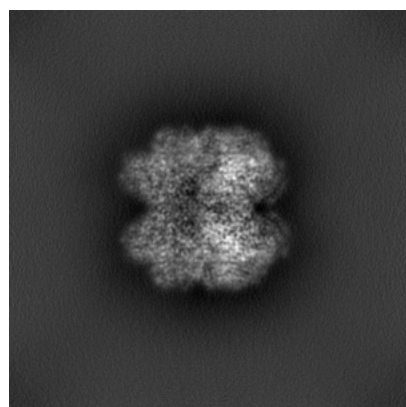


Y

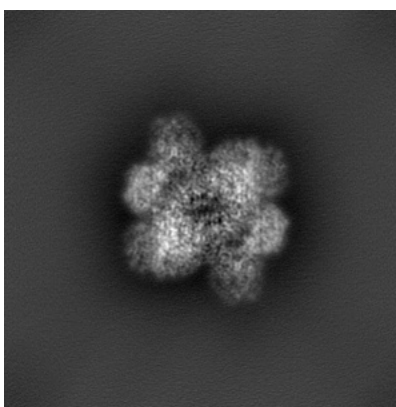


Z

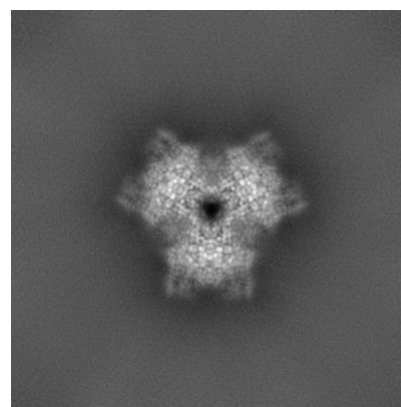
6.1.2 Raw map



X



Y



Z

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

6.2 Central slices [i](#)

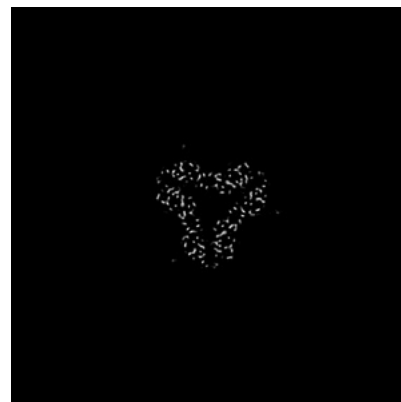
6.2.1 Primary map



X Index: 200

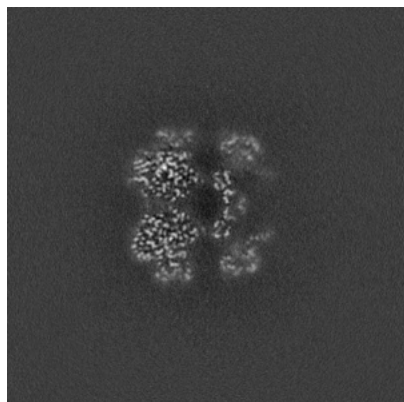


Y Index: 200

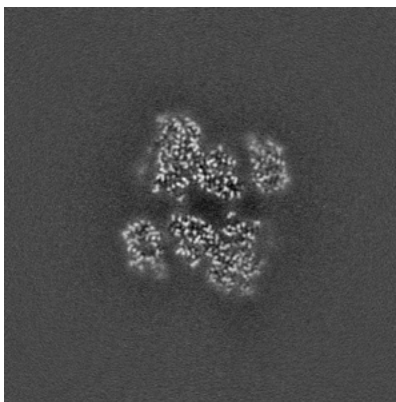


Z Index: 200

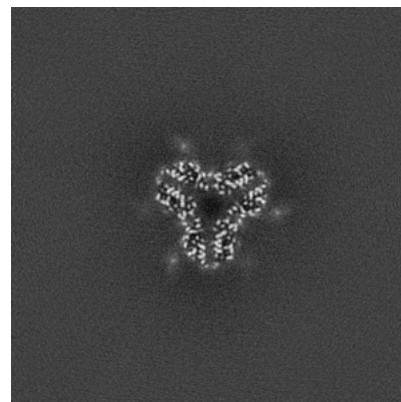
6.2.2 Raw map



X Index: 200



Y Index: 200



Z Index: 200

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: 180

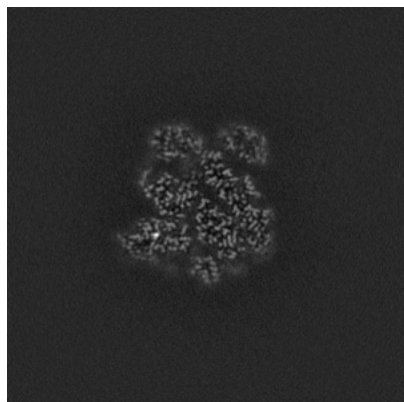


Y Index: 217

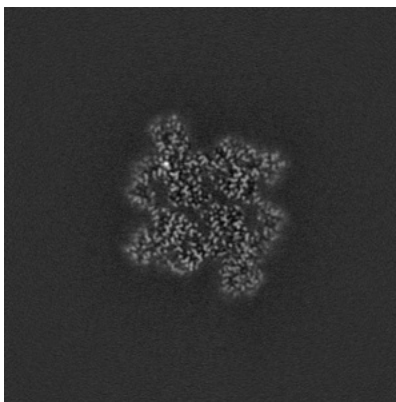


Z Index: 168

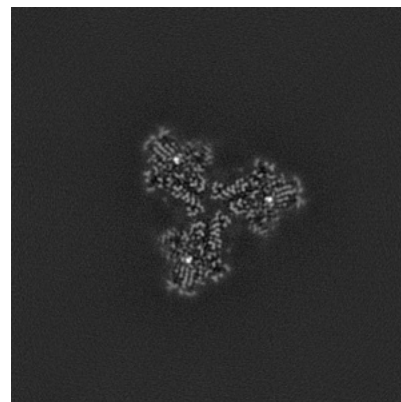
6.3.2 Raw map



X Index: 180



Y Index: 217

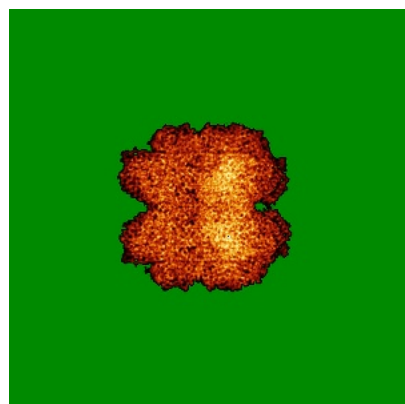


Z Index: 169

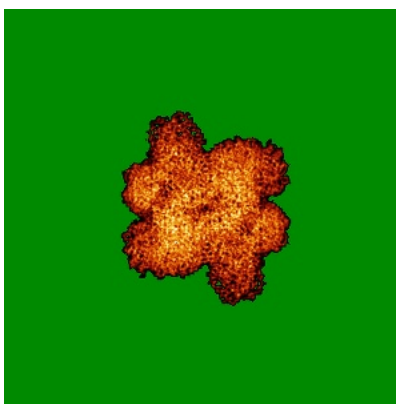
The images above show the largest variance slices of the map in three orthogonal directions.

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

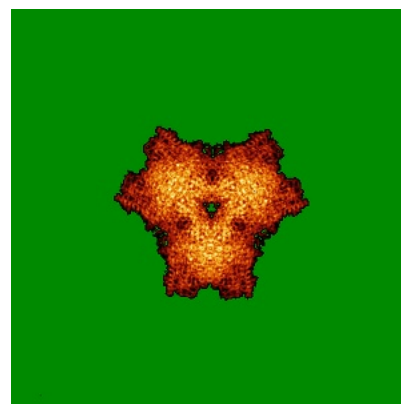
6.4.1 Primary map



X

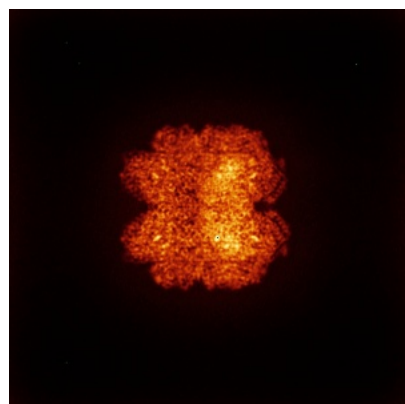


Y

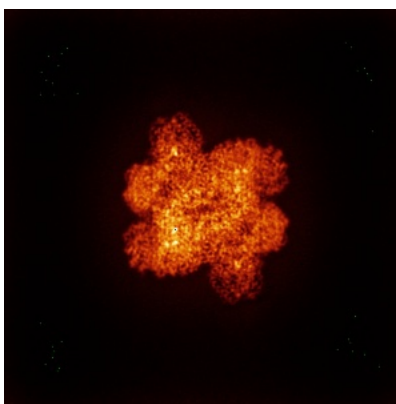


Z

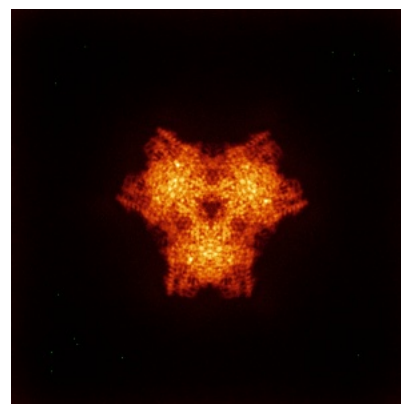
6.4.2 Raw map



X



Y

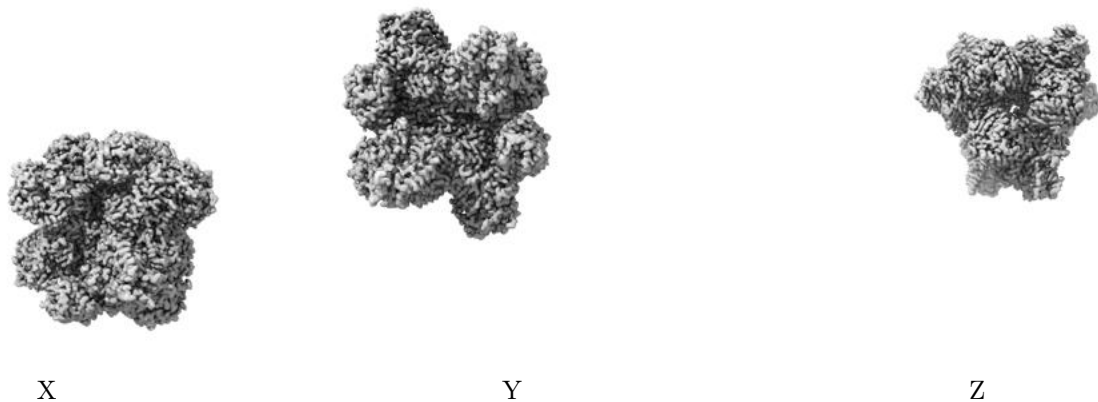


Z

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.

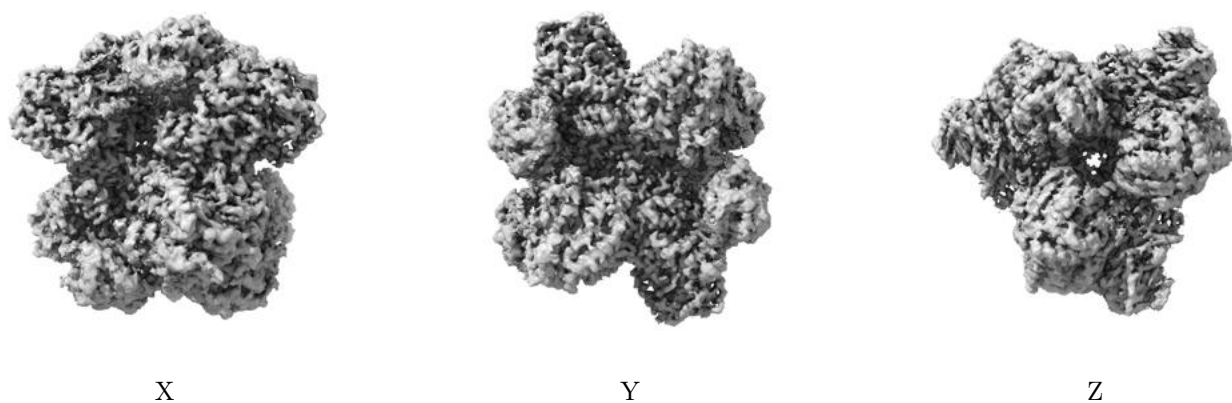
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0141. 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.

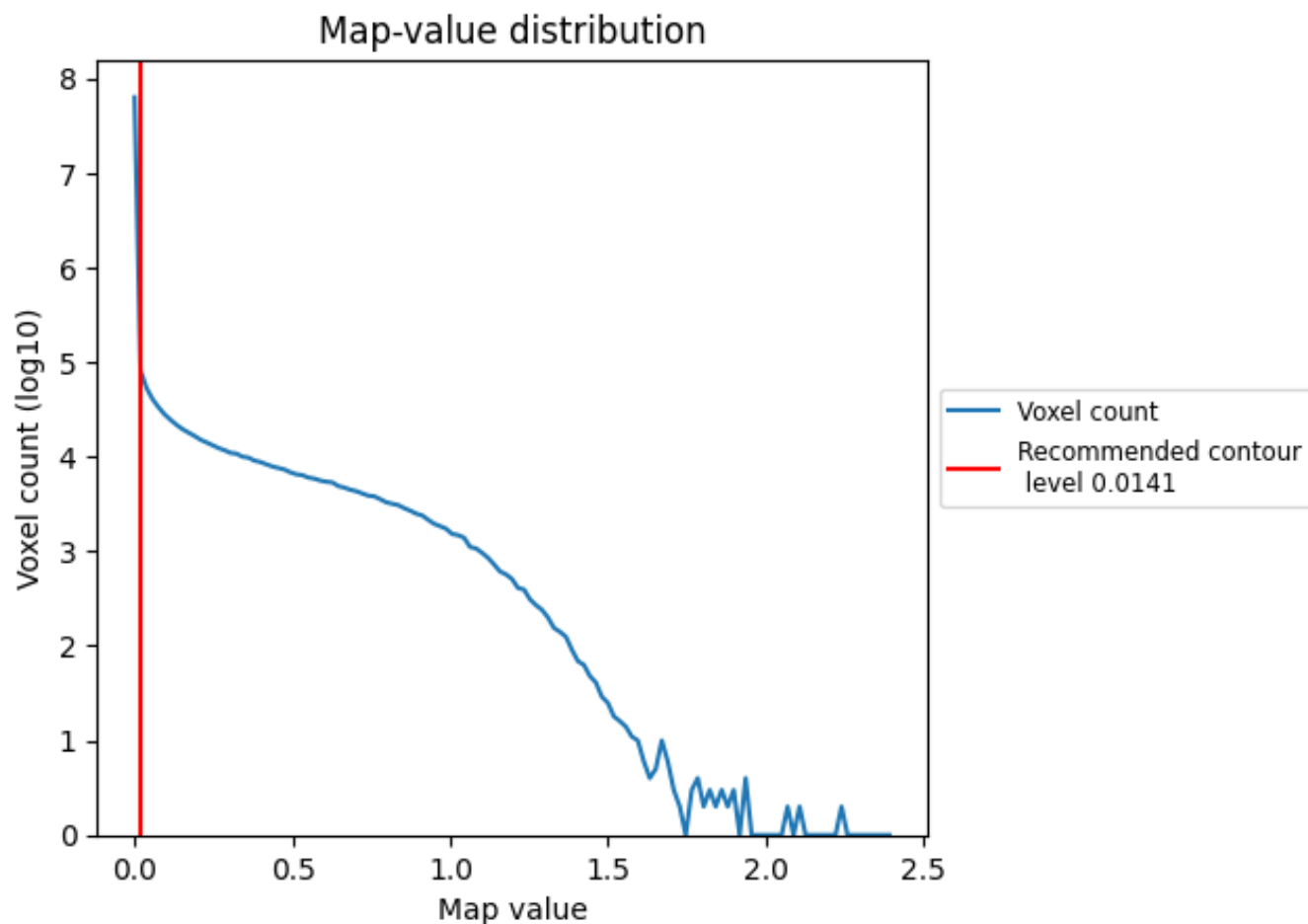
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

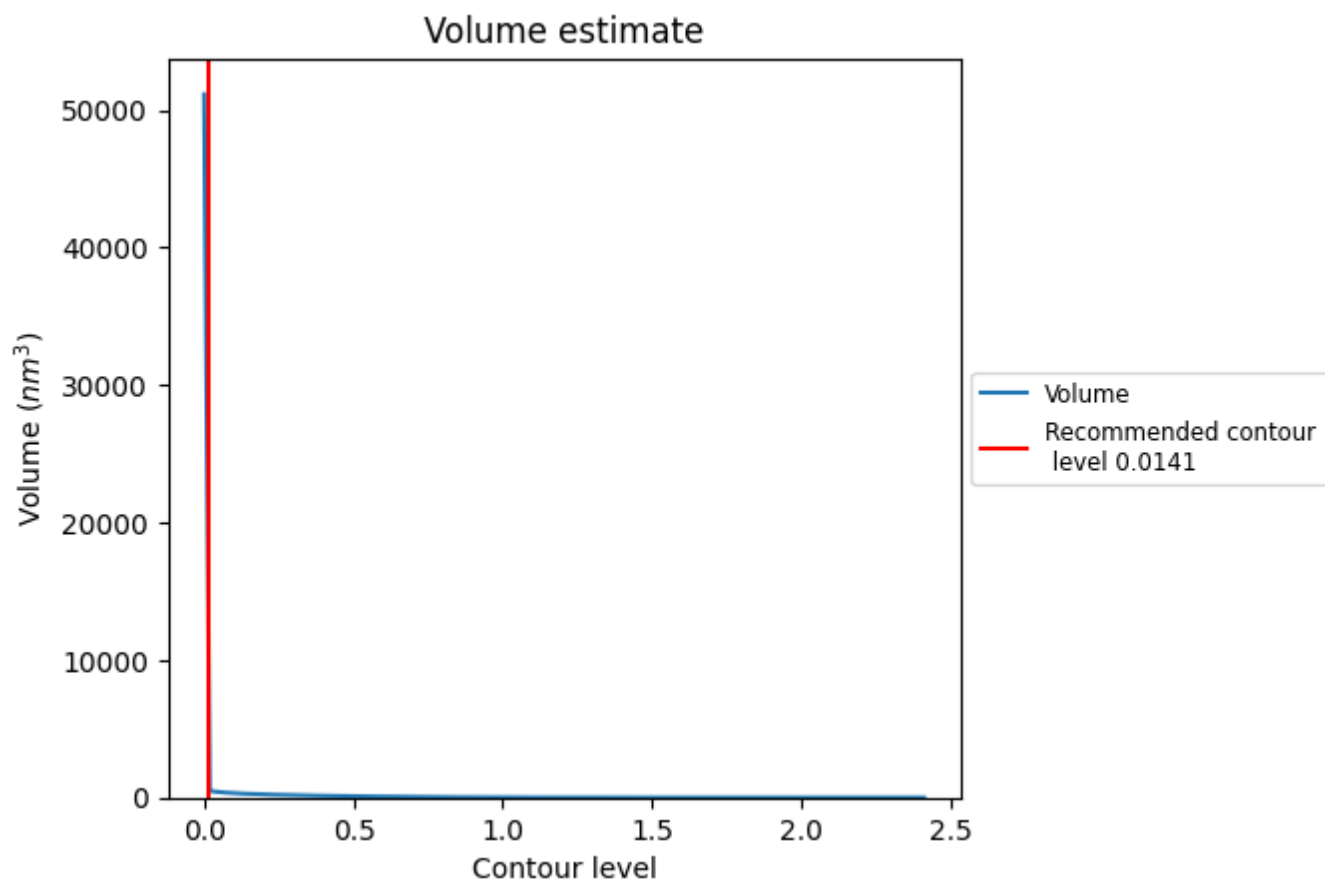
This section contains the results of statistical analysis of the map.

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.

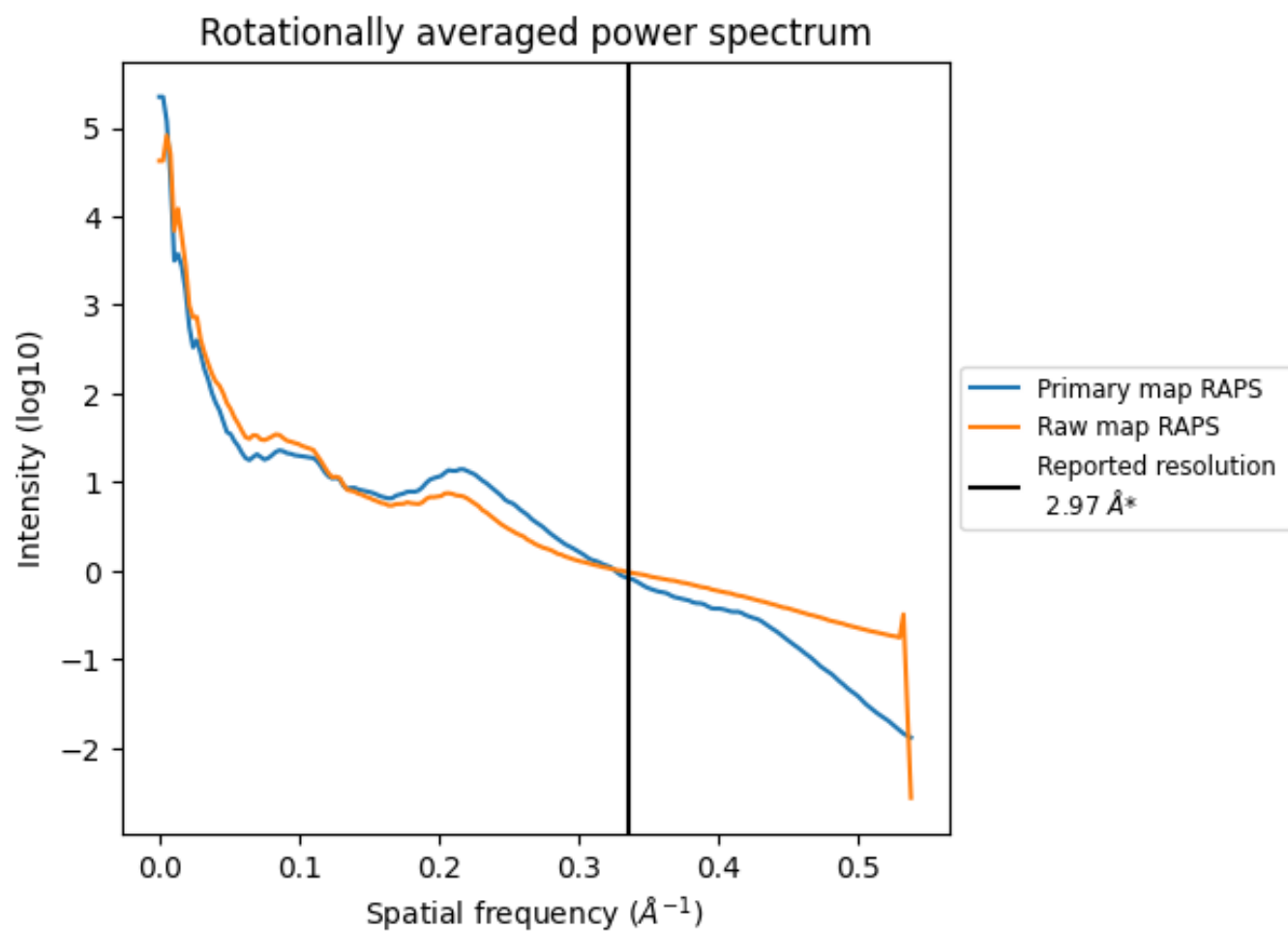
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 8528 nm³; this corresponds to an approximate mass of 7703 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 ⓘ

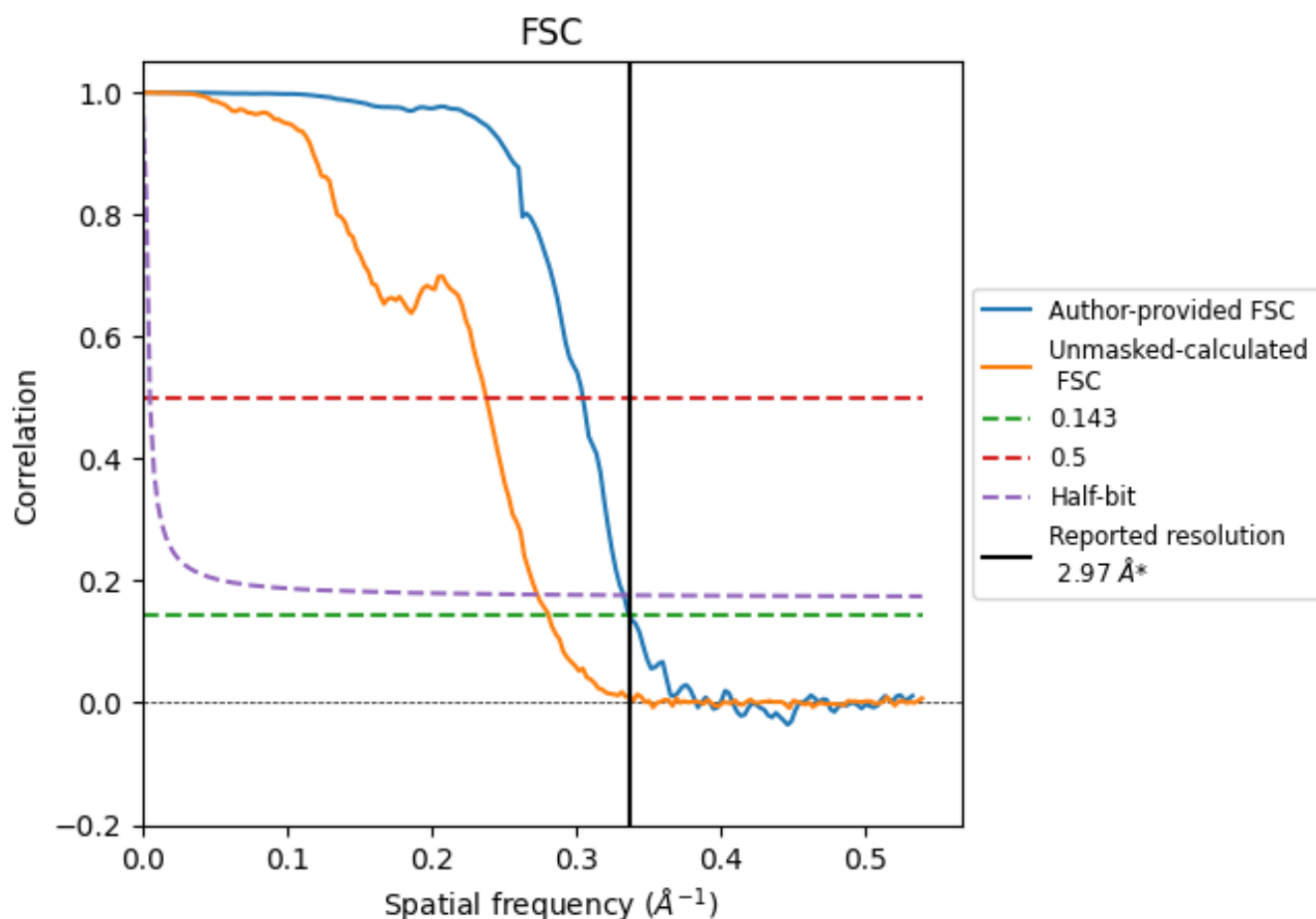


*Reported resolution corresponds to spatial frequency of $0.337 \text{ \AA}^{-1}$

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 $0.337 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

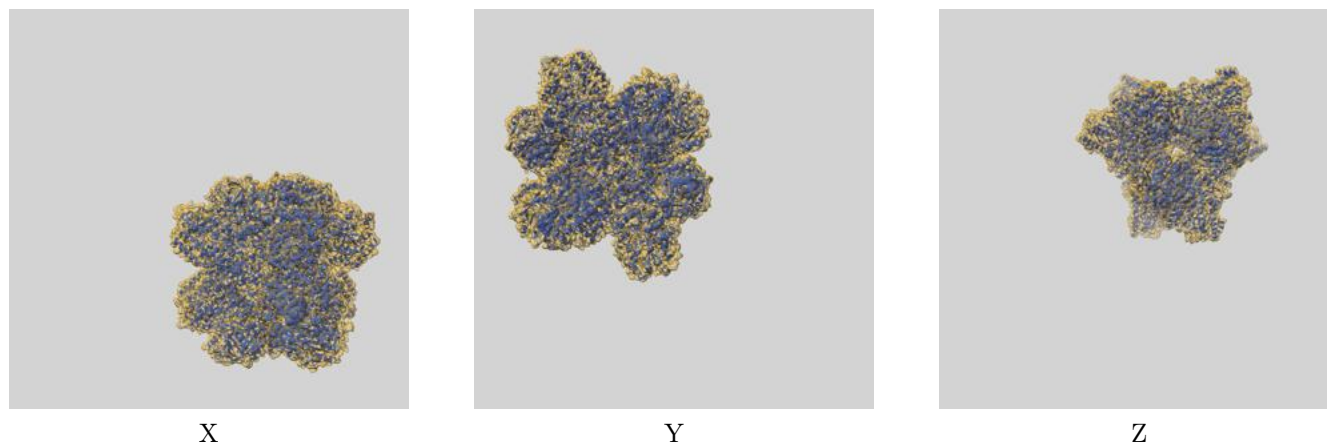
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.97	-	-
Author-provided FSC curve	2.97	3.29	3.01
Unmasked-calculated*	3.56	4.21	3.66

*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 3.56 differs from the reported value 2.97 by more than 10 %

9 Map-model fit [i](#)

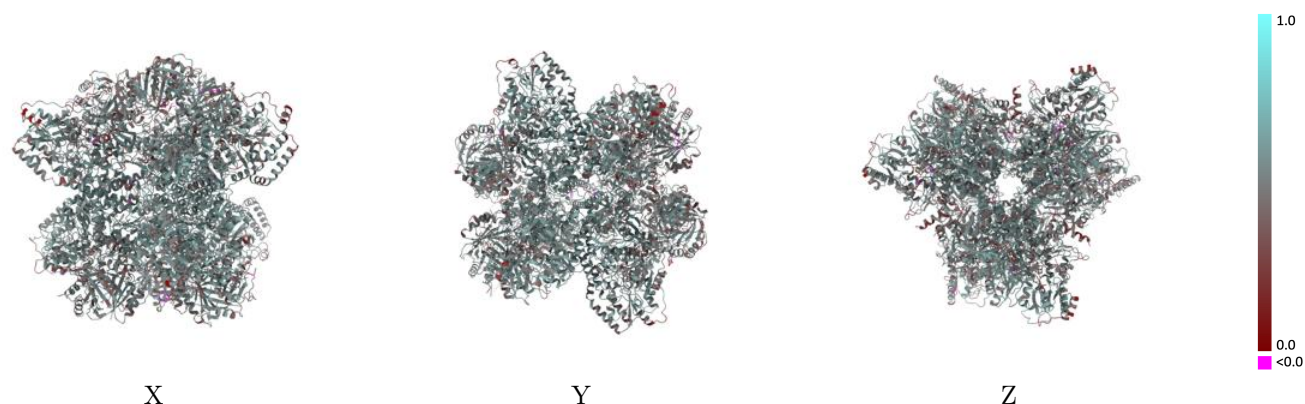
This section contains information regarding the fit between EMDB map EMD-76263 and PDB model 12AH. Per-residue inclusion information can be found in section [3](#) on page [16](#).

9.1 Map-model overlay [i](#)



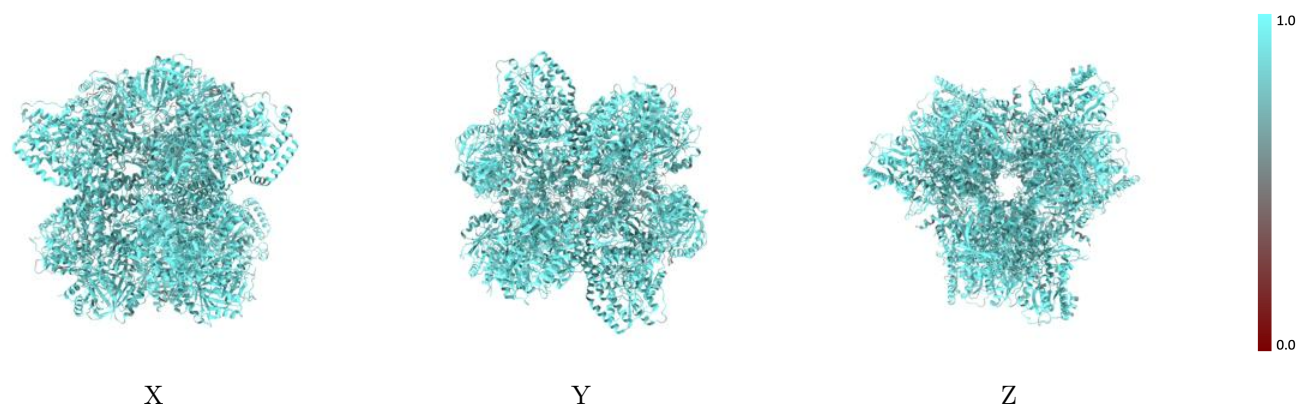
The images above show the 3D surface view of the map at the recommended contour level 0.0141 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



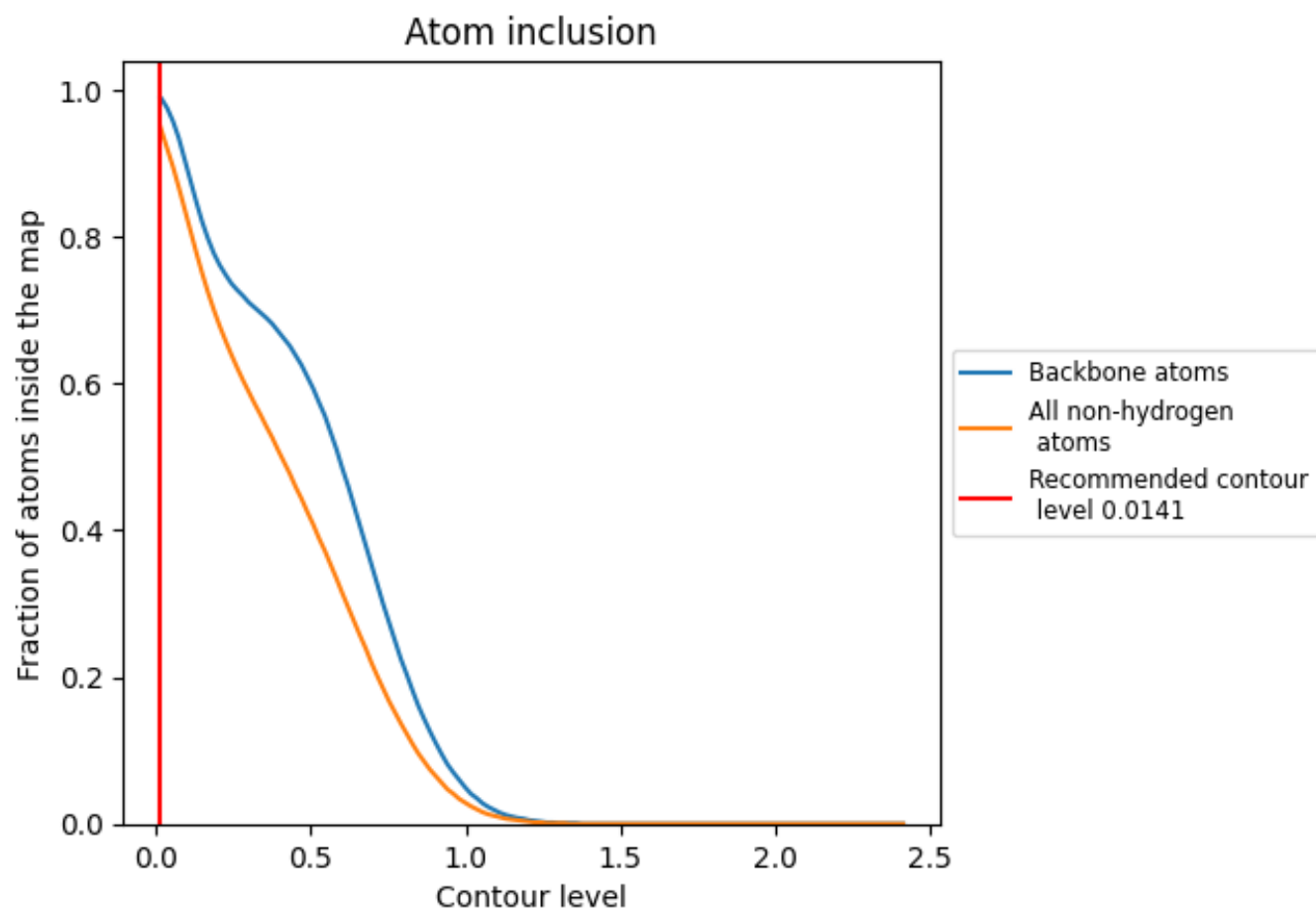
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0141).

9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 95% 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 (0.0141) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9490	 0.5150
B	 0.9770	 0.5600
D	 0.9700	 0.5470
F	 0.9200	 0.4720
H	 0.9260	 0.4920
M	 0.9790	 0.5600
N	 0.9700	 0.5420
P	 0.9120	 0.4710
Q	 0.9280	 0.4860
T	 0.9230	 0.4960
W	 0.9770	 0.5610
X	 0.9720	 0.5500
Z	 0.9260	 0.4800
a	 0.9500	 0.4890
b	 0.9320	 0.5060
e	 0.9580	 0.5230
f	 0.9500	 0.5020
g	 0.8880	 0.4570
h	 0.9200	 0.4770
i	 0.8620	 0.4380
j	 0.9050	 0.4620
k	 0.9520	 0.5220
l	 0.9470	 0.4960
m	 0.8970	 0.4480
n	 0.8940	 0.4380
o	 0.9050	 0.4640
p	 0.9570	 0.5240
q	 0.9470	 0.5000
r	 0.8980	 0.4630
s	 0.8970	 0.4580
t	 0.8960	 0.4510

