



wwPDB EM Validation Summary Report ⓘ

Jan 25, 2025 – 12:52 PM EST

PDB ID : 9CU2
EMDB ID : EMD-45926
Title : Azotobacter vinelandii filamentous 2:2:1 MoFeP:FeP:FeSII-Complex (C2 symmetry)
Authors : Narehood, S.M.; Cook, B.D.; Srisantitham, S.; Eng, V.H.; Shiau, A.; Britt, R.D.; Herzik, M.A.; Tezcan, F.A.
Deposited on : 2024-07-25
Resolution : 2.27 Å (reported)
Based on initial model : 7UT7

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.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

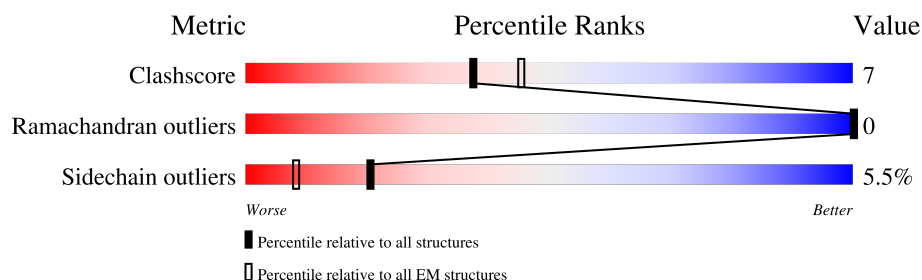
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.27 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	492	
1	C	492	
1	H	492	
1	J	492	
2	B	523	
2	D	523	
2	I	523	
2	K	523	

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Mol	Chain	Length	Quality of chain
3	E	290	
3	F	290	
3	L	290	
3	M	290	
4	G	122	
5	N	122	

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 46276 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 alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	477	Total	C	N	O	S	1	0
			3790	2410	646	709	25		
1	C	477	Total	C	N	O	S	1	0
			3793	2412	646	709	26		
1	H	477	Total	C	N	O	S	0	0
			3787	2408	646	709	24		
1	J	477	Total	C	N	O	S	1	0
			3793	2412	646	709	26		

- Molecule 2 is a protein called Nitrogenase molybdenum-iron protein beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	522	Total	C	N	O	S	0	0
			4174	2666	705	775	28		
2	D	522	Total	C	N	O	S	0	0
			4174	2666	705	775	28		
2	I	522	Total	C	N	O	S	0	0
			4174	2666	705	775	28		
2	K	522	Total	C	N	O	S	0	0
			4174	2666	705	775	28		

- Molecule 3 is a protein called Nitrogenase iron protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	274	Total	C	N	O	S	0	0
			2077	1298	353	405	21		
3	F	283	Total	C	N	O	S	0	0
			2145	1340	363	421	21		
3	L	272	Total	C	N	O	S	0	0
			2060	1288	351	401	20		
3	M	280	Total	C	N	O	S	0	0
			2121	1323	359	418	21		

- Molecule 4 is a protein called Protein FeSII.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	121	Total	C	N	O	S	0	0
			918	574	161	177	6		

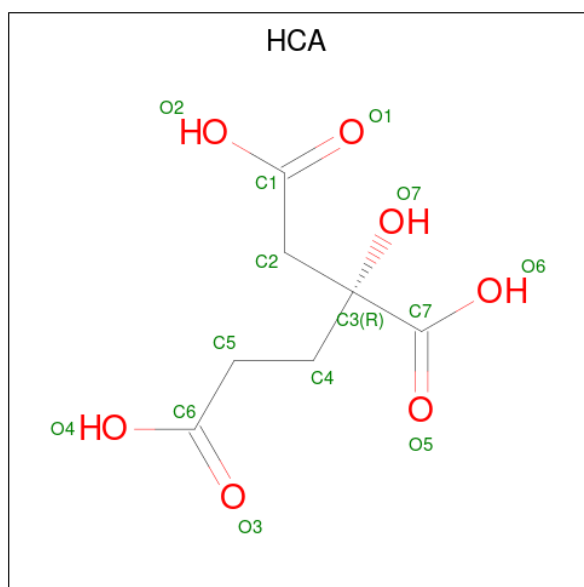
- Molecule 5 is a protein called Protein FeSII.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	N	121	Total	C	N	O	S	0	0
			920	574	163	177	6		

There are 2 discrepancies between the modelled and reference sequences:

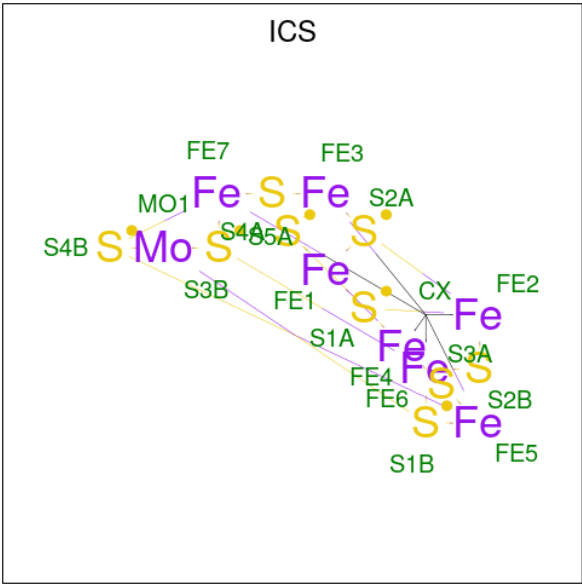
Chain	Residue	Modelled	Actual	Comment	Reference
N	27	LYS	LEU	conflict	UNP Q44501
N	28	LYS	LEU	conflict	UNP Q44501

- Molecule 6 is 3-HYDROXY-3-CARBOXY-ADIPIC ACID (three-letter code: HCA) (formula: $C_7H_{10}O_7$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
6	A	1	Total	C	O	0
			14	7	7	
6	C	1	Total	C	O	0
			14	7	7	
6	H	1	Total	C	O	0
			14	7	7	
6	J	1	Total	C	O	0
			14	7	7	

- Molecule 7 is iron-sulfur-molybdenum cluster with interstitial carbon (three-letter code: ICS) (formula: CFe₇MoS₉) (labeled as "Ligand of Interest" by depositor).

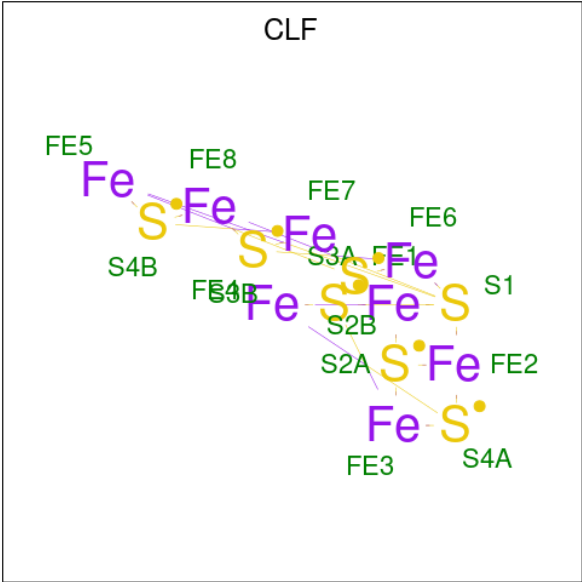


Mol	Chain	Residues	Atoms				AltConf
7	A	1	Total	C	Fe	Mo	S
			18	1	7	1	9
7	C	1	Total	C	Fe	Mo	S
			18	1	7	1	9
7	H	1	Total	C	Fe	Mo	S
			18	1	7	1	9
7	J	1	Total	C	Fe	Mo	S
			18	1	7	1	9

- Molecule 8 is FE (III) ION (three-letter code: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

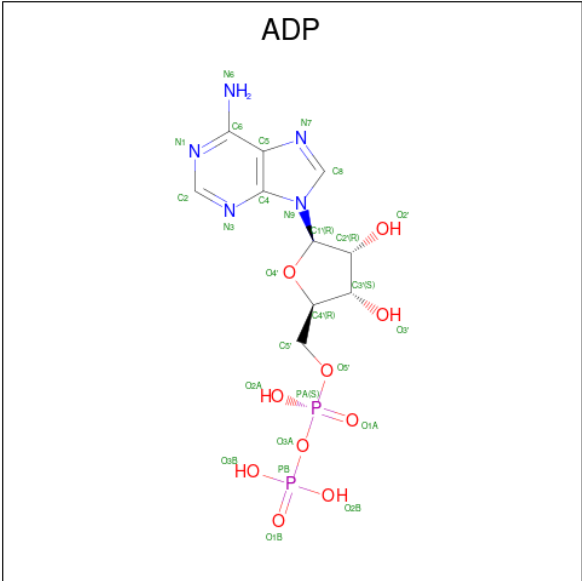
Mol	Chain	Residues	Atoms		AltConf
8	B	2	Total	Fe	0
			2	2	
8	I	1	Total	Fe	0
			1	1	
8	K	1	Total	Fe	0
			1	1	

- Molecule 9 is FE(8)-S(7) CLUSTER (three-letter code: CLF) (formula: Fe₈S₇) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
9	B	1	Total	Fe	S	0
			15	8	7	
9	D	1	Total	Fe	S	0
			15	8	7	
9	H	1	Total	Fe	S	0
			15	8	7	
9	K	1	Total	Fe	S	0
			15	8	7	

- Molecule 10 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).

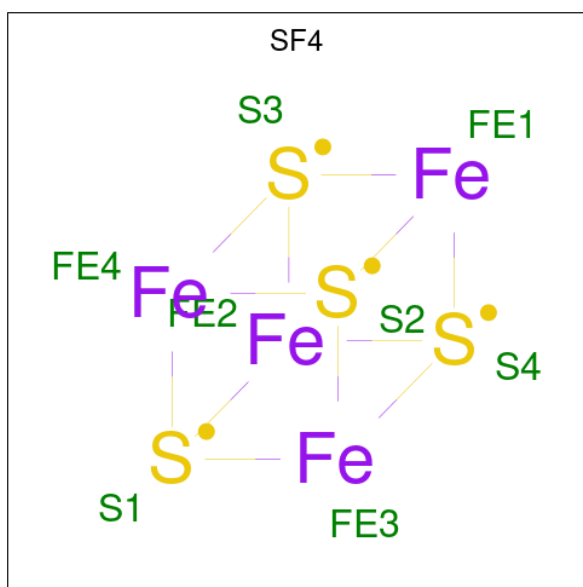


Mol	Chain	Residues	Atoms					AltConf
10	E	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	F	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	L	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	M	1	Total	C	N	O	P	0
			27	10	5	10	2	

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

Mol	Chain	Residues	Atoms		AltConf
11	E	1	Total	Mg	0
			1	1	
11	F	1	Total	Mg	0
			1	1	
11	L	1	Total	Mg	0
			1	1	
11	M	1	Total	Mg	0
			1	1	

- Molecule 12 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄) (labeled as "Ligand of Interest" by depositor).



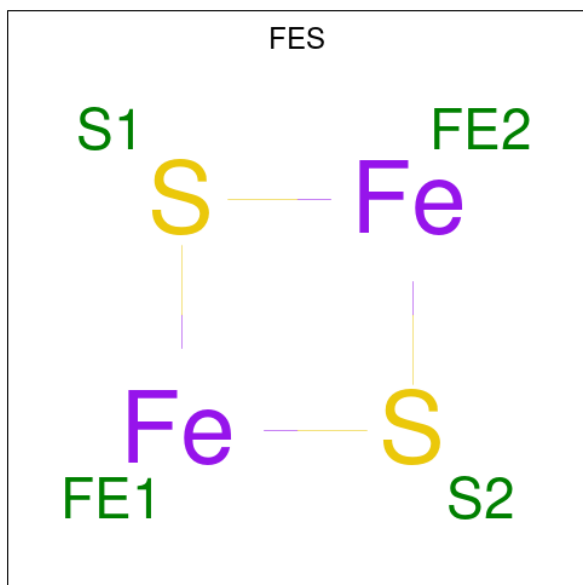
Mol	Chain	Residues	Atoms			AltConf
12	F	1	Total	Fe	S	0
			8	4	4	

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Mol	Chain	Residues	Atoms			AltConf
12	M	1	Total	Fe	S	0
			8	4	4	

- Molecule 13 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
13	G	1	Total	Fe	S	0
			4	2	2	
13	N	1	Total	Fe	S	0
			4	2	2	

- Molecule 14 is water.

Mol	Chain	Residues	Atoms		AltConf
14	A	270	Total	O	0
			270	270	
14	B	346	Total	O	0
			346	346	
14	C	271	Total	O	0
			271	271	
14	D	320	Total	O	0
			320	320	
14	E	290	Total	O	0
			290	290	
14	F	280	Total	O	0
			280	280	

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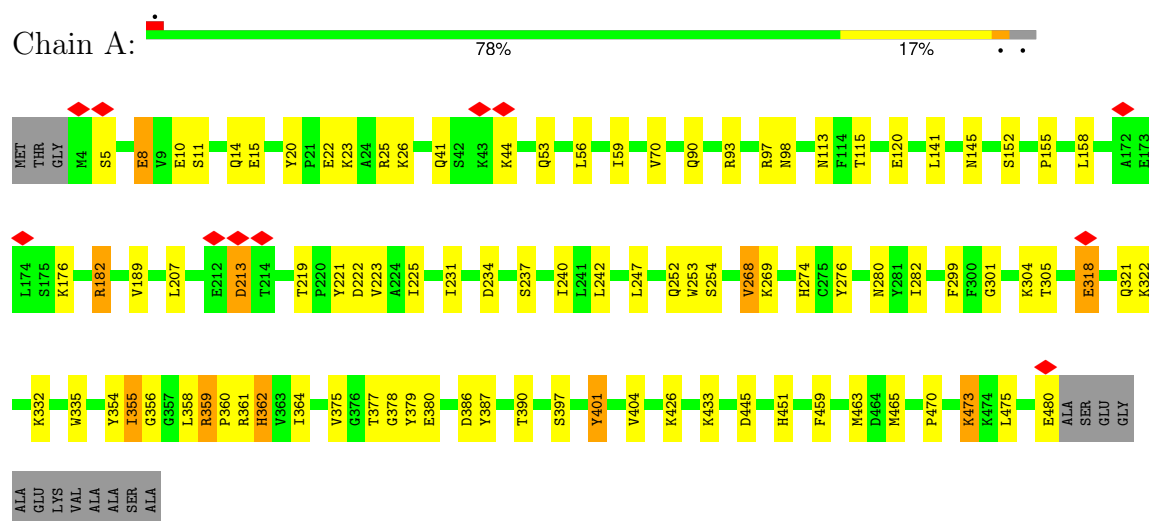
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Mol	Chain	Residues	Atoms		AltConf
14	G	103	Total 103	O 103	0
14	H	256	Total 256	O 256	0
14	I	349	Total 349	O 349	0
14	J	287	Total 287	O 287	0
14	K	368	Total 368	O 368	0
14	L	311	Total 311	O 311	0
14	M	294	Total 294	O 294	0
14	N	103	Total 103	O 103	0

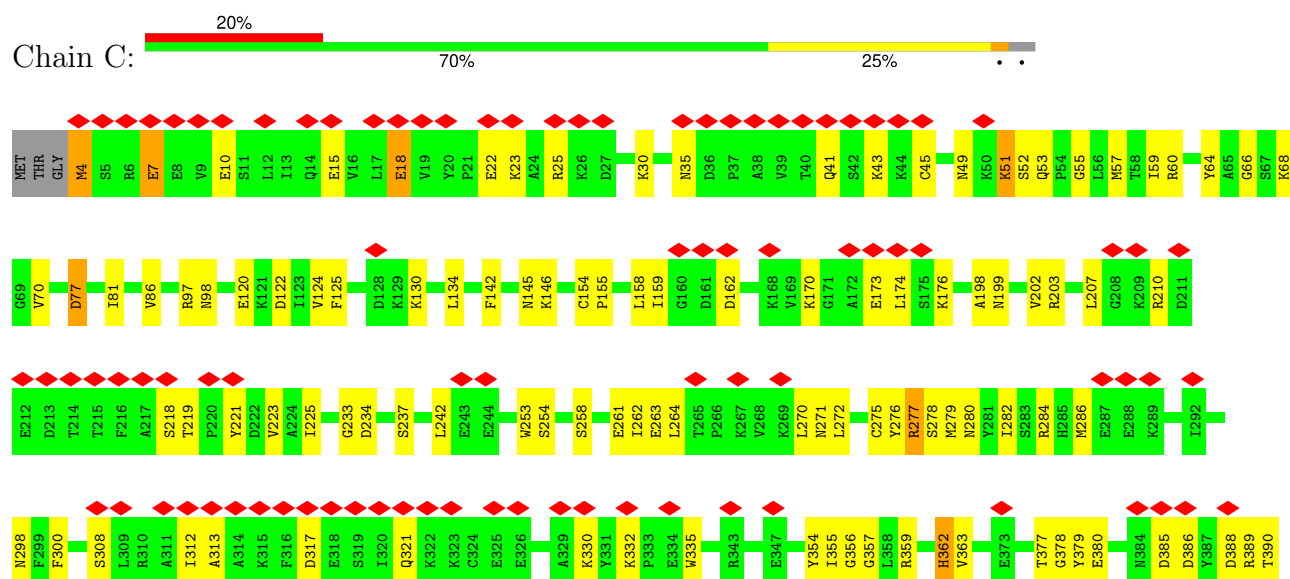
3 Residue-property plots

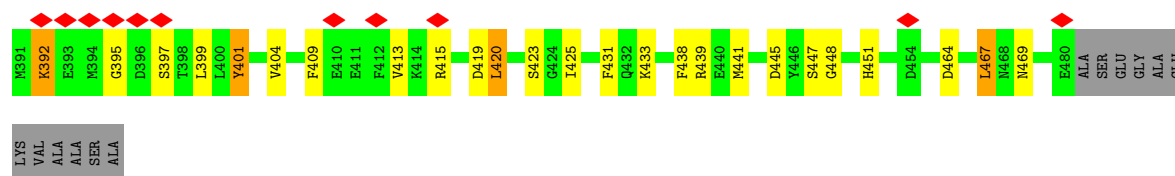
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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



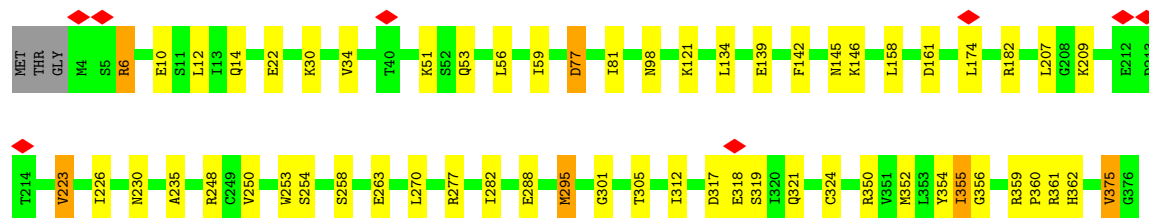
• Molecule 1: Nitrogenase molybdenum-iron protein alpha chain





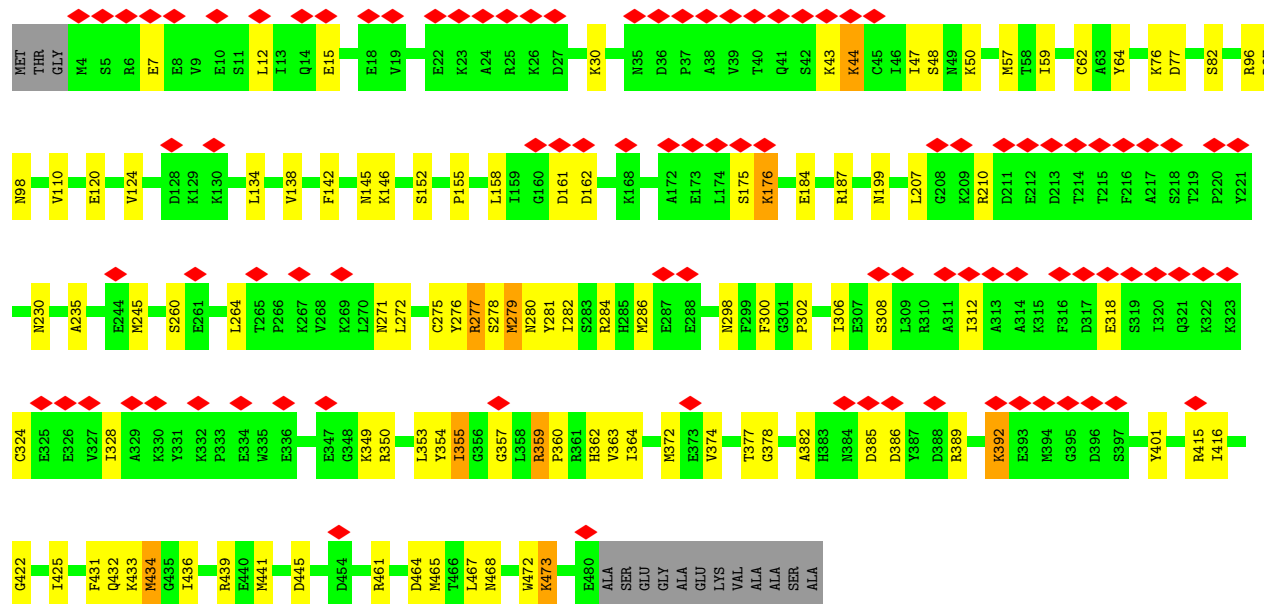
• Molecule 1: Nitrogenase molybdenum-iron protein alpha chain

Chain H: 81% 15% . .



• Molecule 1: Nitrogenase molybdenum-iron protein alpha chain

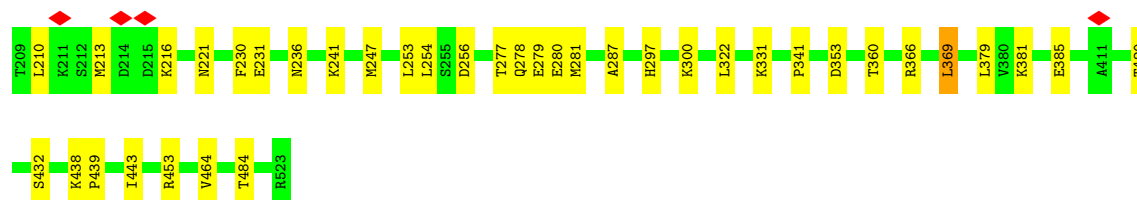
Chain J: 20% 76% 20% . .



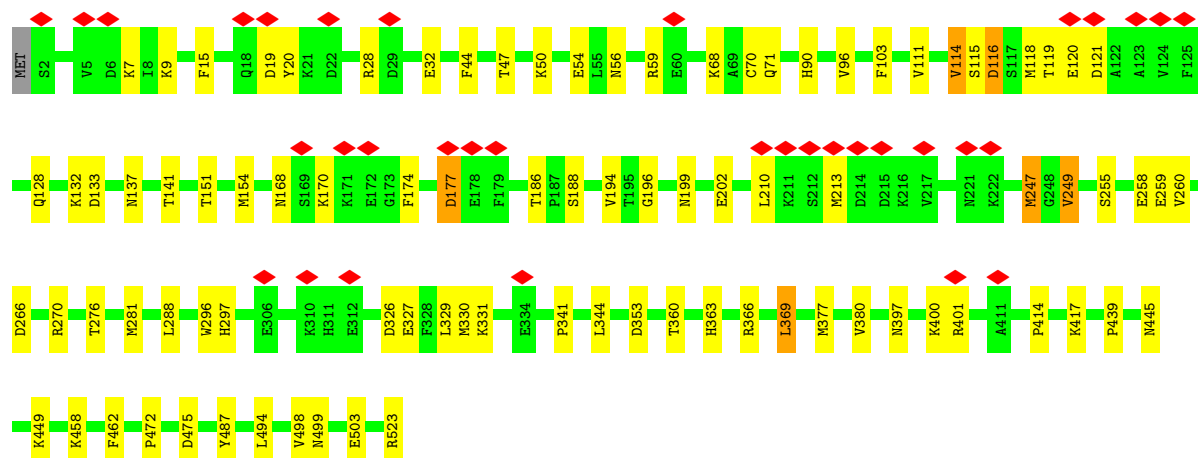
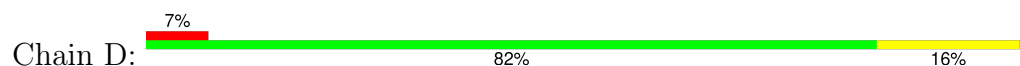
• Molecule 2: Nitrogenase molybdenum-iron protein beta chain

Chain B: 87% 13%

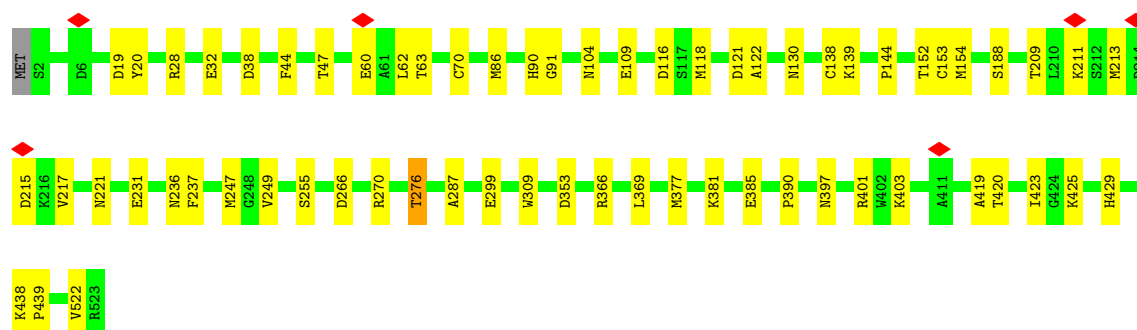
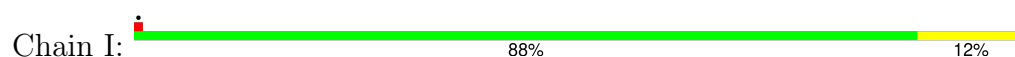




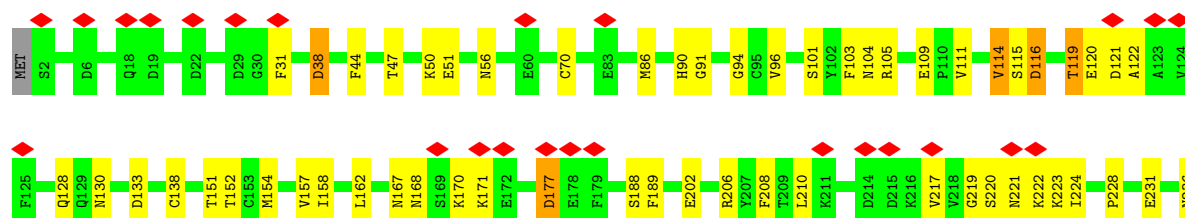
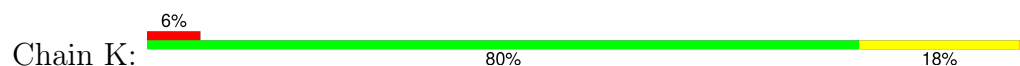
• Molecule 2: Nitrogenase molybdenum-iron protein beta chain

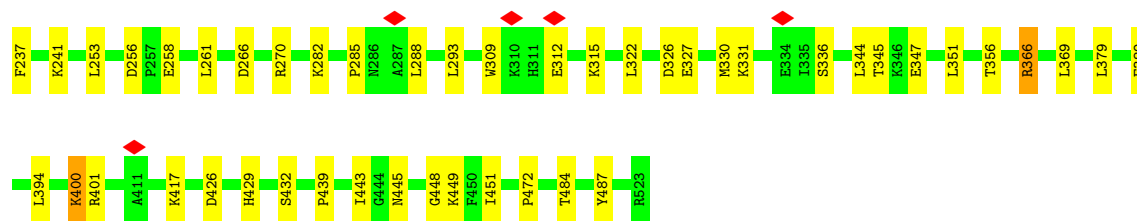


• Molecule 2: Nitrogenase molybdenum-iron protein beta chain

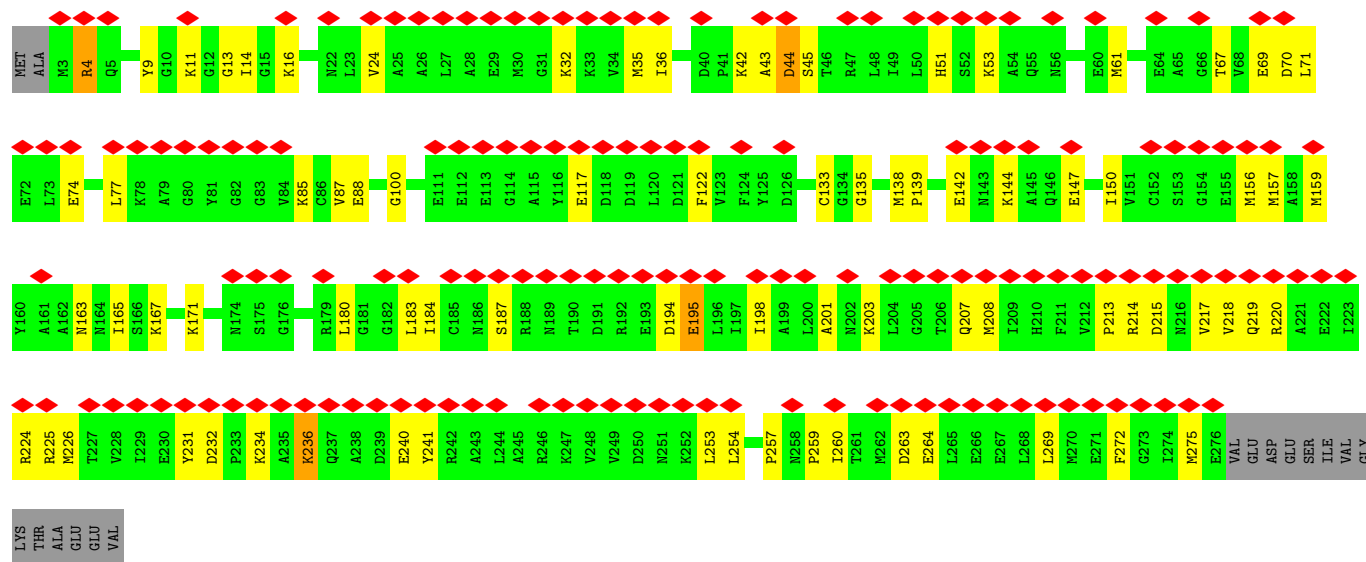


• Molecule 2: Nitrogenase molybdenum-iron protein beta chain

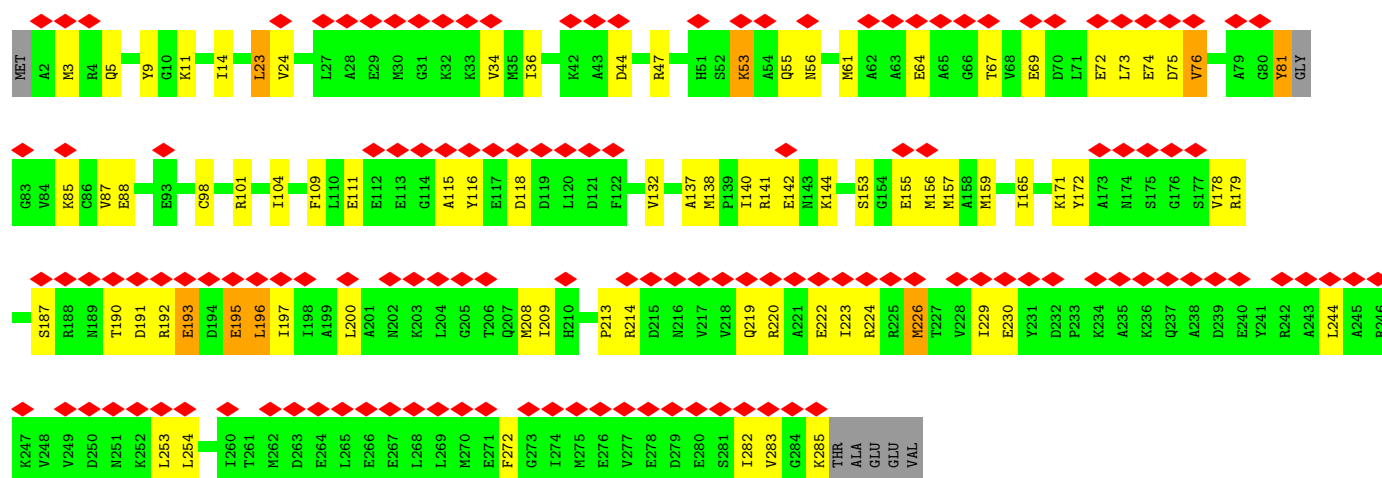




• Molecule 3: Nitrogenase iron protein 1

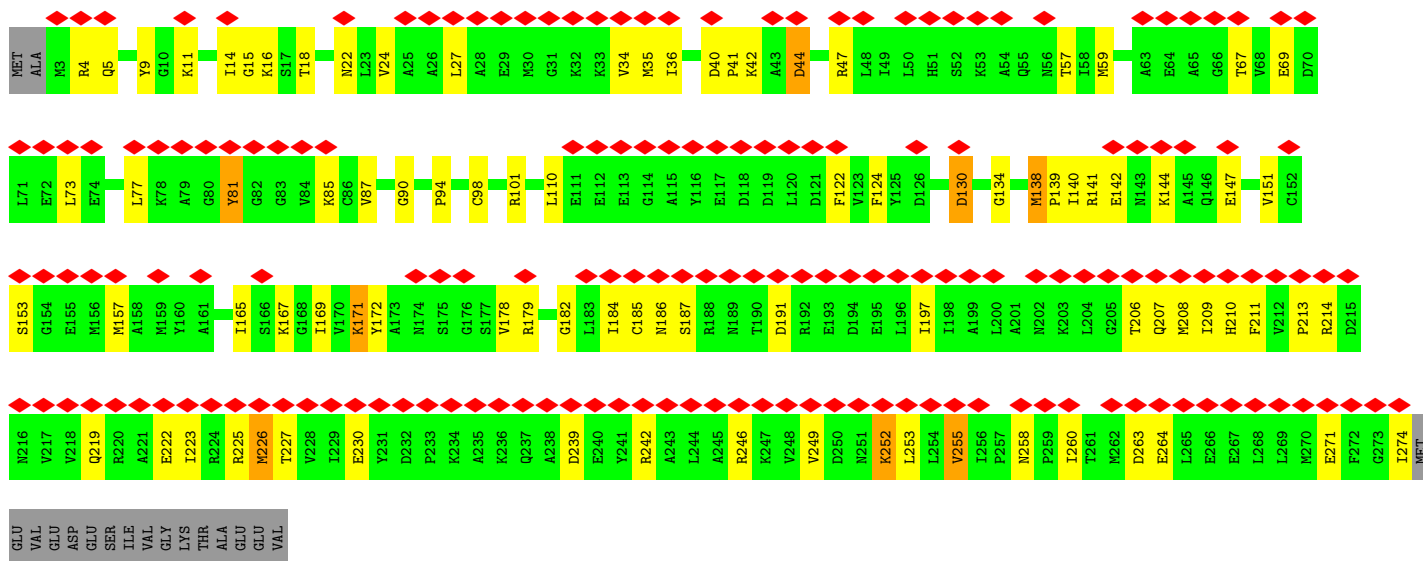


• Molecule 3: Nitrogenase iron protein 1

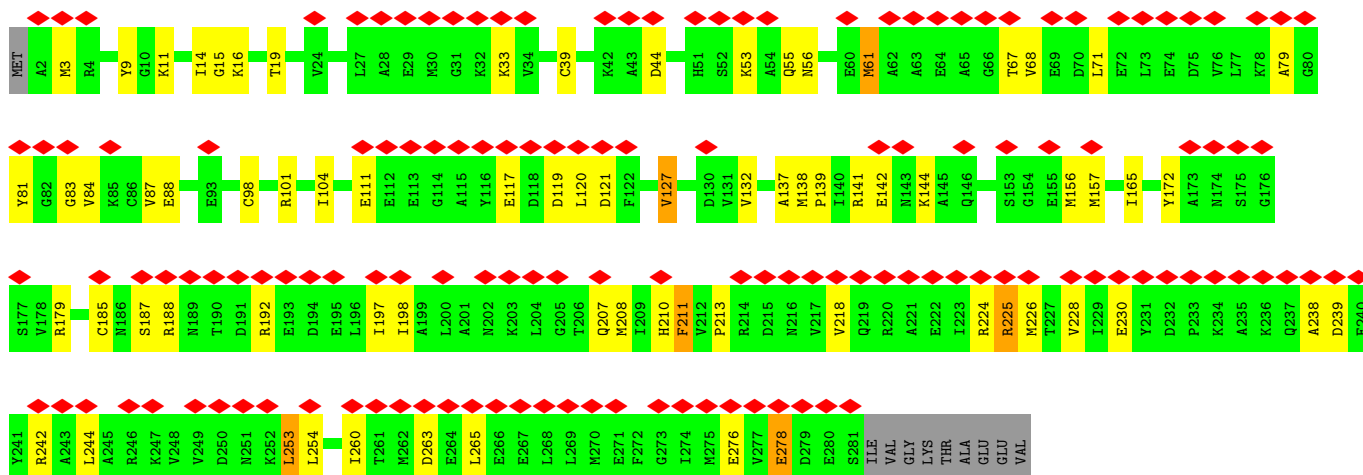
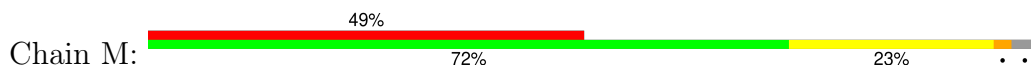


• Molecule 3: Nitrogenase iron protein 1

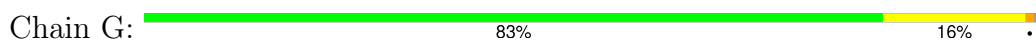




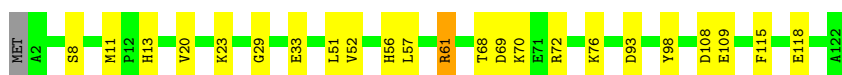
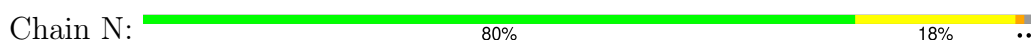
• Molecule 3: Nitrogenase iron protein 1



• Molecule 4: Protein FeSII



• Molecule 5: Protein FeSII



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	414517	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	750	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	165000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.423	Depositor
Minimum map value	-0.183	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.0402	Depositor
Map size (Å)	329.28, 329.28, 329.28	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.735, 0.735, 0.735	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CLF, FES, SF4, MG, HCA, FE, ICS, ADP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.35	0/3881	0.53	0/5234
1	C	0.35	0/3884	0.54	0/5237
1	H	0.33	0/3875	0.51	0/5226
1	J	0.34	0/3884	0.52	0/5237
2	B	0.31	0/4280	0.50	0/5786
2	D	0.35	0/4280	0.51	0/5786
2	I	0.32	0/4280	0.48	0/5786
2	K	0.30	0/4280	0.47	0/5786
3	E	0.35	0/2101	0.55	0/2829
3	F	0.36	0/2169	0.52	0/2921
3	L	0.34	0/2084	0.52	0/2807
3	M	0.36	0/2145	0.57	0/2889
4	G	0.29	0/931	0.51	0/1256
5	N	0.25	0/933	0.49	0/1256
All	All	0.33	0/43007	0.51	0/58036

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
3	E	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	E	117	GLU	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	3790	0	3727	50	0
1	C	3793	0	3735	81	0
1	H	3787	0	3722	39	0
1	J	3793	0	3734	63	0
2	B	4174	0	4088	36	0
2	D	4174	0	4089	50	0
2	I	4174	0	4088	36	0
2	K	4174	0	4088	61	0
3	E	2077	0	2090	54	0
3	F	2145	0	2158	53	0
3	L	2060	0	2075	50	0
3	M	2121	0	2125	49	0
4	G	918	0	936	13	0
5	N	920	0	940	16	0
6	A	14	0	6	0	0
6	C	14	0	7	0	0
6	H	14	0	7	1	0
6	J	14	0	7	0	0
7	A	18	0	0	1	0
7	C	18	0	0	0	0
7	H	18	0	0	0	0
7	J	18	0	0	2	0
8	B	2	0	0	0	0
8	I	1	0	0	0	0
8	K	1	0	0	0	0
9	B	15	0	0	0	0
9	D	15	0	0	0	0
9	H	15	0	0	0	0
9	K	15	0	0	0	0
10	E	27	0	12	3	0
10	F	27	0	12	0	0
10	L	27	0	12	4	0
10	M	27	0	12	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	E	1	0	0	0	0
11	F	1	0	0	0	0
11	L	1	0	0	0	0
11	M	1	0	0	0	0
12	F	8	0	0	1	0
12	M	8	0	0	1	0
13	G	4	0	0	0	0
13	N	4	0	0	0	0
14	A	270	0	0	1	0
14	B	346	0	0	0	0
14	C	271	0	0	5	0
14	D	320	0	0	1	0
14	E	290	0	0	2	0
14	F	280	0	0	1	0
14	G	103	0	0	0	0
14	H	256	0	0	2	0
14	I	349	0	0	0	0
14	J	287	0	0	1	0
14	K	368	0	0	3	0
14	L	311	0	0	2	0
14	M	294	0	0	2	0
14	N	103	0	0	2	0
All	All	46276	0	41670	612	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 612 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:224:ARG:O	3:M:224:ARG:HD3	1.50	1.11
3:M:210:HIS:HE1	14:M:553:HOH:O	1.47	0.96
1:C:22:GLU:N	1:C:22:GLU:OE1	2.07	0.87
3:M:224:ARG:HG3	3:M:226:MET:SD	2.16	0.85
2:I:266:ASP:OD2	2:I:270:ARG:NH2	2.12	0.82

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	476/492 (97%)	461 (97%)	15 (3%)	0	100	100
1	C	476/492 (97%)	460 (97%)	16 (3%)	0	100	100
1	H	475/492 (96%)	462 (97%)	13 (3%)	0	100	100
1	J	476/492 (97%)	462 (97%)	14 (3%)	0	100	100
2	B	520/523 (99%)	510 (98%)	10 (2%)	0	100	100
2	D	520/523 (99%)	510 (98%)	10 (2%)	0	100	100
2	I	520/523 (99%)	513 (99%)	7 (1%)	0	100	100
2	K	520/523 (99%)	510 (98%)	10 (2%)	0	100	100
3	E	272/290 (94%)	262 (96%)	10 (4%)	0	100	100
3	F	281/290 (97%)	275 (98%)	6 (2%)	0	100	100
3	L	270/290 (93%)	265 (98%)	5 (2%)	0	100	100
3	M	278/290 (96%)	268 (96%)	10 (4%)	0	100	100
4	G	119/122 (98%)	117 (98%)	2 (2%)	0	100	100
5	N	119/122 (98%)	117 (98%)	2 (2%)	0	100	100
All	All	5322/5464 (97%)	5192 (98%)	130 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	407/415 (98%)	382 (94%)	25 (6%)	15	20
1	C	408/415 (98%)	377 (92%)	31 (8%)	11	13
1	H	406/415 (98%)	386 (95%)	20 (5%)	21	29
1	J	408/415 (98%)	383 (94%)	25 (6%)	15	20
2	B	454/455 (100%)	442 (97%)	12 (3%)	41	56
2	D	454/455 (100%)	431 (95%)	23 (5%)	20	27
2	I	454/455 (100%)	443 (98%)	11 (2%)	44	59
2	K	454/455 (100%)	432 (95%)	22 (5%)	21	29
3	E	221/234 (94%)	205 (93%)	16 (7%)	12	14
3	F	229/234 (98%)	207 (90%)	22 (10%)	7	7
3	L	219/234 (94%)	195 (89%)	24 (11%)	5	5
3	M	226/234 (97%)	212 (94%)	14 (6%)	15	19
4	G	102/103 (99%)	98 (96%)	4 (4%)	27	39
5	N	102/103 (99%)	100 (98%)	2 (2%)	50	65
All	All	4544/4622 (98%)	4293 (94%)	251 (6%)	20	24

5 of 251 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	F	85	LYS
3	L	208	MET
1	H	295	MET
3	L	179	ARG
3	M	61	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	128	GLN
3	E	216	ASN
3	L	219	GLN
1	J	384	ASN
2	K	168	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 28 ligands modelled in this entry, 8 are monoatomic - leaving 20 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$
6	HCA	C	501	-	13,13,13	1.17	1 (7%)	15,18,18	1.33	3 (20%)
9	CLF	D	601	2,1	0,24,24	-	-	-		
6	HCA	J	501	-	13,13,13	1.17	1 (7%)	15,18,18	1.18	0
10	ADP	E	301	11	24,29,29	0.91	0	29,45,45	1.18	2 (6%)
9	CLF	B	602	2,1	0,24,24	-	-	-		
12	SF4	M	301	3	0,12,12	-	-	-		
6	HCA	H	501	-	13,13,13	1.34	1 (7%)	15,18,18	1.54	3 (20%)
7	ICS	C	502	1	6,30,30	1.74	1 (16%)	-		
9	CLF	H	503	2,1	0,24,24	-	-	-		
13	FES	N	201	5	0,4,4	-	-	-		
7	ICS	J	502	1	6,30,30	1.77	1 (16%)	-		
10	ADP	L	301	11	24,29,29	0.95	1 (4%)	29,45,45	1.23	4 (13%)
13	FES	G	201	4	0,4,4	-	-	-		
7	ICS	H	502	1	6,30,30	1.81	1 (16%)	-		
12	SF4	F	301	3	0,12,12	-	-	-		
6	HCA	A	501	-	13,13,13	1.18	1 (7%)	15,18,18	1.45	3 (20%)
7	ICS	A	502	1	6,30,30	1.74	1 (16%)	-		
9	CLF	K	602	2,1	0,24,24	-	-	-		
10	ADP	F	302	11	24,29,29	0.89	0	29,45,45	1.19	2 (6%)
10	ADP	M	302	11	24,29,29	0.89	0	29,45,45	1.21	2 (6%)

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
6	HCA	C	501	-	-	6/17/17/17	-
9	CLF	D	601	2,1	-	-	0/12/10/10
9	CLF	H	503	2,1	-	-	0/12/10/10
9	CLF	K	602	2,1	-	-	0/12/10/10
13	FES	N	201	5	-	-	0/1/1/1
10	ADP	L	301	11	-	6/12/32/32	0/3/3/3
6	HCA	J	501	-	-	6/17/17/17	-
13	FES	G	201	4	-	-	0/1/1/1
10	ADP	E	301	11	-	6/12/32/32	0/3/3/3
10	ADP	F	302	11	-	3/12/32/32	0/3/3/3
10	ADP	M	302	11	-	3/12/32/32	0/3/3/3
9	CLF	B	602	2,1	-	-	0/12/10/10
12	SF4	M	301	3	-	-	0/6/5/5
6	HCA	H	501	-	-	5/17/17/17	-
12	SF4	F	301	3	-	-	0/6/5/5
6	HCA	A	501	-	-	7/17/17/17	-

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	J	502	ICS	S2B-FE6	-3.60	2.16	2.24
7	C	502	ICS	S2B-FE6	-3.52	2.16	2.24
7	A	502	ICS	S2B-FE6	-3.41	2.16	2.24
7	H	502	ICS	S2B-FE6	-3.37	2.16	2.24
6	C	501	HCA	C3-C7	2.43	1.56	1.53

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	M	302	ADP	N3-C2-N1	-3.67	123.69	128.67
10	F	302	ADP	N3-C2-N1	-3.64	123.73	128.67
10	L	301	ADP	N3-C2-N1	-3.43	124.01	128.67
10	E	301	ADP	N3-C2-N1	-3.38	124.08	128.67
6	H	501	HCA	O5-C7-C3	-3.33	115.63	122.09

There are no chirality outliers.

5 of 42 torsion outliers are listed below:

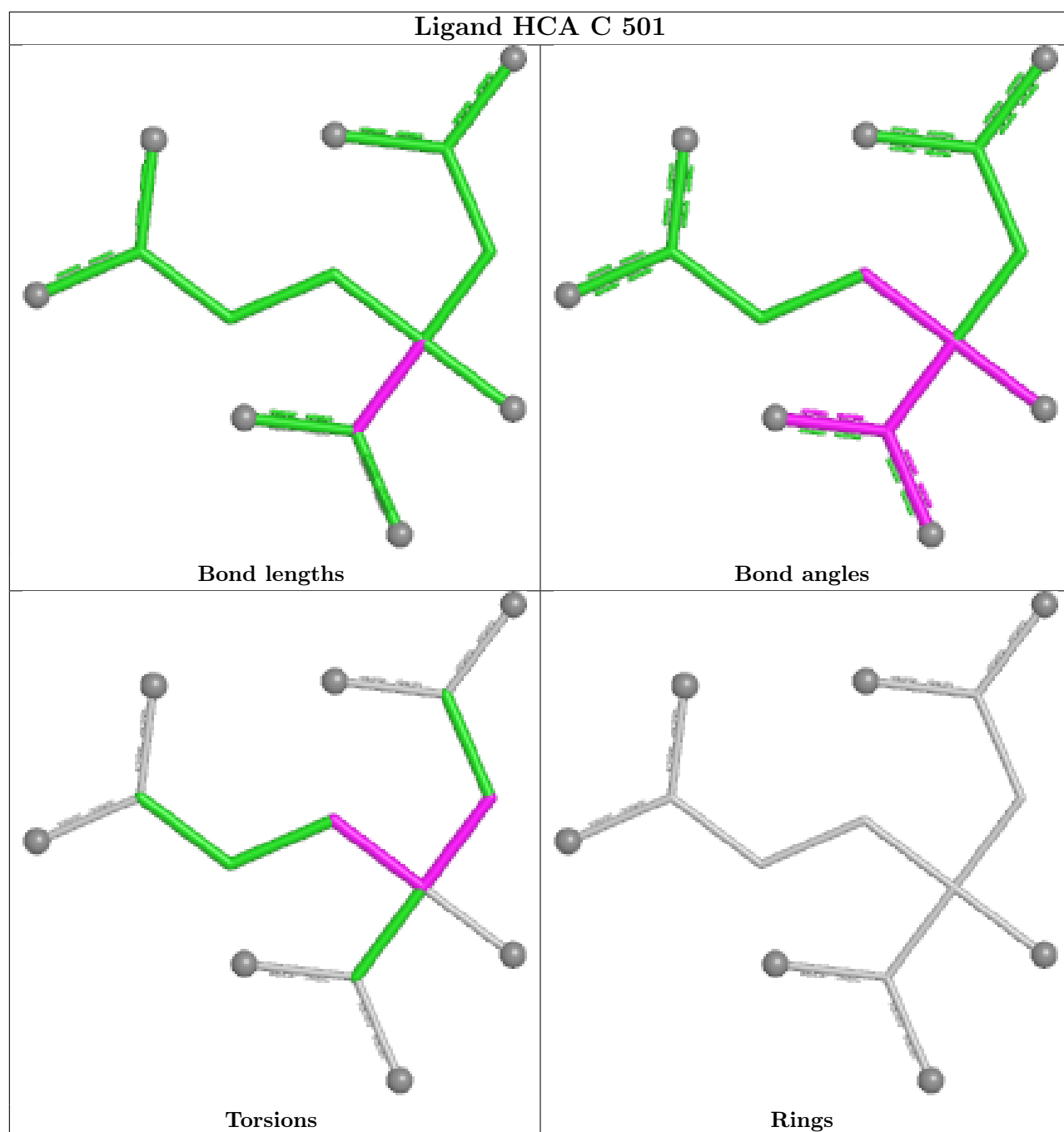
Mol	Chain	Res	Type	Atoms
6	A	501	HCA	C2-C3-C4-C5
6	A	501	HCA	O7-C3-C4-C5
6	C	501	HCA	C2-C3-C4-C5
6	C	501	HCA	O7-C3-C4-C5
6	J	501	HCA	C1-C2-C3-C4

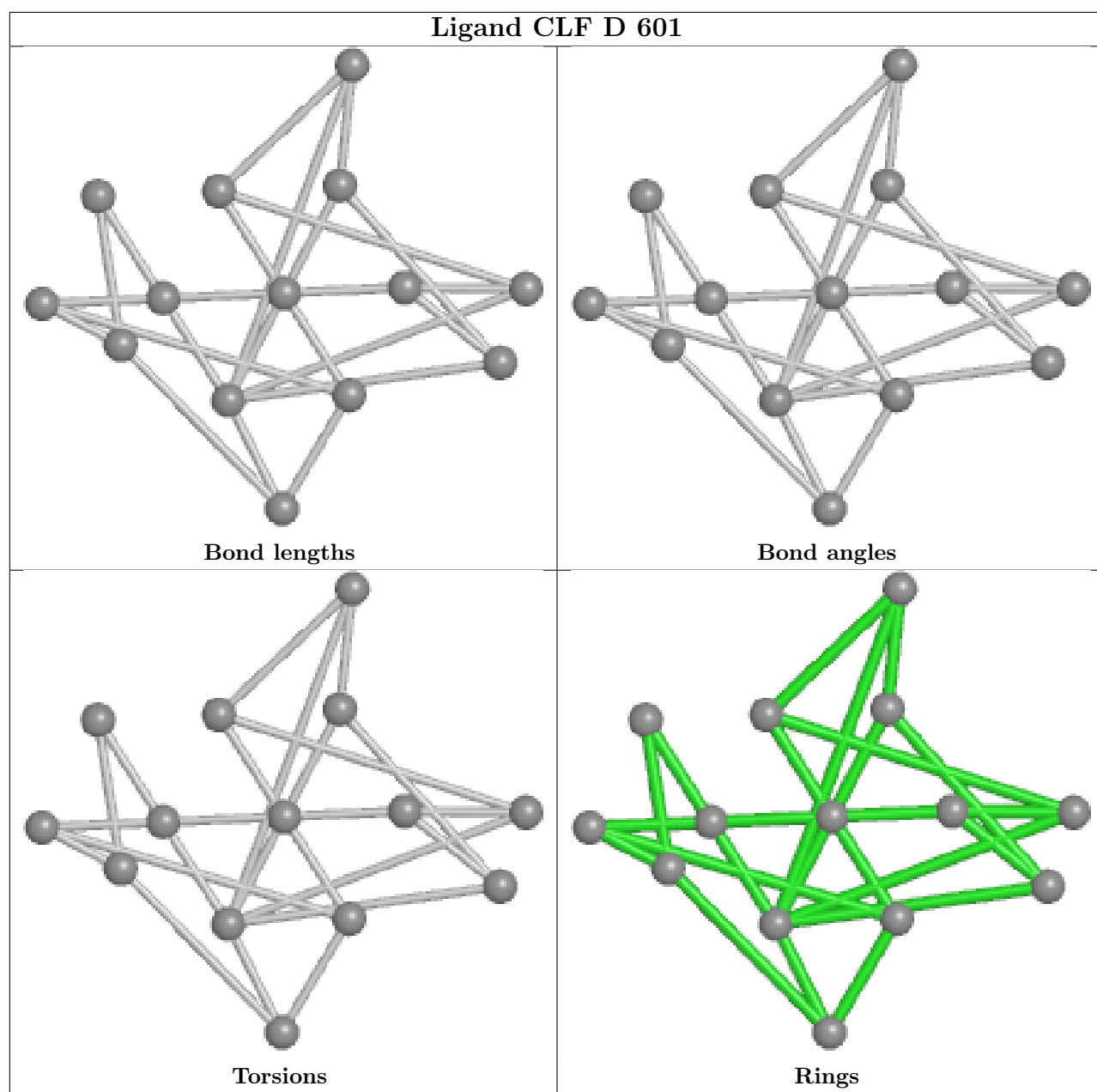
There are no ring outliers.

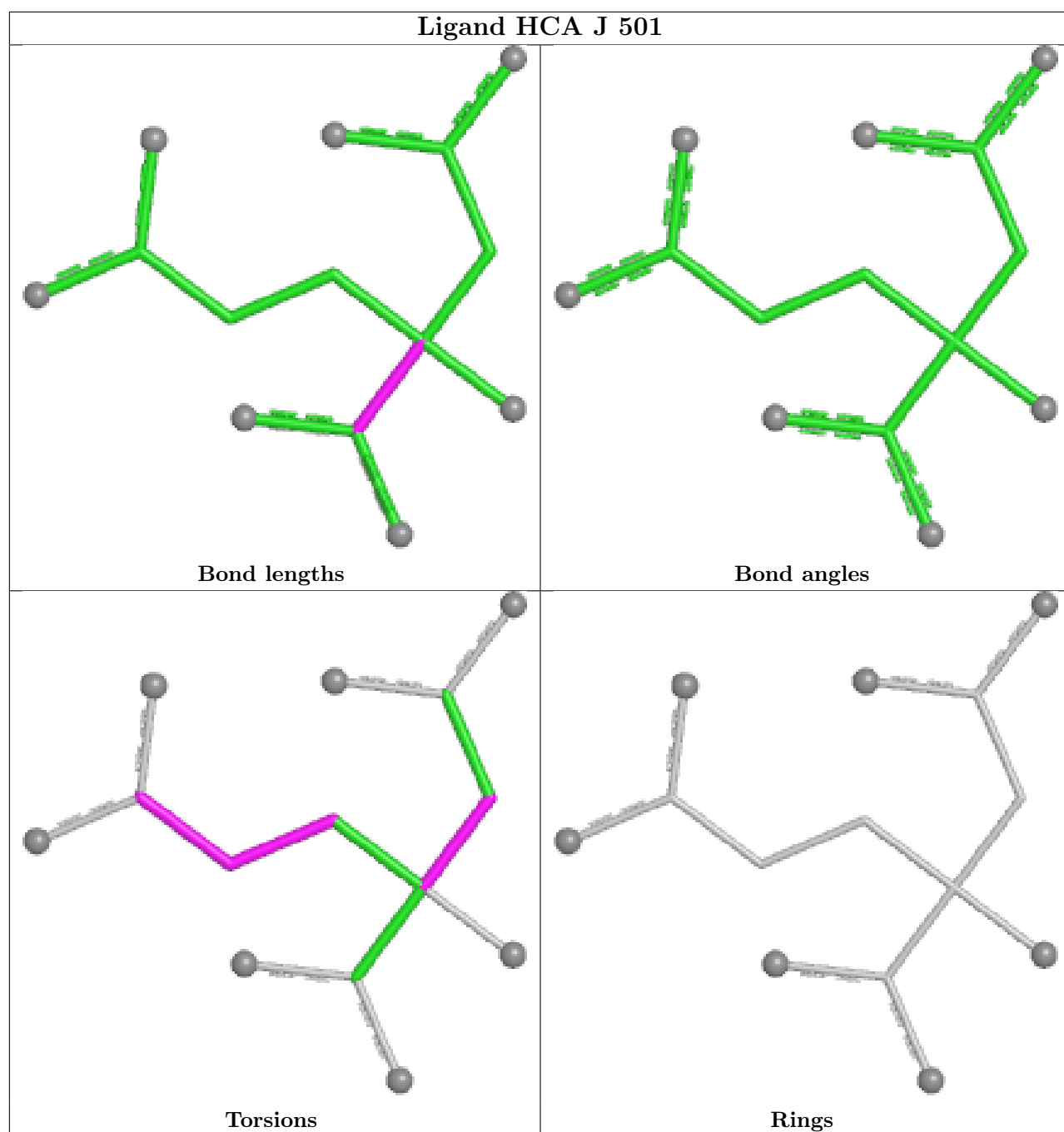
8 monomers are involved in 15 short contacts:

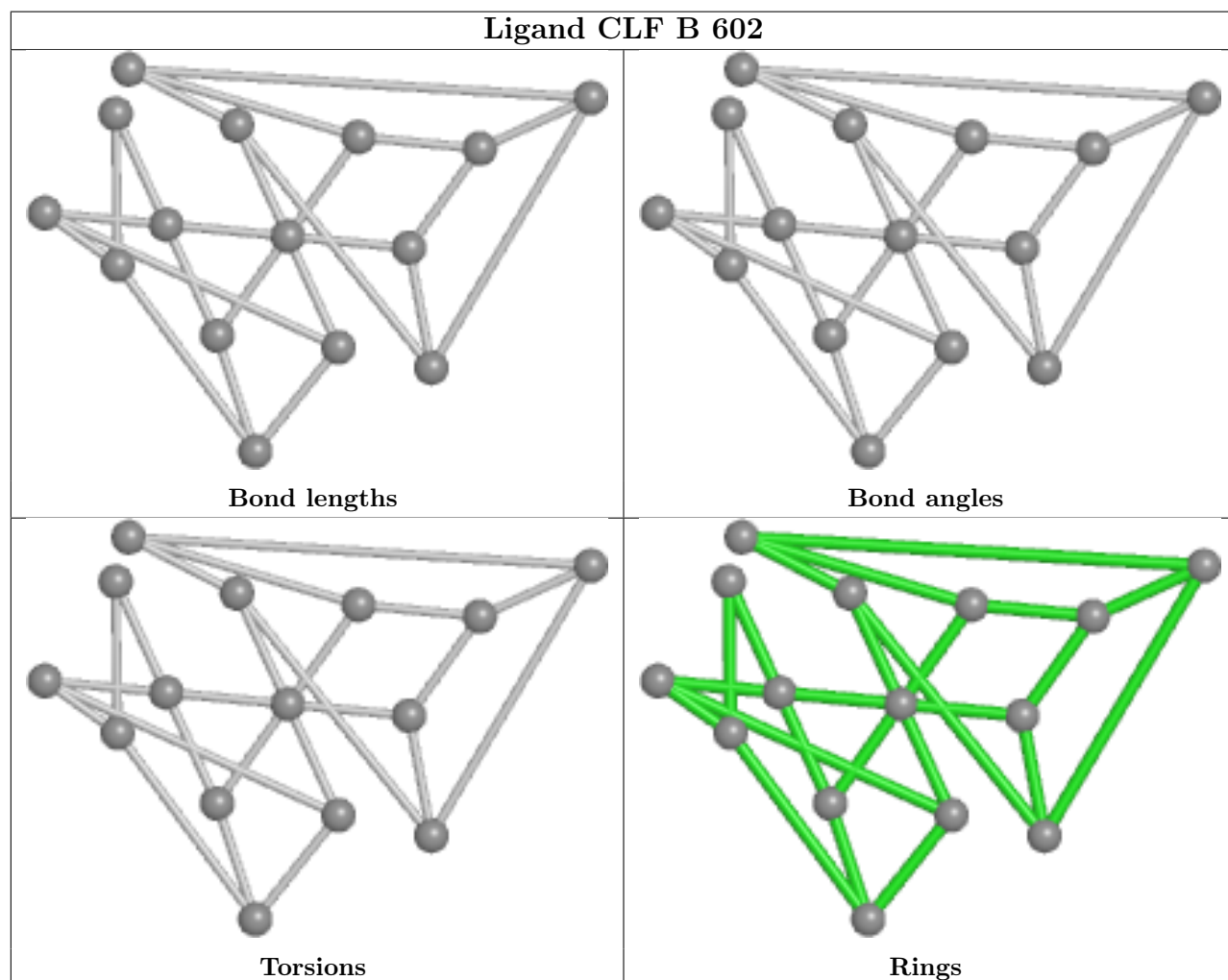
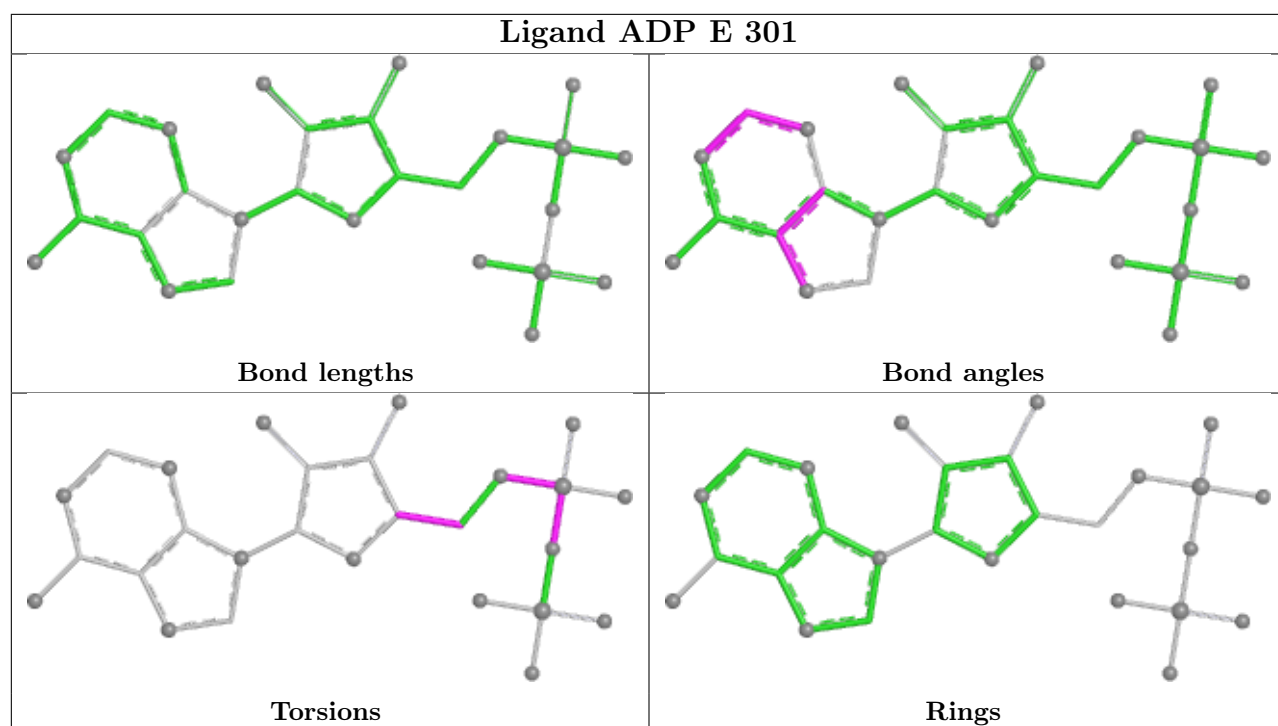
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	E	301	ADP	3	0
12	M	301	SF4	1	0
6	H	501	HCA	1	0
7	J	502	ICS	2	0
10	L	301	ADP	4	0
12	F	301	SF4	1	0
7	A	502	ICS	1	0
10	M	302	ADP	2	0

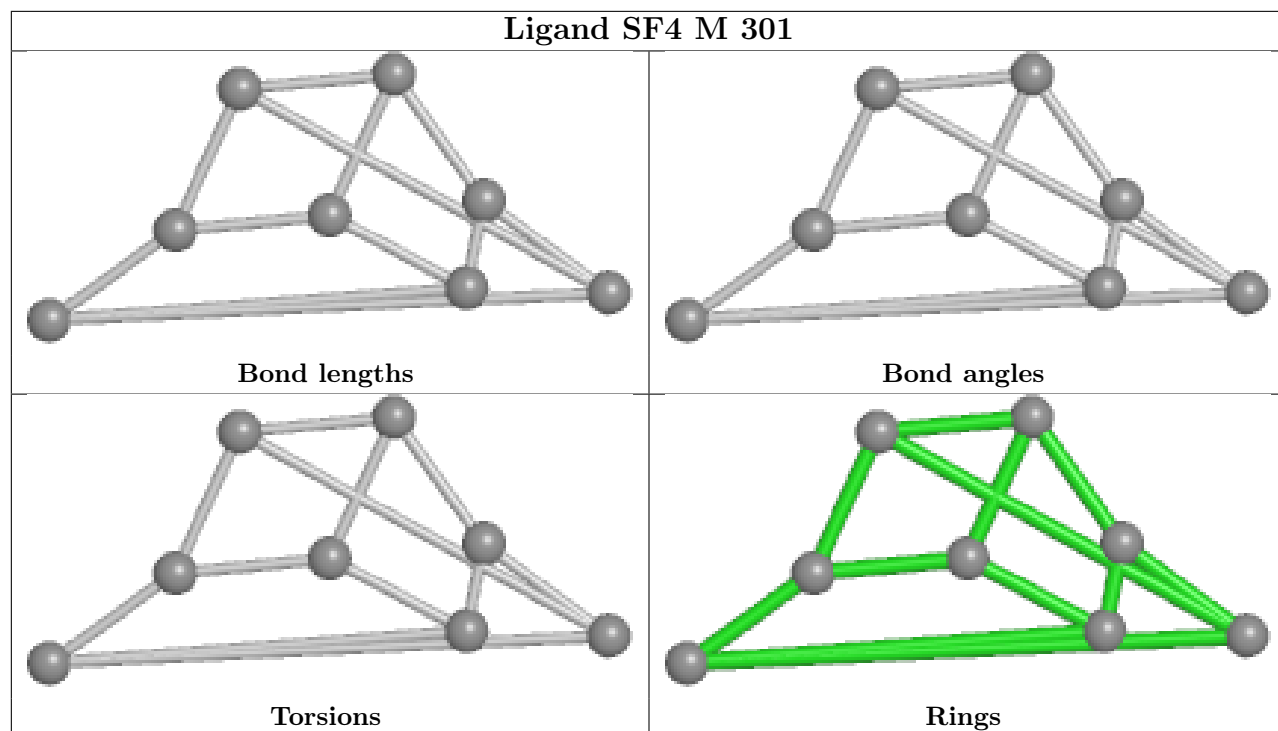
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

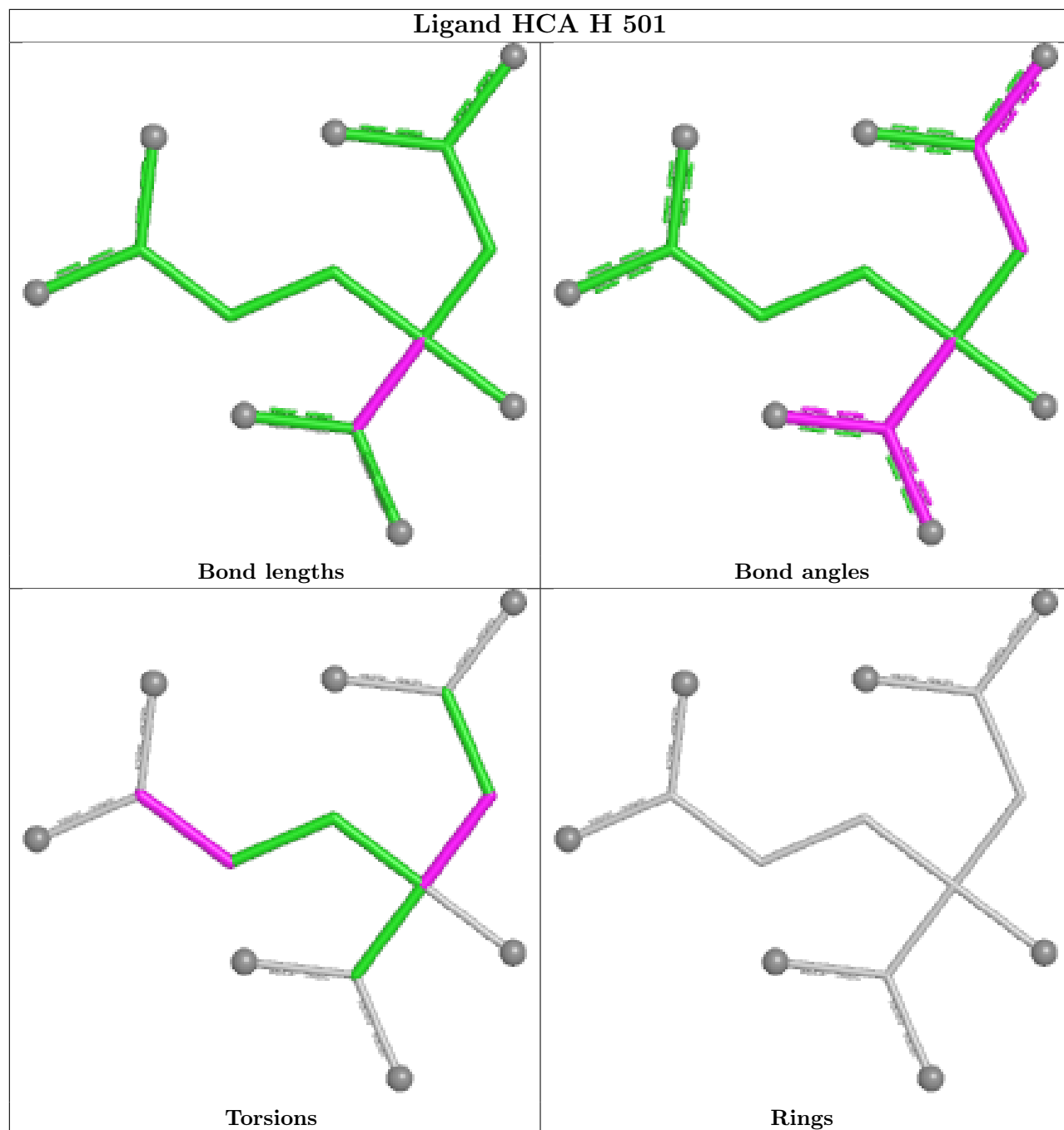


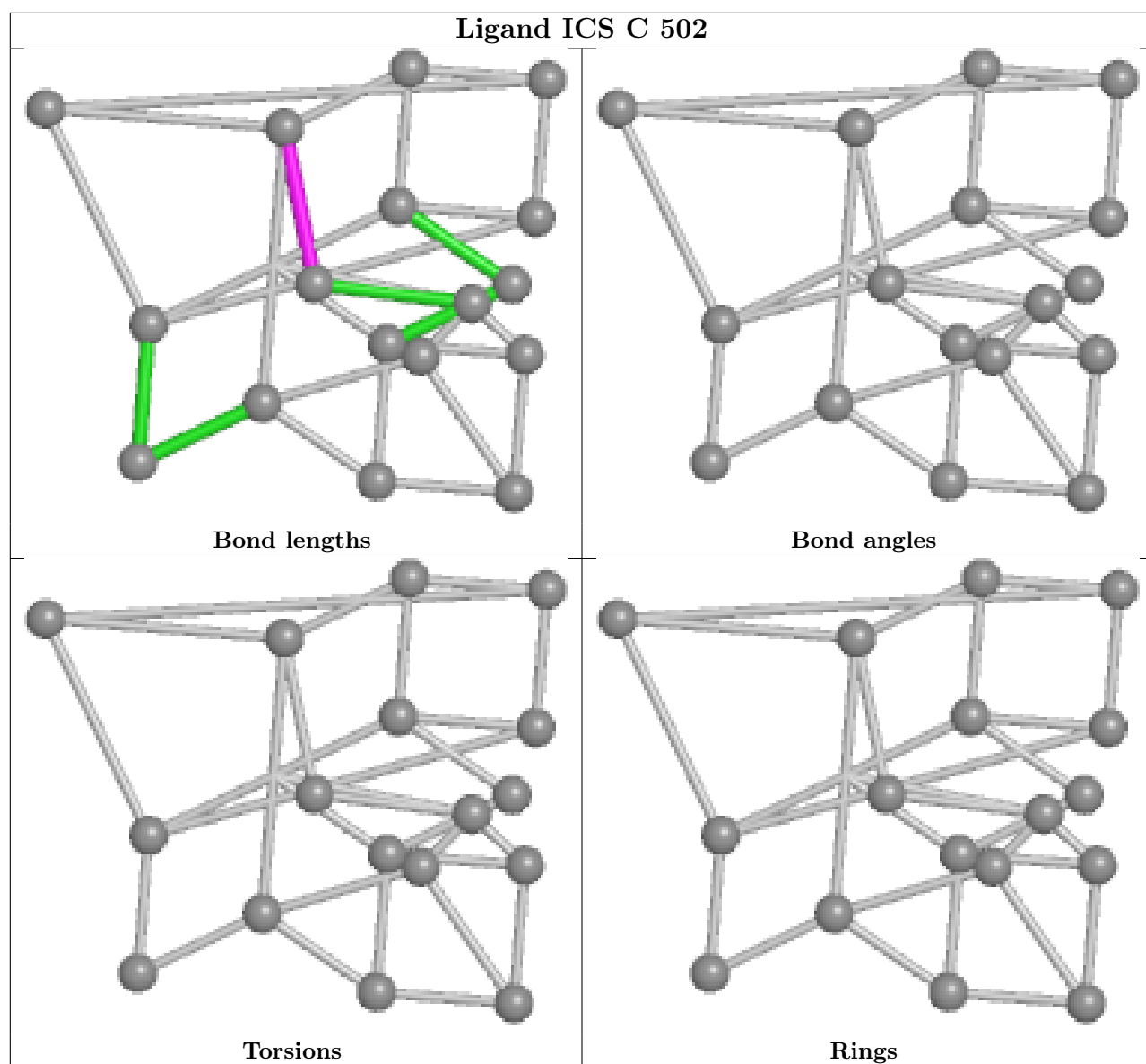


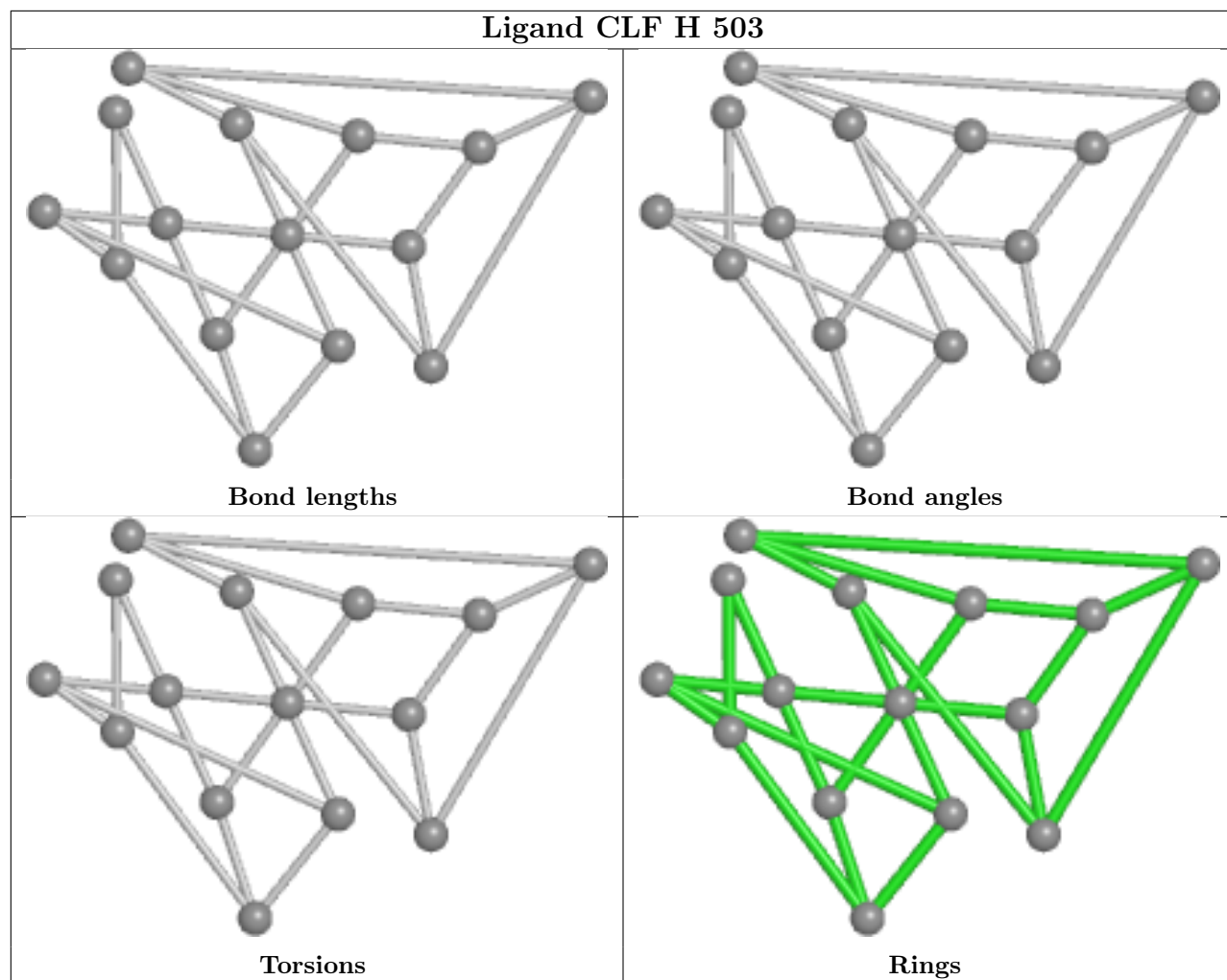


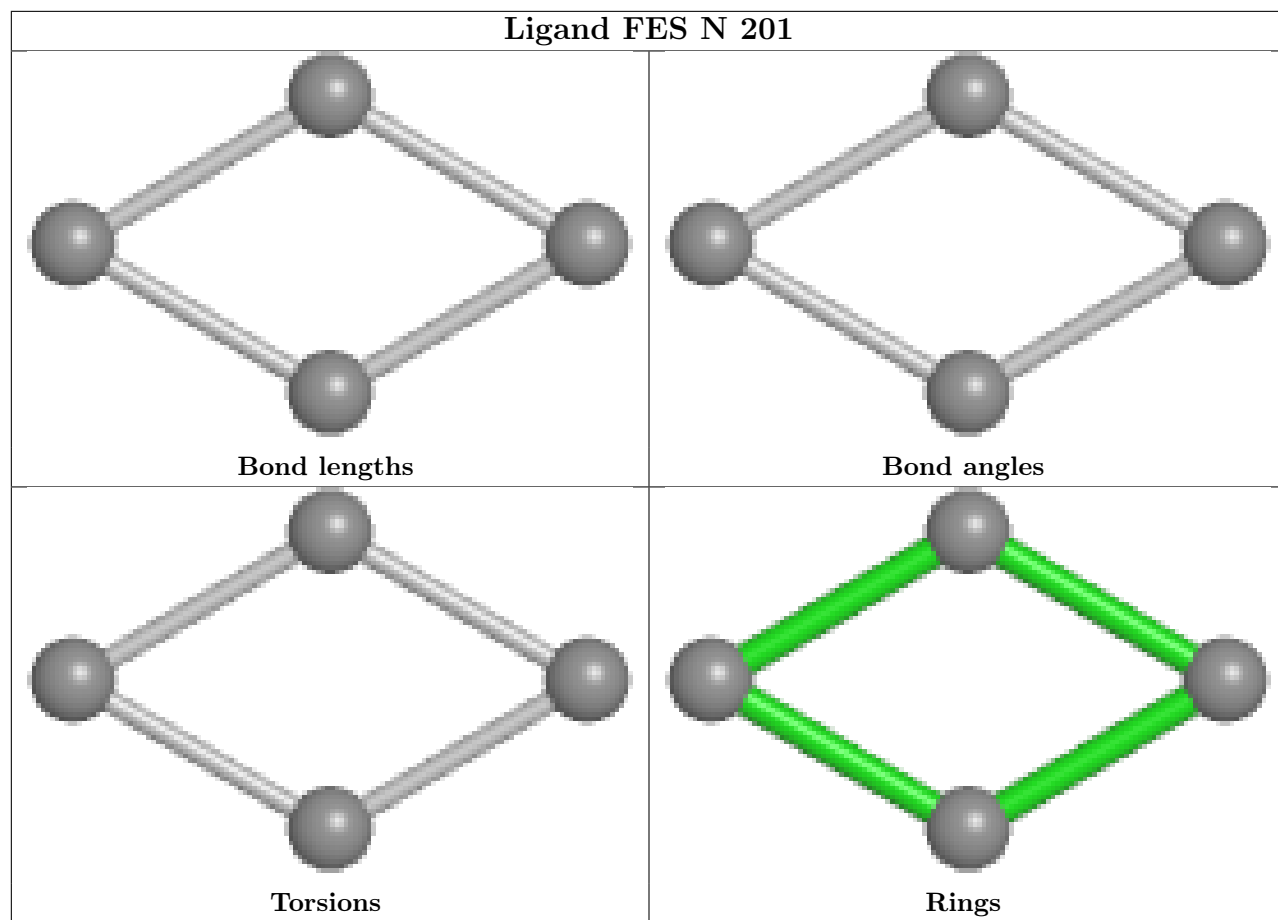




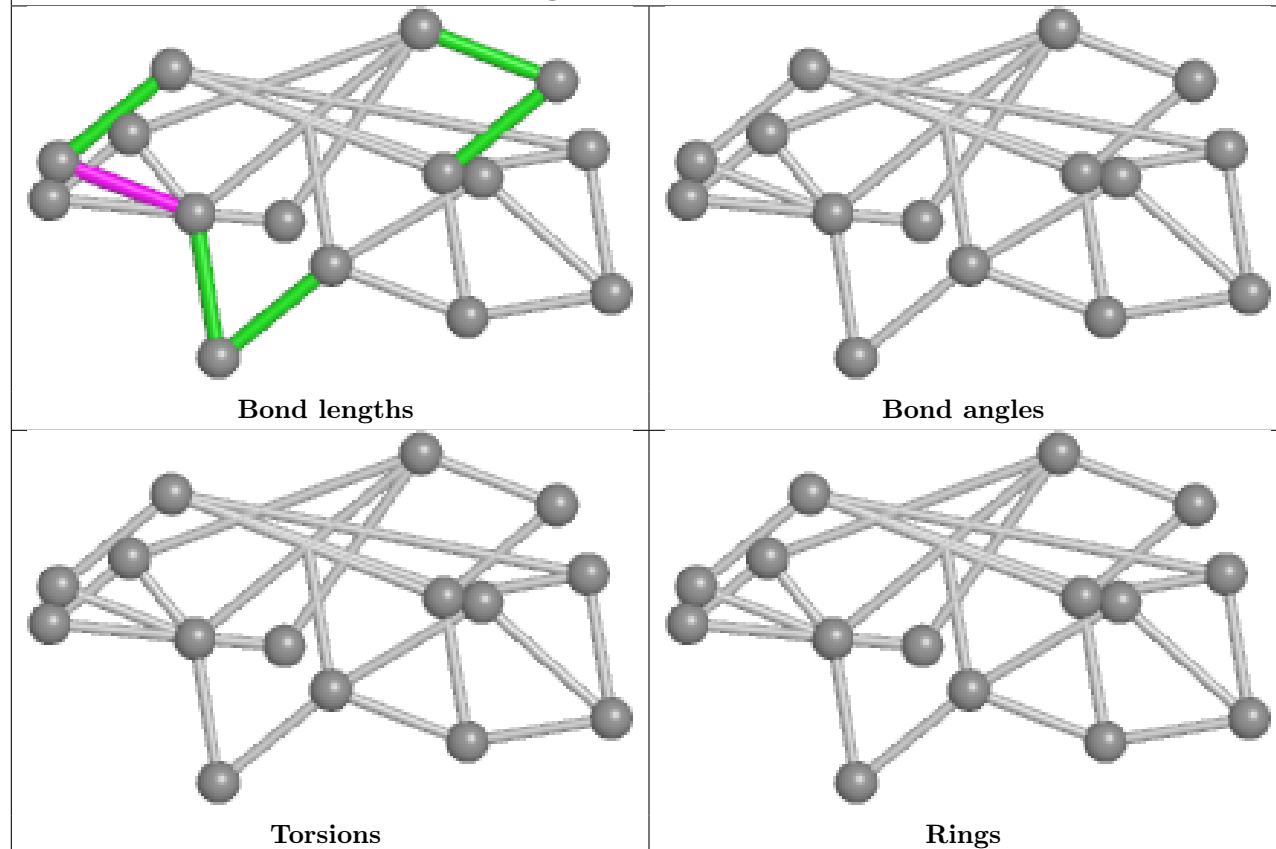




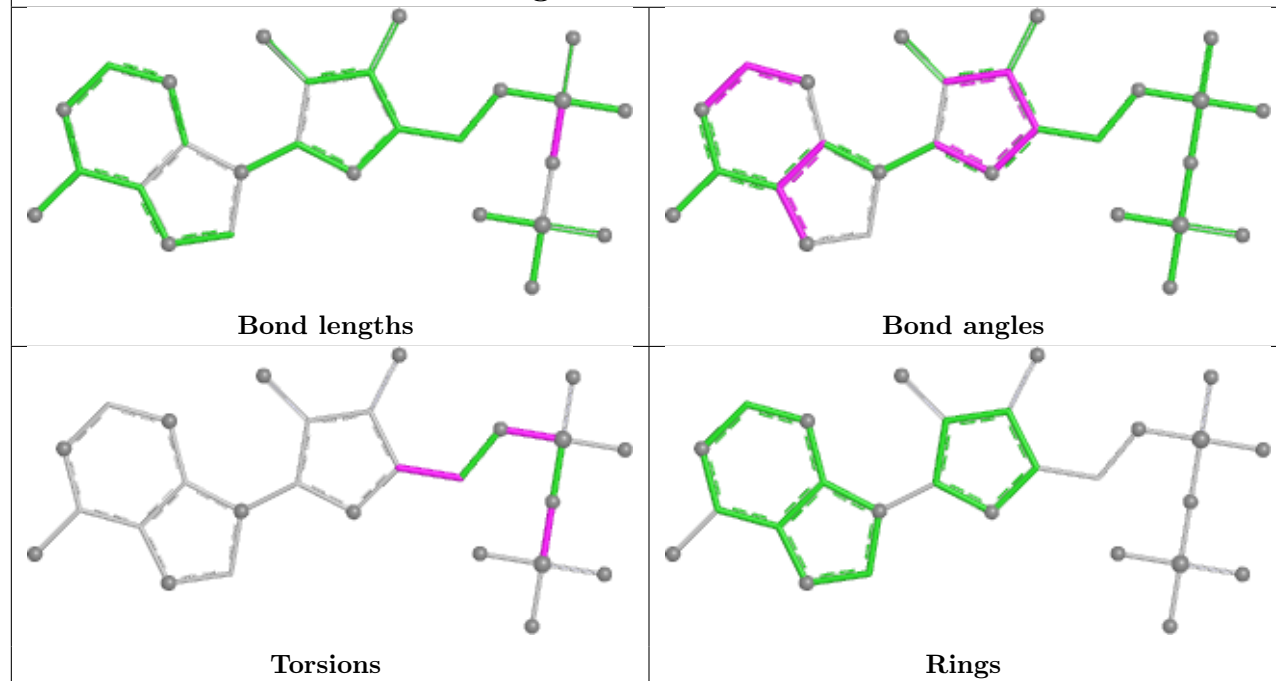


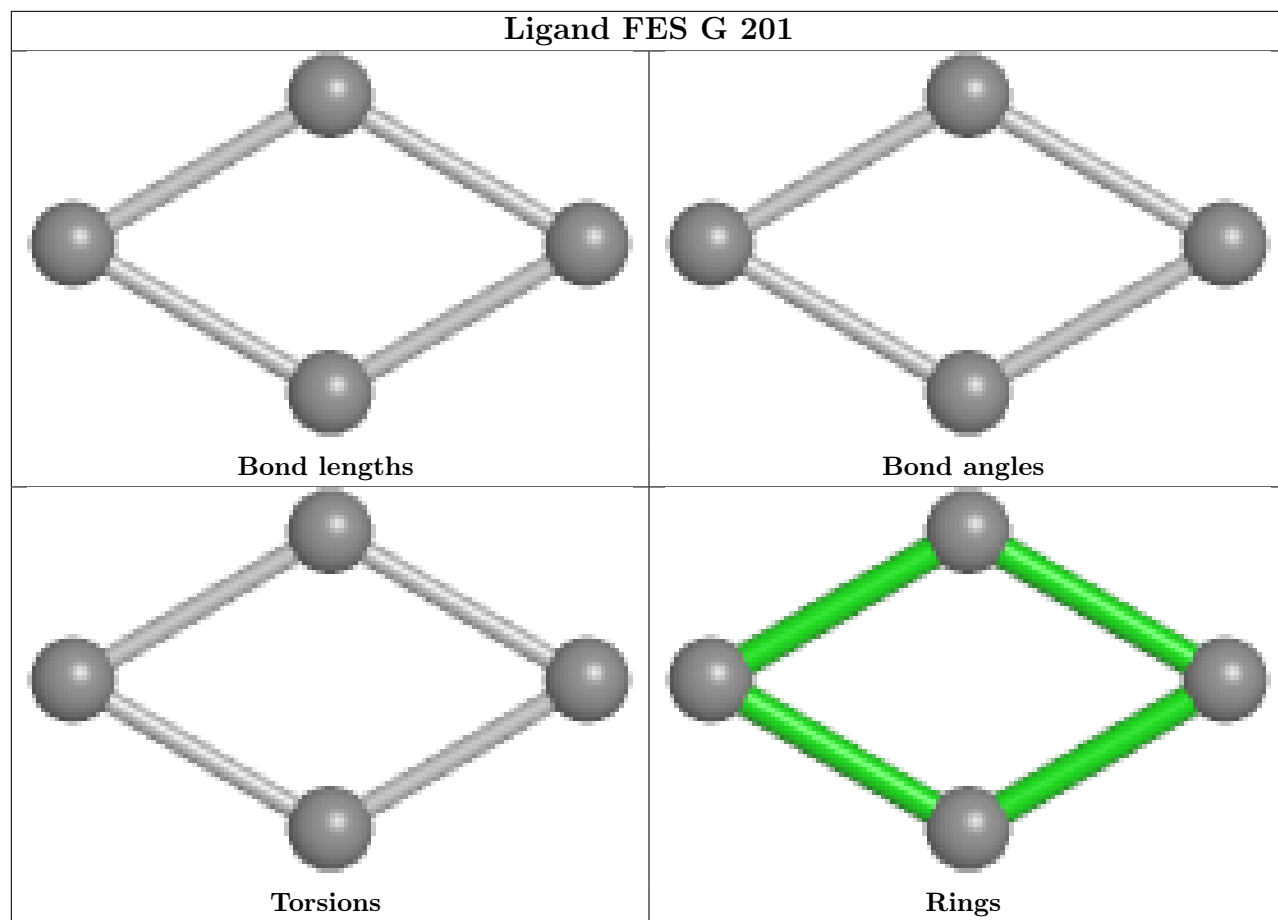


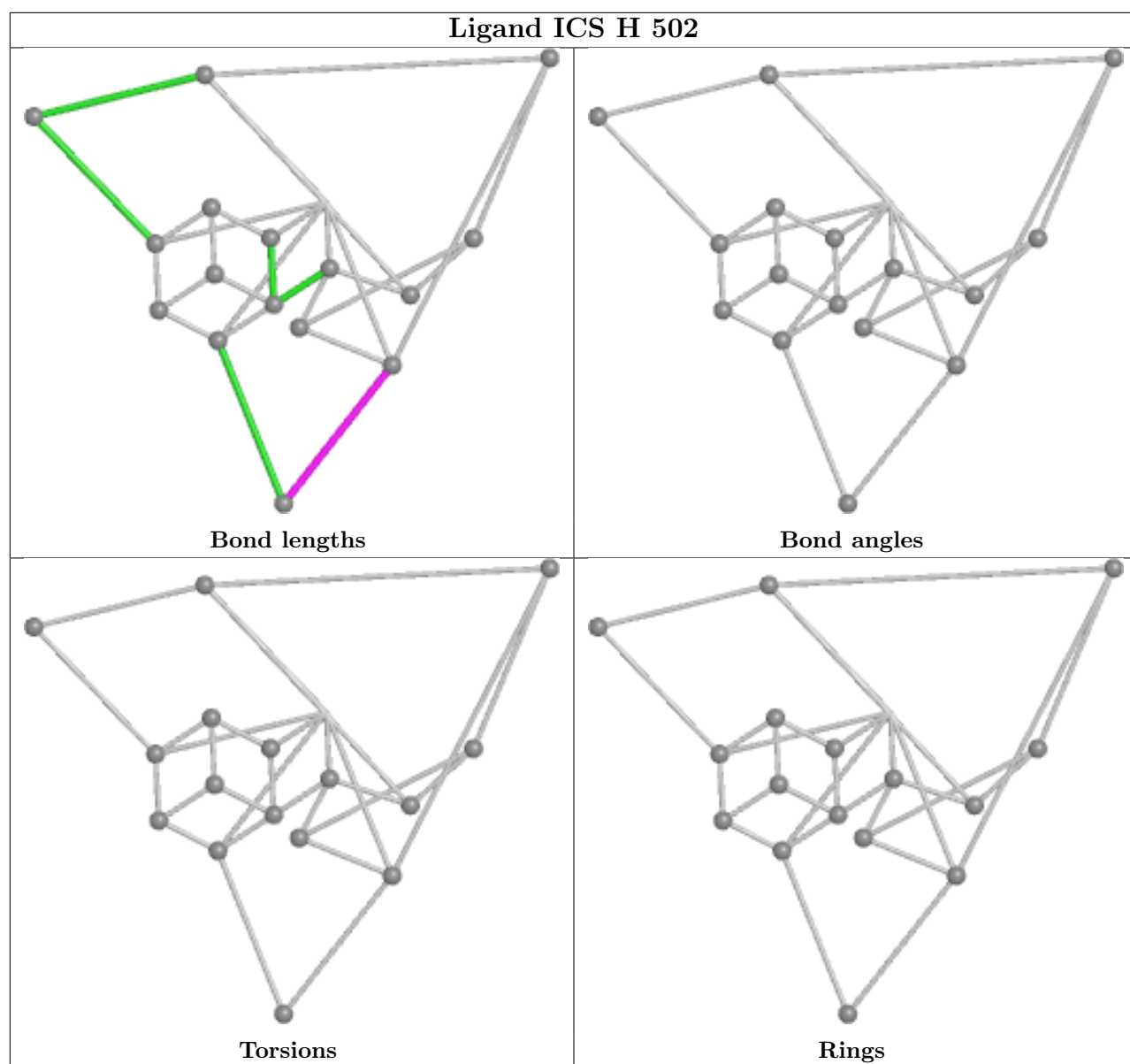
Ligand ICS J 502

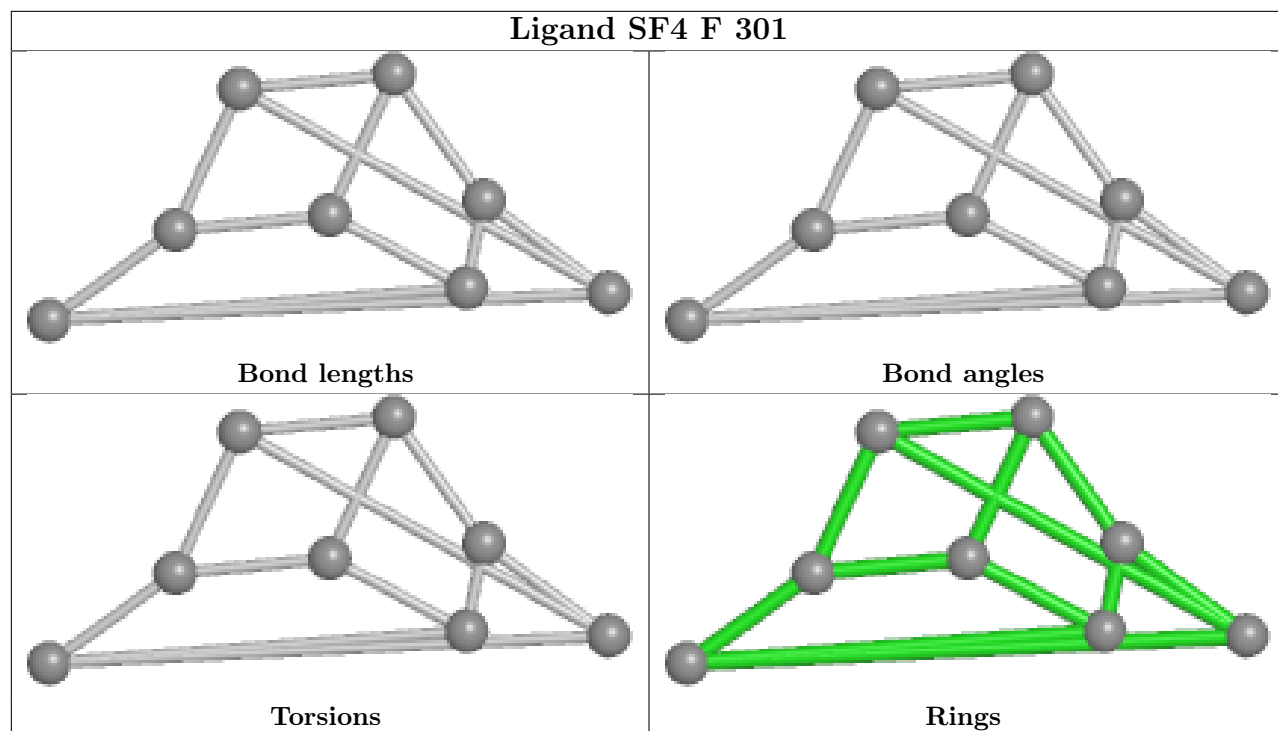


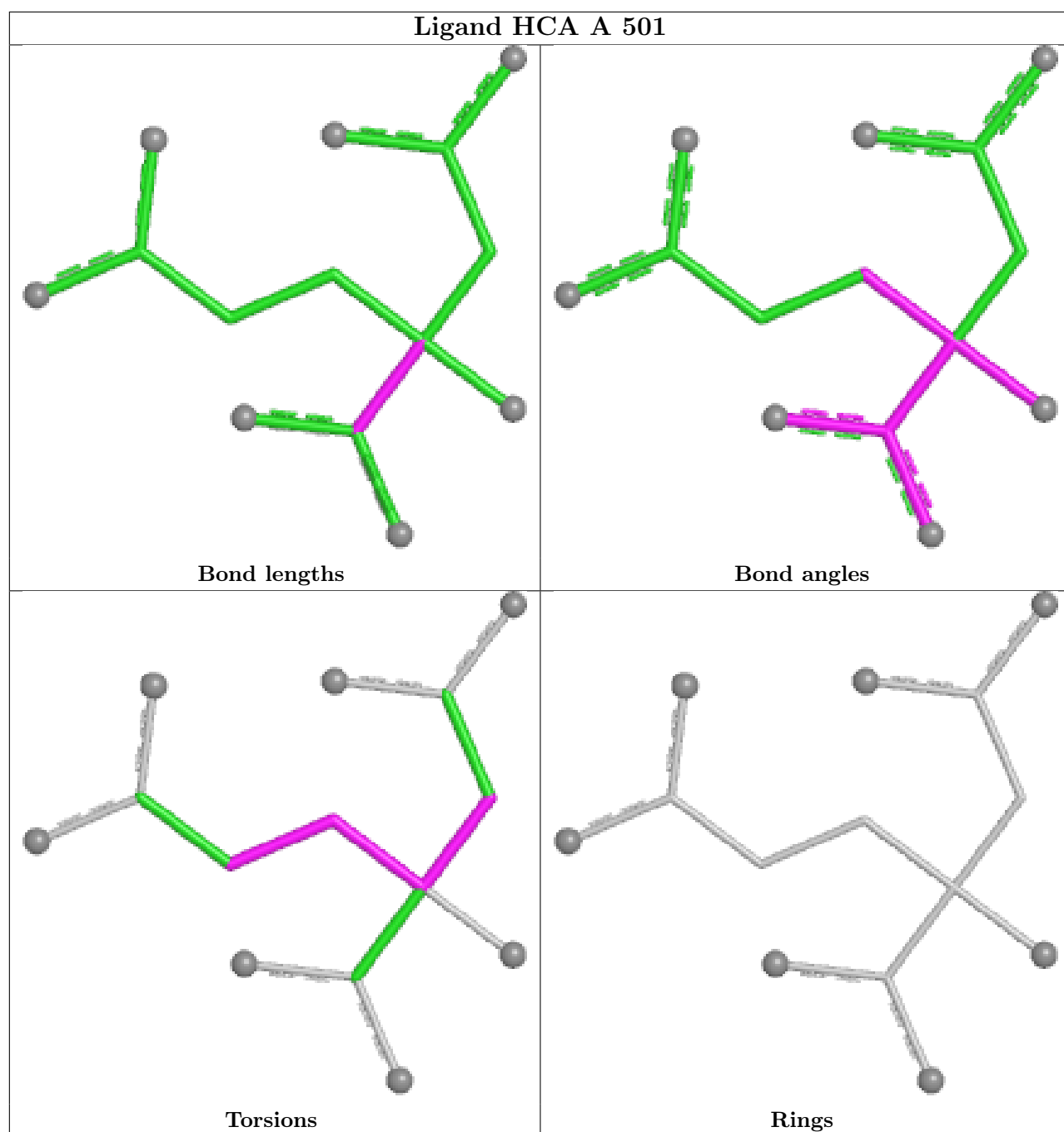
Ligand ADP L 301



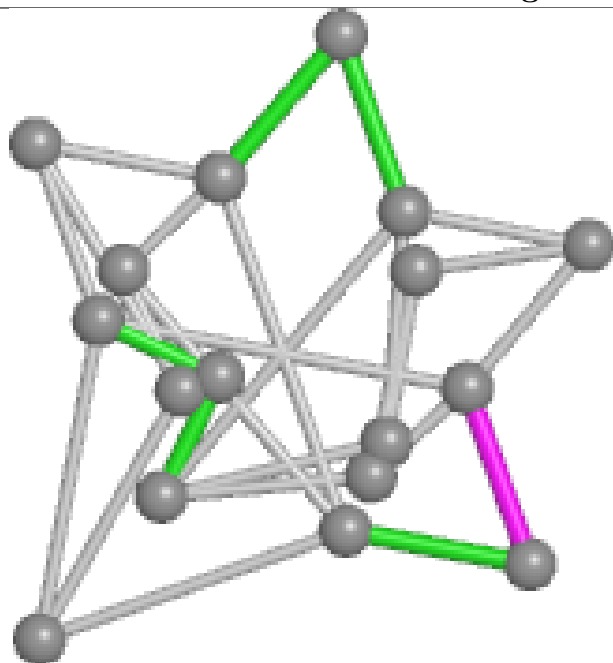




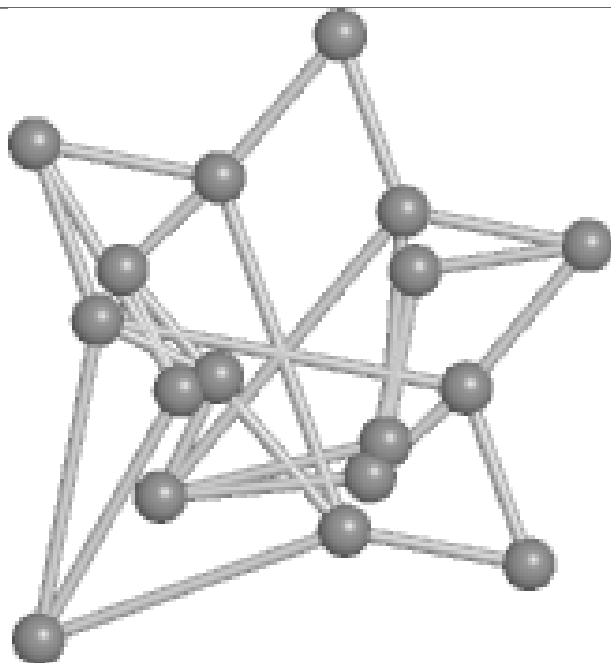




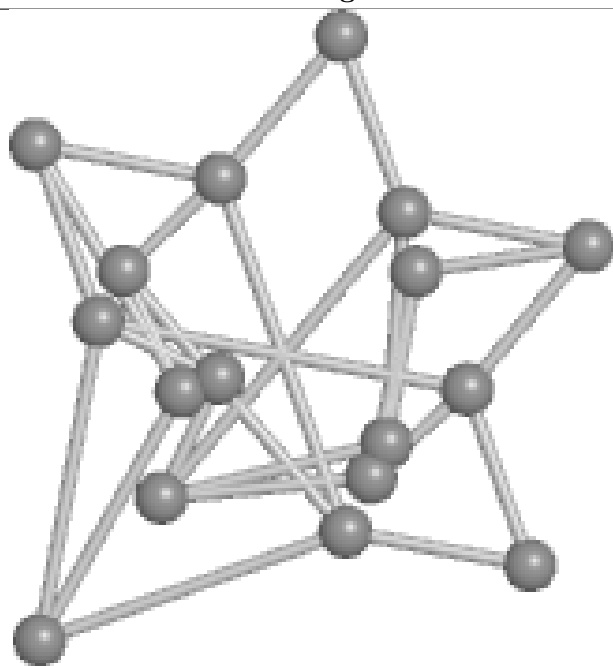
Ligand ICS A 502



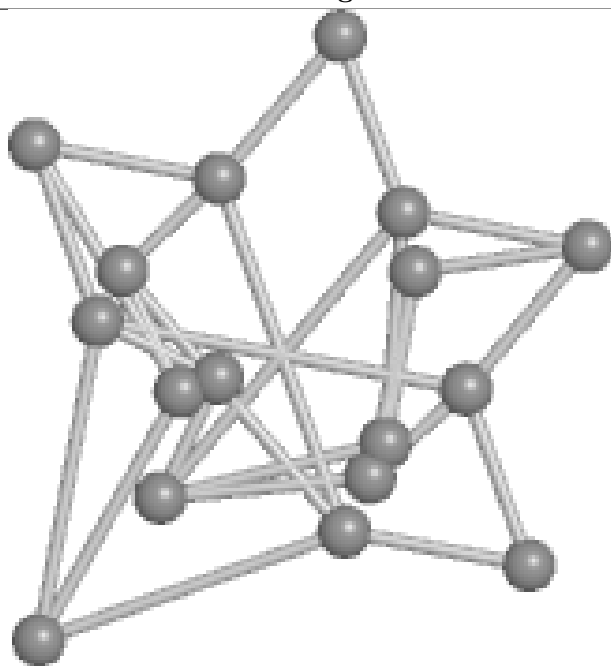
Bond lengths



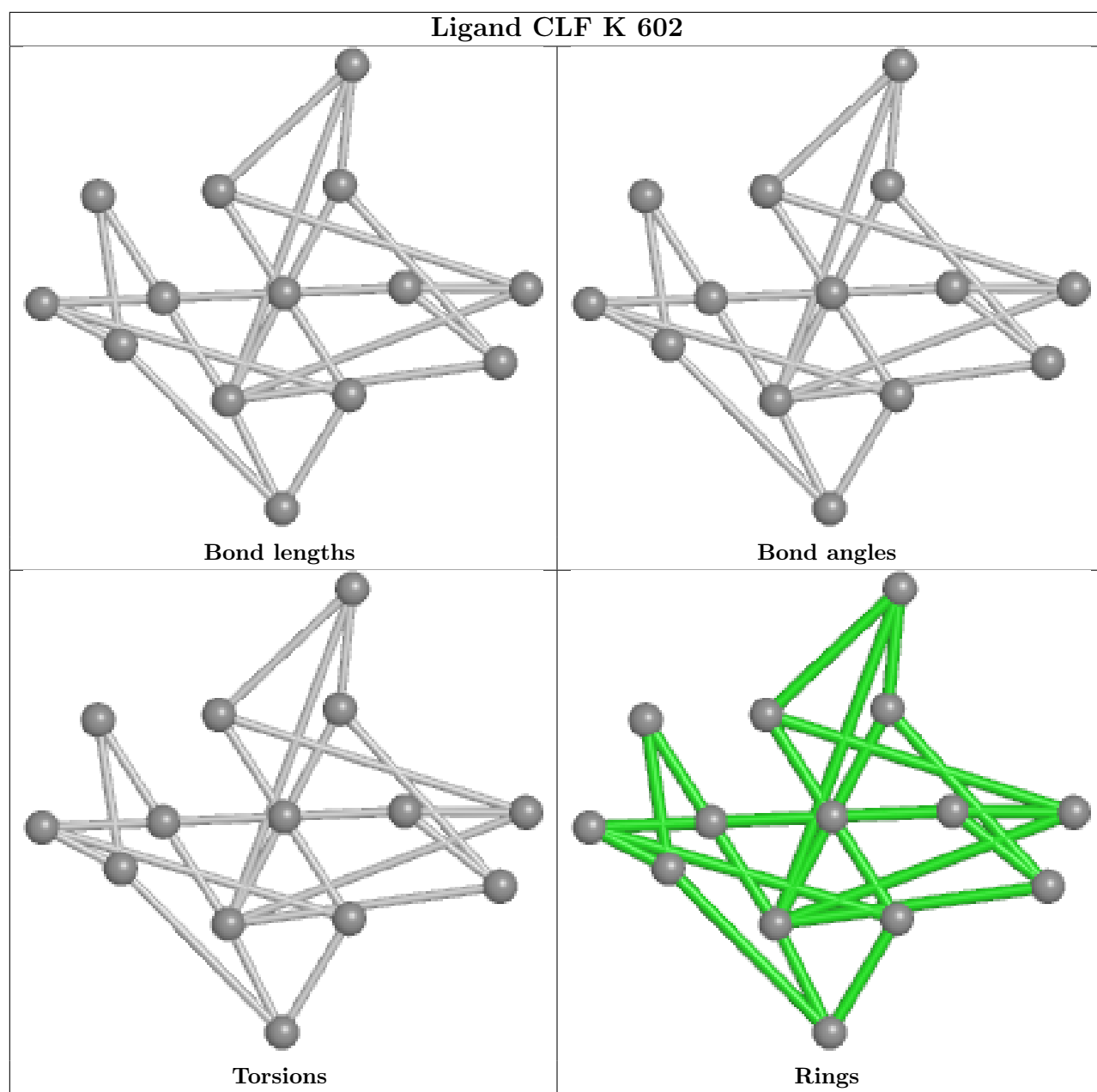
Bond angles

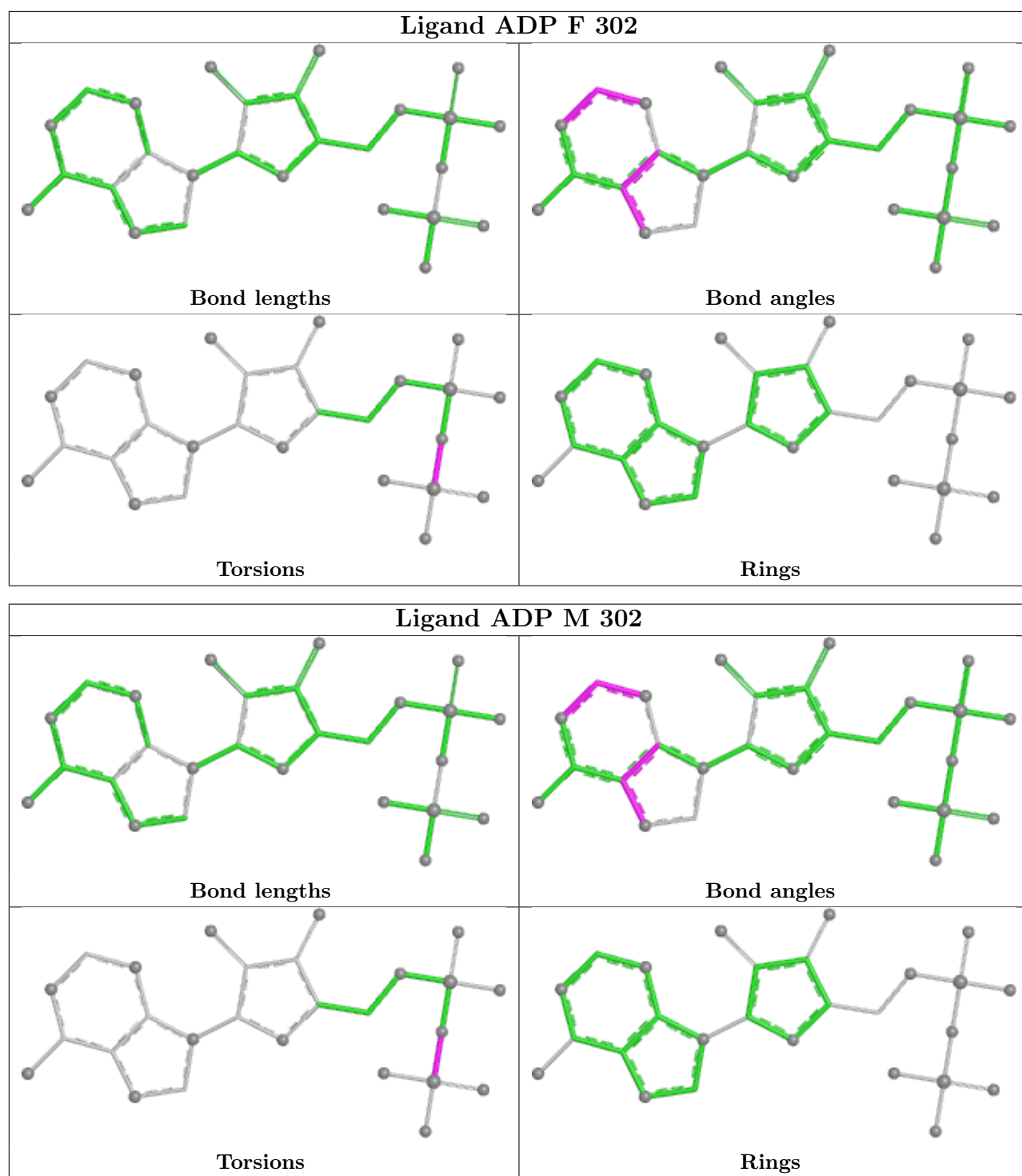


Torsions



Rings





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

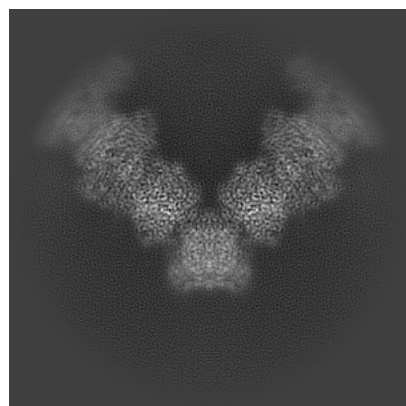
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45926. These allow visual inspection of the internal detail of the map and identification of artifacts.

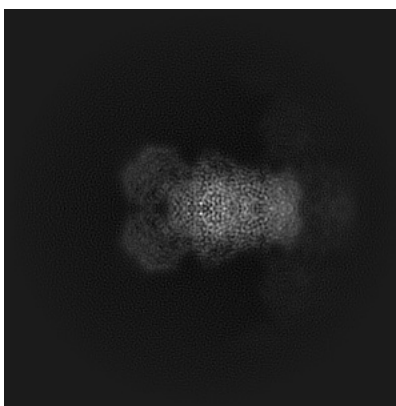
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

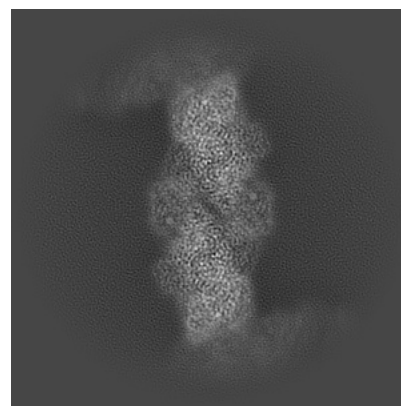
6.1.1 Primary map



X

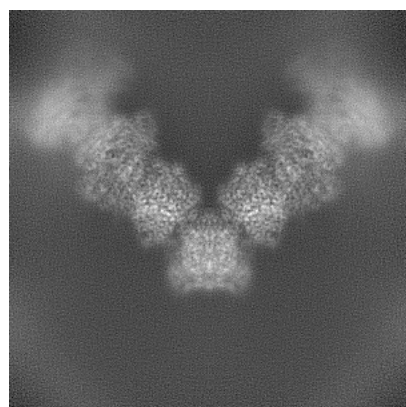


Y

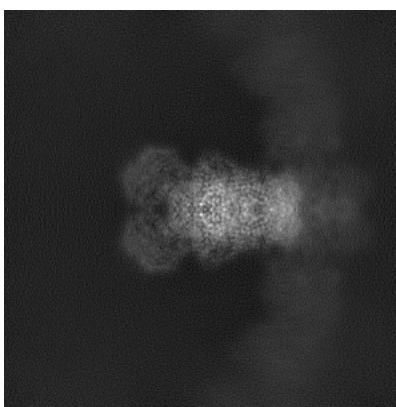


Z

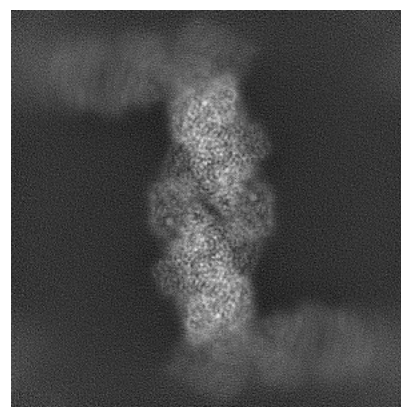
6.1.2 Raw map



X



Y

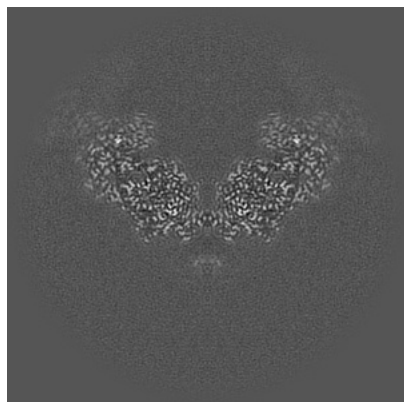


Z

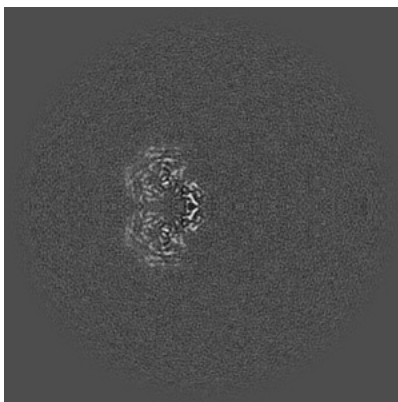
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

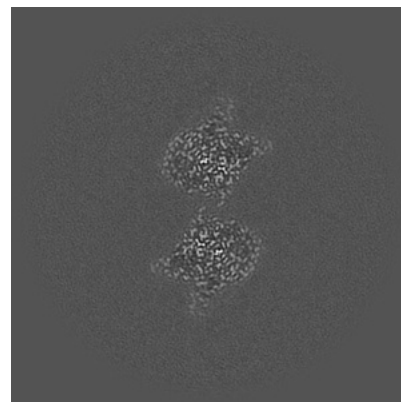
6.2.1 Primary map



X Index: 224

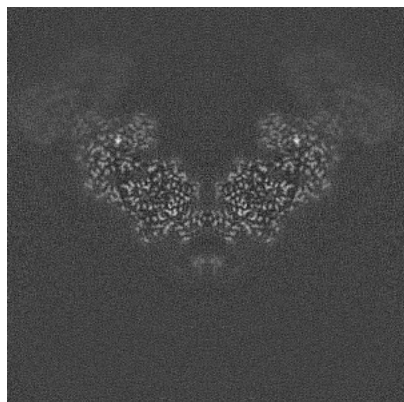


Y Index: 224

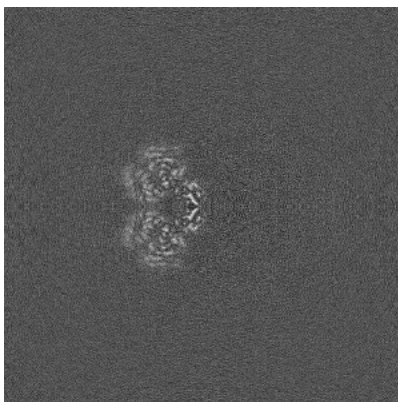


Z Index: 224

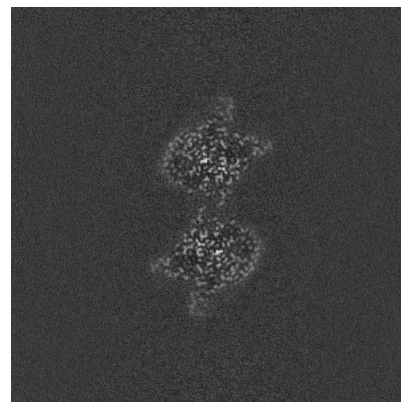
6.2.2 Raw map



X Index: 224



Y Index: 224

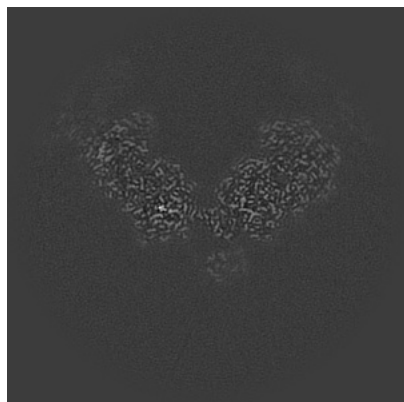


Z Index: 224

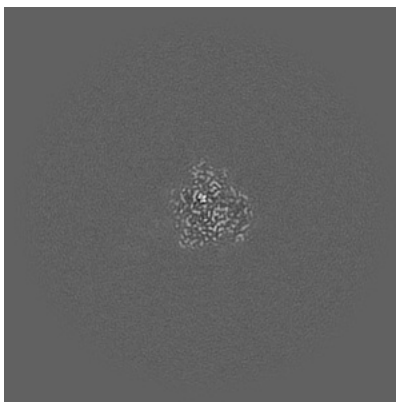
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

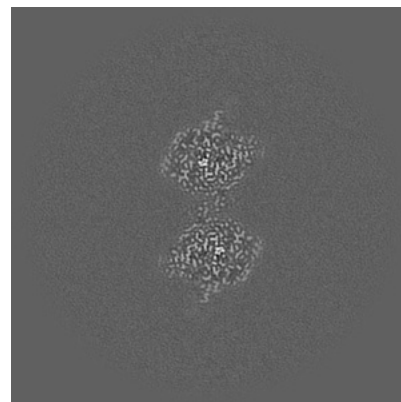
6.3.1 Primary map



X Index: 230

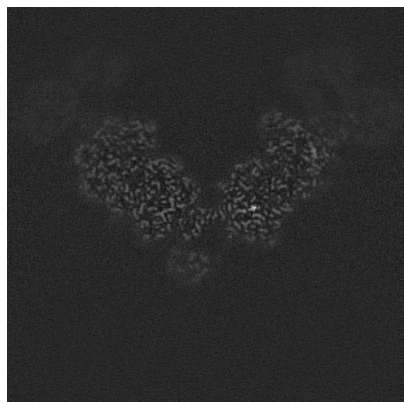


Y Index: 174

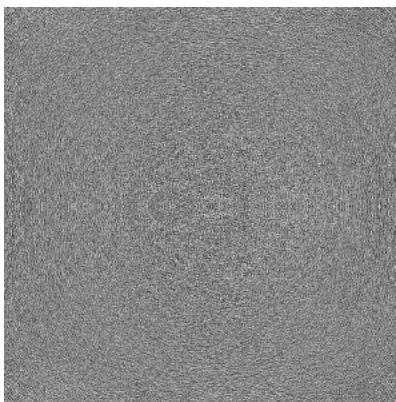


Z Index: 220

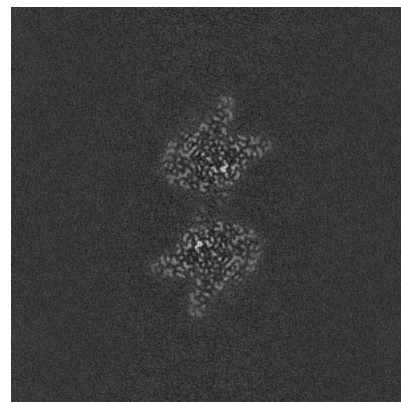
6.3.2 Raw map



X Index: 218



Y Index: 0

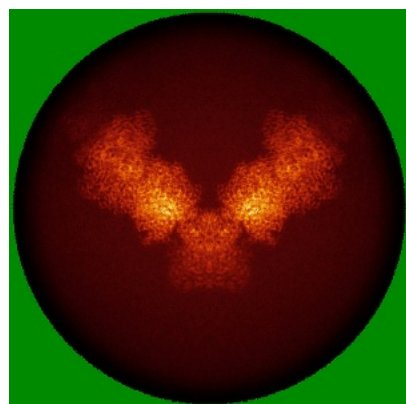


Z Index: 226

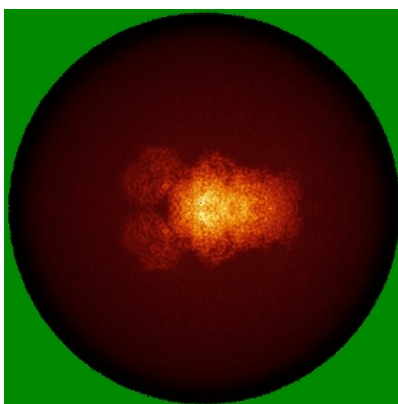
The images above show the largest variance slices of the map in three orthogonal directions.

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

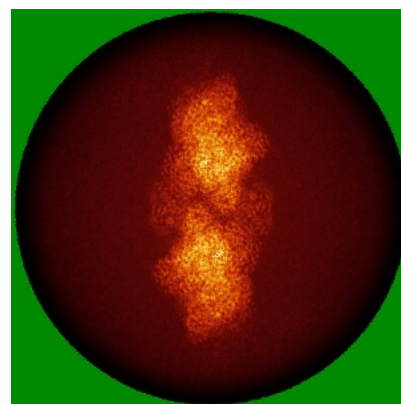
6.4.1 Primary map



X

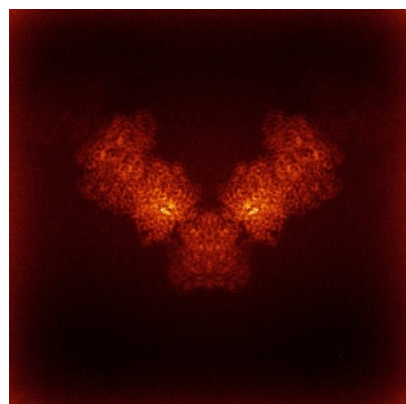


Y

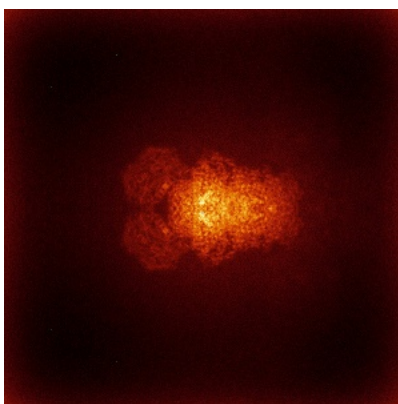


Z

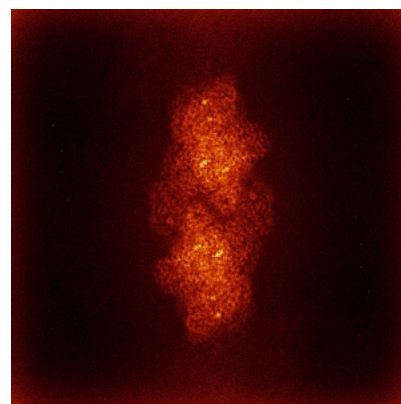
6.4.2 Raw map



X



Y

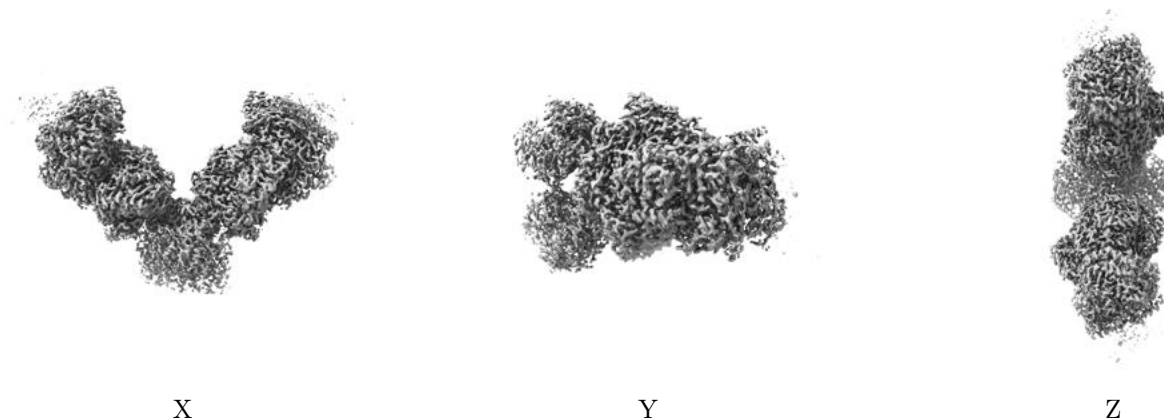


Z

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.

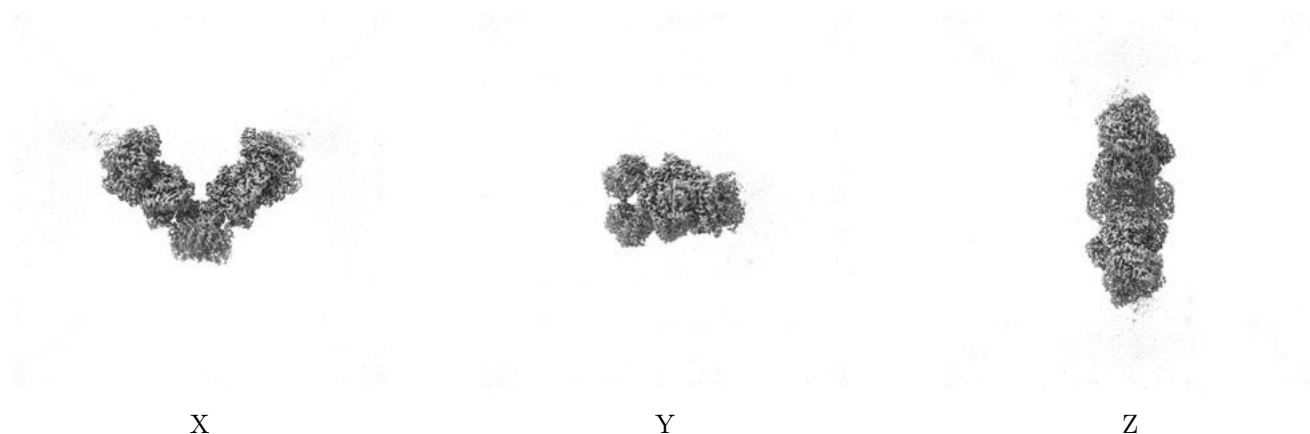
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0402. 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.

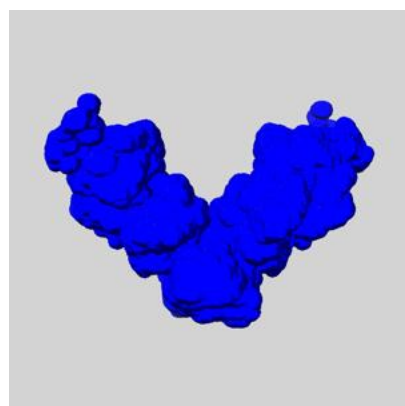
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

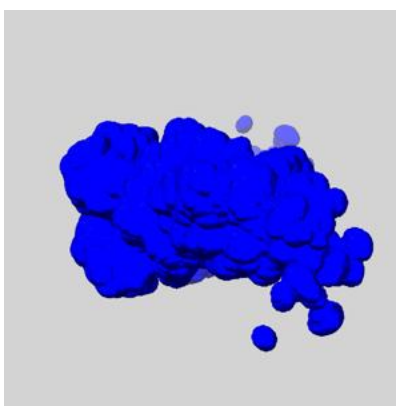
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

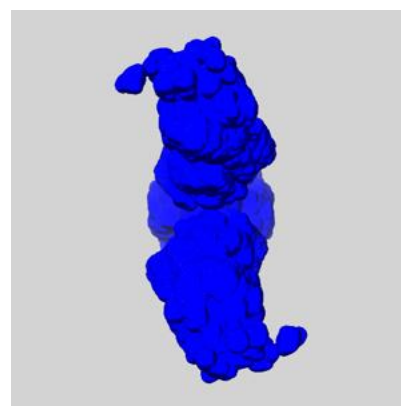
6.6.1 emd_45926_msk_1.map [i](#)



X



Y

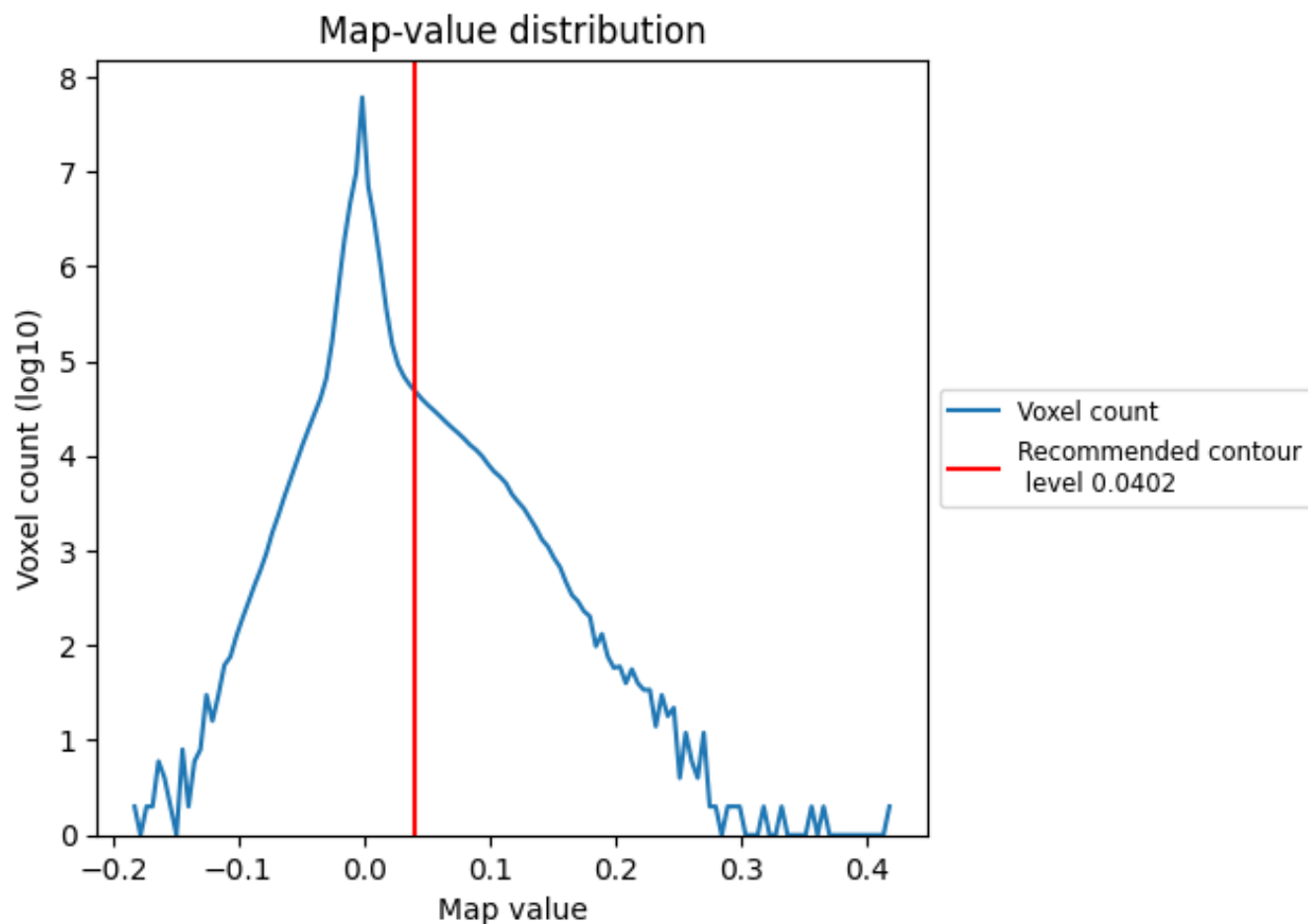


Z

7 Map analysis [i](#)

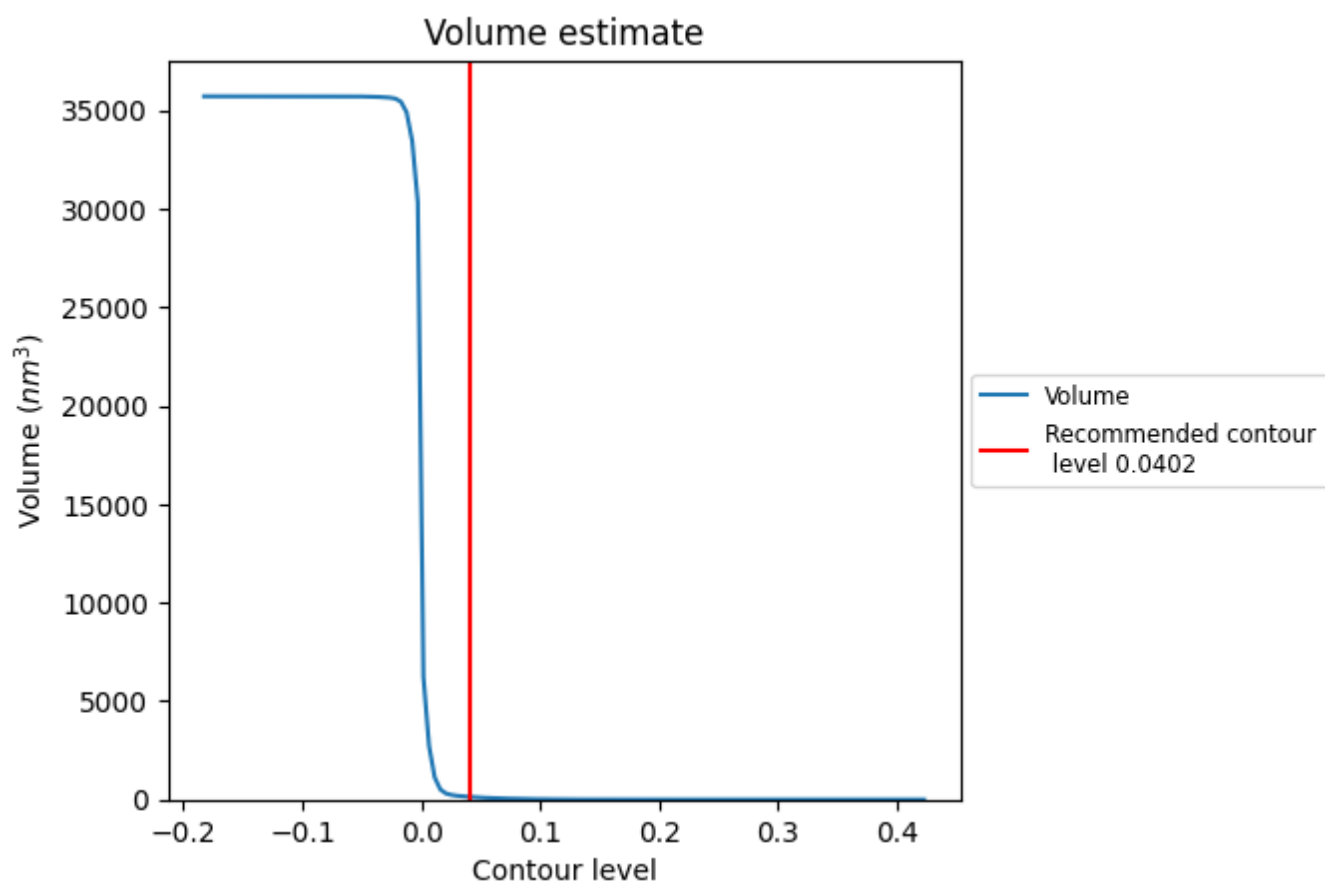
This section contains the results of statistical analysis of the map.

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.

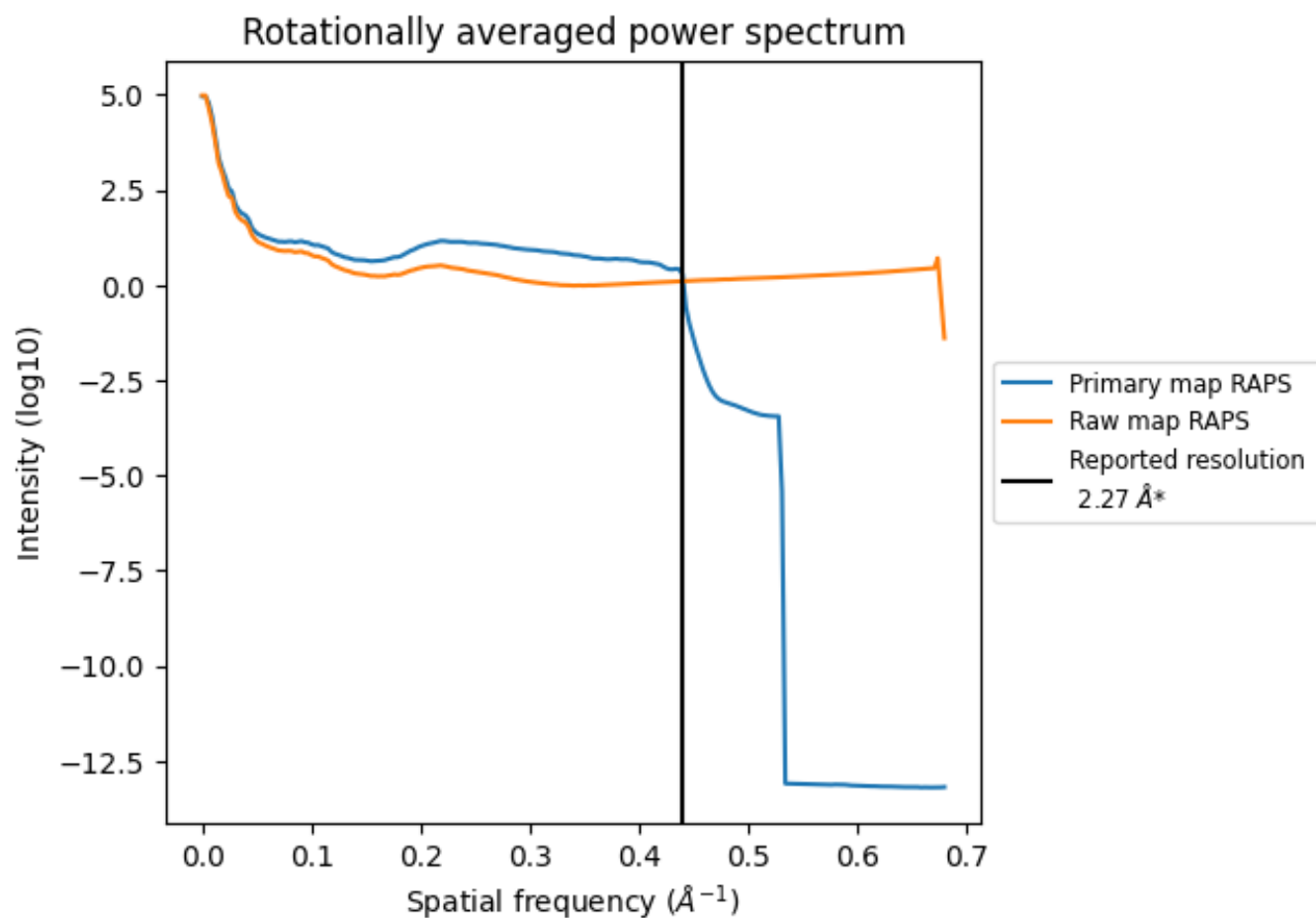
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 137 nm³; this corresponds to an approximate mass of 124 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 ⓘ

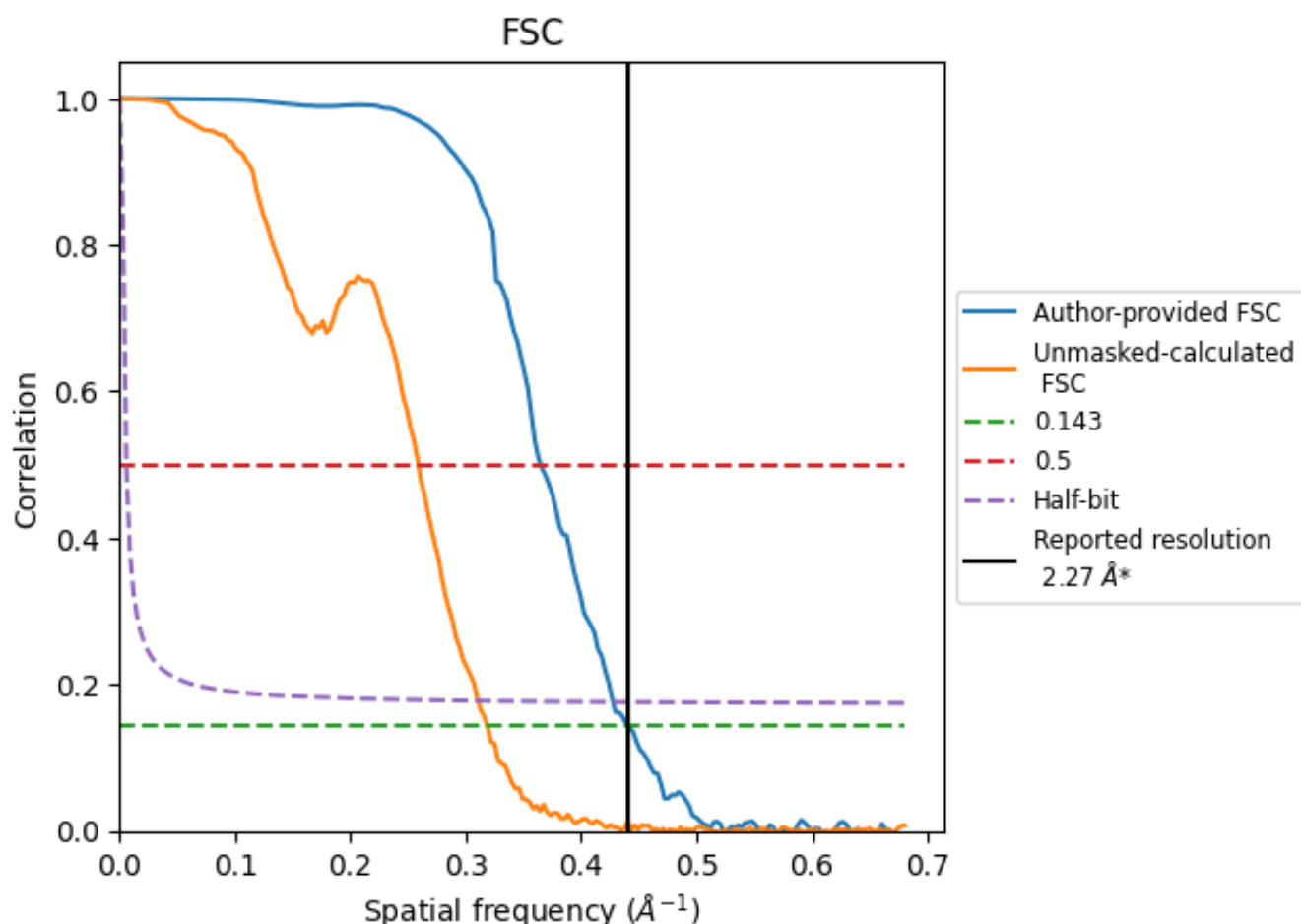


*Reported resolution corresponds to spatial frequency of 0.441 Å⁻¹

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 0.441 \AA^{-1}

8.2 Resolution estimates [i](#)

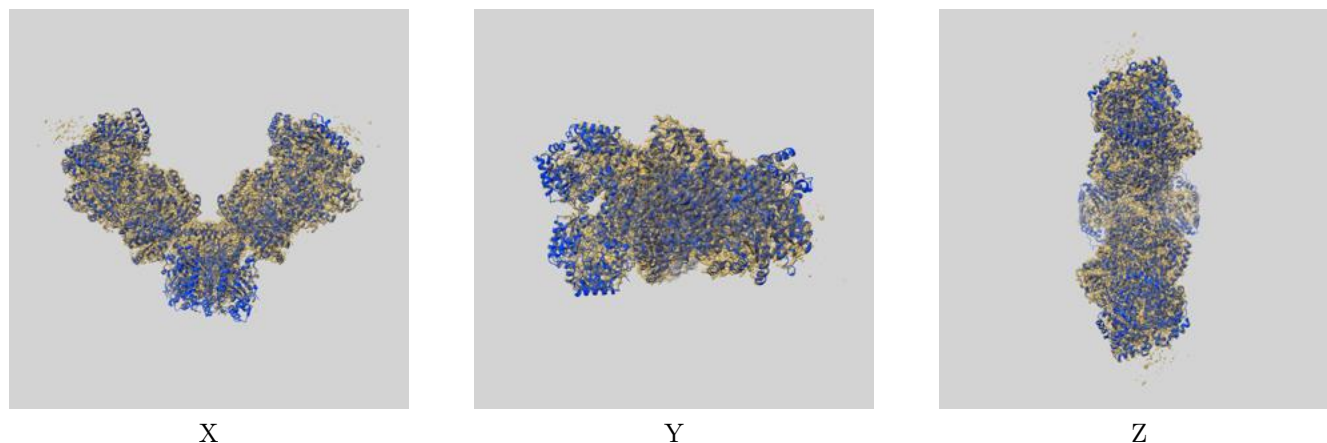
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.27	-	-
Author-provided FSC curve	2.27	2.74	2.34
Unmasked-calculated*	3.14	3.86	3.22

*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 3.14 differs from the reported value 2.27 by more than 10 %

9 Map-model fit [i](#)

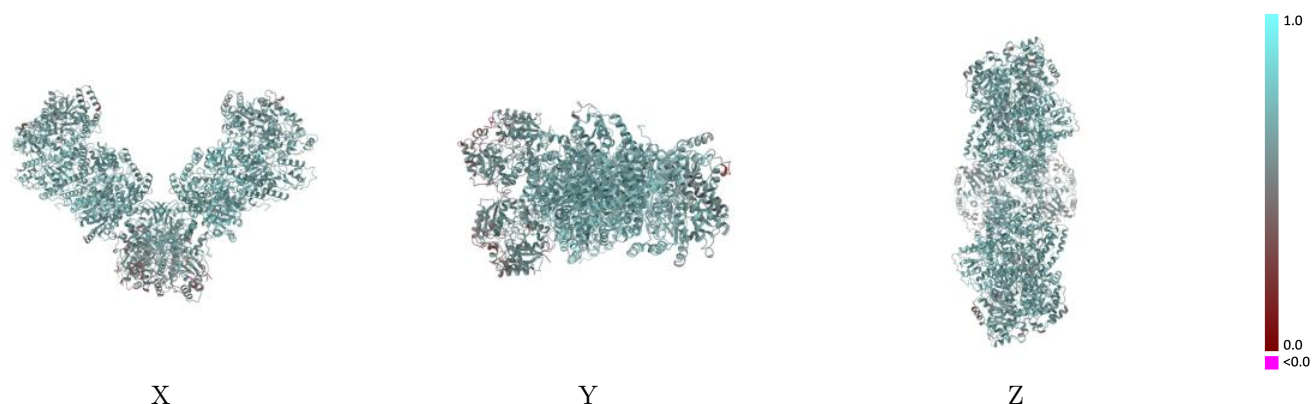
This section contains information regarding the fit between EMDB map EMD-45926 and PDB model 9CU2. Per-residue inclusion information can be found in [section 3](#) on [page 11](#).

9.1 Map-model overlay [i](#)



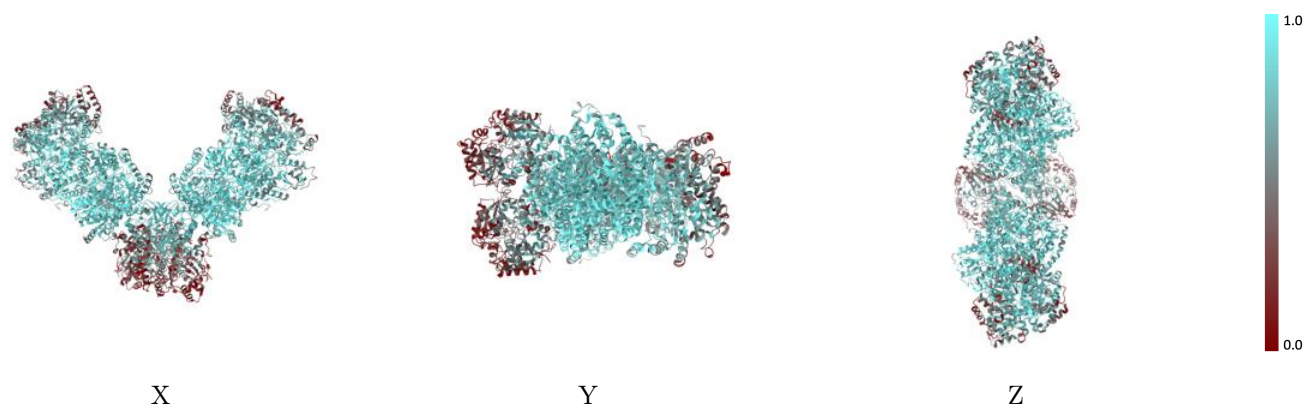
The images above show the 3D surface view of the map at the recommended contour level 0.0402 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



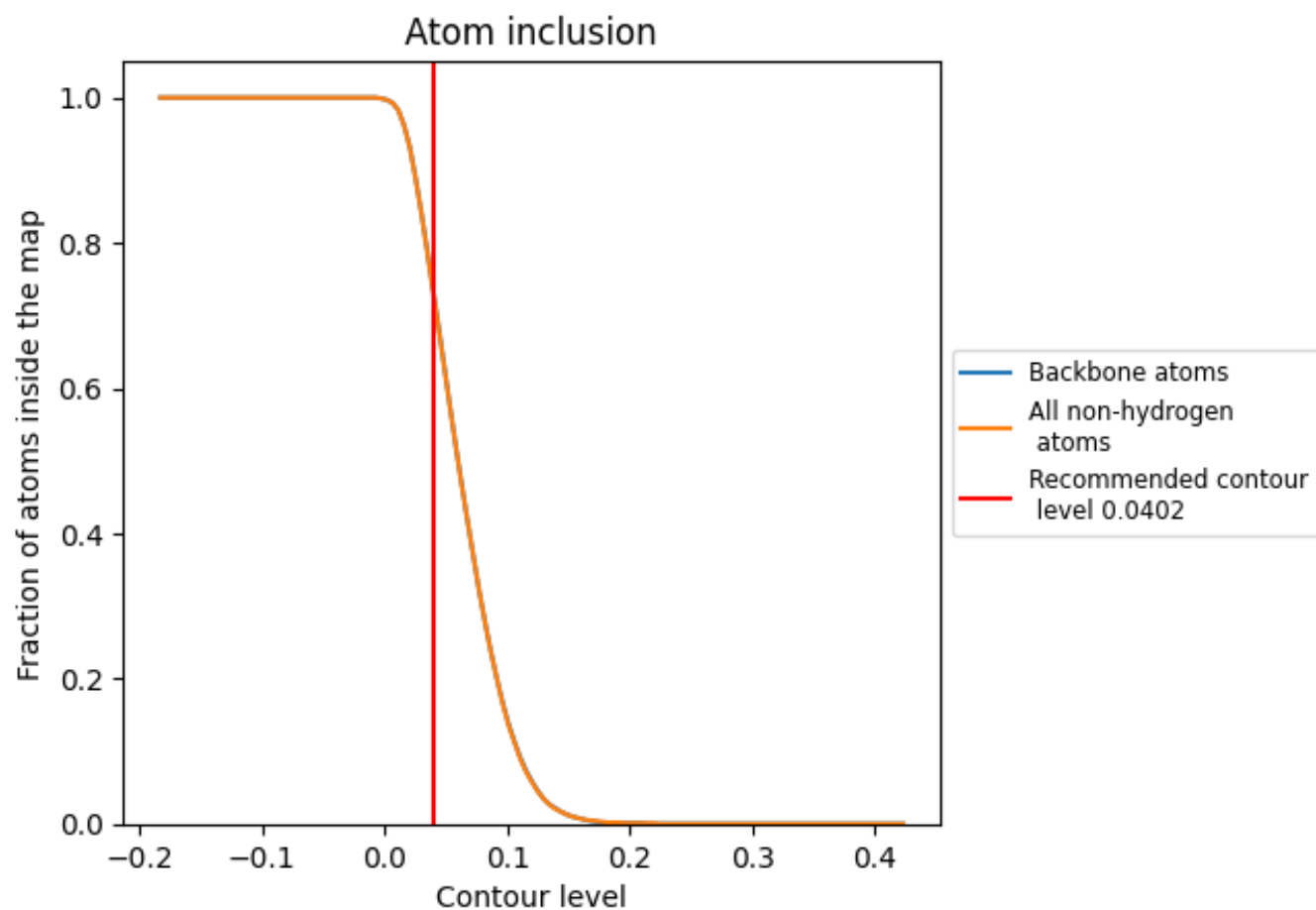
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0402).































9.4 Atom inclusion ⓘ



At the recommended contour level, 73% of all backbone atoms, 73% 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 (0.0402) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7280	 0.6400
A	 0.8850	 0.6750
B	 0.9030	 0.6860
C	 0.6420	 0.6140
D	 0.8010	 0.6610
E	 0.3620	 0.5360
F	 0.4140	 0.5500
G	 0.9200	 0.6930
H	 0.8930	 0.6820
I	 0.9070	 0.6880
J	 0.6450	 0.6190
K	 0.8010	 0.6640
L	 0.3570	 0.5450
M	 0.4230	 0.5460
N	 0.9110	 0.6930

