



Full wwPDB EM Validation Report ⓘ

May 5, 2025 – 10:19 am BST

PDB ID : 8RVU / pdb_00008rvu
EMDB ID : EMD-19533
Title : CryoEM structure of the Elp-Hdr complex of Methanothermobacter marburgensis state 2 (composite structure)
Authors : San Segundo-Acosta, P.; Murphy, B.J.
Deposited on : 2024-02-02
Resolution : 2.22 Å(reported)
Based on initial model : .

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev118
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0rc1
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) : 2.43.1

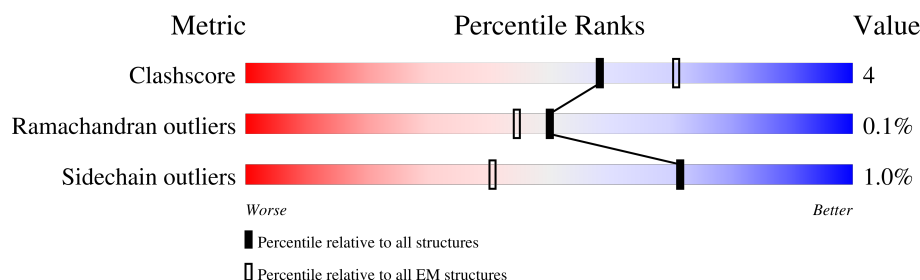
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.22 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	E	380	<div> <div>22%</div> <div>75%</div> <div>19%</div> <div>5%</div> </div>
2	D	342	<div> <div>39%</div> <div>75%</div> <div>21%</div> <div>5%</div> </div>
3	F	136	<div> <div>80%</div> <div>14%</div> <div>5%</div> </div>
4	B	302	<div> <div>20%</div> <div>85%</div> <div>8%</div> <div>6%</div> </div>
4	b	302	<div> <div>16%</div> <div>82%</div> <div>11%</div> <div>6%</div> </div>
5	C	185	<div> <div>10%</div> <div>92%</div> <div>7%</div> </div>
5	c	185	<div> <div>9%</div> <div>88%</div> <div>9%</div> </div>
6	A	659	<div> <div>15%</div> <div>87%</div> <div>8%</div> </div>

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Mol	Chain	Length	Quality of chain
6	a	659	 <div>60% 35%</div>

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 44370 atoms, of which 21804 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 Formate dehydrogenase, beta subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	E	380	Total	C	H	N	O	S	0	0
			5928	1882	2908	515	591	32		

- Molecule 2 is a protein called Formate dehydrogenase, alpha subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	D	339	Total	C	H	N	O	S	0	0
			5094	1632	2515	437	495	15		

- Molecule 3 is a protein called Methyl viologen-reducing hydrogenase, subunit D-related protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	F	129	Total	C	H	N	O	S	0	0
			2026	663	989	179	185	10		

- Molecule 4 is a protein called H(2):CoB-CoM heterodisulfide,ferredoxin reductase subunit B.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	b	284	Total	C	H	N	O	S	0	0
			4357	1387	2161	364	424	21		
4	B	284	Total	C	H	N	O	S	0	0
			4367	1389	2168	364	424	22		

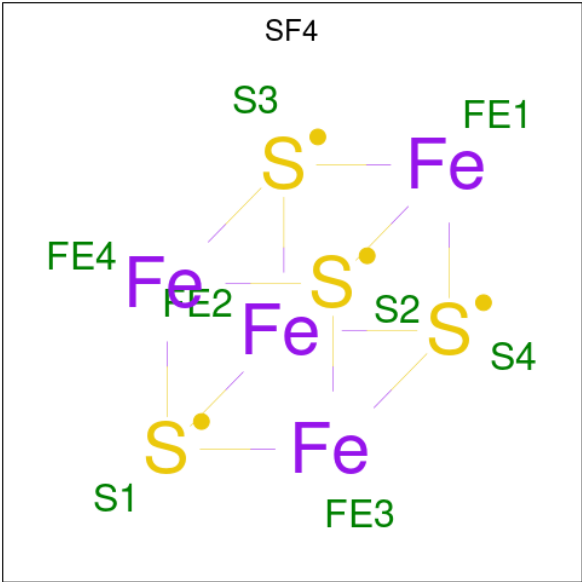
- Molecule 5 is a protein called H(2):CoB-CoM heterodisulfide,ferredoxin reductase subunit C.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	c	184	Total	C	H	N	O	S	0	0
			2853	893	1431	253	265	11		
5	C	183	Total	C	H	N	O	S	0	0
			2847	890	1430	252	264	11		

- Molecule 6 is a protein called H(2):CoB-CoM heterodisulfide,ferredoxin reductase subunit A.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	a	427	Total	C	H	N	O	S	0	0
			6540	2072	3264	537	636	31		
6	A	643	Total	C	H	N	O	S	0	0
			9786	3096	4876	818	948	48		

- Molecule 7 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄) (labeled as "Lig- and of Interest" by depositor).



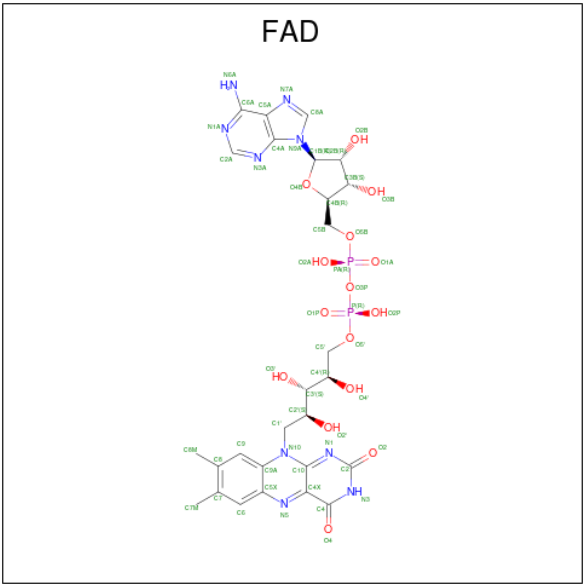
Mol	Chain	Residues	Atoms			AltConf
7	E	1	Total	Fe	S	0
			8	4	4	
7	E	1	Total	Fe	S	0
			8	4	4	
7	E	1	Total	Fe	S	0
			8	4	4	
7	E	1	Total	Fe	S	0
			8	4	4	
7	D	1	Total	Fe	S	0
			8	4	4	
7	c	1	Total	Fe	S	0
			8	4	4	
7	c	1	Total	Fe	S	0
			8	4	4	
7	C	1	Total	Fe	S	0
			8	4	4	

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Mol	Chain	Residues	Atoms			AltConf
7	C	1	Total	Fe	S	0
			8	4	4	
7	a	1	Total	Fe	S	0
			8	4	4	
7	a	1	Total	Fe	S	0
			8	4	4	
7	a	1	Total	Fe	S	0
			8	4	4	
7	A	1	Total	Fe	S	0
			8	4	4	
7	A	1	Total	Fe	S	0
			8	4	4	
7	A	1	Total	Fe	S	0
			8	4	4	
7	A	1	Total	Fe	S	0
			8	4	4	
7	A	1	Total	Fe	S	0
			8	4	4	

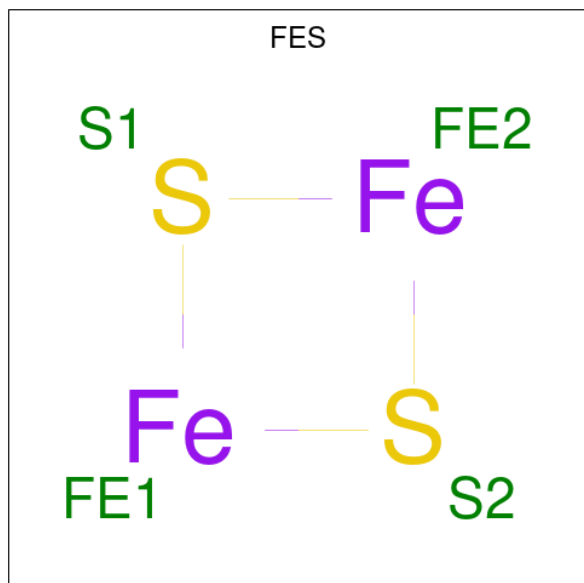
- Molecule 8 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂) (labeled as "Ligand of Interest" by depositor).



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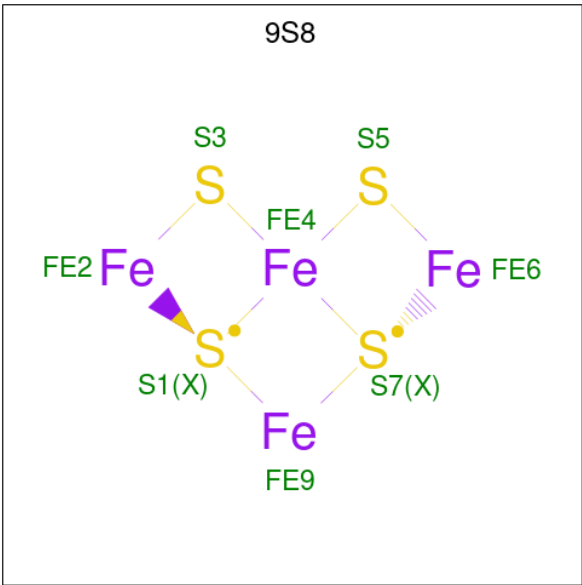
Mol	Chain	Residues	Atoms					AltConf
8	a	1	Total	C	H	N	O	P
			84	27	31	9	15	2
8	A	1	Total	C	H	N	O	P
			84	27	31	9	15	2

- Molecule 9 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
9	F	1	Total	Fe	S	0
			4	2	2	

- Molecule 10 is Non-cubane [4Fe-4S]-cluster (CCD ID: 9S8) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
10	b	1	Total	Fe	S	0
			8	4	4	
10	b	1	Total	Fe	S	0
			8	4	4	
10	B	1	Total	Fe	S	0
			8	4	4	
10	B	1	Total	Fe	S	0
			8	4	4	

- Molecule 11 is water.

Mol	Chain	Residues	Atoms		AltConf
11	E	8	Total	O	0
			8	8	
11	D	7	Total	O	0
			7	7	
11	F	2	Total	O	0
			2	2	
11	b	11	Total	O	0
			11	11	
11	B	14	Total	O	0
			14	14	
11	c	11	Total	O	0
			11	11	
11	C	9	Total	O	0
			9	9	
11	a	60	Total	O	0
			60	60	

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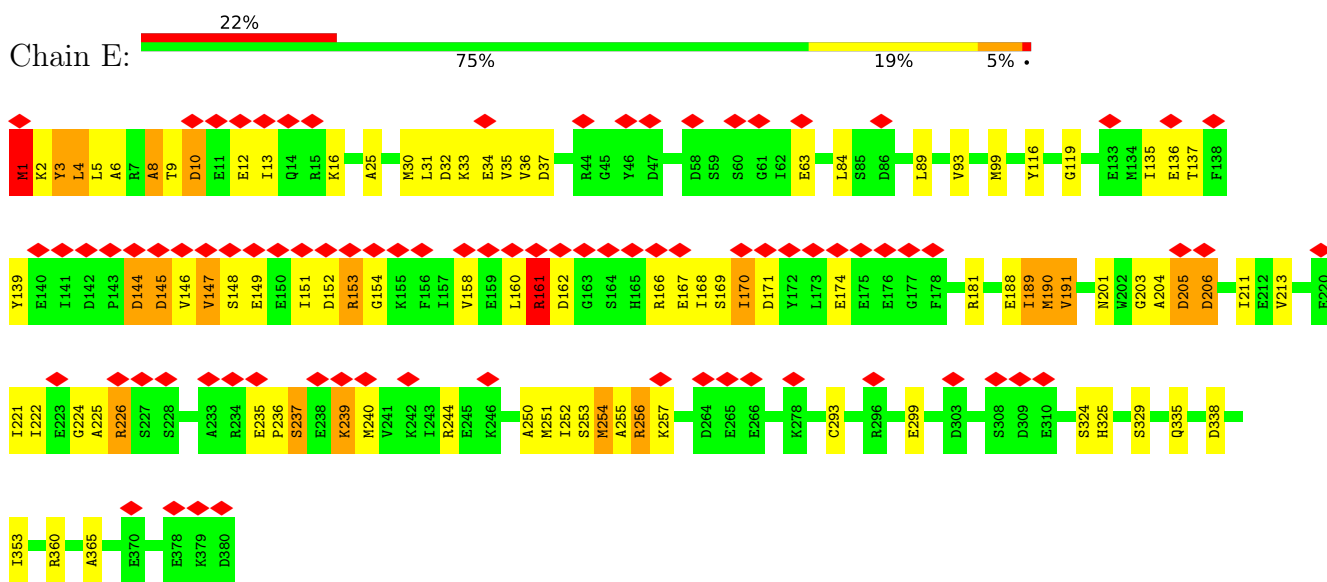
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Mol	Chain	Residues	Atoms		AltConf
11	A	49	Total	O	0
			49	49	

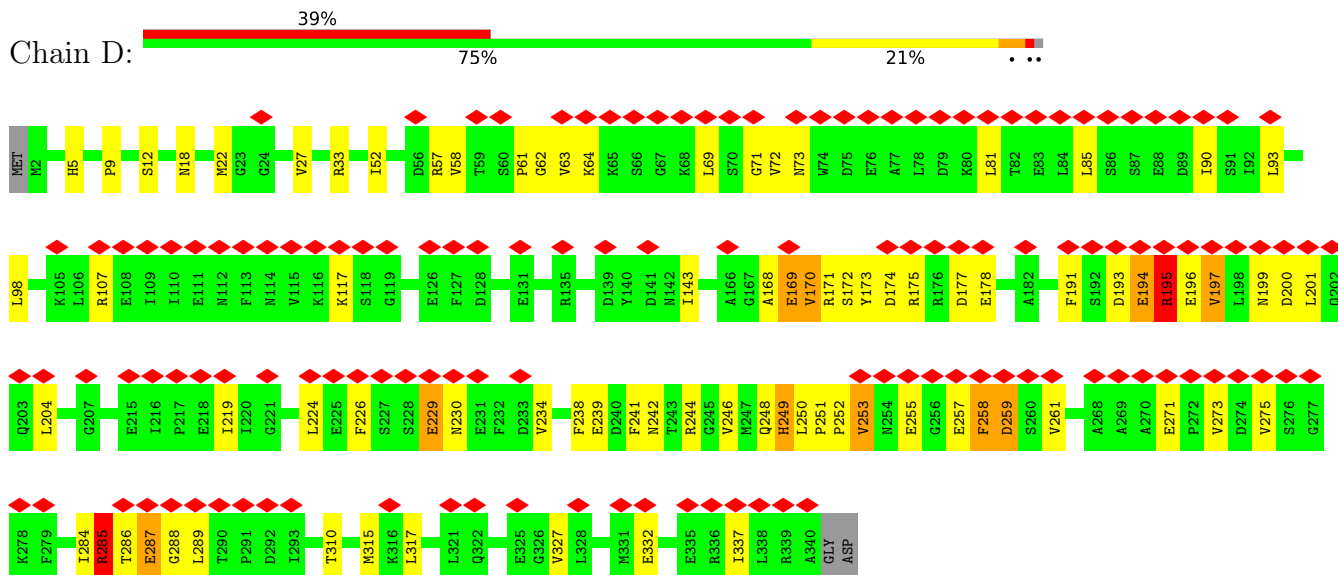
3 Residue-property plots

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: Formate dehydrogenase, beta subunit

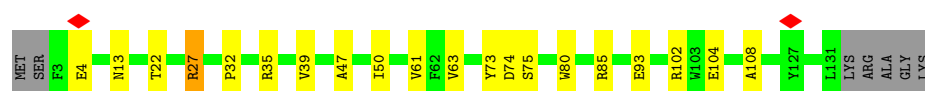


- Molecule 2: Formate dehydrogenase, alpha subunit




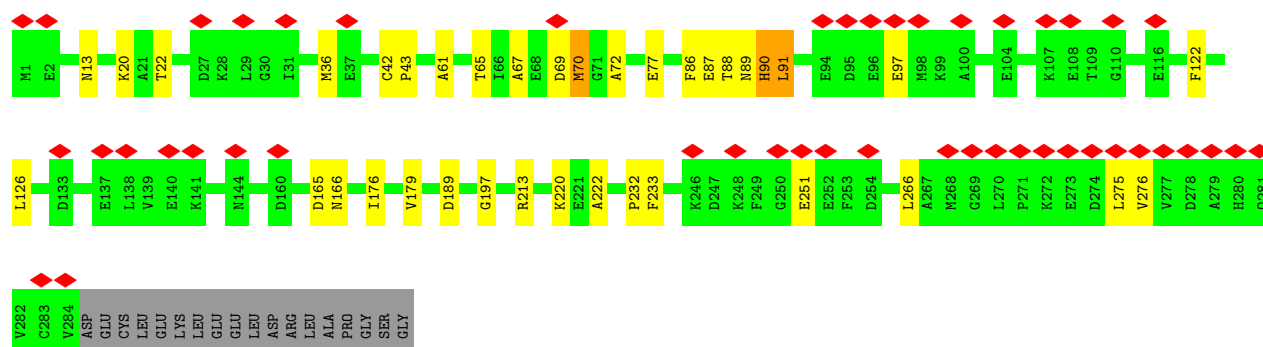
- Molecule 3: Methyl viologen-reducing hydrogenase, subunit D-related protein

Chain F: 




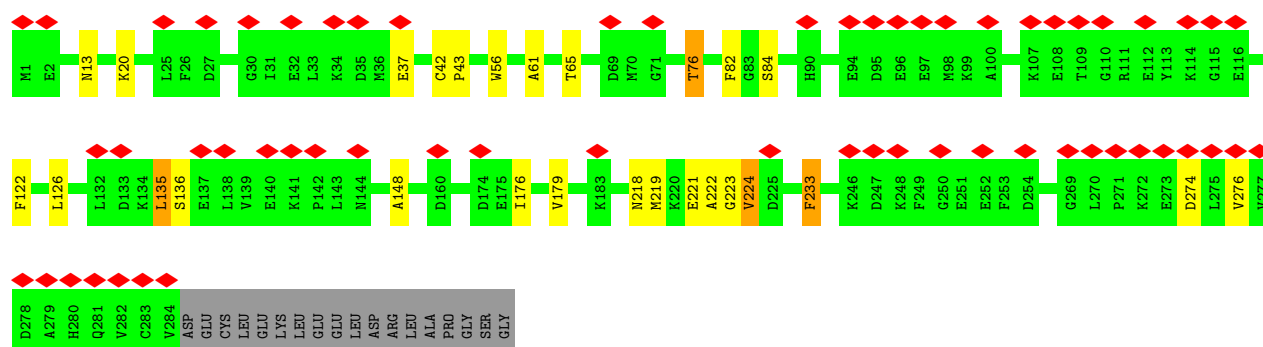
- Molecule 4: H(2):CoB-CoM heterodisulfide,ferredoxin reductase subunit B

Chain b: 




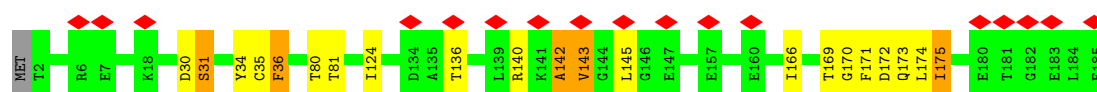
- Molecule 4: H(2):CoB-CoM heterodisulfide,ferredoxin reductase subunit B

Chain B: 

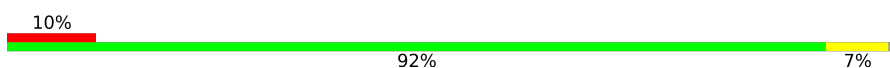


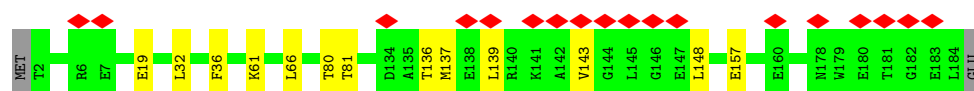
- Molecule 5: H(2):CoB-CoM heterodisulfide,ferredoxin reductase subunit C

Chain c: 

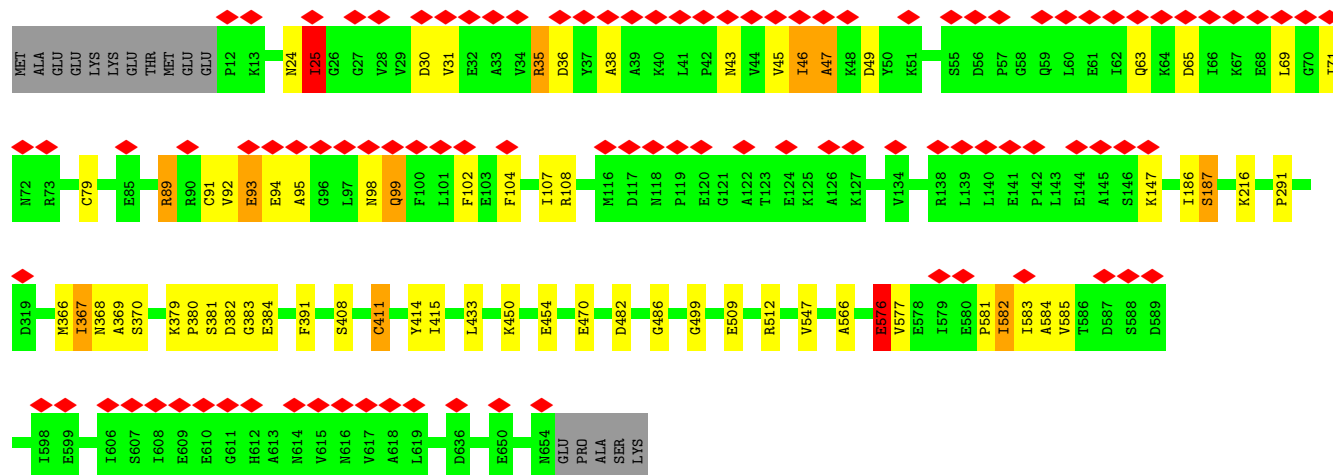
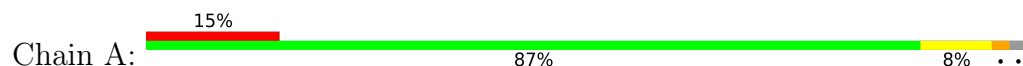


- Molecule 5: H(2):CoB-CoM heterodisulfide,ferredoxin reductase subunit C

Chain C: 



- Chain a:  60% 5% 35%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	234858	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	65	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	57.558	Depositor
Minimum map value	-27.341	Depositor
Average map value	-0.003	Depositor
Map value standard deviation	1.007	Depositor
Recommended contour level	8.39	Depositor
Map size (\AA)	374.976, 374.976, 374.976	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.837, 0.837, 0.837	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FES, FAD, 9S8, SF4

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	E	1.32	49/3076 (1.6%)	1.29	82/4144 (2.0%)
2	D	1.13	28/2632 (1.1%)	1.01	24/3580 (0.7%)
3	F	0.65	6/1066 (0.6%)	0.73	4/1434 (0.3%)
4	B	0.64	10/2236 (0.4%)	0.62	8/3016 (0.3%)
4	b	0.64	9/2233 (0.4%)	0.64	15/3013 (0.5%)
5	C	0.11	0/1442	0.30	0/1944
5	c	1.15	15/1447 (1.0%)	0.96	21/1951 (1.1%)
6	A	0.79	26/4999 (0.5%)	0.74	30/6764 (0.4%)
6	a	0.11	0/3336	0.32	0/4509
All	All	0.85	143/22467 (0.6%)	0.81	184/30355 (0.6%)

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	E	0	6
2	D	0	4
3	F	0	1
5	c	0	1
6	A	0	1
All	All	0	13

All (143) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	251	PRO	C-O	-23.40	1.04	1.24
5	c	35	CYS	C-O	-19.02	1.00	1.23
1	E	254	MET	C-O	-18.03	1.03	1.24
2	D	173	TYR	C-O	-16.24	1.04	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	25	ILE	C-O	-16.06	1.06	1.23
6	A	380	PRO	C-O	-15.97	1.04	1.24
5	c	172	ASP	C-O	-15.52	1.05	1.24
2	D	170	VAL	C-O	-15.50	1.07	1.24
1	E	36	VAL	C-O	-15.29	1.07	1.23
4	B	233	PHE	C-O	-14.69	1.06	1.24
4	b	233	PHE	C-O	-14.44	1.07	1.24
1	E	4	LEU	C-O	-13.83	1.06	1.23
1	E	191	VAL	C-O	-13.71	1.08	1.23
1	E	189	ILE	C-O	-13.63	1.09	1.24
1	E	255	ALA	C-O	-13.58	1.08	1.24
5	c	34	TYR	C-O	-13.42	1.06	1.23
1	E	225	ALA	C-O	-13.31	1.06	1.24
6	A	368	ASN	C-O	-12.74	1.08	1.23
1	E	253	SER	C-O	-12.55	1.09	1.24
2	D	171	ARG	C-O	-12.13	1.08	1.24
1	E	190	MET	C-O	-11.78	1.08	1.24
3	F	73	TYR	C-O	-11.35	1.09	1.24
1	E	2	LYS	C-O	-11.31	1.10	1.24
6	A	583	ILE	C-O	-10.90	1.11	1.23
1	E	13	ILE	C-O	-10.85	1.11	1.24
5	c	36	PHE	C-O	-10.74	1.09	1.24
6	A	577	VAL	C-O	-10.72	1.12	1.23
4	b	89	ASN	C-O	-10.65	1.11	1.24
2	D	285	ARG	C-O	-10.64	1.11	1.23
2	D	169	GLU	CA-C	-10.48	1.40	1.52
5	c	170	GLY	C-O	-10.20	1.10	1.24
2	D	169	GLU	C-O	-10.16	1.11	1.24
6	A	367	ILE	C-O	-10.09	1.10	1.24
6	A	369	ALA	C-O	-9.84	1.12	1.24
4	B	76	THR	C-O	-9.78	1.11	1.24
1	E	35	VAL	C-O	-9.68	1.12	1.24
1	E	169	SER	C-O	-9.66	1.12	1.23
4	b	90	HIS	C-O	-9.65	1.11	1.24
1	E	31	LEU	C-O	-9.61	1.12	1.24
1	E	9	THR	C-O	-9.60	1.12	1.24
6	A	379	LYS	C-O	-9.44	1.11	1.24
1	E	33	LYS	C-O	-9.41	1.11	1.24
1	E	10	ASP	C-O	-9.30	1.12	1.23
1	E	35	VAL	C-N	-9.23	1.21	1.33
6	A	384	GLU	C-O	-9.22	1.12	1.23
2	D	172	SER	C-O	-9.20	1.12	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	225	ALA	CA-CB	-9.20	1.39	1.53
6	A	369	ALA	CA-CB	-9.04	1.39	1.53
2	D	62	GLY	C-O	-8.93	1.11	1.23
6	A	30	ASP	C-O	-8.88	1.12	1.23
1	E	168	ILE	C-O	-8.87	1.15	1.24
5	c	171	PHE	C-O	-8.76	1.13	1.24
2	D	191	PHE	C-O	-8.71	1.13	1.23
2	D	195	ARG	C-O	-8.72	1.12	1.24
4	b	72	ALA	C-O	-8.59	1.12	1.23
3	F	75	SER	C-O	-8.48	1.13	1.24
1	E	250	ALA	C-O	-8.42	1.14	1.24
2	D	170	VAL	N-CA	-8.37	1.36	1.46
5	c	174	LEU	C-O	-8.37	1.14	1.24
1	E	148	SER	C-O	-8.18	1.14	1.23
1	E	251	MET	C-O	-8.16	1.14	1.24
2	D	61	PRO	C-O	-8.10	1.13	1.23
6	A	581	PRO	C-O	-8.07	1.13	1.24
5	c	35	CYS	C-N	-8.05	1.23	1.33
6	A	370	SER	C-O	-8.03	1.13	1.24
6	A	382	ASP	C-O	-7.94	1.14	1.24
2	D	197	VAL	C-O	-7.92	1.14	1.24
2	D	193	ASP	C-O	-7.84	1.14	1.23
6	A	576	GLU	C-O	-7.76	1.14	1.23
5	c	143	VAL	C-O	-7.63	1.12	1.23
1	E	190	MET	C-N	-7.63	1.25	1.33
6	A	584	ALA	C-O	-7.45	1.14	1.23
6	A	584	ALA	CA-CB	-7.44	1.41	1.53
1	E	250	ALA	CA-CB	-7.43	1.41	1.53
4	B	223	GLY	C-O	-7.41	1.14	1.24
1	E	3	TYR	C-O	-7.25	1.15	1.24
4	b	91	LEU	C-O	-7.25	1.15	1.24
2	D	172	SER	CA-CB	-7.13	1.35	1.54
1	E	37	ASP	C-O	-7.11	1.14	1.24
4	B	135	LEU	C-O	-7.11	1.15	1.24
4	B	219	MET	C-O	-7.11	1.15	1.24
5	c	173	GLN	C-O	-7.05	1.15	1.24
1	E	225	ALA	CA-C	-6.89	1.43	1.52
6	A	582	ILE	C-O	-6.83	1.16	1.24
2	D	58	VAL	C-O	-6.81	1.16	1.24
4	B	218	ASN	C-N	-6.73	1.24	1.33
2	D	196	GLU	C-O	-6.72	1.16	1.24
2	D	168	ALA	CA-CB	-6.60	1.42	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	256	ARG	C-O	-6.58	1.16	1.24
6	A	92	VAL	C-O	-6.53	1.16	1.24
2	D	252	PRO	N-CA	-6.48	1.39	1.47
1	E	253	SER	CA-CB	-6.46	1.43	1.53
4	B	224	VAL	C-O	-6.41	1.16	1.24
6	A	370	SER	CA-CB	-6.40	1.42	1.53
3	F	74	ASP	C-O	-6.38	1.16	1.24
2	D	61	PRO	N-CA	-6.35	1.39	1.47
6	A	585	VAL	C-O	-6.32	1.17	1.24
1	E	145	ASP	C-O	-6.27	1.16	1.24
3	F	75	SER	CA-CB	-6.24	1.42	1.53
1	E	36	VAL	C-N	-6.21	1.24	1.33
4	B	221	GLU	C-O	-6.19	1.16	1.24
2	D	250	LEU	C-O	-6.12	1.17	1.24
1	E	149	GLU	C-O	-6.03	1.16	1.23
5	c	175	ILE	C-O	-6.00	1.17	1.24
4	B	222	ALA	CA-CB	-5.99	1.42	1.53
6	A	380	PRO	C-N	-5.99	1.26	1.33
1	E	203	GLY	C-N	-5.95	1.25	1.33
6	A	381	SER	C-O	-5.95	1.17	1.24
1	E	12	GLU	C-O	-5.93	1.17	1.24
1	E	191	VAL	N-CA	-5.89	1.41	1.46
1	E	225	ALA	C-N	-5.89	1.25	1.34
2	D	172	SER	CA-C	-5.87	1.45	1.52
4	B	136	SER	C-O	-5.87	1.17	1.24
1	E	236	PRO	CA-CB	-5.80	1.45	1.53
2	D	170	VAL	C-N	-5.79	1.25	1.33
3	F	27	ARG	C-O	-5.79	1.16	1.23
1	E	189	ILE	C-N	-5.77	1.25	1.33
1	E	34	GLU	C-O	-5.73	1.16	1.23
1	E	170	ILE	C-O	-5.65	1.16	1.24
4	b	72	ALA	C-N	-5.62	1.26	1.33
5	c	140	ARG	C-O	-5.61	1.17	1.24
1	E	235	GLU	C-N	5.59	1.40	1.33
1	E	32	ASP	C-N	-5.58	1.26	1.33
1	E	1	MET	C-O	-5.55	1.12	1.23
1	E	235	GLU	C-O	-5.54	1.16	1.24
1	E	8	ALA	C-O	-5.52	1.17	1.23
6	A	383	GLY	C-O	-5.52	1.15	1.23
2	D	249	HIS	CG-CD2	-5.51	1.29	1.35
1	E	253	SER	CA-C	-5.47	1.45	1.52
5	c	169	THR	C-O	-5.46	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	c	172	ASP	CA-C	-5.42	1.45	1.52
4	b	72	ALA	CA-CB	-5.39	1.43	1.53
4	b	69	ASP	C-O	-5.35	1.17	1.24
6	A	381	SER	CA-CB	-5.33	1.45	1.53
2	D	248	GLN	C-O	-5.25	1.18	1.24
3	F	73	TYR	C-N	-5.23	1.26	1.33
2	D	172	SER	C-N	-5.21	1.25	1.33
1	E	31	LEU	C-N	-5.15	1.26	1.33
4	b	70	MET	C-O	-5.12	1.17	1.24
1	E	226	ARG	C-O	-5.06	1.17	1.24
5	c	142	ALA	C-O	-5.04	1.18	1.24
2	D	173	TYR	C-N	-5.03	1.27	1.33
6	A	47	ALA	C-O	-5.03	1.18	1.23

All (184) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	229	GLU	N-CA-C	-18.61	80.73	110.32
1	E	2	LYS	N-CA-C	-16.87	92.97	111.36
2	D	251	PRO	N-CA-CB	-13.90	95.99	103.22
3	F	27	ARG	CB-CA-C	13.02	129.31	111.86
1	E	144	ASP	N-CA-C	-12.09	92.39	110.28
2	D	251	PRO	N-CA-C	12.09	123.51	110.58
2	D	230	ASN	N-CA-C	11.68	131.48	113.72
2	D	251	PRO	CB-CA-C	-11.62	100.25	111.17
1	E	239	LYS	N-CA-C	-11.54	97.33	112.68
2	D	169	GLU	O-C-N	10.73	135.95	123.29
1	E	135	ILE	O-C-N	-10.44	111.74	121.87
3	F	74	ASP	CA-CB-CG	10.28	122.88	112.60
1	E	137	THR	CA-C-O	-9.74	110.23	120.55
1	E	33	LYS	N-CA-C	-9.53	101.19	112.92
5	c	36	PHE	CA-CB-CG	9.25	123.05	113.80
2	D	168	ALA	CA-C-O	-9.20	110.95	121.81
4	b	91	LEU	N-CA-C	-9.18	101.22	111.14
1	E	191	VAL	CB-CA-C	9.10	120.62	110.52
1	E	5	LEU	N-CA-C	-8.96	94.30	108.90
5	c	36	PHE	CA-C-O	-8.86	109.03	119.48
1	E	3	TYR	N-CA-C	8.82	123.28	108.90
1	E	254	MET	CA-C-N	8.62	131.83	120.28
1	E	254	MET	C-N-CA	8.62	131.83	120.28
5	c	172	ASP	CA-CB-CG	8.61	121.21	112.60
1	E	34	GLU	N-CA-C	8.58	123.21	111.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	99	GLN	N-CA-CB	-8.49	97.15	110.22
6	A	366	MET	O-C-N	-8.30	112.69	122.15
3	F	27	ARG	N-CA-CB	-8.21	99.43	111.91
2	D	169	GLU	CA-C-O	-8.12	111.53	120.38
1	E	255	ALA	CA-C-O	-7.93	112.15	120.55
6	A	366	MET	CA-C-N	7.77	133.54	120.64
6	A	366	MET	C-N-CA	7.77	133.54	120.64
1	E	145	ASP	CA-CB-CG	7.77	120.37	112.60
1	E	10	ASP	CA-C-O	-7.74	113.35	121.55
5	c	36	PHE	CB-CA-C	7.73	123.94	110.64
1	E	250	ALA	CA-C-N	7.70	130.60	120.28
1	E	250	ALA	C-N-CA	7.70	130.60	120.28
4	B	76	THR	CA-CB-OG1	7.69	121.14	109.60
6	A	93	GLU	CB-CA-C	-7.67	98.06	110.79
2	D	170	VAL	N-CA-C	-7.66	97.09	108.12
5	c	145	LEU	N-CA-C	-7.66	100.21	110.55
1	E	144	ASP	CA-C-O	-7.54	112.71	121.16
2	D	251	PRO	O-C-N	-7.54	117.61	121.15
1	E	204	ALA	N-CA-CB	-7.53	98.57	110.69
6	A	381	SER	CA-C-O	-7.52	112.58	120.55
6	A	46	ILE	CA-C-O	-7.51	114.65	120.96
1	E	226	ARG	N-CA-CB	-7.51	98.64	110.28
2	D	61	PRO	N-CA-CB	7.50	110.02	103.27
1	E	206	ASP	CA-C-O	-7.49	112.95	121.19
5	c	173	GLN	CB-CA-C	7.47	123.56	110.85
4	B	233	PHE	CA-C-O	-7.43	112.55	120.42
1	E	31	LEU	CA-C-N	7.42	130.82	120.29
1	E	31	LEU	C-N-CA	7.42	130.82	120.29
6	A	367	ILE	CA-C-N	7.38	131.28	120.95
6	A	367	ILE	C-N-CA	7.38	131.28	120.95
4	B	233	PHE	CA-CB-CG	7.35	121.15	113.80
5	c	34	TYR	CA-C-N	7.31	131.25	120.87
5	c	34	TYR	C-N-CA	7.31	131.25	120.87
1	E	2	LYS	CB-CA-C	7.30	123.27	110.85
1	E	206	ASP	CA-CB-CG	7.30	119.90	112.60
2	D	170	VAL	CB-CA-C	7.15	120.77	110.33
6	A	581	PRO	N-CA-CB	-7.08	95.81	103.25
1	E	9	THR	CA-C-N	6.96	131.25	120.75
1	E	9	THR	C-N-CA	6.96	131.25	120.75
1	E	139	TYR	N-CA-C	-6.91	104.37	114.39
3	F	75	SER	CA-C-O	-6.87	113.31	120.32
1	E	152	ASP	N-CA-C	6.84	119.76	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	289	LEU	CA-C-O	-6.81	113.49	121.46
1	E	33	LYS	CB-CA-C	6.78	122.02	110.56
1	E	226	ARG	CA-C-N	6.76	129.88	120.29
1	E	226	ARG	C-N-CA	6.76	129.88	120.29
5	c	142	ALA	CA-C-O	-6.76	113.39	120.55
2	D	58	VAL	N-CA-C	-6.70	98.21	107.99
4	b	233	PHE	CA-CB-CG	6.69	120.49	113.80
6	A	94	GLU	N-CA-C	-6.68	104.23	112.38
2	D	258	PHE	N-CA-C	6.67	119.40	109.59
4	b	91	LEU	CA-C-O	-6.67	113.83	120.70
5	c	36	PHE	N-CA-C	-6.67	103.54	112.94
1	E	188	GLU	CA-C-N	6.66	131.96	123.10
1	E	188	GLU	C-N-CA	6.66	131.96	123.10
1	E	237	SER	N-CA-C	6.65	118.18	111.07
2	D	288	GLY	N-CA-C	6.65	123.44	111.34
6	A	581	PRO	N-CD-CG	-6.64	93.24	103.20
1	E	253	SER	CA-C-O	-6.63	113.39	120.42
1	E	171	ASP	CA-C-O	-6.58	113.58	120.55
2	D	285	ARG	CB-CA-C	6.54	119.32	110.94
1	E	147	VAL	N-CA-CB	-6.53	103.87	112.36
1	E	236	PRO	CB-CA-C	-6.48	102.47	110.95
6	A	25	ILE	N-CA-C	-6.43	105.56	111.67
6	A	382	ASP	CA-CB-CG	6.41	119.01	112.60
1	E	136	GLU	CA-C-N	6.41	128.87	120.28
1	E	136	GLU	C-N-CA	6.41	128.87	120.28
5	c	31	SER	N-CA-C	6.40	119.07	111.71
2	D	246	VAL	O-C-N	-6.40	114.57	121.80
1	E	170	ILE	N-CA-C	-6.37	103.12	111.09
1	E	9	THR	CA-C-O	-6.32	112.95	120.10
1	E	4	LEU	CA-C-N	6.20	131.74	122.99
1	E	4	LEU	C-N-CA	6.20	131.74	122.99
1	E	205	ASP	CB-CA-C	-6.19	97.00	109.68
1	E	161	ARG	CB-CA-C	-6.17	98.83	110.67
6	A	43	ASN	O-C-N	-6.15	115.41	121.87
4	b	89	ASN	CA-CB-CG	6.09	118.69	112.60
4	B	218	ASN	CA-C-N	6.09	128.94	120.29
4	B	218	ASN	C-N-CA	6.09	128.94	120.29
1	E	5	LEU	N-CA-CB	6.09	120.91	110.68
2	D	171	ARG	CA-C-O	-6.08	114.14	120.70
4	b	89	ASN	CA-C-O	-6.06	114.46	120.82
6	A	581	PRO	CB-CA-C	6.05	121.55	111.56
4	b	233	PHE	CA-C-O	-6.04	114.14	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	25	ILE	CA-C-O	-6.03	114.36	120.69
1	E	235	GLU	CA-C-N	6.02	125.99	120.03
1	E	235	GLU	C-N-CA	6.02	125.99	120.03
6	A	24	ASN	CA-C-O	-6.00	113.58	120.24
5	c	170	GLY	CA-C-N	5.97	128.28	120.28
5	c	170	GLY	C-N-CA	5.97	128.28	120.28
4	b	88	THR	CA-C-N	5.96	128.18	120.44
4	b	88	THR	C-N-CA	5.96	128.18	120.44
2	D	171	ARG	CB-CA-C	5.95	120.73	109.37
1	E	161	ARG	CA-C-O	-5.93	113.15	119.97
1	E	153	ARG	N-CA-CB	5.92	119.50	110.44
1	E	13	ILE	CA-C-N	5.87	128.07	120.44
1	E	13	ILE	C-N-CA	5.87	128.07	120.44
1	E	206	ASP	N-CA-C	-5.85	101.74	110.23
6	A	25	ILE	N-CA-CB	5.85	118.93	110.68
6	A	98	ASN	CA-C-N	5.85	128.70	120.28
6	A	98	ASN	C-N-CA	5.85	128.70	120.28
5	c	140	ARG	CA-C-O	-5.83	114.69	120.70
1	E	252	ILE	CA-C-O	-5.81	114.91	120.95
2	D	248	GLN	CA-C-O	-5.81	114.39	120.55
4	B	219	MET	CA-C-N	5.81	128.06	120.28
4	B	219	MET	C-N-CA	5.81	128.06	120.28
4	B	135	LEU	N-CA-C	-5.80	105.03	111.36
2	D	253	VAL	N-CA-CB	5.72	117.07	110.49
1	E	37	ASP	CA-CB-CG	5.71	118.31	112.60
1	E	239	LYS	CB-CA-C	5.71	119.77	110.24
1	E	256	ARG	CA-C-O	-5.68	114.40	120.42
4	b	90	HIS	CA-C-O	-5.68	113.44	119.97
4	b	233	PHE	CB-CA-C	5.63	120.14	110.79
1	E	224	GLY	O-C-N	-5.63	116.32	122.68
5	c	171	PHE	CA-C-N	5.62	127.81	120.28
5	c	171	PHE	C-N-CA	5.62	127.81	120.28
5	c	171	PHE	CA-C-O	-5.59	114.62	120.55
4	b	220	LYS	N-CA-C	5.59	117.37	111.28
4	b	90	HIS	CA-CB-CG	5.57	119.37	113.80
1	E	30	MET	O-C-N	-5.55	116.23	122.12
1	E	160	LEU	N-CA-C	-5.55	103.16	110.43
5	c	35	CYS	CA-C-N	5.52	130.87	122.37
5	c	35	CYS	C-N-CA	5.52	130.87	122.37
1	E	171	ASP	CB-CA-C	-5.50	101.66	110.79
4	b	222	ALA	N-CA-C	-5.50	106.08	112.89
6	A	89	ARG	O-C-N	-5.46	116.44	122.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	c	140	ARG	CA-C-N	5.42	127.55	120.28
5	c	140	ARG	C-N-CA	5.42	127.55	120.28
6	A	25	ILE	CA-C-N	5.42	126.10	120.03
6	A	25	ILE	C-N-CA	5.42	126.10	120.03
4	b	232	PRO	CA-C-N	5.40	127.52	120.28
4	b	232	PRO	C-N-CA	5.40	127.52	120.28
1	E	205	ASP	CA-CB-CG	5.37	117.97	112.60
6	A	380	PRO	CA-C-N	5.36	127.46	120.28
6	A	380	PRO	C-N-CA	5.36	127.46	120.28
6	A	36	ASP	CA-C-O	-5.35	114.75	120.42
1	E	225	ALA	CA-C-N	5.35	128.44	120.31
1	E	225	ALA	C-N-CA	5.35	128.44	120.31
2	D	287	GLU	N-CA-C	-5.34	99.44	110.80
1	E	225	ALA	N-CA-C	-5.33	105.05	112.45
1	E	148	SER	CA-C-O	-5.31	115.75	121.38
6	A	368	ASN	CA-C-O	-5.31	114.71	120.81
1	E	34	GLU	CA-C-O	-5.29	115.41	121.54
1	E	33	LYS	CA-C-O	-5.28	113.39	119.56
1	E	1	MET	CA-C-O	-5.26	111.86	120.80
1	E	255	ALA	CA-C-N	5.24	127.73	120.29
1	E	255	ALA	C-N-CA	5.24	127.73	120.29
1	E	237	SER	CA-C-O	-5.24	115.32	120.82
1	E	32	ASP	N-CA-C	5.20	117.02	111.36
6	A	92	VAL	N-CA-C	-5.19	105.48	110.72
2	D	195	ARG	N-CA-C	-5.17	106.23	112.54
1	E	161	ARG	CA-C-N	5.17	127.21	120.28
1	E	161	ARG	C-N-CA	5.17	127.21	120.28
6	A	38	ALA	CA-C-O	-5.14	115.11	120.55
1	E	162	ASP	CA-CB-CG	5.08	117.68	112.60
1	E	12	GLU	CA-C-N	5.03	127.34	120.46
1	E	12	GLU	C-N-CA	5.03	127.34	120.46
1	E	31	LEU	N-CA-C	-5.01	105.28	111.40
1	E	149	GLU	CA-C-O	-5.01	115.74	121.40

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	A	35	ARG	Sidechain
2	D	169	GLU	Mainchain
2	D	195	ARG	Sidechain
2	D	285	ARG	Sidechain

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Mol	Chain	Res	Type	Group
2	D	57	ARG	Sidechain
1	E	1	MET	Mainchain
1	E	10	ASP	Mainchain
1	E	161	ARG	Sidechain
1	E	226	ARG	Sidechain
1	E	239	LYS	Mainchain
1	E	256	ARG	Sidechain
3	F	27	ARG	Sidechain
5	c	142	ALA	Mainchain

5.2 Too-close contacts [i](#)

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	E	3020	2908	2908	42	0
2	D	2579	2515	2514	45	0
3	F	1037	989	989	11	0
4	B	2199	2168	2168	15	0
4	b	2196	2161	2161	22	0
5	C	1417	1430	1429	12	0
5	c	1422	1431	1431	7	0
6	A	4910	4876	4872	30	0
6	a	3276	3264	3263	24	0
7	A	48	0	0	0	0
7	C	16	0	0	0	0
7	D	8	0	0	0	0
7	E	32	0	0	0	0
7	a	24	0	0	0	0
7	c	16	0	0	0	0
8	A	53	31	31	0	0
8	E	53	0	31	3	0
8	a	53	31	31	0	0
9	F	4	0	0	0	0
10	B	16	0	0	0	0
10	b	16	0	0	1	0
11	A	49	0	0	2	0
11	B	14	0	0	0	0
11	C	9	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	D	7	0	0	1	0
11	E	8	0	0	1	0
11	F	2	0	0	0	0
11	a	60	0	0	3	0
11	b	11	0	0	0	0
11	c	11	0	0	0	0
All	All	22566	21804	21828	198	0

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

All (198) 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)
1:E:205:ASP:OD2	1:E:206:ASP:O	1.68	1.11
4:b:87:GLU:HA	4:b:90:HIS:CE1	1.86	1.09
2:D:226:PHE:O	2:D:229:GLU:O	1.69	1.07
4:b:213:ARG:HD2	4:b:251:GLU:OE1	1.65	0.96
1:E:254:MET:SD	1:E:257:LYS:NZ	2.44	0.91
1:E:254:MET:CE	1:E:257:LYS:HZ3	1.88	0.87
2:D:93:LEU:HD11	2:D:258:PHE:CE2	2.09	0.87
6:a:308:ASP:OD1	6:a:316:VAL:HG11	1.75	0.85
6:a:308:ASP:OD1	6:a:316:VAL:CG1	2.26	0.83
1:E:299:GLU:OE1	1:E:325:HIS:CE1	2.34	0.81
4:b:67:ALA:HA	4:b:70:MET:HE3	1.61	0.81
4:B:148:ALA:HB2	4:B:224:VAL:HG11	1.62	0.81
6:A:45:VAL:HG23	6:A:71:ILE:HD11	1.63	0.80
2:D:195:ARG:HG3	2:D:199:ASN:OD1	1.81	0.80
1:E:151:ILE:HG22	1:E:151:ILE:O	1.82	0.78
4:b:36:MET:HG2	4:b:70:MET:HE1	1.67	0.76
4:b:61:ALA:O	4:b:65:THR:HG23	1.86	0.75
1:E:158:VAL:HG22	1:E:166:ARG:HB2	1.69	0.75
1:E:154:GLY:O	1:E:170:ILE:HG22	1.87	0.74
1:E:293:CYS:O	11:E:501:HOH:O	2.07	0.71
6:a:241:LYS:HG3	6:a:326:GLU:OE1	1.89	0.71
6:a:482:ASP:OD1	11:a:801:HOH:O	2.08	0.71
6:a:241:LYS:HG2	6:a:326:GLU:HG2	1.74	0.70
4:B:61:ALA:O	4:B:65:THR:HG23	1.92	0.69
5:C:157:GLU:OE2	5:C:157:GLU:N	2.22	0.69
1:E:153:ARG:NH1	1:E:167:GLU:OE2	2.26	0.68
1:E:254:MET:HE1	1:E:257:LYS:NZ	2.09	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:12:SER:HB2	2:D:310:THR:HG23	1.75	0.68
6:a:190:MET:HG2	6:a:207:LEU:HD22	1.76	0.68
6:A:291:PRO:O	11:A:802:HOH:O	2.13	0.67
6:A:470:GLU:OE2	11:A:801:HOH:O	2.12	0.67
4:B:276:VAL:HG22	5:C:143:VAL:HG11	1.77	0.67
4:b:13:ASN:C	5:c:136:THR:HG21	2.19	0.67
6:a:428:ASP:O	6:a:428:ASP:OD1	2.14	0.65
1:E:116:TYR:HD2	1:E:221:ILE:HD11	1.60	0.65
2:D:93:LEU:HD11	2:D:258:PHE:CD2	2.32	0.65
1:E:254:MET:CE	1:E:257:LYS:NZ	2.61	0.63
2:D:85:LEU:HD22	2:D:90:ILE:HD13	1.81	0.62
1:E:1:MET:SD	1:E:213:VAL:HG21	2.39	0.62
4:b:213:ARG:HH11	4:b:251:GLU:CD	2.07	0.62
1:E:299:GLU:OE1	1:E:325:HIS:NE2	2.33	0.60
4:b:213:ARG:CD	4:b:251:GLU:OE1	2.46	0.60
2:D:93:LEU:CD1	2:D:258:PHE:CE2	2.81	0.60
6:a:244:LYS:NZ	6:a:251:GLU:OE2	2.34	0.60
3:F:85:ARG:O	3:F:85:ARG:NH1	2.35	0.59
4:b:97:GLU:OE1	4:b:97:GLU:N	2.23	0.59
6:a:241:LYS:CG	6:a:326:GLU:OE1	2.49	0.59
4:B:13:ASN:C	5:C:136:THR:HG21	2.27	0.59
2:D:194:GLU:HB2	2:D:219:ILE:HD13	1.87	0.56
6:a:492:ASP:O	11:a:802:HOH:O	2.18	0.56
6:A:45:VAL:CG2	6:A:71:ILE:HD11	2.33	0.56
2:D:284:ILE:HD11	2:D:285:ARG:NH1	2.20	0.55
2:D:143:ILE:O	2:D:170:VAL:HA	2.06	0.55
2:D:9:PRO:O	11:D:501:HOH:O	2.17	0.55
2:D:52:ILE:HG23	2:D:285:ARG:HH12	1.71	0.55
2:D:332:GLU:HA	2:D:332:GLU:OE1	2.07	0.55
3:F:32:PRO:O	3:F:35:ARG:NH1	2.39	0.54
4:b:276:VAL:HG22	5:c:143:VAL:HG11	1.88	0.54
4:b:86:PHE:O	4:b:90:HIS:ND1	2.38	0.54
6:a:531:LYS:NZ	11:a:804:HOH:O	2.40	0.54
2:D:253:VAL:HG22	2:D:255:GLU:H	1.73	0.53
4:b:22:THR:OG1	4:b:77:GLU:OE1	2.26	0.53
4:B:276:VAL:CG2	5:C:143:VAL:HG11	2.37	0.53
6:a:527:GLU:OE1	6:a:549:GLN:NE2	2.39	0.53
1:E:84:LEU:HB3	1:E:89:LEU:HD11	1.89	0.53
4:B:122:PHE:CZ	4:B:126:LEU:HD11	2.44	0.53
2:D:238:PHE:H	2:D:310:THR:HG21	1.74	0.53
4:b:87:GLU:HA	4:b:90:HIS:HE1	1.59	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:286:THR:O	2:D:287:GLU:C	2.52	0.52
2:D:244:ARG:NH1	2:D:310:THR:O	2.42	0.52
2:D:238:PHE:CD2	2:D:310:THR:HG22	2.44	0.52
8:E:405:FAD:H2'	8:E:405:FAD:N1	2.24	0.52
6:A:216:LYS:NZ	6:A:216:LYS:HB2	2.25	0.52
2:D:117:LYS:NZ	2:D:257:GLU:O	2.37	0.51
4:b:165:ASP:OD1	4:b:166:ASN:N	2.42	0.51
2:D:200:ASP:O	2:D:200:ASP:OD1	2.29	0.51
1:E:99:MET:HE2	1:E:189:ILE:HG21	1.92	0.51
4:B:76:THR:OG1	4:B:82:PHE:HB2	2.11	0.51
1:E:254:MET:SD	1:E:257:LYS:CE	3.00	0.50
4:B:20:LYS:NZ	4:B:274:ASP:OD1	2.43	0.50
5:C:137:MET:HE3	5:C:148:LEU:HD21	1.92	0.50
6:A:25:ILE:HG21	6:A:107:ILE:HD12	1.94	0.50
6:A:46:ILE:HB	6:A:69:LEU:HD22	1.93	0.50
6:A:89:ARG:HB3	6:A:99:GLN:HG3	1.93	0.50
5:c:30:ASP:OD1	5:c:31:SER:N	2.44	0.50
6:A:391:PHE:HB2	6:A:433:LEU:HD22	1.93	0.50
2:D:107:ARG:HH21	2:D:249:HIS:HA	1.77	0.50
2:D:64:LYS:HA	2:D:69:LEU:HA	1.94	0.49
6:a:566:ALA:HB2	6:A:566:ALA:HB2	1.93	0.49
6:A:147:LYS:HB3	6:A:576:GLU:HG2	1.95	0.49
4:B:126:LEU:HD22	4:B:135:LEU:HD21	1.95	0.49
2:D:261:VAL:HG12	2:D:275:VAL:HG13	1.93	0.49
2:D:71:GLY:O	2:D:72:VAL:HG23	2.13	0.49
4:b:42:CYS:N	4:b:43:PRO:HA	2.28	0.49
6:A:450:LYS:NZ	6:A:454:GLU:OE1	2.46	0.49
5:C:19:GLU:CD	5:C:19:GLU:H	2.20	0.49
4:b:13:ASN:O	5:c:136:THR:HG21	2.14	0.48
6:A:46:ILE:HG21	6:A:65:ASP:OD2	2.13	0.48
6:A:35:ARG:HG2	6:A:47:ALA:HB1	1.95	0.48
1:E:237:SER:HB2	1:E:240:MET:HG2	1.95	0.48
2:D:224:LEU:CD2	2:D:234:VAL:HG11	2.43	0.48
5:C:139:LEU:O	5:C:143:VAL:HG13	2.13	0.48
1:E:191:VAL:HG11	1:E:244:ARG:NH2	2.29	0.48
4:b:266:LEU:HG	4:b:275:LEU:HD21	1.96	0.48
2:D:174:ASP:OD1	2:D:175:ARG:N	2.46	0.48
5:c:80:THR:O	5:c:81:THR:OG1	2.27	0.48
6:a:308:ASP:OD1	6:a:316:VAL:CB	2.60	0.48
2:D:52:ILE:HG23	2:D:285:ARG:NH1	2.29	0.48
3:F:22:THR:OG1	3:F:108:ALA:O	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:81:LEU:HD23	2:D:337:ILE:HD11	1.95	0.47
5:C:137:MET:HE3	5:C:148:LEU:CD2	2.44	0.47
2:D:315:MET:HE2	2:D:317:LEU:HD21	1.96	0.47
4:B:56:TRP:NE1	4:B:84:SER:OG	2.47	0.47
1:E:4:LEU:HG	1:E:211:ILE:HB	1.96	0.47
3:F:102:ARG:NE	3:F:104:GLU:OE2	2.45	0.47
4:B:42:CYS:N	4:B:43:PRO:HA	2.29	0.47
6:A:186:ILE:O	6:A:187:SER:CB	2.62	0.47
4:b:176:ILE:O	4:b:179:VAL:HG22	2.15	0.47
6:a:308:ASP:OD1	6:a:316:VAL:HB	2.15	0.47
6:A:415:ILE:HD11	6:A:499:GLY:HA3	1.97	0.47
1:E:299:GLU:OE1	1:E:325:HIS:HE1	1.92	0.47
6:a:186:ILE:O	6:a:187:SER:HB3	2.15	0.47
2:D:271:GLU:O	2:D:273:VAL:HG13	2.16	0.46
6:a:186:ILE:O	6:a:187:SER:CB	2.62	0.46
6:a:411:CYS:HA	6:a:414:TYR:CE2	2.50	0.46
2:D:178:GLU:N	2:D:178:GLU:OE2	2.49	0.46
1:E:158:VAL:CG2	1:E:166:ARG:HB2	2.41	0.46
3:F:63:VAL:HG11	3:F:80:TRP:CE2	2.50	0.46
1:E:4:LEU:HD12	1:E:6:ALA:HB2	1.98	0.45
6:A:547:VAL:HG12	6:A:547:VAL:O	2.16	0.45
6:a:212:VAL:HG12	6:a:216:LYS:HD2	1.97	0.45
2:D:12:SER:HA	2:D:241:PHE:HA	1.98	0.45
6:a:391:PHE:HB2	6:a:433:LEU:HD22	1.98	0.45
1:E:147:VAL:CG1	1:E:161:ARG:HH11	2.29	0.45
2:D:98:LEU:O	2:D:242:ASN:ND2	2.44	0.45
1:E:353:ILE:HD11	3:F:93:GLU:HG3	1.99	0.45
5:C:80:THR:O	5:C:81:THR:OG1	2.25	0.45
6:A:186:ILE:O	6:A:187:SER:HB3	2.16	0.45
1:E:205:ASP:CG	1:E:206:ASP:N	2.75	0.45
4:B:13:ASN:O	5:C:136:THR:HG21	2.17	0.45
2:D:81:LEU:O	2:D:85:LEU:HG	2.16	0.44
6:a:547:VAL:HG12	6:a:547:VAL:O	2.17	0.44
6:A:49:ASP:OD1	6:A:49:ASP:O	2.35	0.44
2:D:72:VAL:HG12	2:D:73:ASN:O	2.18	0.44
1:E:335:GLN:OE1	2:D:33:ARG:NH2	2.50	0.44
2:D:239:GLU:OE1	2:D:239:GLU:N	2.50	0.44
6:A:25:ILE:CD1	6:A:108:ARG:HB2	2.48	0.44
4:b:20:LYS:HE2	5:c:143:VAL:O	2.18	0.44
1:E:93:VAL:O	1:E:119:GLY:HA2	2.18	0.44
4:b:122:PHE:CZ	4:b:126:LEU:HD11	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:181:ARG:NH1	1:E:338:ASP:OD2	2.51	0.43
8:E:405:FAD:H8A	8:E:405:FAD:H2B	1.84	0.43
1:E:8:ALA:HB2	1:E:25:ALA:HB2	1.99	0.43
3:F:4:GLU:OE2	3:F:4:GLU:HA	2.17	0.43
1:E:16:LYS:HD3	1:E:63:GLU:O	2.18	0.43
3:F:13:ASN:N	3:F:39:VAL:O	2.52	0.43
1:E:147:VAL:CG1	1:E:161:ARG:HG2	2.49	0.43
2:D:143:ILE:HB	2:D:170:VAL:HG22	2.00	0.43
1:E:170:ILE:HG13	1:E:174:GLU:OE2	2.19	0.43
3:F:50:ILE:HD12	3:F:61:VAL:HG11	2.01	0.43
1:E:237:SER:HB2	1:E:240:MET:H	1.84	0.43
2:D:5:HIS:ND1	2:D:18:ASN:OD1	2.38	0.42
2:D:107:ARG:NH2	2:D:249:HIS:HA	2.33	0.42
5:C:61:LYS:HG2	5:C:66:LEU:HD12	2.01	0.42
1:E:324:SER:HB2	3:F:47:ALA:HB3	2.00	0.42
4:B:176:ILE:O	4:B:179:VAL:HG22	2.19	0.42
4:B:37:GLU:OE2	4:B:37:GLU:HA	2.20	0.42
2:D:259:ASP:OD1	2:D:259:ASP:C	2.63	0.42
5:c:124:ILE:HD12	5:c:175:ILE:HD11	2.00	0.42
1:E:4:LEU:HD11	1:E:222:ILE:HD12	2.00	0.42
1:E:254:MET:SD	1:E:257:LYS:HE2	2.60	0.42
8:E:405:FAD:H1'1	8:E:405:FAD:H9	1.71	0.42
2:D:201:LEU:HD23	2:D:204:LEU:HD11	2.01	0.42
6:A:411:CYS:HA	6:A:414:TYR:CE2	2.53	0.42
1:E:147:VAL:HG12	1:E:161:ARG:HH11	1.85	0.42
6:A:25:ILE:HD12	6:A:108:ARG:HB2	2.02	0.42
6:A:414:TYR:CD1	6:A:414:TYR:C	2.97	0.42
2:D:238:PHE:H	2:D:310:THR:CG2	2.32	0.41
6:A:482:ASP:O	6:A:486:GLY:N	2.52	0.41
6:a:385:LYS:HB3	6:a:426:MET:HE3	2.01	0.41
6:A:79:CYS:O	6:A:104:PHE:CE1	2.73	0.41
4:B:42:CYS:SG	4:B:43:PRO:C	3.04	0.41
2:D:22:MET:HB2	2:D:27:VAL:HG11	2.02	0.41
2:D:177:ASP:OD1	2:D:177:ASP:O	2.39	0.41
6:a:414:TYR:CD1	6:a:414:TYR:C	2.99	0.41
6:A:63:GLN:HG2	6:A:95:ALA:HB2	2.02	0.41
4:b:197:GLY:HA3	10:b:401:9S8:S3	2.61	0.41
5:C:32:LEU:HD12	5:C:32:LEU:C	2.46	0.41
1:E:147:VAL:HG11	1:E:161:ARG:HG2	2.02	0.41
1:E:201:ASN:OD1	1:E:201:ASN:C	2.64	0.41
6:A:45:VAL:CG2	6:A:71:ILE:CD1	2.99	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:31:VAL:O	6:A:31:VAL:HG12	2.21	0.40
6:A:408:SER:HB2	6:A:411:CYS:SG	2.61	0.40
1:E:360:ARG:HD3	3:F:85:ARG:HH21	1.86	0.40
6:a:563:GLY:O	6:a:567:ARG:HG2	2.22	0.40
6:A:509:GLU:OE2	6:A:512:ARG:NH2	2.50	0.40
1:E:329:SER:HA	1:E:365:ALA:HB2	2.02	0.40
4:b:42:CYS:SG	4:b:43:PRO:C	3.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	378/380 (100%)	366 (97%)	11 (3%)	1 (0%)	37	41
2	D	337/342 (98%)	327 (97%)	10 (3%)	0	100	100
3	F	127/136 (93%)	125 (98%)	2 (2%)	0	100	100
4	B	282/302 (93%)	278 (99%)	4 (1%)	0	100	100
4	b	282/302 (93%)	280 (99%)	2 (1%)	0	100	100
5	C	181/185 (98%)	177 (98%)	4 (2%)	0	100	100
5	c	182/185 (98%)	179 (98%)	3 (2%)	0	100	100
6	A	641/659 (97%)	627 (98%)	13 (2%)	1 (0%)	44	51
6	a	425/659 (64%)	415 (98%)	9 (2%)	1 (0%)	44	51
All	All	2835/3150 (90%)	2774 (98%)	58 (2%)	3 (0%)	50	56

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	145	ASP

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Mol	Chain	Res	Type
6	a	187	SER
6	A	187	SER

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	E	328/329 (100%)	324 (99%)	4 (1%)	67	79
2	D	277/292 (95%)	272 (98%)	5 (2%)	54	67
3	F	107/112 (96%)	107 (100%)	0	100	100
4	B	240/255 (94%)	239 (100%)	1 (0%)	89	94
4	b	239/255 (94%)	237 (99%)	2 (1%)	79	87
5	C	153/155 (99%)	152 (99%)	1 (1%)	81	89
5	c	153/155 (99%)	151 (99%)	2 (1%)	65	77
6	A	533/547 (97%)	525 (98%)	8 (2%)	60	73
6	a	356/547 (65%)	354 (99%)	2 (1%)	84	91
All	All	2386/2647 (90%)	2361 (99%)	25 (1%)	71	83

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	3	TYR
1	E	144	ASP
1	E	146	VAL
1	E	190	MET
2	D	63	VAL
2	D	194	GLU
2	D	197	VAL
2	D	259	ASP
2	D	327	VAL
4	b	91	LEU
4	b	189	ASP
4	B	233	PHE

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Mol	Chain	Res	Type
5	c	36	PHE
5	c	166	ILE
5	C	36	PHE
6	a	370	SER
6	a	411	CYS
6	A	25	ILE
6	A	91	CYS
6	A	93	GLU
6	A	102	PHE
6	A	367	ILE
6	A	411	CYS
6	A	576	GLU
6	A	582	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	249	ASN
2	D	249	HIS
3	F	46	ASN
3	F	72	HIS
6	A	99	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

26 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	$\# Z > 2$
7	SF4	A	706	6	0,12,12	-	-	-		
7	SF4	E	404	1	0,12,12	-	-	-		
7	SF4	A	704	6	0,12,12	-	-	-		
9	FES	F	201	3	0,4,4	-	-	-		
7	SF4	A	705	6	0,12,12	-	-	-		
7	SF4	A	701	6	0,12,12	-	-	-		
7	SF4	E	402	1	0,12,12	-	-	-		
8	FAD	A	707	-	53,58,58	0.62	0	68,89,89	0.78	3 (4%)
7	SF4	A	702	6	0,12,12	-	-	-		
8	FAD	E	405	-	53,58,58	1.43	6 (11%)	68,89,89	1.28	10 (14%)
8	FAD	a	701	-	53,58,58	0.62	0	68,89,89	0.79	3 (4%)
7	SF4	E	401	1	0,12,12	-	-	-		
7	SF4	C	201	5	0,12,12	-	-	-		
7	SF4	c	202	5	0,12,12	-	-	-		
10	9S8	b	401	4	2,10,10	5.65	2 (100%)	-		
7	SF4	D	401	2	0,12,12	-	-	-		
7	SF4	E	403	1	0,12,12	-	-	-		
7	SF4	C	202	5	0,12,12	-	-	-		
7	SF4	a	704	6	0,12,12	-	-	-		
7	SF4	A	703	6	0,12,12	-	-	-		
10	9S8	B	400	4	2,10,10	5.68	2 (100%)	-		
7	SF4	c	201	5	0,12,12	-	-	-		
7	SF4	a	702	6	0,12,12	-	-	-		
10	9S8	B	401	4	2,10,10	4.92	2 (100%)	-		
10	9S8	b	400	4	2,10,10	5.44	2 (100%)	-		
7	SF4	a	703	6	0,12,12	-	-	-		

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
7	SF4	A	706	6	-	-	0/6/5/5
7	SF4	E	404	1	-	-	0/6/5/5
7	SF4	A	704	6	-	-	0/6/5/5
9	FES	F	201	3	-	-	0/1/1/1
7	SF4	A	705	6	-	-	0/6/5/5
7	SF4	A	701	6	-	-	0/6/5/5
7	SF4	E	402	1	-	-	0/6/5/5
8	FAD	A	707	-	-	1/30/50/50	0/6/6/6
7	SF4	A	702	6	-	-	0/6/5/5
8	FAD	E	405	-	-	11/30/50/50	0/6/6/6
8	FAD	a	701	-	-	1/30/50/50	0/6/6/6
7	SF4	E	401	1	-	-	0/6/5/5
7	SF4	C	201	5	-	-	0/6/5/5
7	SF4	c	202	5	-	-	0/6/5/5
10	9S8	b	401	4	-	-	0/3/3/3
7	SF4	D	401	2	-	-	0/6/5/5
7	SF4	E	403	1	-	-	0/6/5/5
7	SF4	C	202	5	-	-	0/6/5/5
7	SF4	a	704	6	-	-	0/6/5/5
7	SF4	A	703	6	-	-	0/6/5/5
10	9S8	B	400	4	-	-	0/3/3/3
7	SF4	c	201	5	-	-	0/6/5/5
7	SF4	a	702	6	-	-	0/6/5/5
10	9S8	B	401	4	-	-	0/3/3/3
10	9S8	b	400	4	-	-	0/3/3/3
7	SF4	a	703	6	-	-	0/6/5/5

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	b	401	9S8	S3-FE4	-7.73	2.06	2.24
10	B	400	9S8	S3-FE4	-7.04	2.08	2.24
10	B	401	9S8	S3-FE4	-6.60	2.09	2.24
10	b	400	9S8	S3-FE4	-6.26	2.10	2.24
10	b	400	9S8	S5-FE4	-4.48	2.14	2.24
10	B	400	9S8	S5-FE4	-3.85	2.15	2.24
8	E	405	FAD	C2-N3	-3.55	1.30	1.39
8	E	405	FAD	C1'-C2'	-3.38	1.47	1.52
8	E	405	FAD	C2-N1	-2.91	1.29	1.36
8	E	405	FAD	C8A-N7A	-2.71	1.29	1.34
8	E	405	FAD	C9-C8	-2.51	1.35	1.39
10	B	401	9S8	S5-FE4	-2.19	2.19	2.24
8	E	405	FAD	P-O2P	-2.14	1.45	1.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	b	401	9S8	S5-FE4	-2.03	2.20	2.24

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	E	405	FAD	C5'-C4'-C3'	-3.53	105.39	112.20
8	E	405	FAD	P-O3P-PA	3.02	143.17	132.83
8	E	405	FAD	C5A-C6A-N6A	2.78	124.58	120.35
8	E	405	FAD	O3'-C3'-C4'	-2.72	102.23	108.81
8	E	405	FAD	O2'-C2'-C3'	2.66	115.57	109.10
8	E	405	FAD	O5'-C5'-C4'	-2.58	102.47	109.36
8	E	405	FAD	C1'-C2'-C3'	-2.56	102.62	109.79
8	E	405	FAD	O2P-P-O1P	2.47	124.44	112.24
8	a	701	FAD	C5A-C6A-N6A	2.28	123.82	120.35
8	E	405	FAD	C4X-C4-N3	2.25	118.89	113.19
8	A	707	FAD	C5A-C6A-N6A	2.24	123.76	120.35
8	E	405	FAD	O2A-PA-O1A	2.14	122.84	112.24
8	A	707	FAD	O4B-C1B-C2B	-2.11	103.84	106.93
8	a	701	FAD	O4B-C1B-C2B	-2.10	103.86	106.93
8	a	701	FAD	C4-N3-C2	-2.06	121.84	125.64
8	A	707	FAD	C4-N3-C2	-2.04	121.88	125.64

There are no chirality outliers.

All (13) torsion outliers are listed below:

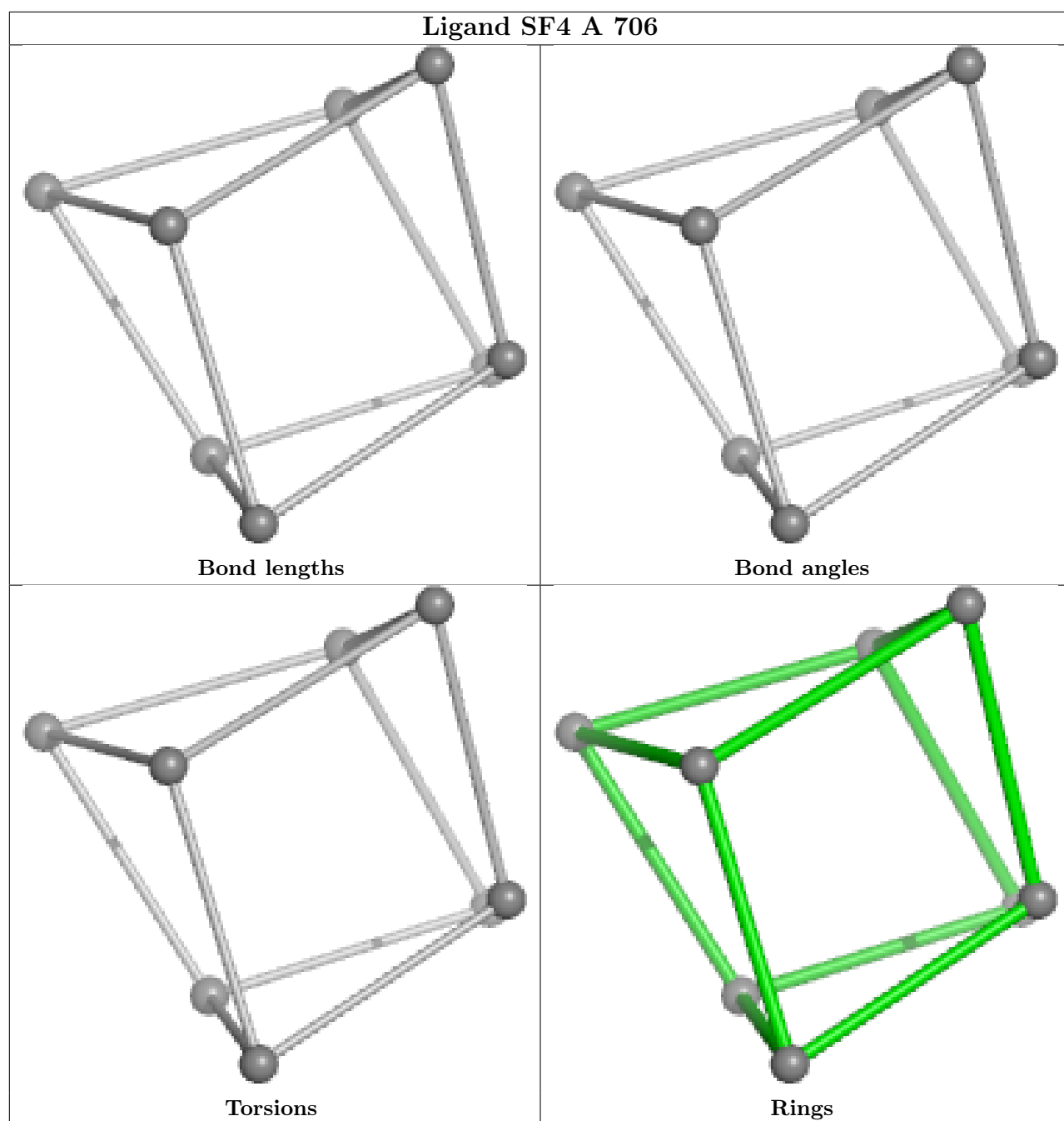
Mol	Chain	Res	Type	Atoms
8	E	405	FAD	C5B-O5B-PA-O2A
8	E	405	FAD	C5B-O5B-PA-O3P
8	E	405	FAD	C1'-C2'-C3'-O3'
8	E	405	FAD	C1'-C2'-C3'-C4'
8	E	405	FAD	O4B-C4B-C5B-O5B
8	E	405	FAD	C3B-C4B-C5B-O5B
8	E	405	FAD	O2'-C2'-C3'-C4'
8	E	405	FAD	O2'-C2'-C3'-O3'
8	E	405	FAD	C2'-C1'-N10-C10
8	E	405	FAD	C4'-C5'-O5'-P
8	a	701	FAD	O4B-C4B-C5B-O5B
8	A	707	FAD	O4B-C4B-C5B-O5B
8	E	405	FAD	C5'-O5'-P-O1P

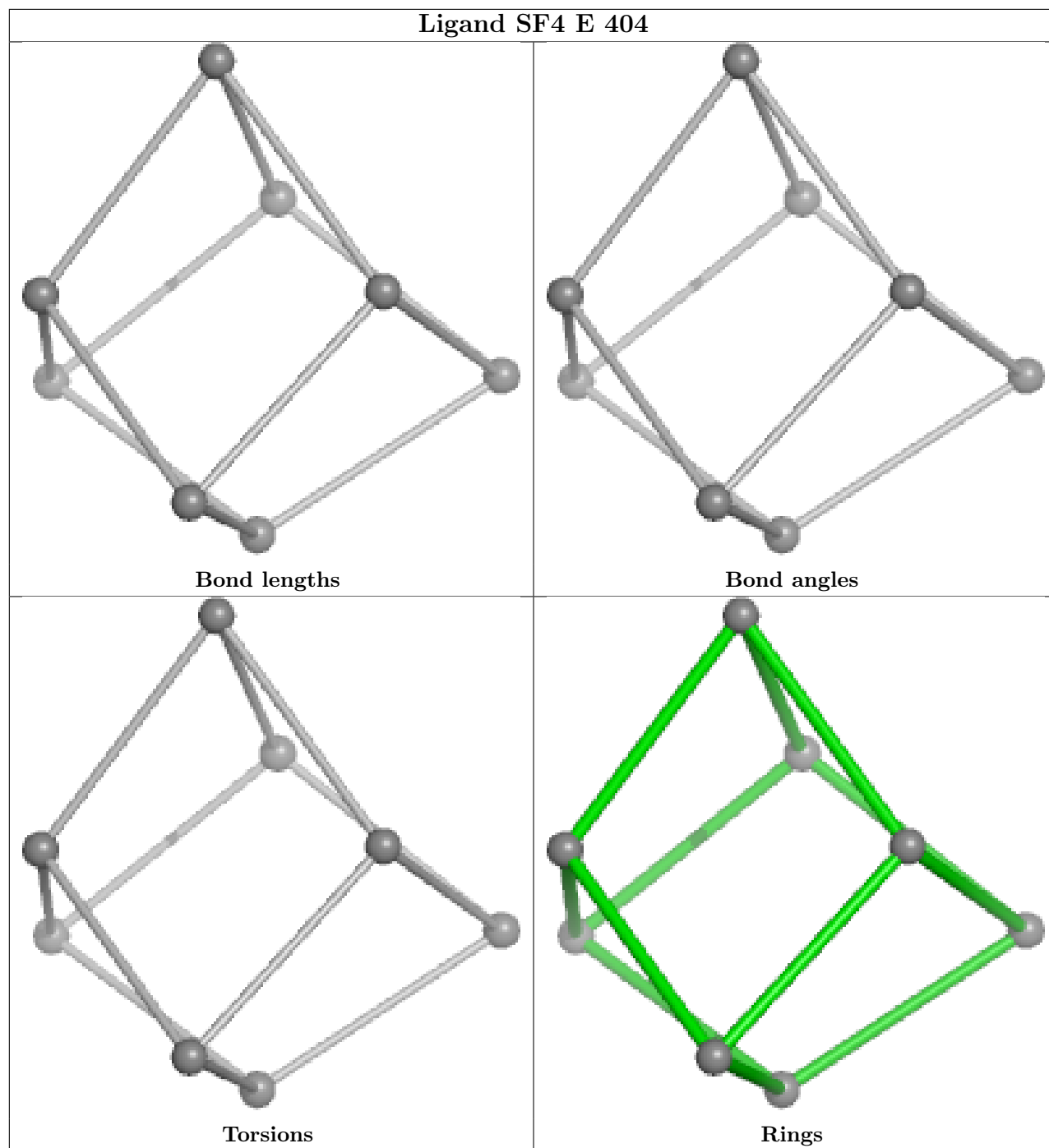
There are no ring outliers.

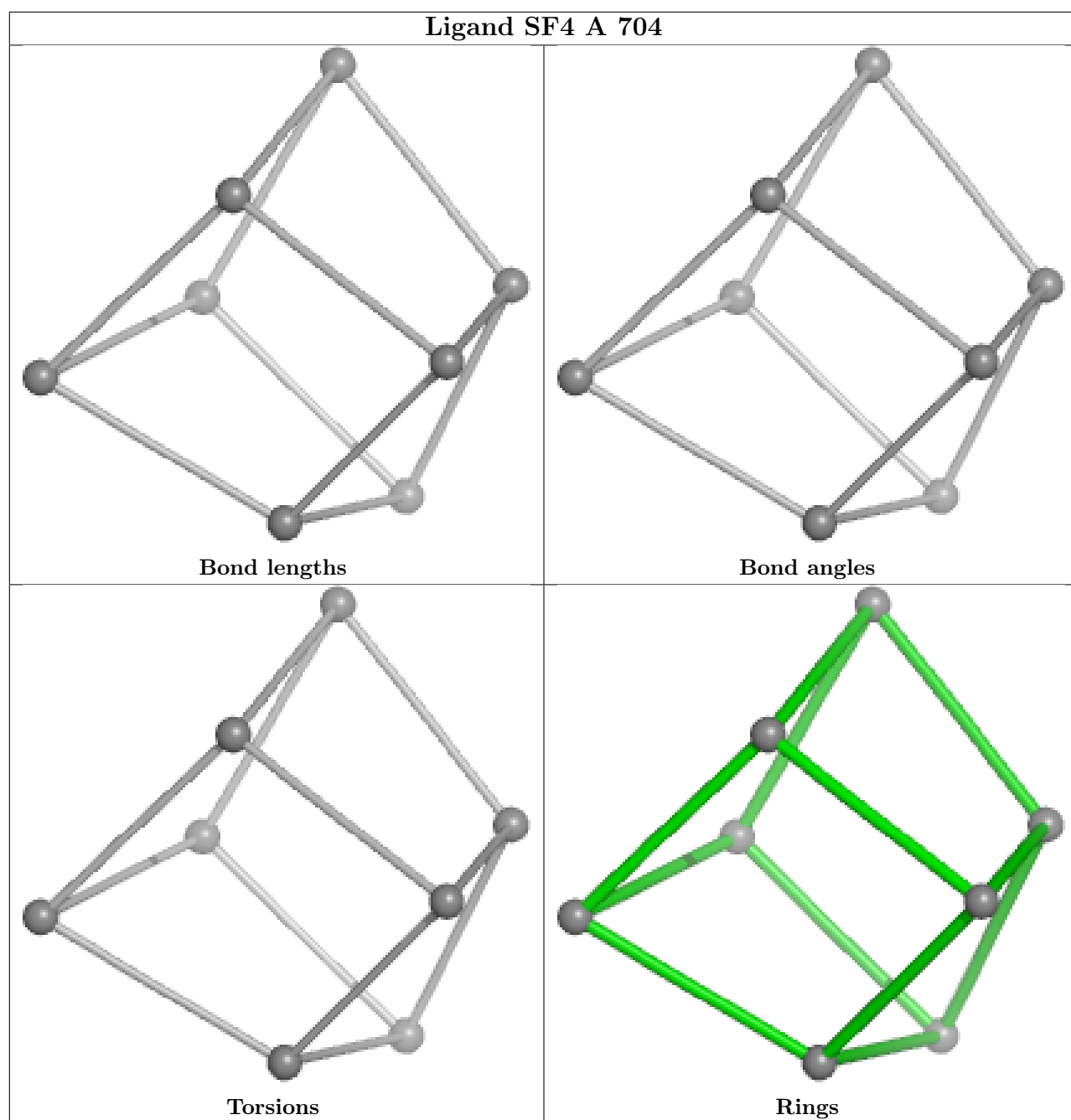
2 monomers are involved in 4 short contacts:

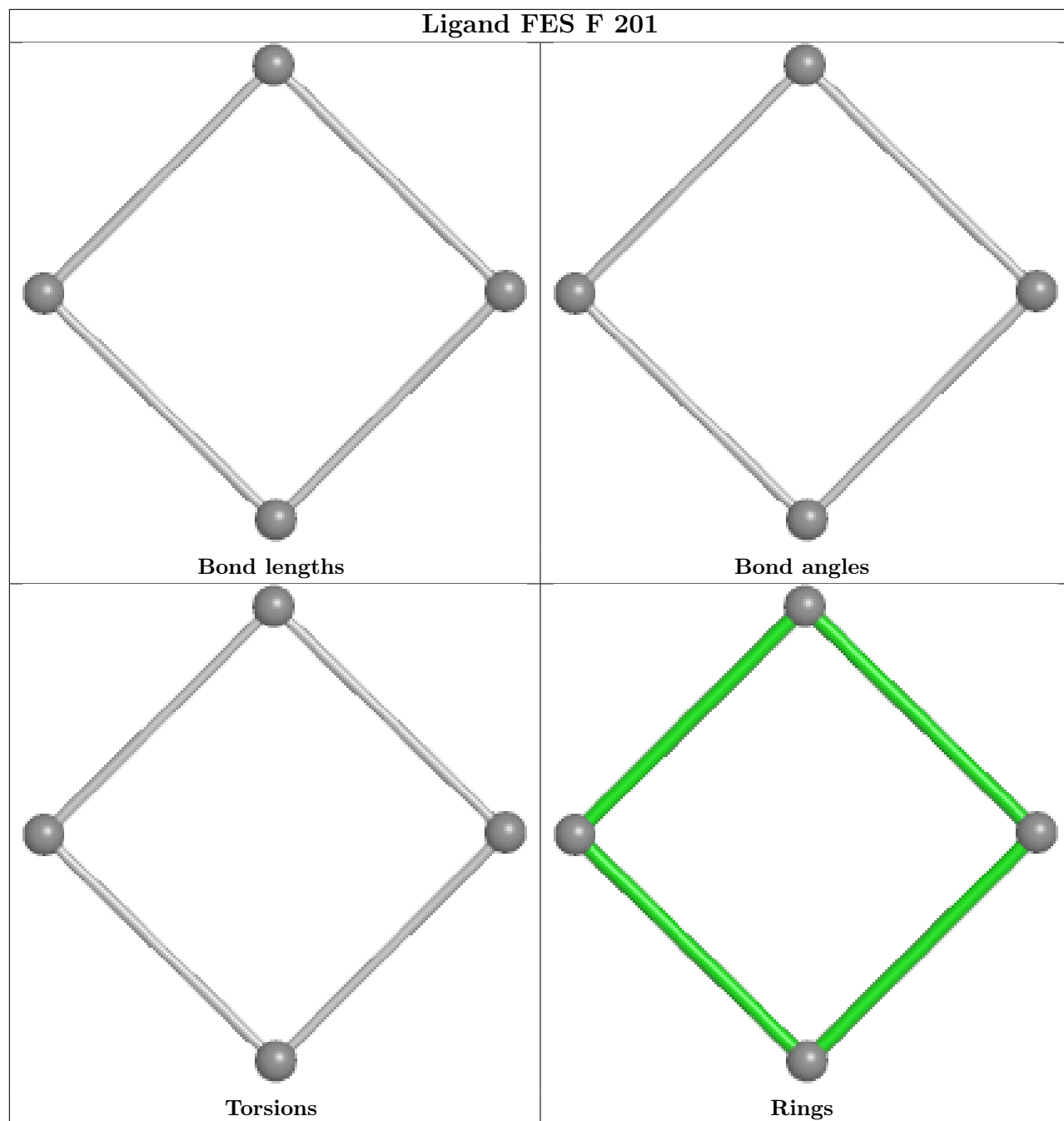
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	E	405	FAD	3	0
10	b	401	9S8	1	0

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.

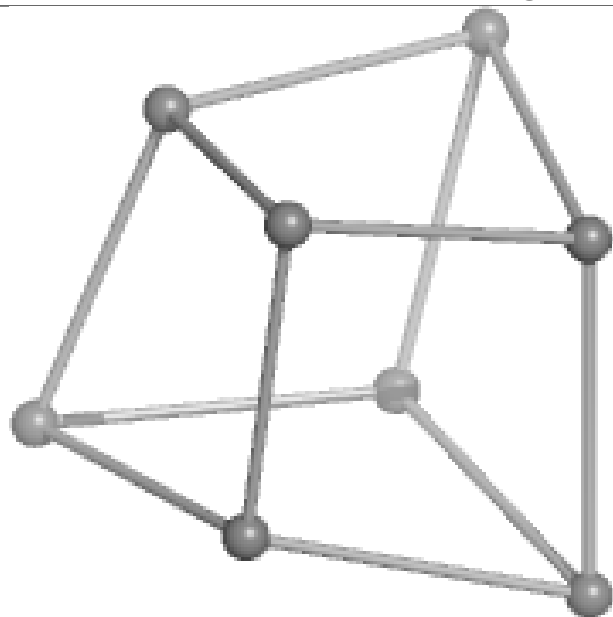




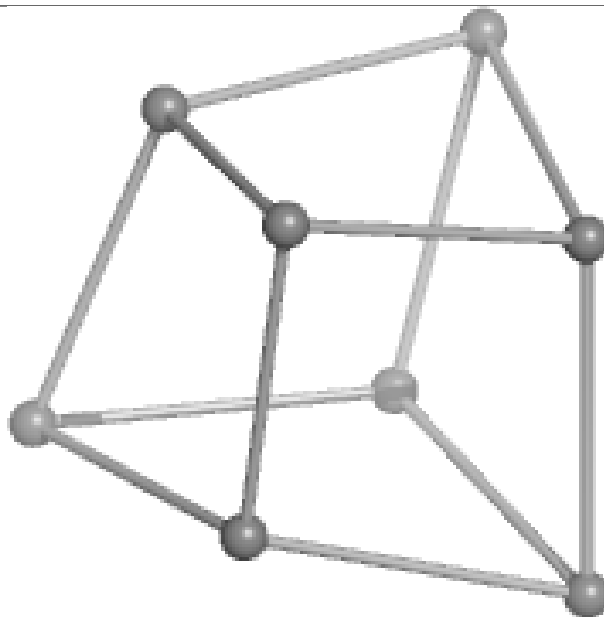




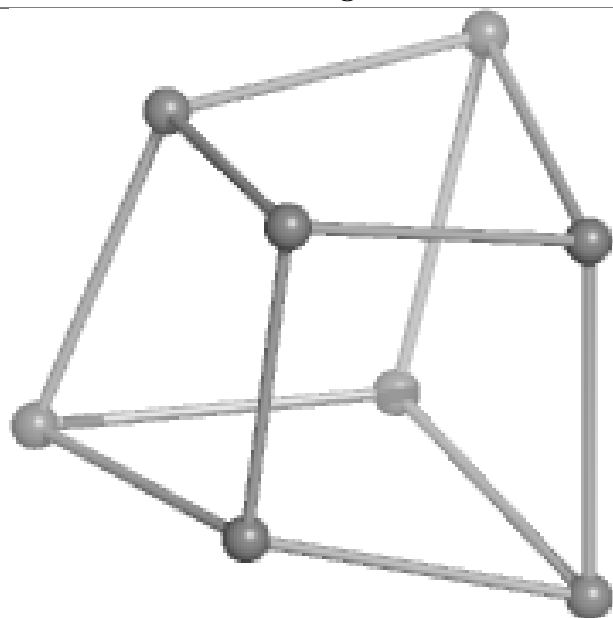
Ligand SF4 A 705



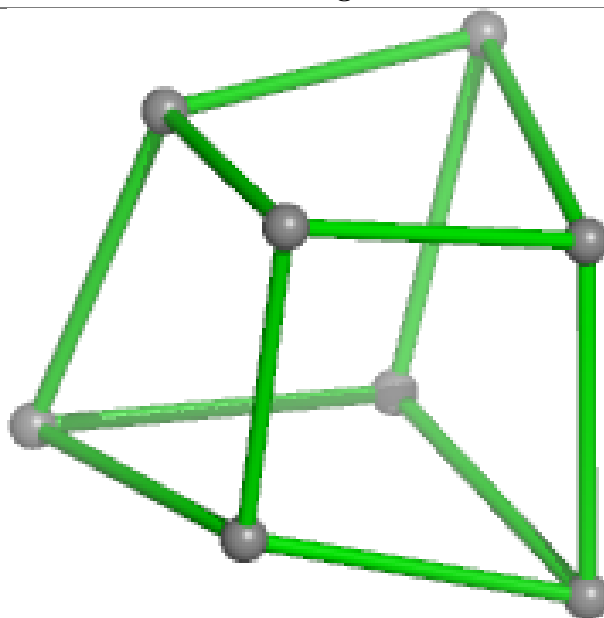
Bond lengths



Bond angles

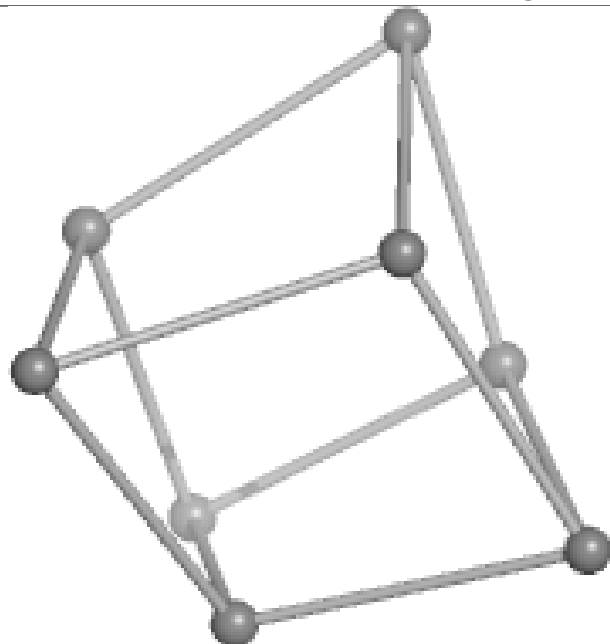


Torsions

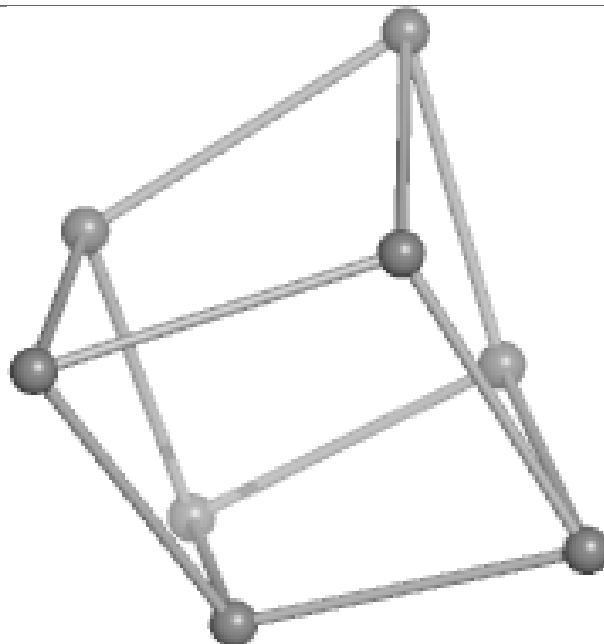


Rings

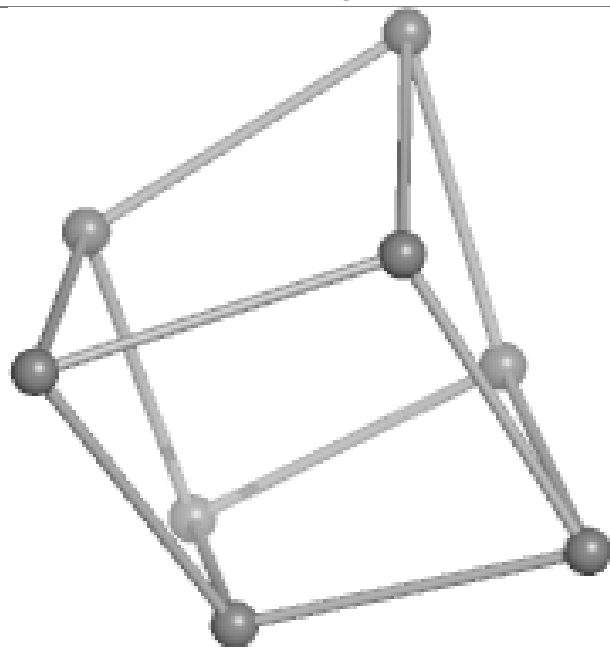
Ligand SF4 A 701



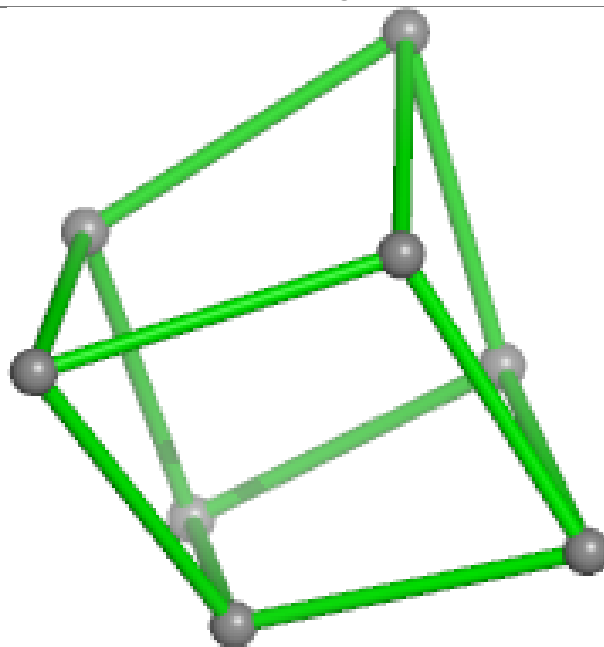
Bond lengths



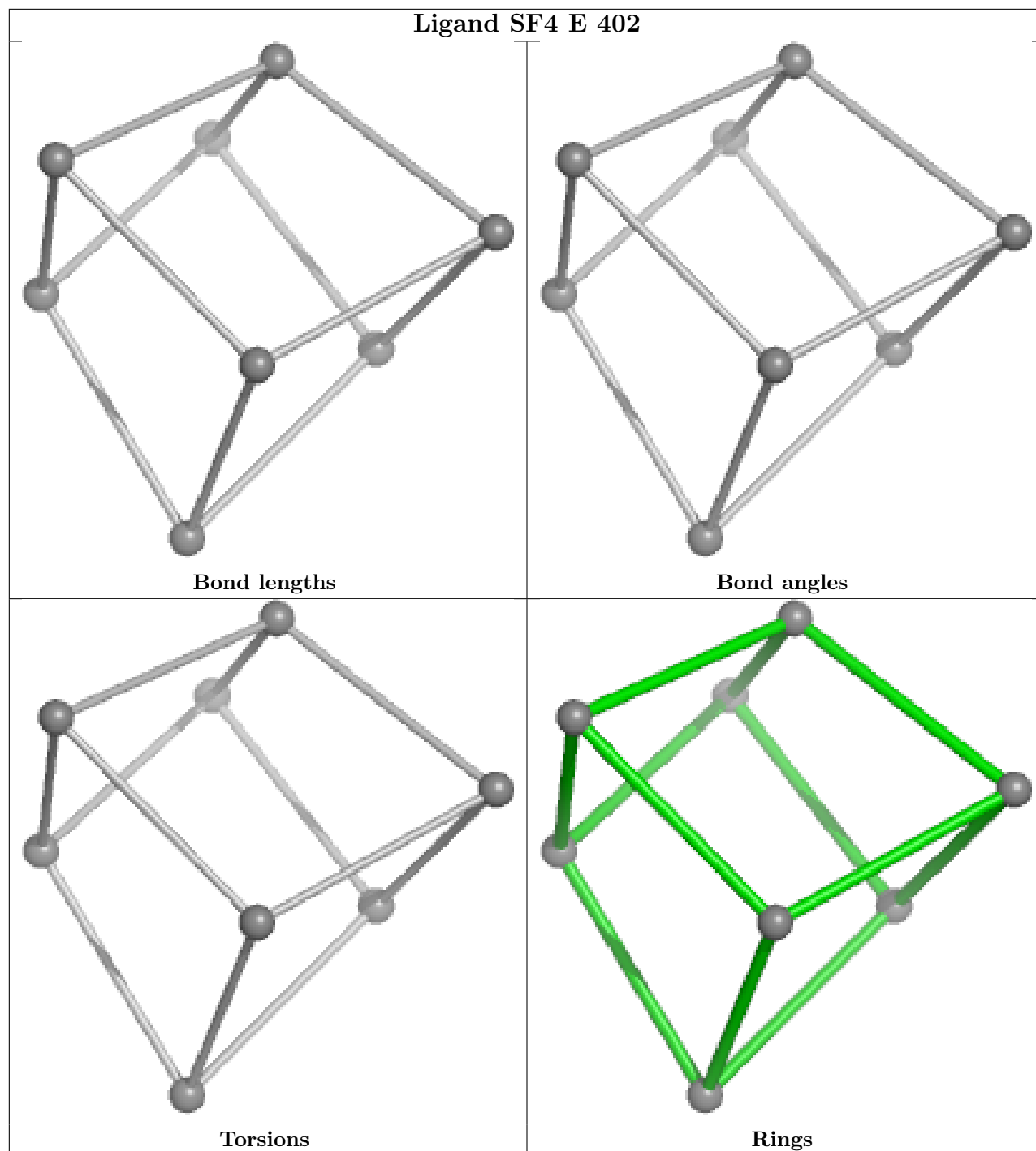
Bond angles

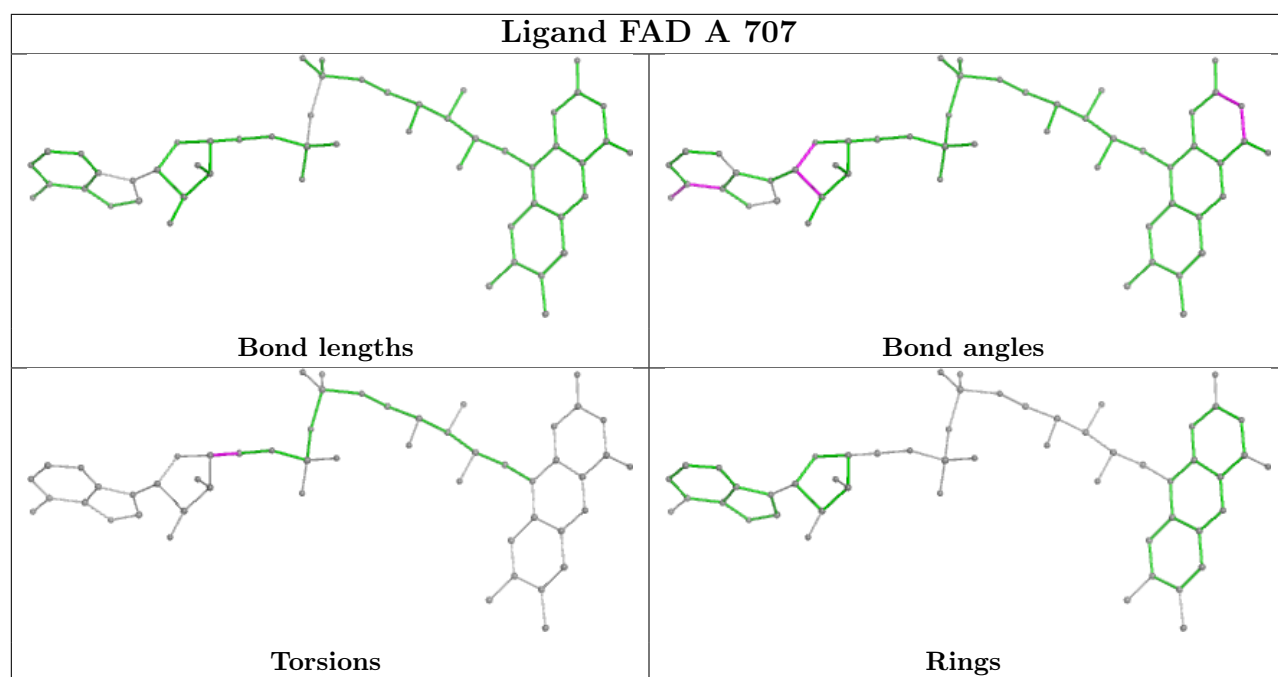


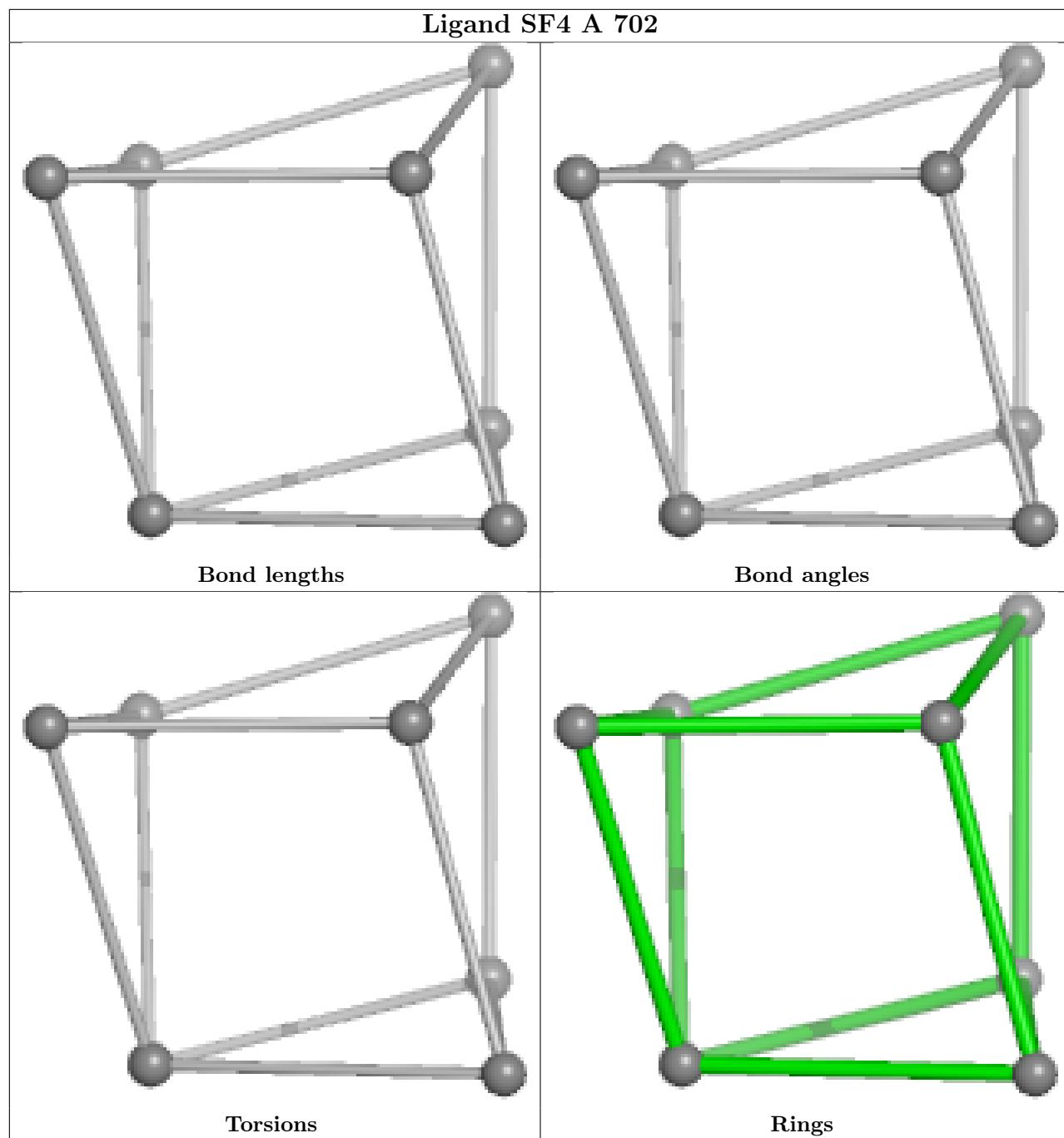
Torsions

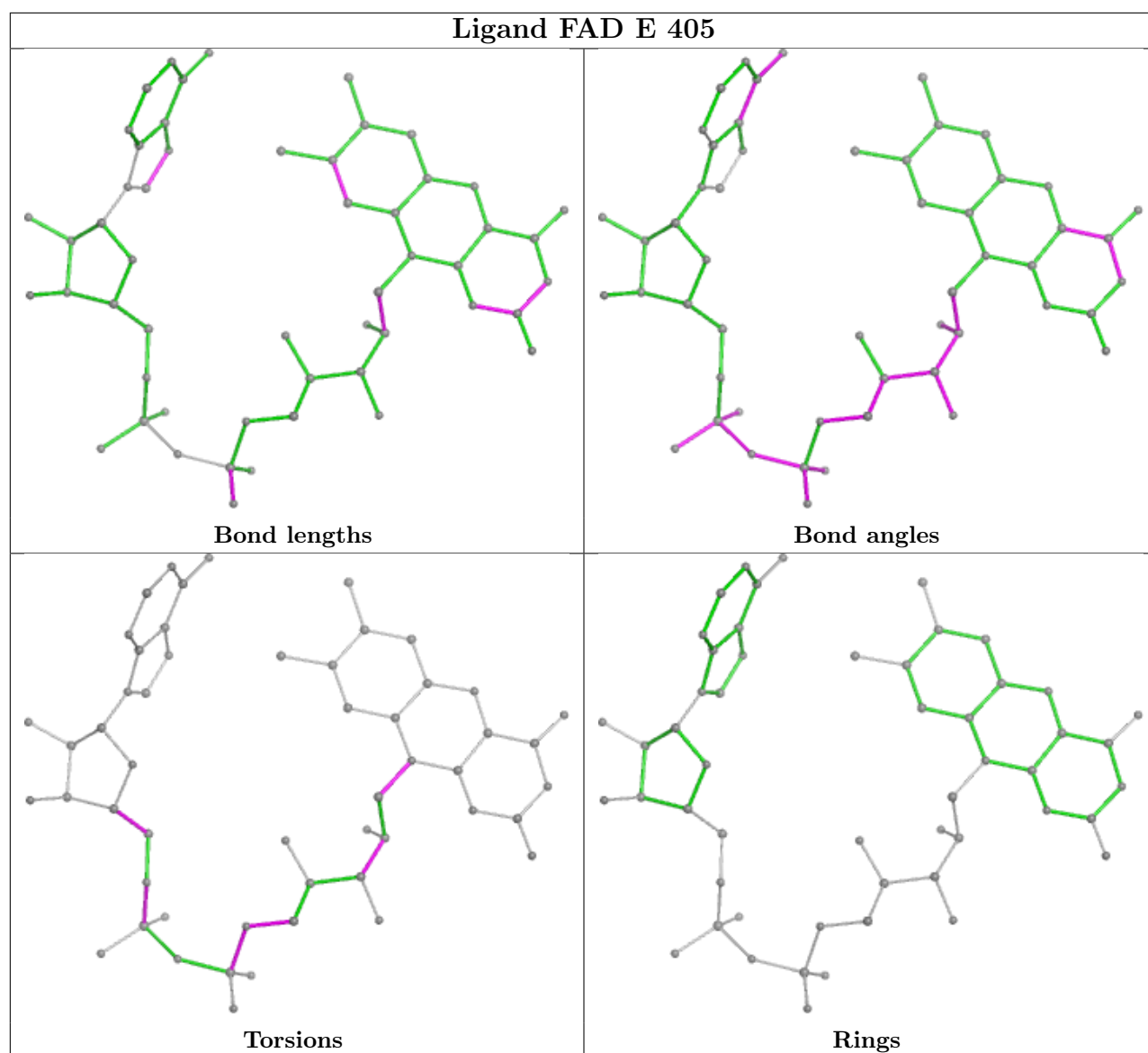


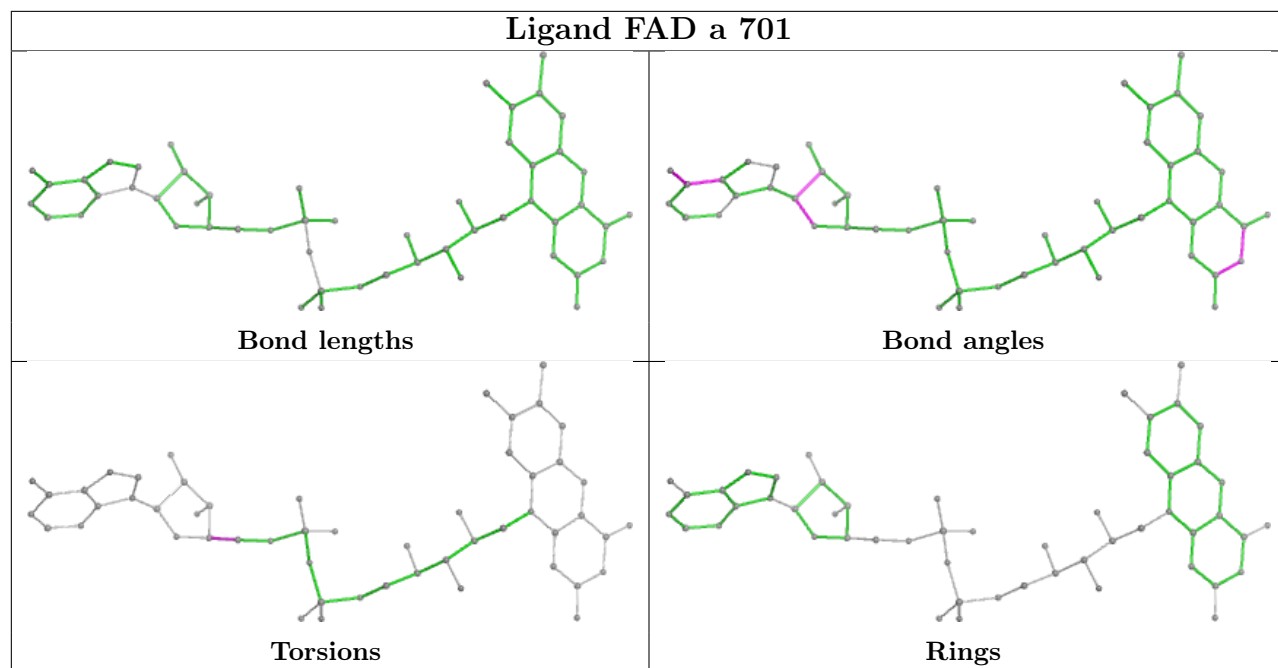
Rings



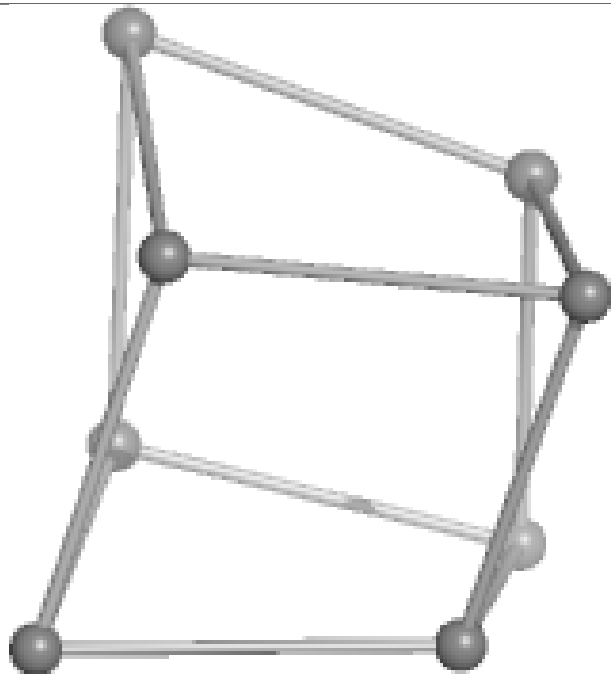




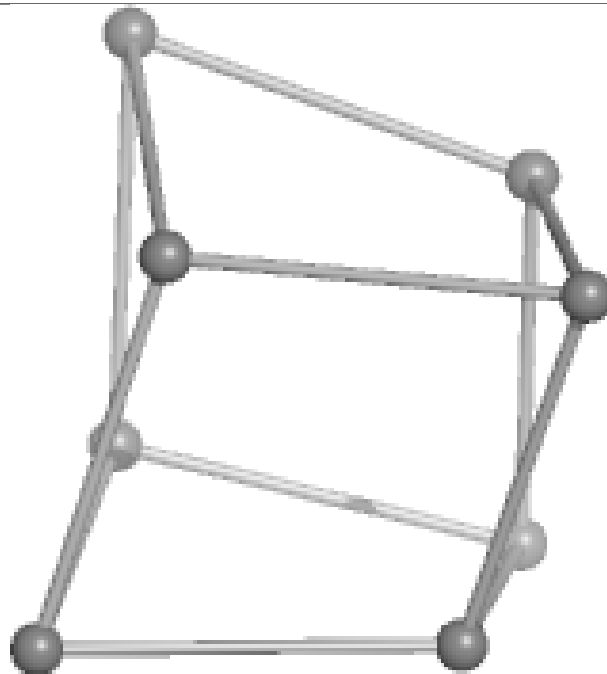




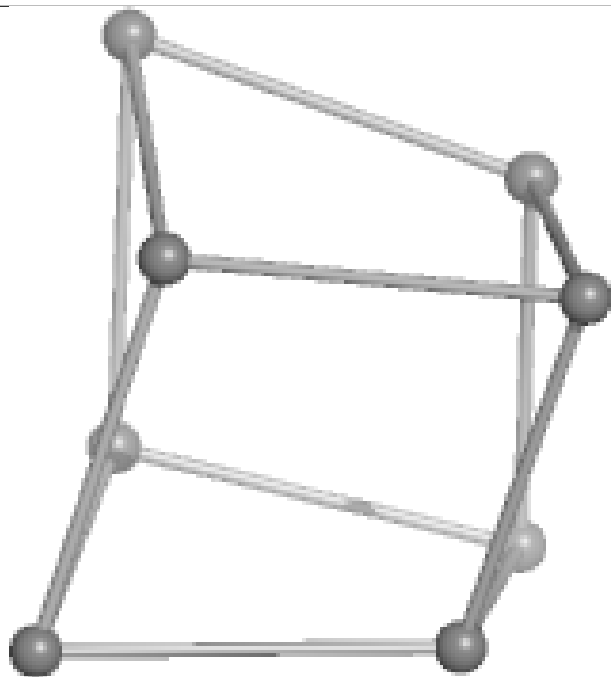
Ligand SF4 E 401



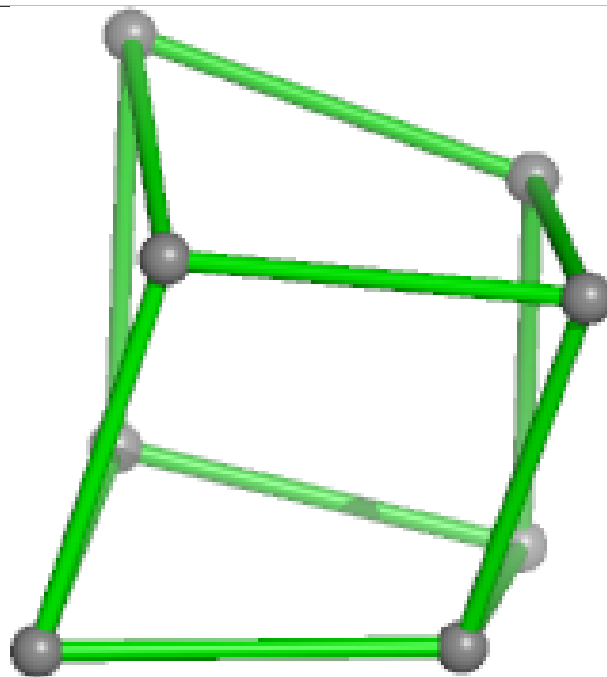
Bond lengths



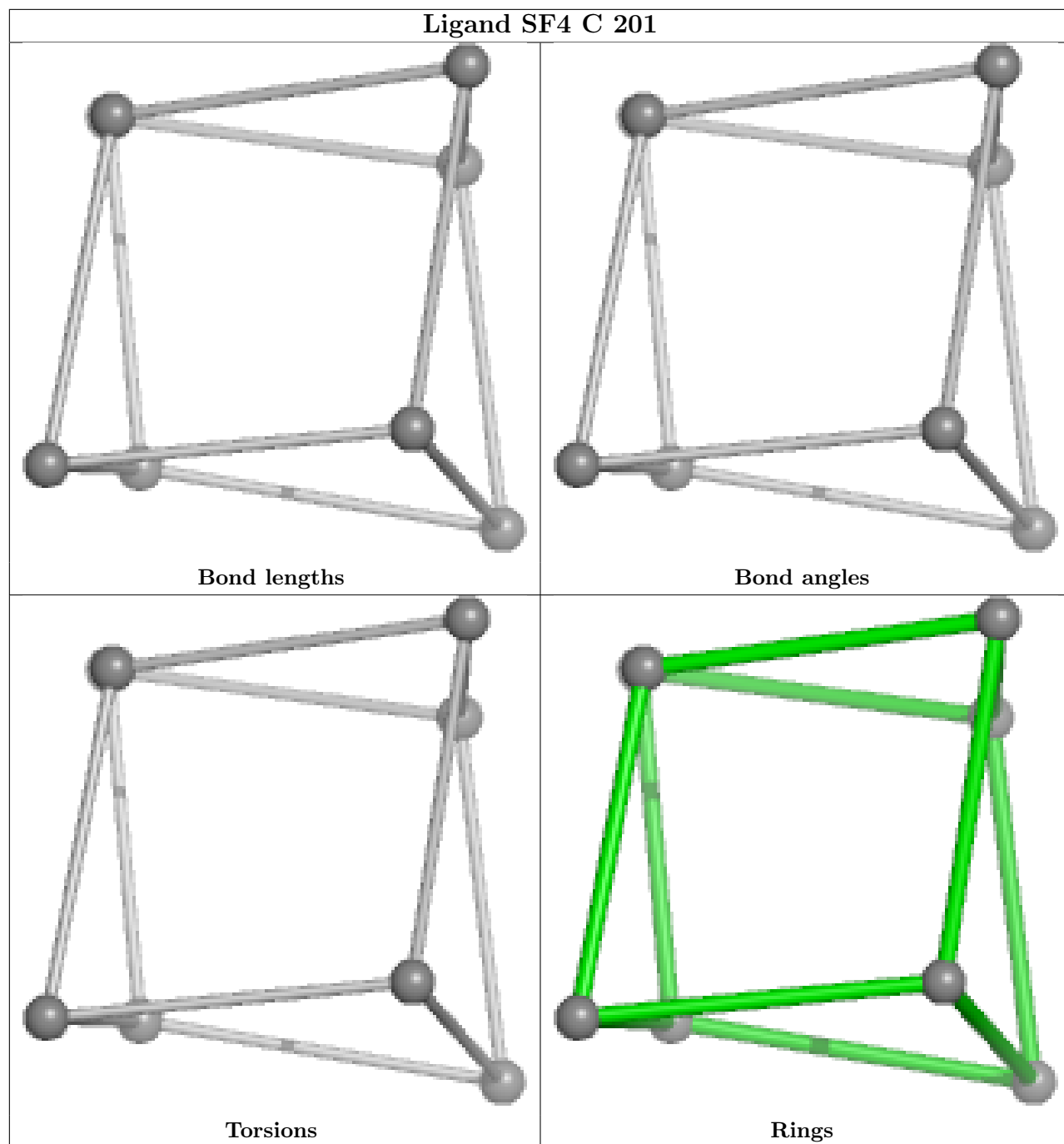
Bond angles



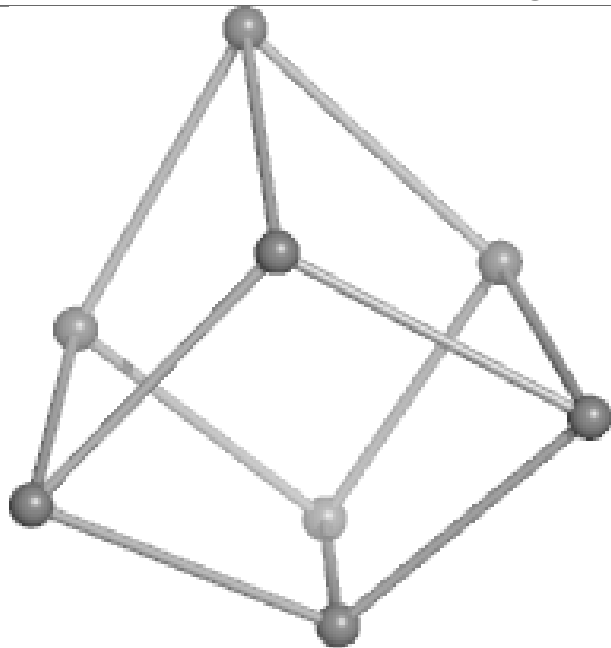
Torsions



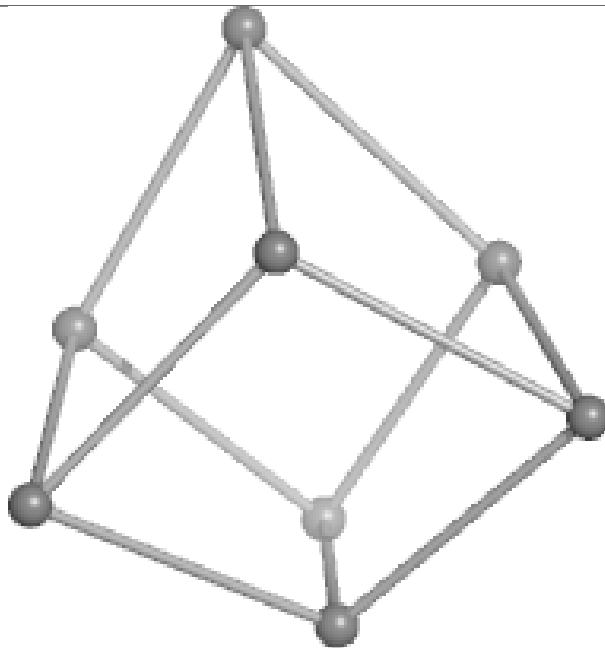
Rings



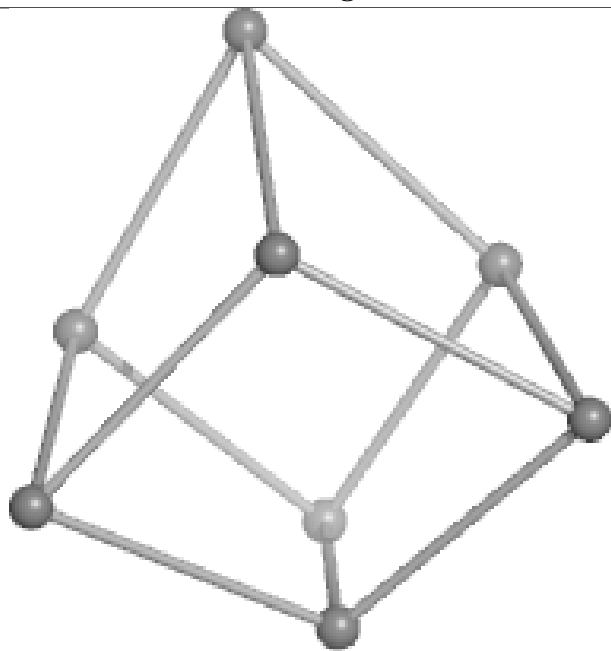
Ligand SF4 c 202



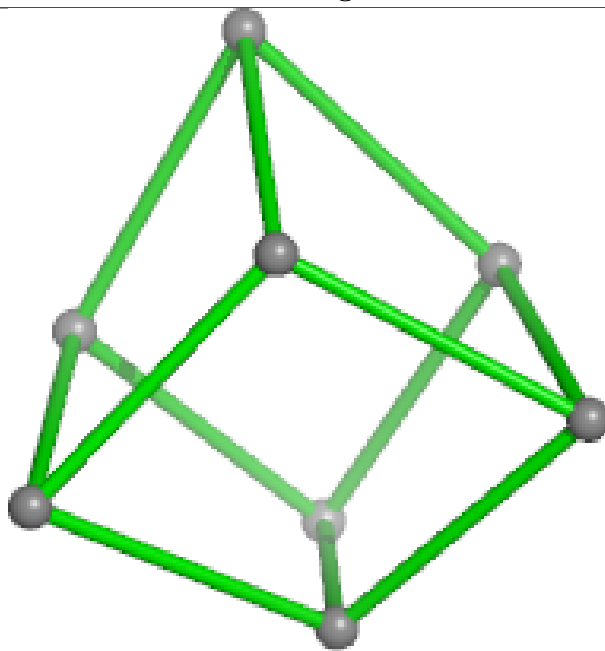
Bond lengths



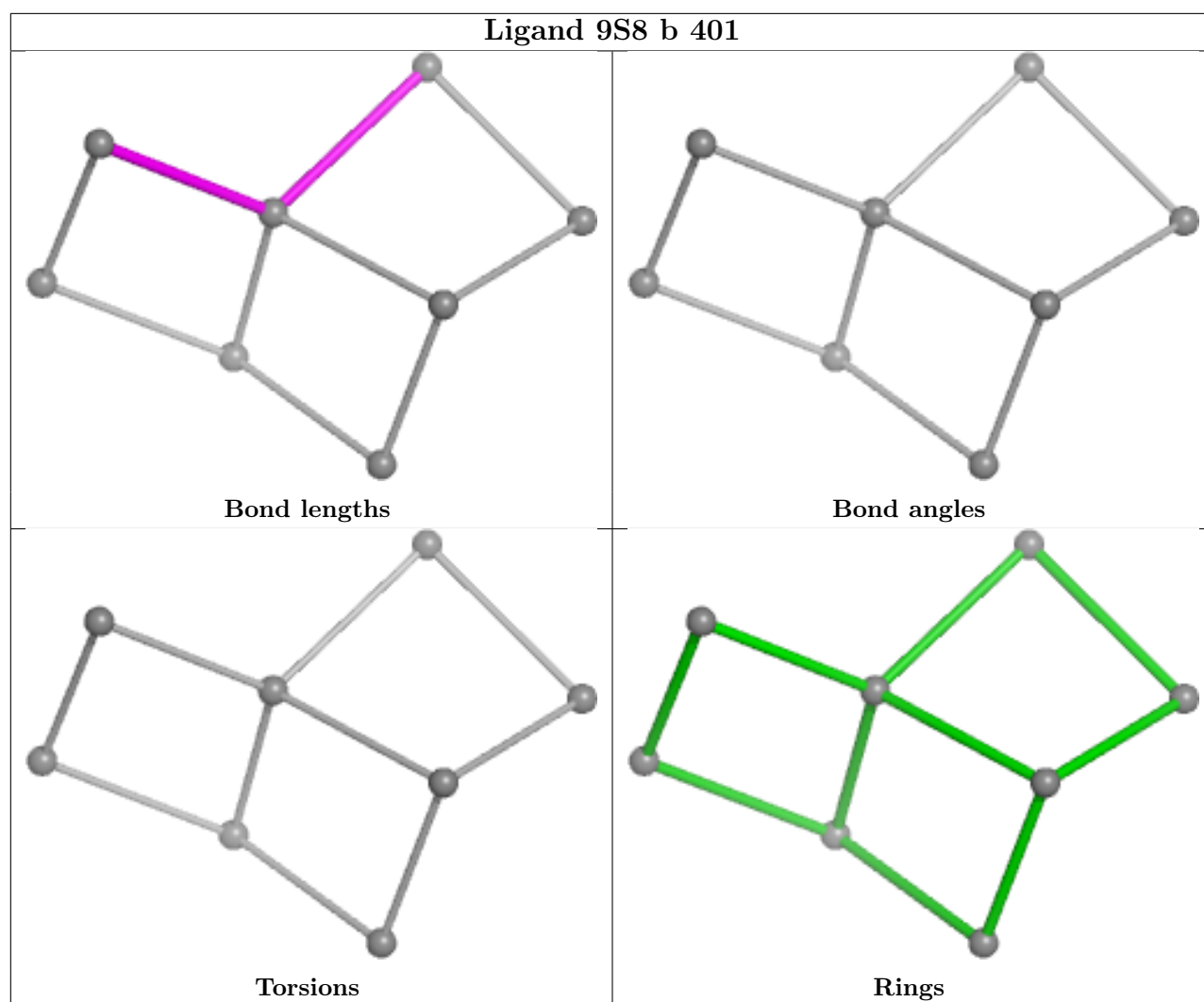
Bond angles

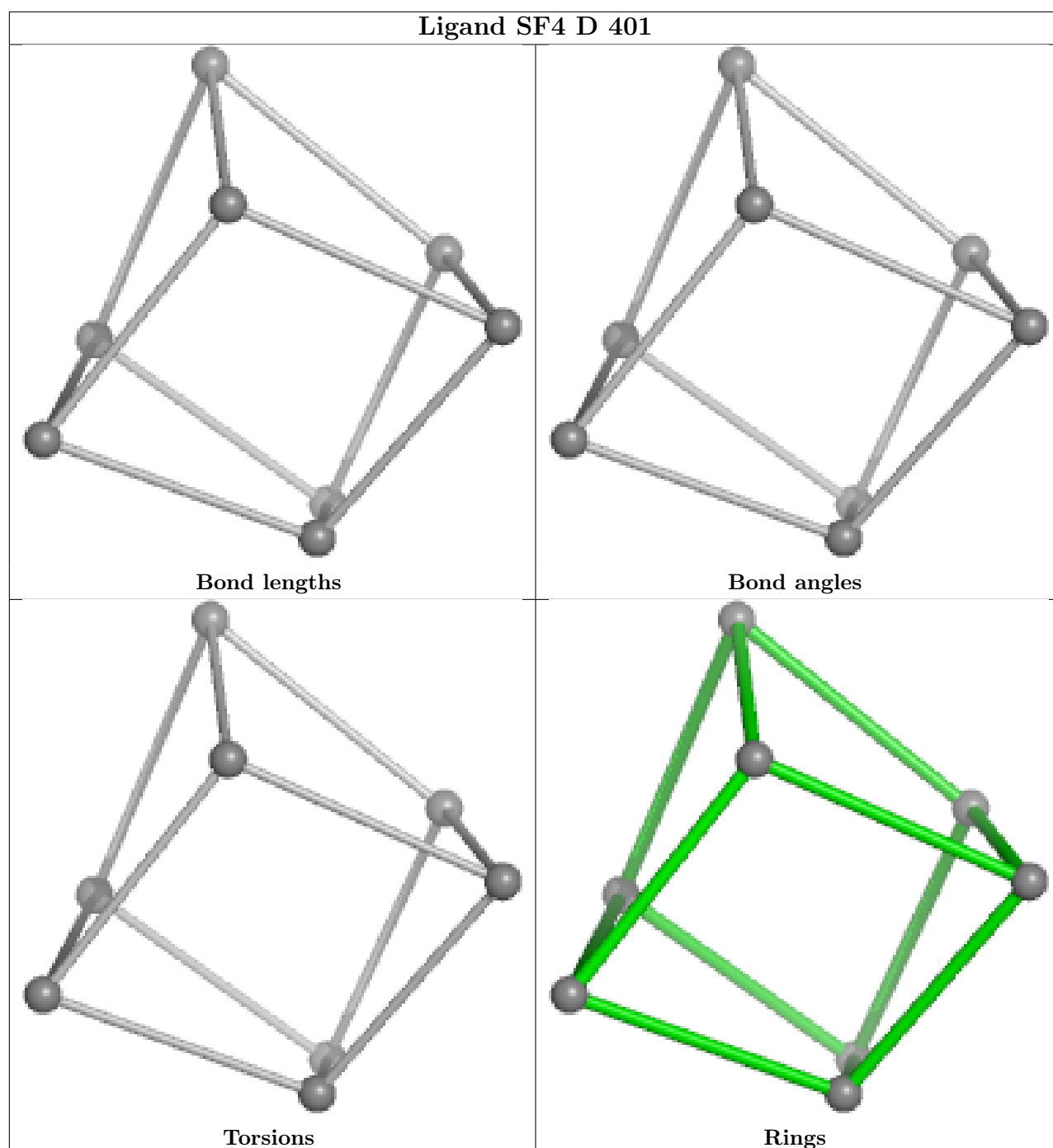


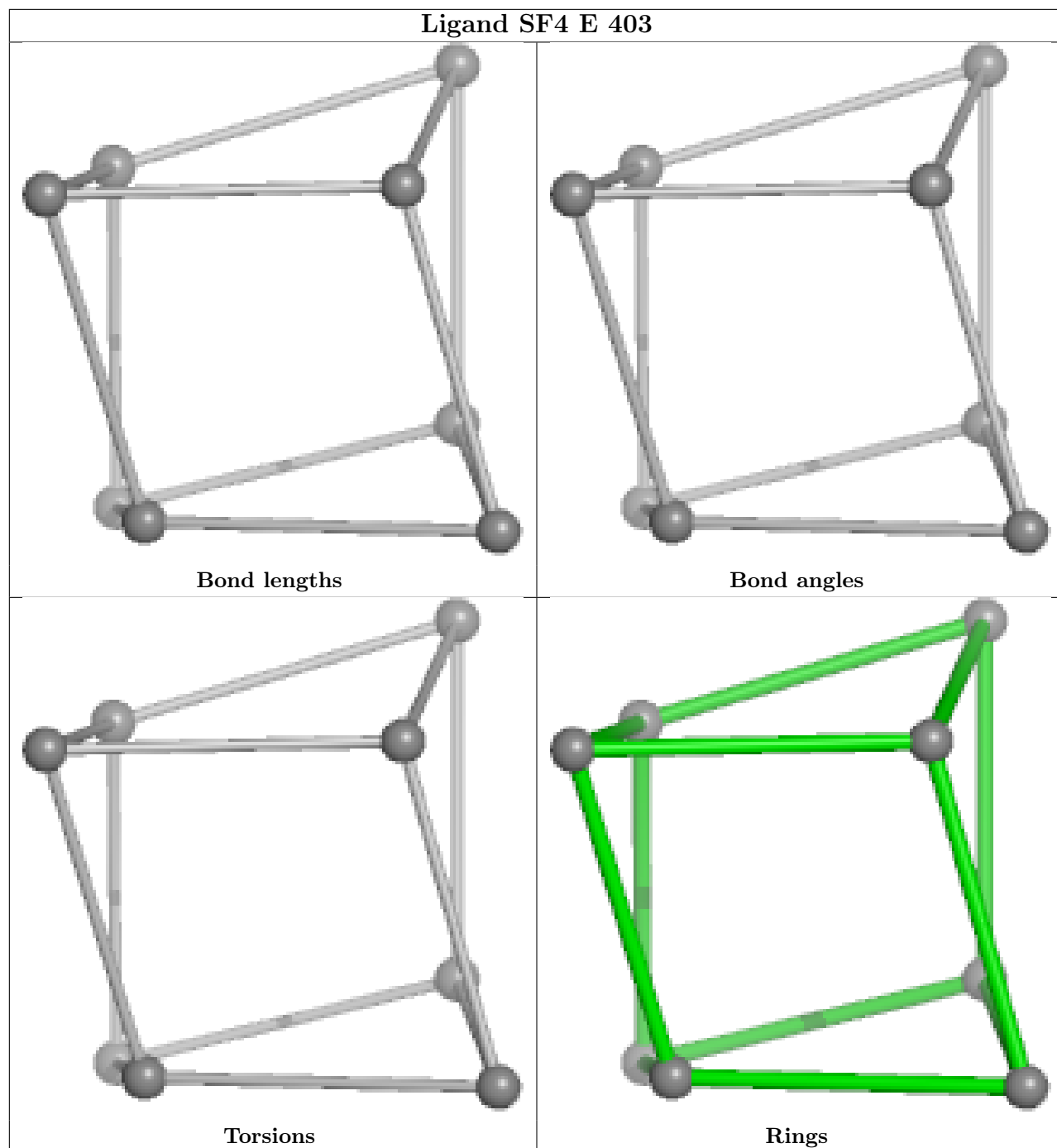
Torsions



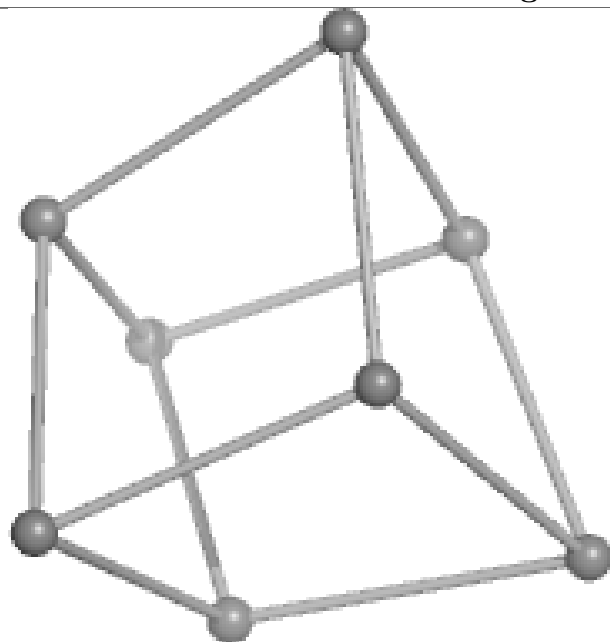
Rings



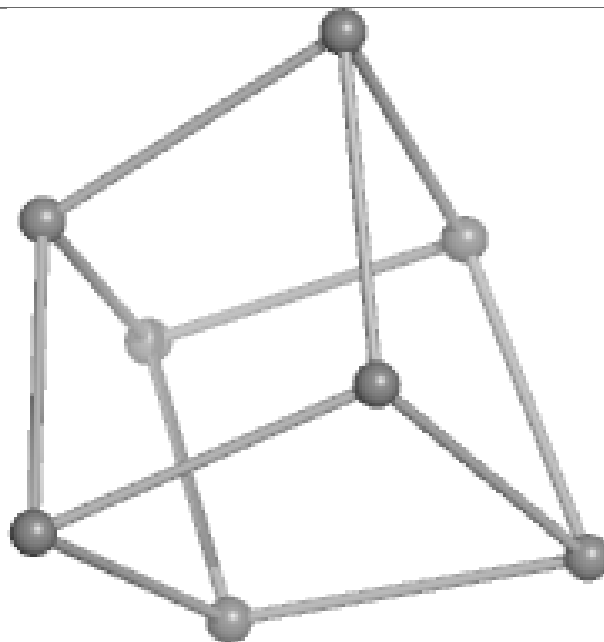




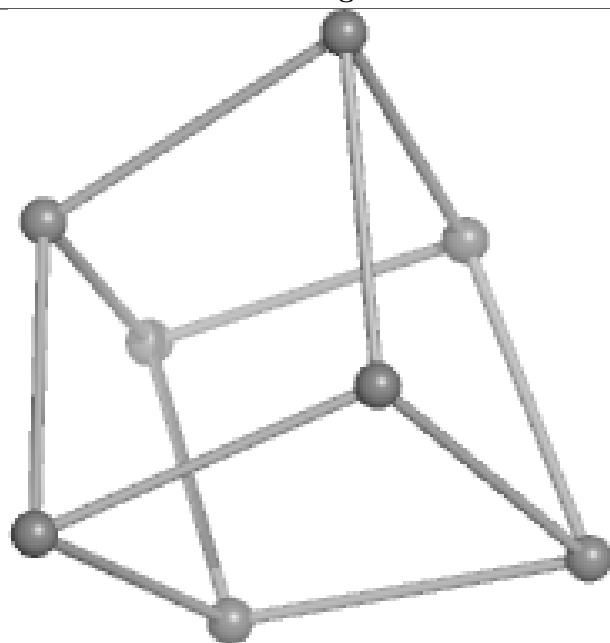
Ligand SF4 C 202



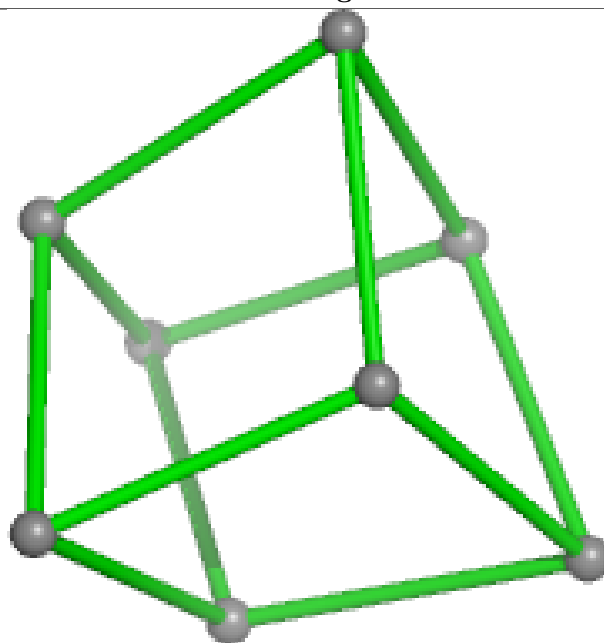
Bond lengths



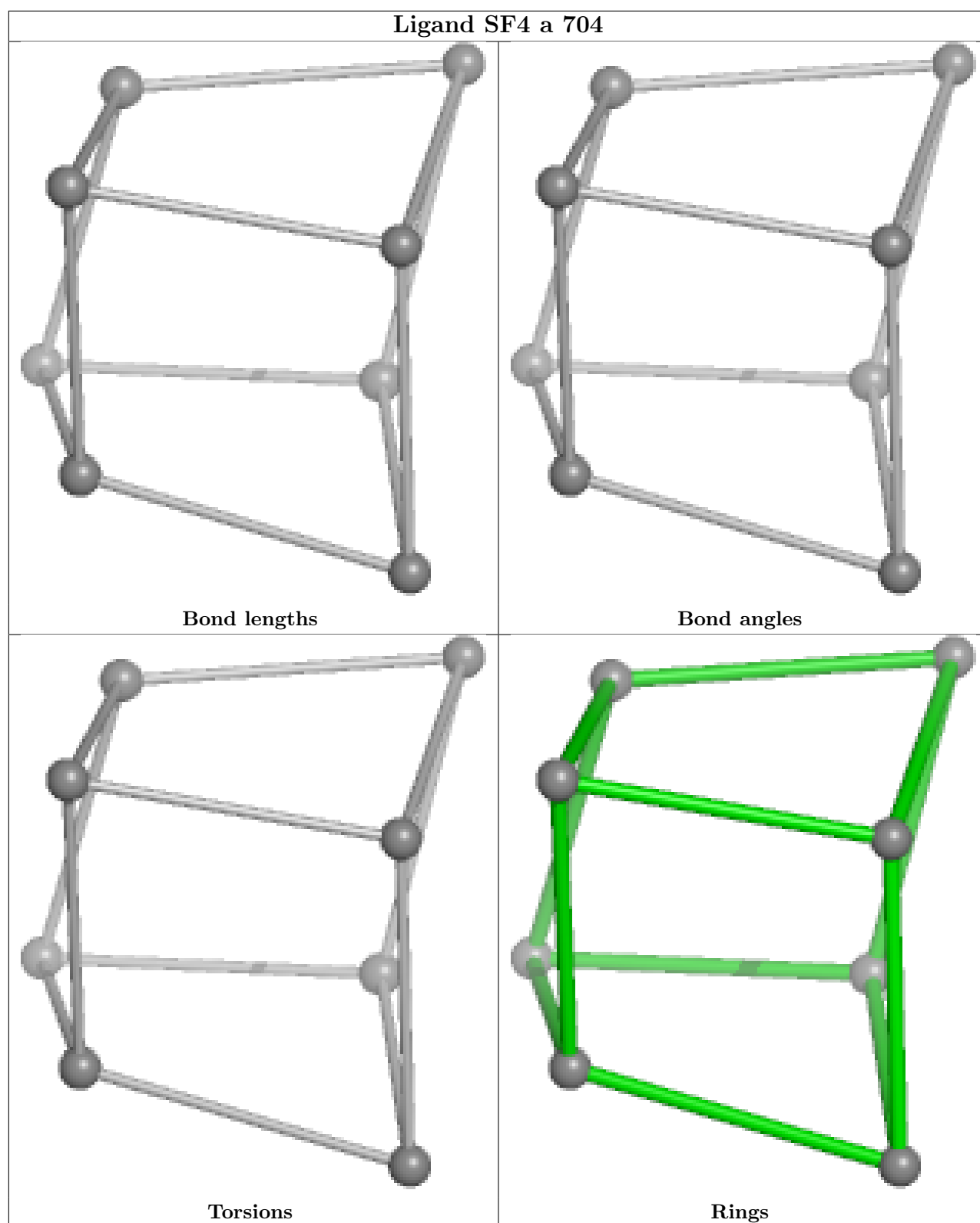
Bond angles

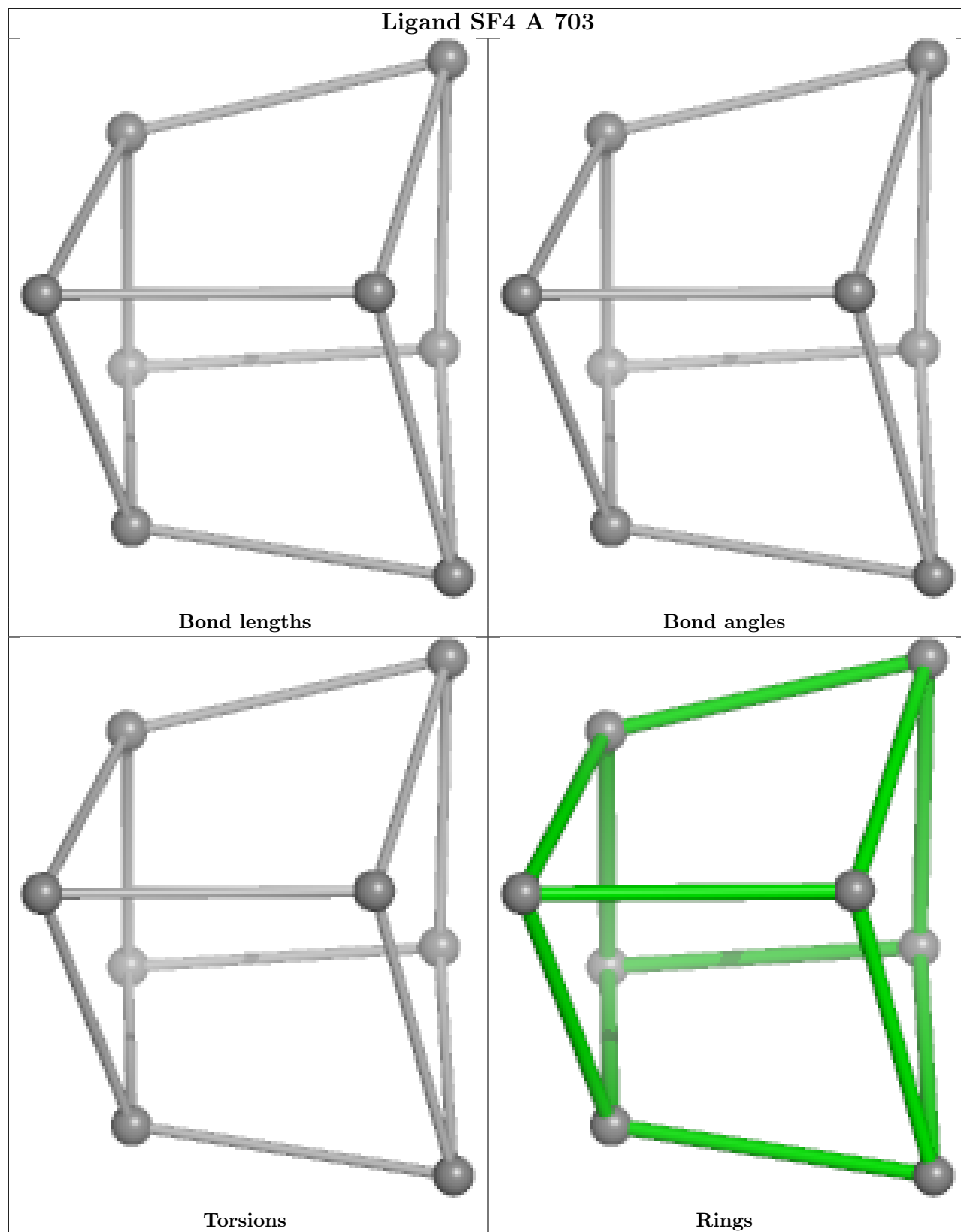


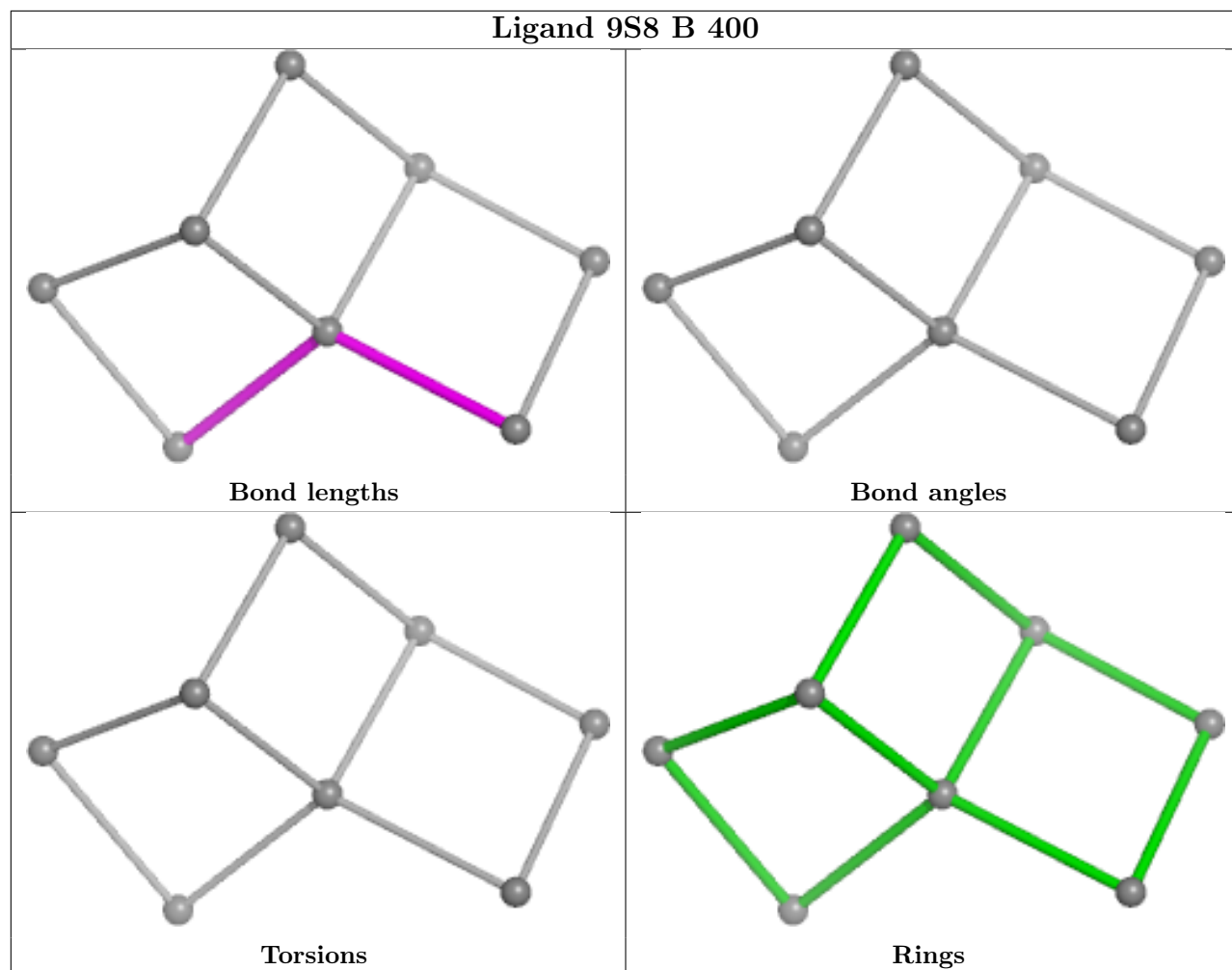
Torsions

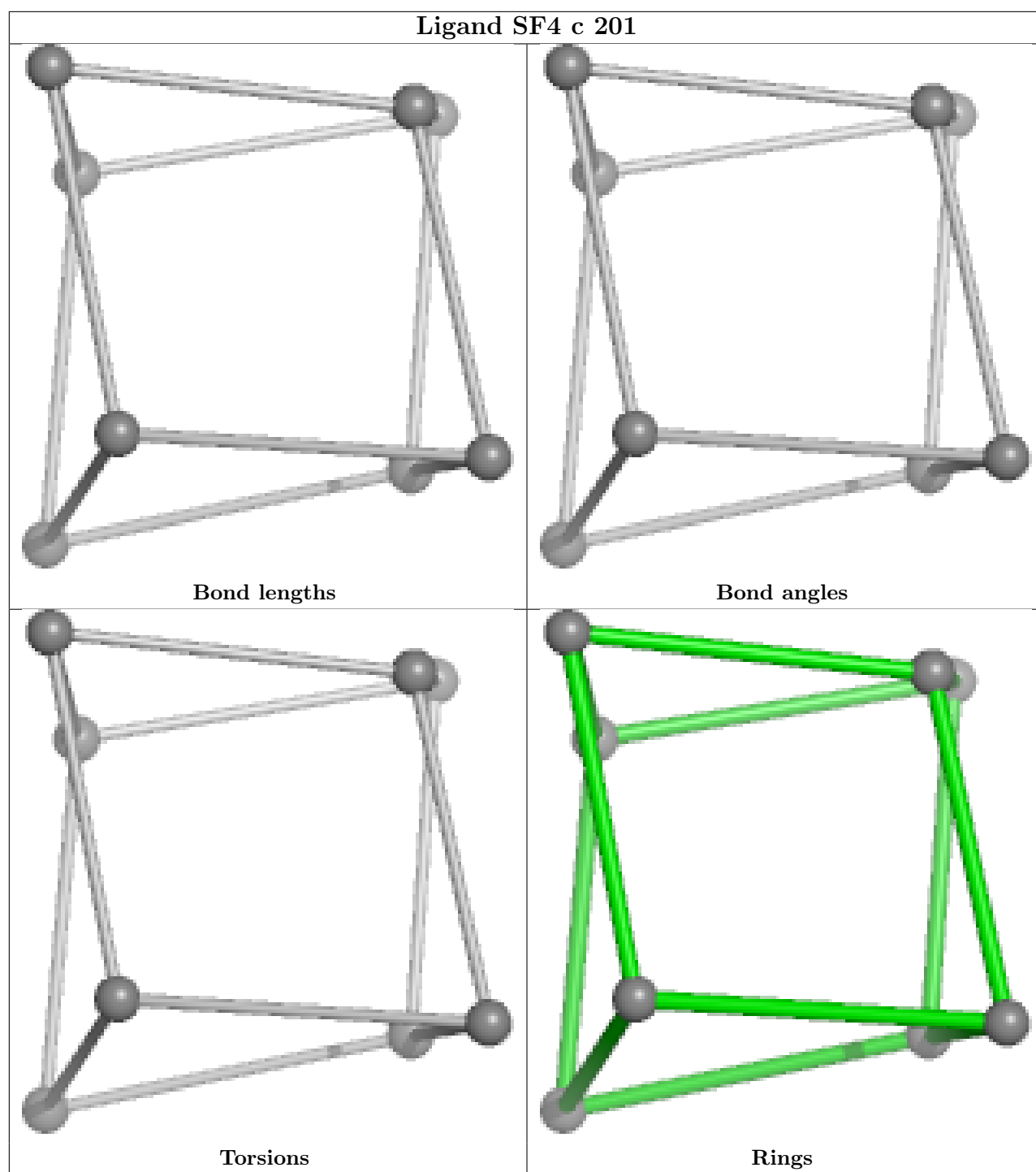


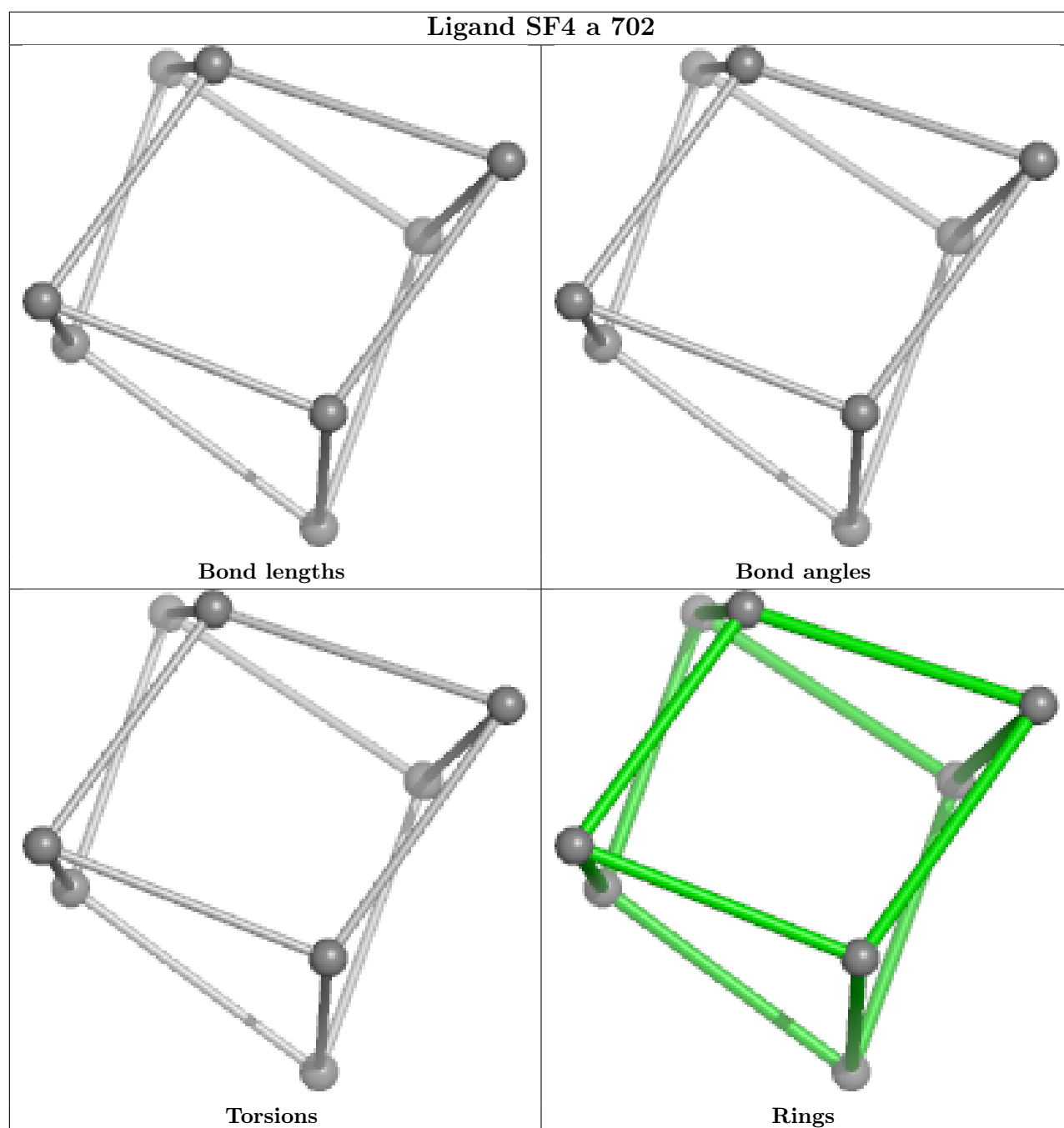
Rings

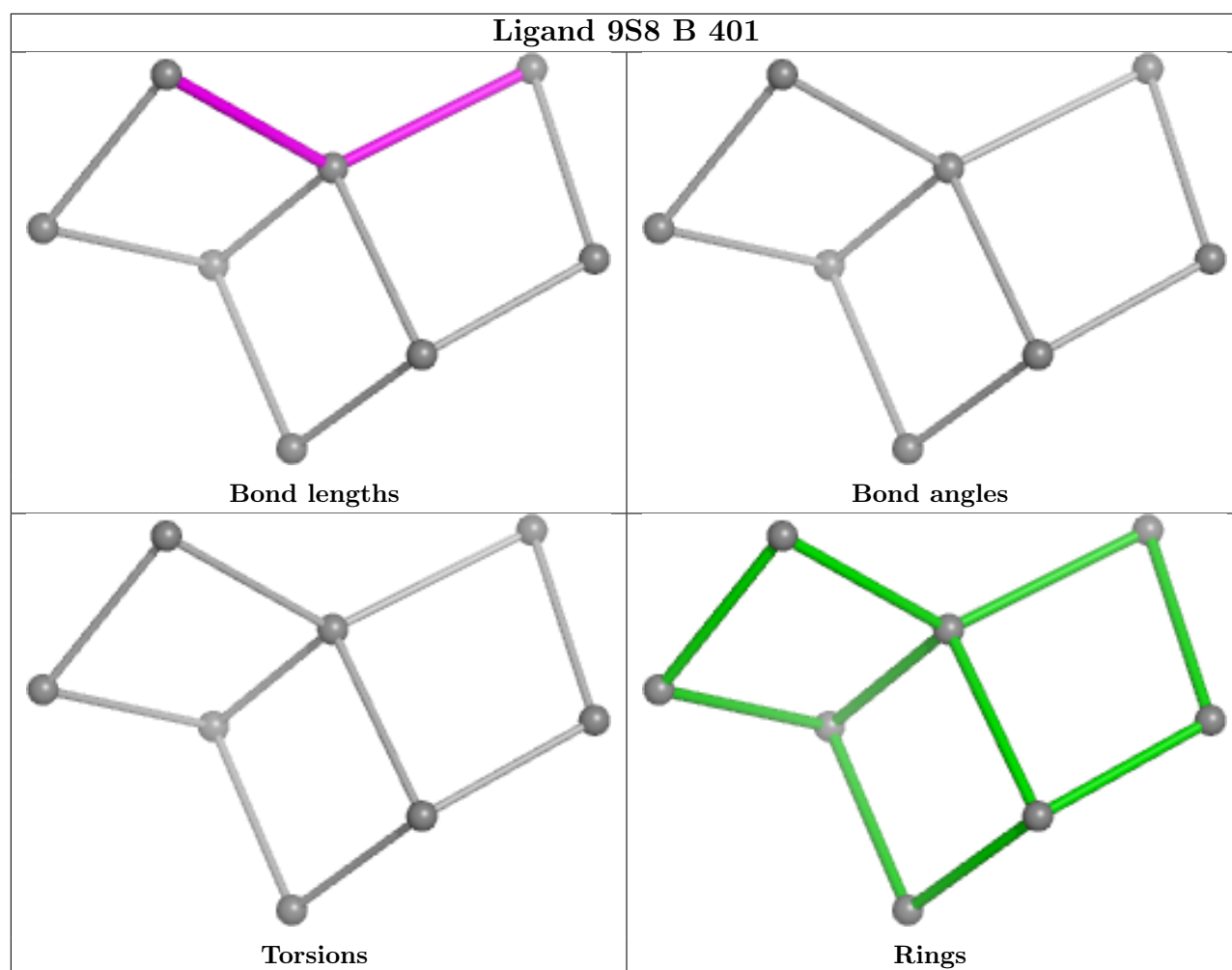


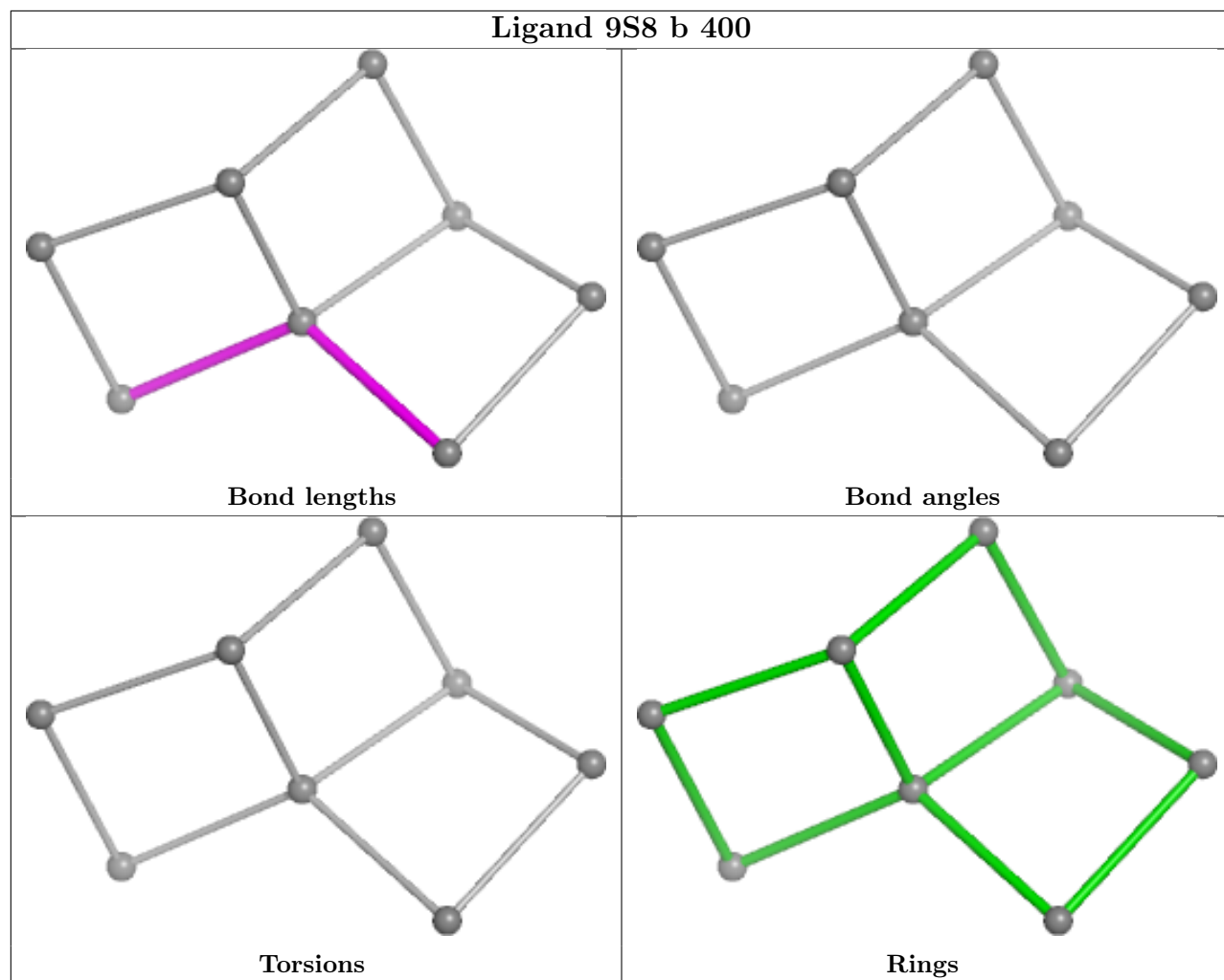


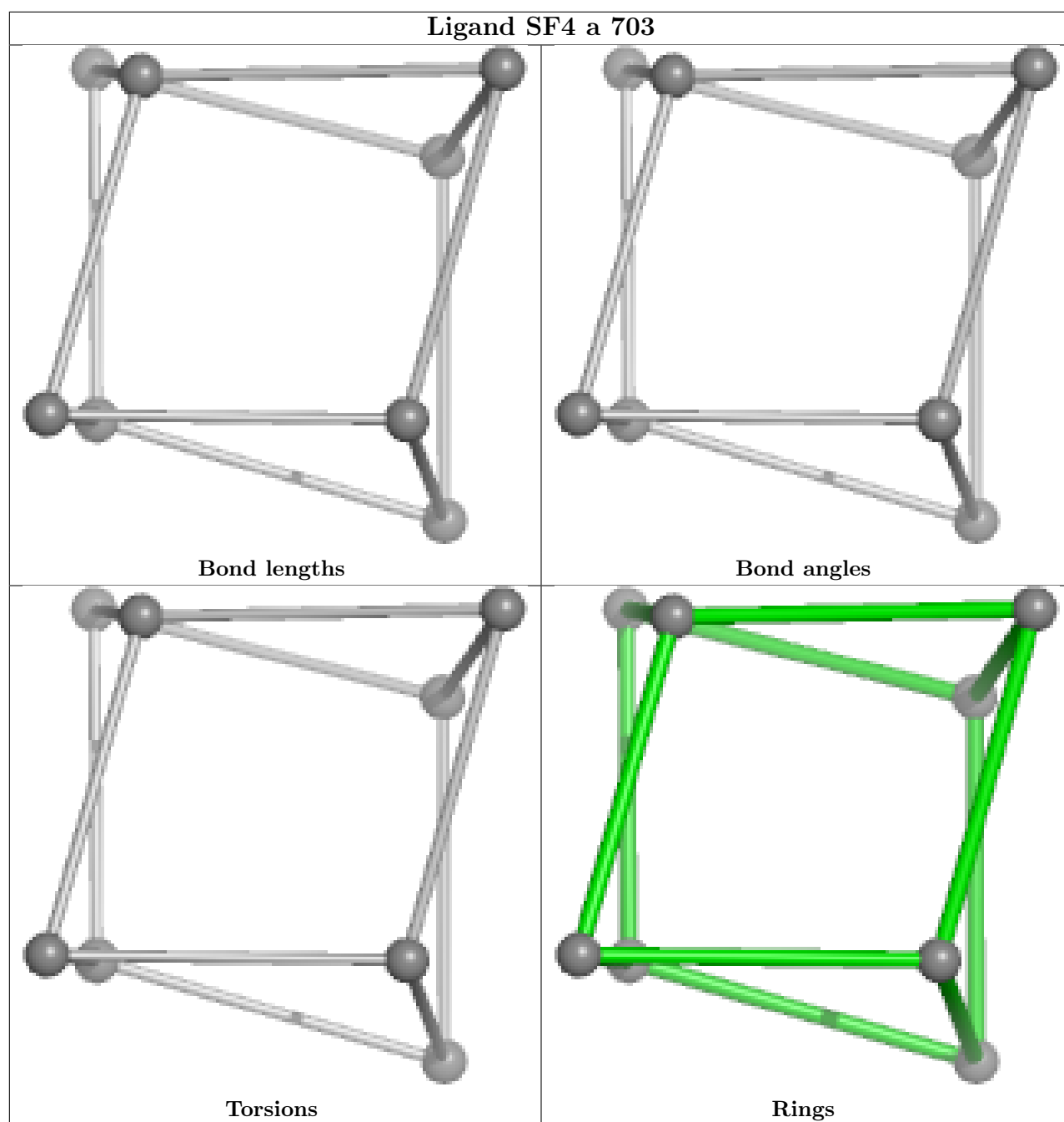












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

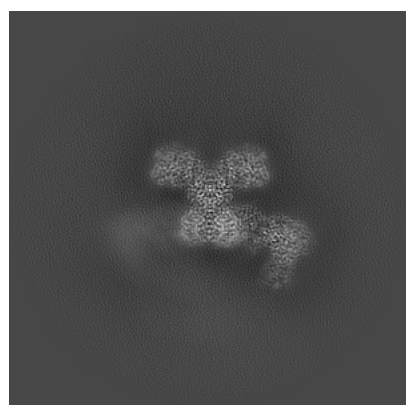
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19533. These allow visual inspection of the internal detail of the map and identification of artifacts.

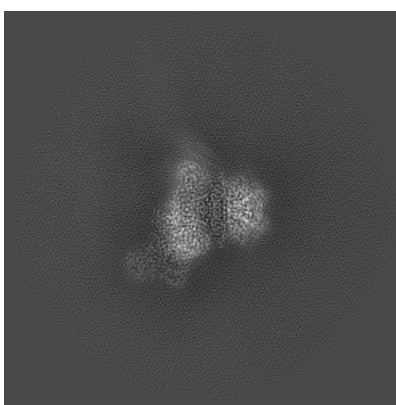
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

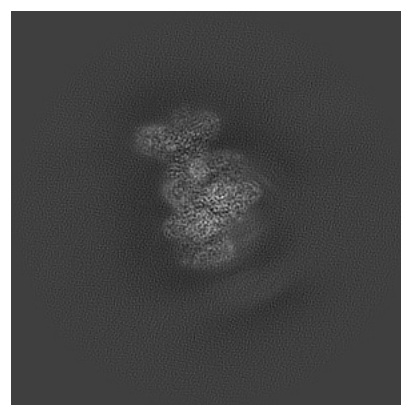
6.1.1 Primary map



X



Y

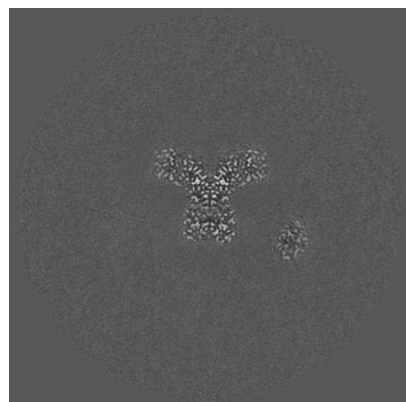


Z

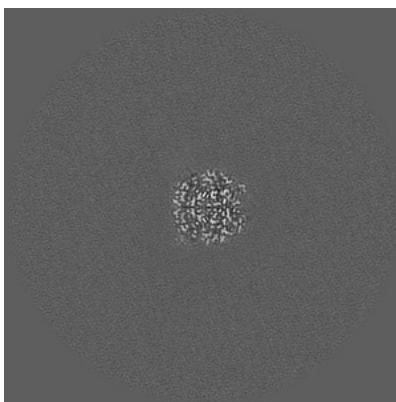
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

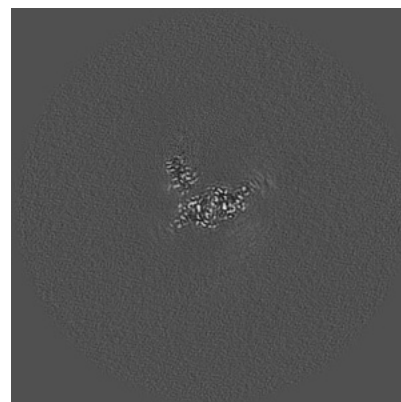
6.2.1 Primary map



X Index: 224



Y Index: 224

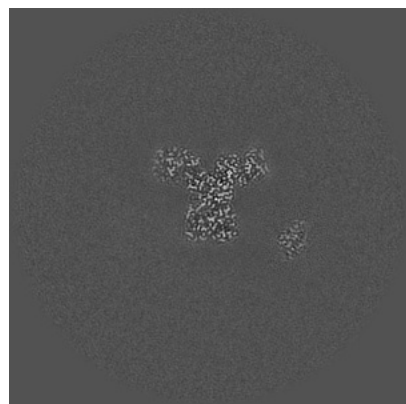


Z Index: 224

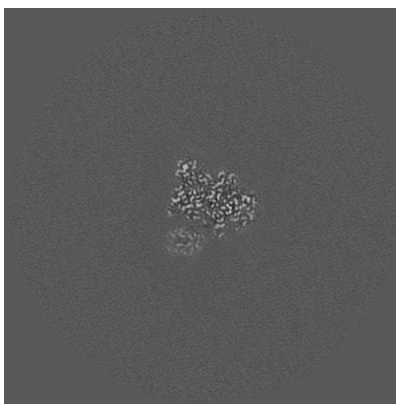
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

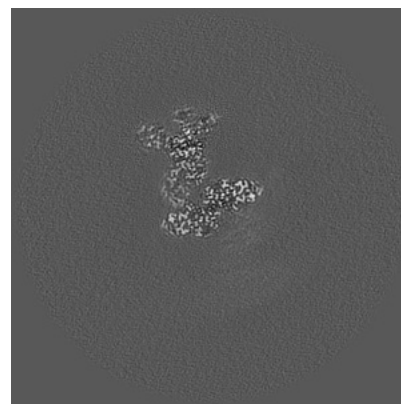
6.3.1 Primary map



X Index: 227



Y Index: 237

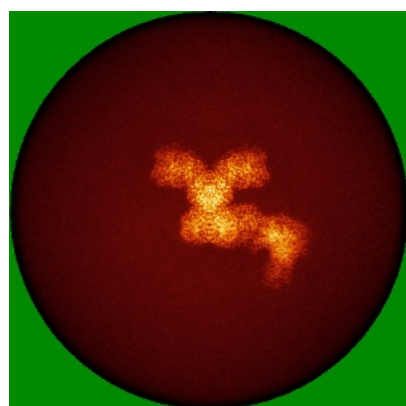


Z Index: 203

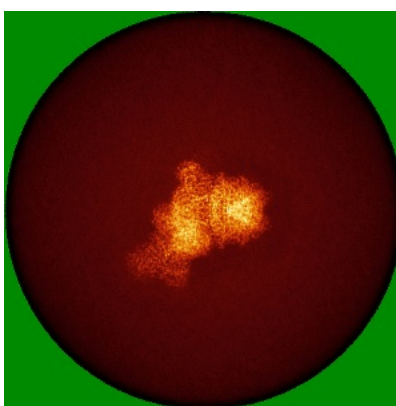
The images above show the largest variance slices of the map in three orthogonal directions.

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

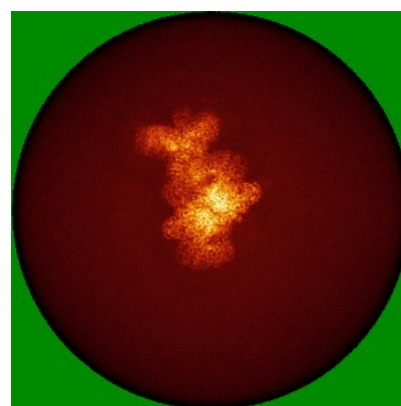
6.4.1 Primary map



X



Y

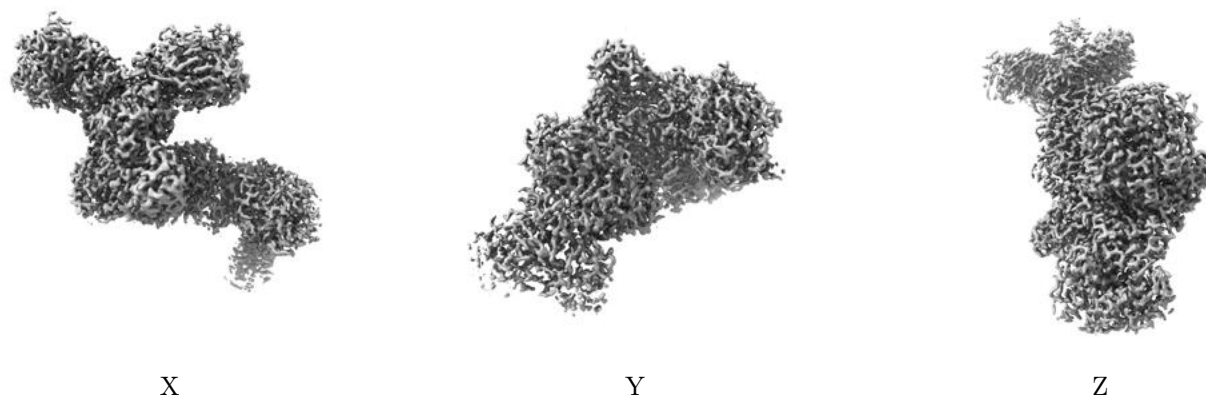


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 8.39. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

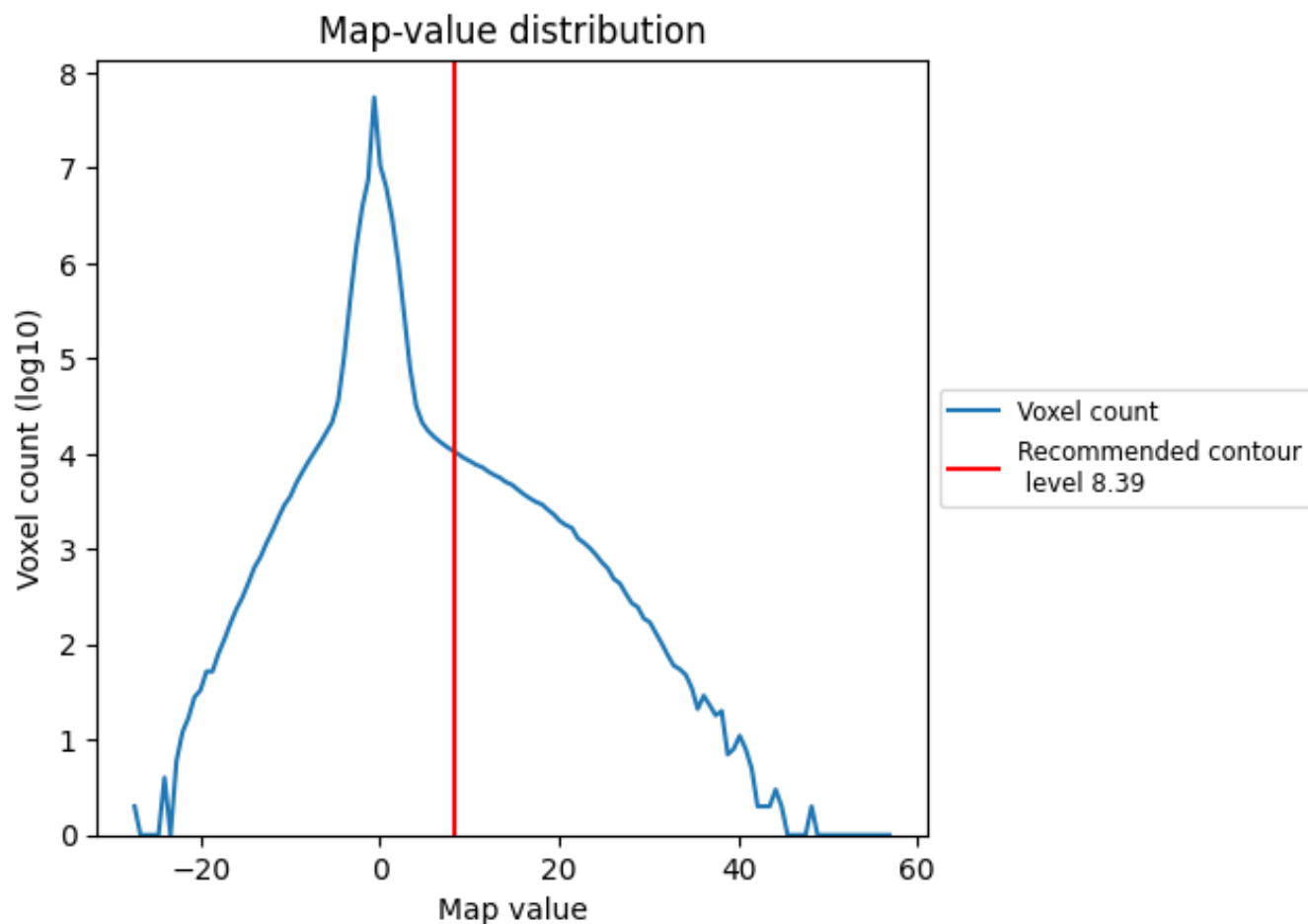
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

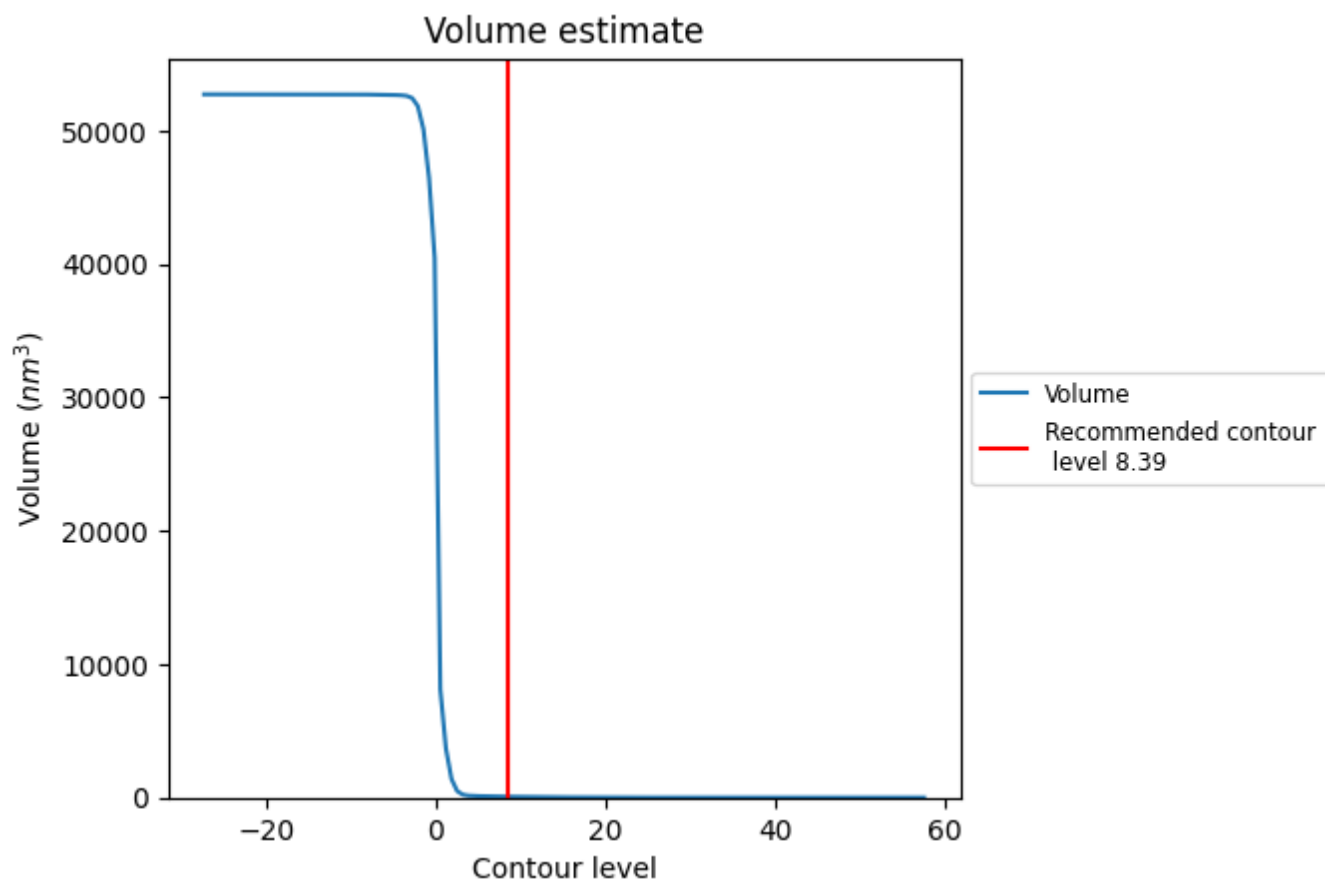
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

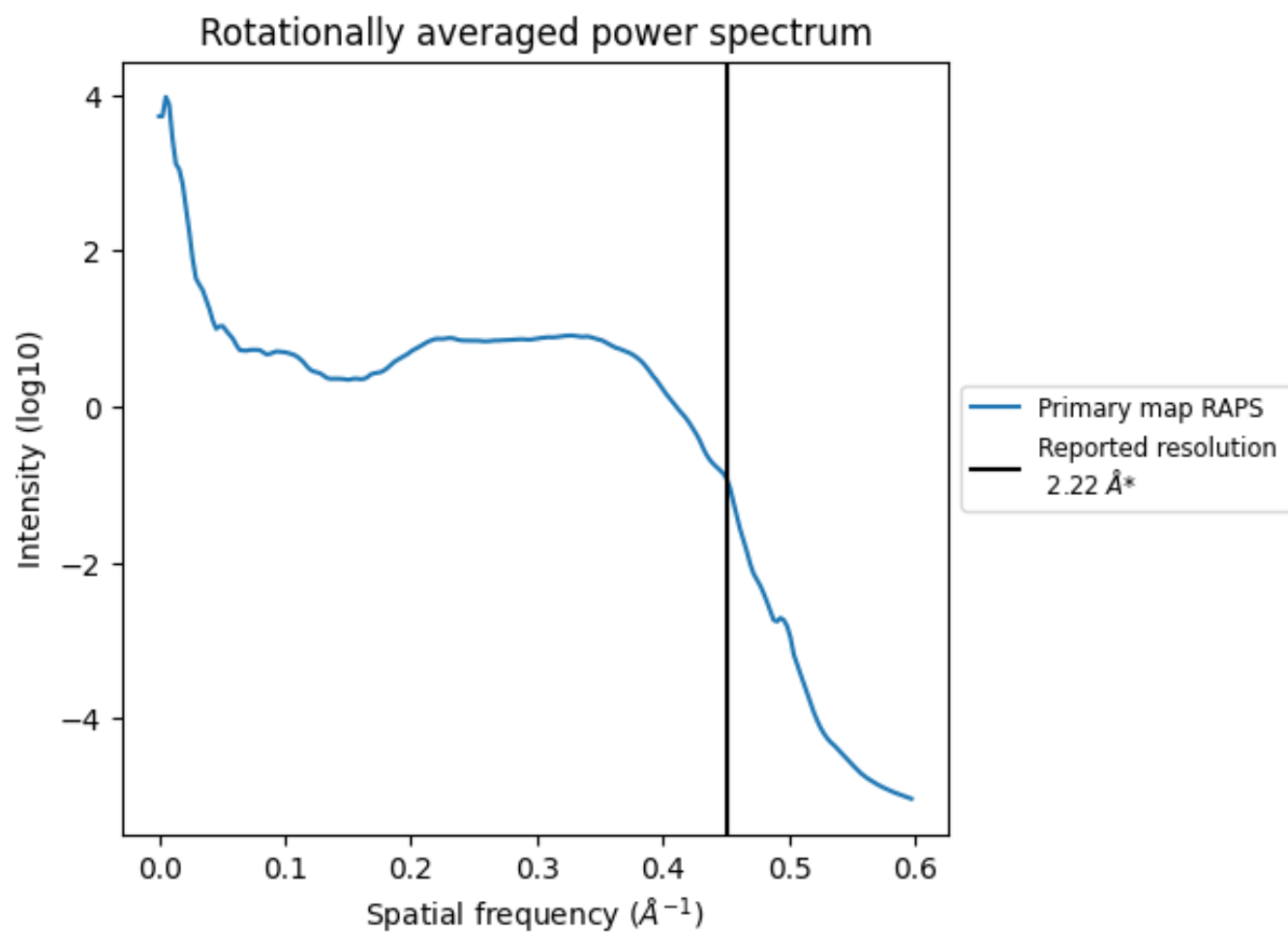
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 66 nm³; this corresponds to an approximate mass of 60 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 0.450 Å⁻¹

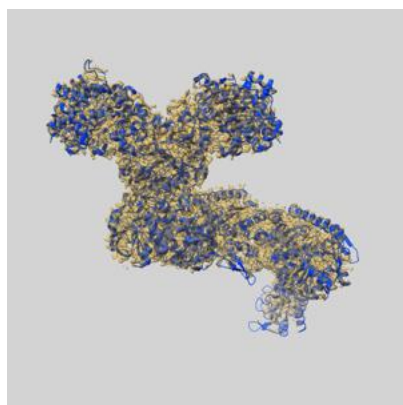
8 Fourier-Shell correlation ⓘ

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

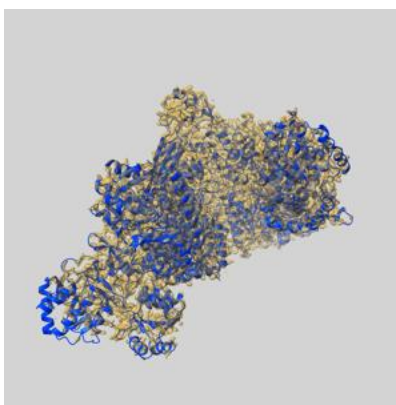
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-19533 and PDB model 8RVU. Per-residue inclusion information can be found in section 3 on page 10.

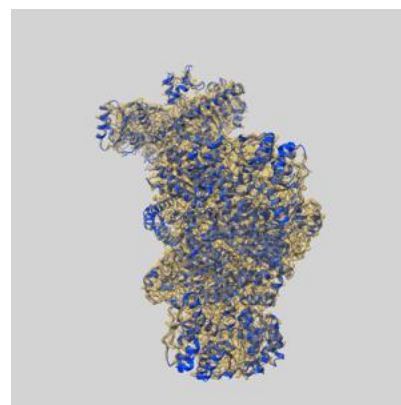
9.1 Map-model overlay [i](#)



X



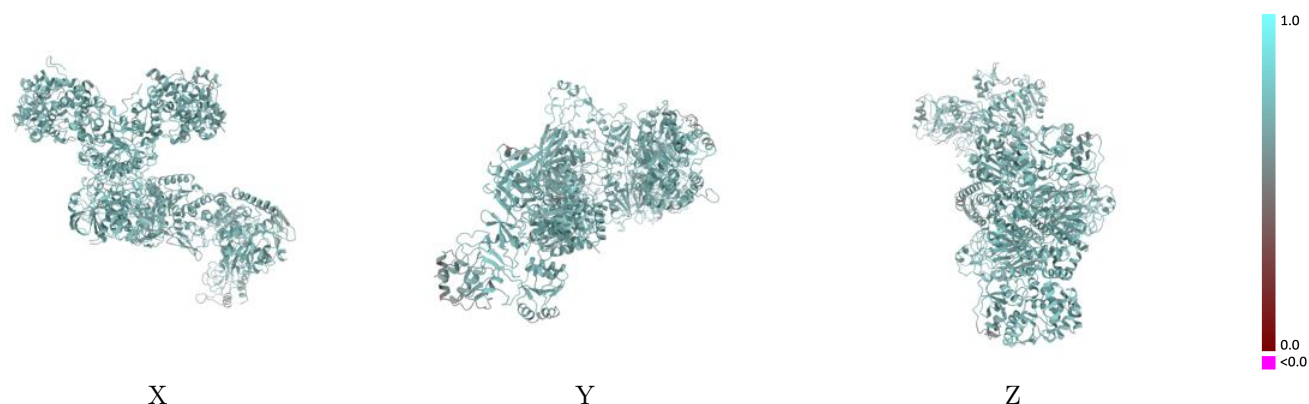
Y



Z

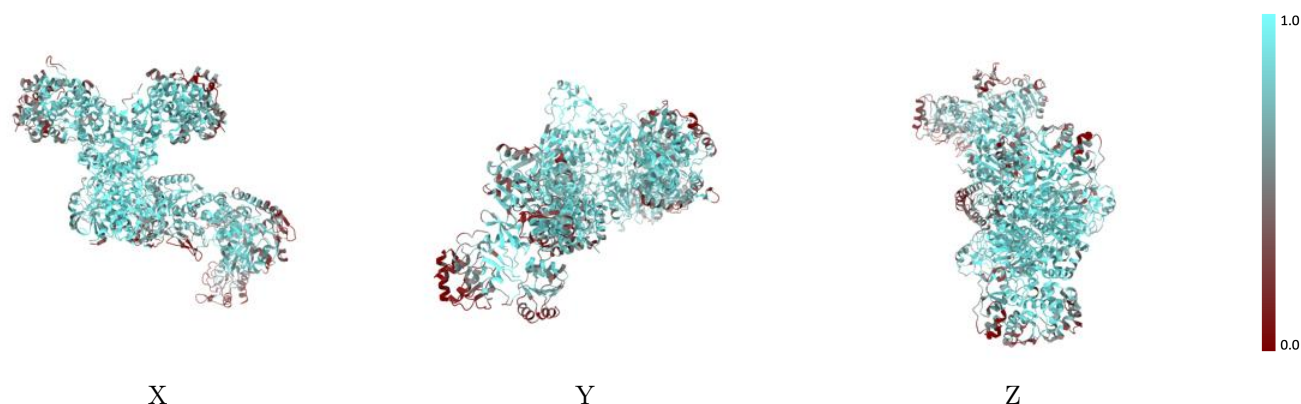
The images above show the 3D surface view of the map at the recommended contour level 8.39 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



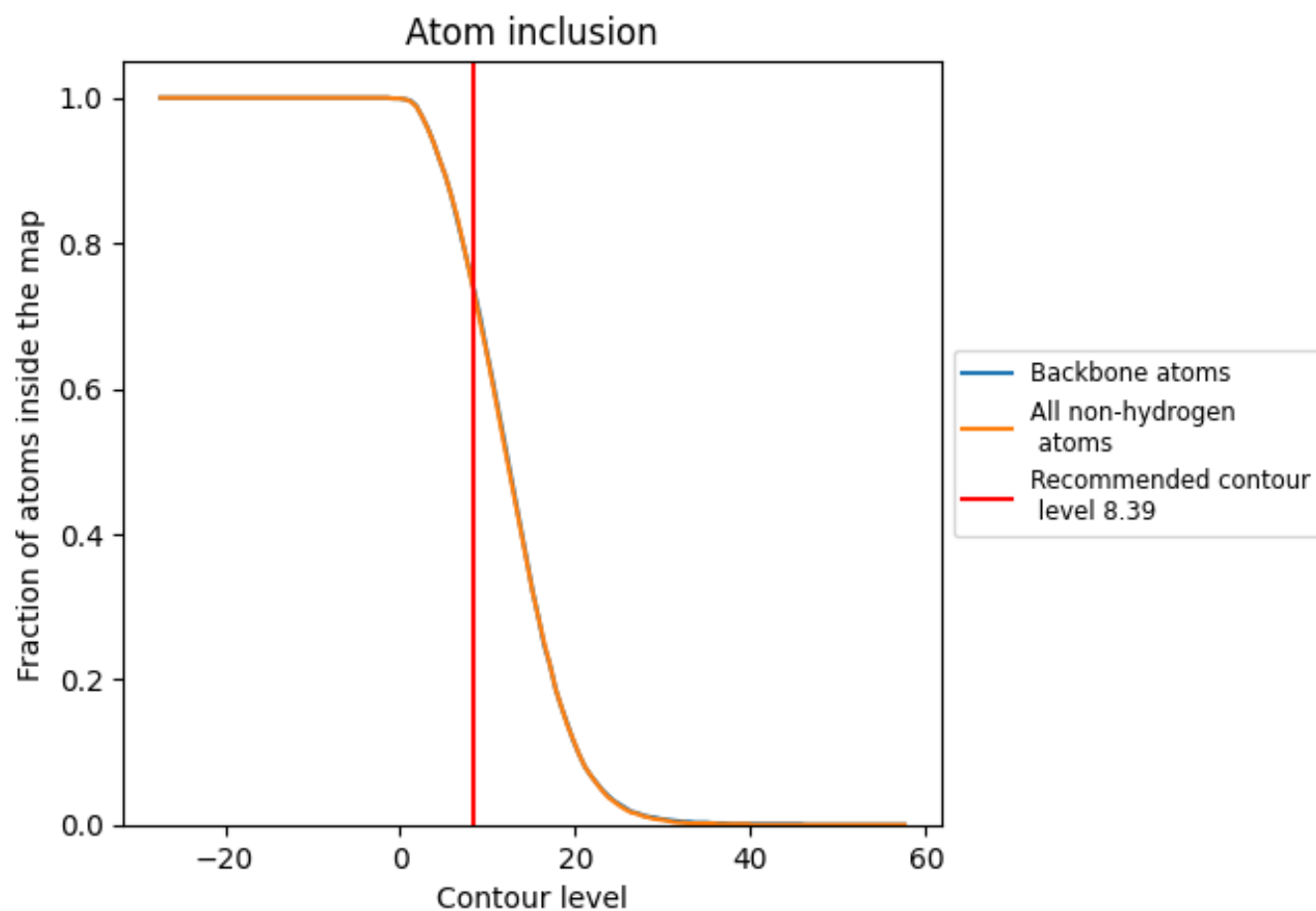
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (8.39).

9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 74% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (8.39) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7350	<div></div> 0.6760
A	<div></div> 0.7600	<div></div> 0.6740
B	<div></div> 0.6730	<div></div> 0.6780
C	<div></div> 0.7690	<div></div> 0.6910
D	<div></div> 0.5220	<div></div> 0.6340
E	<div></div> 0.6890	<div></div> 0.6700
F	<div></div> 0.8850	<div></div> 0.7030
a	<div></div> 0.8710	<div></div> 0.7020
b	<div></div> 0.7050	<div></div> 0.6660
c	<div></div> 0.7890	<div></div> 0.6810

1.0

0.0

<0.0