



Full wwPDB EM Validation Report ⓘ

Apr 20, 2026 – 07:54 pm BST

PDB ID : 9SW5 / pdb_00009sw5
EMDB ID : EMD-55298
Title : Structure of the MvhAGD-HdrABC dimer of *M. marburgensis* under state 1
substate b (composite structure)
Authors : San Segundo-Acosta, P.; Murphy, B.J.
Deposited on : 2025-10-04
Resolution : 3.29 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:

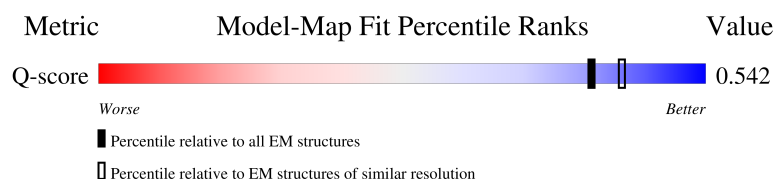
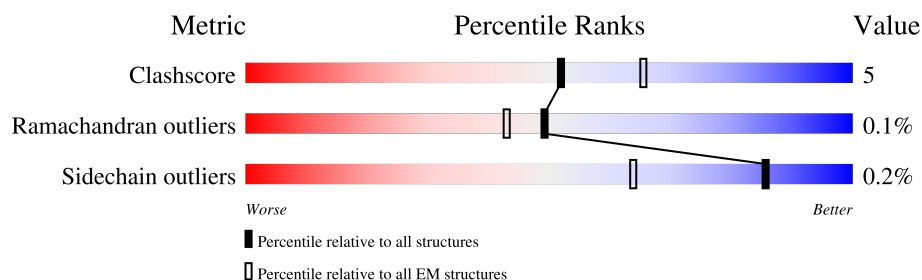
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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



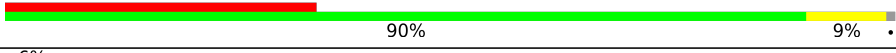

The reported resolution of this entry is 3.29 Å.

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





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14466 (2.79 - 3.79)

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	659	
2	B	302	
3	C	185	
4	F	472	

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Mol	Chain	Length	Quality of chain
5	E	308	
6	D	141	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	NFU	F	501	-	-	X	-

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 30901 atoms, of which 15231 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 H(2):CoB-CoM heterodisulfide,ferredoxin reductase subunit A.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	647	Total	C	H	N	O	S	0	0
			9812	3114	4872	822	956	48		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	291	Total	C	H	N	O	S	0	0
			4405	1422	2152	372	437	22		

- Molecule 3 is a protein called H(2):CoB-CoM heterodisulfide,ferredoxin reductase subunit C.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	184	Total	C	H	N	O	S	0	0
			2854	893	1432	253	265	11		

- Molecule 4 is a protein called F420-non-reducing hydrogenase subunit A.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	F	445	Total	C	H	N	O	S	0	0
			6934	2227	3430	600	659	18		

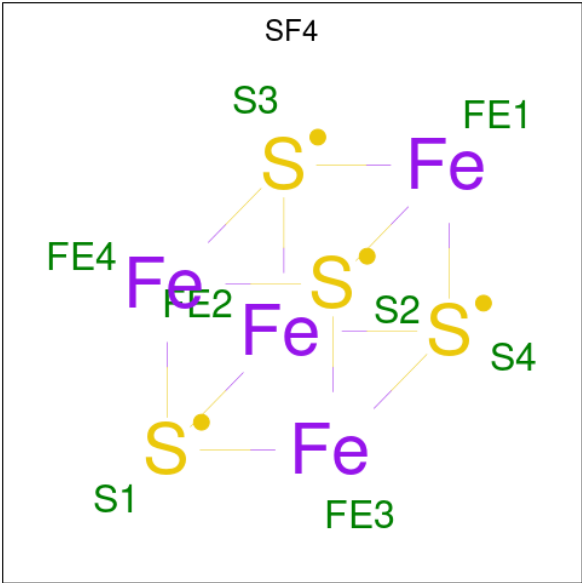
- Molecule 5 is a protein called F420-non-reducing hydrogenase subunit G.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	E	301	Total	C	H	N	O	S	0	0
			4555	1462	2250	365	458	20		

- Molecule 6 is a protein called F420-non-reducing hydrogenase iron-sulfur subunit D.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	D	136	Total	C	H	N	O	S	0	0
			2139	675	1063	198	191	12		

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



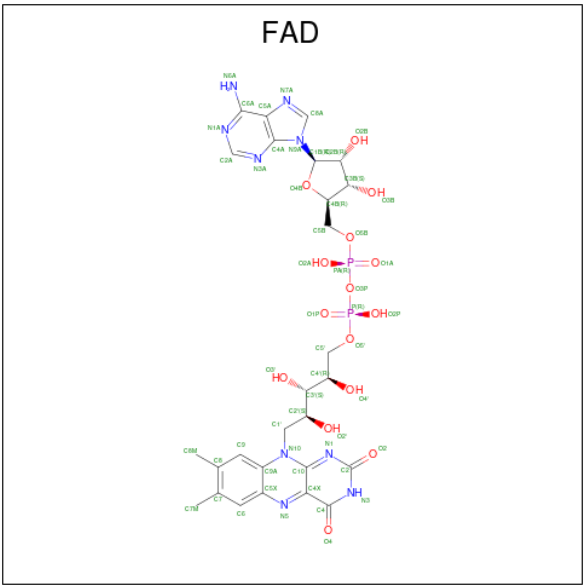
Mol	Chain	Residues	Atoms			AltConf
7	A	1	Total	Fe	S	0
			8	4	4	
7	A	1	Total	Fe	S	0
			8	4	4	
7	A	1	Total	Fe	S	0
			8	4	4	
7	A	1	Total	Fe	S	0
			8	4	4	
7	A	1	Total	Fe	S	0
			8	4	4	
7	A	1	Total	Fe	S	0
			8	4	4	
7	C	1	Total	Fe	S	0
			8	4	4	
7	C	1	Total	Fe	S	0
			8	4	4	
7	E	1	Total	Fe	S	0
			8	4	4	
7	E	1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

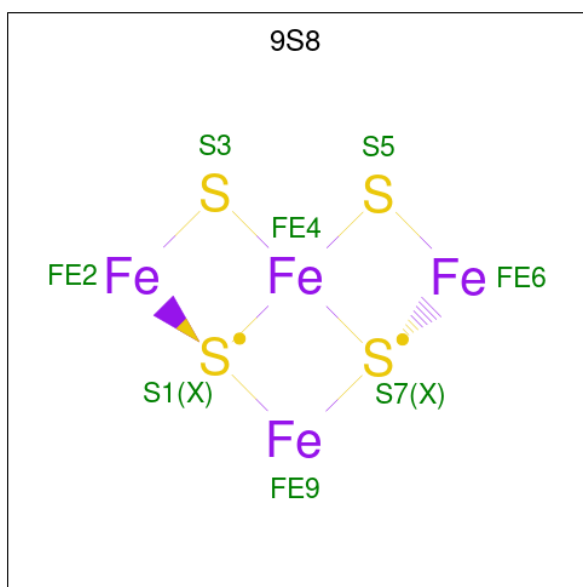
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Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
7	E	1	8	4	4	0

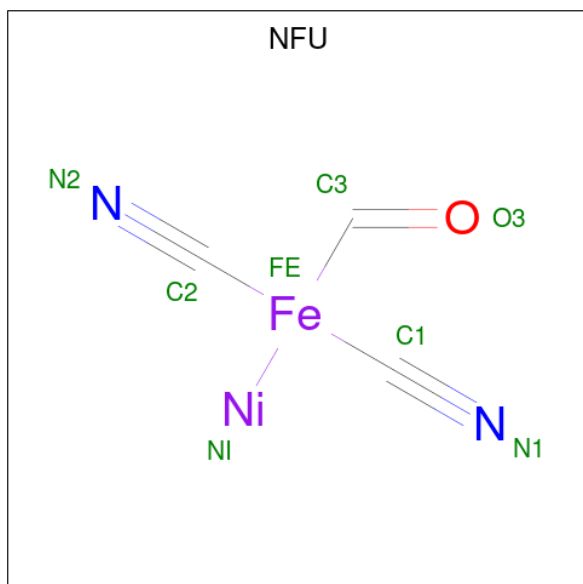
- Molecule 8 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂) (labeled as "Ligand of Interest" by depositor).





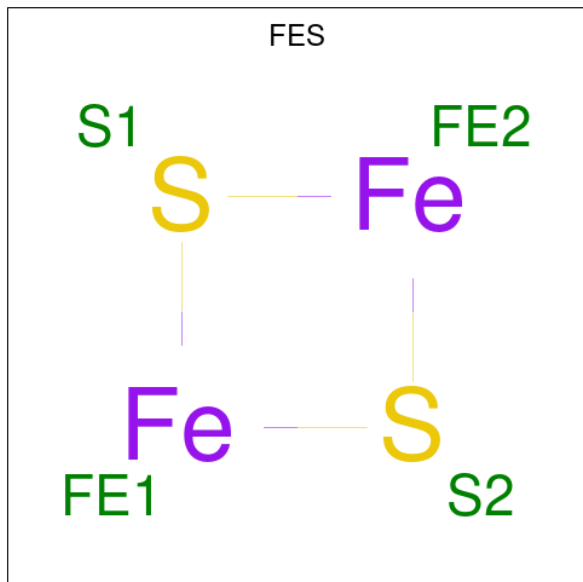
Mol	Chain	Residues	Atoms			AltConf
9	B	1	Total	Fe	S	0
			8	4	4	
9	B	1	Total	Fe	S	0
			8	4	4	

- Molecule 10 is formyl[bis(hydrocyanato-1kappaC)]ironnickel(Fe-Ni) (CCD ID: NFU) (formula: $\text{C}_3\text{HFeN}_2\text{NiO}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms							AltConf
10	F	1	Total	C	Fe	H	N	Ni	O	0
			9	3	1	1	2	1	1	

- Molecule 11 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
11	D	1	Total	Fe	S	0
			4	2	2	

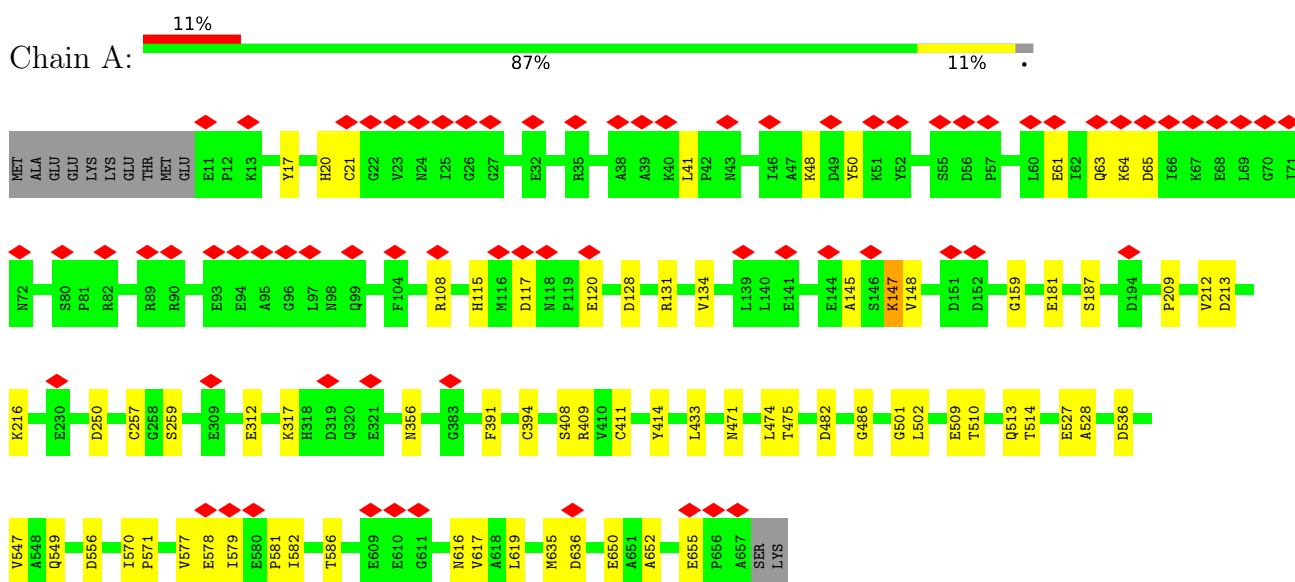
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		AltConf
12	F	1	Total	O	0
			1	1	

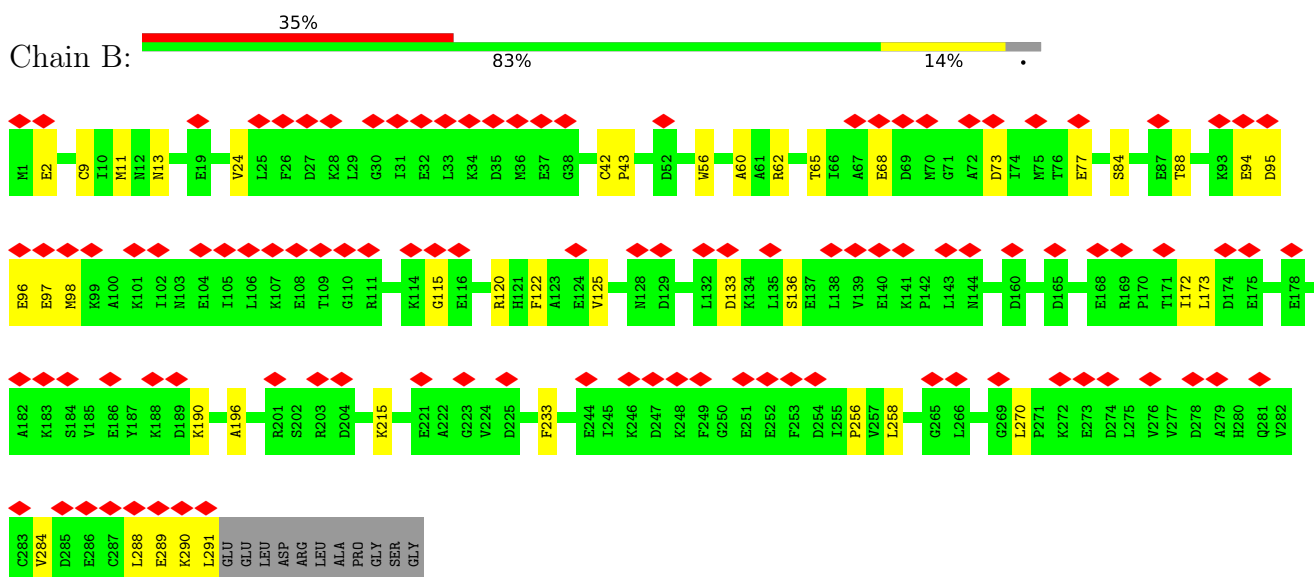
3 Residue-property plots

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

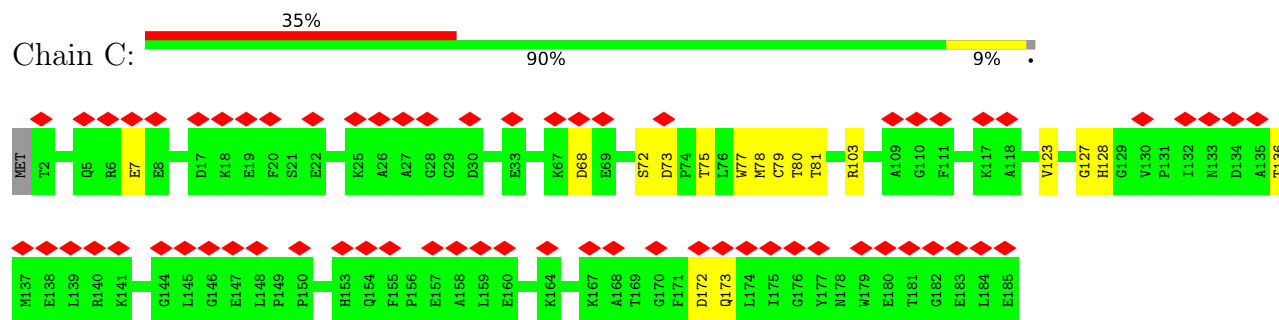
- Molecule 1: H(2):CoB-CoM heterodisulfide,ferredoxin reductase subunit A



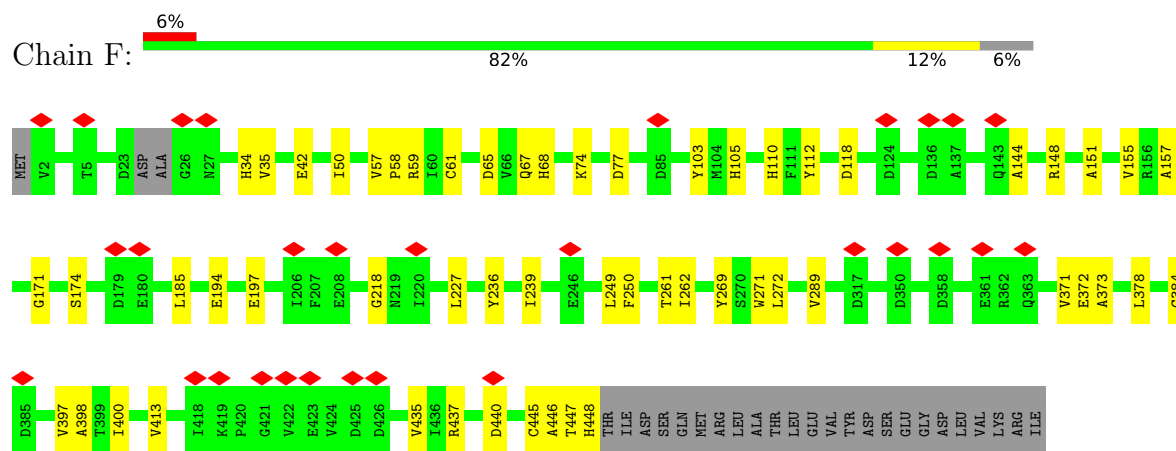
- Molecule 2: H(2):CoB-CoM heterodisulfide,ferredoxin reductase subunit B



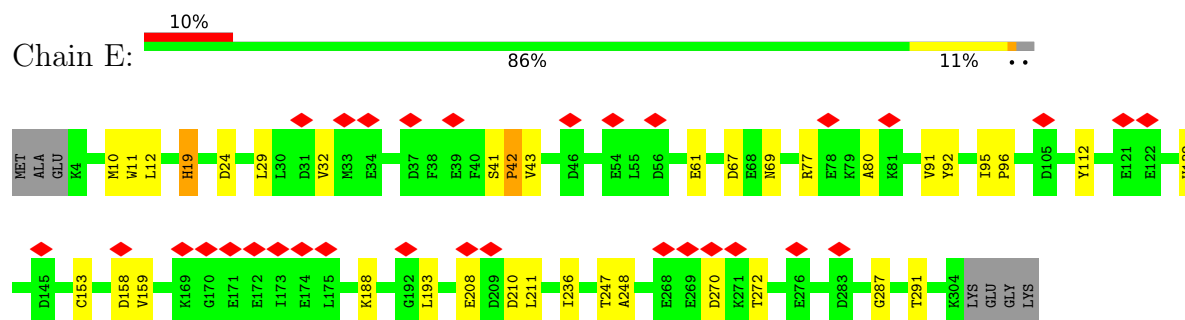
- Molecule 3: H(2):CoB-CoM heterodisulfide,ferredoxin reductase subunit C



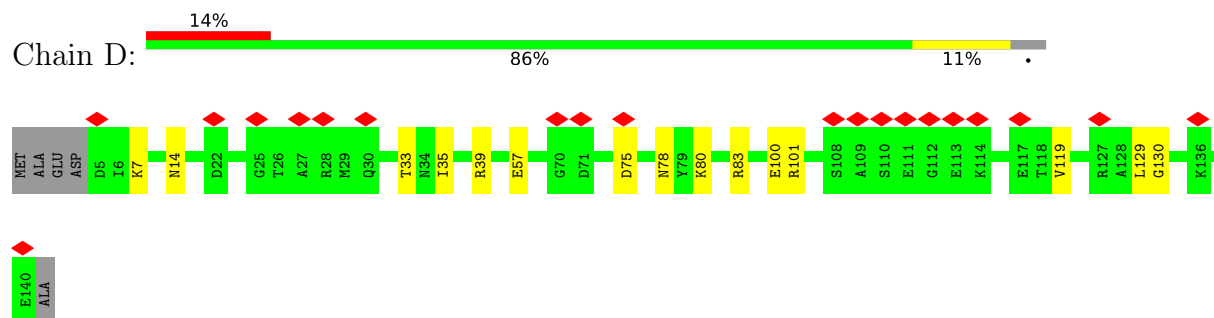
- Molecule 4: F420-non-reducing hydrogenase subunit A



- Molecule 5: F420-non-reducing hydrogenase subunit G



- Molecule 6: F420-non-reducing hydrogenase iron-sulfur subunit D



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	17398	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)	700	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	43.899	Depositor
Minimum map value	-14.687	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.917	Depositor
Recommended contour level	6.07	Depositor
Map size (Å)	401.1, 401.1, 401.1	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.835625, 0.835625, 0.835625	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.17	0/5030	0.32	1/6808 (0.0%)
2	B	0.11	0/2290	0.28	0/3089
3	C	0.09	0/1447	0.21	0/1951
4	F	0.19	1/3583 (0.0%)	0.32	0/4859
5	E	0.63	4/2352 (0.2%)	0.69	5/3195 (0.2%)
6	D	0.11	0/1098	0.31	0/1474
All	All	0.28	5/15800 (0.0%)	0.39	6/21376 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	42	PRO	CB-CG	20.92	2.54	1.49
5	E	42	PRO	CG-CD	-18.77	0.86	1.50
5	E	42	PRO	CA-CB	-6.57	1.45	1.54
5	E	42	PRO	N-CD	6.22	1.56	1.47
4	F	218	GLY	C-O	-6.02	1.17	1.24

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	42	PRO	CB-CG-CD	-27.71	17.43	106.10
5	E	42	PRO	N-CA-CB	-11.91	88.66	102.60
5	E	42	PRO	N-CD-CG	-10.43	87.55	103.20
5	E	42	PRO	CA-CB-CG	-8.37	88.60	104.50
5	E	42	PRO	CA-N-CD	-7.21	101.91	112.00
1	A	582	ILE	N-CA-C	-5.54	97.83	109.34

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4940	4872	4895	45	0
2	B	2253	2152	2217	28	0
3	C	1422	1432	1431	12	0
4	F	3504	3430	3443	43	0
5	E	2305	2250	2258	36	0
6	D	1076	1063	1062	13	0
7	A	48	0	0	1	0
7	C	16	0	0	0	0
7	E	24	0	0	0	0
8	A	53	31	31	0	0
9	B	16	0	0	0	0
10	F	8	1	0	3	0
11	D	4	0	0	0	0
12	F	1	0	0	1	0
All	All	15670	15231	15337	166	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (166) 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)
5:E:42:PRO:CG	5:E:42:PRO:N	1.75	1.42
5:E:42:PRO:CD	5:E:42:PRO:HG3	1.64	1.12
5:E:42:PRO:CG	5:E:42:PRO:HD2	1.55	1.06
5:E:42:PRO:CD	5:E:42:PRO:HG2	1.64	1.06
5:E:42:PRO:CG	5:E:42:PRO:HD3	1.55	1.04
5:E:41:SER:CA	5:E:42:PRO:HG2	1.93	0.99
5:E:41:SER:HA	5:E:42:PRO:HG2	1.43	0.98
4:F:372:GLU:N	4:F:372:GLU:OE1	2.04	0.91
5:E:42:PRO:CG	5:E:42:PRO:CD	0.86	0.86
5:E:42:PRO:CG	5:E:42:PRO:CB	2.54	0.85
4:F:227:LEU:HD22	4:F:372:GLU:OE2	1.79	0.83
5:E:41:SER:C	5:E:42:PRO:HG2	2.04	0.83
5:E:41:SER:C	5:E:42:PRO:CG	2.54	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:445:CYS:SG	10:F:501:NFU:O3	2.37	0.80
1:A:17:TYR:OH	1:A:65:ASP:OD2	2.01	0.79
1:A:586:THR:OG1	1:A:635:MET:SD	2.40	0.78
3:C:68:ASP:O	3:C:72:SER:OG	2.02	0.76
4:F:77:ASP:OD1	4:F:171:GLY:N	2.20	0.74
4:F:151:ALA:O	4:F:155:VAL:HG23	1.88	0.74
2:B:77:GLU:OE1	2:B:77:GLU:N	2.22	0.72
4:F:42:GLU:OE2	12:F:601:HOH:O	2.07	0.72
1:A:652:ALA:O	6:D:7:LYS:NZ	2.22	0.72
3:C:73:ASP:OD2	3:C:75:THR:OG1	2.07	0.72
1:A:145:ALA:HB2	1:A:581:PRO:HD3	1.71	0.71
1:A:471:ASN:ND2	1:A:475:THR:O	2.23	0.71
6:D:100:GLU:OE1	6:D:100:GLU:N	2.23	0.71
5:E:270:ASP:OD2	6:D:80:LYS:NZ	2.24	0.70
5:E:12:LEU:O	5:E:69:ASN:ND2	2.24	0.70
1:A:409:ARG:NH2	1:A:556:ASP:OD2	2.25	0.69
6:D:100:GLU:HG2	6:D:129:LEU:HD21	1.75	0.69
2:B:24:VAL:HG11	2:B:270:LEU:HD21	1.73	0.68
2:B:2:GLU:OE1	2:B:2:GLU:N	2.28	0.66
2:B:97:GLU:OE1	2:B:97:GLU:N	2.28	0.66
5:E:19:HIS:ND1	5:E:61:GLU:OE1	2.29	0.66
1:A:48:LYS:NZ	1:A:61:GLU:OE2	2.19	0.66
1:A:527:GLU:OE1	1:A:549:GLN:NE2	2.29	0.65
2:B:13:ASN:C	3:C:136:THR:HG21	2.23	0.64
1:A:145:ALA:HB1	1:A:579:ILE:O	1.98	0.63
4:F:68:HIS:NE2	10:F:501:NFU:O3	2.31	0.63
1:A:655:GLU:N	1:A:655:GLU:OE1	2.33	0.62
1:A:63:GLN:OE1	1:A:64:LYS:N	2.34	0.61
1:A:41:LEU:HD13	1:A:134:VAL:HG11	1.81	0.61
4:F:397:VAL:HG11	4:F:445:CYS:HB3	1.83	0.60
2:B:60:ALA:HB3	2:B:88:THR:HG21	1.82	0.60
1:A:394:CYS:N	7:A:706:SF4:S4	2.75	0.59
4:F:50:ILE:HD12	4:F:384:CYS:HB3	1.85	0.59
1:A:312:GLU:N	1:A:312:GLU:OE1	2.37	0.58
5:E:287:GLY:O	5:E:291:THR:OG1	2.22	0.58
1:A:250:ASP:OD2	1:A:317:LYS:NZ	2.30	0.57
4:F:413:VAL:HG21	4:F:435:VAL:HG21	1.86	0.57
4:F:118:ASP:OD2	4:F:437:ARG:NH1	2.38	0.57
2:B:284:VAL:O	2:B:288:LEU:HG	2.04	0.56
4:F:397:VAL:HG12	4:F:398:ALA:H	1.71	0.56
4:F:397:VAL:O	4:F:400:ILE:HG22	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:110:HIS:ND1	4:F:440:ASP:OD1	2.39	0.56
2:B:190:LYS:O	2:B:215:LYS:NZ	2.38	0.55
3:C:79:CYS:O	3:C:103:ARG:NH2	2.40	0.55
4:F:174:SER:OG	5:E:236:ILE:O	2.24	0.55
4:F:34:HIS:ND1	4:F:269:TYR:O	2.39	0.55
5:E:210:ASP:O	5:E:211:LEU:HD12	2.07	0.55
2:B:290:LYS:O	2:B:290:LYS:HG2	2.07	0.55
6:D:75:ASP:N	6:D:75:ASP:OD1	2.39	0.54
4:F:61:CYS:CB	4:F:445:CYS:SG	2.96	0.53
5:E:41:SER:HA	5:E:42:PRO:CG	2.28	0.53
6:D:100:GLU:CG	6:D:129:LEU:HD21	2.38	0.53
2:B:95:ASP:OD1	2:B:98:MET:N	2.41	0.53
4:F:372:GLU:N	4:F:372:GLU:CD	2.66	0.53
5:E:270:ASP:OD1	6:D:83:ARG:NH1	2.40	0.52
3:C:172:ASP:OD1	3:C:173:GLN:N	2.42	0.52
2:B:13:ASN:O	3:C:136:THR:HG21	2.09	0.52
5:E:208:GLU:OE1	5:E:208:GLU:N	2.43	0.52
4:F:227:LEU:HB2	4:F:372:GLU:OE2	2.09	0.51
5:E:91:VAL:HG23	5:E:92:TYR:CD2	2.46	0.50
1:A:21:CYS:SG	1:A:108:ARG:NH1	2.82	0.50
4:F:42:GLU:OE2	4:F:448:HIS:HE1	1.93	0.50
4:F:271:TRP:O	5:E:112:TYR:OH	2.22	0.50
4:F:148:ARG:NH2	5:E:24:ASP:OD1	2.45	0.49
1:A:148:VAL:HG22	1:A:577:VAL:HB	1.94	0.49
1:A:636:ASP:N	1:A:636:ASP:OD1	2.44	0.49
5:E:77:ARG:NH2	5:E:80:ALA:O	2.46	0.49
2:B:133:ASP:O	2:B:136:SER:OG	2.27	0.49
1:A:120:GLU:HA	1:A:120:GLU:OE1	2.12	0.49
1:A:145:ALA:HB3	1:A:578:GLU:OE2	2.12	0.49
1:A:528:ALA:N	1:A:536:ASP:O	2.41	0.49
1:A:482:ASP:O	1:A:486:GLY:N	2.45	0.49
6:D:14:ASN:OD1	6:D:39:ARG:NH1	2.38	0.49
1:A:257:CYS:SG	1:A:259:SER:OG	2.66	0.49
2:B:256:PRO:HB3	2:B:284:VAL:HG22	1.95	0.49
4:F:445:CYS:CB	10:F:501:NFU:C2	2.90	0.49
6:D:101:ARG:NH2	6:D:130:GLY:O	2.46	0.49
2:B:96:GLU:OE1	2:B:96:GLU:N	2.46	0.48
5:E:95:ILE:N	5:E:96:PRO:CD	2.77	0.48
4:F:57:VAL:N	4:F:58:PRO:CD	2.77	0.47
2:B:68:GLU:OE2	2:B:115:GLY:N	2.47	0.47
2:B:42:CYS:N	2:B:43:PRO:HA	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:HIS:HD1	1:A:50:TYR:C	2.23	0.47
5:E:95:ILE:HG22	5:E:96:PRO:HD3	1.95	0.47
3:C:78:MET:HE2	3:C:78:MET:HA	1.95	0.47
4:F:397:VAL:HG12	4:F:398:ALA:N	2.30	0.47
2:B:258:LEU:HD21	2:B:284:VAL:HG11	1.97	0.46
1:A:147:LYS:HD2	1:A:578:GLU:OE1	2.15	0.46
1:A:356:ASN:ND2	1:A:474:LEU:O	2.48	0.46
1:A:411:CYS:HA	1:A:414:TYR:CE2	2.49	0.46
4:F:103:TYR:OH	4:F:372:GLU:O	2.26	0.46
4:F:194:GLU:O	4:F:197:GLU:HG2	2.16	0.46
1:A:128:ASP:OD1	1:A:131:ARG:NH2	2.49	0.46
1:A:547:VAL:HG12	1:A:547:VAL:O	2.15	0.46
2:B:11:MET:HE1	2:B:77:GLU:OE2	2.16	0.46
3:C:7:GLU:N	3:C:7:GLU:OE1	2.49	0.46
4:F:289:VAL:O	4:F:289:VAL:HG23	2.16	0.46
4:F:447:THR:O	4:F:448:HIS:C	2.59	0.45
5:E:10:MET:SD	5:E:11:TRP:O	2.75	0.45
2:B:9:CYS:SG	3:C:128:HIS:ND1	2.85	0.45
3:C:80:THR:O	3:C:81:THR:OG1	2.30	0.45
4:F:157:ALA:CB	4:F:185:LEU:HD11	2.47	0.45
6:D:78:ASN:OD1	6:D:78:ASN:N	2.42	0.45
4:F:112:TYR:CG	4:F:144:ALA:HB2	2.51	0.45
6:D:57:GLU:HA	6:D:57:GLU:OE1	2.16	0.44
1:A:145:ALA:CB	1:A:578:GLU:OE2	2.65	0.44
4:F:67:GLN:HG2	4:F:373:ALA:HA	1.99	0.44
2:B:120:ARG:HH21	2:B:125:VAL:HG22	1.83	0.44
4:F:74:LYS:NZ	4:F:236:TYR:O	2.42	0.44
4:F:157:ALA:HB3	4:F:185:LEU:HD11	1.98	0.44
4:F:35:VAL:HG21	4:F:272:LEU:HB2	1.99	0.44
2:B:56:TRP:NE1	2:B:84:SER:OG	2.46	0.44
3:C:77:TRP:C	3:C:78:MET:HE2	2.43	0.44
1:A:408:SER:HB2	1:A:411:CYS:SG	2.58	0.43
4:F:272:LEU:CD1	4:F:446:ALA:HB1	2.48	0.43
5:E:247:THR:HG22	5:E:248:ALA:N	2.33	0.43
1:A:501:GLY:C	1:A:502:LEU:HD12	2.44	0.43
5:E:188:LYS:HE2	5:E:193:LEU:HD13	2.00	0.43
5:E:158:ASP:OD1	5:E:159:VAL:N	2.50	0.43
1:A:209:PRO:O	1:A:213:ASP:OD2	2.36	0.43
4:F:261:THR:C	4:F:262:ILE:HD12	2.43	0.43
4:F:397:VAL:HG21	4:F:445:CYS:O	2.18	0.43
4:F:249:LEU:HD23	4:F:250:PHE:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:196:ALA:HB1	2:B:233:PHE:CD1	2.53	0.42
5:E:43:VAL:HG22	5:E:43:VAL:O	2.18	0.42
1:A:115:HIS:CG	6:D:33:THR:HG22	2.54	0.42
4:F:59:ARG:NH1	5:E:153:CYS:SG	2.92	0.42
1:A:570:ILE:HB	1:A:571:PRO:HD3	2.01	0.42
2:B:94:GLU:HA	2:B:94:GLU:OE1	2.19	0.42
6:D:35:ILE:HG21	6:D:119:VAL:HG13	2.00	0.42
5:E:29:LEU:O	5:E:32:VAL:HG22	2.19	0.42
1:A:616:ASN:ND2	1:A:619:LEU:HD12	2.35	0.42
1:A:159:GLY:N	1:A:181:GLU:OE1	2.52	0.42
2:B:172:ILE:HG23	2:B:173:LEU:N	2.35	0.42
4:F:65:ASP:N	4:F:65:ASP:OD1	2.52	0.42
4:F:371:VAL:O	4:F:378:LEU:HB3	2.20	0.42
2:B:73:ASP:OD1	2:B:73:ASP:N	2.53	0.42
1:A:579:ILE:HD13	1:A:617:VAL:HG12	2.02	0.42
2:B:77:GLU:HB3	2:B:122:PHE:CB	2.50	0.42
1:A:578:GLU:OE1	1:A:578:GLU:HA	2.20	0.41
1:A:650:GLU:OE2	1:A:650:GLU:C	2.64	0.41
3:C:123:VAL:O	3:C:127:GLY:N	2.44	0.41
5:E:67:ASP:OD1	5:E:132:HIS:N	2.52	0.41
5:E:272:THR:O	5:E:272:THR:HG22	2.20	0.41
5:E:41:SER:CA	5:E:42:PRO:CG	2.78	0.41
1:A:117:ASP:OD1	1:A:117:ASP:N	2.53	0.40
1:A:212:VAL:HG12	1:A:216:LYS:HE3	2.03	0.40
1:A:391:PHE:HB2	1:A:433:LEU:HD22	2.02	0.40
1:A:510:THR:O	1:A:514:THR:HG23	2.20	0.40
4:F:239:ILE:O	4:F:239:ILE:HG13	2.21	0.40
1:A:509:GLU:O	1:A:513:GLN:OE1	2.40	0.40
2:B:62:ARG:O	2:B:65:THR:OG1	2.32	0.40
2:B:289:GLU:O	2:B:291:LEU:HG	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	645/659 (98%)	630 (98%)	14 (2%)	1 (0%)	43	71
2	B	289/302 (96%)	279 (96%)	10 (4%)	0	100	100
3	C	182/185 (98%)	180 (99%)	2 (1%)	0	100	100
4	F	441/472 (93%)	425 (96%)	16 (4%)	0	100	100
5	E	299/308 (97%)	290 (97%)	9 (3%)	0	100	100
6	D	134/141 (95%)	134 (100%)	0	0	100	100
All	All	1990/2067 (96%)	1938 (97%)	51 (3%)	1 (0%)	49	75

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	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	A	536/547 (98%)	535 (100%)	1 (0%)	87	88
2	B	246/255 (96%)	246 (100%)	0	100	100
3	C	153/155 (99%)	153 (100%)	0	100	100
4	F	372/396 (94%)	371 (100%)	1 (0%)	86	86
5	E	257/262 (98%)	256 (100%)	1 (0%)	84	84
6	D	112/115 (97%)	112 (100%)	0	100	100
All	All	1676/1730 (97%)	1673 (100%)	3 (0%)	85	88

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	147	LYS

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Mol	Chain	Res	Type
4	F	105	HIS
5	E	19	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	ASN
1	A	471	ASN
1	A	612	HIS
2	B	163	ASN
4	F	448	HIS
6	D	34	ASN
6	D	69	HIS

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](#)

16 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	1	0,12,12	-	-	-		
7	SF4	A	702	1	0,12,12	-	-	-		
10	NFU	F	501	4	2,7,7	0.16	0	-		
9	9S8	B	402	2	2,10,10	1.00	0	-		
7	SF4	E	403	5	0,12,12	-	-	-		
7	SF4	A	701	1	0,12,12	-	-	-		
7	SF4	E	401	5	0,12,12	-	-	-		
9	9S8	B	401	2	2,10,10	1.01	0	-		
7	SF4	A	707	1	0,12,12	-	-	-		
7	SF4	E	402	5	0,12,12	-	-	-		
8	FAD	A	704	-	56,58,58	0.65	1 (1%)	81,89,89	0.83	2 (2%)
7	SF4	A	705	1	0,12,12	-	-	-		
7	SF4	A	703	1	0,12,12	-	-	-		
7	SF4	C	202	3	0,12,12	-	-	-		
11	FES	D	201	6	0,4,4	-	-	-		
7	SF4	C	201	3	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	1	-	-	0/6/5/5
7	SF4	A	702	1	-	-	0/6/5/5
9	9S8	B	402	2	-	-	0/3/3/3
7	SF4	E	403	5	-	-	0/6/5/5
7	SF4	A	701	1	-	-	0/6/5/5
7	SF4	E	401	5	-	-	0/6/5/5
9	9S8	B	401	2	-	-	0/3/3/3
7	SF4	A	707	1	-	-	0/6/5/5
7	SF4	E	402	5	-	-	0/6/5/5
8	FAD	A	704	-	-	4/34/50/50	0/6/6/6
7	SF4	A	705	1	-	-	0/6/5/5
7	SF4	A	703	1	-	-	0/6/5/5
7	SF4	C	202	3	-	-	0/6/5/5
11	FES	D	201	6	-	-	0/1/1/1
7	SF4	C	201	3	-	-	0/6/5/5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	704	FAD	C10-N10	2.36	1.42	1.37

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	704	FAD	C9-C9A-N10	3.10	126.03	121.84
8	A	704	FAD	C4-N3-C2	-2.31	121.38	125.64

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	704	FAD	PA-O3P-P-O5'
8	A	704	FAD	C2B-C1B-N9A-C8A
8	A	704	FAD	O4B-C1B-N9A-C8A
8	A	704	FAD	O4B-C4B-C5B-O5B

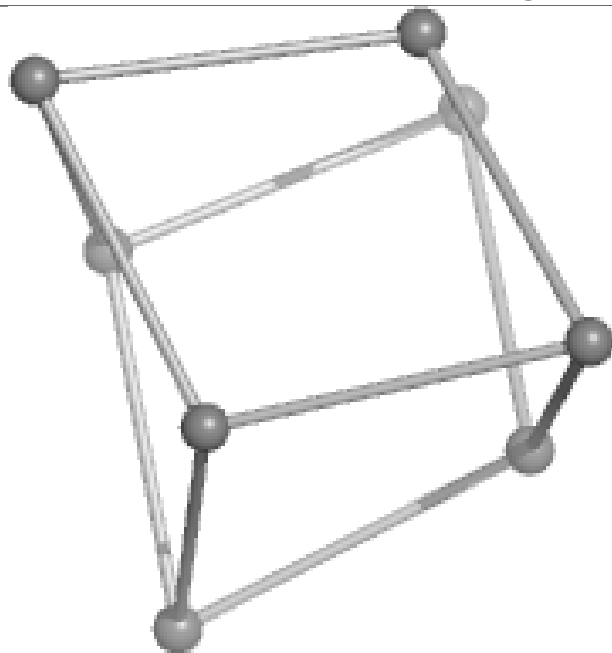
There are no ring outliers.

2 monomers are involved in 4 short contacts:

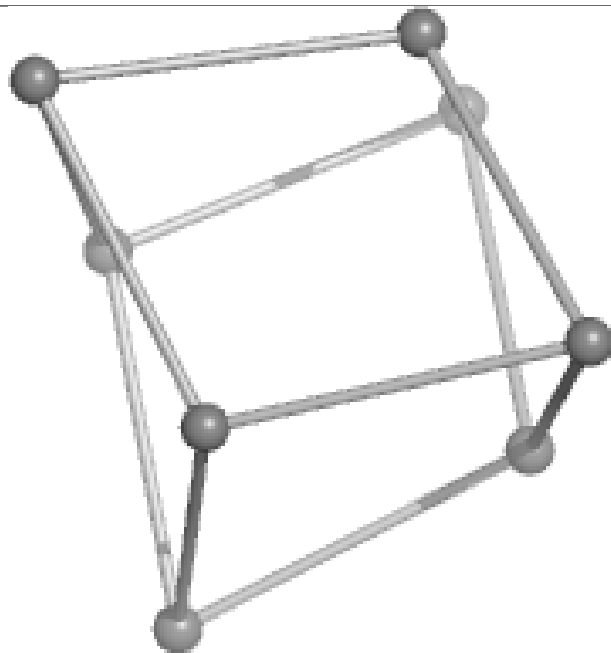
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	706	SF4	1	0
10	F	501	NFU	3	0

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

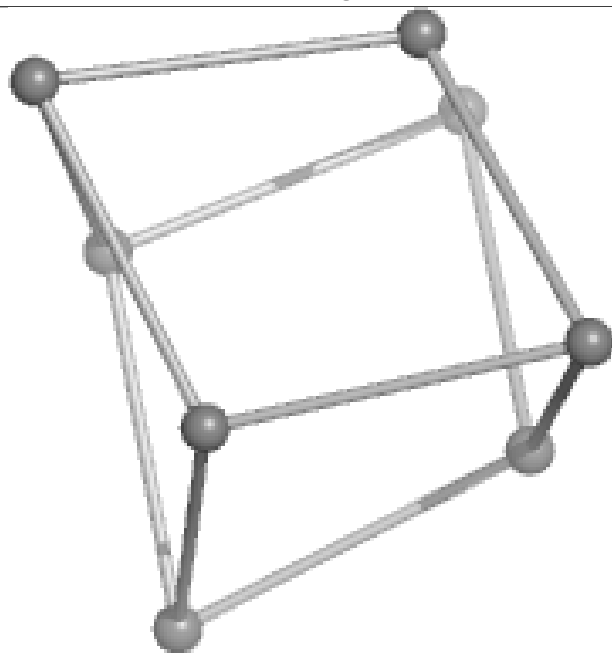
Ligand SF4 A 706



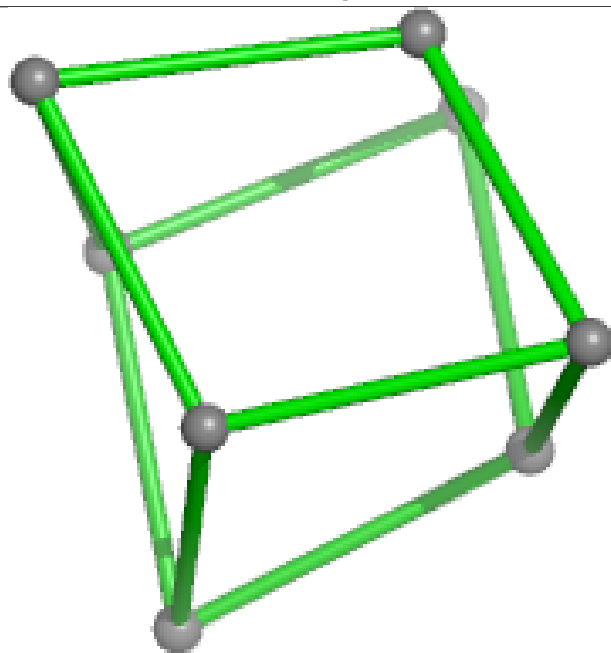
Bond lengths



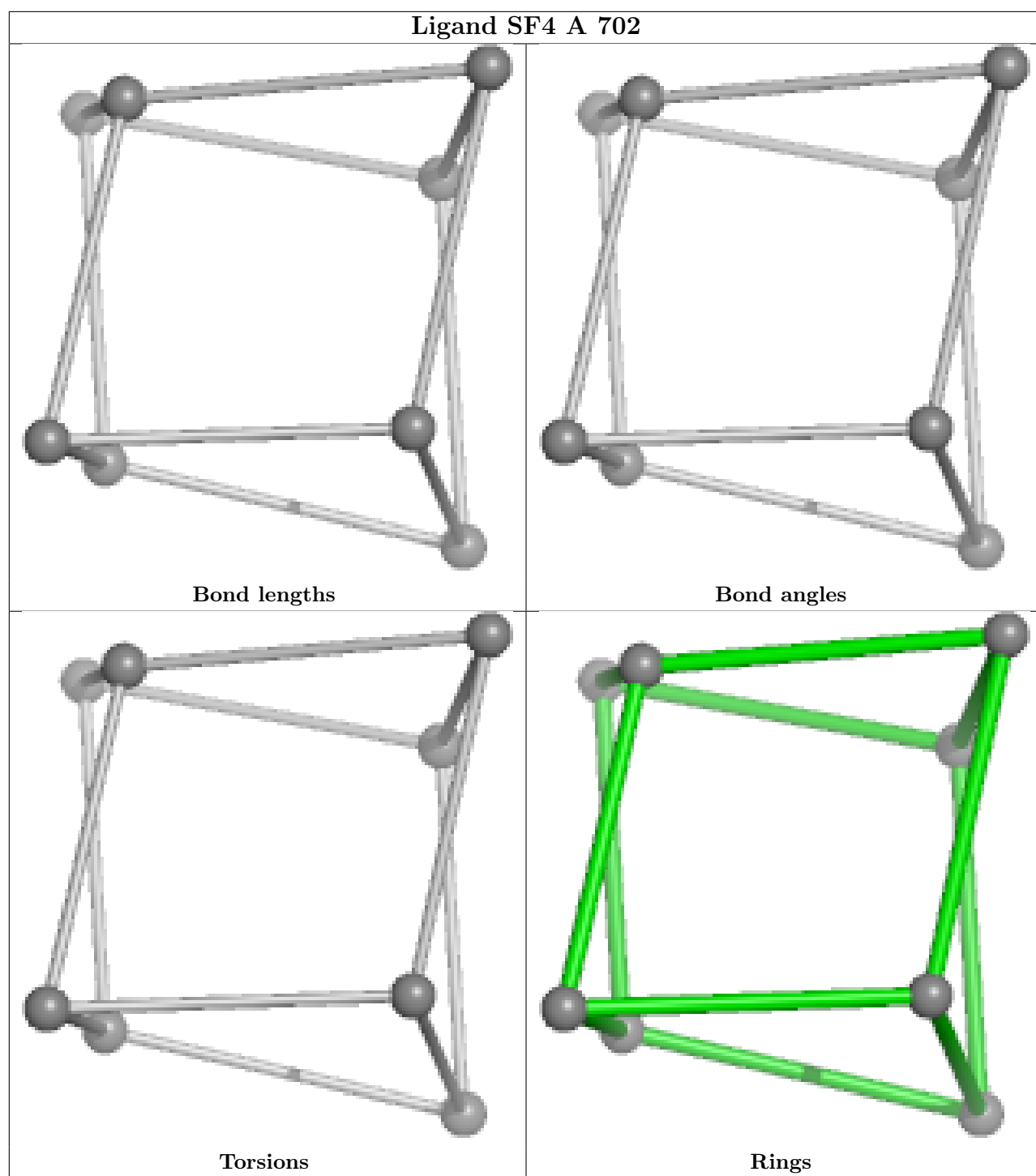
Bond angles

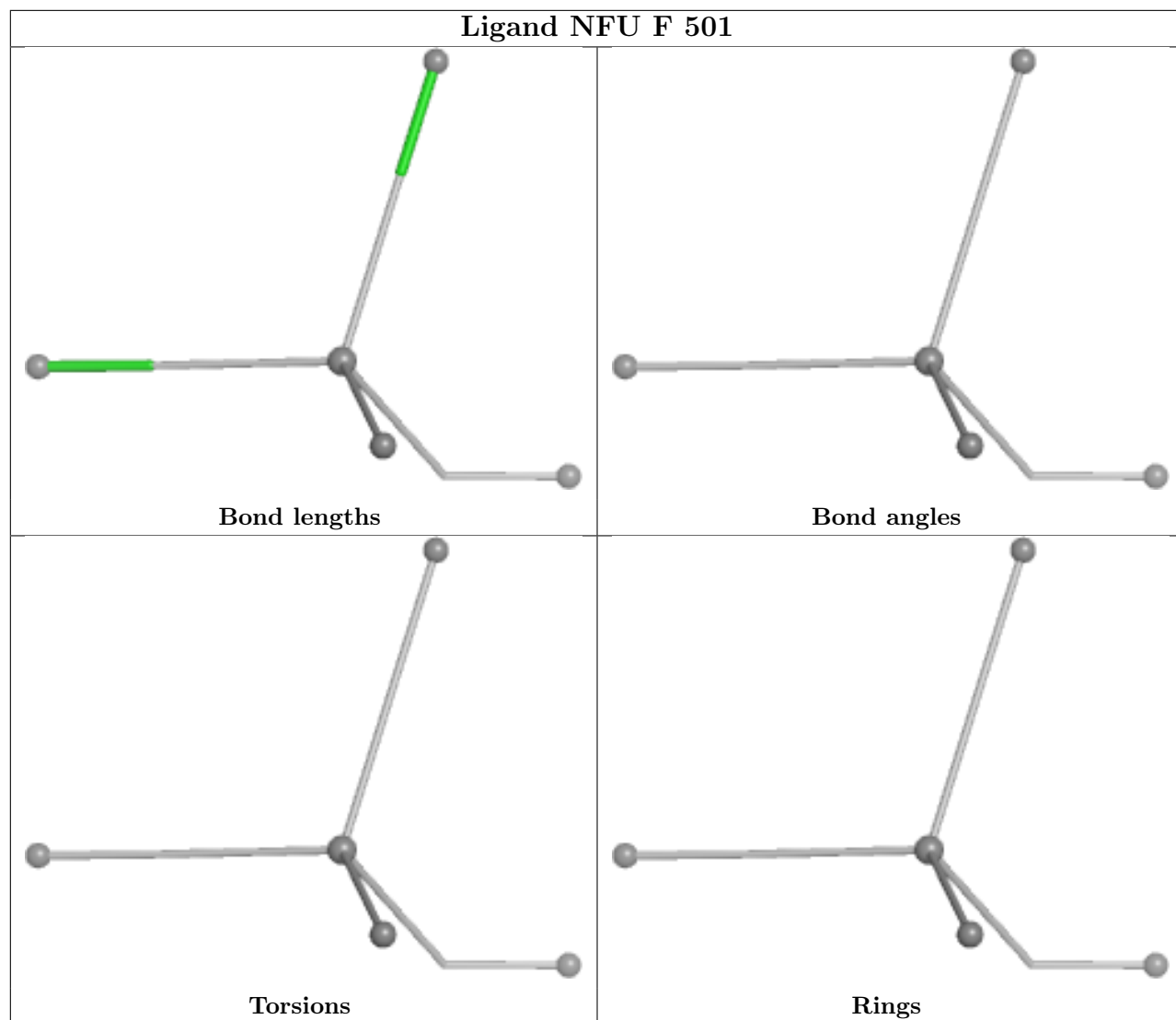


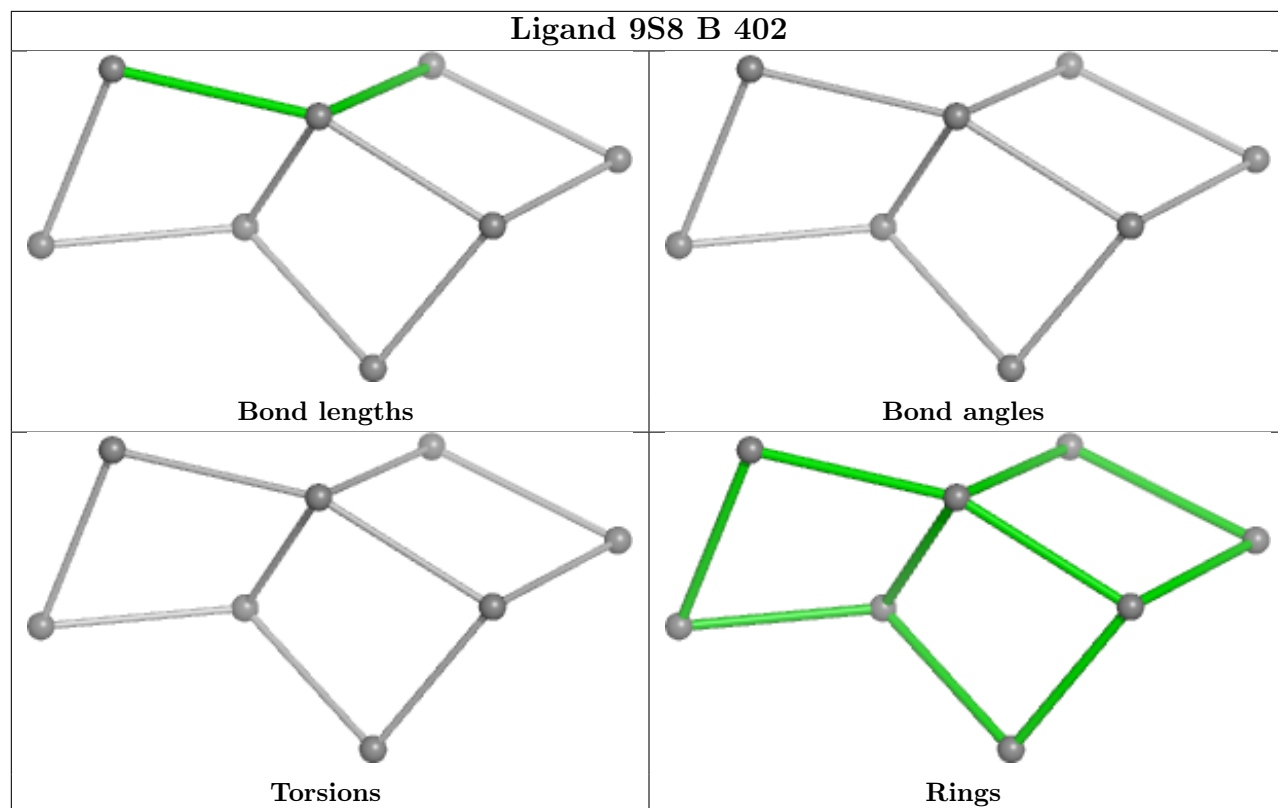
Torsions



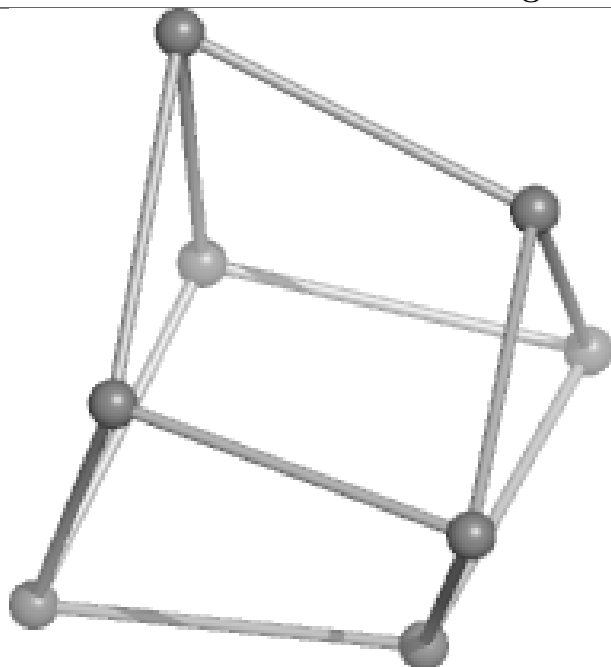
Rings



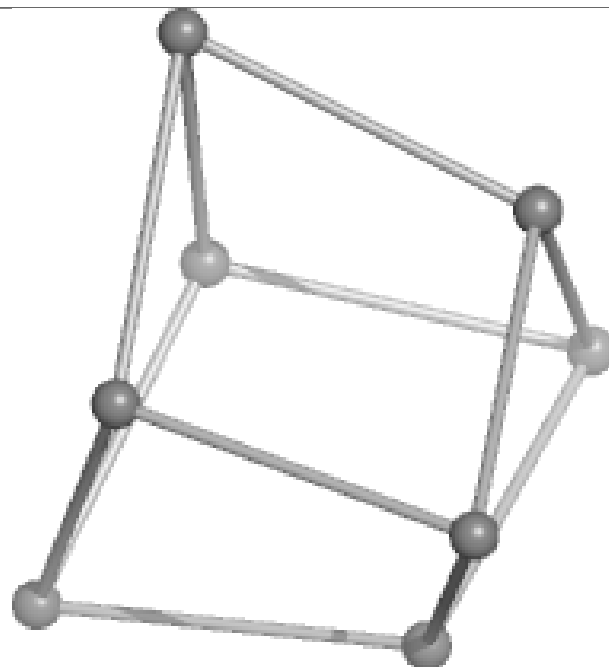




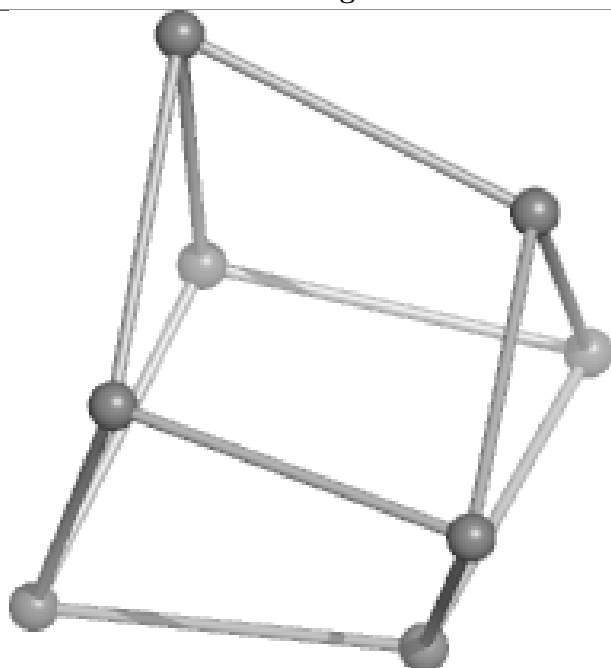
Ligand SF4 E 403



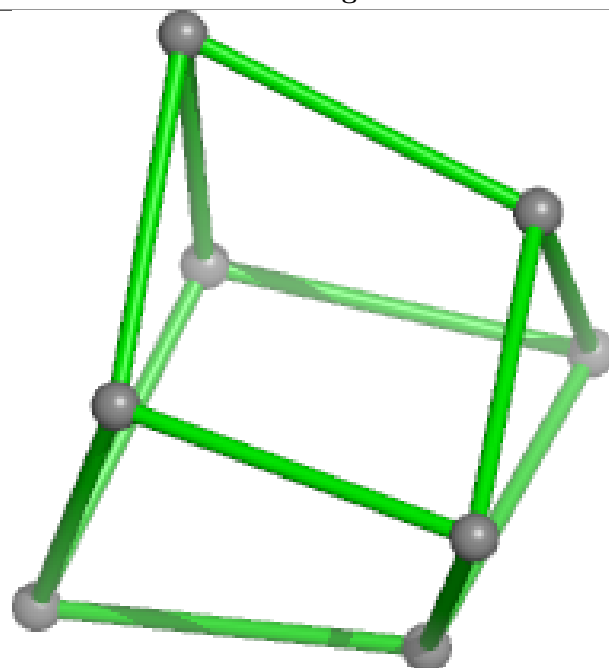
Bond lengths



Bond angles

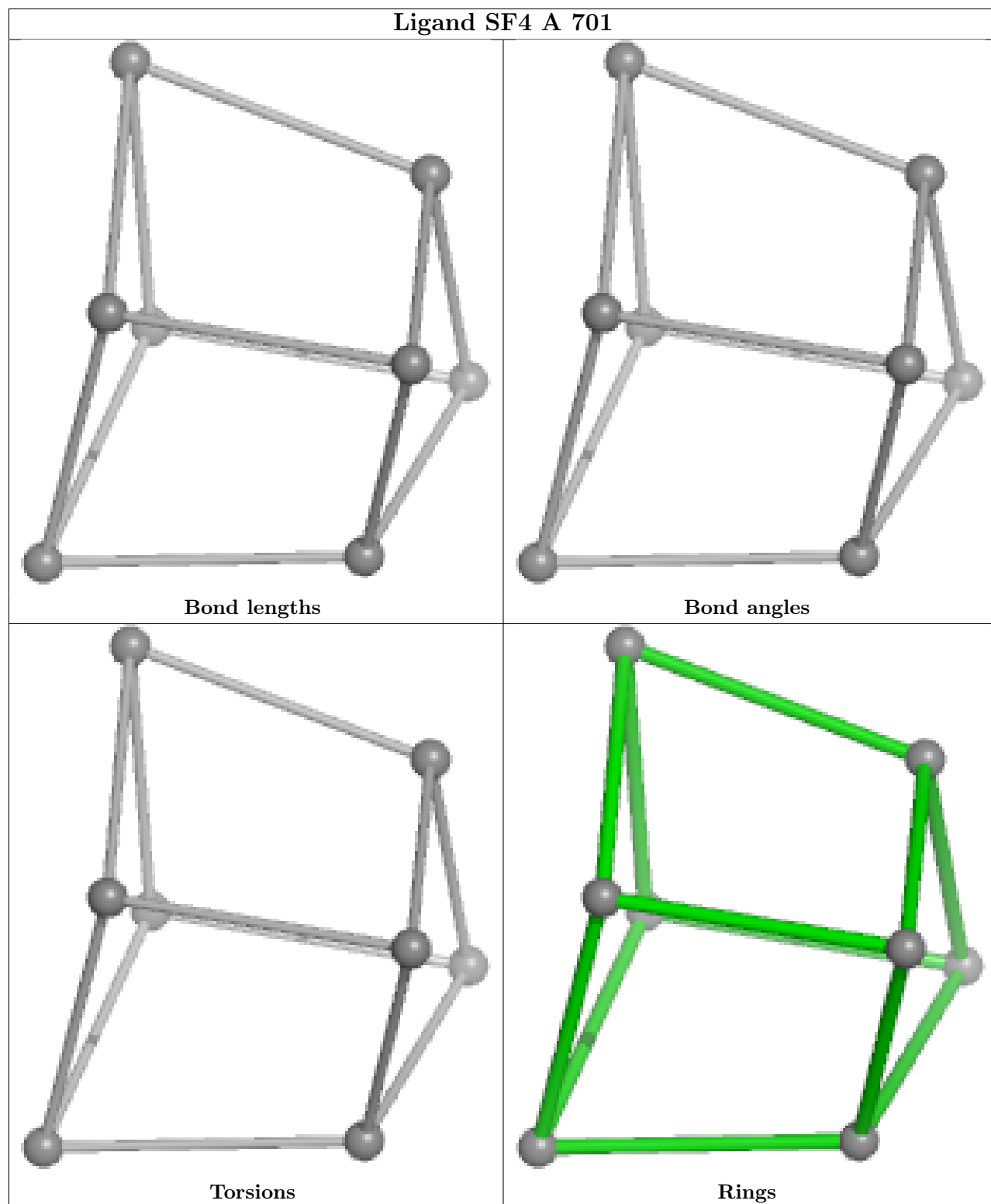


Torsions

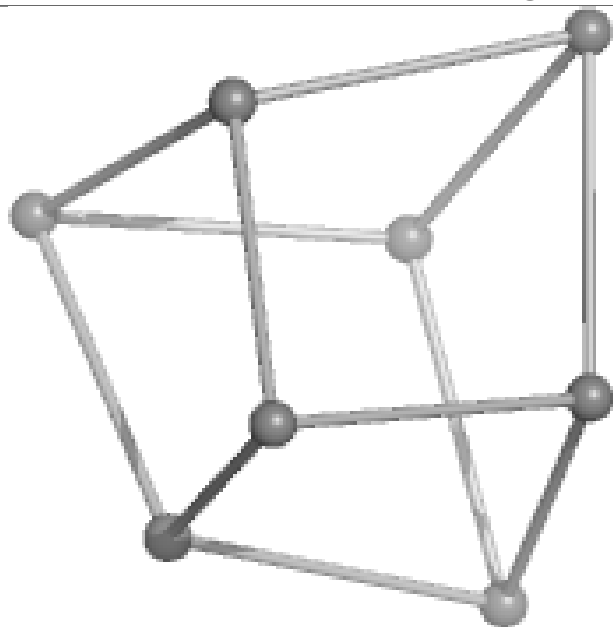


Rings

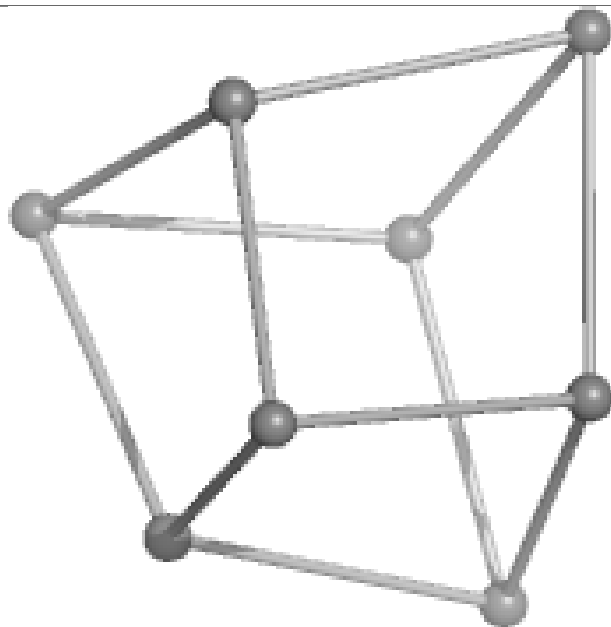
Ligand SF4 A 701



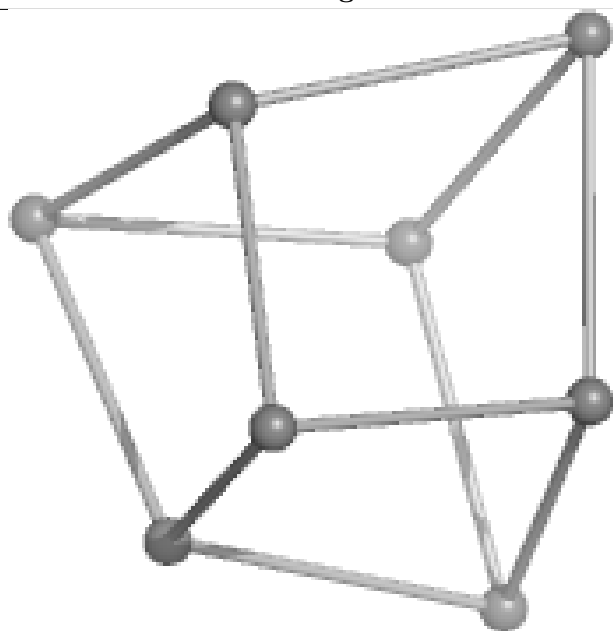
Ligand SF4 E 401



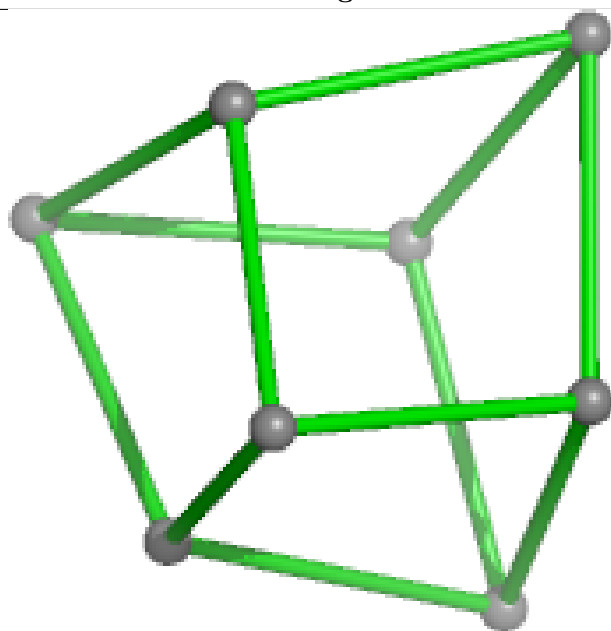
Bond lengths



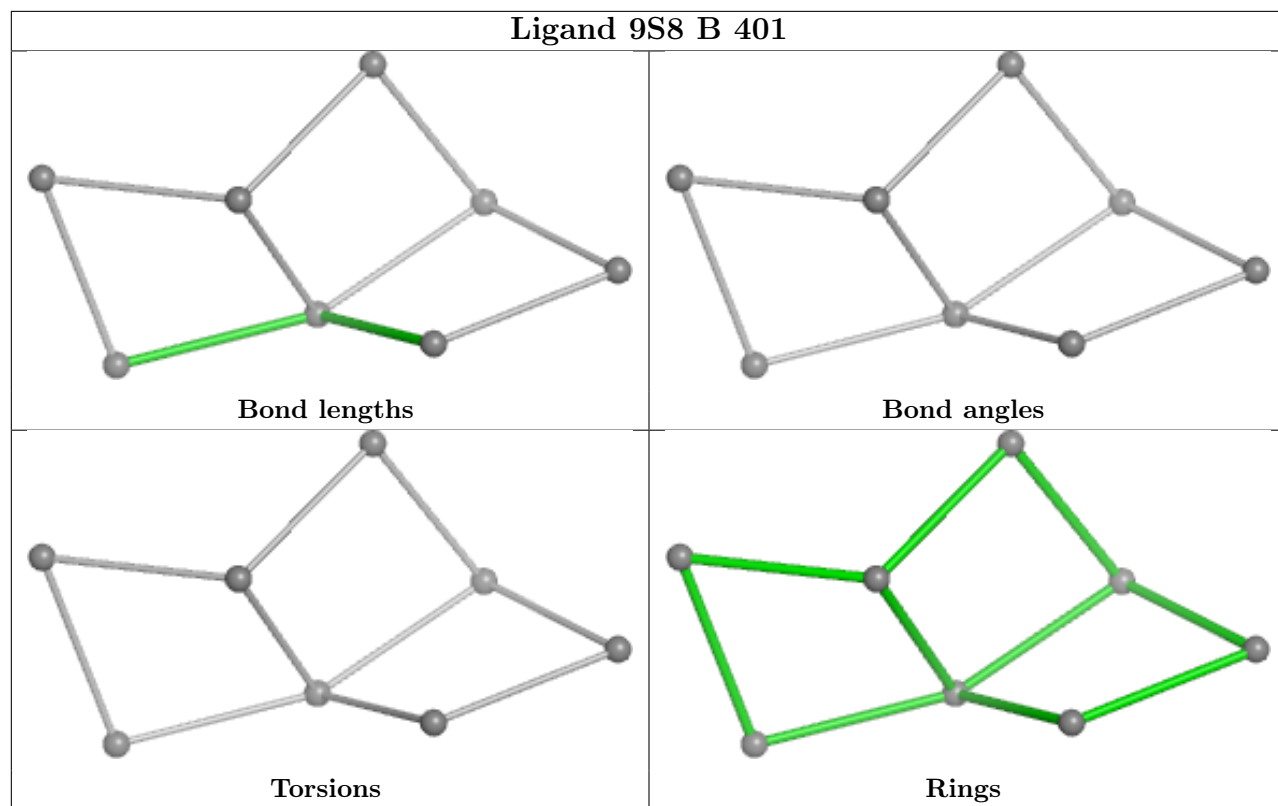
Bond angles



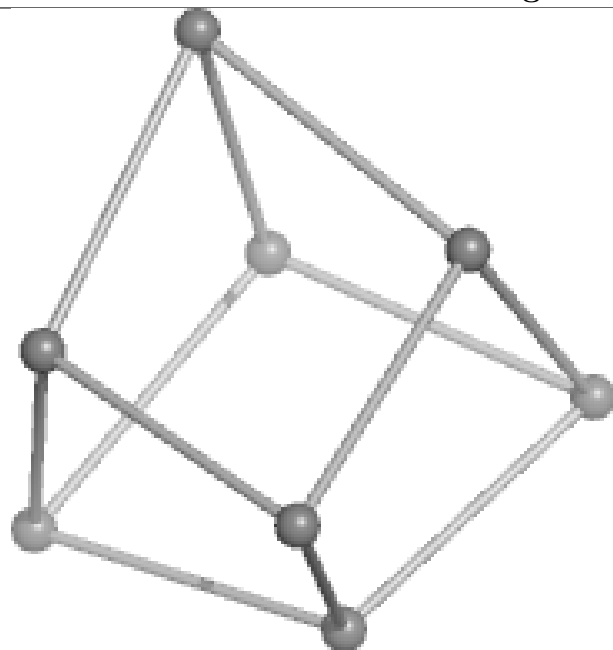
Torsions



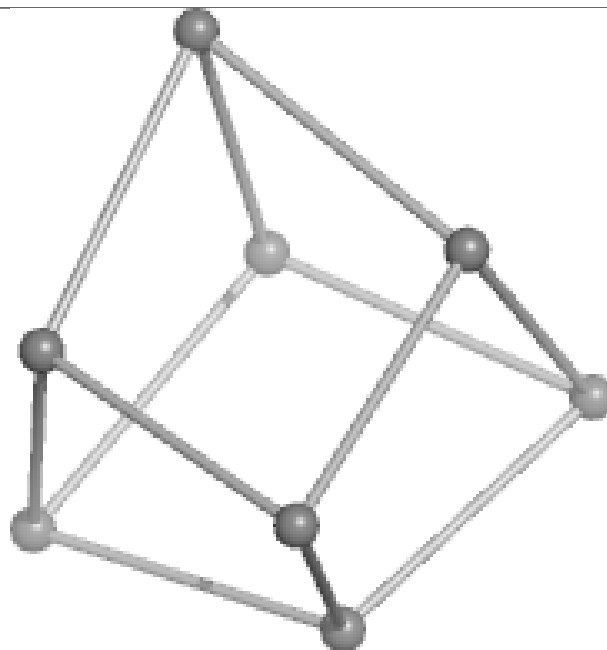
Rings



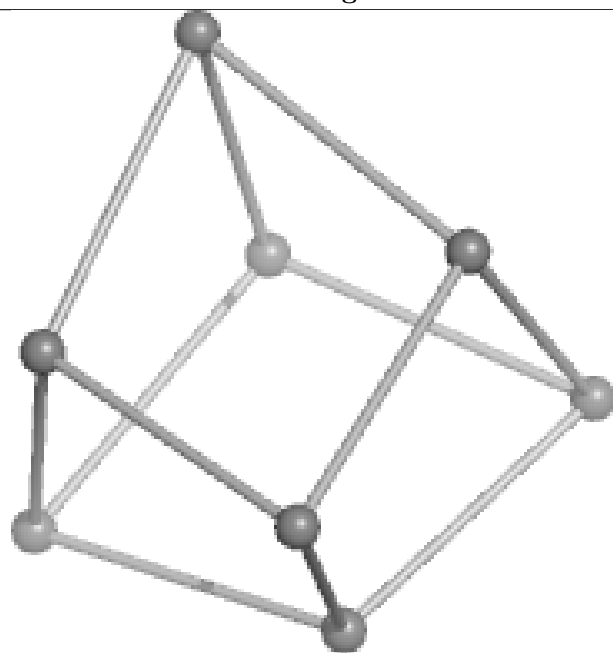
Ligand SF4 A 707



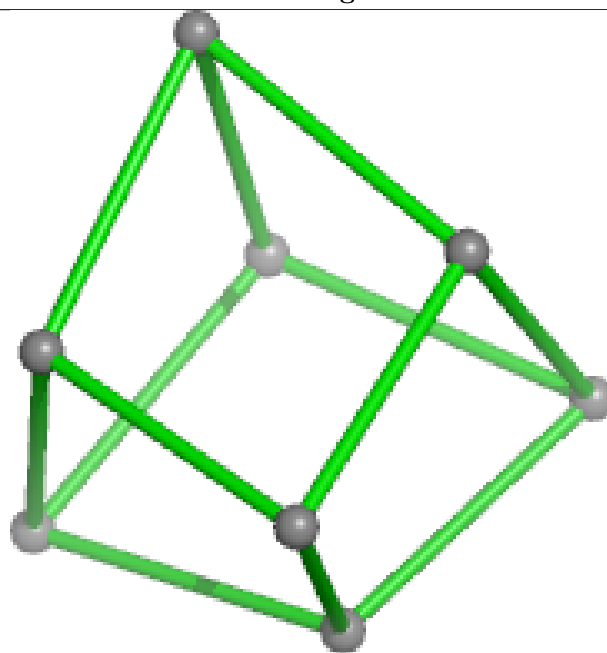
Bond lengths



Bond angles

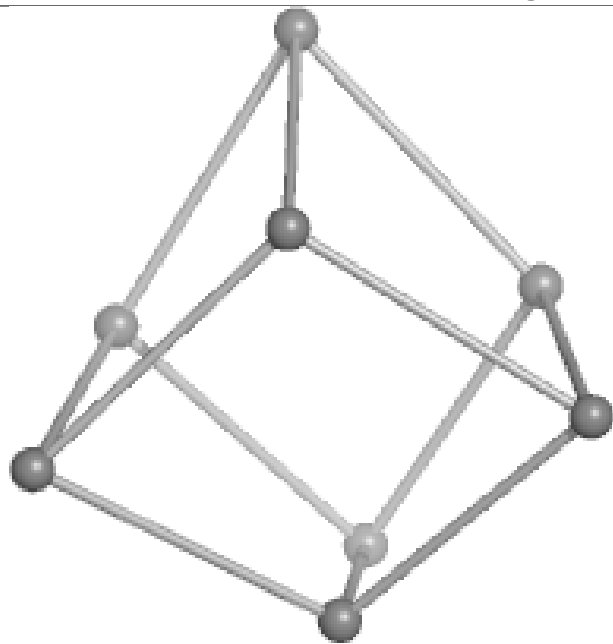


Torsions

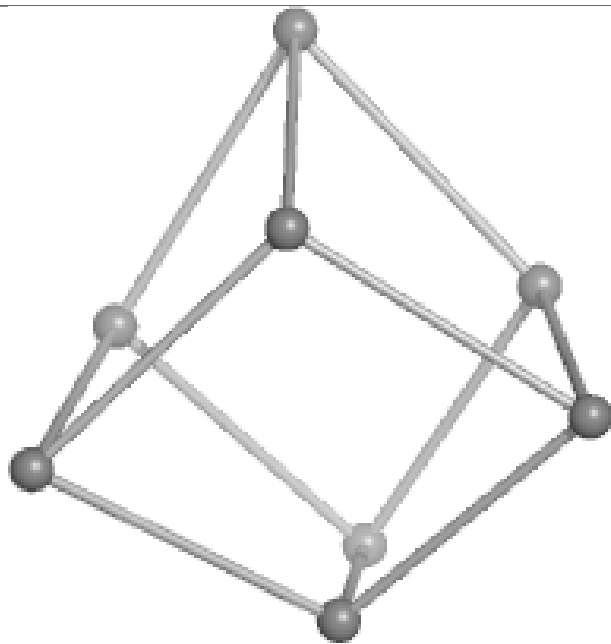


Rings

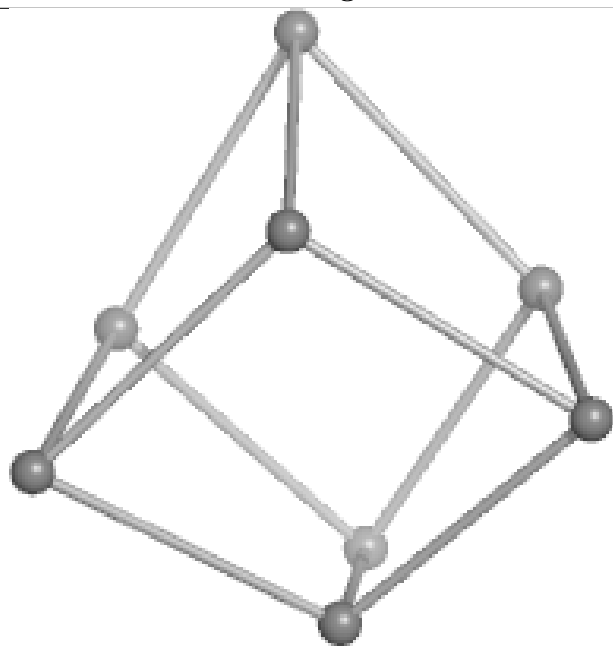
Ligand SF4 E 402



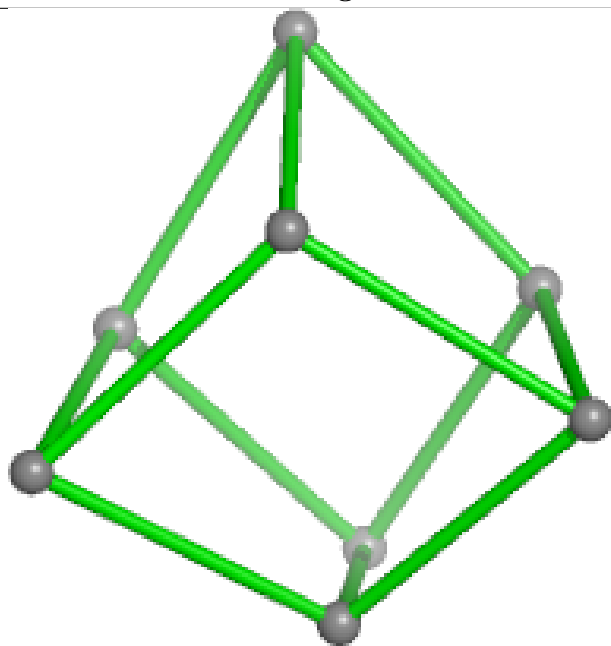
Bond lengths



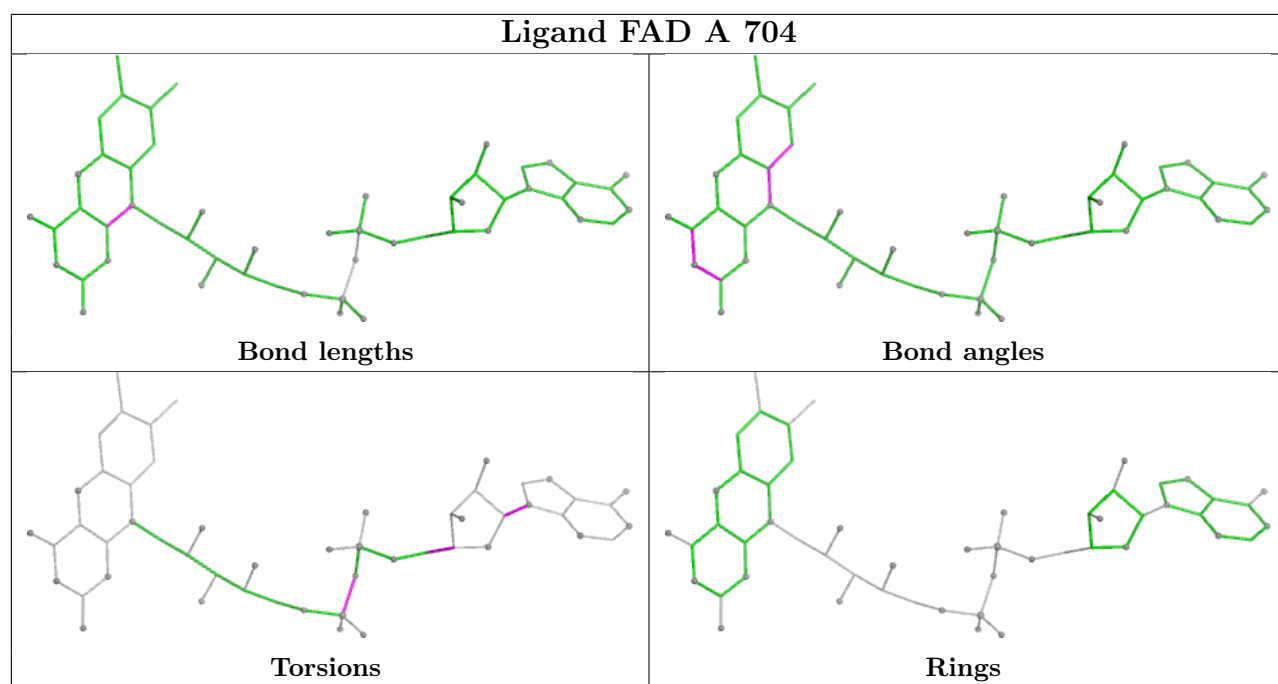
Bond angles

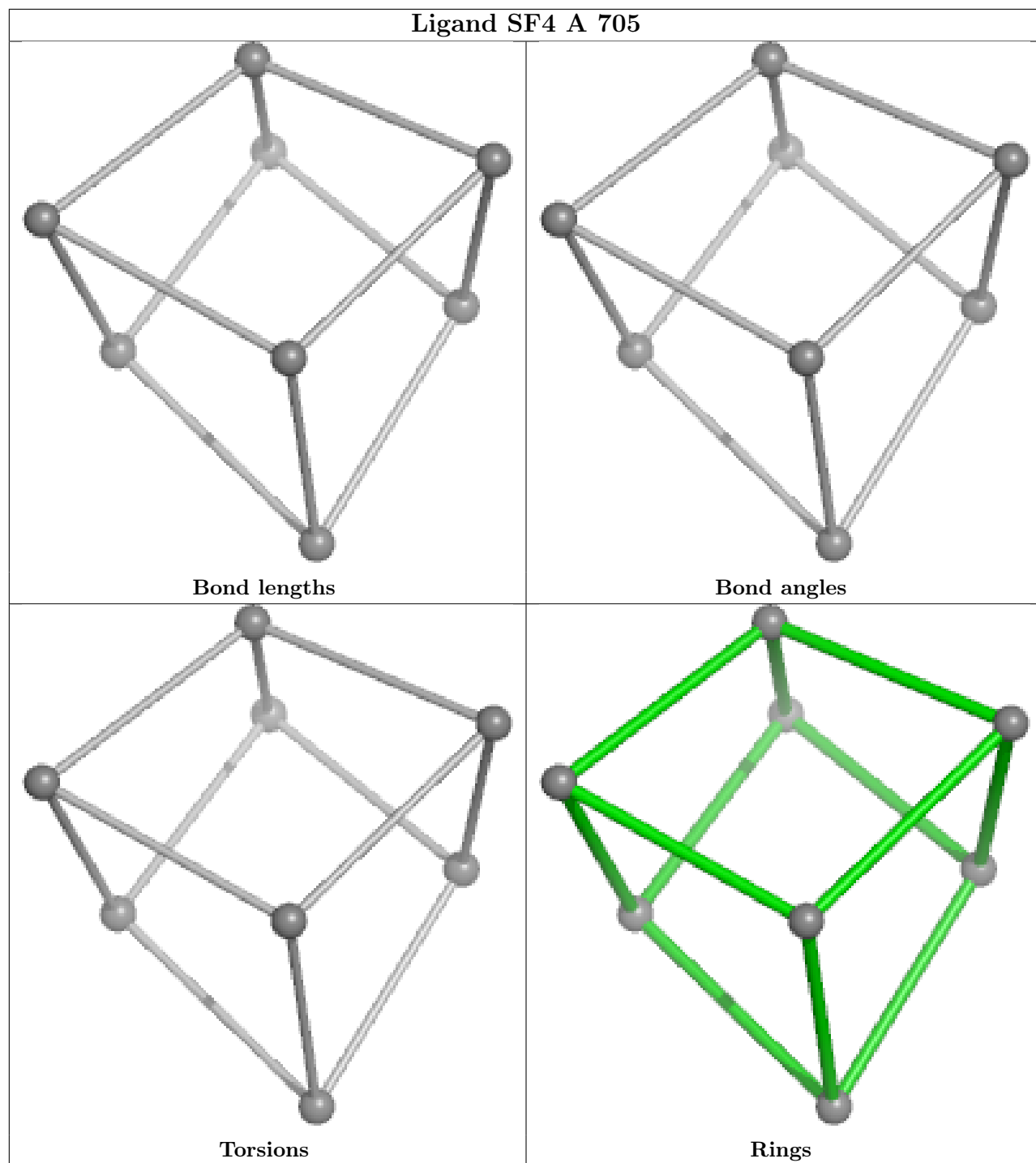


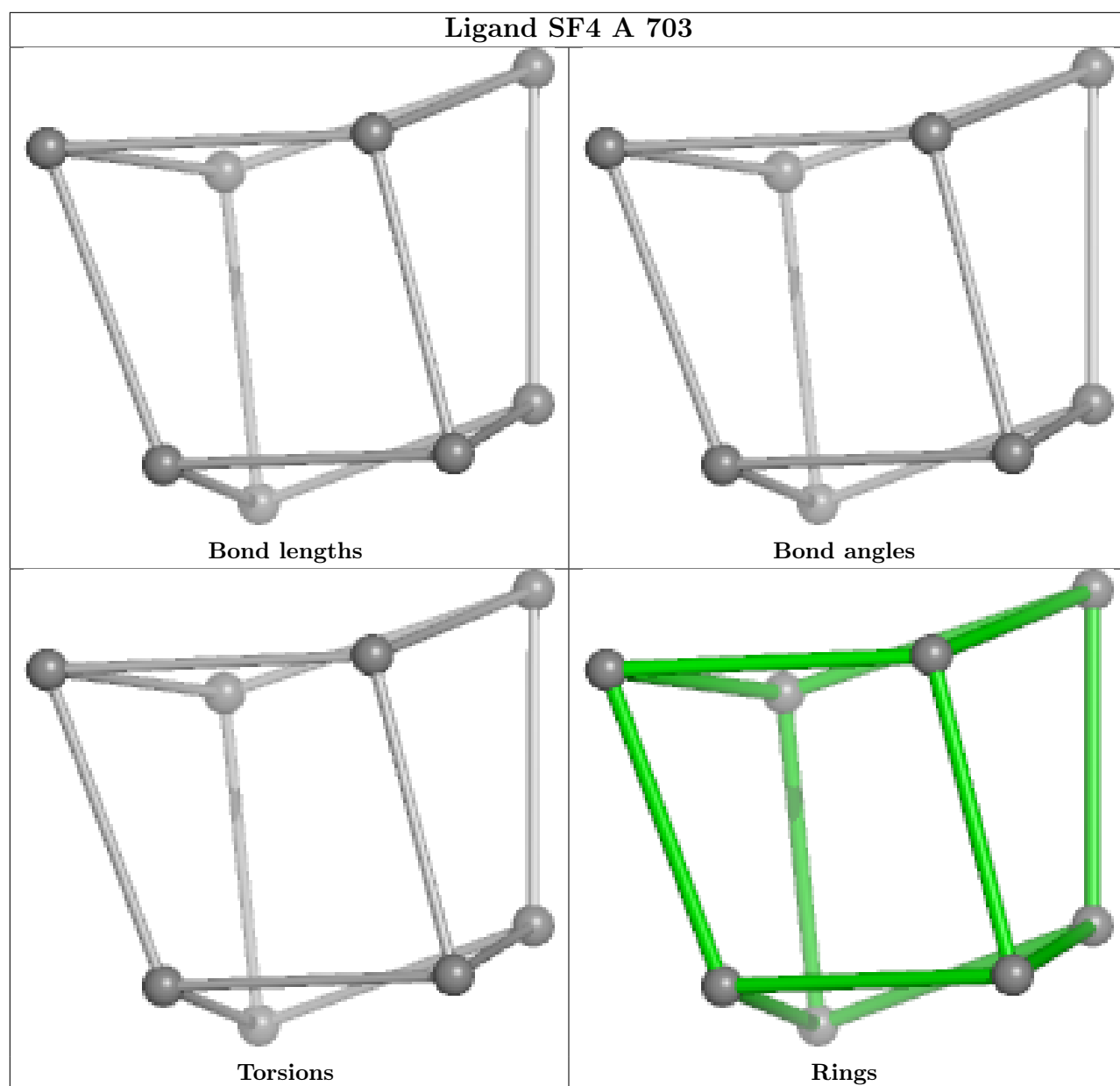
Torsions

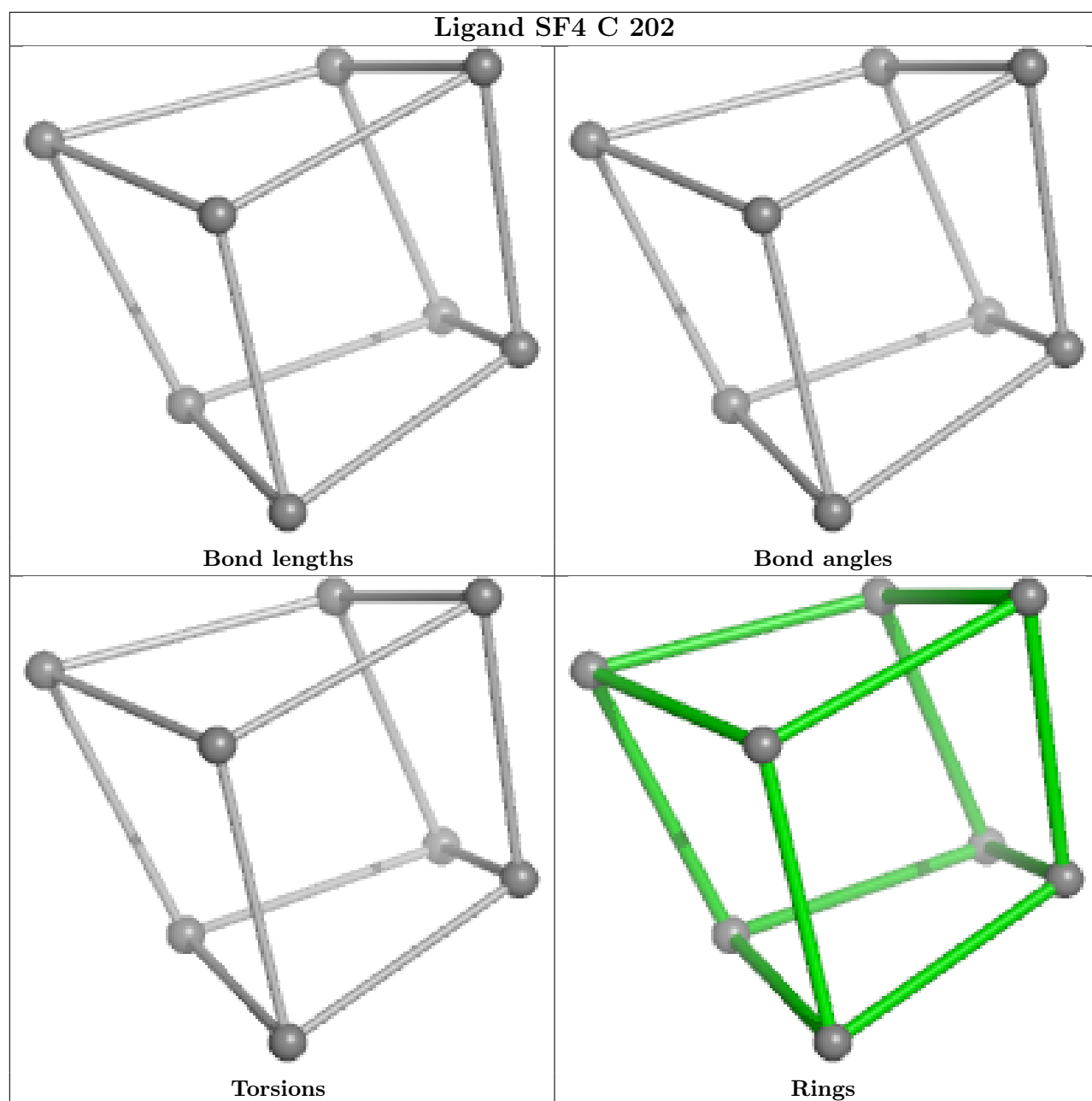


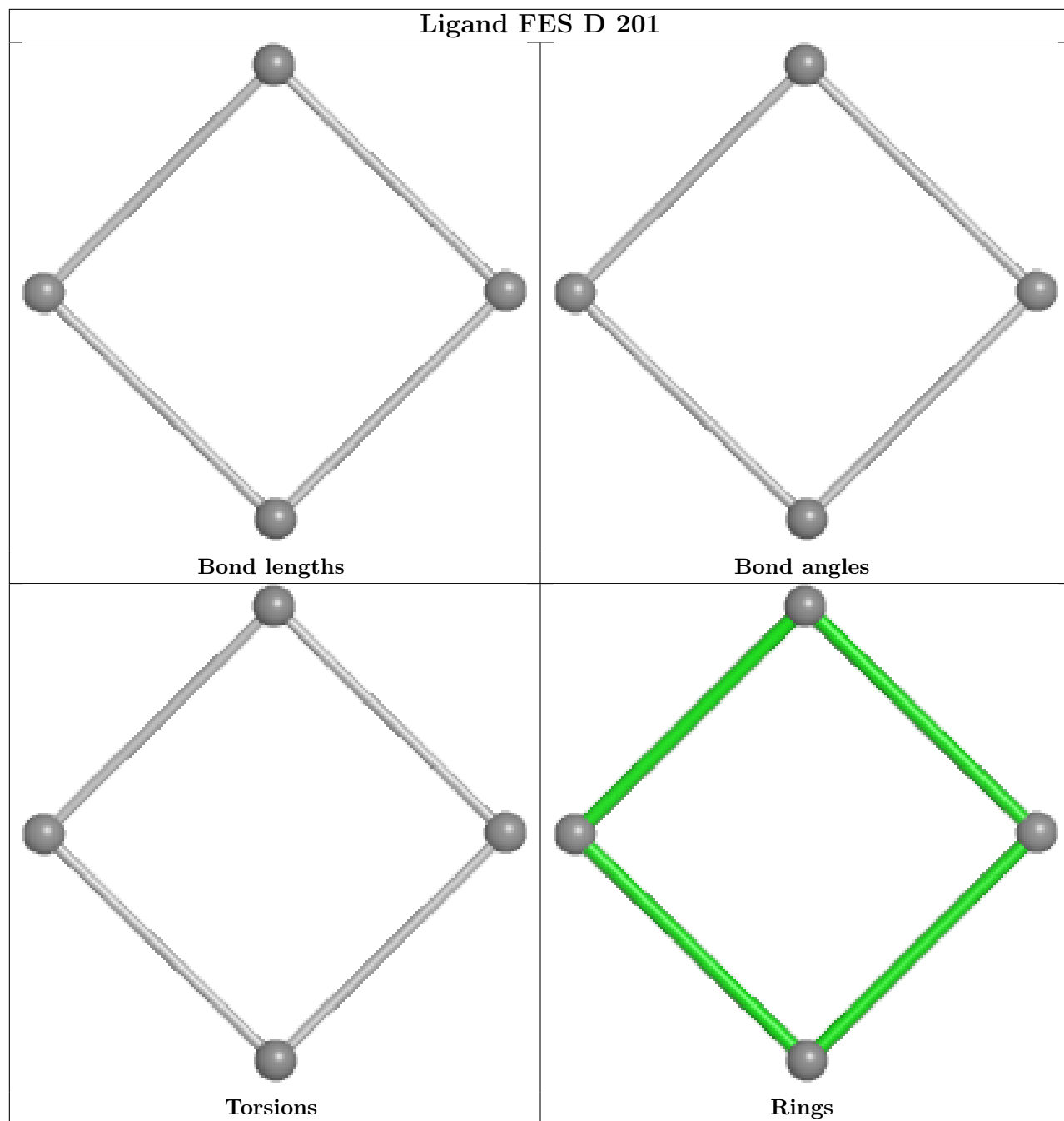
Rings

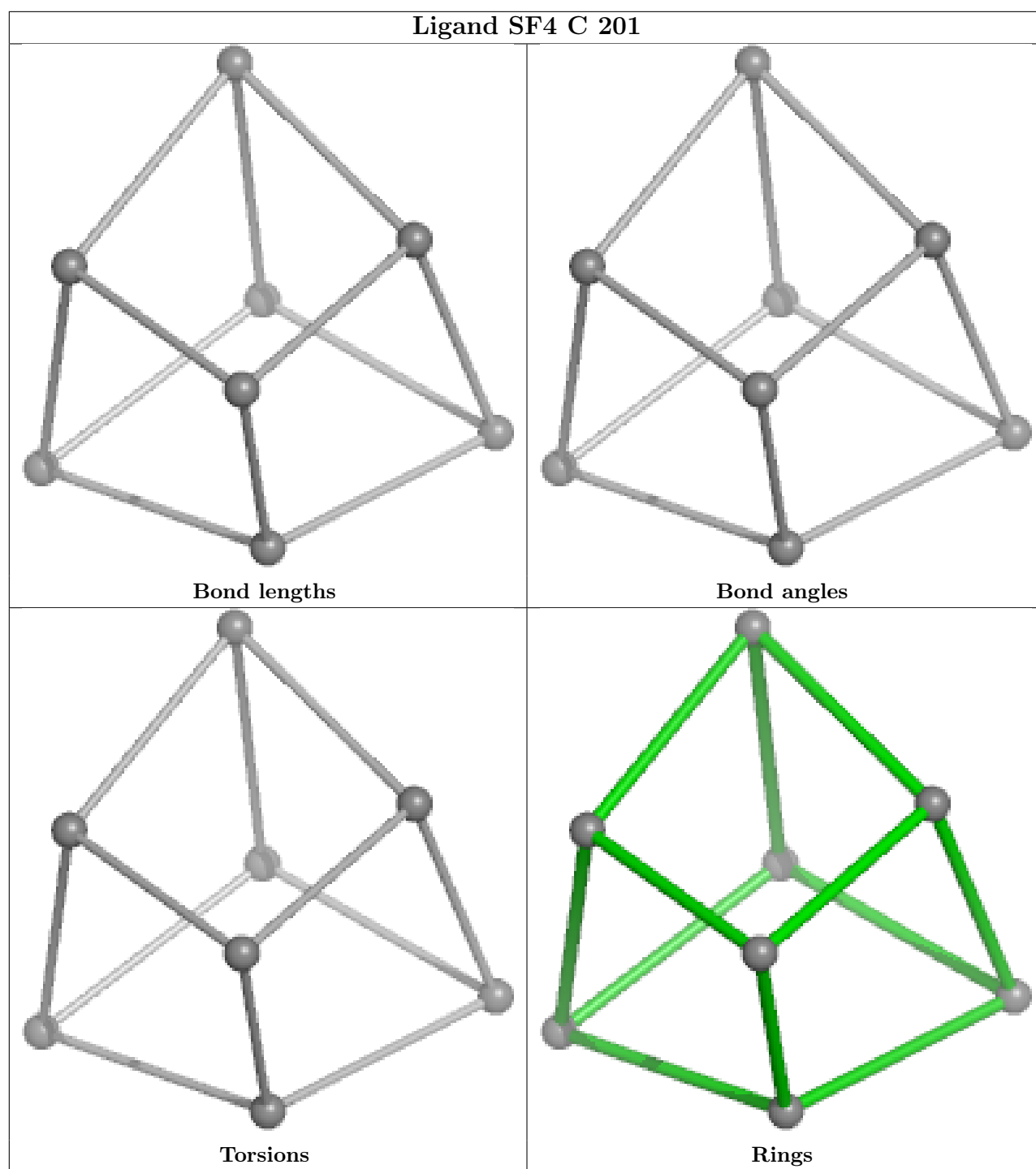












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

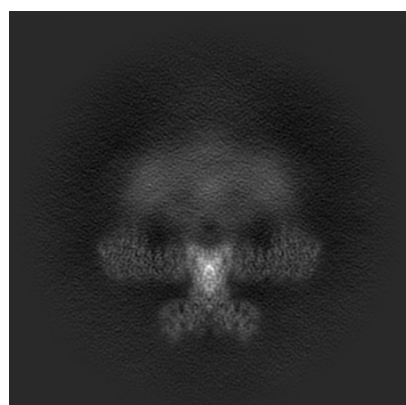
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-55298. These allow visual inspection of the internal detail of the map and identification of artifacts.

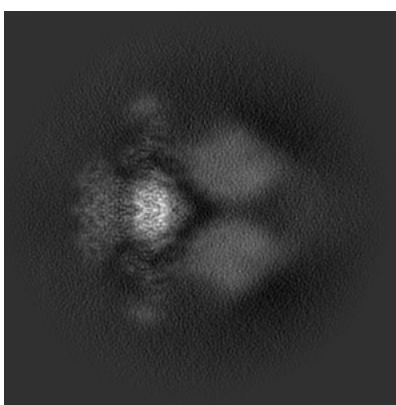
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

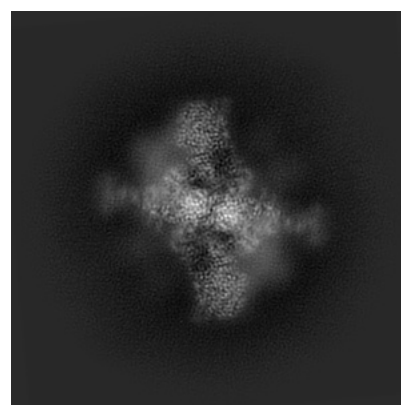
6.1.1 Primary map



X



Y

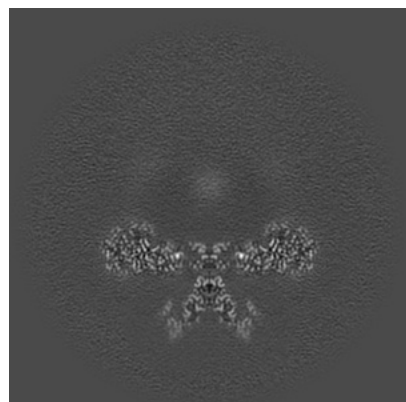


Z

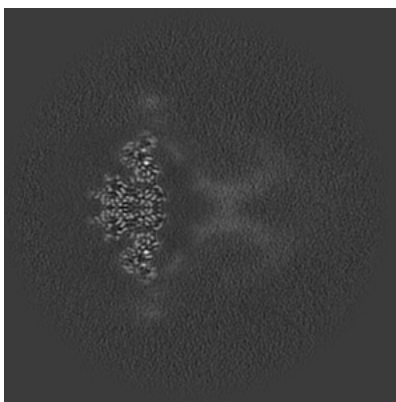
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

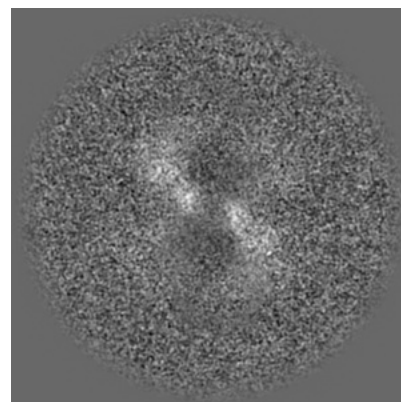
6.2.1 Primary map



X Index: 240



Y Index: 240

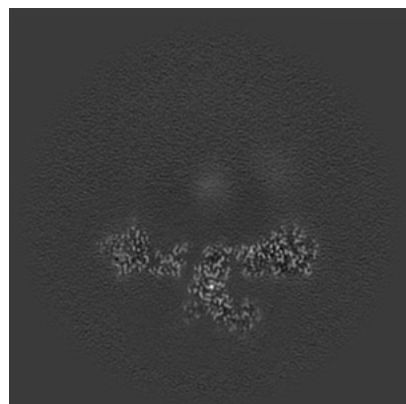


Z Index: 240

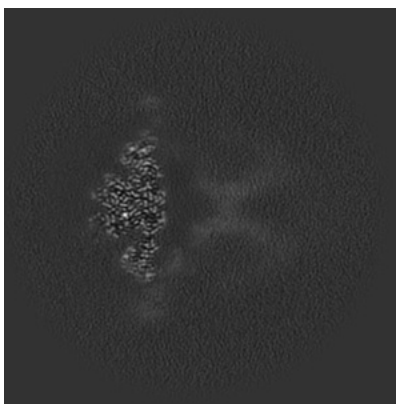
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

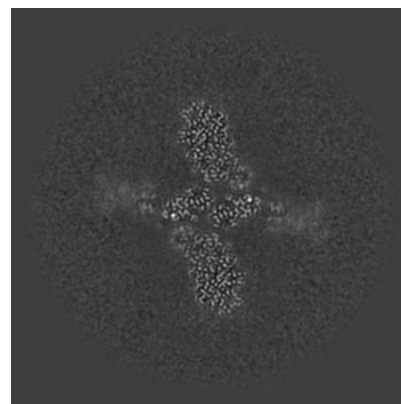
6.3.1 Primary map



X Index: 232



Y Index: 243

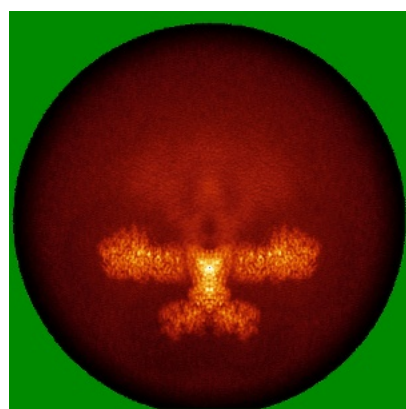


Z Index: 178

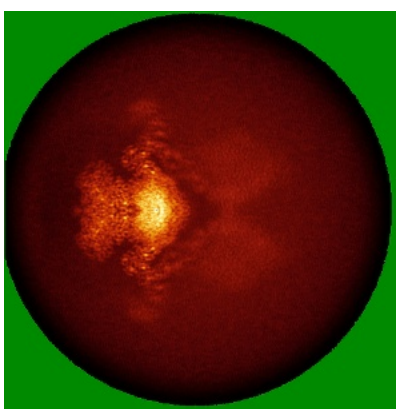
The images above show the largest variance slices of the map in three orthogonal directions.

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

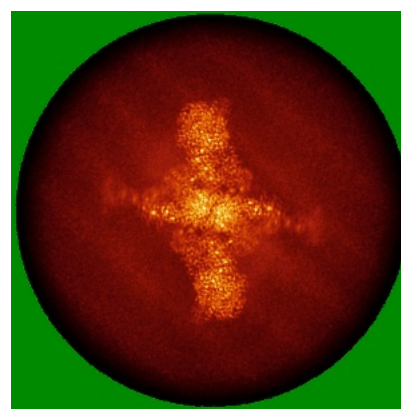
6.4.1 Primary map



X



Y

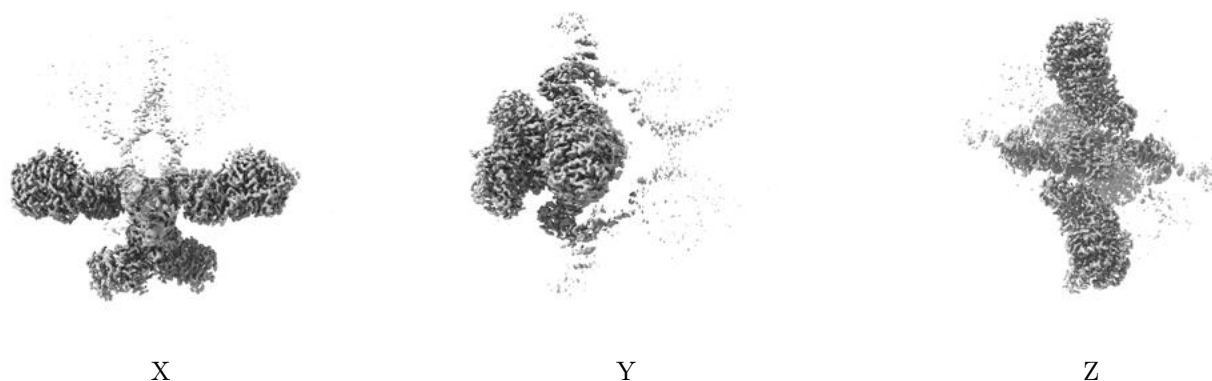


Z

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

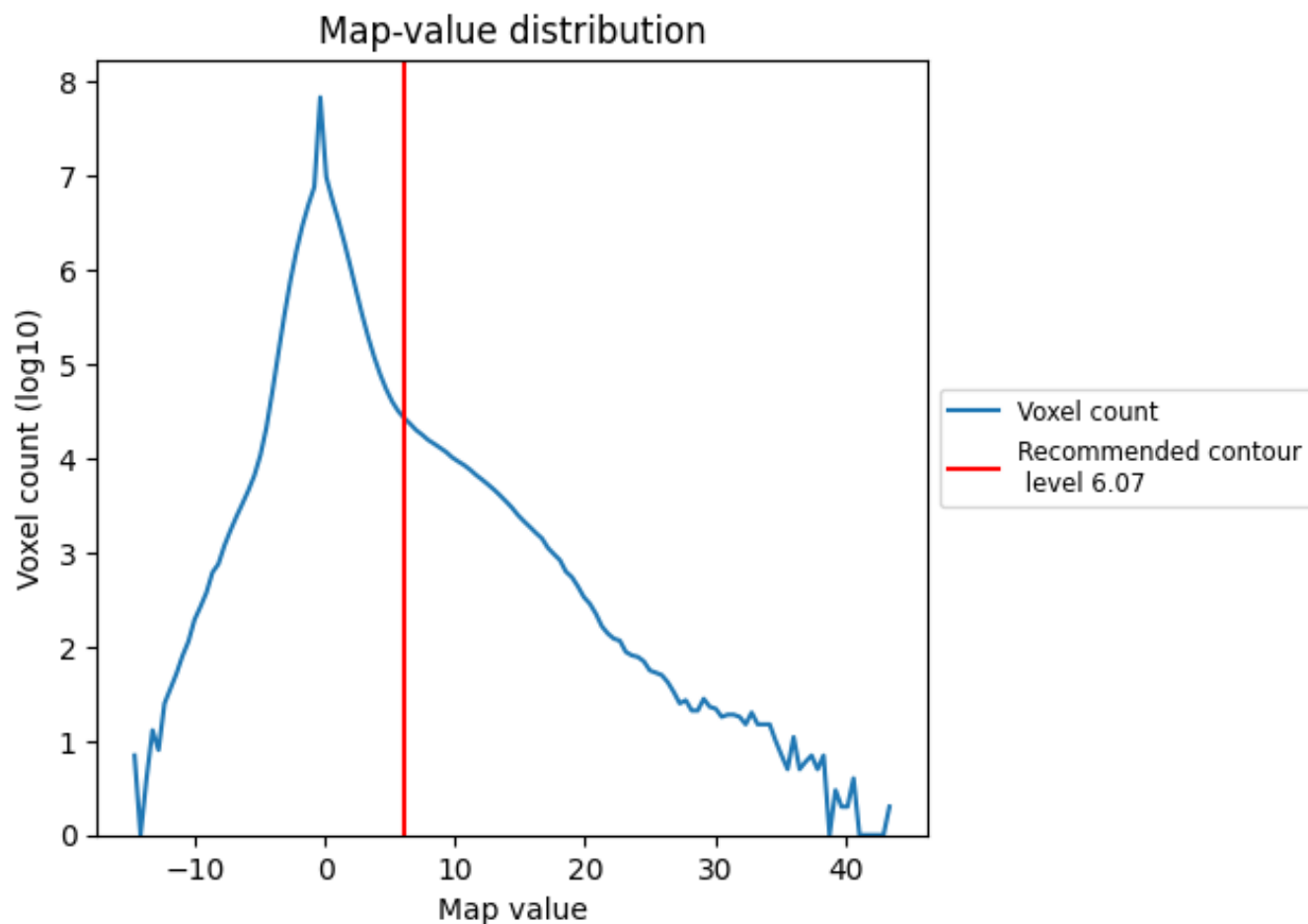
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

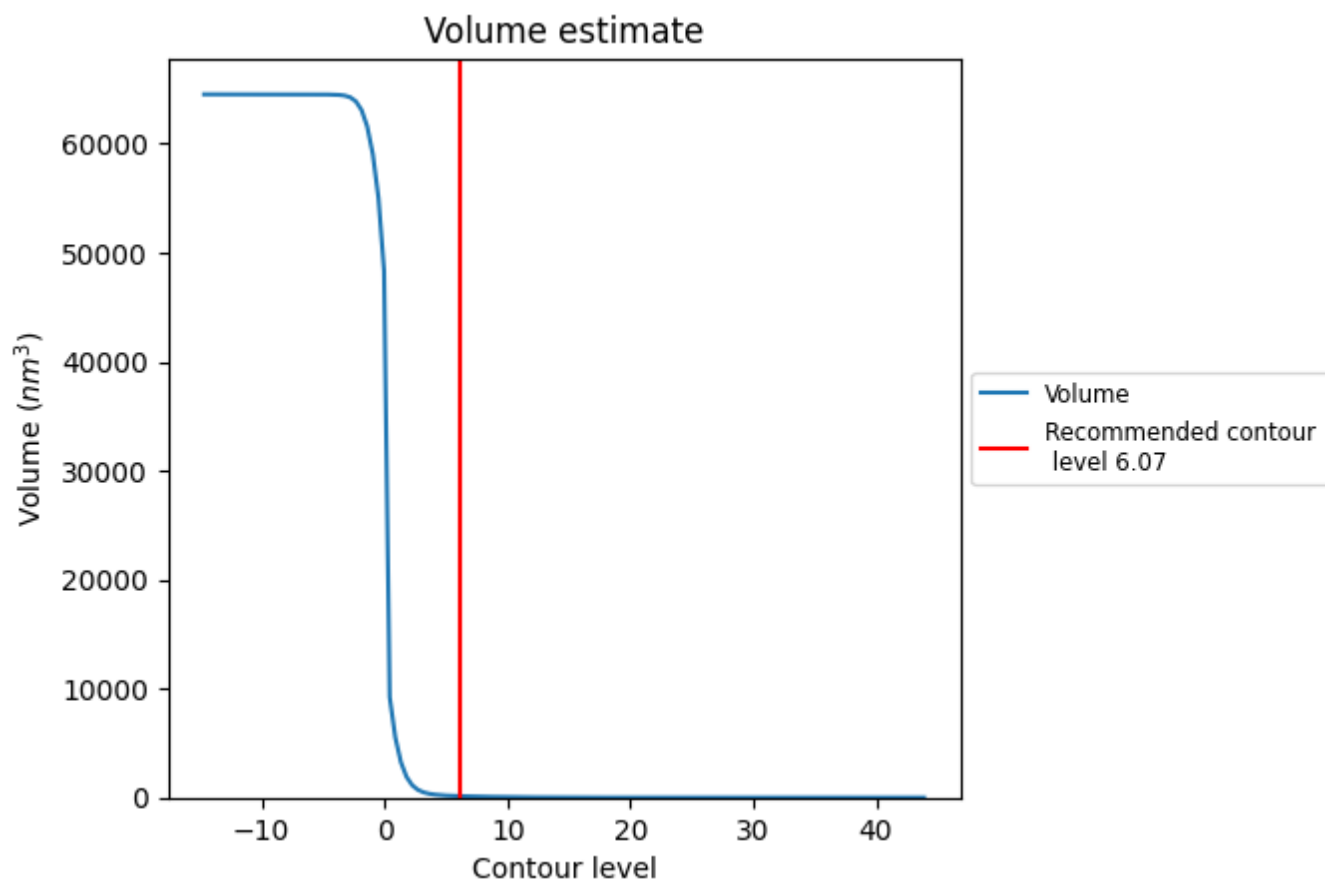
This section contains the results of statistical analysis of the map.

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.

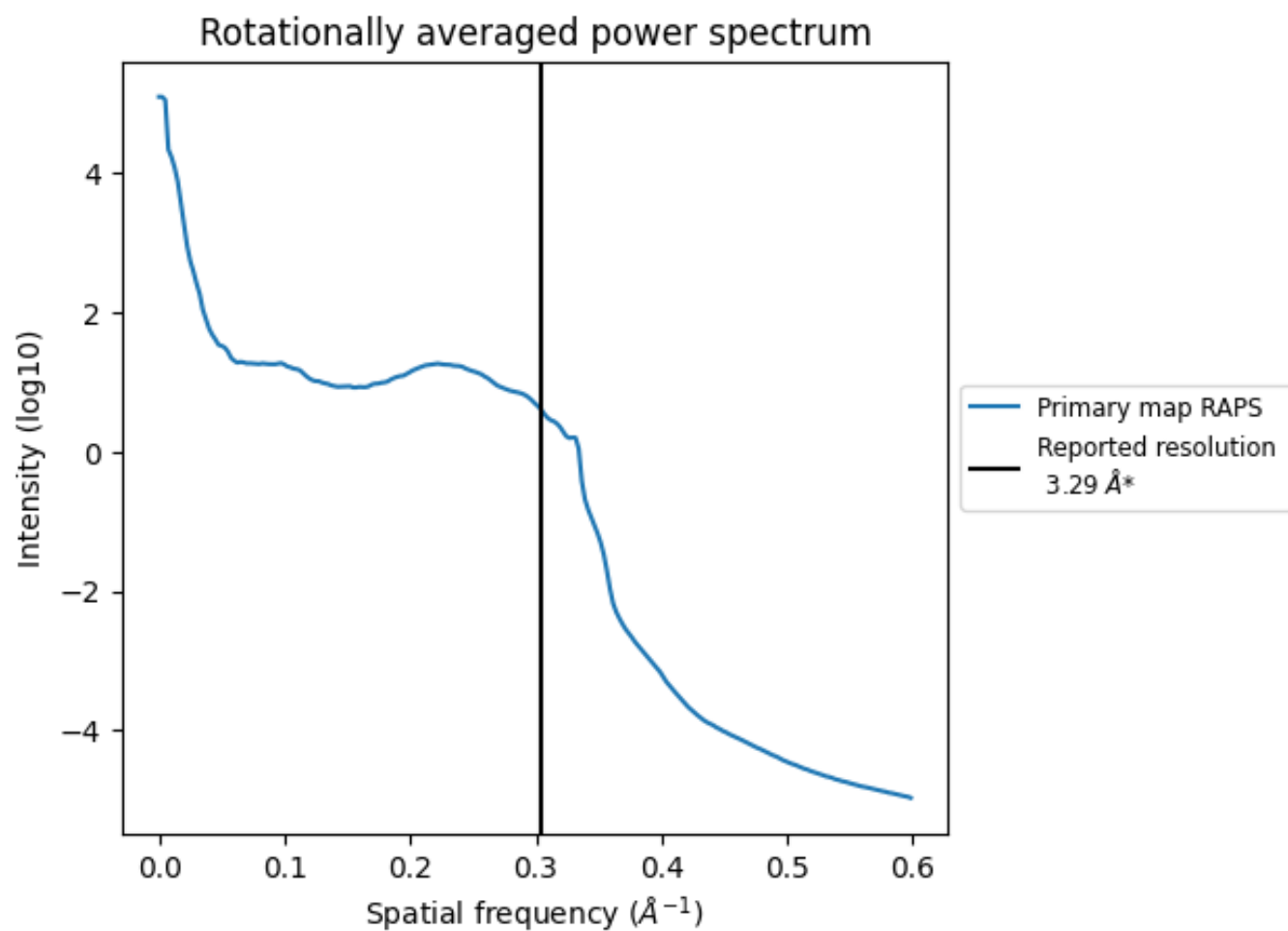
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 133 nm^3 ; this corresponds to an approximate mass of 120 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 0.304 Å⁻¹

8 Fourier-Shell correlation ⓘ

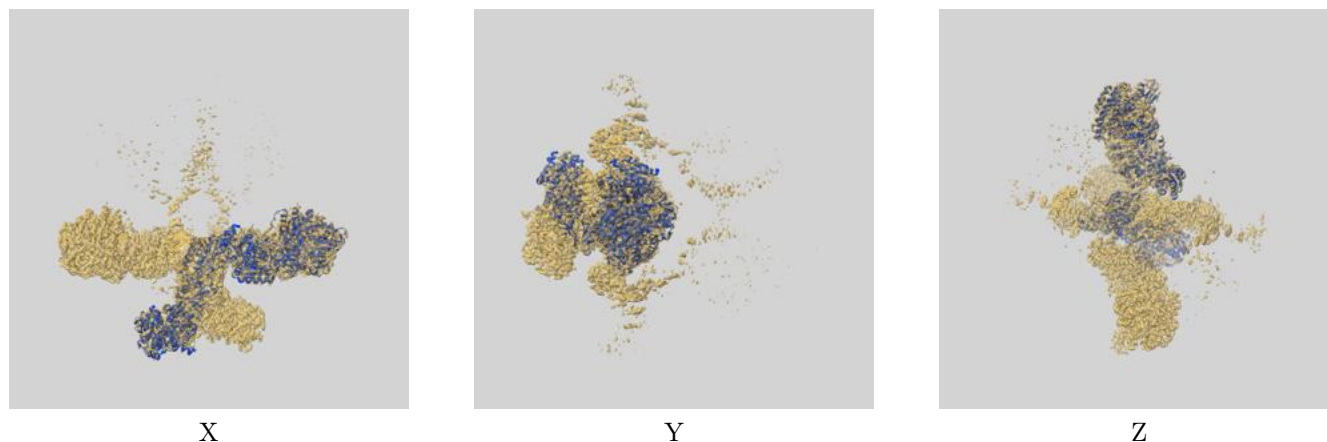
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

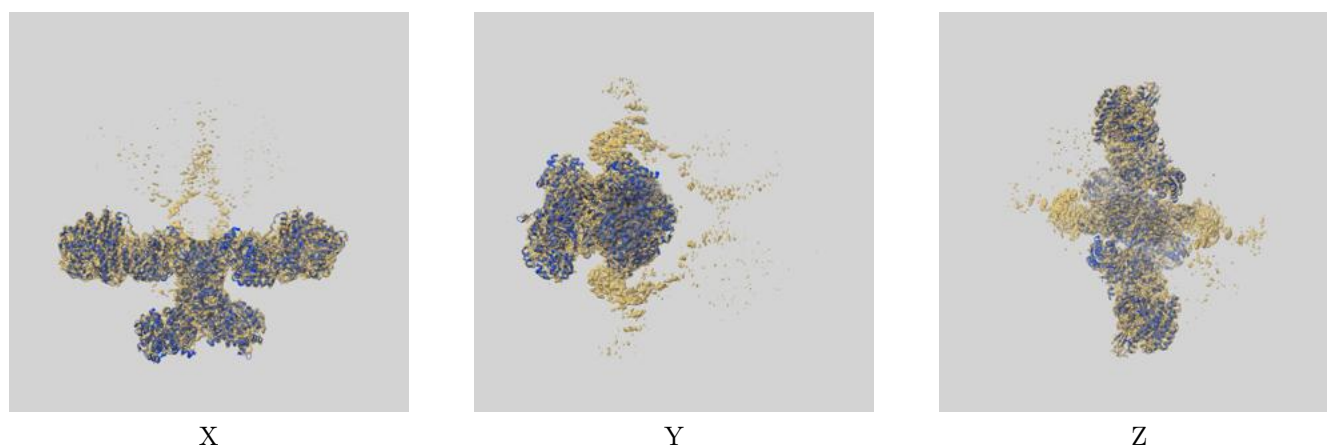
This section contains information regarding the fit between EMDB map EMD-55298 and PDB model 9SW5. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

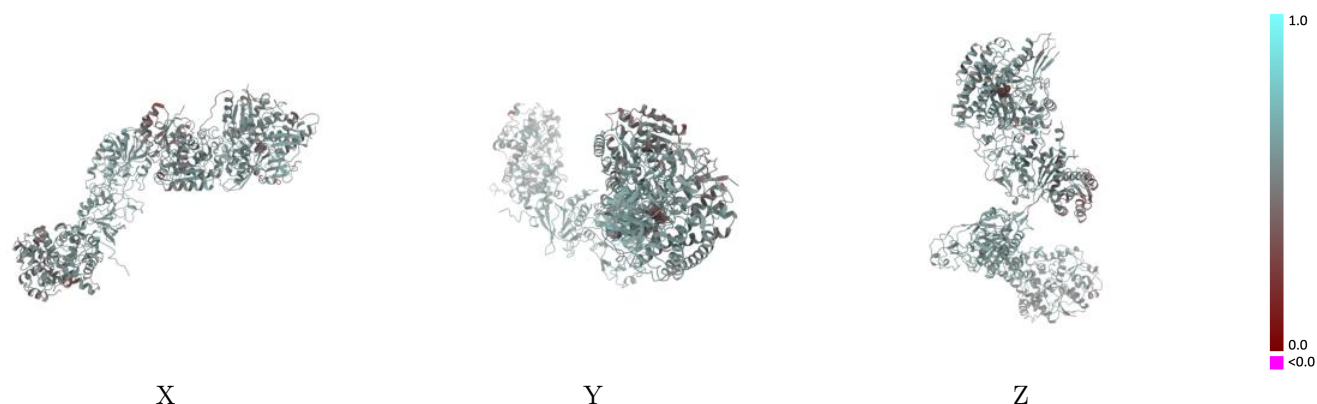


9.1.2 Map-model assembly overlay [i](#)



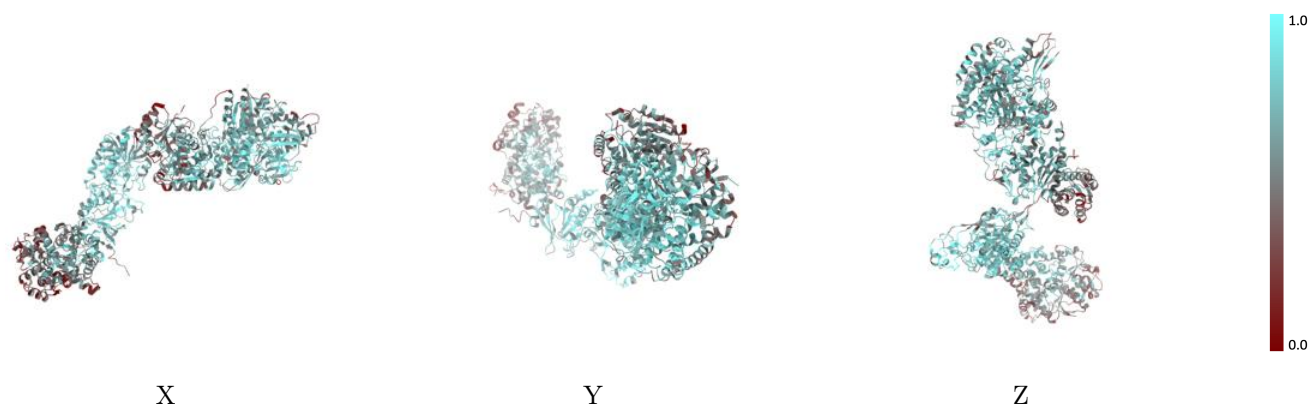
The images above show the 3D surface view of the map at the recommended contour level 6.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



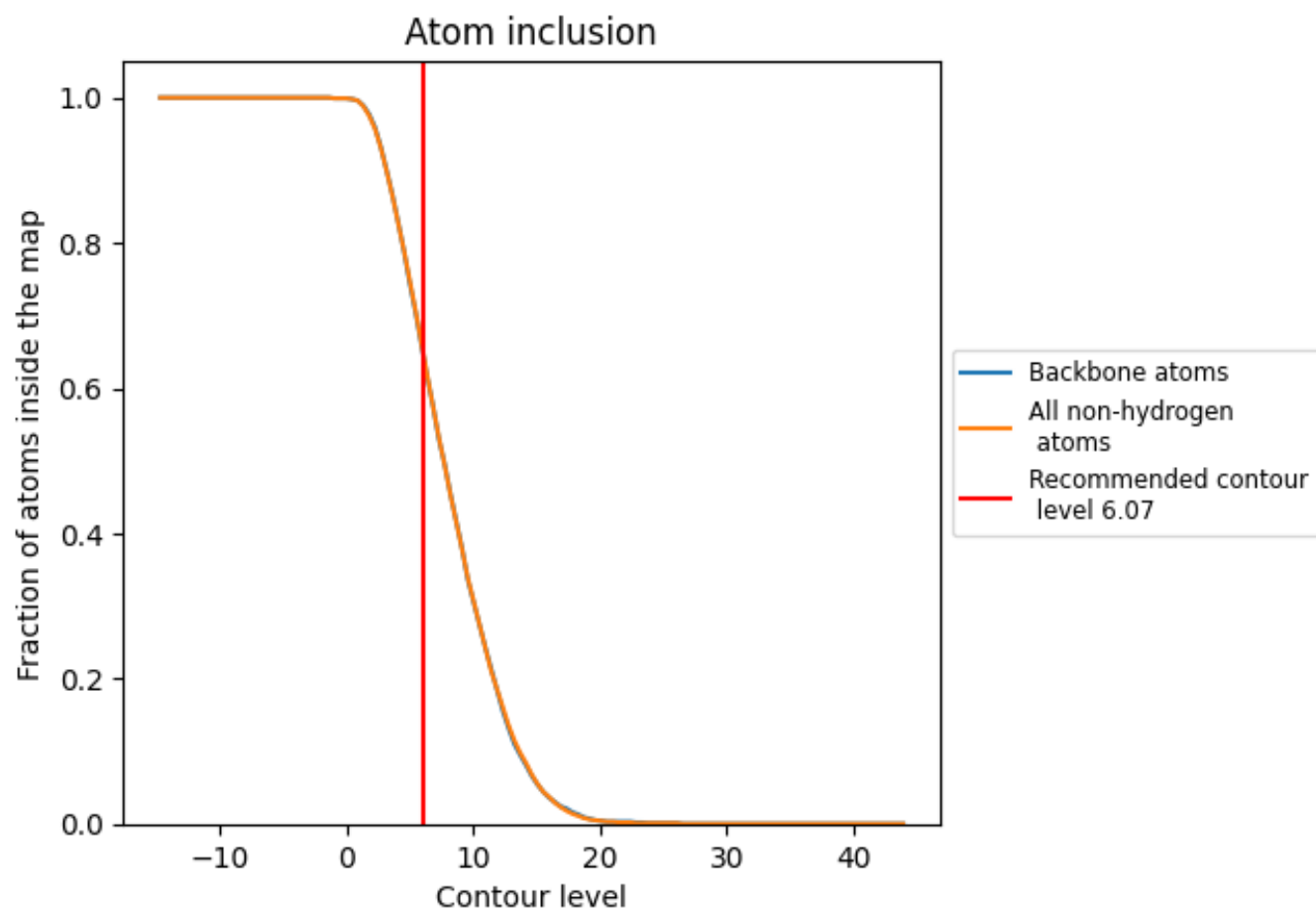
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (6.07).

9.4 Atom inclusion [i](#)



At the recommended contour level, 64% of all backbone atoms, 64% 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 (6.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.6450	<div><div></div></div> 0.5420
A	<div><div></div></div> 0.6880	<div><div></div></div> 0.5460
B	<div><div></div></div> 0.4900	<div><div></div></div> 0.5140
C	<div><div></div></div> 0.5190	<div><div></div></div> 0.5360
D	<div><div></div></div> 0.6460	<div><div></div></div> 0.5500
E	<div><div></div></div> 0.6810	<div><div></div></div> 0.5400
F	<div><div></div></div> 0.7230	<div><div></div></div> 0.5560

1.0

0.0

<0.0