



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 05:19 AM UTC

PDB ID : 7QV7 / pdb_00007qv7
EMDB ID : EMD-14169
Title : Cryo-EM structure of Hydrogen-dependent CO2 reductase.
Authors : Dietrich, H.M.; Righetto, R.D.; Kumar, A.; Wietrzynski, W.; Schuller, S.K.;
Trischler, R.; Wagner, J.; Schwarz, F.M.; Engel, B.D.; Mueller, V.; Schuller,
J.M.
Deposited on : 2022-01-19
Resolution : 3.40 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

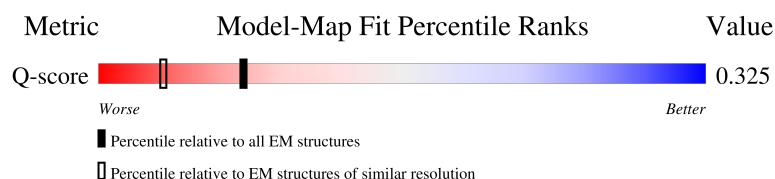
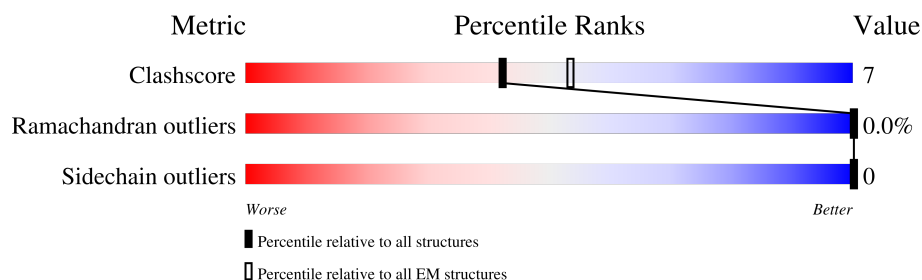
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 3.40 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	14717 (2.90 - 3.90)

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	184	80% 14% 5%
1	G	184	77% 17% • 5%
2	B	210	78% 9% 13%
2	C	210	75% 12% 13%

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Mol	Chain	Length	Quality of chain
2	J	210	
2	N	210	
2	P	210	
2	X	210	
3	D	461	
3	K	461	
3	Q	461	
3	R	461	
3	V	461	
3	Z	461	
4	S	743	
4	Y	743	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	SF4	C	304	-	-	X	-
5	SF4	S	801	-	-	X	-
5	SF4	V	504	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 41236 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Hydrogen dependent carbon dioxide reductase subunit HycB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	174	Total	C	N	O	S	0	0
			1338	844	225	250	19		
1	G	174	Total	C	N	O	S	0	0
			1338	844	225	250	19		

- Molecule 2 is a protein called Hydrogen dependent carbon dioxide reductase subunit HycB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	183	Total	C	N	O	S	0	0
			1378	866	245	248	19		
2	C	183	Total	C	N	O	S	0	0
			1378	866	245	248	19		
2	J	183	Total	C	N	O	S	0	0
			1378	866	245	248	19		
2	N	183	Total	C	N	O	S	0	0
			1378	866	245	248	19		
2	P	183	Total	C	N	O	S	0	0
			1378	866	245	248	19		
2	X	183	Total	C	N	O	S	0	0
			1378	866	245	248	19		

- Molecule 3 is a protein called Hydrogen dependent carbon dioxide reductase subunit HydA2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	448	Total	C	N	O	S	0	0
			3486	2208	592	660	26		
3	K	448	Total	C	N	O	S	0	0
			3486	2208	592	660	26		
3	Q	448	Total	C	N	O	S	0	0
			3486	2208	592	660	26		
3	R	448	Total	C	N	O	S	0	0
			3486	2208	592	660	26		
3	V	448	Total	C	N	O	S	0	0
			3486	2208	592	660	26		

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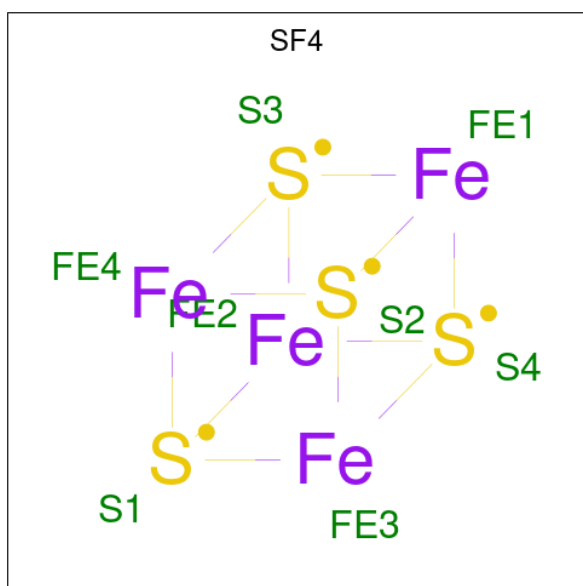
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Mol	Chain	Residues	Atoms					AltConf	Trace
3	Z	448	Total	C	N	O	S	0	0
			3486	2208	592	660	26		

- Molecule 4 is a protein called Hydrogen dependent carbon dioxide reductase subunit FdhF.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	S	571	Total	C	N	O	S	0	0
			4429	2819	768	818	24		
4	Y	571	Total	C	N	O	S	0	0
			4429	2819	768	818	24		

- Molecule 5 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



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

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Mol	Chain	Residues	Atoms			AltConf
5	B	1	Total 8	Fe 4	S 4	0
5	B	1	Total 8	Fe 4	S 4	0
5	C	1	Total 8	Fe 4	S 4	0
5	C	1	Total 8	Fe 4	S 4	0
5	C	1	Total 8	Fe 4	S 4	0
5	C	1	Total 8	Fe 4	S 4	0
5	D	1	Total 8	Fe 4	S 4	0
5	D	1	Total 8	Fe 4	S 4	0
5	D	1	Total 8	Fe 4	S 4	0
5	G	1	Total 8	Fe 4	S 4	0
5	G	1	Total 8	Fe 4	S 4	0
5	G	1	Total 8	Fe 4	S 4	0
5	G	1	Total 8	Fe 4	S 4	0
5	J	1	Total 8	Fe 4	S 4	0
5	J	1	Total 8	Fe 4	S 4	0
5	J	1	Total 8	Fe 4	S 4	0
5	J	1	Total 8	Fe 4	S 4	0
5	K	1	Total 8	Fe 4	S 4	0
5	K	1	Total 8	Fe 4	S 4	0
5	K	1	Total 8	Fe 4	S 4	0
5	N	1	Total 8	Fe 4	S 4	0

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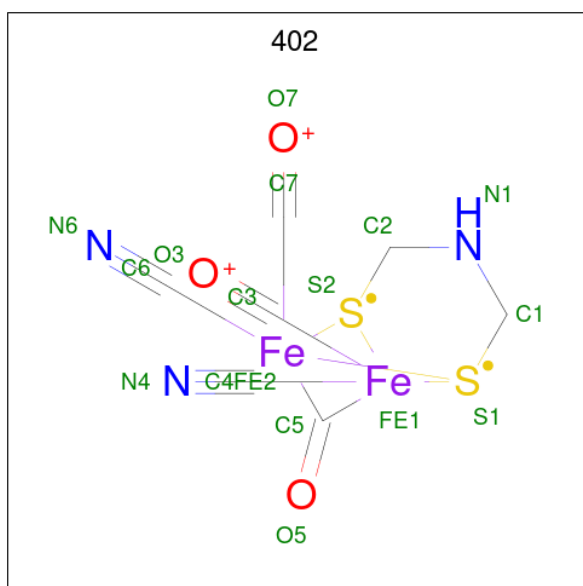
Mol	Chain	Residues	Atoms			AltConf
5	N	1	Total 8	Fe 4	S 4	0
5	N	1	Total 8	Fe 4	S 4	0
5	N	1	Total 8	Fe 4	S 4	0
5	P	1	Total 8	Fe 4	S 4	0
5	P	1	Total 8	Fe 4	S 4	0
5	P	1	Total 8	Fe 4	S 4	0
5	P	1	Total 8	Fe 4	S 4	0
5	Q	1	Total 8	Fe 4	S 4	0
5	Q	1	Total 8	Fe 4	S 4	0
5	Q	1	Total 8	Fe 4	S 4	0
5	R	1	Total 8	Fe 4	S 4	0
5	R	1	Total 8	Fe 4	S 4	0
5	R	1	Total 8	Fe 4	S 4	0
5	S	1	Total 8	Fe 4	S 4	0
5	V	1	Total 8	Fe 4	S 4	0
5	V	1	Total 8	Fe 4	S 4	0
5	V	1	Total 8	Fe 4	S 4	0
5	X	1	Total 8	Fe 4	S 4	0
5	X	1	Total 8	Fe 4	S 4	0
5	X	1	Total 8	Fe 4	S 4	0
5	X	1	Total 8	Fe 4	S 4	0

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Mol	Chain	Residues	Atoms			AltConf
5	Y	1	Total	Fe	S	0
			8	4	4	
5	Z	1	Total	Fe	S	0
			8	4	4	
5	Z	1	Total	Fe	S	0
			8	4	4	
5	Z	1	Total	Fe	S	0
			8	4	4	

- Molecule 6 is dicarbonyl[bis(cyanide-kappaC)]-mu-(iminodimethanethiolato-1kappaS:2kappaS)-mu-(oxomethylidene)diiron(2+) (CCD ID: 402) (formula: $C_7H_5Fe_2N_3O_3S_2$) (labeled as "Ligand of Interest" by depositor).

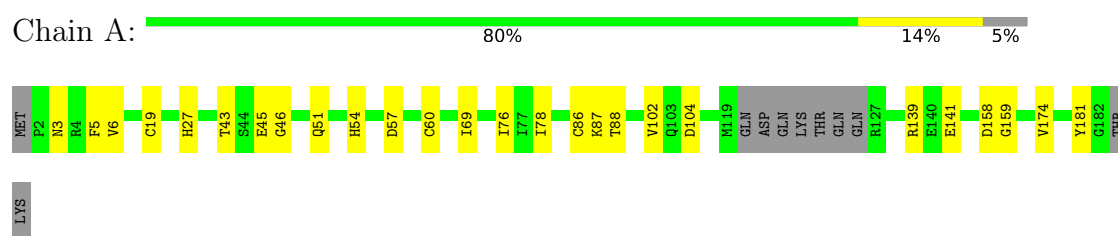


Mol	Chain	Residues	Atoms						AltConf
6	D	1	Total	C	Fe	N	O	S	0
			17	7	2	3	3	2	
6	K	1	Total	C	Fe	N	O	S	0
			17	7	2	3	3	2	
6	Q	1	Total	C	Fe	N	O	S	0
			17	7	2	3	3	2	
6	R	1	Total	C	Fe	N	O	S	0
			17	7	2	3	3	2	
6	V	1	Total	C	Fe	N	O	S	0
			17	7	2	3	3	2	
6	Z	1	Total	C	Fe	N	O	S	0
			17	7	2	3	3	2	

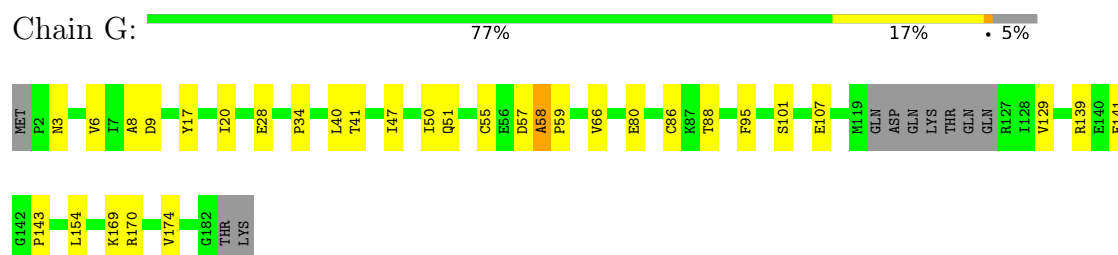
3 Residue-property plots

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.

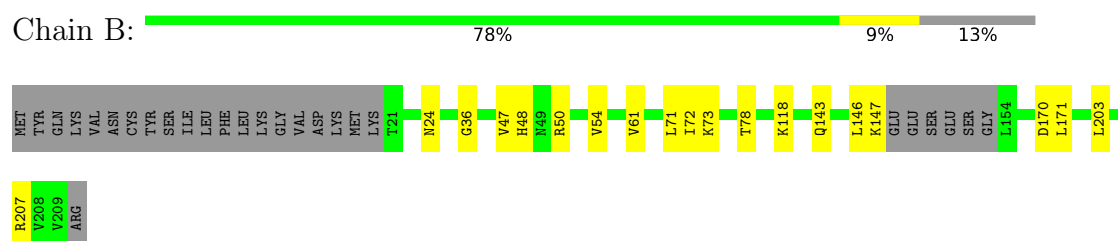
- Molecule 1: Hydrogen dependent carbon dioxide reductase subunit HycB3



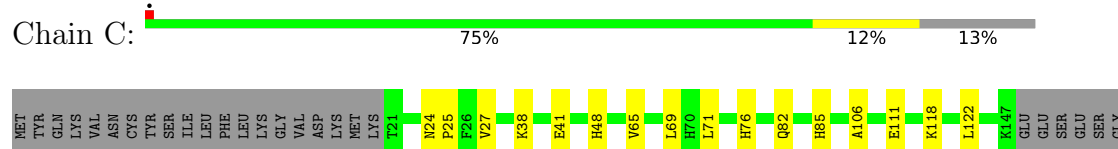
- Molecule 1: Hydrogen dependent carbon dioxide reductase subunit HycB3

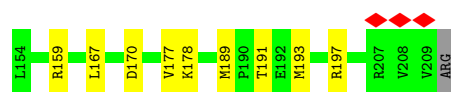


- Molecule 2: Hydrogen dependent carbon dioxide reductase subunit HycB4



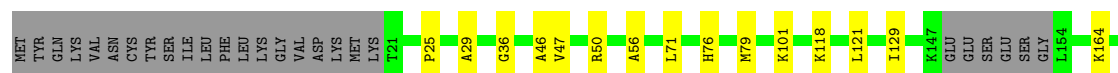
- Molecule 2: Hydrogen dependent carbon dioxide reductase subunit HycB4





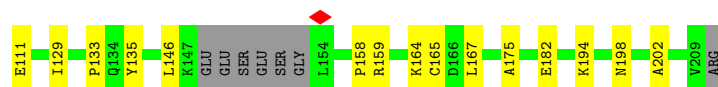
- Molecule 2: Hydrogen dependent carbon dioxide reductase subunit HycB4

Chain J: 78% 9% 13%



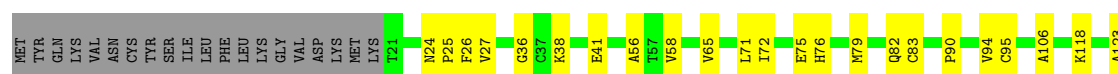
- Molecule 2: Hydrogen dependent carbon dioxide reductase subunit HycB4

Chain N: 70% 17% 13%



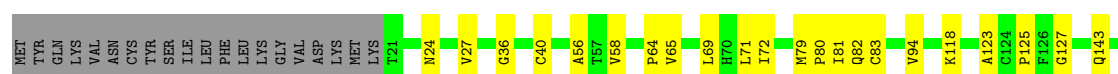
- Molecule 2: Hydrogen dependent carbon dioxide reductase subunit HycB4

Chain P: 72% 15% 13%



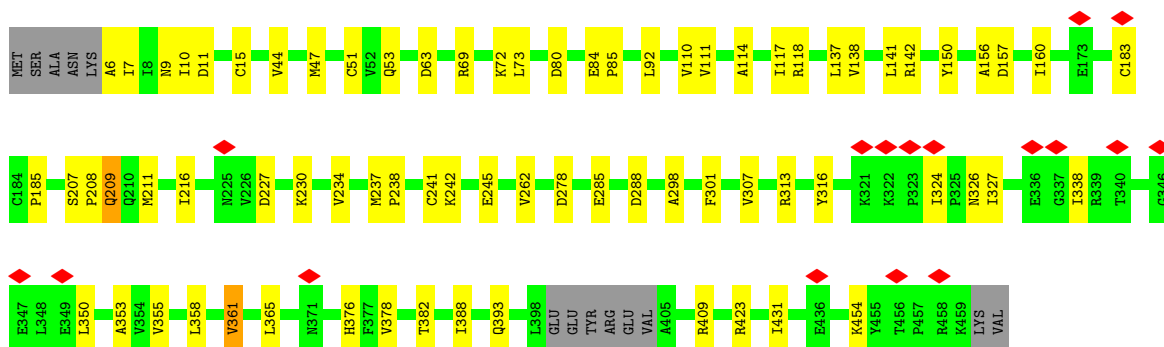
- Molecule 2: Hydrogen dependent carbon dioxide reductase subunit HycB4

Chain X: 74% 13% 13%

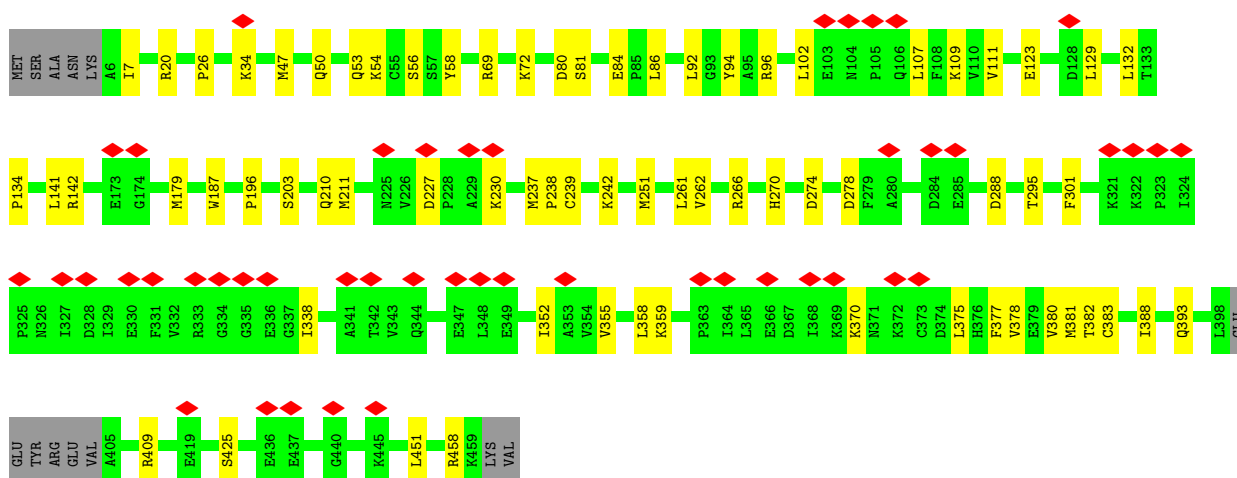
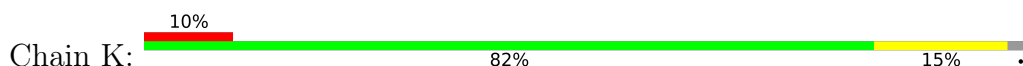


- Molecule 3: Hydrogen dependent carbon dioxide reductase subunit HydA2

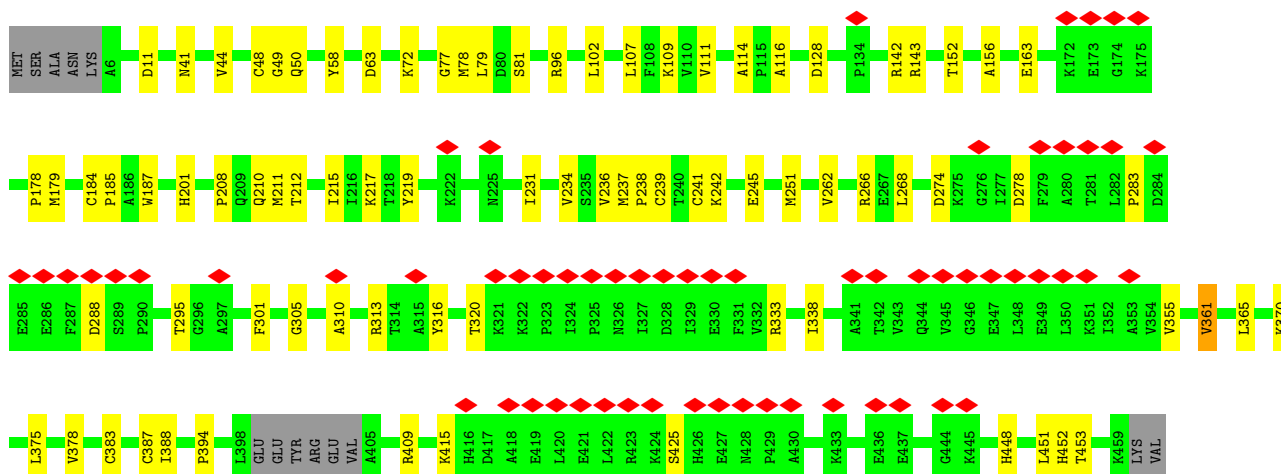
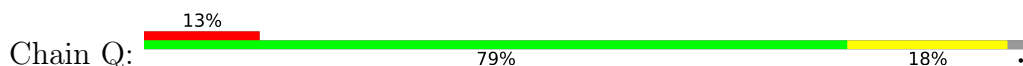
Chain D: 81% 16% 3%



• Molecule 3: Hydrogen dependent carbon dioxide reductase subunit HydA2

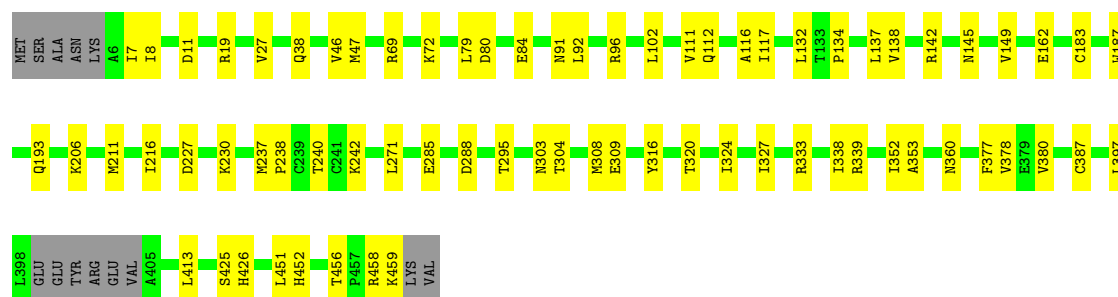


• Molecule 3: Hydrogen dependent carbon dioxide reductase subunit HydA2



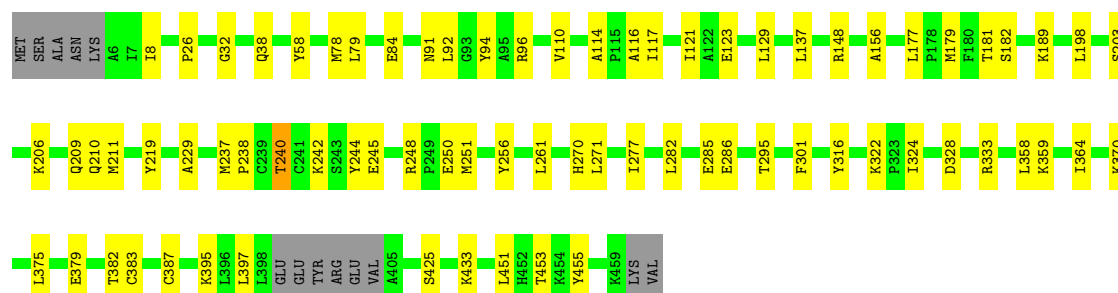
• Molecule 3: Hydrogen dependent carbon dioxide reductase subunit HydA2

Chain R:  82% 16%



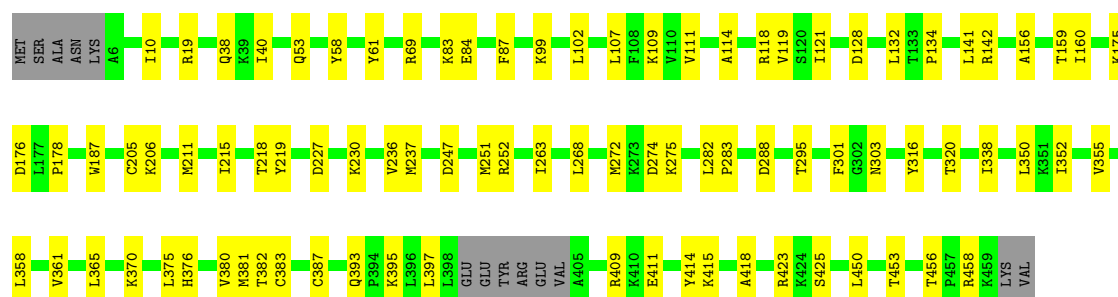
- Molecule 3: Hydrogen dependent carbon dioxide reductase subunit HydA2

Chain V:  81% 16%



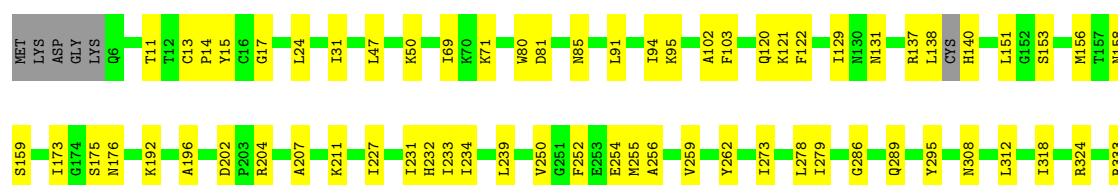
- Molecule 3: Hydrogen dependent carbon dioxide reductase subunit HydA2

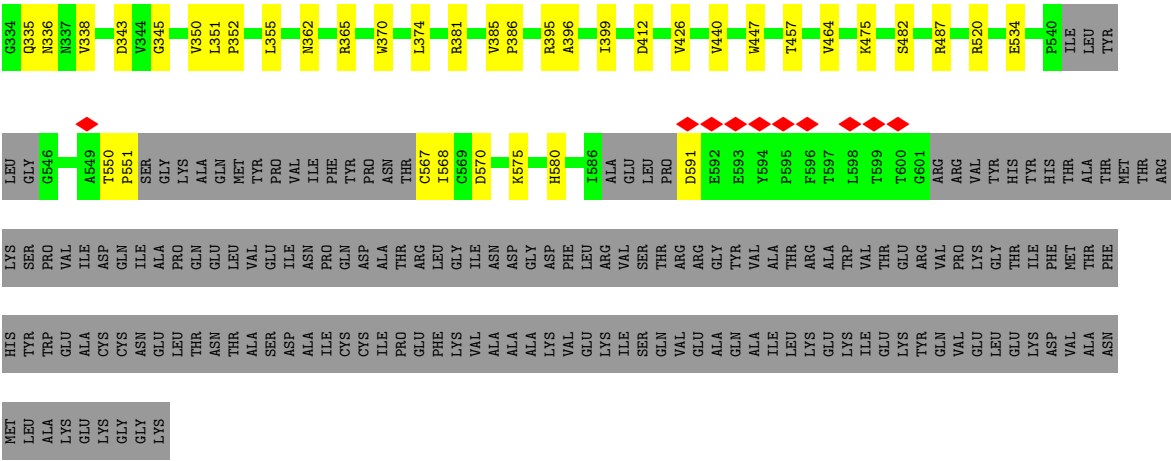
Chain Z:  78% 19%



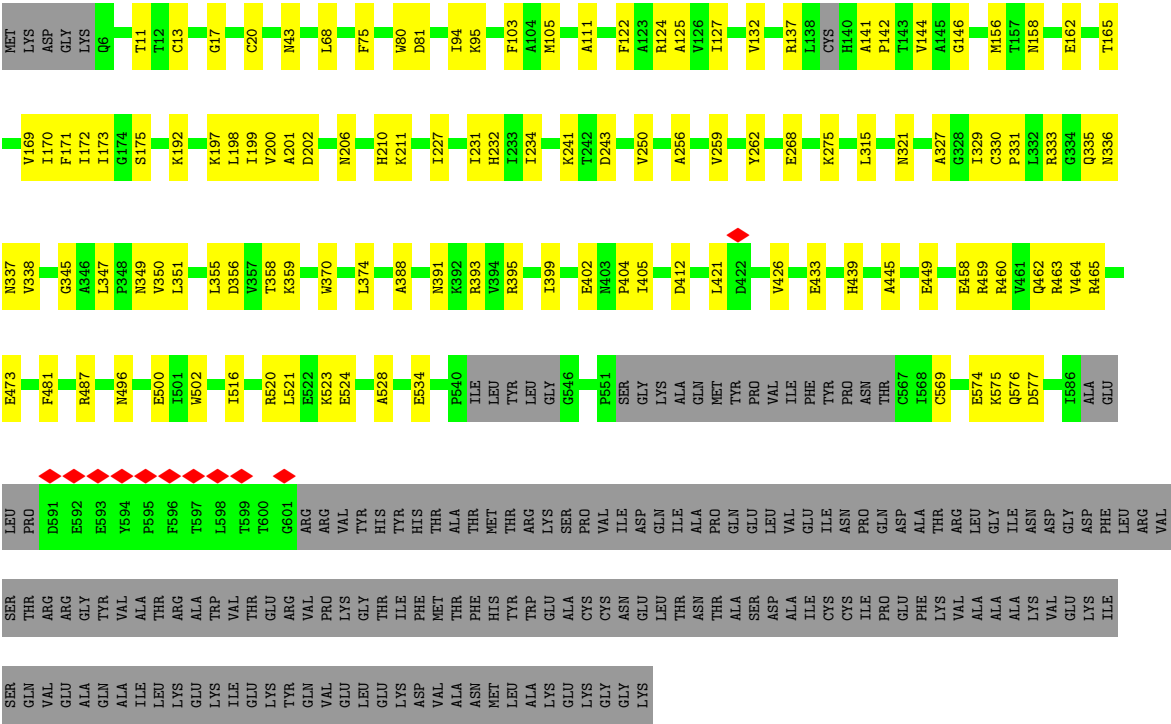
- Molecule 4: Hydrogen dependent carbon dioxide reductase subunit FdhF

Chain S:  63% 14% 23%





● Molecule 4: Hydrogen dependent carbon dioxide reductase subunit FdhF



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	719937	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 ($e^-/\text{\AA}^2$)	52	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	5500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.398	Depositor
Minimum map value	-0.780	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.029	Depositor
Recommended contour level	0.07	Depositor
Map size ($\text{\AA}$)	383.68002, 383.68002, 383.68002	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.09, 1.09, 1.09	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 402, 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	A	0.16	0/1359	0.39	0/1832
1	G	0.16	0/1359	0.42	0/1832
2	B	0.13	0/1400	0.35	0/1898
2	C	0.14	0/1400	0.40	0/1898
2	J	0.16	0/1400	0.36	0/1898
2	N	0.14	0/1400	0.37	0/1898
2	P	0.16	0/1400	0.38	0/1898
2	X	0.14	0/1400	0.35	0/1898
3	D	0.15	0/3548	0.43	4/4788 (0.1%)
3	K	0.13	0/3548	0.35	0/4788
3	Q	0.13	0/3548	0.40	2/4788 (0.0%)
3	R	0.14	0/3548	0.38	0/4788
3	V	0.17	0/3548	0.43	1/4788 (0.0%)
3	Z	0.14	0/3548	0.40	0/4788
4	S	0.15	0/4526	0.41	1/6136 (0.0%)
4	Y	0.13	0/4526	0.37	0/6136
All	All	0.14	0/41458	0.39	8/56052 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	D	0	1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Q	361	VAL	CA-C-N	6.66	124.43	120.24
3	Q	361	VAL	C-N-CA	6.66	124.43	120.24
3	D	361	VAL	CA-C-N	6.38	124.26	120.24
3	D	361	VAL	C-N-CA	6.38	124.26	120.24
3	D	209	GLN	CB-CA-C	6.00	120.79	110.23
3	D	44	VAL	N-CA-C	-5.58	107.84	113.20
3	V	240	THR	N-CA-C	-5.55	104.71	112.25
4	S	551	PRO	CA-N-CD	-5.18	104.74	112.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	208	PRO	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1338	0	1333	23	0
1	G	1338	0	1333	27	0
2	B	1378	0	1401	15	0
2	C	1378	0	1401	19	0
2	J	1378	0	1401	15	0
2	N	1378	0	1401	25	0
2	P	1378	0	1401	27	0
2	X	1378	0	1401	22	0
3	D	3486	0	3527	48	0
3	K	3486	0	3527	44	0
3	Q	3486	0	3527	50	0
3	R	3486	0	3527	42	0
3	V	3486	0	3527	49	0
3	Z	3486	0	3526	57	0
4	S	4429	0	4414	65	0
4	Y	4429	0	4414	71	0
5	A	32	0	0	2	0
5	B	32	0	0	1	0
5	C	32	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	24	0	0	1	0
5	G	32	0	0	1	0
5	J	32	0	0	0	0
5	K	24	0	0	1	0
5	N	32	0	0	1	0
5	P	32	0	0	2	0
5	Q	24	0	0	0	0
5	R	24	0	0	1	0
5	S	8	0	0	2	0
5	V	24	0	0	2	0
5	X	32	0	0	1	0
5	Y	8	0	0	1	0
5	Z	24	0	0	1	0
6	D	17	0	5	3	0
6	K	17	0	5	1	0
6	Q	17	0	5	2	0
6	R	17	0	5	2	0
6	V	17	0	5	3	0
6	Z	17	0	3	4	0
All	All	41236	0	41089	552	0

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

All (552) 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)
2:J:118:LYS:NZ	2:P:24:ASN:O	2.14	0.81
3:K:239:CYS:HB2	5:K:504:SF4:S3	2.26	0.74
4:Y:137:ARG:O	4:Y:141:ALA:HB2	1.89	0.71
3:Z:206:LYS:HB2	3:Z:211:MET:HE3	1.75	0.68
2:N:27:VAL:HG23	2:N:82:GLN:HE21	1.60	0.67
2:P:83:CYS:SG	2:P:164:LYS:NZ	2.68	0.66
4:S:399:ILE:HB	4:S:426:VAL:HG12	1.76	0.65
3:V:110:VAL:HG12	3:V:148:ARG:HB2	1.76	0.65
4:Y:13:CYS:HB3	5:Y:801:SF4:S4	2.37	0.65
4:Y:122:PHE:HD2	4:Y:481:PHE:HB3	1.62	0.65
4:Y:202:ASP:OD2	4:Y:206:ASN:ND2	2.30	0.64
3:R:316:TYR:HE2	3:R:324:ILE:HD12	1.62	0.64
4:Y:175:SER:O	4:Y:206:ASN:ND2	2.31	0.64
3:Q:78:MET:HE3	3:Q:79:LEU:H	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:50:GLN:NE2	3:K:383:CYS:SG	2.70	0.64
2:C:76:HIS:HB2	2:X:206:LEU:HD13	1.79	0.63
3:Z:159:THR:OG1	3:Z:205:CYS:SG	2.57	0.63
4:S:158:ASN:OD1	4:S:159:SER:N	2.32	0.63
1:G:174:VAL:HG13	2:X:79:MET:HE2	1.81	0.63
3:V:358:LEU:HD13	3:V:382:THR:HG22	1.80	0.63
3:Z:338:ILE:HG22	3:Z:355:VAL:HG12	1.79	0.63
3:Z:114:ALA:O	3:Z:118:ARG:NH1	2.32	0.62
3:Q:50:GLN:NE2	3:Q:383:CYS:SG	2.72	0.62
4:Y:335:GLN:HB2	4:Y:338:VAL:HG23	1.82	0.62
3:V:211:MET:HG2	3:V:451:LEU:HD22	1.81	0.62
4:S:129:ILE:HG23	4:S:131:ASN:H	1.63	0.62
2:C:27:VAL:HG23	2:C:82:GLN:HE21	1.64	0.62
3:R:295:THR:HG21	3:R:425:SER:HA	1.81	0.61
1:G:3:ASN:O	2:X:118:LYS:NZ	2.33	0.61
4:S:13:CYS:HB3	5:S:801:SF4:S4	2.39	0.61
3:V:387:CYS:CB	6:V:503:402:C4	2.78	0.61
1:A:19:CYS:HB3	5:A:201:SF4:S3	2.39	0.61
2:B:36:GLY:HA2	2:B:71:LEU:HD11	1.83	0.61
3:Q:338:ILE:HG22	3:Q:355:VAL:HG12	1.81	0.60
2:B:48:HIS:CD2	5:B:304:SF4:S1	2.84	0.60
4:Y:459:ARG:HG2	4:Y:528:ALA:HB1	1.84	0.60
3:Z:19:ARG:NH1	3:Z:38:GLN:OE1	2.34	0.60
2:N:33:LYS:NZ	2:N:182:GLU:O	2.35	0.60
4:S:91:LEU:HD13	4:S:94:ILE:HD11	1.84	0.60
4:S:232:HIS:ND1	4:S:262:TYR:O	2.34	0.60
4:S:239:LEU:HD13	4:S:286:GLY:HA3	1.84	0.59
3:Z:132:LEU:HG	3:Z:134:PRO:HD3	1.82	0.59
3:Q:116:ALA:HB3	3:Q:238:PRO:HG2	1.85	0.59
3:Z:301:PHE:HB3	6:Z:504:402:H11	1.84	0.59
4:S:103:PHE:HB3	4:S:396:ALA:HB3	1.84	0.59
4:Y:405:ILE:HG21	4:Y:433:GLU:HB3	1.84	0.59
4:S:14:PRO:O	4:S:336:ASN:ND2	2.36	0.58
3:Z:69:ARG:HH12	3:Z:83:LYS:HG2	1.68	0.58
3:V:277:ILE:HD11	3:V:282:LEU:HD21	1.86	0.58
4:Y:523:LYS:HG3	4:Y:524:GLU:HG2	1.86	0.58
4:Y:172:ILE:HD13	4:Y:200:VAL:HG22	1.86	0.58
3:Z:387:CYS:CB	6:Z:504:402:C4	2.82	0.58
3:V:248:ARG:HB2	3:V:251:MET:HB2	1.86	0.58
3:V:219:TYR:OH	3:V:433:LYS:NZ	2.37	0.57
2:P:38:LYS:HG3	2:P:71:LEU:HD13	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:106:ALA:HB2	2:C:167:LEU:HD13	1.86	0.57
3:D:338:ILE:HG22	3:D:355:VAL:HG12	1.86	0.57
3:Q:355:VAL:HG21	3:Q:361:VAL:HG22	1.86	0.57
3:V:209:GLN:HB3	3:V:237:MET:HE3	1.86	0.57
3:Z:381:MET:HE1	6:Z:504:402:H7	1.85	0.57
2:C:24:ASN:ND2	2:C:85:HIS:O	2.38	0.57
2:X:58:VAL:HB	3:Z:395:LYS:HB2	1.86	0.57
4:Y:20:CYS:HB3	4:Y:43:ASN:HD22	1.69	0.57
3:Q:370:LYS:HG3	3:Q:375:LEU:HD12	1.85	0.57
3:Z:383:CYS:HB2	5:Z:503:SF4:S3	2.45	0.57
3:V:382:THR:OG1	5:V:504:SF4:S4	2.63	0.57
3:Z:53:GLN:NE2	3:Z:393:GLN:O	2.37	0.57
3:D:11:ASP:OD2	3:D:72:LYS:NZ	2.37	0.57
2:P:173:GLU:OE2	2:P:178:LYS:NZ	2.35	0.57
3:K:266:ARG:O	3:K:270:HIS:ND1	2.30	0.56
3:K:20:ARG:HE	2:N:37:CYS:HB2	1.70	0.56
2:C:38:LYS:HG3	2:C:71:LEU:HD13	1.87	0.56
4:S:15:TYR:HB3	4:S:50:LYS:HD2	1.88	0.56
3:V:328:ASP:OD1	3:V:333:ARG:NH1	2.39	0.56
4:Y:156:MET:HG3	4:Y:330:CYS:HA	1.86	0.56
3:Z:175:LYS:NZ	3:Z:176:ASP:OD2	2.38	0.56
3:Q:11:ASP:OD2	3:Q:72:LYS:NZ	2.39	0.56
3:D:350:LEU:HB3	3:D:376:HIS:HD2	1.70	0.56
3:K:196:PRO:O	3:K:458:ARG:NH1	2.38	0.56
4:Y:520:ARG:NH1	4:Y:534:GLU:O	2.39	0.56
3:D:157:ASP:HB3	3:D:431:ILE:HD11	1.87	0.56
3:V:210:GLN:NE2	3:V:245:GLU:OE1	2.37	0.56
4:Y:232:HIS:ND1	4:Y:262:TYR:O	2.37	0.56
2:P:41:GLU:OE1	3:V:58:TYR:OH	2.23	0.56
3:K:26:PRO:HA	3:K:359:LYS:HE3	1.88	0.56
3:Q:236:VAL:HG21	3:Q:268:LEU:HD22	1.87	0.56
3:Q:251:MET:HE1	3:Q:453:THR:HG21	1.88	0.56
2:B:50:ARG:HH21	2:B:54:VAL:HG23	1.71	0.56
3:D:110:VAL:HG11	3:D:216:ILE:HG21	1.88	0.56
3:R:69:ARG:NH2	3:R:84:GLU:O	2.39	0.56
4:Y:402:GLU:HG3	4:Y:404:PRO:HD3	1.88	0.56
3:R:142:ARG:NH2	3:R:288:ASP:OD1	2.39	0.55
4:S:520:ARG:NH1	4:S:534:GLU:O	2.39	0.55
2:C:25:PRO:HG2	2:C:167:LEU:HD11	1.88	0.55
3:R:187:TRP:CG	3:R:380:VAL:HG21	2.41	0.55
4:S:362:ASN:HA	4:S:365:ARG:HE	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:6:VAL:HG13	1:G:51:GLN:HE21	1.72	0.55
3:K:295:THR:HG21	3:K:425:SER:HA	1.88	0.55
2:X:83:CYS:SG	2:X:164:LYS:NZ	2.76	0.55
3:R:80:ASP:OD1	3:R:96:ARG:NH1	2.38	0.55
4:Y:569:CYS:HB2	4:Y:574:GLU:HB3	1.88	0.55
3:Z:227:ASP:OD1	3:Z:230:LYS:NZ	2.37	0.55
3:D:183:CYS:C	6:D:503:402:H8	2.31	0.55
3:Q:210:GLN:NE2	3:Q:251:MET:O	2.40	0.55
3:Q:388:ILE:O	3:Q:409:ARG:NH1	2.40	0.55
3:R:183:CYS:HB3	6:R:503:402:H8	1.88	0.55
1:A:3:ASN:O	2:P:118:LYS:NZ	2.40	0.55
3:Q:361:VAL:HG12	3:Q:365:LEU:HB2	1.89	0.54
4:S:256:ALA:HA	4:S:259:VAL:HG12	1.90	0.54
4:Y:169:VAL:HG22	4:Y:197:LYS:HB2	1.89	0.54
1:A:57:ASP:OD1	2:P:143:GLN:NE2	2.39	0.54
1:A:69:ILE:HG12	1:A:78:ILE:HD12	1.89	0.54
4:Y:463:ARG:HG2	4:Y:521:LEU:HG	1.88	0.54
3:Z:456:THR:OG1	3:Z:458:ARG:NH1	2.41	0.54
2:C:122:LEU:HD23	2:X:193:MET:HE1	1.90	0.54
1:A:57:ASP:HA	2:P:143:GLN:HE22	1.72	0.54
2:C:25:PRO:HB3	2:C:189:MET:HB2	1.90	0.54
3:Z:121:ILE:HD11	3:Z:272:MET:HE1	1.89	0.54
3:D:47:MET:HG3	3:D:241:CYS:HA	1.90	0.54
2:C:118:LYS:NZ	2:X:24:ASN:O	2.31	0.54
3:D:183:CYS:O	6:D:503:402:H8	2.08	0.54
2:J:56:ALA:HA	3:R:397:LEU:HD12	1.88	0.54
4:S:121:LYS:NZ	4:S:370:TRP:O	2.41	0.54
4:Y:144:VAL:HB	4:Y:333:ARG:HH22	1.71	0.54
4:Y:399:ILE:HB	4:Y:426:VAL:HG12	1.90	0.54
3:Z:393:GLN:OE1	3:Z:409:ARG:NH1	2.41	0.54
4:S:17:GLY:HA2	4:S:336:ASN:HA	1.89	0.53
3:Z:215:ILE:HG23	3:Z:219:TYR:HB3	1.90	0.53
3:Q:310:ALA:HA	3:Q:313:ARG:HD2	1.89	0.53
2:J:129:ILE:HG12	2:J:164:LYS:HB3	1.90	0.53
3:Q:185:PRO:HG3	3:Q:245:GLU:HB2	1.89	0.53
3:Q:387:CYS:HB2	6:Q:504:402:C4	2.38	0.53
4:Y:111:ALA:O	4:Y:337:ASN:ND2	2.28	0.53
3:D:7:ILE:HG13	3:D:92:LEU:HB3	1.90	0.53
4:S:156:MET:HE3	4:S:158:ASN:H	1.72	0.53
1:A:5:PHE:HE1	2:P:118:LYS:HD2	1.74	0.53
2:B:72:ILE:HD13	2:N:198:ASN:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:185:PRO:HG2	3:Q:241:CYS:HB2	1.90	0.53
3:K:7:ILE:HG12	3:K:92:LEU:HD22	1.91	0.53
4:Y:17:GLY:HA2	4:Y:336:ASN:HA	1.91	0.53
4:Y:463:ARG:O	4:Y:465:ARG:NH1	2.42	0.53
2:N:106:ALA:HB2	2:N:167:LEU:HD23	1.90	0.53
4:S:102:ALA:HB1	4:S:395:ARG:HB2	1.91	0.53
3:Z:350:LEU:HB3	3:Z:352:ILE:HD11	1.91	0.53
2:B:47:VAL:HG22	2:B:171:LEU:HD13	1.91	0.53
3:R:387:CYS:CB	6:R:503:402:C4	2.88	0.52
3:Z:247:ASP:HA	3:Z:252:ARG:HH22	1.74	0.52
3:D:313:ARG:HH12	3:D:326:ASN:H	1.57	0.52
2:P:36:GLY:HA2	2:P:71:LEU:HD11	1.92	0.52
3:Z:370:LYS:HG3	3:Z:375:LEU:HD12	1.91	0.52
1:A:43:THR:OG1	1:A:46:GLY:O	2.26	0.52
2:C:27:VAL:O	2:C:82:GLN:NE2	2.43	0.52
3:K:237:MET:HG3	3:K:242:LYS:HG3	1.90	0.52
4:S:69:ILE:HG22	4:S:440:VAL:HG13	1.91	0.52
3:Q:48:CYS:SG	3:Q:49:GLY:N	2.83	0.52
3:V:94:TYR:HB3	3:V:261:LEU:HD13	1.91	0.52
3:Z:114:ALA:HB2	3:Z:237:MET:HB2	1.91	0.52
4:S:231:ILE:HG21	4:S:255:MET:HE2	1.92	0.52
2:X:71:LEU:HA	2:X:80:PRO:HA	1.92	0.52
1:A:27:HIS:NE2	5:A:204:SF4:S4	2.70	0.52
3:K:132:LEU:HG	3:K:134:PRO:HD3	1.91	0.52
3:K:142:ARG:NH2	3:K:288:ASP:OD1	2.42	0.52
1:A:174:VAL:HG22	2:P:79:MET:HE3	1.91	0.52
2:J:46:ALA:O	2:J:50:ARG:NH1	2.42	0.52
3:R:8:ILE:HD11	3:R:240:THR:HG21	1.91	0.52
3:K:370:LYS:HG3	3:K:375:LEU:HD12	1.92	0.51
3:Q:305:GLY:O	3:Q:333:ARG:NH1	2.43	0.51
3:R:338:ILE:HD11	3:R:360:ASN:HB3	1.92	0.51
3:V:78:MET:O	3:V:96:ARG:NH1	2.42	0.51
1:A:46:GLY:H	4:Y:210:HIS:CE1	2.28	0.51
3:Q:239:CYS:HB3	3:Q:242:LYS:HG2	1.92	0.51
3:R:11:ASP:OD2	3:R:72:LYS:NZ	2.43	0.51
3:V:198:LEU:HD13	3:V:370:LYS:HZ3	1.75	0.51
3:Z:236:VAL:HG11	3:Z:268:LEU:HD22	1.92	0.51
3:D:63:ASP:OD1	3:D:63:ASP:N	2.44	0.51
3:K:72:LYS:HD3	3:K:86:LEU:HD12	1.92	0.51
4:Y:391:ASN:ND2	4:Y:391:ASN:O	2.44	0.51
1:G:50:ILE:HD11	2:J:202:ALA:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:56:ALA:HA	3:V:397:LEU:HD12	1.92	0.51
3:K:69:ARG:NH2	3:K:84:GLU:O	2.44	0.51
3:Q:387:CYS:CB	6:Q:504:402:C4	2.89	0.51
4:S:102:ALA:O	4:S:396:ALA:N	2.41	0.51
4:S:231:ILE:HA	4:S:234:ILE:HG12	1.91	0.51
4:S:333:ARG:HB2	4:S:457:THR:HG22	1.92	0.51
3:V:116:ALA:HB3	3:V:238:PRO:HG2	1.93	0.51
3:R:132:LEU:HG	3:R:134:PRO:HD3	1.93	0.51
4:S:175:SER:H	4:S:202:ASP:HB3	1.76	0.51
4:Y:158:ASN:O	4:Y:459:ARG:NH1	2.36	0.51
3:D:117:ILE:HG22	3:D:137:LEU:HD11	1.93	0.51
4:S:153:SER:OG	4:S:570:ASP:OD2	2.29	0.51
3:K:338:ILE:HG22	3:K:355:VAL:HG12	1.91	0.50
4:S:138:LEU:O	4:S:140:HIS:N	2.44	0.50
2:P:106:ALA:HB2	2:P:167:LEU:HD23	1.91	0.50
3:R:227:ASP:OD1	3:R:230:LYS:NZ	2.42	0.50
4:S:173:ILE:HB	4:S:295:TYR:HB3	1.92	0.50
2:X:40:CYS:HB3	5:X:301:SF4:S3	2.51	0.50
2:C:48:HIS:NE2	5:C:304:SF4:S1	2.74	0.50
3:D:242:LYS:NZ	6:D:503:402:S2	2.77	0.50
3:R:116:ALA:HB3	3:R:238:PRO:HG2	1.92	0.50
4:Y:11:THR:HG23	4:Y:464:VAL:HG13	1.92	0.50
1:G:9:ASP:N	1:G:9:ASP:OD1	2.42	0.50
4:S:120:GLN:HE22	4:S:352:PRO:HD3	1.77	0.50
4:Y:241:LYS:HZ3	4:Y:243:ASP:HB2	1.77	0.50
1:G:95:PHE:O	2:J:198:ASN:ND2	2.44	0.50
3:V:206:LYS:HB2	3:V:211:MET:HE3	1.94	0.50
3:D:111:VAL:HG11	3:D:141:LEU:HD22	1.94	0.50
3:D:207:SER:O	3:D:211:MET:HG2	2.12	0.50
1:A:5:PHE:CE1	2:P:118:LYS:HD2	2.47	0.50
3:K:107:LEU:O	3:K:109:LYS:NZ	2.40	0.50
3:Z:142:ARG:NH2	3:Z:288:ASP:OD1	2.45	0.50
2:X:176:CYS:HB2	2:X:185:LEU:HD13	1.92	0.49
3:V:206:LYS:HD3	3:V:251:MET:HE1	1.95	0.49
3:Z:282:LEU:HD12	3:Z:283:PRO:HD2	1.92	0.49
3:K:20:ARG:NH1	3:K:54:LYS:O	2.45	0.49
3:Q:266:ARG:HD3	3:Q:394:PRO:HA	1.94	0.49
3:V:285:GLU:HG2	3:V:286:GLU:H	1.77	0.49
2:B:170:ASP:N	2:B:170:ASP:OD1	2.45	0.49
3:Q:81:SER:OG	3:Q:274:ASP:OD1	2.30	0.49
3:Q:242:LYS:HB2	3:Q:262:VAL:HG21	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:327:ILE:HD12	3:R:327:ILE:H	1.77	0.49
1:A:6:VAL:O	1:A:51:GLN:NE2	2.46	0.49
3:Q:375:LEU:HD22	3:Q:378:VAL:HG21	1.93	0.49
4:S:151:LEU:HB3	4:S:568:ILE:HD11	1.94	0.49
4:S:254:GLU:O	4:S:580:HIS:NE2	2.46	0.49
4:Y:370:TRP:HD1	4:Y:374:LEU:HD21	1.77	0.49
2:X:36:GLY:HA2	2:X:71:LEU:HD11	1.94	0.49
4:Y:94:ILE:HG23	4:Y:395:ARG:HE	1.77	0.49
3:Z:361:VAL:HG12	3:Z:365:LEU:HB2	1.95	0.49
3:K:123:GLU:HG2	3:K:129:LEU:HA	1.95	0.49
3:R:304:THR:OG1	3:R:339:ARG:NH2	2.45	0.49
1:A:45:GLU:OE2	2:B:207:ARG:NH1	2.46	0.48
3:K:81:SER:OG	3:K:274:ASP:OD1	2.31	0.48
2:P:129:ILE:HD11	2:P:162:ALA:HB1	1.94	0.48
4:S:192:LYS:NZ	4:S:211:LYS:O	2.46	0.48
4:S:412:ASP:OD1	4:S:412:ASP:N	2.46	0.48
3:D:353:ALA:HB3	3:D:378:VAL:HG22	1.95	0.48
4:Y:520:ARG:HE	4:Y:523:LYS:HZ1	1.61	0.48
4:Y:496:ASN:ND2	4:Y:500:GLU:OE2	2.46	0.48
3:Q:107:LEU:O	3:Q:109:LYS:NZ	2.42	0.48
4:Y:103:PHE:HZ	4:Y:127:ILE:HG21	1.78	0.48
4:Y:576:GLN:NE2	4:Y:577:ASP:O	2.46	0.48
3:R:308:MET:HE1	3:R:352:ILE:HD12	1.95	0.48
4:S:176:ASN:HB2	4:S:204:ARG:HH21	1.79	0.48
4:S:207:ALA:O	4:S:211:LYS:NZ	2.41	0.48
3:D:227:ASP:OD1	3:D:230:LYS:NZ	2.47	0.48
3:Q:128:ASP:OD1	3:Q:128:ASP:N	2.47	0.48
3:R:309:GLU:OE1	3:R:333:ARG:NH2	2.46	0.48
3:V:8:ILE:HD11	3:V:240:THR:HG21	1.96	0.48
4:S:335:GLN:HB2	4:S:338:VAL:HG23	1.95	0.48
2:J:36:GLY:HA2	2:J:71:LEU:HD11	1.95	0.48
3:Z:303:ASN:ND2	3:Z:414:TYR:OH	2.47	0.48
3:R:456:THR:OG1	3:R:458:ARG:NE	2.47	0.48
3:K:278:ASP:OD1	3:K:278:ASP:N	2.47	0.48
3:K:352:ILE:HG22	3:K:377:PHE:HB3	1.96	0.48
4:S:370:TRP:HE1	4:S:374:LEU:HD21	1.78	0.48
3:V:189:LYS:HD3	3:V:244:TYR:HE2	1.79	0.48
3:V:295:THR:HG21	3:V:425:SER:HA	1.96	0.48
4:S:289:GLN:OE1	4:S:324:ARG:NH2	2.47	0.47
1:G:28:GLU:HG3	1:G:34:PRO:HB3	1.96	0.47
3:Z:206:LYS:HE2	3:Z:453:THR:HB	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:V:316:TYR:CE2	3:V:324:ILE:HB	2.49	0.47
4:Y:81:ASP:OD1	4:Y:487:ARG:NH2	2.47	0.47
4:Y:388:ALA:HB1	4:Y:393:ARG:HB2	1.96	0.47
1:A:54:HIS:CE1	1:A:76:ILE:H	2.32	0.47
1:G:80:GLU:HG3	1:G:129:VAL:HG21	1.97	0.47
2:N:194:LYS:NZ	2:N:198:ASN:OD1	2.48	0.47
3:R:19:ARG:NH1	3:R:38:GLN:OE1	2.46	0.47
4:Y:421:LEU:HD11	4:Y:439:HIS:HB2	1.95	0.47
3:Z:295:THR:HG21	3:Z:425:SER:HA	1.97	0.47
3:Q:142:ARG:NH2	3:Q:288:ASP:OD1	2.47	0.47
4:S:343:ASP:OD1	4:S:343:ASP:N	2.48	0.47
3:V:383:CYS:HB2	5:V:504:SF4:S3	2.54	0.47
2:X:56:ALA:HA	3:Z:397:LEU:HD12	1.96	0.47
4:Y:68:LEU:HB3	4:Y:75:PHE:HB3	1.97	0.47
4:Y:227:ILE:HG13	4:Y:315:LEU:HD12	1.96	0.47
4:Y:329:ILE:HG22	4:Y:331:PRO:HD3	1.95	0.47
2:C:111:GLU:O	2:C:159:ARG:NH2	2.47	0.47
1:G:17:TYR:OH	1:G:107:GLU:OE2	2.32	0.47
1:G:57:ASP:O	2:X:143:GLN:NE2	2.44	0.47
2:P:58:VAL:HB	3:V:395:LYS:HB2	1.96	0.47
3:Q:295:THR:HG21	3:Q:425:SER:HA	1.96	0.47
3:R:303:ASN:OD1	3:R:304:THR:N	2.48	0.47
4:S:351:LEU:HB3	4:S:355:LEU:HB2	1.95	0.47
3:V:322:LYS:HE3	3:V:322:LYS:HA	1.95	0.47
3:V:364:ILE:HB	3:V:375:LEU:HD11	1.97	0.47
4:Y:162:GLU:O	4:Y:165:THR:OG1	2.31	0.47
4:Y:458:GLU:O	4:Y:459:ARG:HD3	2.14	0.47
3:Z:251:MET:O	3:Z:251:MET:HG3	2.15	0.47
3:Q:217:LYS:NZ	3:Q:231:ILE:O	2.47	0.47
3:R:206:LYS:HB2	3:R:211:MET:HE2	1.97	0.47
2:B:73:LYS:HZ2	2:B:78:THR:HG1	1.56	0.47
3:D:185:PRO:HG3	3:D:245:GLU:HB2	1.96	0.47
3:D:207:SER:HB2	3:D:209:GLN:HG3	1.96	0.47
3:D:242:LYS:HB2	3:D:262:VAL:HG21	1.95	0.47
2:P:75:GLU:OE2	2:P:76:HIS:ND1	2.48	0.47
4:S:14:PRO:HG3	4:S:447:TRP:CG	2.50	0.47
3:V:209:GLN:HE22	3:V:242:LYS:HB3	1.79	0.47
1:A:181:TYR:HE1	1:G:66:VAL:HG23	1.80	0.46
3:V:179:MET:HE2	3:V:203:SER:HB2	1.97	0.46
3:Q:77:GLY:HA2	3:Q:96:ARG:HH21	1.79	0.46
4:Y:137:ARG:O	4:Y:141:ALA:CB	2.62	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Z:102:LEU:HD23	3:Z:109:LYS:HD2	1.96	0.46
1:A:174:VAL:HG21	2:P:72:ILE:HG21	1.98	0.46
3:Z:107:LEU:O	3:Z:109:LYS:NZ	2.36	0.46
3:K:375:LEU:HD22	3:K:378:VAL:HG21	1.98	0.46
4:Y:321:ASN:HB3	4:Y:327:ALA:HB1	1.96	0.46
3:V:316:TYR:HE2	3:V:324:ILE:HB	1.80	0.46
2:J:29:ALA:HB3	2:J:79:MET:HE3	1.97	0.46
4:Y:80:TRP:HE1	4:Y:473:GLU:HB3	1.79	0.46
3:D:150:TYR:HE1	3:D:288:ASP:HB2	1.81	0.46
3:K:80:ASP:OD1	3:K:96:ARG:NH1	2.42	0.46
3:V:250:GLU:OE1	3:V:453:THR:OG1	2.33	0.46
4:Y:94:ILE:HD12	4:Y:395:ARG:HE	1.80	0.46
3:R:79:LEU:HD11	3:R:271:LEU:HD23	1.98	0.46
2:X:94:VAL:HG21	2:X:123:ALA:HB2	1.97	0.46
1:G:139:ARG:HD3	1:G:141:GLU:HB3	1.98	0.46
2:J:25:PRO:HG2	2:J:167:LEU:HD21	1.98	0.46
2:J:121:LEU:HD12	2:P:190:PRO:HB2	1.97	0.46
3:K:301:PHE:HB3	6:K:503:402:H11	1.98	0.46
2:B:118:LYS:NZ	2:N:85:HIS:O	2.46	0.45
3:D:51:CYS:HB3	5:D:502:SF4:S3	2.56	0.45
3:D:237:MET:HG3	3:D:242:LYS:HG3	1.96	0.45
1:G:170:ARG:HG3	2:X:81:ILE:HD11	1.98	0.45
2:P:94:VAL:HG21	2:P:123:ALA:HB2	1.98	0.45
3:Q:102:LEU:HD23	3:Q:109:LYS:HD2	1.98	0.45
3:V:91:ASN:OD1	3:V:92:LEU:N	2.50	0.45
4:Y:351:LEU:N	4:Y:355:LEU:O	2.46	0.45
1:G:8:ALA:HB2	1:G:154:LEU:HG	1.99	0.45
3:V:84:GLU:OE1	3:V:270:HIS:NE2	2.37	0.45
3:K:358:LEU:HB2	3:K:382:THR:HG23	1.97	0.45
3:K:102:LEU:HD23	3:K:109:LYS:HD2	1.98	0.45
3:Z:236:VAL:HG22	3:Z:263:ILE:HD11	1.98	0.45
1:A:158:ASP:OD1	1:A:159:GLY:N	2.41	0.45
3:D:388:ILE:O	3:D:409:ARG:NH1	2.49	0.45
3:K:111:VAL:HG11	3:K:141:LEU:HD22	1.98	0.45
2:N:133:PRO:HB3	2:N:158:PRO:HB2	1.98	0.45
4:S:351:LEU:HD23	4:S:355:LEU:HD12	1.99	0.45
4:Y:250:VAL:HG12	4:Y:575:LYS:HD3	1.99	0.45
4:Y:445:ALA:HB1	4:Y:449:GLU:HG3	1.98	0.45
3:Z:156:ALA:HB1	3:Z:301:PHE:CE2	2.51	0.45
2:B:147:LYS:HE2	2:N:103:GLU:HA	1.99	0.45
2:N:83:CYS:HB3	2:N:165:CYS:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:V:182:SER:HG	3:V:455:TYR:HH	1.54	0.45
3:D:316:TYR:HE2	3:D:324:ILE:HB	1.81	0.45
1:G:41:THR:HG21	2:J:198:ASN:HB3	1.98	0.45
3:V:121:ILE:HG21	3:V:137:LEU:HD12	1.99	0.45
1:A:86:CYS:O	1:A:88:THR:N	2.45	0.45
3:D:6:ALA:HA	3:D:9:ASN:HD21	1.82	0.45
3:D:454:LYS:HE3	3:D:454:LYS:HA	1.98	0.45
3:K:56:SER:OG	2:N:38:LYS:O	2.35	0.45
3:Q:278:ASP:OD1	3:Q:278:ASP:N	2.47	0.45
4:S:351:LEU:N	4:S:355:LEU:O	2.47	0.45
3:D:301:PHE:CD1	3:D:307:VAL:HG22	2.52	0.45
3:Q:63:ASP:OD1	3:Q:63:ASP:N	2.49	0.45
4:Y:268:GLU:HG3	4:Y:275:LYS:HB3	1.98	0.45
1:G:41:THR:HG21	1:G:50:ILE:HD12	1.99	0.44
3:Z:316:TYR:O	3:Z:320:THR:HG22	2.17	0.44
3:Z:387:CYS:HB2	6:Z:504:402:C4	2.46	0.44
2:C:69:LEU:HD23	5:C:304:SF4:S4	2.57	0.44
1:G:20:ILE:HD11	1:G:40:LEU:HB2	1.98	0.44
3:Q:111:VAL:HA	3:Q:234:VAL:O	2.17	0.44
4:S:227:ILE:HD12	4:S:312:LEU:HD23	1.99	0.44
2:X:64:PRO:HB3	3:Z:61:TYR:HE1	1.81	0.44
3:Z:99:LYS:NZ	3:Z:274:ASP:OD2	2.44	0.44
1:A:87:LYS:NZ	2:B:24:ASN:O	2.45	0.44
1:A:60:CYS:HB3	1:A:69:ILE:HD13	1.99	0.44
3:D:327:ILE:HD11	3:D:423:ARG:HG3	2.00	0.44
4:Y:171:PHE:HD1	4:Y:199:ILE:HB	1.82	0.44
2:B:54:VAL:HG12	2:B:61:VAL:HG22	1.99	0.44
3:K:34:LYS:HE3	3:K:34:LYS:HA	1.99	0.44
3:R:237:MET:HG3	3:R:242:LYS:HG3	1.98	0.44
4:Y:142:PRO:O	4:Y:146:GLY:N	2.51	0.44
3:Z:358:LEU:HB2	3:Z:382:THR:HG23	1.98	0.44
3:K:53:GLN:HE22	3:K:393:GLN:HB2	1.81	0.44
3:Q:143:ARG:HH12	3:Q:283:PRO:HD2	1.83	0.44
1:G:86:CYS:O	1:G:88:THR:N	2.49	0.44
2:N:69:LEU:HD23	5:N:304:SF4:S4	2.58	0.44
3:R:352:ILE:HG22	3:R:377:PHE:HB3	2.00	0.44
3:V:123:GLU:HG2	3:V:129:LEU:HA	2.00	0.44
3:D:69:ARG:NH1	3:D:84:GLU:O	2.51	0.44
1:G:55:CYS:HB2	1:G:58:ALA:HA	2.00	0.44
3:Q:215:ILE:HG23	3:Q:219:TYR:HB3	2.00	0.44
3:R:353:ALA:HB3	3:R:378:VAL:HG22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:S:80:TRP:CD1	4:S:475:LYS:HZ1	2.36	0.44
4:S:81:ASP:O	4:S:85:ASN:ND2	2.40	0.44
1:A:139:ARG:HD3	1:A:141:GLU:HB3	1.98	0.44
2:C:170:ASP:OD1	2:C:170:ASP:N	2.51	0.44
4:S:370:TRP:NE1	4:S:374:LEU:HD21	2.33	0.44
4:S:385:VAL:HG23	4:S:386:PRO:HD3	2.00	0.44
3:Z:111:VAL:HG11	3:Z:141:LEU:HD22	1.99	0.44
3:D:157:ASP:HA	3:D:160:ILE:HD12	2.00	0.43
3:K:187:TRP:CD1	3:K:380:VAL:HG21	2.53	0.43
4:S:273:ILE:HD11	4:S:278:LEU:HD11	2.00	0.43
3:Z:118:ARG:HG3	3:Z:119:VAL:HG13	2.00	0.43
3:Z:128:ASP:OD1	3:Z:128:ASP:N	2.50	0.43
3:K:227:ASP:OD1	3:K:230:LYS:NZ	2.47	0.43
3:Z:418:ALA:HA	3:Z:423:ARG:HH21	1.83	0.43
3:D:10:ILE:HD11	3:D:15:CYS:HB2	2.01	0.43
2:N:36:GLY:HA3	2:N:73:LYS:HZ3	1.82	0.43
2:N:129:ILE:HG22	2:N:164:LYS:HB3	2.00	0.43
3:Q:178:PRO:HG2	3:Q:201:HIS:CE1	2.52	0.43
3:Q:448:HIS:HA	3:Q:452:HIS:HB2	2.00	0.43
4:S:47:LEU:HB3	5:S:801:SF4:S2	2.58	0.43
4:S:137:ARG:HH12	4:S:381:ARG:HG2	1.84	0.43
4:Y:170:ILE:HB	4:Y:198:LEU:HD23	2.00	0.43
3:V:32:GLY:HA3	3:V:38:GLN:HG3	2.01	0.43
1:G:170:ARG:NH2	2:X:127:GLY:O	2.40	0.43
2:N:36:GLY:HA3	2:N:73:LYS:NZ	2.34	0.43
2:P:90:PRO:HD2	5:P:302:SF4:S1	2.59	0.43
3:Z:350:LEU:HA	3:Z:376:HIS:CD2	2.53	0.43
1:G:6:VAL:HG13	1:G:51:GLN:NE2	2.34	0.43
3:R:211:MET:SD	3:R:451:LEU:HG	2.59	0.43
4:S:24:LEU:HD22	4:S:31:ILE:HD13	2.00	0.43
3:Q:114:ALA:HA	3:Q:152:THR:HG22	2.00	0.43
4:S:192:LYS:HA	4:S:196:ALA:HB3	2.01	0.43
4:S:308:ASN:C	4:S:308:ASN:HD22	2.27	0.43
3:Z:156:ALA:O	3:Z:160:ILE:HG12	2.18	0.43
1:A:102:VAL:HG12	1:A:104:ASP:H	1.83	0.43
3:K:7:ILE:HB	3:K:47:MET:HE1	2.01	0.43
2:X:27:VAL:HG23	2:X:82:GLN:NE2	2.33	0.43
4:Y:105:MET:SD	4:Y:132:VAL:HG23	2.59	0.43
3:D:361:VAL:O	3:D:365:LEU:N	2.49	0.43
2:N:146:LEU:HD23	2:N:146:LEU:HA	1.92	0.43
2:P:25:PRO:HG2	2:P:167:LEU:HD21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:193:GLN:HA	3:R:459:LYS:HE3	2.00	0.43
2:X:69:LEU:HB3	2:X:82:GLN:HB3	1.99	0.43
2:C:177:VAL:O	2:C:178:LYS:HG2	2.18	0.42
2:C:193:MET:SD	2:C:197:ARG:NH1	2.91	0.42
3:D:138:VAL:HG13	3:D:285:GLU:HB2	2.01	0.42
3:D:393:GLN:OE1	3:D:409:ARG:NH1	2.51	0.42
2:N:36:GLY:HA2	2:N:71:LEU:HD11	2.01	0.42
2:N:43:ALA:HB1	2:N:175:ALA:HB1	2.01	0.42
4:S:345:GLY:HA2	4:S:350:VAL:HG13	2.01	0.42
4:Y:349:ASN:OD1	4:Y:349:ASN:N	2.51	0.42
3:Z:10:ILE:HG13	3:Z:40:ILE:HD11	2.01	0.42
2:B:203:LEU:HD23	2:B:203:LEU:HA	1.87	0.42
2:N:31:PRO:HG3	2:N:79:MET:HE1	2.00	0.42
4:S:591:ASP:OD1	4:S:591:ASP:N	2.53	0.42
3:V:301:PHE:HB3	6:V:503:402:H11	2.01	0.42
3:D:114:ALA:O	3:D:118:ARG:NH1	2.52	0.42
3:V:114:ALA:HB3	3:V:117:ILE:HG12	2.01	0.42
2:C:41:GLU:OE2	3:Q:58:TYR:OH	2.31	0.42
3:D:142:ARG:NH2	3:D:288:ASP:OD1	2.53	0.42
3:D:238:PRO:HB3	3:D:393:GLN:HE21	1.83	0.42
3:K:58:TYR:HD2	2:N:65:VAL:HG11	1.84	0.42
2:N:133:PRO:HB2	2:N:135:TYR:HE2	1.83	0.42
3:R:27:VAL:HG21	3:R:46:VAL:HB	2.01	0.42
3:K:381:MET:HA	3:K:381:MET:HE2	2.01	0.42
4:S:250:VAL:HG12	4:S:575:LYS:HD3	2.01	0.42
3:V:26:PRO:HA	3:V:359:LYS:HE3	2.00	0.42
4:Y:125:ALA:HB2	4:Y:370:TRP:CD1	2.54	0.42
3:Z:187:TRP:CD2	3:Z:380:VAL:HG21	2.55	0.42
2:B:143:GLN:HG2	2:B:146:LEU:HD12	2.02	0.42
1:G:170:ARG:HG2	2:X:72:ILE:HD13	2.02	0.42
4:Y:192:LYS:NZ	4:Y:211:LYS:O	2.52	0.42
2:B:72:ILE:HD11	2:N:202:ALA:HB2	2.00	0.42
3:D:111:VAL:HA	3:D:234:VAL:O	2.20	0.42
1:G:169:LYS:HD2	2:X:125:PRO:HA	2.02	0.42
3:Q:316:TYR:O	3:Q:320:THR:HG22	2.20	0.42
3:V:181:THR:HG21	3:V:379:GLU:HG3	2.02	0.42
3:D:156:ALA:HB3	3:D:298:ALA:HB1	2.02	0.42
2:J:101:LYS:HE2	2:J:101:LYS:HB3	1.92	0.42
3:K:94:TYR:HB3	3:K:261:LEU:HD13	2.01	0.42
3:Q:41:ASN:HB3	3:Q:44:VAL:HG12	2.01	0.42
3:V:79:LEU:HD11	3:V:271:LEU:HD23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Y:95:LYS:HE2	4:Y:127:ILE:HG12	2.01	0.42
2:C:65:VAL:HG11	3:Q:58:TYR:HD2	1.84	0.42
3:D:358:LEU:HD12	3:D:382:THR:HG23	2.00	0.42
3:K:7:ILE:HG23	3:K:92:LEU:HB2	2.02	0.42
3:Q:208:PRO:O	3:Q:212:THR:OG1	2.27	0.42
4:S:233:ILE:HD13	4:S:279:ILE:HD13	2.02	0.42
4:Y:370:TRP:CD1	4:Y:374:LEU:HD21	2.55	0.42
3:Z:87:PHE:CE2	3:Z:395:LYS:HE2	2.55	0.42
2:J:76:HIS:HB2	2:P:206:LEU:HD13	2.02	0.41
4:Y:345:GLY:HA2	4:Y:350:VAL:HG13	2.01	0.41
2:C:189:MET:HE1	2:C:191:THR:HB	2.02	0.41
2:X:65:VAL:HG11	3:Z:58:TYR:HD2	1.85	0.41
2:P:27:VAL:HG23	2:P:82:GLN:HE21	1.85	0.41
3:R:7:ILE:HG21	3:R:47:MET:HE3	2.02	0.41
4:Y:460:ARG:HD2	4:Y:462:GLN:HE21	1.85	0.41
3:R:112:GLN:HE21	3:R:216:ILE:HD12	1.84	0.41
4:S:11:THR:HG23	4:S:464:VAL:HG13	2.01	0.41
4:Y:124:ARG:HB3	4:Y:374:LEU:HD22	2.02	0.41
3:K:211:MET:HE2	3:K:451:LEU:HG	2.03	0.41
3:K:242:LYS:HB3	3:K:262:VAL:HG11	2.02	0.41
2:N:48:HIS:CE1	2:N:68:ARG:HG3	2.56	0.41
2:P:65:VAL:HG11	3:V:58:TYR:HD2	1.85	0.41
3:D:69:ARG:HH12	3:D:85:PRO:HA	1.86	0.41
2:P:95:CYS:HB2	5:P:303:SF4:S2	2.59	0.41
3:Q:237:MET:HG3	3:Q:242:LYS:HG3	2.01	0.41
4:S:95:LYS:HE2	4:S:95:LYS:HB3	1.91	0.41
4:Y:137:ARG:HE	4:Y:347:LEU:HD22	1.85	0.41
1:G:101:SER:OG	1:G:129:VAL:N	2.48	0.41
1:G:139:ARG:NH1	1:G:141:GLU:OE1	2.54	0.41
3:Q:415:LYS:HD3	3:Q:415:LYS:HA	1.90	0.41
3:V:177:LEU:O	3:V:179:MET:N	2.53	0.41
3:D:73:LEU:HD13	3:D:80:ASP:HA	2.03	0.41
3:D:118:ARG:HG3	3:D:137:LEU:HD13	2.01	0.41
3:K:210:GLN:HE21	3:K:251:MET:HE2	1.85	0.41
3:R:46:VAL:HG12	5:R:502:SF4:S4	2.61	0.41
3:V:245:GLU:O	3:V:251:MET:HG2	2.20	0.41
4:Y:359:LYS:HE3	4:Y:359:LYS:HB2	1.86	0.41
3:Z:411:GLU:O	3:Z:415:LYS:HG2	2.21	0.41
3:D:278:ASP:OD1	3:D:278:ASP:N	2.45	0.41
1:G:143:PRO:HB3	5:G:204:SF4:S1	2.61	0.41
3:K:388:ILE:O	3:K:409:ARG:NH1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:163:GLU:OE2	3:Q:179:MET:HE1	2.21	0.41
3:Q:184:CYS:HB3	3:Q:187:TRP:CE2	2.55	0.41
3:Q:211:MET:SD	3:Q:451:LEU:HG	2.61	0.41
3:R:316:TYR:O	3:R:320:THR:HG22	2.20	0.41
4:S:71:LYS:HA	4:S:71:LYS:HD2	1.83	0.41
4:S:252:PHE:HE1	4:S:318:ILE:HD11	1.85	0.41
4:S:550:THR:O	4:S:567:CYS:HB3	2.21	0.41
4:Y:122:PHE:CD2	4:Y:481:PHE:HB3	2.50	0.41
3:Z:69:ARG:NH2	3:Z:84:GLU:O	2.54	0.41
3:Z:99:LYS:HE3	3:Z:275:LYS:HE2	2.03	0.41
3:Z:178:PRO:HB3	3:Z:375:LEU:HB2	2.02	0.41
3:D:237:MET:HA	3:D:238:PRO:HD3	1.94	0.41
2:J:118:LYS:HE3	2:P:26:PHE:CE1	2.56	0.41
2:N:111:GLU:O	2:N:159:ARG:NH2	2.54	0.41
3:R:102:LEU:HD11	3:R:145:ASN:HB2	2.03	0.41
3:R:111:VAL:HG13	3:R:149:VAL:HG23	2.02	0.41
4:S:85:ASN:CG	4:S:487:ARG:HH12	2.29	0.41
4:S:122:PHE:HE2	4:S:482:SER:HA	1.86	0.41
4:Y:256:ALA:HA	4:Y:259:VAL:HG22	2.03	0.41
4:Y:502:TRP:NE1	4:Y:516:ILE:O	2.48	0.41
1:G:47:ILE:HD13	4:S:207:ALA:HA	2.01	0.40
3:R:117:ILE:HG22	3:R:137:LEU:HD11	2.02	0.40
4:S:17:GLY:O	4:S:457:THR:HG23	2.21	0.40
4:Y:173:ILE:HD13	4:Y:201:ALA:HB3	2.02	0.40
4:Y:356:ASP:HB3	4:Y:358:THR:HG22	2.02	0.40
3:Z:218:THR:HG21	3:Z:450:LEU:HD13	2.03	0.40
3:Z:268:LEU:HG	3:Z:272:MET:HE2	2.03	0.40
1:A:6:VAL:HG13	1:A:51:GLN:NE2	2.35	0.40
3:D:53:GLN:NE2	3:D:393:GLN:O	2.52	0.40
3:D:316:TYR:CE2	3:D:324:ILE:HB	2.56	0.40
2:J:47:VAL:HG22	2:J:171:LEU:HD22	2.02	0.40
3:R:91:ASN:OD1	3:R:92:LEU:N	2.55	0.40
3:V:156:ALA:HB1	3:V:301:PHE:CE2	2.56	0.40
3:V:229:ALA:HA	3:V:256:TYR:HE2	1.86	0.40
3:K:210:GLN:HB3	3:K:251:MET:HE2	2.02	0.40
3:R:413:LEU:HD23	3:R:413:LEU:HA	1.93	0.40
3:R:138:VAL:HG13	3:R:285:GLU:HB2	2.03	0.40
3:R:426:HIS:O	3:R:426:HIS:ND1	2.54	0.40
4:Y:231:ILE:HA	4:Y:234:ILE:HG12	2.03	0.40
3:K:179:MET:SD	3:K:203:SER:HB2	2.62	0.40
3:K:237:MET:HA	3:K:238:PRO:HD3	1.97	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:45:PHE:CD2	2:N:65:VAL:HG23	2.57	0.40
3:Q:156:ALA:HB1	3:Q:301:PHE:CE2	2.56	0.40
3:R:162:GLU:OE1	3:R:452:HIS:NE2	2.55	0.40
3:V:387:CYS:HB2	6:V:503:402:C4	2.50	0.40
4:Y:412:ASP:N	4:Y:412:ASP:OD1	2.53	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	A	170/184 (92%)	162 (95%)	8 (5%)	0	100	100
1	G	170/184 (92%)	159 (94%)	9 (5%)	2 (1%)	10	35
2	B	179/210 (85%)	169 (94%)	10 (6%)	0	100	100
2	C	179/210 (85%)	166 (93%)	13 (7%)	0	100	100
2	J	179/210 (85%)	171 (96%)	8 (4%)	0	100	100
2	N	179/210 (85%)	172 (96%)	7 (4%)	0	100	100
2	P	179/210 (85%)	173 (97%)	6 (3%)	0	100	100
2	X	179/210 (85%)	172 (96%)	7 (4%)	0	100	100
3	D	444/461 (96%)	419 (94%)	25 (6%)	0	100	100
3	K	444/461 (96%)	420 (95%)	24 (5%)	0	100	100
3	Q	444/461 (96%)	420 (95%)	24 (5%)	0	100	100
3	R	444/461 (96%)	419 (94%)	25 (6%)	0	100	100
3	V	444/461 (96%)	413 (93%)	31 (7%)	0	100	100
3	Z	444/461 (96%)	420 (95%)	24 (5%)	0	100	100
4	S	561/743 (76%)	527 (94%)	34 (6%)	0	100	100
4	Y	561/743 (76%)	534 (95%)	27 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	5200/5880 (88%)	4916 (94%)	282 (5%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	58	ALA
1	G	59	PRO

5.3.2 Protein sidechains [i](#)

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	151/161 (94%)	151 (100%)	0	100	100
1	G	151/161 (94%)	151 (100%)	0	100	100
2	B	154/179 (86%)	154 (100%)	0	100	100
2	C	154/179 (86%)	154 (100%)	0	100	100
2	J	154/179 (86%)	154 (100%)	0	100	100
2	N	154/179 (86%)	154 (100%)	0	100	100
2	P	154/179 (86%)	154 (100%)	0	100	100
2	X	154/179 (86%)	154 (100%)	0	100	100
3	D	384/396 (97%)	384 (100%)	0	100	100
3	K	384/396 (97%)	384 (100%)	0	100	100
3	Q	384/396 (97%)	384 (100%)	0	100	100
3	R	384/396 (97%)	384 (100%)	0	100	100
3	V	384/396 (97%)	384 (100%)	0	100	100
3	Z	384/396 (97%)	384 (100%)	0	100	100
4	S	470/616 (76%)	470 (100%)	0	100	100
4	Y	470/616 (76%)	470 (100%)	0	100	100
All	All	4470/5004 (89%)	4470 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	30	ASN
3	D	9	ASN
3	D	360	ASN
3	D	376	HIS
2	J	145	ASN
2	J	156	GLN
3	K	9	ASN
3	K	53	GLN
3	K	210	GLN
2	P	24	ASN
2	P	48	HIS
2	P	143	GLN
3	Q	74	GLN
3	Q	210	GLN
3	Q	360	ASN
3	R	9	ASN
3	R	74	GLN
3	R	360	ASN
4	S	113	ASN
4	S	120	GLN
4	S	228	ASN
4	S	301	GLN
4	S	308	ASN
4	S	413	HIS
3	V	9	ASN
3	V	106	GLN
3	V	165	ASN
3	V	209	GLN
3	V	326	ASN
3	V	344	GLN
3	V	416	HIS
3	V	446	GLN
2	X	198	ASN
4	Y	89	ASN
4	Y	130	ASN
4	Y	206	ASN
4	Y	228	ASN
4	Y	248	HIS
4	Y	308	ASN

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Mol	Chain	Res	Type
4	Y	314	ASN
4	Y	321	ASN
4	Y	576	GLN
3	Z	165	ASN
3	Z	326	ASN

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](#)

58 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	$\# Z > 2$
5	SF4	C	303	2	0,12,12	-	-	-		
5	SF4	S	801	4	0,12,12	-	-	-		
5	SF4	K	504	3	0,12,12	-	-	-		
5	SF4	K	502	3	0,12,12	-	-	-		
5	SF4	V	504	6,3	0,12,12	-	-	-		
5	SF4	C	302	2	0,12,12	-	-	-		
5	SF4	K	501	3	0,12,12	-	-	-		
5	SF4	A	204	1	0,12,12	-	-	-		
5	SF4	D	501	3	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	SF4	N	303	2	0,12,12	-	-	-		
5	SF4	Q	503	3	0,12,12	-	-	-		
6	402	V	503	5,3	15,19,19	2.76	11 (73%)	1,36,36	0.02	0
5	SF4	P	301	2	0,12,12	-	-	-		
5	SF4	N	304	2	0,12,12	-	-	-		
5	SF4	P	303	2	0,12,12	-	-	-		
5	SF4	A	203	1	0,12,12	-	-	-		
5	SF4	B	302	2	0,12,12	-	-	-		
5	SF4	A	201	1	0,12,12	-	-	-		
5	SF4	N	302	2	0,12,12	-	-	-		
5	SF4	V	501	3	0,12,12	-	-	-		
5	SF4	Z	501	3	0,12,12	-	-	-		
5	SF4	N	301	2	0,12,12	-	-	-		
5	SF4	Z	503	3	0,12,12	-	-	-		
5	SF4	D	502	3	0,12,12	-	-	-		
5	SF4	R	502	3	0,12,12	-	-	-		
5	SF4	R	504	3	0,12,12	-	-	-		
5	SF4	A	202	1	0,12,12	-	-	-		
5	SF4	C	304	2	0,12,12	-	-	-		
5	SF4	D	504	3	0,12,12	-	-	-		
5	SF4	X	301	2	0,12,12	-	-	-		
5	SF4	J	303	2	0,12,12	-	-	-		
5	SF4	G	203	1	0,12,12	-	-	-		
5	SF4	G	202	1	0,12,12	-	-	-		
6	402	Z	504	3	15,19,19	2.76	12 (80%)	1,36,36	0.26	0
5	SF4	Y	801	4	0,12,12	-	-	-		
5	SF4	Z	502	3	0,12,12	-	-	-		
5	SF4	Q	501	3	0,12,12	-	-	-		
5	SF4	X	303	2	0,12,12	-	-	-		
6	402	D	503	3	15,19,19	2.62	10 (66%)	1,36,36	0.14	0
5	SF4	J	304	2	0,12,12	-	-	-		
6	402	K	503	3	15,19,19	2.79	13 (86%)	1,36,36	0.07	0
5	SF4	X	302	2	0,12,12	-	-	-		
5	SF4	B	301	2	0,12,12	-	-	-		
5	SF4	G	201	1	0,12,12	-	-	-		
5	SF4	X	304	2	0,12,12	-	-	-		
5	SF4	R	501	3	0,12,12	-	-	-		
6	402	Q	504	3	15,19,19	2.78	13 (86%)	1,36,36	0.19	0
6	402	R	503	3	15,19,19	2.74	12 (80%)	1,36,36	0.09	0
5	SF4	Q	502	3	0,12,12	-	-	-		
5	SF4	J	302	2	0,12,12	-	-	-		
5	SF4	B	303	2	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	SF4	J	301	2	0,12,12	-	-	-		
5	SF4	P	304	2	0,12,12	-	-	-		
5	SF4	B	304	2	0,12,12	-	-	-		
5	SF4	G	204	1	0,12,12	-	-	-		
5	SF4	C	301	2	0,12,12	-	-	-		
5	SF4	V	502	3	0,12,12	-	-	-		
5	SF4	P	302	2	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
5	SF4	C	303	2	-	-	0/6/5/5
5	SF4	S	801	4	-	-	0/6/5/5
5	SF4	K	504	3	-	-	0/6/5/5
5	SF4	K	502	3	-	-	0/6/5/5
5	SF4	V	504	6,3	-	-	0/6/5/5
5	SF4	C	302	2	-	-	0/6/5/5
5	SF4	K	501	3	-	-	0/6/5/5
5	SF4	A	204	1	-	-	0/6/5/5
5	SF4	D	501	3	-	-	0/6/5/5
5	SF4	N	303	2	-	-	0/6/5/5
5	SF4	Q	503	3	-	-	0/6/5/5
6	402	V	503	5,3	-	-	0/5/3/3
5	SF4	P	301	2	-	-	0/6/5/5
5	SF4	N	304	2	-	-	0/6/5/5
5	SF4	P	303	2	-	-	0/6/5/5
5	SF4	A	203	1	-	-	0/6/5/5
5	SF4	B	302	2	-	-	0/6/5/5
5	SF4	A	201	1	-	-	0/6/5/5
5	SF4	N	302	2	-	-	0/6/5/5
5	SF4	V	501	3	-	-	0/6/5/5
5	SF4	Z	501	3	-	-	0/6/5/5
5	SF4	N	301	2	-	-	0/6/5/5
5	SF4	Z	503	3	-	-	0/6/5/5
5	SF4	D	502	3	-	-	0/6/5/5
5	SF4	R	502	3	-	-	0/6/5/5
5	SF4	R	504	3	-	-	0/6/5/5
5	SF4	A	202	1	-	-	0/6/5/5
5	SF4	C	304	2	-	-	0/6/5/5
5	SF4	D	504	3	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	SF4	X	301	2	-	-	0/6/5/5
5	SF4	J	303	2	-	-	0/6/5/5
5	SF4	G	203	1	-	-	0/6/5/5
5	SF4	G	202	1	-	-	0/6/5/5
6	402	Z	504	3	-	-	0/5/3/3
5	SF4	Y	801	4	-	-	0/6/5/5
5	SF4	Z	502	3	-	-	0/6/5/5
5	SF4	Q	501	3	-	-	0/6/5/5
5	SF4	X	303	2	-	-	0/6/5/5
6	402	D	503	3	-	-	0/5/3/3
5	SF4	J	304	2	-	-	0/6/5/5
6	402	K	503	3	-	-	0/5/3/3
5	SF4	X	302	2	-	-	0/6/5/5
5	SF4	B	301	2	-	-	0/6/5/5
5	SF4	G	201	1	-	-	0/6/5/5
5	SF4	X	304	2	-	-	0/6/5/5
5	SF4	R	501	3	-	-	0/6/5/5
6	402	Q	504	3	-	-	0/5/3/3
6	402	R	503	3	-	-	0/5/3/3
5	SF4	Q	502	3	-	-	0/6/5/5
5	SF4	J	302	2	-	-	0/6/5/5
5	SF4	B	303	2	-	-	0/6/5/5
5	SF4	J	301	2	-	-	0/6/5/5
5	SF4	P	304	2	-	-	0/6/5/5
5	SF4	B	304	2	-	-	0/6/5/5
5	SF4	G	204	1	-	-	0/6/5/5
5	SF4	C	301	2	-	-	0/6/5/5
5	SF4	V	502	3	-	-	0/6/5/5
5	SF4	P	302	2	-	-	0/6/5/5

All (71) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	V	503	402	C4-N4	3.51	1.20	1.15
6	Q	504	402	C1-N1	3.49	1.50	1.40
6	Z	504	402	C1-N1	3.46	1.50	1.40
6	D	503	402	C2-N1	3.45	1.50	1.40
6	Q	504	402	C2-N1	3.45	1.50	1.40
6	V	503	402	C2-N1	3.45	1.50	1.40
6	Z	504	402	C2-N1	3.45	1.50	1.40
6	R	503	402	C4-N4	3.45	1.20	1.15
6	V	503	402	C1-N1	3.44	1.50	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	R	503	402	C1-N1	3.43	1.50	1.40
6	K	503	402	C2-N1	3.43	1.50	1.40
6	Q	504	402	C4-N4	3.42	1.20	1.15
6	K	503	402	C1-N1	3.41	1.50	1.40
6	D	503	402	S1-FE2	3.40	2.30	2.26
6	Z	504	402	C4-N4	3.39	1.20	1.15
6	D	503	402	C1-N1	3.38	1.50	1.40
6	K	503	402	C4-N4	3.38	1.20	1.15
6	R	503	402	C2-N1	3.37	1.50	1.40
6	V	503	402	C6-N6	-3.29	1.10	1.15
6	D	503	402	C4-N4	3.29	1.20	1.15
6	R	503	402	C6-N6	-3.19	1.10	1.15
6	Z	504	402	C6-N6	-3.15	1.10	1.15
6	Q	504	402	C6-N6	-3.12	1.10	1.15
6	K	503	402	S1-FE2	3.11	2.30	2.26
6	K	503	402	S1-FE1	3.09	2.30	2.26
6	K	503	402	C6-N6	-3.08	1.10	1.15
6	Q	504	402	S1-FE2	3.07	2.30	2.26
6	Z	504	402	S2-FE2	3.07	2.30	2.26
6	K	503	402	S2-FE1	3.04	2.30	2.26
6	R	503	402	S2-FE2	3.02	2.30	2.26
6	Z	504	402	S1-FE2	3.02	2.30	2.26
6	V	503	402	C3-FE1	-3.01	1.70	1.79
6	V	503	402	S2-FE2	3.01	2.30	2.26
6	Q	504	402	S1-FE1	3.00	2.30	2.26
6	Z	504	402	S2-FE1	3.00	2.30	2.26
6	Q	504	402	S2-FE1	2.99	2.30	2.26
6	R	503	402	C3-FE1	-2.95	1.70	1.79
6	K	503	402	S2-FE2	2.95	2.30	2.26
6	Z	504	402	C3-FE1	-2.95	1.70	1.79
6	R	503	402	S1-FE2	2.94	2.30	2.26
6	D	503	402	C3-FE1	-2.93	1.70	1.79
6	Q	504	402	C2-S2	2.93	1.90	1.85
6	Q	504	402	S2-FE2	2.91	2.30	2.26
6	Q	504	402	C3-FE1	-2.90	1.70	1.79
6	V	503	402	S1-FE2	2.87	2.30	2.26
6	D	503	402	C2-S2	2.87	1.90	1.85
6	R	503	402	S1-FE1	2.87	2.30	2.26
6	K	503	402	C3-FE1	-2.87	1.70	1.79
6	K	503	402	C2-S2	2.83	1.90	1.85
6	Z	504	402	C2-S2	2.82	1.90	1.85
6	V	503	402	S2-FE1	2.82	2.30	2.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	V	503	402	S1-FE1	2.81	2.30	2.26
6	D	503	402	S1-FE1	2.81	2.30	2.26
6	V	503	402	C2-S2	2.79	1.90	1.85
6	R	503	402	S2-FE1	2.78	2.30	2.26
6	D	503	402	S2-FE1	2.77	2.30	2.26
6	R	503	402	C2-S2	2.76	1.90	1.85
6	D	503	402	S2-FE2	2.70	2.30	2.26
6	V	503	402	C1-S1	-2.67	1.80	1.85
6	D	503	402	C1-S1	-2.66	1.80	1.85
6	Z	504	402	C1-S1	-2.65	1.80	1.85
6	R	503	402	C1-S1	-2.57	1.80	1.85
6	Q	504	402	C1-S1	-2.54	1.80	1.85
6	K	503	402	C1-S1	-2.53	1.80	1.85
6	Z	504	402	S1-FE1	2.53	2.29	2.26
6	Z	504	402	O7-C7	2.08	1.20	1.15
6	Q	504	402	O7-C7	2.04	1.20	1.15
6	K	503	402	O5-C5	2.04	1.21	1.17
6	R	503	402	O3-C3	2.03	1.20	1.15
6	K	503	402	O3-C3	2.02	1.20	1.15
6	Q	504	402	O3-C3	2.01	1.20	1.15

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

22 monomers are involved in 34 short contacts:

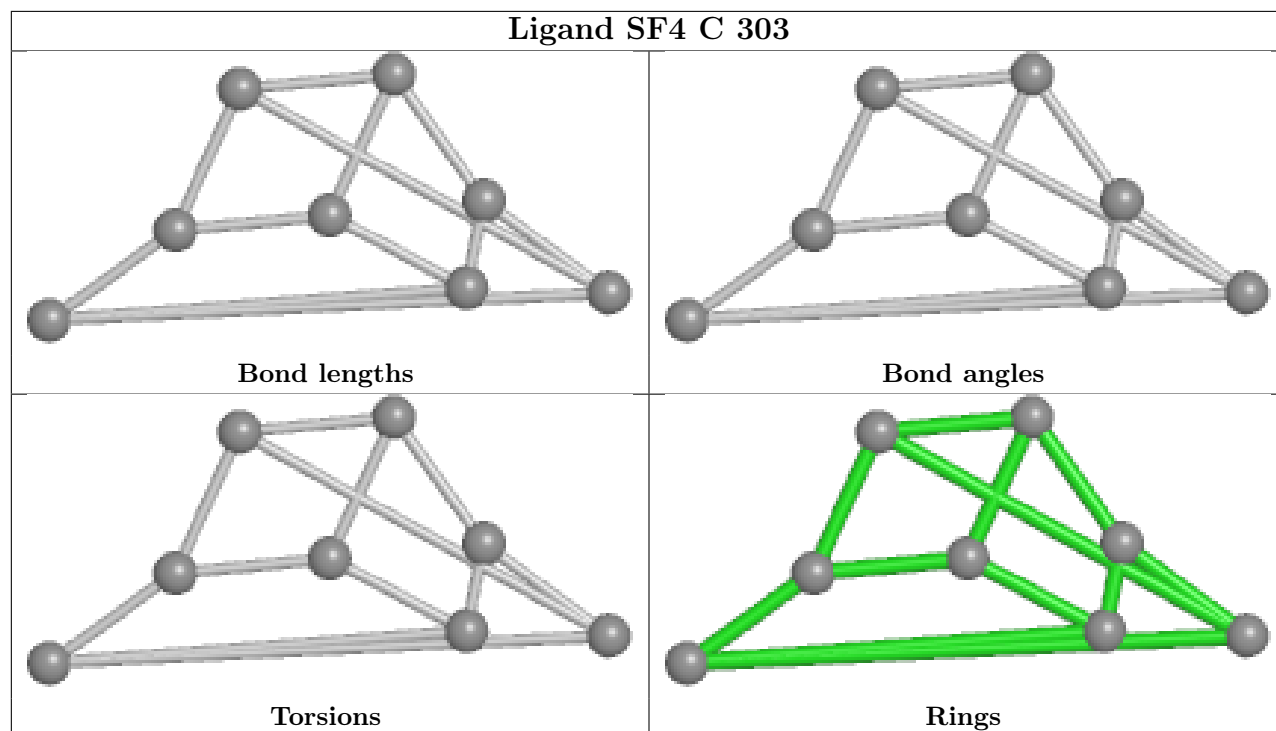
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	S	801	SF4	2	0
5	K	504	SF4	1	0
5	V	504	SF4	2	0
5	A	204	SF4	1	0
6	V	503	402	3	0
5	N	304	SF4	1	0
5	P	303	SF4	1	0
5	A	201	SF4	1	0
5	Z	503	SF4	1	0
5	D	502	SF4	1	0
5	R	502	SF4	1	0
5	C	304	SF4	2	0
5	X	301	SF4	1	0

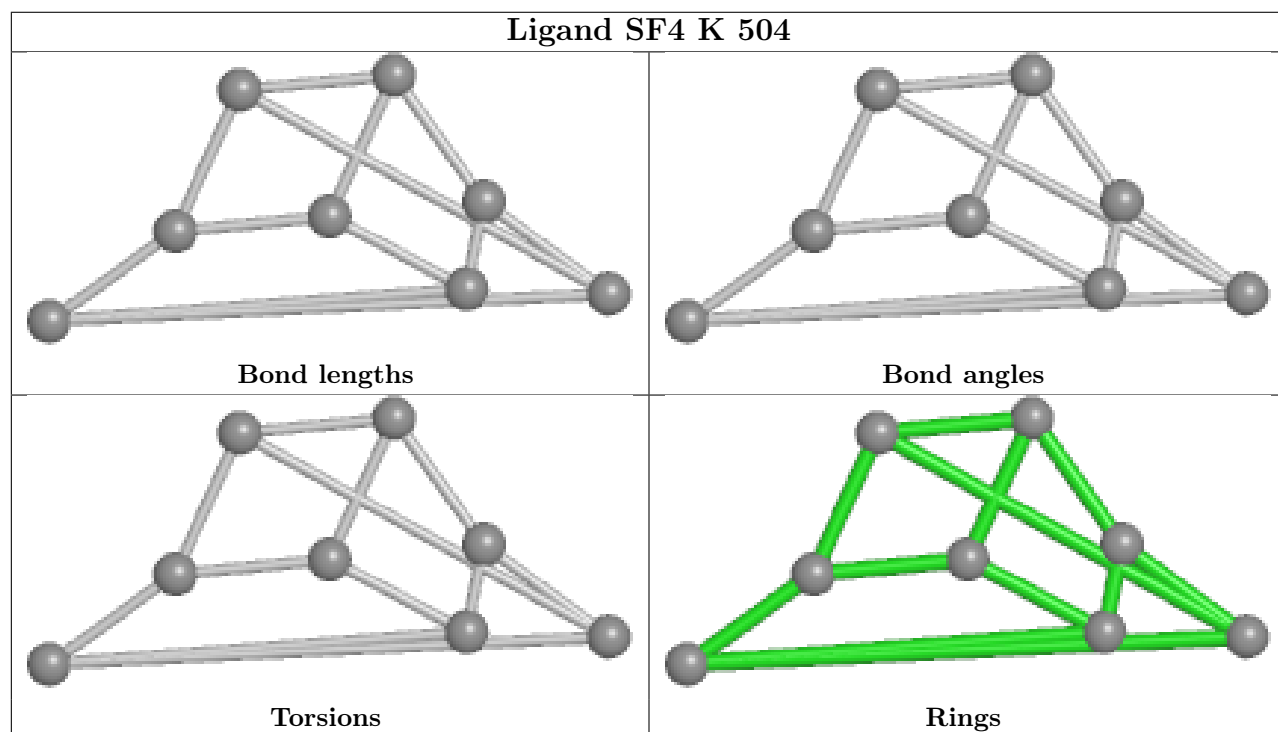
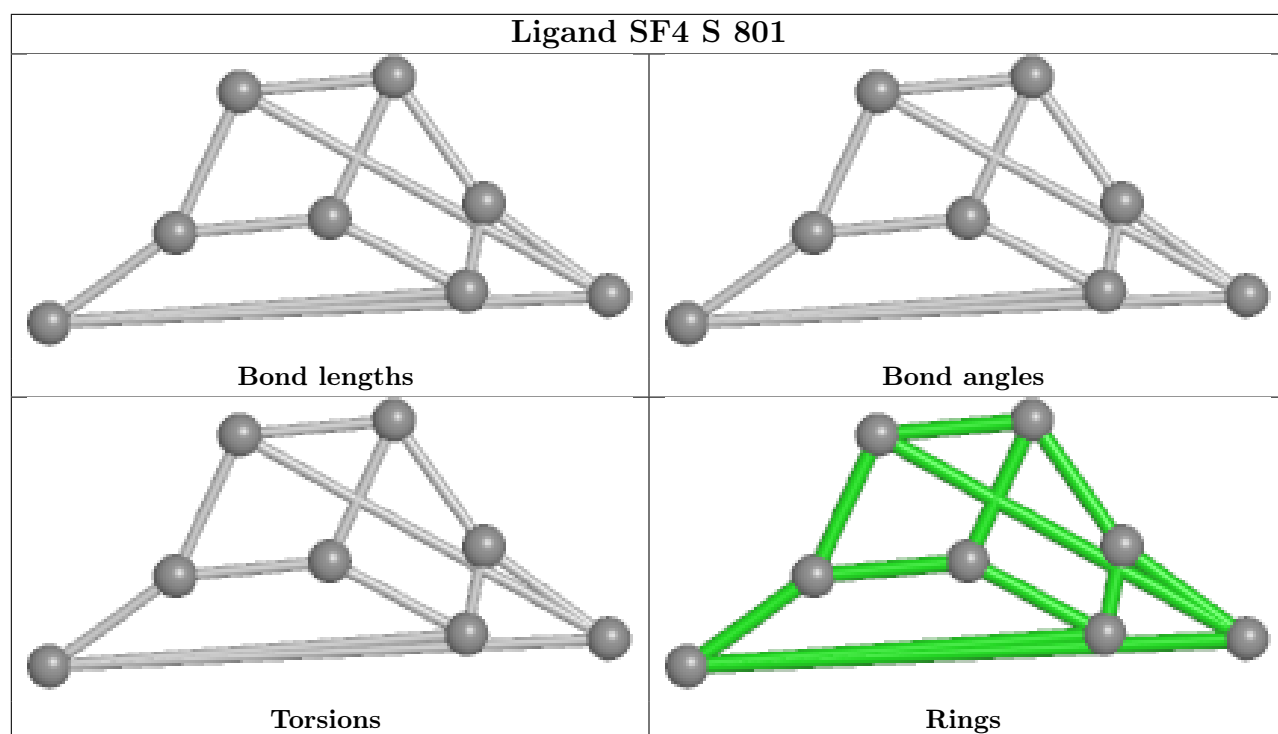
Continued on next page...

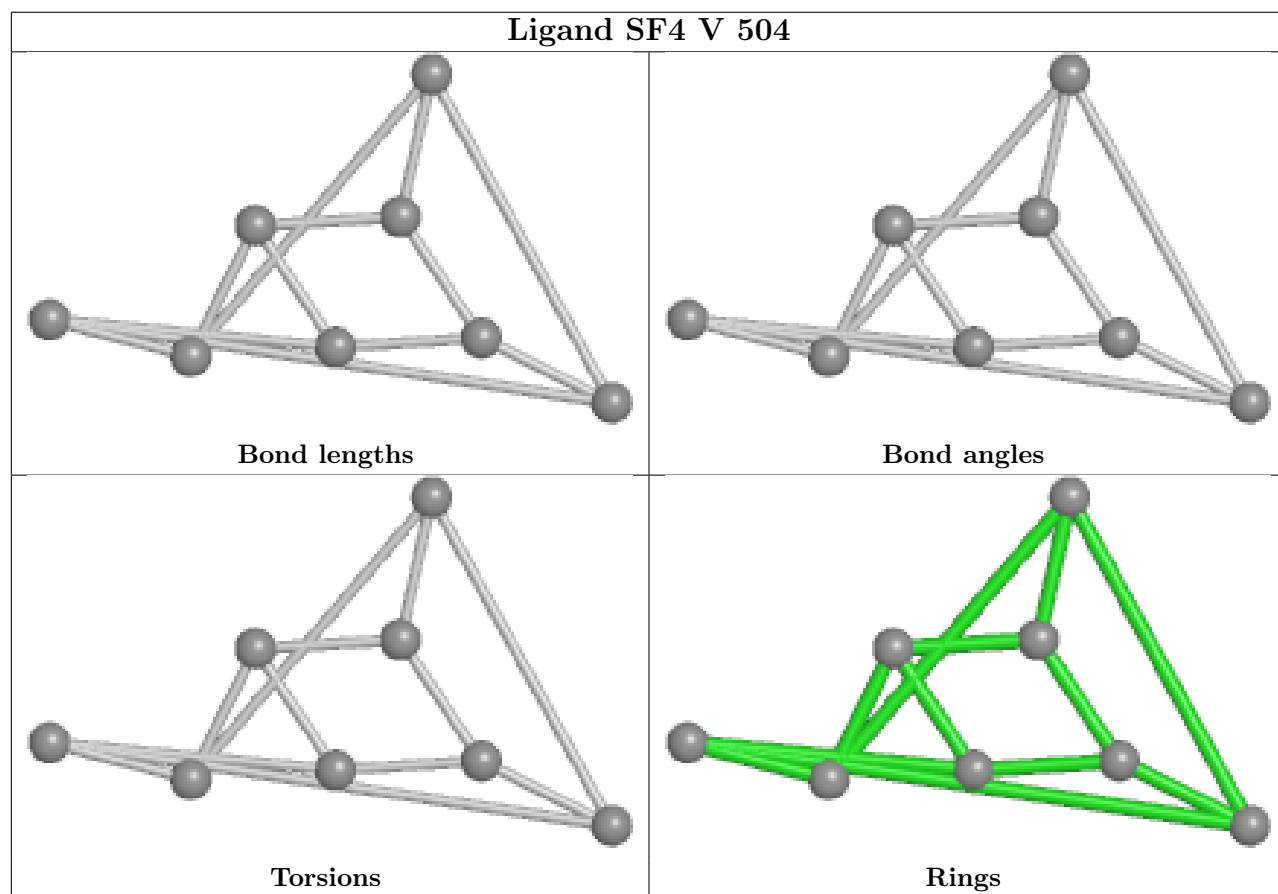
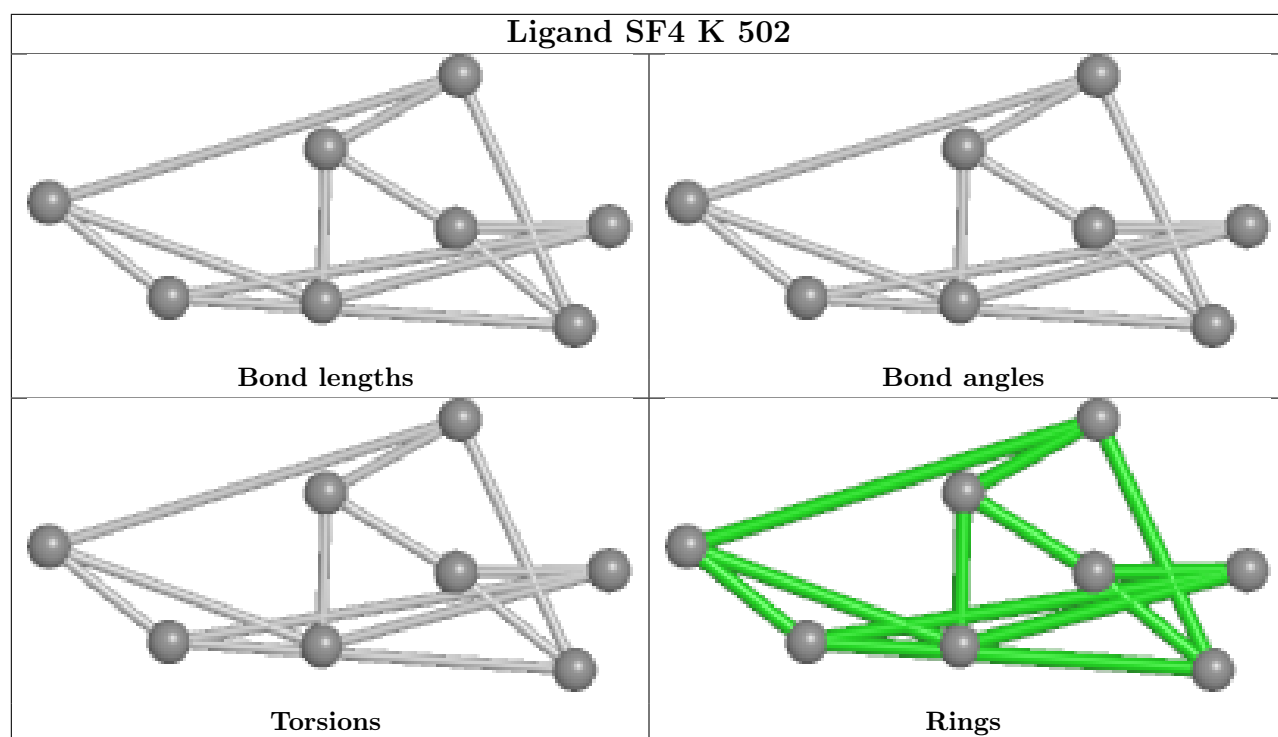
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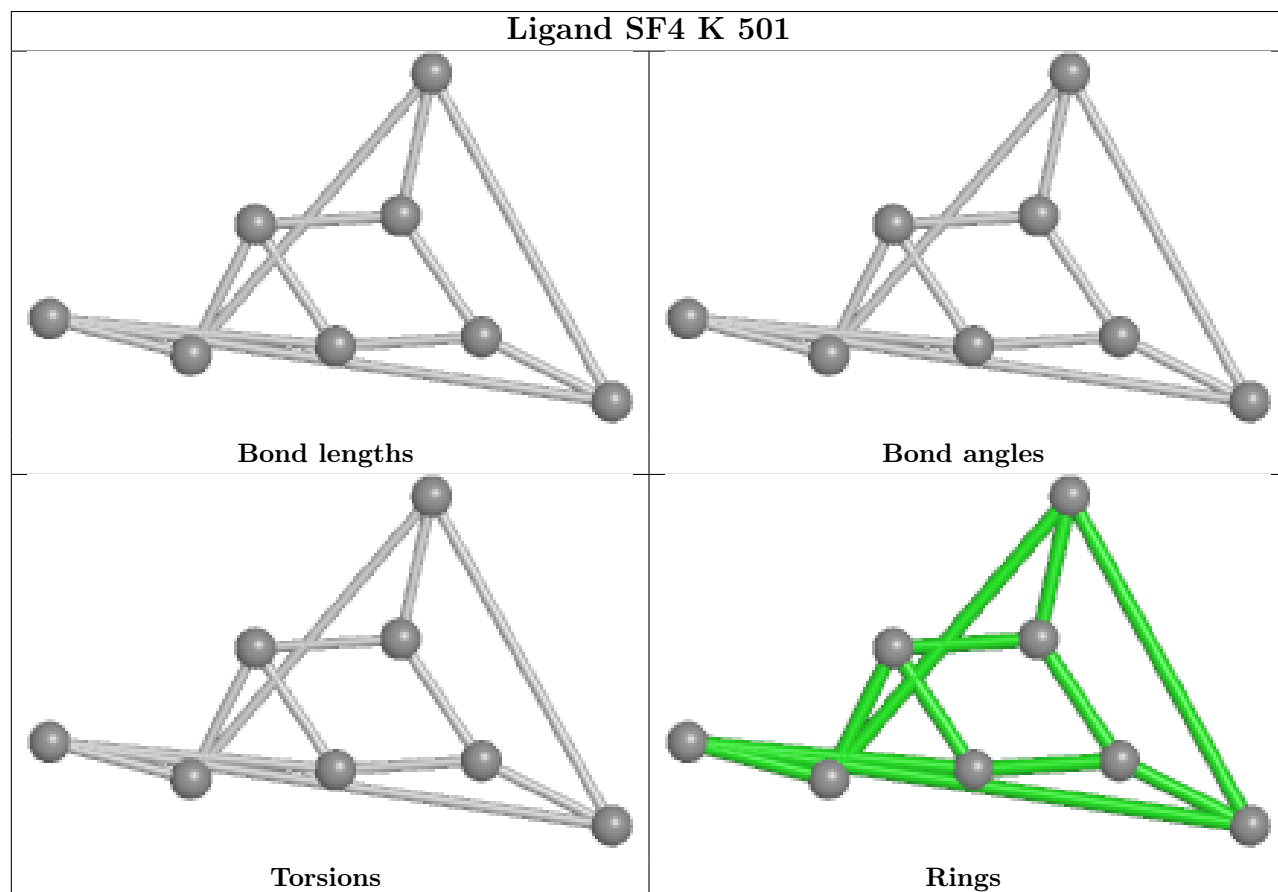
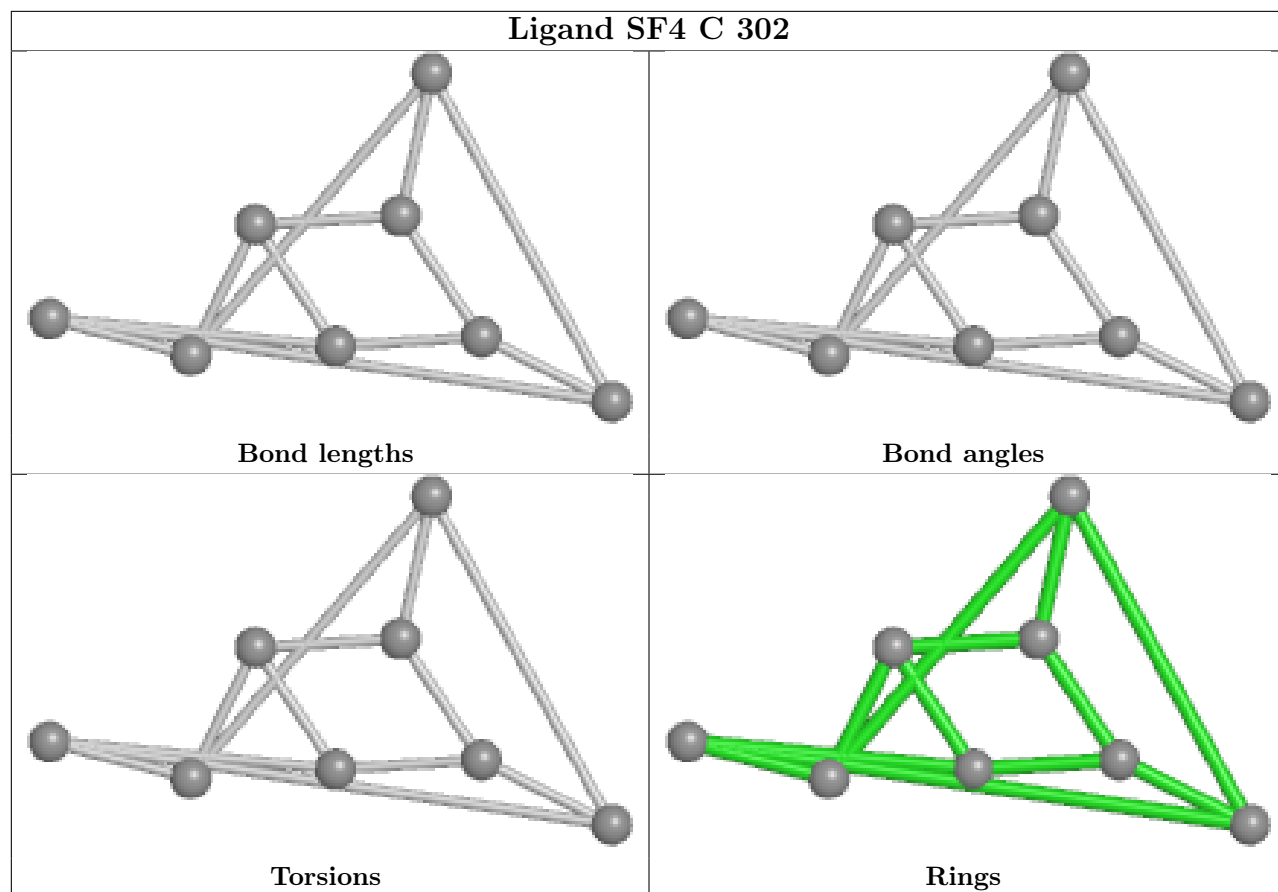
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	Z	504	402	4	0
5	Y	801	SF4	1	0
6	D	503	402	3	0
6	K	503	402	1	0
6	Q	504	402	2	0
6	R	503	402	2	0
5	B	304	SF4	1	0
5	G	204	SF4	1	0
5	P	302	SF4	1	0

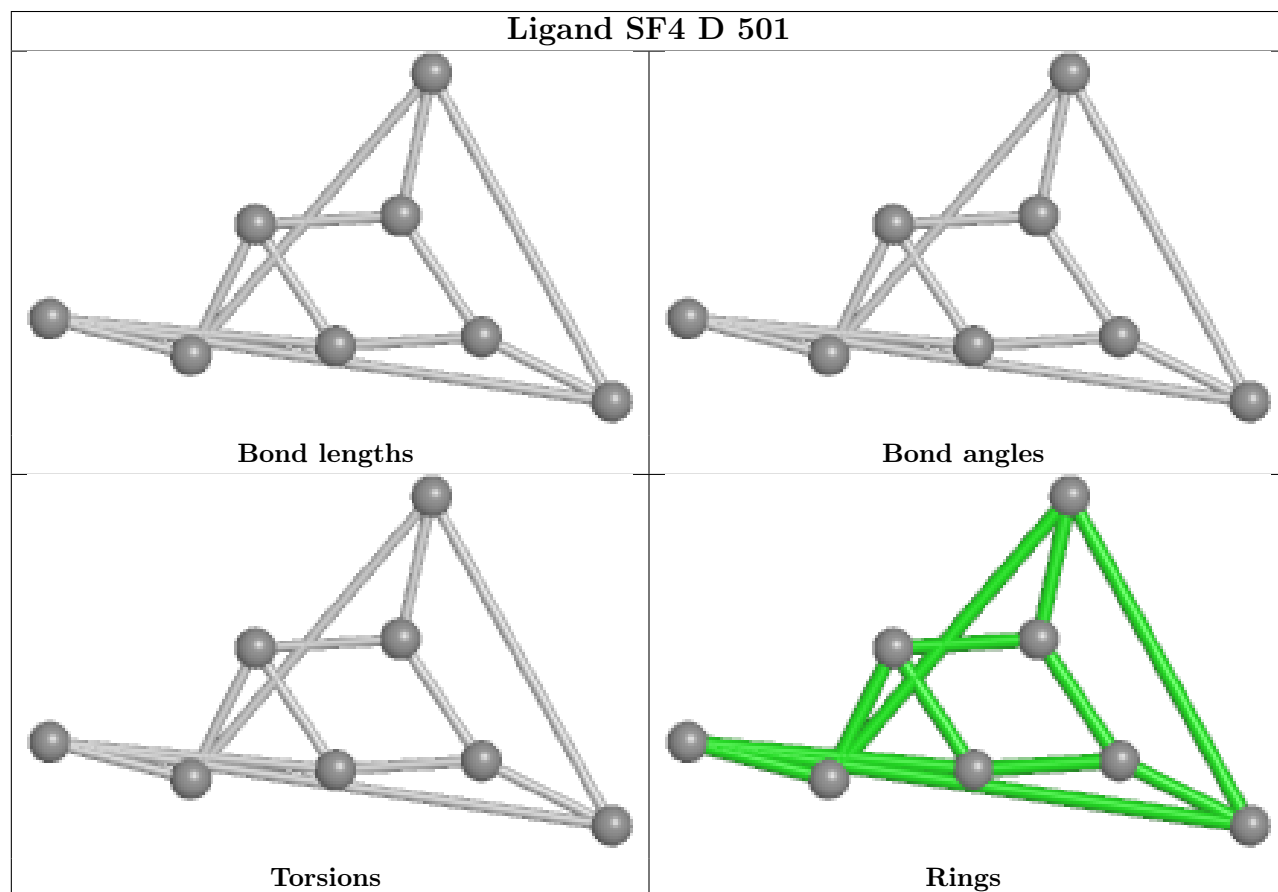
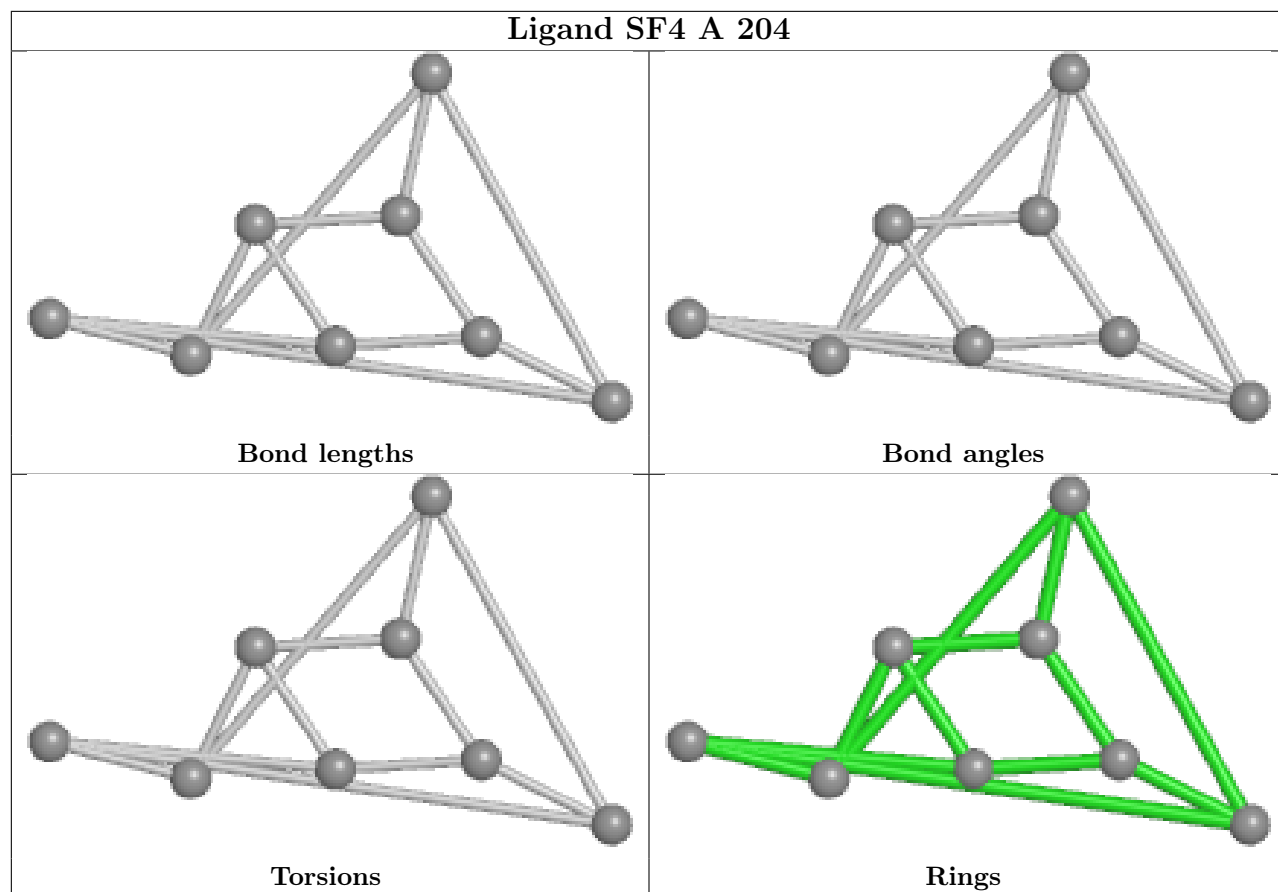
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

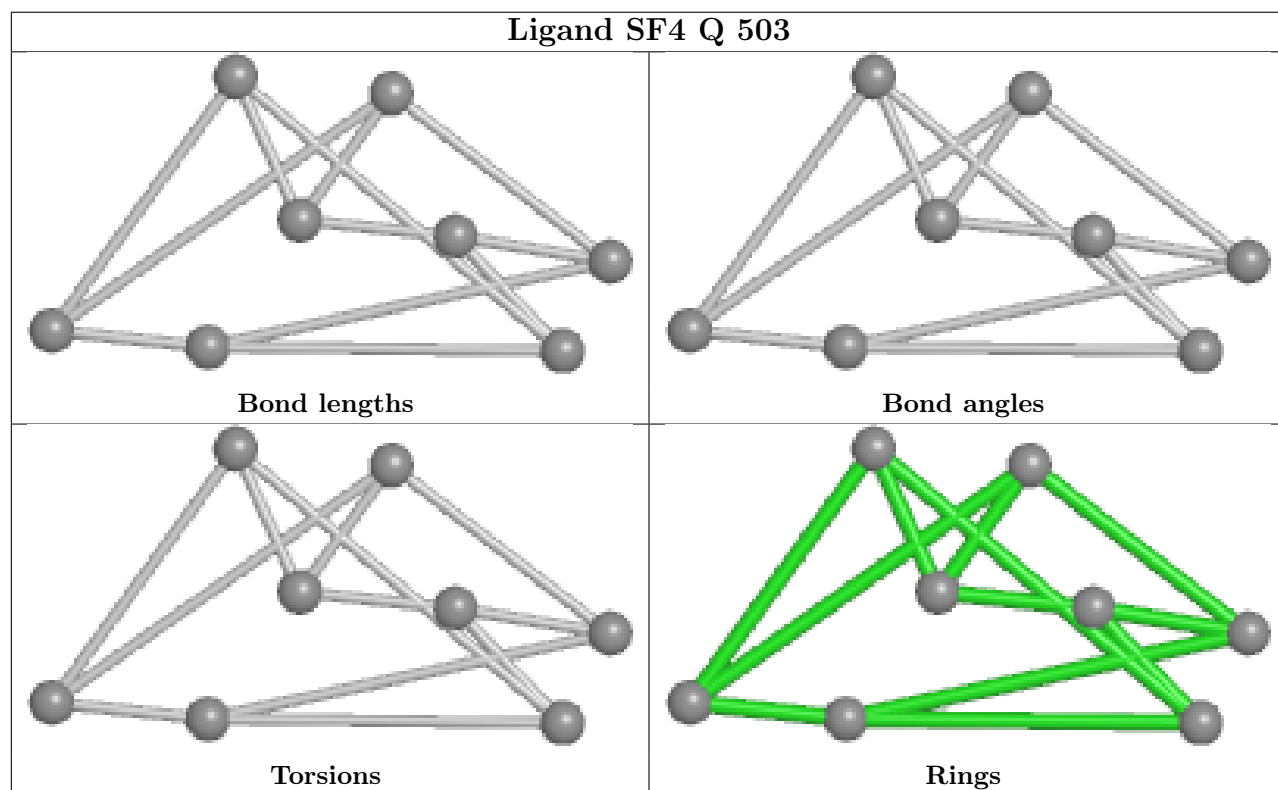
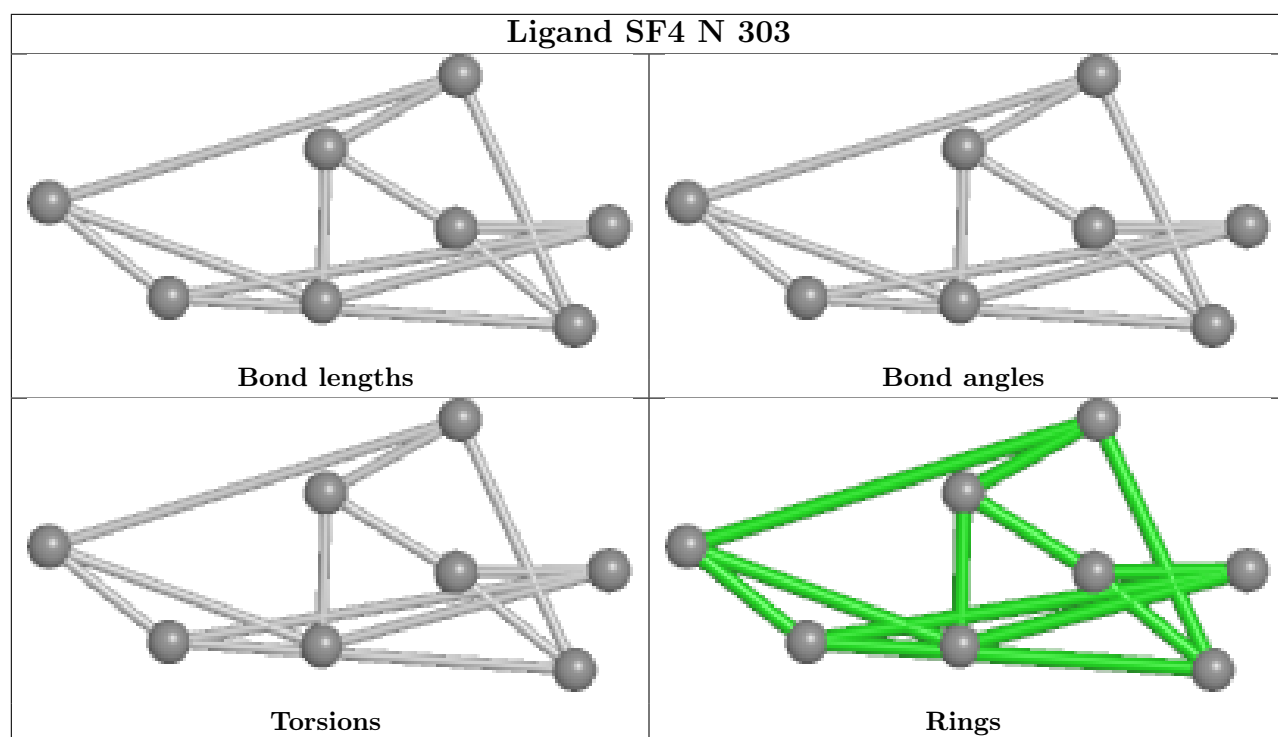


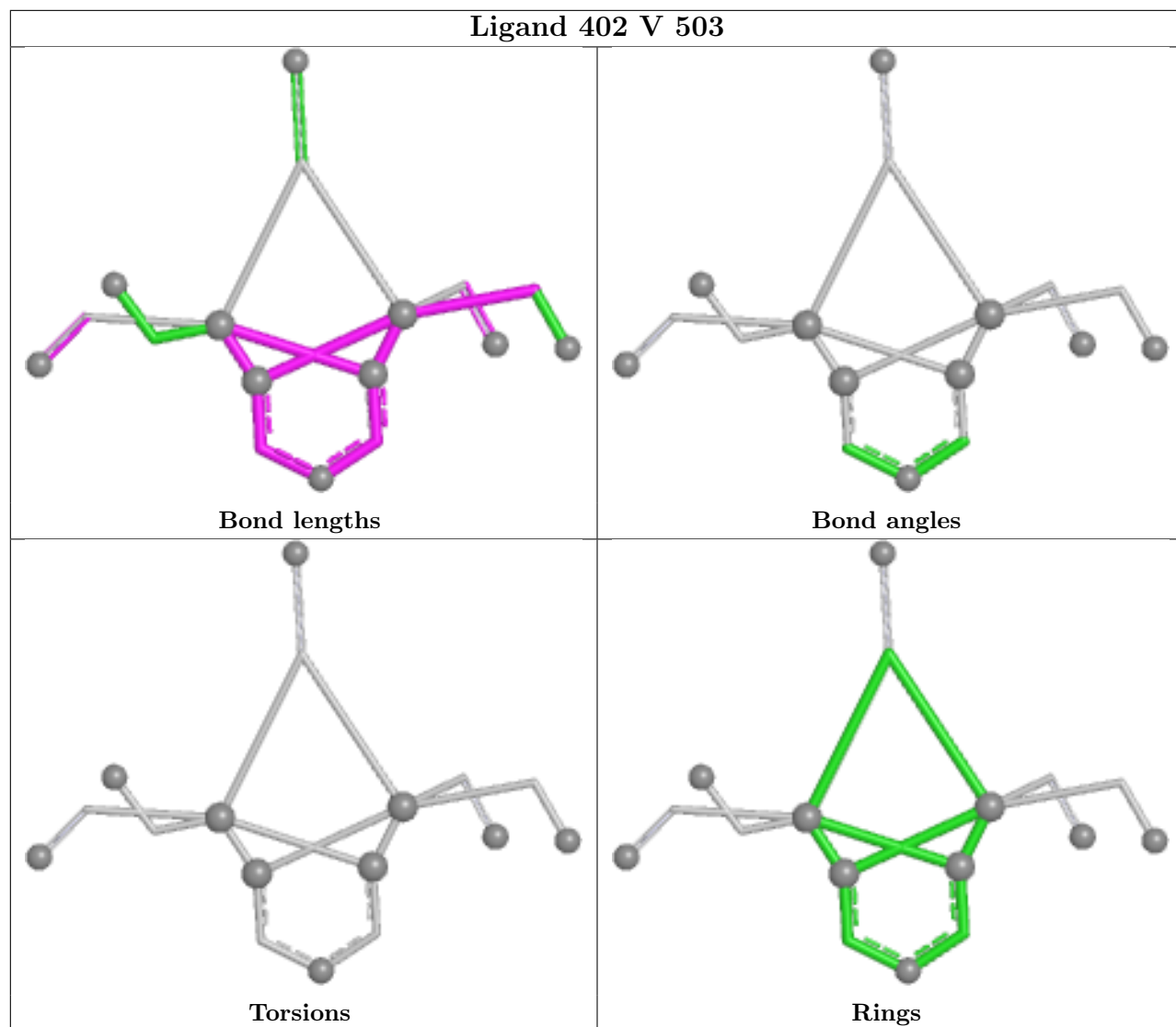




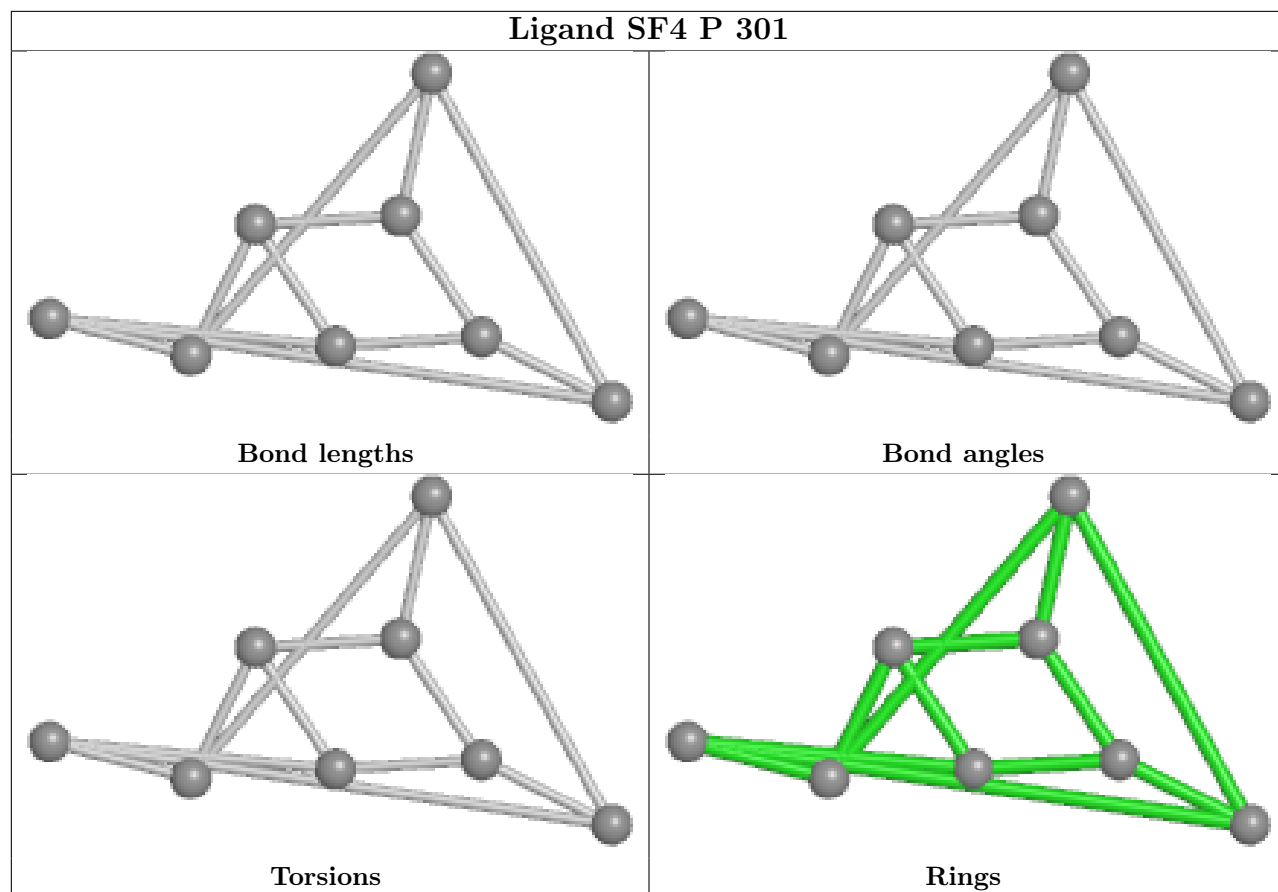




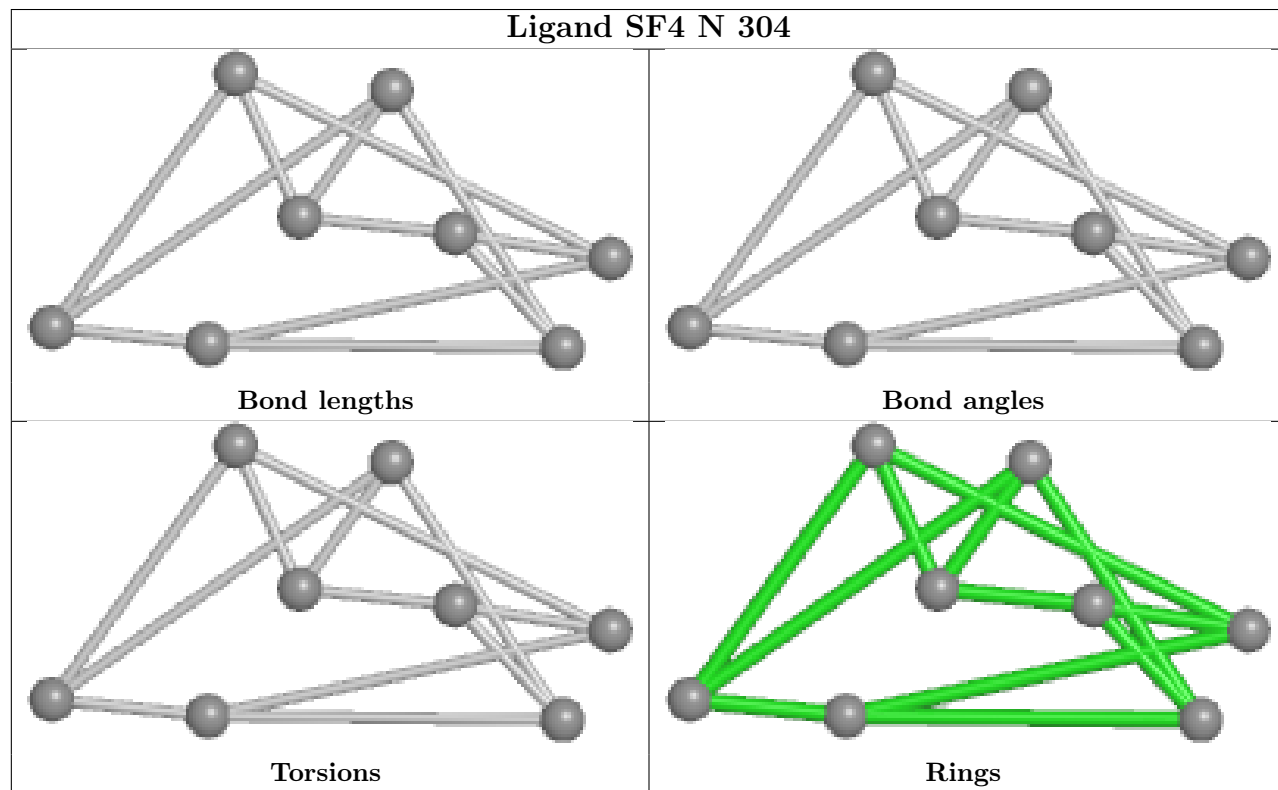


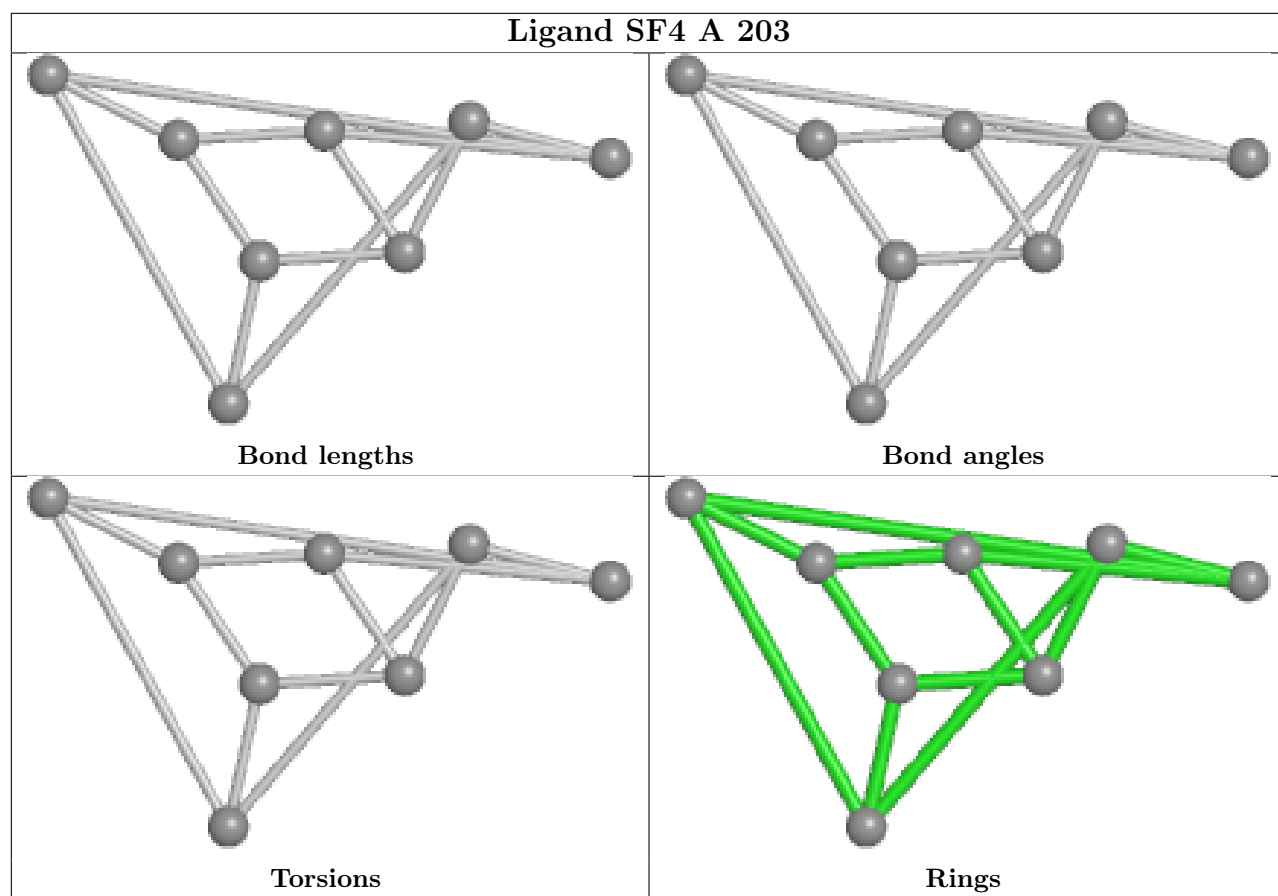
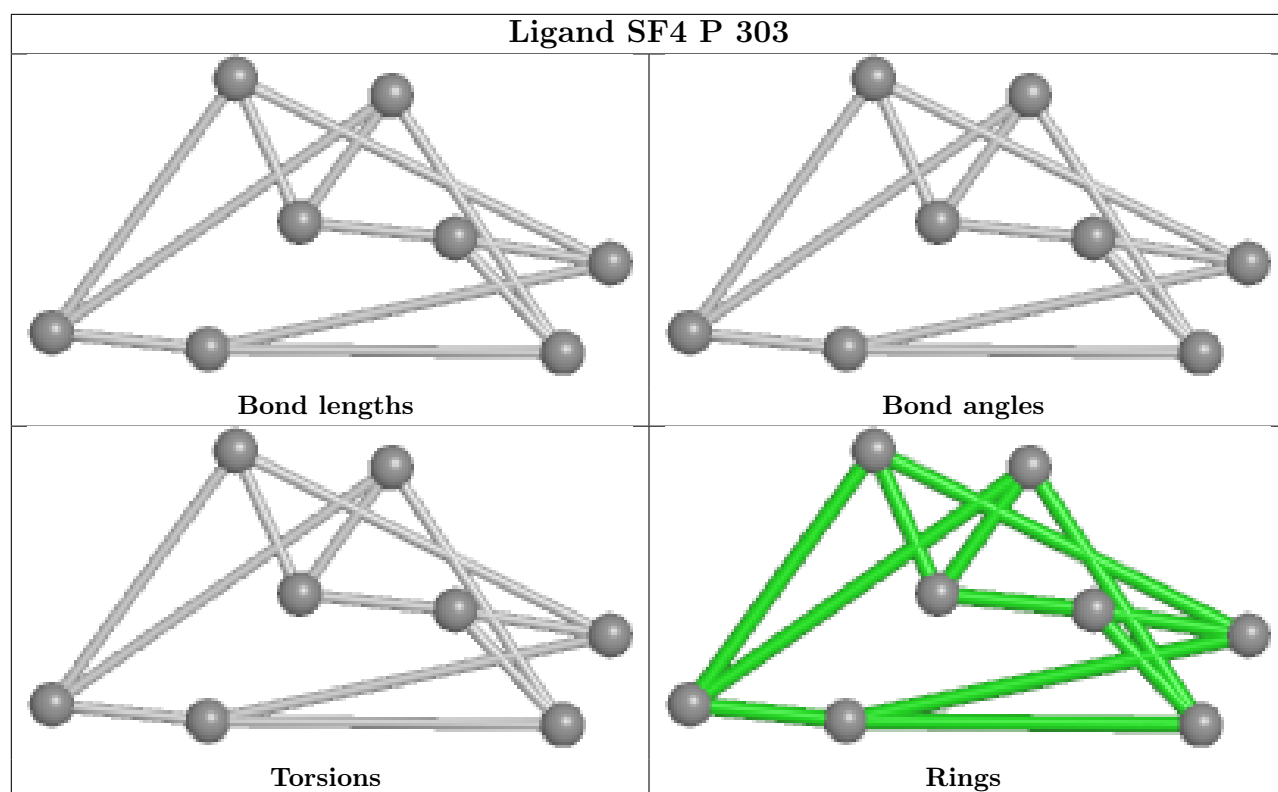


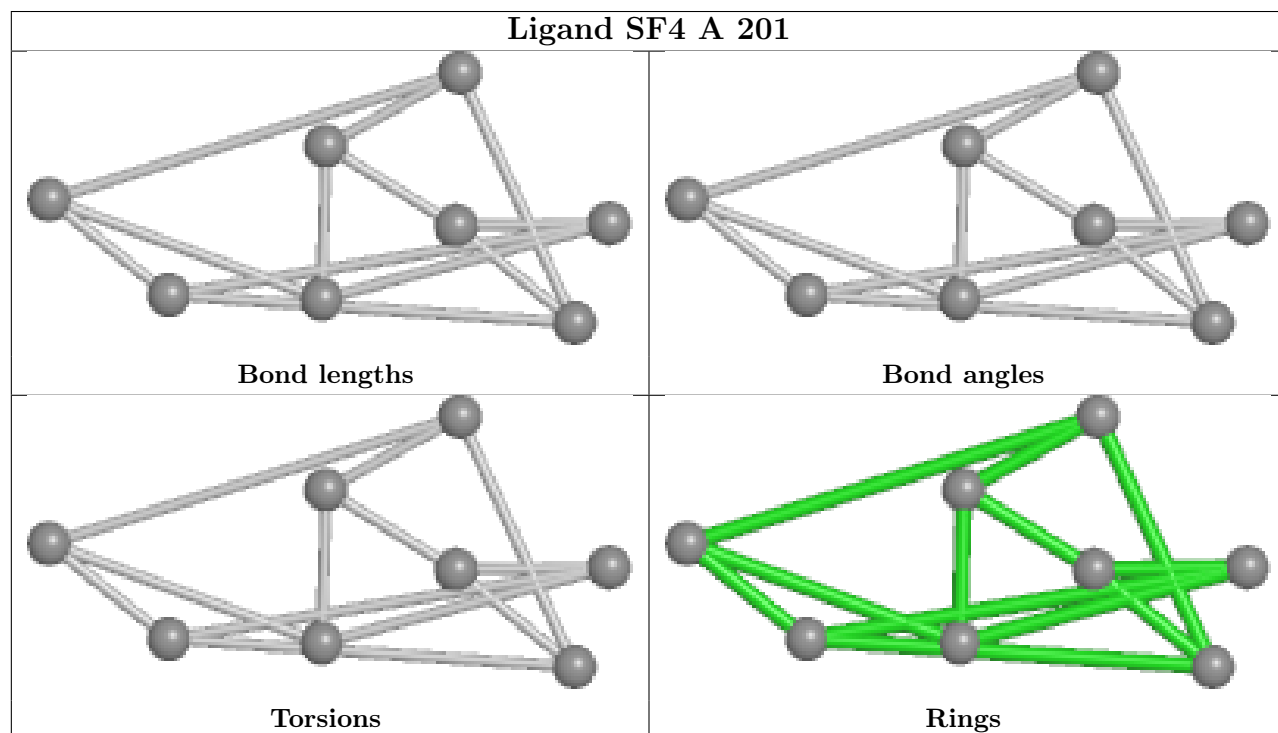
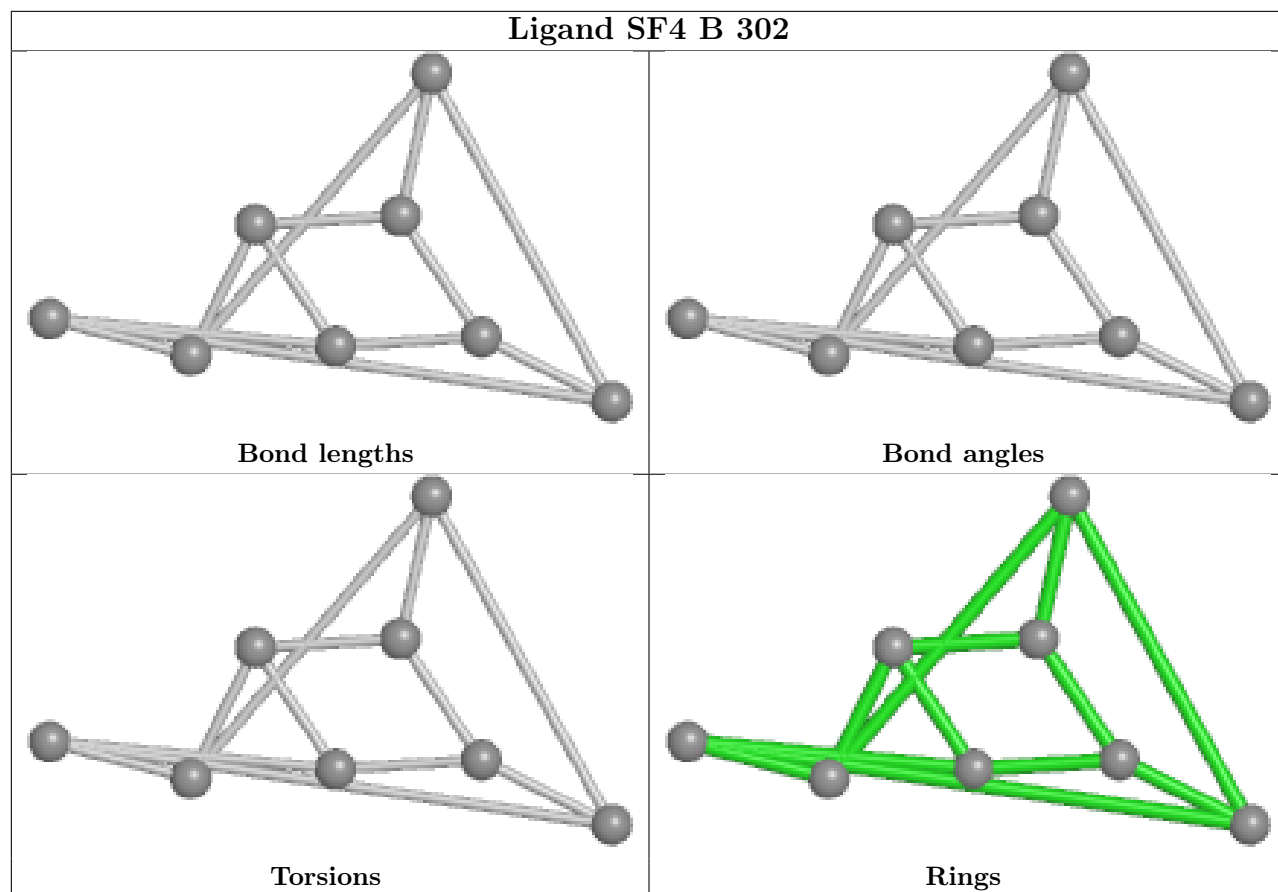
Ligand SF4 P 301



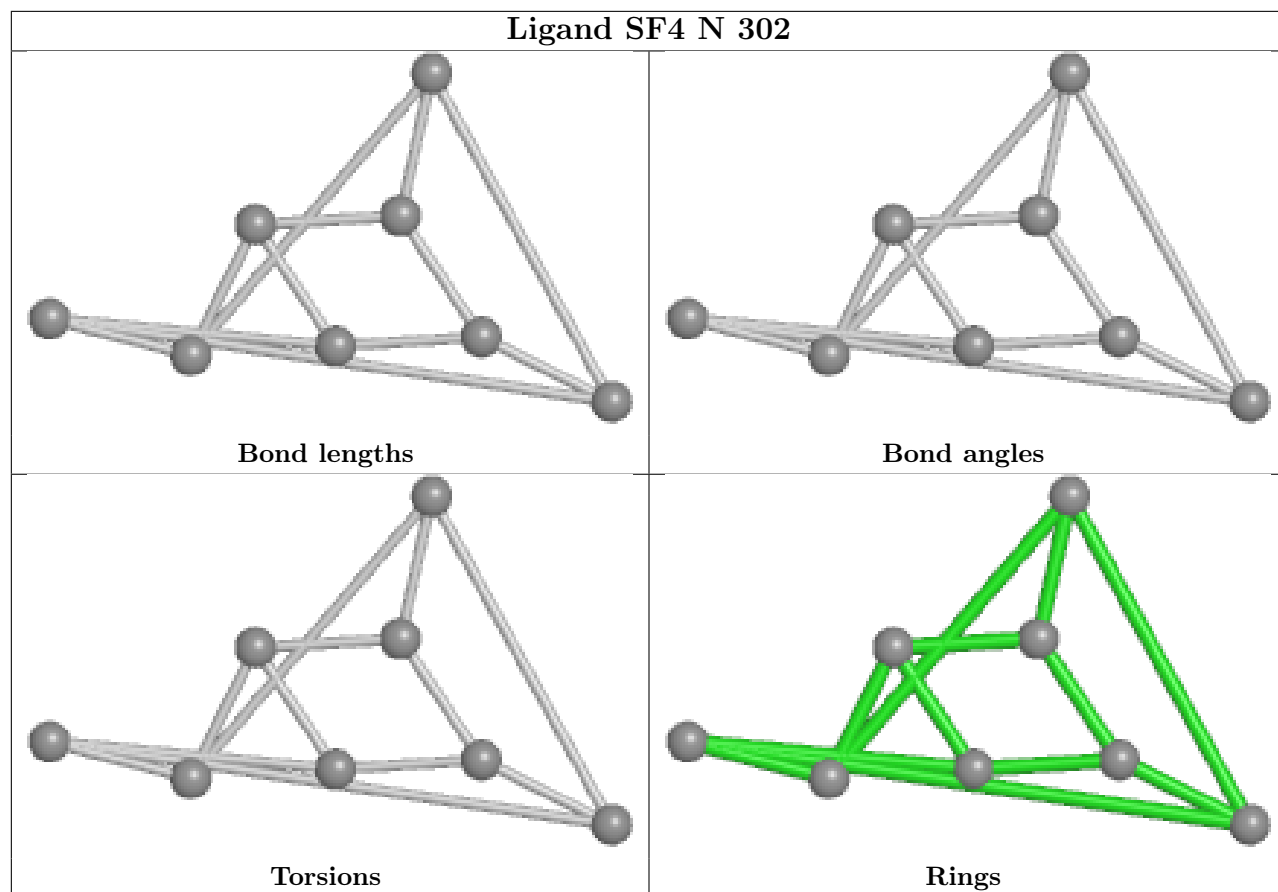
Ligand SF4 N 304



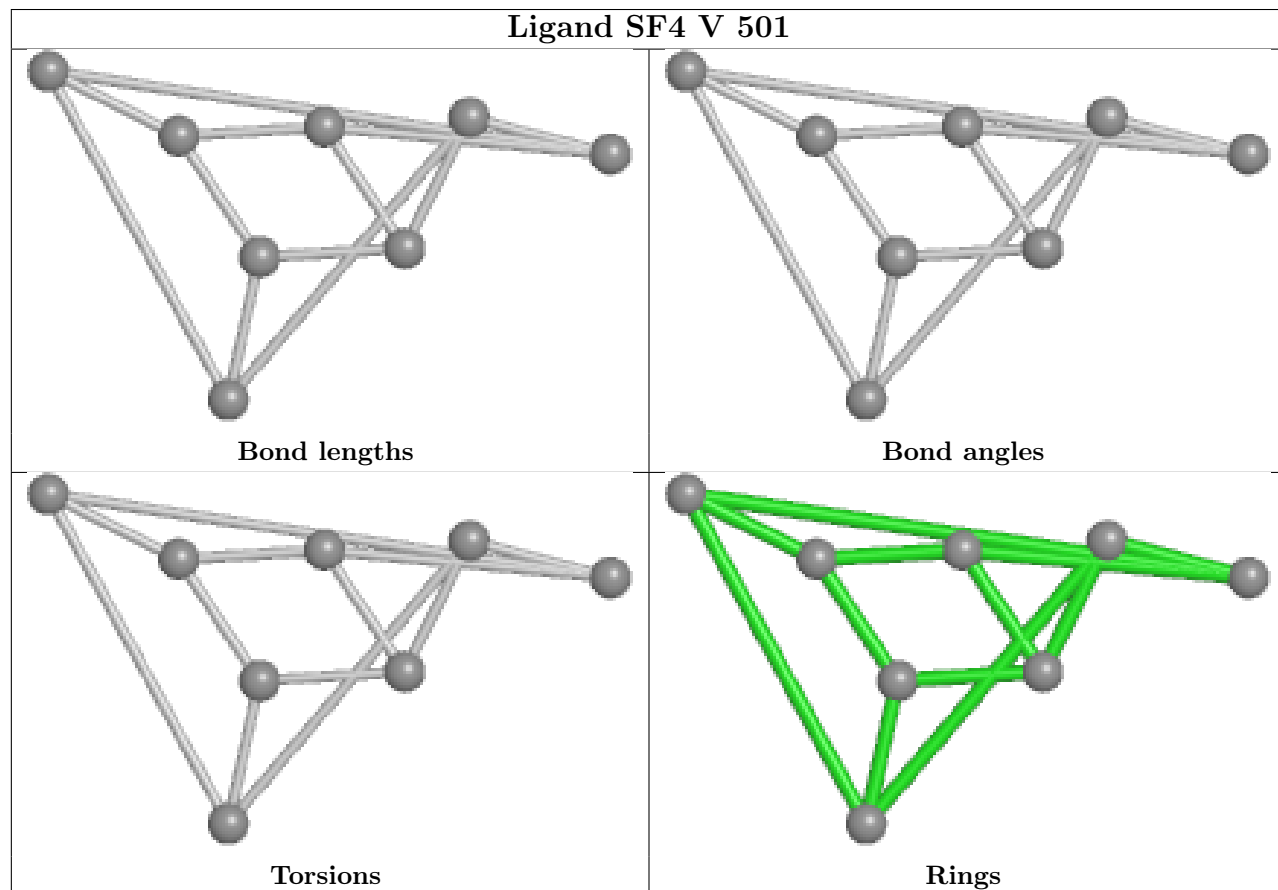


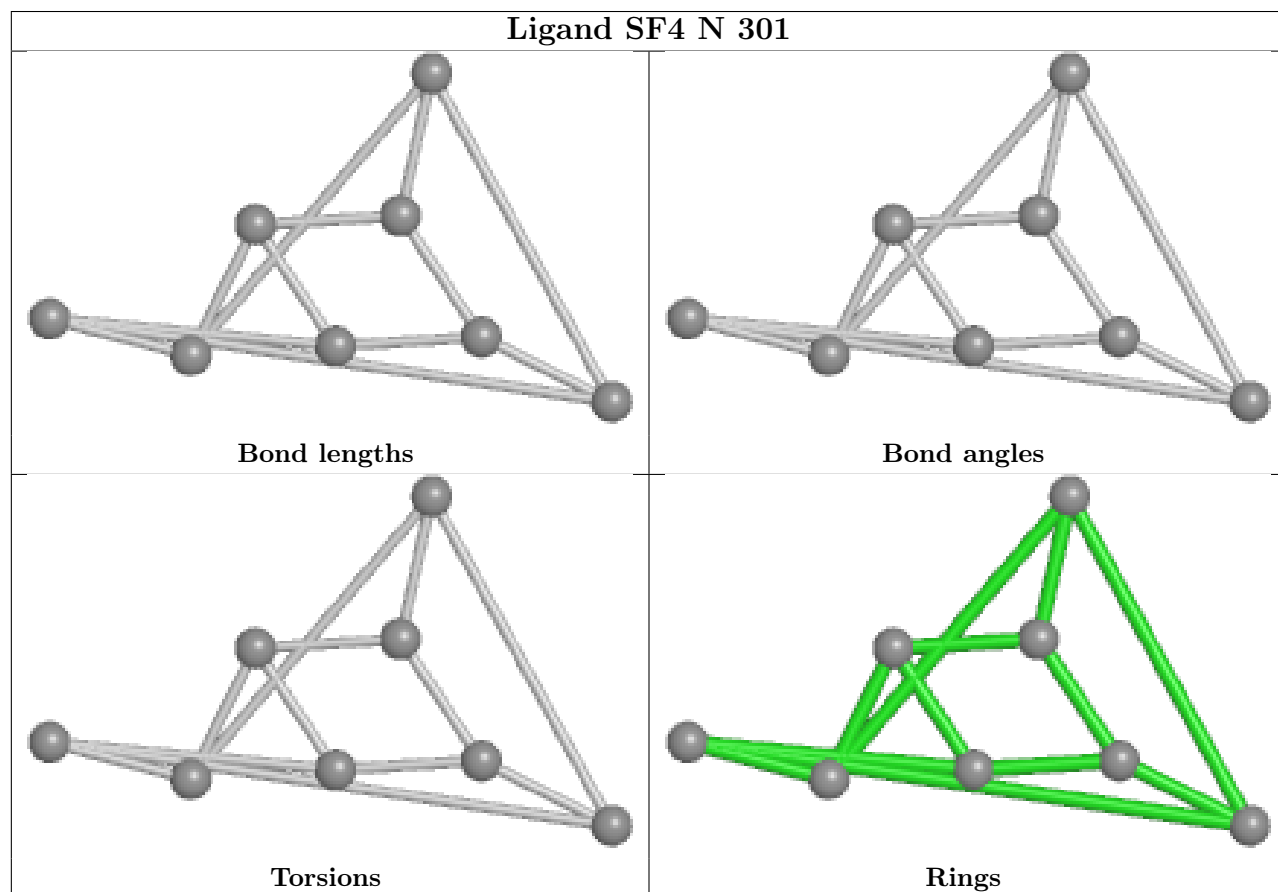
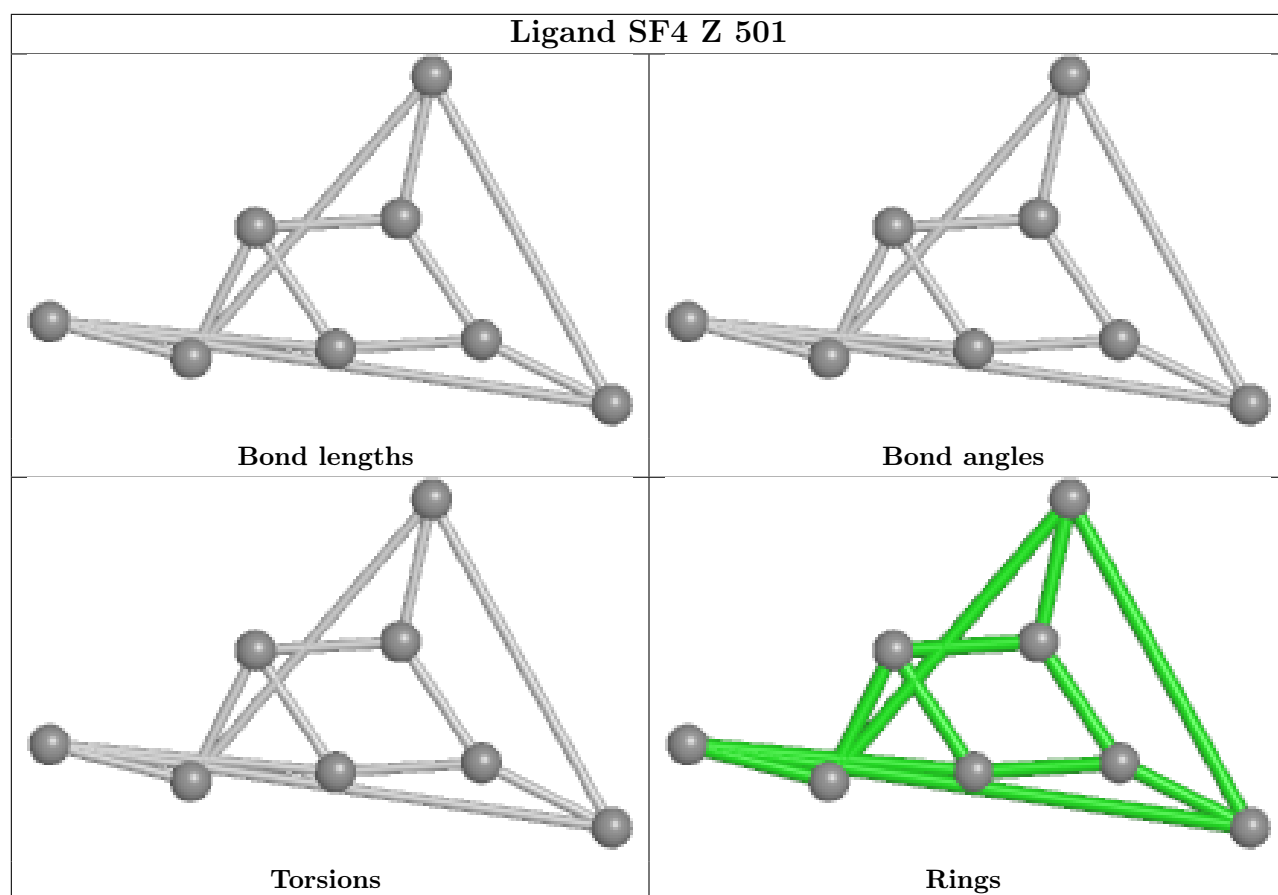


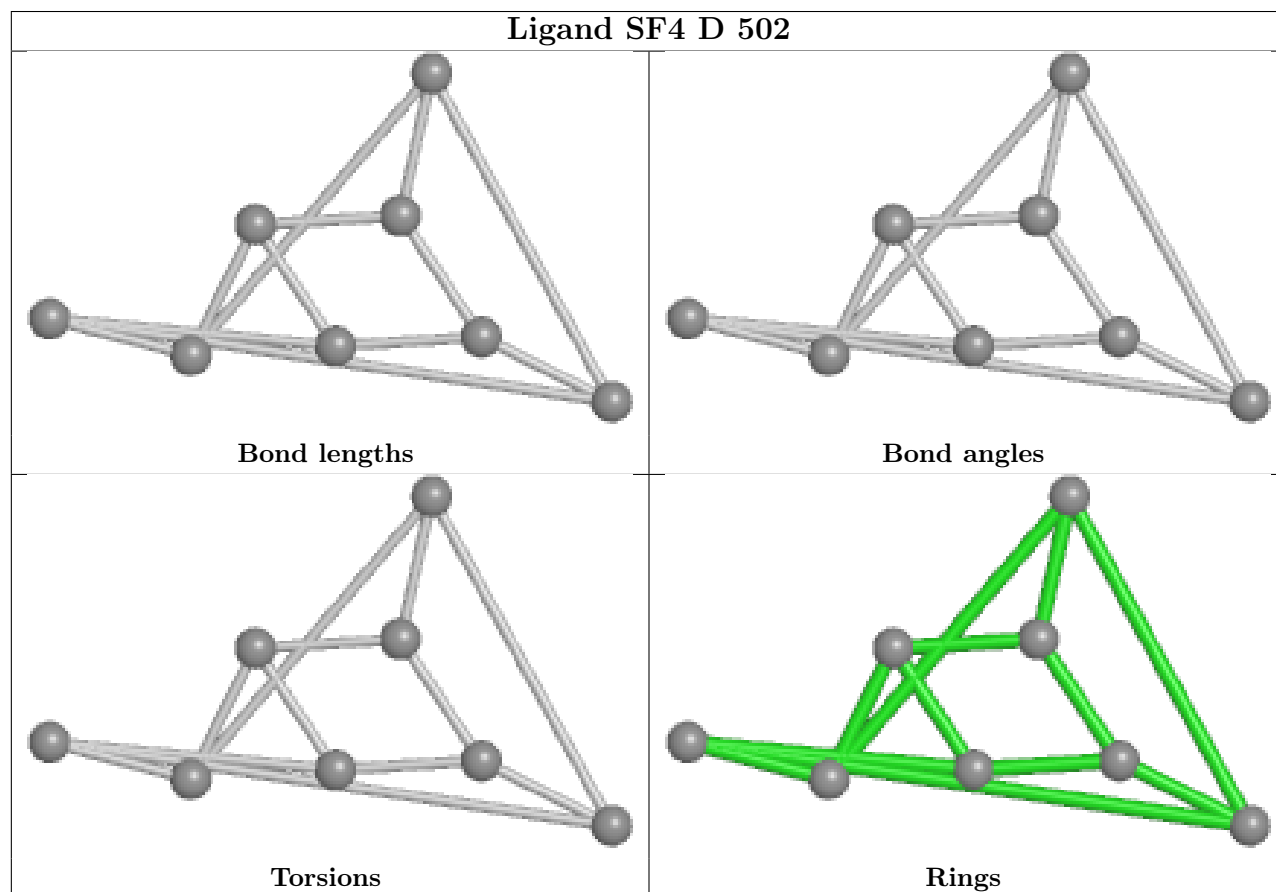
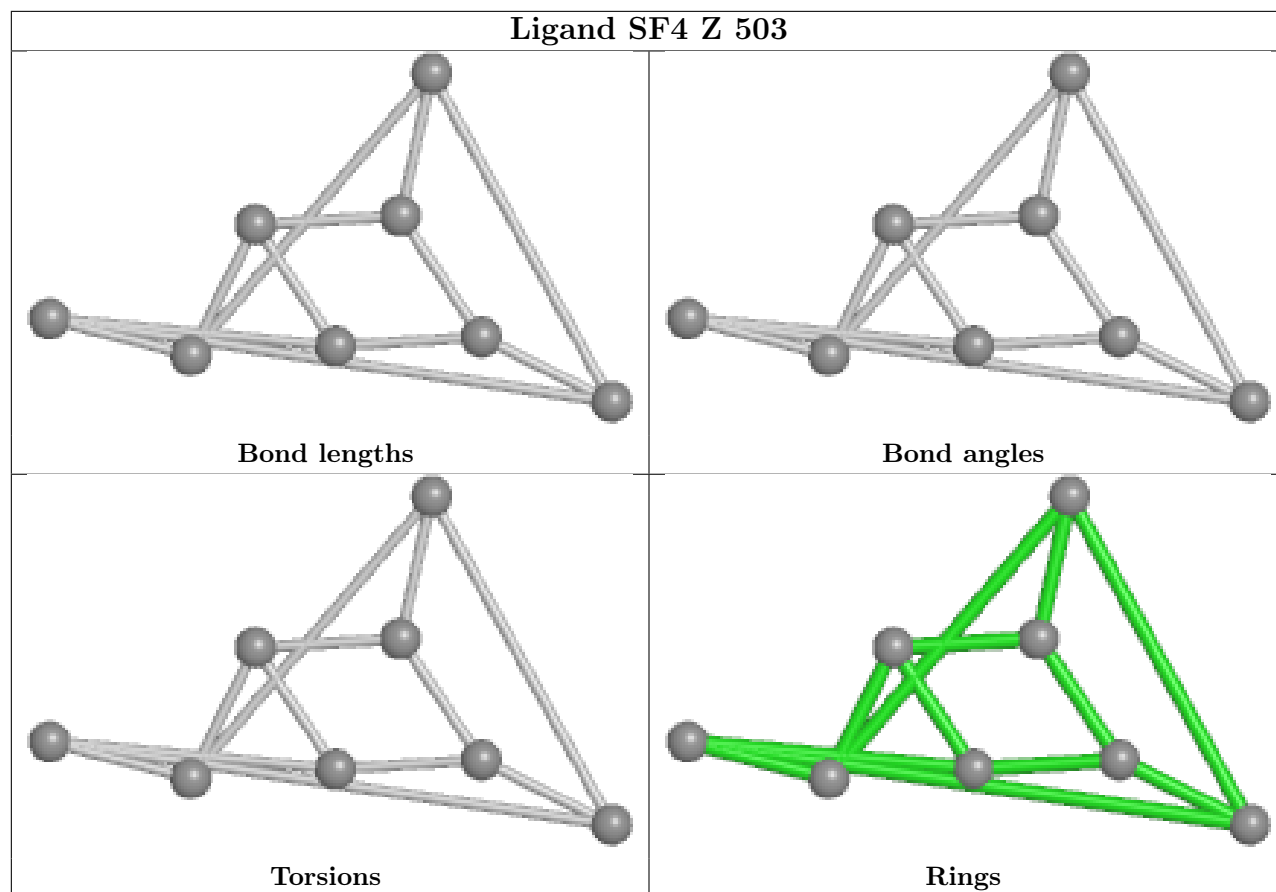
Ligand SF4 N 302

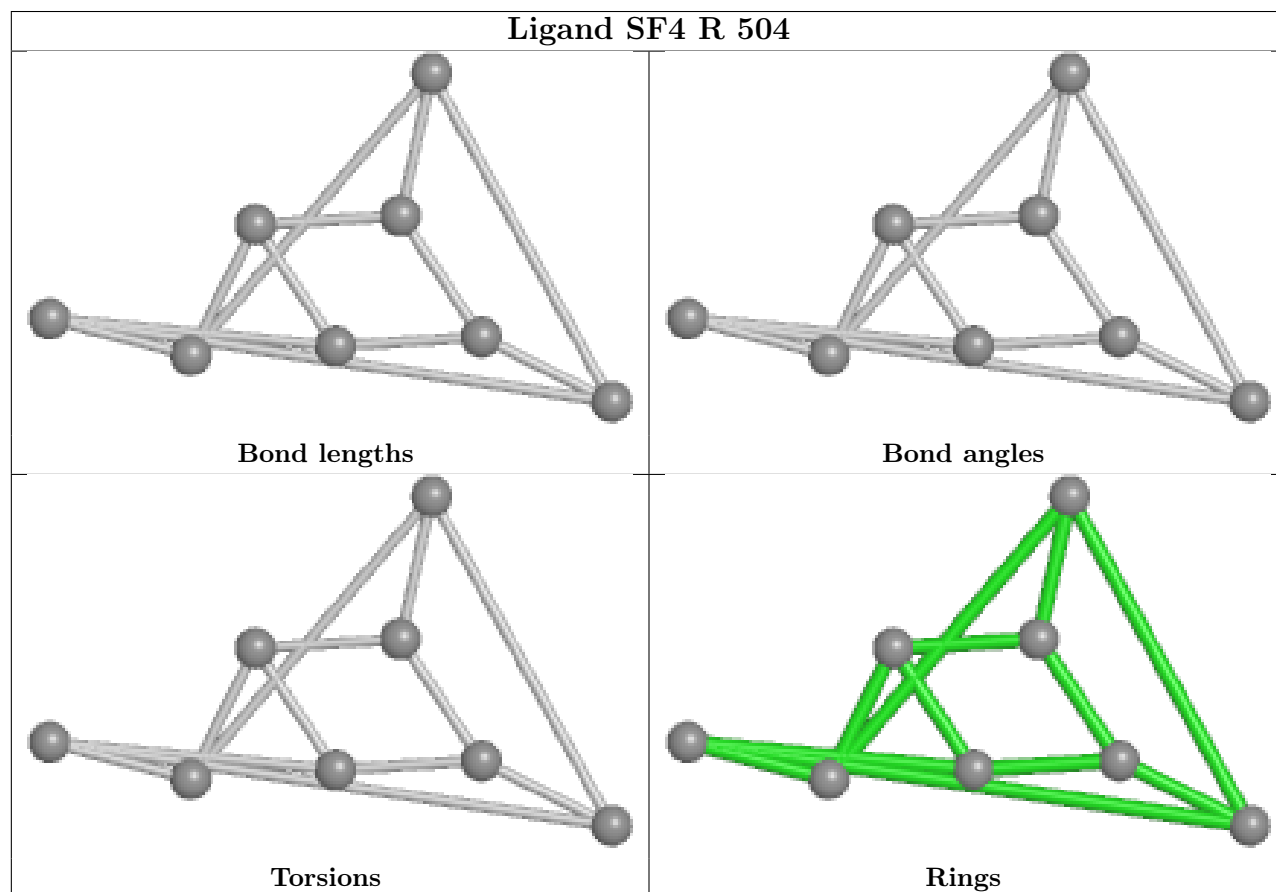
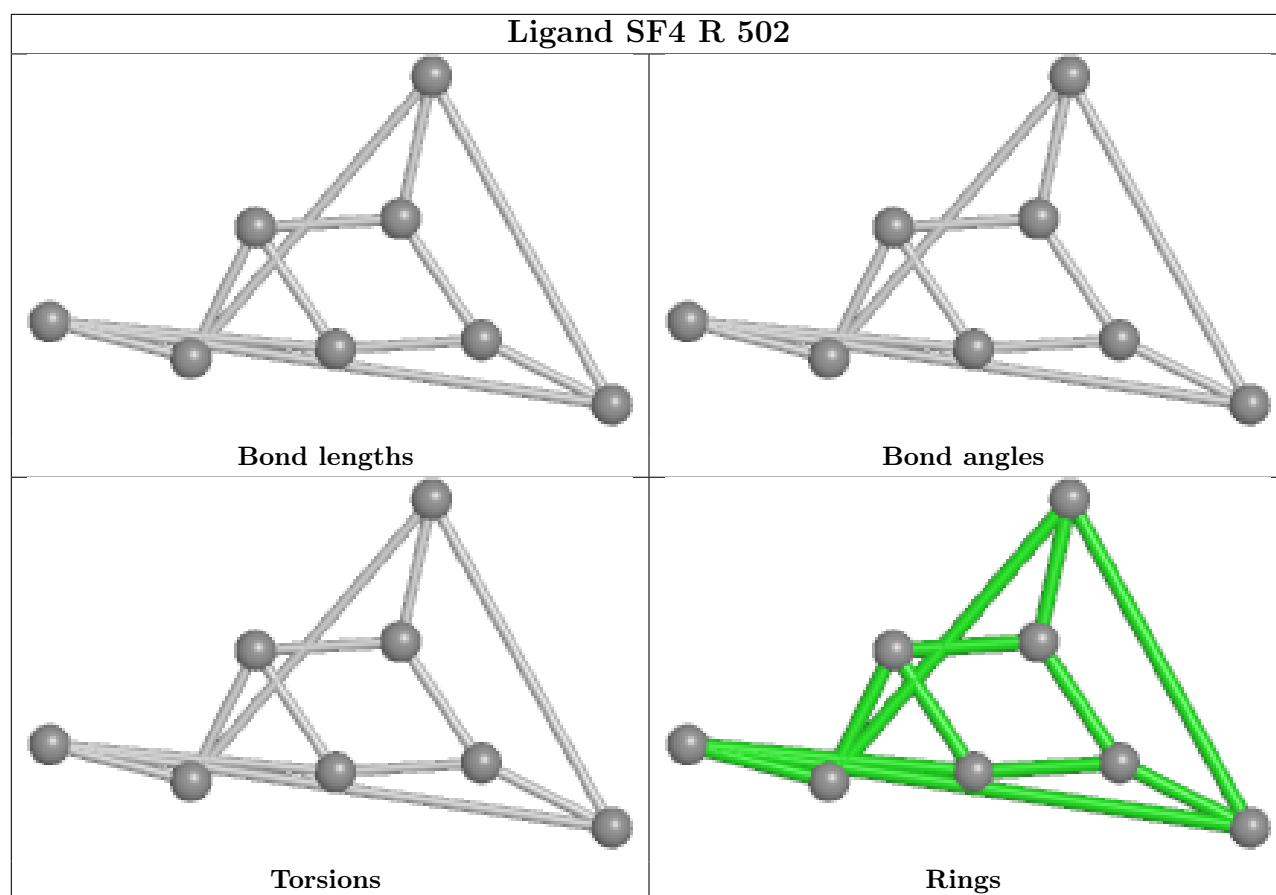


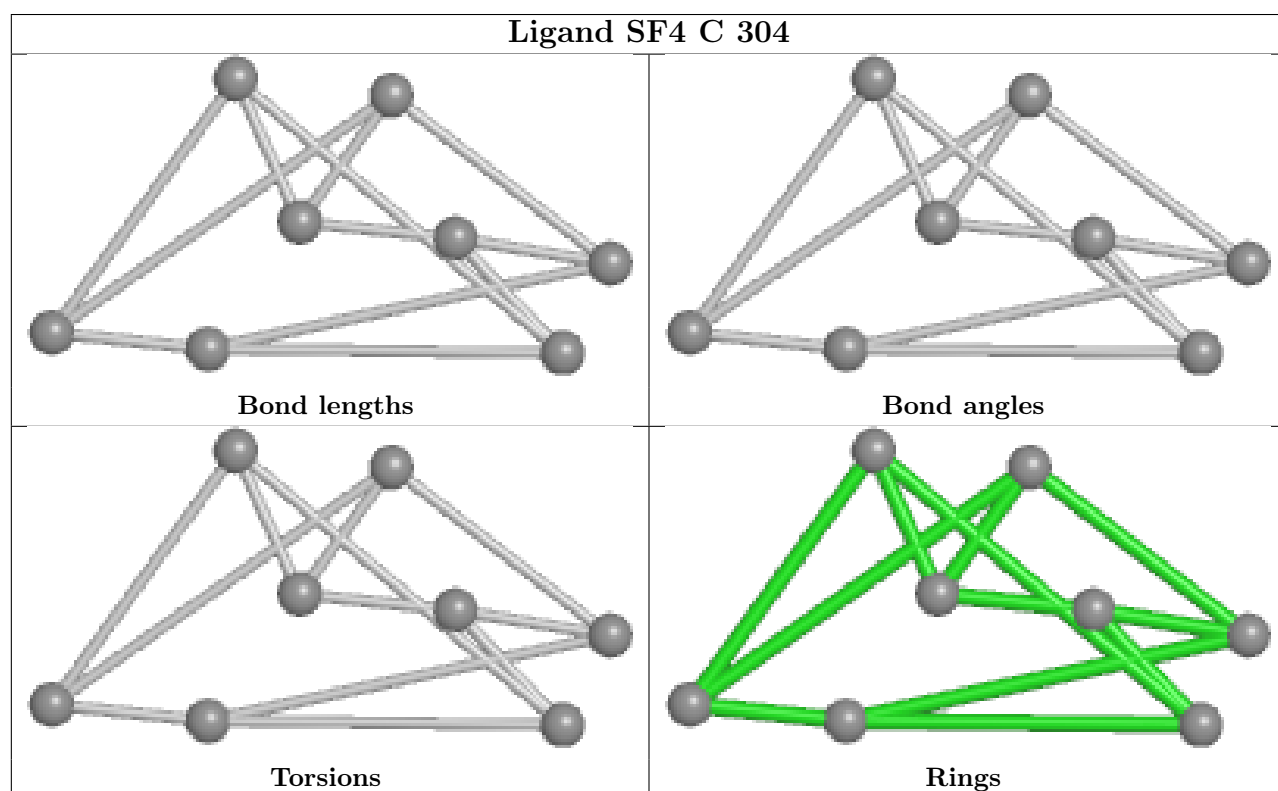
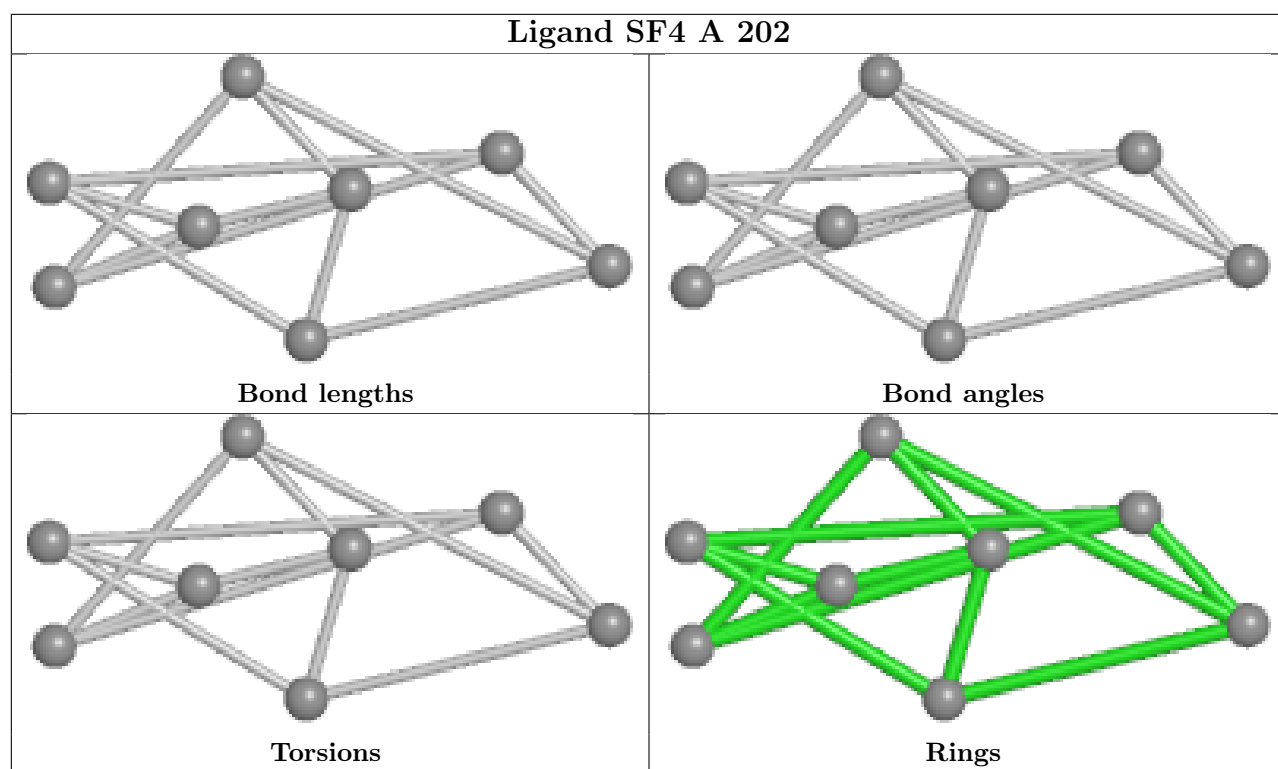
Ligand SF4 V 501

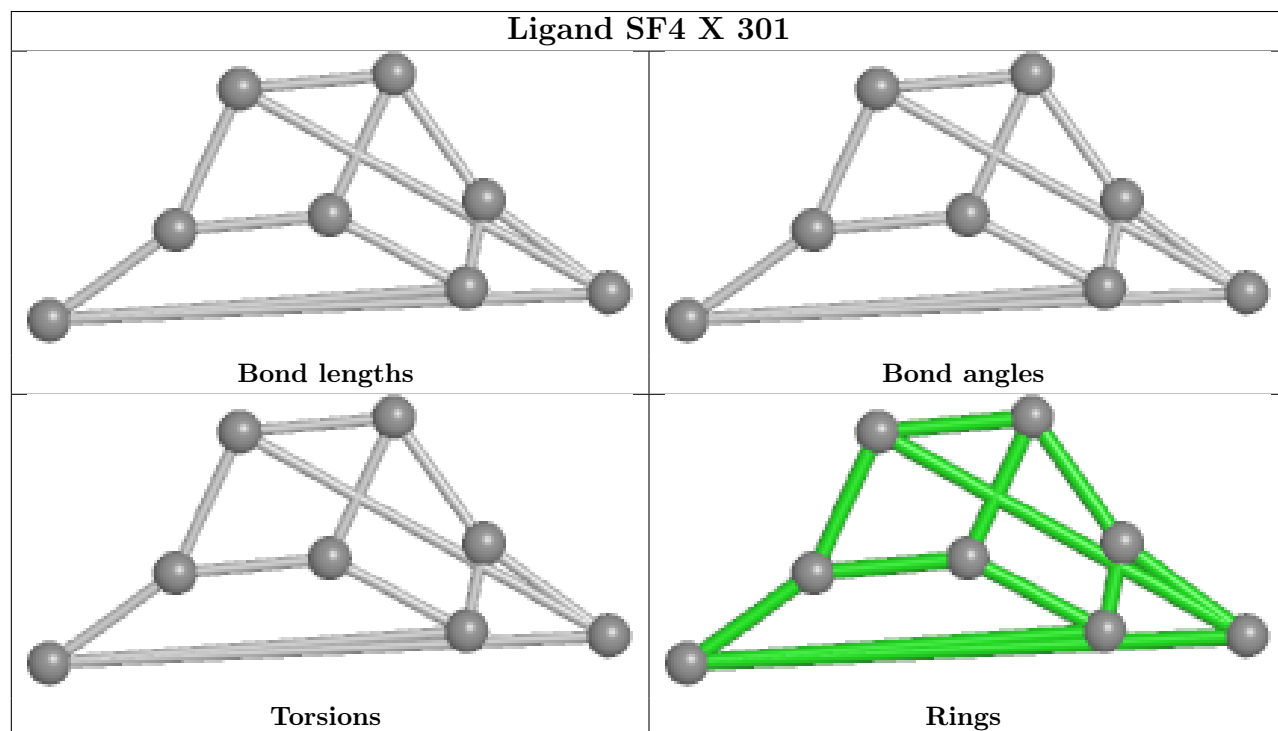
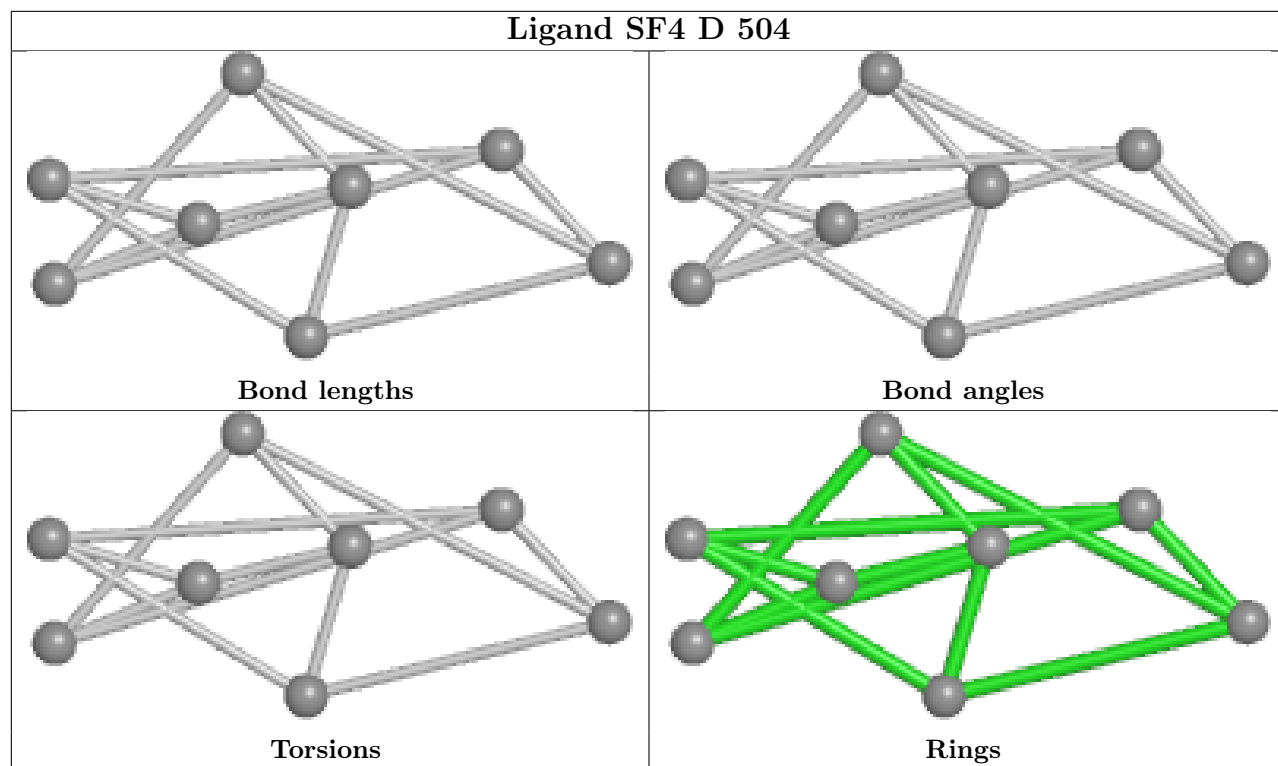


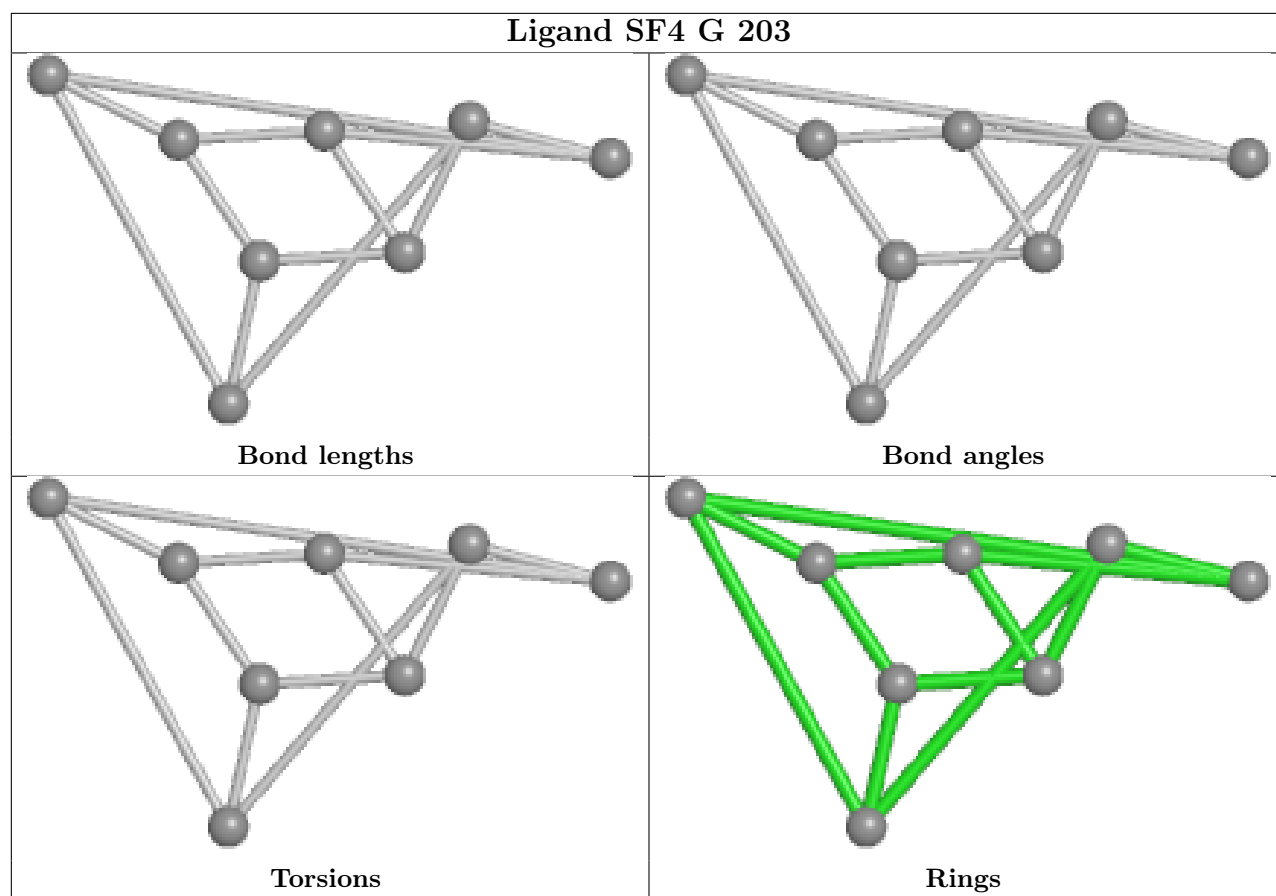
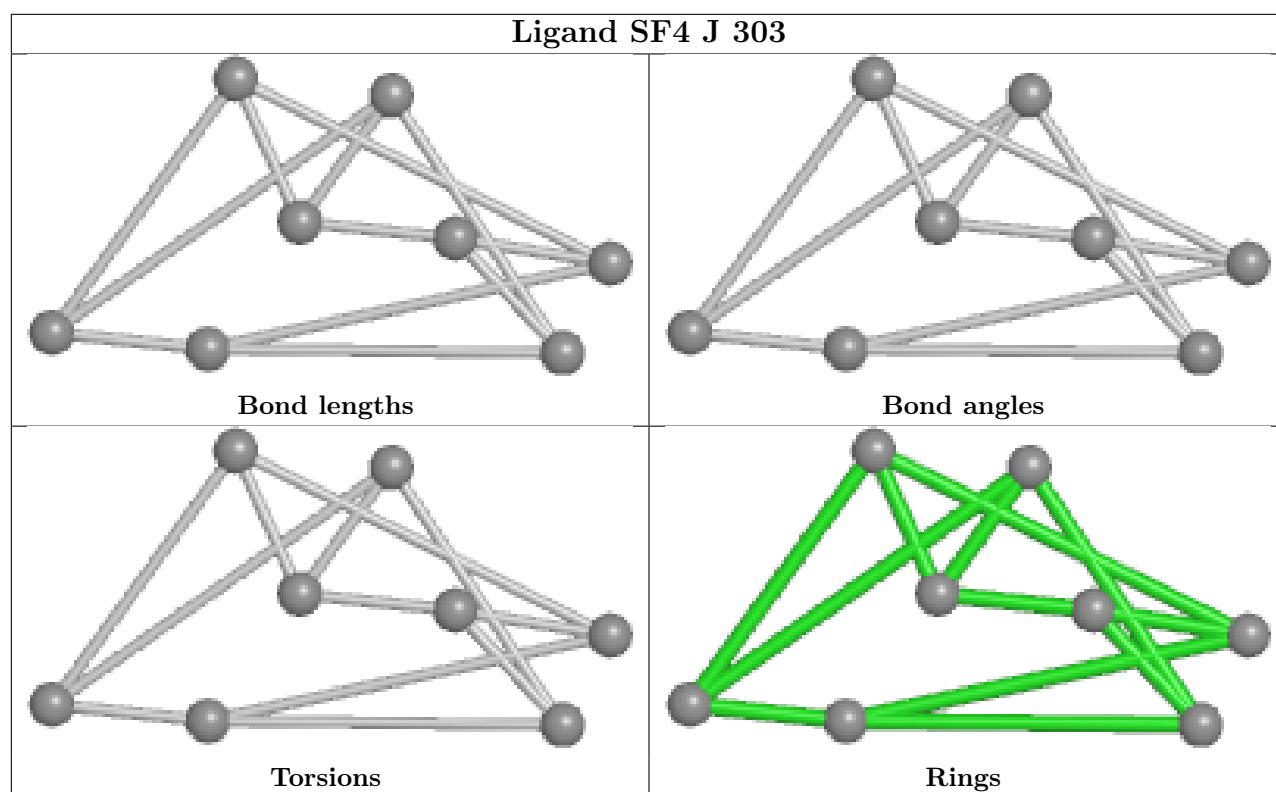


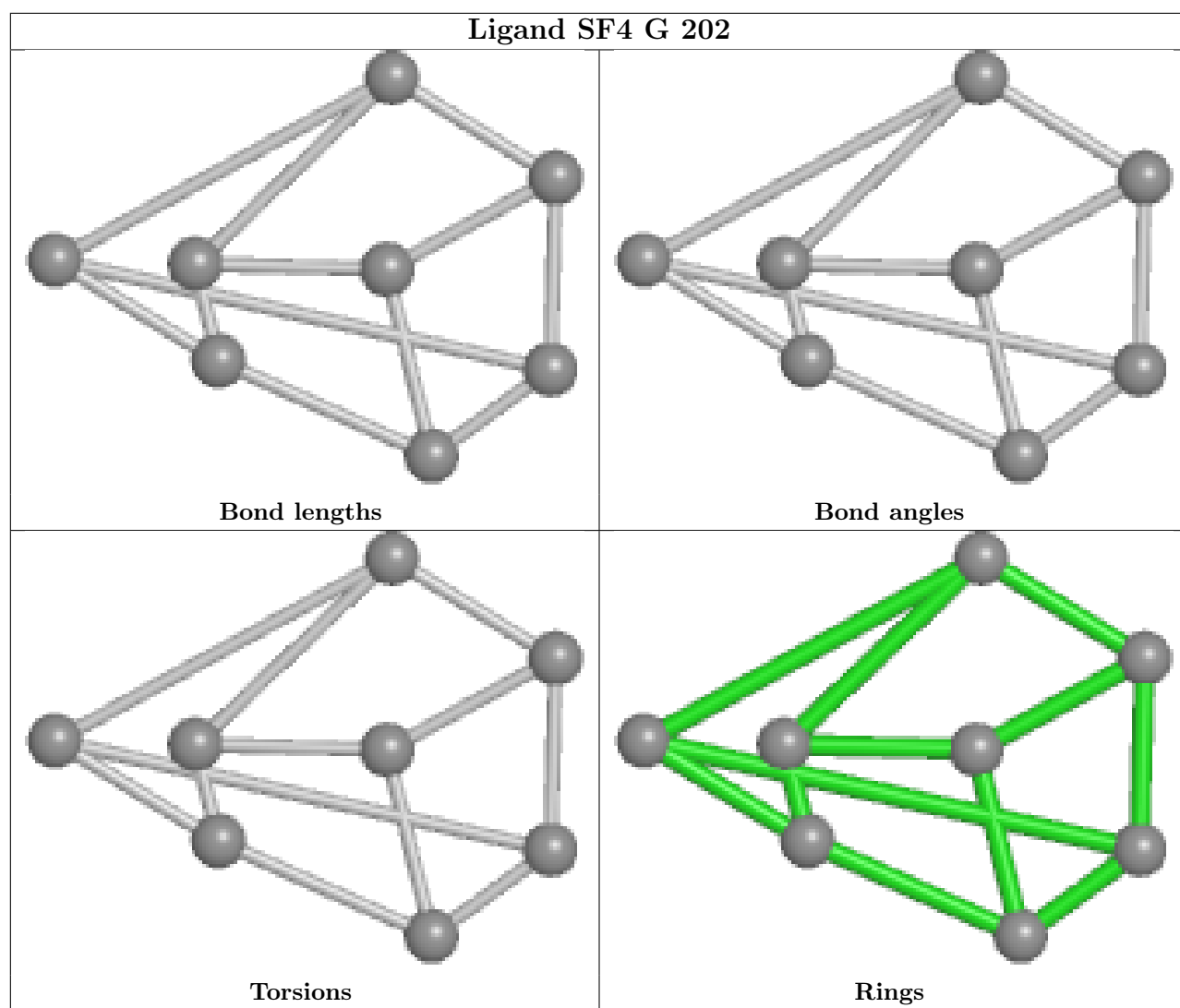




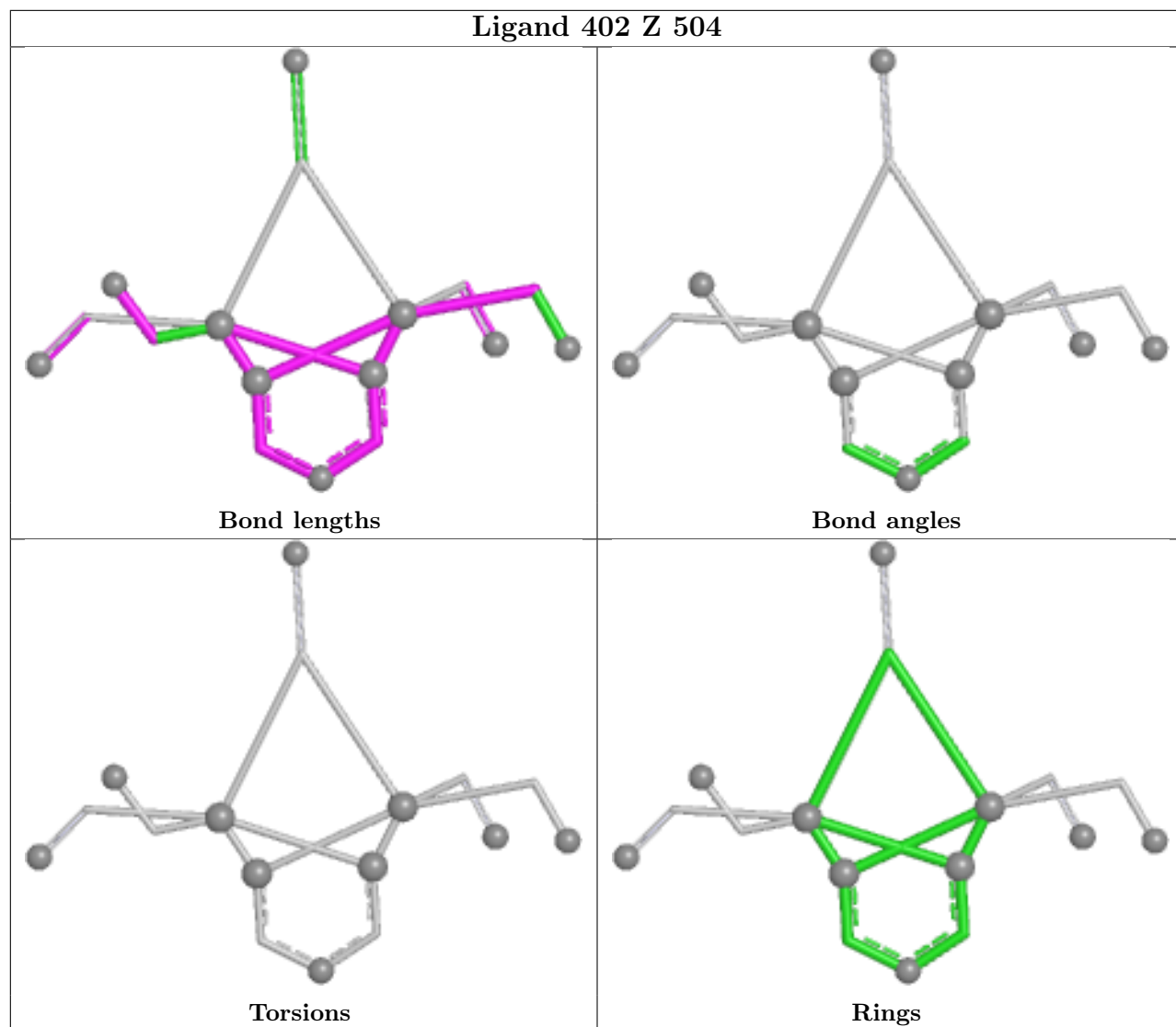




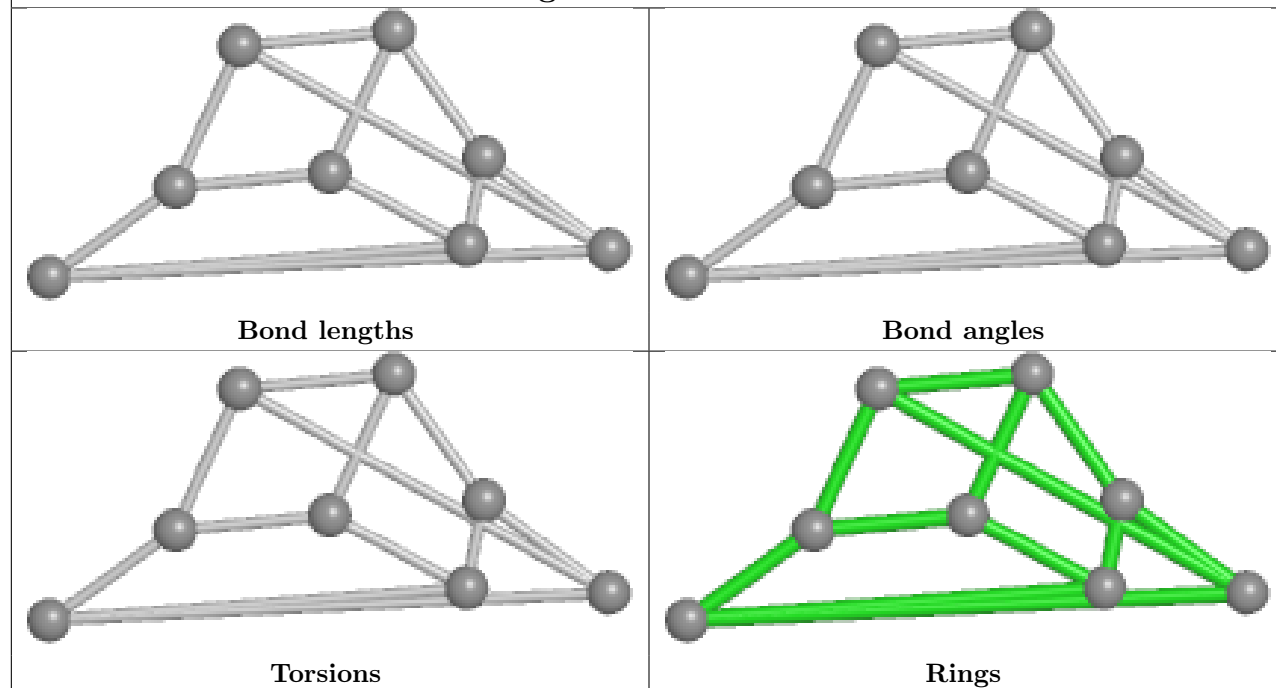




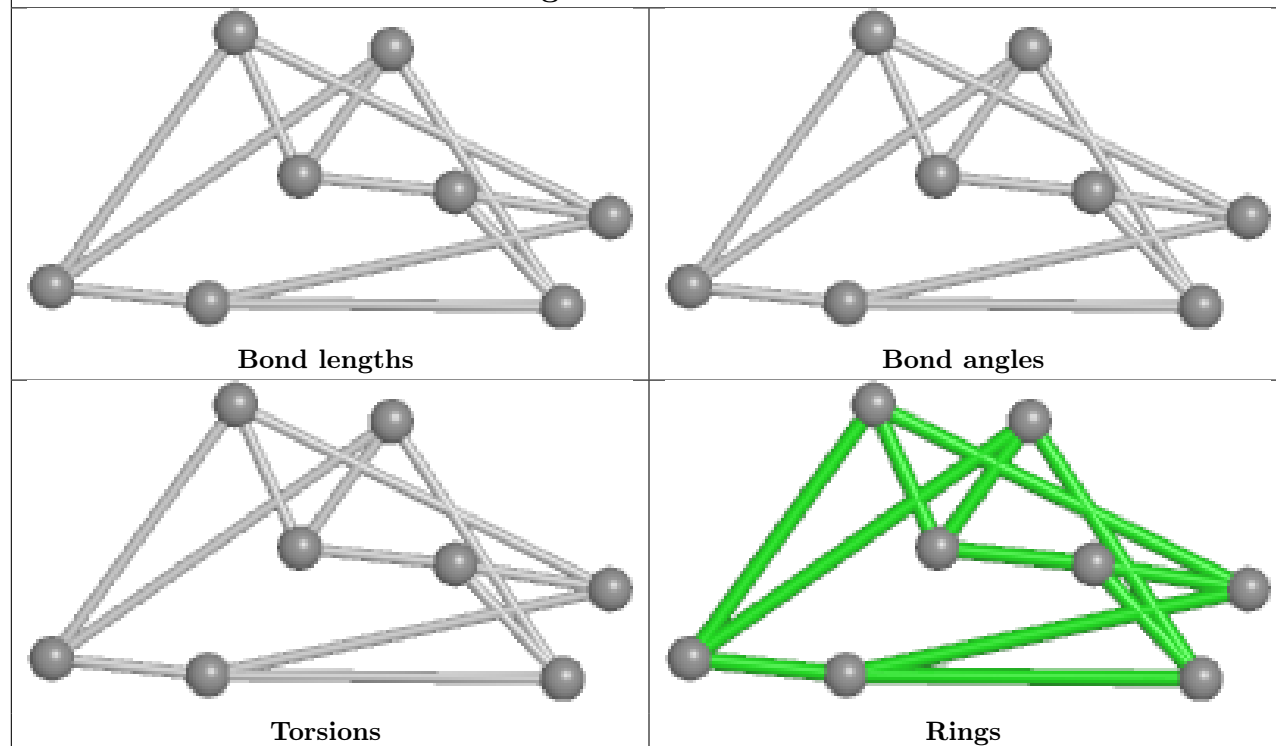
Ligand 402 Z 504

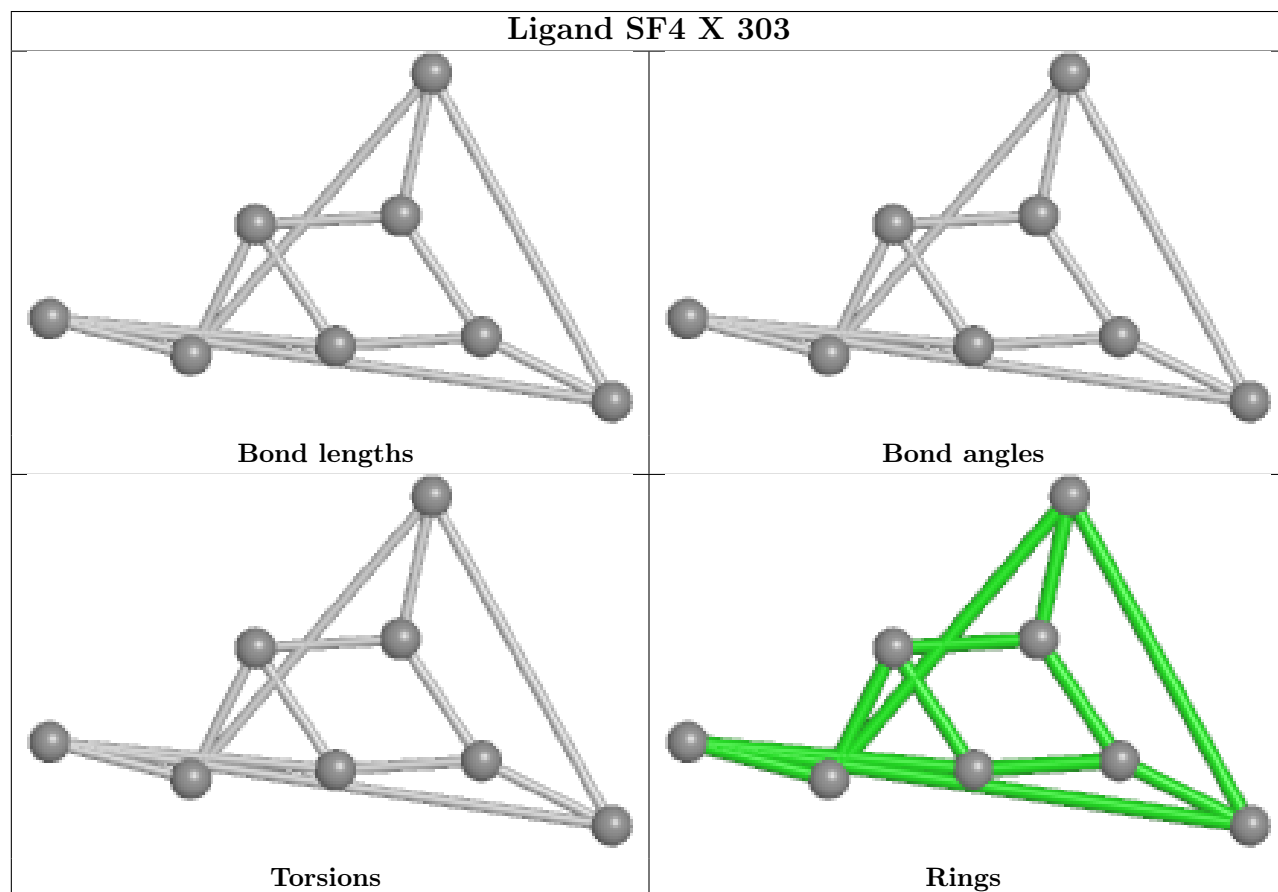
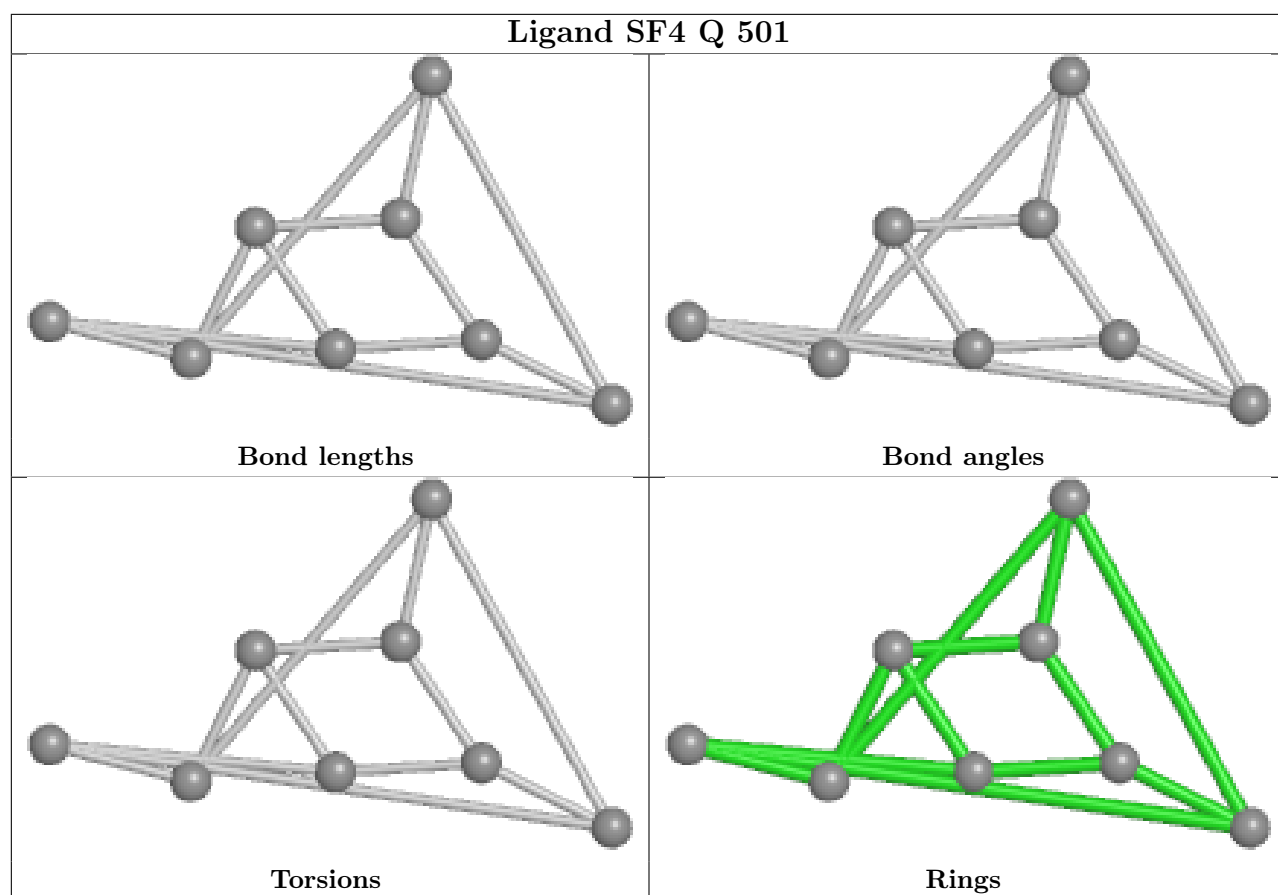


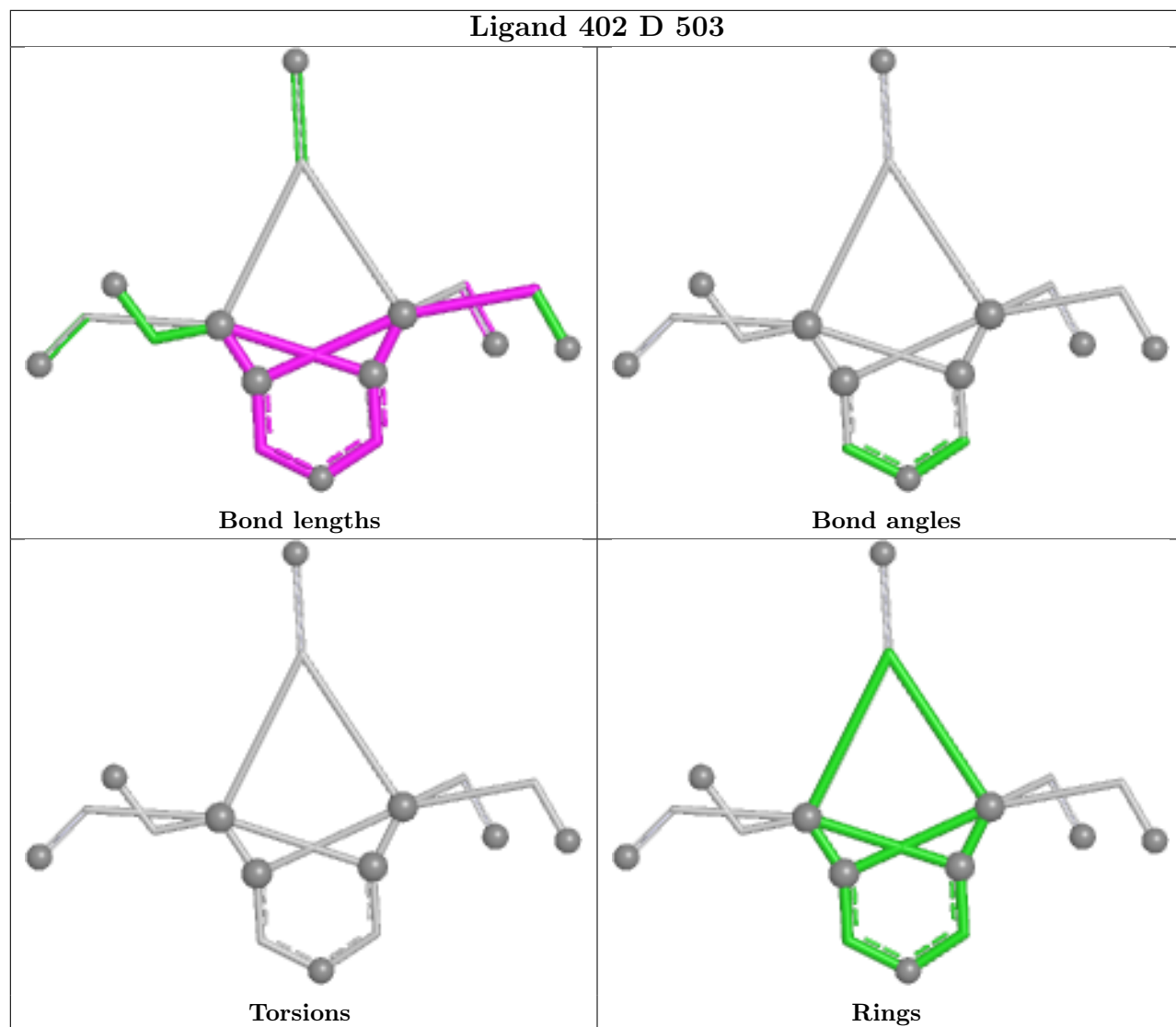
Ligand SF4 Y 801

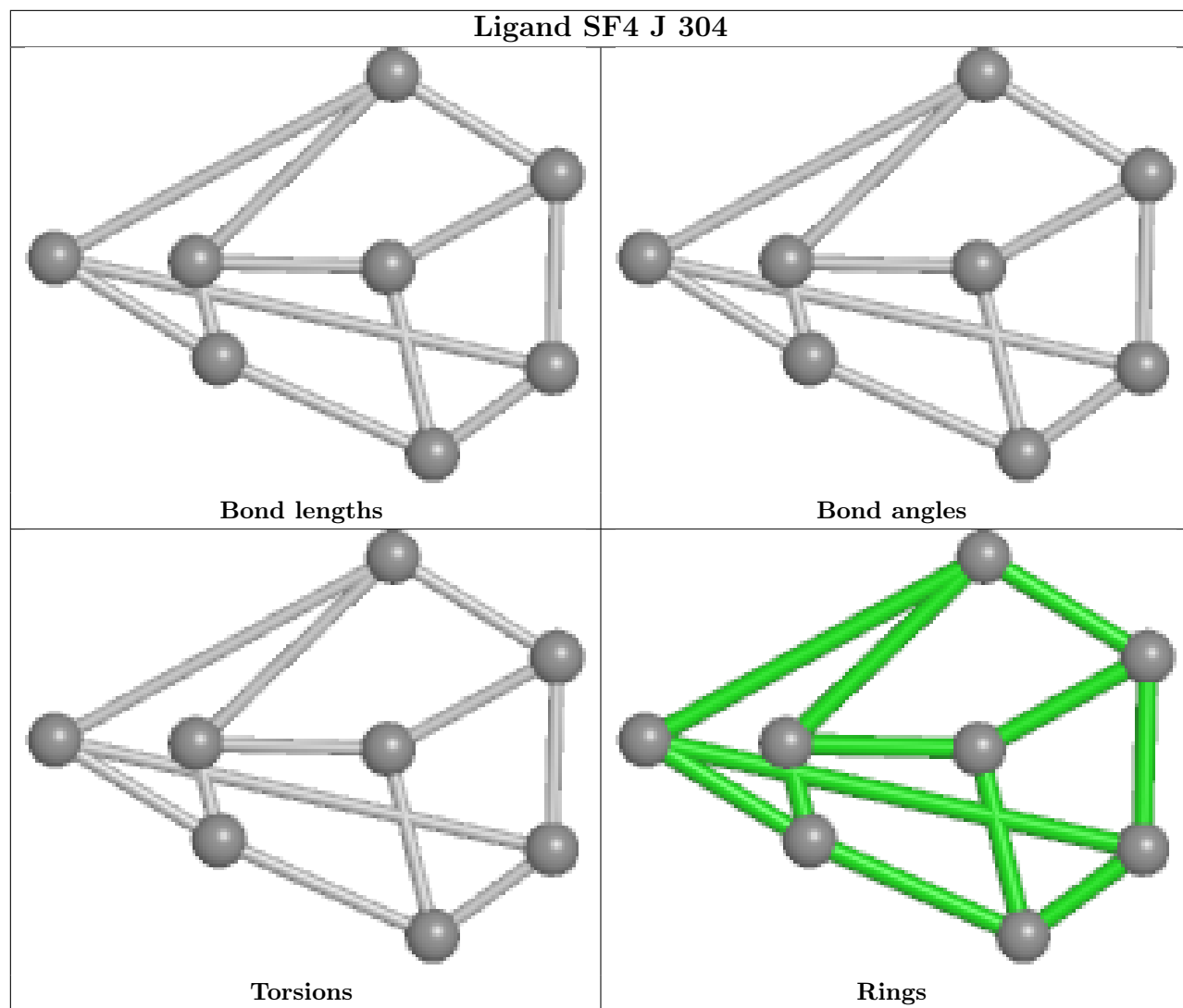


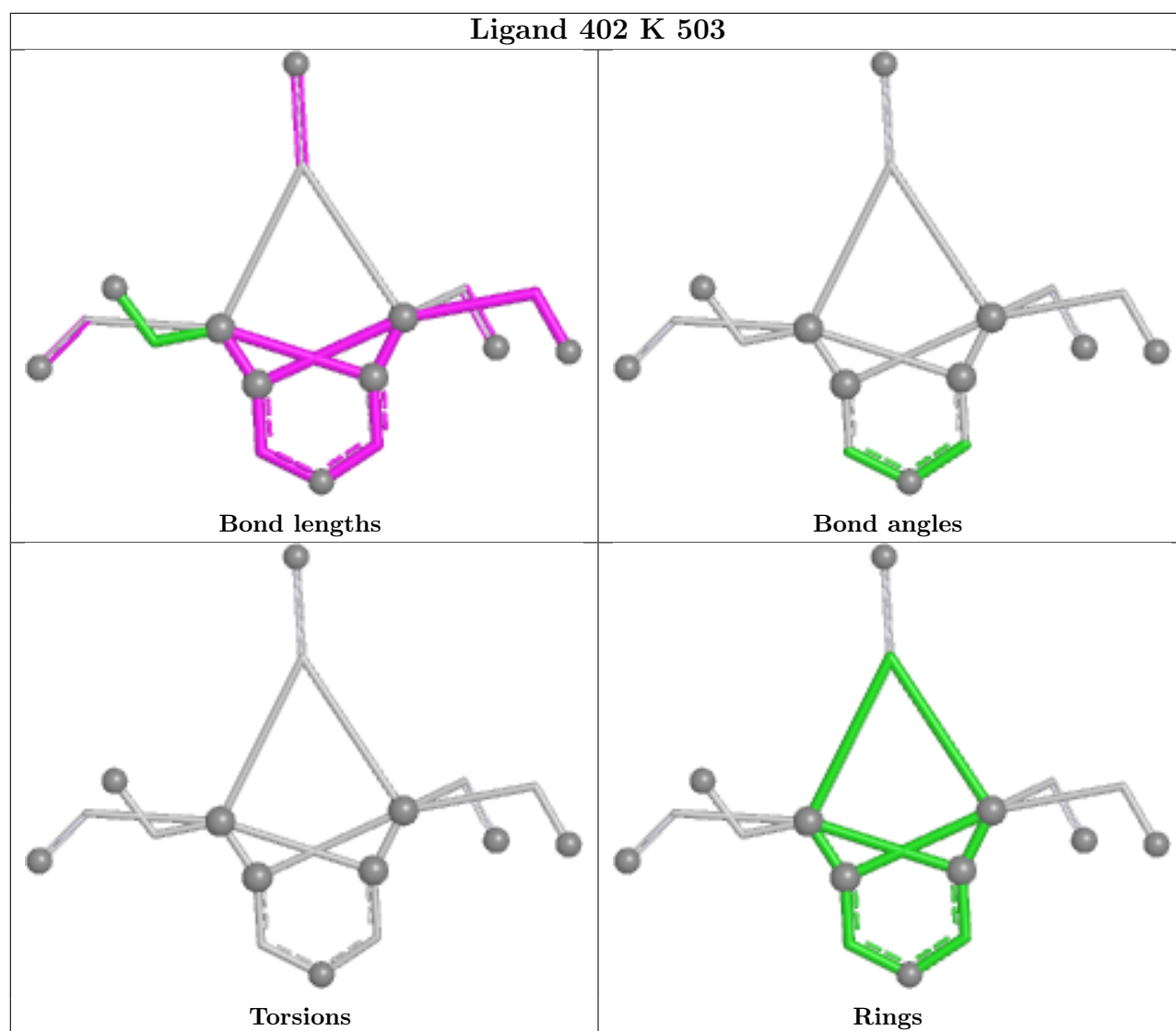
Ligand SF4 Z 502

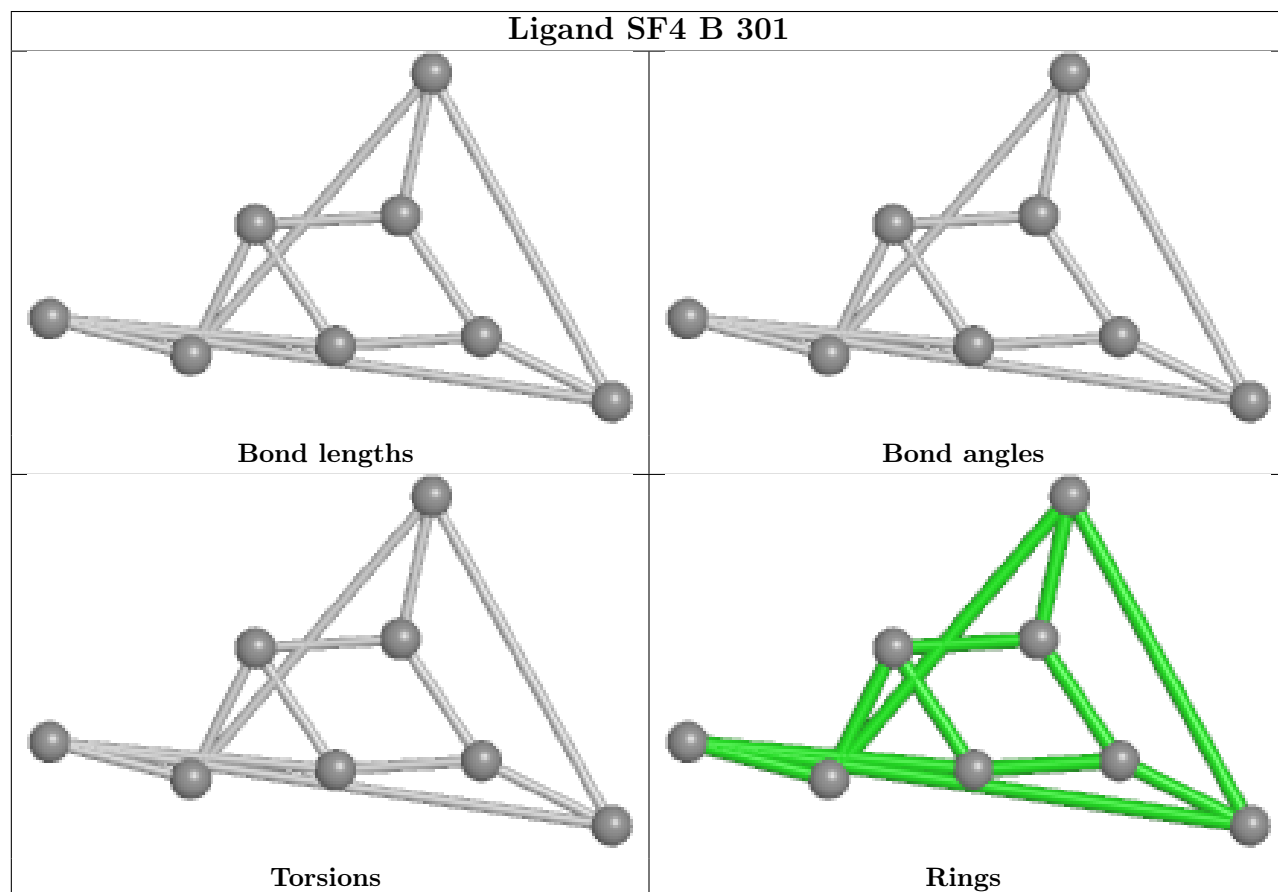
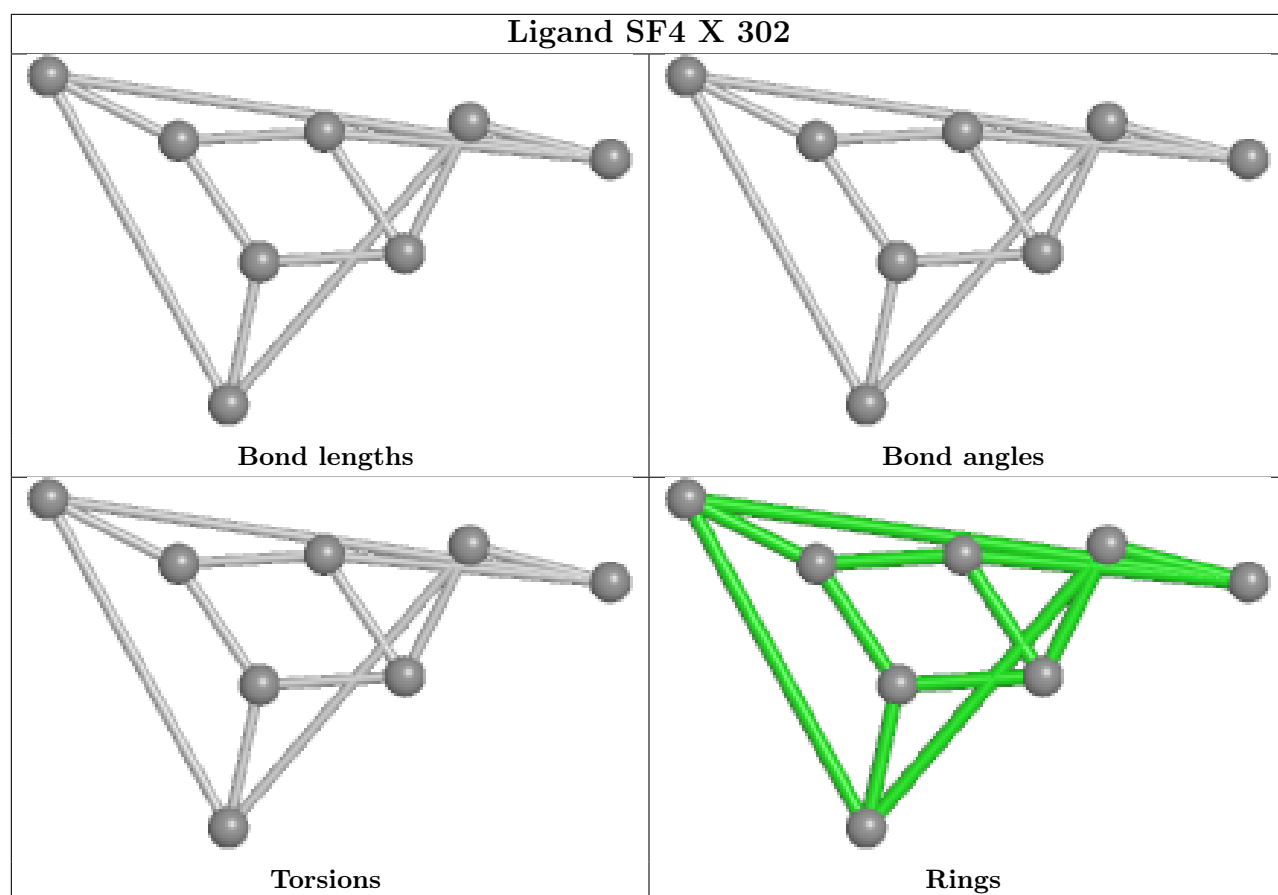


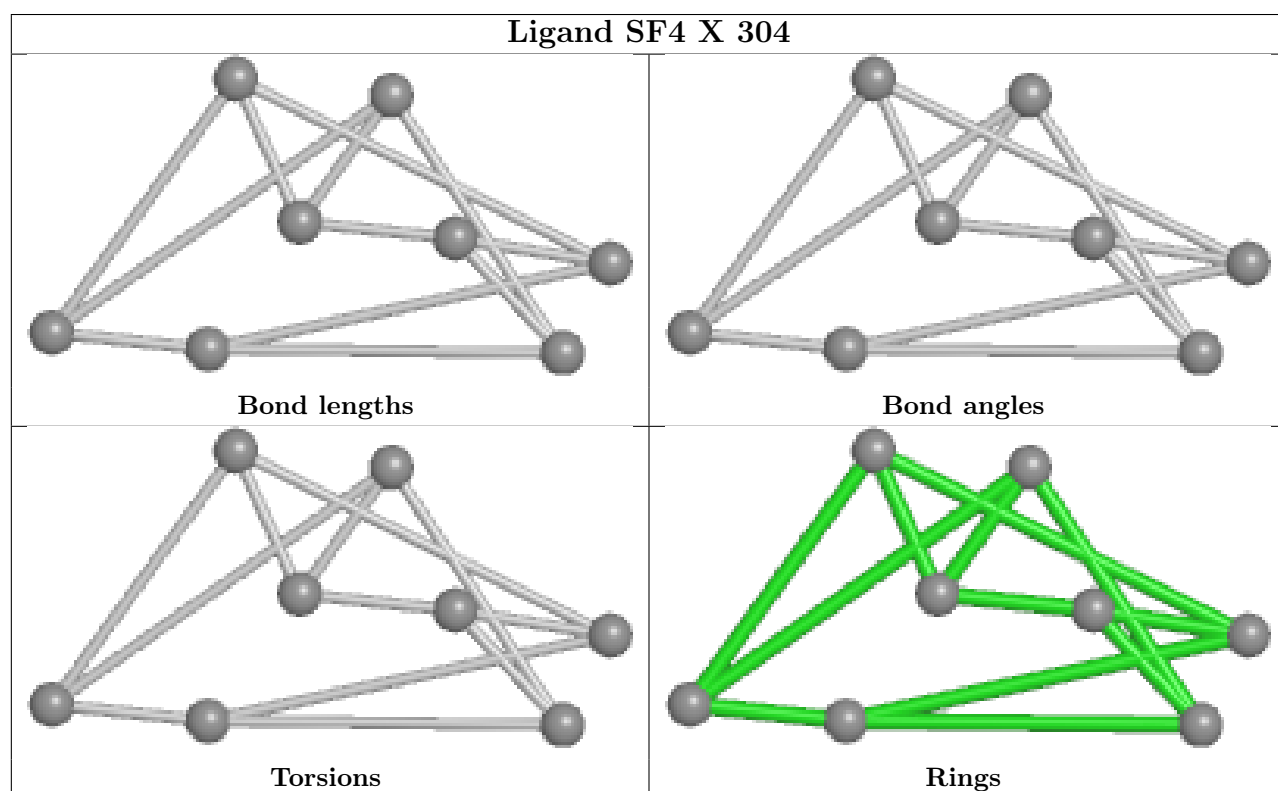
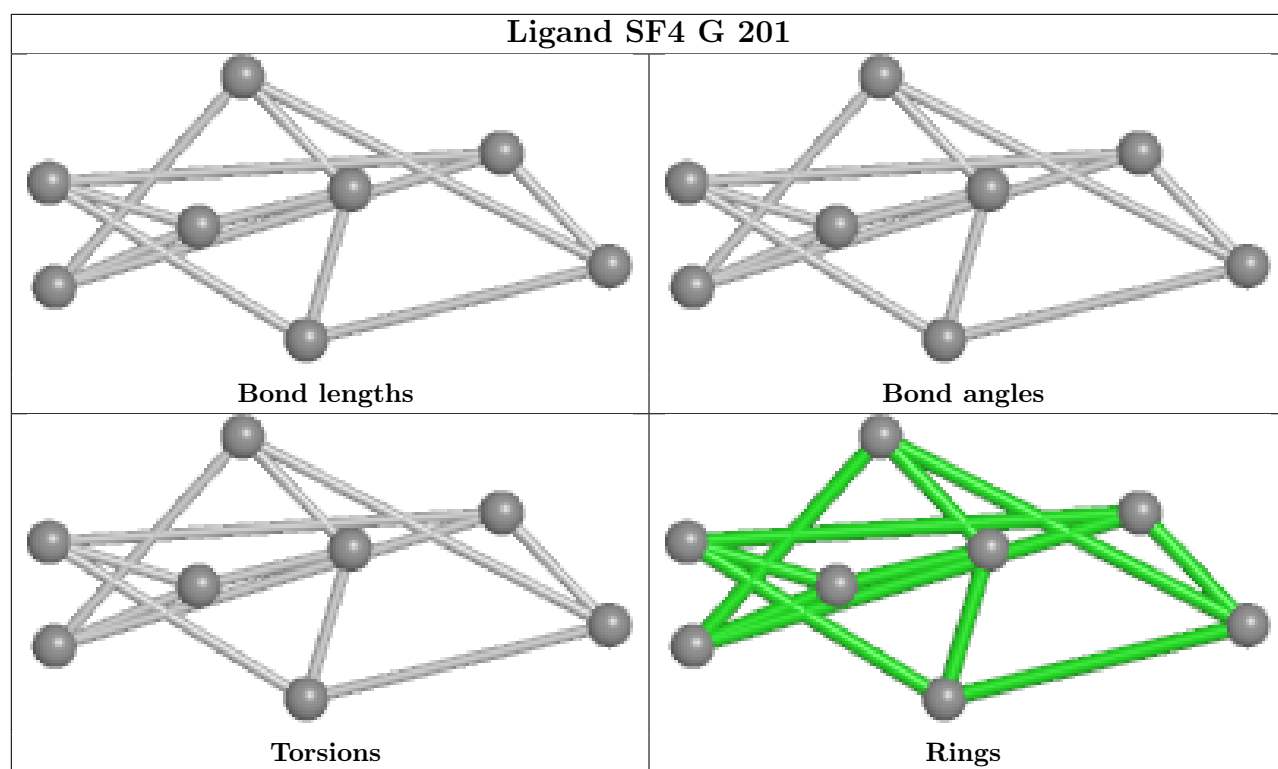


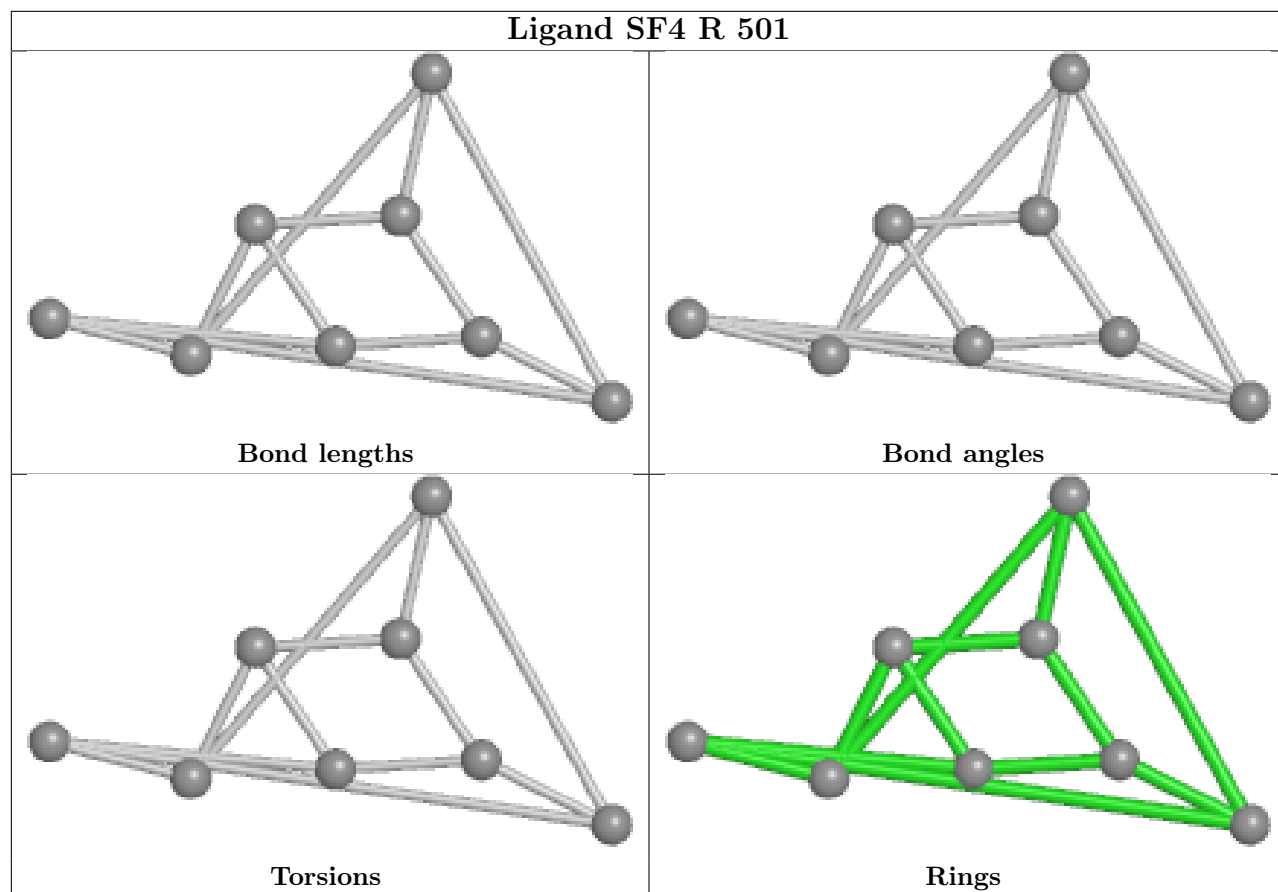


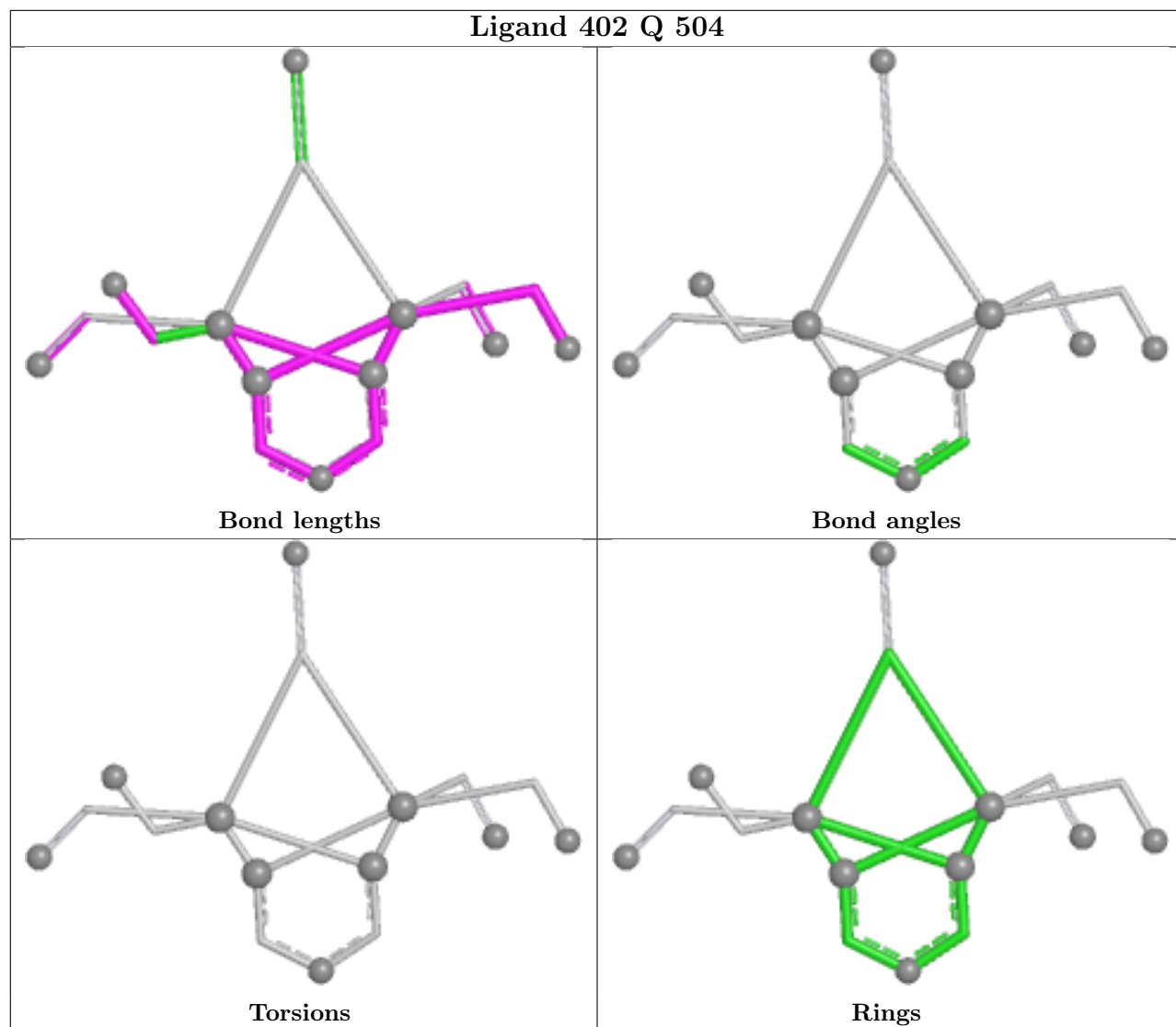


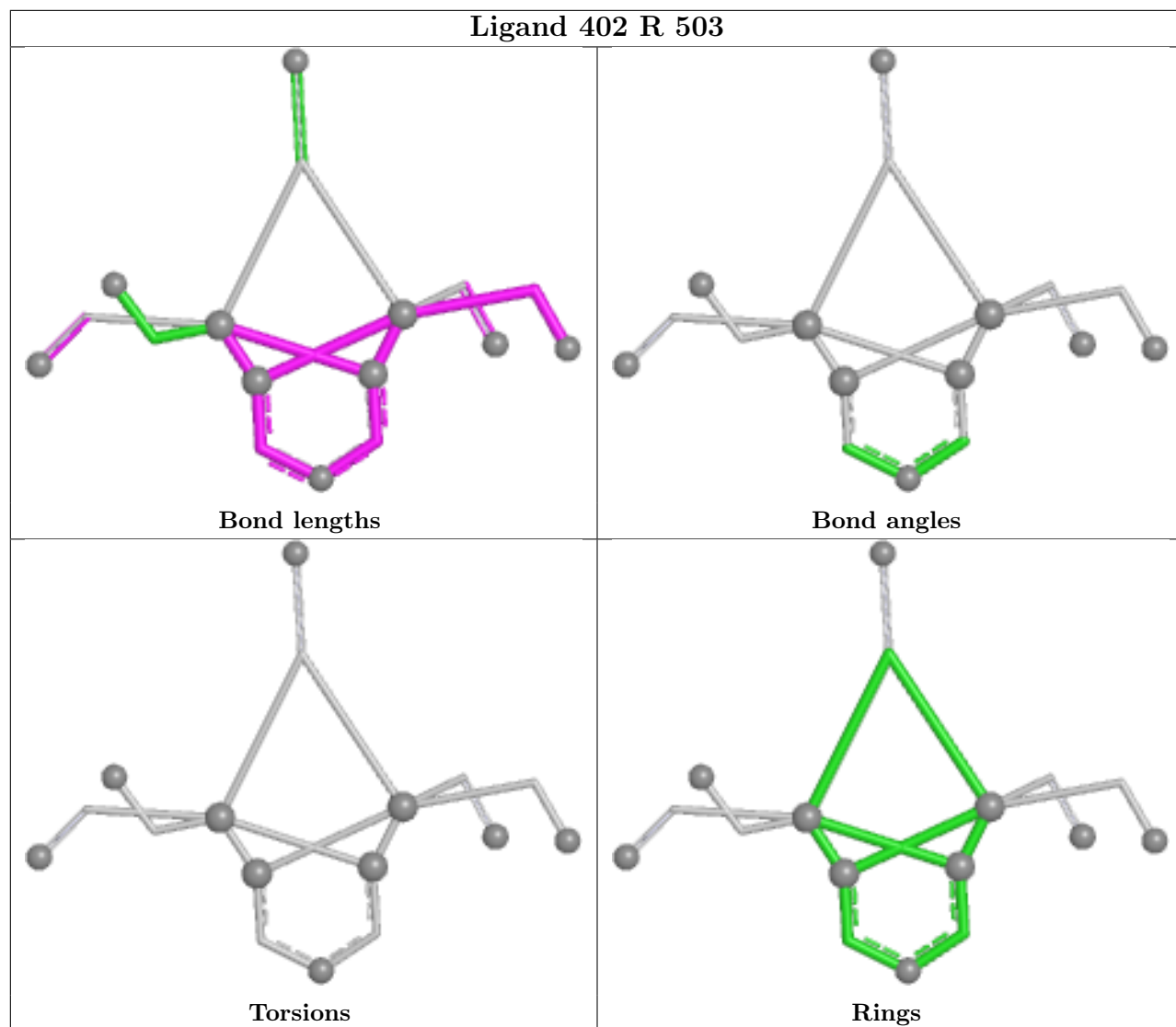


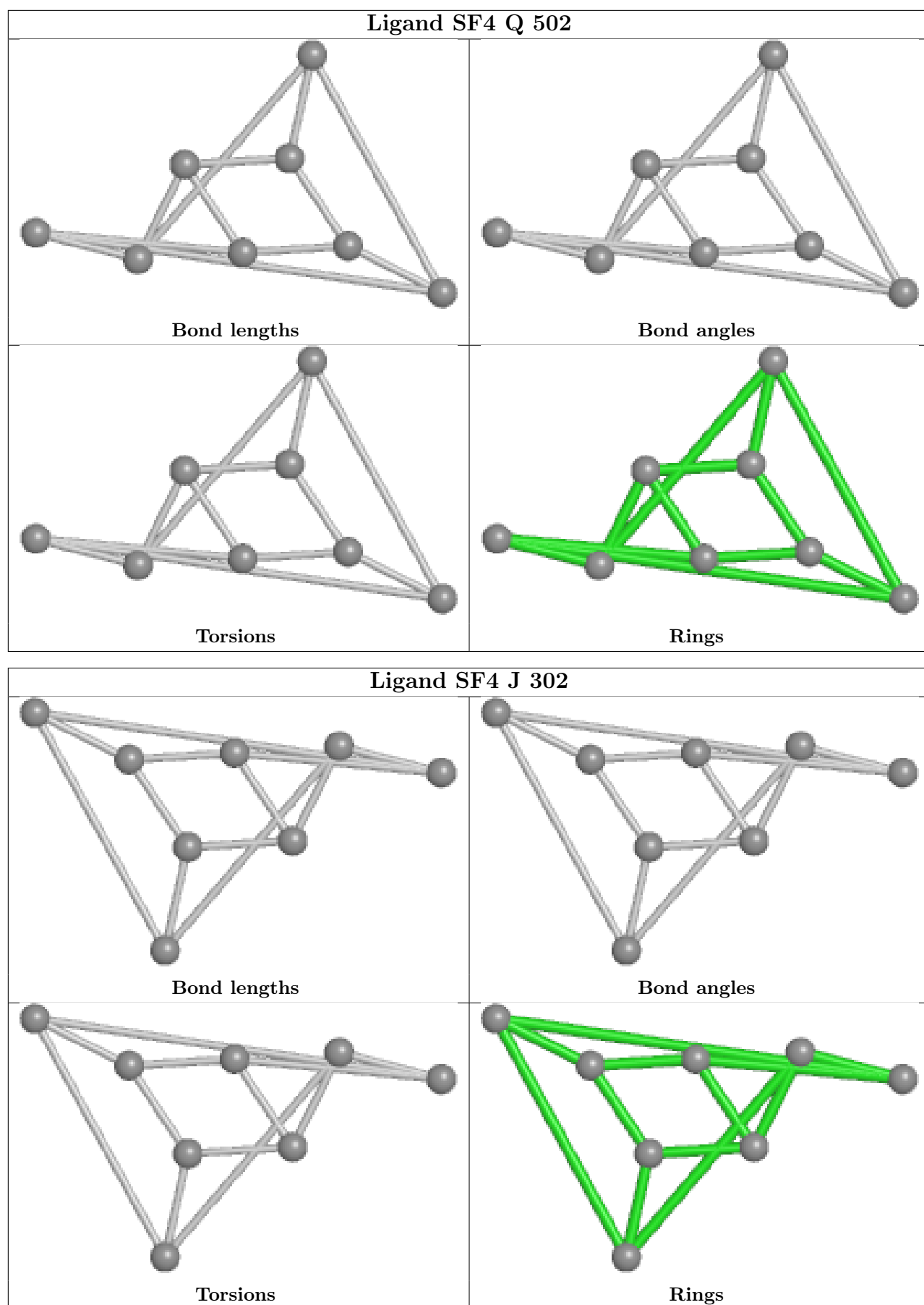


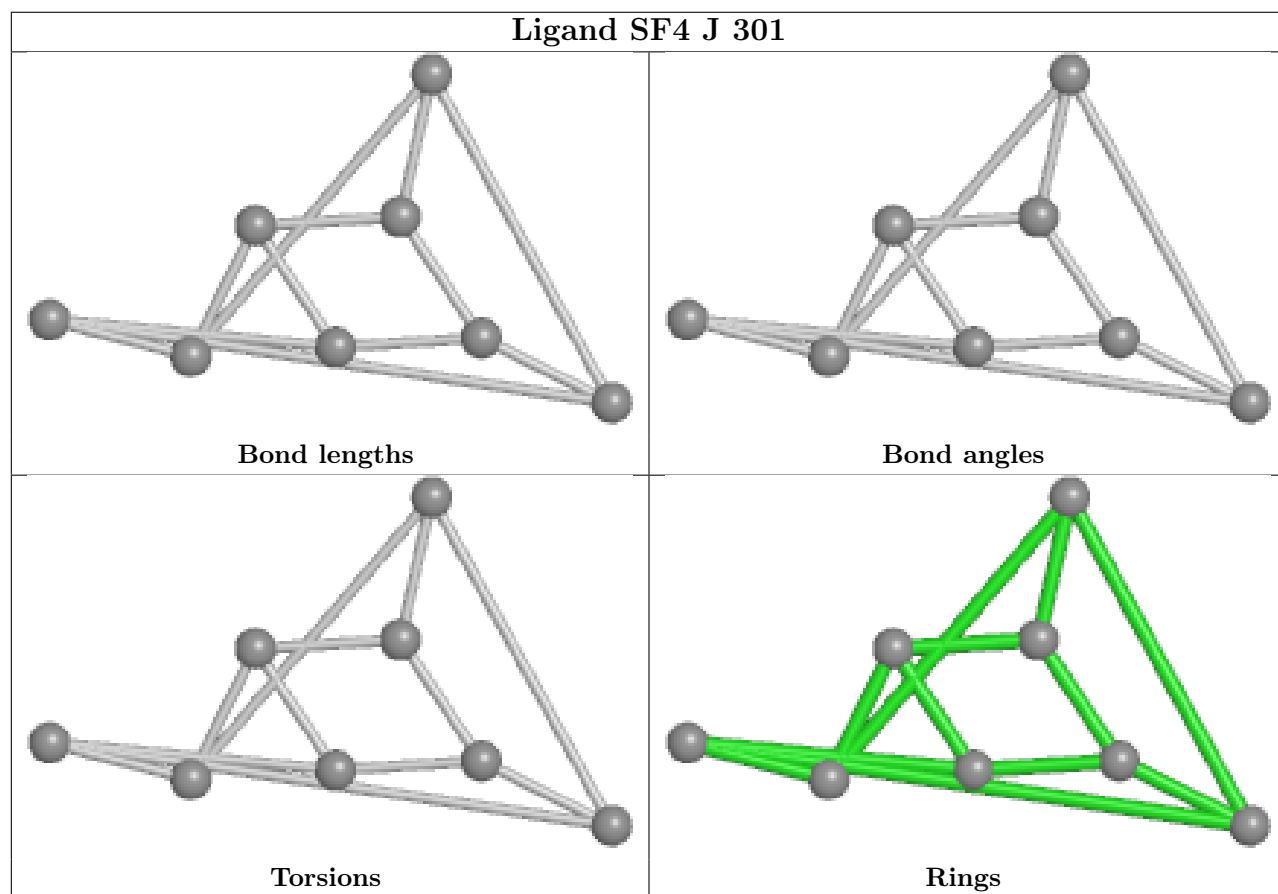
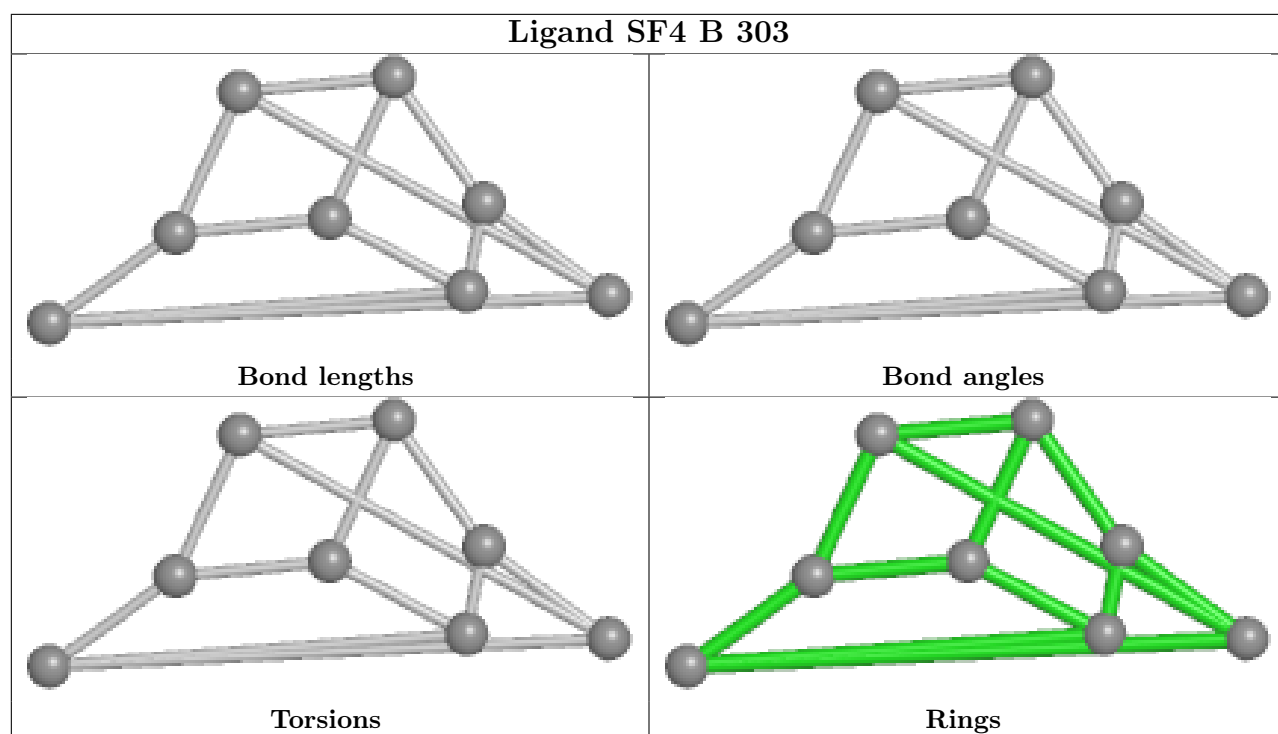


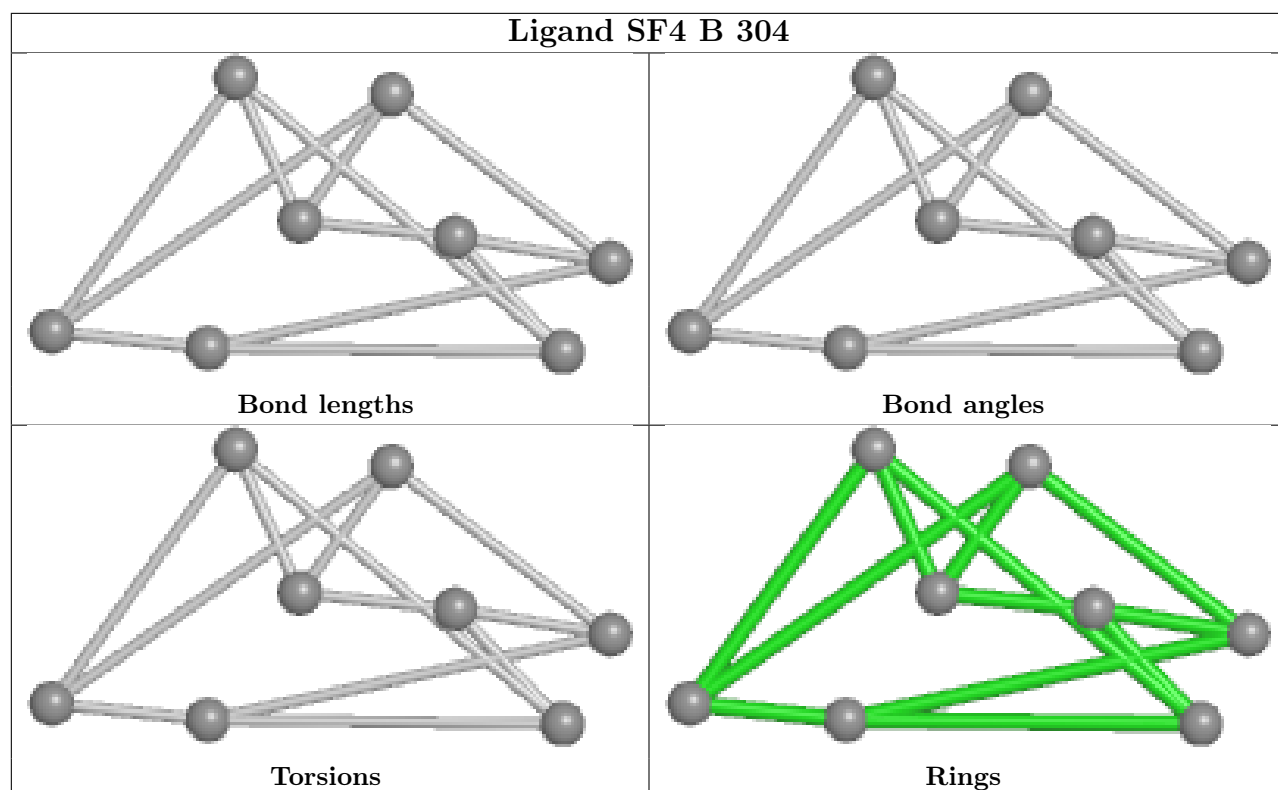
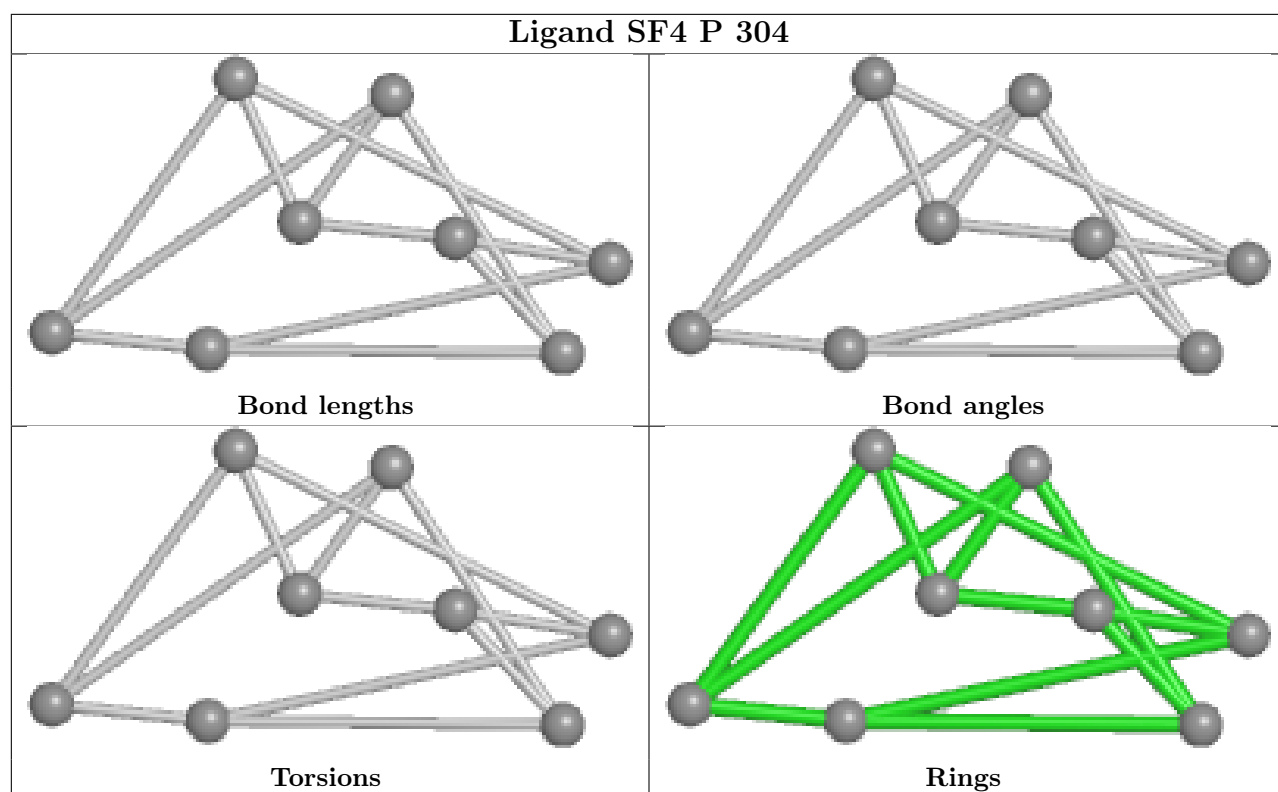


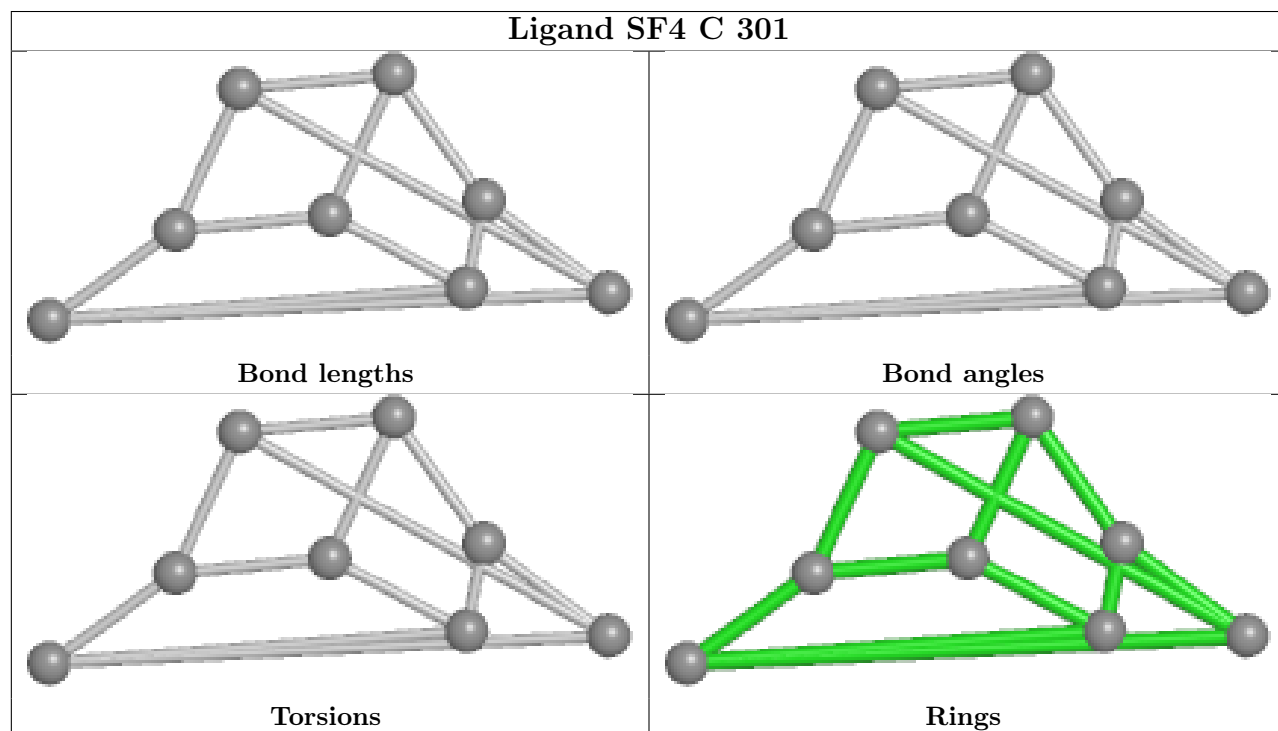
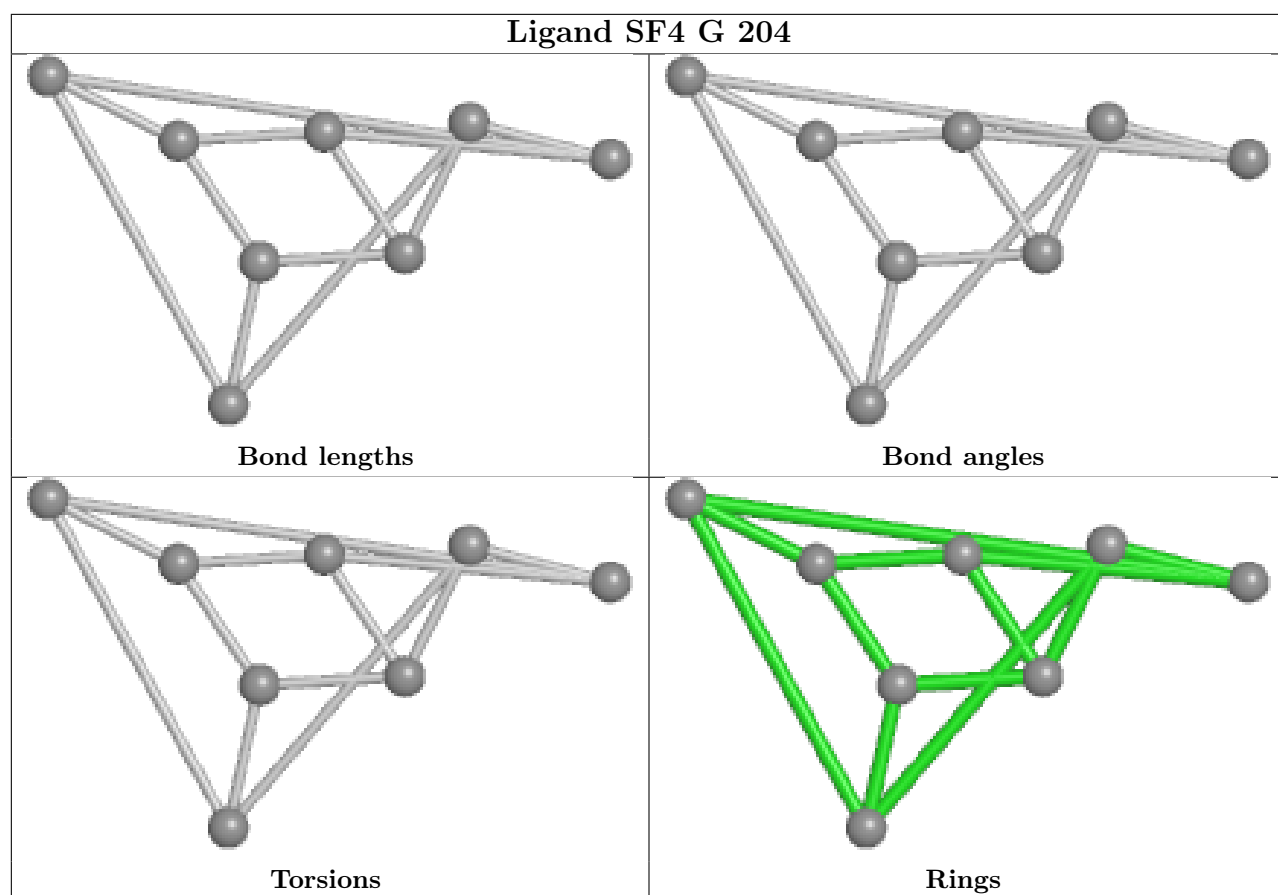


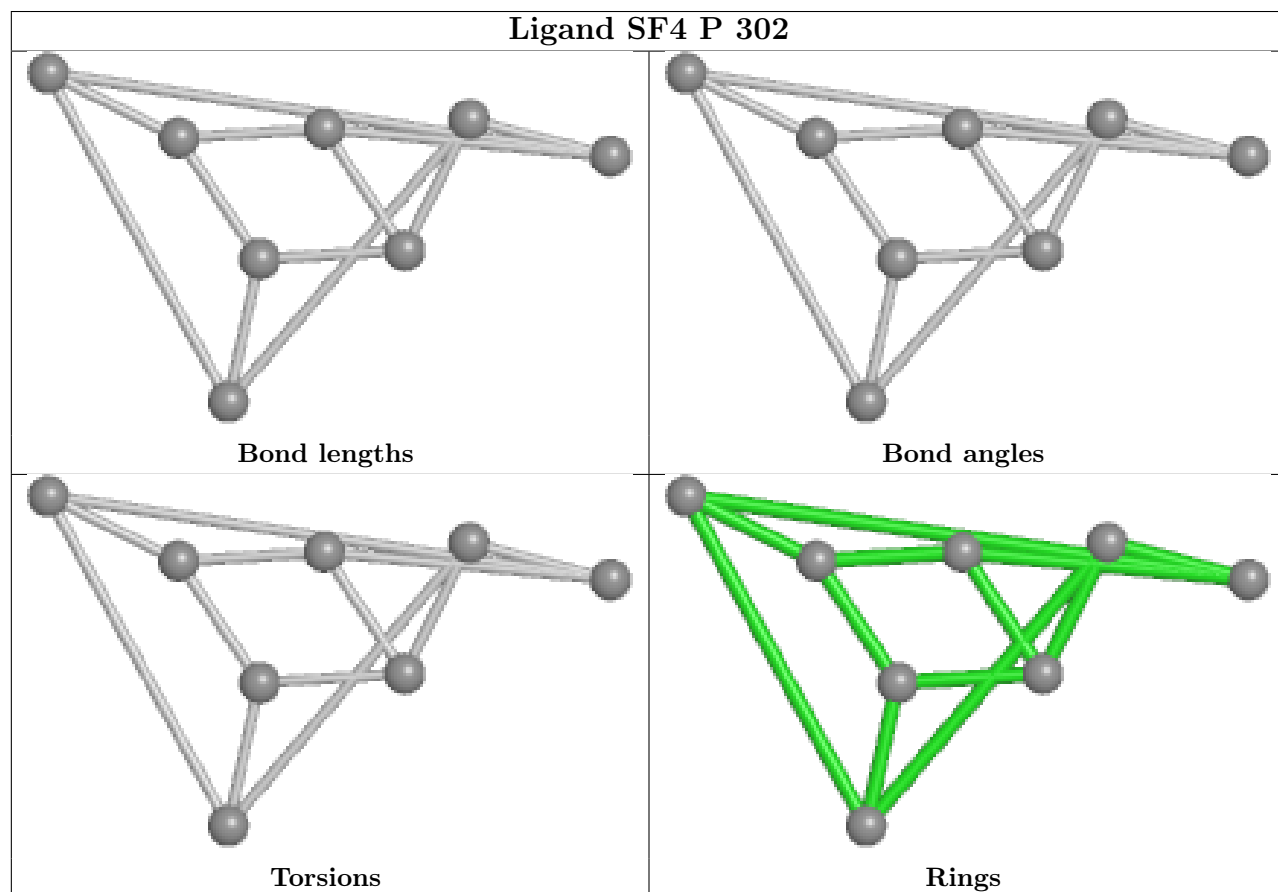
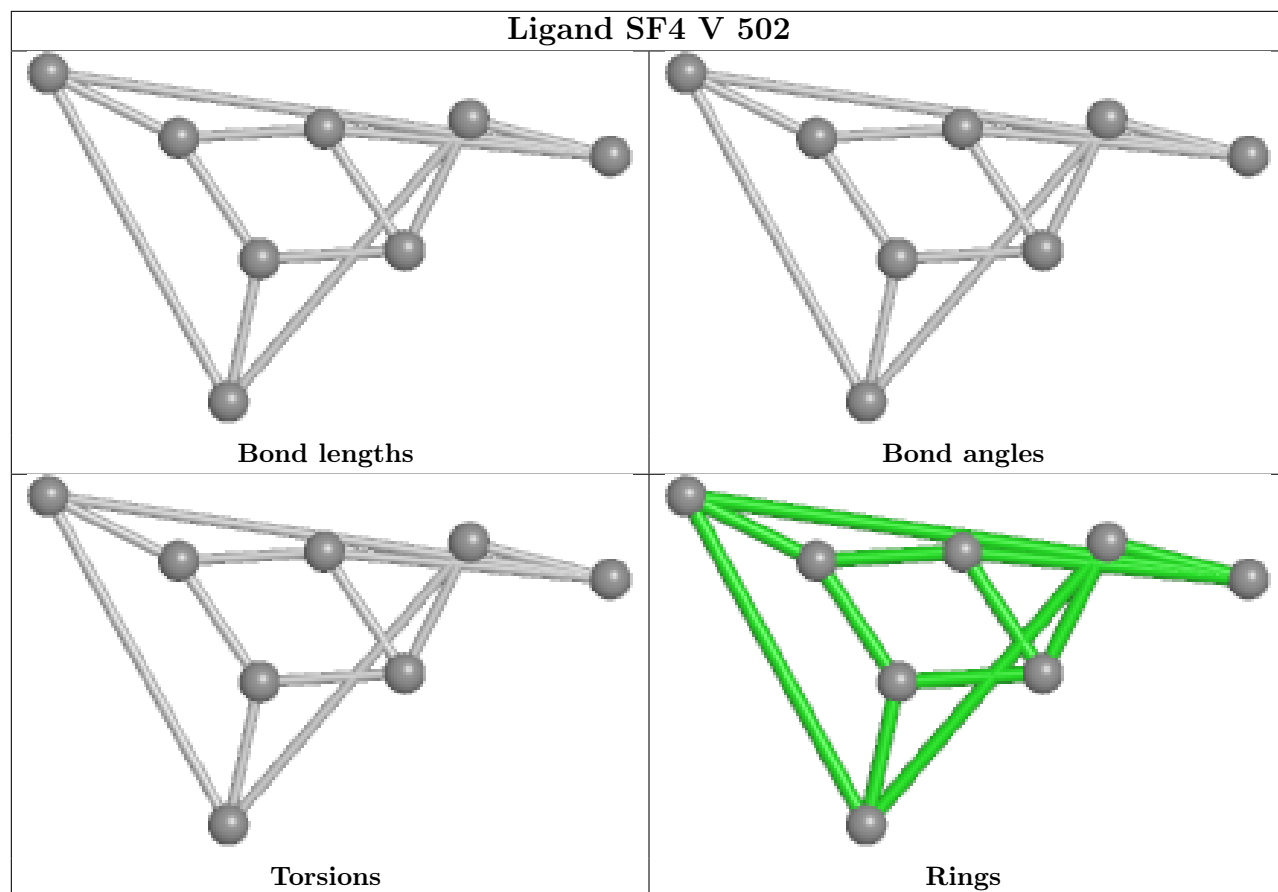












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

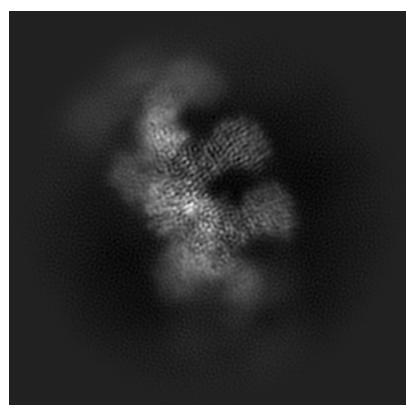
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14169. These allow visual inspection of the internal detail of the map and identification of artifacts.

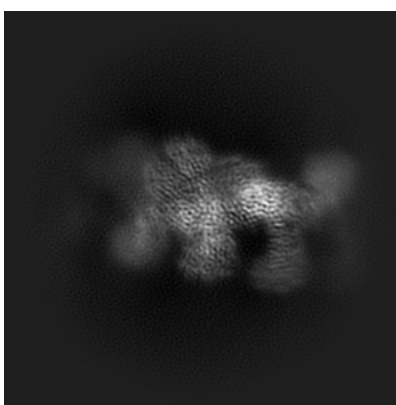
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

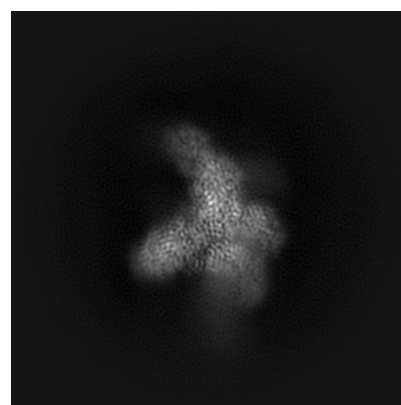
6.1.1 Primary map



X



Y

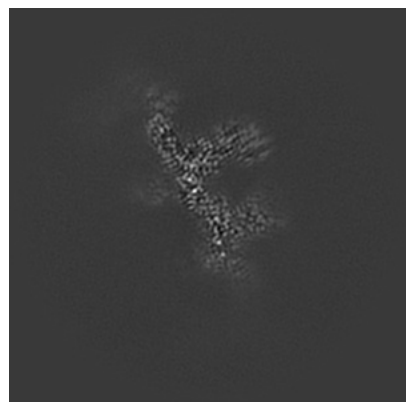


Z

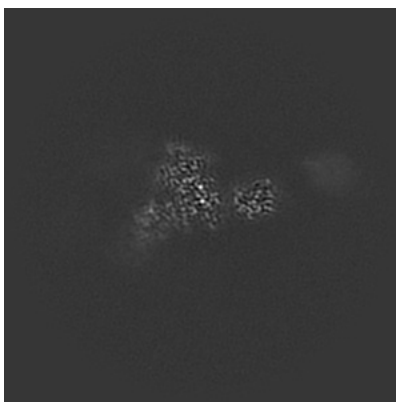
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

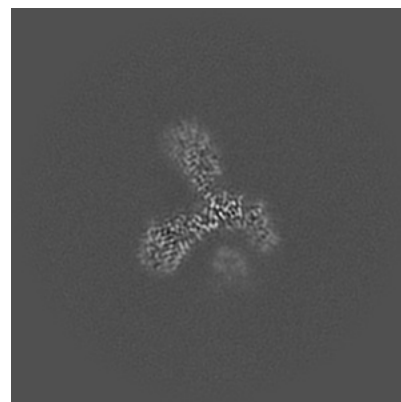
6.2.1 Primary map



X Index: 176



Y Index: 176

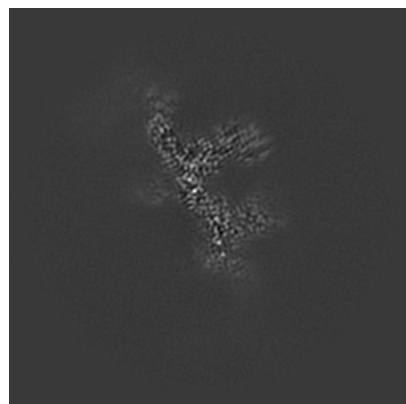


Z Index: 176

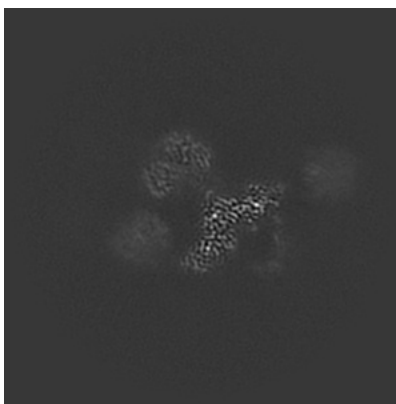
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

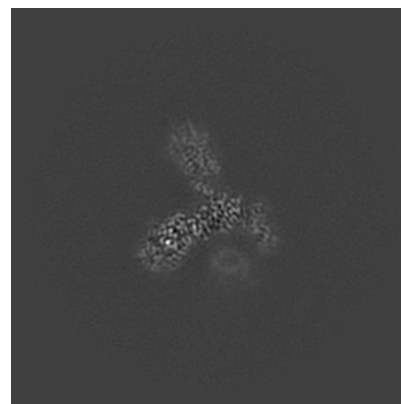
6.3.1 Primary map



X Index: 176



Y Index: 155

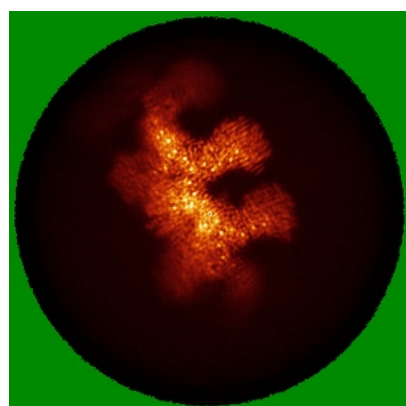


Z Index: 178

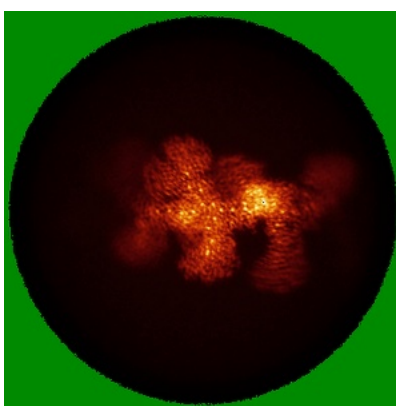
The images above show the largest variance slices of the map in three orthogonal directions.

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

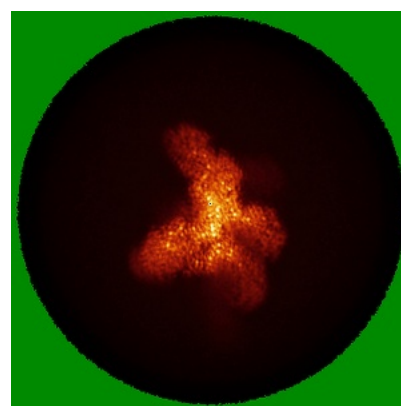
6.4.1 Primary map



X



Y

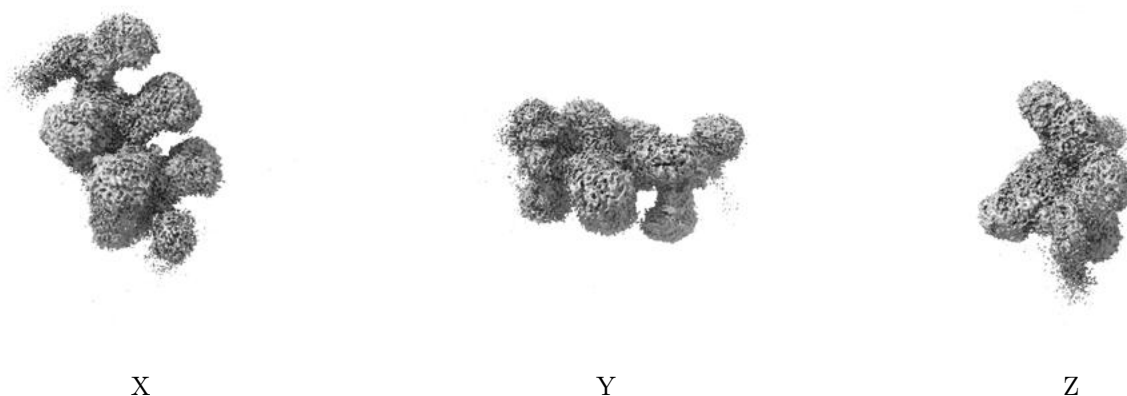


Z

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

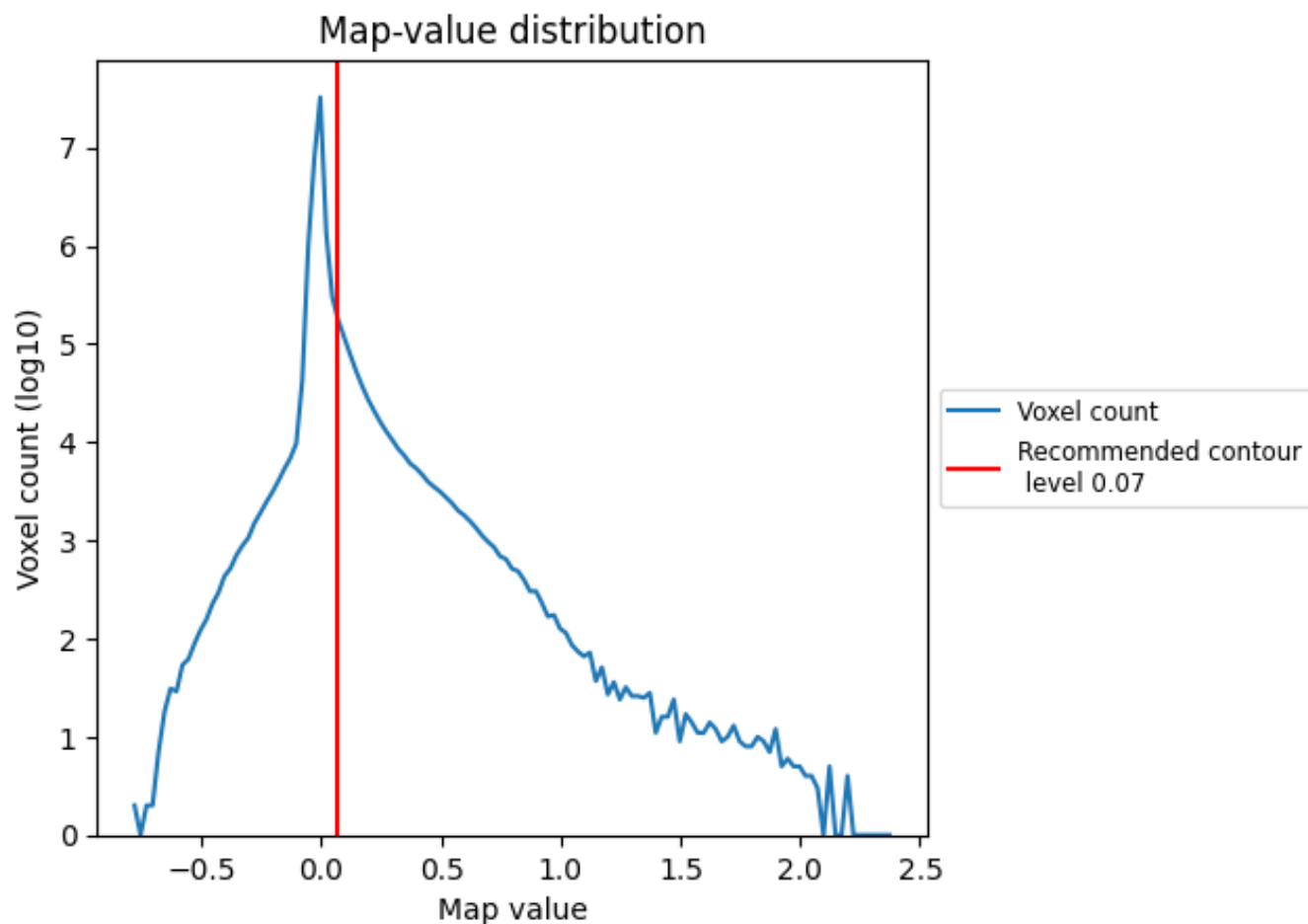
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

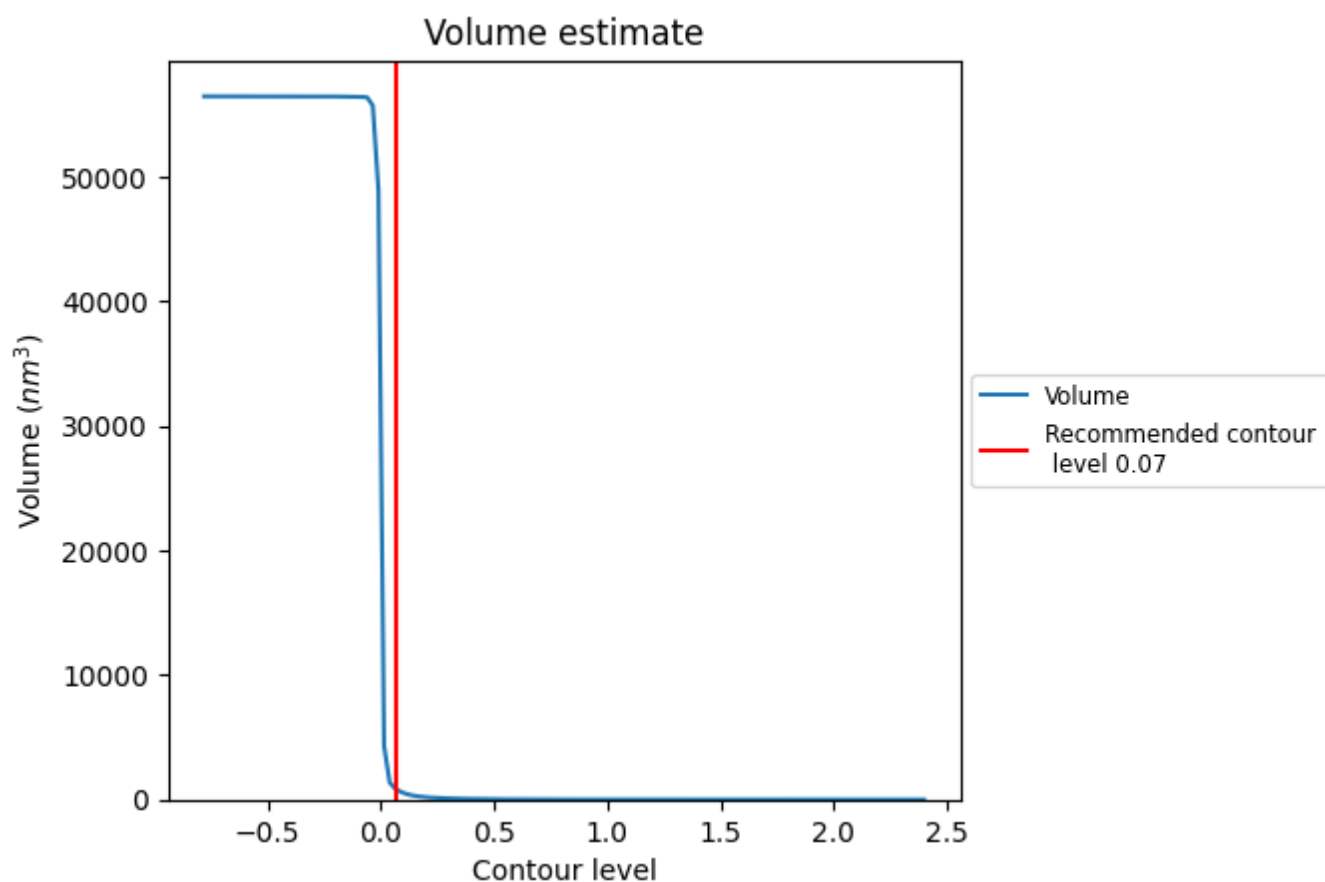
This section contains the results of statistical analysis of the map.

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.

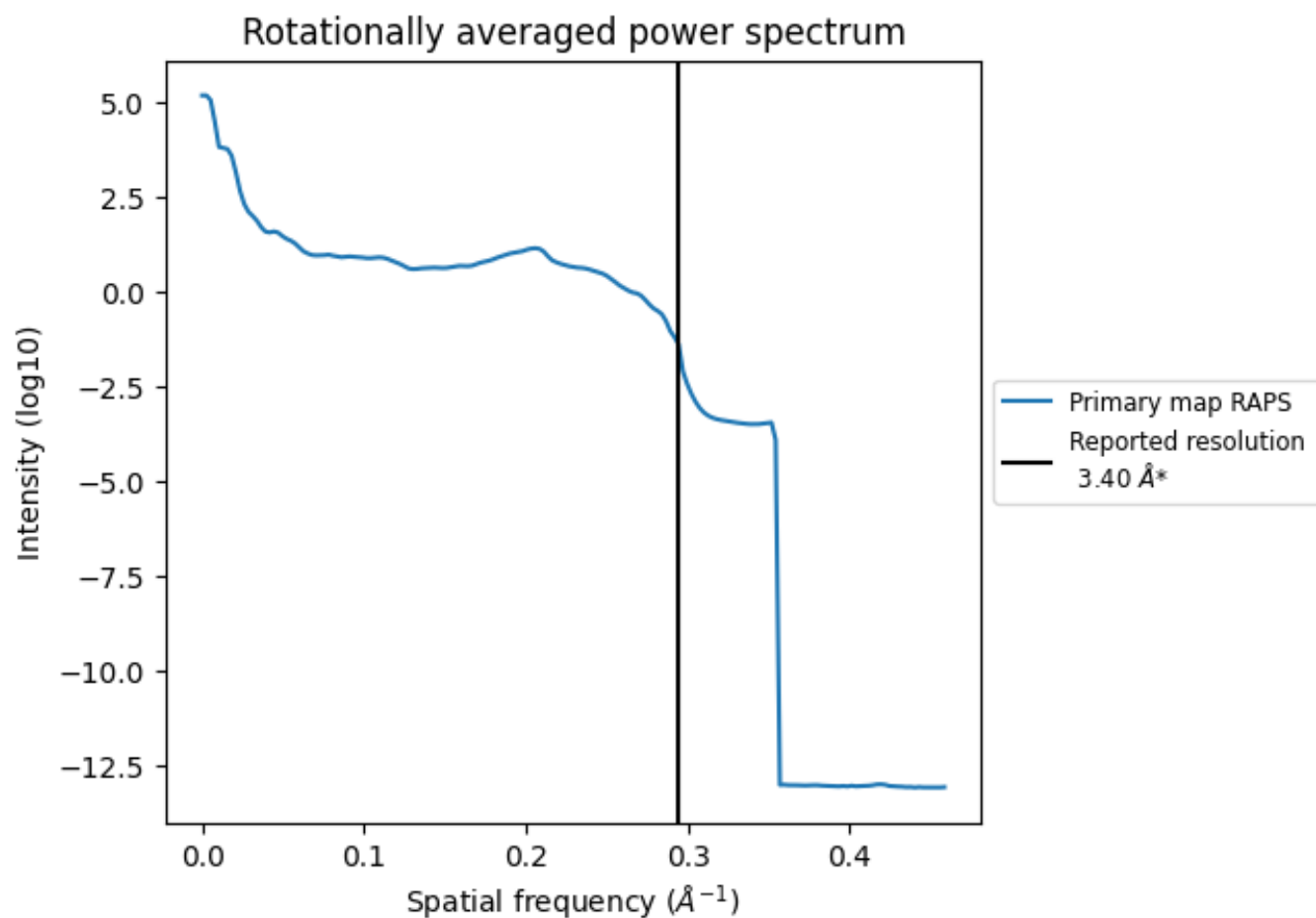
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 811 nm³; this corresponds to an approximate mass of 733 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 0.294 Å⁻¹

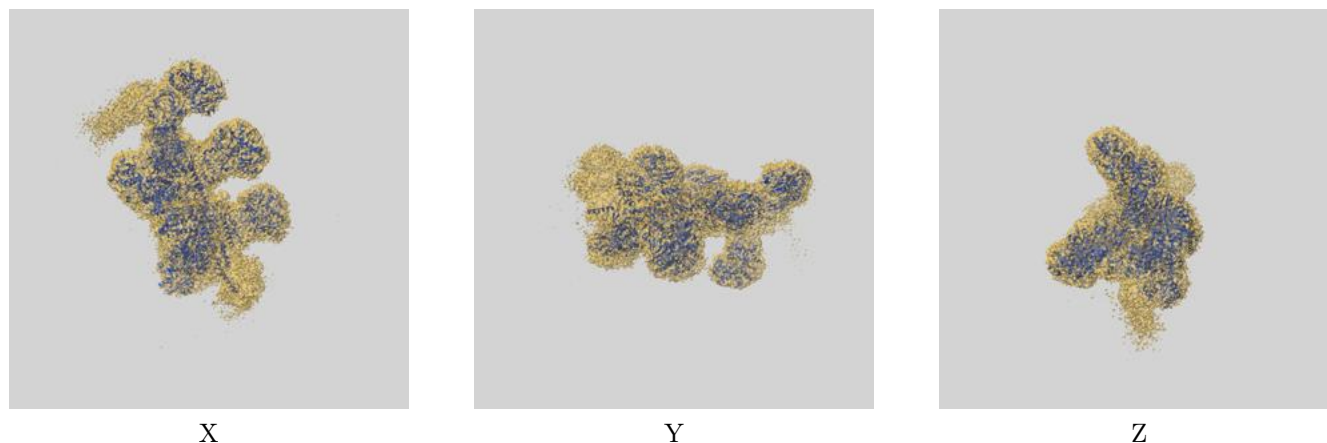
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

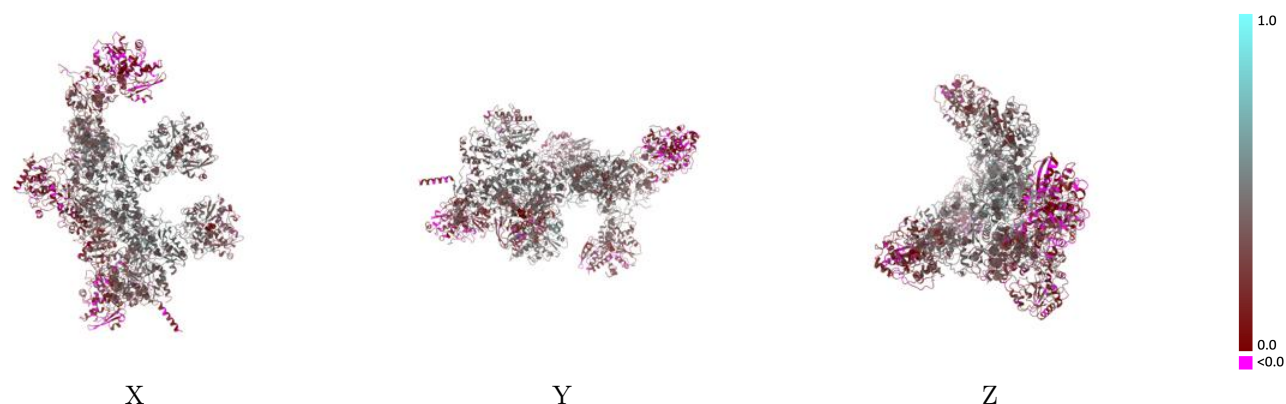
This section contains information regarding the fit between EMDB map EMD-14169 and PDB model 7QV7. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



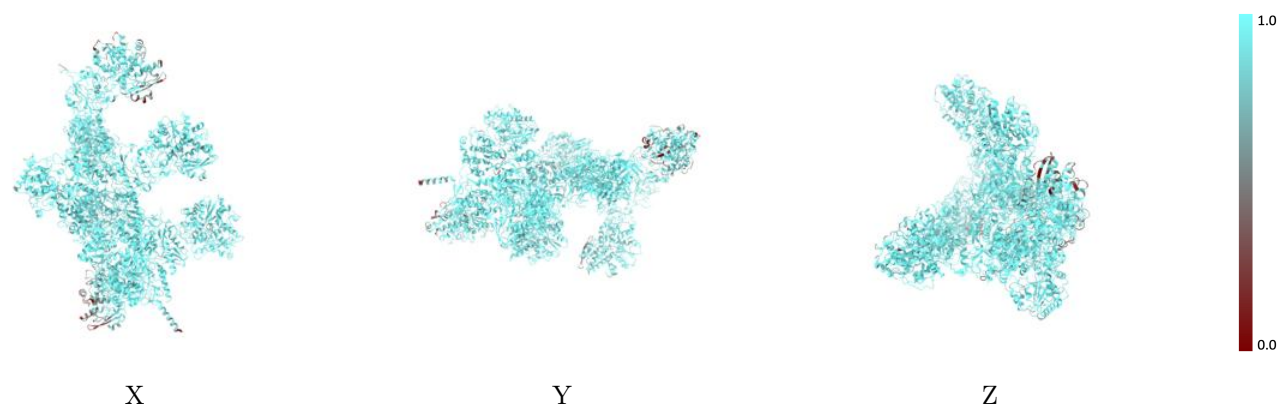
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



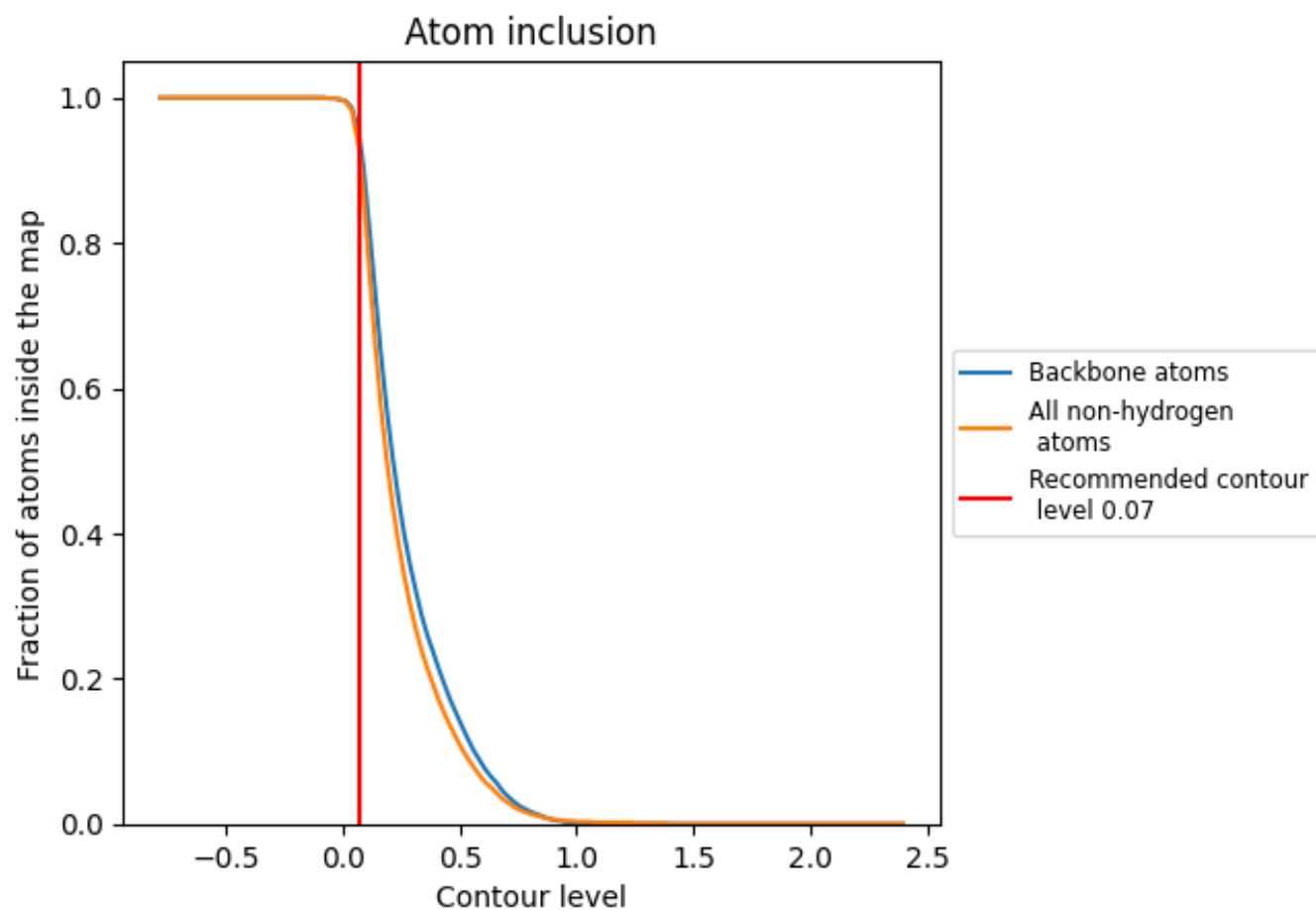
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.07).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 93% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9310	 0.3250
A	 0.9870	 0.4770
B	 0.9800	 0.4420
C	 0.9450	 0.3570
D	 0.9070	 0.2310
G	 0.9920	 0.4950
J	 0.9870	 0.5030
K	 0.8170	 0.0890
N	 0.9380	 0.2840
P	 0.9850	 0.4920
Q	 0.8020	 0.1520
R	 0.9710	 0.4300
S	 0.9530	 0.3500
V	 0.9600	 0.4220
X	 0.9910	 0.4700
Y	 0.9360	 0.2520
Z	 0.9580	 0.3250

