



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 04:51 PM UTC

PDB ID : 7Q4V / pdb_00007q4v
EMDB ID : EMD-13818
Title : Electron bifurcating hydrogenase - HydABC from A. woodii
Authors : Katsyv, A.; Kumar, A.; Saura, P.; Poeverlein, M.C.; Freibert, S.A.; Stripp, S.; Jain, S.; Gamiz-Hernandez, A.P.; Kaila, V.R.I.; Mueller, V.; Schuller, J.M.
Deposited on : 2021-11-02
Resolution : 4.70 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:

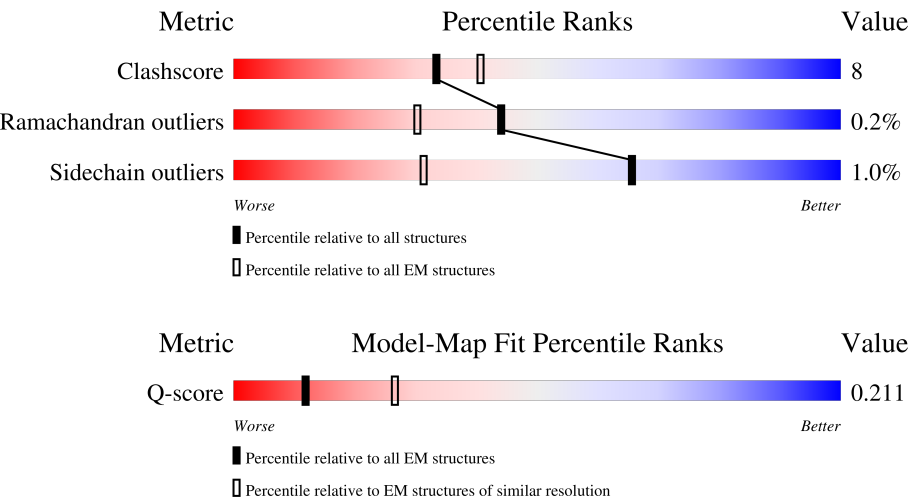
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 i

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

The reported resolution of this entry is 4.70 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	1989 (4.20 - 5.20)

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	583	
1	E	583	
2	B	599	
2	F	599	

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Mol	Chain	Length	Quality of chain
3	C	156	
3	G	156	

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
4	SF4	A	603	-	-	X	-
4	SF4	B	606	-	-	X	-
5	FES	C	201	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 19303 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 Iron hydrogenase HydA1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	583	Total	C	N	O	S	0	0
			4442	2774	766	865	37		
1	E	583	Total	C	N	O	S	0	0
			4442	2774	766	865	37		

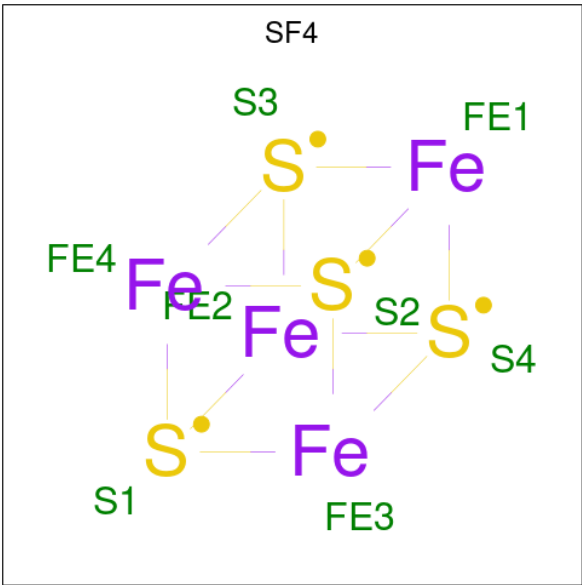
- Molecule 2 is a protein called Iron hydrogenase HydB.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	599	Total	C	N	O	S	0	0
			4510	2849	762	862	37		
2	F	470	Total	C	N	O	S	0	0
			3513	2216	592	676	29		

- Molecule 3 is a protein called Iron hydrogenase HydC.

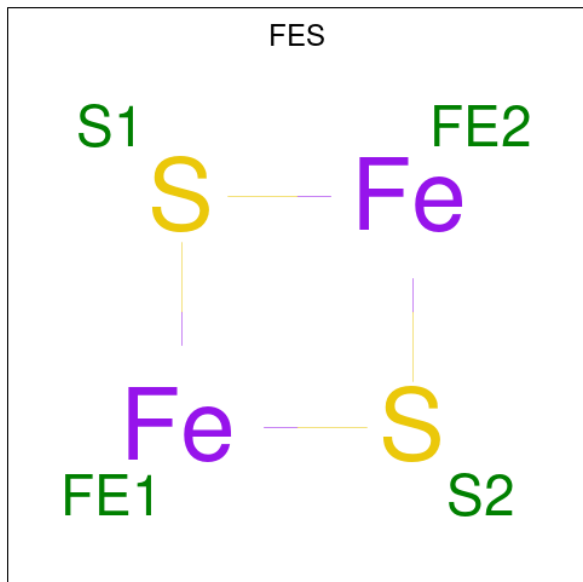
Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	156	Total	C	N	O	S	0	0
			1188	761	190	228	9		
3	G	129	Total	C	N	O	S	0	0
			968	620	156	183	9		

- Molecule 4 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 5 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).

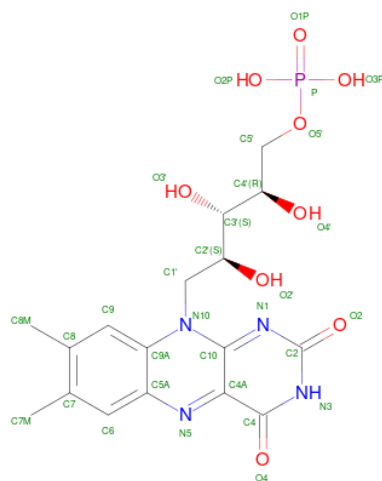


Mol	Chain	Residues	Atoms			AltConf
5	A	1	Total	Fe	S	0
			4	2	2	
5	B	1	Total	Fe	S	0
			4	2	2	
5	C	1	Total	Fe	S	0
			4	2	2	
5	E	1	Total	Fe	S	0
			4	2	2	
5	G	1	Total	Fe	S	0
			4	2	2	

- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

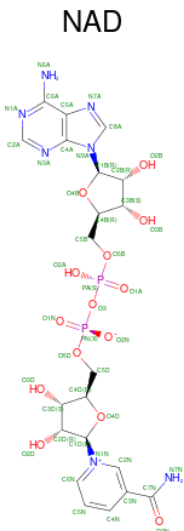
Mol	Chain	Residues	Atoms		AltConf
6	B	1	Total	Zn	0
			1	1	
6	F	1	Total	Zn	0
			1	1	

- Molecule 7 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $\text{C}_{17}\text{H}_{21}\text{N}_4\text{O}_9\text{P}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
7	B	1	Total 31	C 17	N 4	O 9	P 1	0
7	F	1	Total 31	C 17	N 4	O 9	P 1	0

- Molecule 8 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $\text{C}_{21}\text{H}_{27}\text{N}_7\text{O}_{14}\text{P}_2$) (labeled as "Ligand of Interest" by depositor).

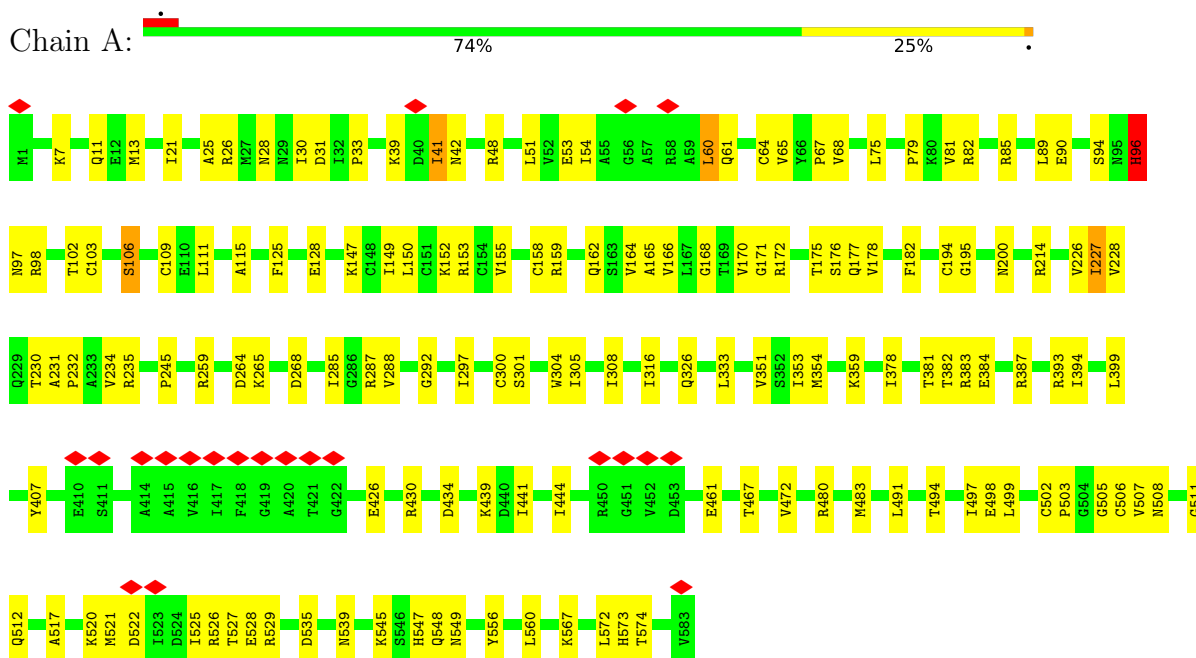


Mol	Chain	Residues	Atoms					AltConf
8	F	1	Total 44	C 21	N 7	O 14	P 2	0

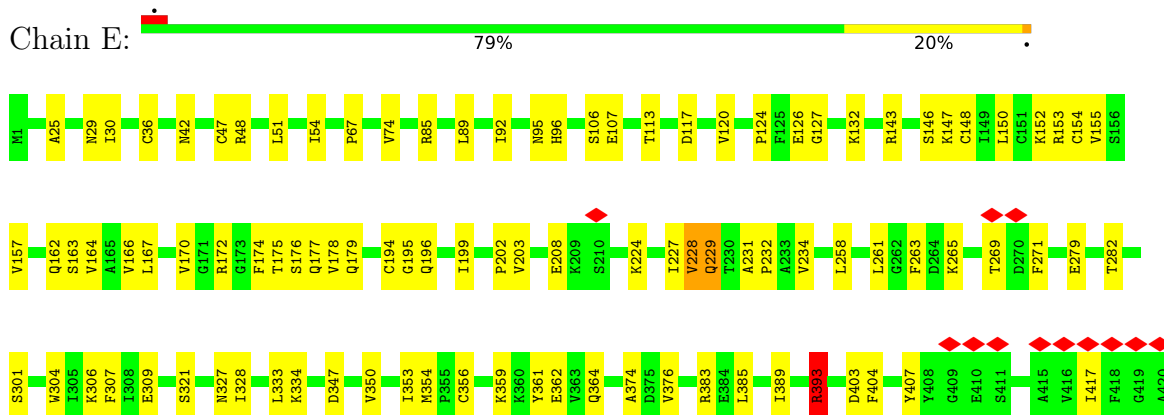
3 Residue-property plots

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

• Molecule 1: Iron hydrogenase HydA1

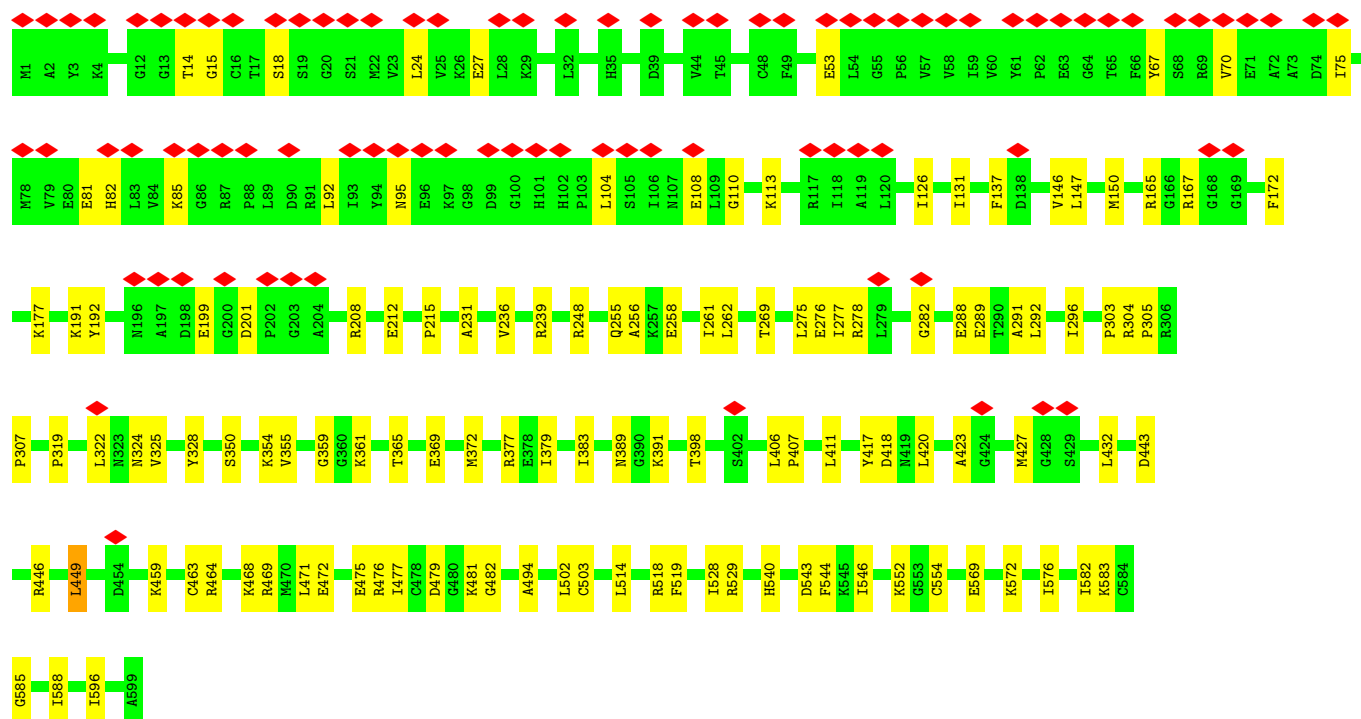
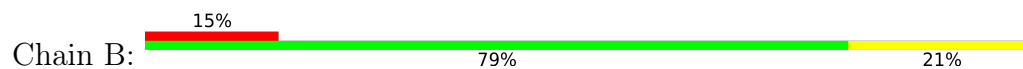


• Molecule 1: Iron hydrogenase HydA1

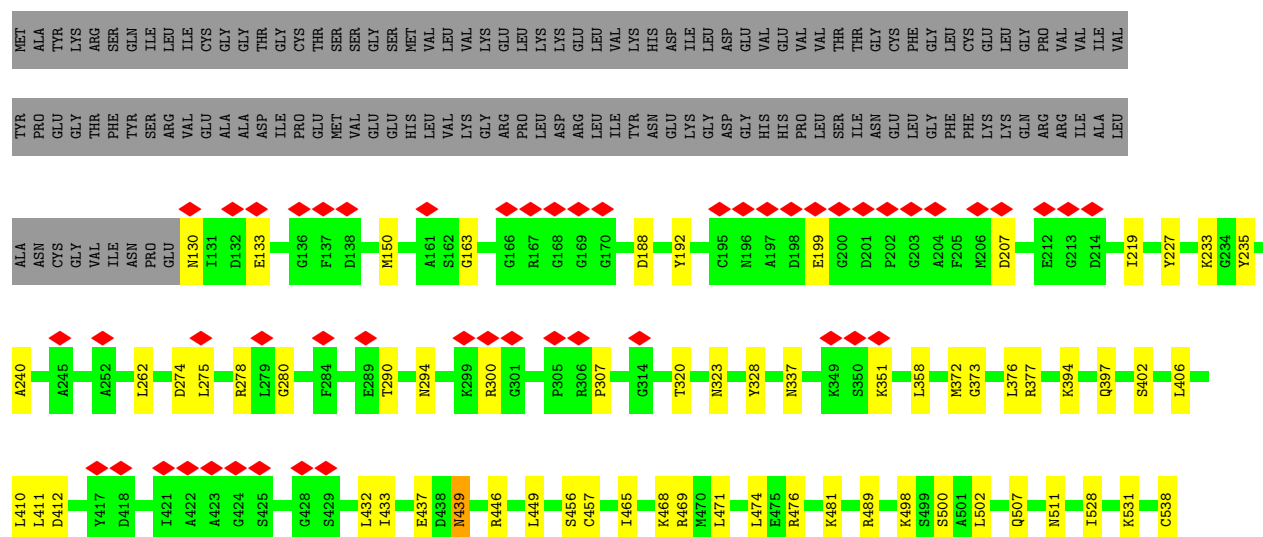


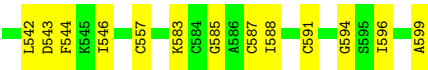


• Molecule 2: Iron hydrogenase HydB

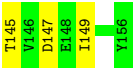
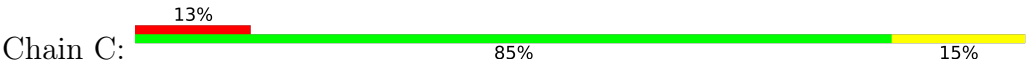


• Molecule 2: Iron hydrogenase HydB

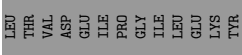
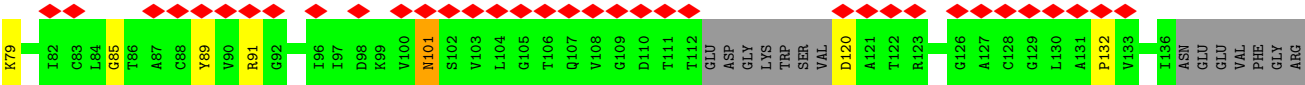




• Molecule 3: Iron hydrogenase HydC



• Molecule 3: Iron hydrogenase HydC



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	559245	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 ($e^-/\text{\AA}^2$)	55	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.025	Depositor
Minimum map value	-0.007	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.00114	Depositor
Map size ($\text{\AA}$)	218.0, 218.0, 218.0	wwPDB
Map dimensions	200, 200, 200	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: FES, NAD, ZN, FMN, 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	0.44	7/4507 (0.2%)	0.72	11/6105 (0.2%)
1	E	0.33	4/4507 (0.1%)	0.63	2/6105 (0.0%)
2	B	0.25	0/4592	0.53	4/6195 (0.1%)
2	F	0.22	1/3577 (0.0%)	0.52	0/4825
3	C	0.25	0/1207	0.66	2/1638 (0.1%)
3	G	0.37	1/981 (0.1%)	0.74	0/1330
All	All	0.32	13/19371 (0.1%)	0.62	19/26198 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	E	0	2
2	F	0	1
3	G	0	1
All	All	0	6

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	573	HIS	CA-C	8.81	1.63	1.52
1	A	245	PRO	CG-CD	-7.96	1.23	1.50
1	A	549	ASN	CA-C	7.12	1.61	1.52
1	A	96	HIS	N-CA	-6.74	1.38	1.46
1	A	574	THR	N-CA	6.62	1.55	1.46
1	E	573	HIS	CA-C	5.81	1.59	1.52
1	A	574	THR	CA-C	5.54	1.61	1.53
1	E	229	GLN	CD-OE1	5.16	1.33	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	101	ASN	CG-OD1	5.16	1.33	1.23
1	E	564	ASN	CG-OD1	5.10	1.33	1.23
1	E	327	ASN	CG-OD1	5.06	1.33	1.23
2	F	439	ASN	CG-OD1	5.06	1.33	1.23
1	A	177	GLN	CD-OE1	5.05	1.33	1.23

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	245	PRO	CA-N-CD	-11.61	95.75	112.00
1	A	245	PRO	N-CD-CG	-8.94	89.79	103.20
1	A	574	THR	N-CA-C	8.81	123.39	109.65
1	A	96	HIS	CA-CB-CG	-7.88	105.92	113.80
1	A	573	HIS	N-CA-CB	-6.57	100.85	110.84
1	A	90	GLU	N-CA-CB	5.72	119.15	110.28
2	B	582	ILE	N-CA-C	-5.67	106.96	112.29
1	A	245	PRO	CA-CB-CG	-5.64	93.79	104.50
3	C	136	ILE	O-C-N	-5.63	117.23	123.03
1	A	96	HIS	CB-CG-ND1	-5.58	114.32	122.70
2	B	303	PRO	CA-C-N	5.57	128.22	120.65
2	B	303	PRO	C-N-CA	5.57	128.22	120.65
1	E	393	ARG	CG-CD-NE	-5.49	99.92	112.00
1	A	96	HIS	N-CA-C	5.39	117.02	108.67
1	A	393	ARG	CA-CB-CG	5.35	124.80	114.10
1	E	95	ASN	N-CA-C	5.29	118.07	111.24
2	B	449	LEU	CA-CB-CG	5.27	134.75	116.30
3	C	33	GLU	N-CA-CB	5.18	118.30	110.28
1	A	572	LEU	N-CA-C	5.16	119.44	113.20

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	407	TYR	Peptide
1	A	96	HIS	Sidechain
1	E	393	ARG	Sidechain
1	E	407	TYR	Peptide
2	F	538	CYS	Peptide
3	G	23	VAL	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	4442	0	4463	94	0
1	E	4442	0	4462	81	0
2	B	4510	0	4495	81	0
2	F	3513	0	3481	49	0
3	C	1188	0	1211	14	0
3	G	968	0	1000	23	0
4	A	32	0	0	4	0
4	B	24	0	0	3	0
4	E	32	0	0	2	0
4	F	24	0	0	0	0
5	A	4	0	0	0	0
5	B	4	0	0	0	0
5	C	4	0	0	2	0
5	E	4	0	0	0	0
5	G	4	0	0	0	0
6	B	1	0	0	0	0
6	F	1	0	0	0	0
7	B	31	0	19	2	0
7	F	31	0	19	0	0
8	F	44	0	26	0	0
All	All	19303	0	19176	321	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 8.

All (321) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:3:GLU:HB2	3:G:8:GLU:OE2	1.56	1.05
1:A:545:LYS:HB2	1:A:548:GLN:OE1	1.56	1.05
1:E:170:VAL:O	1:E:176:SER:HA	1.59	1.03
1:A:170:VAL:O	1:A:176:SER:HA	1.61	0.97
1:A:103:CYS:HB2	4:A:603:SF4:S4	2.05	0.96
2:B:503:CYS:HB2	4:B:606:SF4:S1	2.09	0.92
3:G:3:GLU:CB	3:G:8:GLU:OE2	2.18	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:545:LYS:HB2	1:A:548:GLN:CD	1.97	0.87
2:B:468:LYS:HA	2:B:471:LEU:HD13	1.67	0.74
1:E:279:GLU:OE1	1:E:573:HIS:CE1	2.42	0.73
3:C:128:CYS:HB3	5:C:201:FES:S2	2.28	0.72
2:B:569:GLU:H	2:B:572:LYS:HE3	1.57	0.69
2:F:446:ARG:HB3	2:F:474:LEU:HD11	1.74	0.69
1:E:328:ILE:HD12	1:E:572:LEU:CD1	2.23	0.68
3:G:3:GLU:HB2	3:G:8:GLU:CD	2.18	0.68
1:E:279:GLU:OE1	1:E:573:HIS:HE1	1.77	0.68
2:B:110:GLY:HA2	2:B:113:LYS:HD3	1.74	0.68
1:A:526:ARG:NH1	1:A:527:THR:OG1	2.27	0.67
2:B:463:CYS:HB2	4:B:606:SF4:S2	2.35	0.67
1:E:147:LYS:NZ	4:E:603:SF4:S2	2.66	0.67
1:E:354:MET:HE3	1:E:356:CYS:HB2	1.75	0.67
1:A:109:CYS:HB2	4:A:603:SF4:S3	2.35	0.67
3:G:5:ILE:O	3:G:9:ASN:OD1	2.13	0.66
1:A:81:VAL:HG23	1:A:85:ARG:HH22	1.60	0.65
2:B:503:CYS:CB	4:B:606:SF4:S1	2.86	0.64
2:F:468:LYS:HA	2:F:471:LEU:HD13	1.79	0.63
1:A:89:LEU:HD21	1:A:115:ALA:HA	1.81	0.63
1:E:433:ALA:HB1	1:E:439:LYS:HB3	1.79	0.63
2:F:498:LYS:HD2	2:F:507:GLN:HB2	1.79	0.63
2:F:476:ARG:HB3	2:F:481:LYS:HB3	1.81	0.63
2:B:546:ILE:HG23	2:B:576:ILE:HD11	1.80	0.62
2:B:423:ALA:O	2:B:518:ARG:NH2	2.32	0.62
2:B:239:ARG:HE	2:B:282:GLY:HA2	1.64	0.62
2:F:163:GLY:HA3	2:F:351:LYS:HD2	1.80	0.62
1:E:472:VAL:HA	1:E:498:GLU:HB3	1.80	0.62
2:B:292:LEU:HD11	2:B:322:LEU:HD11	1.82	0.62
1:E:430:ARG:NH2	1:E:544:ARG:O	2.33	0.62
1:E:67:PRO:HD2	2:F:307:PRO:HG2	1.81	0.62
2:B:191:LYS:NZ	2:B:192:TYR:O	2.33	0.61
3:C:128:CYS:CB	5:C:201:FES:S2	2.88	0.61
1:A:125:PHE:HB3	2:B:469:ARG:HH12	1.65	0.61
3:G:28:MET:HA	3:G:31:LEU:HD12	1.82	0.61
1:E:124:PRO:O	2:F:489:ARG:NH2	2.34	0.61
1:E:143:ARG:HH12	1:E:179:GLN:HA	1.64	0.61
1:A:194:CYS:SG	1:A:195:GLY:N	2.74	0.60
1:E:417:ILE:HA	1:E:533:LEU:HD21	1.84	0.60
1:E:258:LEU:HD13	1:E:261:LEU:HD12	1.83	0.59
2:B:146:VAL:HA	2:B:150:MET:HB2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:542:LEU:O	2:F:583:LYS:NZ	2.35	0.59
1:E:126:GLU:O	2:F:469:ARG:NH1	2.35	0.59
1:E:153:ARG:HH22	1:E:202:PRO:HB3	1.68	0.59
2:F:372:MET:HE3	2:F:373:GLY:H	1.69	0.58
1:E:389:ILE:O	1:E:393:ARG:N	2.34	0.58
2:B:389:ASN:HB3	2:B:391:LYS:HE2	1.85	0.58
1:E:571:ILE:HG13	1:E:572:LEU:HD22	1.86	0.57
1:A:103:CYS:O	1:A:106:SER:OG	2.21	0.57
3:C:21:ARG:HH12	3:C:53:LEU:HA	1.69	0.57
1:A:430:ARG:HH21	1:A:444:ILE:HD12	1.69	0.57
1:A:384:GLU:OE2	1:A:387:ARG:NH1	2.38	0.57
1:A:434:ASP:OD2	1:A:547:HIS:NE2	2.37	0.57
1:E:194:CYS:N	4:E:601:SF4:S3	2.76	0.57
3:G:22:GLU:HB3	3:G:25:GLY:HA3	1.86	0.57
1:A:556:TYR:HA	1:A:560:LEU:HB2	1.85	0.57
2:B:528:ILE:HG22	2:B:529:ARG:HE	1.70	0.57
2:F:397:GLN:HB3	2:F:433:ILE:HB	1.86	0.56
3:G:3:GLU:HB3	3:G:8:GLU:OE2	2.05	0.56
1:A:81:VAL:HB	1:A:85:ARG:HH12	1.71	0.56
1:A:300:CYS:SG	1:A:301:SER:N	2.79	0.56
1:E:148:CYS:HA	1:E:203:VAL:HG21	1.86	0.56
1:E:232:PRO:HD3	1:E:269:THR:HB	1.88	0.56
2:F:290:THR:O	2:F:294:ASN:ND2	2.37	0.56
3:G:31:LEU:O	3:G:34:THR:OG1	2.17	0.56
2:B:476:ARG:HD3	2:B:482:GLY:HA2	1.88	0.56
1:A:525:ILE:HG23	1:A:529:ARG:HH12	1.70	0.56
2:B:305:PRO:HG3	2:B:502:LEU:HD21	1.86	0.56
2:F:588:ILE:HA	2:F:596:ILE:HD12	1.88	0.56
2:B:262:LEU:HD21	2:B:275:LEU:HB2	1.88	0.56
2:F:233:LYS:HD2	2:F:274:ASP:HB2	1.88	0.56
1:A:172:ARG:N	1:A:175:THR:OG1	2.37	0.55
1:E:127:GLY:HA3	2:F:469:ARG:HH22	1.70	0.55
1:E:150:LEU:HD11	1:E:177:GLN:HA	1.89	0.55
2:F:543:ASP:O	2:F:599:ALA:N	2.39	0.55
1:A:94:SER:OG	2:B:469:ARG:NH1	2.40	0.55
1:A:354:MET:HG3	1:A:359:LYS:HG2	1.88	0.55
2:B:191:LYS:HB3	2:B:231:ALA:HA	1.88	0.55
1:A:54:ILE:HD13	1:A:61:GLN:HB2	1.88	0.55
2:F:358:LEU:HA	2:F:432:LEU:HB3	1.88	0.55
3:G:50:ALA:O	3:G:54:GLY:N	2.38	0.55
1:E:321:SER:OG	1:E:573:HIS:HB3	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:VAL:HG23	1:A:228:VAL:O	2.06	0.55
1:E:224:LYS:NZ	1:E:347:ASP:OD1	2.40	0.54
1:E:51:LEU:O	1:E:85:ARG:NH2	2.41	0.54
1:A:382:THR:OG1	1:A:511:GLY:O	2.22	0.54
2:B:131:ILE:HD12	2:B:255:GLN:HB3	1.89	0.54
3:C:145:THR:HG23	3:C:147:ASP:H	1.73	0.54
2:B:379:ILE:HA	2:B:383:ILE:HD12	1.90	0.54
1:E:170:VAL:HA	3:G:65:THR:HG21	1.90	0.54
2:B:126:ILE:HG22	2:B:137:PHE:HD2	1.73	0.53
2:F:394:LYS:HE2	2:F:437:GLU:HA	1.90	0.53
1:E:359:LYS:NZ	1:E:362:GLU:OE2	2.38	0.53
2:F:150:MET:O	2:F:227:TYR:OH	2.24	0.53
2:F:528:ILE:O	2:F:531:LYS:NZ	2.36	0.53
1:E:196:GLN:HA	1:E:199:ILE:HG22	1.91	0.53
2:B:377:ARG:N	2:B:411:LEU:O	2.43	0.52
3:G:91:ARG:HG2	3:G:132:PRO:HD3	1.92	0.52
2:F:588:ILE:HG13	2:F:596:ILE:HB	1.92	0.52
2:B:288:GLU:OE1	2:B:291:ALA:N	2.42	0.52
1:E:36:CYS:HB3	1:E:47:CYS:H	1.74	0.52
1:A:150:LEU:HB3	1:A:152:LYS:HZ2	1.75	0.52
1:A:159:ARG:HA	1:A:165:ALA:HB2	1.92	0.52
1:A:545:LYS:CB	1:A:548:GLN:OE1	2.44	0.52
1:A:439:LYS:HE2	1:A:441:ILE:HD11	1.92	0.52
2:B:81:GLU:HA	2:B:85:LYS:HD2	1.92	0.52
1:A:64:CYS:SG	1:A:65:VAL:N	2.83	0.52
1:E:350:VAL:HG13	1:E:376:VAL:HG23	1.92	0.52
2:F:544:PHE:HE2	2:F:585:GLY:HA2	1.75	0.52
1:A:259:ARG:HH22	1:A:265:LYS:HA	1.74	0.52
1:A:158:CYS:HA	1:A:162:GLN:HG3	1.92	0.51
2:B:27:GLU:HB3	2:B:75:ILE:HG21	1.93	0.51
3:G:42:PRO:HB2	3:G:45:LEU:HB2	1.93	0.51
1:A:39:LYS:NZ	1:A:520:LYS:O	2.44	0.51
1:A:103:CYS:SG	1:A:147:LYS:NZ	2.72	0.51
2:B:494:ALA:HB1	2:B:514:LEU:HD21	1.92	0.51
1:A:491:LEU:HD12	1:A:494:THR:HB	1.91	0.51
1:E:328:ILE:HD12	1:E:572:LEU:HD12	1.91	0.51
3:G:85:GLY:O	3:G:89:TYR:N	2.41	0.51
1:E:48:ARG:NH1	2:F:500:SER:O	2.44	0.51
2:F:377:ARG:HB3	2:F:411:LEU:HB3	1.93	0.51
2:B:544:PHE:HE2	2:B:585:GLY:HA2	1.76	0.50
2:F:402:SER:O	2:F:511:ASN:ND2	2.39	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:147:LEU:HB3	2:B:269:THR:HG21	1.93	0.50
2:B:546:ILE:HG22	2:B:596:ILE:HG12	1.94	0.50
1:E:163:SER:O	1:E:480:ARG:NH2	2.44	0.50
1:E:429:VAL:HA	1:E:432:VAL:HG12	1.93	0.50
1:A:67:PRO:HD2	2:B:307:PRO:HG2	1.92	0.50
1:A:25:ALA:HB1	1:A:30:ILE:HB	1.92	0.50
1:A:305:ILE:HA	1:A:308:ILE:HG22	1.93	0.50
2:B:53:GLU:HB2	2:B:365:THR:H	1.77	0.50
3:C:141:PHE:HB2	3:C:144:LEU:HD11	1.94	0.50
1:A:26:ARG:NH2	1:A:522:ASP:OD1	2.44	0.49
2:B:70:VAL:HG22	2:B:92:LEU:HD13	1.93	0.49
2:B:201:ASP:OD1	2:B:201:ASP:N	2.46	0.49
1:A:232:PRO:HA	1:A:235:ARG:HH22	1.77	0.49
1:E:132:LYS:HE2	1:E:146:SER:HB2	1.93	0.49
1:E:227:ILE:HG12	1:E:265:LYS:HB3	1.93	0.49
1:A:301:SER:OG	4:A:605:SF4:S1	2.67	0.49
1:E:42:ASN:C	1:E:42:ASN:HD22	2.19	0.49
3:G:29:GLN:O	3:G:32:GLN:NE2	2.44	0.49
2:B:191:LYS:HE2	2:B:319:PRO:HB2	1.93	0.49
3:G:27:LEU:HA	3:G:30:ILE:HG12	1.95	0.49
1:E:282:THR:HG21	1:E:563:PRO:HB2	1.95	0.49
1:A:297:ILE:HG22	1:A:497:ILE:HB	1.94	0.48
2:F:406:LEU:HB3	2:F:410:LEU:HD11	1.95	0.48
2:B:476:ARG:O	2:B:481:LYS:N	2.45	0.48
2:B:552:LYS:HD2	2:B:554:CYS:HB3	1.95	0.48
2:F:377:ARG:HD2	2:F:412:ASP:HA	1.95	0.48
1:A:226:VAL:HG23	1:A:264:ASP:H	1.77	0.48
2:B:276:GLU:HG2	2:B:278:ARG:HH12	1.77	0.48
1:E:167:LEU:HD12	1:E:178:VAL:HG22	1.95	0.48
1:E:445:ASP:OD1	1:E:445:ASP:N	2.46	0.48
2:B:199:GLU:O	2:B:239:ARG:NH1	2.47	0.48
2:B:398:THR:HG21	2:B:420:LEU:HD21	1.95	0.48
2:B:14:THR:HG22	3:C:127:ALA:HB2	1.95	0.48
3:C:35:GLN:NE2	3:C:39:GLY:O	2.46	0.48
1:E:25:ALA:HB1	1:E:30:ILE:HB	1.94	0.48
1:E:403:ASP:OD1	1:E:404:PHE:N	2.45	0.48
1:A:439:LYS:NZ	1:A:461:GLU:OE2	2.40	0.48
2:B:355:VAL:HG13	2:B:369:GLU:HG3	1.96	0.48
2:B:354:LYS:NZ	2:B:372:MET:SD	2.87	0.48
2:B:406:LEU:HD21	2:B:420:LEU:HD11	1.96	0.48
2:B:543:ASP:OD1	2:B:543:ASP:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:282:THR:HG22	1:E:564:ASN:HD22	1.79	0.48
2:F:300:ARG:HD2	3:G:66:PHE:HB2	1.96	0.48
1:E:549:ASN:OD1	1:E:551:SER:OG	2.28	0.48
2:B:324:ASN:ND2	7:B:605:FMN:O2	2.47	0.48
2:B:359:GLY:N	2:B:432:LEU:O	2.47	0.48
1:E:54:ILE:HA	1:E:74:VAL:HG12	1.96	0.48
2:F:235:TYR:HB3	2:F:278:ARG:HG2	1.96	0.47
2:B:199:GLU:OE2	2:B:208:ARG:NH1	2.43	0.47
1:A:526:ARG:HA	1:A:529:ARG:HG2	1.96	0.47
1:E:157:VAL:O	1:E:162:GLN:HG2	2.15	0.47
1:A:155:VAL:O	1:A:159:ARG:HB2	2.14	0.47
2:B:350:SER:HB2	2:B:372:MET:HE1	1.95	0.47
1:A:33:PRO:HD3	1:E:393:ARG:CZ	2.45	0.47
2:B:24:LEU:HD22	2:B:75:ILE:HD11	1.97	0.47
2:B:304:ARG:HD2	2:B:305:PRO:HD2	1.97	0.47
2:B:459:LYS:O	2:B:464:ARG:NH2	2.35	0.47
2:B:278:ARG:HD3	2:B:296:ILE:HD12	1.97	0.46
2:F:262:LEU:HD21	2:F:275:LEU:HB2	1.97	0.46
2:F:278:ARG:NH2	3:G:22:GLU:OE2	2.48	0.46
2:F:372:MET:HE3	2:F:373:GLY:N	2.30	0.46
1:A:301:SER:HB3	1:A:304:TRP:CD1	2.50	0.46
2:B:588:ILE:HG13	2:B:596:ILE:HB	1.96	0.46
1:E:334:LYS:NZ	1:E:374:ALA:O	2.34	0.46
2:B:104:LEU:N	2:B:108:GLU:OE1	2.48	0.46
1:E:361:TYR:O	1:E:364:GLN:HB3	2.16	0.46
1:A:31:ASP:O	1:E:393:ARG:NH2	2.48	0.46
2:B:472:GLU:HA	2:B:475:GLU:HG3	1.97	0.46
2:B:477:ILE:HD12	2:B:528:ILE:HG12	1.96	0.46
1:A:228:VAL:HG12	1:A:351:VAL:CG1	2.45	0.46
1:E:42:ASN:C	1:E:42:ASN:ND2	2.74	0.46
2:F:557:CYS:HB2	2:F:587:CYS:HB2	1.97	0.46
1:A:79:PRO:HA	1:A:82:ARG:HD2	1.98	0.46
1:E:571:ILE:HG13	1:E:572:LEU:CD2	2.45	0.46
3:C:125:VAL:HG13	3:C:127:ALA:H	1.80	0.46
1:E:359:LYS:O	1:E:362:GLU:HG3	2.16	0.45
2:F:476:ARG:O	2:F:481:LYS:N	2.46	0.45
3:G:101:ASN:OD1	3:G:101:ASN:O	2.34	0.45
1:A:164:VAL:HG12	1:A:166:VAL:HG13	1.97	0.45
1:E:475:GLY:HA2	1:E:503:PRO:HG3	1.98	0.45
1:A:53:GLU:OE2	1:A:75:LEU:HB3	2.16	0.45
1:A:535:ASP:O	1:A:539:ASN:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:ARG:HD3	1:A:292:GLY:HA3	1.97	0.45
1:E:301:SER:HB3	1:E:304:TRP:CD1	2.51	0.45
2:F:188:ASP:OD1	2:F:188:ASP:N	2.50	0.45
3:G:67:TYR:HB3	3:G:69:GLN:HG3	1.99	0.45
1:A:60:LEU:N	1:A:60:LEU:HD22	2.31	0.45
1:E:89:LEU:HA	1:E:92:ILE:HG22	1.98	0.45
1:E:328:ILE:HD12	1:E:572:LEU:HD13	1.99	0.45
1:E:172:ARG:HH21	2:F:457:CYS:HA	1.81	0.45
3:G:79:LYS:NZ	3:G:120:ASP:OD2	2.36	0.44
1:A:41:ILE:HD12	1:A:42:ASN:HB2	1.98	0.44
1:A:383:ARG:NH1	1:A:512:GLN:O	2.51	0.44
2:B:427:MET:SD	2:B:427:MET:N	2.90	0.44
1:E:208:GLU:OE2	1:E:383:ARG:NH2	2.38	0.44
2:F:337:ASN:O	2:F:337:ASN:ND2	2.50	0.44
3:G:120:ASP:N	3:G:120:ASP:OD1	2.50	0.44
1:A:472:VAL:HG22	1:A:498:GLU:HB3	1.99	0.44
1:E:306:LYS:HA	1:E:309:GLU:HG2	1.98	0.44
2:F:199:GLU:OE2	2:F:207:ASP:N	2.50	0.44
2:B:165:ARG:HE	2:B:417:TYR:HE1	1.64	0.44
2:B:446:ARG:HA	2:B:449:LEU:HB3	2.00	0.44
1:E:113:THR:O	1:E:117:ASP:HB2	2.17	0.44
1:A:13:MET:SD	1:A:28:ASN:ND2	2.85	0.44
1:A:381:THR:OG1	1:A:382:THR:N	2.48	0.44
1:A:39:LYS:HG3	1:A:521:MET:HE1	2.00	0.44
1:A:353:ILE:O	1:A:354:MET:HE2	2.17	0.44
1:E:194:CYS:SG	1:E:195:GLY:N	2.91	0.44
1:A:168:GLY:O	1:A:178:VAL:HA	2.18	0.44
3:G:47:GLY:HA2	3:G:57:LEU:HD21	1.99	0.43
1:A:525:ILE:O	1:A:528:GLU:HG3	2.17	0.43
1:A:567:LYS:HA	1:A:567:LYS:HD3	1.78	0.43
1:E:271:PHE:HE1	1:E:552:VAL:HB	1.83	0.43
1:A:171:GLY:O	1:A:172:ARG:NH1	2.51	0.43
1:A:234:VAL:HG13	1:A:235:ARG:HG3	2.00	0.43
1:A:503:PRO:O	1:A:508:ASN:HB2	2.19	0.43
2:B:67:TYR:OH	2:B:82:HIS:ND1	2.45	0.43
2:B:255:GLN:HA	2:B:258:GLU:HB2	2.00	0.43
1:E:154:CYS:SG	1:E:155:VAL:N	2.92	0.43
2:F:240:ALA:N	2:F:280:GLY:O	2.52	0.43
1:A:7:LYS:HA	1:A:11:GLN:O	2.18	0.43
3:C:112:THR:OG1	3:C:114:ASP:OD1	2.35	0.43
1:E:48:ARG:HH22	2:F:502:LEU:HA	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:164:VAL:HG12	1:E:166:VAL:HG13	2.00	0.43
1:E:150:LEU:O	1:E:152:LYS:NZ	2.52	0.43
2:F:130:ASN:HB3	2:F:133:GLU:HB2	2.00	0.43
1:E:227:ILE:HG21	1:E:333:LEU:HD21	2.00	0.43
1:A:60:LEU:N	1:A:60:LEU:CD2	2.82	0.43
1:A:545:LYS:O	1:A:548:GLN:HG2	2.19	0.43
2:F:323:ASN:HB2	2:F:328:TYR:CZ	2.54	0.43
1:A:304:TRP:CE3	1:A:499:LEU:HD22	2.54	0.43
1:A:502:CYS:SG	1:A:505:GLY:O	2.78	0.42
1:A:21:ILE:HG13	1:A:68:VAL:HG12	2.01	0.42
1:A:517:ALA:O	1:A:521:MET:HG2	2.19	0.42
2:B:208:ARG:O	2:B:212:GLU:N	2.38	0.42
2:B:325:VAL:HA	2:B:328:TYR:HD2	1.84	0.42
2:F:446:ARG:HA	2:F:449:LEU:HG	2.00	0.42
1:E:228:VAL:HG11	1:E:263:PHE:CD2	2.54	0.42
2:B:540:HIS:O	2:B:583:LYS:NZ	2.39	0.42
3:C:29:GLN:O	3:C:32:GLN:HG3	2.19	0.42
1:A:301:SER:HB3	1:A:304:TRP:HD1	1.85	0.42
2:B:15:GLY:O	2:B:18:SER:OG	2.34	0.42
2:B:167:ARG:NH2	2:B:427:MET:HB2	2.34	0.42
2:B:215:PRO:HD3	2:B:248:ARG:HH21	1.84	0.42
2:B:443:ASP:OD1	2:B:443:ASP:N	2.53	0.42
1:A:383:ARG:HH22	1:A:511:GLY:HA2	1.85	0.42
1:A:394:ILE:HG22	1:A:399:LEU:HD21	2.02	0.42
2:B:420:LEU:HD12	2:B:423:ALA:HB3	2.00	0.42
1:E:29:ASN:C	1:E:29:ASN:HD22	2.27	0.42
1:E:328:ILE:HG23	1:E:572:LEU:HD11	2.01	0.42
1:A:231:ALA:O	1:A:235:ARG:NH1	2.49	0.42
2:F:192:TYR:HB2	2:F:320:THR:HG22	2.02	0.41
1:A:96:HIS:CD2	1:A:111:LEU:HD23	2.55	0.41
1:E:172:ARG:NH2	2:F:456:SER:O	2.48	0.41
1:E:304:TRP:HA	1:E:307:PHE:HB3	2.02	0.41
1:A:426:GLU:O	1:A:430:ARG:HG2	2.19	0.41
2:B:172:PHE:HB3	2:B:177:LYS:HZ1	1.85	0.41
1:E:174:PHE:HE1	2:F:465:ILE:HA	1.84	0.41
3:G:32:GLN:HA	3:G:35:GLN:HG3	2.01	0.41
2:B:407:PRO:HG2	2:B:519:PHE:CD1	2.55	0.41
1:E:554:ARG:O	1:E:558:GLU:HB2	2.20	0.41
1:A:426:GLU:OE1	1:A:430:ARG:NH2	2.53	0.41
2:B:236:VAL:HG23	2:B:277:ILE:HD12	2.02	0.41
2:B:262:LEU:HD11	2:B:275:LEU:HD23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:75:LYS:HE3	3:C:75:LYS:HA	2.02	0.41
2:B:479:ASP:HA	2:B:540:HIS:HB3	2.03	0.41
2:F:376:LEU:HB2	2:F:411:LEU:HA	2.02	0.41
1:E:172:ARG:N	1:E:175:THR:OG1	2.52	0.41
1:A:48:ARG:HE	1:A:51:LEU:HD21	1.86	0.41
1:A:227:ILE:HG21	1:A:333:LEU:HD21	2.03	0.41
2:B:256:ALA:O	2:B:261:ILE:N	2.54	0.41
2:B:361:LYS:HE2	2:B:361:LYS:HB2	1.89	0.41
2:F:591:CYS:SG	2:F:594:GLY:N	2.92	0.41
1:A:102:THR:HG22	1:E:120:VAL:HG13	2.02	0.41
1:A:128:GLU:HB2	2:B:468:LYS:NZ	2.35	0.41
1:A:214:ARG:HG2	1:A:378:ILE:HD11	2.03	0.41
1:A:480:ARG:HA	1:A:483:MET:HE2	2.02	0.41
3:C:109:GLY:H	3:C:119:VAL:HG13	1.86	0.40
1:A:285:ILE:HA	1:A:288:VAL:HG22	2.02	0.40
1:A:461:GLU:HB3	1:A:467:THR:HG22	2.03	0.40
3:C:96:ILE:HD13	3:C:149:ILE:HD11	2.02	0.40
1:E:231:ALA:HB3	1:E:234:VAL:HG13	2.03	0.40
2:B:588:ILE:HA	2:B:596:ILE:HD12	2.03	0.40
1:A:153:ARG:NH2	1:A:200:ASN:O	2.54	0.40
1:E:334:LYS:HB3	1:E:334:LYS:HE2	1.83	0.40
1:A:103:CYS:CB	4:A:603:SF4:S4	2.87	0.40
1:A:182:PHE:CZ	3:C:43:LEU:HB3	2.56	0.40
1:A:230:THR:HG22	1:A:268:ASP:HA	2.04	0.40
2:B:289:GLU:OE1	7:B:605:FMN:O2'	2.38	0.40
1:E:353:ILE:HG21	1:E:385:LEU:HD12	2.03	0.40
2:F:546:ILE:HD12	2:F:546:ILE:HA	1.92	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	581/583 (100%)	547 (94%)	32 (6%)	2 (0%)	36	72
1	E	581/583 (100%)	556 (96%)	24 (4%)	1 (0%)	43	78
2	B	597/599 (100%)	587 (98%)	10 (2%)	0	100	100
2	F	468/599 (78%)	454 (97%)	14 (3%)	0	100	100
3	C	154/156 (99%)	146 (95%)	8 (5%)	0	100	100
3	G	125/156 (80%)	105 (84%)	19 (15%)	1 (1%)	16	53
All	All	2506/2676 (94%)	2395 (96%)	107 (4%)	4 (0%)	44	78

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	106	SER
1	E	106	SER
1	A	97	ASN
3	G	24	PRO

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	492/492 (100%)	483 (98%)	9 (2%)	51	67
1	E	492/492 (100%)	487 (99%)	5 (1%)	68	76
2	B	480/480 (100%)	478 (100%)	2 (0%)	84	83
2	F	369/480 (77%)	367 (100%)	2 (0%)	81	82
3	C	130/130 (100%)	129 (99%)	1 (1%)	73	78
3	G	106/130 (82%)	104 (98%)	2 (2%)	50	66
All	All	2069/2204 (94%)	2048 (99%)	21 (1%)	65	76

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	ILE

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Mol	Chain	Res	Type
1	A	60	LEU
1	A	98	ARG
1	A	149	ILE
1	A	227	ILE
1	A	316	ILE
1	A	326	GLN
1	A	506	CYS
1	A	507	VAL
2	B	95	ASN
2	B	418	ASP
3	C	30	ILE
1	E	96	HIS
1	E	107	GLU
1	E	228	VAL
1	E	229	GLN
1	E	574	THR
2	F	219	ILE
2	F	439	ASN
3	G	10	LEU
3	G	16	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	ASN
1	A	364	GLN
2	B	102	HIS
2	B	247	ASN
2	B	397	GLN
3	C	9	ASN
3	C	94	GLN
1	E	29	ASN
1	E	42	ASN
1	E	162	GLN
1	E	200	ASN
1	E	290	ASN
1	E	327	ASN
1	E	469	ASN
1	E	485	GLN
1	E	564	ASN
1	E	573	HIS
2	F	255	GLN

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Mol	Chain	Res	Type
2	F	337	ASN
2	F	439	ASN
3	G	9	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](#)

Of 24 ligands modelled in this entry, 2 are monoatomic - leaving 22 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	SF4	F	601	2	0,12,12	-	-	-		
4	SF4	F	602	2	0,12,12	-	-	-		
4	SF4	A	603	1	0,12,12	-	-	-		
7	FMN	B	605	-	33,33,33	2.20	14 (42%)	48,50,50	2.75	15 (31%)
8	NAD	F	605	-	46,48,48	1.56	5 (10%)	64,73,73	1.49	4 (6%)
5	FES	G	201	3	0,4,4	-	-	-		
4	SF4	A	605	1	0,12,12	-	-	-		
4	SF4	A	602	1	0,12,12	-	-	-		
5	FES	A	604	1	0,4,4	-	-	-		
4	SF4	E	605	1	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SF4	A	601	1	0,12,12	-	-	-		
4	SF4	B	606	2	0,12,12	-	-	-		
4	SF4	F	606	2	0,12,12	-	-	-		
4	SF4	E	603	1	0,12,12	-	-	-		
4	SF4	B	603	2	0,12,12	-	-	-		
7	FMN	F	604	-	33,33,33	2.17	15 (45%)	48,50,50	2.73	18 (37%)
4	SF4	E	601	1	0,12,12	-	-	-		
4	SF4	E	602	1	0,12,12	-	-	-		
5	FES	E	604	1	0,4,4	-	-	-		
4	SF4	B	602	2	0,12,12	-	-	-		
5	FES	C	201	3	0,4,4	-	-	-		
5	FES	B	601	2	0,4,4	-	-	-		

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
4	SF4	F	601	2	-	-	0/6/5/5
4	SF4	F	602	2	-	-	0/6/5/5
4	SF4	A	603	1	-	-	0/6/5/5
7	FMN	B	605	-	-	11/18/18/18	0/3/3/3
8	NAD	F	605	-	-	12/30/62/62	0/5/5/5
5	FES	G	201	3	-	-	0/1/1/1
4	SF4	A	605	1	-	-	0/6/5/5
4	SF4	A	602	1	-	-	0/6/5/5
5	FES	A	604	1	-	-	0/1/1/1
4	SF4	E	605	1	-	-	0/6/5/5
4	SF4	A	601	1	-	-	0/6/5/5
4	SF4	B	606	2	-	-	0/6/5/5
4	SF4	F	606	2	-	-	0/6/5/5
4	SF4	E	603	1	-	-	0/6/5/5
7	FMN	F	604	-	-	7/18/18/18	0/3/3/3
4	SF4	B	603	2	-	-	0/6/5/5
4	SF4	E	601	1	-	-	0/6/5/5
4	SF4	E	602	1	-	-	0/6/5/5
5	FES	E	604	1	-	-	0/1/1/1
4	SF4	B	602	2	-	-	0/6/5/5
5	FES	C	201	3	-	-	0/1/1/1
5	FES	B	601	2	-	-	0/1/1/1

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	F	605	NAD	C4N-C3N	7.18	1.50	1.39
8	F	605	NAD	C5N-C4N	5.86	1.48	1.38
7	F	604	FMN	C10-N1	4.66	1.42	1.33
7	B	605	FMN	C10-N1	4.62	1.42	1.33
7	B	605	FMN	C9A-C5A	3.82	1.47	1.41
7	F	604	FMN	C9A-C5A	3.69	1.47	1.41
7	B	605	FMN	C2-N3	-3.48	1.31	1.39
7	F	604	FMN	C4-N3	-3.43	1.32	1.38
7	B	605	FMN	C4-N3	-3.39	1.32	1.38
7	F	604	FMN	C2-N3	-3.33	1.31	1.39
7	F	604	FMN	C2-N1	3.09	1.43	1.36
7	B	605	FMN	C4A-C4	3.08	1.55	1.44
7	F	604	FMN	C4A-C4	3.03	1.55	1.44
7	B	605	FMN	C2-N1	2.94	1.43	1.36
7	B	605	FMN	C9-C8	-2.74	1.35	1.39
8	F	605	NAD	C3N-C7N	-2.69	1.46	1.50
8	F	605	NAD	C6N-C5N	-2.69	1.33	1.38
7	F	604	FMN	C9-C8	-2.49	1.36	1.39
7	F	604	FMN	C1'-C2'	-2.39	1.49	1.52
7	F	604	FMN	C5A-N5	-2.32	1.35	1.39
7	B	605	FMN	C5A-N5	-2.29	1.35	1.39
8	F	605	NAD	C2N-C3N	-2.26	1.35	1.39
7	B	605	FMN	C6-C7	-2.21	1.36	1.39
7	B	605	FMN	C9A-N10	-2.16	1.37	1.41
7	F	604	FMN	C2'-C3'	-2.16	1.49	1.53
7	B	605	FMN	P-O2P	-2.13	1.46	1.54
7	F	604	FMN	C6-C7	-2.12	1.36	1.39
7	F	604	FMN	P-O2P	-2.12	1.46	1.54
7	F	604	FMN	C4'-C3'	-2.10	1.49	1.53
7	B	605	FMN	C1'-C2'	-2.08	1.49	1.52
7	B	605	FMN	C4A-C10	2.07	1.50	1.44
7	F	604	FMN	C4A-C10	2.05	1.50	1.44
7	F	604	FMN	C9A-N10	-2.04	1.37	1.41
7	B	605	FMN	C4'-C3'	-2.02	1.49	1.53

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	F	605	NAD	C5N-C4N-C3N	-10.33	110.21	120.36
7	F	604	FMN	C4A-C10-N1	-8.84	102.91	124.59
7	B	605	FMN	C4A-C10-N1	-8.76	103.11	124.59
7	B	605	FMN	C10-N1-C2	8.17	134.55	116.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	F	604	FMN	C10-N1-C2	8.13	134.45	116.85
7	B	605	FMN	C4A-C10-N10	7.13	126.69	116.48
7	F	604	FMN	C4A-C10-N10	7.12	126.67	116.48
7	F	604	FMN	C10-C4A-N5	-4.83	114.94	124.81
7	B	605	FMN	C10-C4A-N5	-4.79	115.04	124.81
7	F	604	FMN	N10-C10-N1	4.05	130.42	118.51
7	B	605	FMN	N10-C10-N1	3.97	130.21	118.51
7	B	605	FMN	C9A-N10-C10	-3.58	115.29	120.75
7	F	604	FMN	C9A-N10-C10	-3.57	115.30	120.75
7	B	605	FMN	C4A-C4-N3	3.53	122.23	113.25
7	B	605	FMN	C4-N3-C2	-3.49	119.44	125.64
7	B	605	FMN	C4-C4A-N5	3.44	122.95	118.21
7	F	604	FMN	C4A-C4-N3	3.38	121.84	113.25
7	F	604	FMN	C4-N3-C2	-3.37	119.65	125.64
7	F	604	FMN	C4-C4A-C10	3.29	122.58	116.93
7	F	604	FMN	C4-C4A-N5	3.09	122.48	118.21
7	B	605	FMN	C4-C4A-C10	2.96	122.01	116.93
8	F	605	NAD	C2N-C3N-C4N	2.90	121.63	118.26
7	B	605	FMN	C1'-N10-C9A	2.87	126.21	120.63
7	F	604	FMN	C1'-N10-C9A	2.84	126.16	120.63
7	F	604	FMN	O2'-C2'-C3'	-2.77	102.77	109.25
8	F	605	NAD	C6N-C5N-C4N	2.71	123.36	119.45
7	B	605	FMN	O2'-C2'-C3'	-2.63	103.09	109.25
7	B	605	FMN	C1'-C2'-C3'	2.41	116.19	109.66
7	B	605	FMN	C4'-C3'-C2'	2.40	117.57	113.57
7	F	604	FMN	C1'-C2'-C3'	2.31	115.93	109.66
7	F	604	FMN	O3'-C3'-C2'	-2.25	103.82	108.93
7	B	605	FMN	O3'-C3'-C2'	-2.20	103.92	108.93
8	F	605	NAD	C6N-N1N-C2N	-2.19	120.02	121.88
7	F	604	FMN	C4'-C3'-C2'	2.17	117.19	113.57
7	F	604	FMN	O2'-C2'-C1'	-2.17	101.30	110.20
7	F	604	FMN	O3P-P-O2P	2.03	115.41	107.80
7	F	604	FMN	O4-C4-C4A	-2.01	121.23	126.53

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	605	FMN	N10-C1'-C2'-O2'
7	B	605	FMN	N10-C1'-C2'-C3'
7	B	605	FMN	C1'-C2'-C3'-O3'
7	B	605	FMN	C1'-C2'-C3'-C4'

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Mol	Chain	Res	Type	Atoms
7	B	605	FMN	C3'-C4'-C5'-O5'
7	B	605	FMN	O4'-C4'-C5'-O5'
7	B	605	FMN	C5'-O5'-P-O1P
7	B	605	FMN	C5'-O5'-P-O3P
7	F	604	FMN	N10-C1'-C2'-O2'
7	F	604	FMN	N10-C1'-C2'-C3'
7	F	604	FMN	C3'-C4'-C5'-O5'
7	F	604	FMN	O4'-C4'-C5'-O5'
7	F	604	FMN	C5'-O5'-P-O1P
7	F	604	FMN	C5'-O5'-P-O2P
7	F	604	FMN	C5'-O5'-P-O3P
8	F	605	NAD	O4B-C4B-C5B-O5B
8	F	605	NAD	C3B-C4B-C5B-O5B
8	F	605	NAD	O4D-C1D-N1N-C2N
8	F	605	NAD	C2D-C1D-N1N-C2N
8	F	605	NAD	O4D-C4D-C5D-O5D
8	F	605	NAD	C3D-C4D-C5D-O5D
7	B	605	FMN	C5'-O5'-P-O2P
8	F	605	NAD	PA-O3-PN-O2N
8	F	605	NAD	C4B-C5B-O5B-PA
7	B	605	FMN	O2'-C2'-C3'-C4'
8	F	605	NAD	C4D-C5D-O5D-PN
8	F	605	NAD	C2D-C1D-N1N-C6N
7	B	605	FMN	O2'-C2'-C3'-O3'
8	F	605	NAD	O4D-C1D-N1N-C6N
8	F	605	NAD	PA-O3-PN-O1N

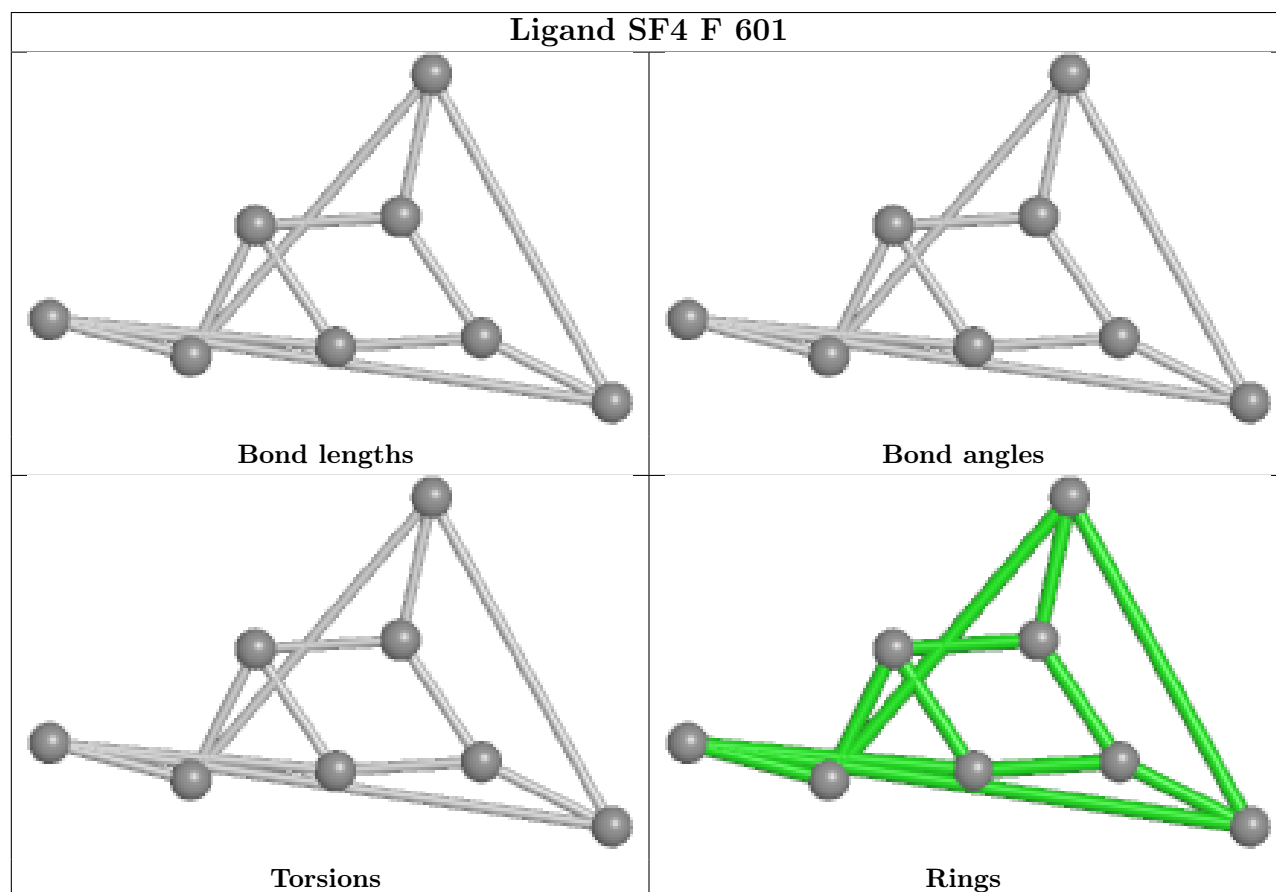
There are no ring outliers.

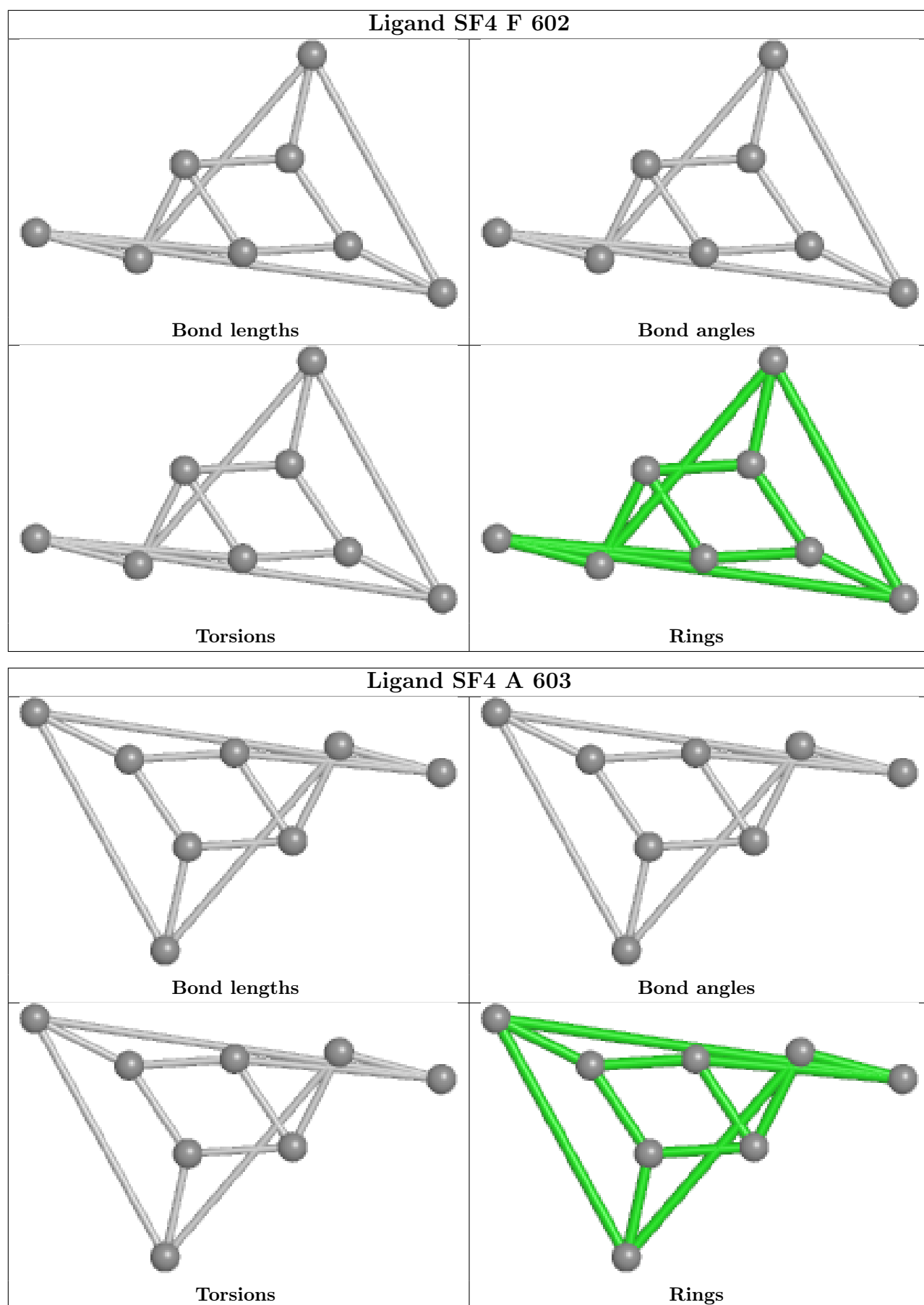
7 monomers are involved in 13 short contacts:

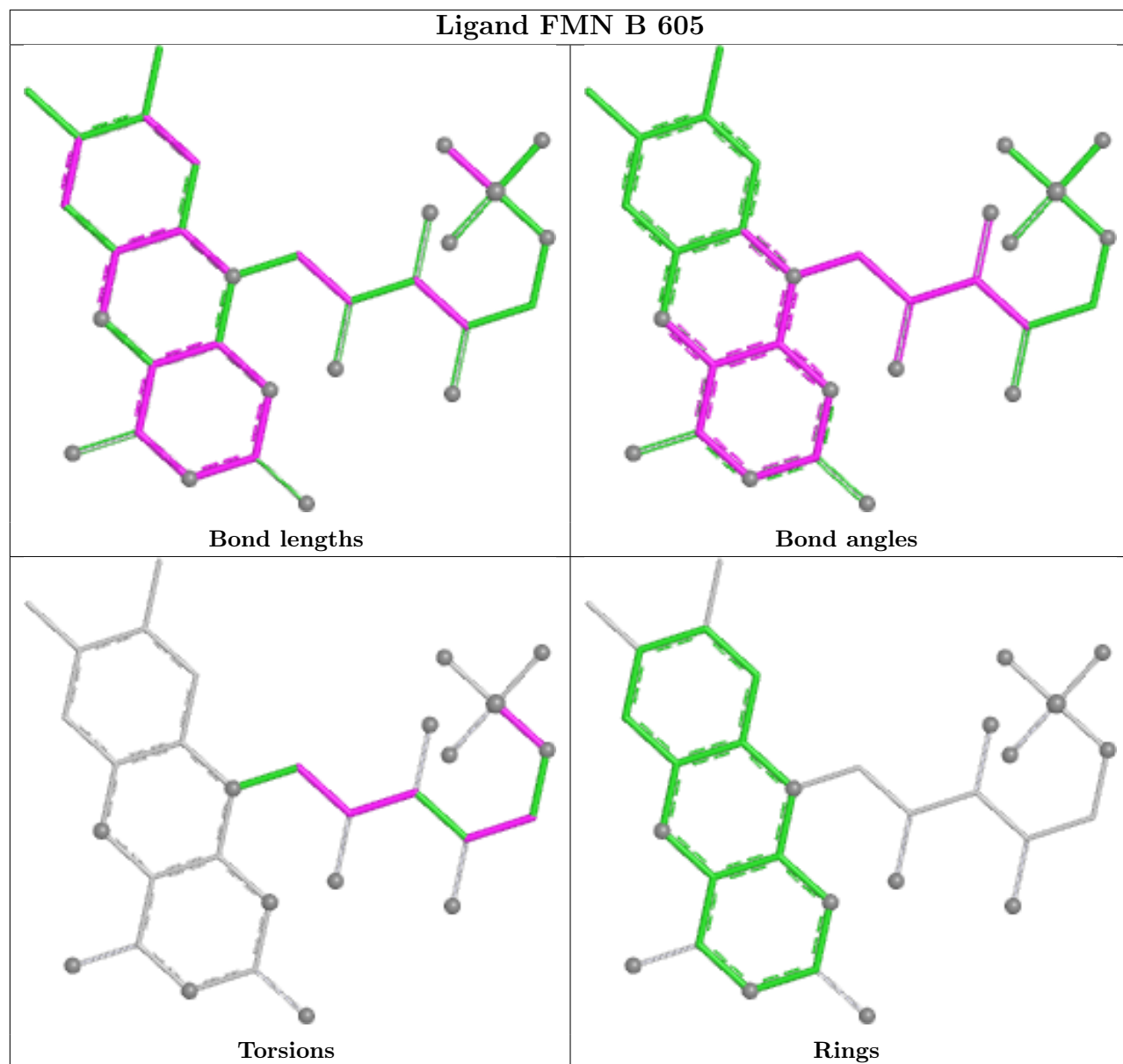
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	603	SF4	3	0
7	B	605	FMN	2	0
4	A	605	SF4	1	0
4	B	606	SF4	3	0
4	E	603	SF4	1	0
4	E	601	SF4	1	0
5	C	201	FES	2	0

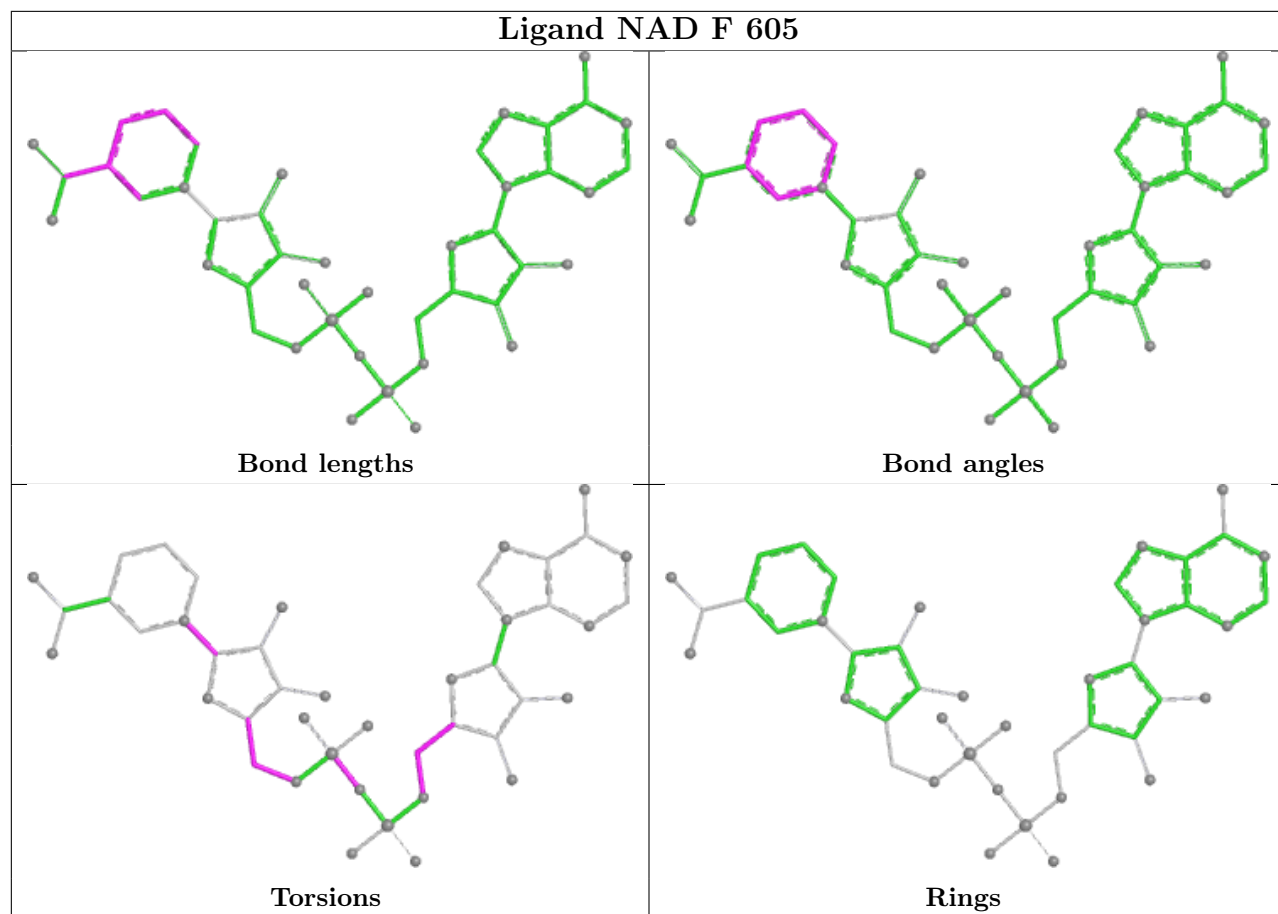
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

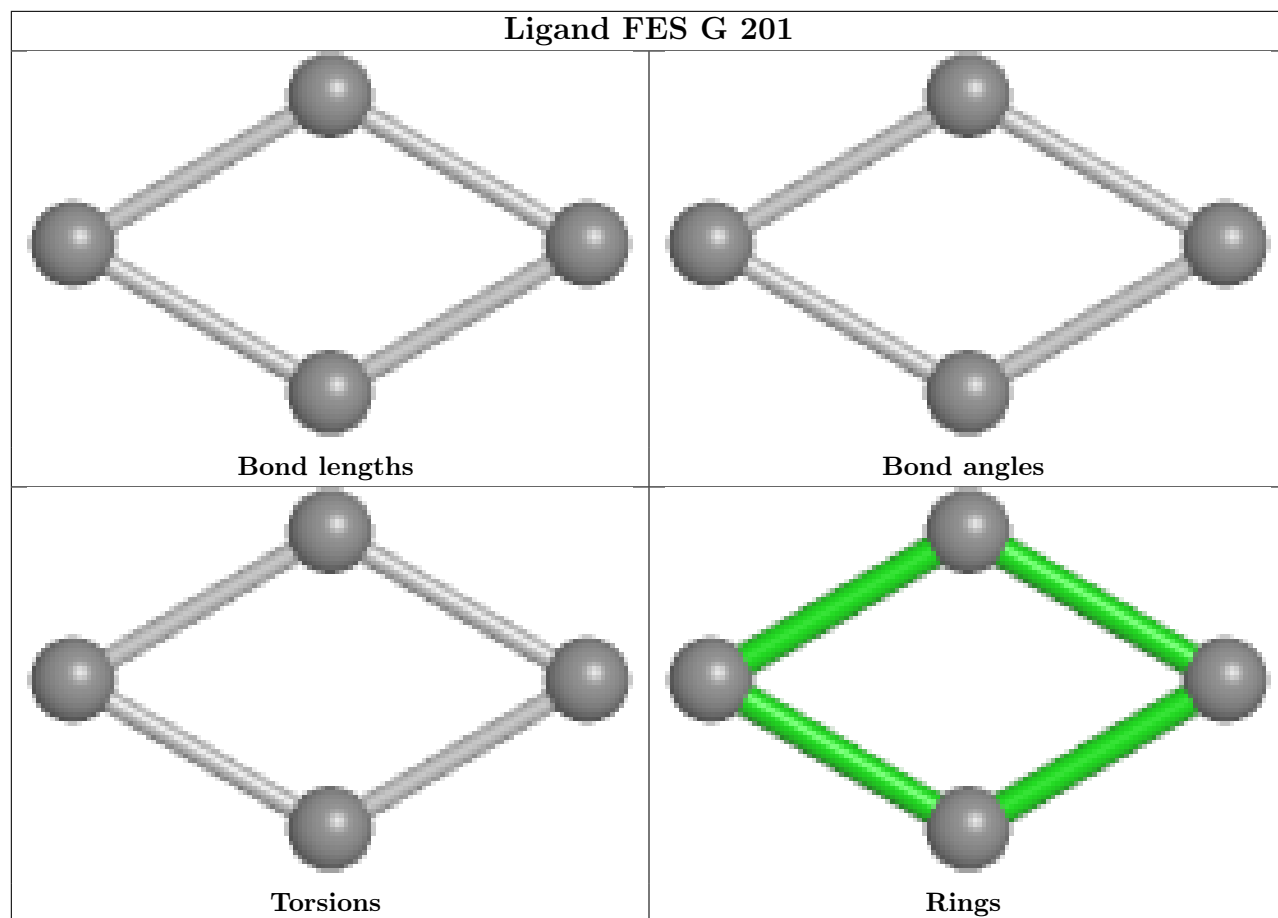
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

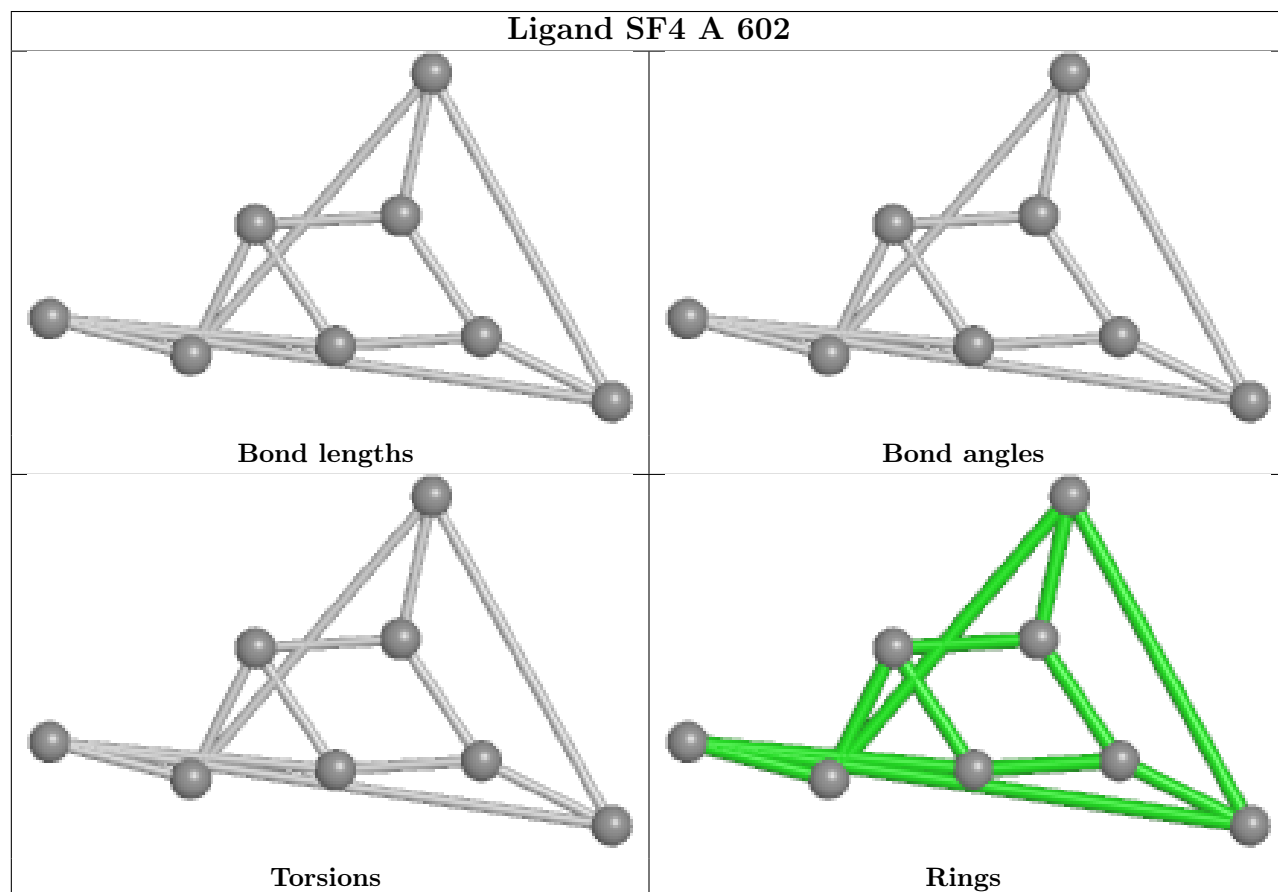
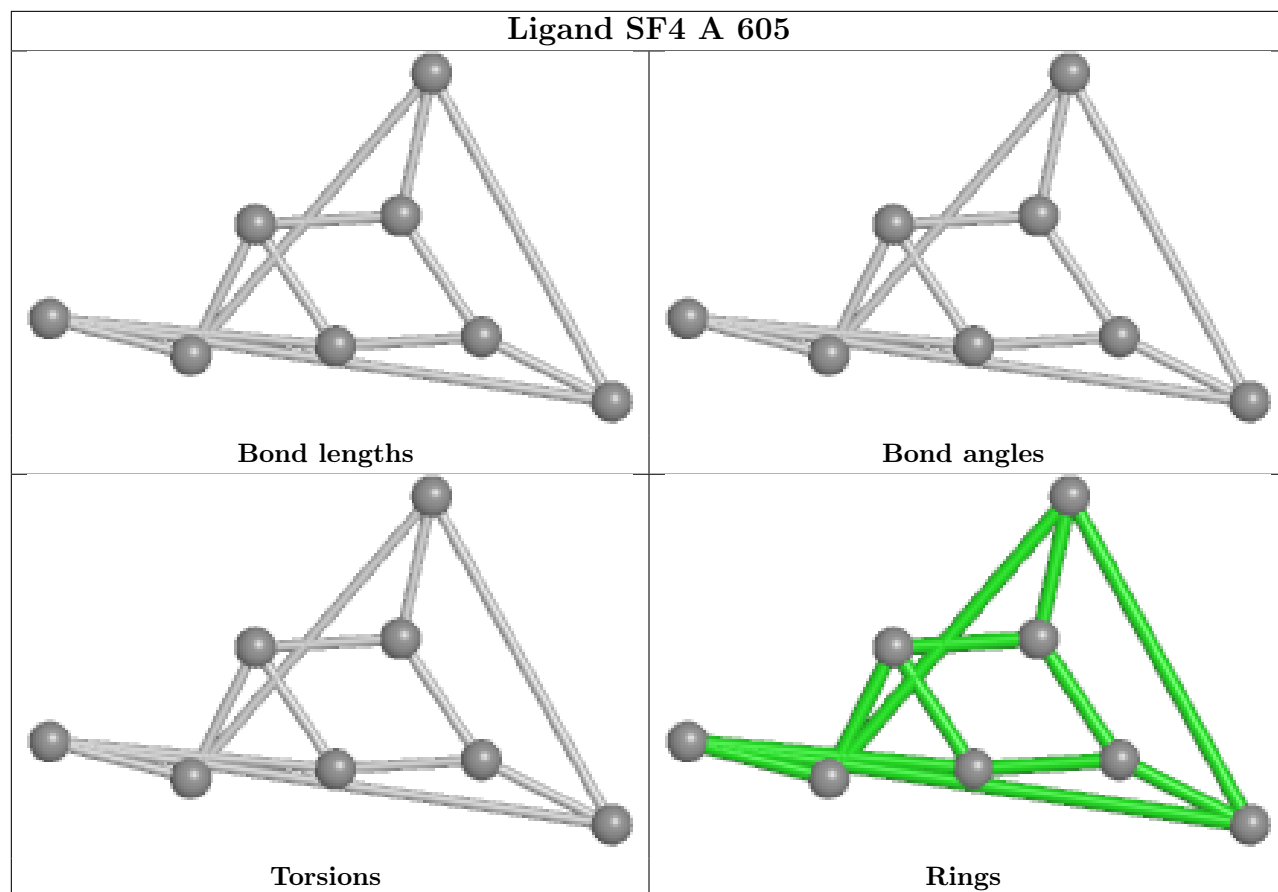


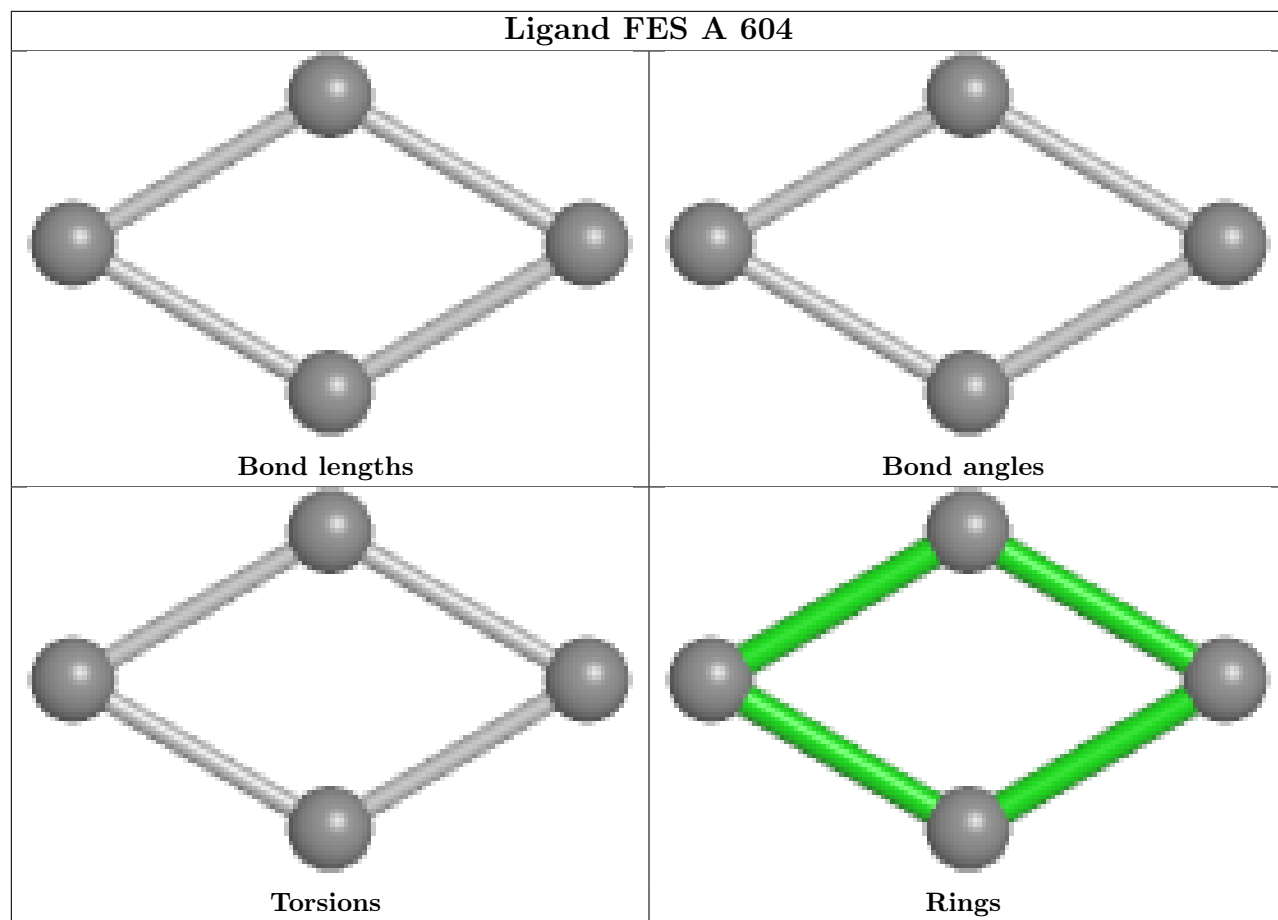


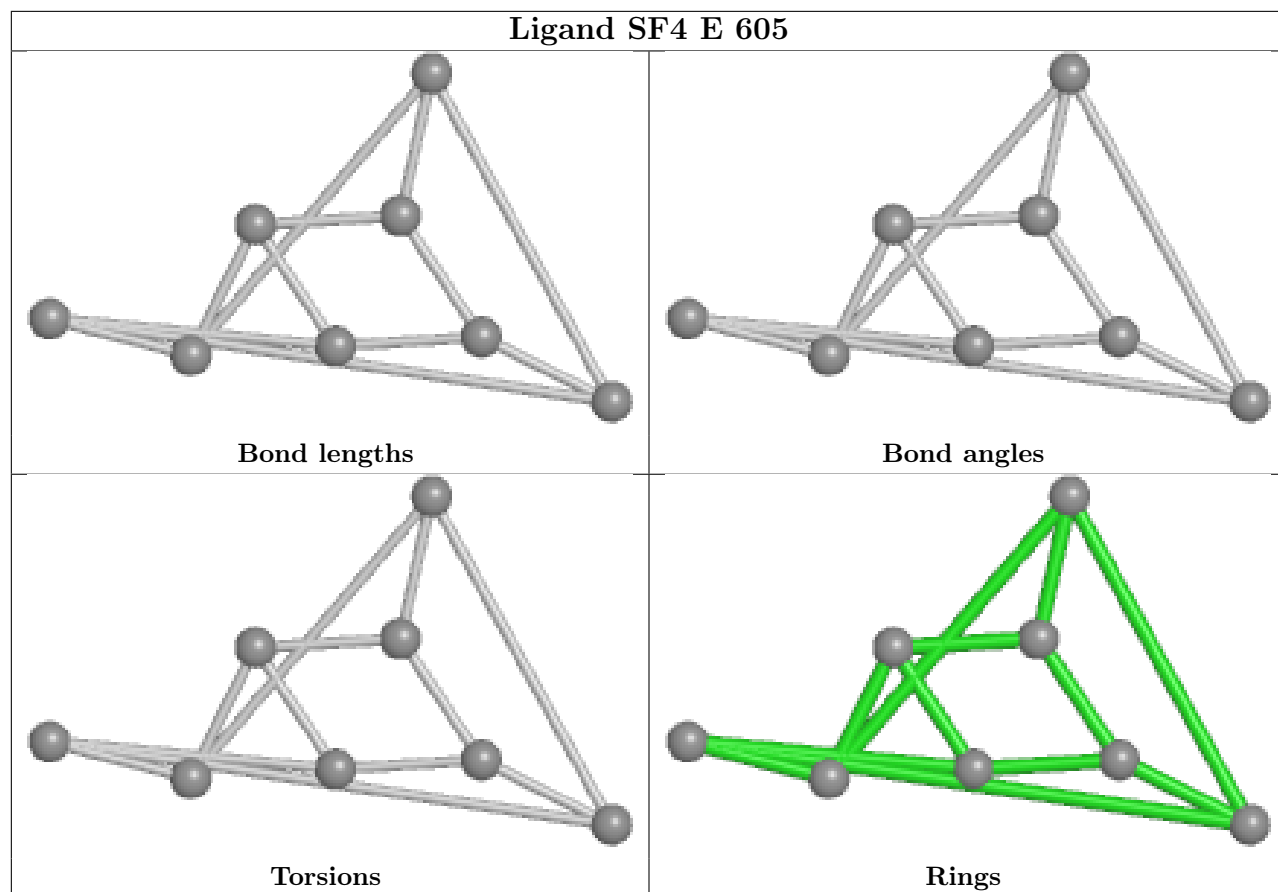


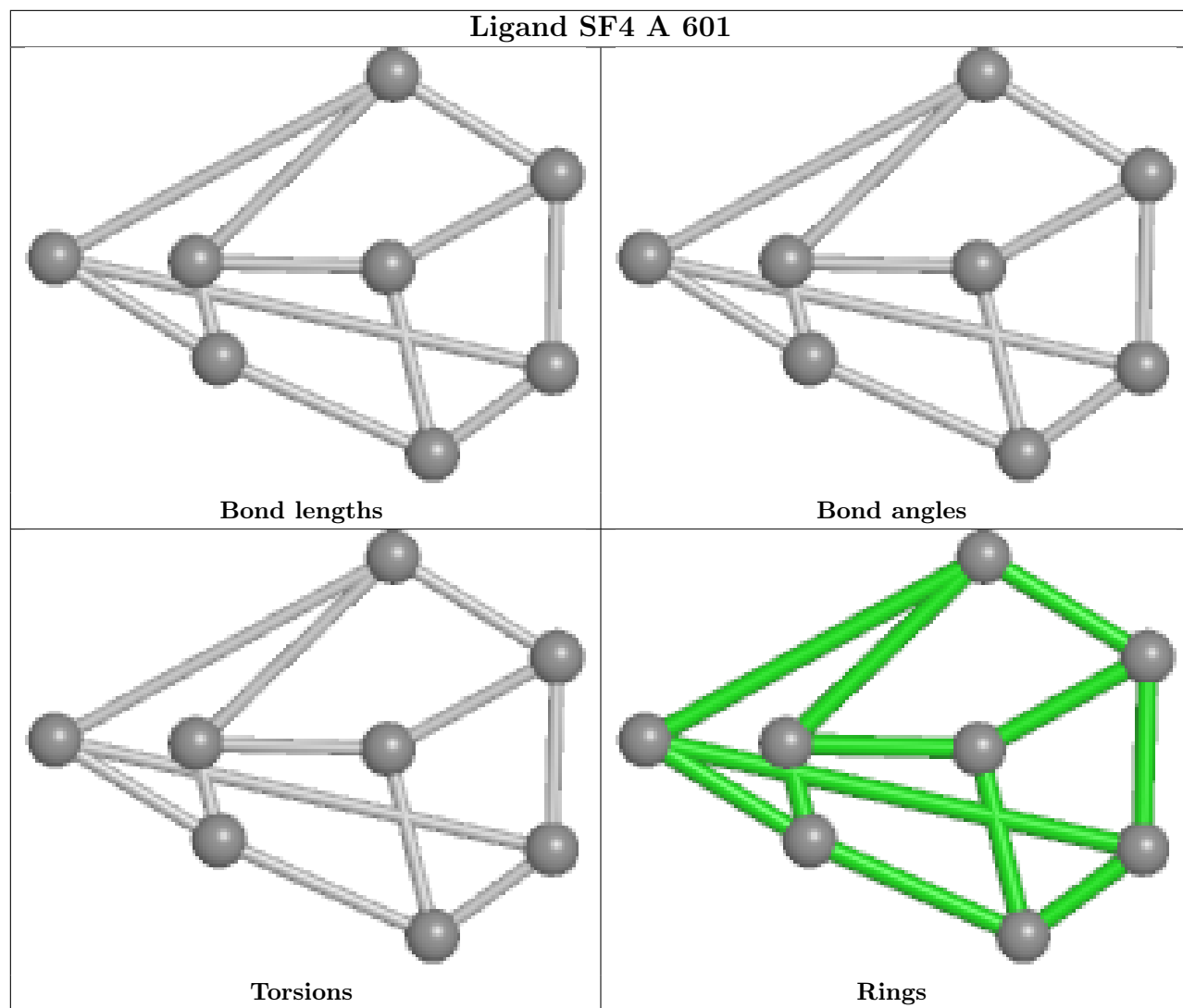


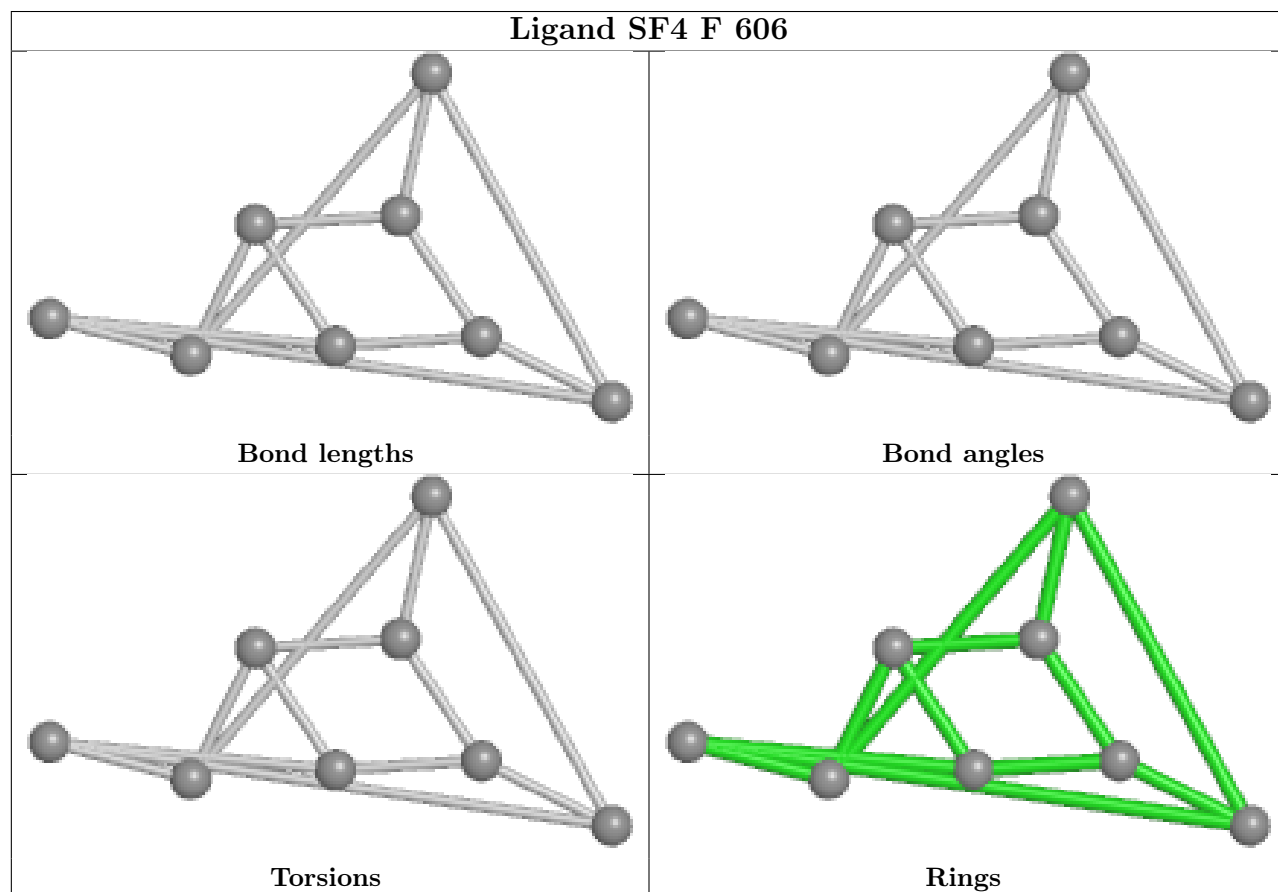
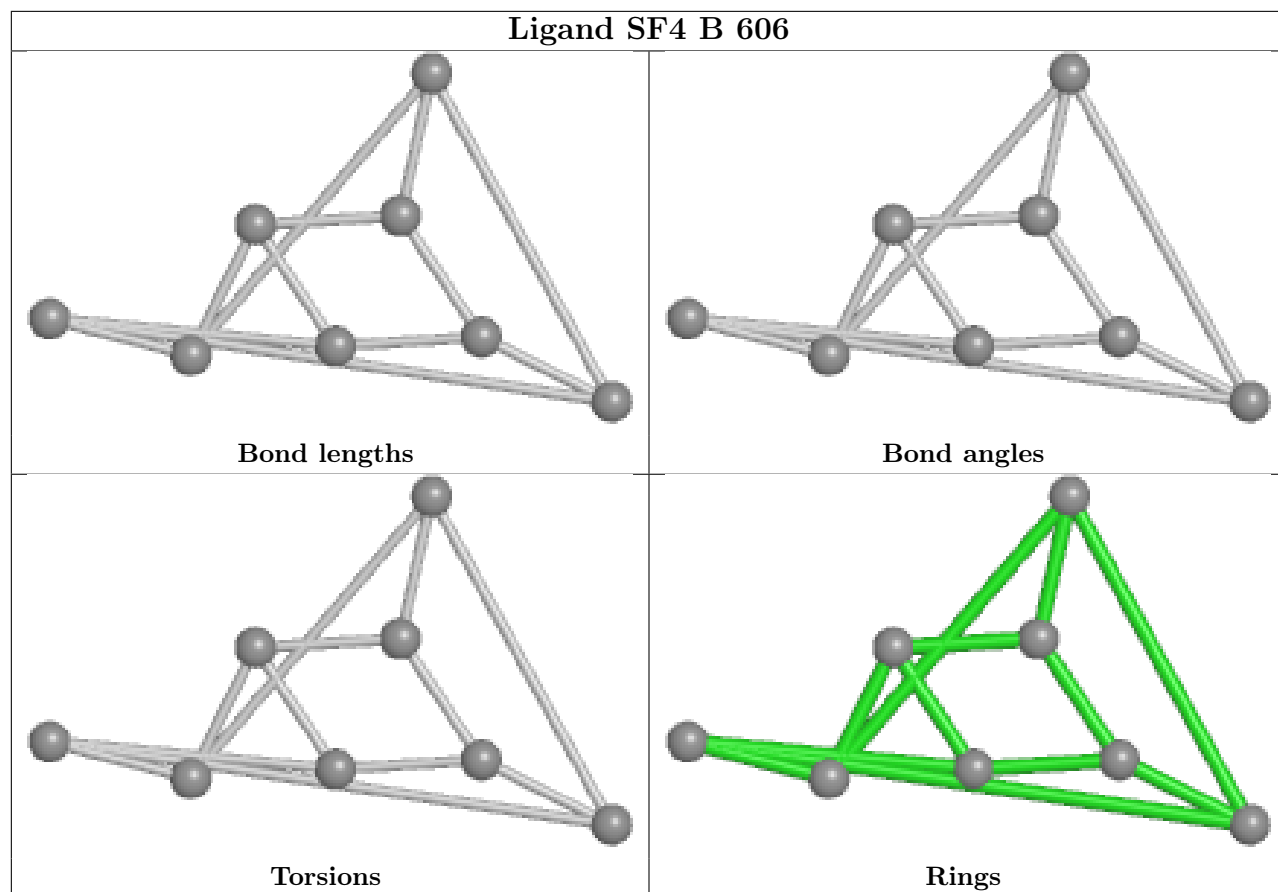


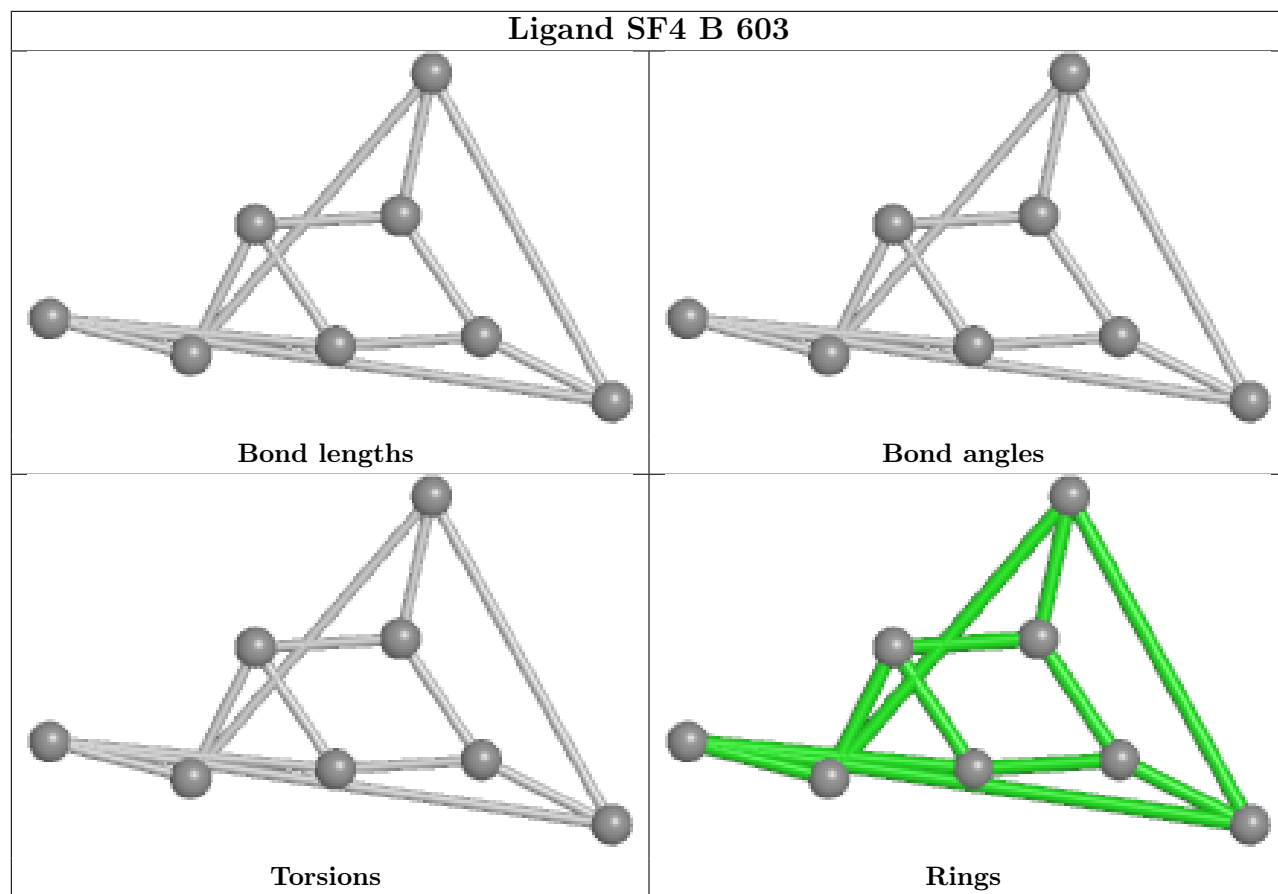
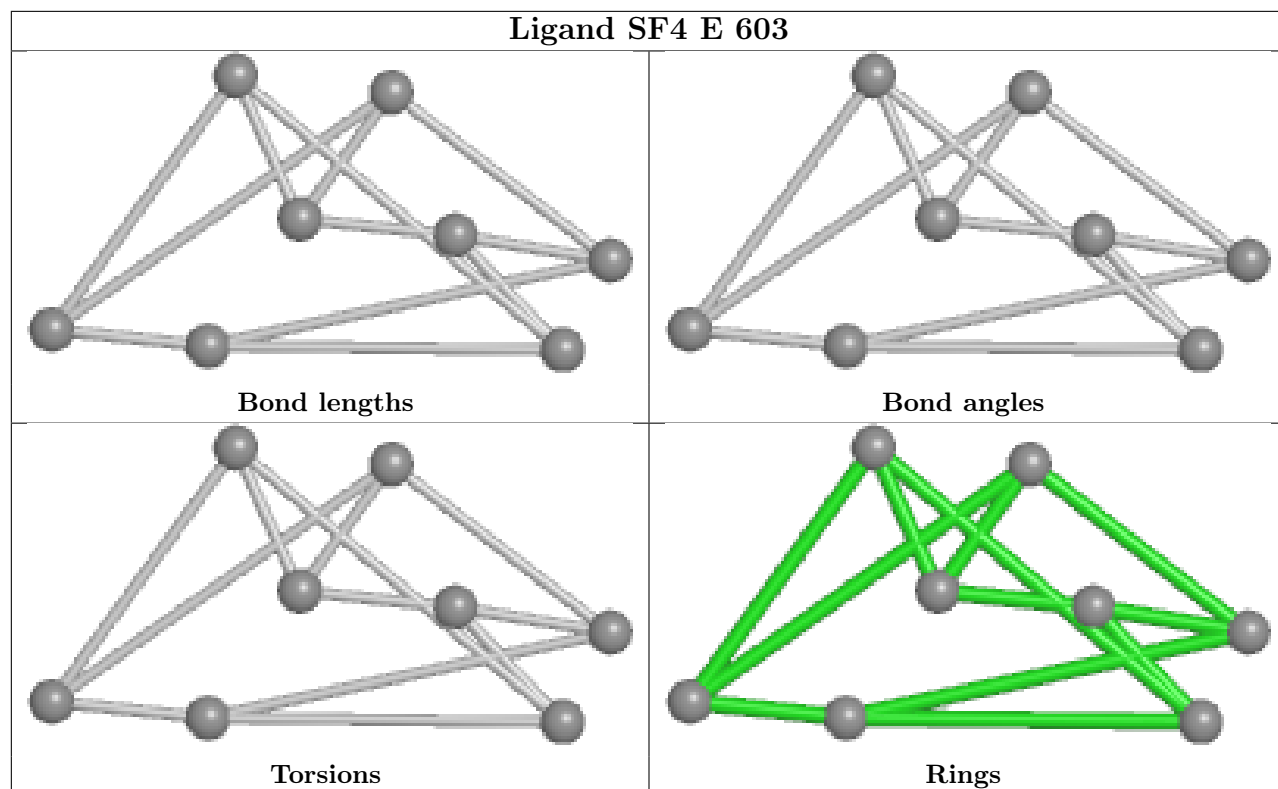


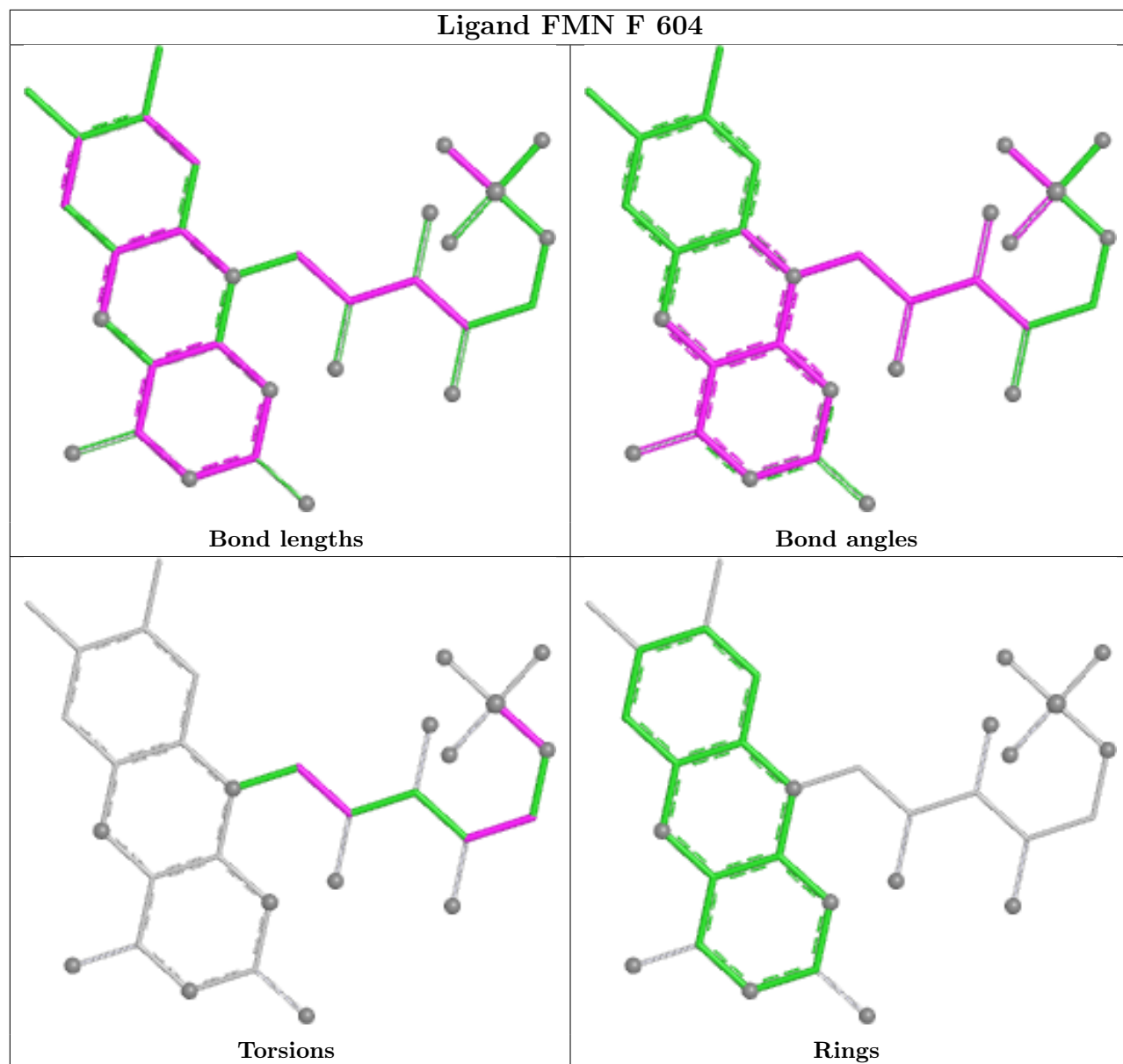


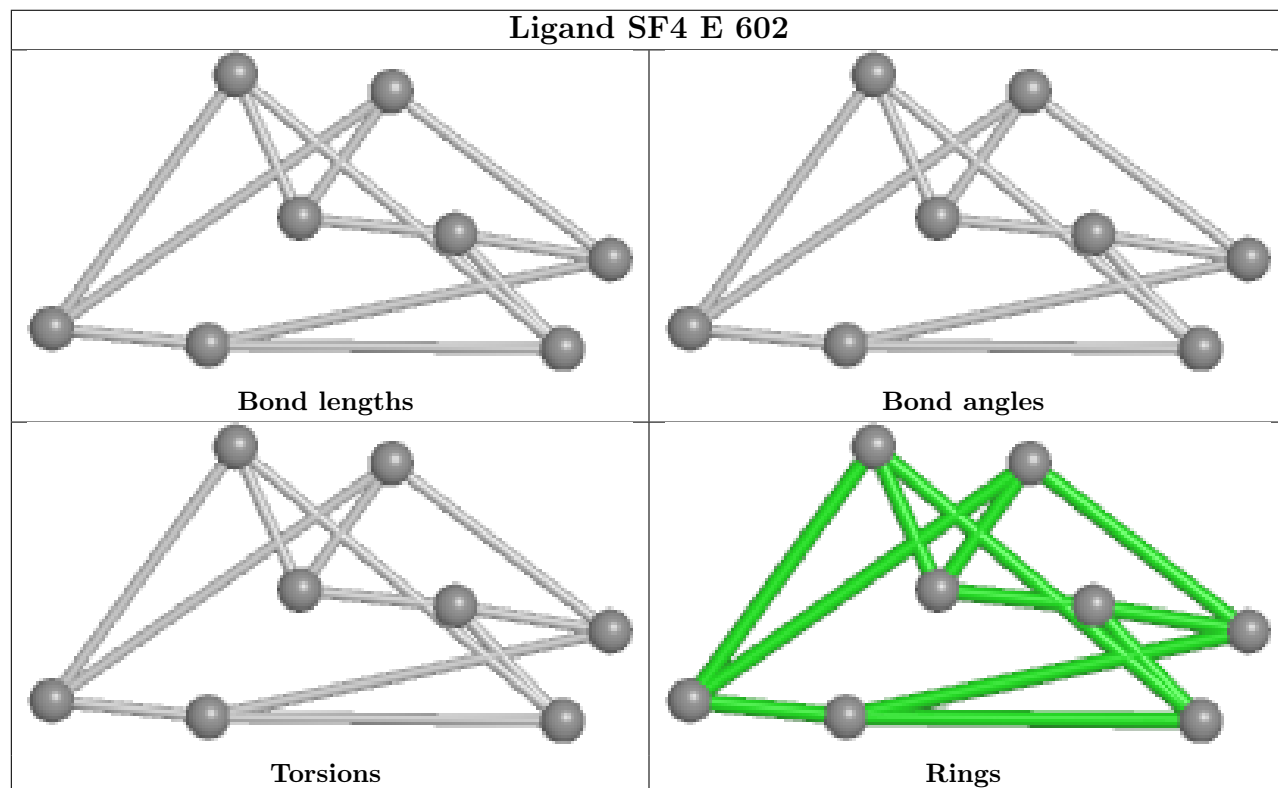
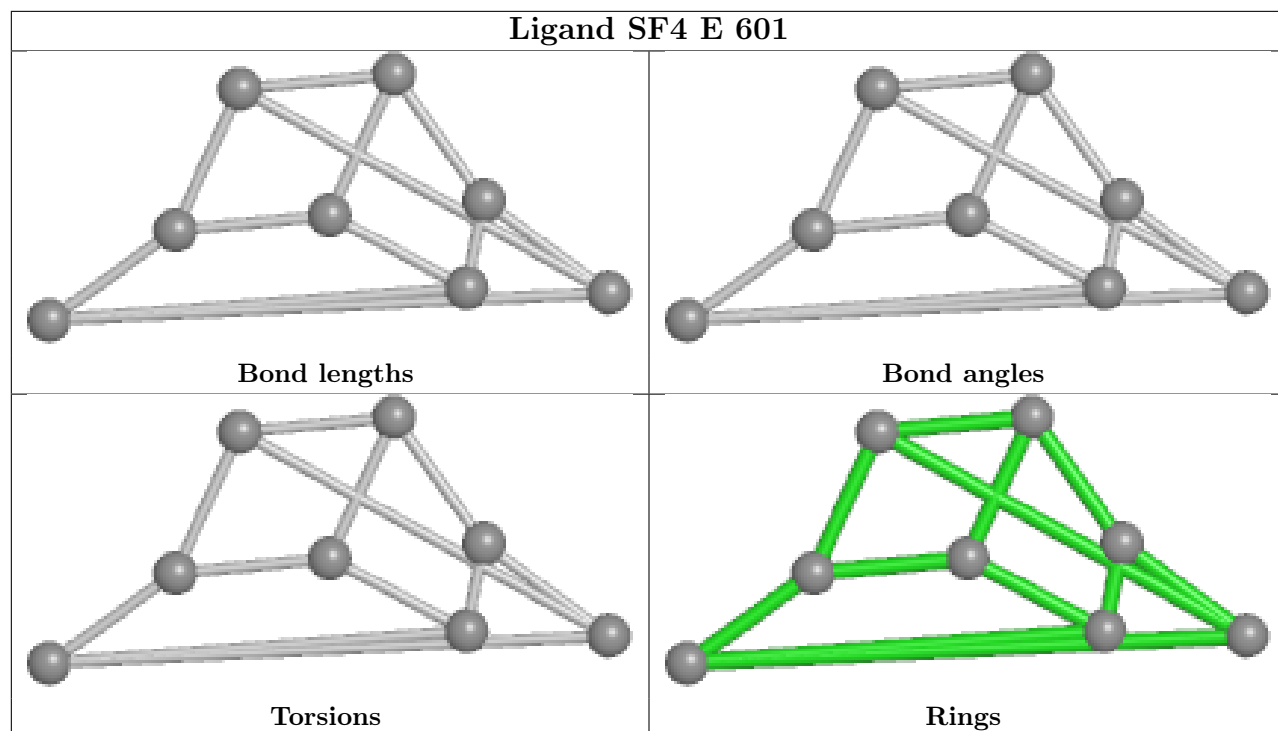


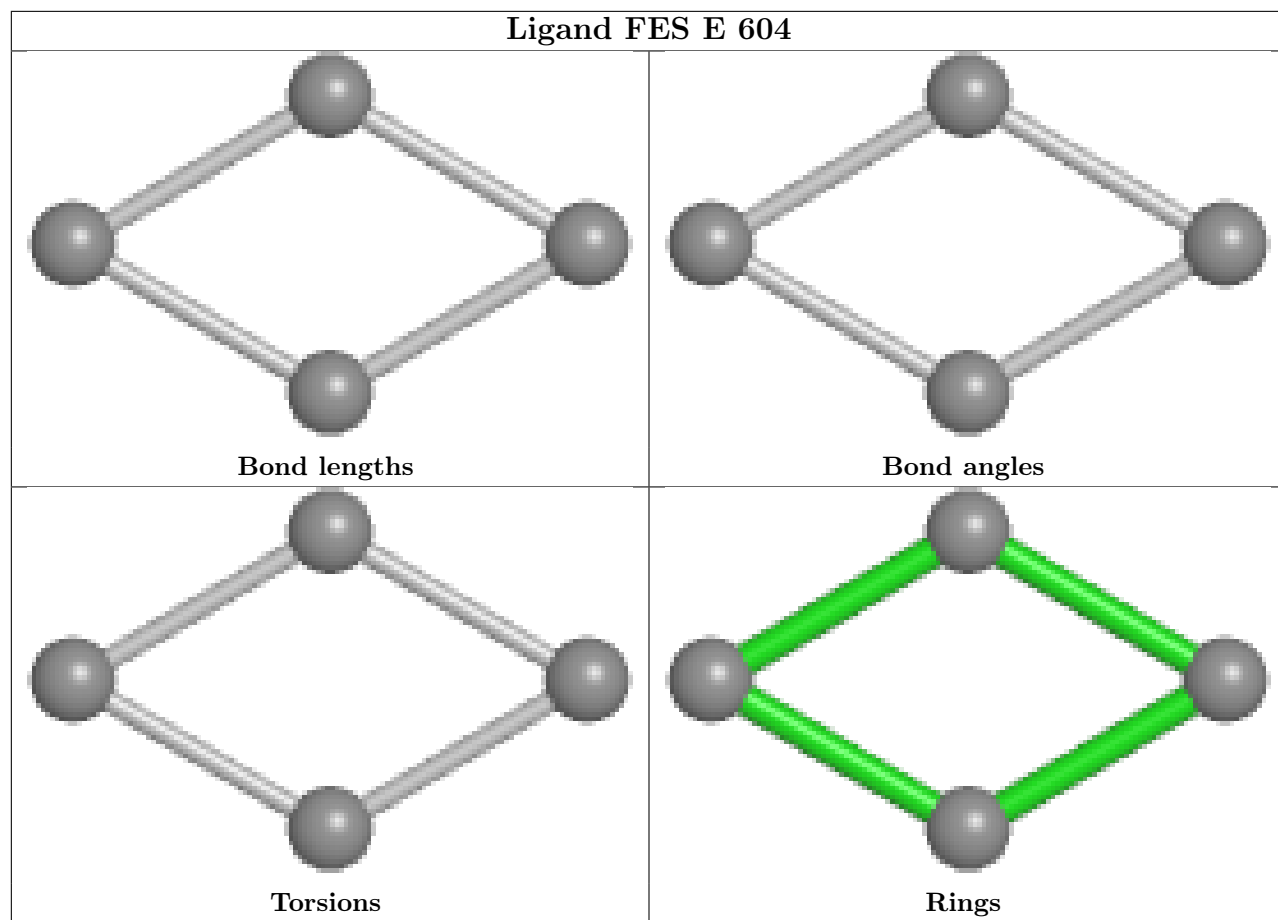


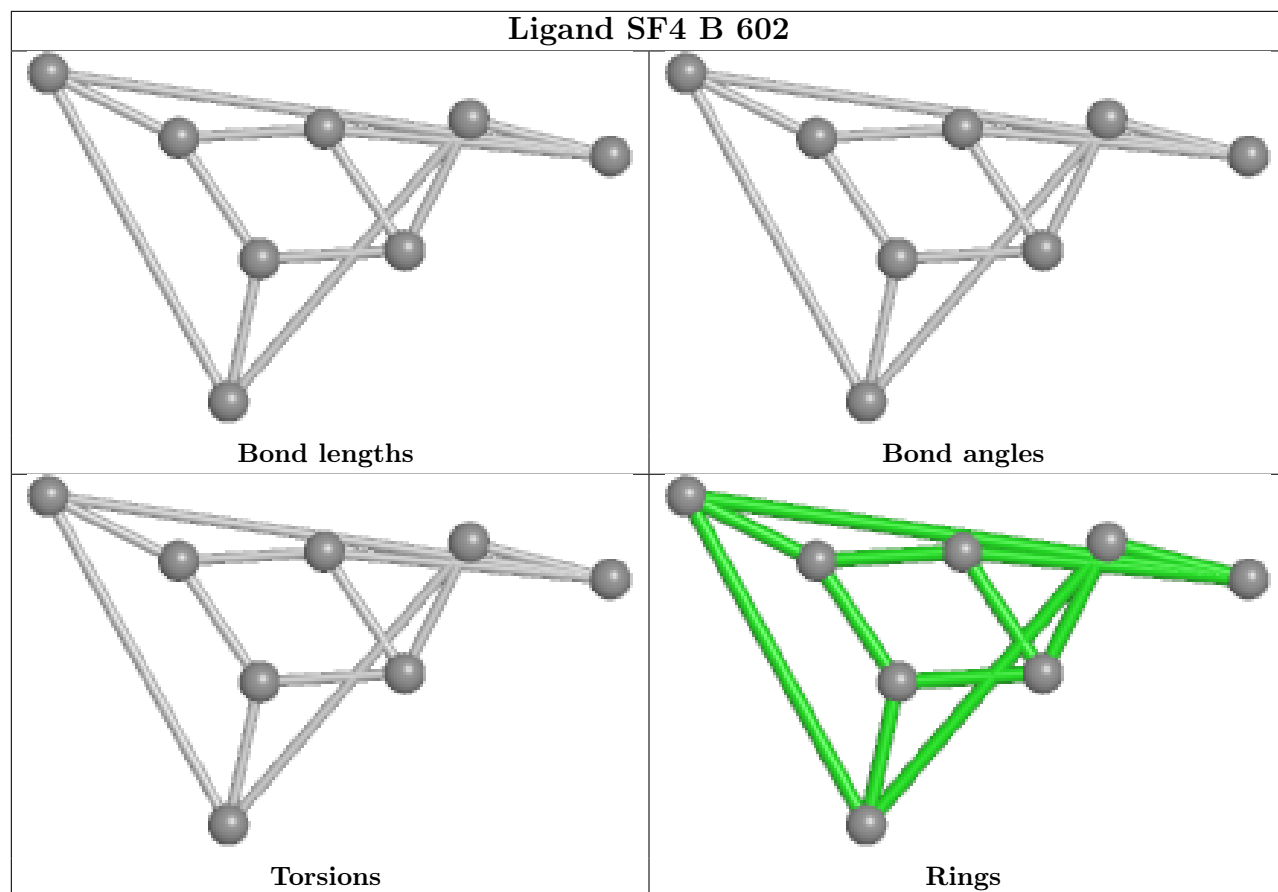


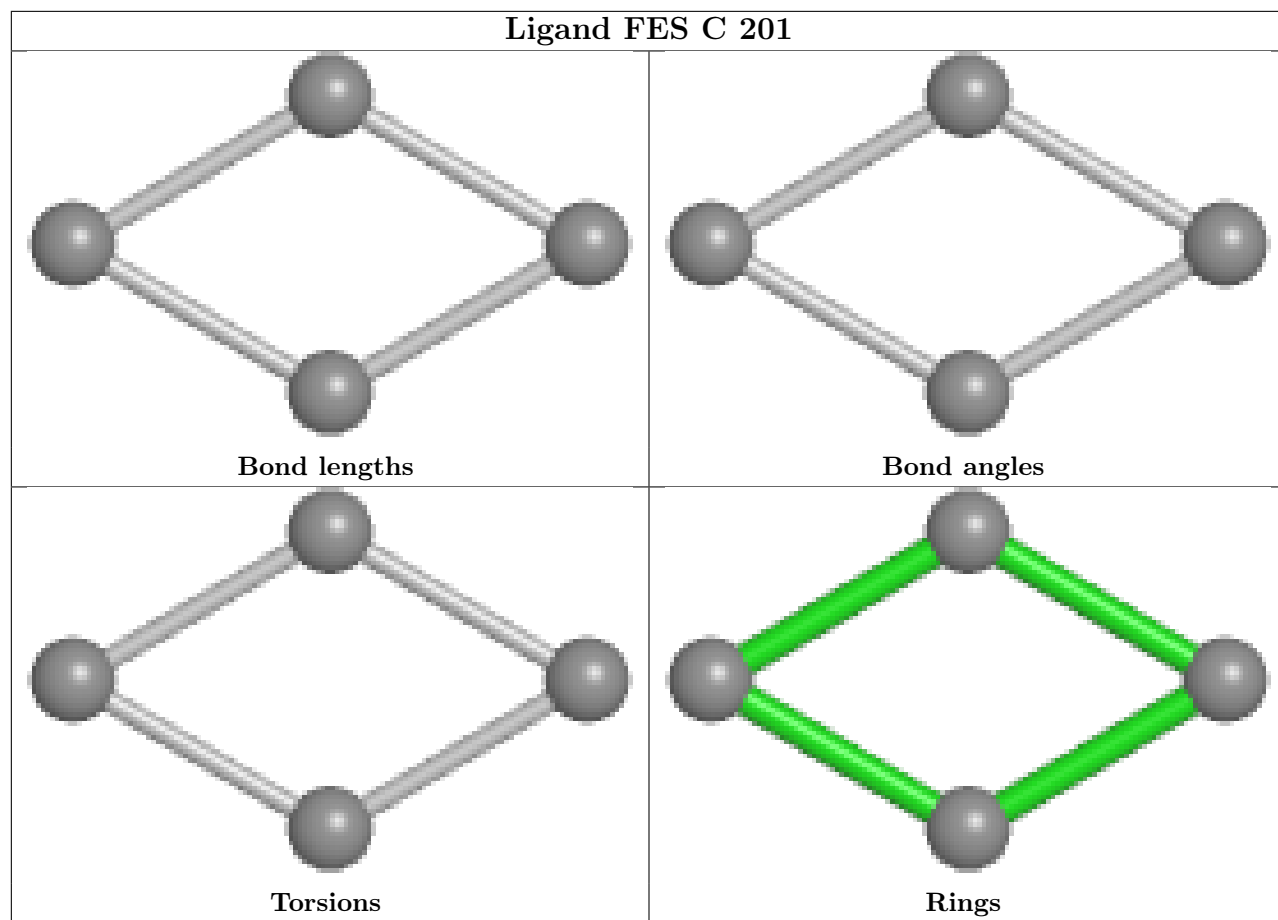


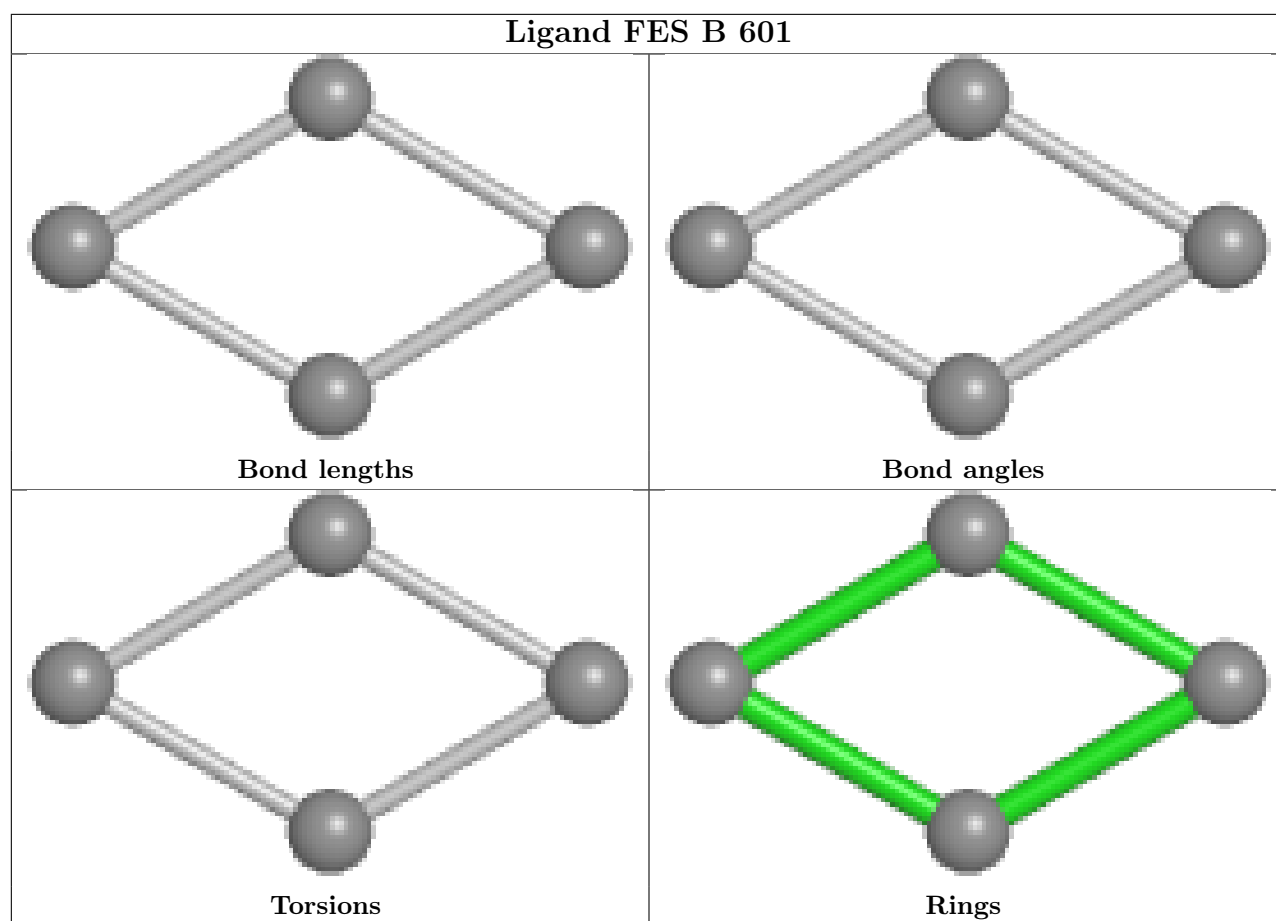












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

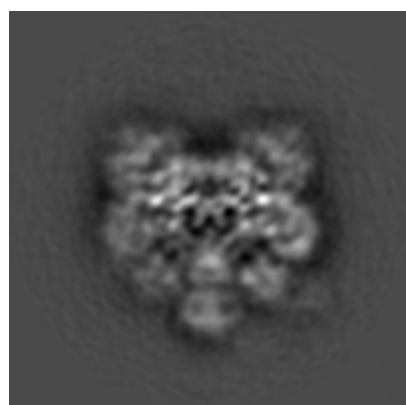
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13818. These allow visual inspection of the internal detail of the map and identification of artifacts.

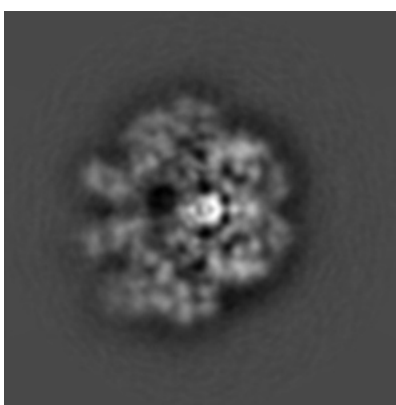
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

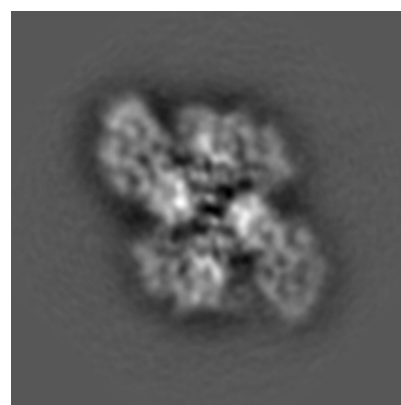
6.1.1 Primary map



X



Y

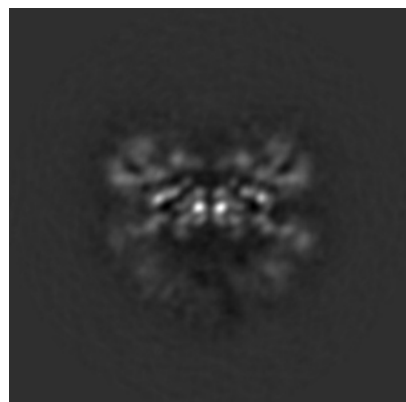


Z

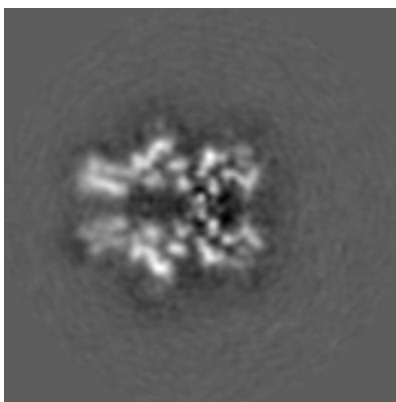
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

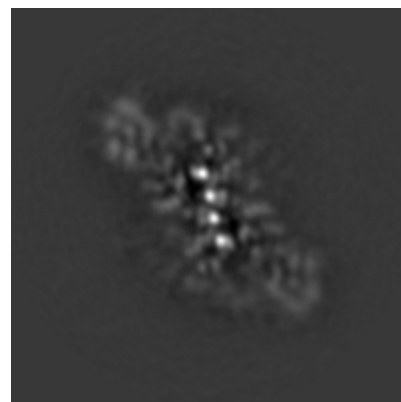
6.2.1 Primary map



X Index: 100



Y Index: 100

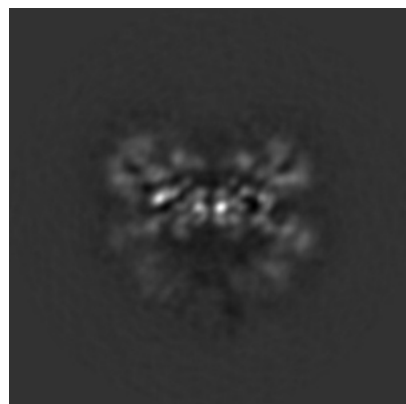


Z Index: 100

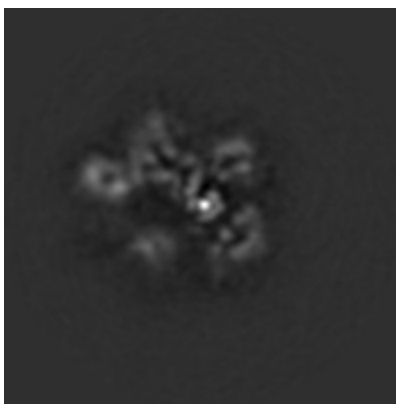
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

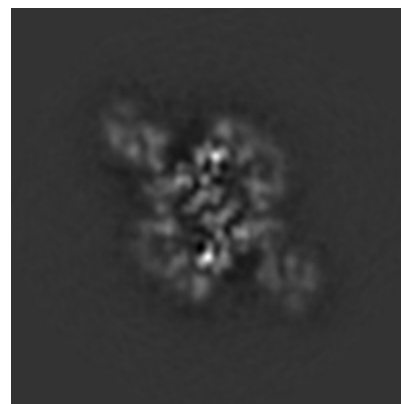
6.3.1 Primary map



X Index: 99



Y Index: 94

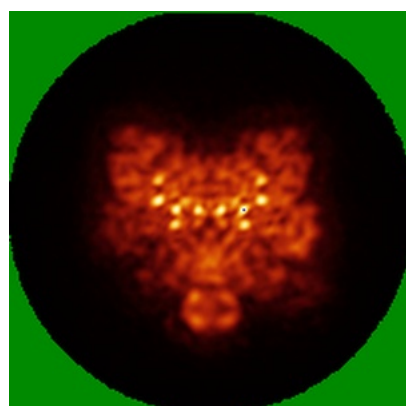


Z Index: 105

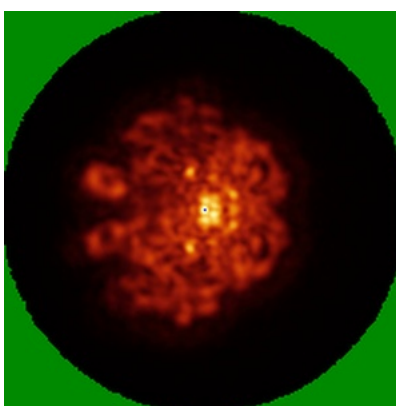
The images above show the largest variance slices of the map in three orthogonal directions.

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

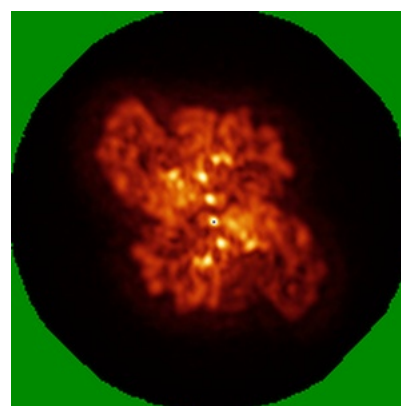
6.4.1 Primary map



X



Y

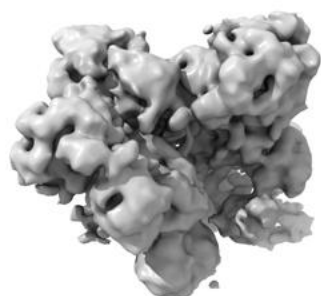


Z

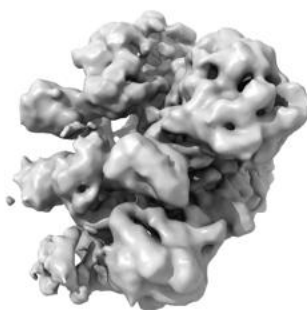
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

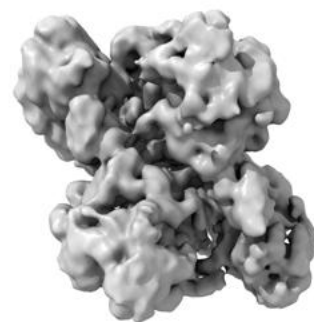
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.00114. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

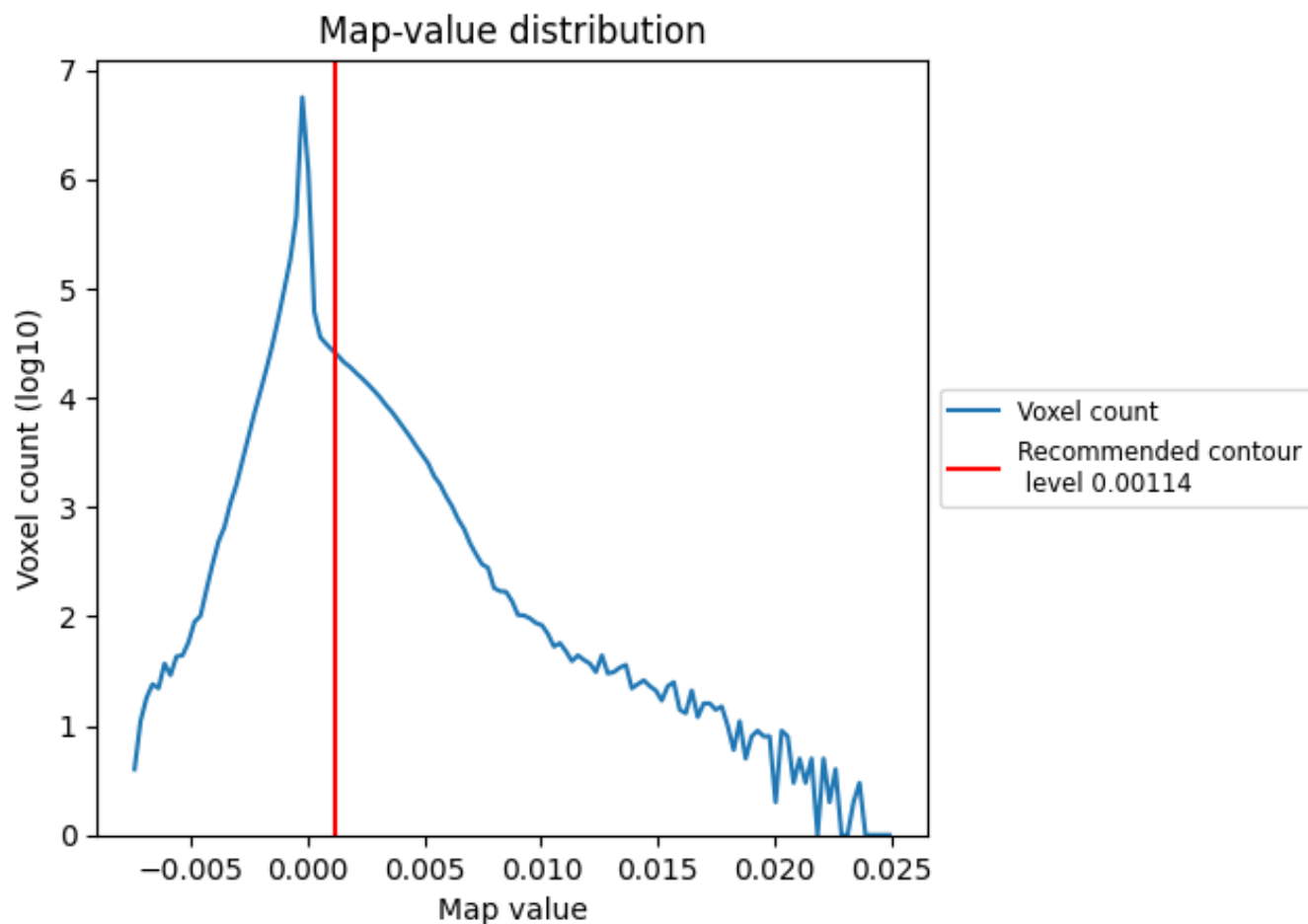
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

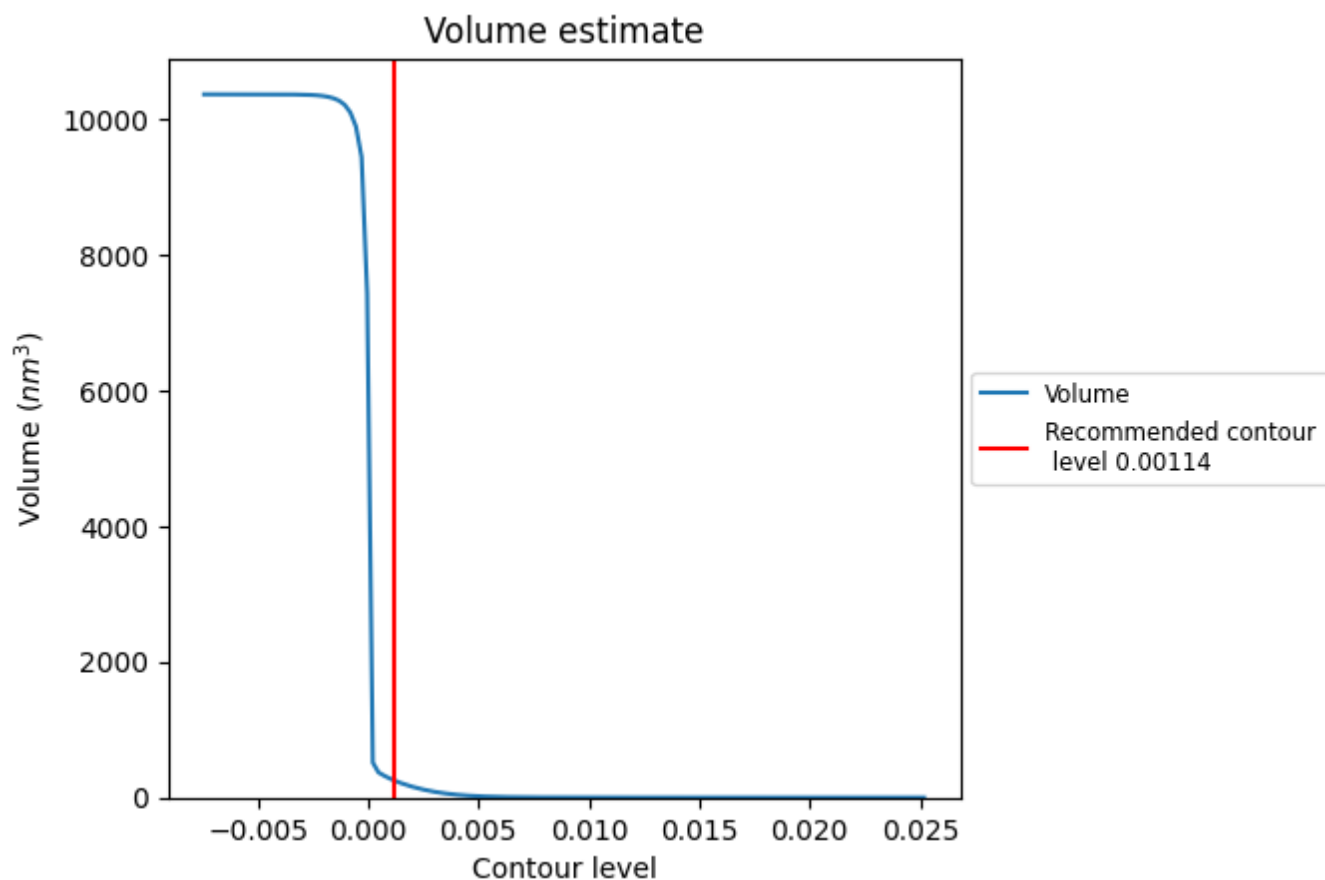
This section contains the results of statistical analysis of the map.

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.

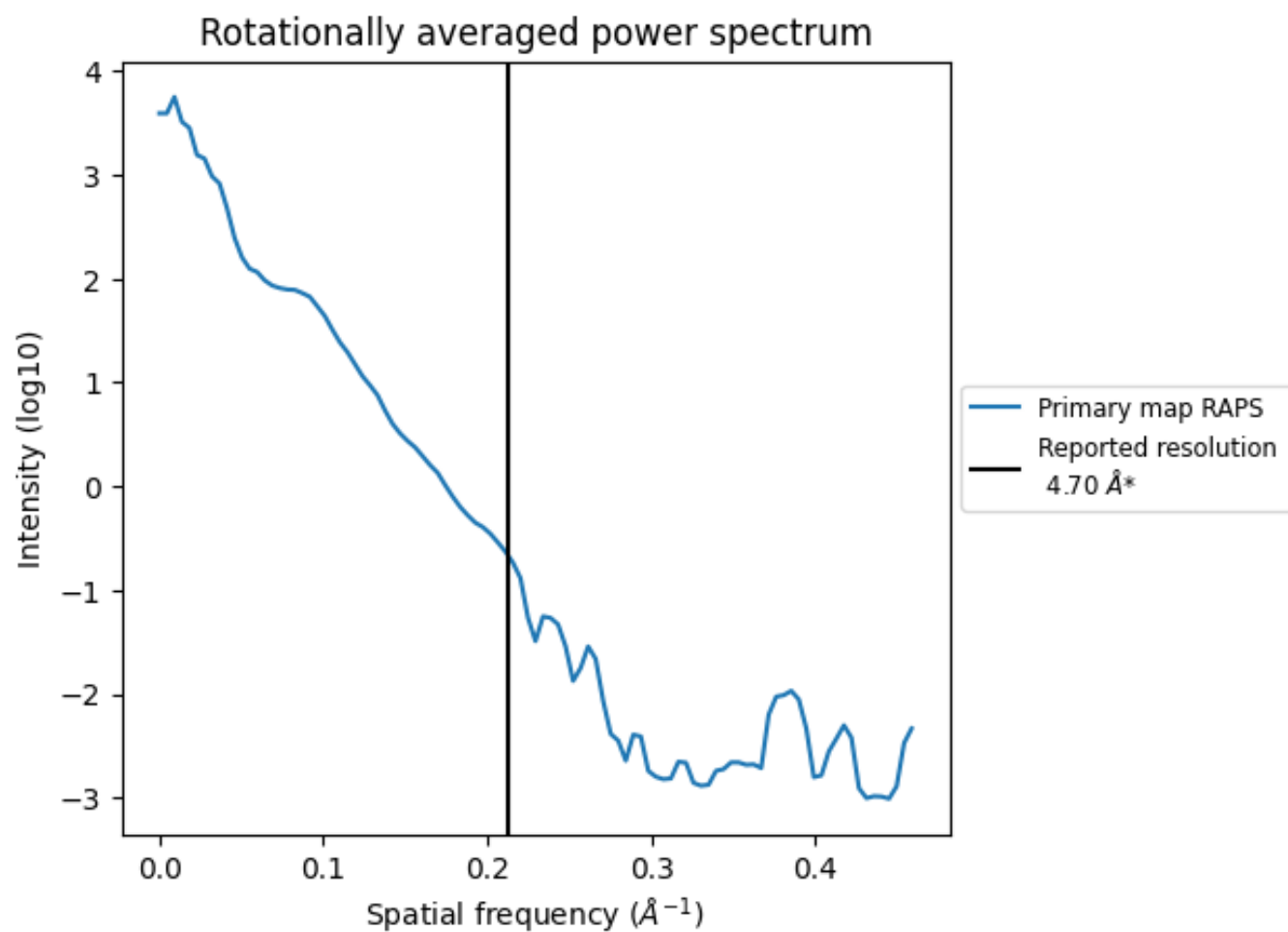
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 259 nm³; this corresponds to an approximate mass of 234 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 0.213 Å⁻¹

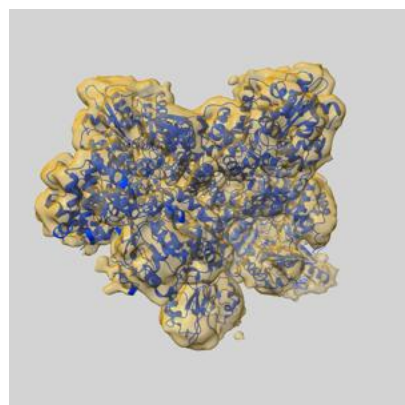
8 Fourier-Shell correlation ⓘ

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

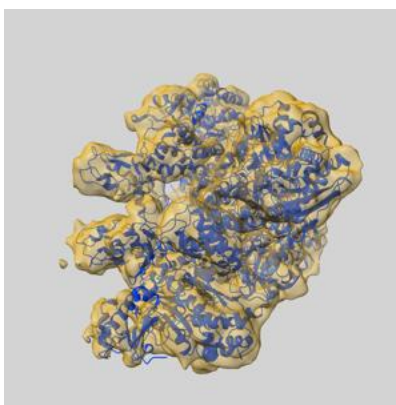
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-13818 and PDB model 7Q4V. Per-residue inclusion information can be found in section [3](#) on page [8](#).

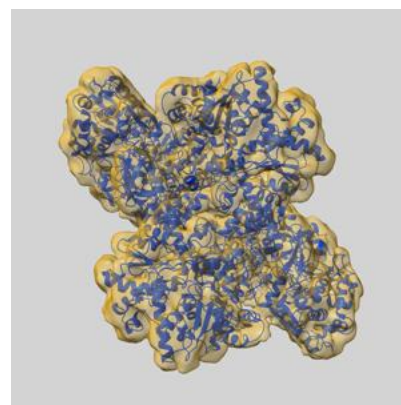
9.1 Map-model overlay [i](#)



X



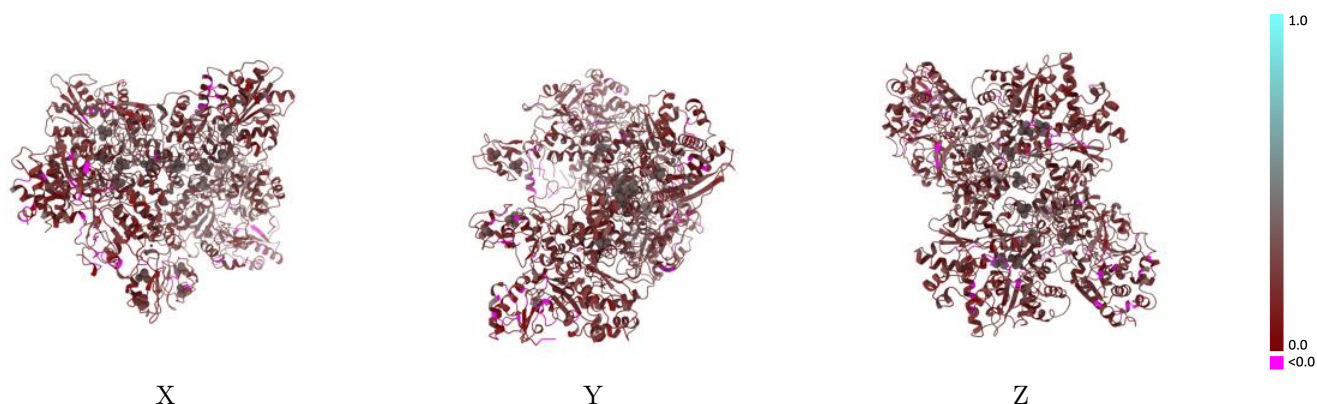
Y



Z

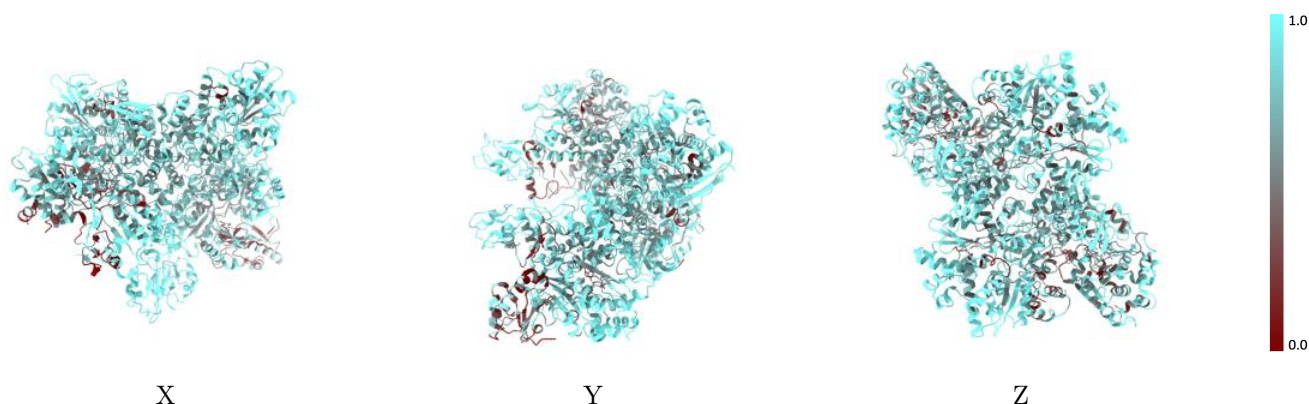
The images above show the 3D surface view of the map at the recommended contour level 0.00114 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



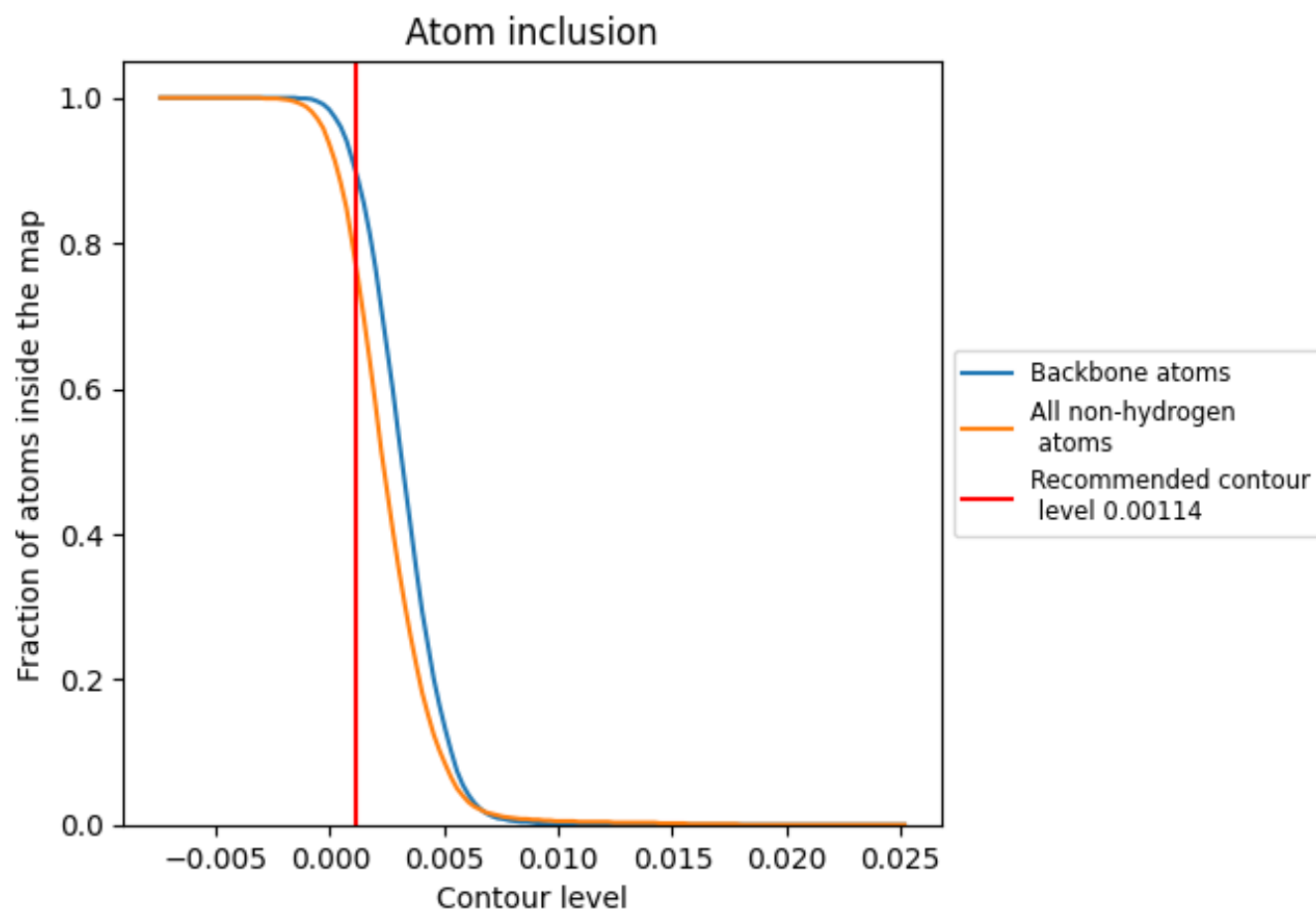
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00114).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 77% 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 (0.00114) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7700	0.2110
A	0.8070	0.2400
B	0.7520	0.1860
C	0.7710	0.2090
E	0.8230	0.2340
F	0.7660	0.1970
G	0.4600	0.1530

1.0

0.0

<0.0