



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 03:22 AM UTC

PDB ID : 9NF0 / pdb_00009nf0
EMDB ID : EMD-49341
Title : Structure of the NADPH-bound *Pyrococcus furiosus* SHI complex
Authors : Xiao, X.; Li, H.
Deposited on : 2025-02-20
Resolution : 3.06 Å (reported)
Based on initial model : .

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

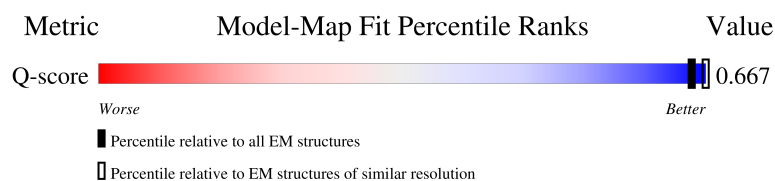
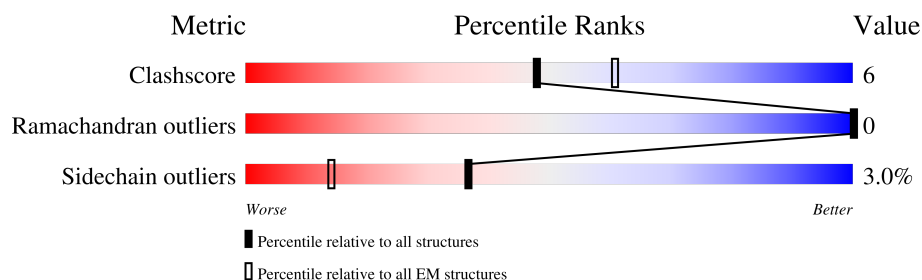
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.06 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	13976 (2.56 - 3.56)

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	261	
1	E	261	
2	B	367	
2	F	367	

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Mol	Chain	Length	Quality of chain
3	C	292	 78% 22%
3	G	292	 79% 21%
4	D	428	 78% 18% ..
4	H	428	 77% 21% ..

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	B	403	-	-	X	-
5	SF4	F	404	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 21344 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 Sulphydrogenase 1 subunit delta.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	255	Total	C	N	O	S	0	0
			2006	1290	327	369	20		
1	E	255	Total	C	N	O	S	0	0
			2006	1290	327	369	20		

- Molecule 2 is a protein called Sulphydrogenase 1 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	339	Total	C	N	O	S	0	0
			2841	1824	487	508	22		
2	F	339	Total	C	N	O	S	0	0
			2841	1824	487	508	22		

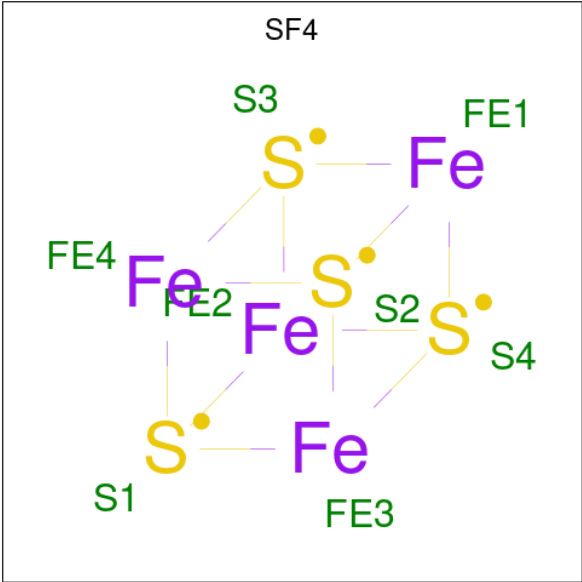
- Molecule 3 is a protein called Sulphydrogenase 1 subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	292	Total	C	N	O	S	0	0
			2325	1505	391	412	17		
3	G	292	Total	C	N	O	S	0	0
			2325	1505	391	412	17		

- Molecule 4 is a protein called Sulphydrogenase 1 subunit alpha.

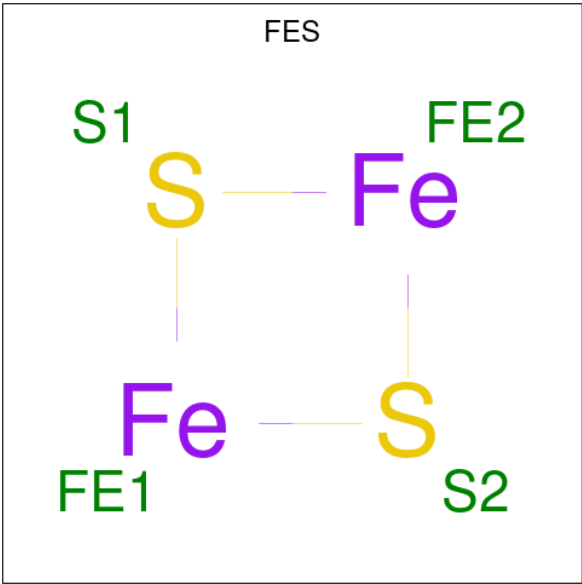
Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	419	Total	C	N	O	S	0	0
			3324	2140	554	615	15		
4	H	420	Total	C	N	O	S	0	0
			3336	2149	555	617	15		

- Molecule 5 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄) (labeled as "Ligand of Interest" by depositor).



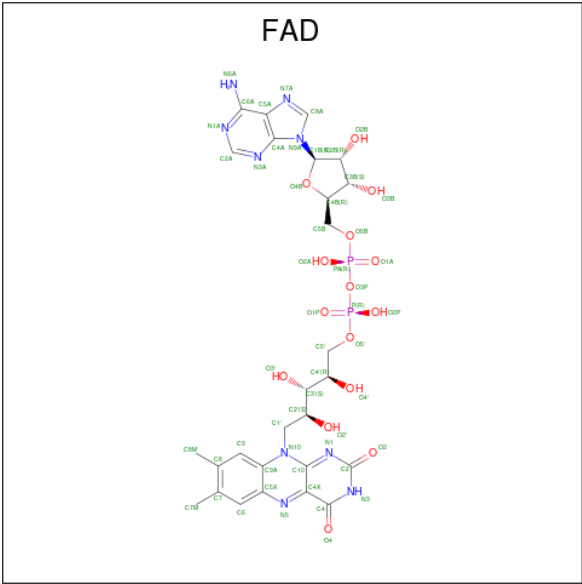
Mol	Chain	Residues	Atoms			AltConf
5	A	1	Total	Fe	S	0
			8	4	4	
5	A	1	Total	Fe	S	
			8	4	4	
5	A	1	Total	Fe	S	0
			8	4	4	
5	B	1	Total	Fe	S	
			8	4	4	
5	B	1	Total	Fe	S	0
			8	4	4	
5	B	1	Total	Fe	S	
			8	4	4	
5	B	1	Total	Fe	S	0
			8	4	4	
5	E	1	Total	Fe	S	
			8	4	4	
5	E	1	Total	Fe	S	0
			8	4	4	
5	E	1	Total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

- Molecule 6 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



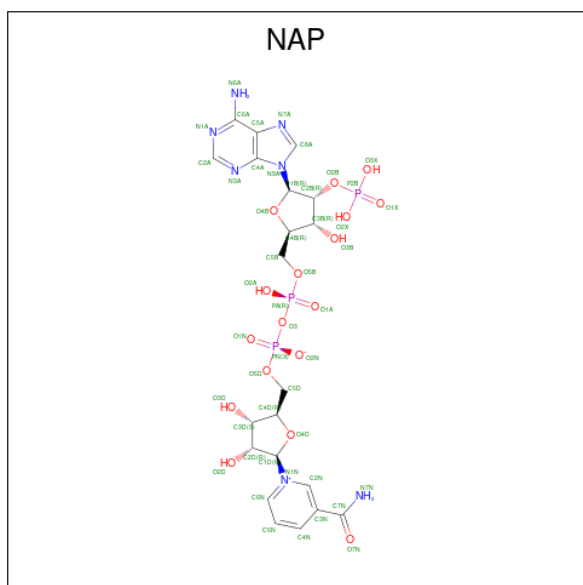
Mol	Chain	Residues	Atoms			AltConf
6	C	1	Total	Fe	S	0
			4	2	2	
6	G	1	Total	Fe	S	0
			4	2	2	

- Molecule 7 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $\text{C}_{27}\text{H}_{33}\text{N}_9\text{O}_{15}\text{P}_2$) (labeled as "Ligand of Interest" by depositor).



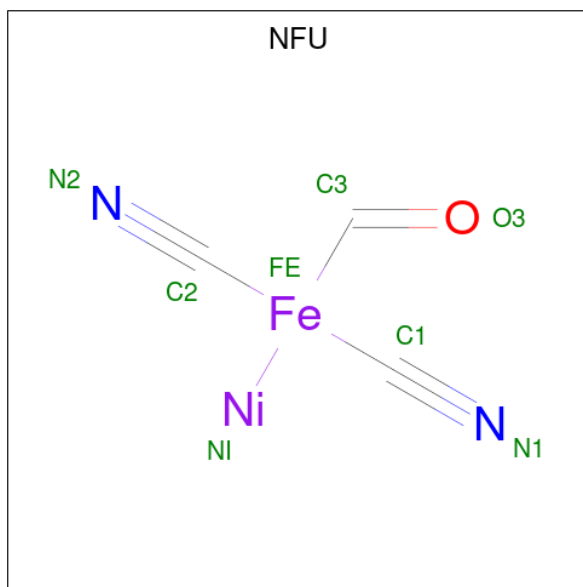
Mol	Chain	Residues	Atoms					AltConf
7	C	1	Total 53	C 27	N 9	O 15	P 2	0
7	G	1	Total 53	C 27	N 9	O 15	P 2	0

- Molecule 8 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
8	C	1	Total 48	C 21	N 7	O 17	P 3	0
8	G	1	Total 48	C 21	N 7	O 17	P 3	0

- Molecule 9 is formyl[bis(hydrocyanato-1kappaC)]ironnickel(Fe-Ni) (CCD ID: NFU) (formula: C₃HFeN₂NiO) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
9	D	1	Total	C	Fe	N	Ni	O	0
			8	3	1	2	1	1	
9	H	1	Total	C	Fe	N	Ni	O	0
			8	3	1	2	1	1	

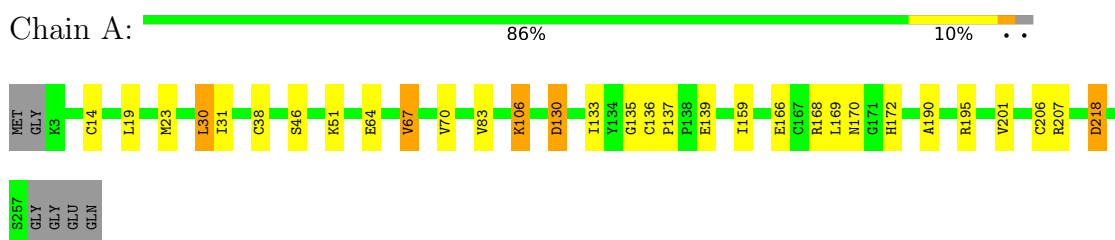
- Molecule 10 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
10	D	1	Total	Mg	0
			1	1	
10	H	1	Total	Mg	0
			1	1	

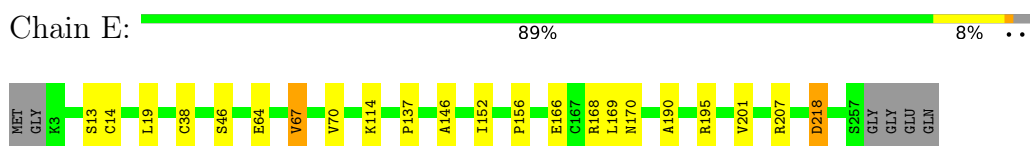
3 Residue-property plots

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

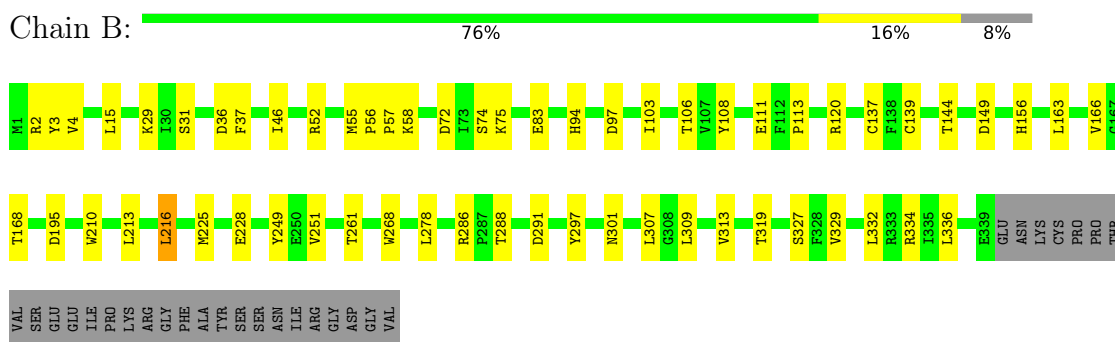
- Molecule 1: Sulphydrogenase 1 subunit delta



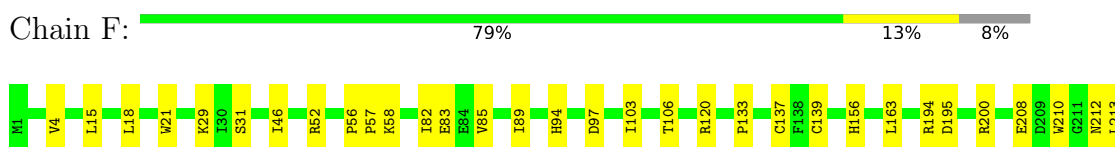
- Molecule 1: Sulphydrogenase 1 subunit delta

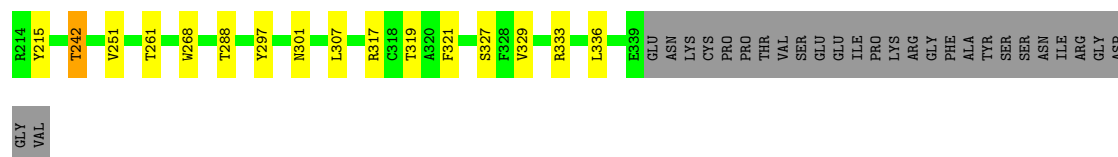


- Molecule 2: Sulphydrogenase 1 subunit beta



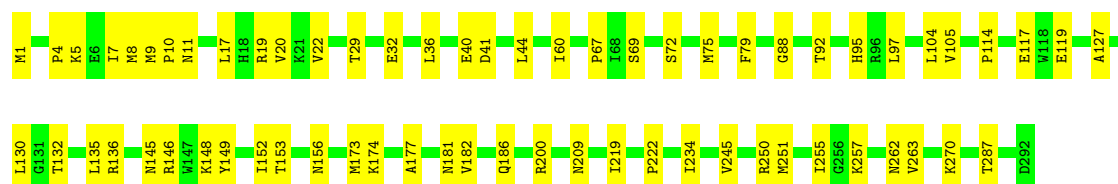
- Molecule 2: Sulphydrogenase 1 subunit beta





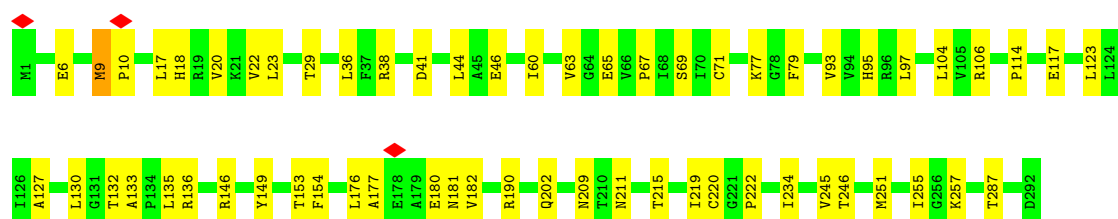
• Molecule 3: Sulfhydrogenase 1 subunit gamma

Chain C: 78% 22%



• Molecule 3: Sulfhydrogenase 1 subunit gamma

Chain G: 79% 21%



• Molecule 4: Sulfhydrogenase 1 subunit alpha

Chain D: 78% 18% ..



• Molecule 4: Sulfhydrogenase 1 subunit alpha

Chain H: 77% 21% ..



K134	R135	E136	I137	E138	I139	K142	L146	G147	T148	M151	S156	R157	A158	I159	H160	Q161	E162	K182	L185	L191	Y224	G225	I226	H260	R275	V276	A280	Q310	E313	Y316	F317	A321	D326	K331	K335	D338	E339	V340	E341	I342	
K343	D344	G345	F346	T350	T351	E352	A353	P354	V359	Y360	A361	L362	K363	G367	Y371	A372	D373	L382	M385	E386	E387	H388	M391	M392	H396	D399	D400	L404	K405	I406	L407	R413	A414	Y415	D416	I419	H424	VAL	VAL	ARG	LEU

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	313849	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	19.719	Depositor
Minimum map value	0.000	Depositor
Average map value	0.044	Depositor
Map value standard deviation	0.581	Depositor
Recommended contour level	0.7	Depositor
Map size (Å)	317.952, 317.952, 317.952	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.828, 0.828, 0.828	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.12	0/2049	0.28	0/2762
1	E	0.13	0/2049	0.31	0/2762
2	B	0.12	0/2917	0.28	0/3929
2	F	0.12	0/2917	0.28	0/3929
3	C	0.12	0/2386	0.27	0/3232
3	G	0.13	0/2386	0.30	0/3232
4	D	0.14	0/3394	0.29	0/4584
4	H	0.14	0/3407	0.29	0/4602
All	All	0.13	0/21505	0.29	0/29032

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2006	0	2002	23	0
1	E	2006	0	2002	13	0
2	B	2841	0	2746	32	0
2	F	2841	0	2746	26	0
3	C	2325	0	2348	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	2325	0	2348	30	0
4	D	3324	0	3355	47	0
4	H	3336	0	3364	57	0
5	A	24	0	0	2	0
5	B	32	0	0	2	0
5	E	24	0	0	1	0
5	F	32	0	0	2	0
6	C	4	0	0	0	0
6	G	4	0	0	0	0
7	C	53	0	31	1	0
7	G	53	0	31	1	0
8	C	48	0	23	4	0
8	G	48	0	25	4	0
9	D	8	0	0	0	0
9	H	8	0	0	0	0
10	D	1	0	0	0	0
10	H	1	0	0	0	0
All	All	21344	0	21021	249	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 6.

All (249) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:301:SF4:S1	4:D:160:HIS:CD2	2.72	0.83
1:A:168:ARG:NH2	1:A:172:HIS:O	2.23	0.71
4:H:43:ARG:NH2	4:H:63:ARG:O	2.27	0.68
4:D:226:ILE:HG22	4:D:351:THR:HG22	1.77	0.67
1:A:168:ARG:NH1	5:A:303:SF4:S3	2.69	0.66
4:H:310:GLN:NE2	4:H:416:ASP:OD2	2.28	0.66
3:C:174:LYS:HA	3:C:177:ALA:HB3	1.78	0.64
4:H:18:GLY:HA3	4:H:419:ILE:HB	1.80	0.64
2:F:208:GLU:OE2	2:F:333:ARG:NH1	2.30	0.63
4:D:310:GLN:NE2	4:D:416:ASP:OD2	2.30	0.63
2:B:94:HIS:ND1	5:B:403:SF4:S2	2.72	0.62
2:F:52:ARG:NH2	2:F:137:CYS:SG	2.72	0.62
4:H:14:ALA:O	4:H:413:ARG:NH1	2.33	0.62
4:H:89:ARG:NH2	4:H:335:LYS:O	2.32	0.62
4:H:104:MET:HE3	4:H:354:PRO:HA	1.82	0.61
1:E:195:ARG:HD3	4:H:156:SER:HB3	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:177:ALA:HB1	3:C:182:VAL:HB	1.83	0.61
2:B:83:GLU:OE2	2:B:120:ARG:NH2	2.34	0.61
1:E:146:ALA:HA	1:E:156:PRO:HG3	1.83	0.61
3:G:46:GLU:OE1	3:G:77:LYS:NZ	2.34	0.61
2:B:52:ARG:NH2	2:B:137:CYS:SG	2.74	0.60
3:G:176:LEU:O	3:G:180:GLU:HB2	2.01	0.60
1:E:38:CYS:HA	1:E:46:SER:HB2	1.82	0.60
4:D:14:ALA:O	4:D:413:ARG:NH1	2.35	0.60
1:A:169:LEU:HD11	2:B:268:TRP:HB2	1.83	0.60
3:C:219:ILE:HB	3:C:245:VAL:HG12	1.84	0.59
3:G:130:LEU:H	8:G:303:NAP:H51N	1.67	0.59
2:B:156:HIS:HB2	2:B:163:LEU:HB3	1.84	0.59
4:H:275:ARG:HD3	4:H:352:GLU:HG2	1.84	0.59
3:C:19:ARG:NH1	3:C:40:GLU:OE1	2.36	0.59
3:G:146:ARG:NH1	3:G:149:TYR:O	2.35	0.58
3:G:219:ILE:HB	3:G:245:VAL:HG12	1.85	0.58
4:H:65:CYS:SG	4:H:66:SER:N	2.77	0.58
3:G:125:LEU:HB2	3:G:154:PHE:HD1	1.68	0.58
2:B:139:CYS:HB3	5:B:403:SF4:S4	2.42	0.58
4:D:275:ARG:HH11	4:D:352:GLU:HG3	1.67	0.58
3:G:41:ASP:HB3	3:G:44:LEU:HB3	1.85	0.58
3:C:41:ASP:HB3	3:C:44:LEU:HB3	1.85	0.58
4:D:146:LEU:HD21	4:D:185:LEU:HD23	1.86	0.57
3:G:71:CYS:HB3	3:G:133:ALA:HB1	1.85	0.57
4:D:104:MET:HG3	4:D:354:PRO:HG3	1.85	0.57
4:D:101:ILE:HG21	4:D:321:ALA:HB2	1.86	0.57
1:A:218:ASP:OD1	1:A:218:ASP:N	2.34	0.57
2:F:83:GLU:OE2	2:F:120:ARG:NH2	2.38	0.57
3:G:132:THR:O	3:G:136:ARG:N	2.37	0.56
3:C:20:VAL:HG21	3:C:105:VAL:HB	1.87	0.56
2:F:156:HIS:HB2	2:F:163:LEU:HB3	1.87	0.56
4:H:275:ARG:HH11	4:H:352:GLU:HG3	1.69	0.56
4:H:344:ASP:OD1	4:H:344:ASP:N	2.38	0.56
2:B:288:THR:OG1	2:B:291:ASP:OD1	2.24	0.56
1:E:14:CYS:HB3	4:H:43:ARG:HH22	1.71	0.56
1:E:169:LEU:HD21	2:F:268:TRP:HB2	1.87	0.56
2:B:228:GLU:OE2	2:B:334:ARG:NH1	2.38	0.56
4:D:15:ARG:HH21	4:D:119:ASP:HB3	1.70	0.56
4:H:104:MET:HG2	4:H:354:PRO:HG3	1.88	0.56
4:D:101:ILE:HG23	4:D:317:PHE:HB3	1.87	0.55
1:E:166:GLU:O	1:E:170:ASN:ND2	2.34	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:146:LEU:HD21	4:H:185:LEU:HD23	1.88	0.55
1:A:139:GLU:OE2	1:A:195:ARG:NH2	2.32	0.55
1:A:14:CYS:SG	4:D:160:HIS:CE1	3.00	0.55
4:H:148:THR:HG23	4:H:158:ALA:HB2	1.88	0.55
2:F:297:TYR:O	2:F:301:ASN:ND2	2.35	0.55
4:H:89:ARG:NH1	4:H:338:ASP:OD1	2.40	0.55
1:E:218:ASP:OD1	1:E:218:ASP:N	2.33	0.55
3:C:67:PRO:HG3	3:C:251:MET:HB2	1.90	0.54
3:G:6:GLU:O	3:G:18:HIS:NE2	2.38	0.54
3:C:130:LEU:H	8:C:303:NAP:H51N	1.72	0.54
3:G:222:PRO:HG2	8:G:303:NAP:H52A	1.90	0.54
4:H:101:ILE:HG21	4:H:321:ALA:HB2	1.90	0.54
3:C:130:LEU:O	8:C:303:NAP:N7N	2.39	0.54
2:B:15:LEU:HD13	2:B:46:ILE:HD12	1.89	0.54
3:C:127:ALA:HB2	3:C:135:LEU:HD12	1.90	0.54
3:G:17:LEU:HB3	3:G:104:LEU:HB3	1.88	0.54
4:D:224:TYR:HB3	4:D:316:TYR:CZ	2.43	0.53
4:D:17:GLU:HB3	4:D:418:CYS:HA	1.90	0.53
4:D:344:ASP:OD1	4:D:344:ASP:N	2.40	0.53
4:H:59:ALA:O	4:H:63:ARG:NH1	2.41	0.53
4:H:363:LYS:HB3	4:H:371:TYR:HB3	1.90	0.53
4:D:8:ILE:HD12	4:D:404:LEU:HD23	1.91	0.53
4:D:75:THR:HG22	4:D:360:TYR:HB2	1.91	0.53
2:B:216:LEU:HD23	2:B:336:LEU:HA	1.90	0.53
3:G:255:ILE:HG13	3:G:257:LYS:HG2	1.91	0.53
4:D:361:ALA:HB3	4:D:373:ASP:HB3	1.89	0.53
4:H:90:GLU:OE1	4:H:331:LYS:NZ	2.42	0.53
2:F:242:THR:HG22	2:F:317:ARG:HD3	1.91	0.53
3:C:60:ILE:HD11	3:C:97:LEU:HD11	1.90	0.53
3:G:67:PRO:HG3	3:G:251:MET:HB2	1.90	0.53
3:C:156:ASN:HB3	3:C:186:GLN:HG2	1.90	0.52
4:D:18:GLY:HA3	4:D:419:ILE:HB	1.91	0.52
4:D:350:THR:HG22	4:D:359:VAL:HG22	1.91	0.52
2:F:15:LEU:HD13	2:F:46:ILE:HD12	1.92	0.52
3:G:60:ILE:HD11	3:G:97:LEU:HD11	1.91	0.52
3:C:114:PRO:HB2	3:C:117:GLU:HG2	1.92	0.52
1:A:38:CYS:HA	1:A:46:SER:HB2	1.92	0.52
1:A:137:PRO:HG3	4:D:159:ILE:HB	1.92	0.52
3:C:17:LEU:HB3	3:C:104:LEU:HB3	1.91	0.52
4:D:148:THR:HG23	4:D:158:ALA:HB2	1.91	0.51
4:H:361:ALA:HB3	4:H:373:ASP:HB3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:249:TYR:HE2	3:C:257:LYS:HB3	1.75	0.51
1:A:166:GLU:O	1:A:170:ASN:ND2	2.34	0.51
4:D:139:ILE:HG13	4:D:191:LEU:HD22	1.93	0.51
4:D:342:ILE:HG21	4:D:367:GLY:HA2	1.92	0.51
4:D:260:HIS:NE2	4:D:386:GLU:OE2	2.44	0.51
1:E:19:LEU:HD11	4:H:110:LEU:HD21	1.93	0.51
2:F:94:HIS:ND1	5:F:404:SF4:S4	2.82	0.51
3:G:130:LEU:HB3	8:G:303:NAP:H2D	1.93	0.51
2:B:297:TYR:O	2:B:301:ASN:ND2	2.37	0.50
4:D:59:ALA:O	4:D:63:ARG:NH1	2.44	0.50
4:H:224:TYR:HB3	4:H:316:TYR:CZ	2.46	0.50
3:C:132:THR:O	3:C:136:ARG:N	2.42	0.50
3:G:114:PRO:HB2	3:G:117:GLU:HG2	1.92	0.50
4:H:182:LYS:NZ	4:H:326:ASP:OD1	2.43	0.50
4:D:276:VAL:O	4:D:280:ALA:HB2	2.12	0.49
3:C:4:PRO:HA	3:C:7:ILE:HG22	1.94	0.49
4:H:350:THR:HG22	4:H:359:VAL:HG22	1.93	0.49
2:B:2:ARG:HB3	2:B:166:VAL:HB	1.93	0.49
4:D:207:GLU:OE1	4:D:207:GLU:N	2.44	0.49
4:D:13:ILE:HD11	4:D:22:VAL:HG13	1.94	0.49
4:H:67:PHE:O	4:H:107:SER:OG	2.30	0.48
2:F:210:TRP:HH2	2:F:329:VAL:HG23	1.78	0.48
4:H:15:ARG:HH21	4:H:119:ASP:HB3	1.79	0.48
2:B:286:ARG:NH1	3:C:262:ASN:OD1	2.47	0.48
4:D:388:HIS:HA	4:D:391:MET:HG2	1.94	0.48
2:F:319:THR:HG23	2:F:327:SER:HA	1.95	0.48
3:G:9:MET:HG3	3:G:10:PRO:HD2	1.95	0.48
3:G:190:ARG:NE	8:G:303:NAP:O3X	2.46	0.48
4:H:139:ILE:HG13	4:H:191:LEU:HB3	1.95	0.48
4:D:111:HIS:NE2	4:D:416:ASP:OD1	2.47	0.48
1:E:137:PRO:HG3	4:H:159:ILE:HB	1.94	0.48
4:D:275:ARG:HE	4:D:313:GLU:CD	2.21	0.48
3:G:177:ALA:HB1	3:G:182:VAL:HB	1.96	0.48
1:A:19:LEU:HD11	4:D:110:LEU:HD21	1.96	0.48
2:B:74:SER:O	2:B:75:LYS:HG3	2.14	0.48
4:H:101:ILE:HG23	4:H:317:PHE:HB3	1.95	0.48
4:H:49:THR:HG22	4:H:60:ILE:HD11	1.96	0.48
3:C:153:THR:OG1	3:C:209:ASN:OD1	2.31	0.48
4:H:388:HIS:HA	4:H:391:MET:HG2	1.96	0.48
3:C:146:ARG:NH1	3:C:149:TYR:O	2.47	0.47
4:D:156:SER:HB3	4:D:163:ASN:HB2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:57:PRO:HG2	2:F:97:ASP:HB3	1.96	0.47
3:G:153:THR:OG1	3:G:209:ASN:OD1	2.32	0.47
2:B:108:TYR:HA	3:C:257:LYS:HE3	1.96	0.47
3:G:36:LEU:HD11	3:G:79:PHE:HB3	1.95	0.47
2:B:57:PRO:HG2	2:B:97:ASP:HB3	1.95	0.47
4:D:45:PHE:HA	4:D:48:ILE:HG12	1.97	0.47
3:C:152:ILE:HB	3:C:182:VAL:HG22	1.97	0.46
3:C:255:ILE:HG13	3:C:257:LYS:HD3	1.97	0.46
2:F:139:CYS:HB3	5:F:404:SF4:S3	2.56	0.46
4:D:21:GLY:O	4:D:37:ASN:N	2.49	0.46
4:D:275:ARG:HD3	4:D:352:GLU:HG2	1.97	0.46
2:B:319:THR:HG23	2:B:327:SER:HA	1.97	0.46
2:F:85:VAL:HG21	2:F:120:ARG:HG2	1.96	0.46
3:G:127:ALA:HB2	3:G:135:LEU:HD12	1.98	0.46
2:B:103:ILE:O	2:B:106:THR:OG1	2.33	0.46
3:C:9:MET:O	3:C:11:ASN:N	2.48	0.46
4:H:75:THR:HG22	4:H:360:TYR:HB2	1.97	0.45
1:A:130:ASP:OD1	1:A:130:ASP:N	2.49	0.45
3:C:36:LEU:HD11	3:C:79:PHE:HB3	1.98	0.45
2:F:21:TRP:HB3	2:F:89:ILE:HD11	1.98	0.45
4:H:388:HIS:ND1	4:H:415:TYR:OH	2.48	0.45
2:B:113:PRO:HD2	3:C:8:MET:HE1	1.99	0.45
4:H:342:ILE:HG21	4:H:367:GLY:HA2	1.98	0.45
3:C:1:MET:SD	3:C:1:MET:N	2.75	0.45
4:D:89:ARG:NH2	4:D:335:LYS:O	2.50	0.45
2:F:213:LEU:HA	2:F:336:LEU:HD21	1.99	0.45
4:H:399:ASP:OD1	4:H:400:ASP:N	2.42	0.45
4:H:275:ARG:HE	4:H:313:GLU:CD	2.22	0.45
1:A:23:MET:HG2	4:D:144:LYS:HD2	1.99	0.45
2:B:210:TRP:HH2	2:B:329:VAL:HG23	1.81	0.45
3:C:119:GLU:HG3	3:C:148:LYS:HG3	1.99	0.45
4:D:70:ALA:HB3	4:D:103:ASP:HB2	1.99	0.45
4:H:70:ALA:HB3	4:H:103:ASP:HB2	1.99	0.45
3:C:222:PRO:HG3	8:C:303:NAP:H52A	1.98	0.44
4:D:58:LEU:HD13	4:D:77:LEU:HD23	1.97	0.44
3:G:211:ASN:O	3:G:215:THR:OG1	2.23	0.44
1:E:190:ALA:O	1:E:207:ARG:NE	2.50	0.44
2:F:29:LYS:HG2	2:F:31:SER:O	2.18	0.44
3:G:65:GLU:OE2	3:G:106:ARG:NH2	2.49	0.44
4:H:8:ILE:HD12	4:H:404:LEU:HD23	2.00	0.44
4:H:10:ILE:HG12	4:H:405:LYS:NZ	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:144:THR:OG1	2:B:313:VAL:O	2.36	0.44
1:A:136:CYS:HB3	1:A:206:CYS:HB2	1.99	0.44
2:B:225:MET:HA	2:B:228:GLU:HG2	1.99	0.44
3:C:173:MET:HG2	3:C:174:LYS:H	1.83	0.44
4:H:139:ILE:HD11	4:H:191:LEU:O	2.18	0.43
1:A:135:GLY:HA2	1:A:207:ARG:HG2	2.00	0.43
4:D:363:LYS:HB3	4:D:371:TYR:HB3	1.99	0.43
4:H:151:MET:HE2	4:H:161:GLN:NE2	2.32	0.43
4:H:260:HIS:NE2	4:H:386:GLU:OE2	2.46	0.43
4:H:392:MET:HE3	4:H:407:LEU:HD23	2.00	0.43
1:A:31:ILE:HD11	4:D:127:LEU:HD22	1.99	0.43
1:A:83:VAL:HG22	1:A:133:ILE:HD12	1.99	0.43
3:C:135:LEU:HD23	3:C:135:LEU:HA	1.86	0.43
4:H:28:ASP:OD1	4:H:28:ASP:N	2.52	0.43
1:A:67:VAL:HA	1:A:70:VAL:HG22	2.01	0.43
2:B:29:LYS:HG2	2:B:31:SER:O	2.19	0.43
3:C:29:THR:OG1	3:C:32:GLU:OE1	2.25	0.42
2:F:133:PRO:HD3	2:F:200:ARG:HG3	2.00	0.42
4:H:346:PHE:HD1	4:H:363:LYS:HB2	1.84	0.42
4:H:121:ARG:HD2	4:H:133:TYR:CZ	2.54	0.42
1:A:64:GLU:HA	1:A:67:VAL:HG13	2.02	0.42
4:H:65:CYS:SG	4:H:67:PHE:N	2.87	0.42
4:D:38:ILE:HB	4:D:256:SER:HB2	2.02	0.42
3:G:23:LEU:HD11	3:G:38:ARG:HD2	2.02	0.42
3:C:146:ARG:NH2	3:C:181:ASN:HB2	2.35	0.42
2:F:56:PRO:HG2	2:F:58:LYS:HG2	2.02	0.42
4:H:275:ARG:NE	4:H:313:GLU:OE2	2.41	0.42
4:H:156:SER:HB2	4:H:162:GLU:H	1.85	0.42
4:H:276:VAL:O	4:H:280:ALA:HB2	2.19	0.42
3:C:263:VAL:HG23	3:C:270:LYS:HB2	2.01	0.41
3:C:75:MET:HE3	3:C:145:ASN:HD21	1.85	0.41
1:E:67:VAL:HA	1:E:70:VAL:HG22	2.01	0.41
2:F:210:TRP:CH2	2:F:329:VAL:HG23	2.55	0.41
1:A:30:LEU:HD23	1:A:30:LEU:HA	1.92	0.41
3:C:146:ARG:HA	3:C:146:ARG:HD2	1.89	0.41
1:E:13:SER:HB2	5:E:302:SF4:S3	2.61	0.41
3:G:146:ARG:HH21	3:G:181:ASN:HB2	1.85	0.41
4:H:129:MET:O	4:H:137:ILE:HG13	2.20	0.41
3:C:88:GLY:O	3:C:92:THR:OG1	2.35	0.41
2:B:3:TYR:OH	2:F:215:TYR:HB3	2.20	0.41
2:B:278:LEU:O	3:C:250:ARG:HD2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:5:LYS:HE3	3:C:10:PRO:HG3	2.03	0.41
3:G:63:VAL:HG21	3:G:93:VAL:HG21	2.03	0.41
4:H:142:LYS:HE2	4:H:142:LYS:HB3	1.94	0.41
1:A:195:ARG:NE	4:D:157:ARG:HG3	2.36	0.41
2:B:216:LEU:HD21	2:F:194:ARG:HD3	2.03	0.41
3:C:200:ARG:HH12	8:C:303:NAP:P2B	2.43	0.41
4:H:58:LEU:HD13	4:H:77:LEU:HD23	2.02	0.41
2:B:56:PRO:HG2	2:B:58:LYS:HG2	2.02	0.41
2:B:111:GLU:O	2:B:113:PRO:HD3	2.21	0.41
4:D:416:ASP:OD1	4:D:416:ASP:N	2.54	0.41
3:G:220:CYS:SG	3:G:246:THR:OG1	2.73	0.41
4:D:166:LEU:HB3	4:D:340:VAL:HG11	2.03	0.41
4:H:36:LEU:HD23	4:H:382:LEU:HD22	2.02	0.41
1:A:106:LYS:HE2	4:D:50:ILE:HG13	2.03	0.40
2:F:103:ILE:O	2:F:106:THR:OG1	2.31	0.40
2:F:242:THR:HG21	2:F:321:PHE:CD2	2.56	0.40
3:G:69:SER:OG	7:G:302:FAD:H6	2.21	0.40
1:E:64:GLU:HA	1:E:67:VAL:HG13	2.03	0.40
4:H:382:LEU:HD23	4:H:382:LEU:HA	1.93	0.40
1:A:51:LYS:HE3	1:A:51:LYS:HB2	1.99	0.40
1:A:190:ALA:O	1:A:207:ARG:NE	2.54	0.40
2:B:36:ASP:OD1	2:B:37:PHE:N	2.53	0.40
3:C:69:SER:OG	7:C:302:FAD:H6	2.21	0.40
2:F:212:ASN:HA	2:F:215:TYR:HD2	1.86	0.40
4:H:135:ARG:O	4:H:139:ILE:HG22	2.22	0.40
2:B:149:ASP:OD1	2:B:149:ASP:N	2.55	0.40
2:B:213:LEU:HD21	2:B:332:LEU:HD13	2.04	0.40
2:F:15:LEU:HD23	2:F:18:LEU:HD12	2.02	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	253/261 (97%)	245 (97%)	8 (3%)	0	100	100
1	E	253/261 (97%)	242 (96%)	11 (4%)	0	100	100
2	B	337/367 (92%)	330 (98%)	7 (2%)	0	100	100
2	F	337/367 (92%)	331 (98%)	6 (2%)	0	100	100
3	C	290/292 (99%)	281 (97%)	9 (3%)	0	100	100
3	G	290/292 (99%)	279 (96%)	11 (4%)	0	100	100
4	D	417/428 (97%)	406 (97%)	11 (3%)	0	100	100
4	H	418/428 (98%)	410 (98%)	8 (2%)	0	100	100
All	All	2595/2696 (96%)	2524 (97%)	71 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	217/220 (99%)	210 (97%)	7 (3%)	34	60
1	E	217/220 (99%)	211 (97%)	6 (3%)	38	63
2	B	307/331 (93%)	297 (97%)	10 (3%)	33	60
2	F	307/331 (93%)	299 (97%)	8 (3%)	40	65
3	C	253/253 (100%)	248 (98%)	5 (2%)	48	69
3	G	253/253 (100%)	244 (96%)	9 (4%)	31	58
4	D	350/359 (98%)	337 (96%)	13 (4%)	30	57
4	H	351/359 (98%)	342 (97%)	9 (3%)	40	65
All	All	2255/2326 (97%)	2188 (97%)	67 (3%)	37	62

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	LEU
1	A	67	VAL

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Mol	Chain	Res	Type
1	A	106	LYS
1	A	130	ASP
1	A	159	ILE
1	A	201	VAL
1	A	218	ASP
2	B	4	VAL
2	B	55	MET
2	B	72	ASP
2	B	168	THR
2	B	195	ASP
2	B	216	LEU
2	B	251	VAL
2	B	261	THR
2	B	307	LEU
2	B	309	LEU
3	C	22	VAL
3	C	72	SER
3	C	95	HIS
3	C	234	ILE
3	C	287	THR
4	D	16	VAL
4	D	26	ILE
4	D	55	GLU
4	D	60	ILE
4	D	87	VAL
4	D	104	MET
4	D	132	GLU
4	D	277	ILE
4	D	297	LEU
4	D	340	VAL
4	D	344	ASP
4	D	351	THR
4	D	416	ASP
1	E	67	VAL
1	E	114	LYS
1	E	152	ILE
1	E	168	ARG
1	E	201	VAL
1	E	218	ASP
2	F	4	VAL
2	F	82	ILE
2	F	195	ASP

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Mol	Chain	Res	Type
2	F	242	THR
2	F	251	VAL
2	F	261	THR
2	F	288	THR
2	F	307	LEU
3	G	9	MET
3	G	20	VAL
3	G	22	VAL
3	G	29	THR
3	G	95	HIS
3	G	123	LEU
3	G	202	GLN
3	G	234	ILE
3	G	287	THR
4	H	55	GLU
4	H	139	ILE
4	H	226	ILE
4	H	340	VAL
4	H	344	ASP
4	H	351	THR
4	H	385	MET
4	H	396	HIS
4	H	416	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	172	HIS
2	B	178	ASN
3	C	181	ASN
4	D	366	ASN
2	F	178	ASN
3	G	54	GLN
3	G	151	ASN
4	H	111	HIS
4	H	366	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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	$\# Z > 2$
5	SF4	F	403	2	0,12,12	-	-	-		
8	NAP	C	303	-	50,52,52	0.60	1 (2%)	71,80,80	0.93	3 (4%)
5	SF4	F	404	2	0,12,12	-	-	-		
7	FAD	C	302	-	58,58,58	0.33	0	85,89,89	0.32	0
5	SF4	A	303	1	0,12,12	-	-	-		
9	NFU	D	501	4	2,7,7	0.12	0	-		
5	SF4	B	401	2	0,12,12	-	-	-		
7	FAD	G	302	-	58,58,58	0.32	0	85,89,89	0.30	0
5	SF4	B	404	2	0,12,12	-	-	-		
5	SF4	E	302	1	0,12,12	-	-	-		
6	FES	C	301	3	0,4,4	-	-	-		
5	SF4	A	301	4,1	0,12,12	-	-	-		
9	NFU	H	501	4	2,7,7	0.15	0	-		
5	SF4	F	402	2	0,12,12	-	-	-		
5	SF4	B	403	2	0,12,12	-	-	-		
5	SF4	B	402	2	0,12,12	-	-	-		
8	NAP	G	303	-	50,52,52	0.65	1 (2%)	71,80,80	0.97	3 (4%)
5	SF4	E	303	1	0,12,12	-	-	-		
6	FES	G	301	3	0,4,4	-	-	-		
5	SF4	E	301	1	0,12,12	-	-	-		
5	SF4	F	401	2	0,12,12	-	-	-		
5	SF4	A	302	1	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	F	403	2	-	-	0/6/5/5
8	NAP	C	303	-	-	14/35/67/67	0/5/5/5
5	SF4	F	404	2	-	-	0/6/5/5
5	SF4	A	303	1	-	-	0/6/5/5
7	FAD	C	302	-	-	9/34/50/50	0/6/6/6
5	SF4	B	401	2	-	-	0/6/5/5
7	FAD	G	302	-	-	4/34/50/50	0/6/6/6
5	SF4	B	404	2	-	-	0/6/5/5
5	SF4	E	302	1	-	-	0/6/5/5
6	FES	C	301	3	-	-	0/1/1/1
5	SF4	A	301	4,1	-	-	0/6/5/5
5	SF4	F	402	2	-	-	0/6/5/5
5	SF4	B	403	2	-	-	0/6/5/5
5	SF4	B	402	2	-	-	0/6/5/5
8	NAP	G	303	-	-	13/35/67/67	0/5/5/5
5	SF4	E	303	1	-	-	0/6/5/5
6	FES	G	301	3	-	-	0/1/1/1
5	SF4	E	301	1	-	-	0/6/5/5
5	SF4	F	401	2	-	-	0/6/5/5
5	SF4	A	302	1	-	-	0/6/5/5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	G	303	NAP	C2N-N1N	2.60	1.37	1.35
8	C	303	NAP	C2N-N1N	2.17	1.37	1.35

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	303	NAP	P2B-O2B-C2B	-5.29	109.31	123.43
8	G	303	NAP	P2B-O2B-C2B	-5.27	109.35	123.43
8	G	303	NAP	C6N-N1N-C2N	-2.81	119.49	121.88
8	C	303	NAP	C6N-N1N-C2N	-2.42	119.82	121.88
8	G	303	NAP	C3B-C2B-C1B	-2.31	98.38	102.81
8	C	303	NAP	C3B-C2B-C1B	-2.24	98.51	102.81

There are no chirality outliers.

All (40) torsion outliers are listed below:

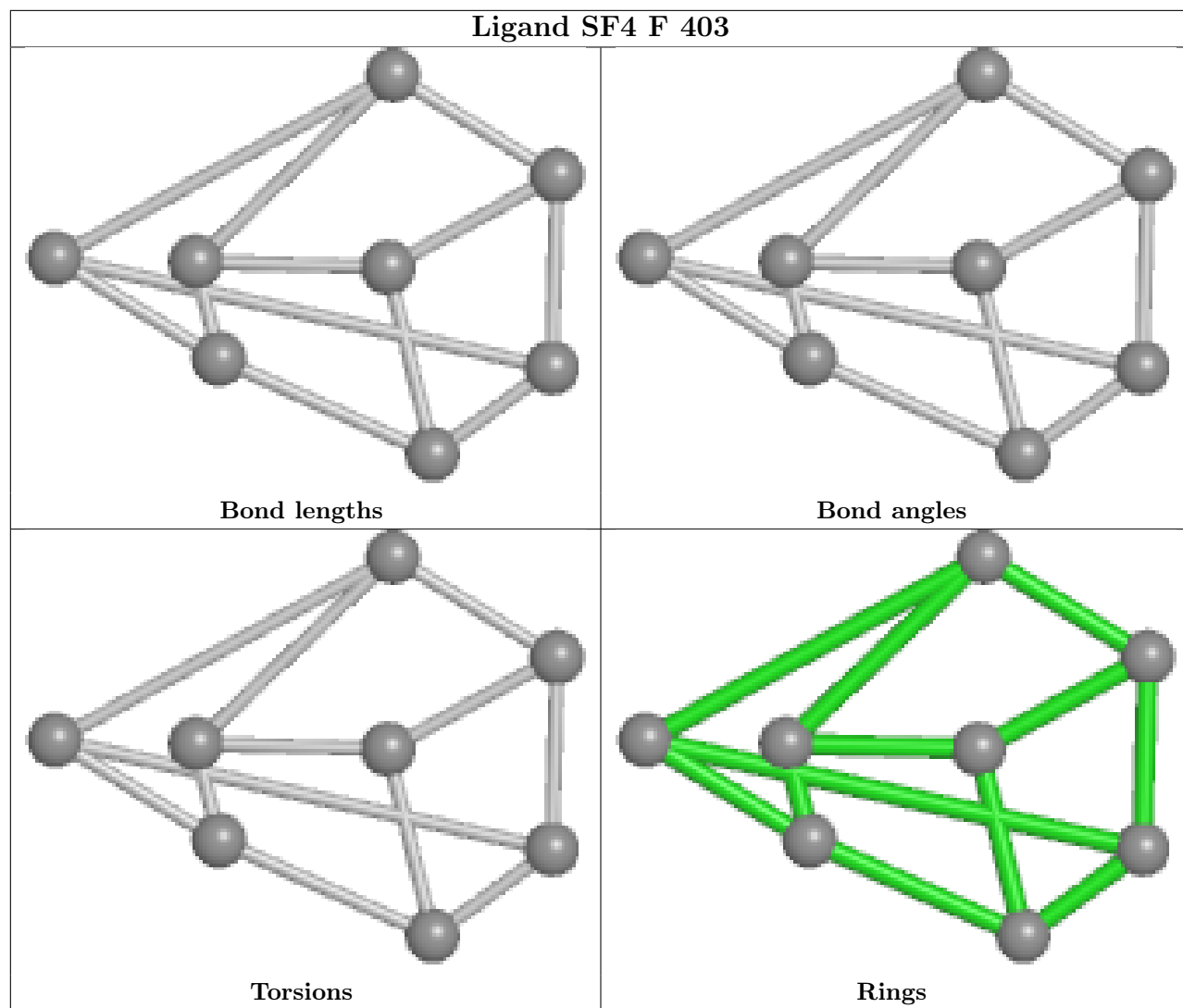
Mol	Chain	Res	Type	Atoms
7	C	302	FAD	C5B-O5B-PA-O1A
7	C	302	FAD	C5B-O5B-PA-O2A
7	C	302	FAD	C3'-C4'-C5'-O5'
7	G	302	FAD	O4B-C4B-C5B-O5B
7	G	302	FAD	C3'-C4'-C5'-O5'
7	G	302	FAD	O4'-C4'-C5'-O5'
8	C	303	NAP	C5B-O5B-PA-O1A
8	C	303	NAP	O4D-C4D-C5D-O5D
8	C	303	NAP	O4D-C1D-N1N-C2N
8	C	303	NAP	O4D-C1D-N1N-C6N
8	C	303	NAP	C2D-C1D-N1N-C2N
8	C	303	NAP	C2D-C1D-N1N-C6N
8	G	303	NAP	O4D-C4D-C5D-O5D
8	G	303	NAP	O4D-C1D-N1N-C2N
8	G	303	NAP	O4D-C1D-N1N-C6N
8	G	303	NAP	C2D-C1D-N1N-C6N
7	C	302	FAD	O4B-C4B-C5B-O5B
7	C	302	FAD	C3B-C4B-C5B-O5B
8	C	303	NAP	C3D-C4D-C5D-O5D
8	G	303	NAP	C3D-C4D-C5D-O5D
8	C	303	NAP	C4B-C5B-O5B-PA
7	C	302	FAD	O4'-C4'-C5'-O5'
7	G	302	FAD	C3B-C4B-C5B-O5B
8	C	303	NAP	C4N-C3N-C7N-N7N
8	C	303	NAP	C4N-C3N-C7N-O7N
8	C	303	NAP	C4D-C5D-O5D-PN
8	G	303	NAP	C4B-C5B-O5B-PA
8	G	303	NAP	C4D-C5D-O5D-PN
8	C	303	NAP	C2N-C3N-C7N-O7N
8	C	303	NAP	C2N-C3N-C7N-N7N
7	C	302	FAD	C5B-O5B-PA-O3P
8	G	303	NAP	C5B-O5B-PA-O1A
8	G	303	NAP	C5D-O5D-PN-O1N
8	G	303	NAP	C2D-C1D-N1N-C2N
8	G	303	NAP	O4B-C1B-N9A-C8A
8	G	303	NAP	C2B-C1B-N9A-C4A
8	G	303	NAP	C2B-C1B-N9A-C8A
7	C	302	FAD	PA-O3P-P-O2P
8	C	303	NAP	O4B-C1B-N9A-C8A
7	C	302	FAD	PA-O3P-P-O1P

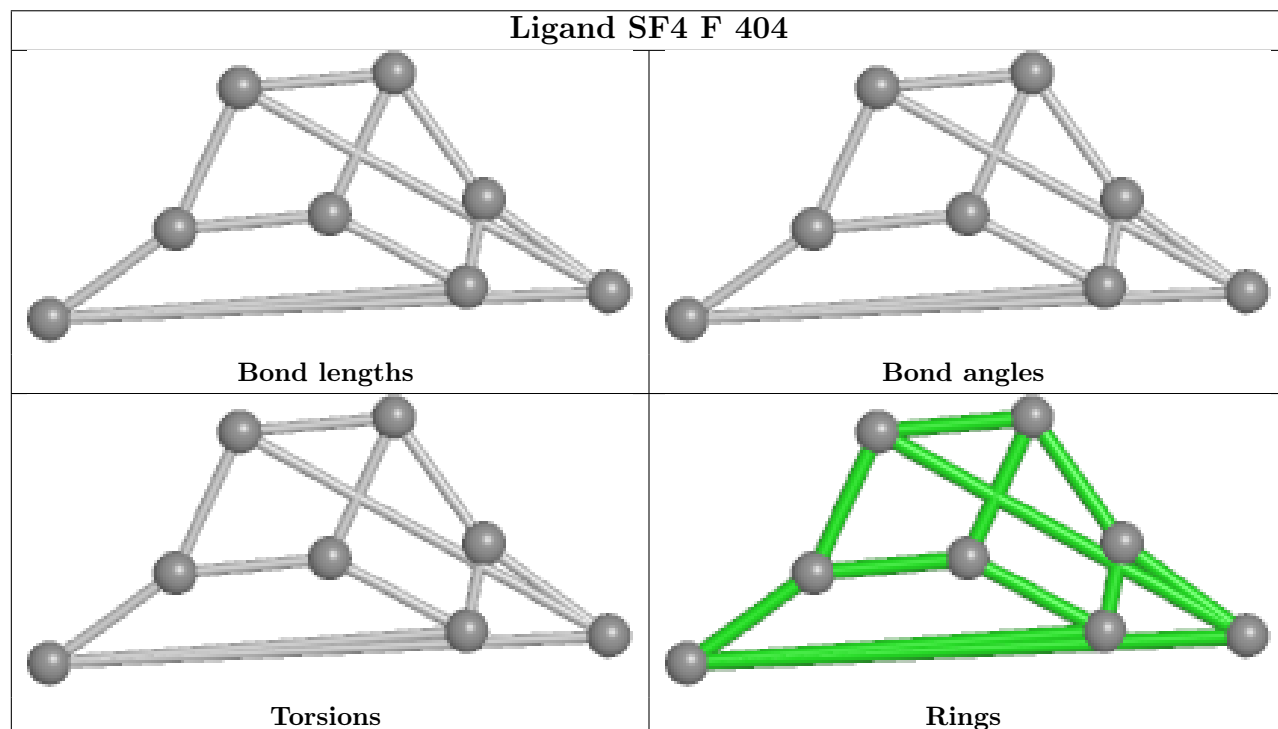
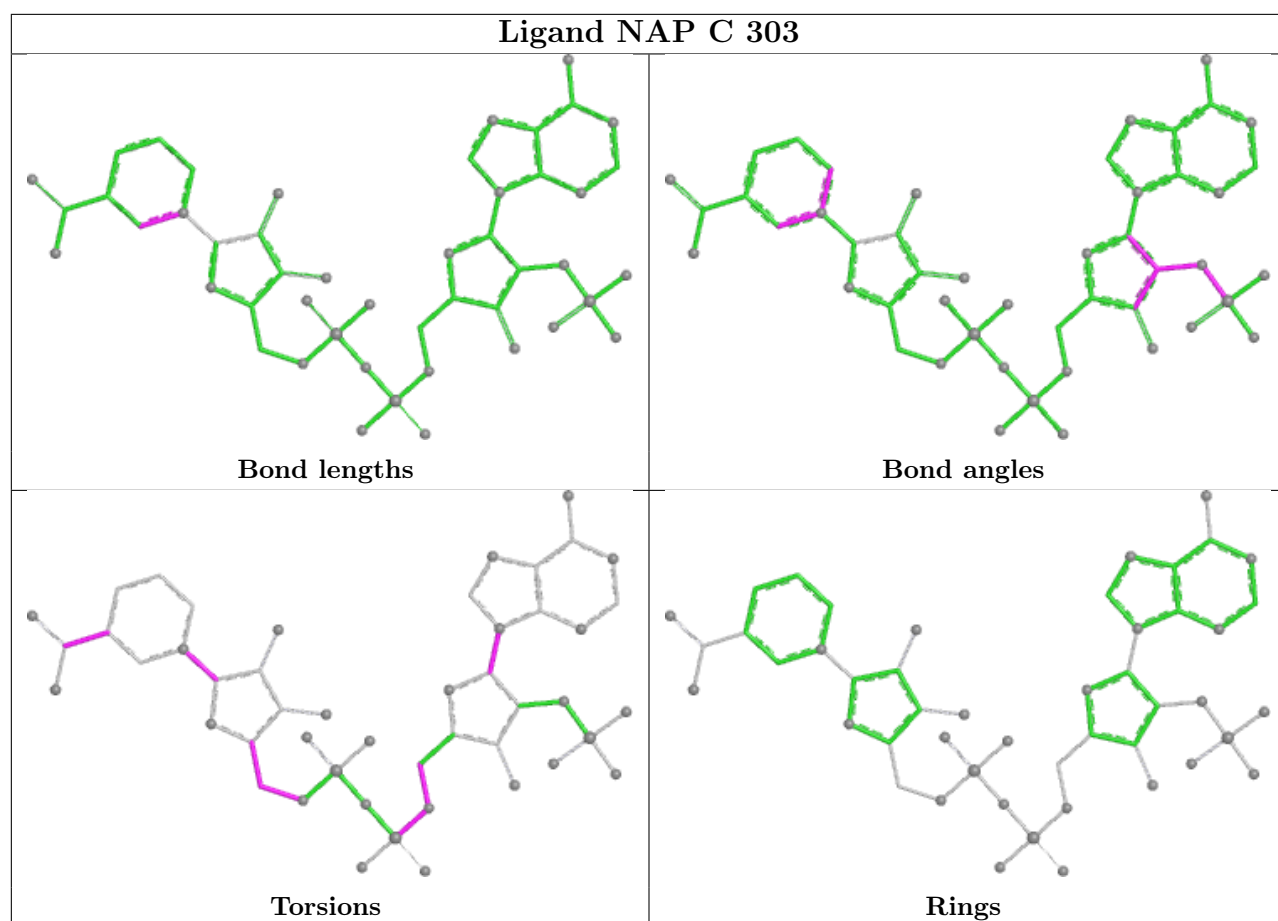
There are no ring outliers.

9 monomers are involved in 17 short contacts:

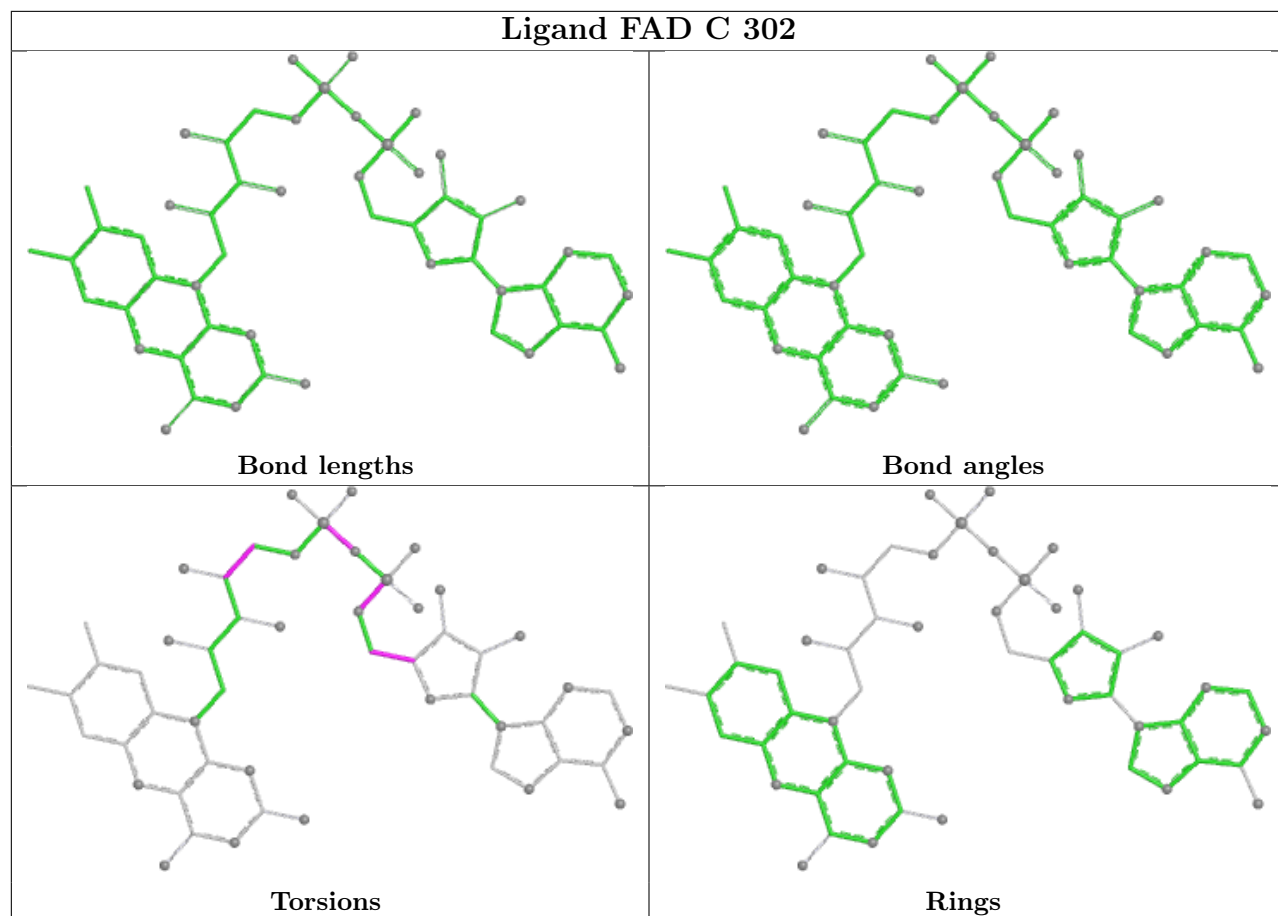
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	303	NAP	4	0
5	F	404	SF4	2	0
7	C	302	FAD	1	0
5	A	303	SF4	1	0
7	G	302	FAD	1	0
5	E	302	SF4	1	0
5	A	301	SF4	1	0
5	B	403	SF4	2	0
8	G	303	NAP	4	0

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.

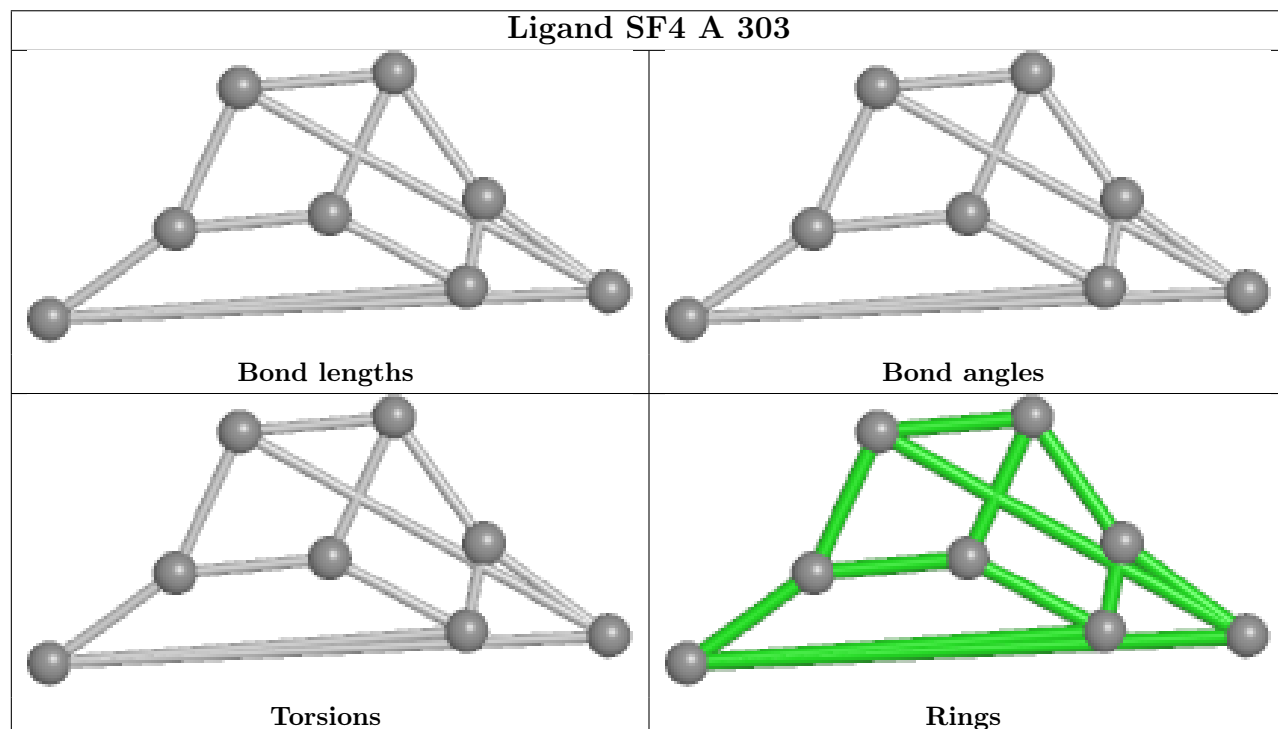


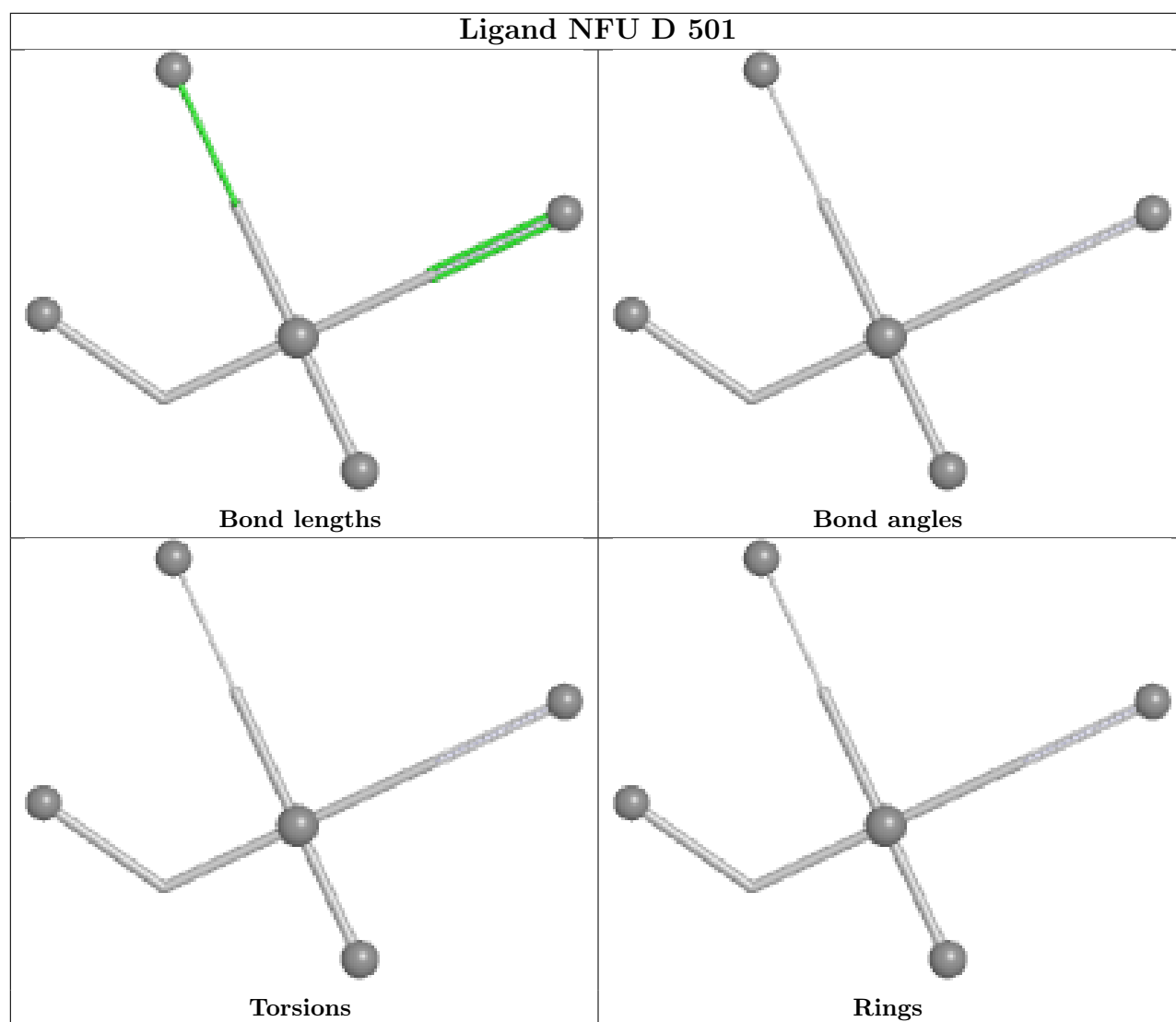


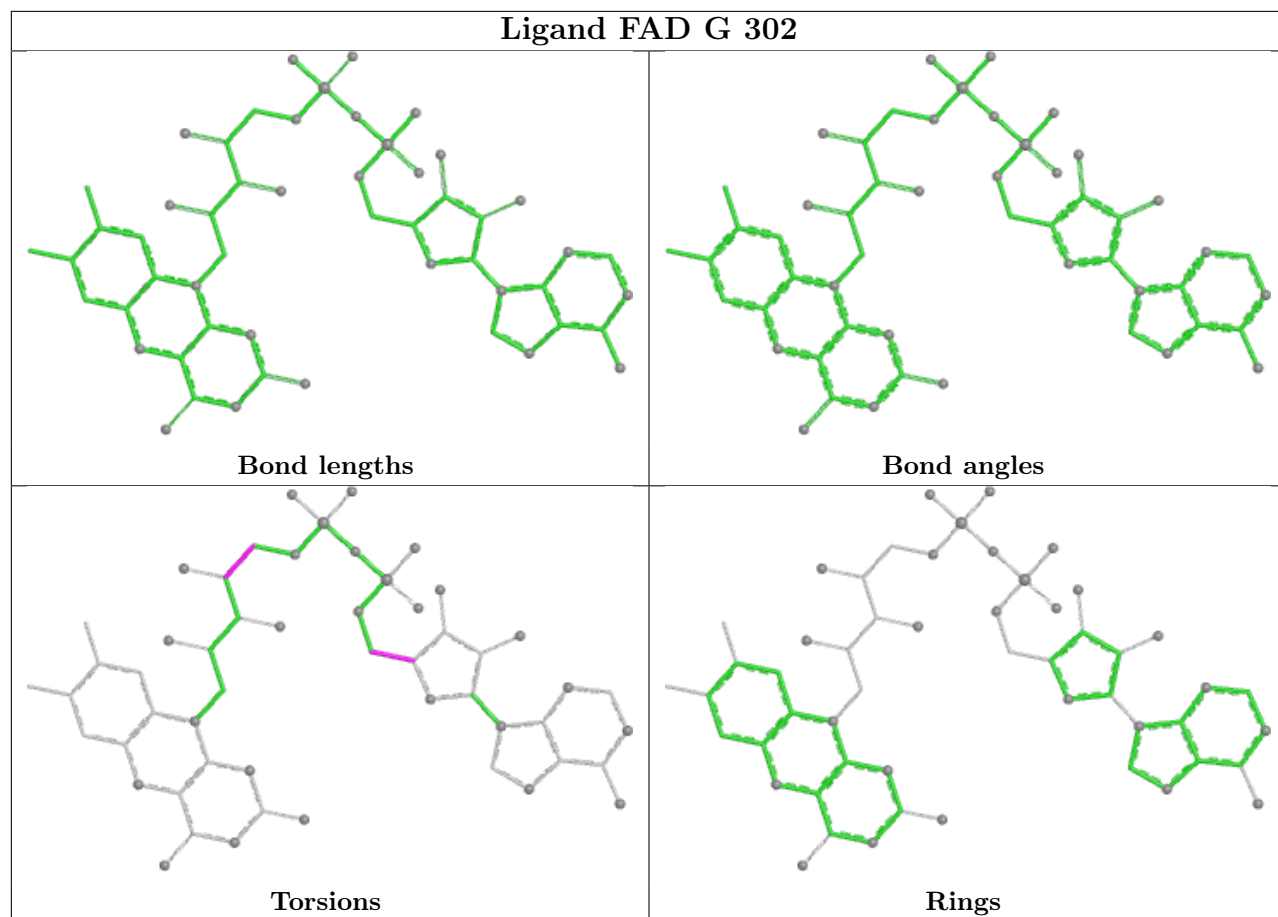
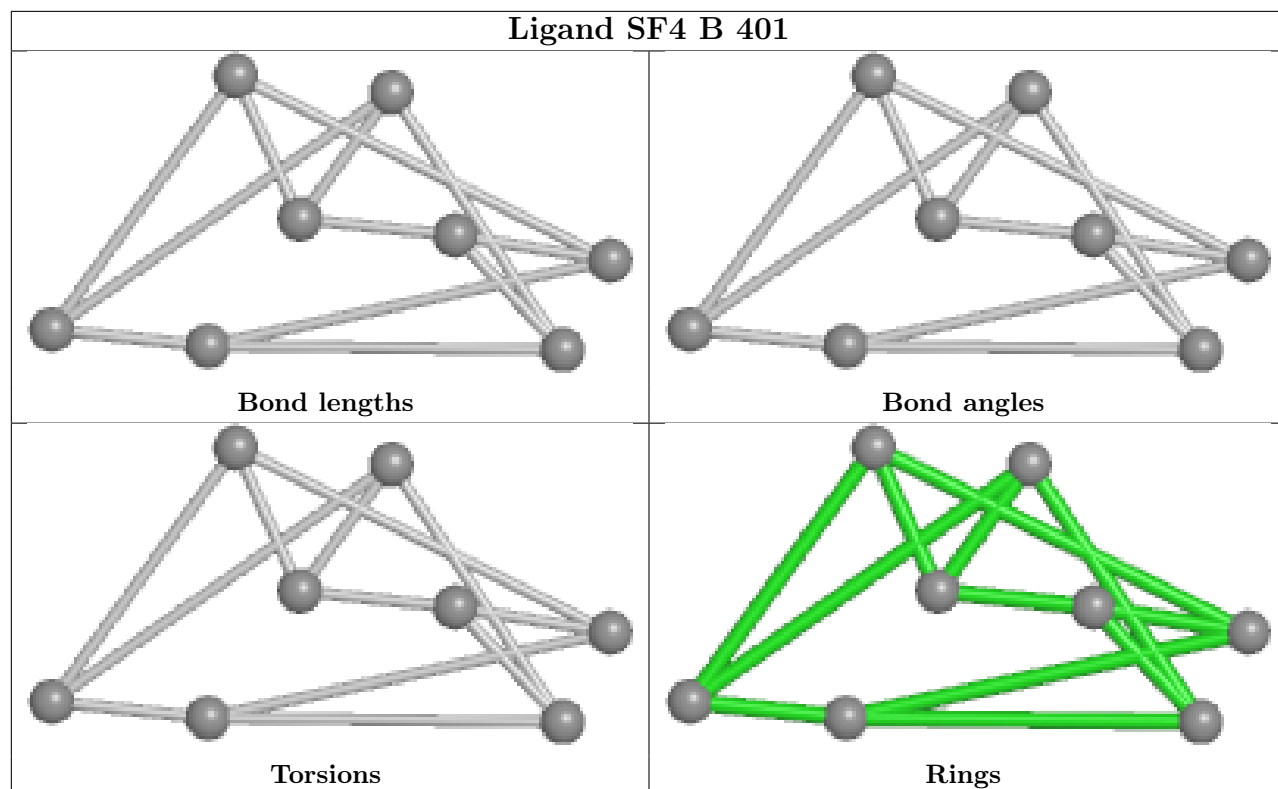
Ligand FAD C 302

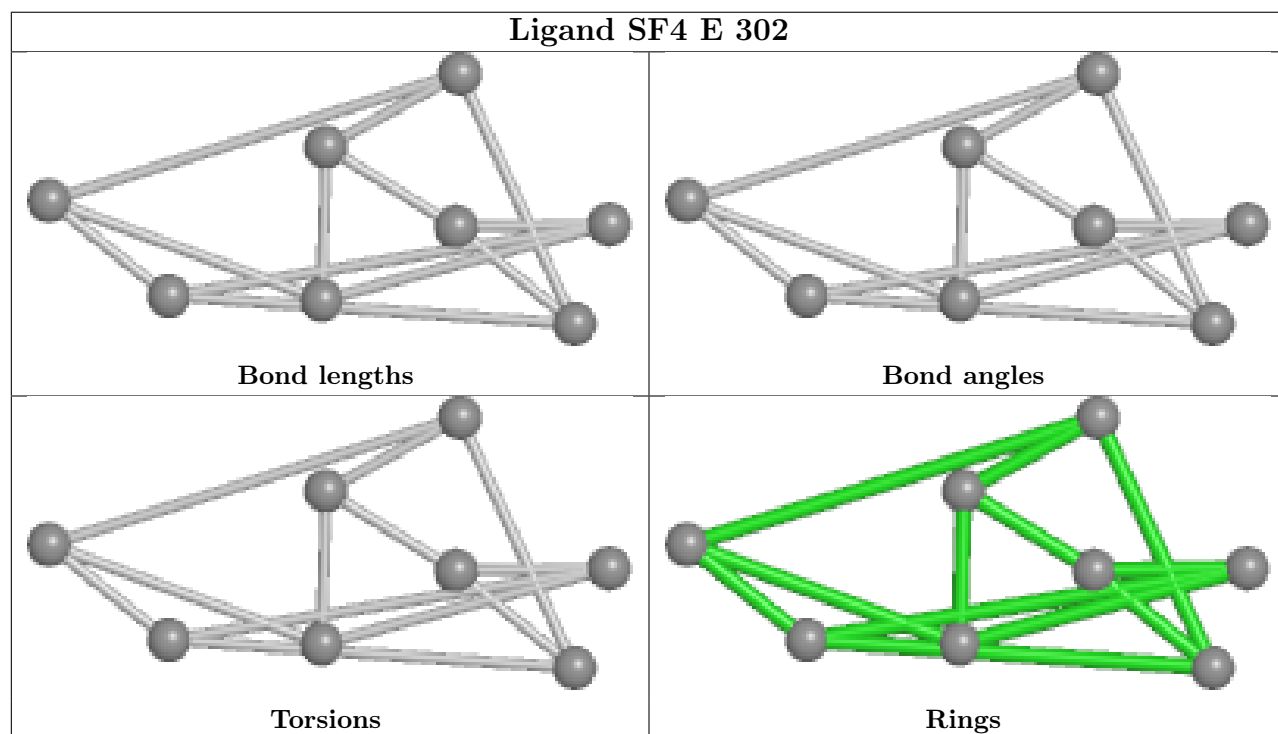
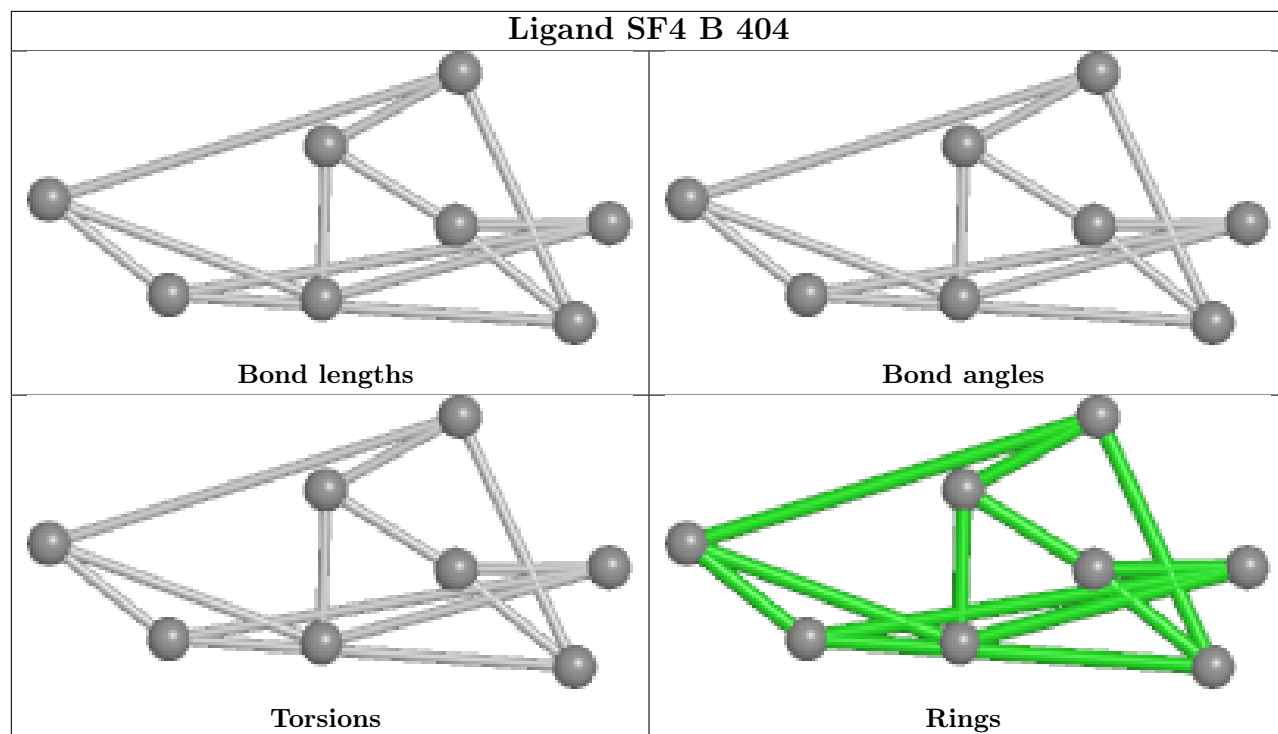


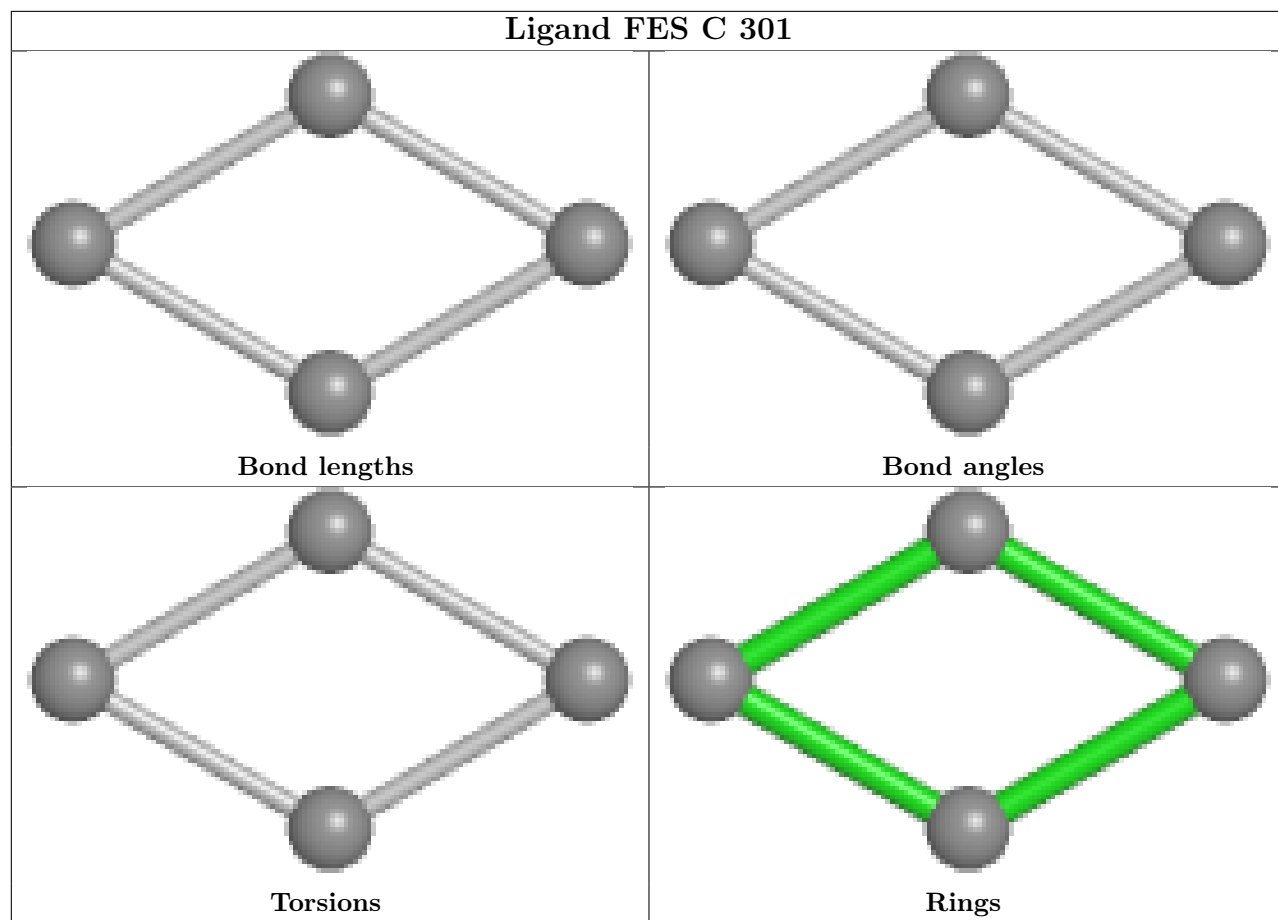
Ligand SF4 A 303

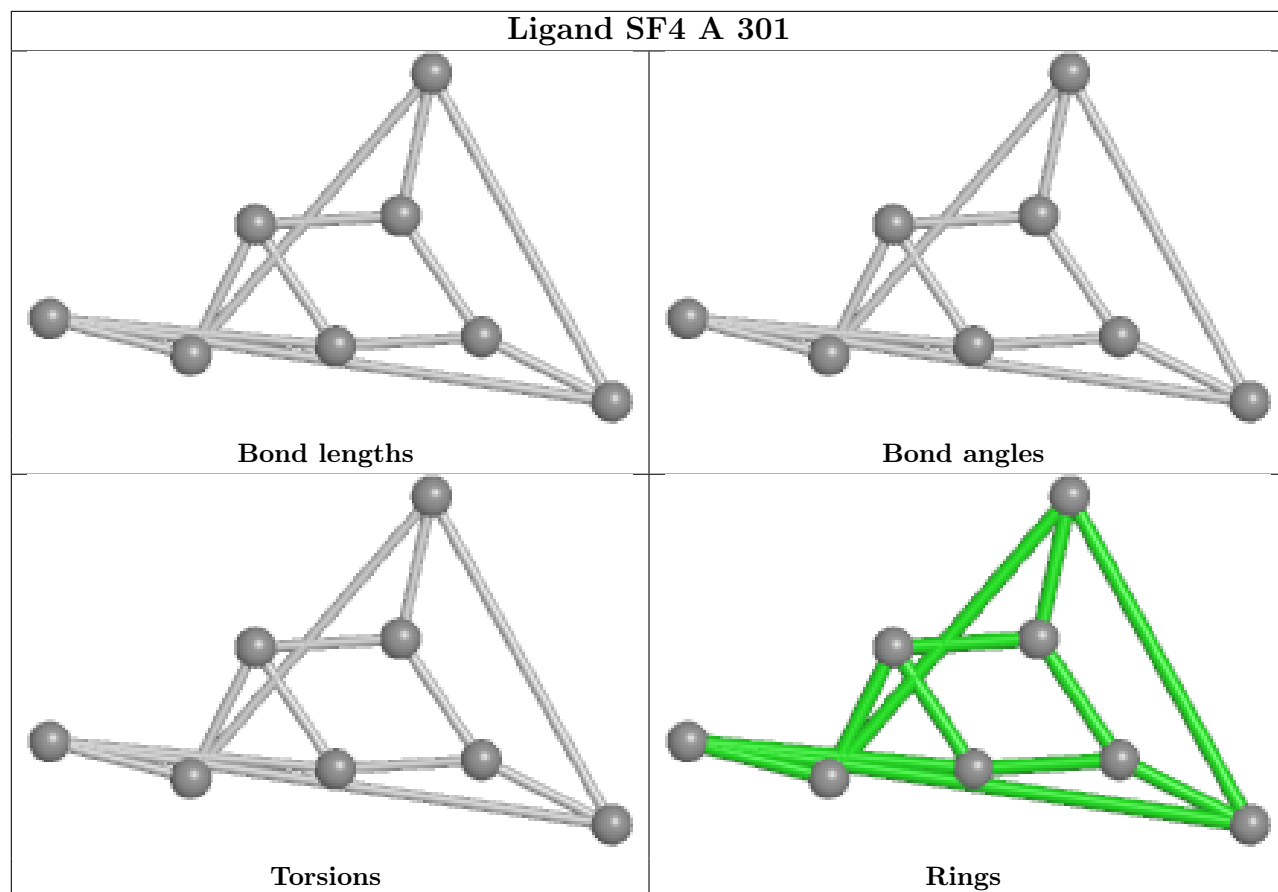


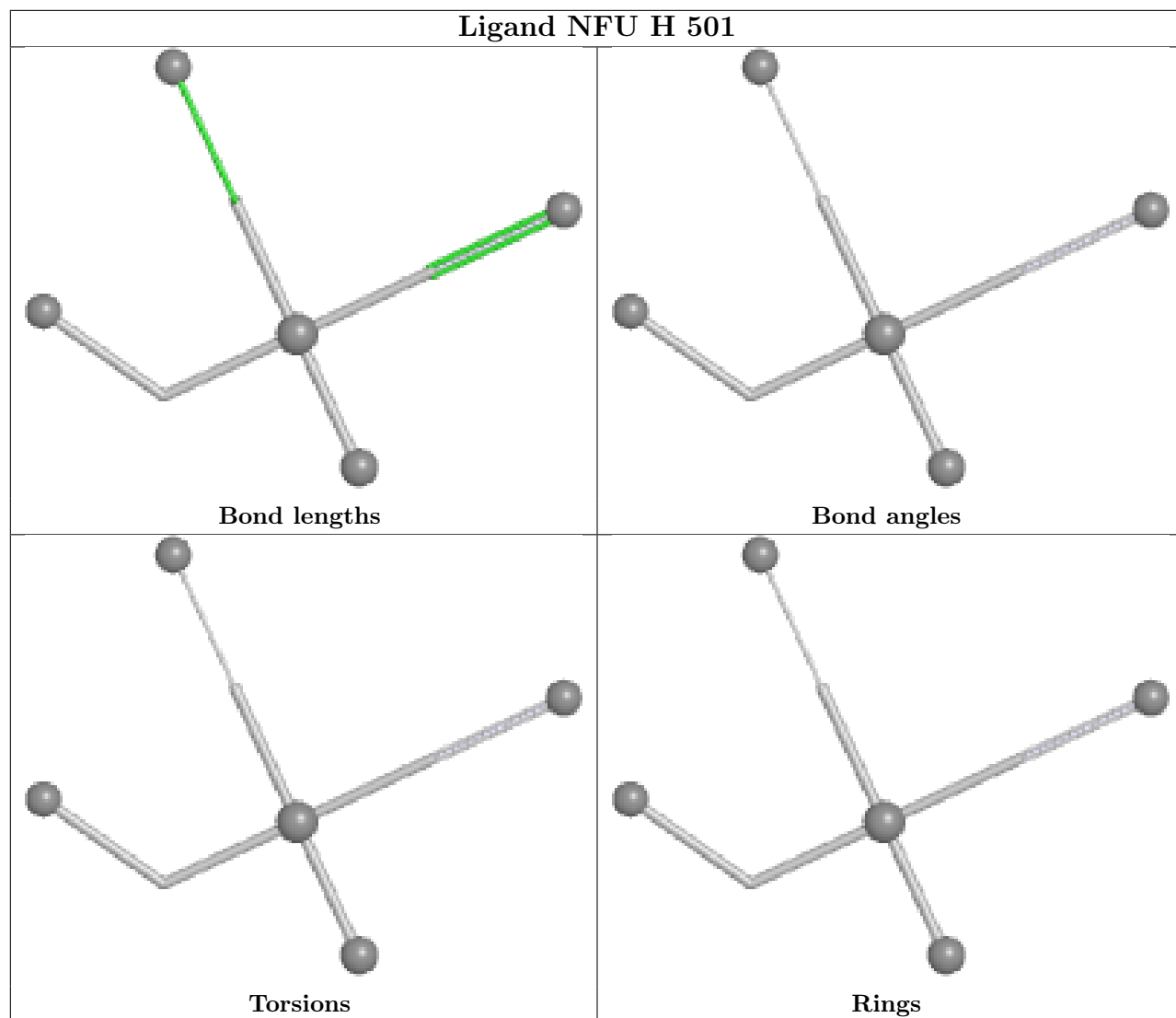


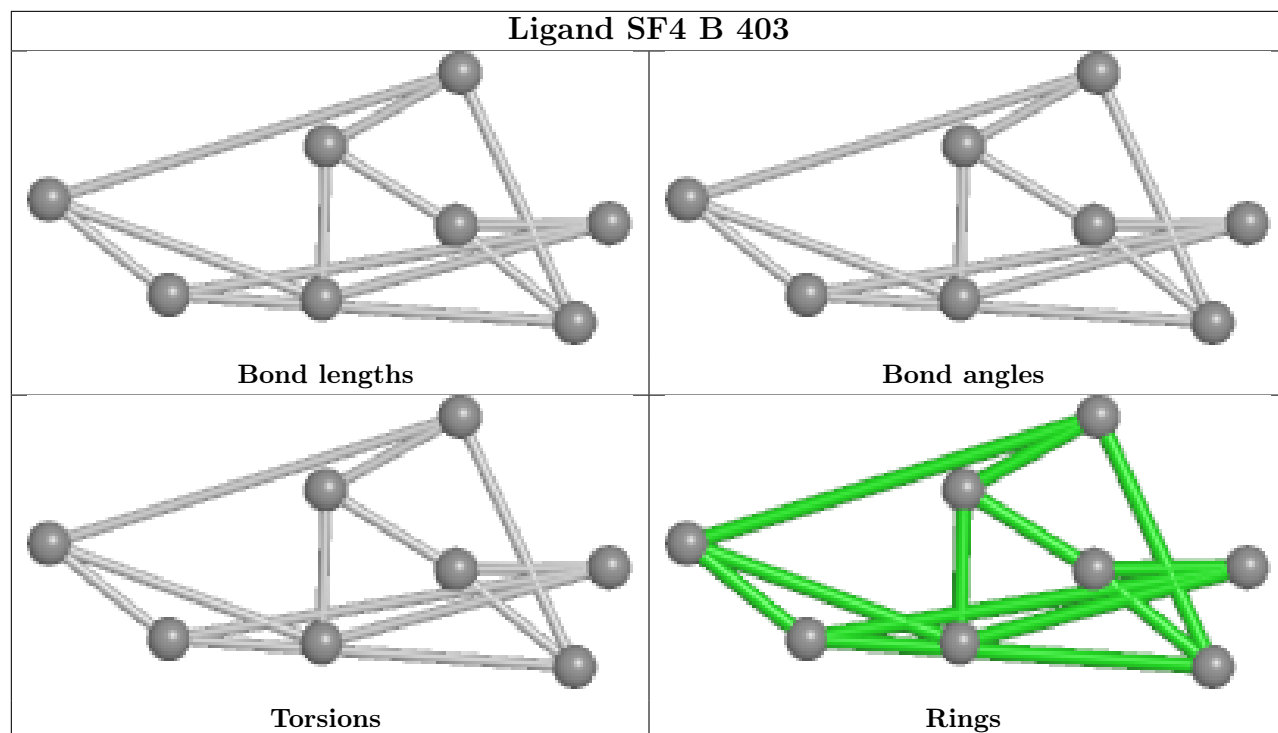
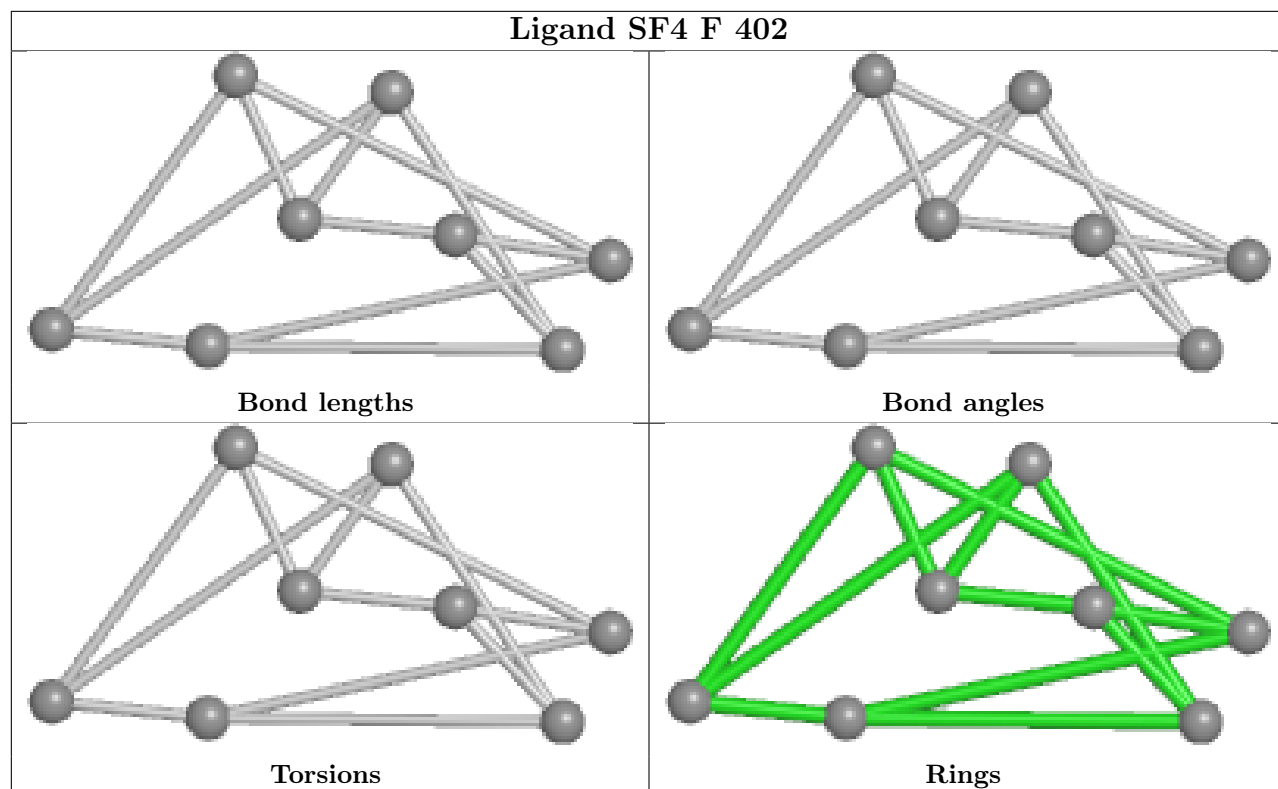


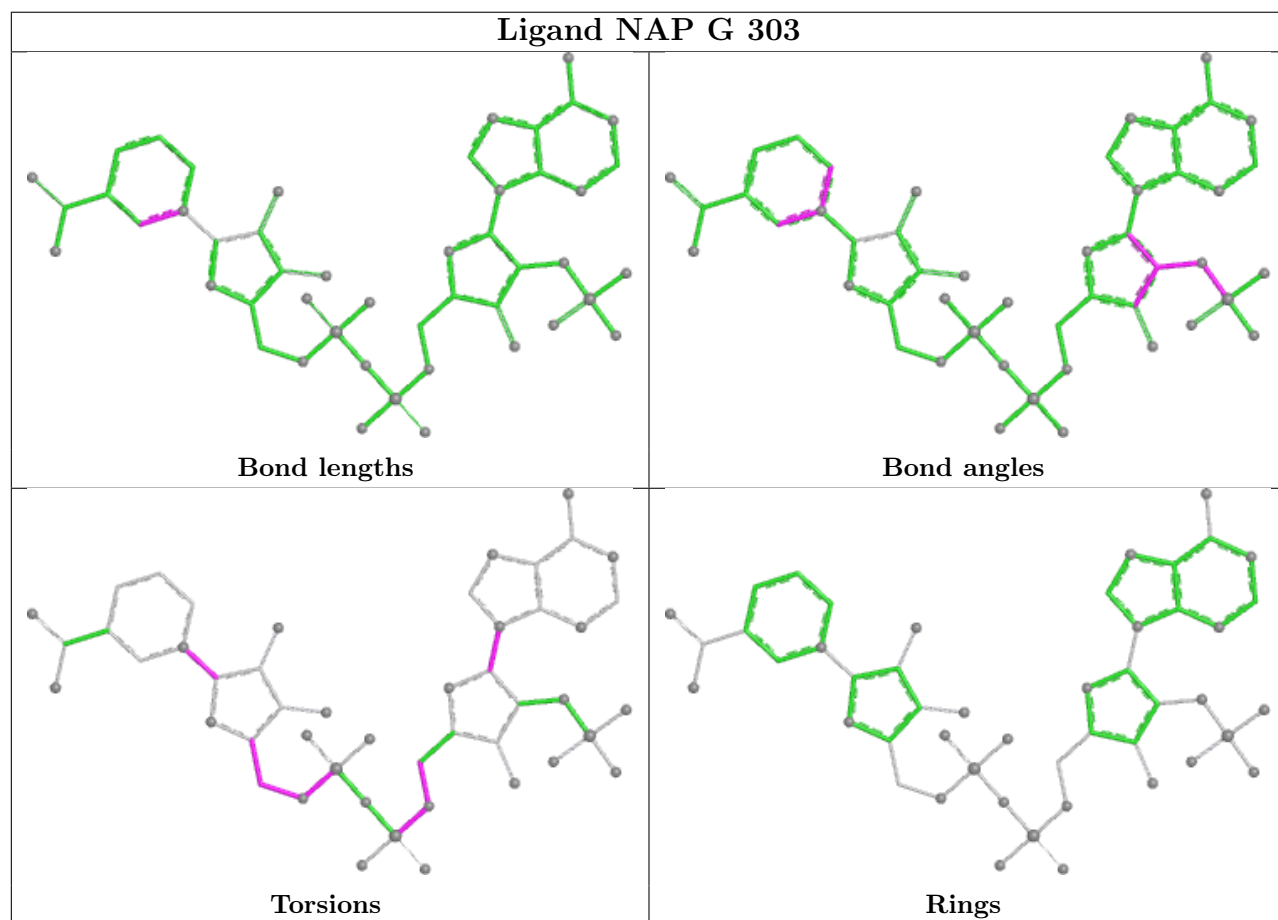
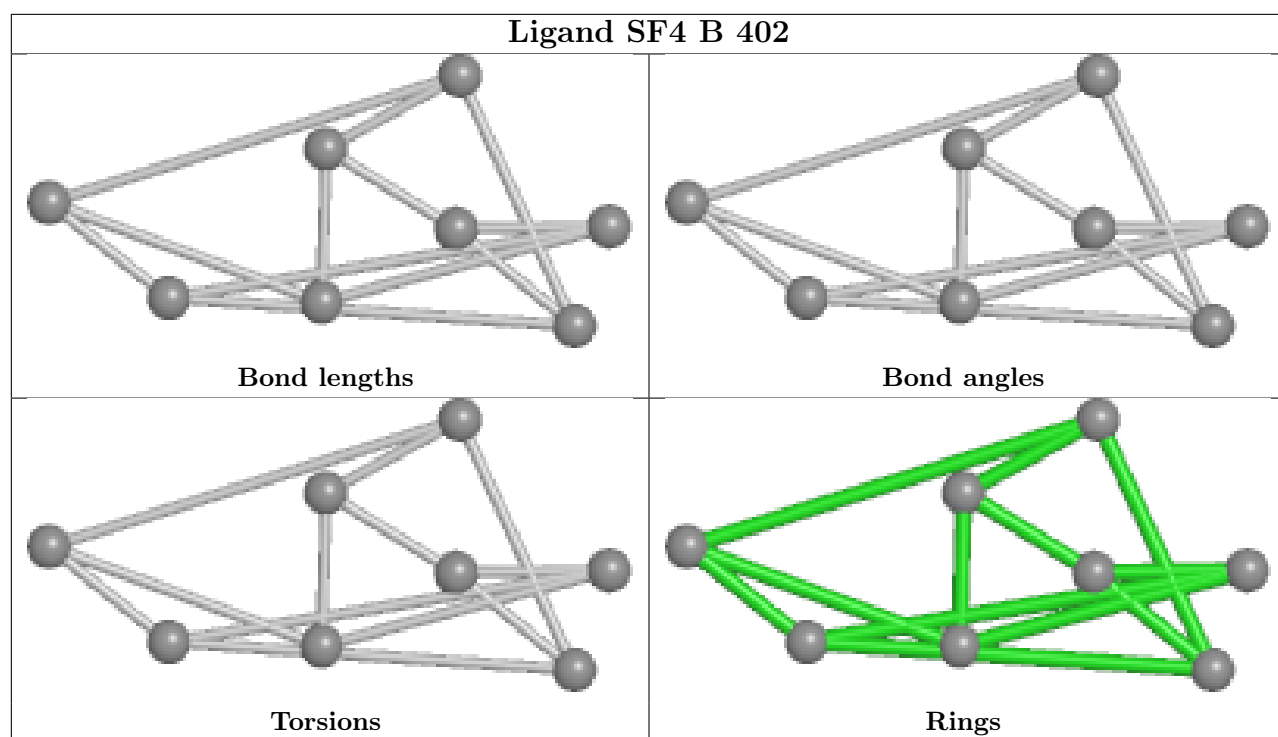


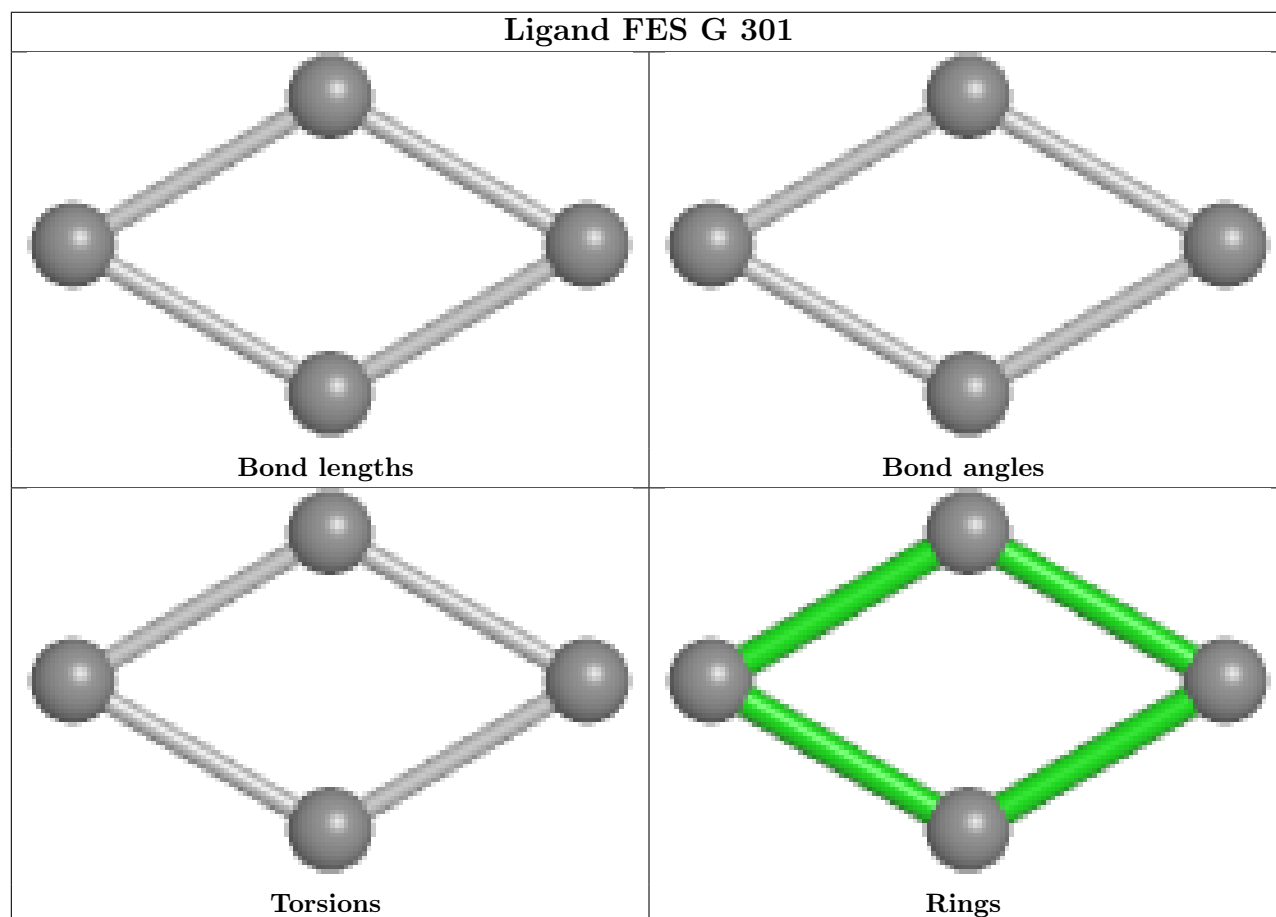
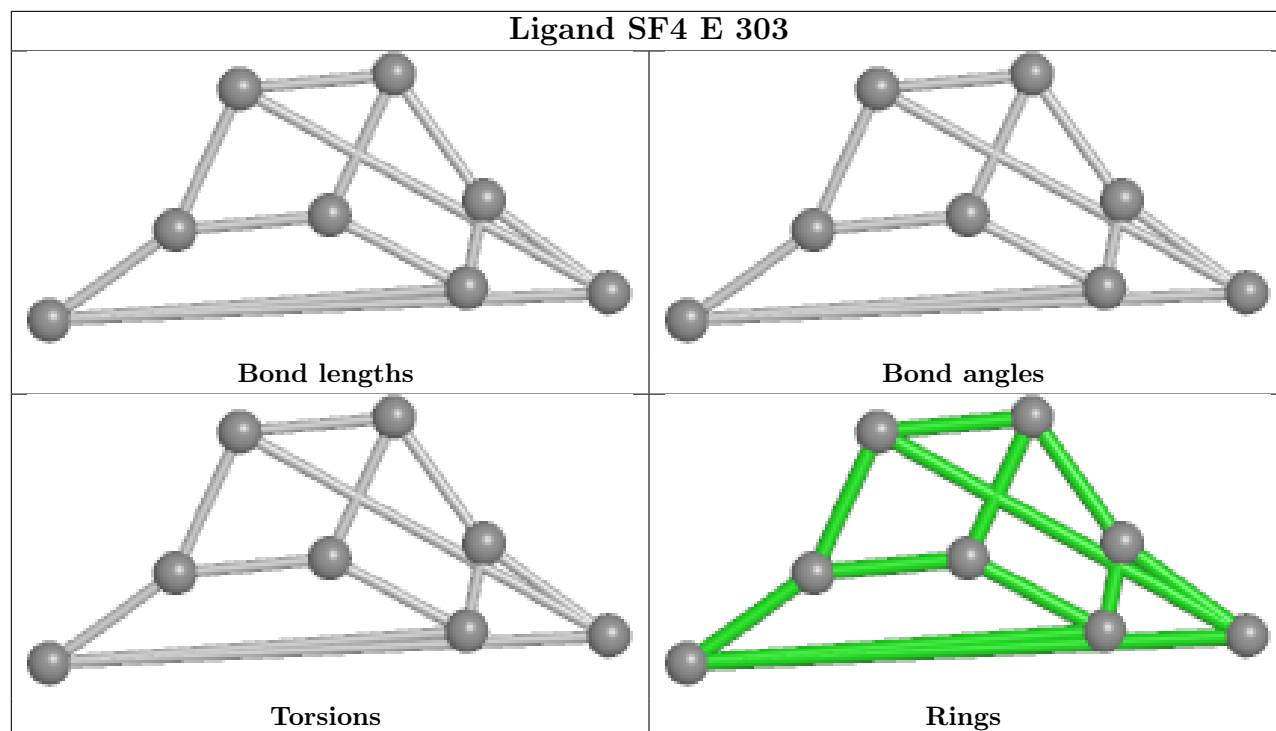


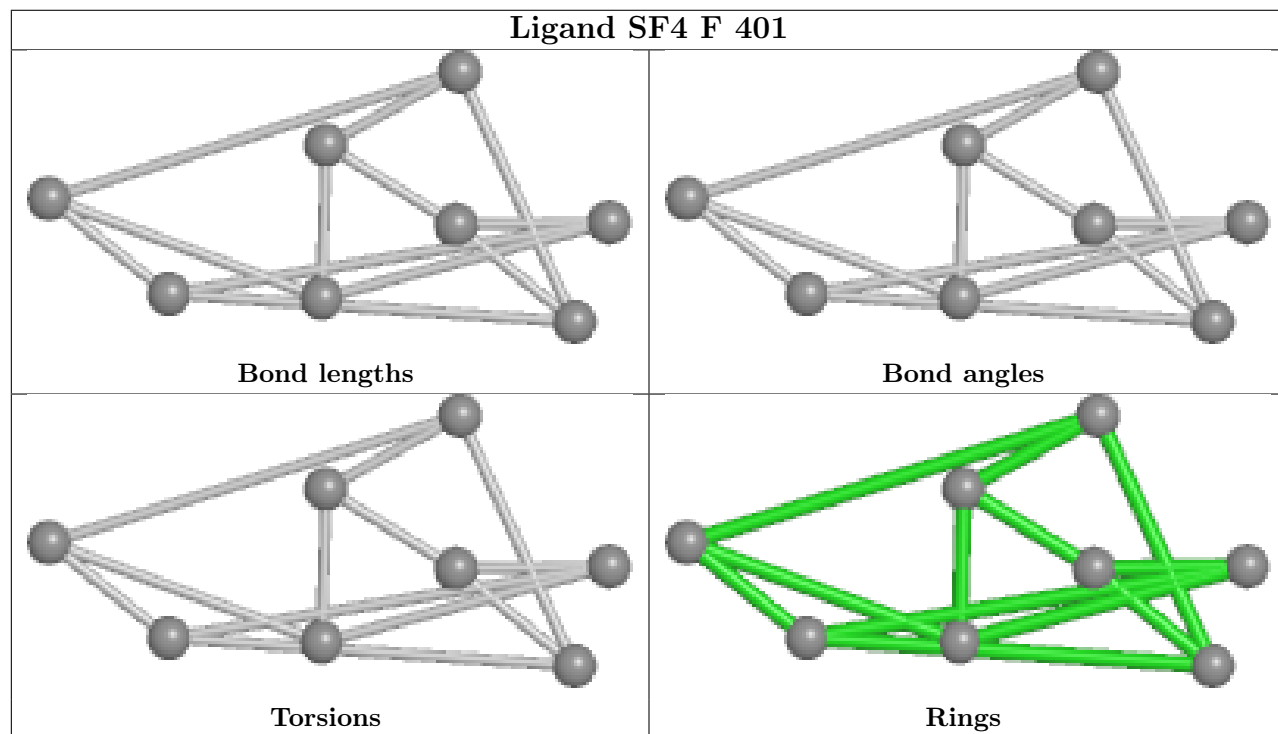
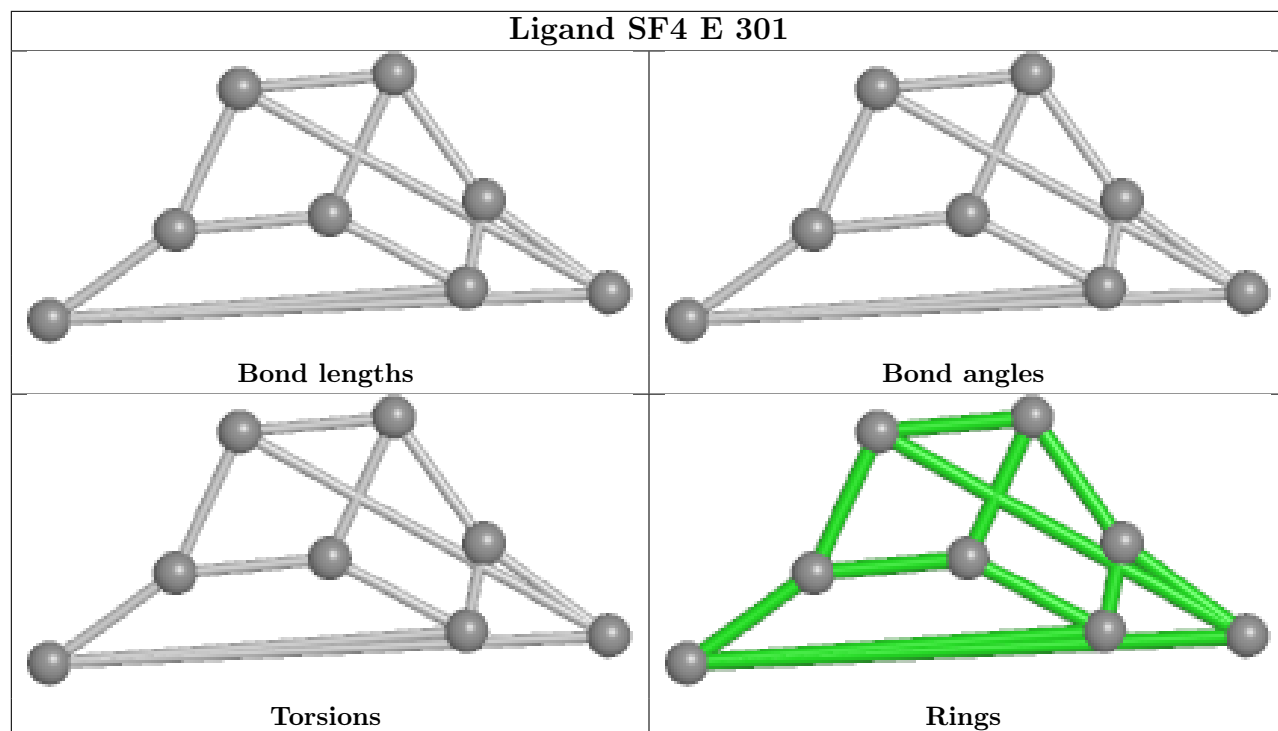


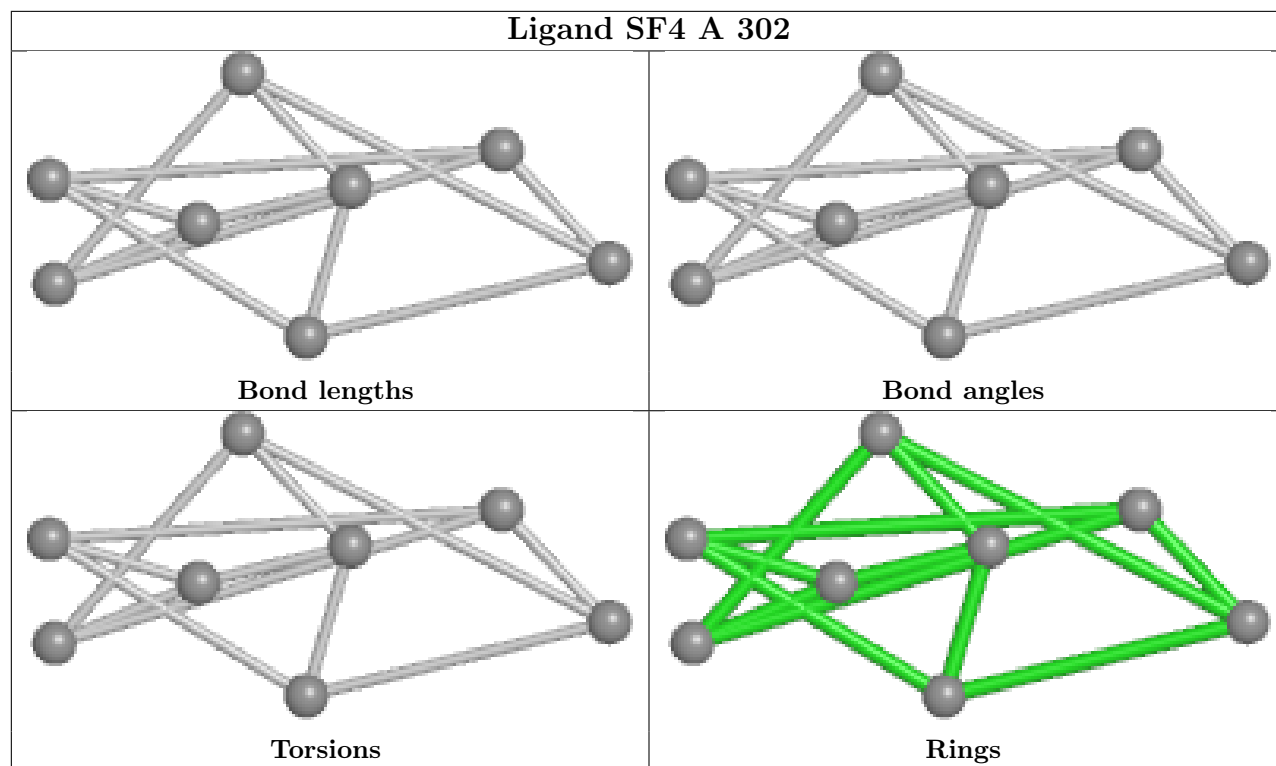












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

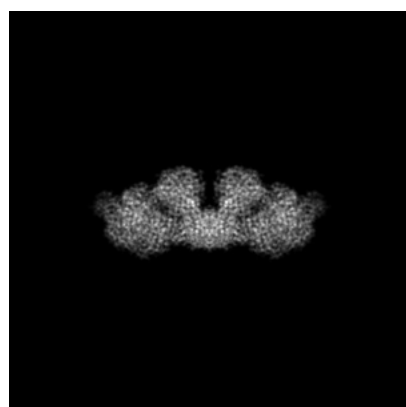
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-49341. These allow visual inspection of the internal detail of the map and identification of artifacts.

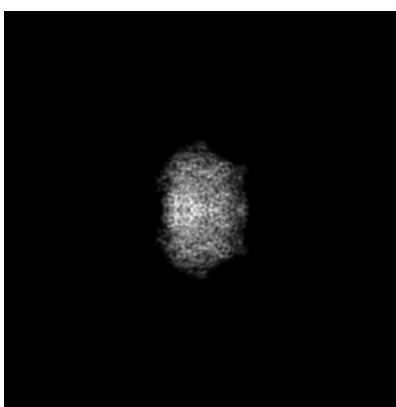
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

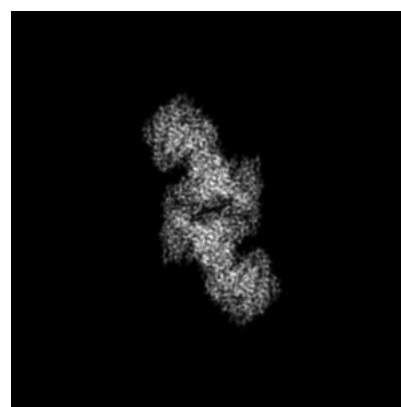
6.1.1 Primary map



X



Y

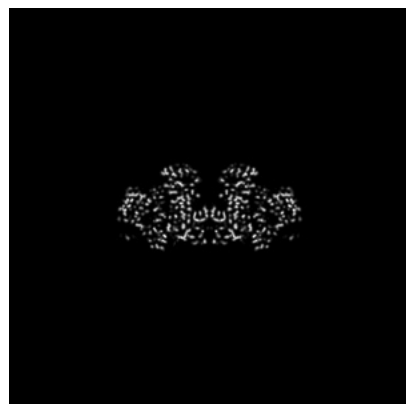


Z

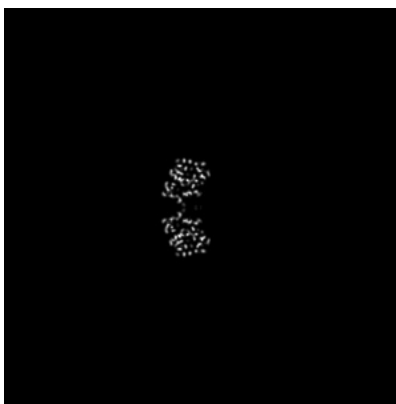
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

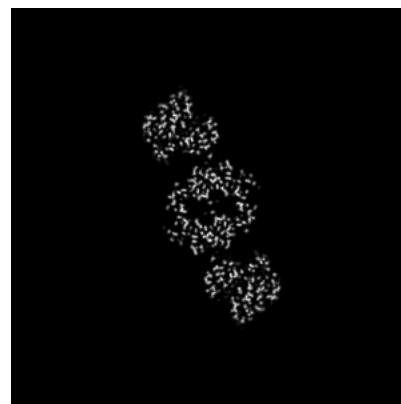
6.2.1 Primary map



X Index: 192



Y Index: 192



Z Index: 192

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

6.3 Largest variance slices [i](#)

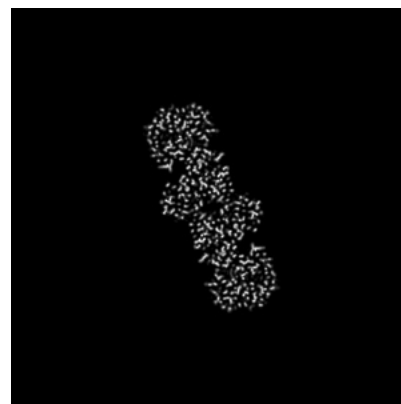
6.3.1 Primary map



X Index: 197



Y Index: 209

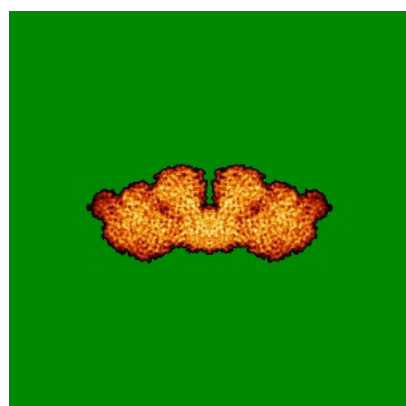


Z Index: 178

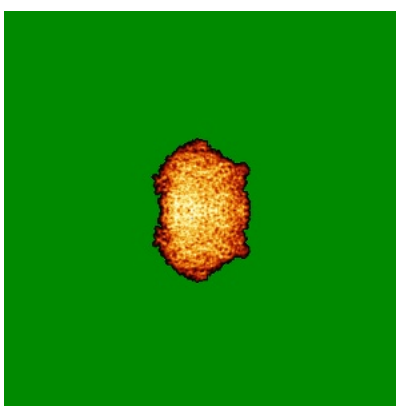
The images above show the largest variance slices of the map in three orthogonal directions.

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

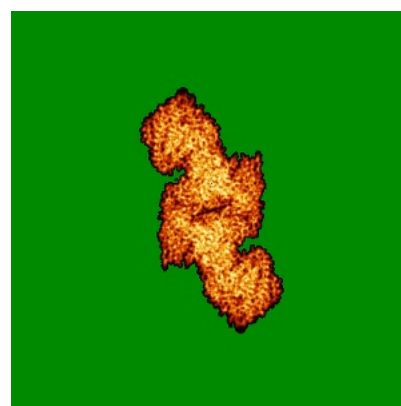
6.4.1 Primary map



X



Y

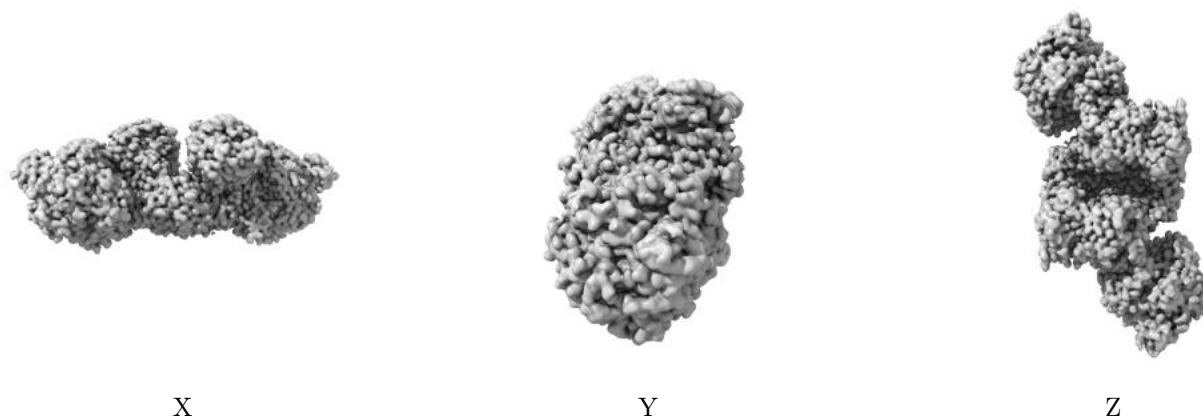


Z

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

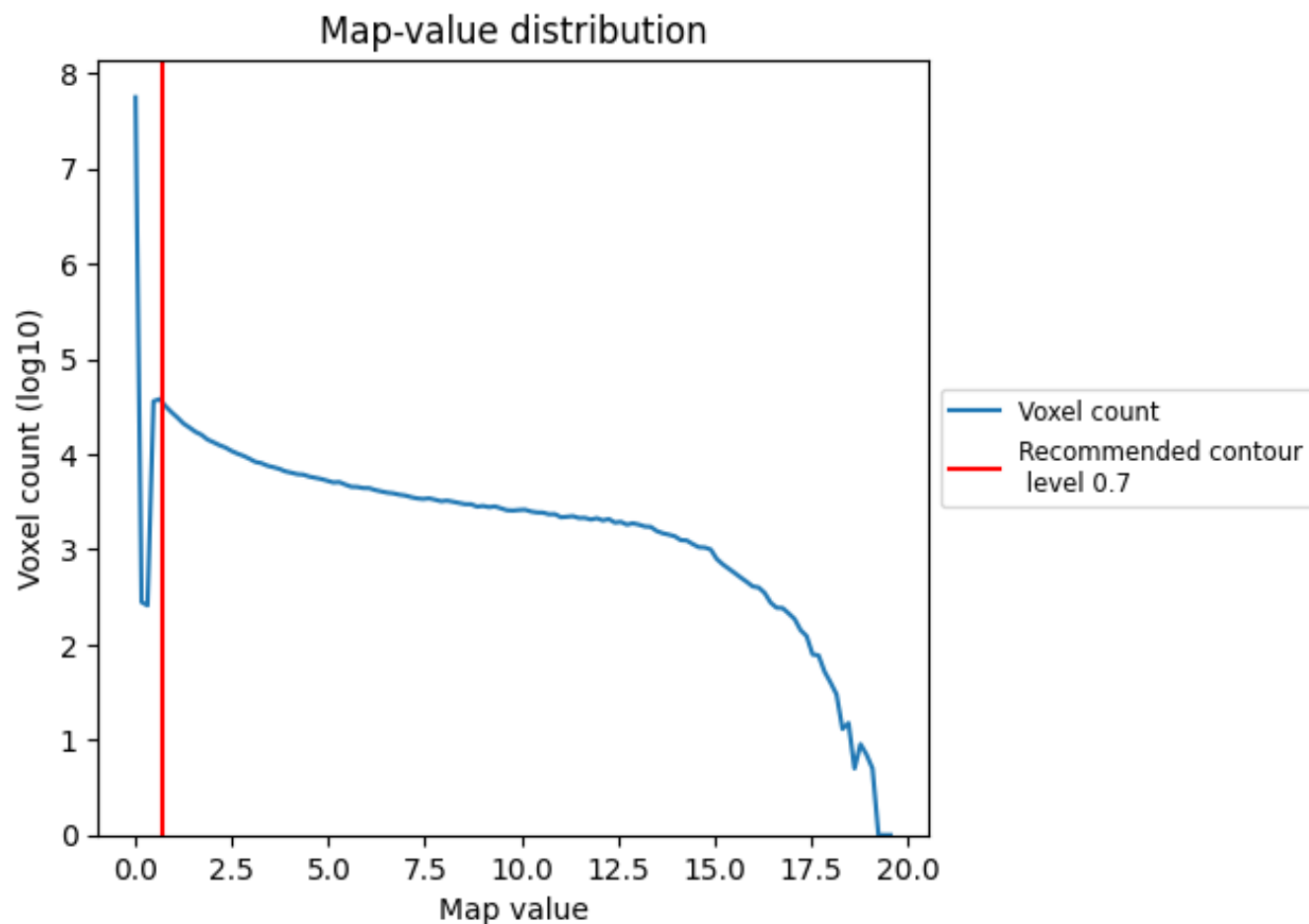
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

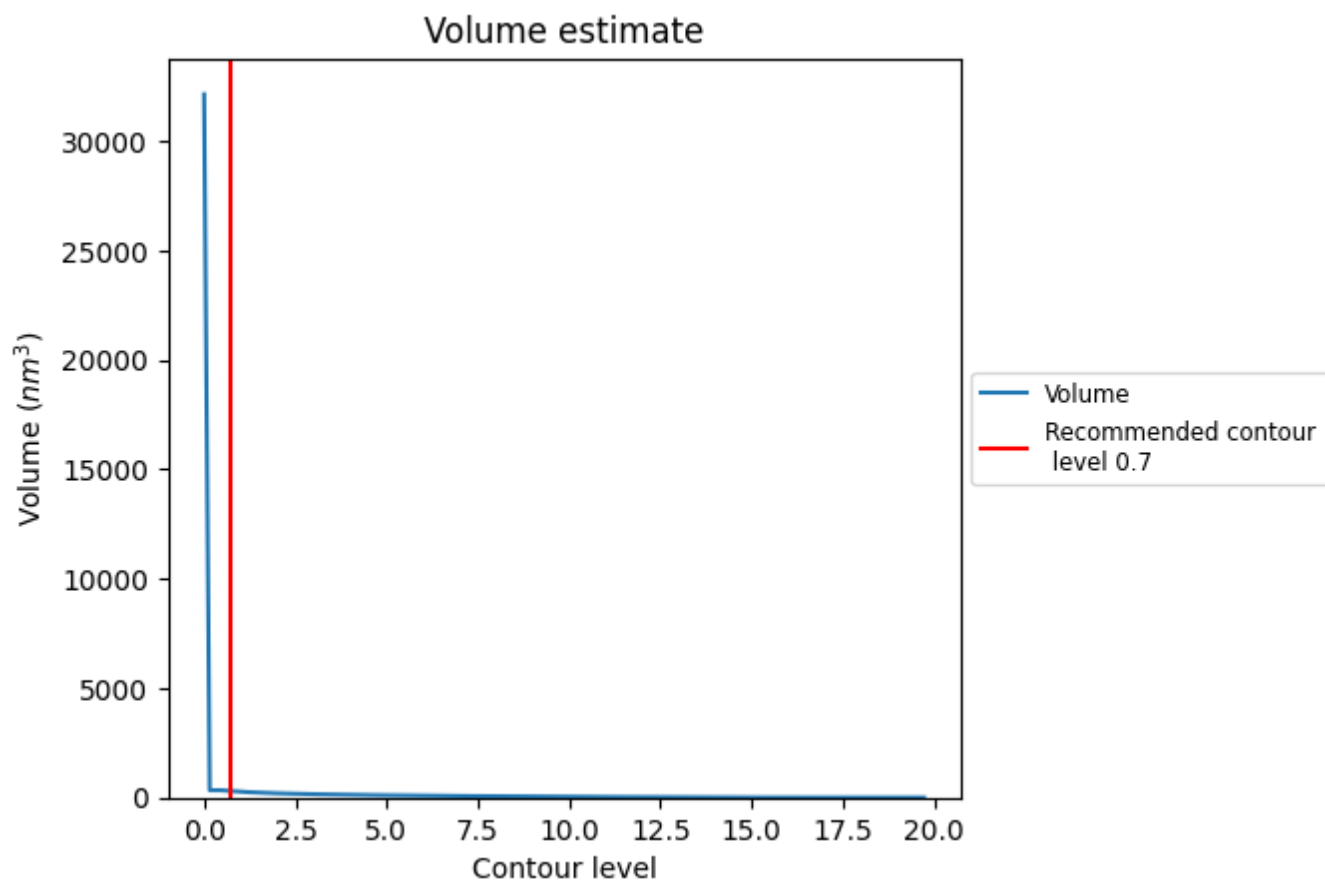
This section contains the results of statistical analysis of the map.

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.

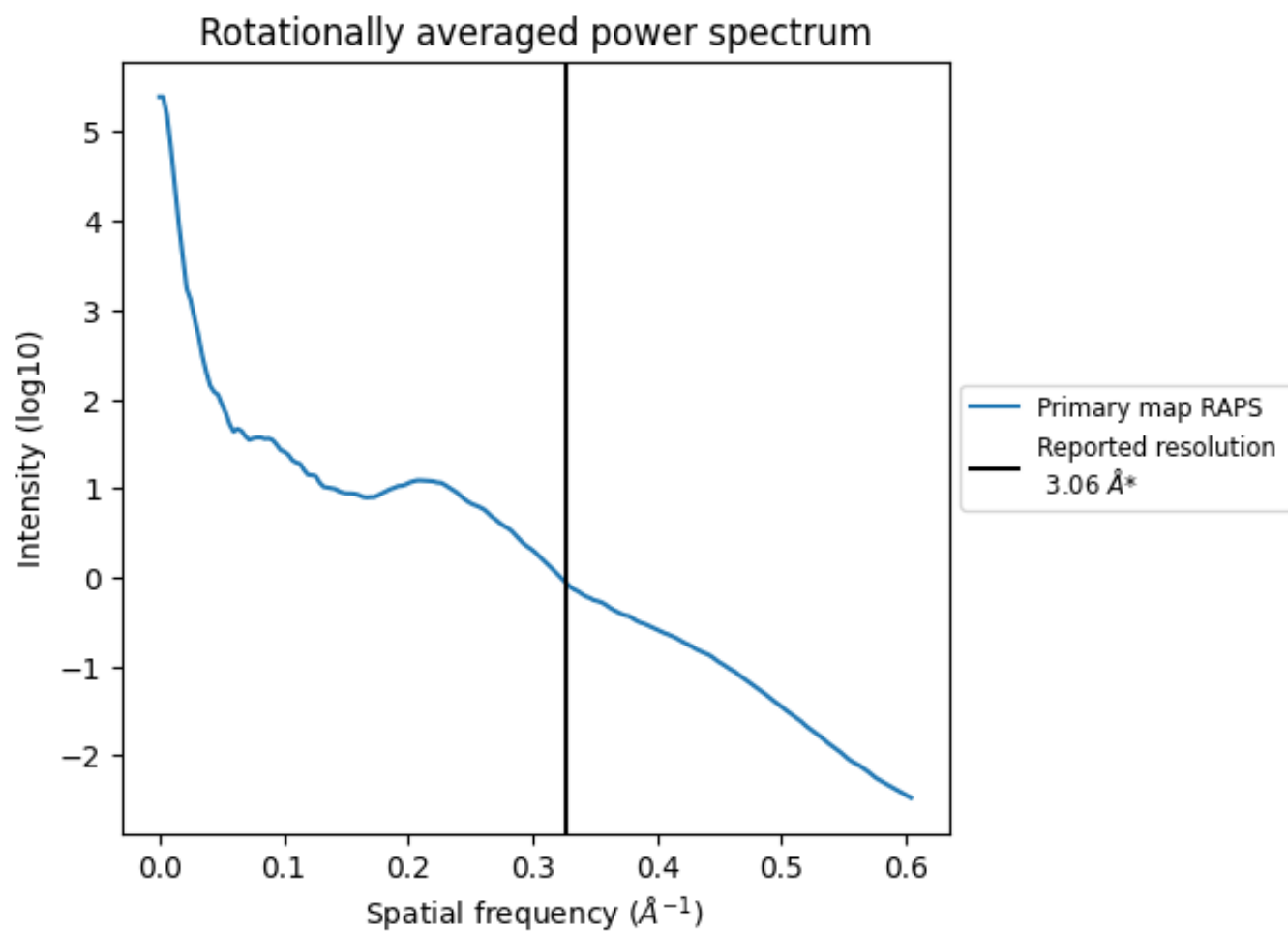
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 302 nm³; this corresponds to an approximate mass of 273 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 ⓘ

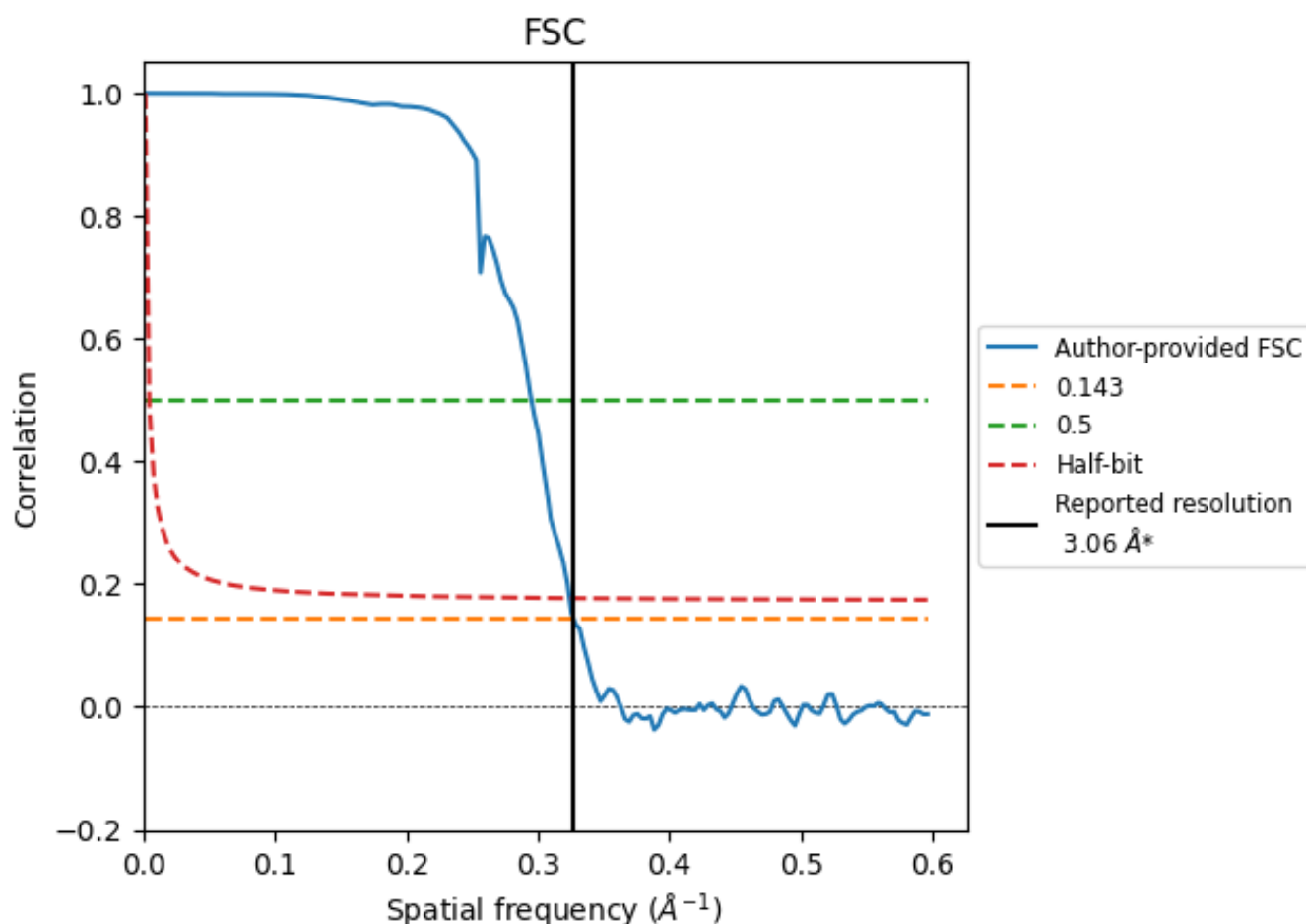


*Reported resolution corresponds to spatial frequency of 0.327 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.327 Å⁻¹

8.2 Resolution estimates [i](#)

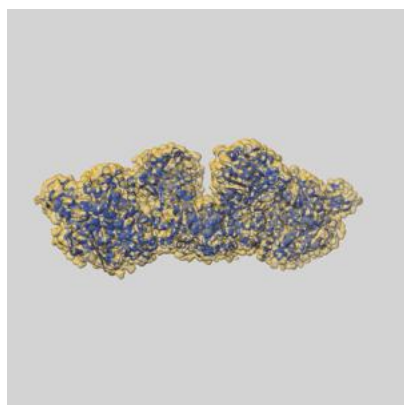
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.06	-	-
Author-provided FSC curve	3.06	3.39	3.09
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

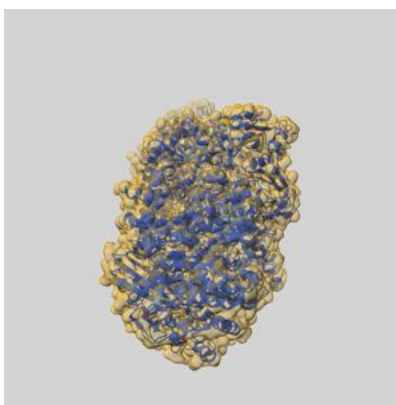
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-49341 and PDB model 9NF0. Per-residue inclusion information can be found in section [3](#) on page [9](#).

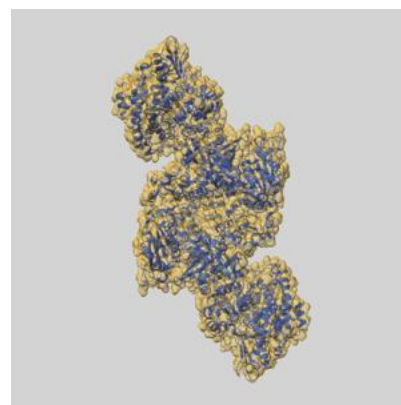
9.1 Map-model overlay [i](#)



X



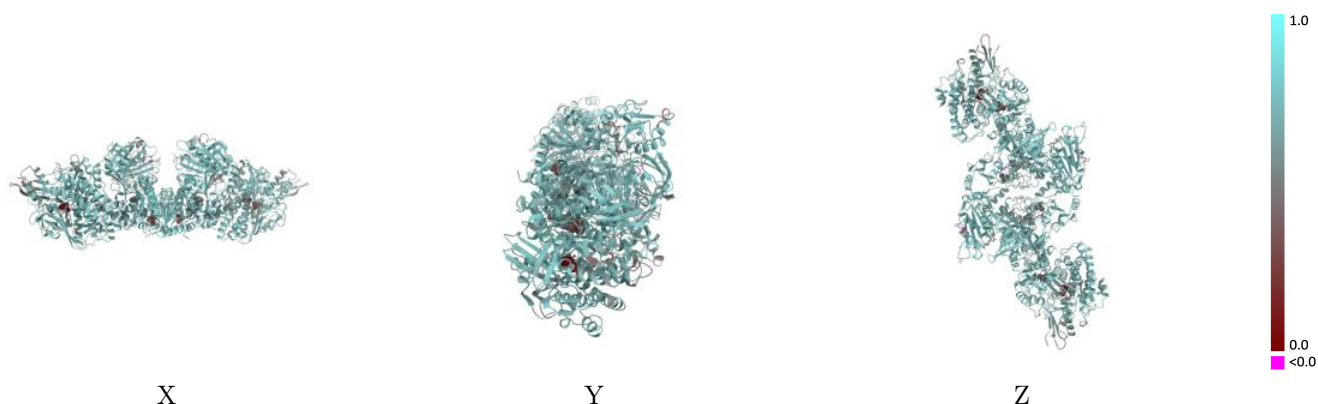
Y



Z

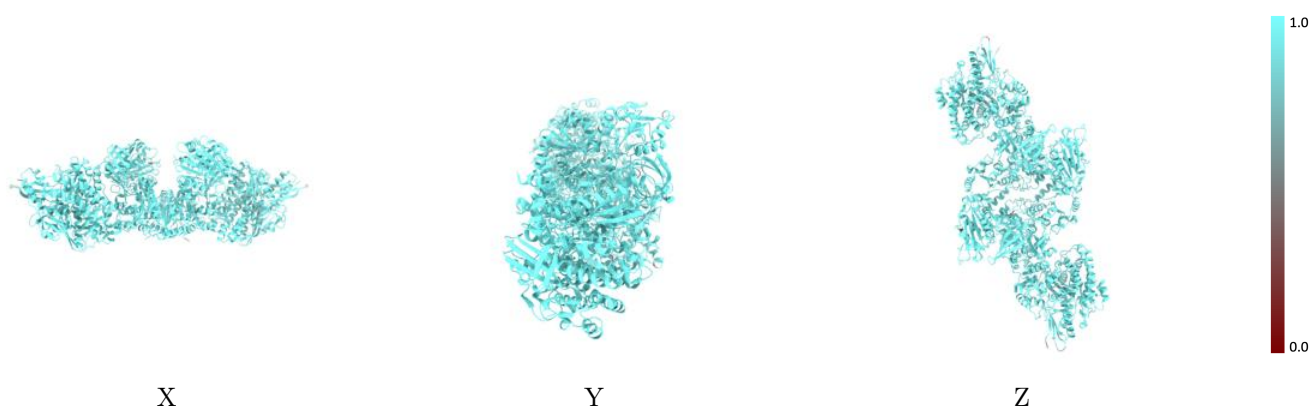
The images above show the 3D surface view of the map at the recommended contour level 0.7 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



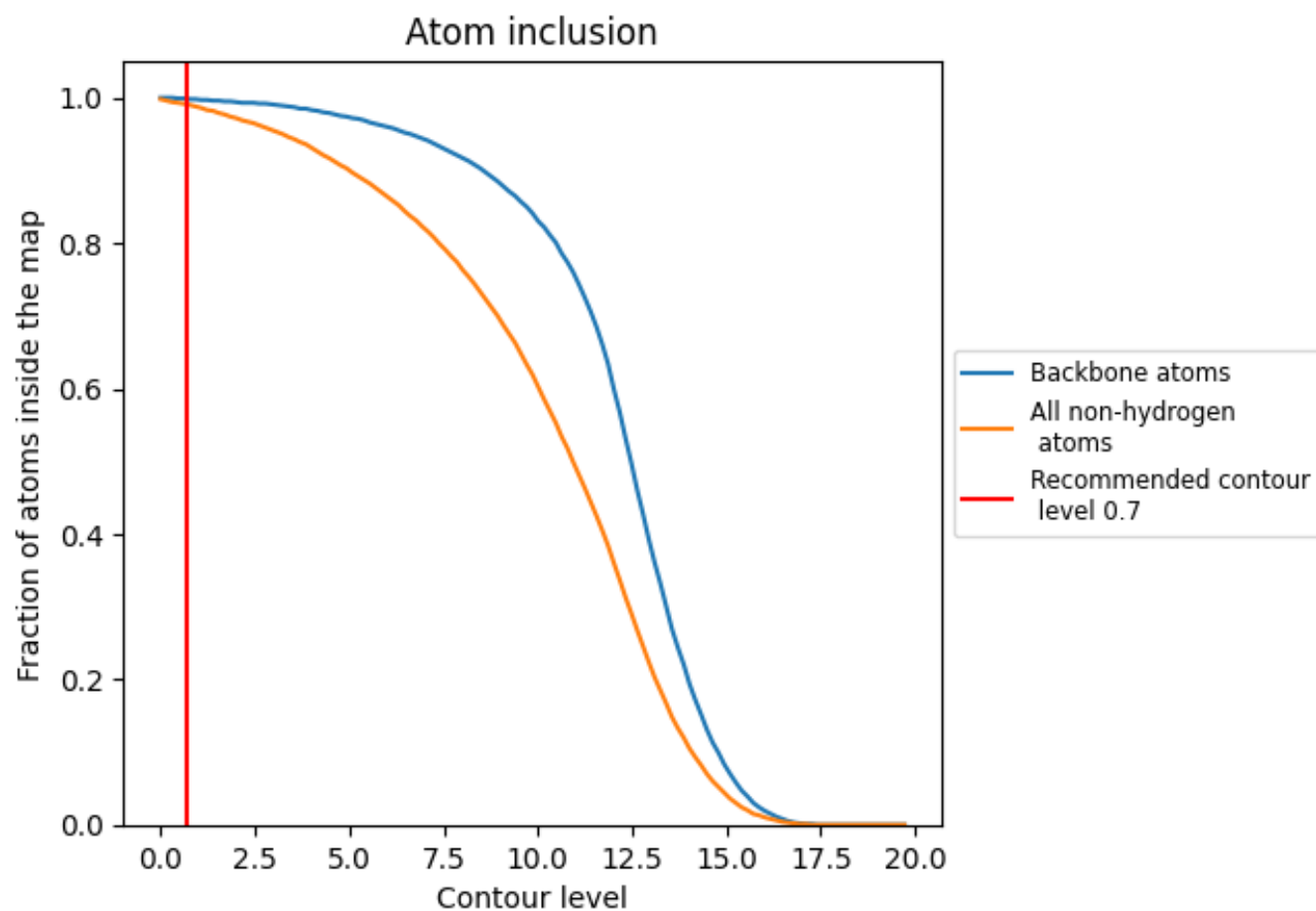
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.7).

9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 99% 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 (0.7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9910	0.6670
A	0.9980	0.6770
B	0.9940	0.6930
C	0.9870	0.6620
D	0.9880	0.6430
E	0.9980	0.6790
F	0.9960	0.6940
G	0.9880	0.6600
H	0.9860	0.6430

