



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 07:50 AM UTC

PDB ID : 8D1O / pdb_00008d1o
EMDB ID : EMD-27137
Title : hBest1_345 Ca2+-bound open state
Authors : Owji, A.P.; Kittredge, A.; Hendrickson, W.A.; Tingting, Y.
Deposited on : 2022-05-27
Resolution : 2.44 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

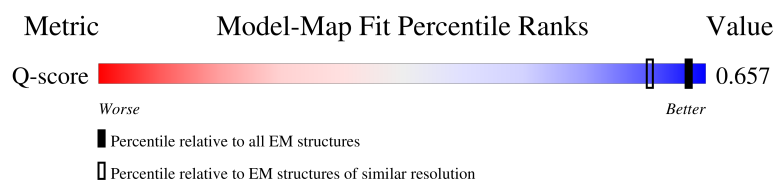
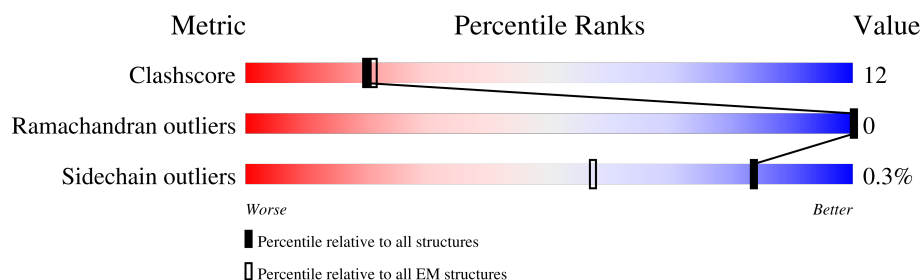
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.44 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	5856 (1.94 - 2.94)

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	345	 76% 21% .
1	B	345	 77% 20% .
1	C	345	 76% 22% .
1	D	345	 76% 22% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	E	345	76% 22%

2 Entry composition ⓘ

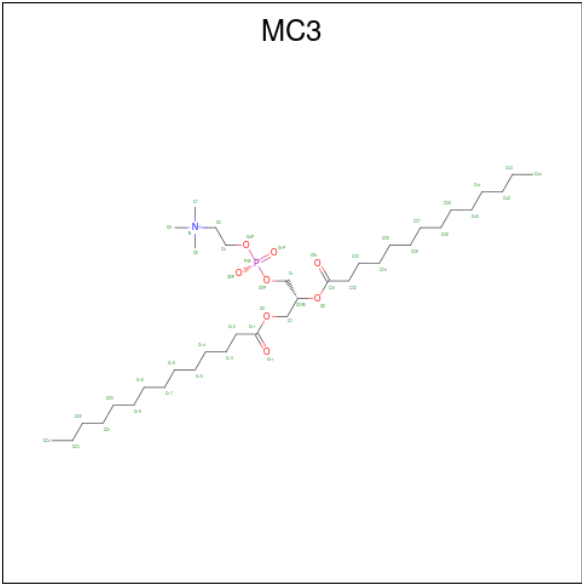
There are 4 unique types of molecules in this entry. The entry contains 15015 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Bestrophin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	E	338	Total	C	N	O	S	0	0
			2814	1859	459	482	14		
1	A	338	Total	C	N	O	S	0	0
			2814	1859	459	482	14		
1	B	338	Total	C	N	O	S	0	0
			2814	1859	459	482	14		
1	C	338	Total	C	N	O	S	0	0
			2814	1859	459	482	14		
1	D	338	Total	C	N	O	S	0	0
			2814	1859	459	482	14		

- Molecule 2 is 1,2-DIMYRISTOYL-RAC-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: MC3) (formula: C₃₆H₇₂NO₈P).



Mol	Chain	Residues	Atoms		AltConf
2	E	1	Total	C	0
			5	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
2	E	1	Total	C	O	P	0
			38	29	8	1	
2	E	1	Total	C			0
			14	14			
2	E	1	Total	C			0
			12	12			
2	E	1	Total	C			0
			14	14			
2	E	1	Total	C			0
			10	10			
2	E	1	Total	C			0
			14	14			
2	E	1	Total	C	O		0
			35	31	4		
2	A	1	Total	C	O		0
			35	31	4		
2	A	1	Total	C			0
			5	5			
2	A	1	Total	C	O	P	0
			38	29	8	1	
2	A	1	Total	C			0
			14	14			
2	A	1	Total	C			0
			12	12			
2	A	1	Total	C			0
			14	14			
2	A	1	Total	C			0
			10	10			
2	A	1	Total	C			0
			14	14			
2	B	1	Total	C	O		0
			35	31	4		
2	B	1	Total	C			0
			5	5			
2	B	1	Total	C	O	P	0
			38	29	8	1	
2	B	1	Total	C			0
			14	14			
2	B	1	Total	C			0
			12	12			
2	B	1	Total	C			0
			14	14			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
2	B	1	Total C 10 10	0
2	B	1	Total C 14 14	0
2	C	1	Total C O 35 31 4	0
2	C	1	Total C 5 5	0
2	C	1	Total C O P 38 29 8 1	0
2	C	1	Total C 14 14	0
2	C	1	Total C 12 12	0
2	C	1	Total C 14 14	0
2	C	1	Total C 10 10	0
2	C	1	Total C 14 14	0
2	D	1	Total C O 35 31 4	0
2	D	1	Total C 5 5	0
2	D	1	Total C O P 38 29 8 1	0
2	D	1	Total C 14 14	0
2	D	1	Total C 12 12	0
2	D	1	Total C 14 14	0
2	D	1	Total C 10 10	0
2	D	1	Total C 14 14	0

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
3	E	1	Total Ca 1 1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total 1	Ca 1	0
3	B	1	Total 1	Ca 1	0
3	C	1	Total 1	Ca 1	0
3	D	1	Total 1	Ca 1	0

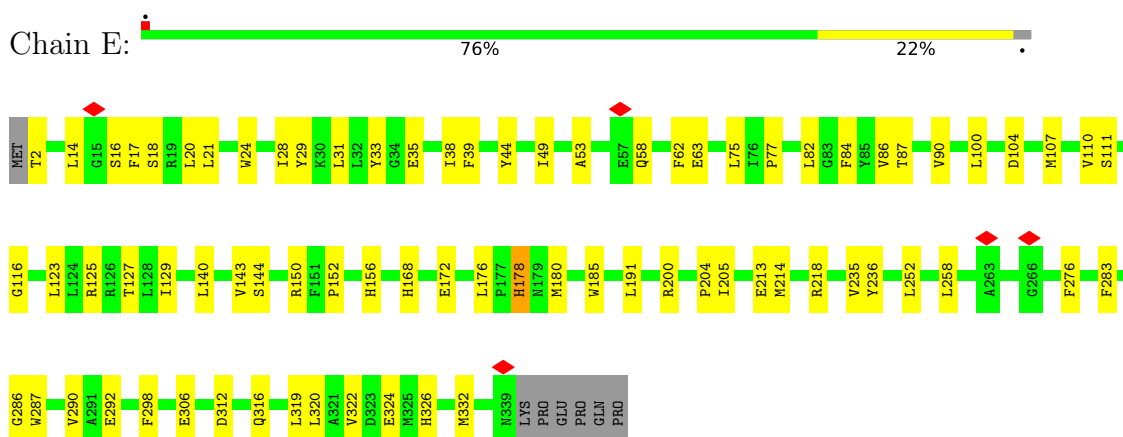
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		AltConf
4	E	46	Total 46	O 46	0
4	A	46	Total 46	O 46	0
4	B	46	Total 46	O 46	0
4	C	46	Total 46	O 46	0
4	D	46	Total 46	O 46	0

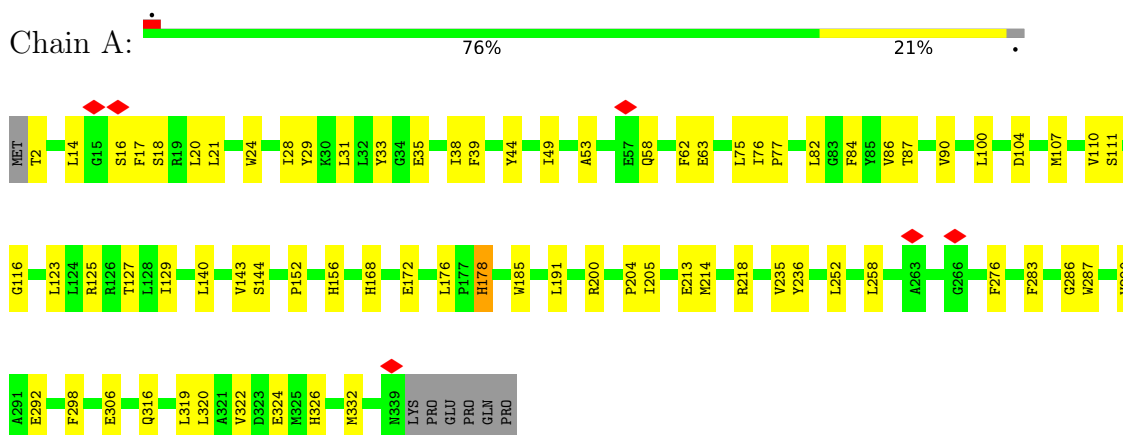
3 Residue-property plots

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.

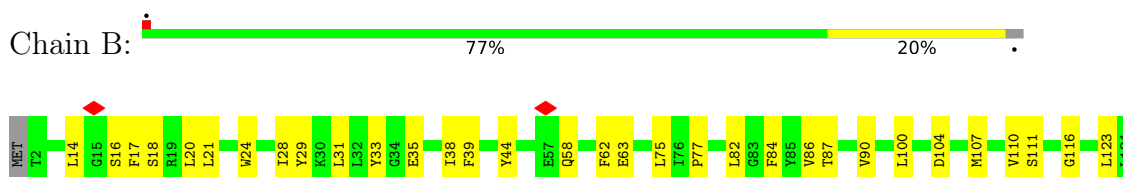
• Molecule 1: Bestrophin-1

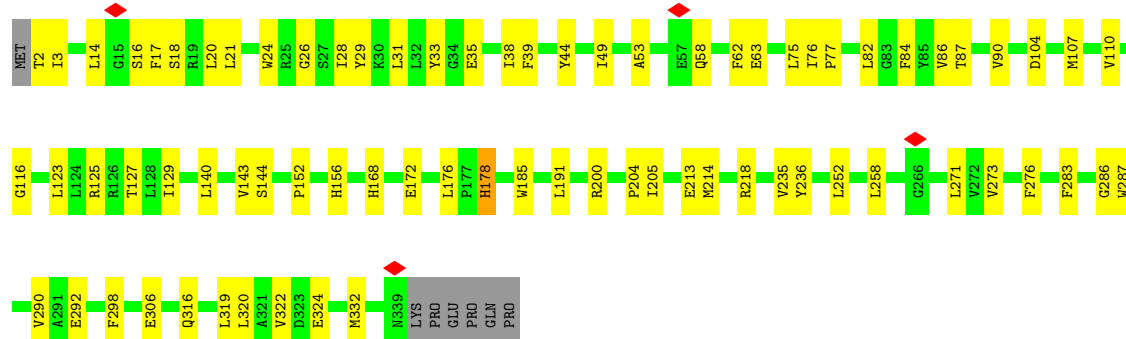


• Molecule 1: Bestrophin-1



• Molecule 1: Bestrophin-1





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	25050	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	58	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	6.649	Depositor
Minimum map value	-4.059	Depositor
Average map value	-0.021	Depositor
Map value standard deviation	0.611	Depositor
Recommended contour level	0.9	Depositor
Map size ($\text{\AA}$)	102.92, 102.92, 122.84	wwPDB
Map dimensions	124, 124, 148	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.83, 0.83, 0.83	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: CA, MC3

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	1.05	2/2899 (0.1%)	1.19	0/3952
1	B	1.06	2/2899 (0.1%)	1.19	0/3952
1	C	1.06	2/2899 (0.1%)	1.19	0/3952
1	D	1.06	2/2899 (0.1%)	1.19	0/3952
1	E	1.06	2/2899 (0.1%)	1.19	0/3952
All	All	1.06	10/14495 (0.1%)	1.19	0/19760

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	21	LEU	C-O	-6.28	1.16	1.24
1	A	21	LEU	C-O	-6.28	1.16	1.24
1	B	21	LEU	C-O	-6.28	1.16	1.24
1	D	21	LEU	C-O	-6.26	1.16	1.24
1	C	21	LEU	C-O	-6.23	1.16	1.24
1	E	213	GLU	C-O	5.83	1.30	1.24
1	D	213	GLU	C-O	5.83	1.30	1.24
1	C	213	GLU	C-O	5.83	1.30	1.24
1	B	213	GLU	C-O	5.82	1.30	1.24
1	A	213	GLU	C-O	5.75	1.30	1.24

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	2814	0	2800	91	0
1	B	2814	0	2800	92	0
1	C	2814	0	2800	94	0
1	D	2814	0	2800	93	0
1	E	2814	0	2800	95	0
2	A	142	0	235	17	0
2	B	142	0	235	17	0
2	C	142	0	235	18	0
2	D	142	0	235	16	0
2	E	142	0	235	18	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
4	A	46	0	0	0	0
4	B	46	0	0	0	0
4	C	46	0	0	0	0
4	D	46	0	0	0	0
4	E	46	0	0	0	0
All	All	15015	0	15175	371	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 12.

All (371) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:129:ILE:HD13	1:C:322:VAL:CG2	1.93	0.99
1:B:129:ILE:HD13	1:B:322:VAL:CG2	1.93	0.99
1:D:129:ILE:HD13	1:D:322:VAL:CG2	1.93	0.99
1:E:129:ILE:HD13	1:E:322:VAL:CG2	1.93	0.98
1:A:129:ILE:HD13	1:A:322:VAL:CG2	1.93	0.98
1:A:129:ILE:HD13	1:A:322:VAL:HG21	1.44	0.96
1:B:129:ILE:HD13	1:B:322:VAL:HG21	1.44	0.96
1:C:129:ILE:HD13	1:C:322:VAL:HG21	1.44	0.96
1:D:129:ILE:HD13	1:D:322:VAL:HG21	1.44	0.96
1:E:129:ILE:HD13	1:E:322:VAL:HG21	1.44	0.95
1:A:38:ILE:CG1	2:A:409:MC3:H431	2.05	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:ILE:CG1	2:B:409:MC3:H431	2.05	0.87
1:E:38:ILE:CG1	2:E:608:MC3:H431	2.05	0.87
1:C:38:ILE:CG1	2:C:409:MC3:H431	2.05	0.86
1:D:38:ILE:CG1	2:D:409:MC3:H431	2.05	0.85
1:A:129:ILE:CD1	1:A:322:VAL:HG21	2.09	0.82
1:B:129:ILE:CD1	1:B:322:VAL:HG21	2.09	0.82
1:C:129:ILE:CD1	1:C:322:VAL:HG21	2.09	0.82
1:D:129:ILE:CD1	1:D:322:VAL:HG21	2.09	0.82
1:E:129:ILE:CD1	1:E:322:VAL:HG21	2.09	0.80
1:C:292:GLU:OE1	1:D:16:SER:CB	2.31	0.79
1:E:16:SER:CB	1:D:292:GLU:OE1	2.30	0.79
1:B:292:GLU:OE1	1:C:16:SER:CB	2.31	0.79
1:A:292:GLU:OE1	1:B:16:SER:CB	2.31	0.78
1:E:292:GLU:OE1	1:A:16:SER:CB	2.31	0.78
1:C:38:ILE:HG13	2:C:409:MC3:H431	1.68	0.75
1:B:38:ILE:HG13	2:B:409:MC3:H431	1.68	0.75
1:E:129:ILE:CD1	1:E:322:VAL:CG2	2.65	0.74
1:A:129:ILE:CD1	1:A:322:VAL:CG2	2.65	0.74
1:D:286:GLY:O	1:D:290:VAL:HG23	1.88	0.74
1:D:129:ILE:CD1	1:D:322:VAL:CG2	2.65	0.74
1:E:286:GLY:O	1:E:290:VAL:HG23	1.88	0.73
1:C:286:GLY:O	1:C:290:VAL:HG23	1.88	0.73
1:D:38:ILE:HG13	2:D:409:MC3:H431	1.68	0.73
1:A:38:ILE:HG13	2:A:409:MC3:H431	1.68	0.73
1:A:286:GLY:O	1:A:290:VAL:HG23	1.88	0.73
1:B:129:ILE:CD1	1:B:322:VAL:CG2	2.65	0.73
1:B:286:GLY:O	1:B:290:VAL:HG23	1.88	0.72
1:E:38:ILE:HG13	2:E:608:MC3:H431	1.68	0.72
1:C:129:ILE:CD1	1:C:322:VAL:CG2	2.65	0.71
1:E:127:THR:HG21	1:A:332:MET:SD	2.31	0.71
1:A:129:ILE:HD13	1:A:322:VAL:HG22	1.72	0.70
1:E:332:MET:SD	1:D:127:THR:HG21	2.31	0.70
1:A:127:THR:HG21	1:B:332:MET:SD	2.31	0.70
1:B:129:ILE:HD13	1:B:322:VAL:HG22	1.72	0.70
1:B:127:THR:HG21	1:C:332:MET:SD	2.31	0.69
1:C:127:THR:HG21	1:D:332:MET:SD	2.31	0.69
1:C:129:ILE:HD13	1:C:322:VAL:HG22	1.72	0.69
1:E:129:ILE:HD13	1:E:322:VAL:HG22	1.72	0.68
1:C:38:ILE:HG12	2:C:409:MC3:H431	1.76	0.67
1:D:129:ILE:HD13	1:D:322:VAL:HG22	1.72	0.67
1:D:38:ILE:HG12	2:D:409:MC3:H431	1.76	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:ILE:HG12	2:A:409:MC3:H431	1.76	0.67
1:B:38:ILE:HG12	2:B:409:MC3:H431	1.76	0.66
1:E:38:ILE:HG12	2:E:608:MC3:H431	1.76	0.66
1:B:168:HIS:NE2	1:B:172:GLU:OE2	2.29	0.66
1:A:168:HIS:NE2	1:A:172:GLU:OE2	2.29	0.65
1:C:168:HIS:NE2	1:C:172:GLU:OE2	2.29	0.65
1:B:292:GLU:CD	1:C:16:SER:HB3	2.22	0.65
1:E:168:HIS:NE2	1:E:172:GLU:OE2	2.29	0.65
1:A:292:GLU:CD	1:B:16:SER:HB3	2.22	0.64
1:C:292:GLU:CD	1:D:16:SER:HB3	2.22	0.64
1:D:168:HIS:NE2	1:D:172:GLU:OE2	2.29	0.64
1:A:17:PHE:HA	1:A:20:LEU:HD12	1.79	0.64
1:C:17:PHE:HA	1:C:20:LEU:HD12	1.79	0.64
1:D:17:PHE:HA	1:D:20:LEU:HD12	1.79	0.64
1:E:17:PHE:HA	1:E:20:LEU:HD12	1.79	0.64
1:E:16:SER:HB3	1:D:292:GLU:CD	2.22	0.63
1:E:292:GLU:CD	1:A:16:SER:HB3	2.22	0.63
1:E:16:SER:CB	1:D:292:GLU:CD	2.72	0.63
1:B:17:PHE:HA	1:B:20:LEU:HD12	1.79	0.63
1:A:86:VAL:HG21	1:A:287:TRP:CD1	2.34	0.62
1:B:86:VAL:HG21	1:B:287:TRP:CD1	2.34	0.62
1:A:292:GLU:CD	1:B:16:SER:CB	2.73	0.62
1:B:292:GLU:CD	1:C:16:SER:CB	2.73	0.62
1:C:292:GLU:CD	1:D:16:SER:CB	2.73	0.62
1:E:86:VAL:HG21	1:E:287:TRP:CD1	2.34	0.62
1:C:86:VAL:HG21	1:C:287:TRP:CD1	2.34	0.62
1:E:292:GLU:CD	1:A:16:SER:CB	2.73	0.62
1:D:86:VAL:HG21	1:D:287:TRP:CD1	2.34	0.61
1:E:75:LEU:HD22	1:A:276:PHE:HB3	1.83	0.60
1:A:75:LEU:HD22	1:B:276:PHE:HB3	1.83	0.60
1:C:75:LEU:HD22	1:D:276:PHE:HB3	1.83	0.60
1:E:276:PHE:HB3	1:D:75:LEU:HD22	1.83	0.60
1:B:75:LEU:HD22	1:C:276:PHE:HB3	1.83	0.59
1:B:82:LEU:HG	1:B:287:TRP:HD1	1.69	0.58
1:A:82:LEU:HG	1:A:287:TRP:HD1	1.69	0.58
1:E:235:VAL:HG21	1:A:290:VAL:HG13	1.86	0.58
1:C:82:LEU:HG	1:C:287:TRP:HD1	1.69	0.57
1:E:16:SER:HB3	1:D:292:GLU:OE2	2.05	0.57
1:A:235:VAL:HG21	1:B:290:VAL:HG13	1.86	0.57
1:A:292:GLU:OE2	1:B:16:SER:HB3	2.05	0.57
1:B:235:VAL:HG21	1:C:290:VAL:HG13	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:290:VAL:HG13	1:D:235:VAL:HG21	1.86	0.57
1:E:292:GLU:OE2	1:A:16:SER:HB3	2.05	0.57
1:C:104:ASP:HA	1:C:107:MET:HG2	1.87	0.57
1:C:235:VAL:HG21	1:D:290:VAL:HG13	1.86	0.57
1:D:104:ASP:HA	1:D:107:MET:HG2	1.87	0.57
1:A:104:ASP:HA	1:A:107:MET:HG2	1.87	0.57
1:B:104:ASP:HA	1:B:107:MET:HG2	1.87	0.56
1:D:82:LEU:HG	1:D:287:TRP:HD1	1.69	0.56
1:E:84:PHE:HZ	1:A:90:VAL:HG21	1.70	0.56
1:C:292:GLU:OE2	1:D:16:SER:HB3	2.05	0.56
1:E:82:LEU:HG	1:E:287:TRP:HD1	1.69	0.56
1:A:84:PHE:HZ	1:B:90:VAL:HG21	1.71	0.56
1:C:252:LEU:HD11	2:D:401:MC3:H443	1.88	0.56
1:E:90:VAL:HG21	1:D:84:PHE:HZ	1.71	0.56
2:E:609:MC3:H443	1:D:252:LEU:HD11	1.88	0.56
1:B:252:LEU:HD11	2:C:401:MC3:H443	1.88	0.56
1:E:252:LEU:HD11	2:A:401:MC3:H443	1.88	0.56
1:C:292:GLU:OE1	1:D:16:SER:HB2	2.06	0.56
1:A:292:GLU:OE1	1:B:16:SER:HB2	2.06	0.56
1:B:292:GLU:OE1	1:C:16:SER:HB2	2.06	0.56
1:E:104:ASP:HA	1:E:107:MET:HG2	1.87	0.56
1:B:84:PHE:HZ	1:C:90:VAL:HG21	1.71	0.56
1:B:292:GLU:OE2	1:C:16:SER:HB3	2.05	0.56
1:A:252:LEU:HD11	2:B:401:MC3:H443	1.88	0.55
1:C:84:PHE:HZ	1:D:90:VAL:HG21	1.71	0.55
1:E:292:GLU:OE1	1:A:16:SER:HB2	2.06	0.54
1:B:116:GLY:HA3	1:B:200:ARG:HH21	1.72	0.54
1:D:116:GLY:HA3	1:D:200:ARG:HH21	1.72	0.54
1:A:116:GLY:HA3	1:A:200:ARG:HH21	1.72	0.54
1:C:116:GLY:HA3	1:C:200:ARG:HH21	1.72	0.54
1:E:116:GLY:HA3	1:E:200:ARG:HH21	1.72	0.54
1:E:16:SER:HB2	1:D:292:GLU:OE1	2.05	0.53
1:A:62:PHE:HD2	2:A:404:MC3:H352	1.74	0.53
1:B:62:PHE:HD2	2:B:404:MC3:H352	1.74	0.53
1:C:62:PHE:HD2	2:C:404:MC3:H352	1.74	0.52
1:E:290:VAL:HG11	1:D:236:TYR:CZ	2.45	0.52
2:E:602:MC3:H412	2:E:602:MC3:H201	1.91	0.52
1:E:62:PHE:HD2	2:E:603:MC3:H352	1.74	0.52
1:E:236:TYR:CZ	1:A:290:VAL:HG11	2.44	0.52
1:C:236:TYR:CZ	1:D:290:VAL:HG11	2.45	0.52
2:C:403:MC3:H201	2:C:403:MC3:H412	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:403:MC3:H201	2:D:403:MC3:H412	1.91	0.52
1:D:62:PHE:HD2	2:D:404:MC3:H352	1.74	0.52
2:A:403:MC3:H201	2:A:403:MC3:H412	1.91	0.51
2:B:403:MC3:H201	2:B:403:MC3:H412	1.91	0.51
1:B:236:TYR:CZ	1:C:290:VAL:HG11	2.45	0.51
1:D:28:ILE:HD11	1:D:286:GLY:CA	2.41	0.51
1:A:236:TYR:CZ	1:B:290:VAL:HG11	2.45	0.51
1:E:16:SER:HB3	1:D:292:GLU:OE1	2.10	0.51
1:C:28:ILE:HD11	1:C:286:GLY:CA	2.40	0.51
1:E:28:ILE:HD11	1:E:286:GLY:CA	2.40	0.51
1:B:28:ILE:HD11	1:B:286:GLY:CA	2.40	0.50
1:E:58:GLN:HG2	2:E:603:MC3:C31	2.42	0.50
1:D:58:GLN:HG2	2:D:404:MC3:C31	2.42	0.50
1:A:28:ILE:HD11	1:A:286:GLY:CA	2.41	0.50
1:A:176:LEU:HD13	1:A:178:HIS:HE1	1.77	0.50
1:B:185:TRP:CD1	1:B:214:MET:HE3	2.47	0.49
1:D:129:ILE:HD11	1:D:319:LEU:HD23	1.94	0.49
1:E:129:ILE:HD11	1:E:319:LEU:HD23	1.94	0.49
1:E:185:TRP:CD1	1:E:214:MET:HE3	2.47	0.49
1:E:176:LEU:HD13	1:E:178:HIS:HE1	1.77	0.49
1:E:218:ARG:HH21	1:A:104:ASP:CG	2.21	0.49
1:A:218:ARG:HH21	1:B:104:ASP:CG	2.21	0.49
1:B:129:ILE:HD11	1:B:319:LEU:HD23	1.94	0.49
1:C:185:TRP:CD1	1:C:214:MET:HE3	2.47	0.49
1:E:292:GLU:OE1	1:A:16:SER:HB3	2.10	0.49
1:B:176:LEU:HD13	1:B:178:HIS:HE1	1.77	0.49
1:D:185:TRP:CD1	1:D:214:MET:HE3	2.47	0.49
1:E:104:ASP:CG	1:D:218:ARG:HH21	2.21	0.49
1:B:58:GLN:HG2	2:B:404:MC3:C31	2.42	0.49
1:C:58:GLN:HG2	2:C:404:MC3:C31	2.42	0.49
1:A:58:GLN:HG2	2:A:404:MC3:C31	2.42	0.49
1:C:144:SER:HB2	1:C:298:PHE:HB3	1.95	0.49
1:C:218:ARG:HH21	1:D:104:ASP:CG	2.21	0.49
1:A:129:ILE:HD11	1:A:319:LEU:HD23	1.94	0.48
1:B:218:ARG:HH21	1:C:104:ASP:CG	2.21	0.48
1:A:123:LEU:HG	1:B:332:MET:HG2	1.96	0.48
1:A:185:TRP:CD1	1:A:214:MET:HE3	2.47	0.48
1:B:144:SER:HB2	1:B:298:PHE:HB3	1.95	0.48
1:E:283:PHE:CD2	1:D:77:PRO:HD2	2.49	0.48
1:B:123:LEU:HG	1:C:332:MET:HG2	1.96	0.48
1:C:84:PHE:O	1:C:87:THR:HG22	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:176:LEU:HD13	1:C:178:HIS:HE1	1.77	0.48
1:D:176:LEU:HD13	1:D:178:HIS:HE1	1.77	0.48
1:D:84:PHE:O	1:D:87:THR:HG22	2.14	0.48
1:E:77:PRO:HD2	1:A:283:PHE:CD2	2.49	0.48
1:C:123:LEU:HG	1:D:332:MET:HG2	1.96	0.48
1:E:144:SER:HB2	1:E:298:PHE:HB3	1.95	0.47
1:E:332:MET:HG2	1:D:123:LEU:HG	1.95	0.47
1:B:39:PHE:HD1	2:C:401:MC3:H421	1.79	0.47
1:B:77:PRO:HD2	1:C:283:PHE:CD2	2.49	0.47
1:C:129:ILE:HD11	1:C:319:LEU:HD23	1.94	0.47
2:C:401:MC3:H242	2:C:401:MC3:H212	1.73	0.47
1:B:84:PHE:O	1:B:87:THR:HG22	2.14	0.47
1:E:123:LEU:HG	1:A:332:MET:HG2	1.96	0.47
1:A:144:SER:HB2	1:A:298:PHE:HB3	1.95	0.47
1:E:84:PHE:O	1:E:87:THR:HG22	2.14	0.47
1:A:39:PHE:HD1	2:B:401:MC3:H421	1.79	0.47
1:C:39:PHE:HD1	2:D:401:MC3:H421	1.79	0.47
1:E:44:TYR:CE2	2:E:605:MC3:H402	2.50	0.47
1:E:283:PHE:O	1:E:287:TRP:HB2	2.15	0.47
1:A:44:TYR:CE2	2:A:406:MC3:H402	2.50	0.47
1:A:77:PRO:HD2	1:B:283:PHE:CD2	2.49	0.47
1:A:84:PHE:O	1:A:87:THR:HG22	2.14	0.47
1:B:44:TYR:CE2	2:B:406:MC3:H402	2.50	0.47
1:D:144:SER:HB2	1:D:298:PHE:HB3	1.95	0.47
1:B:283:PHE:O	1:B:287:TRP:HB2	2.15	0.47
1:B:185:TRP:CD1	1:B:214:MET:HG3	2.50	0.47
1:A:185:TRP:CD1	1:A:214:MET:HG3	2.50	0.47
1:B:24:TRP:HB2	2:B:403:MC3:H351	1.97	0.47
1:D:24:TRP:HB2	2:D:403:MC3:H351	1.97	0.47
1:D:185:TRP:CD1	1:D:214:MET:HG3	2.50	0.47
1:D:283:PHE:O	1:D:287:TRP:HB2	2.15	0.47
2:E:609:MC3:H421	1:D:39:PHE:HD1	1.79	0.46
1:C:77:PRO:HD2	1:D:283:PHE:CD2	2.49	0.46
1:C:283:PHE:O	1:C:287:TRP:HB2	2.15	0.46
1:C:185:TRP:CD1	1:C:214:MET:HG3	2.50	0.46
1:A:111:SER:O	1:A:326:HIS:ND1	2.36	0.46
1:C:44:TYR:CE2	2:C:406:MC3:H402	2.50	0.46
1:E:39:PHE:HD1	2:A:401:MC3:H421	1.79	0.46
1:E:185:TRP:CD1	1:E:214:MET:HG3	2.50	0.46
1:E:24:TRP:HB2	2:E:602:MC3:H351	1.97	0.46
1:B:235:VAL:HG11	1:C:31:LEU:HD12	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:44:TYR:CE2	2:D:406:MC3:H402	2.50	0.46
1:A:235:VAL:HG11	1:B:31:LEU:HD12	1.98	0.46
1:B:129:ILE:HG21	1:B:322:VAL:HG11	1.98	0.46
1:A:28:ILE:HD11	1:A:286:GLY:HA3	1.98	0.46
1:A:292:GLU:OE1	1:B:16:SER:HB3	2.10	0.46
1:B:63:GLU:HG2	1:B:258:LEU:HD22	1.98	0.46
1:C:129:ILE:HG21	1:C:322:VAL:HG11	1.98	0.46
1:E:235:VAL:HG11	1:A:31:LEU:HD12	1.98	0.46
1:A:283:PHE:O	1:A:287:TRP:HB2	2.15	0.46
1:E:28:ILE:HD11	1:E:286:GLY:HA3	1.98	0.45
1:A:129:ILE:HG21	1:A:322:VAL:HG11	1.98	0.45
1:C:24:TRP:HB2	2:C:403:MC3:H351	1.97	0.45
1:D:63:GLU:HG2	1:D:258:LEU:HD22	1.98	0.45
1:A:24:TRP:HB2	2:A:403:MC3:H351	1.97	0.45
1:C:235:VAL:HG11	1:D:31:LEU:HD12	1.98	0.45
1:E:129:ILE:HG21	1:E:322:VAL:HG11	1.98	0.45
1:E:14:LEU:HD12	1:D:35:GLU:HG3	1.99	0.45
1:E:84:PHE:CE2	1:A:86:VAL:HG12	2.52	0.45
1:A:204:PRO:HB2	1:B:205:ILE:HG21	1.99	0.45
1:C:84:PHE:CE2	1:D:86:VAL:HG12	2.52	0.45
1:C:127:THR:HG23	1:C:191:LEU:HD21	1.99	0.45
1:D:129:ILE:HG21	1:D:322:VAL:HG11	1.98	0.45
1:E:205:ILE:HG21	1:D:204:PRO:HB2	1.99	0.45
1:B:204:PRO:HB2	1:C:205:ILE:HG21	1.99	0.45
1:D:127:THR:HG23	1:D:191:LEU:HD21	1.99	0.45
1:E:31:LEU:HD12	1:D:235:VAL:HG11	1.98	0.45
1:E:204:PRO:HB2	1:A:205:ILE:HG21	1.99	0.45
1:A:63:GLU:HG2	1:A:258:LEU:HD22	1.98	0.45
1:B:292:GLU:OE1	1:C:16:SER:HB3	2.10	0.45
1:C:63:GLU:HG2	1:C:258:LEU:HD22	1.98	0.45
1:C:204:PRO:HB2	1:D:205:ILE:HG21	1.99	0.45
1:A:29:TYR:HB3	2:A:403:MC3:H201	1.99	0.45
1:B:35:GLU:HG3	1:C:14:LEU:HD12	1.99	0.45
1:B:84:PHE:CE2	1:C:86:VAL:HG12	2.52	0.45
1:A:24:TRP:CZ3	2:A:403:MC3:H141	2.52	0.45
1:A:84:PHE:CE2	1:B:86:VAL:HG12	2.52	0.45
1:B:28:ILE:HD11	1:B:286:GLY:HA3	1.98	0.45
1:C:35:GLU:HG3	1:D:14:LEU:HD12	1.99	0.45
1:E:127:THR:HG23	1:E:191:LEU:HD21	1.99	0.44
1:C:28:ILE:HD11	1:C:286:GLY:HA3	1.98	0.44
1:D:320:LEU:HD12	1:D:324:GLU:HB2	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:86:VAL:HG12	1:D:84:PHE:CE2	2.52	0.44
1:B:127:THR:HG23	1:B:191:LEU:HD21	1.99	0.44
1:A:35:GLU:HG3	1:B:14:LEU:HD12	1.99	0.44
1:E:63:GLU:HG2	1:E:258:LEU:HD22	1.98	0.44
1:B:29:TYR:HB3	2:B:403:MC3:H201	1.99	0.44
1:C:292:GLU:OE1	1:D:16:SER:HB3	2.10	0.44
1:E:24:TRP:CZ3	2:E:602:MC3:H141	2.52	0.44
1:E:29:TYR:HB3	2:E:602:MC3:H201	1.99	0.44
1:D:24:TRP:CZ3	2:D:403:MC3:H141	2.52	0.44
1:C:24:TRP:CZ3	2:C:403:MC3:H141	2.52	0.44
1:E:35:GLU:HG3	1:A:14:LEU:HD12	1.99	0.44
1:E:320:LEU:HD12	1:E:324:GLU:HB2	1.99	0.44
1:C:24:TRP:CE3	2:C:403:MC3:H141	2.53	0.44
2:E:609:MC3:H242	2:E:609:MC3:H212	1.73	0.44
1:B:24:TRP:CE3	2:B:403:MC3:H141	2.53	0.44
1:C:320:LEU:HD12	1:C:324:GLU:HB2	1.99	0.44
1:D:29:TYR:CZ	2:D:403:MC3:H392	2.53	0.44
1:D:33:TYR:HB3	2:D:403:MC3:H211	2.00	0.44
1:D:110:VAL:HG12	1:D:125:ARG:HG2	2.00	0.44
1:A:29:TYR:CZ	2:A:403:MC3:H392	2.53	0.44
1:B:24:TRP:CZ3	2:B:403:MC3:H141	2.52	0.44
1:D:28:ILE:HD11	1:D:286:GLY:HA3	1.98	0.44
1:A:16:SER:C	1:A:18:SER:H	2.26	0.43
1:A:127:THR:HG23	1:A:191:LEU:HD21	1.99	0.43
1:A:320:LEU:HD12	1:A:324:GLU:HB2	1.99	0.43
1:B:110:VAL:HG12	1:B:125:ARG:HG2	2.00	0.43
1:B:320:LEU:HD12	1:B:324:GLU:HB2	1.99	0.43
1:C:29:TYR:CZ	2:C:403:MC3:H392	2.53	0.43
1:D:24:TRP:CE3	2:D:403:MC3:H141	2.53	0.43
1:B:29:TYR:HB3	2:B:403:MC3:C20	2.49	0.43
1:B:111:SER:O	1:B:326:HIS:ND1	2.36	0.43
1:C:16:SER:C	1:C:18:SER:H	2.26	0.43
1:D:16:SER:C	1:D:18:SER:H	2.27	0.43
1:E:29:TYR:CZ	2:E:602:MC3:H392	2.53	0.43
1:D:29:TYR:HB3	2:D:403:MC3:H201	1.99	0.43
1:A:24:TRP:CE3	2:A:403:MC3:H141	2.53	0.43
1:A:33:TYR:HB3	2:A:403:MC3:H211	2.00	0.43
1:E:29:TYR:HB3	2:E:602:MC3:C20	2.49	0.43
1:B:29:TYR:CZ	2:B:403:MC3:H392	2.53	0.43
1:E:24:TRP:CE3	2:E:602:MC3:H141	2.53	0.43
1:C:29:TYR:HB3	2:C:403:MC3:C20	2.49	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:178:HIS:NE2	1:D:316:GLN:OE1	2.52	0.43
1:C:110:VAL:HG12	1:C:125:ARG:HG2	2.00	0.43
1:D:129:ILE:CD1	1:D:322:VAL:HG22	2.42	0.43
1:E:110:VAL:HG12	1:E:125:ARG:HG2	2.00	0.43
1:A:75:LEU:HD22	1:B:276:PHE:CB	2.48	0.43
1:C:29:TYR:HB3	2:C:403:MC3:H201	1.99	0.43
1:A:178:HIS:NE2	1:B:316:GLN:OE1	2.52	0.42
1:E:316:GLN:OE1	1:D:178:HIS:NE2	2.52	0.42
1:B:33:TYR:HB3	2:B:403:MC3:H211	2.00	0.42
1:B:178:HIS:NE2	1:C:316:GLN:OE1	2.52	0.42
1:D:29:TYR:HB3	2:D:403:MC3:C20	2.49	0.42
1:E:16:SER:C	1:E:18:SER:H	2.27	0.42
1:E:33:TYR:HB3	2:E:602:MC3:H211	2.00	0.42
1:A:140:LEU:HA	1:A:143:VAL:HG22	2.02	0.42
1:A:110:VAL:HG12	1:A:125:ARG:HG2	2.00	0.42
1:B:75:LEU:HD22	1:C:276:PHE:CB	2.48	0.42
1:E:75:LEU:HD22	1:A:276:PHE:CB	2.48	0.42
1:C:33:TYR:HB3	2:C:403:MC3:H211	2.00	0.42
1:C:100:LEU:HD21	1:C:298:PHE:HE1	1.85	0.42
1:C:111:SER:O	1:C:326:HIS:ND1	2.36	0.42
1:E:178:HIS:NE2	1:A:316:GLN:OE1	2.52	0.42
1:A:29:TYR:HB3	2:A:403:MC3:C20	2.49	0.42
1:B:100:LEU:HD21	1:B:298:PHE:HE1	1.85	0.42
1:C:129:ILE:CD1	1:C:322:VAL:HG22	2.42	0.41
1:B:16:SER:C	1:B:18:SER:H	2.27	0.41
1:E:49:ILE:O	1:E:53:ALA:HB3	2.21	0.41
1:D:3:ILE:HG13	1:D:26:GLY:HA3	2.03	0.41
1:E:16:SER:C	1:E:18:SER:N	2.78	0.41
1:E:140:LEU:HA	1:E:143:VAL:HG22	2.02	0.41
1:B:140:LEU:HA	1:B:143:VAL:HG22	2.02	0.41
1:D:76:ILE:HA	1:D:77:PRO:HD3	1.90	0.41
1:E:100:LEU:HD21	1:E:298:PHE:HE1	1.85	0.41
1:C:16:SER:C	1:C:18:SER:N	2.78	0.41
1:A:49:ILE:O	1:A:53:ALA:HB3	2.21	0.41
1:B:16:SER:C	1:B:18:SER:N	2.78	0.41
1:B:292:GLU:HG2	1:C:17:PHE:CZ	2.56	0.41
1:A:76:ILE:HA	1:A:77:PRO:HD3	1.90	0.41
1:C:75:LEU:HD22	1:D:276:PHE:CB	2.48	0.41
1:C:180:MET:HE3	1:C:180:MET:HB3	1.97	0.41
1:D:49:ILE:O	1:D:53:ALA:HB3	2.21	0.41
1:E:276:PHE:CB	1:D:75:LEU:HD22	2.48	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:GLU:HG2	1:B:17:PHE:CZ	2.56	0.41
1:E:82:LEU:HG	1:E:287:TRP:CD1	2.54	0.41
1:E:111:SER:O	1:E:326:HIS:ND1	2.36	0.41
1:E:150:ARG:NH2	1:E:312:ASP:OD1	2.47	0.41
1:E:180:MET:HE3	1:E:180:MET:HB3	1.97	0.41
2:E:602:MC3:H352	2:E:602:MC3:H162	2.03	0.41
1:A:100:LEU:HD21	1:A:298:PHE:HE1	1.85	0.41
1:A:152:PRO:HD2	1:A:156:HIS:CD2	2.56	0.41
1:C:2:THR:N	1:C:306:GLU:OE2	2.54	0.41
1:C:140:LEU:HA	1:C:143:VAL:HG22	2.02	0.41
2:C:403:MC3:H352	2:C:403:MC3:H162	2.03	0.41
1:B:152:PRO:HD2	1:B:156:HIS:CD2	2.56	0.41
1:D:140:LEU:HA	1:D:143:VAL:HG22	2.02	0.41
2:B:401:MC3:H242	2:B:401:MC3:H212	1.73	0.40
1:D:152:PRO:HD2	1:D:156:HIS:CD2	2.56	0.40
1:A:2:THR:N	1:A:306:GLU:OE2	2.54	0.40
1:B:129:ILE:CD1	1:B:322:VAL:HG22	2.42	0.40
1:C:49:ILE:O	1:C:53:ALA:HB3	2.21	0.40
1:E:2:THR:N	1:E:306:GLU:OE2	2.54	0.40
1:E:17:PHE:CZ	1:D:292:GLU:HG2	2.56	0.40
1:E:129:ILE:CD1	1:E:322:VAL:HG22	2.42	0.40
1:D:2:THR:N	1:D:306:GLU:OE2	2.54	0.40
1:E:152:PRO:HD2	1:E:156:HIS:CD2	2.56	0.40
1:E:292:GLU:HG2	1:A:17:PHE:CZ	2.56	0.40
2:A:403:MC3:H352	2:A:403:MC3:H162	2.03	0.40
1:B:82:LEU:HG	1:B:287:TRP:CD1	2.54	0.40
1:C:152:PRO:HD2	1:C:156:HIS:CD2	2.56	0.40
1:D:16:SER:C	1:D:18:SER:N	2.78	0.40
1:B:292:GLU:O	1:B:295:ILE:HG22	2.22	0.40
1:C:3:ILE:HG13	1:C:26:GLY:HA3	2.03	0.40
1:C:292:GLU:HG2	1:D:17:PHE:CZ	2.56	0.40
1:D:271:LEU:O	1:D:273:VAL:N	2.47	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	336/345 (97%)	328 (98%)	8 (2%)	0	100	100
1	B	336/345 (97%)	328 (98%)	8 (2%)	0	100	100
1	C	336/345 (97%)	328 (98%)	8 (2%)	0	100	100
1	D	336/345 (97%)	328 (98%)	8 (2%)	0	100	100
1	E	336/345 (97%)	328 (98%)	8 (2%)	0	100	100
All	All	1680/1725 (97%)	1640 (98%)	40 (2%)	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	306/313 (98%)	305 (100%)	1 (0%)	86	91
1	B	306/313 (98%)	305 (100%)	1 (0%)	86	91
1	C	306/313 (98%)	305 (100%)	1 (0%)	86	91
1	D	306/313 (98%)	305 (100%)	1 (0%)	86	91
1	E	306/313 (98%)	305 (100%)	1 (0%)	86	91
All	All	1530/1565 (98%)	1525 (100%)	5 (0%)	84	91

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	178	HIS
1	A	178	HIS
1	B	178	HIS
1	C	178	HIS
1	D	178	HIS

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

Mol	Chain	Res	Type
1	E	208	GLN
1	A	208	GLN
1	B	208	GLN
1	C	208	GLN
1	D	208	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 45 ligands modelled in this entry, 5 are monoatomic - leaving 40 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	$\# Z > 2$
2	MC3	E	604	-	11,11,45	0.18	0	10,10,53	0.13	0
2	MC3	B	407	-	9,9,45	0.23	0	8,8,53	0.26	0
2	MC3	A	403	-	37,37,45	0.44	0	40,42,53	0.49	0
2	MC3	E	606	-	9,9,45	0.22	0	8,8,53	0.26	0
2	MC3	B	405	-	11,11,45	0.19	0	10,10,53	0.13	0
2	MC3	C	406	-	13,13,45	0.16	0	12,12,53	0.16	0
2	MC3	C	403	-	37,37,45	0.44	0	40,42,53	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MC3	E	609	-	34,34,45	0.31	0	36,36,53	0.26	0
2	MC3	B	402	-	4,4,45	0.17	0	3,3,53	0.24	0
2	MC3	C	409	-	13,13,45	0.23	0	12,12,53	0.15	0
2	MC3	D	409	-	13,13,45	0.23	0	12,12,53	0.15	0
2	MC3	D	406	-	13,13,45	0.16	0	12,12,53	0.16	0
2	MC3	E	603	-	13,13,45	0.17	0	12,12,53	0.23	0
2	MC3	C	401	-	34,34,45	0.31	0	36,36,53	0.27	0
2	MC3	D	402	-	4,4,45	0.17	0	3,3,53	0.24	0
2	MC3	D	405	-	11,11,45	0.18	0	10,10,53	0.13	0
2	MC3	C	407	-	9,9,45	0.23	0	8,8,53	0.26	0
2	MC3	B	404	-	13,13,45	0.17	0	12,12,53	0.23	0
2	MC3	E	608	-	13,13,45	0.23	0	12,12,53	0.15	0
2	MC3	D	404	-	13,13,45	0.17	0	12,12,53	0.23	0
2	MC3	B	409	-	13,13,45	0.23	0	12,12,53	0.15	0
2	MC3	A	401	-	34,34,45	0.32	0	36,36,53	0.27	0
2	MC3	D	403	-	37,37,45	0.44	0	40,42,53	0.50	0
2	MC3	A	406	-	13,13,45	0.16	0	12,12,53	0.16	0
2	MC3	B	401	-	34,34,45	0.31	0	36,36,53	0.26	0
2	MC3	E	601	-	4,4,45	0.17	0	3,3,53	0.24	0
2	MC3	D	407	-	9,9,45	0.23	0	8,8,53	0.26	0
2	MC3	A	407	-	9,9,45	0.22	0	8,8,53	0.26	0
2	MC3	A	409	-	13,13,45	0.23	0	12,12,53	0.15	0
2	MC3	E	602	-	37,37,45	0.44	0	40,42,53	0.50	0
2	MC3	B	403	-	37,37,45	0.44	0	40,42,53	0.49	0
2	MC3	C	405	-	11,11,45	0.18	0	10,10,53	0.13	0
2	MC3	E	605	-	13,13,45	0.16	0	12,12,53	0.16	0
2	MC3	A	402	-	4,4,45	0.17	0	3,3,53	0.24	0
2	MC3	A	404	-	13,13,45	0.17	0	12,12,53	0.23	0
2	MC3	A	405	-	11,11,45	0.18	0	10,10,53	0.13	0
2	MC3	D	401	-	34,34,45	0.31	0	36,36,53	0.27	0
2	MC3	B	406	-	13,13,45	0.16	0	12,12,53	0.16	0
2	MC3	C	402	-	4,4,45	0.17	0	3,3,53	0.24	0
2	MC3	C	404	-	13,13,45	0.17	0	12,12,53	0.23	0

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
2	MC3	E	604	-	-	6/9/9/49	-
2	MC3	B	407	-	-	5/7/7/49	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MC3	A	403	-	-	18/39/39/49	-
2	MC3	E	606	-	-	5/7/7/49	-
2	MC3	B	405	-	-	6/9/9/49	-
2	MC3	C	406	-	-	7/11/11/49	-
2	MC3	C	403	-	-	18/39/39/49	-
2	MC3	E	609	-	-	24/35/35/49	-
2	MC3	B	402	-	-	1/2/2/49	-
2	MC3	C	409	-	-	4/11/11/49	-
2	MC3	D	409	-	-	4/11/11/49	-
2	MC3	D	406	-	-	7/11/11/49	-
2	MC3	E	603	-	-	6/11/11/49	-
2	MC3	C	401	-	-	24/35/35/49	-
2	MC3	D	402	-	-	1/2/2/49	-
2	MC3	D	405	-	-	6/9/9/49	-
2	MC3	C	407	-	-	5/7/7/49	-
2	MC3	B	404	-	-	6/11/11/49	-
2	MC3	E	608	-	-	4/11/11/49	-
2	MC3	D	404	-	-	6/11/11/49	-
2	MC3	B	409	-	-	4/11/11/49	-
2	MC3	A	401	-	-	24/35/35/49	-
2	MC3	D	403	-	-	18/39/39/49	-
2	MC3	A	406	-	-	7/11/11/49	-
2	MC3	B	401	-	-	24/35/35/49	-
2	MC3	E	601	-	-	1/2/2/49	-
2	MC3	D	407	-	-	5/7/7/49	-
2	MC3	A	407	-	-	5/7/7/49	-
2	MC3	A	409	-	-	4/11/11/49	-
2	MC3	E	602	-	-	18/39/39/49	-
2	MC3	B	403	-	-	18/39/39/49	-
2	MC3	C	405	-	-	6/9/9/49	-
2	MC3	E	605	-	-	7/11/11/49	-
2	MC3	A	402	-	-	1/2/2/49	-
2	MC3	A	404	-	-	6/11/11/49	-
2	MC3	A	405	-	-	6/9/9/49	-
2	MC3	D	401	-	-	24/35/35/49	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MC3	B	406	-	-	7/11/11/49	-
2	MC3	C	402	-	-	1/2/2/49	-
2	MC3	C	404	-	-	6/11/11/49	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (355) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	602	MC3	C32-C31-O2-C2
2	E	609	MC3	C32-C31-O2-C2
2	A	401	MC3	C32-C31-O2-C2
2	A	403	MC3	C32-C31-O2-C2
2	B	401	MC3	C32-C31-O2-C2
2	B	403	MC3	C32-C31-O2-C2
2	C	401	MC3	C32-C31-O2-C2
2	C	403	MC3	C32-C31-O2-C2
2	D	401	MC3	C32-C31-O2-C2
2	D	403	MC3	C32-C31-O2-C2
2	E	602	MC3	O31-C31-O2-C2
2	A	403	MC3	O31-C31-O2-C2
2	B	403	MC3	O31-C31-O2-C2
2	C	403	MC3	O31-C31-O2-C2
2	D	403	MC3	O31-C31-O2-C2
2	E	609	MC3	O11-C11-O3-C3
2	A	401	MC3	O11-C11-O3-C3
2	B	401	MC3	O11-C11-O3-C3
2	C	401	MC3	O11-C11-O3-C3
2	D	401	MC3	O11-C11-O3-C3
2	E	609	MC3	O31-C31-O2-C2
2	A	401	MC3	O31-C31-O2-C2
2	B	401	MC3	O31-C31-O2-C2
2	C	401	MC3	O31-C31-O2-C2
2	D	401	MC3	O31-C31-O2-C2
2	E	609	MC3	C12-C11-O3-C3
2	A	401	MC3	C12-C11-O3-C3
2	B	401	MC3	C12-C11-O3-C3
2	C	401	MC3	C12-C11-O3-C3
2	D	401	MC3	C12-C11-O3-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	E	602	MC3	C37-C38-C39-C40
2	A	403	MC3	C37-C38-C39-C40
2	B	403	MC3	C37-C38-C39-C40
2	C	403	MC3	C37-C38-C39-C40
2	D	403	MC3	C37-C38-C39-C40
2	E	602	MC3	C31-C32-C33-C34
2	A	403	MC3	C31-C32-C33-C34
2	B	403	MC3	C31-C32-C33-C34
2	C	403	MC3	C31-C32-C33-C34
2	D	403	MC3	C31-C32-C33-C34
2	E	609	MC3	C39-C40-C41-C42
2	A	401	MC3	C39-C40-C41-C42
2	B	401	MC3	C33-C34-C35-C36
2	B	401	MC3	C39-C40-C41-C42
2	C	401	MC3	C33-C34-C35-C36
2	C	401	MC3	C39-C40-C41-C42
2	D	401	MC3	C39-C40-C41-C42
2	E	609	MC3	C33-C34-C35-C36
2	A	401	MC3	C33-C34-C35-C36
2	D	401	MC3	C33-C34-C35-C36
2	E	609	MC3	C11-C12-C13-C14
2	A	401	MC3	C11-C12-C13-C14
2	B	401	MC3	C11-C12-C13-C14
2	C	401	MC3	C11-C12-C13-C14
2	D	401	MC3	C11-C12-C13-C14
2	C	404	MC3	C37-C38-C39-C40
2	E	602	MC3	C36-C37-C38-C39
2	E	603	MC3	C37-C38-C39-C40
2	E	609	MC3	C34-C35-C36-C37
2	A	401	MC3	C34-C35-C36-C37
2	A	404	MC3	C37-C38-C39-C40
2	B	401	MC3	C34-C35-C36-C37
2	B	403	MC3	C36-C37-C38-C39
2	B	404	MC3	C37-C38-C39-C40
2	C	401	MC3	C34-C35-C36-C37
2	C	403	MC3	C36-C37-C38-C39
2	D	401	MC3	C34-C35-C36-C37
2	D	403	MC3	C36-C37-C38-C39
2	A	403	MC3	C36-C37-C38-C39
2	D	404	MC3	C37-C38-C39-C40
2	E	602	MC3	C19-C20-C21-C22
2	A	403	MC3	C19-C20-C21-C22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	B	403	MC3	C19-C20-C21-C22
2	C	403	MC3	C19-C20-C21-C22
2	D	403	MC3	C19-C20-C21-C22
2	E	609	MC3	C17-C18-C19-C20
2	A	401	MC3	C17-C18-C19-C20
2	B	401	MC3	C17-C18-C19-C20
2	C	401	MC3	C17-C18-C19-C20
2	E	608	MC3	C32-C33-C34-C35
2	A	409	MC3	C32-C33-C34-C35
2	B	409	MC3	C32-C33-C34-C35
2	C	409	MC3	C32-C33-C34-C35
2	D	401	MC3	C17-C18-C19-C20
2	D	409	MC3	C32-C33-C34-C35
2	E	604	MC3	C40-C41-C42-C43
2	A	405	MC3	C40-C41-C42-C43
2	B	405	MC3	C40-C41-C42-C43
2	C	405	MC3	C40-C41-C42-C43
2	D	405	MC3	C40-C41-C42-C43
2	D	404	MC3	C34-C35-C36-C37
2	E	603	MC3	C34-C35-C36-C37
2	A	404	MC3	C34-C35-C36-C37
2	B	404	MC3	C34-C35-C36-C37
2	C	401	MC3	C19-C20-C21-C22
2	C	404	MC3	C34-C35-C36-C37
2	D	401	MC3	C19-C20-C21-C22
2	E	609	MC3	C19-C20-C21-C22
2	E	609	MC3	C38-C39-C40-C41
2	A	401	MC3	C19-C20-C21-C22
2	A	401	MC3	C38-C39-C40-C41
2	B	401	MC3	C19-C20-C21-C22
2	B	401	MC3	C38-C39-C40-C41
2	C	401	MC3	C38-C39-C40-C41
2	D	401	MC3	C38-C39-C40-C41
2	E	602	MC3	C12-C13-C14-C15
2	A	403	MC3	C12-C13-C14-C15
2	B	403	MC3	C12-C13-C14-C15
2	C	403	MC3	C12-C13-C14-C15
2	D	403	MC3	C12-C13-C14-C15
2	E	609	MC3	C40-C41-C42-C43
2	A	401	MC3	C40-C41-C42-C43
2	B	401	MC3	C40-C41-C42-C43
2	B	406	MC3	C32-C33-C34-C35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	C	401	MC3	C40-C41-C42-C43
2	D	401	MC3	C40-C41-C42-C43
2	E	605	MC3	C32-C33-C34-C35
2	A	406	MC3	C32-C33-C34-C35
2	C	406	MC3	C32-C33-C34-C35
2	D	406	MC3	C32-C33-C34-C35
2	D	401	MC3	C37-C38-C39-C40
2	E	609	MC3	C37-C38-C39-C40
2	A	401	MC3	C37-C38-C39-C40
2	B	401	MC3	C37-C38-C39-C40
2	C	401	MC3	C37-C38-C39-C40
2	E	606	MC3	C35-C36-C37-C38
2	A	407	MC3	C35-C36-C37-C38
2	B	407	MC3	C35-C36-C37-C38
2	D	407	MC3	C35-C36-C37-C38
2	C	407	MC3	C35-C36-C37-C38
2	E	603	MC3	C38-C39-C40-C41
2	A	404	MC3	C38-C39-C40-C41
2	B	404	MC3	C38-C39-C40-C41
2	C	404	MC3	C38-C39-C40-C41
2	D	404	MC3	C38-C39-C40-C41
2	E	609	MC3	C20-C21-C22-C23
2	A	401	MC3	C20-C21-C22-C23
2	B	401	MC3	C20-C21-C22-C23
2	C	401	MC3	C20-C21-C22-C23
2	D	401	MC3	C20-C21-C22-C23
2	E	604	MC3	C33-C34-C35-C36
2	E	609	MC3	C21-C22-C23-C24
2	A	401	MC3	C21-C22-C23-C24
2	A	405	MC3	C33-C34-C35-C36
2	B	401	MC3	C21-C22-C23-C24
2	B	405	MC3	C33-C34-C35-C36
2	C	401	MC3	C21-C22-C23-C24
2	C	405	MC3	C33-C34-C35-C36
2	D	401	MC3	C21-C22-C23-C24
2	D	405	MC3	C33-C34-C35-C36
2	E	602	MC3	O2-C2-C3-O3
2	A	403	MC3	O2-C2-C3-O3
2	B	403	MC3	O2-C2-C3-O3
2	C	403	MC3	O2-C2-C3-O3
2	D	403	MC3	O2-C2-C3-O3
2	A	405	MC3	C35-C36-C37-C38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	E	604	MC3	C35-C36-C37-C38
2	E	609	MC3	C12-C13-C14-C15
2	A	401	MC3	C12-C13-C14-C15
2	B	401	MC3	C12-C13-C14-C15
2	B	405	MC3	C35-C36-C37-C38
2	C	401	MC3	C12-C13-C14-C15
2	C	405	MC3	C35-C36-C37-C38
2	D	401	MC3	C12-C13-C14-C15
2	D	405	MC3	C35-C36-C37-C38
2	E	605	MC3	C40-C41-C42-C43
2	A	406	MC3	C40-C41-C42-C43
2	B	406	MC3	C40-C41-C42-C43
2	C	406	MC3	C40-C41-C42-C43
2	D	406	MC3	C40-C41-C42-C43
2	E	602	MC3	C18-C19-C20-C21
2	A	403	MC3	C18-C19-C20-C21
2	B	403	MC3	C18-C19-C20-C21
2	C	403	MC3	C18-C19-C20-C21
2	D	403	MC3	C18-C19-C20-C21
2	E	609	MC3	C36-C37-C38-C39
2	C	401	MC3	C36-C37-C38-C39
2	A	401	MC3	C36-C37-C38-C39
2	B	401	MC3	C36-C37-C38-C39
2	D	401	MC3	C36-C37-C38-C39
2	E	604	MC3	C37-C38-C39-C40
2	A	405	MC3	C37-C38-C39-C40
2	B	405	MC3	C37-C38-C39-C40
2	C	405	MC3	C37-C38-C39-C40
2	D	405	MC3	C37-C38-C39-C40
2	A	409	MC3	C36-C37-C38-C39
2	E	604	MC3	C39-C40-C41-C42
2	E	608	MC3	C36-C37-C38-C39
2	A	405	MC3	C39-C40-C41-C42
2	B	405	MC3	C39-C40-C41-C42
2	B	409	MC3	C36-C37-C38-C39
2	C	405	MC3	C39-C40-C41-C42
2	C	409	MC3	C36-C37-C38-C39
2	D	405	MC3	C39-C40-C41-C42
2	D	409	MC3	C36-C37-C38-C39
2	E	608	MC3	C39-C40-C41-C42
2	B	409	MC3	C39-C40-C41-C42
2	C	409	MC3	C39-C40-C41-C42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	D	409	MC3	C39-C40-C41-C42
2	A	409	MC3	C39-C40-C41-C42
2	E	604	MC3	C38-C39-C40-C41
2	A	405	MC3	C38-C39-C40-C41
2	B	405	MC3	C38-C39-C40-C41
2	C	405	MC3	C38-C39-C40-C41
2	D	405	MC3	C38-C39-C40-C41
2	E	609	MC3	C1-C2-C3-O3
2	A	401	MC3	C1-C2-C3-O3
2	B	401	MC3	C1-C2-C3-O3
2	C	401	MC3	C1-C2-C3-O3
2	D	401	MC3	C1-C2-C3-O3
2	E	602	MC3	C1-C2-C3-O3
2	A	403	MC3	C1-C2-C3-O3
2	B	403	MC3	C1-C2-C3-O3
2	C	403	MC3	C1-C2-C3-O3
2	D	403	MC3	C1-C2-C3-O3
2	B	401	MC3	C32-C33-C34-C35
2	C	401	MC3	C32-C33-C34-C35
2	A	401	MC3	C32-C33-C34-C35
2	D	401	MC3	C32-C33-C34-C35
2	E	609	MC3	C32-C33-C34-C35
2	E	601	MC3	C32-C33-C34-C35
2	A	402	MC3	C32-C33-C34-C35
2	B	402	MC3	C32-C33-C34-C35
2	C	402	MC3	C32-C33-C34-C35
2	D	402	MC3	C32-C33-C34-C35
2	E	609	MC3	O2-C2-C3-O3
2	A	401	MC3	O2-C2-C3-O3
2	B	401	MC3	O2-C2-C3-O3
2	C	401	MC3	O2-C2-C3-O3
2	D	401	MC3	O2-C2-C3-O3
2	C	407	MC3	C36-C37-C38-C39
2	D	407	MC3	C36-C37-C38-C39
2	E	606	MC3	C36-C37-C38-C39
2	A	407	MC3	C36-C37-C38-C39
2	B	407	MC3	C36-C37-C38-C39
2	A	401	MC3	C16-C17-C18-C19
2	C	401	MC3	C16-C17-C18-C19
2	D	401	MC3	C16-C17-C18-C19
2	B	403	MC3	C39-C40-C41-C42
2	D	403	MC3	C39-C40-C41-C42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	E	609	MC3	C16-C17-C18-C19
2	B	401	MC3	C16-C17-C18-C19
2	E	602	MC3	C39-C40-C41-C42
2	A	403	MC3	C39-C40-C41-C42
2	C	403	MC3	C39-C40-C41-C42
2	A	403	MC3	C34-C35-C36-C37
2	E	602	MC3	C34-C35-C36-C37
2	B	403	MC3	C34-C35-C36-C37
2	D	403	MC3	C34-C35-C36-C37
2	C	403	MC3	C34-C35-C36-C37
2	A	406	MC3	C33-C34-C35-C36
2	E	605	MC3	C33-C34-C35-C36
2	B	406	MC3	C33-C34-C35-C36
2	D	406	MC3	C33-C34-C35-C36
2	C	406	MC3	C33-C34-C35-C36
2	B	407	MC3	C38-C39-C40-C41
2	C	407	MC3	C38-C39-C40-C41
2	E	609	MC3	C13-C14-C15-C16
2	A	401	MC3	C13-C14-C15-C16
2	B	401	MC3	C13-C14-C15-C16
2	C	401	MC3	C13-C14-C15-C16
2	D	401	MC3	C13-C14-C15-C16
2	D	407	MC3	C38-C39-C40-C41
2	E	606	MC3	C38-C39-C40-C41
2	A	407	MC3	C38-C39-C40-C41
2	E	609	MC3	C3-C2-O2-C31
2	A	401	MC3	C3-C2-O2-C31
2	B	401	MC3	C3-C2-O2-C31
2	C	401	MC3	C3-C2-O2-C31
2	D	401	MC3	C3-C2-O2-C31
2	E	606	MC3	C39-C40-C41-C42
2	A	407	MC3	C39-C40-C41-C42
2	E	602	MC3	C1-O3P-P-O1P
2	A	403	MC3	C1-O3P-P-O1P
2	B	403	MC3	C1-O3P-P-O1P
2	C	403	MC3	C1-O3P-P-O1P
2	D	403	MC3	C1-O3P-P-O1P
2	B	407	MC3	C39-C40-C41-C42
2	C	407	MC3	C39-C40-C41-C42
2	D	407	MC3	C39-C40-C41-C42
2	E	602	MC3	C14-C15-C16-C17
2	B	403	MC3	C14-C15-C16-C17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	D	403	MC3	C14-C15-C16-C17
2	C	403	MC3	C14-C15-C16-C17
2	A	403	MC3	C14-C15-C16-C17
2	B	404	MC3	C39-C40-C41-C42
2	D	404	MC3	C39-C40-C41-C42
2	C	404	MC3	C39-C40-C41-C42
2	E	603	MC3	C39-C40-C41-C42
2	A	404	MC3	C39-C40-C41-C42
2	E	602	MC3	C15-C16-C17-C18
2	C	403	MC3	C15-C16-C17-C18
2	B	403	MC3	C15-C16-C17-C18
2	A	403	MC3	C15-C16-C17-C18
2	D	403	MC3	C15-C16-C17-C18
2	E	609	MC3	C31-C32-C33-C34
2	B	401	MC3	C31-C32-C33-C34
2	C	401	MC3	C31-C32-C33-C34
2	D	401	MC3	C31-C32-C33-C34
2	A	401	MC3	C31-C32-C33-C34
2	A	406	MC3	C34-C35-C36-C37
2	E	605	MC3	C34-C35-C36-C37
2	A	404	MC3	C32-C33-C34-C35
2	B	406	MC3	C34-C35-C36-C37
2	E	603	MC3	C32-C33-C34-C35
2	B	404	MC3	C32-C33-C34-C35
2	C	404	MC3	C32-C33-C34-C35
2	D	404	MC3	C32-C33-C34-C35
2	D	406	MC3	C34-C35-C36-C37
2	C	406	MC3	C34-C35-C36-C37
2	B	406	MC3	C35-C36-C37-C38
2	C	406	MC3	C35-C36-C37-C38
2	E	605	MC3	C35-C36-C37-C38
2	A	406	MC3	C35-C36-C37-C38
2	D	406	MC3	C35-C36-C37-C38
2	C	407	MC3	C34-C35-C36-C37
2	A	407	MC3	C34-C35-C36-C37
2	E	606	MC3	C34-C35-C36-C37
2	D	407	MC3	C34-C35-C36-C37
2	B	407	MC3	C34-C35-C36-C37
2	D	406	MC3	C36-C37-C38-C39
2	C	406	MC3	C36-C37-C38-C39
2	E	605	MC3	C36-C37-C38-C39
2	A	406	MC3	C36-C37-C38-C39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	B	406	MC3	C36-C37-C38-C39
2	E	602	MC3	O3-C11-C12-C13
2	A	403	MC3	O3-C11-C12-C13
2	B	403	MC3	O3-C11-C12-C13
2	C	403	MC3	O3-C11-C12-C13
2	D	403	MC3	O3-C11-C12-C13
2	E	602	MC3	C11-C12-C13-C14
2	A	403	MC3	C11-C12-C13-C14
2	B	403	MC3	C11-C12-C13-C14
2	C	403	MC3	C11-C12-C13-C14
2	D	403	MC3	C11-C12-C13-C14
2	E	605	MC3	C31-C32-C33-C34
2	A	406	MC3	C31-C32-C33-C34
2	B	406	MC3	C31-C32-C33-C34
2	D	406	MC3	C31-C32-C33-C34
2	C	406	MC3	C31-C32-C33-C34
2	A	404	MC3	C35-C36-C37-C38
2	B	404	MC3	C35-C36-C37-C38
2	C	404	MC3	C35-C36-C37-C38
2	D	404	MC3	C35-C36-C37-C38
2	E	603	MC3	C35-C36-C37-C38
2	B	409	MC3	C31-C32-C33-C34
2	E	608	MC3	C31-C32-C33-C34
2	C	409	MC3	C31-C32-C33-C34
2	D	409	MC3	C31-C32-C33-C34
2	A	409	MC3	C31-C32-C33-C34
2	E	602	MC3	C33-C34-C35-C36
2	A	403	MC3	C33-C34-C35-C36
2	C	403	MC3	C33-C34-C35-C36
2	B	403	MC3	C33-C34-C35-C36
2	D	403	MC3	C33-C34-C35-C36

There are no ring outliers.

25 monomers are involved in 86 short contacts:

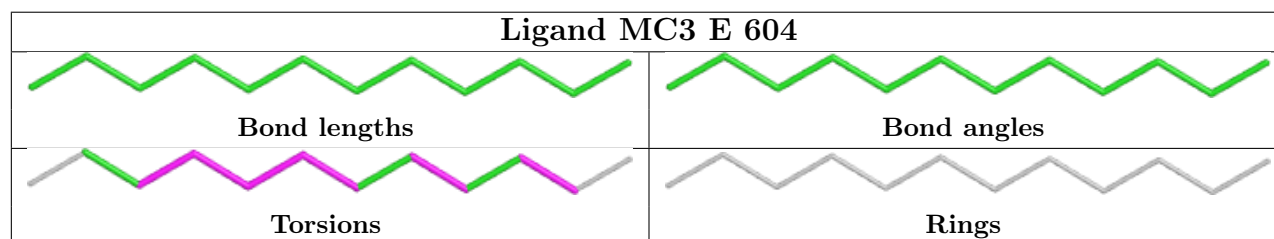
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	403	MC3	9	0
2	C	406	MC3	1	0
2	C	403	MC3	9	0
2	E	609	MC3	3	0
2	C	409	MC3	3	0
2	D	409	MC3	3	0

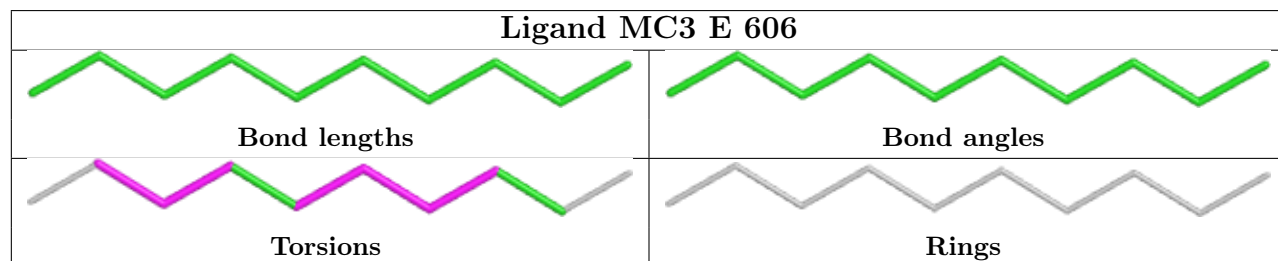
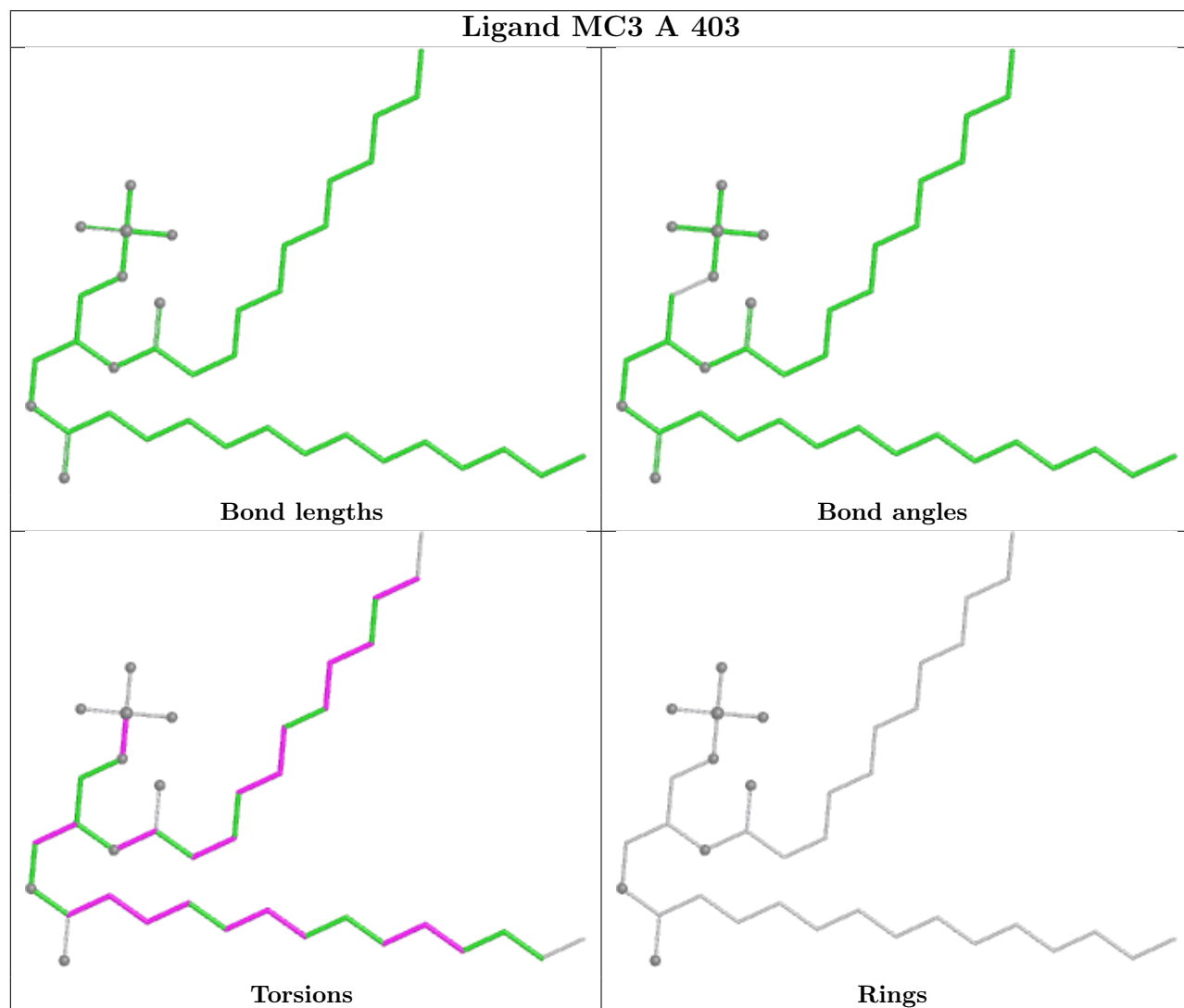
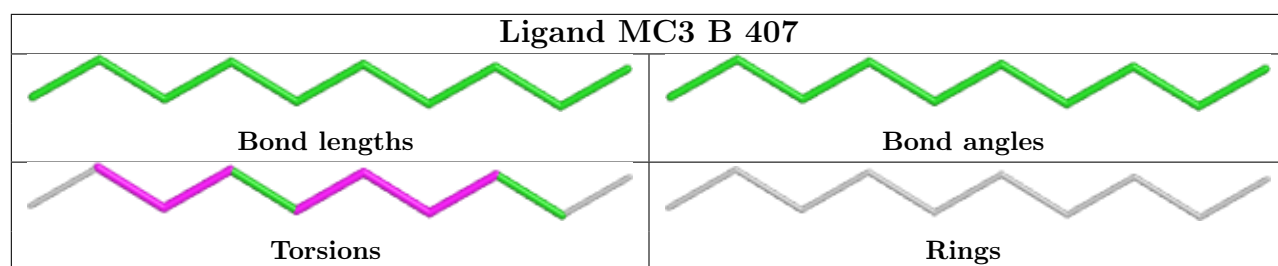
Continued on next page...

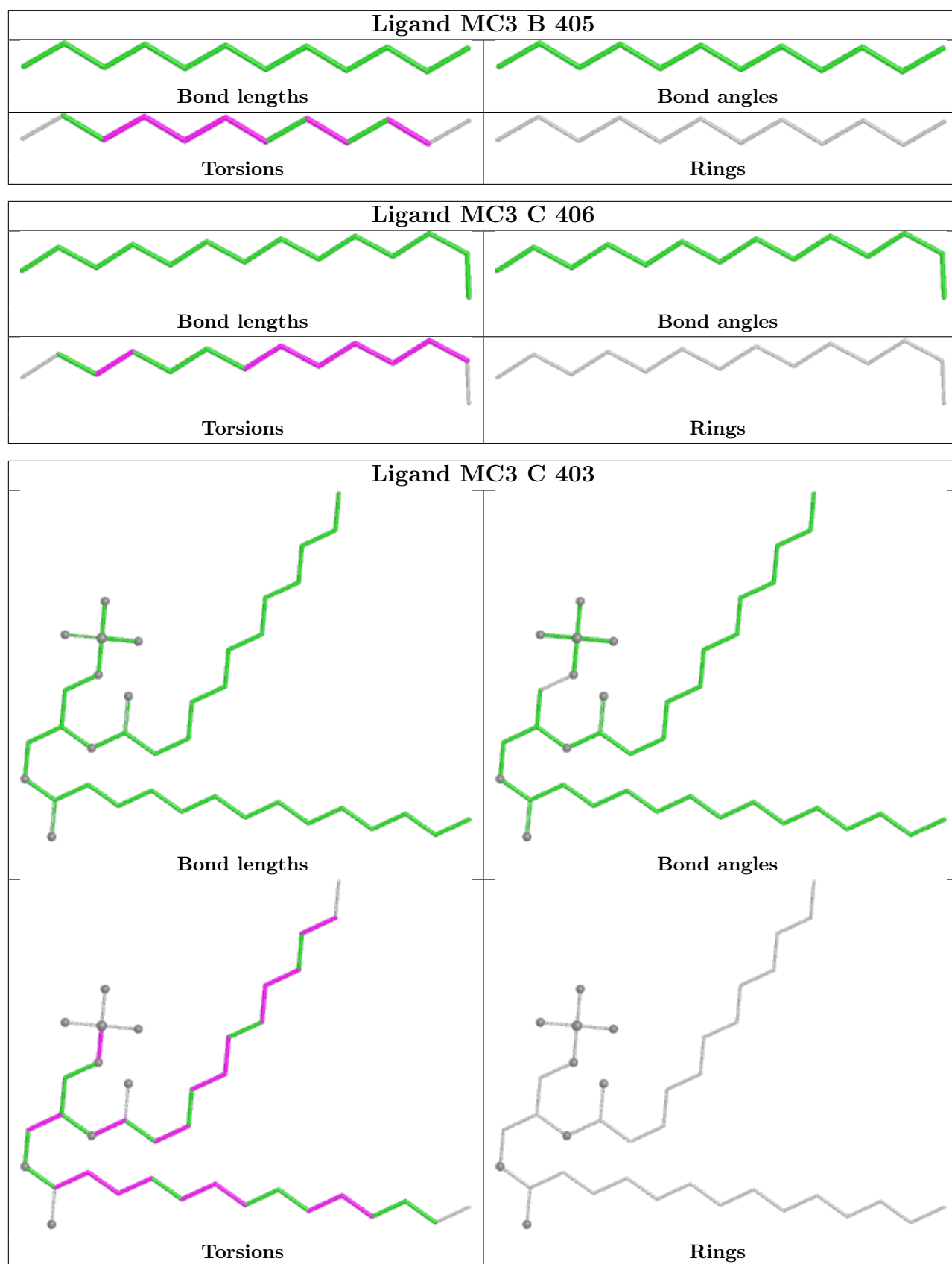
Continued from previous page...

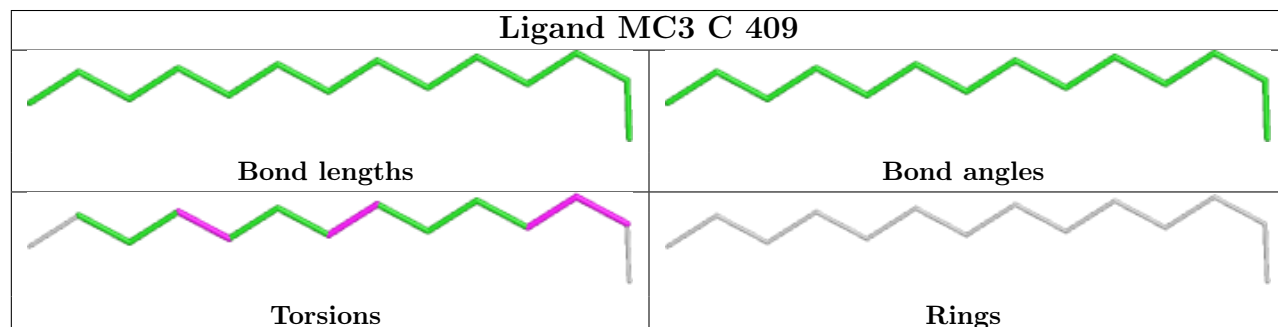
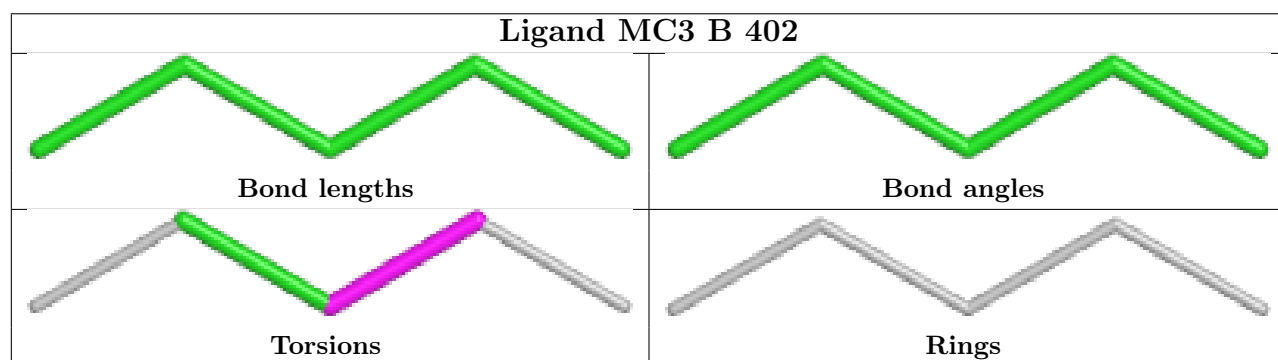
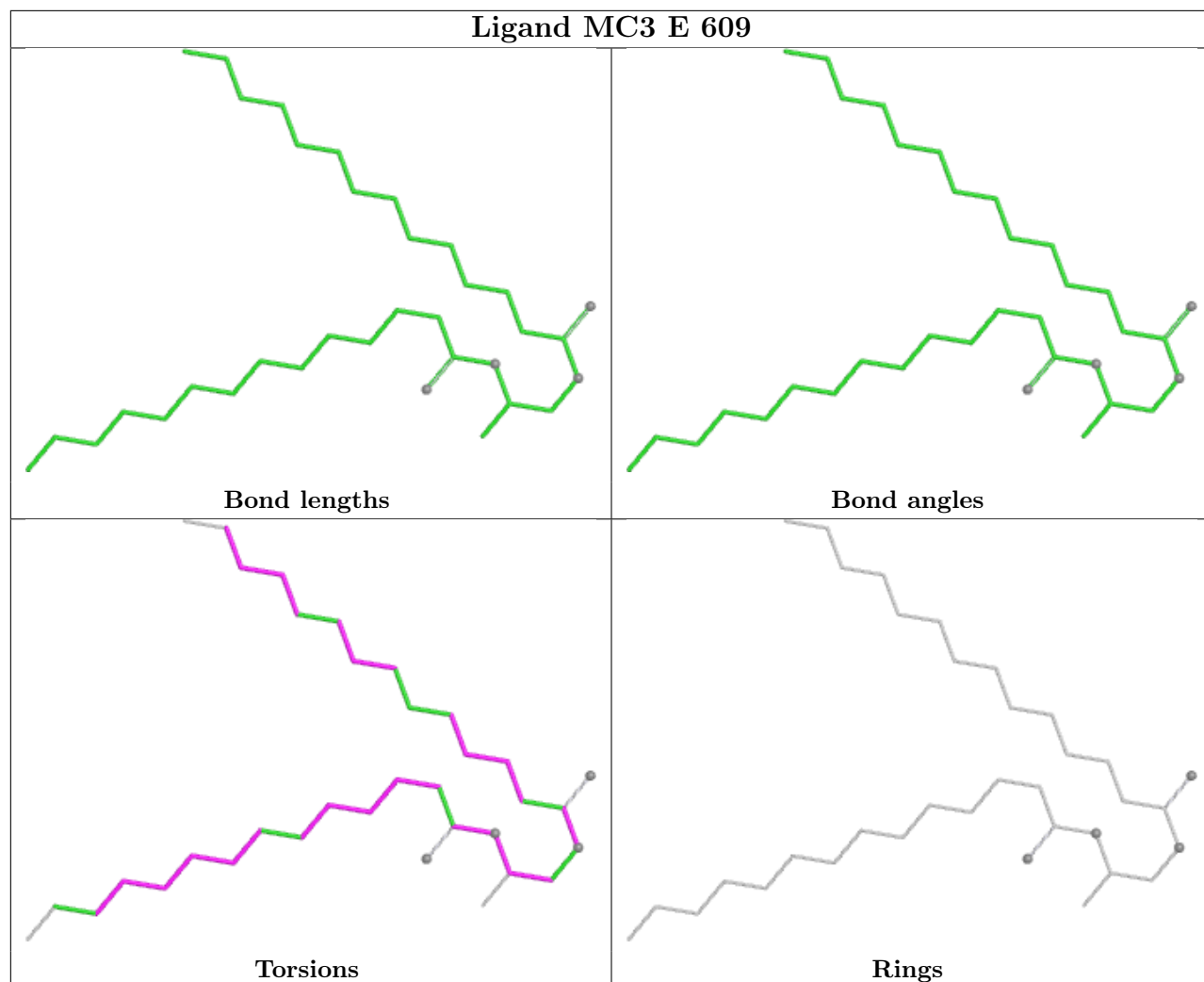
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	406	MC3	1	0
2	E	603	MC3	2	0
2	C	401	MC3	3	0
2	B	404	MC3	2	0
2	E	608	MC3	3	0
2	D	404	MC3	2	0
2	B	409	MC3	3	0
2	A	401	MC3	2	0
2	D	403	MC3	8	0
2	A	406	MC3	1	0
2	B	401	MC3	3	0
2	A	409	MC3	3	0
2	E	602	MC3	9	0
2	B	403	MC3	8	0
2	E	605	MC3	1	0
2	A	404	MC3	2	0
2	D	401	MC3	2	0
2	B	406	MC3	1	0
2	C	404	MC3	2	0

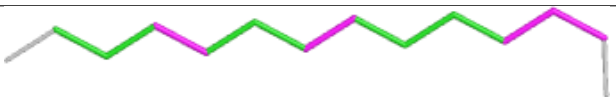
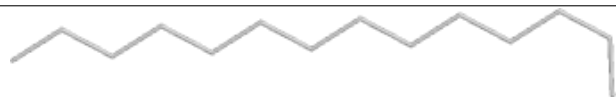
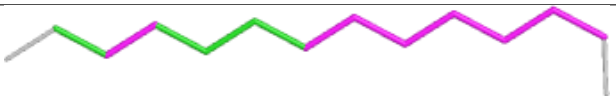
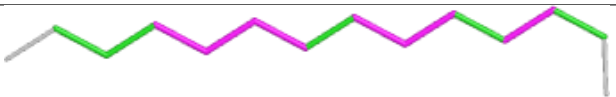
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

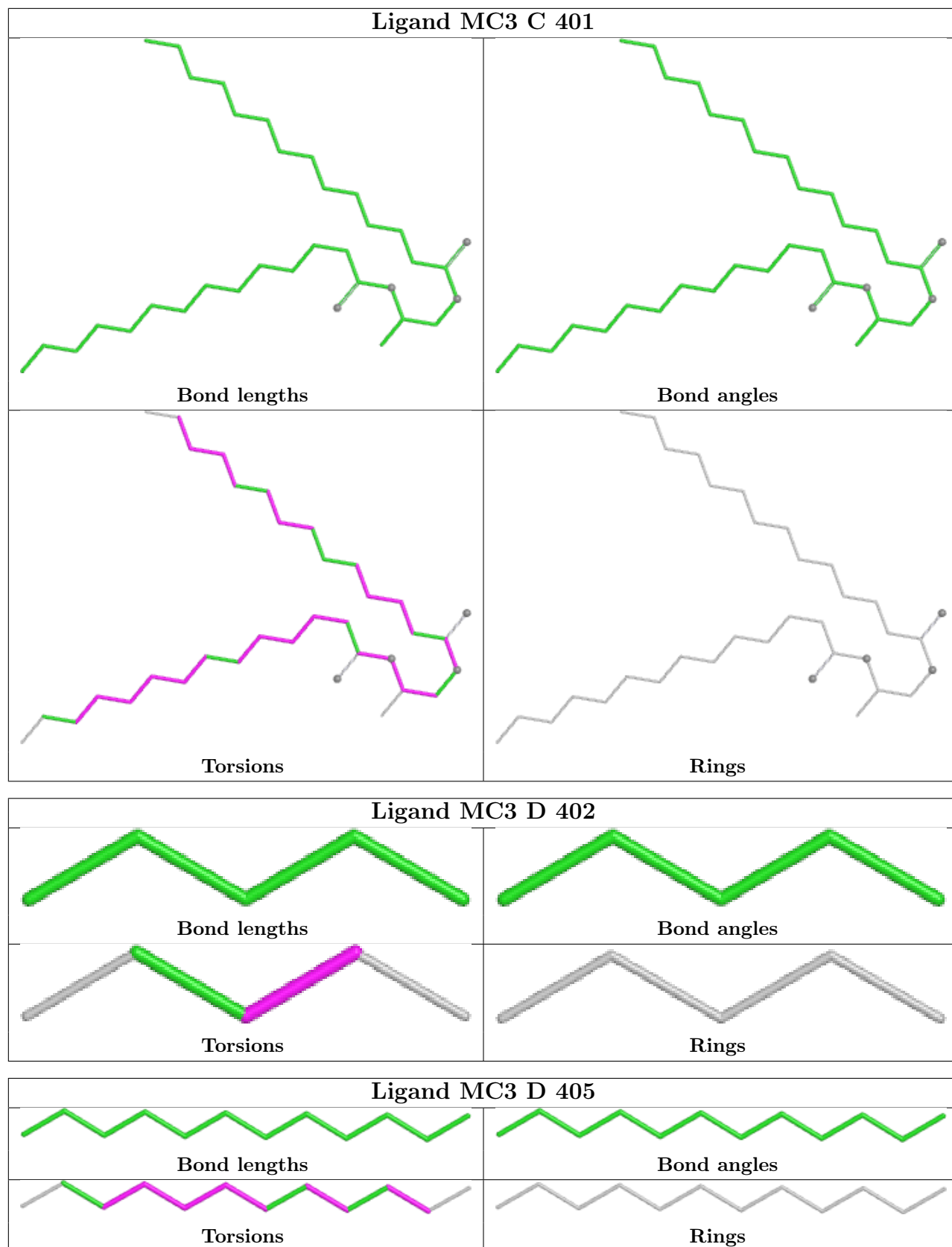


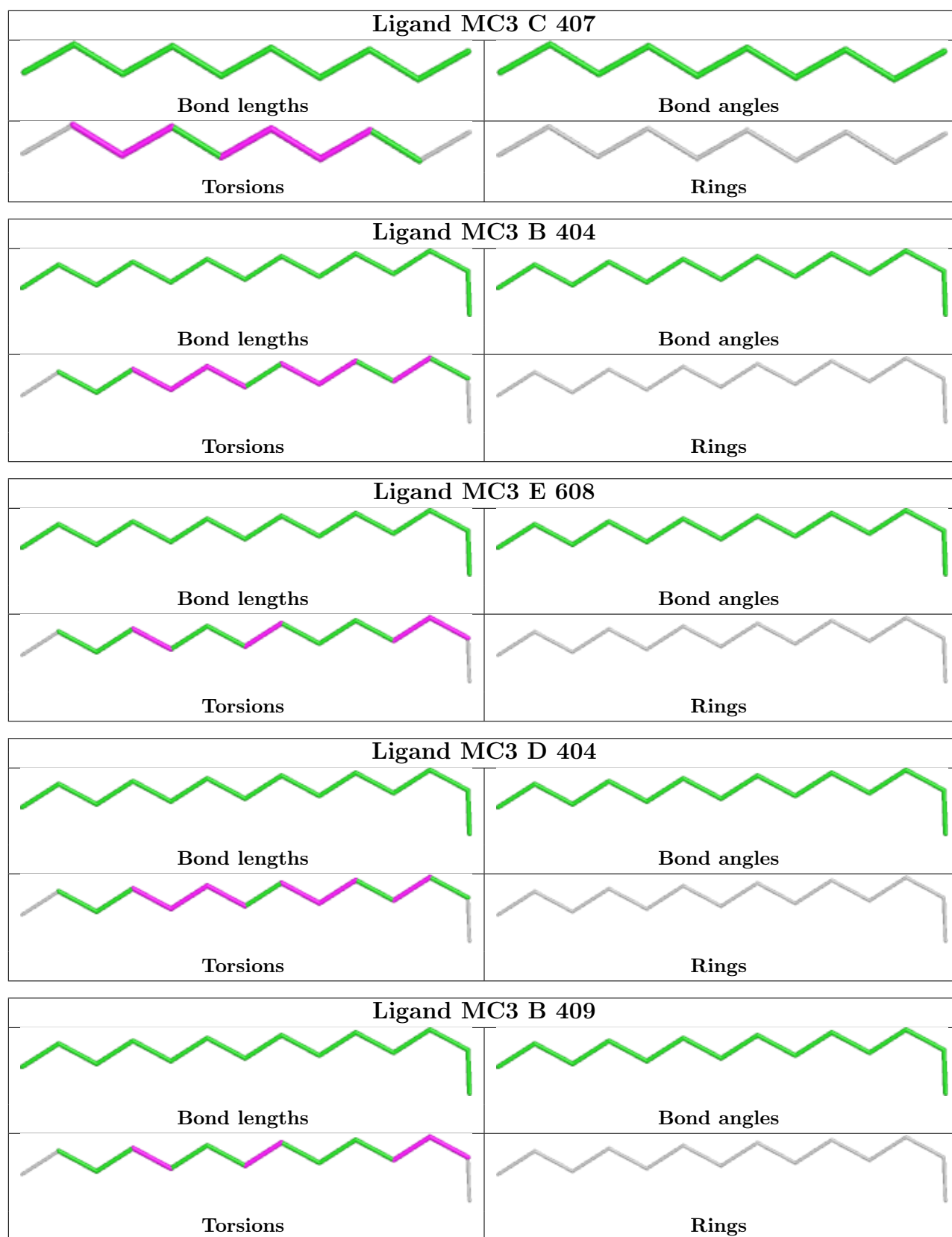


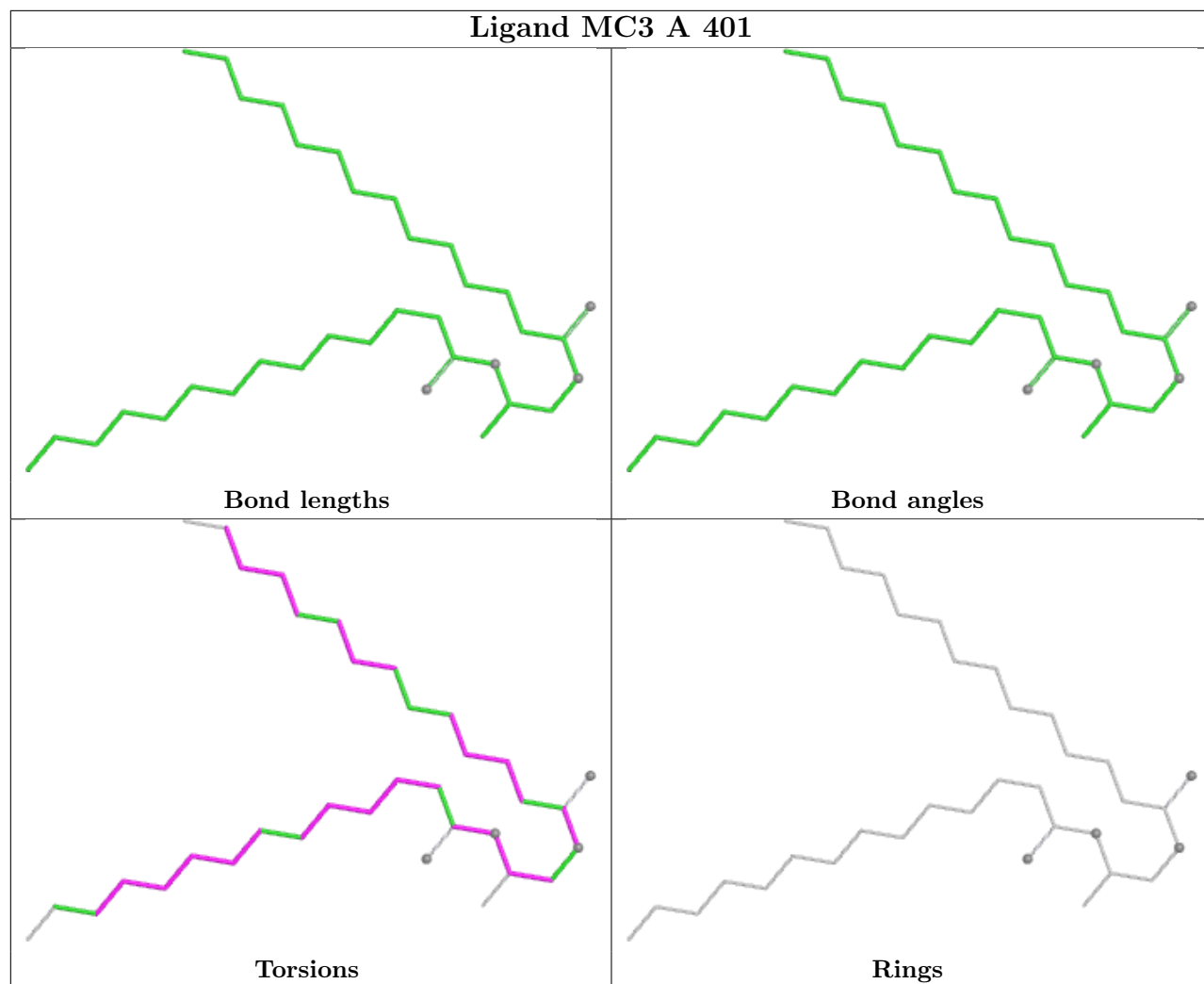


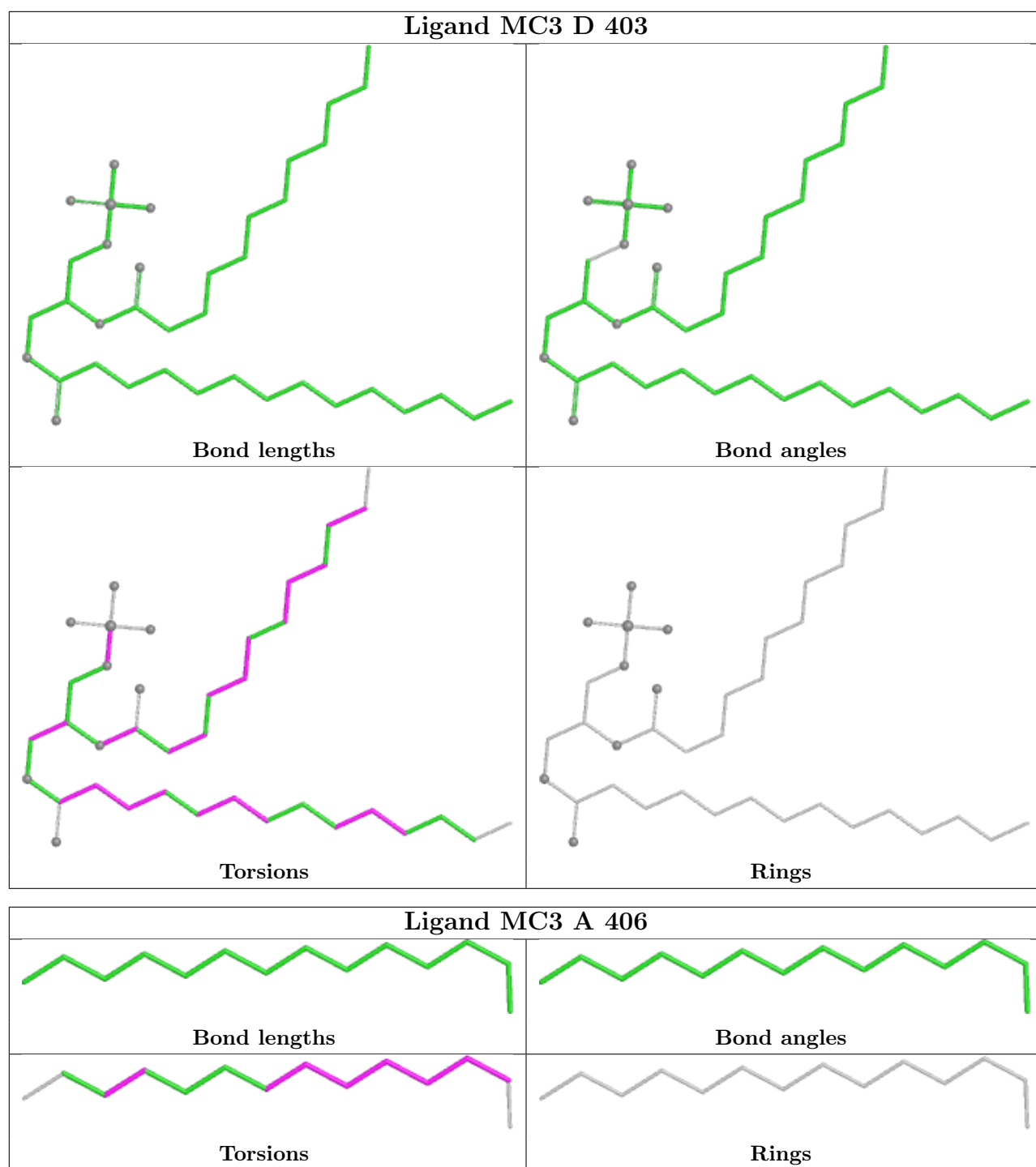


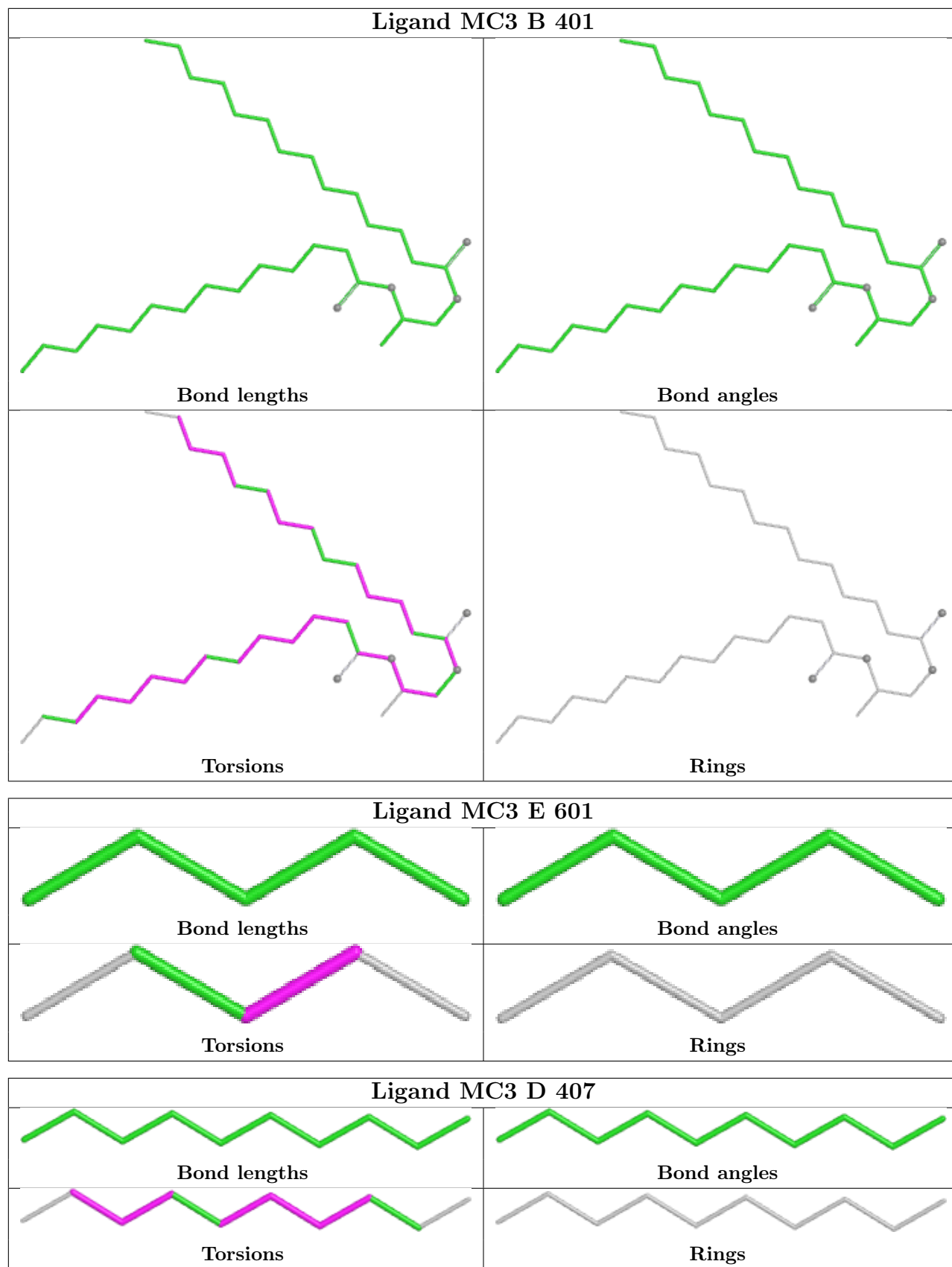
Ligand MC3 D 409			
 Bond lengths		 Bond angles	
 Torsions		 Rings	
Ligand MC3 D 406			
 Bond lengths		 Bond angles	
 Torsions		 Rings	
Ligand MC3 E 603			
 Bond lengths		 Bond angles	
 Torsions		 Rings	

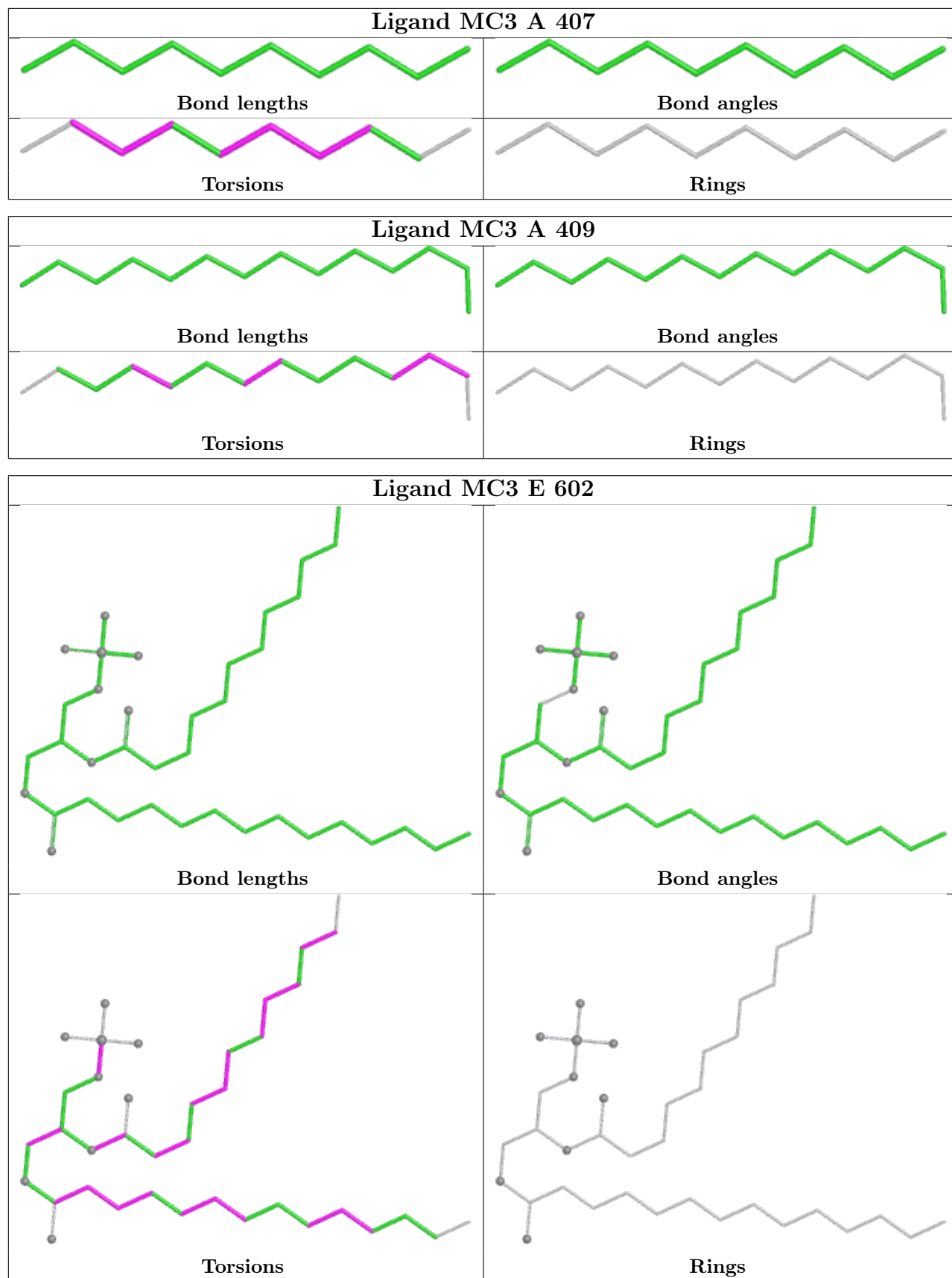


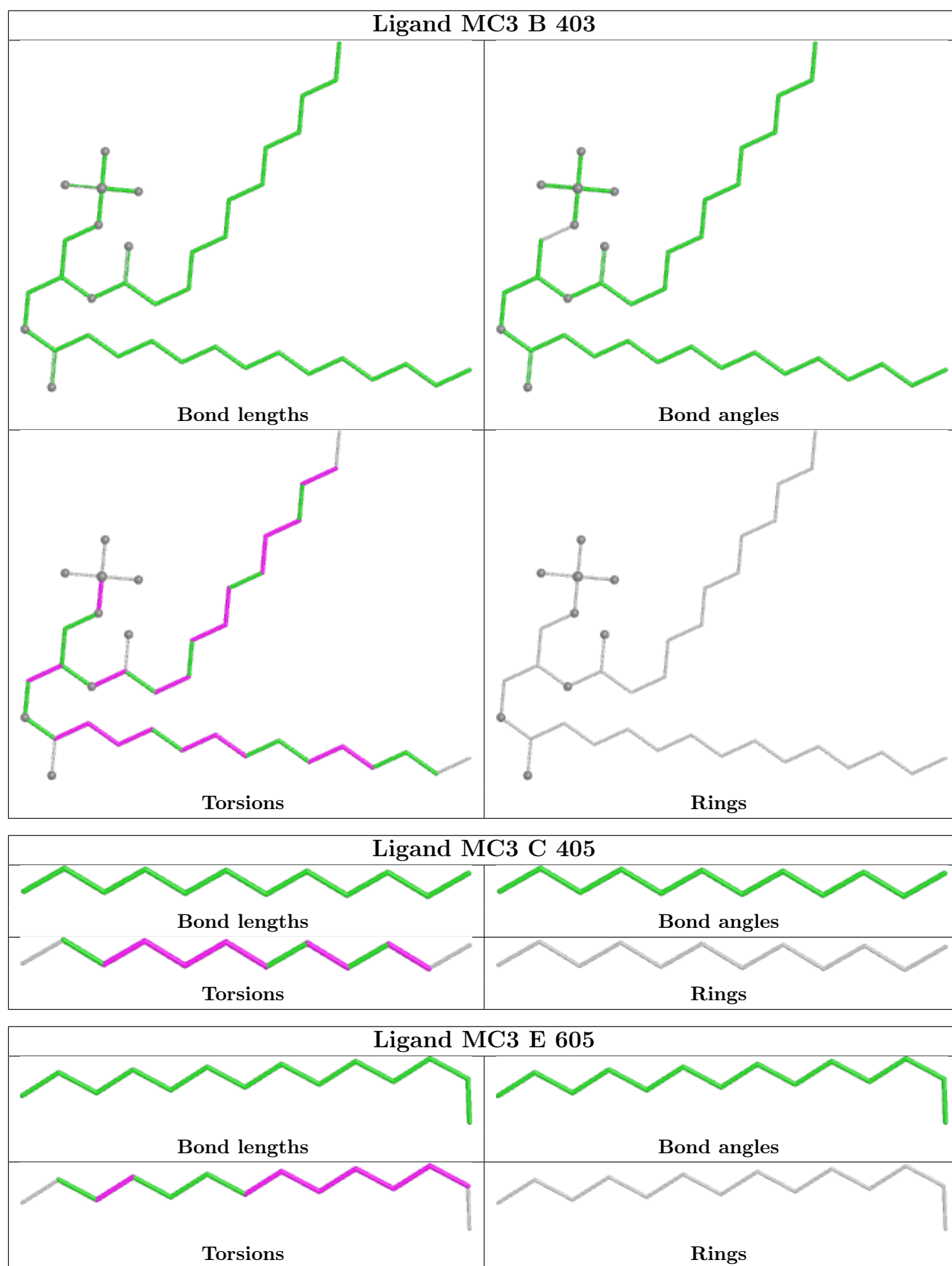


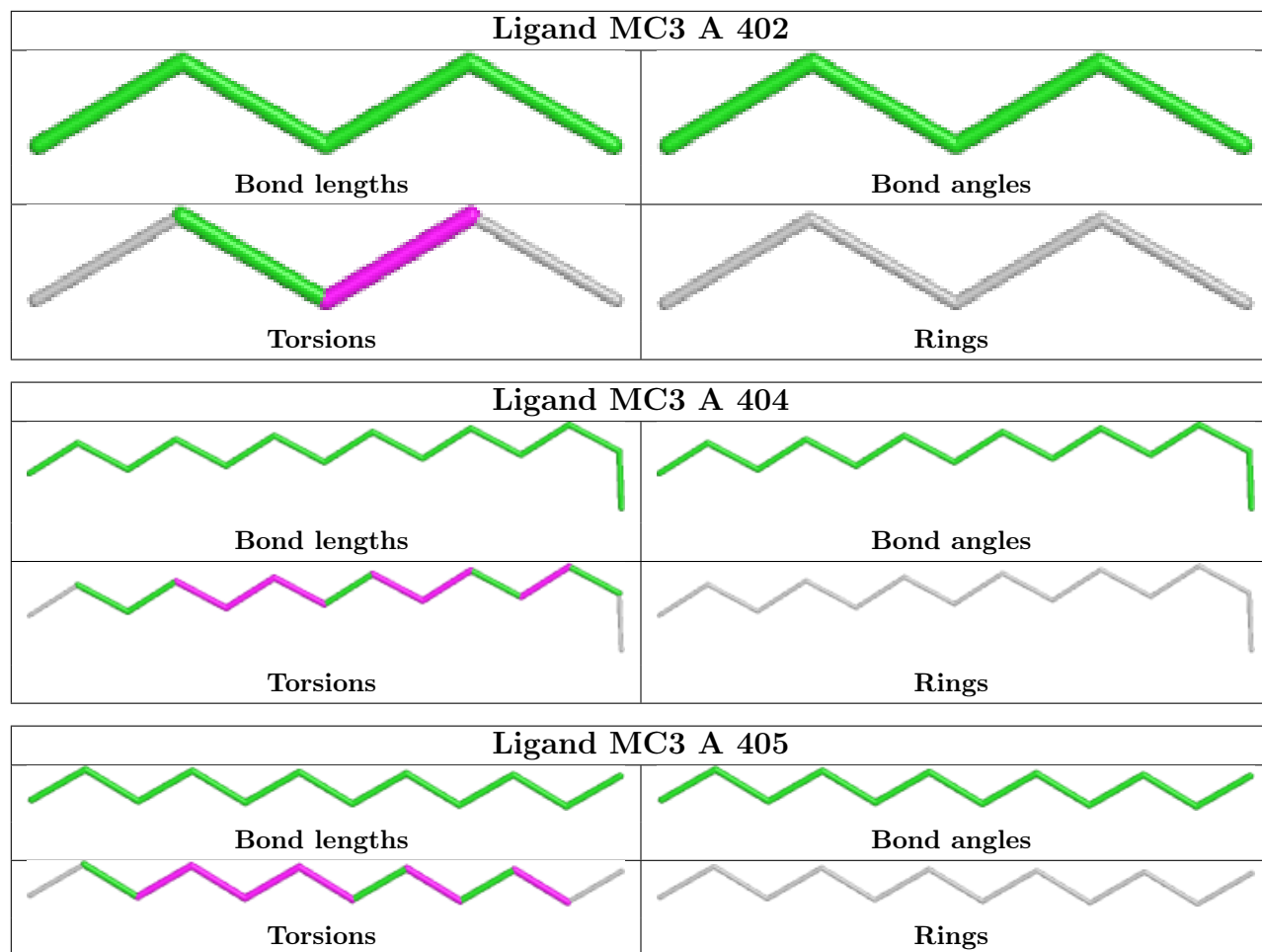


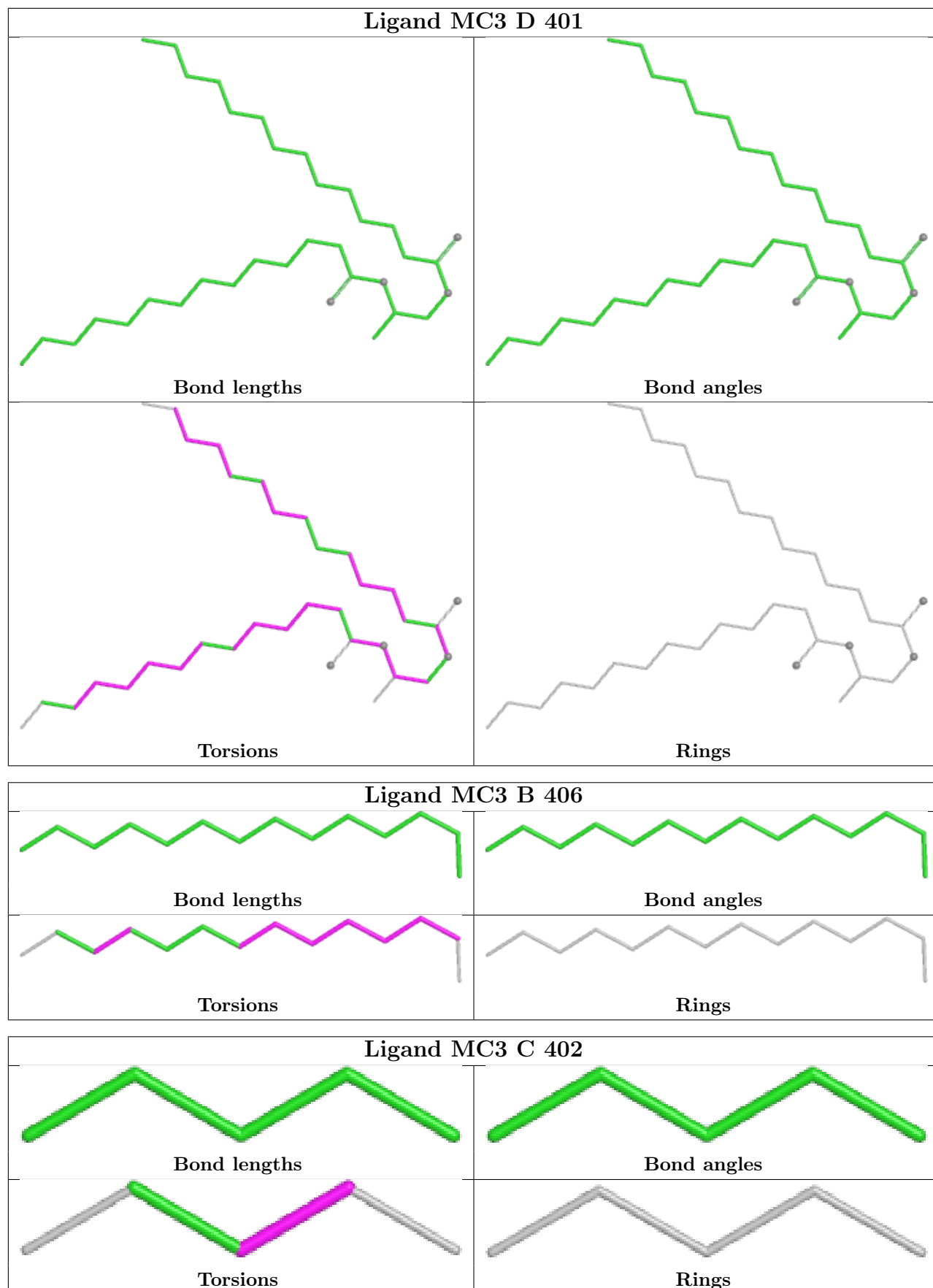


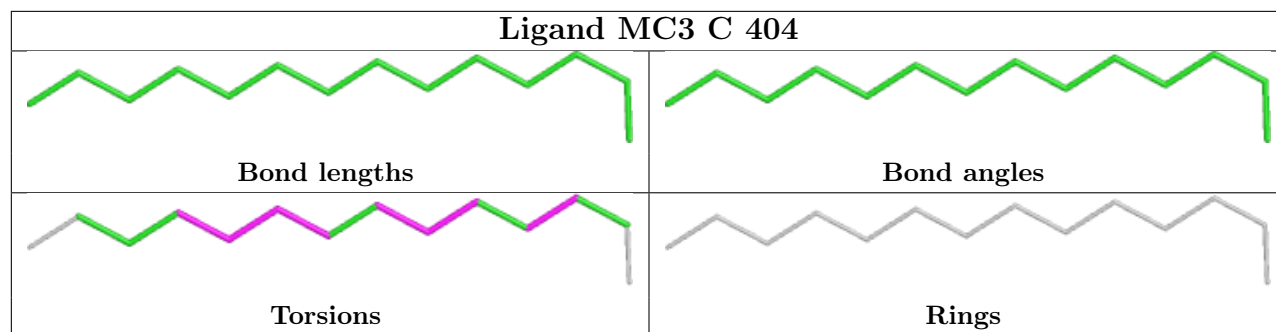












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

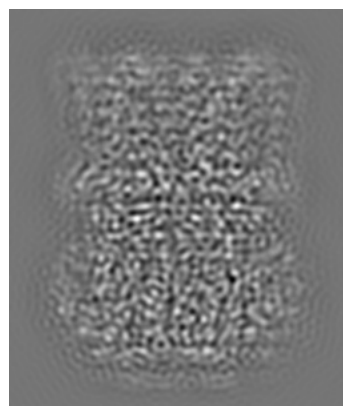
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27137. These allow visual inspection of the internal detail of the map and identification of artifacts.

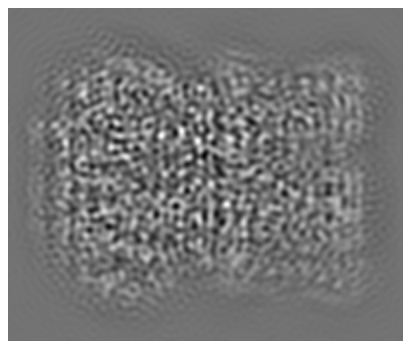
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

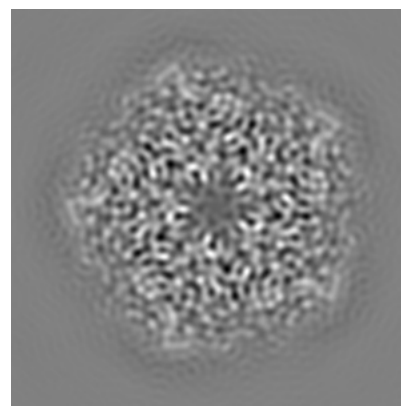
6.1.1 Primary map



X

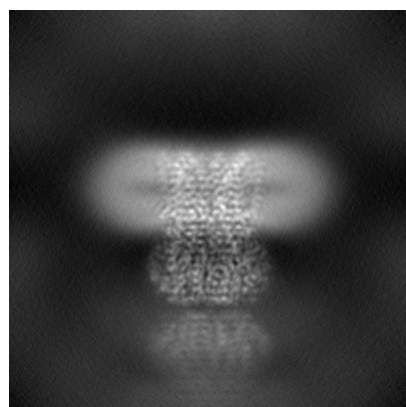


Y

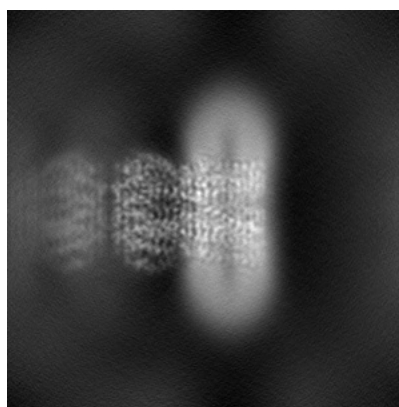


Z

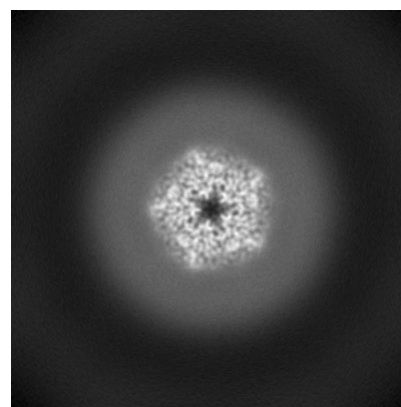
6.1.2 Raw map



X



Y

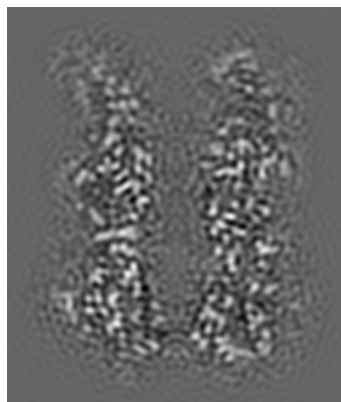


Z

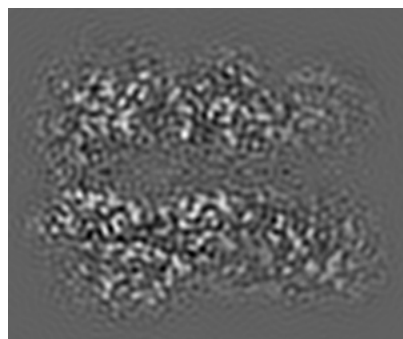
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

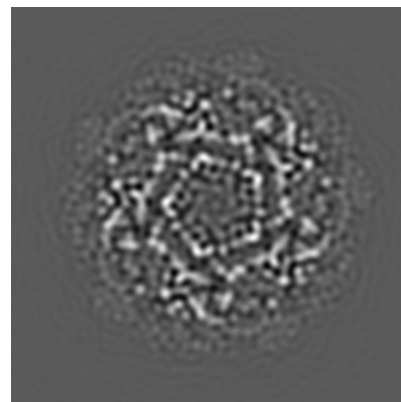
6.2.1 Primary map



X Index: 62

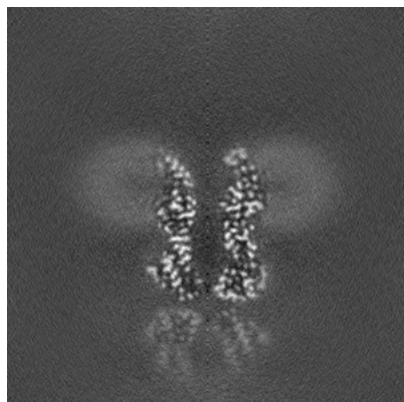


Y Index: 62

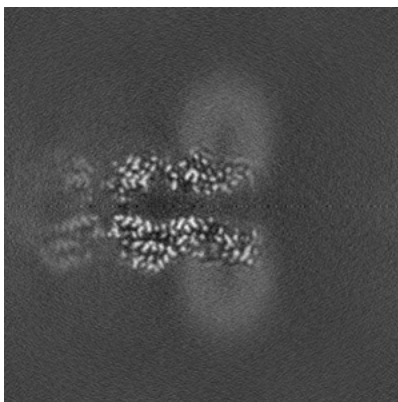


Z Index: 74

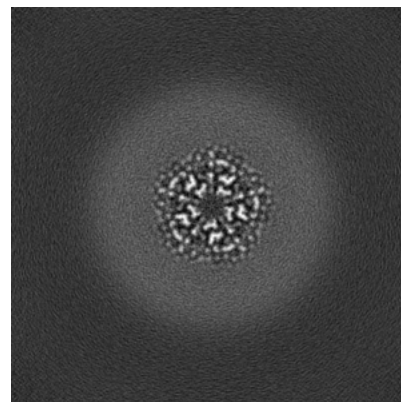
6.2.2 Raw map



X Index: 150



Y Index: 150

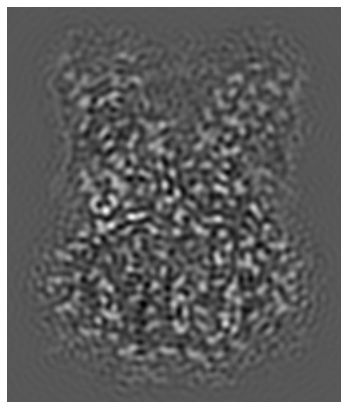


Z Index: 150

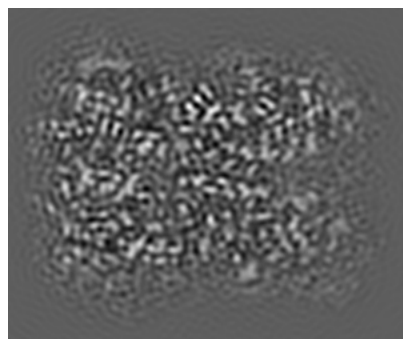
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

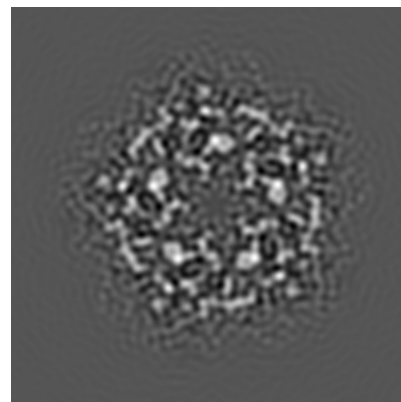
6.3.1 Primary map



X Index: 51

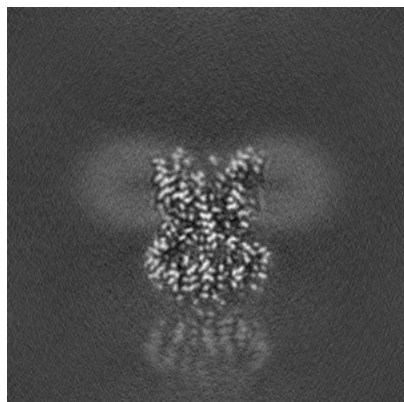


Y Index: 74

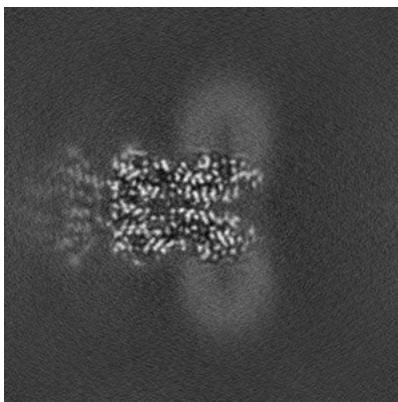


Z Index: 70

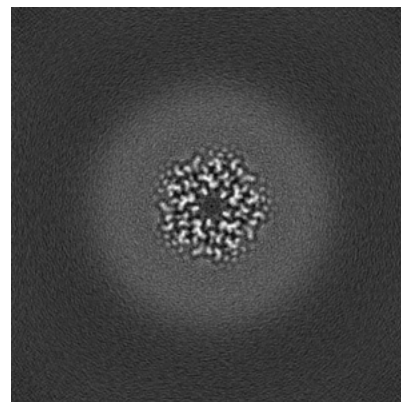
6.3.2 Raw map



X Index: 136



Y Index: 161

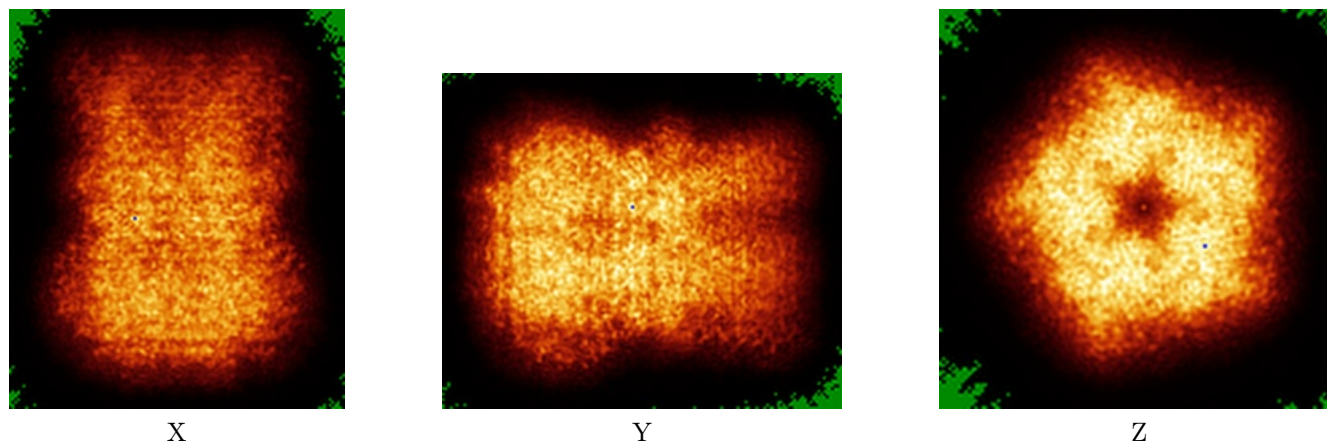


Z Index: 148

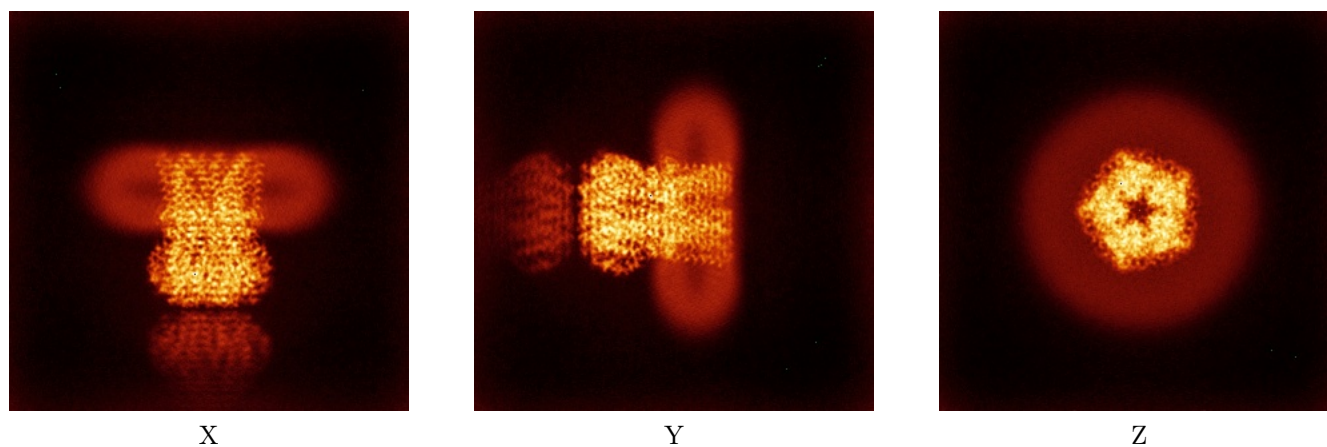
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



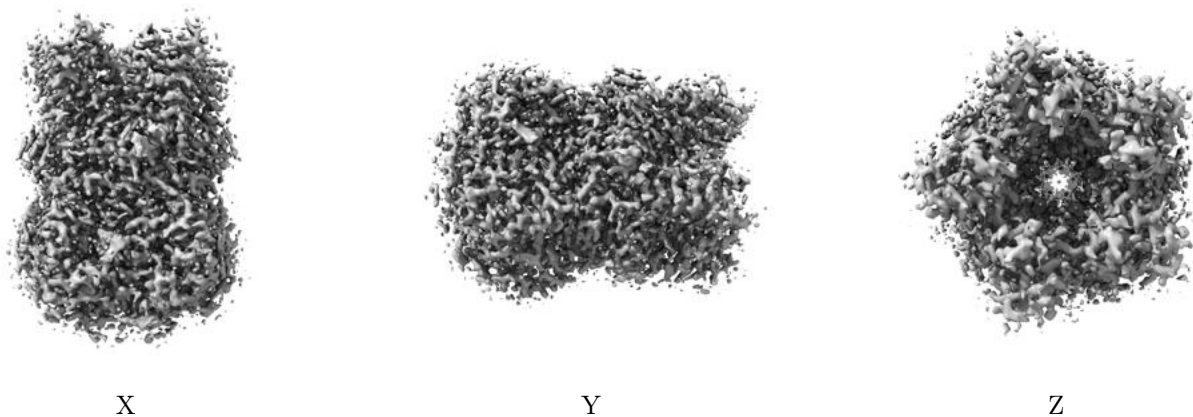
6.4.2 Raw map



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.

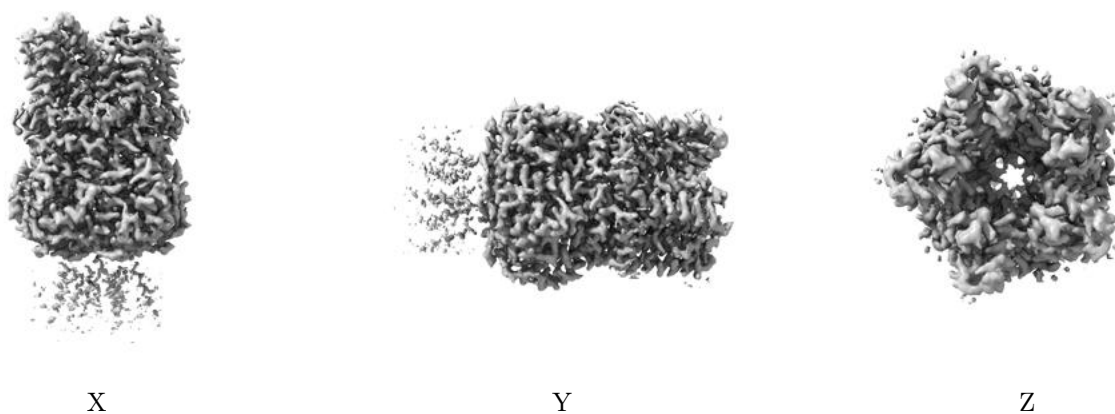
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.9. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

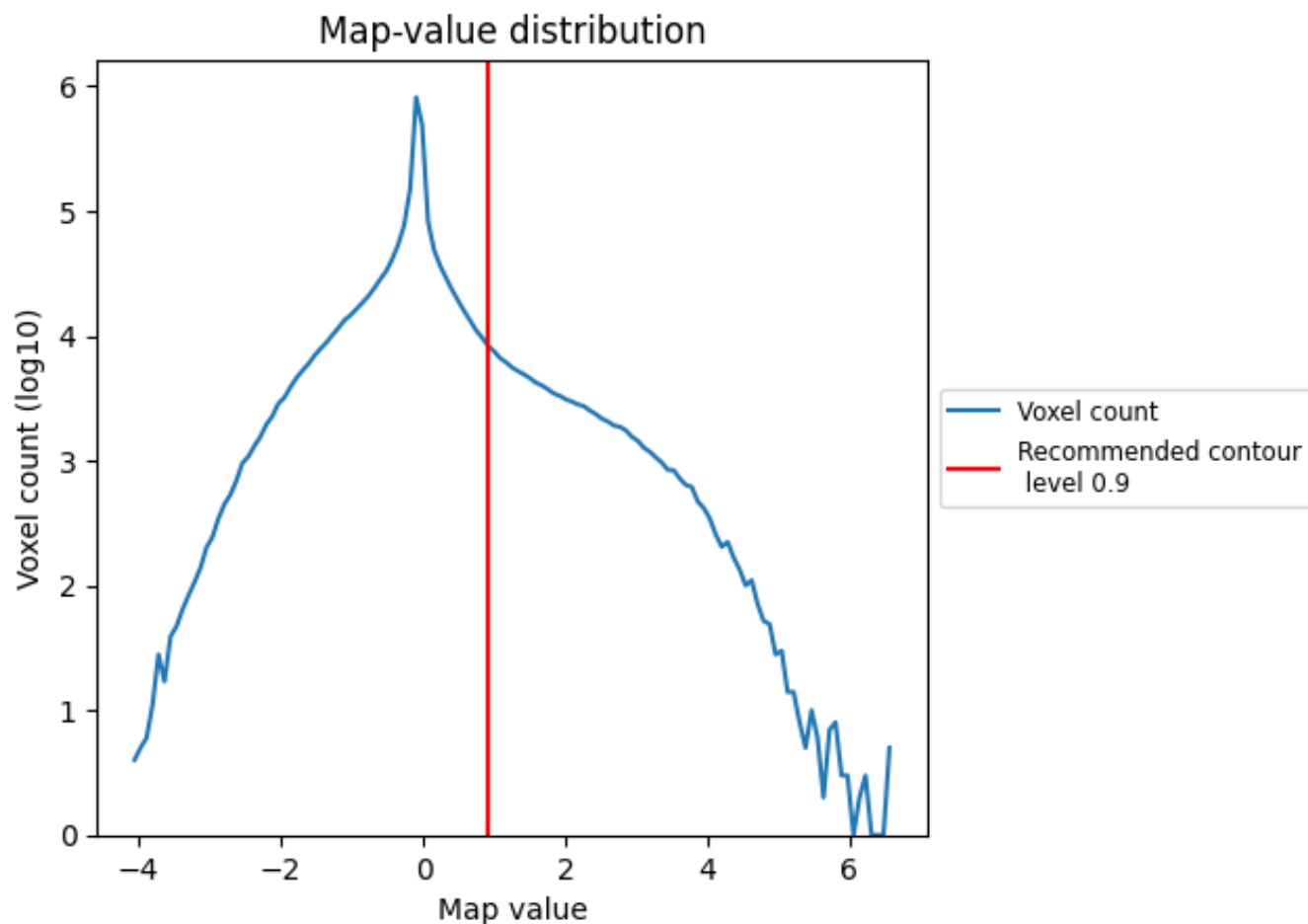
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

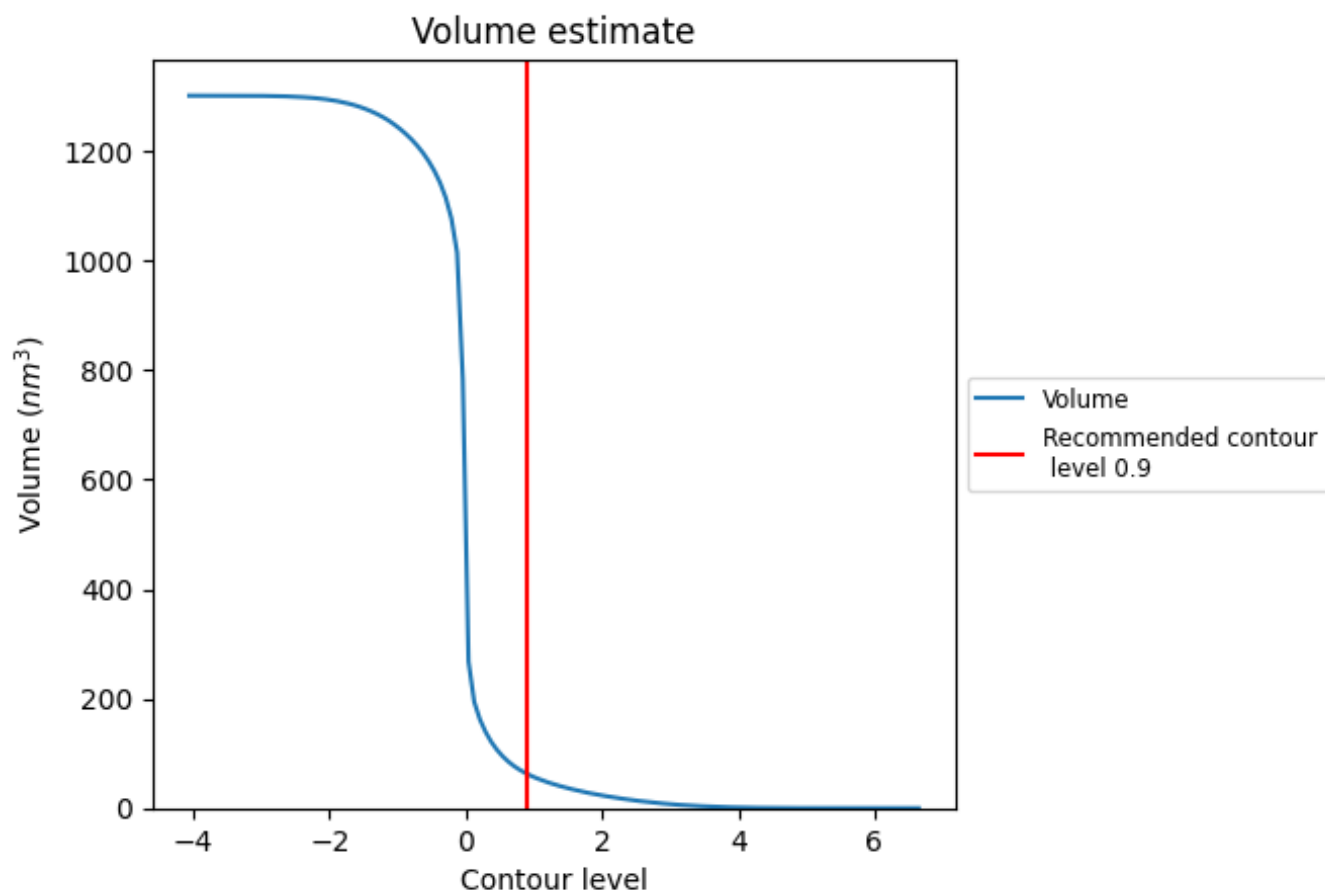
This section contains the results of statistical analysis of the map.

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 63 nm³; this corresponds to an approximate mass of 57 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.

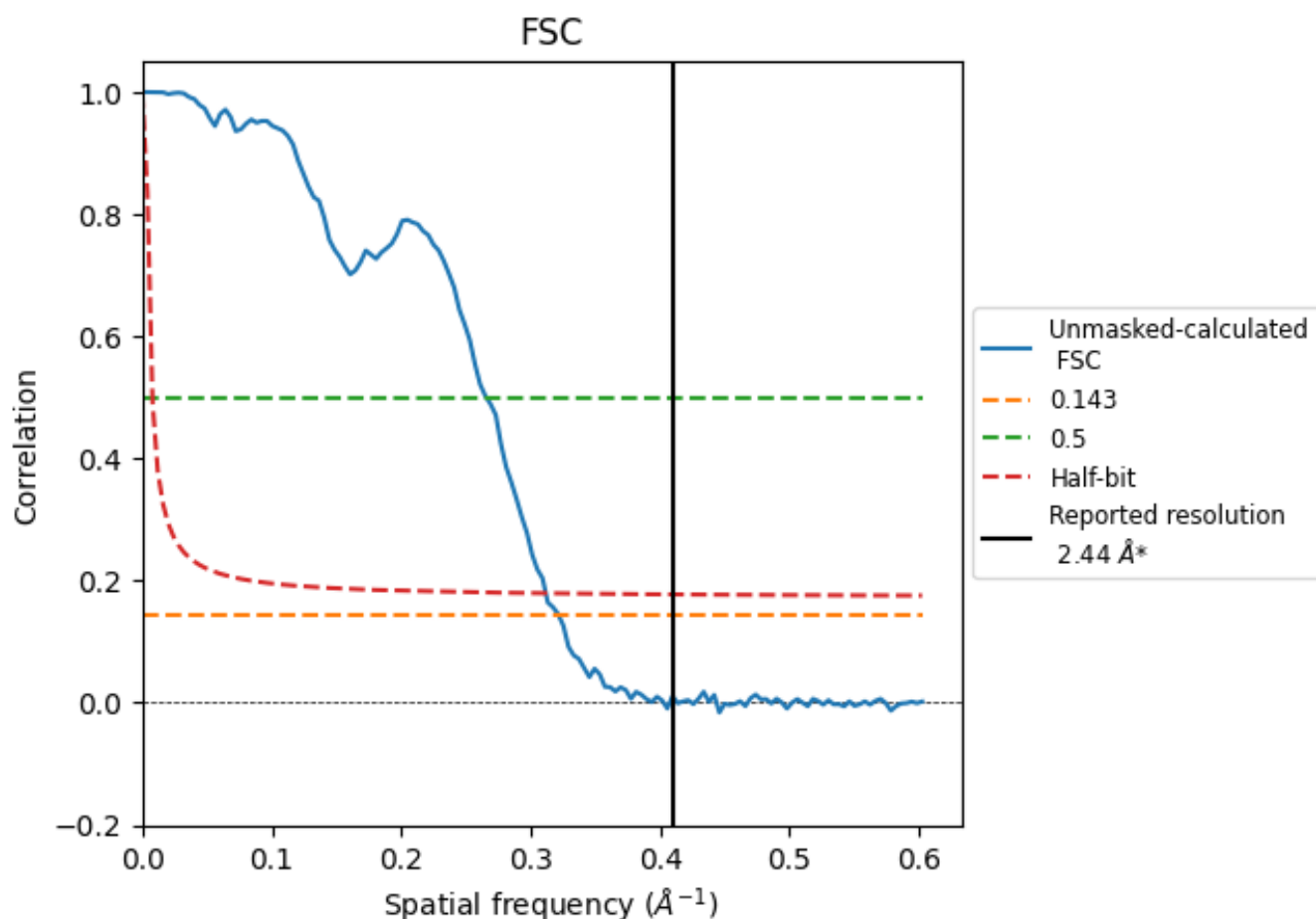
7.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

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 $0.410 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

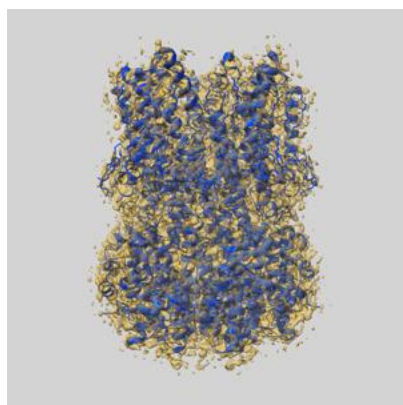
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.44	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.11	3.76	3.21

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.11 differs from the reported value 2.44 by more than 10 %

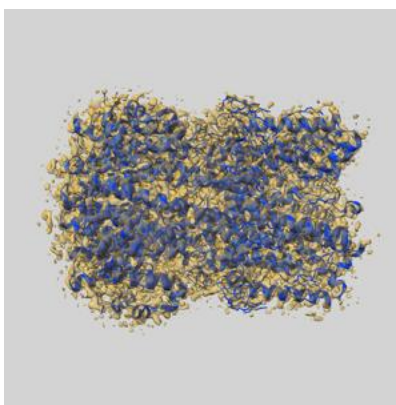
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-27137 and PDB model 8D1O. Per-residue inclusion information can be found in section 3 on page 8.

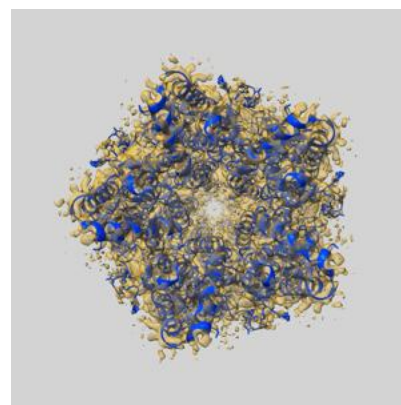
9.1 Map-model overlay [i](#)



X



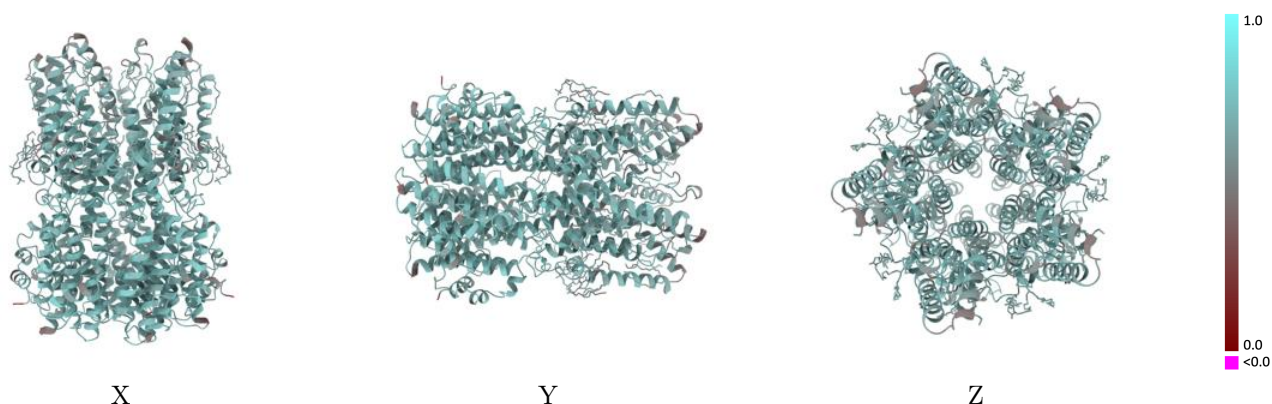
Y



Z

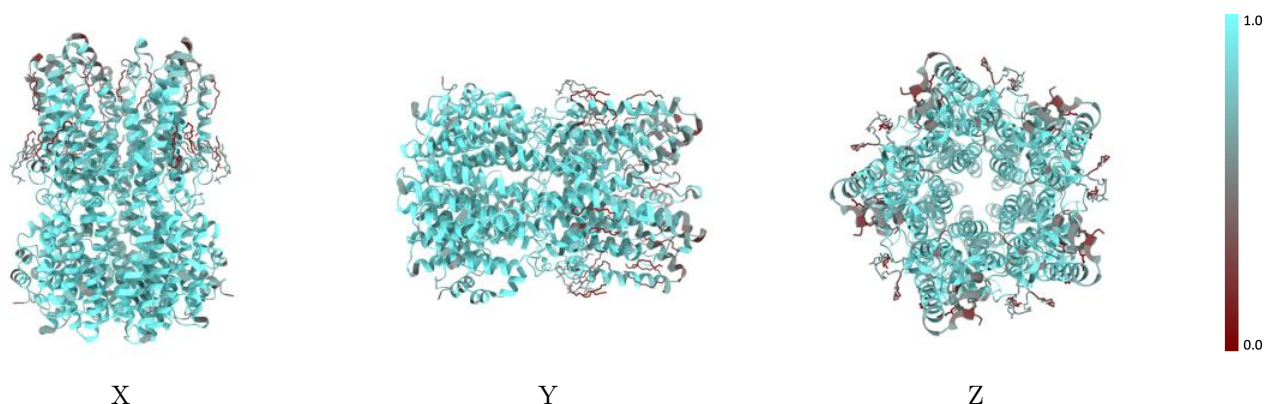
The images above show the 3D surface view of the map at the recommended contour level 0.9 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



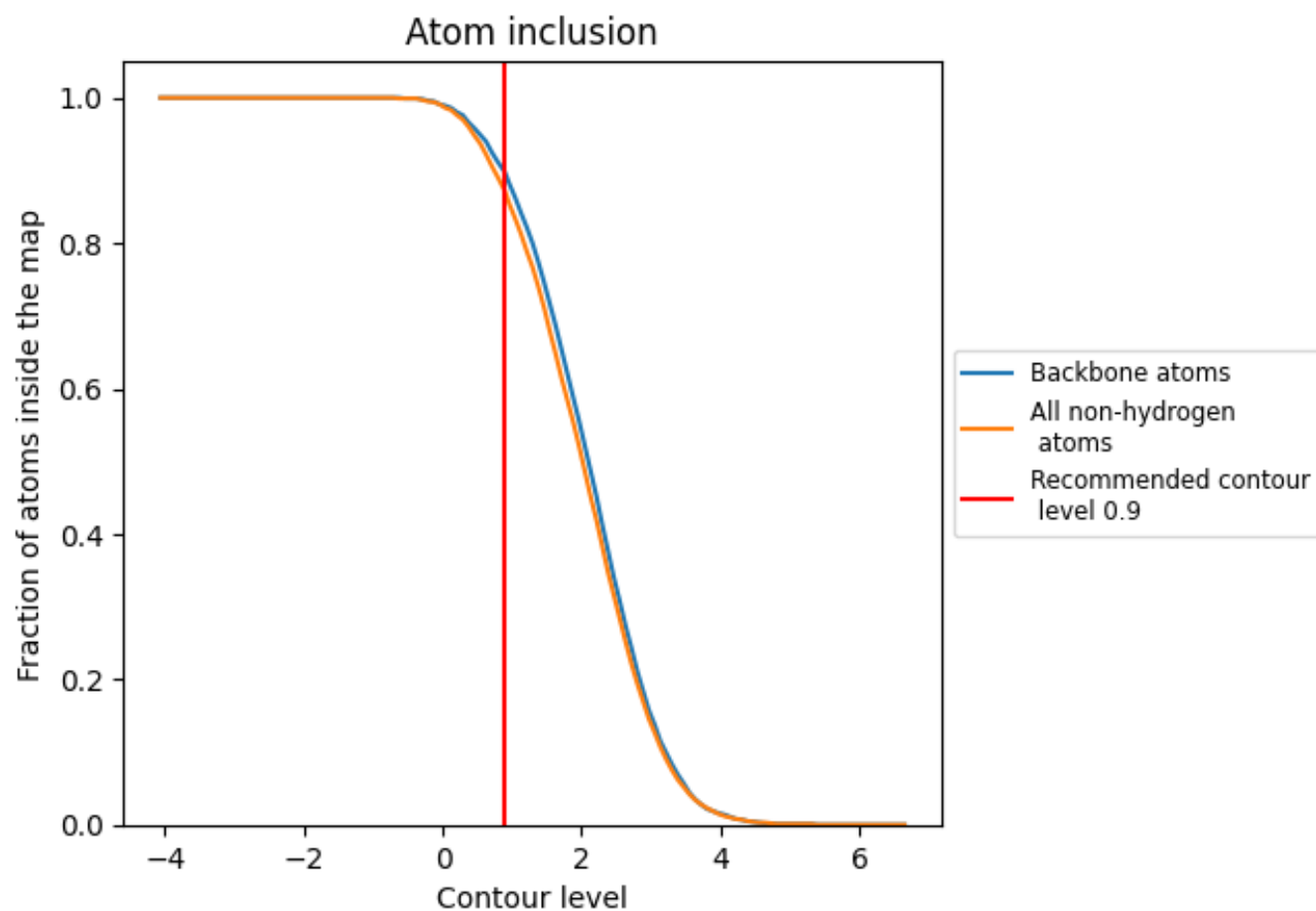
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.9).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 87% 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 (0.9) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8710	0.6570
A	0.8740	0.6570
B	0.8770	0.6570
C	0.8740	0.6570
D	0.8730	0.6560
E	0.8750	0.6570

