



Full wwPDB EM Validation Report ⓘ

Nov 27, 2023 – 10:16 PM JST

PDB ID : 7YNF
EMDB ID : EMD-33960
Title : CCA-bound alpha-synuclein fibrils
Authors : Tao, Y.Q.; Zhao, Q.Y.; Liu, C.; Li, D.
Deposited on : 2022-07-30
Resolution : 2.50 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:

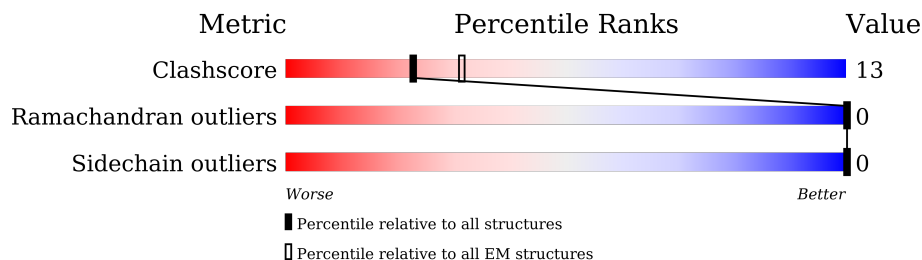
EMDB validation analysis : 0.0.1.dev70
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

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 2.50 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	140	38% 7% 55%
1	B	140	40% 5% 55%
1	C	140	38% 7% 55%
1	D	140	40% 5% 55%
1	E	140	39% 6% 55%
1	F	140	39% 6% 55%

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
2	V79	A	201	X	-	-	-
2	V79	A	202	X	-	-	-
2	V79	A	203	X	-	-	-
2	V79	A	204	X	-	-	-
2	V79	C	201	X	-	-	-
2	V79	C	202	X	-	-	-
2	V79	C	203	X	-	-	-
2	V79	D	201	X	-	-	-

2 Entry composition [i](#)

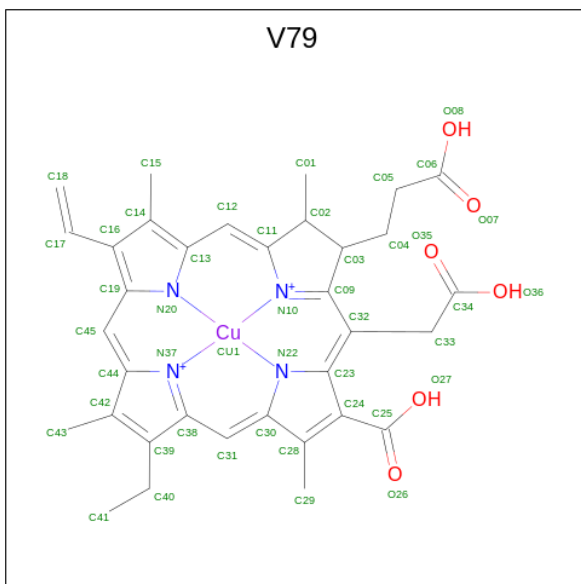
There are 2 unique types of molecules in this entry. The entry contains 2988 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Alpha-synuclein.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	A	63	Total 438	C 274	N 76	O 88	0	0
1	B	63	Total 438	C 274	N 76	O 88	0	0
1	C	63	Total 438	C 274	N 76	O 88	0	0
1	D	63	Total 438	C 274	N 76	O 88	0	0
1	E	63	Total 438	C 274	N 76	O 88	0	0
1	F	63	Total 438	C 274	N 76	O 88	0	0

- Molecule 2 is copper;trisodium;18-(2-carboxylatoethyl)-20-(carboxylatomethyl)-12-ethenyl-7-ethyl-3,8,13,17-tetramethyl-17,18-dihydroporphyrin-21,23-diide-2-carboxylate (three-letter code: V79) (formula: $C_{34}H_{34}CuN_4O_6$) (labeled as "Ligand of Interest" by depositor).




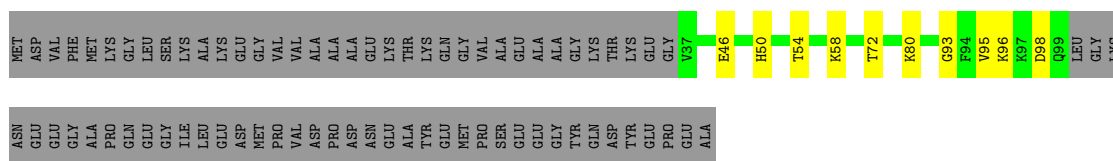
Mol	Chain	Residues	Atoms				AltConf	
2	A	1	Total	C	Cu	N	O	0
			45	34	1	4	6	
2	A	1	Total	C	Cu	N	O	0
			45	34	1	4	6	
2	A	1	Total	C	Cu	N	O	0
			45	34	1	4	6	
2	A	1	Total	C	Cu	N	O	0
			45	34	1	4	6	
2	C	1	Total	C	Cu	N	O	0
			45	34	1	4	6	
2	C	1	Total	C	Cu	N	O	0
			45	34	1	4	6	
2	C	1	Total	C	Cu	N	O	0
			45	34	1	4	6	
2	D	1	Total	C	Cu	N	O	0
			45	34	1	4	6	

3 Residue-property plots [i](#)


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.

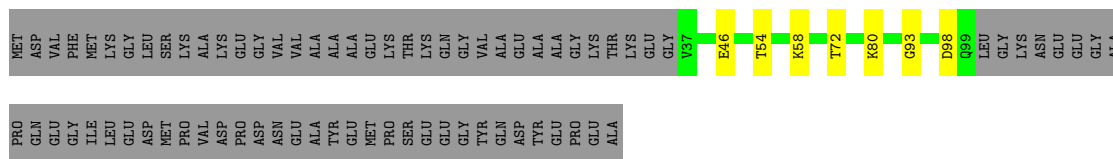
- Molecule 1: Alpha-synuclein

Chain A: 




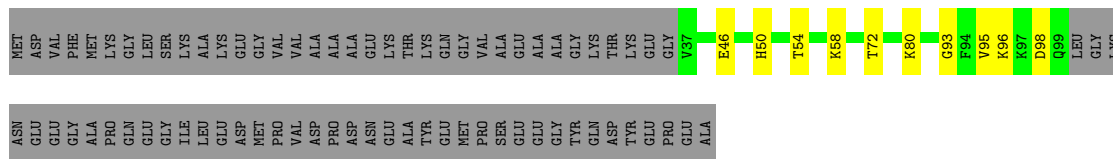
- Molecule 1: Alpha-synuclein

Chain B: 




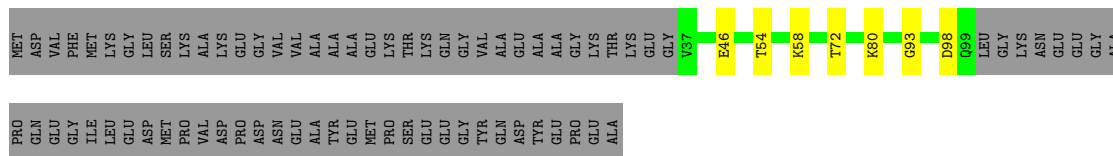
- Molecule 1: Alpha-synuclein

Chain C: 



- Molecule 1: Alpha-synuclein

Chain D: 



4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=179.56°, rise=2.43 Å, axial sym=C1	Depositor
Number of segments used	213959	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{Å}^2$)	55	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.097	Depositor
Minimum map value	-0.047	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.004	Depositor
Map size (Å)	305.27997, 305.27997, 305.27997	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	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: V79

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	0.40	0/440	0.53	0/595
1	B	0.40	0/440	0.53	0/595
1	C	0.40	0/440	0.53	0/595
1	D	0.40	0/440	0.53	0/595
1	E	0.40	0/440	0.53	0/595
1	F	0.40	0/440	0.53	0/595
All	All	0.40	0/2640	0.53	0/3570

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	438	0	459	13	0
1	B	438	0	459	6	0
1	C	438	0	459	13	0
1	D	438	0	459	6	0
1	E	438	0	459	7	0
1	F	438	0	459	7	0
2	A	180	0	0	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	135	0	0	13	0
2	D	45	0	0	9	0
All	All	2988	0	2754	72	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 13.

All (72) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:202:V79:O36	2:A:202:V79:C05	2.15	0.94
2:D:201:V79:C05	2:D:201:V79:O36	2.20	0.90
1:B:46:GLU:OE2	1:B:80:LYS:NZ	2.31	0.58
1:E:46:GLU:OE2	1:E:80:LYS:NZ	2.31	0.58
1:A:46:GLU:OE2	1:A:80:LYS:NZ	2.31	0.57
2:A:202:V79:O36	2:A:202:V79:O08	2.23	0.57
1:F:46:GLU:OE2	1:F:80:LYS:NZ	2.31	0.57
2:A:202:V79:O36	2:A:202:V79:C06	2.53	0.56
1:C:95:VAL:HG21	2:C:201:V79:O26	2.07	0.54
1:A:95:VAL:HG21	2:A:201:V79:O26	2.07	0.54
1:D:46:GLU:OE2	1:D:80:LYS:NZ	2.31	0.53
1:C:58:LYS:O	1:E:58:LYS:HA	2.09	0.53
1:A:58:LYS:O	1:F:58:LYS:HA	2.09	0.53
1:C:72:THR:OG1	1:E:72:THR:HG22	2.09	0.53
2:D:201:V79:O36	2:D:201:V79:O08	2.27	0.53
1:C:46:GLU:OE2	1:C:80:LYS:NZ	2.31	0.52
1:A:72:THR:OG1	1:F:72:THR:HG22	2.09	0.52
1:A:54:THR:OG1	1:F:54:THR:HG22	2.11	0.51
2:A:202:V79:O36	2:A:202:V79:C04	2.59	0.51
1:C:54:THR:OG1	1:E:54:THR:HG22	2.11	0.51
2:D:201:V79:O36	2:D:201:V79:C06	2.59	0.51
2:A:202:V79:O35	2:A:202:V79:C25	2.59	0.50
2:A:203:V79:C25	2:A:203:V79:C33	2.90	0.50
2:A:201:V79:C25	2:A:201:V79:C33	2.90	0.50
1:C:72:THR:HG22	1:D:72:THR:OG1	2.11	0.50
2:D:201:V79:C33	2:D:201:V79:C25	2.90	0.50
1:A:72:THR:HG22	1:B:72:THR:OG1	2.11	0.50
1:C:58:LYS:HA	1:D:58:LYS:O	2.12	0.49
2:C:202:V79:C33	2:C:202:V79:C25	2.90	0.49
1:A:58:LYS:HA	1:B:58:LYS:O	2.12	0.49
2:C:201:V79:C33	2:C:201:V79:C25	2.90	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:THR:HG22	1:B:54:THR:OG1	2.13	0.48
1:C:93:GLY:O	1:E:93:GLY:HA3	2.13	0.48
2:A:202:V79:C25	2:A:202:V79:C33	2.90	0.48
2:C:203:V79:C25	2:C:203:V79:C33	2.90	0.48
1:C:54:THR:HG22	1:D:54:THR:OG1	2.13	0.48
1:A:93:GLY:O	1:F:93:GLY:HA3	2.13	0.47
1:C:93:GLY:HA3	1:D:93:GLY:O	2.14	0.47
2:A:204:V79:C33	2:A:204:V79:C25	2.90	0.47
2:D:201:V79:C25	2:D:201:V79:O35	2.63	0.46
2:A:202:V79:C04	2:A:202:V79:C33	2.94	0.46
2:D:201:V79:C33	2:D:201:V79:C04	2.94	0.46
2:A:203:V79:C33	2:A:203:V79:C04	2.94	0.46
2:A:204:V79:C33	2:A:204:V79:C04	2.94	0.46
1:A:93:GLY:HA3	1:B:93:GLY:O	2.14	0.46
2:A:201:V79:C33	2:A:201:V79:C04	2.94	0.46
2:C:203:V79:C33	2:C:203:V79:C04	2.94	0.46
2:A:202:V79:C04	2:A:202:V79:C34	2.94	0.46
2:C:202:V79:C04	2:C:202:V79:C34	2.94	0.46
2:C:203:V79:C04	2:C:203:V79:C34	2.94	0.46
2:C:201:V79:C33	2:C:201:V79:C04	2.94	0.45
2:D:201:V79:O36	2:D:201:V79:C04	2.64	0.45
2:D:201:V79:C04	2:D:201:V79:C34	2.94	0.45
2:C:202:V79:C33	2:C:202:V79:C04	2.94	0.45
2:A:201:V79:C04	2:A:201:V79:C34	2.94	0.45
2:A:203:V79:C04	2:A:203:V79:C34	2.94	0.45
2:A:201:V79:C25	2:A:201:V79:C34	2.95	0.45
2:A:204:V79:C04	2:A:204:V79:C34	2.94	0.45
2:A:203:V79:C25	2:A:203:V79:C34	2.95	0.44
2:C:201:V79:C04	2:C:201:V79:C34	2.94	0.44
2:A:202:V79:C25	2:A:202:V79:C34	2.95	0.44
2:C:201:V79:C25	2:C:201:V79:C34	2.95	0.44
2:A:204:V79:C25	2:A:204:V79:C34	2.95	0.44
2:C:203:V79:C25	2:C:203:V79:C34	2.95	0.44
2:C:202:V79:C25	2:C:202:V79:C34	2.95	0.43
2:D:201:V79:C25	2:D:201:V79:C34	2.95	0.43
1:C:96:LYS:HE3	1:D:98:ASP:OD2	2.20	0.41
1:A:96:LYS:HE3	1:B:98:ASP:OD2	2.20	0.41
1:C:98:ASP:OD2	1:E:96:LYS:HE3	2.21	0.41
1:C:50:HIS:HA	1:E:50:HIS:O	2.22	0.40
1:A:50:HIS:HA	1:F:50:HIS:O	2.22	0.40
1:A:98:ASP:OD2	1:F:96:LYS:HE3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	61/140 (44%)	57 (93%)	4 (7%)	0	100	100
1	B	61/140 (44%)	57 (93%)	4 (7%)	0	100	100
1	C	61/140 (44%)	57 (93%)	4 (7%)	0	100	100
1	D	61/140 (44%)	57 (93%)	4 (7%)	0	100	100
1	E	61/140 (44%)	57 (93%)	4 (7%)	0	100	100
1	F	61/140 (44%)	57 (93%)	4 (7%)	0	100	100
All	All	366/840 (44%)	342 (93%)	24 (7%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	45/103 (44%)	45 (100%)	0	100	100
1	B	45/103 (44%)	45 (100%)	0	100	100
1	C	45/103 (44%)	45 (100%)	0	100	100
1	D	45/103 (44%)	45 (100%)	0	100	100
1	E	45/103 (44%)	45 (100%)	0	100	100
1	F	45/103 (44%)	45 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	270/618 (44%)	270 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	GLN
1	B	99	GLN
1	C	99	GLN
1	D	99	GLN
1	E	99	GLN
1	F	99	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	V79	A	204	-	45,52,52	5.01	28 (62%)	51,86,86	2.51	18 (35%)
2	V79	A	203	-	45,52,52	5.01	28 (62%)	51,86,86	2.51	18 (35%)
2	V79	C	202	-	45,52,52	5.01	28 (62%)	51,86,86	2.51	18 (35%)
2	V79	C	201	-	45,52,52	5.01	28 (62%)	51,86,86	2.50	18 (35%)
2	V79	A	202	-	45,52,52	5.01	28 (62%)	51,86,86	2.51	18 (35%)
2	V79	C	203	-	45,52,52	5.01	28 (62%)	51,86,86	2.51	18 (35%)
2	V79	D	201	-	45,52,52	5.00	28 (62%)	51,86,86	2.51	18 (35%)
2	V79	A	201	-	45,52,52	5.01	28 (62%)	51,86,86	2.51	18 (35%)

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	V79	A	204	-	5/5/15/19	10/15/101/101	-
2	V79	A	203	-	5/5/15/19	10/15/101/101	-
2	V79	C	202	-	5/5/15/19	10/15/101/101	-
2	V79	C	201	-	5/5/15/19	10/15/101/101	-
2	V79	A	202	-	5/5/15/19	9/15/101/101	-
2	V79	C	203	-	5/5/15/19	10/15/101/101	-
2	V79	D	201	-	5/5/15/19	9/15/101/101	-
2	V79	A	201	-	5/5/15/19	10/15/101/101	-

All (224) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	203	V79	C11-N10	-12.89	1.14	1.36
2	A	201	V79	C11-N10	-12.87	1.14	1.36
2	C	202	V79	C11-N10	-12.87	1.14	1.36
2	A	204	V79	C11-N10	-12.86	1.14	1.36
2	A	202	V79	C11-N10	-12.85	1.14	1.36
2	C	201	V79	C11-N10	-12.84	1.14	1.36
2	D	201	V79	C11-N10	-12.83	1.14	1.36
2	C	203	V79	C11-N10	-12.80	1.14	1.36
2	A	202	V79	C02-C03	-11.57	1.22	1.54
2	A	204	V79	C02-C03	-11.56	1.22	1.54
2	C	202	V79	C02-C03	-11.56	1.22	1.54
2	C	201	V79	C02-C03	-11.55	1.22	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	203	V79	C02-C03	-11.55	1.22	1.54
2	A	201	V79	C02-C03	-11.55	1.22	1.54
2	D	201	V79	C02-C03	-11.55	1.22	1.54
2	C	203	V79	C02-C03	-11.54	1.22	1.54
2	A	201	V79	C16-C14	11.33	1.56	1.40
2	C	202	V79	C16-C14	11.32	1.56	1.40
2	A	204	V79	C16-C14	11.31	1.56	1.40
2	C	201	V79	C16-C14	11.31	1.56	1.40
2	A	202	V79	C16-C14	11.29	1.56	1.40
2	A	203	V79	C16-C14	11.28	1.56	1.40
2	C	203	V79	C16-C14	11.25	1.56	1.40
2	D	201	V79	C16-C14	11.22	1.55	1.40
2	A	201	V79	C33-C32	-10.87	1.35	1.51
2	A	203	V79	C33-C32	-10.85	1.35	1.51
2	A	204	V79	C33-C32	-10.84	1.35	1.51
2	C	202	V79	C33-C32	-10.84	1.35	1.51
2	C	201	V79	C33-C32	-10.82	1.35	1.51
2	C	203	V79	C33-C32	-10.80	1.35	1.51
2	A	202	V79	C33-C32	-10.80	1.35	1.51
2	D	201	V79	C33-C32	-10.77	1.35	1.51
2	A	204	V79	C44-N37	-9.36	1.21	1.38
2	C	203	V79	C44-N37	-9.36	1.21	1.38
2	C	202	V79	C44-N37	-9.36	1.21	1.38
2	A	201	V79	C44-N37	-9.36	1.21	1.38
2	A	202	V79	C44-N37	-9.35	1.21	1.38
2	D	201	V79	C44-N37	-9.35	1.21	1.38
2	A	203	V79	C44-N37	-9.34	1.21	1.38
2	C	201	V79	C44-N37	-9.33	1.21	1.38
2	C	203	V79	C16-C17	8.55	1.65	1.47
2	A	201	V79	C16-C17	8.54	1.65	1.47
2	C	202	V79	C16-C17	8.54	1.65	1.47
2	A	203	V79	C16-C17	8.53	1.65	1.47
2	C	201	V79	C16-C17	8.53	1.65	1.47
2	A	202	V79	C16-C17	8.53	1.65	1.47
2	D	201	V79	C16-C17	8.52	1.65	1.47
2	A	204	V79	C16-C17	8.50	1.65	1.47
2	C	201	V79	C30-C28	-7.66	1.30	1.45
2	C	203	V79	C30-C28	-7.66	1.30	1.45
2	A	201	V79	C30-C28	-7.65	1.30	1.45
2	D	201	V79	C30-C28	-7.64	1.30	1.45
2	A	202	V79	C30-C28	-7.62	1.30	1.45
2	A	204	V79	C30-C28	-7.61	1.30	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	202	V79	C30-C28	-7.60	1.30	1.45
2	A	203	V79	C30-C28	-7.60	1.30	1.45
2	A	203	V79	C38-N37	7.06	1.50	1.37
2	C	202	V79	C38-N37	7.04	1.50	1.37
2	C	201	V79	C38-N37	7.03	1.50	1.37
2	A	204	V79	C38-N37	7.01	1.50	1.37
2	C	203	V79	C38-N37	6.99	1.50	1.37
2	A	202	V79	C38-N37	6.99	1.50	1.37
2	A	201	V79	C38-N37	6.98	1.50	1.37
2	D	201	V79	C38-N37	6.97	1.50	1.37
2	C	203	V79	C15-C14	6.39	1.64	1.51
2	D	201	V79	C15-C14	6.37	1.64	1.51
2	A	203	V79	C15-C14	6.36	1.64	1.51
2	A	204	V79	C15-C14	6.35	1.64	1.51
2	C	202	V79	C15-C14	6.35	1.64	1.51
2	C	201	V79	C15-C14	6.34	1.64	1.51
2	A	202	V79	C15-C14	6.33	1.64	1.51
2	A	201	V79	C15-C14	6.33	1.64	1.51
2	A	201	V79	C04-C03	5.69	1.64	1.54
2	A	204	V79	C04-C03	5.68	1.64	1.54
2	A	203	V79	C04-C03	5.67	1.64	1.54
2	C	202	V79	C04-C03	5.66	1.64	1.54
2	A	202	V79	C04-C03	5.66	1.64	1.54
2	C	203	V79	C04-C03	5.65	1.64	1.54
2	D	201	V79	C04-C03	5.64	1.64	1.54
2	C	201	V79	C04-C03	5.63	1.64	1.54
2	A	203	V79	C03-C09	-5.35	1.40	1.52
2	C	203	V79	C03-C09	-5.34	1.40	1.52
2	A	201	V79	C03-C09	-5.34	1.40	1.52
2	C	202	V79	C03-C09	-5.33	1.40	1.52
2	A	202	V79	C03-C09	-5.33	1.40	1.52
2	C	201	V79	C03-C09	-5.32	1.40	1.52
2	A	204	V79	C03-C09	-5.31	1.40	1.52
2	D	201	V79	C03-C09	-5.30	1.40	1.52
2	C	203	V79	O36-C34	5.17	1.48	1.30
2	A	204	V79	O36-C34	5.16	1.48	1.30
2	D	201	V79	O36-C34	5.15	1.48	1.30
2	C	202	V79	O36-C34	5.14	1.48	1.30
2	A	201	V79	O36-C34	5.14	1.48	1.30
2	C	201	V79	O36-C34	5.14	1.48	1.30
2	A	203	V79	O36-C34	5.13	1.48	1.30
2	A	202	V79	O36-C34	5.13	1.48	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	202	V79	C44-C42	4.97	1.54	1.44
2	C	203	V79	C44-C42	4.97	1.54	1.44
2	C	201	V79	C44-C42	4.96	1.54	1.44
2	A	201	V79	C44-C42	4.95	1.54	1.44
2	A	202	V79	C44-C42	4.94	1.54	1.44
2	A	203	V79	C44-C42	4.94	1.54	1.44
2	D	201	V79	C44-C42	4.92	1.54	1.44
2	A	204	V79	C44-C42	4.92	1.54	1.44
2	C	201	V79	C33-C34	-4.20	1.44	1.51
2	A	203	V79	C33-C34	-4.19	1.44	1.51
2	C	203	V79	C33-C34	-4.19	1.44	1.51
2	D	201	V79	C33-C34	-4.19	1.44	1.51
2	A	202	V79	C33-C34	-4.17	1.44	1.51
2	C	202	V79	C33-C34	-4.17	1.44	1.51
2	C	203	V79	O27-C25	-4.16	1.18	1.30
2	A	204	V79	C33-C34	-4.16	1.44	1.51
2	A	203	V79	O27-C25	-4.15	1.18	1.30
2	A	204	V79	O27-C25	-4.15	1.18	1.30
2	C	201	V79	O27-C25	-4.15	1.18	1.30
2	A	202	V79	O27-C25	-4.15	1.18	1.30
2	C	202	V79	O27-C25	-4.14	1.18	1.30
2	D	201	V79	O27-C25	-4.14	1.18	1.30
2	A	201	V79	C33-C34	-4.13	1.44	1.51
2	A	201	V79	O27-C25	-4.13	1.18	1.30
2	C	201	V79	C23-C32	-4.13	1.26	1.38
2	A	203	V79	C23-C32	-4.11	1.26	1.38
2	C	202	V79	C23-C32	-4.09	1.26	1.38
2	A	202	V79	C23-C32	-4.09	1.26	1.38
2	D	201	V79	C23-C32	-4.09	1.26	1.38
2	C	203	V79	C23-C32	-4.09	1.26	1.38
2	A	204	V79	C23-C32	-4.08	1.26	1.38
2	A	201	V79	C23-C32	-4.08	1.26	1.38
2	D	201	V79	C24-C28	3.97	1.50	1.39
2	C	201	V79	C24-C28	3.95	1.49	1.39
2	A	202	V79	C24-C28	3.95	1.49	1.39
2	C	202	V79	C24-C28	3.95	1.49	1.39
2	C	203	V79	C24-C28	3.94	1.49	1.39
2	A	201	V79	C24-C28	3.94	1.49	1.39
2	A	203	V79	C24-C28	3.93	1.49	1.39
2	A	204	V79	C24-C28	3.92	1.49	1.39
2	C	203	V79	C24-C23	-3.27	1.36	1.44
2	D	201	V79	C24-C23	-3.26	1.36	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	202	V79	C24-C23	-3.26	1.36	1.44
2	C	201	V79	C24-C23	-3.26	1.36	1.44
2	A	201	V79	C24-C23	-3.26	1.36	1.44
2	C	202	V79	C24-C23	-3.25	1.36	1.44
2	A	204	V79	C24-C23	-3.24	1.36	1.44
2	A	203	V79	C24-C23	-3.23	1.36	1.44
2	A	202	V79	O35-C34	-3.04	1.12	1.22
2	D	201	V79	O35-C34	-3.03	1.12	1.22
2	C	203	V79	O35-C34	-3.02	1.12	1.22
2	A	203	V79	O35-C34	-3.02	1.12	1.22
2	A	201	V79	O35-C34	-3.02	1.12	1.22
2	C	201	V79	O35-C34	-3.01	1.12	1.22
2	A	204	V79	O35-C34	-3.01	1.12	1.22
2	C	202	V79	O35-C34	-3.00	1.12	1.22
2	A	203	V79	C13-N20	2.97	1.41	1.35
2	C	203	V79	C13-N20	2.94	1.41	1.35
2	A	204	V79	C13-N20	2.94	1.41	1.35
2	A	201	V79	C13-N20	2.93	1.41	1.35
2	A	202	V79	C13-N20	2.93	1.41	1.35
2	C	202	V79	C13-N20	2.93	1.41	1.35
2	D	201	V79	C13-N20	2.92	1.41	1.35
2	C	201	V79	C13-N20	2.91	1.41	1.35
2	A	204	V79	C05-C06	-2.83	1.44	1.50
2	A	201	V79	C05-C06	-2.82	1.44	1.50
2	C	203	V79	C05-C06	-2.82	1.44	1.50
2	C	202	V79	C05-C06	-2.81	1.44	1.50
2	C	202	V79	C38-C39	-2.80	1.40	1.45
2	A	203	V79	C05-C06	-2.80	1.44	1.50
2	A	202	V79	C05-C06	-2.80	1.44	1.50
2	A	203	V79	C38-C39	-2.79	1.40	1.45
2	D	201	V79	C05-C06	-2.79	1.44	1.50
2	C	201	V79	C05-C06	-2.78	1.44	1.50
2	A	201	V79	C38-C39	-2.77	1.40	1.45
2	C	201	V79	C38-C39	-2.77	1.40	1.45
2	D	201	V79	C38-C39	-2.75	1.40	1.45
2	A	202	V79	C38-C39	-2.74	1.40	1.45
2	C	203	V79	C38-C39	-2.74	1.40	1.45
2	A	204	V79	C38-C39	-2.74	1.40	1.45
2	C	202	V79	C23-N22	2.68	1.43	1.38
2	C	203	V79	C23-N22	2.67	1.43	1.38
2	A	201	V79	C23-N22	2.67	1.43	1.38
2	A	204	V79	C23-N22	2.67	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	201	V79	C23-N22	2.66	1.43	1.38
2	C	201	V79	C23-N22	2.66	1.43	1.38
2	A	203	V79	C23-N22	2.66	1.43	1.38
2	A	202	V79	C23-N22	2.62	1.43	1.38
2	C	201	V79	C40-C39	2.53	1.57	1.51
2	C	202	V79	C40-C39	2.51	1.57	1.51
2	C	203	V79	C40-C39	2.51	1.57	1.51
2	A	201	V79	C40-C39	2.51	1.57	1.51
2	A	204	V79	C40-C39	2.49	1.57	1.51
2	A	203	V79	C40-C39	2.49	1.57	1.51
2	D	201	V79	C40-C39	2.49	1.57	1.51
2	A	202	V79	C40-C39	2.48	1.57	1.51
2	A	202	V79	C19-N20	-2.28	1.31	1.35
2	C	202	V79	C19-N20	-2.26	1.31	1.35
2	C	201	V79	C19-N20	-2.23	1.31	1.35
2	A	203	V79	C13-C12	-2.23	1.34	1.41
2	C	203	V79	C19-N20	-2.23	1.31	1.35
2	A	203	V79	C19-N20	-2.22	1.31	1.35
2	A	202	V79	C13-C12	-2.22	1.34	1.41
2	A	201	V79	C19-N20	-2.22	1.31	1.35
2	A	201	V79	C13-C12	-2.22	1.34	1.41
2	A	204	V79	C19-N20	-2.21	1.31	1.35
2	A	201	V79	O07-C06	2.21	1.29	1.22
2	A	204	V79	O07-C06	2.21	1.29	1.22
2	D	201	V79	C13-C12	-2.20	1.34	1.41
2	D	201	V79	C19-N20	-2.20	1.31	1.35
2	C	201	V79	O07-C06	2.20	1.29	1.22
2	A	204	V79	C13-C12	-2.19	1.34	1.41
2	C	202	V79	C13-C12	-2.19	1.34	1.41
2	C	201	V79	C13-C12	-2.19	1.34	1.41
2	C	203	V79	C13-C12	-2.19	1.34	1.41
2	C	203	V79	O07-C06	2.18	1.29	1.22
2	A	203	V79	O07-C06	2.17	1.29	1.22
2	A	202	V79	O07-C06	2.17	1.29	1.22
2	C	202	V79	O07-C06	2.17	1.29	1.22
2	D	201	V79	O07-C06	2.16	1.29	1.22
2	A	203	V79	C24-C25	2.08	1.52	1.48
2	A	204	V79	C24-C25	2.08	1.52	1.48
2	C	201	V79	C24-C25	2.07	1.52	1.48
2	A	202	V79	C24-C25	2.07	1.52	1.48
2	C	203	V79	C24-C25	2.07	1.52	1.48
2	C	202	V79	C24-C25	2.06	1.52	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	201	V79	C24-C25	2.05	1.52	1.48
2	A	201	V79	C24-C25	2.03	1.52	1.48

All (144) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	203	V79	C04-C03-C09	6.55	133.45	111.97
2	C	201	V79	C04-C03-C09	6.54	133.41	111.97
2	C	202	V79	C04-C03-C09	6.54	133.41	111.97
2	A	204	V79	C04-C03-C09	6.54	133.40	111.97
2	D	201	V79	C04-C03-C09	6.54	133.40	111.97
2	A	201	V79	C04-C03-C09	6.54	133.40	111.97
2	A	203	V79	C04-C03-C09	6.54	133.39	111.97
2	A	202	V79	C04-C03-C09	6.53	133.38	111.97
2	A	204	V79	C01-C02-C11	6.23	128.52	111.77
2	A	201	V79	C01-C02-C11	6.23	128.50	111.77
2	A	203	V79	C01-C02-C11	6.22	128.50	111.77
2	C	202	V79	C01-C02-C11	6.22	128.50	111.77
2	C	201	V79	C01-C02-C11	6.22	128.50	111.77
2	D	201	V79	C01-C02-C11	6.22	128.48	111.77
2	A	202	V79	C01-C02-C11	6.21	128.47	111.77
2	C	203	V79	C01-C02-C11	6.21	128.46	111.77
2	A	204	V79	C13-C12-C11	-5.62	118.98	130.12
2	A	203	V79	C13-C12-C11	-5.62	118.99	130.12
2	A	202	V79	C13-C12-C11	-5.61	119.00	130.12
2	D	201	V79	C13-C12-C11	-5.61	119.01	130.12
2	C	201	V79	C13-C12-C11	-5.61	119.01	130.12
2	C	202	V79	C13-C12-C11	-5.61	119.01	130.12
2	C	203	V79	C13-C12-C11	-5.61	119.02	130.12
2	A	201	V79	C13-C12-C11	-5.60	119.02	130.12
2	A	204	V79	C30-C31-C38	-4.57	116.19	126.06
2	C	203	V79	C30-C31-C38	-4.57	116.20	126.06
2	A	202	V79	C30-C31-C38	-4.57	116.20	126.06
2	D	201	V79	C30-C31-C38	-4.56	116.22	126.06
2	A	201	V79	C30-C31-C38	-4.56	116.23	126.06
2	C	201	V79	C30-C31-C38	-4.55	116.24	126.06
2	C	202	V79	C30-C31-C38	-4.55	116.24	126.06
2	A	203	V79	C30-C31-C38	-4.55	116.24	126.06
2	C	202	V79	C45-C44-C42	-4.53	114.20	126.72
2	A	202	V79	C45-C44-C42	-4.53	114.20	126.72
2	D	201	V79	C45-C44-C42	-4.53	114.20	126.72
2	A	204	V79	C45-C44-C42	-4.52	114.23	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	201	V79	C45-C44-C42	-4.52	114.23	126.72
2	A	203	V79	C45-C44-C42	-4.51	114.24	126.72
2	A	201	V79	C45-C44-C42	-4.51	114.24	126.72
2	C	203	V79	C45-C44-C42	-4.51	114.25	126.72
2	A	202	V79	C31-C30-N22	4.49	130.56	124.63
2	A	203	V79	C31-C30-N22	4.49	130.56	124.63
2	D	201	V79	C31-C30-N22	4.47	130.54	124.63
2	A	204	V79	C31-C30-N22	4.47	130.53	124.63
2	C	202	V79	C31-C30-N22	4.47	130.53	124.63
2	C	201	V79	C31-C30-N22	4.46	130.52	124.63
2	C	203	V79	C31-C30-N22	4.45	130.50	124.63
2	A	201	V79	C31-C30-N22	4.43	130.49	124.63
2	C	203	V79	C31-C38-C39	-3.23	120.09	124.84
2	D	201	V79	C31-C38-C39	-3.23	120.10	124.84
2	A	201	V79	C31-C38-C39	-3.22	120.10	124.84
2	A	202	V79	C31-C38-C39	-3.22	120.10	124.84
2	A	203	V79	C31-C38-C39	-3.21	120.13	124.84
2	A	204	V79	C31-C38-C39	-3.20	120.13	124.84
2	C	202	V79	C31-C38-C39	-3.19	120.15	124.84
2	C	201	V79	C31-C38-C39	-3.19	120.16	124.84
2	A	204	V79	C31-C38-N37	3.16	127.96	124.60
2	C	203	V79	C31-C38-N37	3.16	127.96	124.60
2	A	202	V79	C31-C38-N37	3.14	127.95	124.60
2	A	201	V79	C31-C38-N37	3.14	127.94	124.60
2	A	203	V79	C31-C38-N37	3.11	127.92	124.60
2	C	202	V79	C45-C44-N37	3.11	132.60	124.83
2	A	201	V79	C45-C44-N37	3.11	132.60	124.83
2	C	201	V79	C31-C38-N37	3.11	127.91	124.60
2	D	201	V79	C45-C44-N37	3.11	132.59	124.83
2	A	202	V79	C45-C44-N37	3.11	132.59	124.83
2	C	203	V79	C45-C44-N37	3.10	132.58	124.83
2	D	201	V79	C31-C30-C28	-3.10	118.98	125.48
2	C	202	V79	C31-C38-N37	3.10	127.90	124.60
2	C	201	V79	C45-C44-N37	3.10	132.57	124.83
2	A	203	V79	C45-C44-N37	3.10	132.56	124.83
2	C	202	V79	C31-C30-C28	-3.09	118.99	125.48
2	A	204	V79	C45-C44-N37	3.09	132.55	124.83
2	A	202	V79	C31-C30-C28	-3.09	118.99	125.48
2	D	201	V79	C31-C38-N37	3.09	127.89	124.60
2	A	203	V79	C02-C03-C09	3.09	105.97	101.34
2	A	204	V79	C31-C30-C28	-3.09	119.00	125.48
2	C	201	V79	C31-C30-C28	-3.09	119.00	125.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	202	V79	C02-C03-C09	3.09	105.97	101.34
2	C	202	V79	C02-C03-C09	3.08	105.96	101.34
2	A	201	V79	C31-C30-C28	-3.08	119.01	125.48
2	A	203	V79	C31-C30-C28	-3.08	119.02	125.48
2	C	201	V79	C02-C03-C09	3.08	105.95	101.34
2	C	203	V79	C31-C30-C28	-3.08	119.02	125.48
2	D	201	V79	C02-C03-C09	3.08	105.95	101.34
2	A	201	V79	C02-C03-C09	3.08	105.95	101.34
2	A	204	V79	C02-C03-C09	3.07	105.94	101.34
2	C	203	V79	C02-C03-C09	3.06	105.92	101.34
2	A	203	V79	C01-C02-C03	2.99	125.88	113.83
2	A	202	V79	C01-C02-C03	2.99	125.88	113.83
2	C	201	V79	C01-C02-C03	2.99	125.87	113.83
2	D	201	V79	C01-C02-C03	2.99	125.87	113.83
2	C	202	V79	C01-C02-C03	2.98	125.87	113.83
2	C	203	V79	C01-C02-C03	2.98	125.86	113.83
2	A	201	V79	C01-C02-C03	2.98	125.86	113.83
2	A	204	V79	C01-C02-C03	2.98	125.84	113.83
2	D	201	V79	C25-C24-C28	-2.93	119.02	127.30
2	C	203	V79	C25-C24-C28	-2.92	119.04	127.30
2	A	202	V79	C25-C24-C28	-2.92	119.04	127.30
2	C	202	V79	C25-C24-C28	-2.92	119.04	127.30
2	A	204	V79	C25-C24-C28	-2.92	119.05	127.30
2	C	201	V79	C25-C24-C28	-2.92	119.05	127.30
2	A	203	V79	C25-C24-C28	-2.92	119.05	127.30
2	A	201	V79	C25-C24-C28	-2.91	119.08	127.30
2	A	204	V79	C04-C03-C02	2.88	120.66	112.78
2	A	202	V79	C04-C03-C02	2.88	120.66	112.78
2	A	201	V79	C04-C03-C02	2.88	120.65	112.78
2	D	201	V79	C04-C03-C02	2.88	120.65	112.78
2	A	203	V79	C04-C03-C02	2.87	120.64	112.78
2	C	201	V79	C04-C03-C02	2.87	120.64	112.78
2	C	202	V79	C04-C03-C02	2.87	120.64	112.78
2	C	203	V79	C04-C03-C02	2.87	120.64	112.78
2	C	202	V79	C15-C14-C16	2.54	129.43	124.68
2	D	201	V79	C15-C14-C16	2.53	129.41	124.68
2	A	201	V79	C15-C14-C16	2.53	129.41	124.68
2	C	203	V79	C15-C14-C16	2.52	129.40	124.68
2	A	202	V79	C15-C14-C16	2.52	129.39	124.68
2	C	201	V79	C15-C14-C16	2.51	129.38	124.68
2	A	203	V79	C15-C14-C16	2.51	129.38	124.68
2	A	204	V79	C42-C44-N37	2.50	113.22	109.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	204	V79	C15-C14-C16	2.50	129.35	124.68
2	A	202	V79	C42-C44-N37	2.50	113.21	109.63
2	D	201	V79	C42-C44-N37	2.49	113.21	109.63
2	C	201	V79	C42-C44-N37	2.49	113.20	109.63
2	C	202	V79	C42-C44-N37	2.49	113.20	109.63
2	A	203	V79	C42-C44-N37	2.49	113.20	109.63
2	C	203	V79	C42-C44-N37	2.46	113.17	109.63
2	A	201	V79	C42-C44-N37	2.46	113.15	109.63
2	D	201	V79	C23-C24-C25	2.39	133.88	126.86
2	C	203	V79	C23-C24-C25	2.38	133.85	126.86
2	C	201	V79	C23-C24-C25	2.37	133.82	126.86
2	A	202	V79	C23-C24-C25	2.37	133.82	126.86
2	A	201	V79	C23-C24-C25	2.37	133.81	126.86
2	C	202	V79	C23-C24-C25	2.37	133.81	126.86
2	A	204	V79	C23-C24-C25	2.36	133.81	126.86
2	A	203	V79	C23-C24-C25	2.36	133.80	126.86
2	C	203	V79	C03-C02-C11	2.36	105.68	101.87
2	A	202	V79	C03-C02-C11	2.34	105.65	101.87
2	D	201	V79	C03-C02-C11	2.34	105.65	101.87
2	A	204	V79	C03-C02-C11	2.33	105.64	101.87
2	A	201	V79	C03-C02-C11	2.33	105.64	101.87
2	C	201	V79	C03-C02-C11	2.33	105.63	101.87
2	C	202	V79	C03-C02-C11	2.33	105.63	101.87
2	A	203	V79	C03-C02-C11	2.32	105.61	101.87

All (40) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	201	V79	N22
2	A	201	V79	C02
2	A	201	V79	N37
2	A	201	V79	N10
2	A	201	V79	C03
2	A	202	V79	N22
2	A	202	V79	C02
2	A	202	V79	N37
2	A	202	V79	N10
2	A	202	V79	C03
2	A	203	V79	N22
2	A	203	V79	C02
2	A	203	V79	N37
2	A	203	V79	N10

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Mol	Chain	Res	Type	Atom
2	A	203	V79	C03
2	A	204	V79	N22
2	A	204	V79	C02
2	A	204	V79	N37
2	A	204	V79	N10
2	A	204	V79	C03
2	C	201	V79	N22
2	C	201	V79	C02
2	C	201	V79	N37
2	C	201	V79	N10
2	C	201	V79	C03
2	C	202	V79	N22
2	C	202	V79	C02
2	C	202	V79	N37
2	C	202	V79	N10
2	C	202	V79	C03
2	C	203	V79	N22
2	C	203	V79	C02
2	C	203	V79	N37
2	C	203	V79	N10
2	C	203	V79	C03
2	D	201	V79	N22
2	D	201	V79	C02
2	D	201	V79	N37
2	D	201	V79	N10
2	D	201	V79	C03

All (78) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	201	V79	C23-C24-C25-O26
2	A	201	V79	C23-C24-C25-O27
2	A	201	V79	C28-C24-C25-O26
2	A	201	V79	C28-C24-C25-O27
2	A	201	V79	C09-C03-C04-C05
2	A	202	V79	C23-C24-C25-O26
2	A	202	V79	C23-C24-C25-O27
2	A	202	V79	C28-C24-C25-O26
2	A	202	V79	C28-C24-C25-O27
2	A	202	V79	C09-C03-C04-C05
2	A	203	V79	C23-C24-C25-O26
2	A	203	V79	C23-C24-C25-O27

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Mol	Chain	Res	Type	Atoms
2	A	203	V79	C28-C24-C25-O26
2	A	203	V79	C28-C24-C25-O27
2	A	203	V79	C09-C03-C04-C05
2	A	204	V79	C23-C24-C25-O26
2	A	204	V79	C23-C24-C25-O27
2	A	204	V79	C28-C24-C25-O26
2	A	204	V79	C28-C24-C25-O27
2	A	204	V79	C09-C03-C04-C05
2	C	201	V79	C23-C24-C25-O26
2	C	201	V79	C23-C24-C25-O27
2	C	201	V79	C28-C24-C25-O26
2	C	201	V79	C28-C24-C25-O27
2	C	201	V79	C09-C03-C04-C05
2	C	202	V79	C23-C24-C25-O26
2	C	202	V79	C23-C24-C25-O27
2	C	202	V79	C28-C24-C25-O26
2	C	202	V79	C28-C24-C25-O27
2	C	202	V79	C09-C03-C04-C05
2	C	203	V79	C23-C24-C25-O26
2	C	203	V79	C23-C24-C25-O27
2	C	203	V79	C28-C24-C25-O26
2	C	203	V79	C28-C24-C25-O27
2	C	203	V79	C09-C03-C04-C05
2	D	201	V79	C23-C24-C25-O26
2	D	201	V79	C23-C24-C25-O27
2	D	201	V79	C28-C24-C25-O26
2	D	201	V79	C28-C24-C25-O27
2	D	201	V79	C09-C03-C04-C05
2	D	201	V79	C32-C33-C34-O36
2	A	201	V79	C32-C33-C34-O35
2	A	203	V79	C32-C33-C34-O35
2	A	204	V79	C32-C33-C34-O35
2	C	201	V79	C32-C33-C34-O35
2	C	202	V79	C32-C33-C34-O35
2	C	203	V79	C32-C33-C34-O35
2	A	201	V79	C04-C05-C06-O08
2	A	202	V79	C04-C05-C06-O08
2	C	201	V79	C04-C05-C06-O08
2	C	202	V79	C04-C05-C06-O08
2	D	201	V79	C04-C05-C06-O08
2	A	203	V79	C04-C05-C06-O08
2	A	204	V79	C04-C05-C06-O08

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Mol	Chain	Res	Type	Atoms
2	C	203	V79	C04-C05-C06-O08
2	A	201	V79	C02-C03-C04-C05
2	A	202	V79	C02-C03-C04-C05
2	A	203	V79	C02-C03-C04-C05
2	A	204	V79	C02-C03-C04-C05
2	C	201	V79	C02-C03-C04-C05
2	C	202	V79	C02-C03-C04-C05
2	C	203	V79	C02-C03-C04-C05
2	D	201	V79	C02-C03-C04-C05
2	A	201	V79	C04-C05-C06-O07
2	A	203	V79	C04-C05-C06-O07
2	A	204	V79	C04-C05-C06-O07
2	A	201	V79	C32-C33-C34-O36
2	A	202	V79	C32-C33-C34-O36
2	A	203	V79	C32-C33-C34-O36
2	A	204	V79	C32-C33-C34-O36
2	C	201	V79	C32-C33-C34-O36
2	C	202	V79	C32-C33-C34-O36
2	C	203	V79	C32-C33-C34-O36
2	A	202	V79	C04-C05-C06-O07
2	C	201	V79	C04-C05-C06-O07
2	C	202	V79	C04-C05-C06-O07
2	C	203	V79	C04-C05-C06-O07
2	D	201	V79	C04-C05-C06-O07

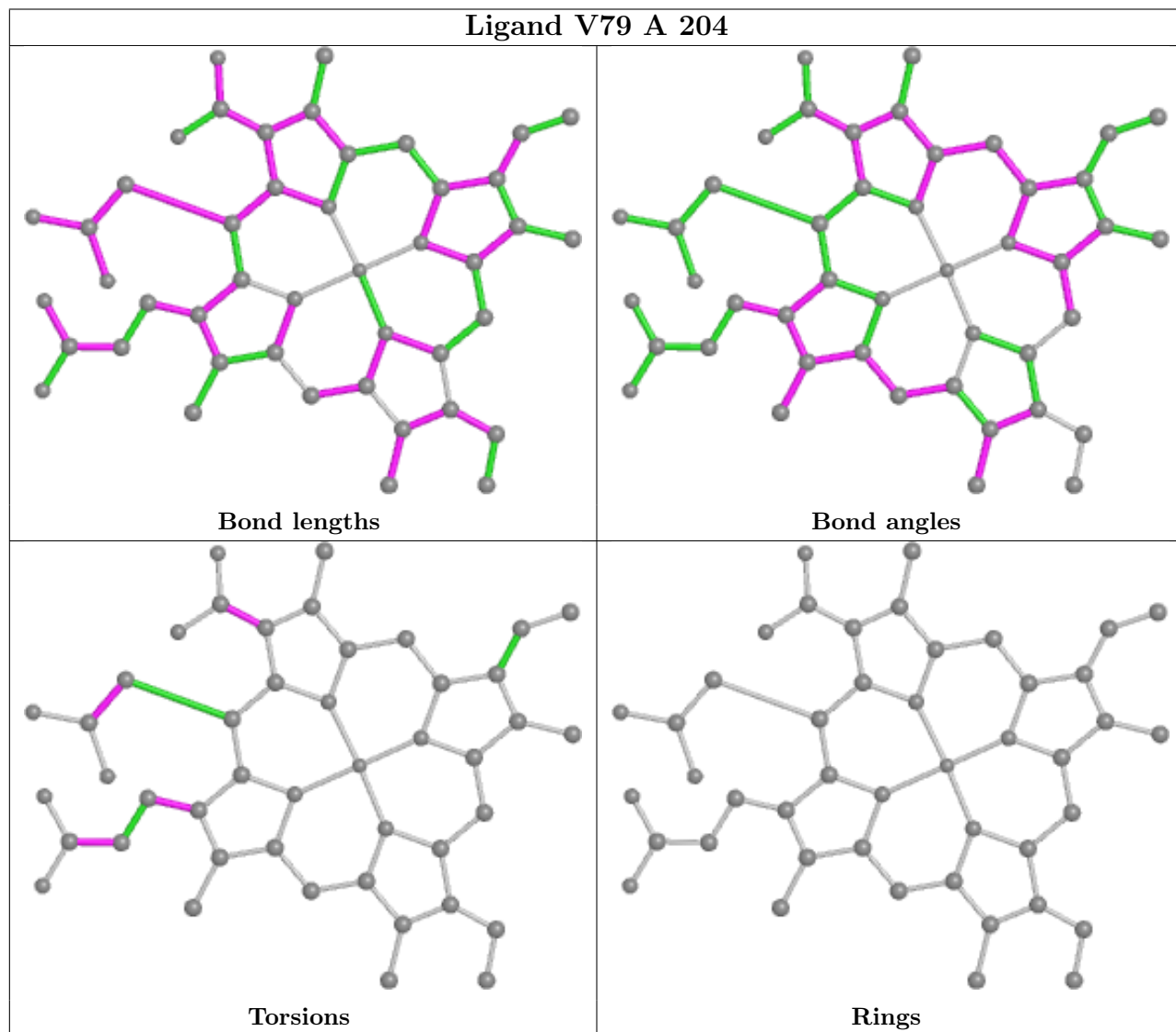
There are no ring outliers.

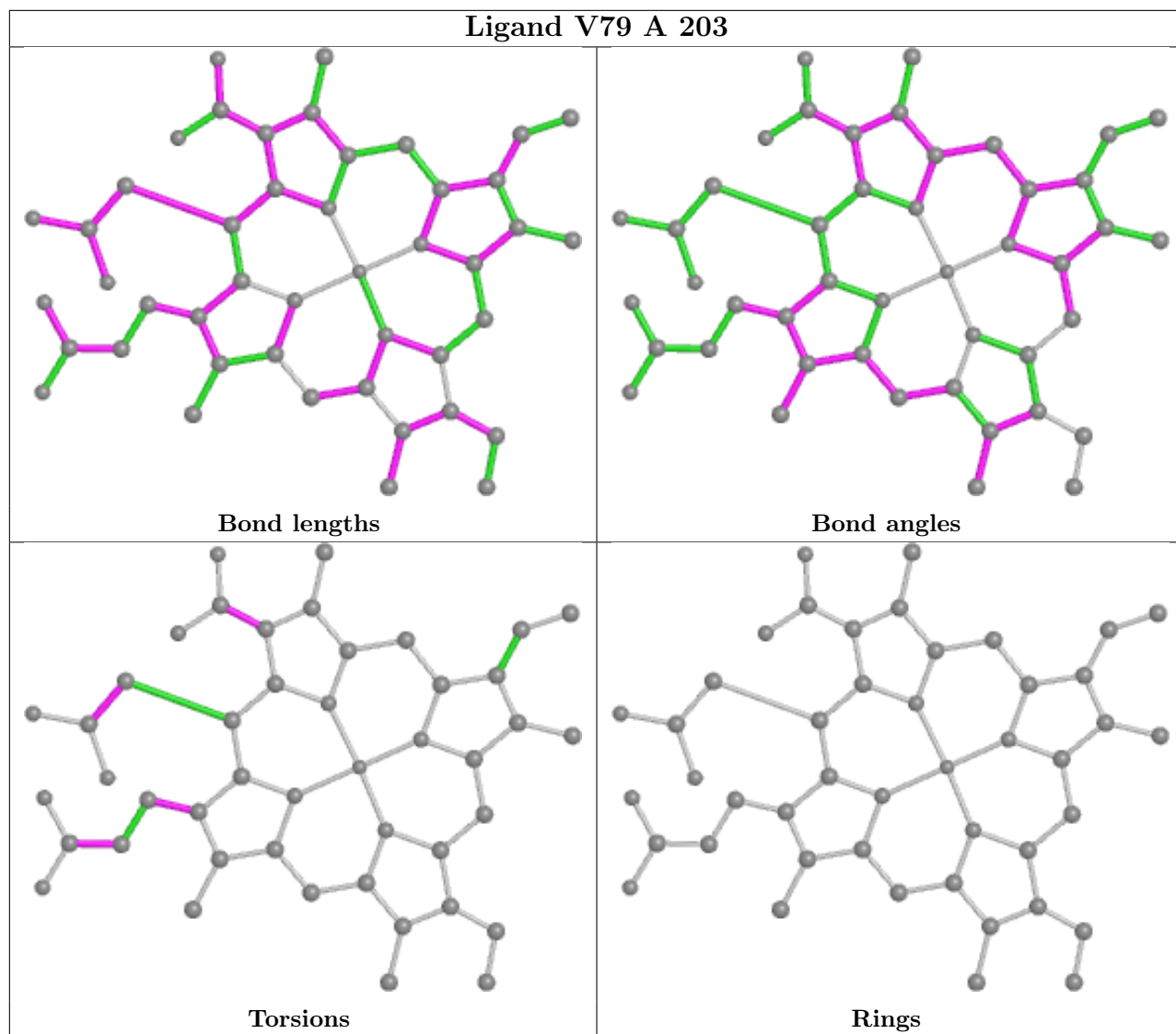
8 monomers are involved in 44 short contacts:

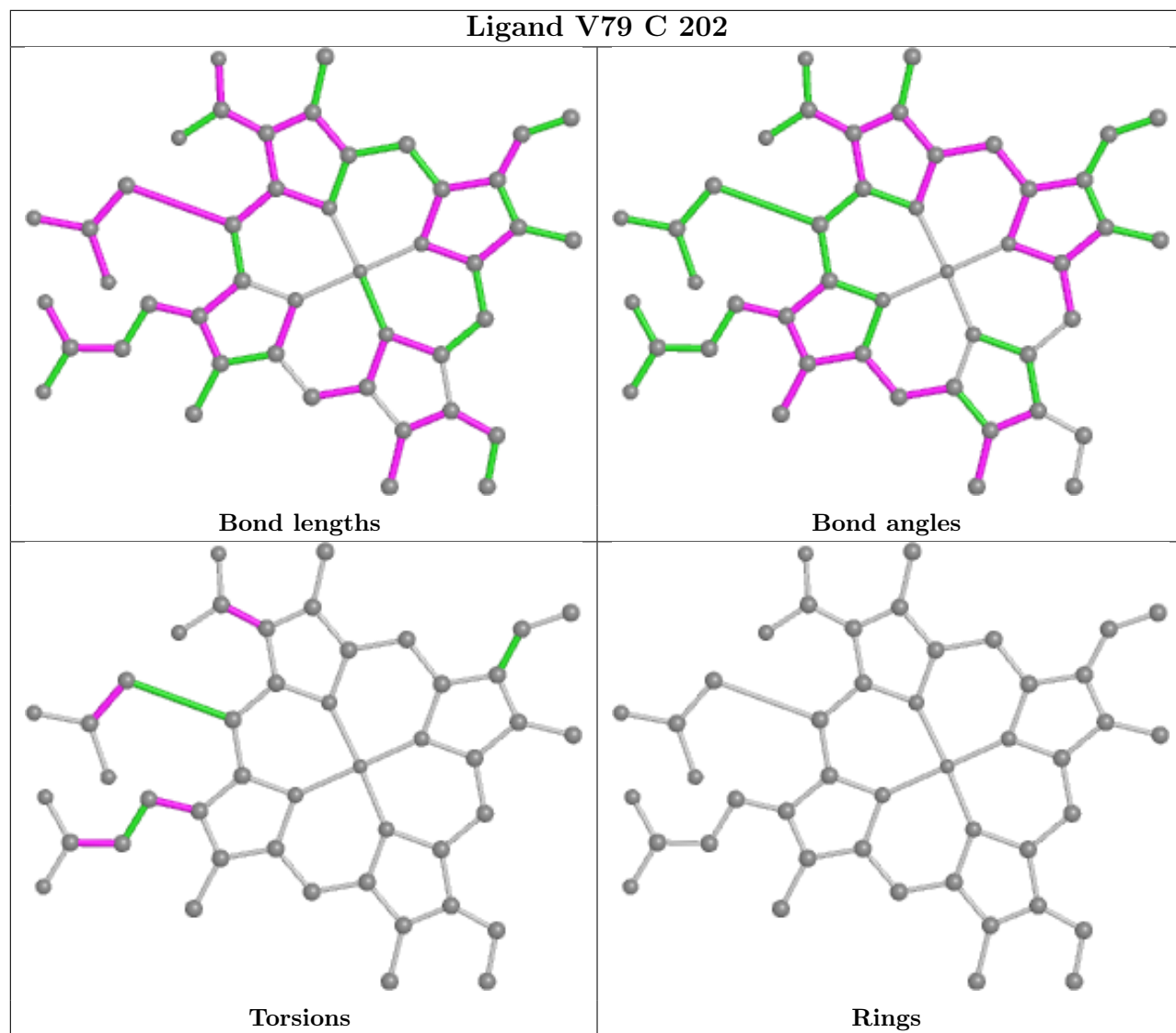
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	204	V79	4	0
2	A	203	V79	4	0
2	C	202	V79	4	0
2	C	201	V79	5	0
2	A	202	V79	9	0
2	C	203	V79	4	0
2	D	201	V79	9	0
2	A	201	V79	5	0

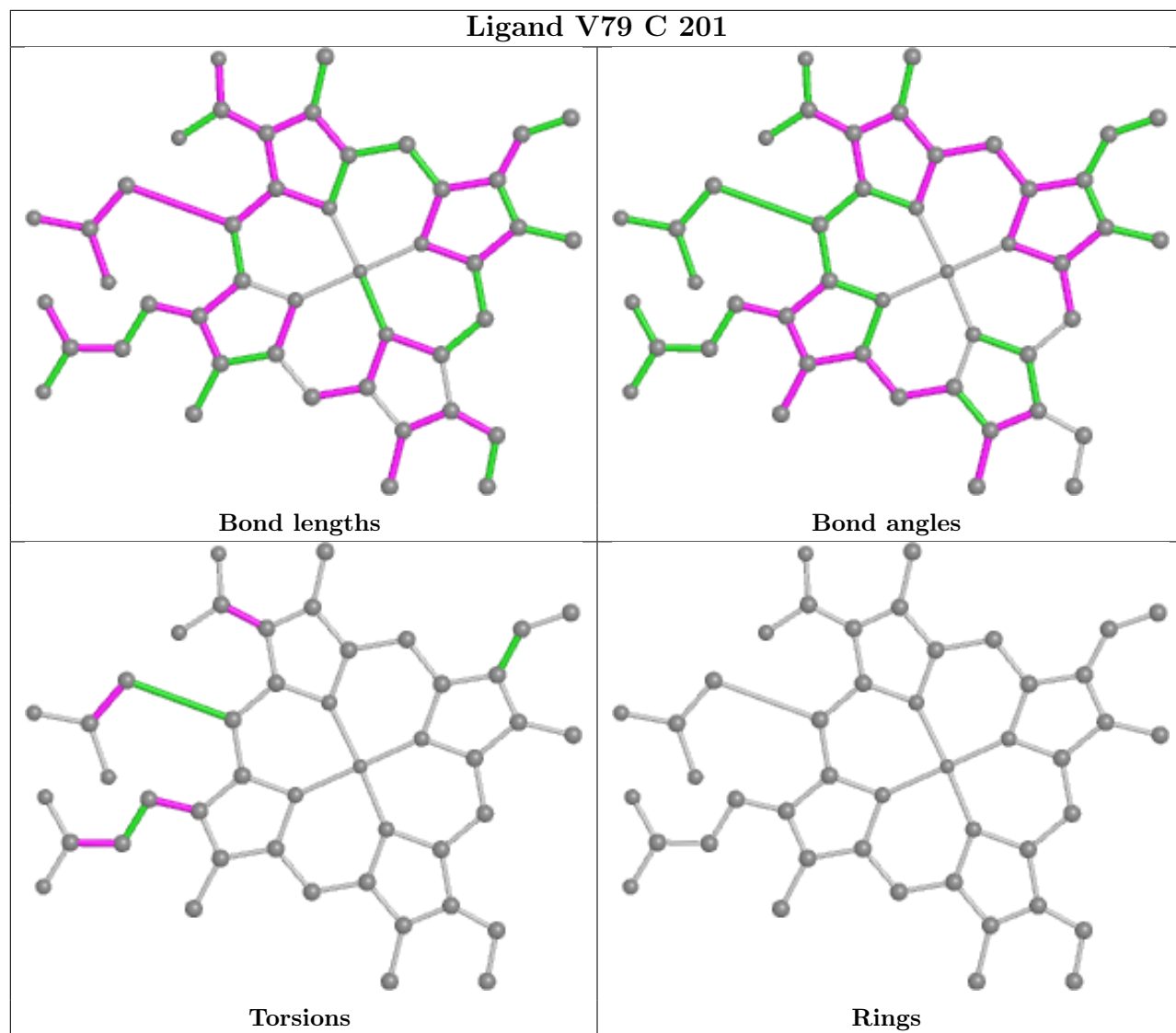
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

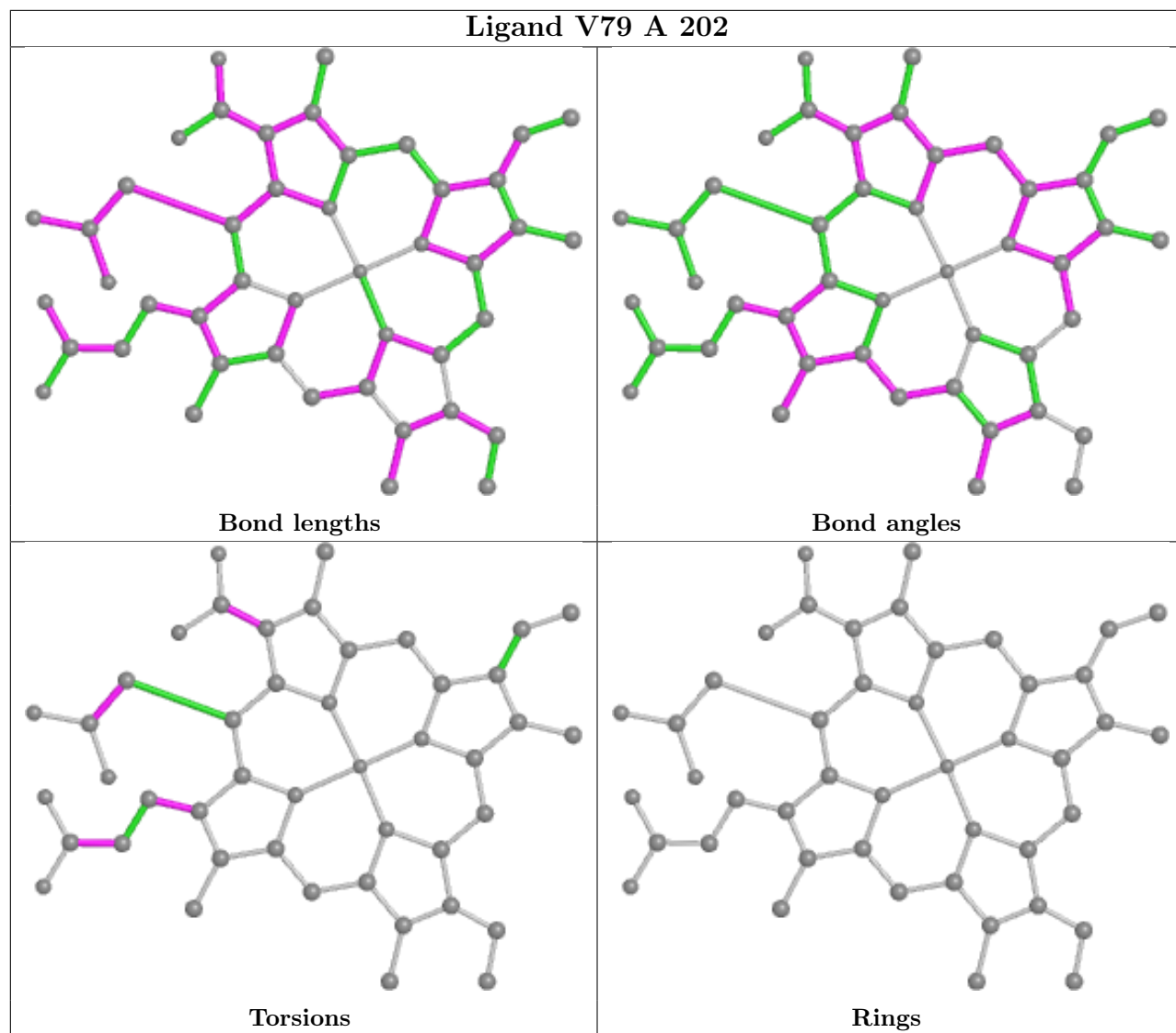
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question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

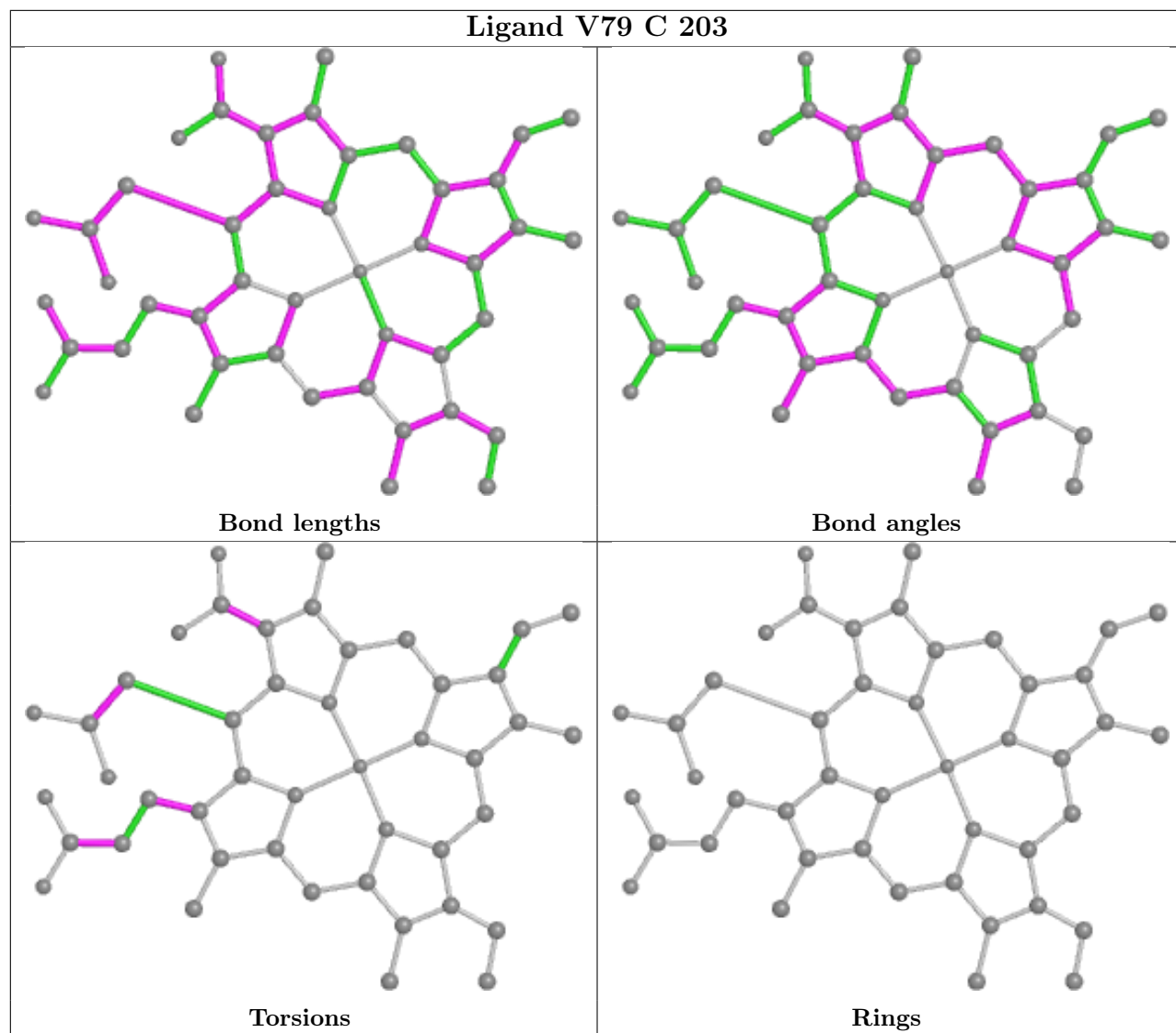


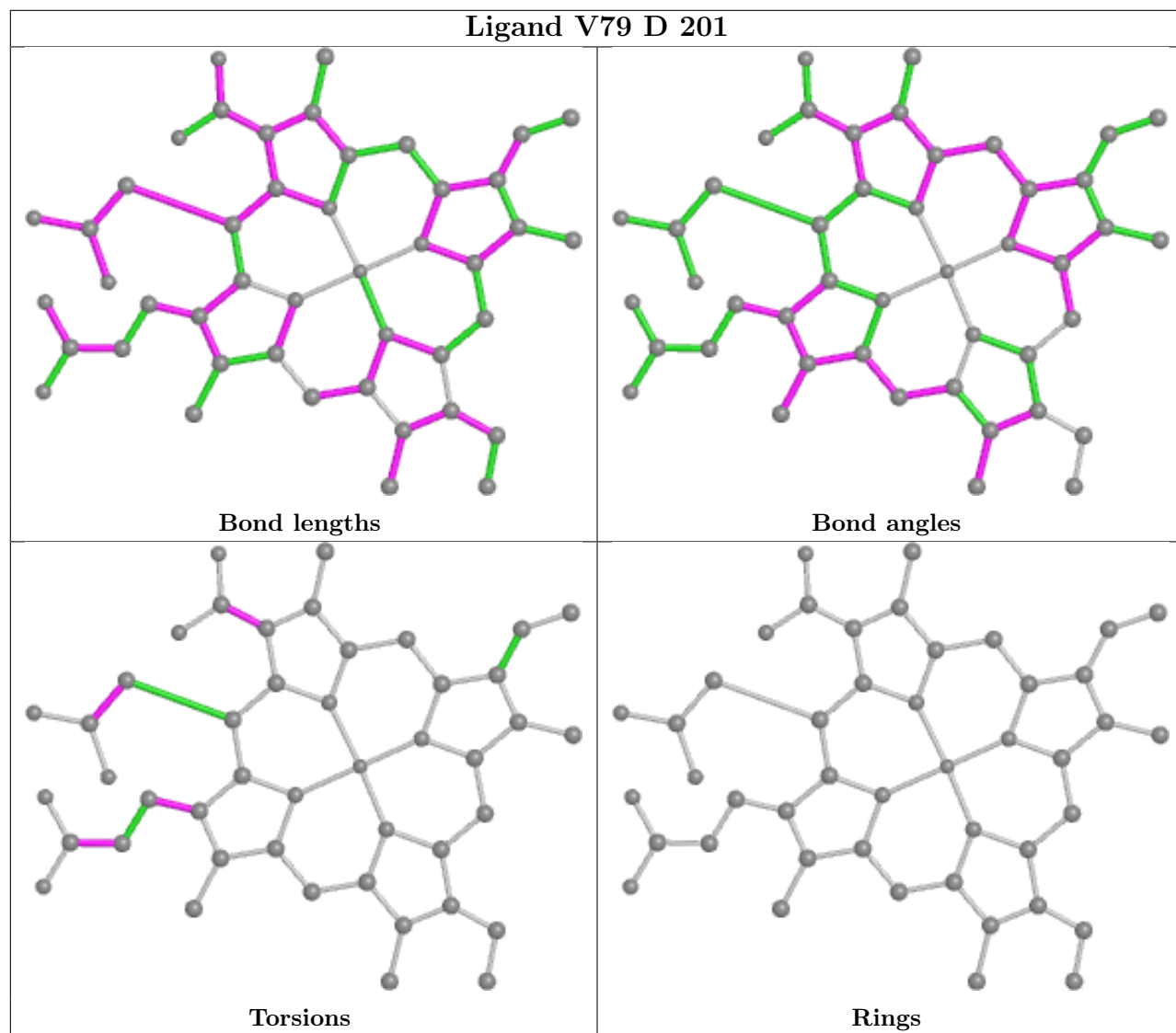


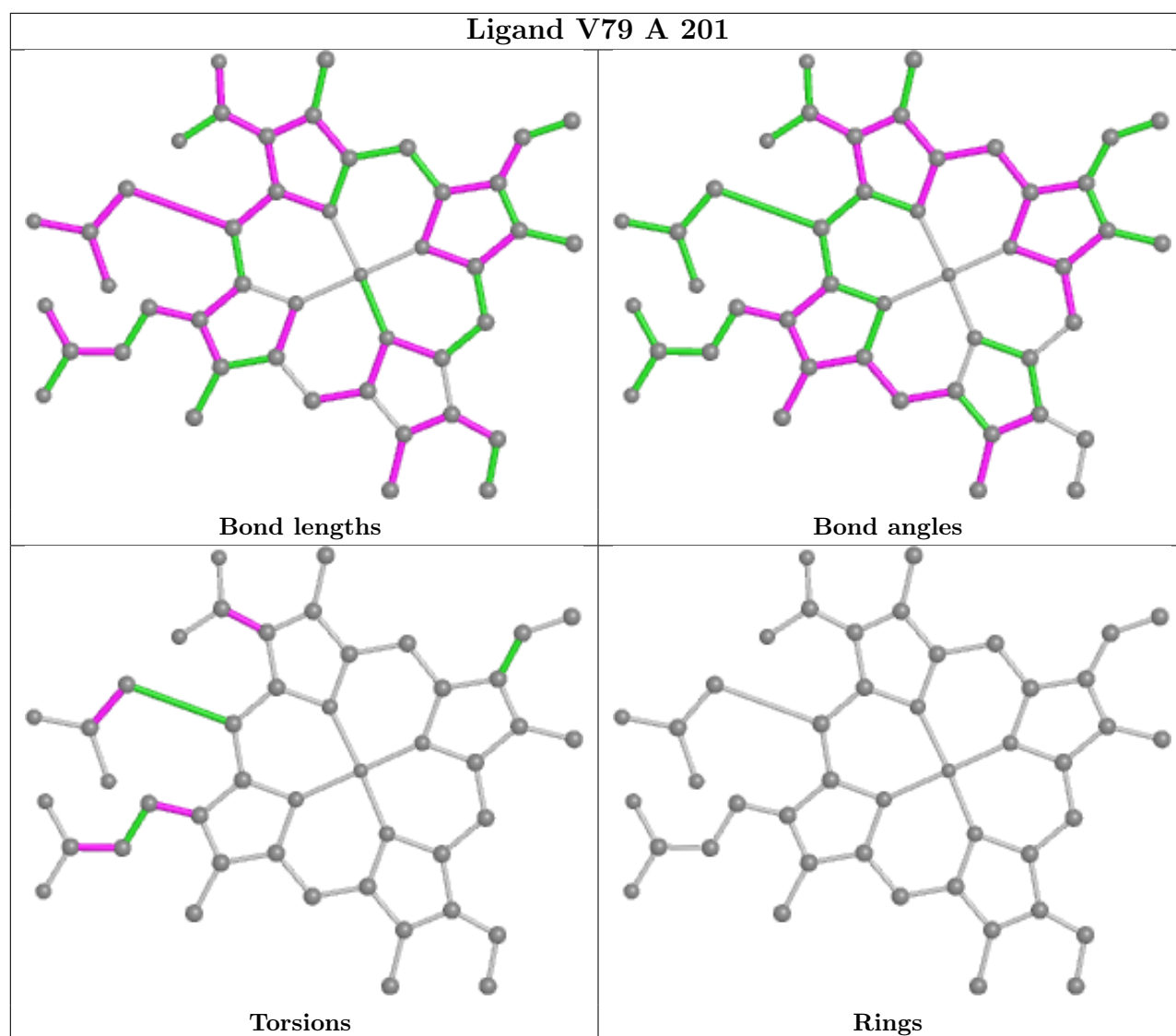












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

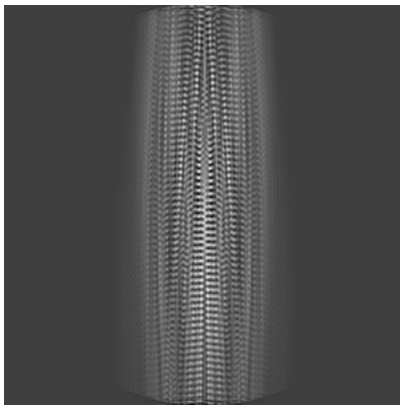
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33960. These allow visual inspection of the internal detail of the map and identification of artifacts.

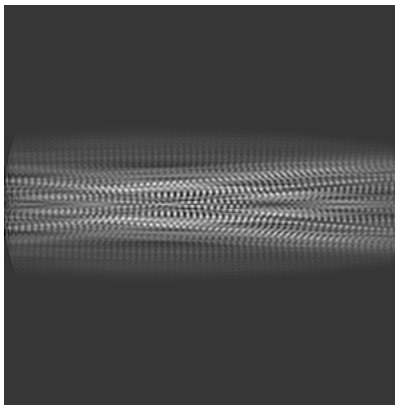
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

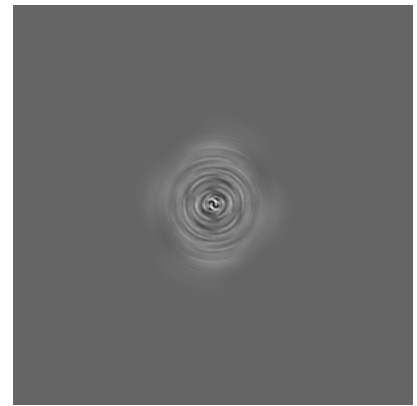
6.1.1 Primary map



X

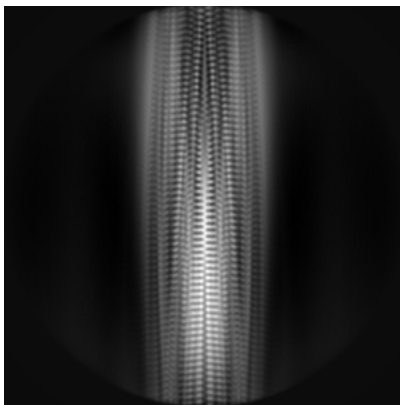


Y

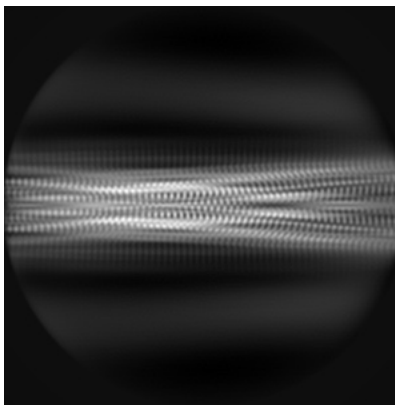


Z

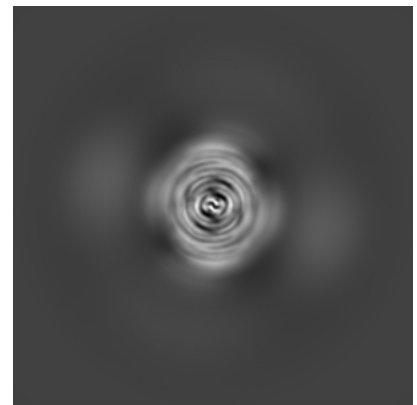
6.1.2 Raw map



X



Y

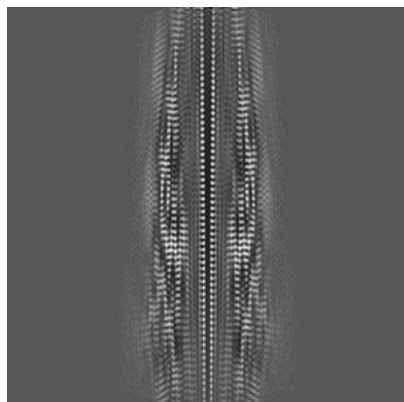


Z

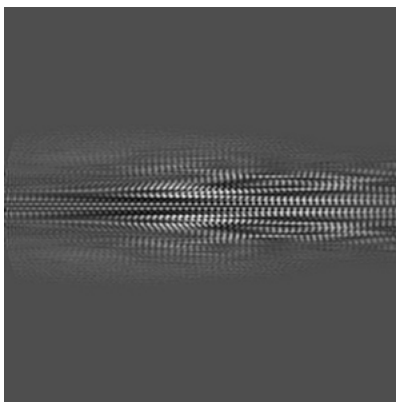
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

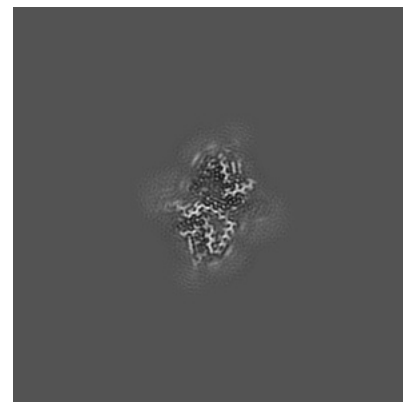
6.2.1 Primary map



X Index: 144

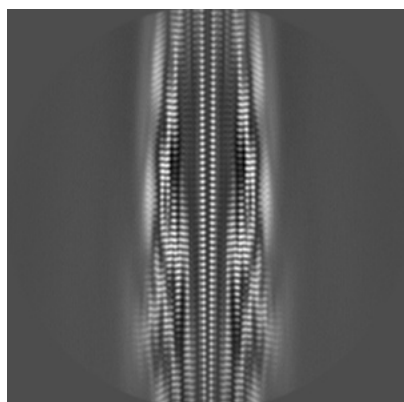


Y Index: 144

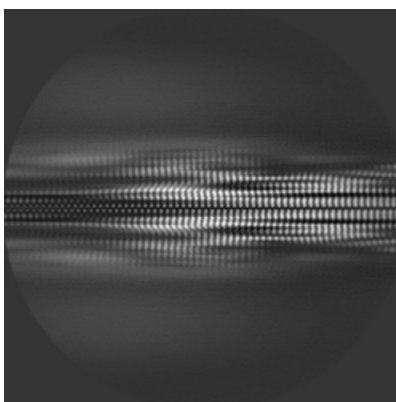


Z Index: 144

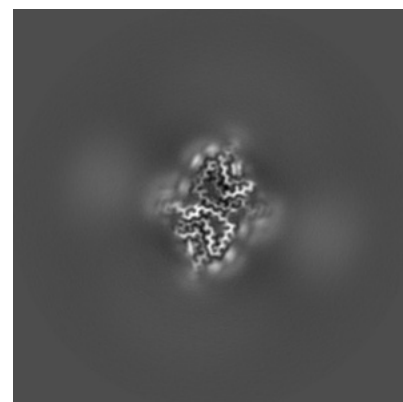
6.2.2 Raw map



X Index: 144



Y Index: 144

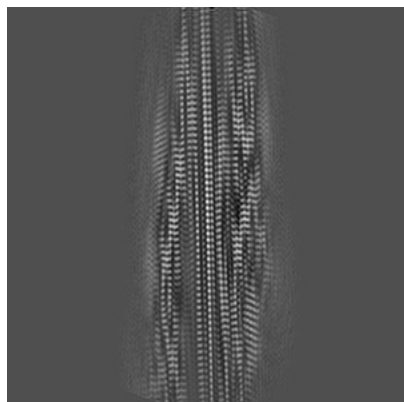


Z Index: 144

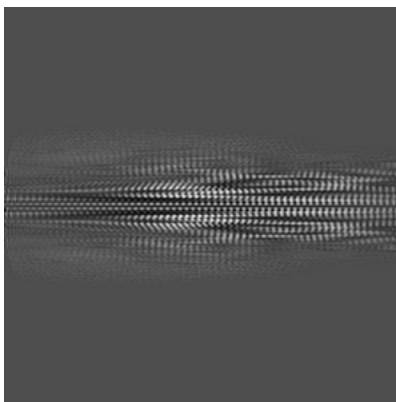
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

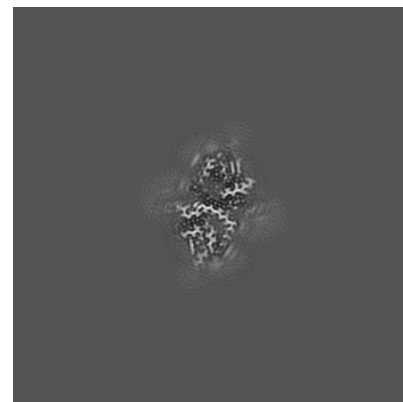
6.3.1 Primary map



X Index: 151

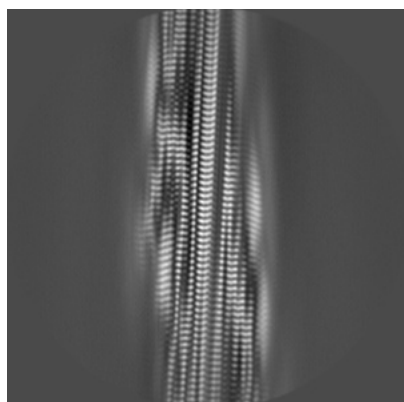


Y Index: 144

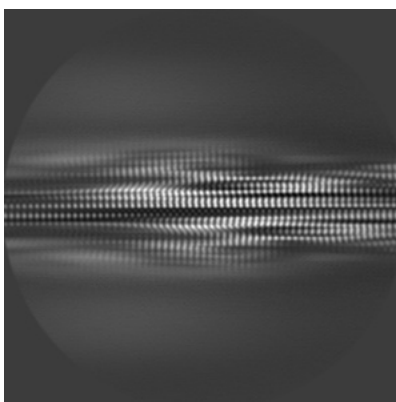


Z Index: 140

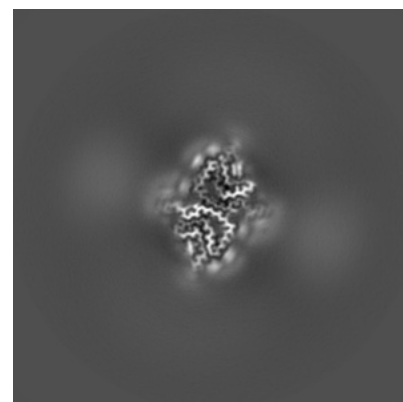
6.3.2 Raw map



X Index: 132



Y Index: 145

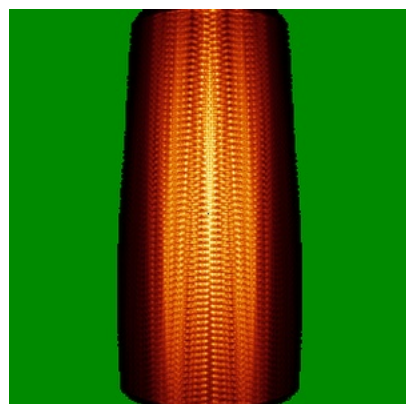


Z Index: 149

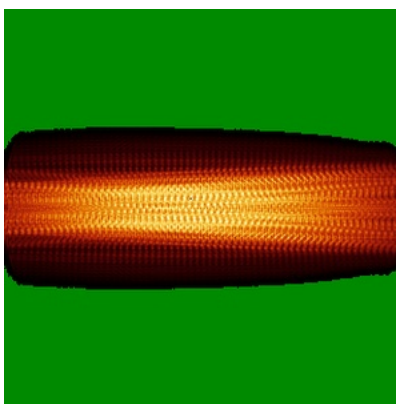
The images above show the largest variance slices of the map in three orthogonal directions.

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

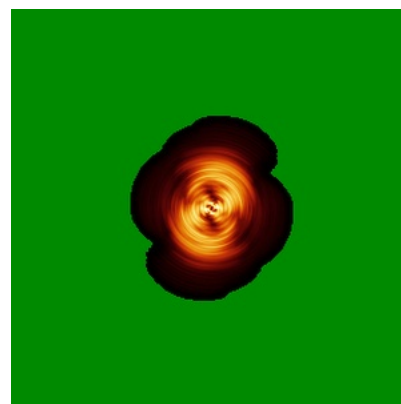
6.4.1 Primary map



X

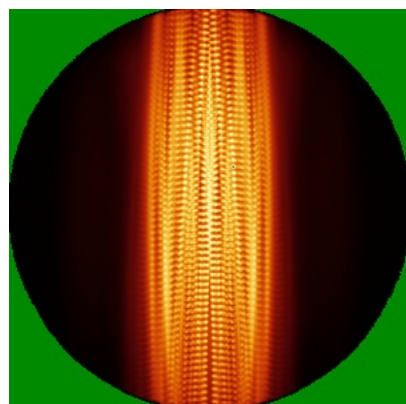


Y

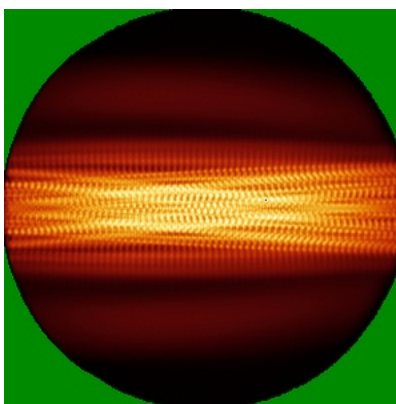


Z

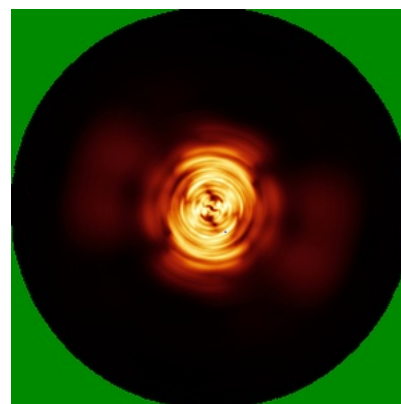
6.4.2 Raw map



X



Y

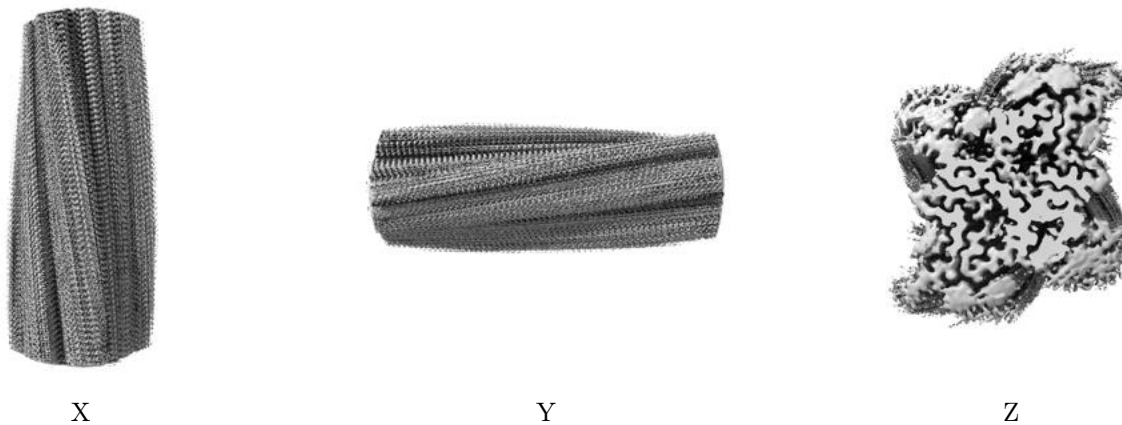


Z

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.

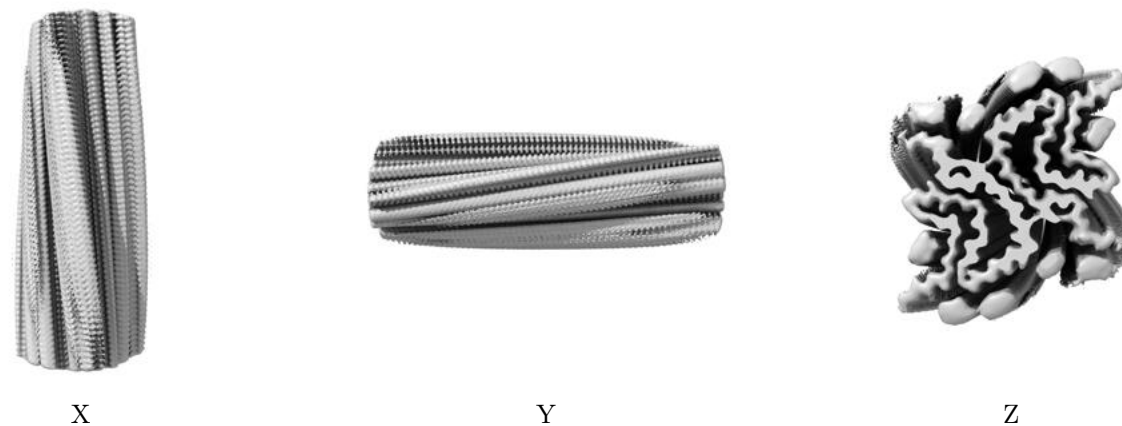
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.004. 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.

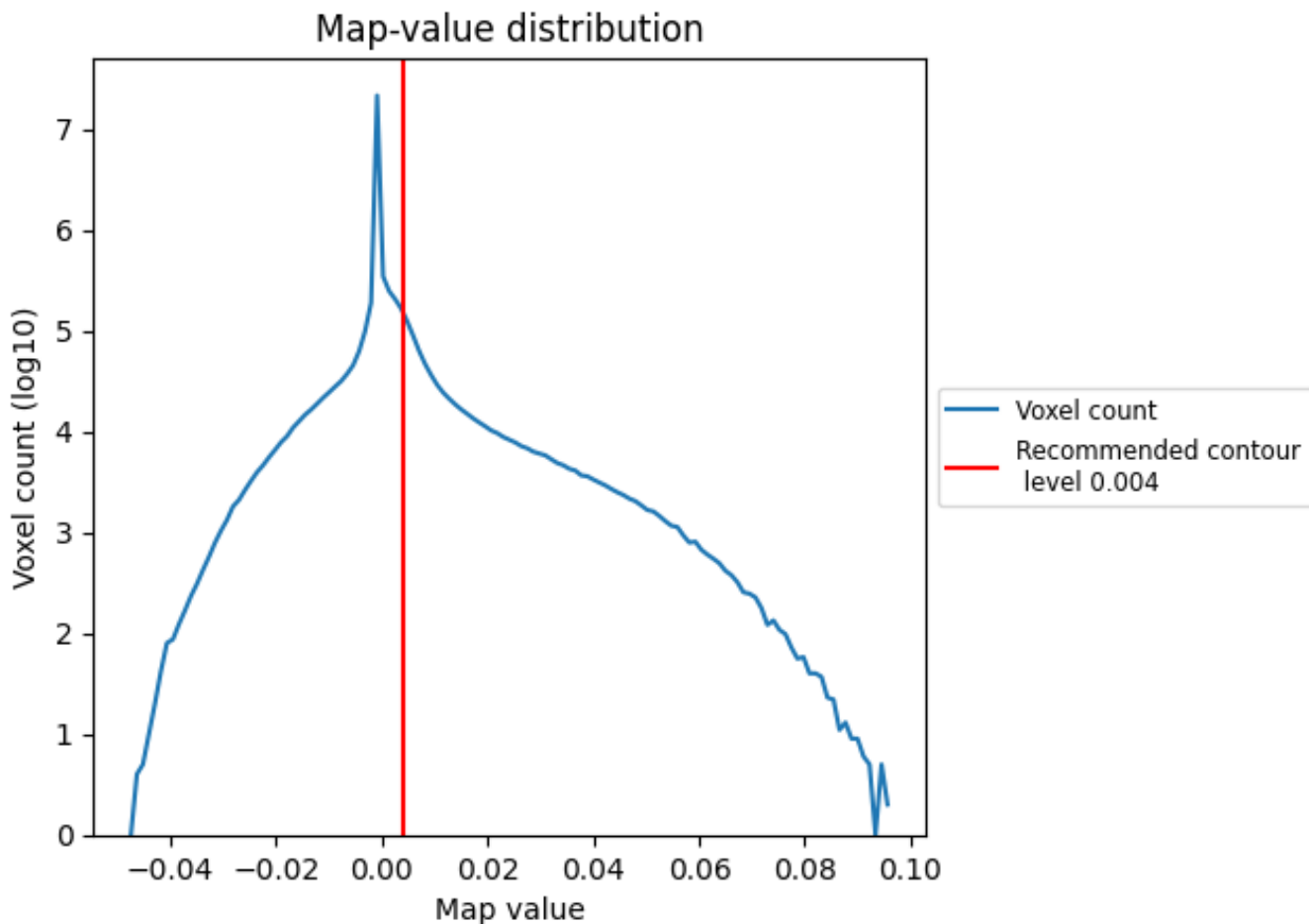
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

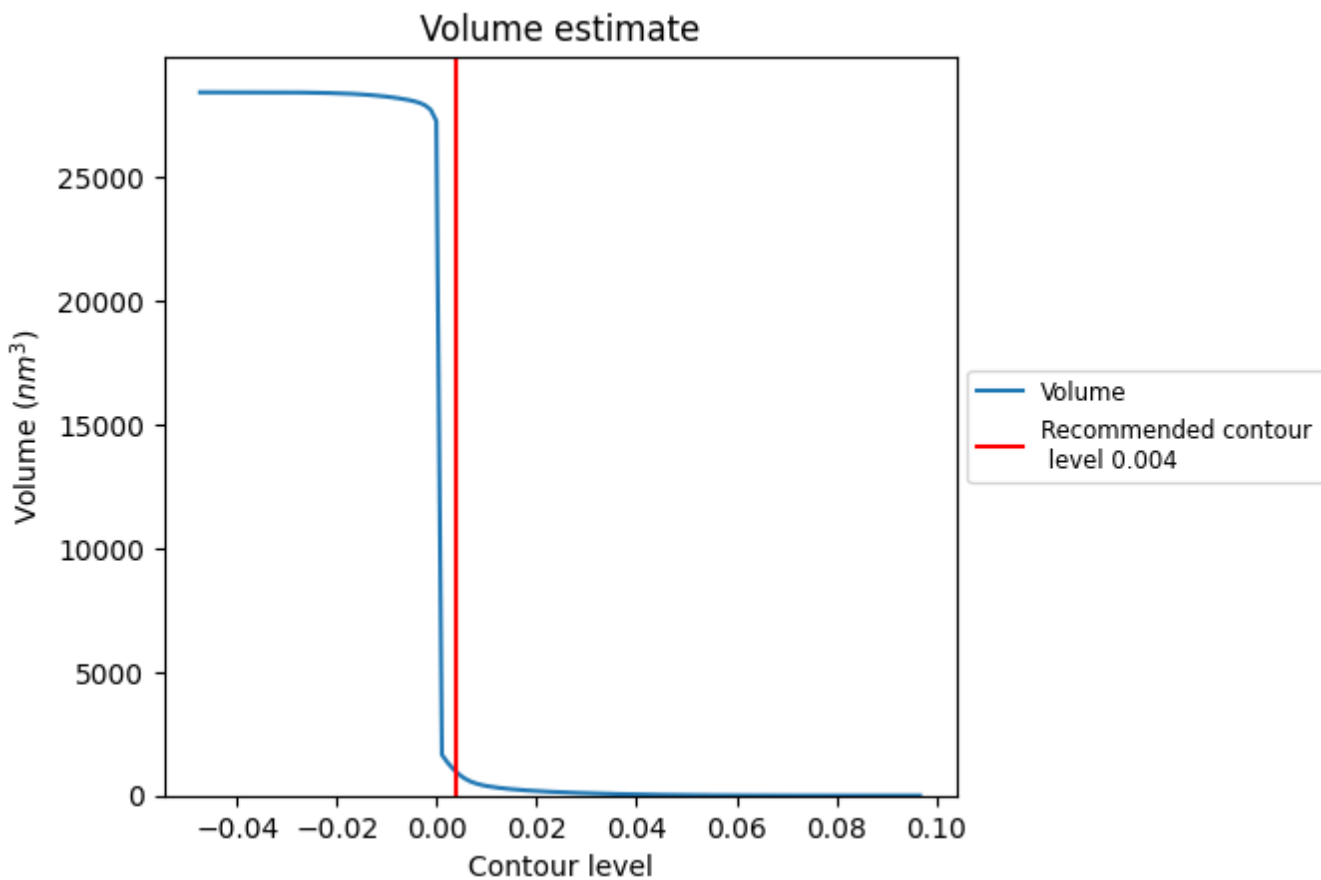
This section contains the results of statistical analysis of the map.

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.

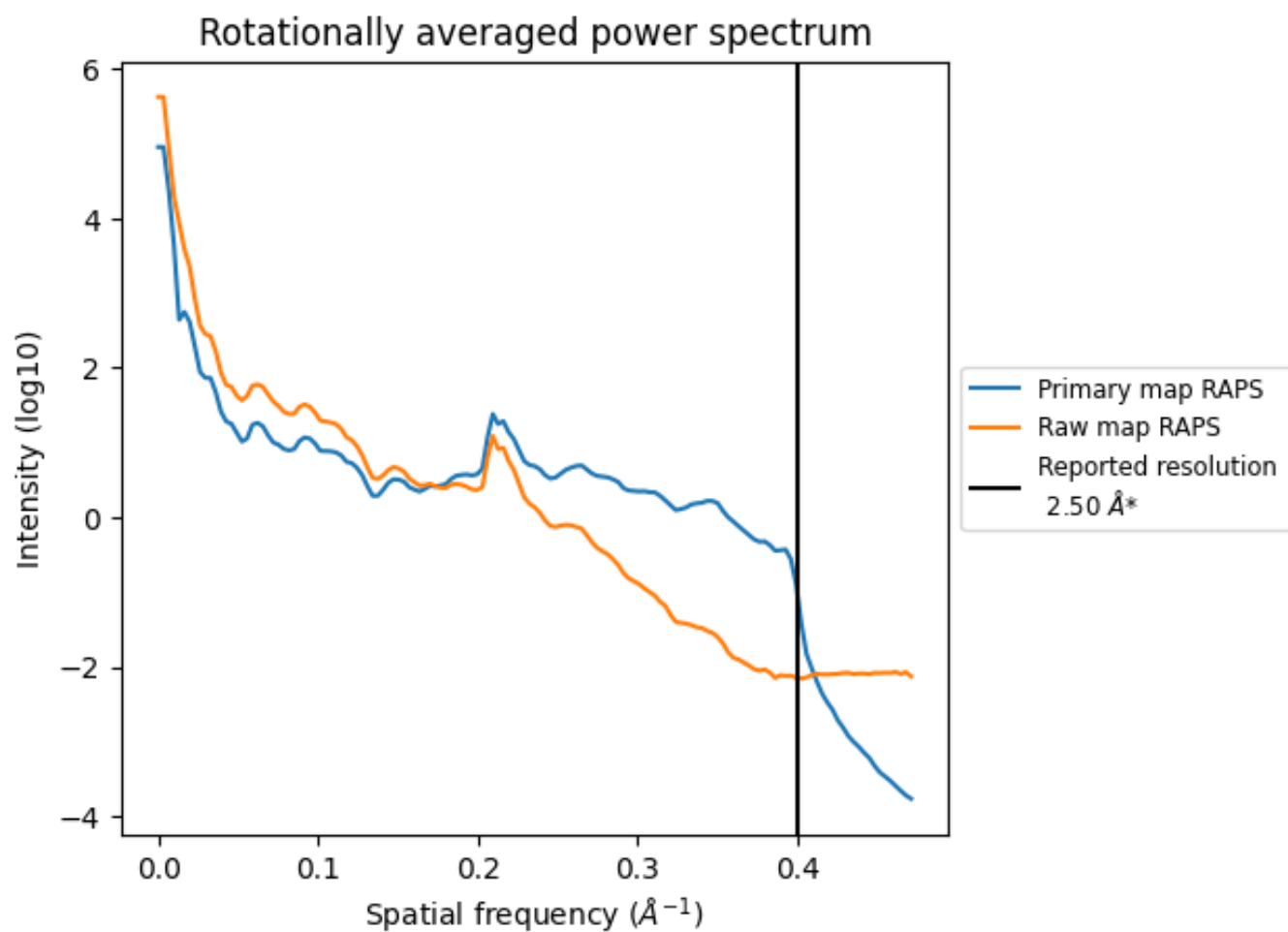
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 941 nm^3 ; this corresponds to an approximate mass of 850 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

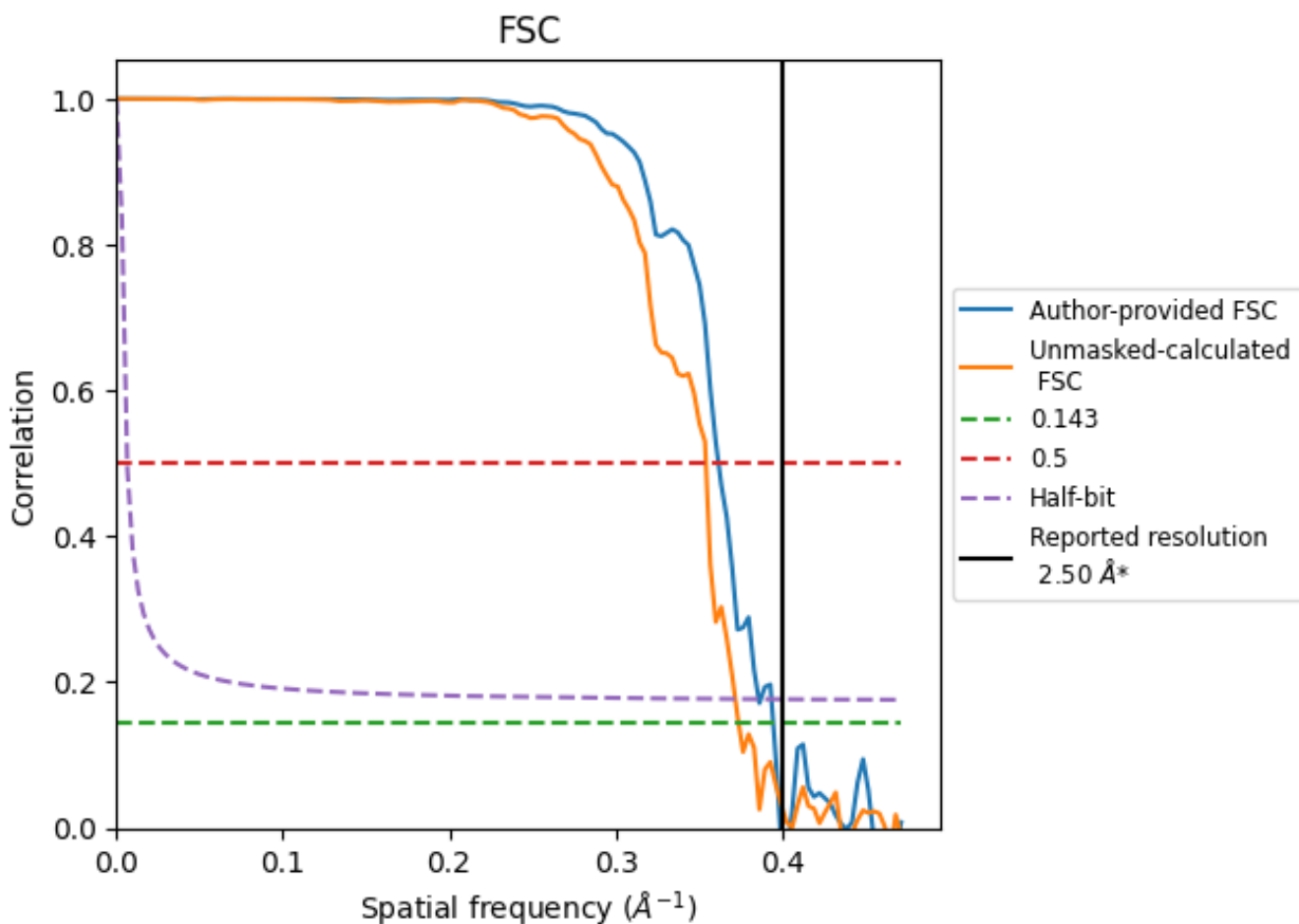


*Reported resolution corresponds to spatial frequency of 0.400 Å⁻¹

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 0.400 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.50	-	-
Author-provided FSC curve	2.53	2.76	2.59
Unmasked-calculated*	2.67	2.82	2.69

*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-33960 and PDB model 7YNF. Per-residue inclusion information can be found in section 3 on page 6.

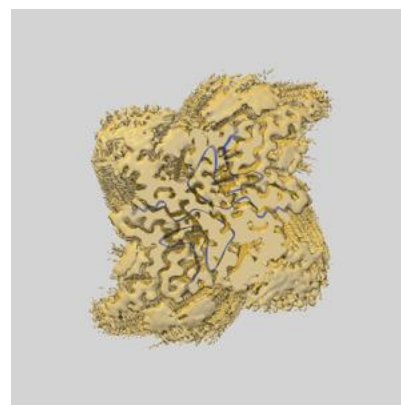
9.1 Map-model overlay [i](#)



X



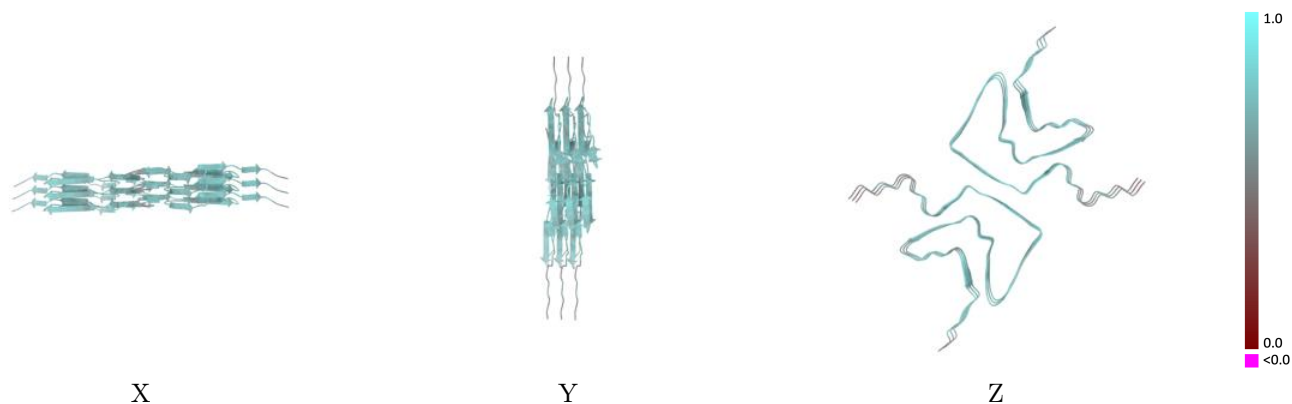
Y



Z

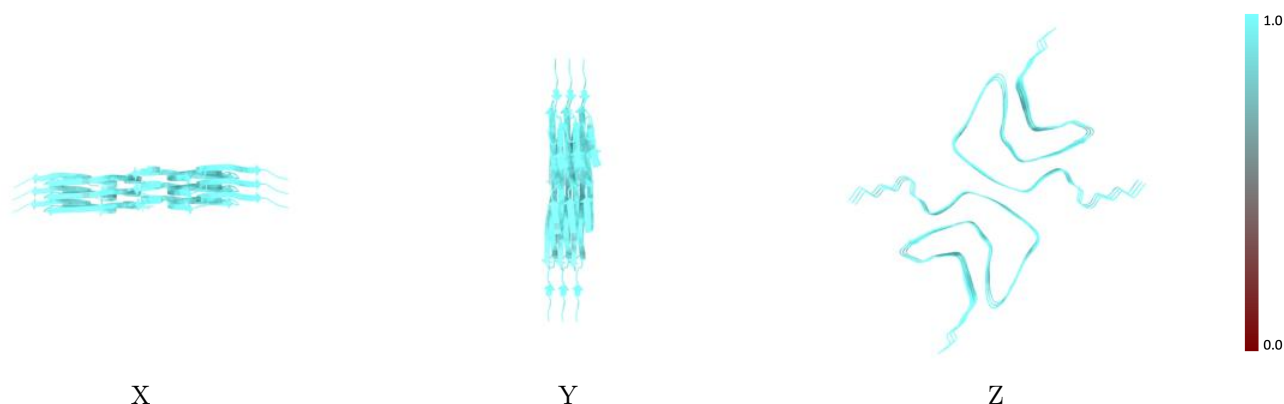
The images above show the 3D surface view of the map at the recommended contour level 0.004 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



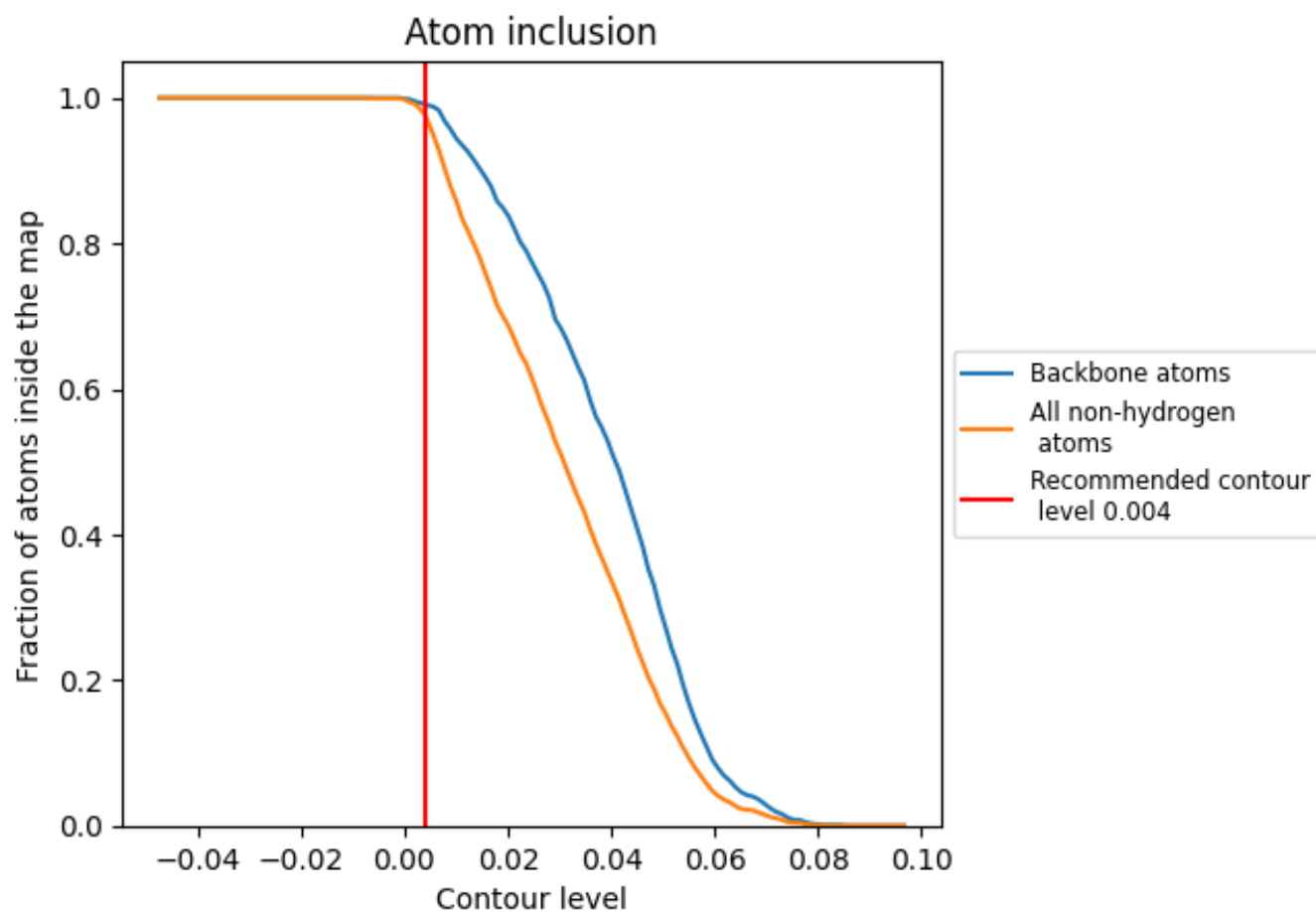
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.004).















9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 98% 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 (0.004) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9770	 0.6180
A	 0.9710	 0.5870
B	 0.9790	 0.6410
C	 0.9740	 0.6010
D	 0.9750	 0.6150
E	 0.9840	 0.6380
F	 0.9820	 0.6430

