



## wwPDB EM Validation Summary Report ⓘ

Dec 27, 2023 – 04:37 PM EST

PDB ID : 8G6E  
EMDB ID : EMD-29764  
Title : Structure of the Plasmodium falciparum 20S proteasome complexed with inhibitor TDI-8304  
Authors : Hsu, H.-C.; Li, H.  
Deposited on : 2023-02-15  
Resolution : 2.18 Å (reported)  
Based on initial model : 6MUW

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

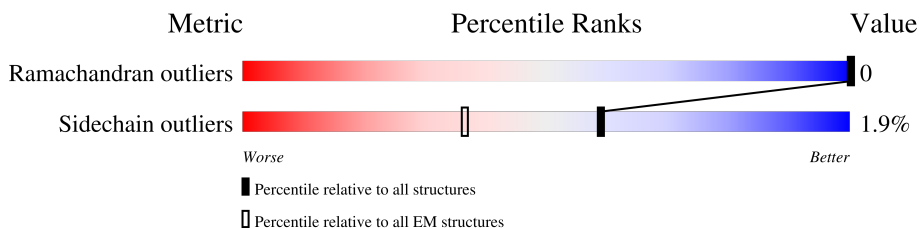
EMDB validation analysis : 0.0.1.dev70  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal 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 2.18 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.



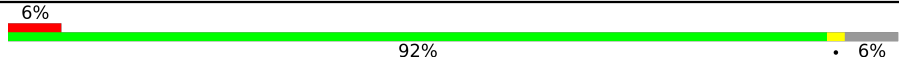
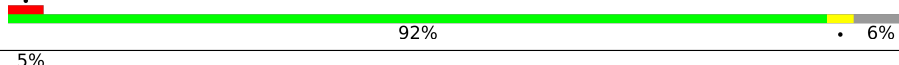
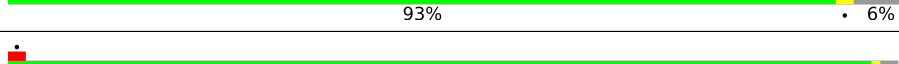
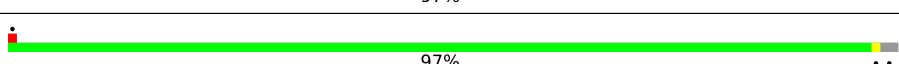
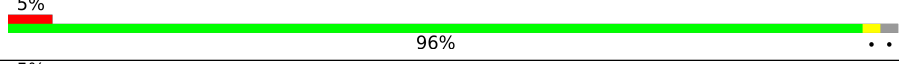
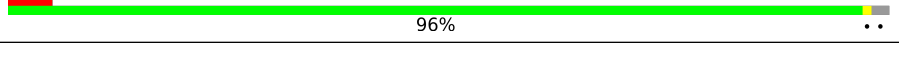
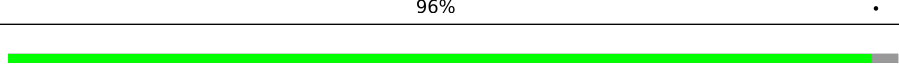
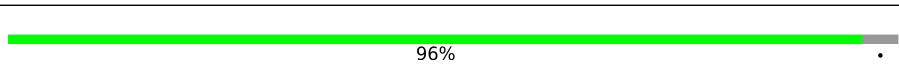
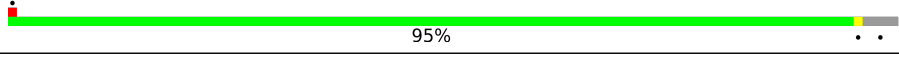
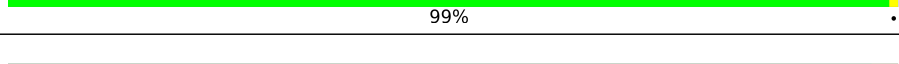
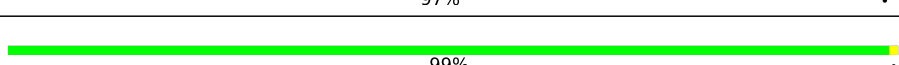
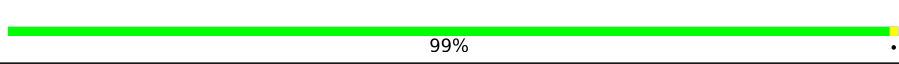
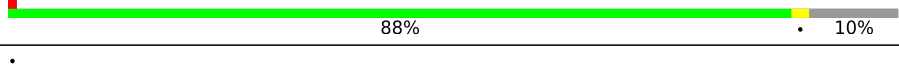

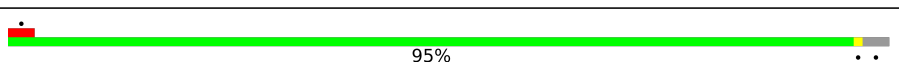




Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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  $\geq 3$ , 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	260	96% ..
1	O	260	96% ..
2	B	235	7% 97% ..
2	P	235	6% 96% ..
3	C	246	97% ..
3	Q	246	97% ..
4	D	241	96% ..
4	R	241	95% ..
5	E	256	6% 91% .. 6%

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Mol	Chain	Length	Quality of chain
5	S	256	 92% 6% 6%
6	F	253	 92% 6% 6%
6	T	253	 93% 5% 6%
7	G	252	 97% ..
7	U	252	 97% ..
8	H	252	 96% ..
8	V	252	 96% ..
9	I	229	 96% .
9	W	229	 97% .
10	J	218	 96% .
10	X	218	 95% ..
11	K	195	 99% .
11	Y	195	 97% .
12	L	211	 99% .
12	Z	211	 99% .
13	M	240	 88% . 10%
13	a	240	 87% . 10%
14	N	265	 96% ..
14	b	265	 95% ..

## 2 Entry composition [i](#)

There are 16 unique types of molecules in this entry. The entry contains 52266 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 Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	253	Total	C	N	O	S	0	0
			2006	1259	337	395	15		
1	O	253	Total	C	N	O	S	0	0
			2006	1259	337	395	15		

- Molecule 2 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	233	Total	C	N	O	S	0	0
			1851	1189	302	353	7		
2	P	233	Total	C	N	O	S	0	0
			1851	1189	302	353	7		

- Molecule 3 is a protein called Proteasome subunit alpha type.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	242	Total	C	N	O	S	0	0
			1938	1241	315	379	3		
3	Q	242	Total	C	N	O	S	0	0
			1938	1241	315	379	3		

- Molecule 4 is a protein called Proteasome subunit alpha type.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	236	Total	C	N	O	S	0	0
			1870	1192	318	352	8		
4	R	236	Total	C	N	O	S	0	0
			1870	1192	318	352	8		

- Molecule 5 is a protein called Proteasome subunit alpha type.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	241	Total	C	N	O	S	0	0
			1867	1175	312	369	11		
5	S	241	Total	C	N	O	S	0	0
			1867	1175	312	369	11		

- Molecule 6 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	239	Total	C	N	O	S	0	0
			1897	1204	313	369	11		
6	T	239	Total	C	N	O	S	0	0
			1897	1204	313	369	11		

- Molecule 7 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	247	Total	C	N	O	S	0	0
			2025	1289	338	385	13		
7	U	247	Total	C	N	O	S	0	0
			2025	1289	338	385	13		

- Molecule 8 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	246	Total	C	N	O	S	0	0
			1991	1257	339	383	12		
8	V	246	Total	C	N	O	S	0	0
			1991	1257	339	383	12		

- Molecule 9 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	221	Total	C	N	O	S	1	0
			1703	1076	297	316	14		
9	W	221	Total	C	N	O	S	1	0
			1703	1076	297	316	14		

- Molecule 10 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	210	Total	C	N	O	S	0	0
			1653	1055	269	315	14		

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	X	210	1653	1055	269	315	14	0	0

- Molecule 11 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	K	195	1614	1042	266	298	8	0	0
11	Y	195	1614	1042	266	298	8	0	0

- Molecule 12 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	L	211	1663	1060	275	320	8	0	0
12	Z	211	1663	1060	275	320	8	0	0

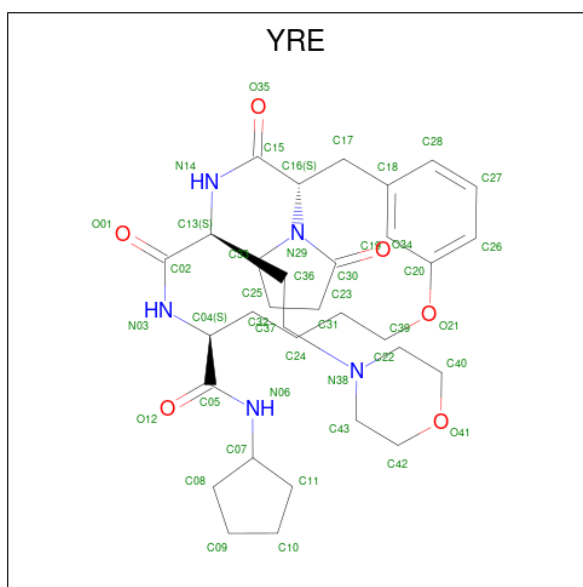
- Molecule 13 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	M	215	1711	1096	285	323	7	0	0
13	a	215	1711	1096	285	323	7	0	0

- Molecule 14 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	N	256	2106	1342	357	397	10	1	0
14	b	256	2106	1342	357	397	10	1	0

- Molecule 15 is (7S,10S,13S)-N-cyclopentyl-10-[2-(morpholin-4-yl)ethyl]-9,12-dioxo-13-(2-oxopyrrolidin-1-yl)-2-oxa-8,11-diazabicyclo[13.3.1]nonadeca-1(19),15,17-triene-7-carboxamide (three-letter code: YRE) (formula: C<sub>32</sub>H<sub>47</sub>N<sub>5</sub>O<sub>6</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf	
			Total	C	N		O
15	C	1	43	32	5	6	0
15	I	1	43	32	5	6	0
15	L	1	43	32	5	6	0
15	Q	1	43	32	5	6	0
15	W	1	43	32	5	6	0
15	Z	1	43	32	5	6	0

- Molecule 16 is water.

Mol	Chain	Residues	Atoms		AltConf
16	A	4	Total	O	0
			4	4	
16	B	4	Total	O	0
			4	4	
16	C	8	Total	O	0
			8	8	
16	D	6	Total	O	0
			6	6	
16	E	7	Total	O	0
			7	7	
16	F	11	Total	O	0
			11	11	

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Mol	Chain	Residues	Atoms	AltConf
16	G	7	Total O 7 7	0
16	H	14	Total O 14 14	0
16	I	7	Total O 7 7	0
16	J	9	Total O 9 9	0
16	K	8	Total O 8 8	0
16	L	5	Total O 5 5	0
16	M	6	Total O 6 6	0
16	N	13	Total O 13 13	0
16	O	5	Total O 5 5	0
16	P	3	Total O 3 3	0
16	Q	11	Total O 11 11	0
16	R	9	Total O 9 9	0
16	S	7	Total O 7 7	0
16	T	11	Total O 11 11	0
16	U	9	Total O 9 9	0
16	V	9	Total O 9 9	0
16	W	7	Total O 7 7	0
16	X	10	Total O 10 10	0
16	Y	7	Total O 7 7	0
16	Z	3	Total O 3 3	0
16	a	7	Total O 7 7	0

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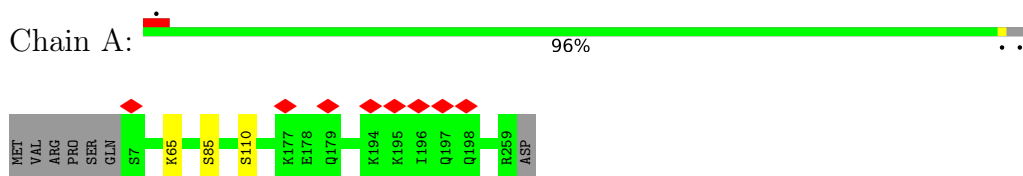
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>AltConf</b>
16	b	11	Total	O	0
			11	11	

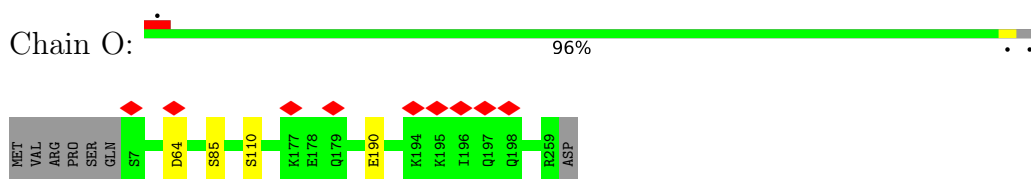
### 3 Residue-property plots [i](#)

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.

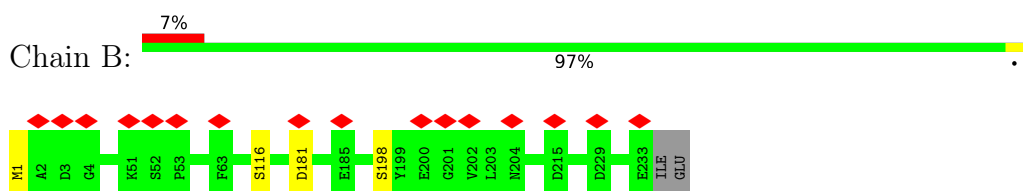
- Molecule 1: Proteasome subunit alpha type-6



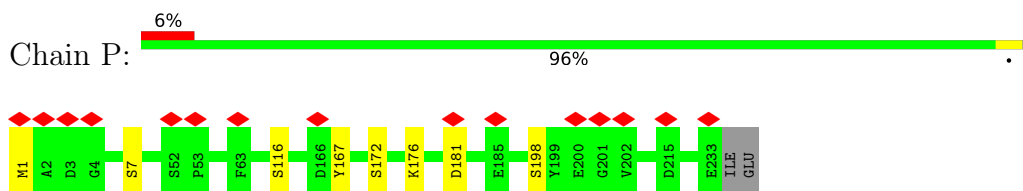
- Molecule 1: Proteasome subunit alpha type-6



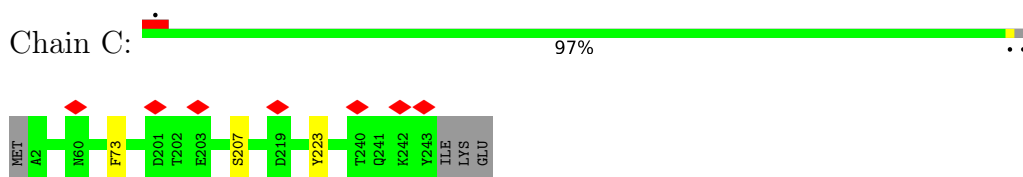
- Molecule 2: Proteasome subunit alpha type-2



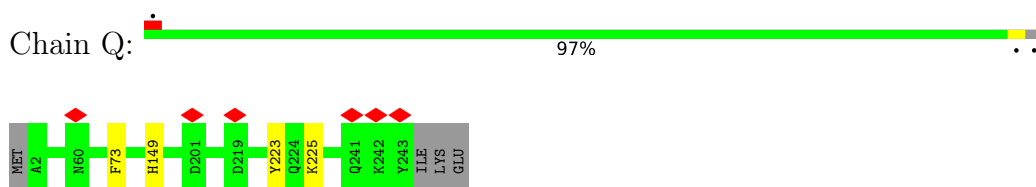
- Molecule 2: Proteasome subunit alpha type-2



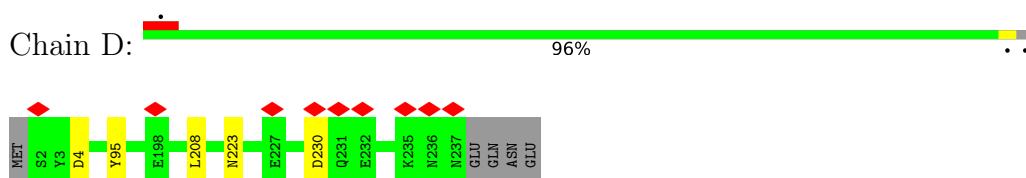
- Molecule 3: Proteasome subunit alpha type



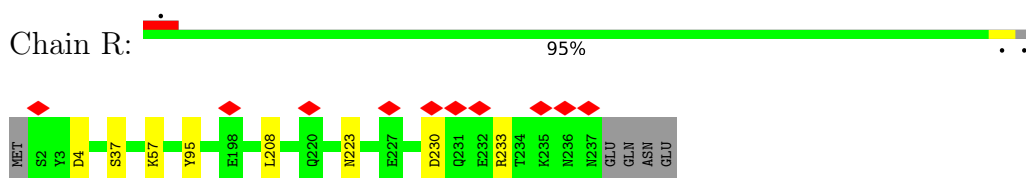
- Molecule 3: Proteasome subunit alpha type



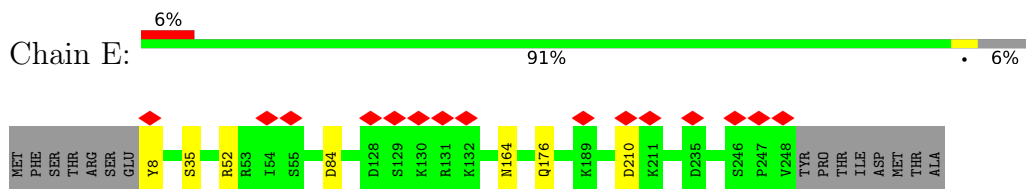
- Molecule 4: Proteasome subunit alpha type



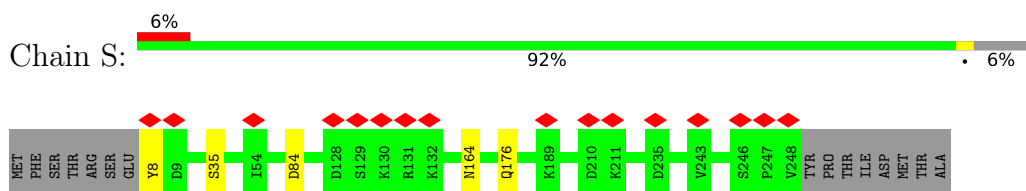
- Molecule 4: Proteasome subunit alpha type



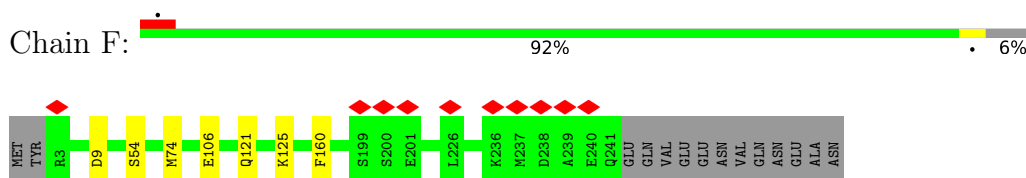
- Molecule 5: Proteasome subunit alpha type



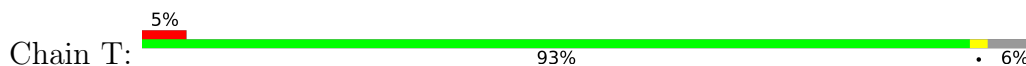
- Molecule 5: Proteasome subunit alpha type

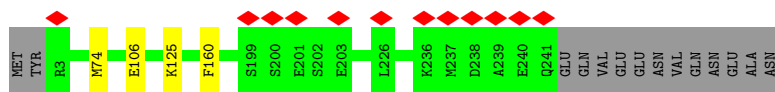


- Molecule 6: Proteasome subunit alpha type-1

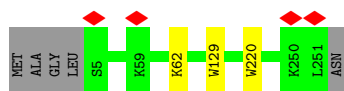


- Molecule 6: Proteasome subunit alpha type-1

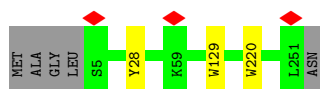




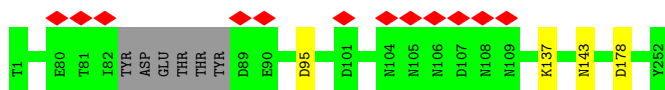
- Molecule 7: Proteasome subunit alpha type-3



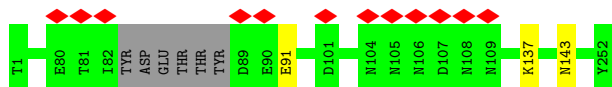
- Molecule 7: Proteasome subunit alpha type-3



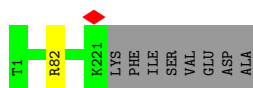
- Molecule 8: Proteasome subunit beta type-6



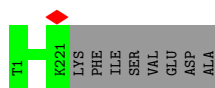
- Molecule 8: Proteasome subunit beta type-6



- Molecule 9: Proteasome subunit beta

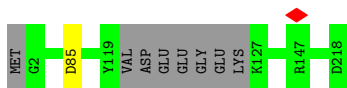


- Molecule 9: Proteasome subunit beta



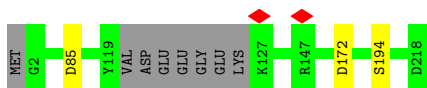
- Molecule 10: Proteasome subunit beta

Chain J:  96%



- Molecule 10: Proteasome subunit beta

Chain X:  95%



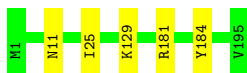
- Molecule 11: Proteasome subunit beta

Chain K:  99%



- Molecule 11: Proteasome subunit beta

Chain Y:  97%



- Molecule 12: Proteasome subunit beta

Chain L:  99%




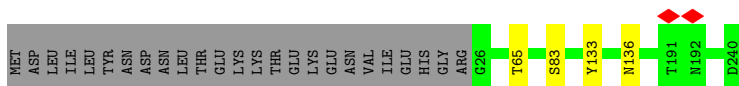
- Molecule 12: Proteasome subunit beta

Chain Z:  99%

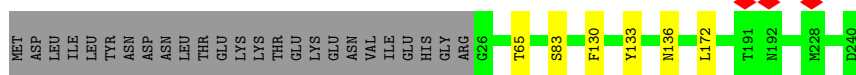
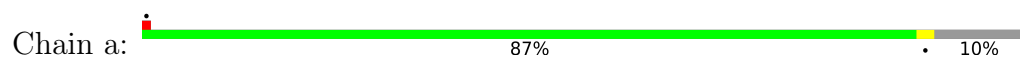


- Molecule 13: Proteasome subunit beta

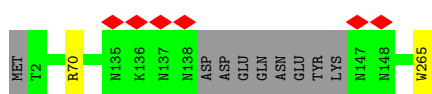
Chain M:  88% 10%



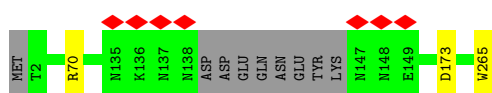
- Molecule 13: Proteasome subunit beta



● Molecule 14: Proteasome subunit beta



● Molecule 14: Proteasome subunit beta



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	305581	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	66	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.200	Depositor
Minimum map value	-0.094	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	317.952, 317.952, 317.952	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.828, 0.828, 0.828	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: YRE

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	0.29	0/2033	0.50	0/2741
1	O	0.29	0/2033	0.50	0/2741
2	B	0.29	0/1885	0.49	0/2545
2	P	0.29	0/1885	0.49	0/2545
3	C	0.30	0/1974	0.50	0/2673
3	Q	0.30	0/1974	0.50	0/2673
4	D	0.29	0/1900	0.48	0/2563
4	R	0.30	0/1900	0.48	0/2563
5	E	0.28	0/1893	0.50	0/2556
5	S	0.28	0/1893	0.51	0/2556
6	F	0.29	0/1931	0.47	0/2600
6	T	0.29	0/1931	0.47	0/2600
7	G	0.30	0/2069	0.47	0/2796
7	U	0.30	0/2069	0.47	0/2796
8	H	0.31	0/2024	0.50	0/2720
8	V	0.31	0/2024	0.50	0/2720
9	I	0.30	0/1740	0.51	0/2365
9	W	0.30	0/1740	0.51	0/2365
10	J	0.31	0/1681	0.51	0/2268
10	X	0.31	0/1681	0.51	0/2268
11	K	0.31	0/1649	0.50	0/2223
11	Y	0.33	0/1649	0.51	0/2223
12	L	0.32	0/1697	0.51	0/2286
12	Z	0.33	0/1697	0.50	0/2286
13	M	0.31	0/1744	0.52	0/2360
13	a	0.31	0/1744	0.52	0/2360
14	N	0.31	0/2152	0.52	0/2910
14	b	0.31	0/2152	0.52	0/2910
All	All	0.30	0/52744	0.50	0/71212

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](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 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	251/260 (96%)	249 (99%)	2 (1%)	0	100	100
1	O	251/260 (96%)	248 (99%)	3 (1%)	0	100	100
2	B	231/235 (98%)	226 (98%)	5 (2%)	0	100	100
2	P	231/235 (98%)	225 (97%)	6 (3%)	0	100	100
3	C	240/246 (98%)	237 (99%)	3 (1%)	0	100	100
3	Q	240/246 (98%)	236 (98%)	4 (2%)	0	100	100
4	D	234/241 (97%)	227 (97%)	7 (3%)	0	100	100
4	R	234/241 (97%)	228 (97%)	6 (3%)	0	100	100
5	E	239/256 (93%)	227 (95%)	12 (5%)	0	100	100
5	S	239/256 (93%)	229 (96%)	10 (4%)	0	100	100
6	F	237/253 (94%)	234 (99%)	3 (1%)	0	100	100
6	T	237/253 (94%)	233 (98%)	4 (2%)	0	100	100
7	G	245/252 (97%)	243 (99%)	2 (1%)	0	100	100
7	U	245/252 (97%)	243 (99%)	2 (1%)	0	100	100
8	H	242/252 (96%)	236 (98%)	6 (2%)	0	100	100
8	V	242/252 (96%)	237 (98%)	5 (2%)	0	100	100
9	I	220/229 (96%)	215 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	W	220/229 (96%)	216 (98%)	4 (2%)	0	100	100
10	J	206/218 (94%)	204 (99%)	2 (1%)	0	100	100
10	X	206/218 (94%)	204 (99%)	2 (1%)	0	100	100
11	K	193/195 (99%)	189 (98%)	4 (2%)	0	100	100
11	Y	193/195 (99%)	188 (97%)	5 (3%)	0	100	100
12	L	209/211 (99%)	206 (99%)	3 (1%)	0	100	100
12	Z	209/211 (99%)	206 (99%)	3 (1%)	0	100	100
13	M	213/240 (89%)	206 (97%)	7 (3%)	0	100	100
13	a	213/240 (89%)	206 (97%)	7 (3%)	0	100	100
14	N	253/265 (96%)	249 (98%)	4 (2%)	0	100	100
14	b	253/265 (96%)	249 (98%)	4 (2%)	0	100	100
All	All	6426/6706 (96%)	6296 (98%)	130 (2%)	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	224/231 (97%)	221 (99%)	3 (1%)	69	79
1	O	224/231 (97%)	220 (98%)	4 (2%)	59	70
2	B	203/205 (99%)	199 (98%)	4 (2%)	55	66
2	P	203/205 (99%)	195 (96%)	8 (4%)	32	38
3	C	209/213 (98%)	206 (99%)	3 (1%)	67	78
3	Q	209/213 (98%)	205 (98%)	4 (2%)	57	68
4	D	202/207 (98%)	197 (98%)	5 (2%)	47	57
4	R	202/207 (98%)	194 (96%)	8 (4%)	31	37
5	E	209/223 (94%)	202 (97%)	7 (3%)	38	46
5	S	209/223 (94%)	204 (98%)	5 (2%)	49	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	213/226 (94%)	206 (97%)	7 (3%)	38	46
6	T	213/226 (94%)	209 (98%)	4 (2%)	57	68
7	G	226/229 (99%)	223 (99%)	3 (1%)	69	79
7	U	226/229 (99%)	223 (99%)	3 (1%)	69	79
8	H	225/231 (97%)	221 (98%)	4 (2%)	59	70
8	V	225/231 (97%)	222 (99%)	3 (1%)	69	79
9	I	188/194 (97%)	187 (100%)	1 (0%)	88	94
9	W	188/194 (97%)	188 (100%)	0	100	100
10	J	184/191 (96%)	183 (100%)	1 (0%)	88	94
10	X	184/191 (96%)	181 (98%)	3 (2%)	62	74
11	K	174/174 (100%)	172 (99%)	2 (1%)	73	83
11	Y	174/174 (100%)	169 (97%)	5 (3%)	42	51
12	L	176/176 (100%)	174 (99%)	2 (1%)	73	83
12	Z	176/176 (100%)	174 (99%)	2 (1%)	73	83
13	M	192/216 (89%)	188 (98%)	4 (2%)	53	64
13	a	192/216 (89%)	186 (97%)	6 (3%)	40	48
14	N	231/239 (97%)	229 (99%)	2 (1%)	78	87
14	b	231/239 (97%)	228 (99%)	3 (1%)	69	79
All	All	5712/5910 (97%)	5606 (98%)	106 (2%)	59	68

5 of 106 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	P	176	LYS
4	R	233	ARG
13	a	130	PHE
2	P	198	SER
4	R	37	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
8	V	104	ASN
8	V	190	GLN
14	b	126	ASN

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Mol	Chain	Res	Type
14	b	112	ASN
14	N	126	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

6 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
15	YRE	W	301	-	47,47,47	0.92	1 (2%)	62,63,63	1.33	5 (8%)
15	YRE	Z	301	-	47,47,47	0.86	1 (2%)	62,63,63	1.18	4 (6%)
15	YRE	C	301	-	47,47,47	0.90	2 (4%)	62,63,63	1.53	8 (12%)
15	YRE	I	301	-	47,47,47	0.88	1 (2%)	62,63,63	1.30	6 (9%)
15	YRE	L	301	-	47,47,47	0.86	1 (2%)	62,63,63	1.18	4 (6%)
15	YRE	Q	301	-	47,47,47	0.90	2 (4%)	62,63,63	1.41	6 (9%)

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
15	YRE	W	301	-	-	14/45/70/70	0/4/5/5
15	YRE	Z	301	-	-	4/45/70/70	0/4/5/5
15	YRE	C	301	-	-	12/45/70/70	0/4/5/5
15	YRE	I	301	-	-	12/45/70/70	0/4/5/5
15	YRE	L	301	-	-	4/45/70/70	0/4/5/5
15	YRE	Q	301	-	-	12/45/70/70	0/4/5/5

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	Q	301	YRE	C30-N29	3.45	1.39	1.34
15	W	301	YRE	C17-C16	3.14	1.60	1.54
15	C	301	YRE	C30-N29	2.98	1.39	1.34
15	I	301	YRE	C17-C16	2.70	1.59	1.54
15	Z	301	YRE	C30-N29	2.56	1.38	1.34

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	Q	301	YRE	C16-N29-C30	6.47	129.93	122.83
15	C	301	YRE	C16-N29-C30	6.18	129.61	122.83
15	Z	301	YRE	C16-N29-C30	6.17	129.60	122.83
15	L	301	YRE	C16-N29-C30	6.12	129.54	122.83
15	W	301	YRE	C33-N29-C30	-4.92	110.28	113.42

There are no chirality outliers.

5 of 58 torsion outliers are listed below:

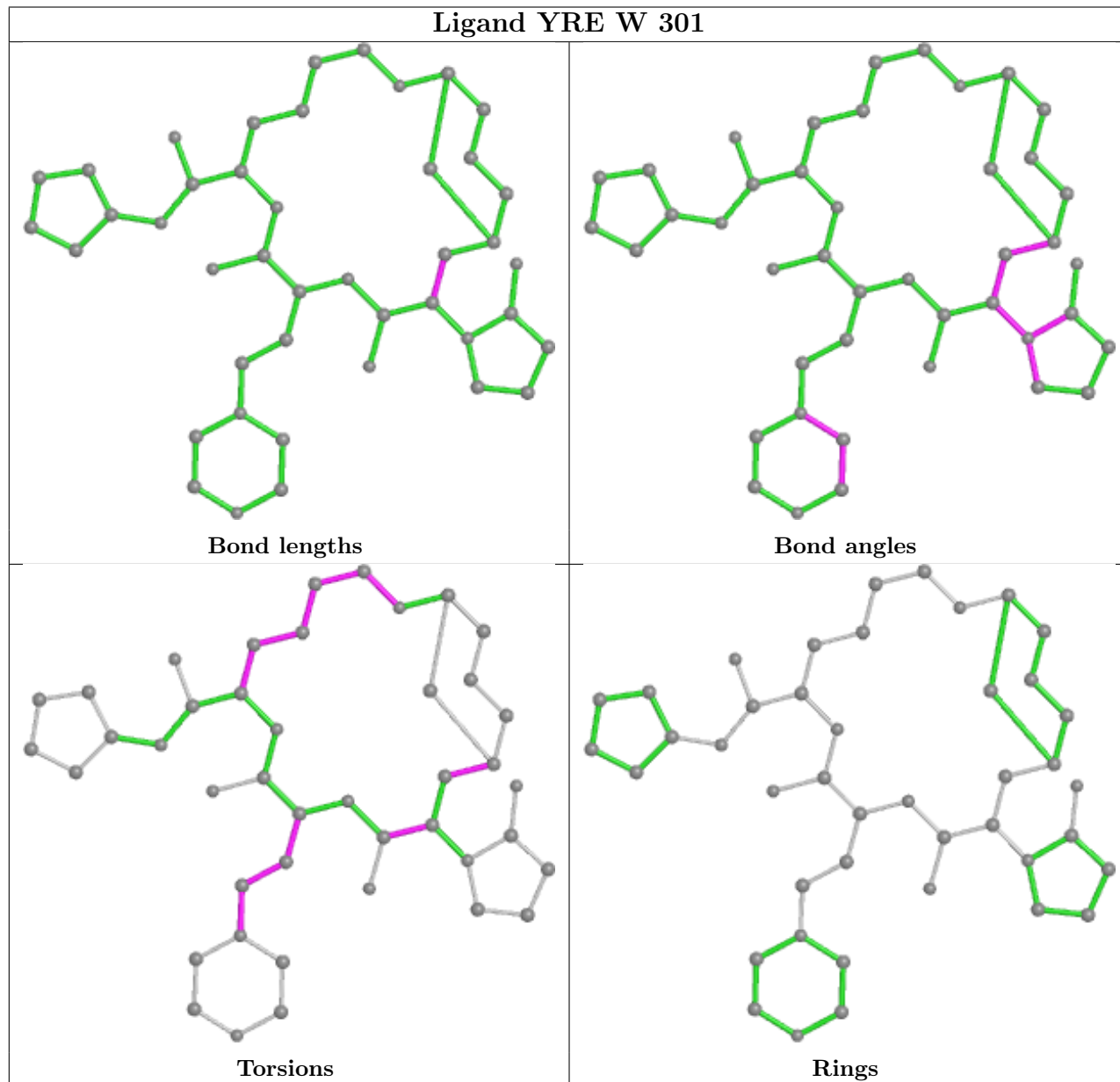
Mol	Chain	Res	Type	Atoms
15	C	301	YRE	C02-C13-C36-C37
15	L	301	YRE	C02-C13-C36-C37
15	L	301	YRE	N14-C13-C36-C37
15	Q	301	YRE	C02-C13-C36-C37
15	W	301	YRE	C23-C24-C25-C04

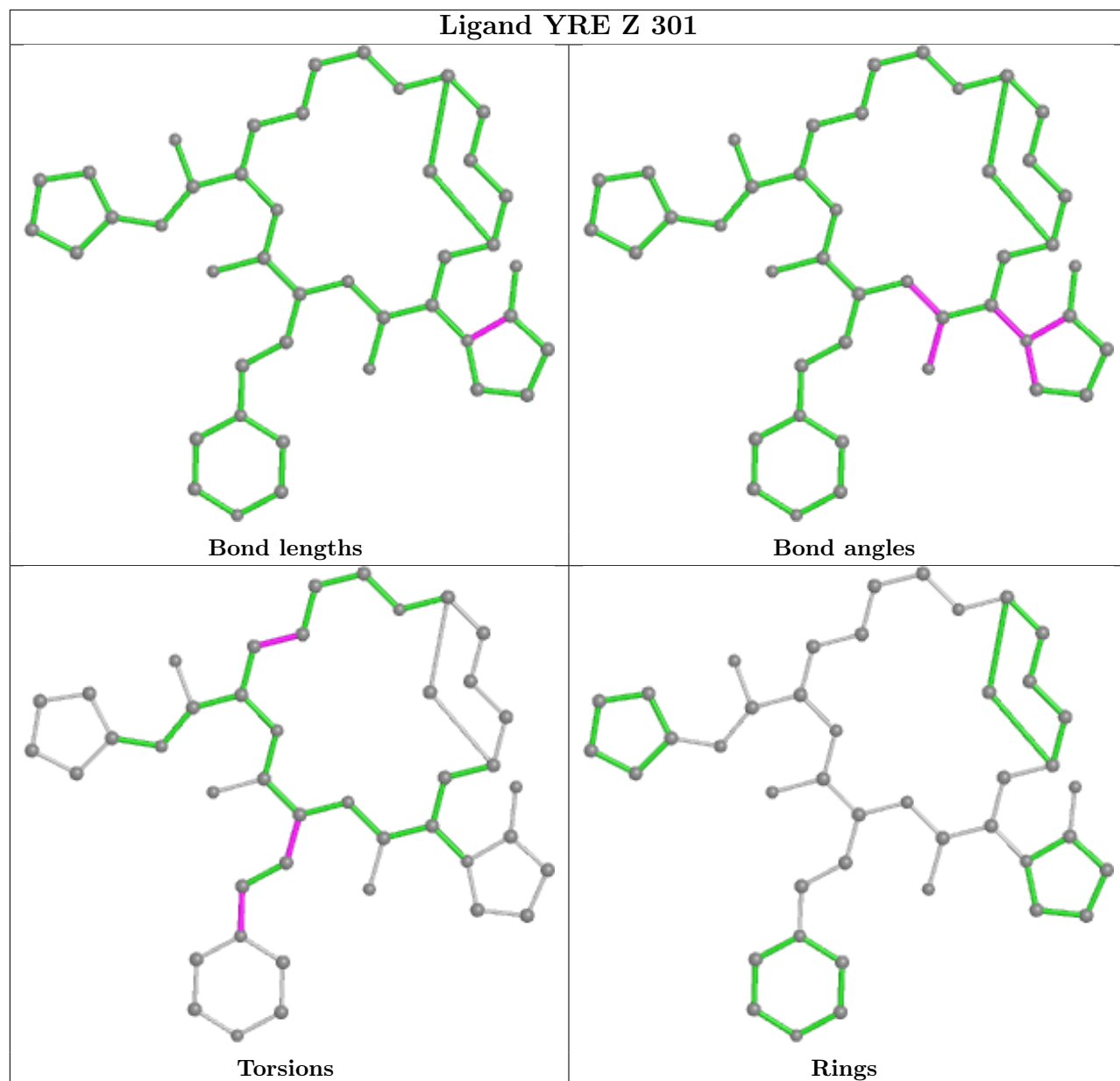
There are no ring outliers.

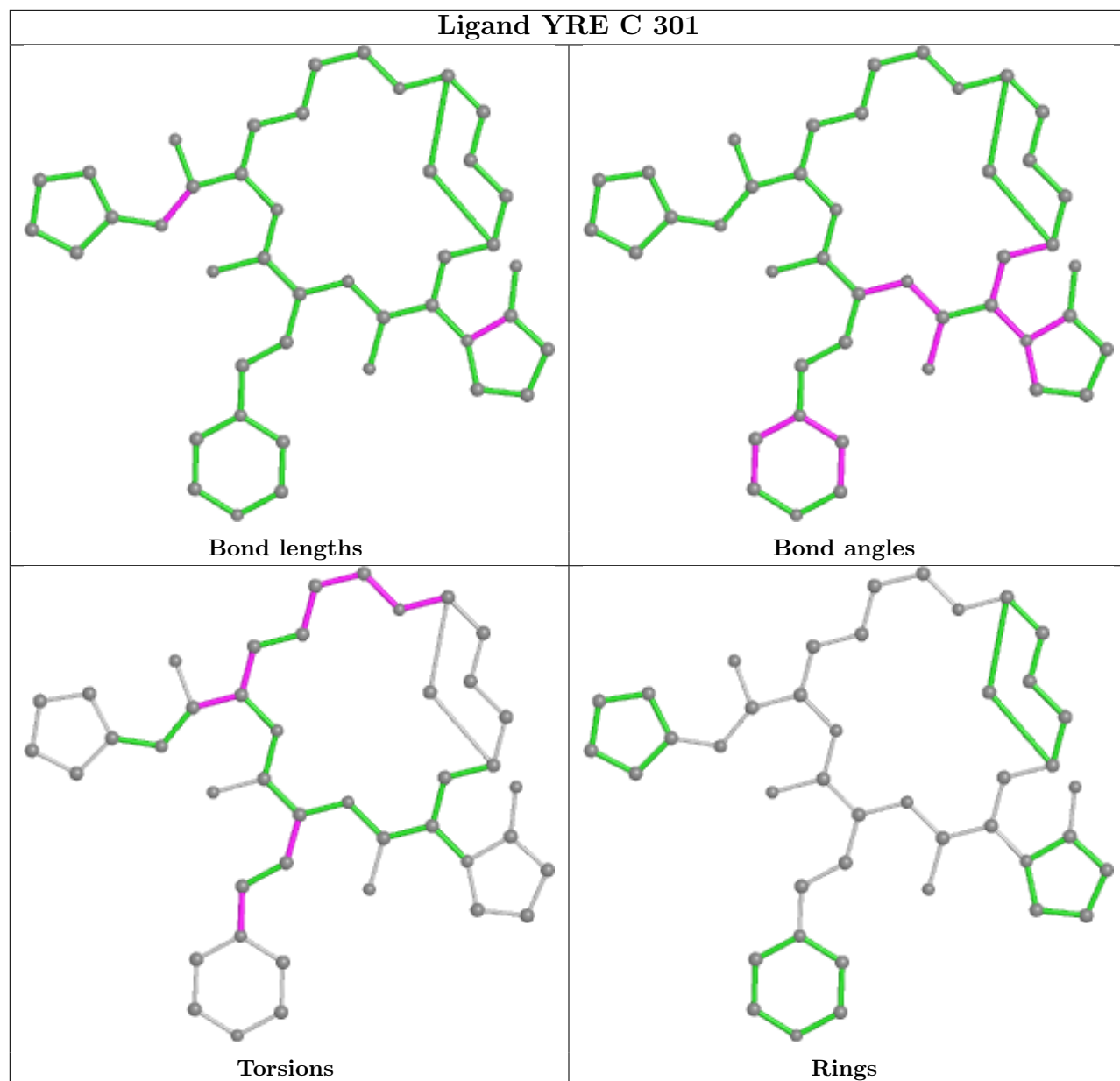
No monomer is involved in short contacts.

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

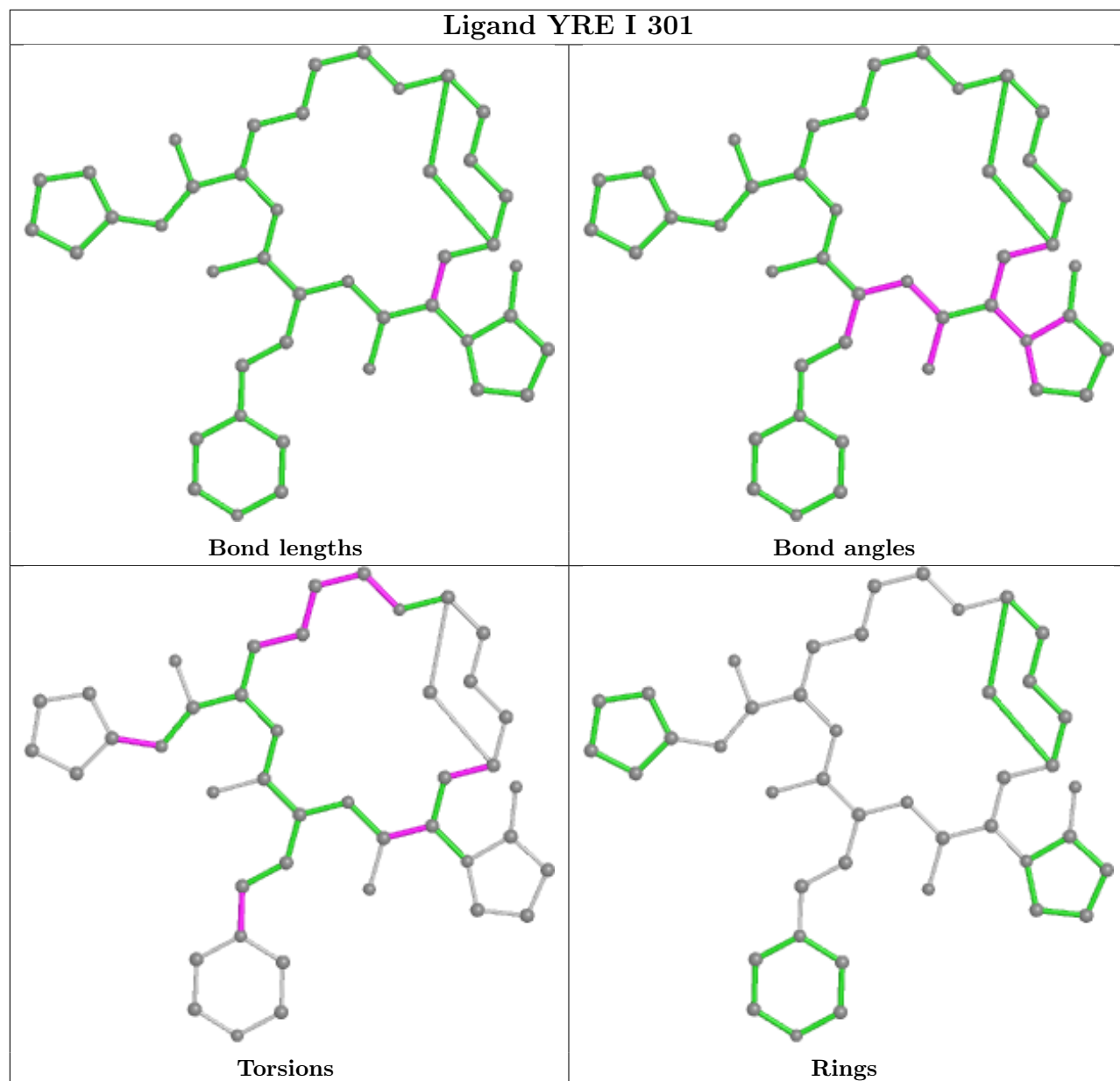
addition, ligands with molecular weight  $> 250$  and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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.

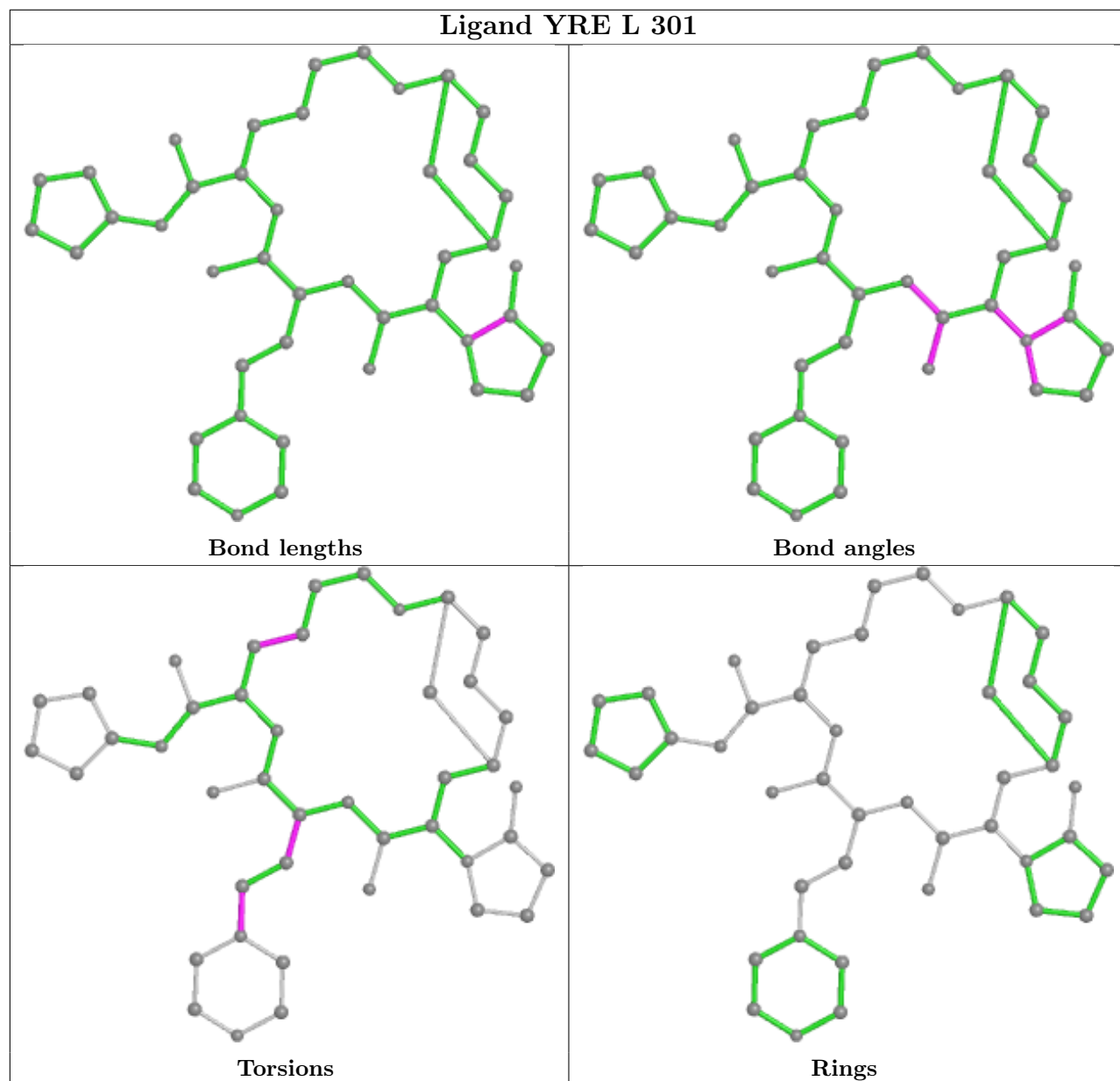


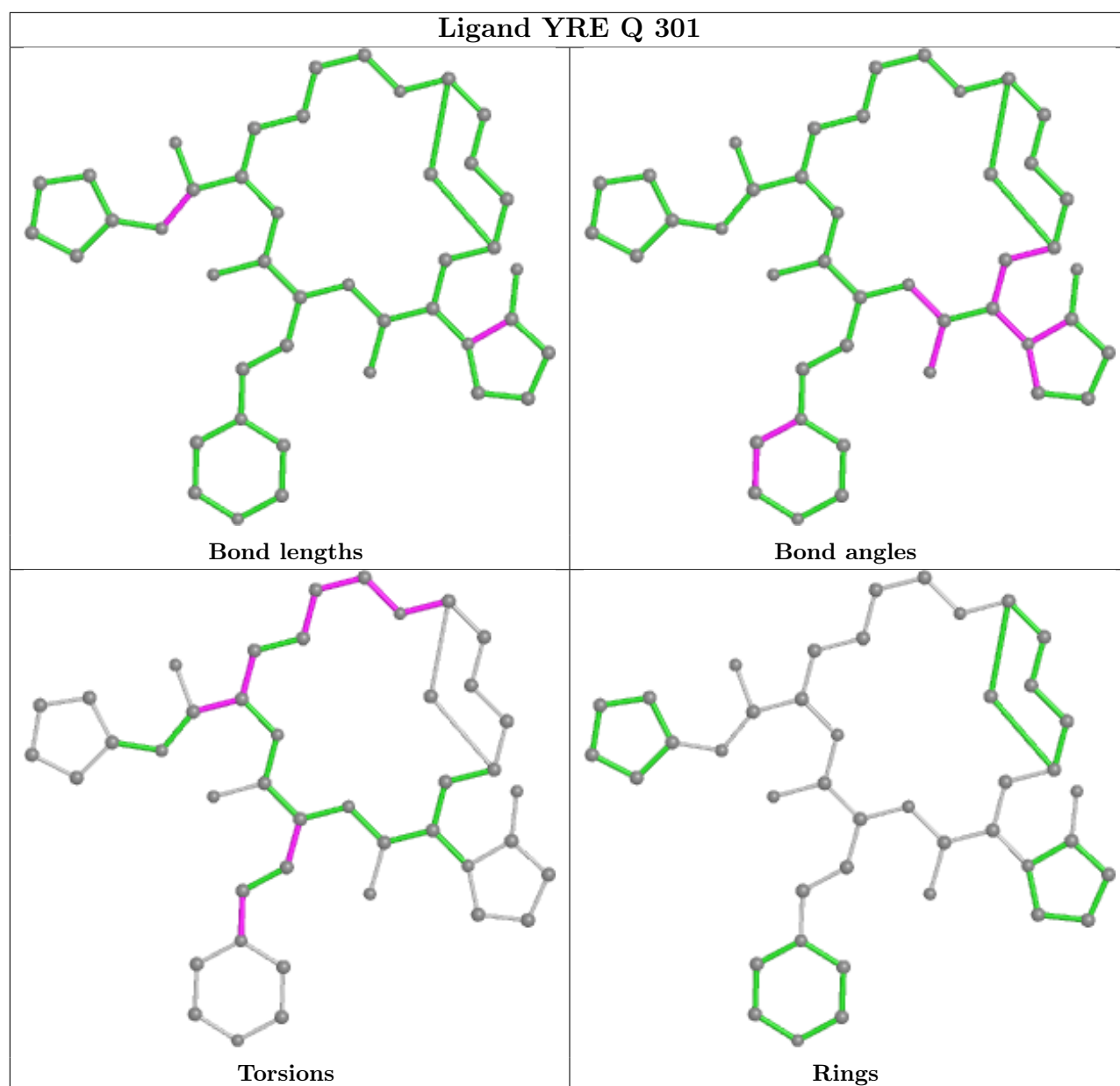












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

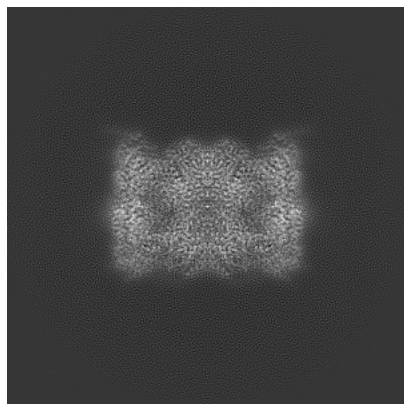
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29764. These allow visual inspection of the internal detail of the map and identification of artifacts.

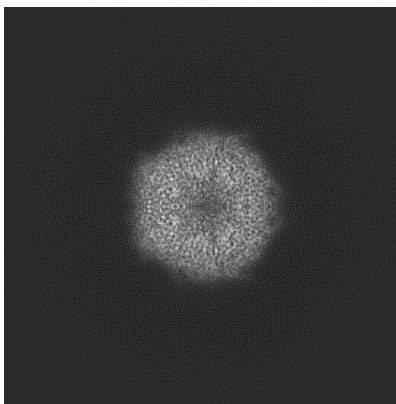
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

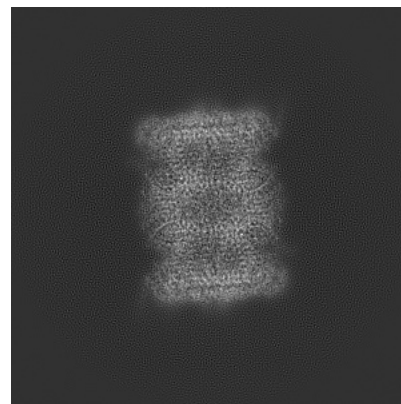
#### 6.1.1 Primary map



X

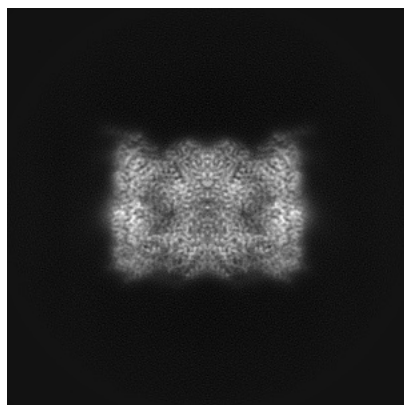


Y

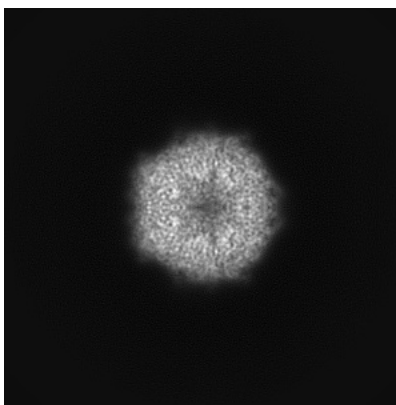


Z

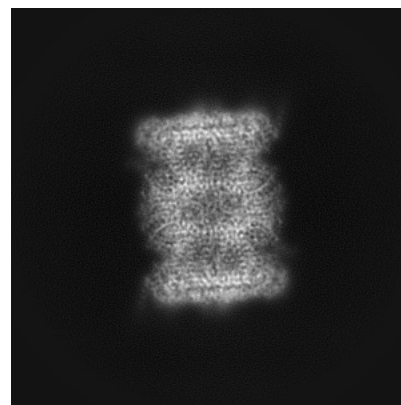
#### 6.1.2 Raw map



X



Y

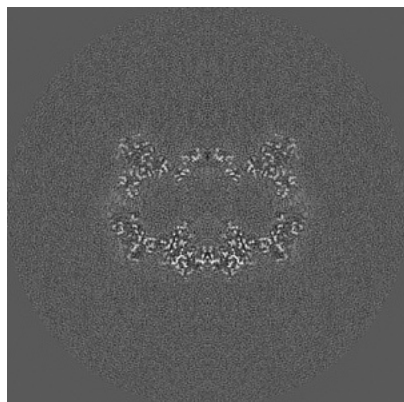


Z

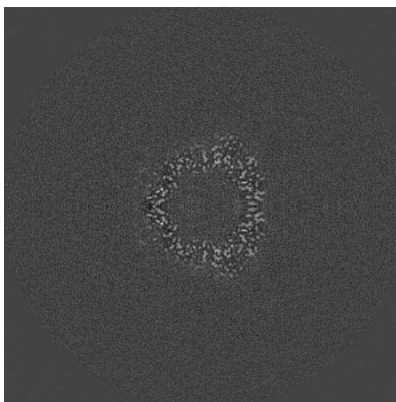
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

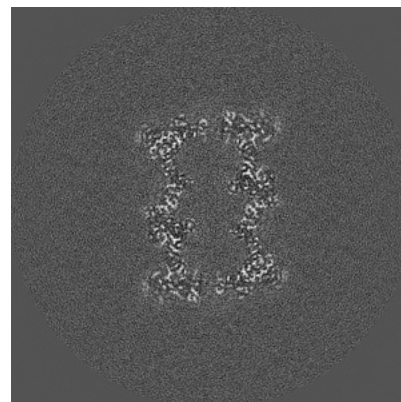
### 6.2.1 Primary map



X Index: 192

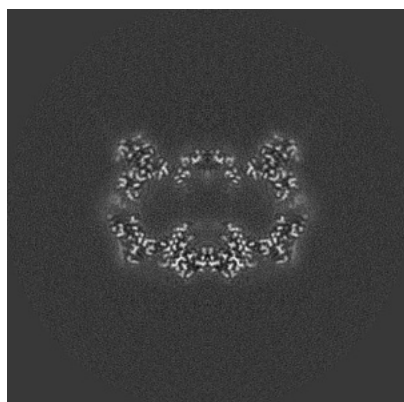


Y Index: 192

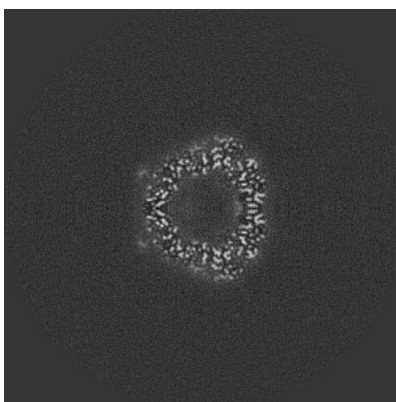


Z Index: 192

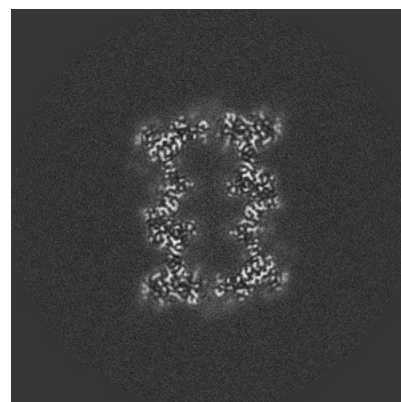
### 6.2.2 Raw map



X Index: 192



Y Index: 192

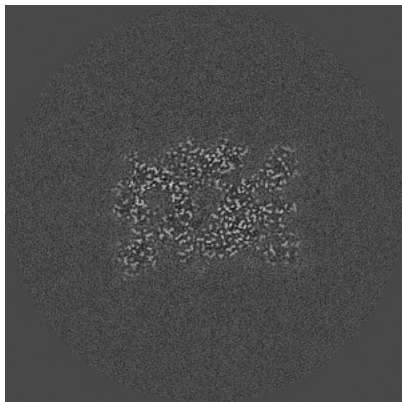


Z Index: 192

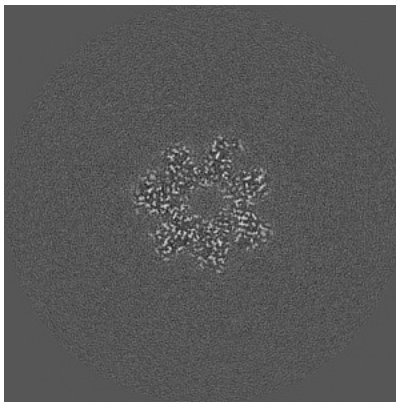
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

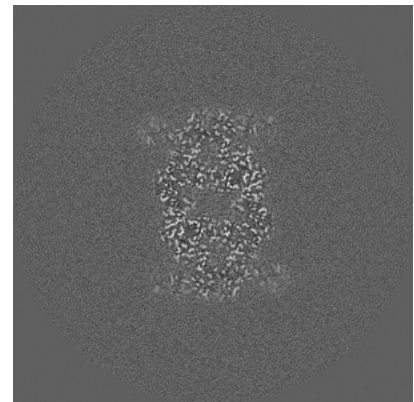
### 6.3.1 Primary map



X Index: 223

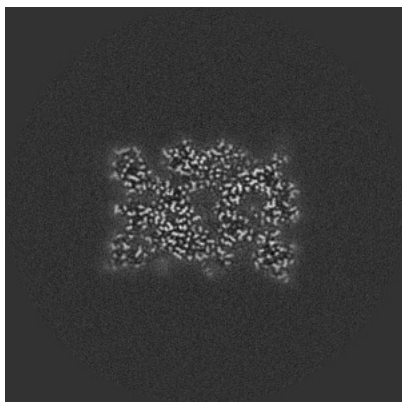


Y Index: 169

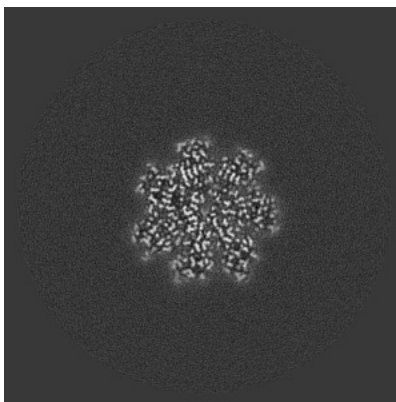


Z Index: 165

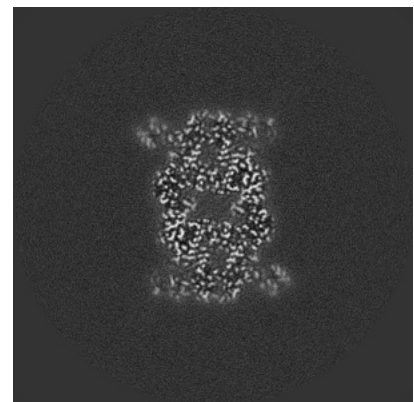
### 6.3.2 Raw map



X Index: 161



Y Index: 263



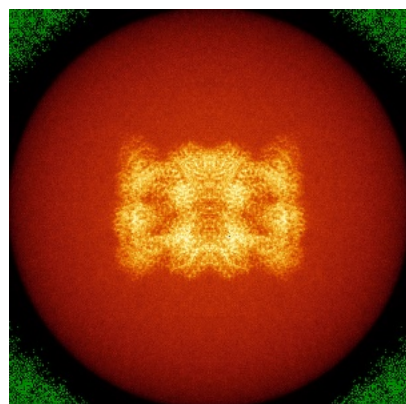
Z Index: 165

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

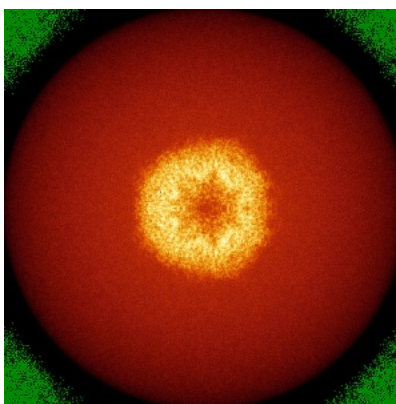


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

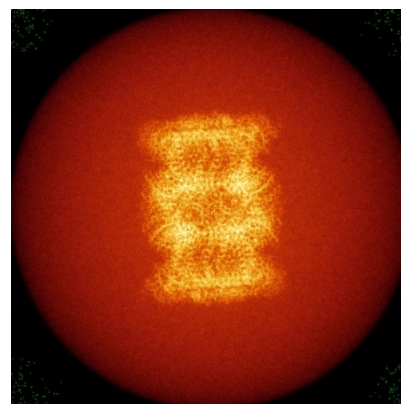
### 6.4.1 Primary map



X

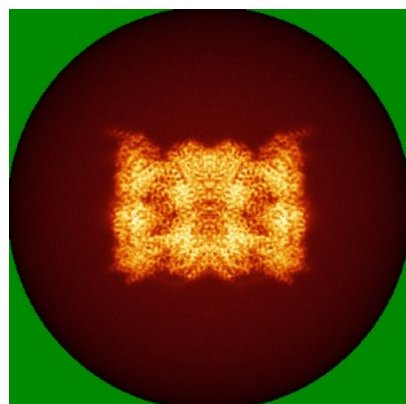


Y

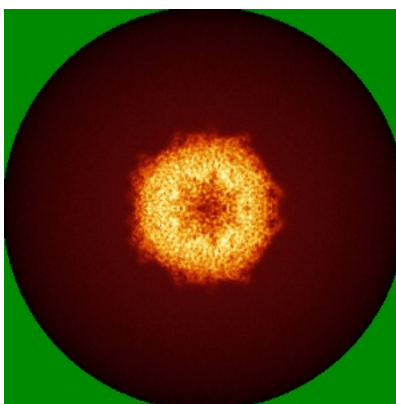


Z

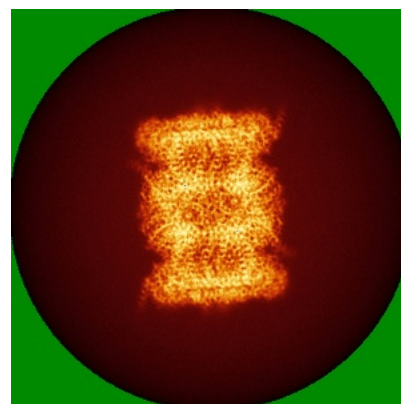
### 6.4.2 Raw map



X



Y

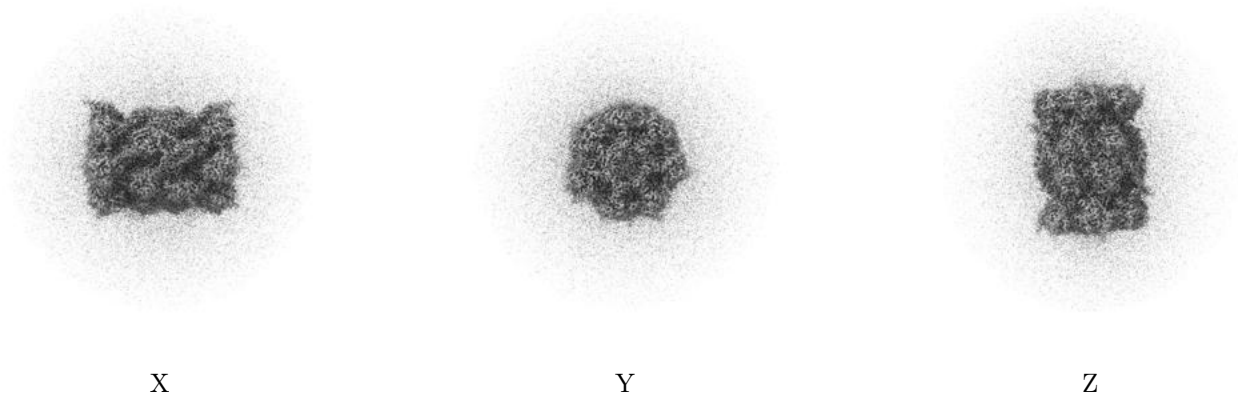


Z

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.

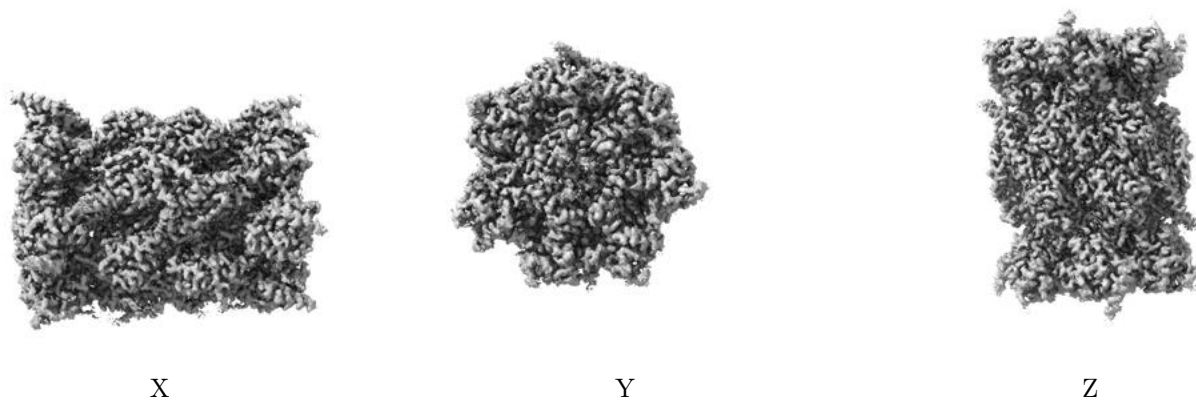
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.025. 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.



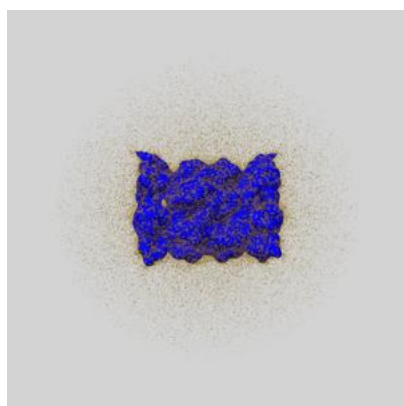
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

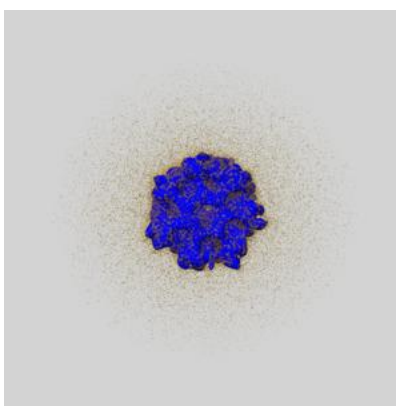
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

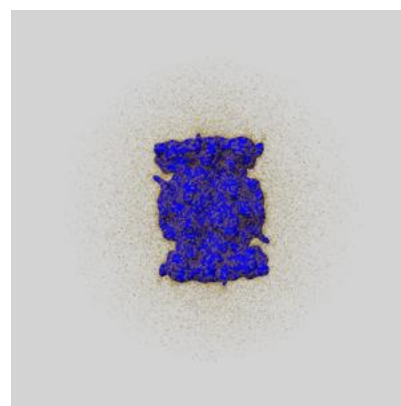
### 6.6.1 emd\_29764\_msk\_1.map [i](#)



X



Y

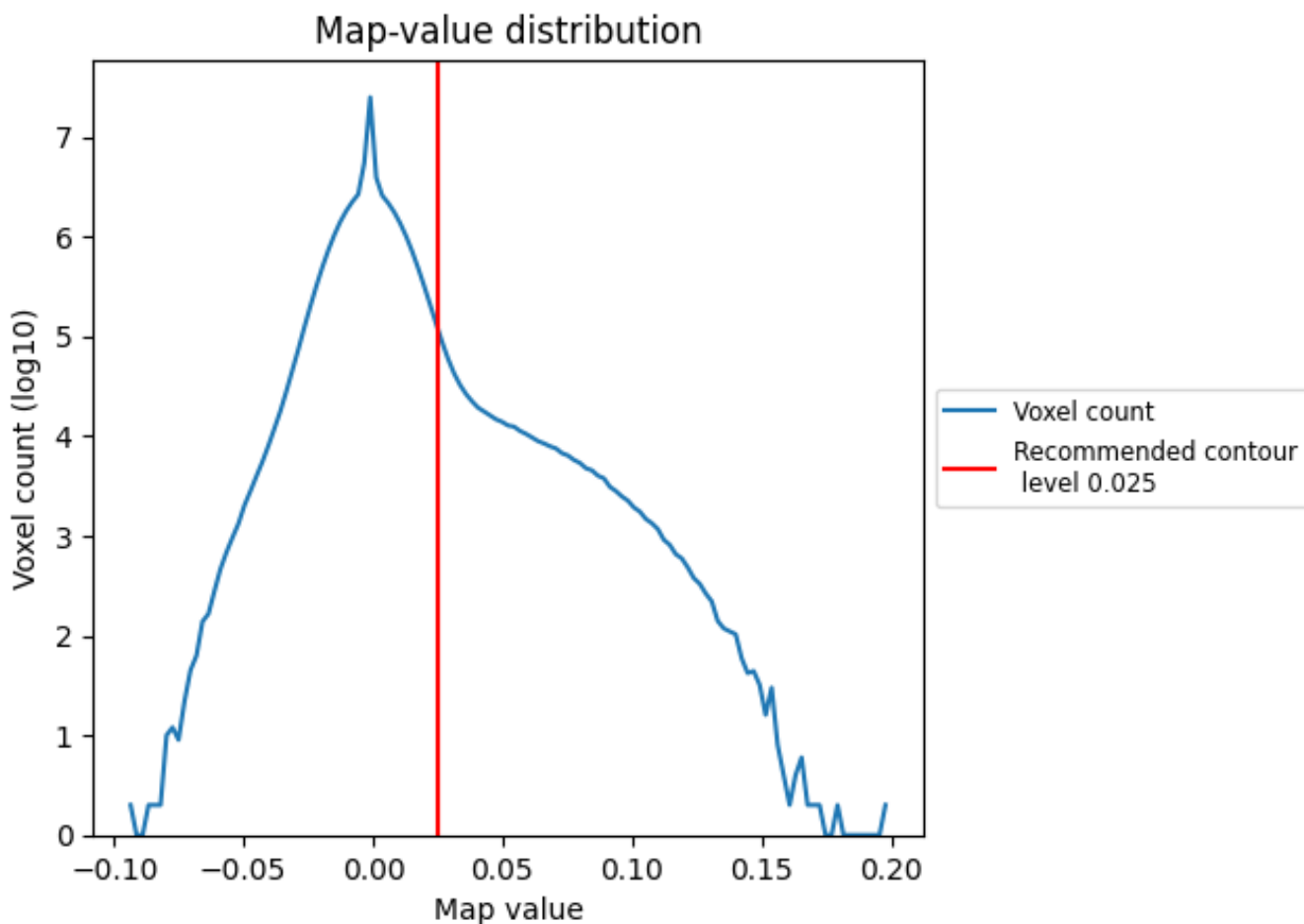


Z

## 7 Map analysis [i](#)

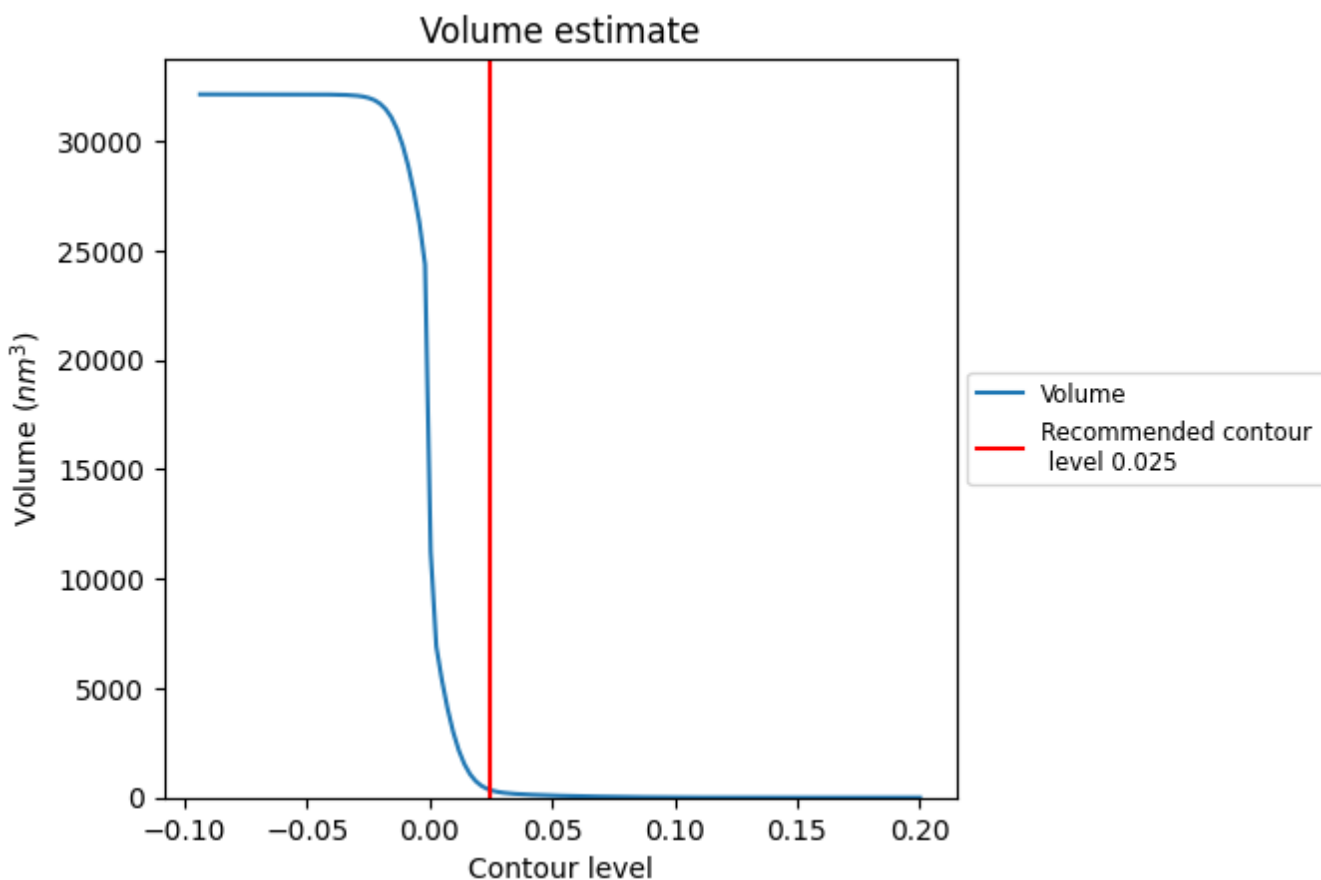
This section contains the results of statistical analysis of the map.

### 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.

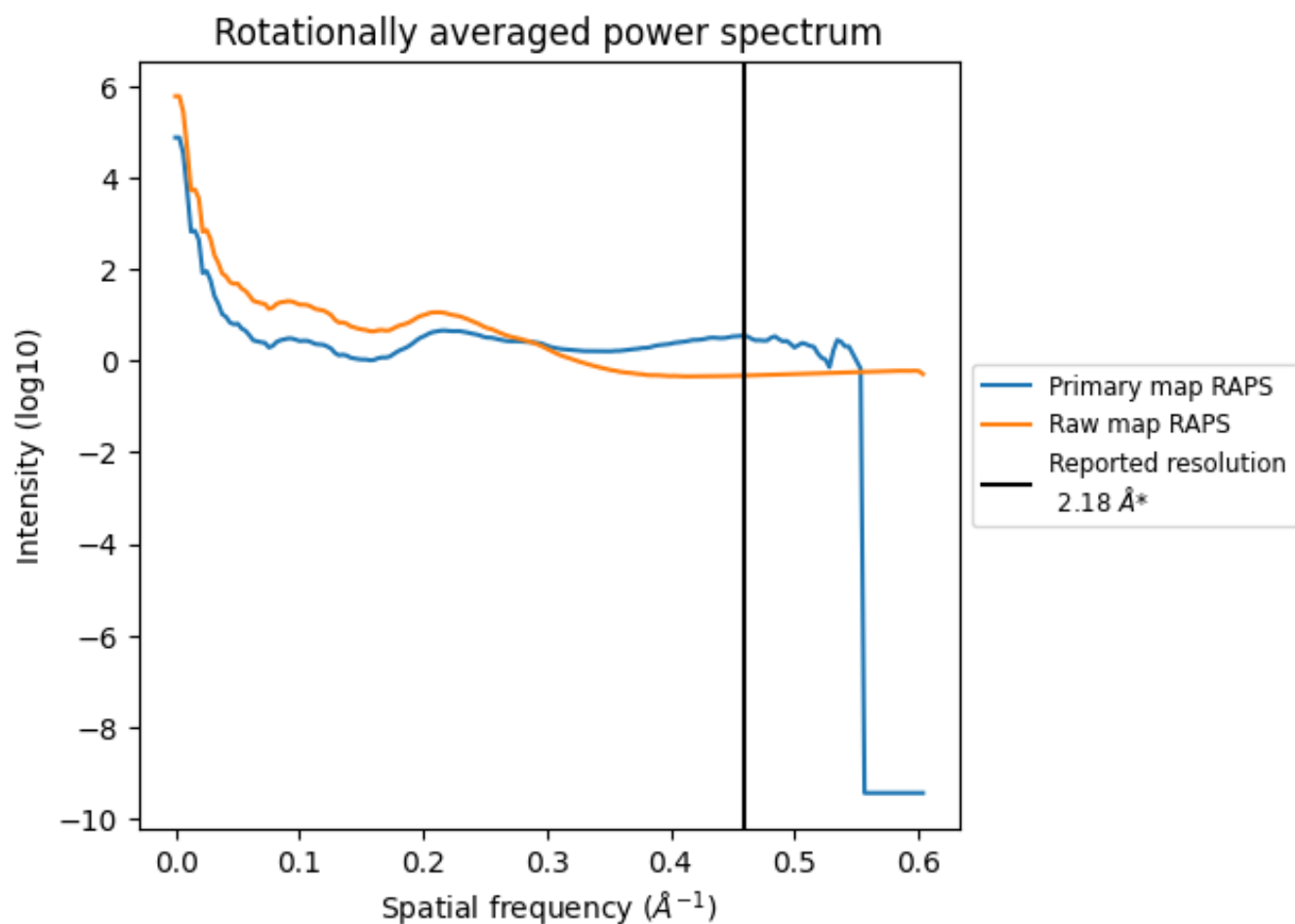
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 343 nm<sup>3</sup>; this corresponds to an approximate mass of 310 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

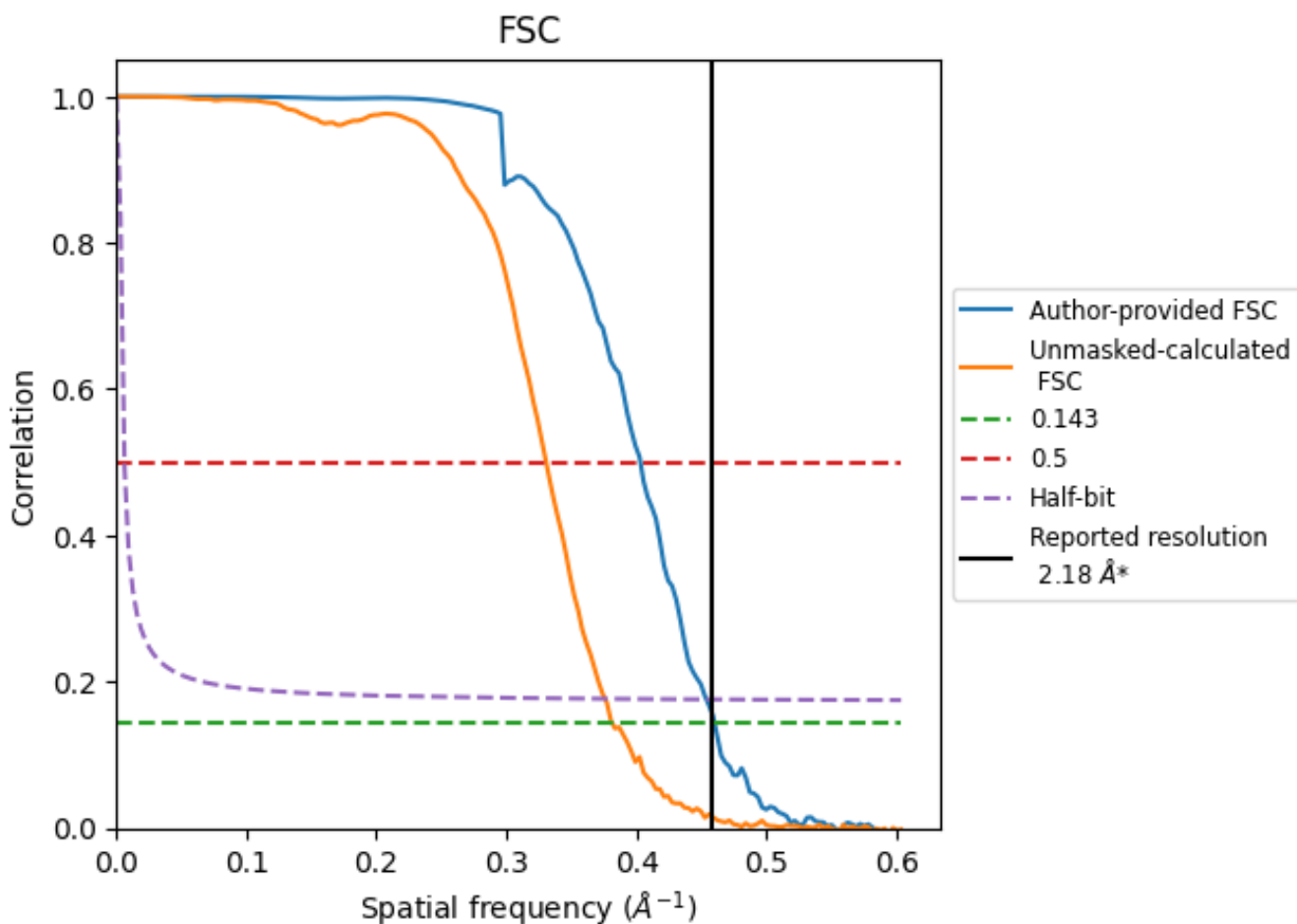


\*Reported resolution corresponds to spatial frequency of 0.459 Å<sup>-1</sup>

## 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 0.459 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

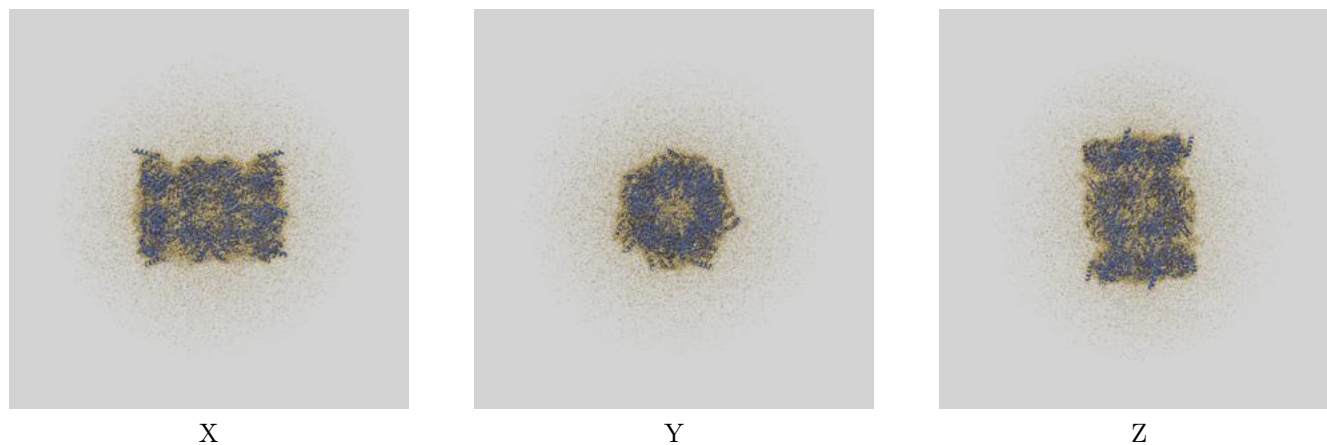
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.18	-	-
Author-provided FSC curve	2.17	2.48	2.20
Unmasked-calculated*	2.62	3.02	2.66

\*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 2.62 differs from the reported value 2.18 by more than 10 %

## 9 Map-model fit [i](#)

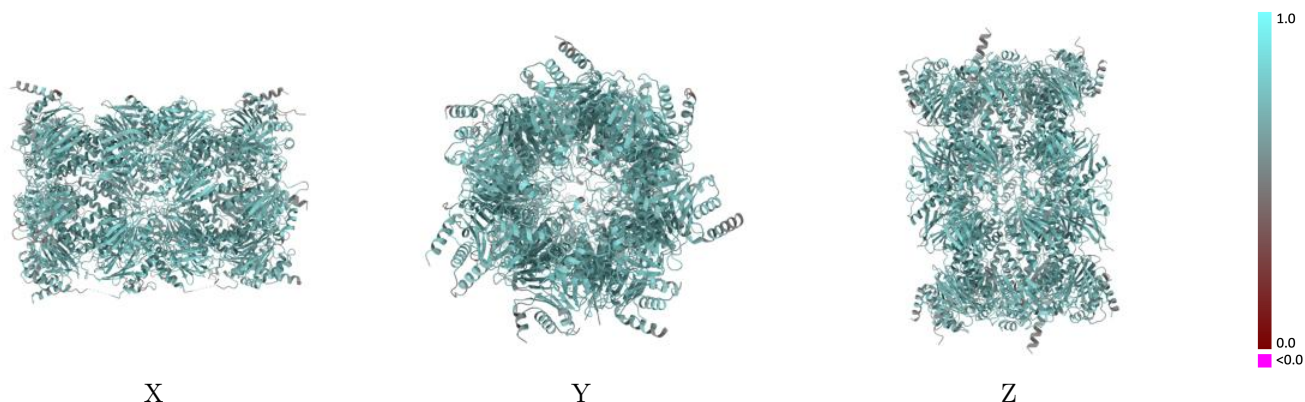
This section contains information regarding the fit between EMDB map EMD-29764 and PDB model 8G6E. Per-residue inclusion information can be found in section 3 on page 10.

### 9.1 Map-model overlay [i](#)



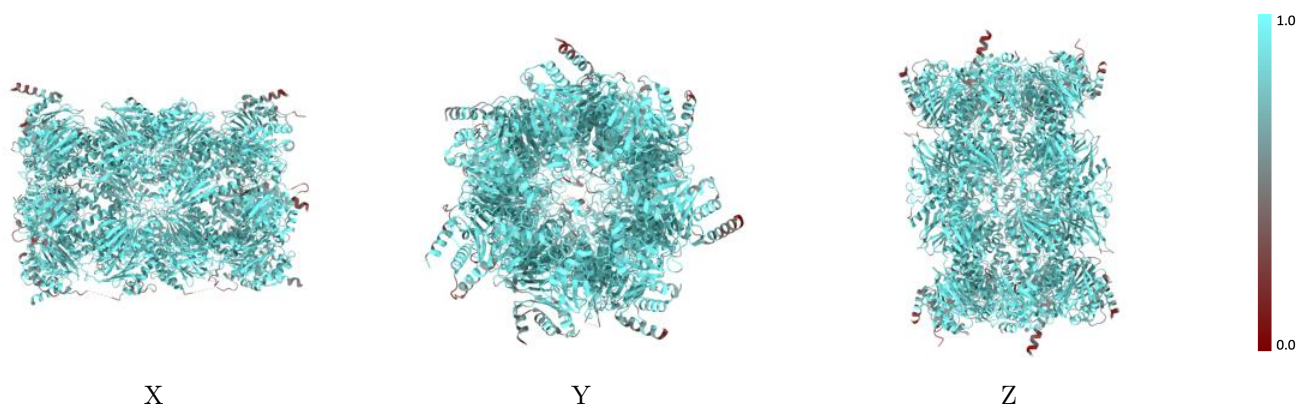
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

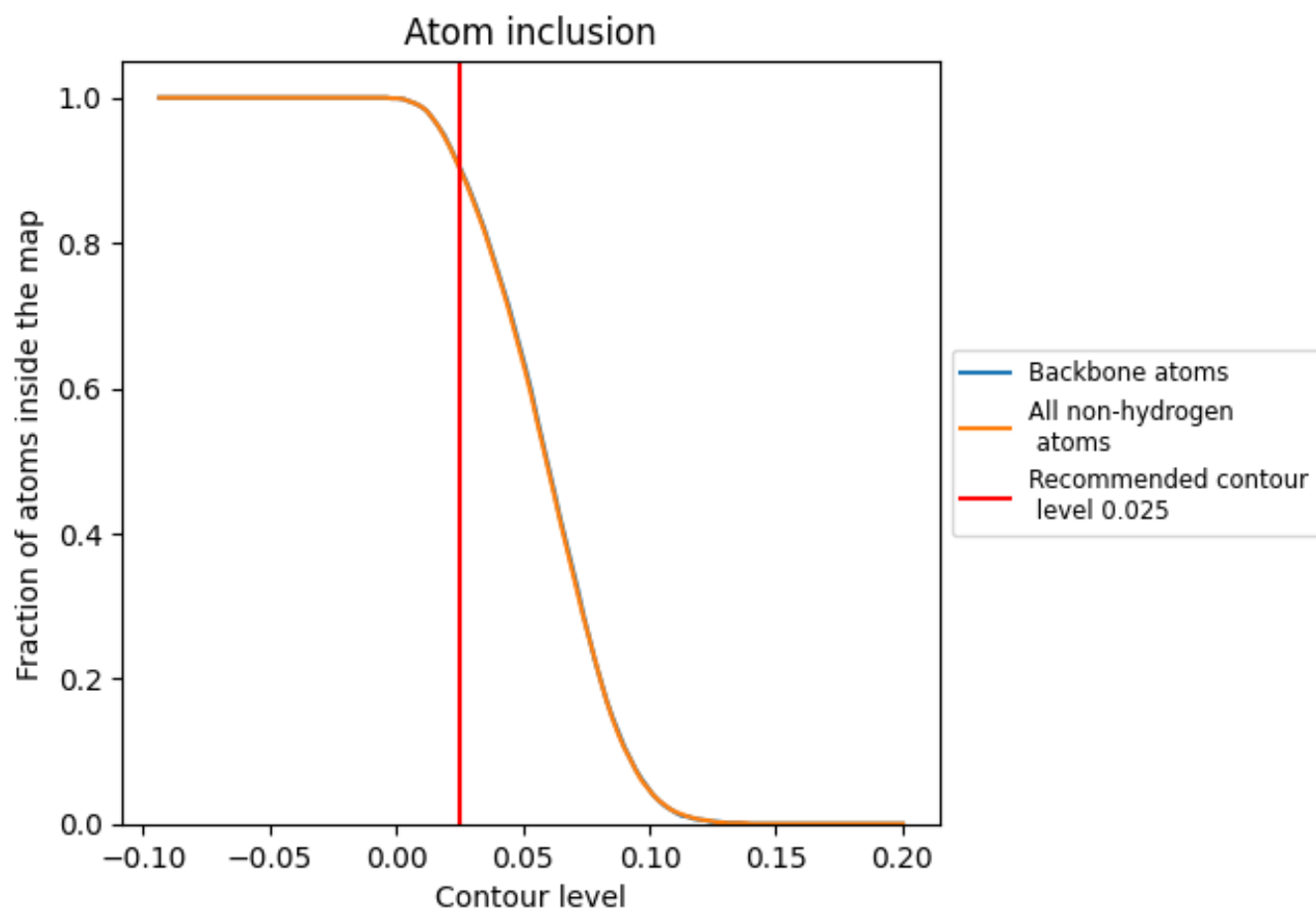
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.025).





























































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 90% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9030	 0.7150
A	 0.8820	 0.7020
B	 0.8420	 0.6740
C	 0.8790	 0.6960
D	 0.8610	 0.6880
E	 0.8490	 0.6760
F	 0.8760	 0.6960
G	 0.9140	 0.7130
H	 0.9170	 0.7300
I	 0.9500	 0.7390
J	 0.9460	 0.7470
K	 0.9460	 0.7360
L	 0.9620	 0.7480
M	 0.9380	 0.7330
N	 0.9350	 0.7380
O	 0.8800	 0.7020
P	 0.8430	 0.6740
Q	 0.8830	 0.6990
R	 0.8580	 0.6890
S	 0.8470	 0.6780
T	 0.8780	 0.6970
U	 0.9150	 0.7140
V	 0.9150	 0.7290
W	 0.9480	 0.7370
X	 0.9450	 0.7450
Y	 0.9480	 0.7360
Z	 0.9610	 0.7480
a	 0.9360	 0.7350
b	 0.9350	 0.7360

