



wwPDB EM Validation Summary Report ⓘ

Dec 30, 2024 – 01:25 PM EST

PDB ID : 8CVR
EMDB ID : EMD-27013
Title : Human 20S proteasome with MG-132
Authors : Zhao, J.
Deposited on : 2022-05-18
Resolution : 2.70 Å(reported)

This is a wwPDB EM Validation Summary 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:

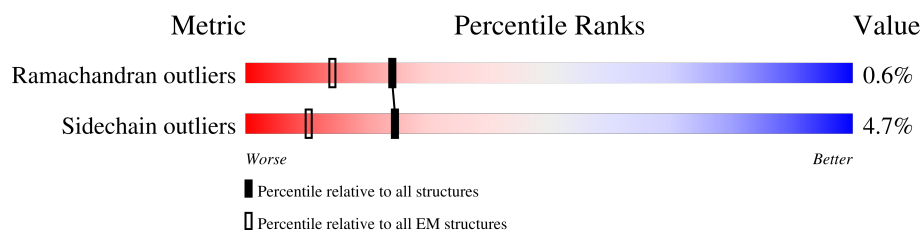
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance

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



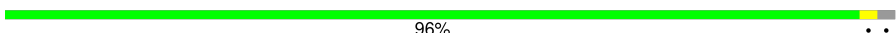
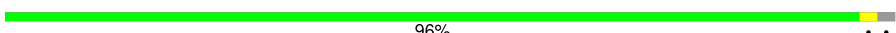





The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



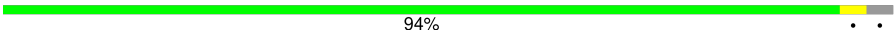




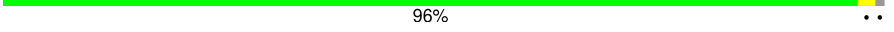
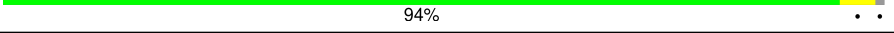


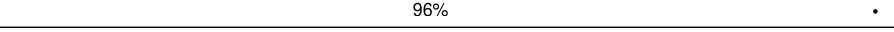
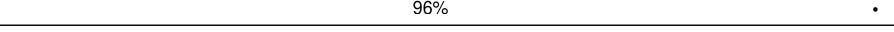
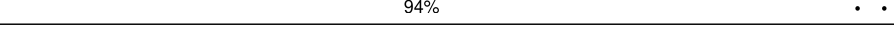
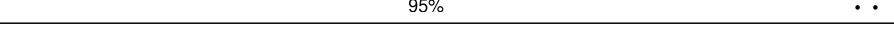
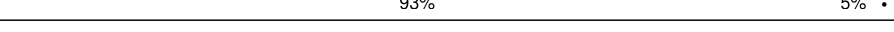





Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	246	 92%5% •
1	O	246	 90%7% •
2	B	234	 96%• •
2	P	234	 96%• •
3	C	261	 91%• 5%
3	Q	261	 91%• 5%
4	D	248	 91%• 6%
4	R	248	 92%• 6%
5	E	241	 92%5% •

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Mol	Chain	Length	Quality of chain
5	S	241	 94% . .
6	F	263	 85% . 11%
6	T	263	 86% . 11%
7	G	255	 91% . 6%
7	U	255	 89% . 6%
8	H	205	 96% . .
8	V	205	 94% . .
9	I	234	 88% 6% 6%
9	W	234	 91% . 6%
10	J	205	 96% .
10	X	205	 96% .
11	K	201	 94% . .
11	Y	201	 95% . .
12	L	204	 93% 5% .
12	Z	204	 91% 7% .
13	M	241	 84% . 12%
13	a	241	 84% . 12%
14	N	264	 78% . 20%
14	b	264	 78% . 20%

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 45586 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
1	A	240	Total	C	N	O	S	0	0
			1738	1106	304	316	12		
1	O	240	Total	C	N	O	S	0	0
			1734	1104	304	314	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	229	Total	C	N	O	S	0	0
			1662	1080	288	288	6		
2	P	229	Total	C	N	O	S	0	0
			1662	1080	288	288	6		

- Molecule 3 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	247	Total	C	N	O	S	0	0
			1786	1143	320	313	10		
3	Q	247	Total	C	N	O	S	0	0
			1786	1143	320	313	10		

- Molecule 4 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	232	Total	C	N	O	S	0	0
			1633	1038	306	284	5		
4	R	232	Total	C	N	O	S	0	0
			1633	1038	306	284	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	233	Total	C	N	O	S	0	0
			1660	1056	287	306	11		
5	S	233	Total	C	N	O	S	0	0
			1660	1056	287	306	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	233	Total	C	N	O	S	0	0
			1704	1087	315	293	9		
6	T	233	Total	C	N	O	S	0	0
			1707	1089	315	293	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	239	Total	C	N	O	S	0	0
			1760	1131	308	311	10		
7	U	239	Total	C	N	O	S	0	0
			1760	1131	308	311	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	202	Total	C	N	O	S	0	0
			1469	928	257	272	12		
8	V	202	Total	C	N	O	S	0	0
			1465	926	256	271	12		

- Molecule 9 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	220	Total	C	N	O	S	0	0
			1580	1005	272	294	9		
9	W	220	Total	C	N	O	S	0	0
			1576	1003	272	292	9		

- Molecule 10 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	204	Total	C	N	O	S	0	0
			1546	992	262	273	19		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	X	204	Total	C	N	O	S	0	0
			1534	987	262	267	18		

- Molecule 11 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	196	Total	C	N	O	S	0	0
			1509	974	259	268	8		
11	Y	196	Total	C	N	O	S	0	0
			1506	973	259	266	8		

- Molecule 12 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	200	Total	C	N	O	S	0	0
			1504	957	271	267	9		
12	Z	200	Total	C	N	O	S	0	0
			1500	954	270	267	9		

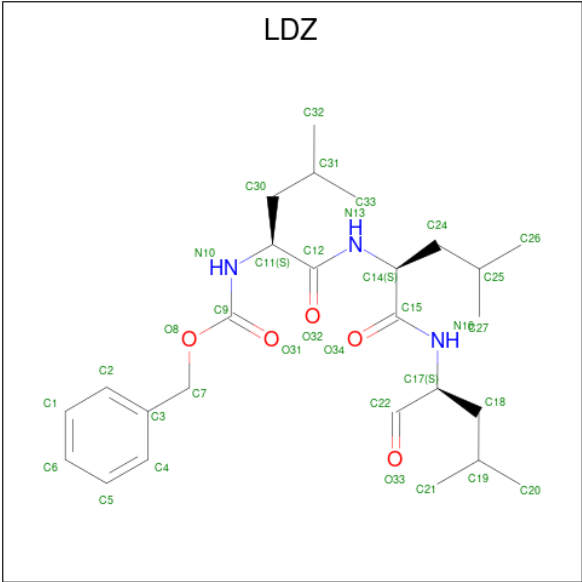
- Molecule 13 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	212	Total	C	N	O	S	0	0
			1584	1016	279	279	10		
13	a	212	Total	C	N	O	S	0	0
			1584	1016	279	279	10		

- Molecule 14 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	212	Total	C	N	O	S	0	0
			1568	998	279	280	11		
14	b	212	Total	C	N	O	S	0	0
			1572	1000	279	282	11		

- Molecule 15 is N-[(benzyloxy)carbonyl]-L-leucyl-N-[(2S)-4-methyl-1-oxopentan-2-yl]-L-leucine amide (three-letter code: LDZ) (formula: C₂₆H₄₁N₃O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
15	H	1	Total	C	N	O	0
			34	26	3	5	
15	I	1	Total	C	N	O	0
			34	26	3	5	
15	L	1	Total	C	N	O	0
			34	26	3	5	
15	V	1	Total	C	N	O	0
			34	26	3	5	
15	W	1	Total	C	N	O	0
			34	26	3	5	
15	Z	1	Total	C	N	O	0
			34	26	3	5	

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

Chain A:  92% 5% •



- Molecule 1: Proteasome subunit alpha type-6

Chain O:  90% 7% •



- Molecule 2: Proteasome subunit alpha type-2

Chain B:  96% • •



- Molecule 2: Proteasome subunit alpha type-2

Chain P:  96% • •




- Molecule 3: Proteasome subunit alpha type-4

Chain C:  91% • 5%



- Molecule 3: Proteasome subunit alpha type-4

Chain Q:  91% • 5%



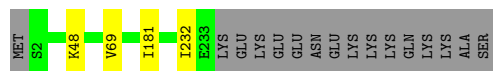
- Molecule 4: Proteasome subunit alpha type-7

Chain D:  91% • 6%



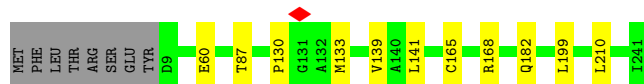
- Molecule 4: Proteasome subunit alpha type-7

Chain R:  92% • 6%



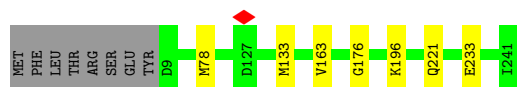
- Molecule 5: Proteasome subunit alpha type-5

Chain E:  92% 5% •




- Molecule 5: Proteasome subunit alpha type-5

Chain S:  94% • •




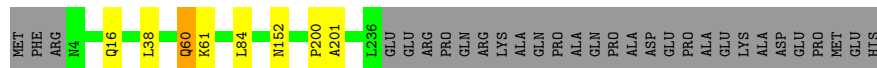
- Molecule 6: Proteasome subunit alpha type-1

Chain F:  85% • 11%



- Molecule 6: Proteasome subunit alpha type-1

Chain T:  86% • 11%




- Molecule 7: Proteasome subunit alpha type-3

Chain G:  91% • 6%



- Molecule 7: Proteasome subunit alpha type-3

Chain U:  89% • 6%



- Molecule 8: Proteasome subunit beta type-6

Chain H:  96% ••




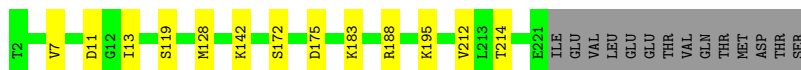
- Molecule 8: Proteasome subunit beta type-6

Chain V:  94% ••



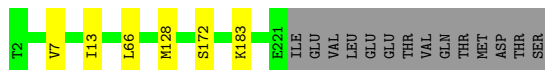
- Molecule 9: Proteasome subunit beta type-7

Chain I:  88% 6% 6%



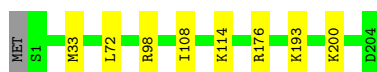
- Molecule 9: Proteasome subunit beta type-7

Chain W:  91% • 6%



- Molecule 10: Proteasome subunit beta type-3

Chain J:  96% •



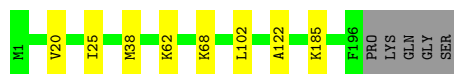
- Molecule 10: Proteasome subunit beta type-3

Chain X:  96% .



- Molecule 11: Proteasome subunit beta type-2

Chain K:  94% . .



- Molecule 11: Proteasome subunit beta type-2

Chain Y:  95% . .



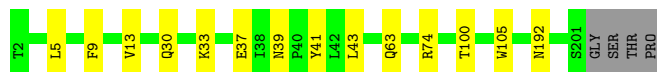
- Molecule 12: Proteasome subunit beta type-5

Chain L:  93% 5% .




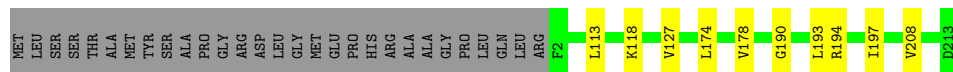
- Molecule 12: Proteasome subunit beta type-5

Chain Z:  91% 7% .




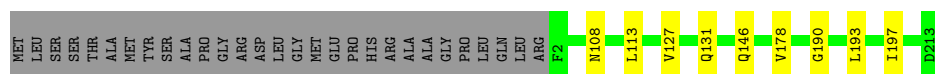
- Molecule 13: Proteasome subunit beta type-1

Chain M:  84% . 12%



- Molecule 13: Proteasome subunit beta type-1

Chain a:  84% . 12%

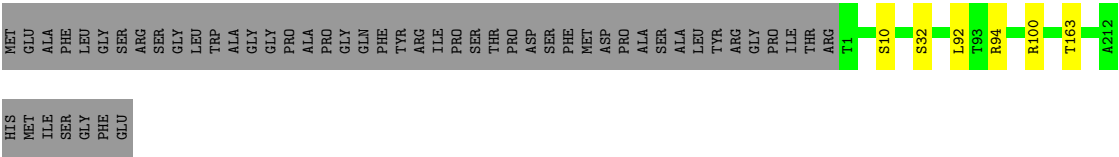


- Molecule 14: Proteasome subunit beta type-4

Chain N:

78%

20%

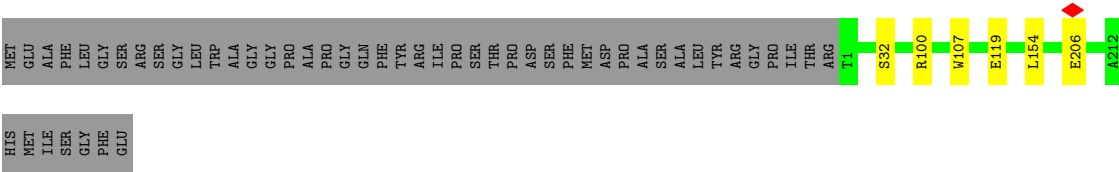


• Molecule 14: Proteasome subunit beta type-4

Chain b:

78%

20%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	214790	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 ($e^-/\text{\AA}^2$)	30	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	0.788	Depositor
Minimum map value	-0.318	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.035	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	339.19998, 339.19998, 339.19998	wwPDB
Map dimensions	320, 320, 320	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: LDZ

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	0.60	0/1767	0.65	0/2398
1	O	0.60	0/1763	0.65	0/2393
2	B	0.60	0/1701	0.63	0/2318
2	P	0.59	0/1701	0.63	0/2318
3	C	0.60	0/1815	0.63	0/2466
3	Q	0.60	0/1815	0.62	0/2466
4	D	0.61	0/1657	0.63	0/2261
4	R	0.62	0/1657	0.63	0/2261
5	E	0.61	0/1686	0.62	0/2290
5	S	0.61	0/1686	0.62	0/2290
6	F	0.60	0/1738	0.63	0/2364
6	T	0.60	0/1741	0.64	0/2367
7	G	0.60	0/1795	0.63	0/2434
7	U	0.60	0/1795	0.62	0/2434
8	H	0.58	0/1495	0.65	0/2026
8	V	0.58	0/1491	0.67	0/2021
9	I	0.58	0/1607	0.68	0/2185
9	W	0.58	0/1603	0.67	0/2180
10	J	0.57	0/1575	0.67	0/2128
10	X	0.57	0/1563	0.68	0/2113
11	K	0.56	0/1541	0.63	0/2092
11	Y	0.56	0/1538	0.64	0/2088
12	L	0.57	0/1535	0.64	0/2080
12	Z	0.58	0/1531	0.64	0/2076
13	M	0.58	0/1614	0.67	0/2178
13	a	0.58	0/1614	0.67	1/2178 (0.0%)
14	N	0.58	0/1598	0.66	0/2170
14	b	0.58	0/1602	0.66	0/2175
All	All	0.59	0/46224	0.64	1/62750 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	a	131	GLN	CB-CA-C	-5.33	99.73	110.40

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	238/246 (97%)	223 (94%)	12 (5%)	3 (1%)	10	26
1	O	238/246 (97%)	221 (93%)	13 (6%)	4 (2%)	7	20
2	B	227/234 (97%)	222 (98%)	5 (2%)	0	100	100
2	P	227/234 (97%)	224 (99%)	3 (1%)	0	100	100
3	C	245/261 (94%)	231 (94%)	9 (4%)	5 (2%)	6	16
3	Q	245/261 (94%)	240 (98%)	4 (2%)	1 (0%)	30	55
4	D	230/248 (93%)	219 (95%)	9 (4%)	2 (1%)	14	35
4	R	230/248 (93%)	220 (96%)	7 (3%)	3 (1%)	10	26
5	E	231/241 (96%)	219 (95%)	11 (5%)	1 (0%)	30	55
5	S	231/241 (96%)	221 (96%)	9 (4%)	1 (0%)	30	55
6	F	231/263 (88%)	217 (94%)	13 (6%)	1 (0%)	30	55
6	T	231/263 (88%)	220 (95%)	7 (3%)	4 (2%)	7	20
7	G	237/255 (93%)	228 (96%)	9 (4%)	0	100	100
7	U	237/255 (93%)	230 (97%)	5 (2%)	2 (1%)	16	38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	H	200/205 (98%)	195 (98%)	5 (2%)	0	100	100
8	V	200/205 (98%)	191 (96%)	8 (4%)	1 (0%)	25	49
9	I	218/234 (93%)	211 (97%)	5 (2%)	2 (1%)	14	35
9	W	218/234 (93%)	210 (96%)	7 (3%)	1 (0%)	25	49
10	J	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
10	X	202/205 (98%)	197 (98%)	5 (2%)	0	100	100
11	K	194/201 (96%)	187 (96%)	5 (3%)	2 (1%)	13	33
11	Y	194/201 (96%)	187 (96%)	6 (3%)	1 (0%)	25	49
12	L	198/204 (97%)	190 (96%)	8 (4%)	0	100	100
12	Z	198/204 (97%)	192 (97%)	6 (3%)	0	100	100
13	M	210/241 (87%)	200 (95%)	9 (4%)	1 (0%)	25	49
13	a	210/241 (87%)	202 (96%)	7 (3%)	1 (0%)	25	49
14	N	210/264 (80%)	194 (92%)	15 (7%)	1 (0%)	25	49
14	b	210/264 (80%)	197 (94%)	11 (5%)	2 (1%)	13	33
All	All	6142/6604 (93%)	5883 (96%)	220 (4%)	39 (1%)	24	45

5 of 39 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	203	VAL
11	K	25	ILE
1	O	191	PHE
4	R	48	LYS
4	R	181	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	164/210 (78%)	154 (94%)	10 (6%)	15	36
1	O	163/210 (78%)	148 (91%)	15 (9%)	7	18

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	150/191 (78%)	146 (97%)	4 (3%)	40	69
2	P	150/191 (78%)	146 (97%)	4 (3%)	40	69
3	C	160/221 (72%)	155 (97%)	5 (3%)	35	64
3	Q	160/221 (72%)	151 (94%)	9 (6%)	17	41
4	D	136/211 (64%)	132 (97%)	4 (3%)	37	67
4	R	136/211 (64%)	135 (99%)	1 (1%)	81	93
5	E	158/203 (78%)	148 (94%)	10 (6%)	15	35
5	S	158/203 (78%)	152 (96%)	6 (4%)	28	56
6	F	160/224 (71%)	151 (94%)	9 (6%)	17	41
6	T	161/224 (72%)	156 (97%)	5 (3%)	35	64
7	G	162/212 (76%)	156 (96%)	6 (4%)	29	58
7	U	162/212 (76%)	153 (94%)	9 (6%)	17	41
8	H	141/159 (89%)	136 (96%)	5 (4%)	31	60
8	V	140/159 (88%)	132 (94%)	8 (6%)	17	40
9	I	158/195 (81%)	147 (93%)	11 (7%)	12	31
9	W	157/195 (80%)	152 (97%)	5 (3%)	34	63
10	J	159/174 (91%)	151 (95%)	8 (5%)	20	46
10	X	155/174 (89%)	147 (95%)	8 (5%)	19	44
11	K	149/171 (87%)	143 (96%)	6 (4%)	27	55
11	Y	148/171 (86%)	144 (97%)	4 (3%)	40	69
12	L	139/159 (87%)	128 (92%)	11 (8%)	10	25
12	Z	138/159 (87%)	124 (90%)	14 (10%)	6	15
13	M	158/199 (79%)	149 (94%)	9 (6%)	17	40
13	a	158/199 (79%)	151 (96%)	7 (4%)	24	51
14	N	149/215 (69%)	144 (97%)	5 (3%)	32	61
14	b	150/215 (70%)	146 (97%)	4 (3%)	40	69
All	All	4279/5488 (78%)	4077 (95%)	202 (5%)	24	49

5 of 202 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	182	LYS
7	U	69	VAL

Continued on next page...

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Mol	Chain	Res	Type
14	b	107	TRP
2	P	91	LYS
3	Q	224	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 64 such sidechains are listed below:

Mol	Chain	Res	Type
11	Y	132	HIS
12	Z	163	GLN
11	K	189	HIS
11	K	132	HIS
12	Z	192	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	LDZ	I	301	-	33,34,34	1.81	7 (21%)	42,44,44	1.34	6 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	LDZ	L	301	-	33,34,34	1.85	7 (21%)	42,44,44	1.53	8 (19%)
15	LDZ	Z	301	-	33,34,34	1.73	7 (21%)	42,44,44	1.16	5 (11%)
15	LDZ	V	301	-	33,34,34	1.80	7 (21%)	42,44,44	1.39	4 (9%)
15	LDZ	H	301	-	33,34,34	1.76	7 (21%)	42,44,44	1.22	4 (9%)
15	LDZ	W	301	-	33,34,34	1.76	7 (21%)	42,44,44	1.17	2 (4%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	LDZ	I	301	-	-	9/38/39/39	0/1/1/1
15	LDZ	L	301	-	-	23/38/39/39	0/1/1/1
15	LDZ	Z	301	-	-	10/38/39/39	0/1/1/1
15	LDZ	V	301	-	-	13/38/39/39	0/1/1/1
15	LDZ	H	301	-	-	15/38/39/39	0/1/1/1
15	LDZ	W	301	-	-	17/38/39/39	0/1/1/1

The worst 5 of 42 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	V	301	LDZ	C15-N16	5.55	1.45	1.34
15	I	301	LDZ	C12-N13	5.52	1.45	1.34
15	L	301	LDZ	C12-N13	5.52	1.45	1.34
15	L	301	LDZ	C15-N16	5.45	1.45	1.34
15	W	301	LDZ	C15-N16	5.29	1.45	1.34

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	L	301	LDZ	O8-C9-N10	5.23	121.64	110.45
15	I	301	LDZ	O8-C9-N10	4.54	120.15	110.45
15	H	301	LDZ	O8-C9-N10	4.27	119.58	110.45
15	V	301	LDZ	O8-C9-N10	4.15	119.33	110.45
15	Z	301	LDZ	O8-C9-N10	4.03	119.07	110.45

There are no chirality outliers.

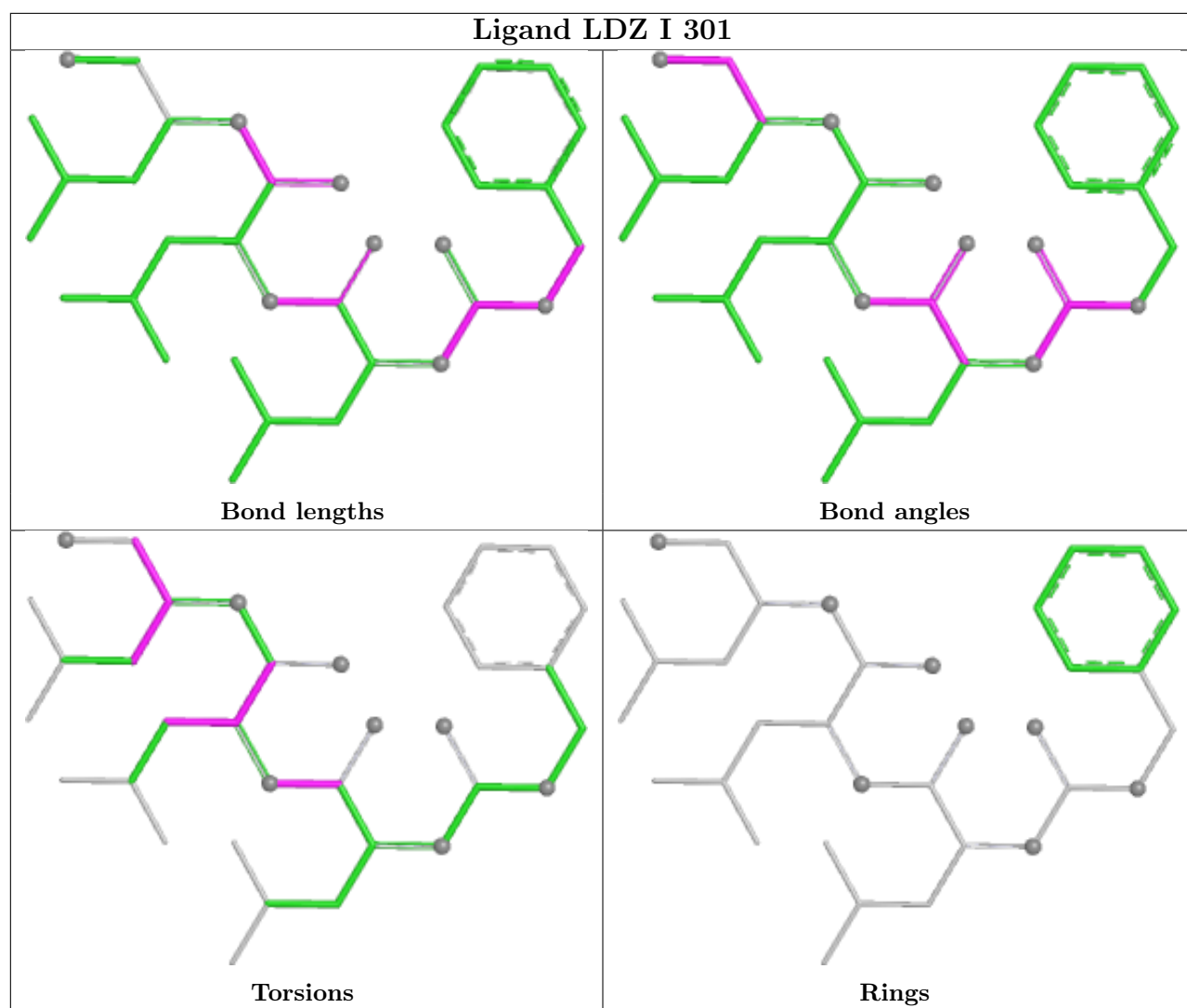
5 of 87 torsion outliers are listed below:

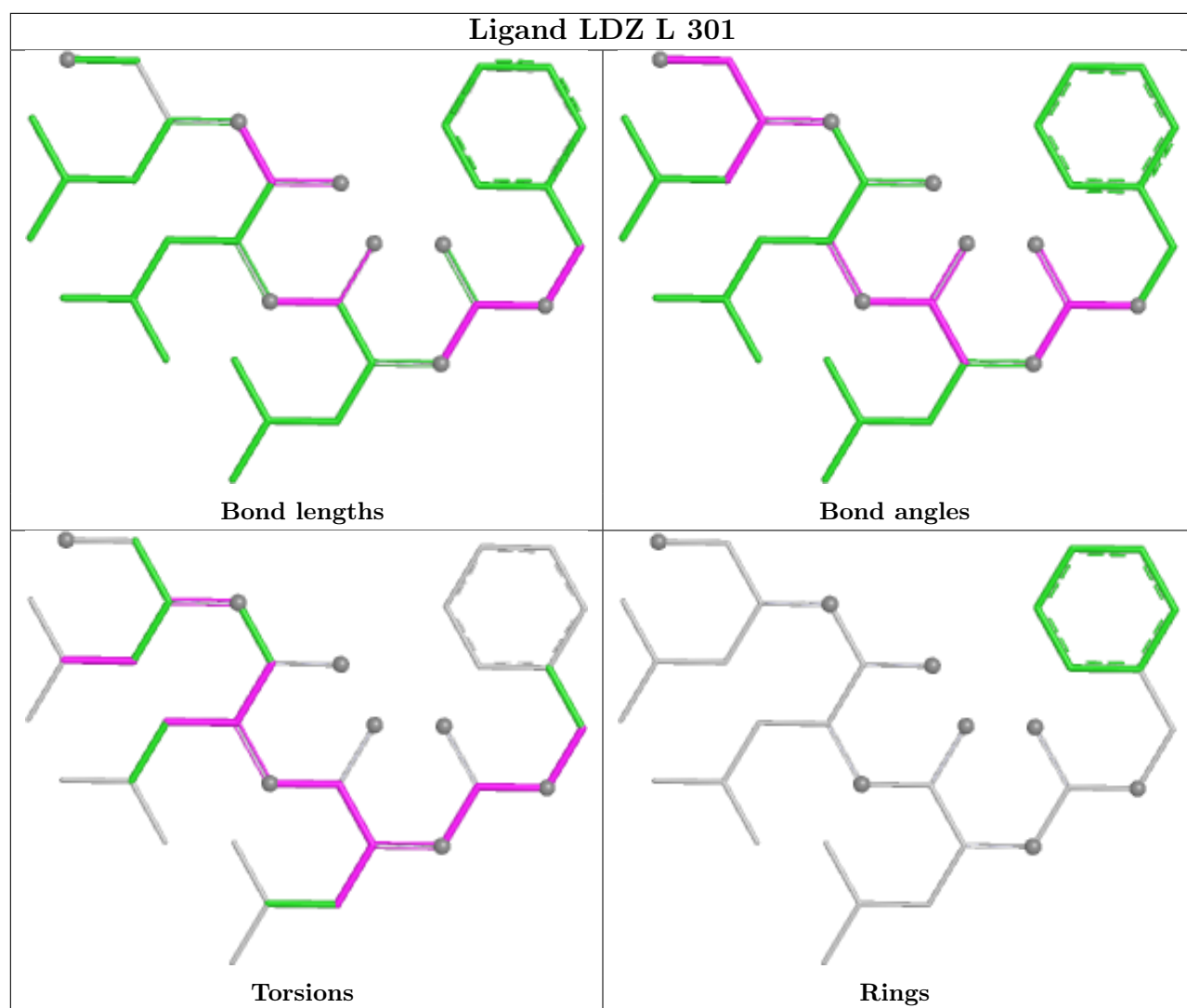
Mol	Chain	Res	Type	Atoms
15	H	301	LDZ	C22-C17-C18-C19
15	I	301	LDZ	C18-C17-C22-O33
15	I	301	LDZ	C22-C17-C18-C19
15	V	301	LDZ	O31-C9-O8-C7
15	V	301	LDZ	N10-C9-O8-C7

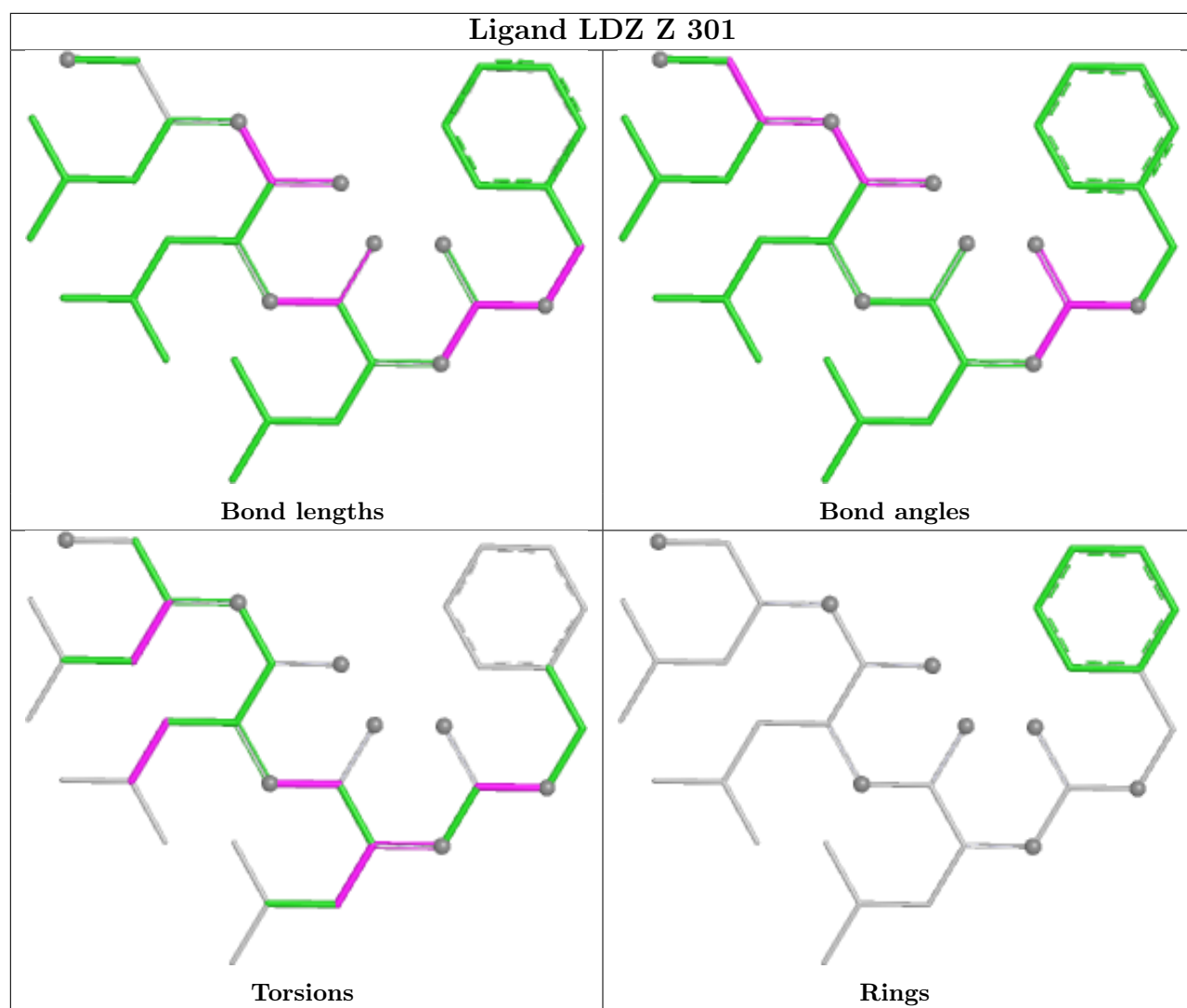
There are no ring outliers.

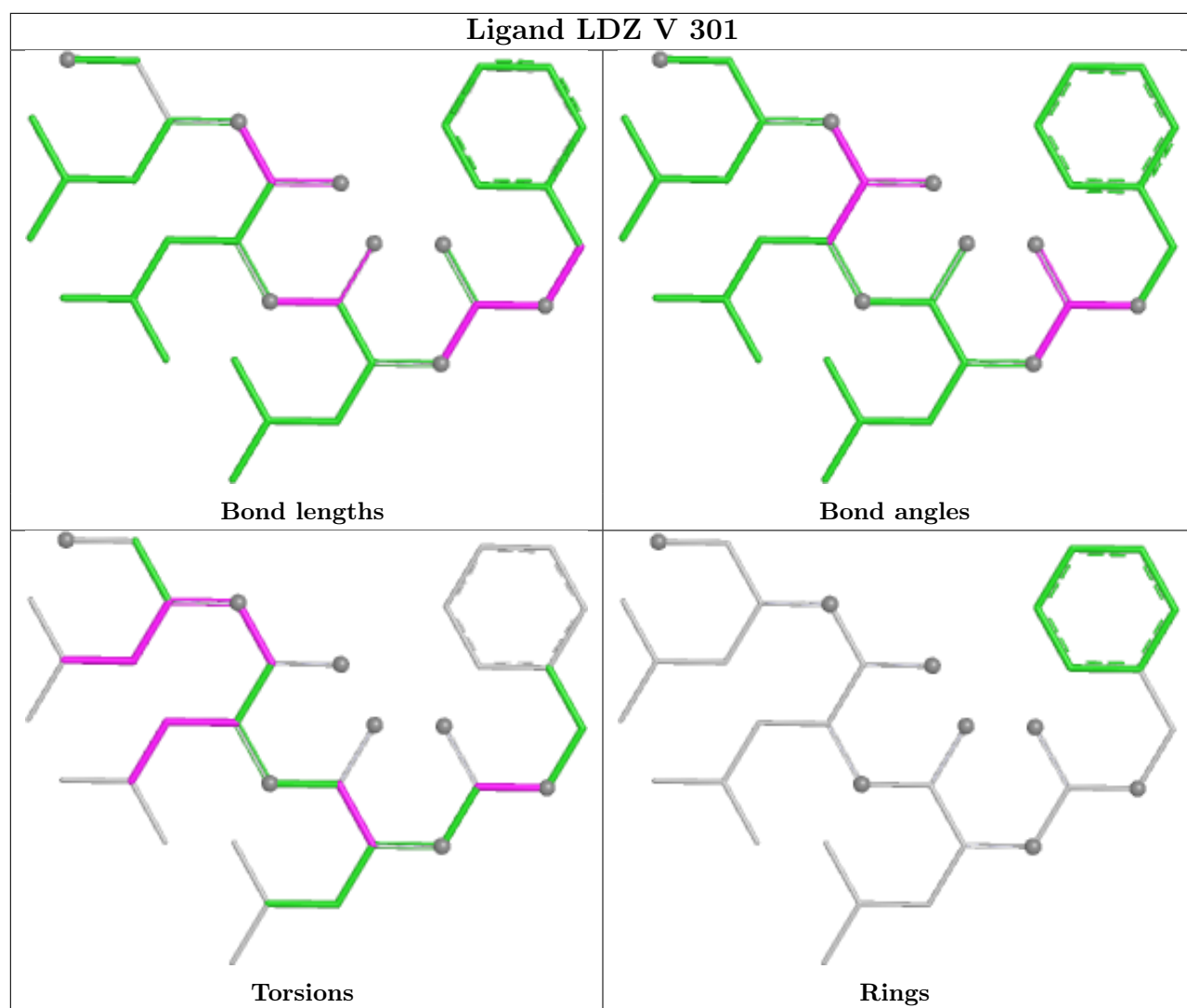
No monomer is involved in short contacts.

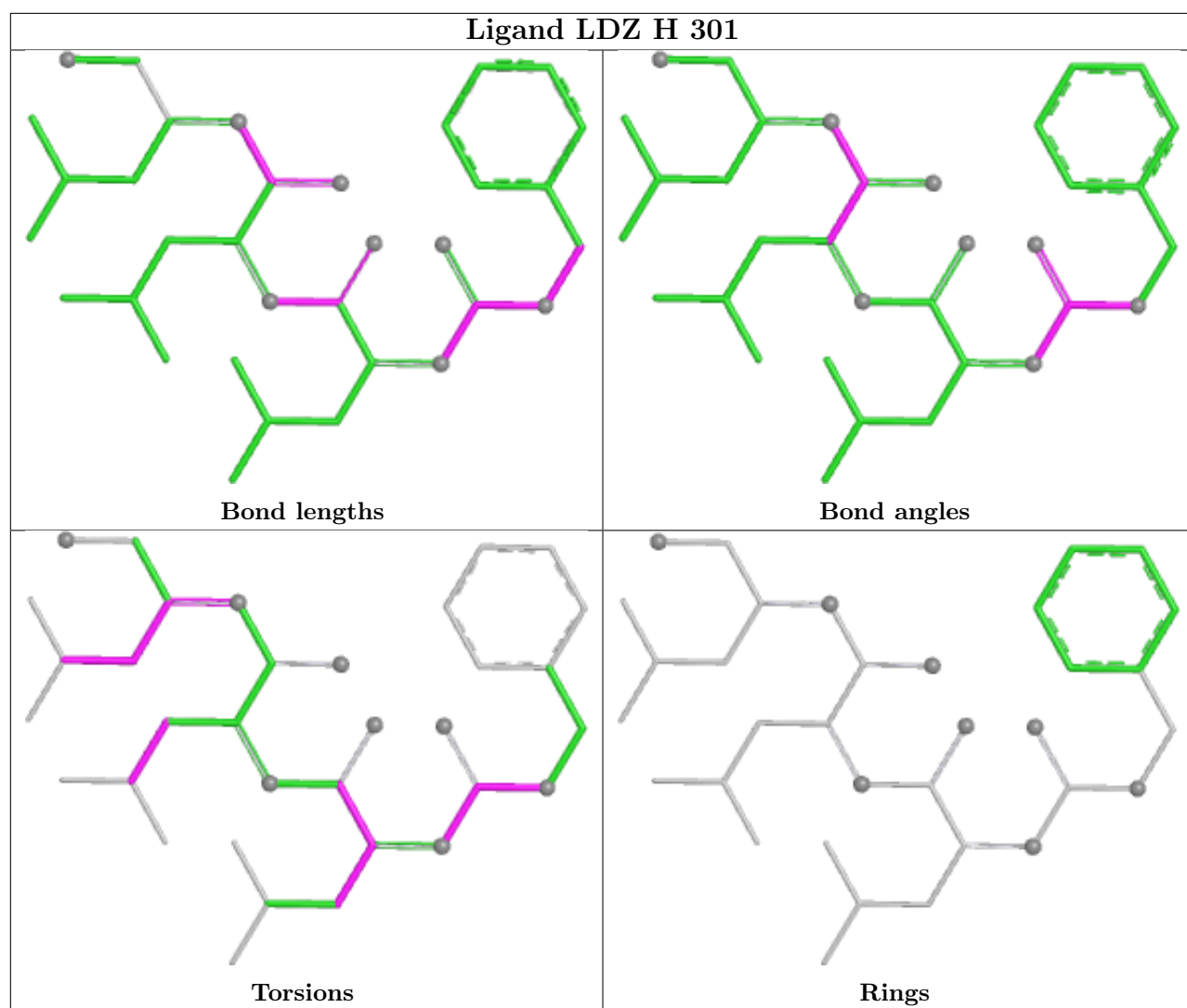
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

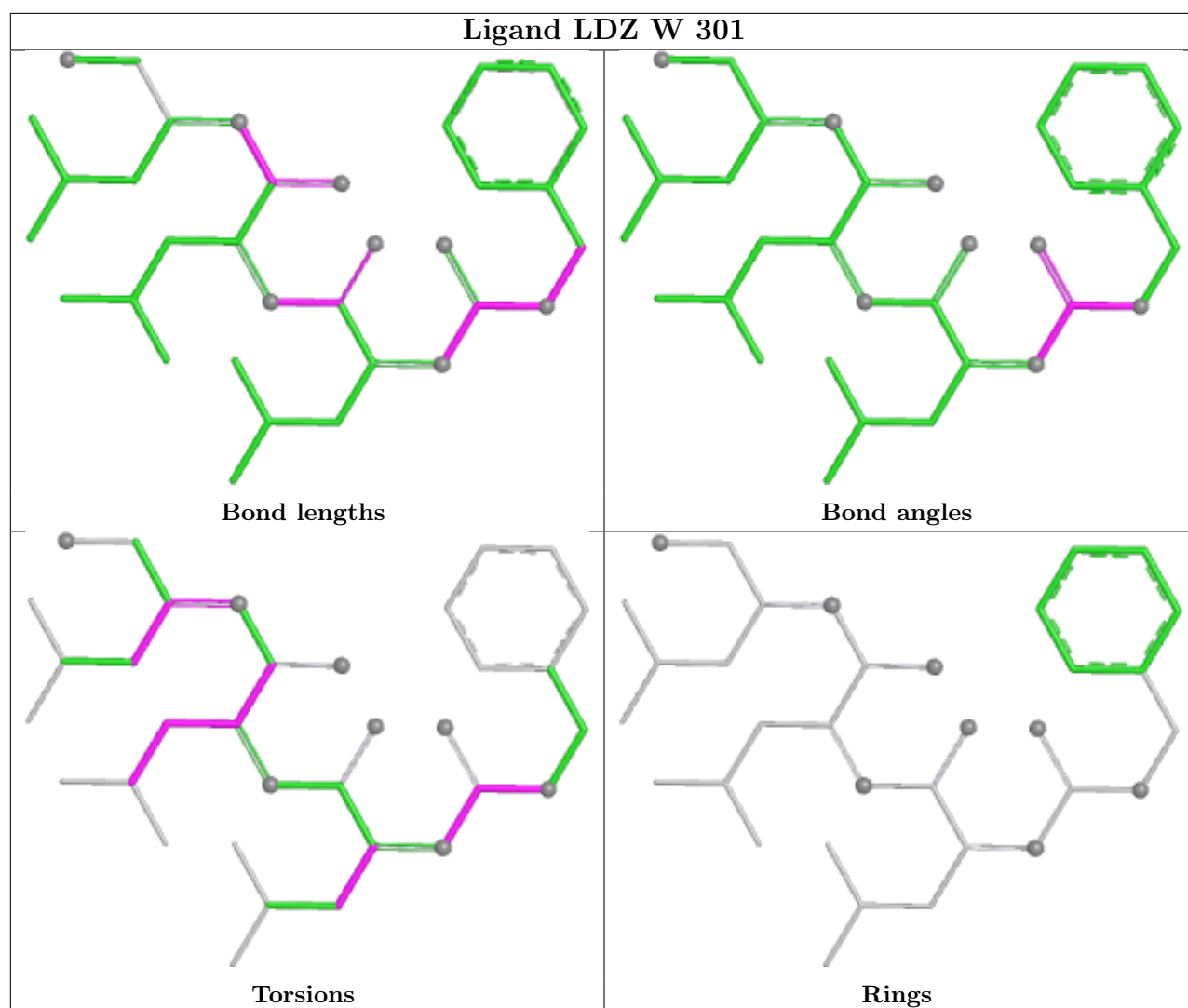












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

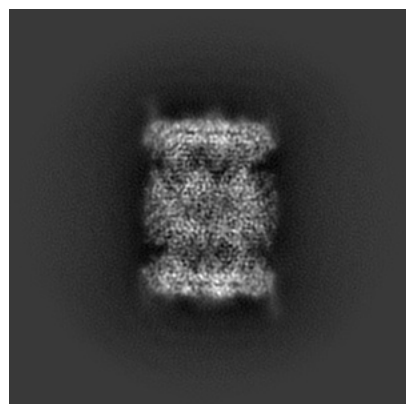
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27013. These allow visual inspection of the internal detail of the map and identification of artifacts.

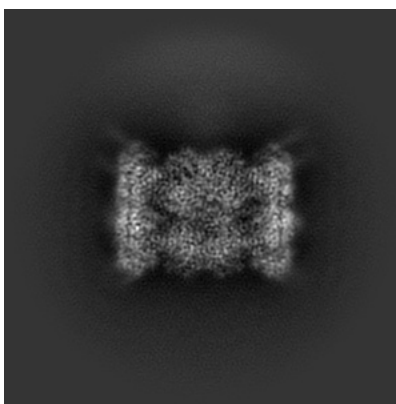
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

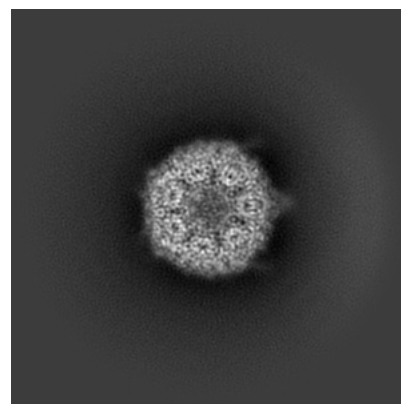
6.1.1 Primary map



X

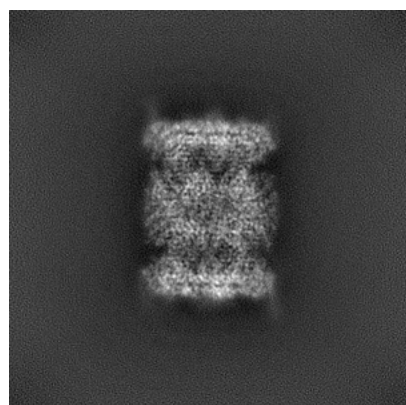


Y

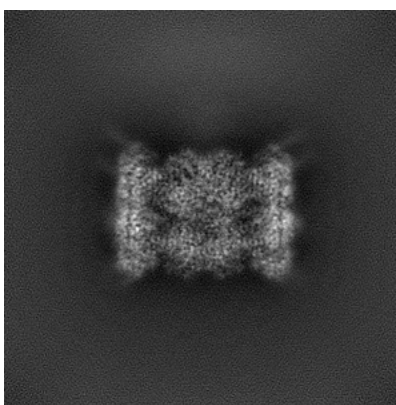


Z

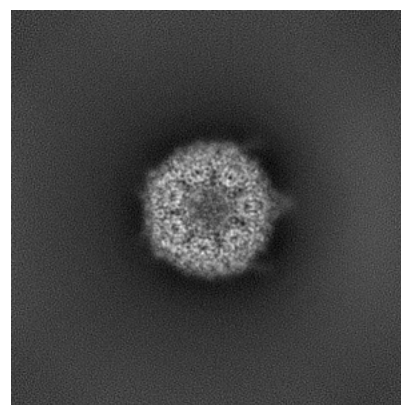
6.1.2 Raw map



X



Y

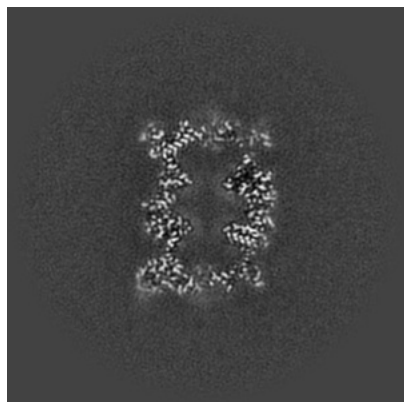


Z

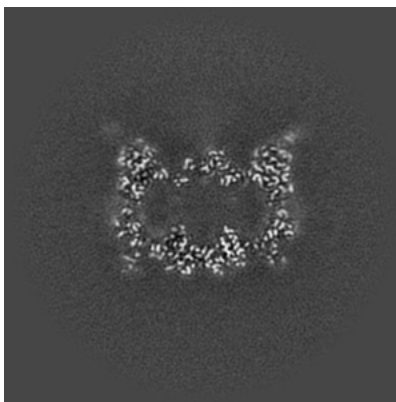
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

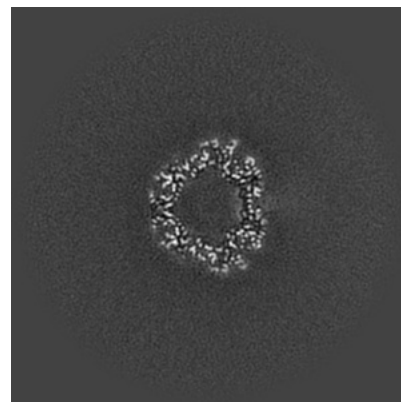
6.2.1 Primary map



X Index: 160

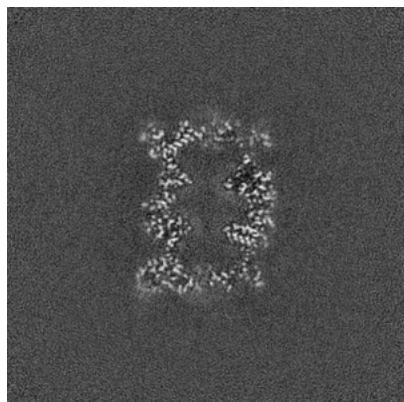


Y Index: 160

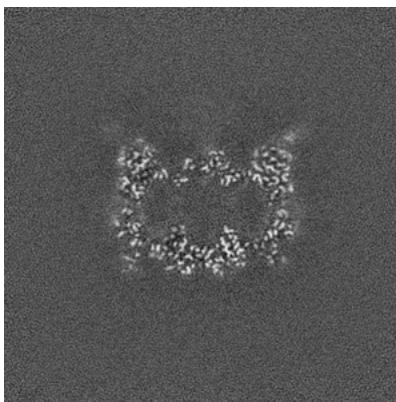


Z Index: 160

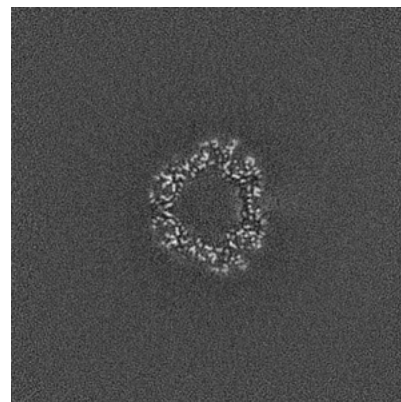
6.2.2 Raw map



X Index: 160



Y Index: 160

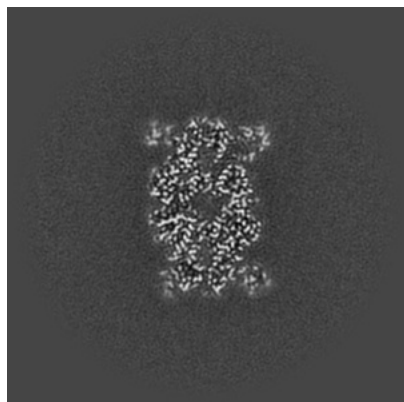


Z Index: 160

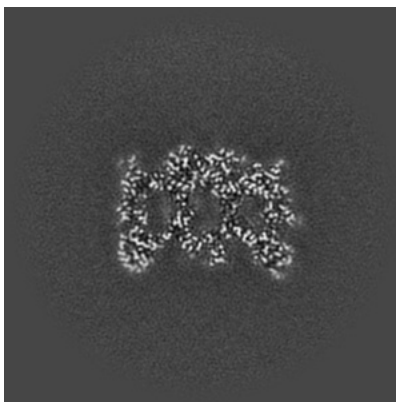
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

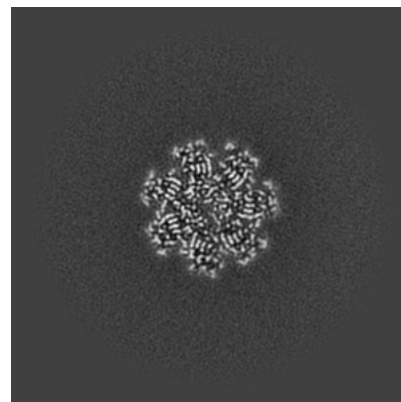
6.3.1 Primary map



X Index: 135

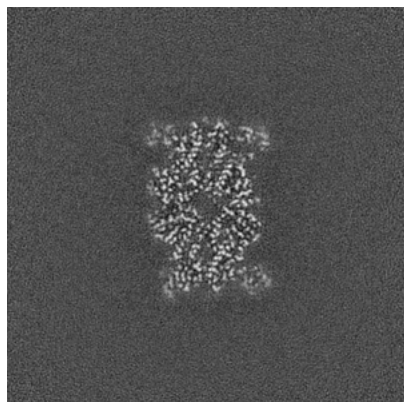


Y Index: 140

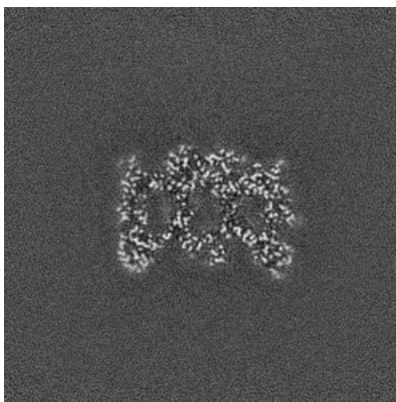


Z Index: 106

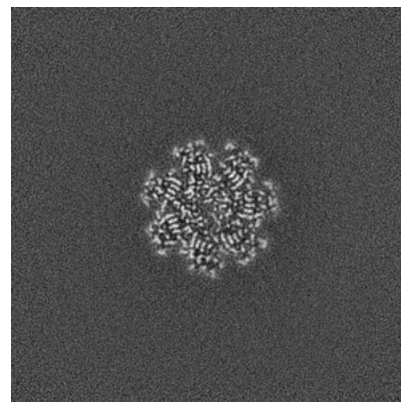
6.3.2 Raw map



X Index: 134



Y Index: 140

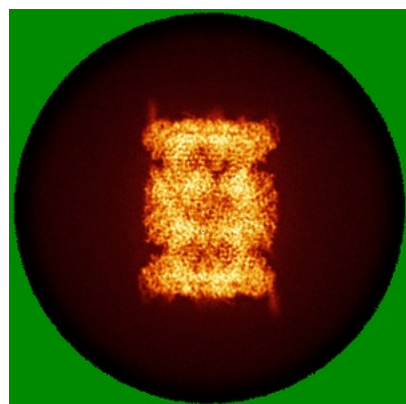


Z Index: 106

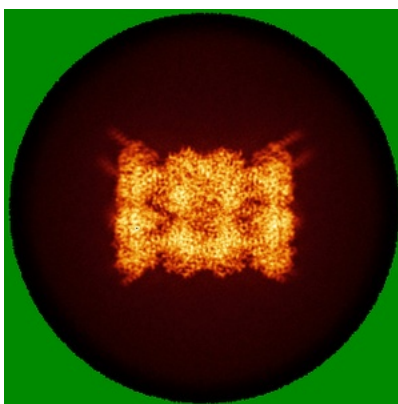
The images above show the largest variance slices of the map in three orthogonal directions.

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

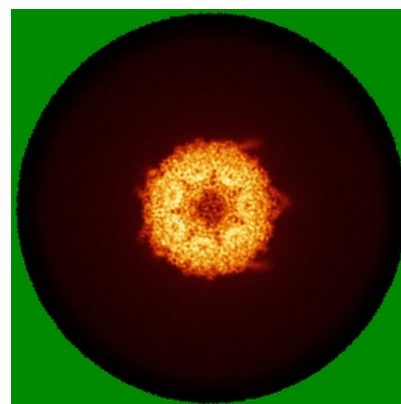
6.4.1 Primary map



X

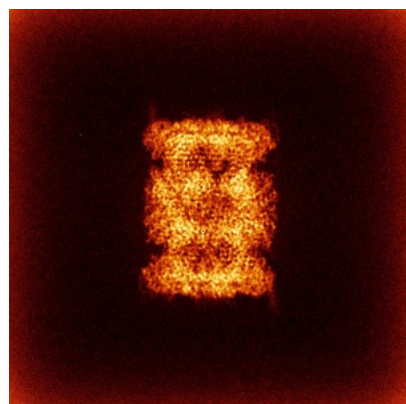


Y

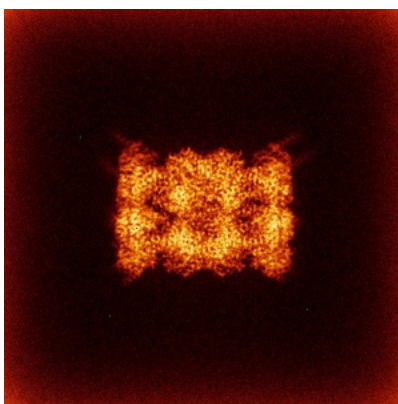


Z

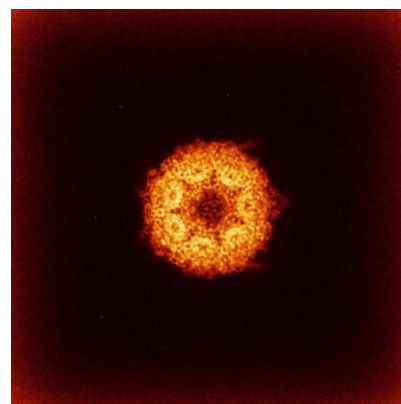
6.4.2 Raw map



X



Y

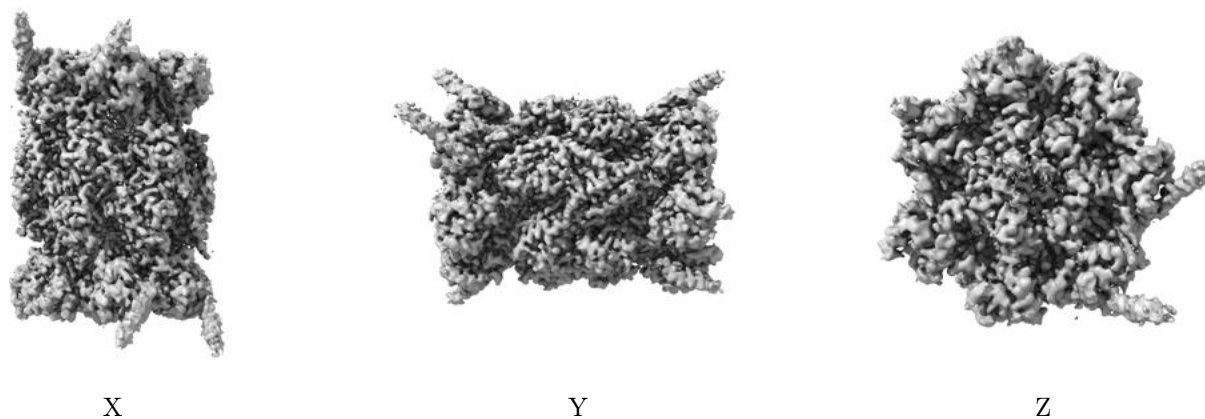


Z

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.

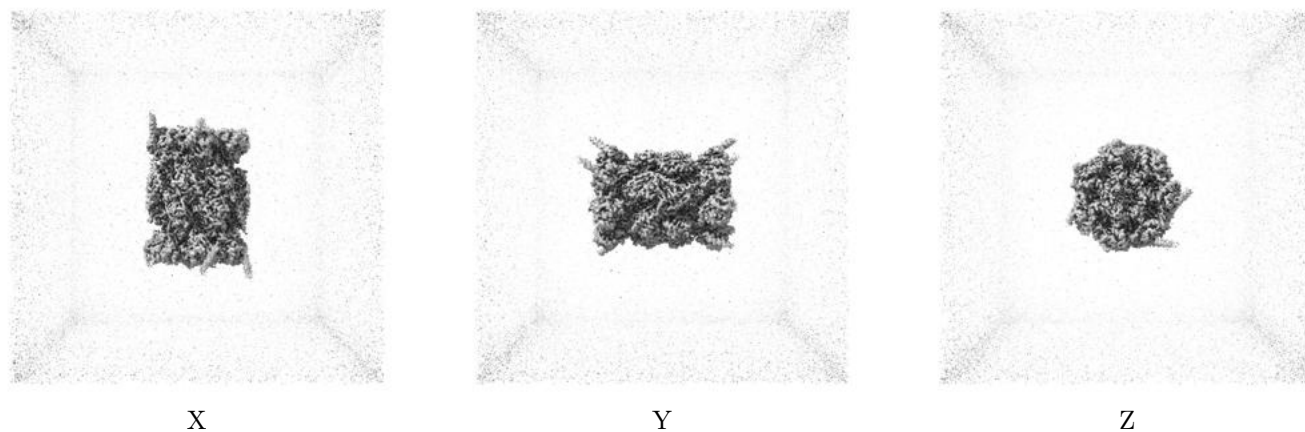
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. 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.

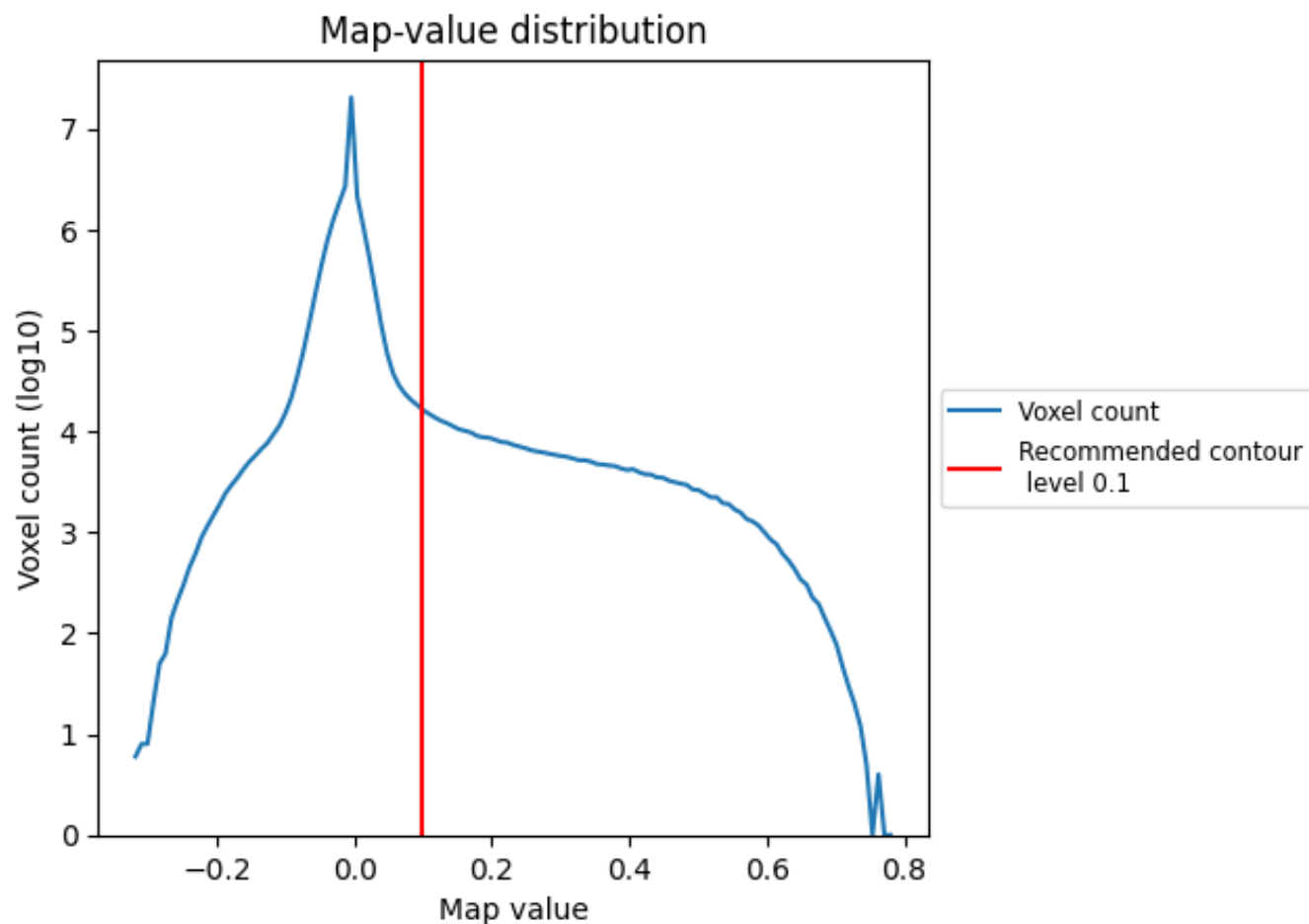
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

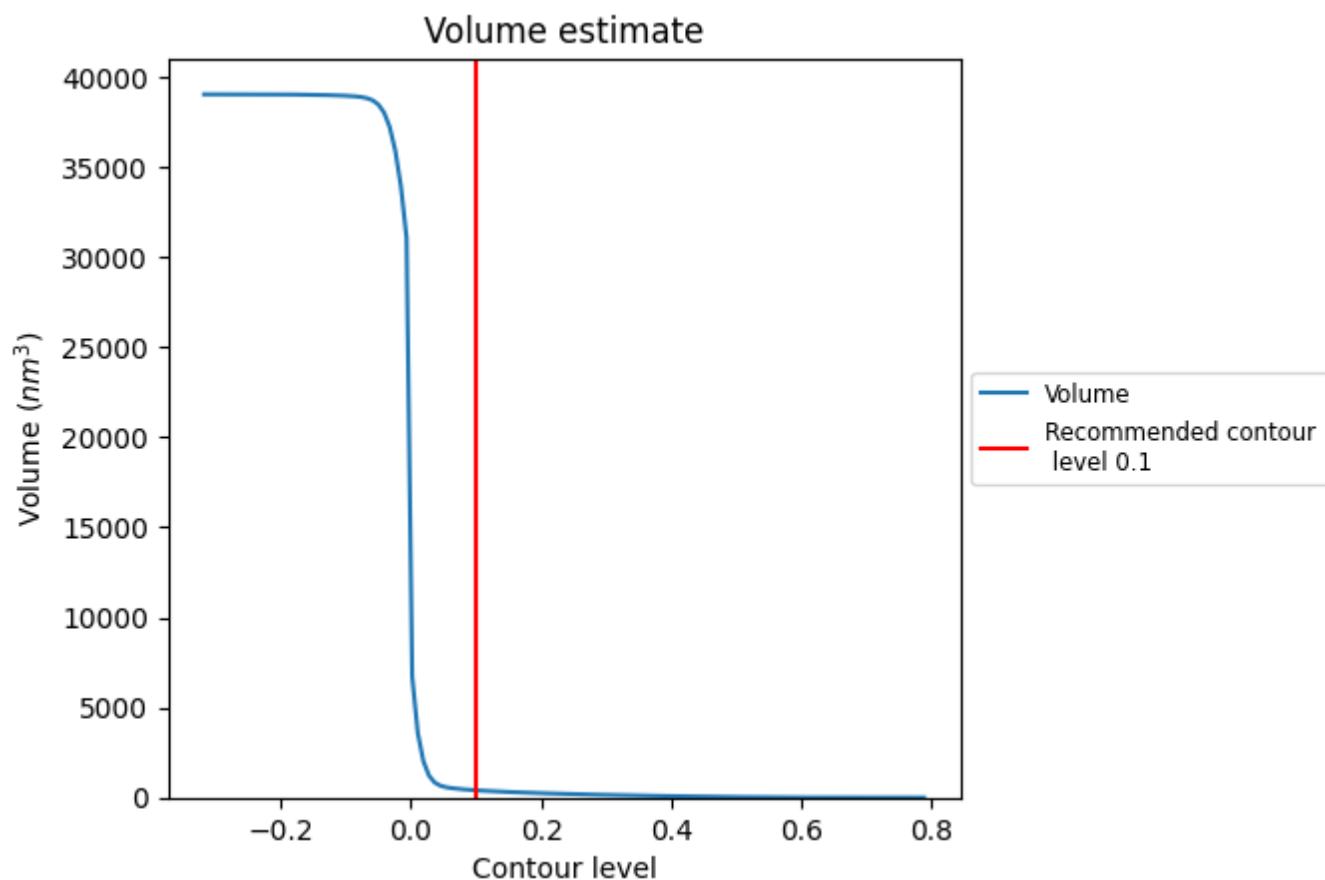
This section contains the results of statistical analysis of the map.

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.

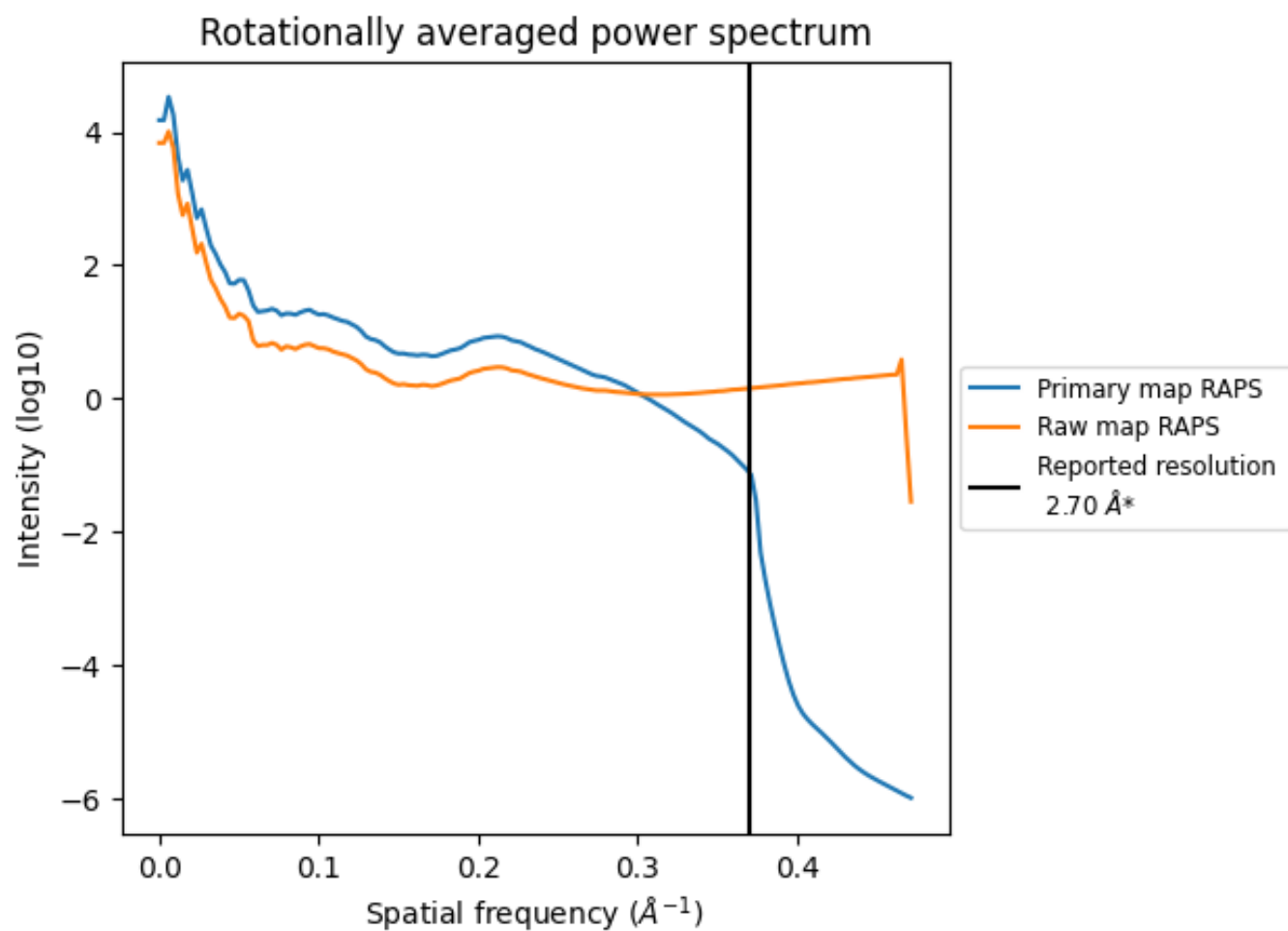
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 403 nm^3 ; this corresponds to an approximate mass of 364 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

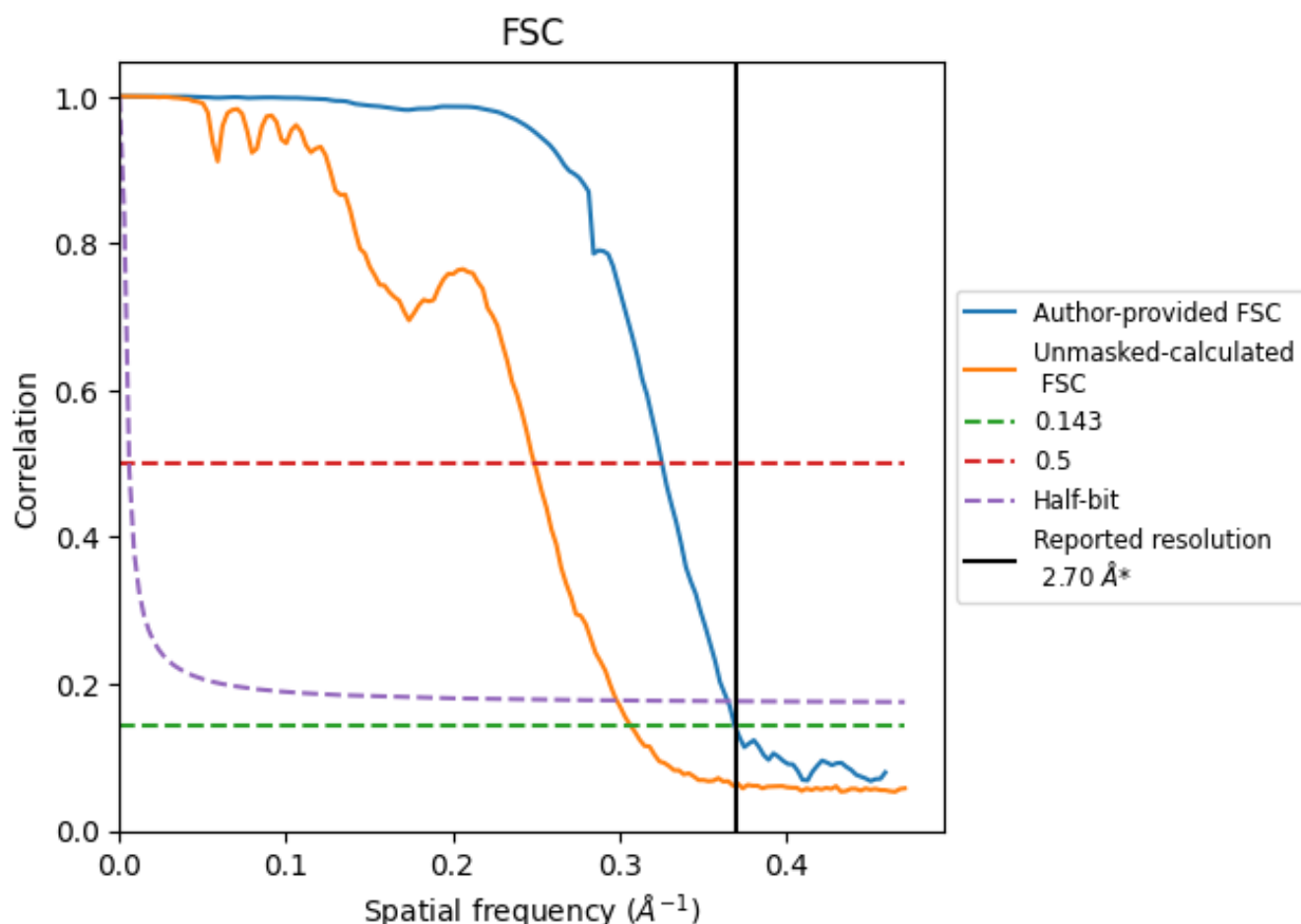


*Reported resolution corresponds to spatial frequency of 0.370 Å⁻¹

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 0.370 \AA^{-1}

8.2 Resolution estimates [i](#)

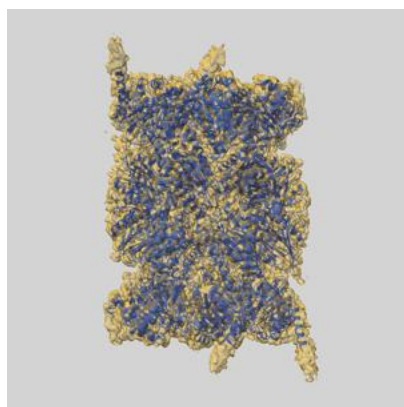
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.71	3.07	2.74
Unmasked-calculated*	3.26	4.01	3.35

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.26 differs from the reported value 2.7 by more than 10 %

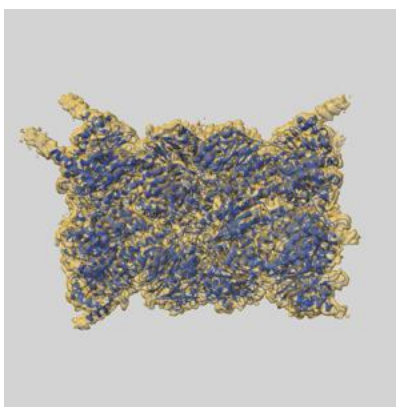
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-27013 and PDB model 8CVR. Per-residue inclusion information can be found in section [3](#) on page [8](#).

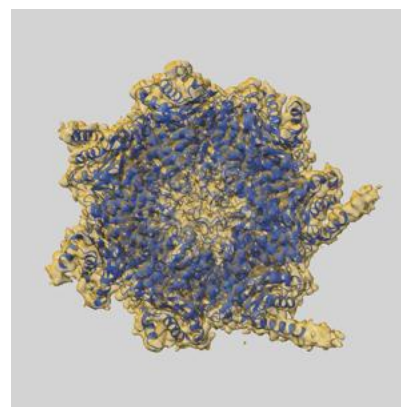
9.1 Map-model overlay [i](#)



X



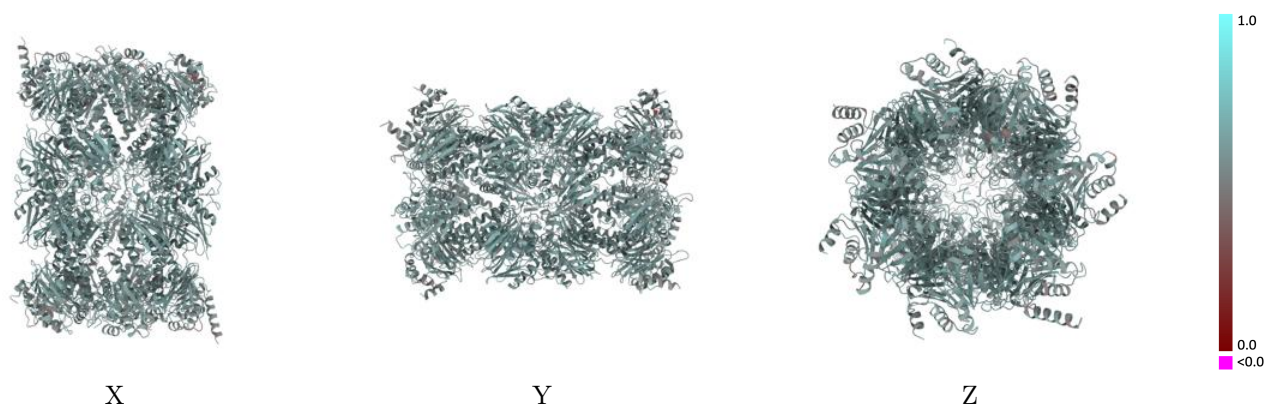
Y



Z

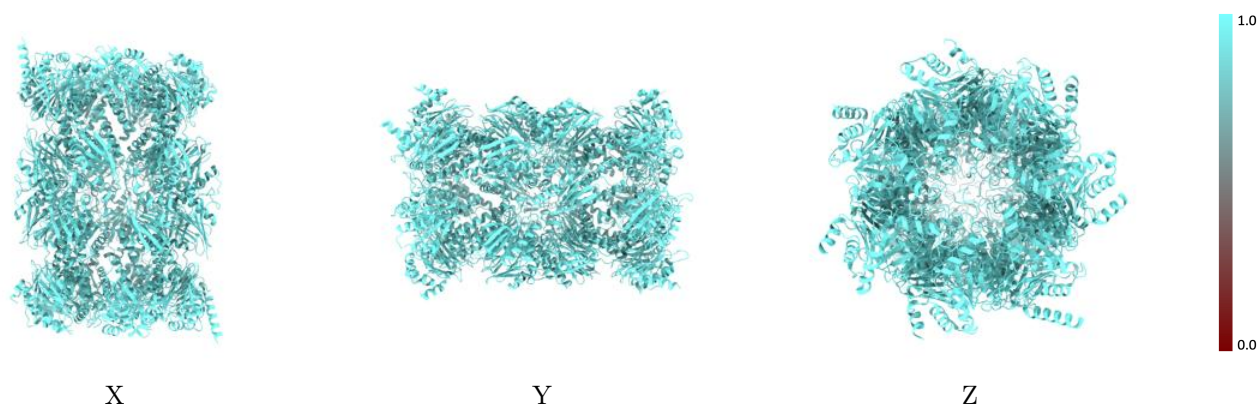
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



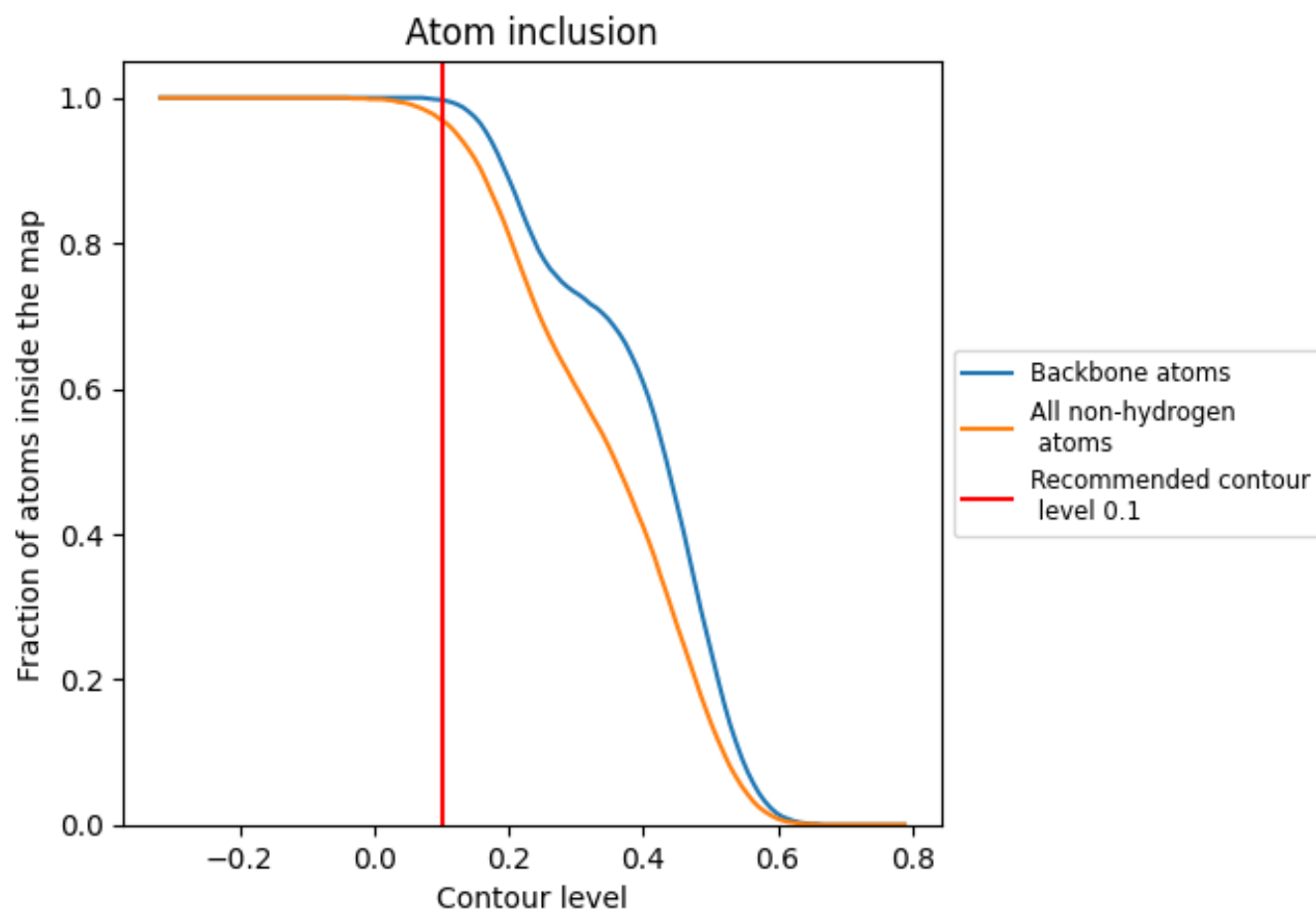
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).



























































9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 97% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9690	 0.5820
A	 0.9760	 0.5720
B	 0.9800	 0.5820
C	 0.9710	 0.5700
D	 0.9720	 0.5680
E	 0.9540	 0.5720
F	 0.9690	 0.5710
G	 0.9760	 0.5750
H	 0.9570	 0.5940
I	 0.9680	 0.5880
J	 0.9700	 0.5930
K	 0.9660	 0.5950
L	 0.9600	 0.5880
M	 0.9740	 0.5970
N	 0.9800	 0.5950
O	 0.9770	 0.5760
P	 0.9810	 0.5810
Q	 0.9650	 0.5710
R	 0.9680	 0.5670
S	 0.9600	 0.5660
T	 0.9720	 0.5720
U	 0.9710	 0.5720
V	 0.9590	 0.5900
W	 0.9700	 0.5920
X	 0.9730	 0.5970
Y	 0.9650	 0.5930
Z	 0.9630	 0.5880
a	 0.9730	 0.5910
b	 0.9720	 0.5950

