



wwPDB EM Validation Summary Report

Oct 24, 2022 – 06:52 PM EDT


PDB ID : 8CVS
EMDB ID : EMD-27015
Title : Human PA200-20S proteasome with MG-132
Authors : Zhao, J.
Deposited on : 2022-05-18
Resolution : 3.10 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:

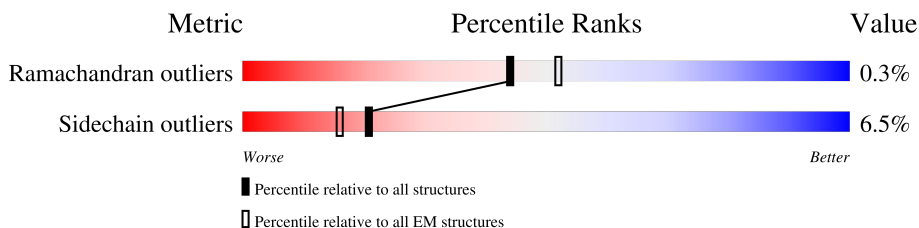
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

1 Overall quality at a glance

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

The reported resolution of this entry is 3.10 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 ≥ 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	234	87% 6% 7%
1	O	234	93% 5% .
2	B	261	82% 6% 12%
2	P	261	91% 5% 5%
3	C	248	82% 9% 9%
3	Q	248	94% . .
4	D	241	90% 5% 5%
4	R	241	94% . .
5	E	263	87% 5% 9%

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Mol	Chain	Length	Quality of chain
5	S	263	87% 10%
6	F	255	90% 5%
6	T	255	91% 6%
7	G	246	91% 5%
7	U	246	94% 5%
8	H	234	89% 5% 6%
8	V	234	87% 7% 6%
9	I	205	96%
9	W	205	94% 6%
10	J	201	91% 7%
10	X	201	92% 6%
11	K	204	93% 5%
11	Y	204	94%
12	L	241	85% 12%
12	Z	241	85% 12%
13	M	264	79% 18%
13	a	264	77% 5% 18%
14	N	205	96%
14	b	205	98%
15	c	1843	92% 6%

2 Entry composition [i](#)

There are 17 unique types of molecules in this entry. The entry contains 61346 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-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	217	Total	C	N	O	S	0	0
			1665	1070	289	300	6		
1	O	230	Total	C	N	O	S	0	0
			1724	1117	296	306	5		

- Molecule 2 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	230	Total	C	N	O	S	0	0
			1721	1089	295	328	9		
2	P	249	Total	C	N	O	S	0	0
			1874	1192	328	344	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	225	Total	C	N	O	S	0	0
			1666	1049	301	311	5		
3	Q	239	Total	C	N	O	S	0	0
			1781	1130	324	322	5		

- Molecule 4 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	229	Total	C	N	O	S	0	0
			1711	1088	285	327	11		
4	R	235	Total	C	N	O	S	0	0
			1711	1089	294	318	10		

- Molecule 5 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	240	1870	1178	340	340	12	0	0
5	S	237	1784	1131	331	312	10	0	0

- Molecule 6 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	244	1867	1189	321	348	9	0	0
6	T	240	1823	1162	317	333	11	0	0

- Molecule 7 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	238	1789	1145	304	327	13	0	0
7	U	243	1840	1172	312	344	12	0	0

- Molecule 8 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	220	1617	1025	275	306	11	0	0
8	V	221	1641	1038	278	314	11	0	0

- Molecule 9 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	204	1562	1000	263	280	19	0	0
9	W	204	1576	1008	264	285	19	0	0

- Molecule 10 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	196	1526	988	261	268	9	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	X	197	Total	C	N	O	S	0	0
			1543	998	265	271	9		

- Molecule 11 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	201	Total	C	N	O	S	0	0
			1545	980	274	282	9		
11	Y	200	Total	C	N	O	S	0	0
			1539	976	272	282	9		

- Molecule 12 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	213	Total	C	N	O	S	0	0
			1623	1032	280	301	10		
12	Z	213	Total	C	N	O	S	0	0
			1617	1032	281	294	10		

- Molecule 13 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	216	Total	C	N	O	S	0	0
			1671	1060	291	308	12		
13	a	216	Total	C	N	O	S	0	0
			1658	1053	290	303	12		

- Molecule 14 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	202	Total	C	N	O	S	0	0
			1481	936	258	275	12		
14	b	203	Total	C	N	O	S	0	0
			1486	939	259	277	11		

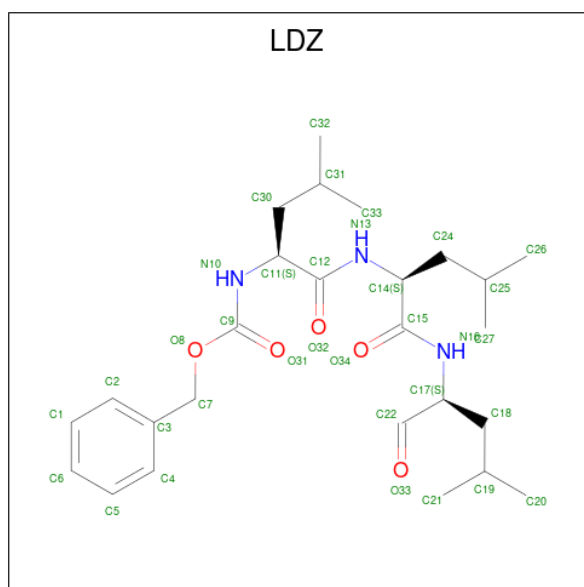
- Molecule 15 is a protein called Proteasome activator complex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	c	1802	Total	C	N	O	S	0	0
			14159	9175	2444	2466	74		

There are 3 discrepancies between the modelled and reference sequences:

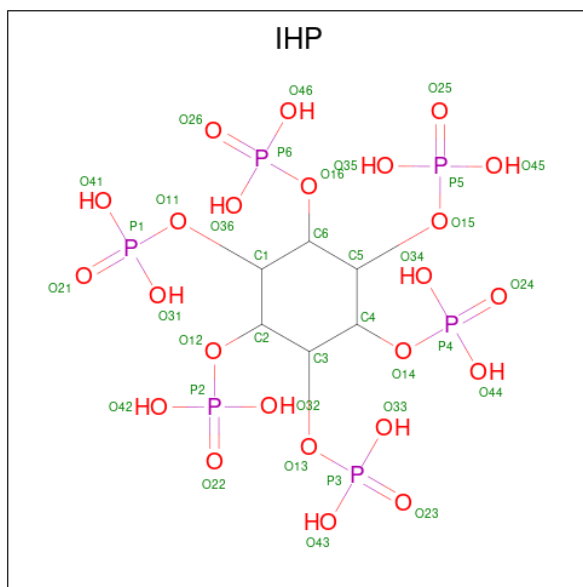
Chain	Residue	Modelled	Actual	Comment	Reference
c	821	ILE	LEU	conflict	UNP Q14997
c	822	LEU	ILE	conflict	UNP Q14997
c	1238	LEU	ILE	conflict	UNP Q14997

- Molecule 16 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
			Total	C	N	O	
16	H	1	Total	C	N	O	0
			34	26	3	5	
16	K	1	Total	C	N	O	0
			34	26	3	5	
16	N	1	Total	C	N	O	0
			34	26	3	5	
16	V	1	Total	C	N	O	0
			34	26	3	5	
16	Y	1	Total	C	N	O	0
			34	26	3	5	
16	b	1	Total	C	N	O	0
			34	26	3	5	

- Molecule 17 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: C₆H₁₈O₂₄P₆).




Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
17	c	1	72	12	48	12	0
17	c	1	72	12	48	12	0

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.

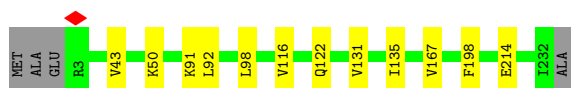
- Molecule 1: Proteasome subunit alpha type-2

Chain A: 




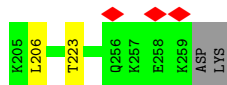
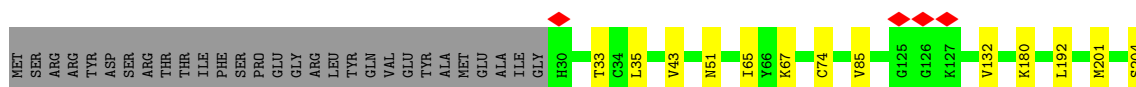
- Molecule 1: Proteasome subunit alpha type-2

Chain O: 



- Molecule 2: Proteasome subunit alpha type-4

Chain B: 




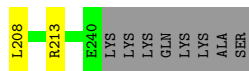
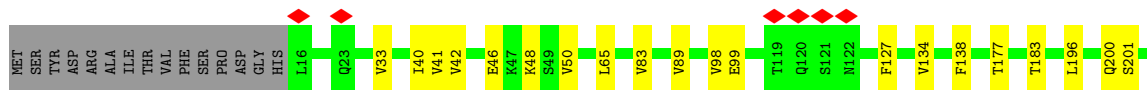
- Molecule 2: Proteasome subunit alpha type-4

Chain P: 



- Molecule 3: Proteasome subunit alpha type-7

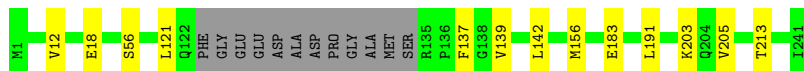
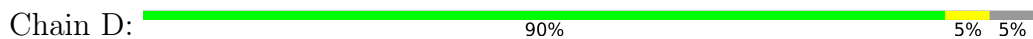
Chain C: 



• Molecule 3: Proteasome subunit alpha type-7



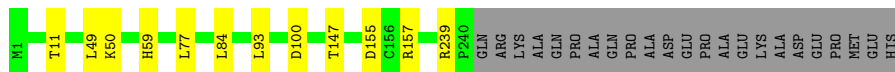
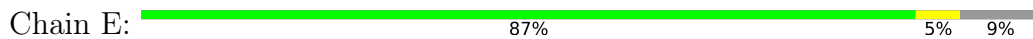
• Molecule 4: Proteasome subunit alpha type-5



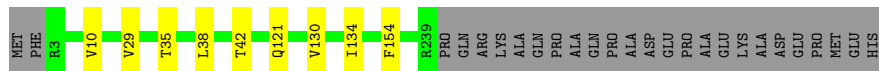
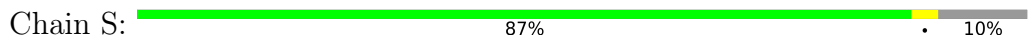
• Molecule 4: Proteasome subunit alpha type-5



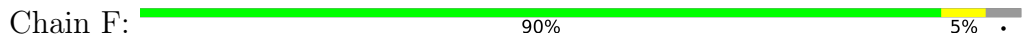
• Molecule 5: Proteasome subunit alpha type-1




• Molecule 5: Proteasome subunit alpha type-1



• Molecule 6: Proteasome subunit alpha type-3



- Molecule 6: Proteasome subunit alpha type-3

Chain T:  91% 6%



- Molecule 7: Proteasome subunit alpha type-6

Chain G:  91% 5%




- Molecule 7: Proteasome subunit alpha type-6

Chain U:  94% 5%




- Molecule 8: Proteasome subunit beta type-7

Chain H:  89% 5% 6%



- Molecule 8: Proteasome subunit beta type-7

Chain V:  87% 7% 6%



- Molecule 9: Proteasome subunit beta type-3

Chain I:  96%



- Molecule 9: Proteasome subunit beta type-3

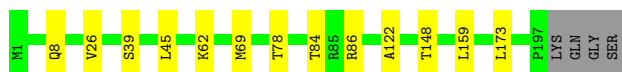
Chain W:  94% 6%



• Molecule 10: Proteasome subunit beta type-2



• Molecule 10: Proteasome subunit beta type-2



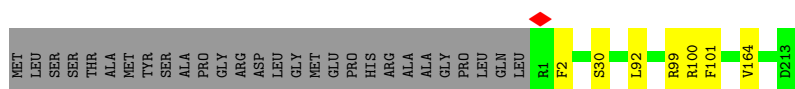
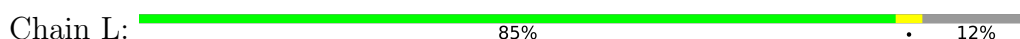
• Molecule 11: Proteasome subunit beta type-5



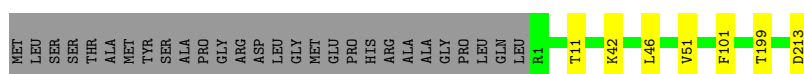
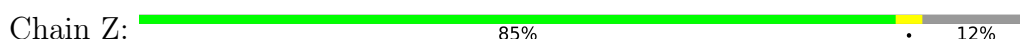
• Molecule 11: Proteasome subunit beta type-5



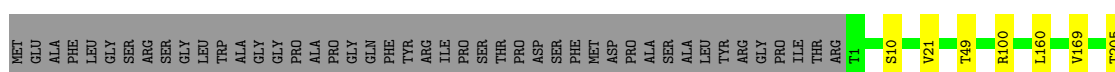
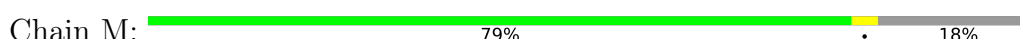
• Molecule 12: Proteasome subunit beta type-1

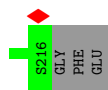


• Molecule 12: Proteasome subunit beta type-1

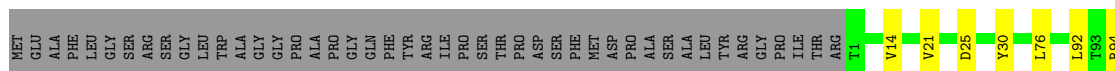
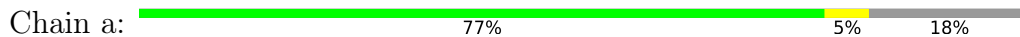


• Molecule 13: Proteasome subunit beta type-4

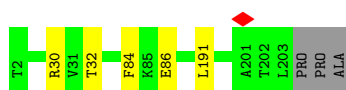




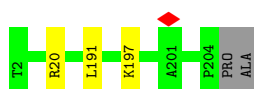
• Molecule 13: Proteasome subunit beta type-4



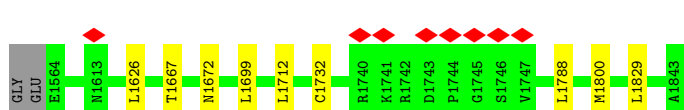
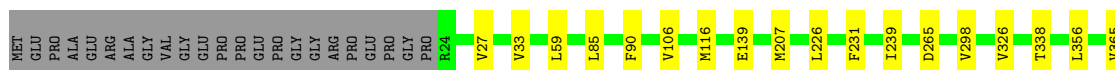
• Molecule 14: Proteasome subunit beta type-6



• Molecule 14: Proteasome subunit beta type-6



• Molecule 15: Proteasome activator complex subunit 4



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	70412	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	1.484	Depositor
Minimum map value	-0.690	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.055	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	317.99997, 317.99997, 317.99997	wwPDB
Map dimensions	300, 300, 300	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, IHP

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	0.57	0/1700	0.68	0/2306
1	O	0.59	0/1763	0.68	0/2400
2	B	0.59	0/1744	0.69	0/2359
2	P	0.59	0/1904	0.66	0/2579
3	C	0.60	0/1686	0.70	0/2287
3	Q	0.60	0/1807	0.68	0/2453
4	D	0.61	0/1737	0.69	0/2352
4	R	0.61	0/1738	0.66	0/2358
5	E	0.58	0/1906	0.70	0/2579
5	S	0.60	0/1818	0.69	0/2467
6	F	0.59	0/1902	0.70	1/2569 (0.0%)
6	T	0.60	0/1858	0.67	0/2512
7	G	0.58	0/1822	0.69	0/2476
7	U	0.59	0/1873	0.67	0/2542
8	H	0.58	0/1644	0.74	0/2234
8	V	0.58	0/1668	0.72	0/2263
9	I	0.56	0/1591	0.72	1/2148 (0.0%)
9	W	0.56	0/1605	0.73	0/2167
10	J	0.56	0/1558	0.68	0/2114
10	X	0.56	0/1576	0.69	0/2137
11	K	0.58	0/1576	0.69	0/2131
11	Y	0.57	0/1570	0.70	0/2125
12	L	0.58	0/1653	0.72	1/2230 (0.0%)
12	Z	0.59	0/1647	0.71	1/2223 (0.0%)
13	M	0.58	0/1704	0.70	0/2309
13	a	0.57	0/1691	0.69	0/2294
14	N	0.58	0/1507	0.68	0/2044
14	b	0.59	0/1513	0.70	0/2054
15	c	0.59	0/14498	0.68	2/19731 (0.0%)
All	All	0.59	0/62259	0.69	6/84443 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
8	V	0	1

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	c	1113	PRO	N-CA-CB	-6.77	95.15	102.60
15	c	1113	PRO	CA-N-CD	-5.80	103.38	111.50
9	I	99	PHE	CB-CA-C	5.57	121.55	110.40
12	Z	101	PHE	CB-CA-C	5.44	121.27	110.40
12	L	101	PHE	CB-CA-C	5.41	121.21	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	V	188	ARG	Peptide

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	215/234 (92%)	214 (100%)	1 (0%)	0	100	100
1	O	228/234 (97%)	225 (99%)	3 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	228/261 (87%)	223 (98%)	4 (2%)	1 (0%)	34	69
2	P	247/261 (95%)	244 (99%)	2 (1%)	1 (0%)	34	69
3	C	223/248 (90%)	216 (97%)	6 (3%)	1 (0%)	34	69
3	Q	237/248 (96%)	237 (100%)	0	0	100	100
4	D	225/241 (93%)	221 (98%)	3 (1%)	1 (0%)	34	69
4	R	233/241 (97%)	232 (100%)	1 (0%)	0	100	100
5	E	238/263 (90%)	234 (98%)	3 (1%)	1 (0%)	34	69
5	S	235/263 (89%)	234 (100%)	1 (0%)	0	100	100
6	F	242/255 (95%)	240 (99%)	1 (0%)	1 (0%)	34	69
6	T	238/255 (93%)	238 (100%)	0	0	100	100
7	G	236/246 (96%)	234 (99%)	2 (1%)	0	100	100
7	U	241/246 (98%)	240 (100%)	1 (0%)	0	100	100
8	H	218/234 (93%)	213 (98%)	4 (2%)	1 (0%)	29	64
8	V	219/234 (94%)	215 (98%)	4 (2%)	0	100	100
9	I	202/205 (98%)	196 (97%)	5 (2%)	1 (0%)	29	64
9	W	202/205 (98%)	196 (97%)	5 (2%)	1 (0%)	29	64
10	J	194/201 (96%)	192 (99%)	1 (0%)	1 (0%)	29	64
10	X	195/201 (97%)	192 (98%)	2 (1%)	1 (0%)	29	64
11	K	199/204 (98%)	198 (100%)	1 (0%)	0	100	100
11	Y	198/204 (97%)	198 (100%)	0	0	100	100
12	L	211/241 (88%)	209 (99%)	2 (1%)	0	100	100
12	Z	211/241 (88%)	208 (99%)	3 (1%)	0	100	100
13	M	214/264 (81%)	210 (98%)	4 (2%)	0	100	100
13	a	214/264 (81%)	210 (98%)	4 (2%)	0	100	100
14	N	200/205 (98%)	197 (98%)	3 (2%)	0	100	100
14	b	201/205 (98%)	198 (98%)	3 (2%)	0	100	100
15	c	1798/1843 (98%)	1750 (97%)	39 (2%)	9 (0%)	29	64
All	All	7942/8447 (94%)	7814 (98%)	108 (1%)	20 (0%)	44	73

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	59	HIS

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Mol	Chain	Res	Type
8	H	189	PRO
15	c	686	VAL
15	c	1113	PRO
2	B	67	LYS

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	167/191 (87%)	153 (92%)	14 (8%)	11	38
1	O	162/191 (85%)	150 (93%)	12 (7%)	13	42
2	B	170/221 (77%)	156 (92%)	14 (8%)	11	38
2	P	181/221 (82%)	170 (94%)	11 (6%)	18	49
3	C	160/211 (76%)	139 (87%)	21 (13%)	4	17
3	Q	169/211 (80%)	162 (96%)	7 (4%)	30	64
4	D	179/203 (88%)	167 (93%)	12 (7%)	16	46
4	R	164/203 (81%)	155 (94%)	9 (6%)	21	53
5	E	195/224 (87%)	184 (94%)	11 (6%)	21	52
5	S	173/224 (77%)	164 (95%)	9 (5%)	23	55
6	F	184/212 (87%)	170 (92%)	14 (8%)	13	41
6	T	176/212 (83%)	167 (95%)	9 (5%)	24	56
7	G	181/210 (86%)	168 (93%)	13 (7%)	14	44
7	U	186/210 (89%)	174 (94%)	12 (6%)	17	47
8	H	166/195 (85%)	155 (93%)	11 (7%)	16	47
8	V	174/195 (89%)	158 (91%)	16 (9%)	9	33
9	I	164/174 (94%)	158 (96%)	6 (4%)	34	66
9	W	165/174 (95%)	154 (93%)	11 (7%)	16	46
10	J	151/171 (88%)	138 (91%)	13 (9%)	10	37
10	X	155/171 (91%)	143 (92%)	12 (8%)	13	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	K	146/159 (92%)	135 (92%)	11 (8%)	13	42
11	Y	145/159 (91%)	136 (94%)	9 (6%)	18	49
12	L	168/199 (84%)	162 (96%)	6 (4%)	35	67
12	Z	163/199 (82%)	157 (96%)	6 (4%)	34	66
13	M	170/215 (79%)	163 (96%)	7 (4%)	30	64
13	a	166/215 (77%)	153 (92%)	13 (8%)	12	40
14	N	143/159 (90%)	138 (96%)	5 (4%)	36	68
14	b	145/159 (91%)	142 (98%)	3 (2%)	53	79
15	c	1489/1673 (89%)	1383 (93%)	106 (7%)	14	44
All	All	6157/7161 (86%)	5754 (94%)	403 (6%)	21	47

5 of 403 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	V	64	LEU
13	a	92	LEU
15	c	1732	CYS
8	V	184	LEU
10	X	78	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 103 such sidechains are listed below:

Mol	Chain	Res	Type
6	T	221	ASN
12	Z	157	ASN
15	c	1521	ASN
7	U	150	GLN
10	X	24	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](#)

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
16	LDZ	b	301	-	33,34,34	2.45	8 (24%)	42,44,44	1.15	2 (4%)
17	IHP	c	1901	-	36,36,36	0.83	0	54,60,60	1.47	7 (12%)
16	LDZ	Y	301	-	33,34,34	2.52	8 (24%)	42,44,44	1.35	6 (14%)
16	LDZ	K	301	-	33,34,34	2.46	8 (24%)	42,44,44	1.27	7 (16%)
16	LDZ	N	301	-	33,34,34	2.50	8 (24%)	42,44,44	1.47	8 (19%)
17	IHP	c	1902	-	36,36,36	0.77	0	54,60,60	1.28	4 (7%)
16	LDZ	H	301	-	33,34,34	2.49	8 (24%)	42,44,44	1.27	5 (11%)
16	LDZ	V	301	-	33,34,34	2.53	8 (24%)	42,44,44	1.66	10 (23%)

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
16	LDZ	b	301	-	-	19/38/39/39	0/1/1/1
17	IHP	c	1901	-	-	5/30/54/54	0/1/1/1
16	LDZ	Y	301	-	-	13/38/39/39	0/1/1/1
16	LDZ	K	301	-	-	14/38/39/39	0/1/1/1
16	LDZ	N	301	-	-	12/38/39/39	0/1/1/1
17	IHP	c	1902	-	-	2/30/54/54	0/1/1/1
16	LDZ	H	301	-	-	10/38/39/39	0/1/1/1
16	LDZ	V	301	-	-	23/38/39/39	0/1/1/1

The worst 5 of 48 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	V	301	LDZ	C15-N16	8.45	1.52	1.34
16	Y	301	LDZ	C15-N16	8.39	1.52	1.34
16	H	301	LDZ	C15-N16	8.27	1.52	1.34
16	N	301	LDZ	C15-N16	8.26	1.52	1.34
16	K	301	LDZ	C15-N16	8.26	1.52	1.34

The worst 5 of 49 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	Y	301	LDZ	O8-C9-N10	4.83	120.33	110.50
16	V	301	LDZ	C14-C15-N16	4.62	126.83	116.70
16	N	301	LDZ	O8-C9-N10	4.52	119.68	110.50
16	H	301	LDZ	O8-C9-N10	4.45	119.55	110.50
17	c	1901	IHP	C6-C5-C4	4.11	119.41	110.41

There are no chirality outliers.

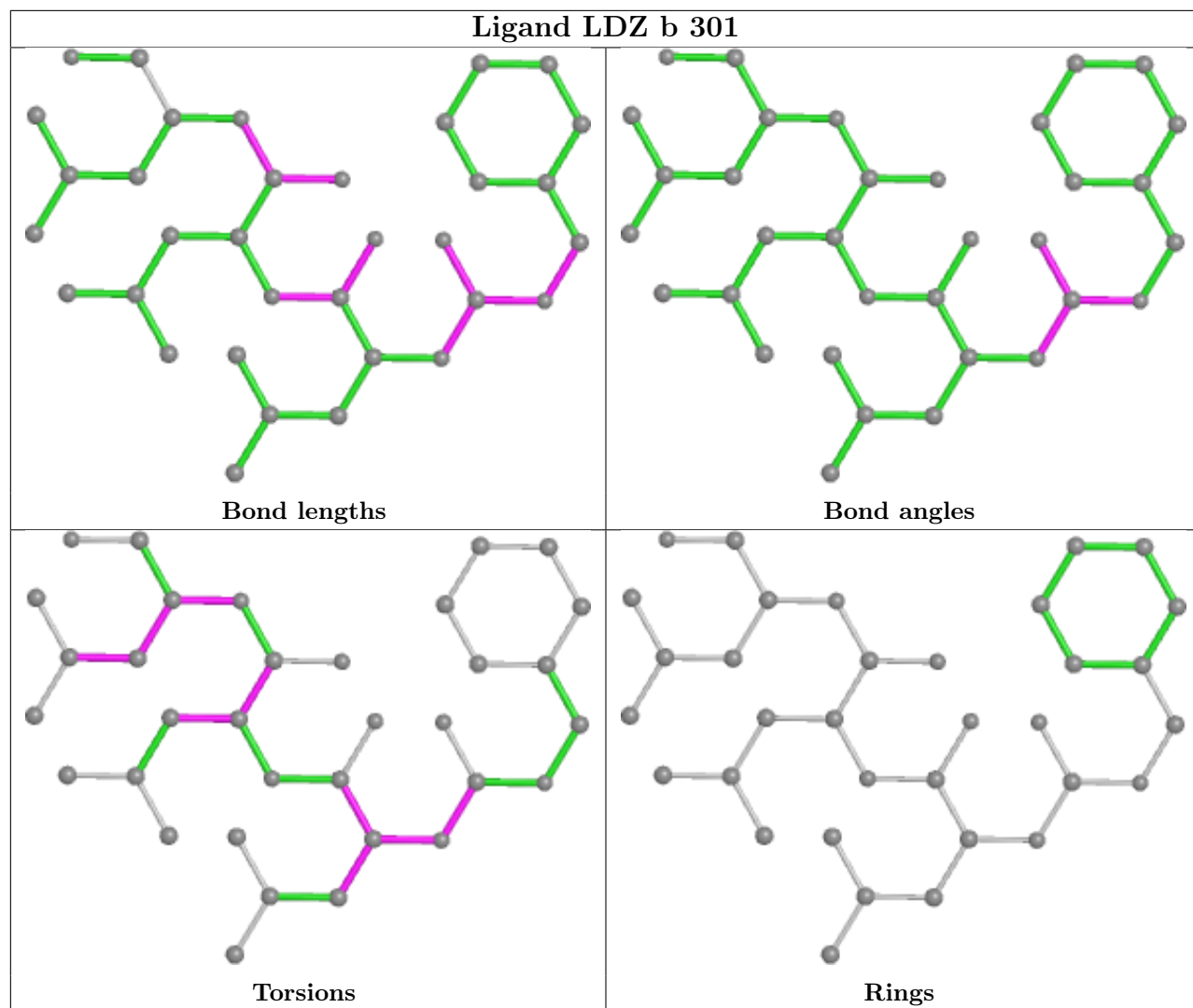
5 of 98 torsion outliers are listed below:

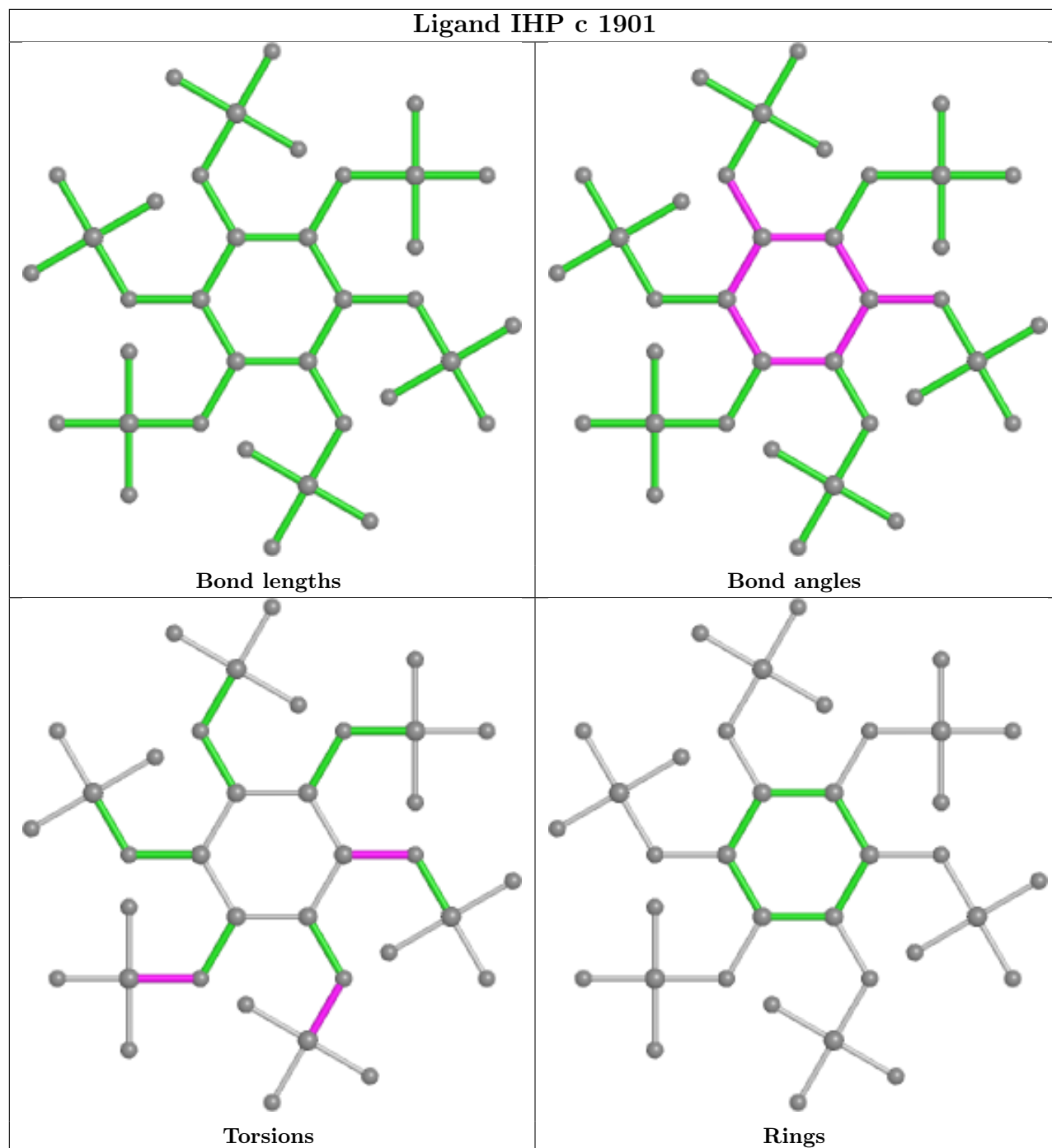
Mol	Chain	Res	Type	Atoms
16	H	301	LDZ	O31-C9-O8-C7
16	H	301	LDZ	N10-C9-O8-C7
16	K	301	LDZ	C30-C11-N10-C9
16	K	301	LDZ	N13-C14-C24-C25
16	K	301	LDZ	C18-C17-N16-C15

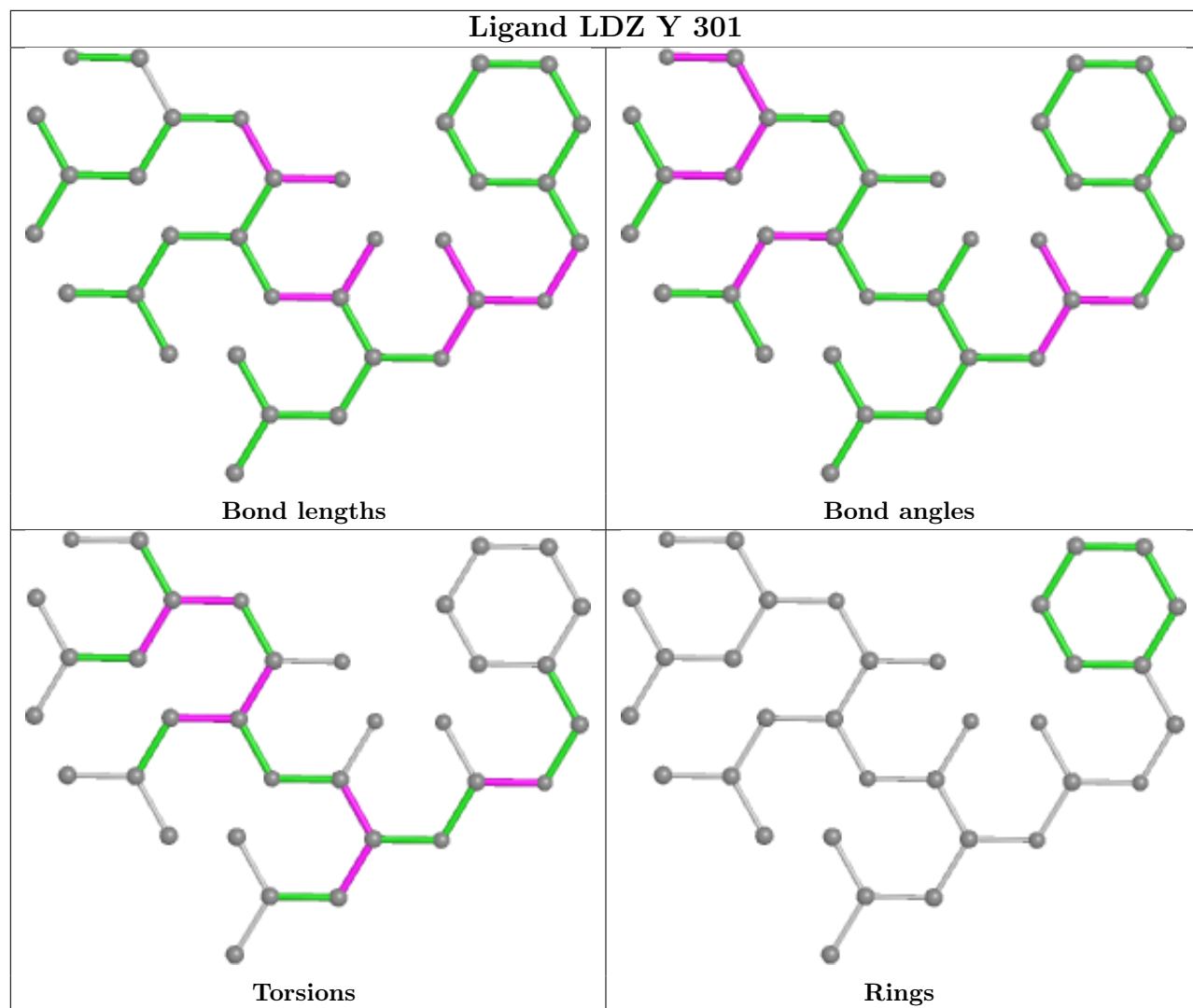
There are no ring outliers.

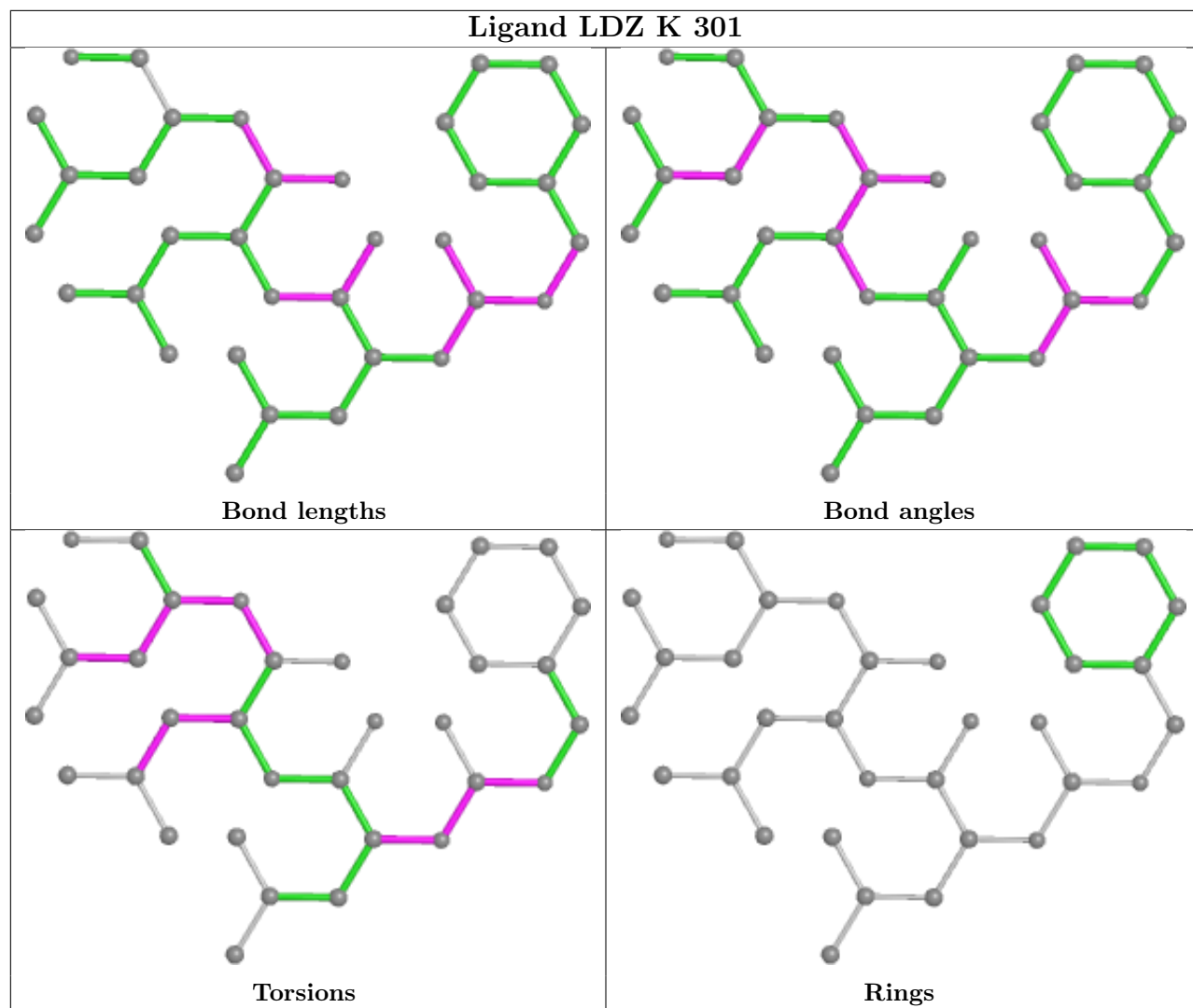
No monomer is involved in short contacts.

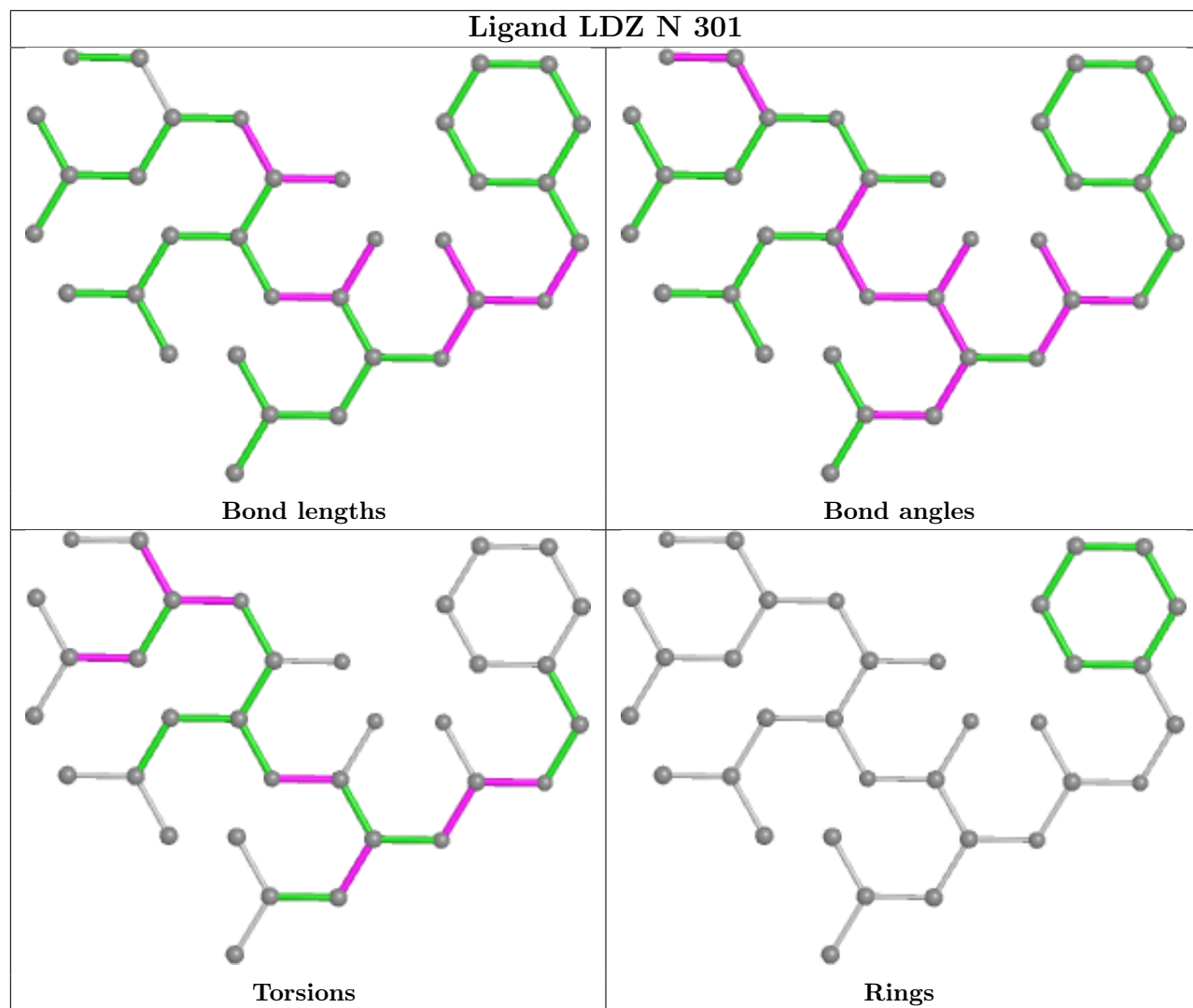
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

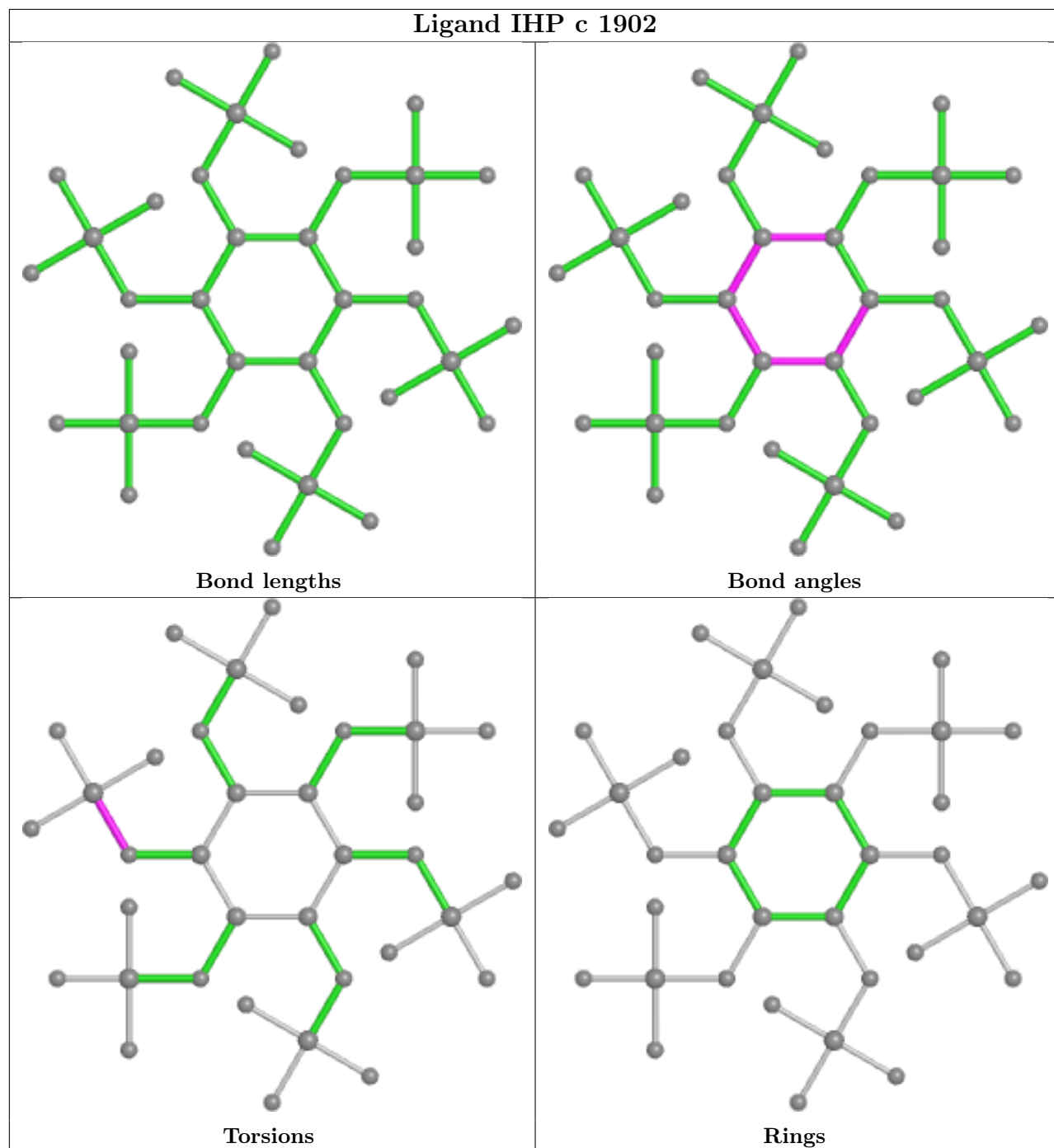


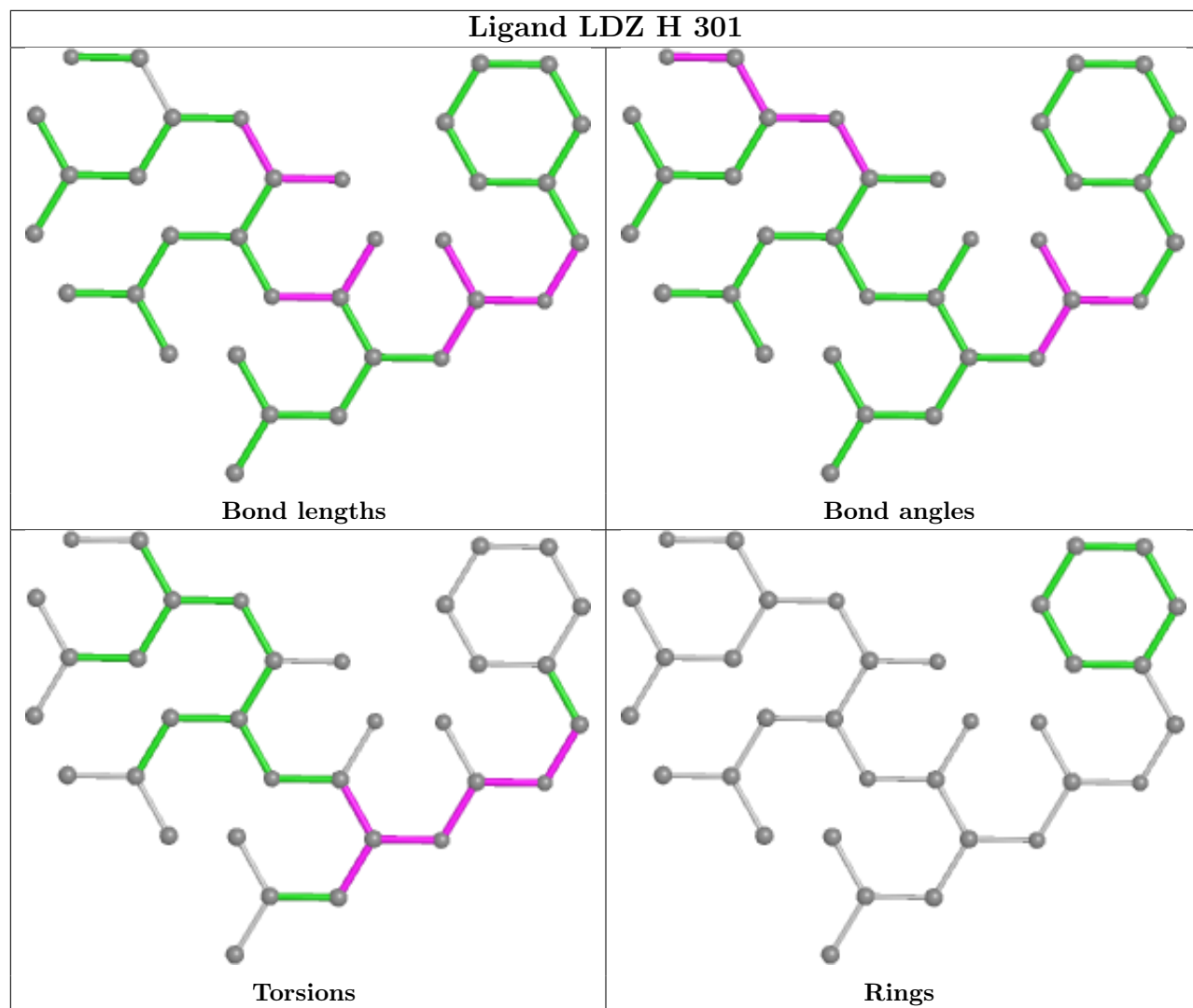


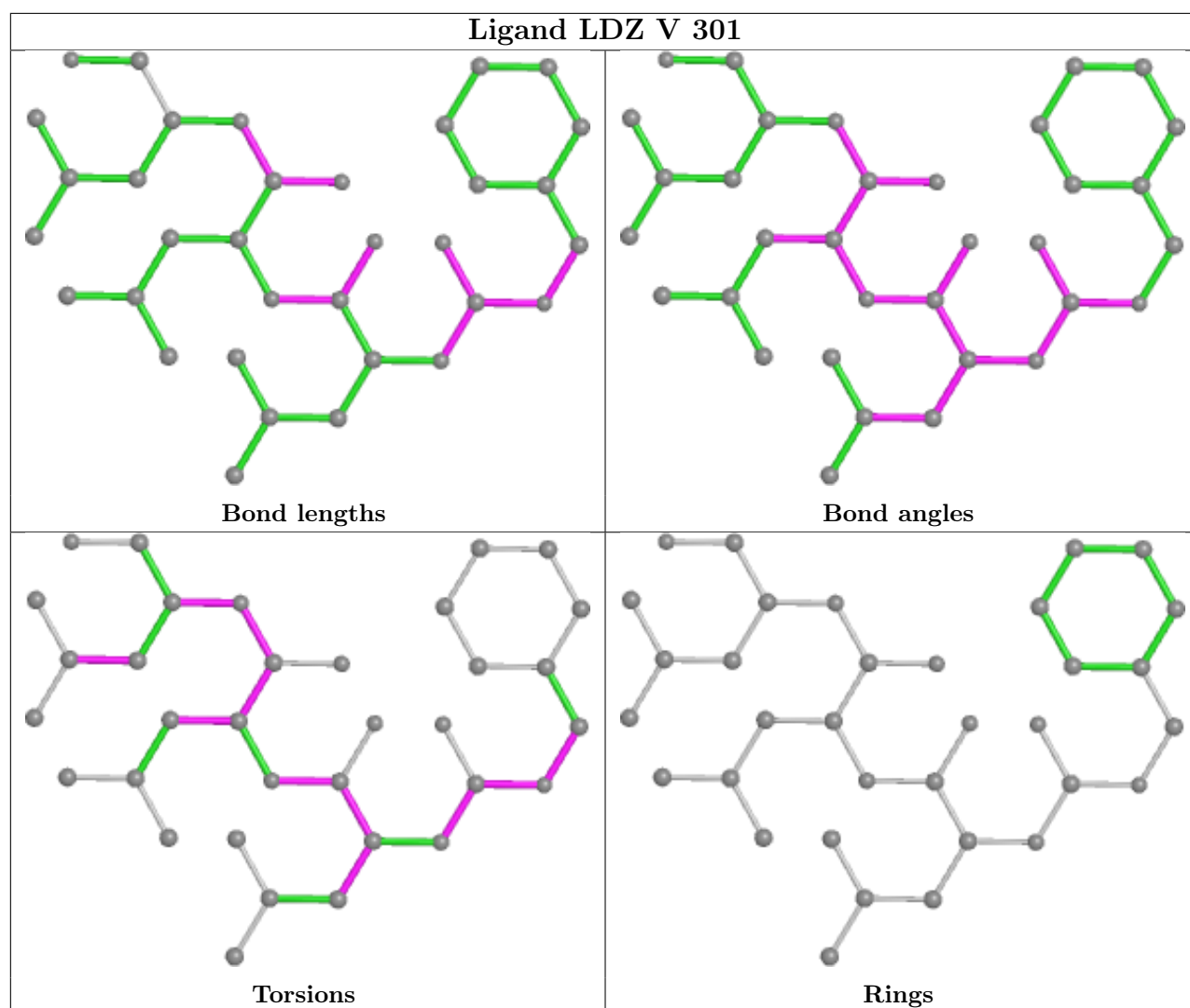












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

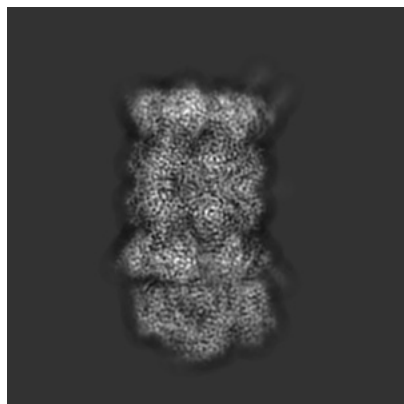
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27015. These allow visual inspection of the internal detail of the map and identification of artifacts.

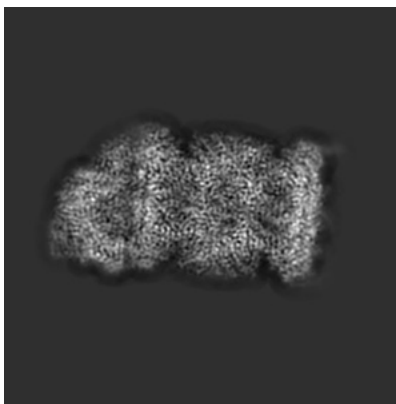
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

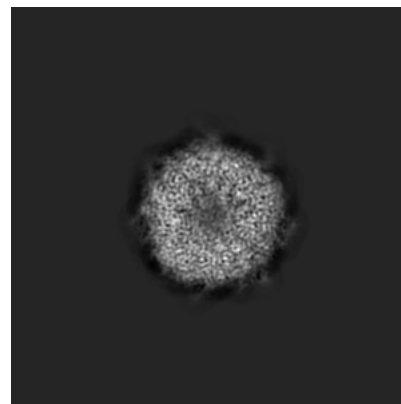
6.1.1 Primary map



X

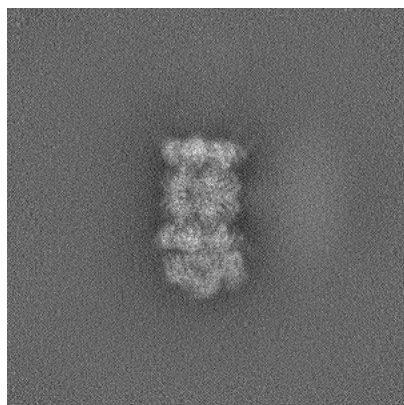


Y

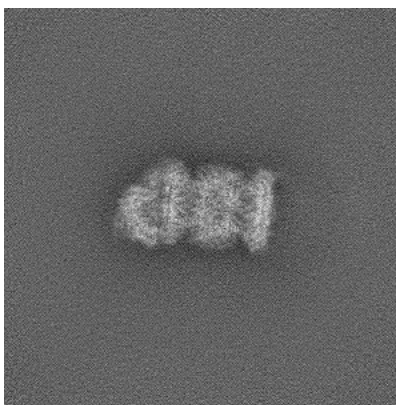


Z

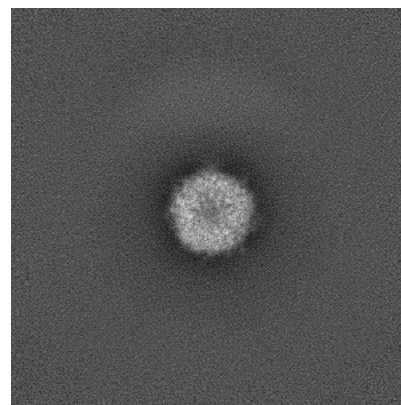
6.1.2 Raw map



X



Y

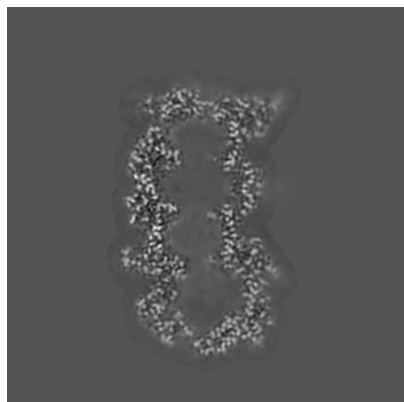


Z

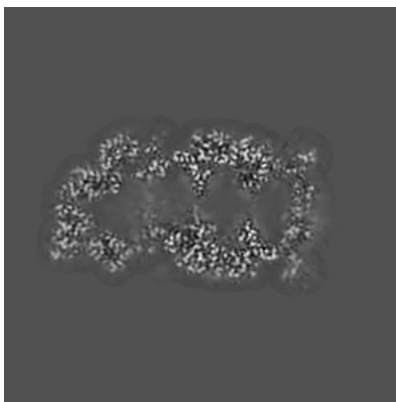
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

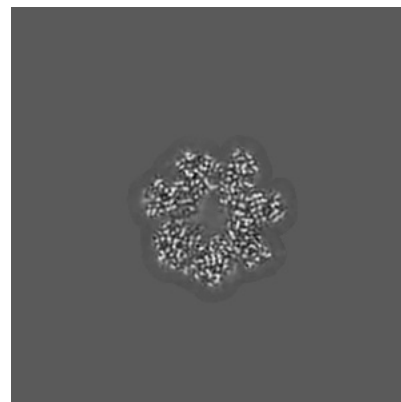
6.2.1 Primary map



X Index: 150

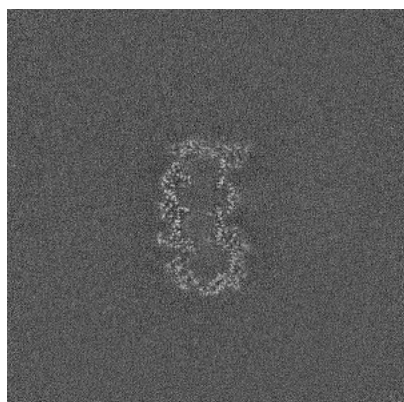


Y Index: 150

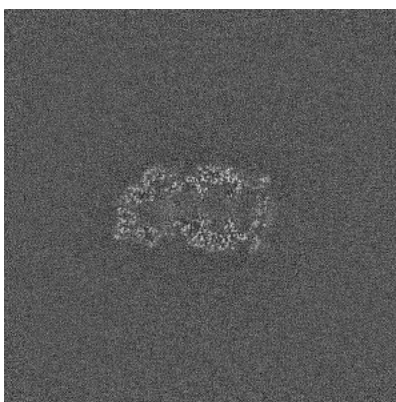


Z Index: 150

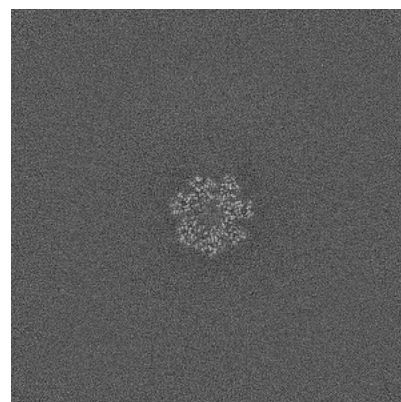
6.2.2 Raw map



X Index: 256



Y Index: 256

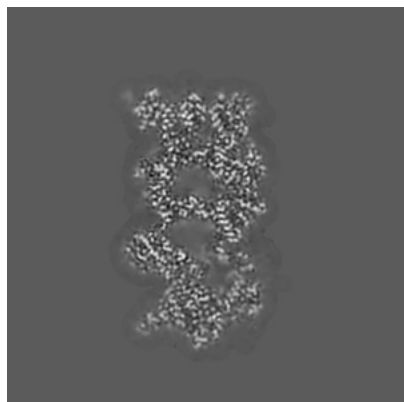


Z Index: 256

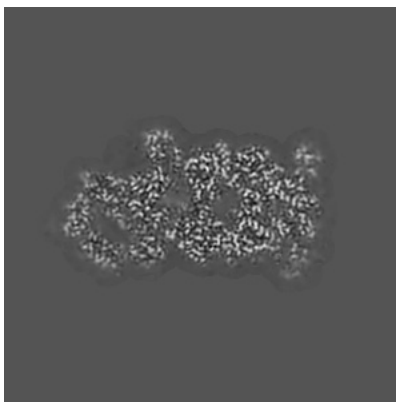
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

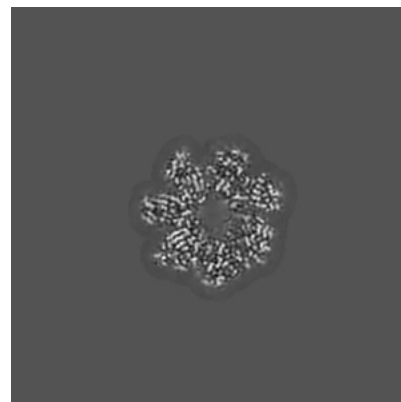
6.3.1 Primary map



X Index: 170

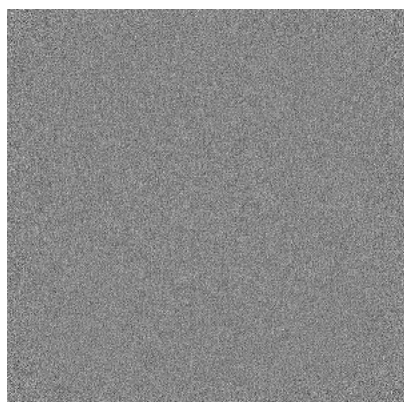


Y Index: 121

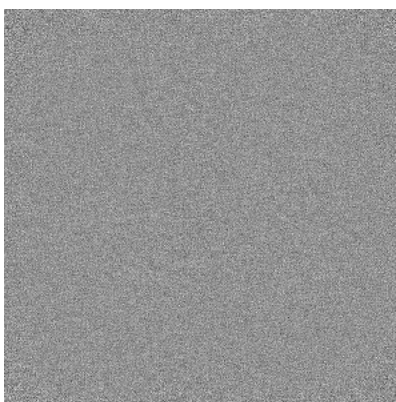


Z Index: 180

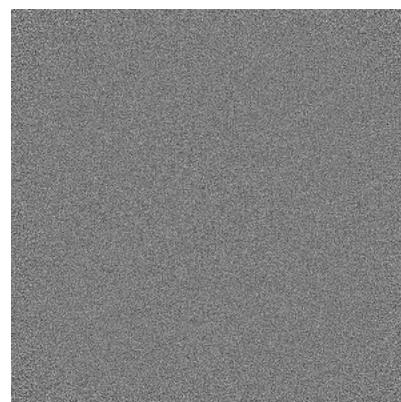
6.3.2 Raw map



X Index: 0



Y Index: 0

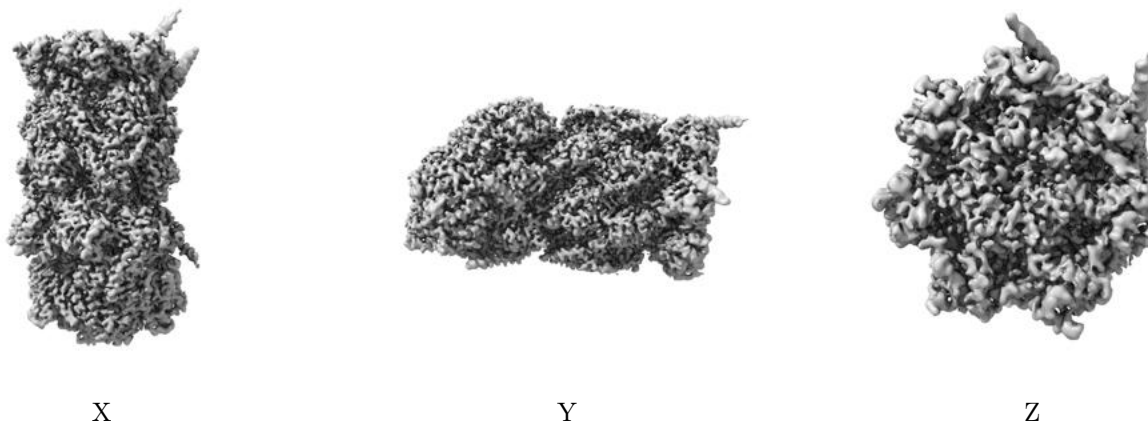


Z Index: 0

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

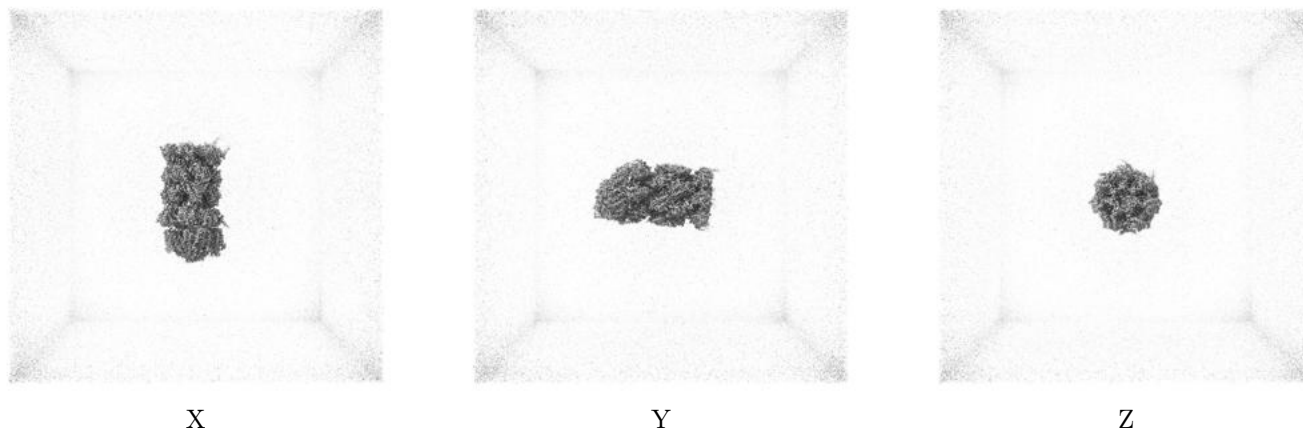
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

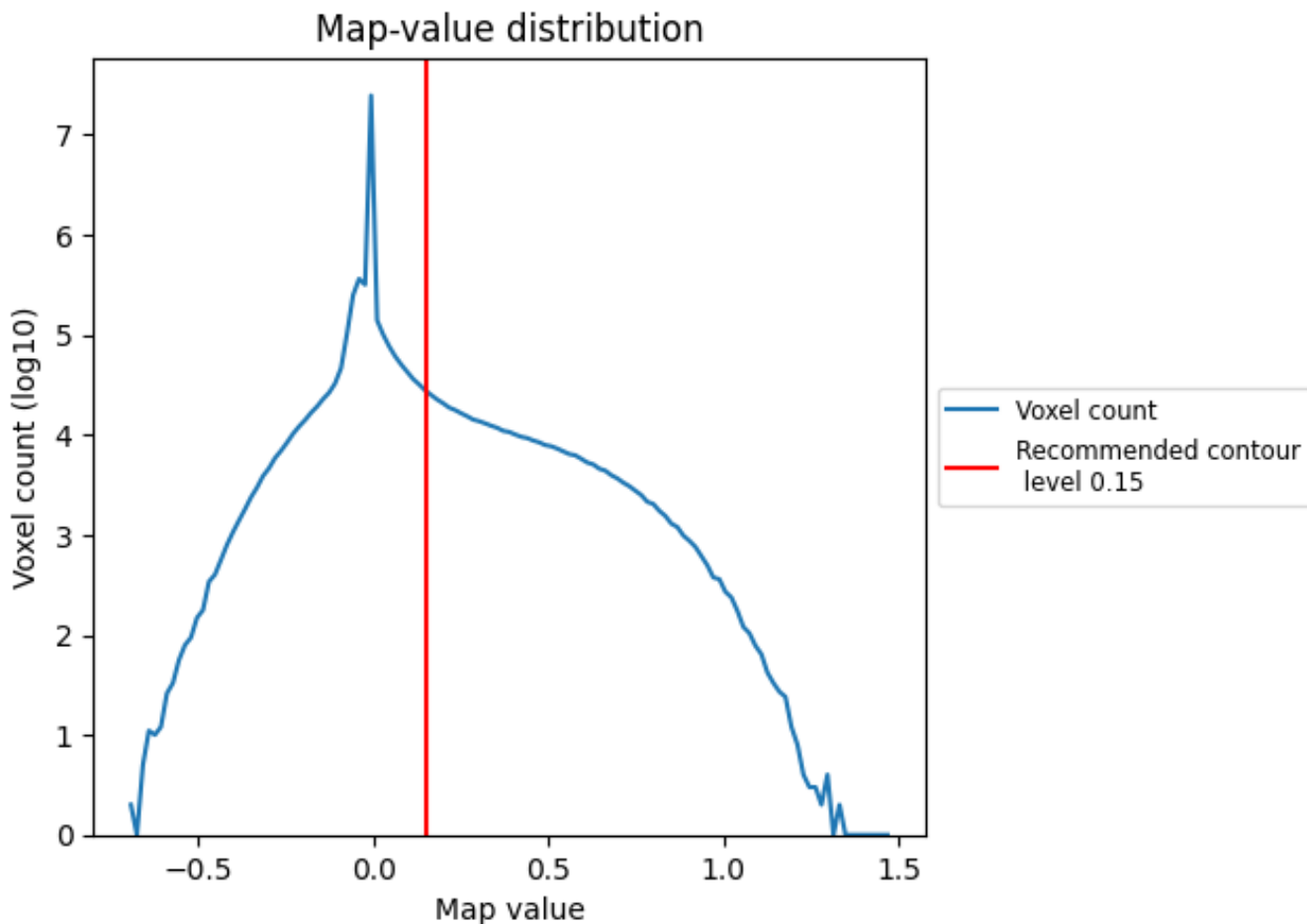
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

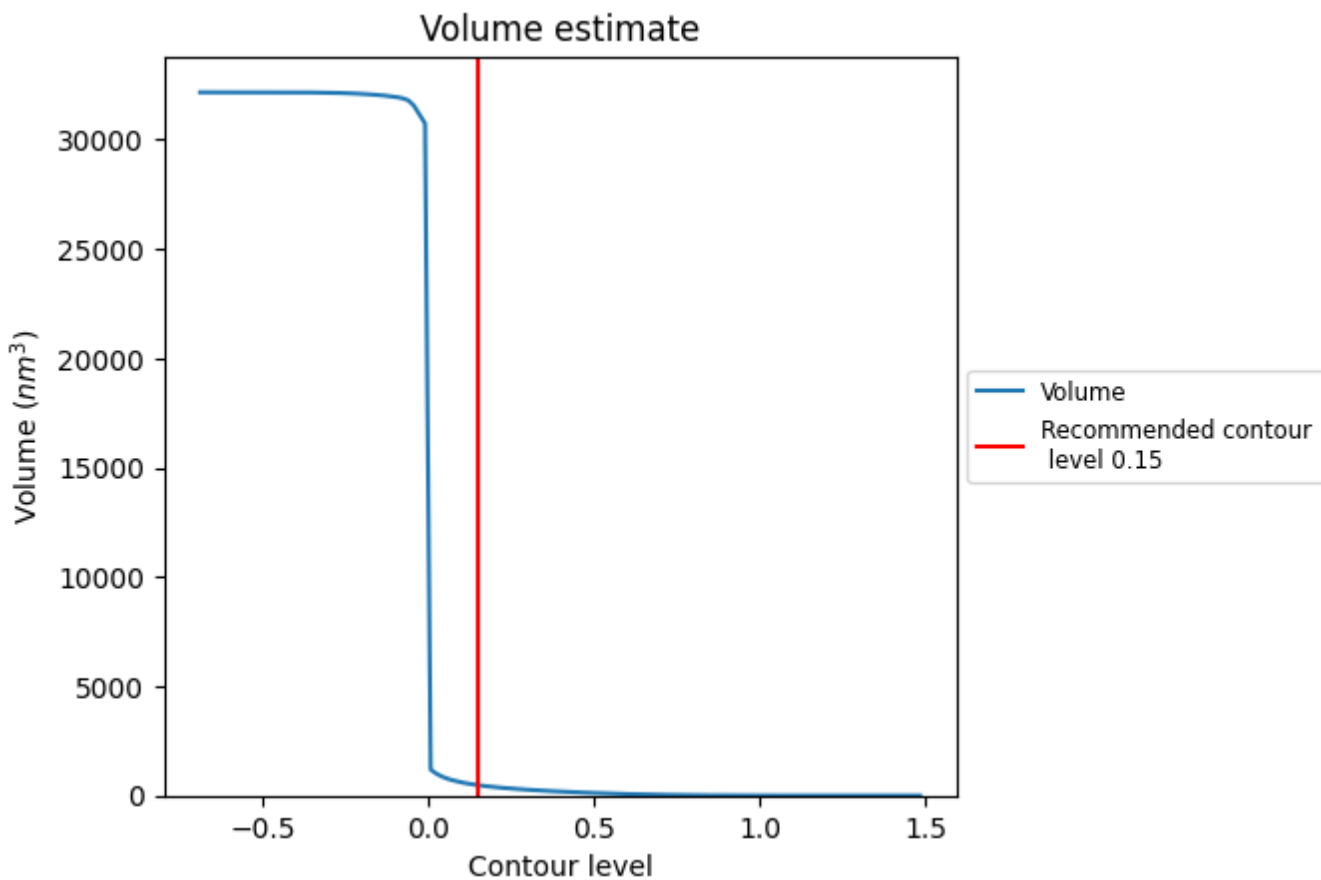
This section contains the results of statistical analysis of the map.

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.

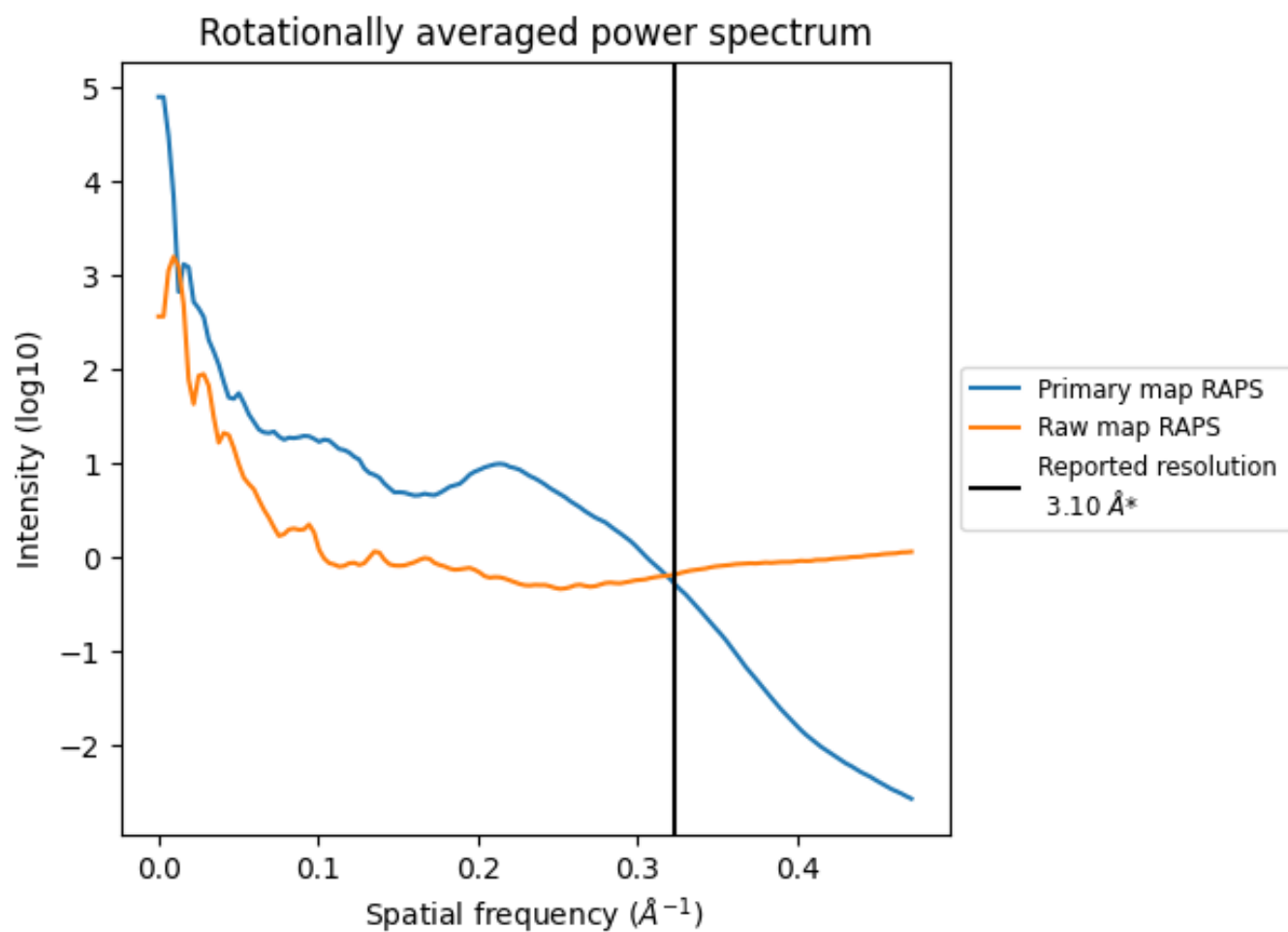
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 474 nm³; this corresponds to an approximate mass of 428 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

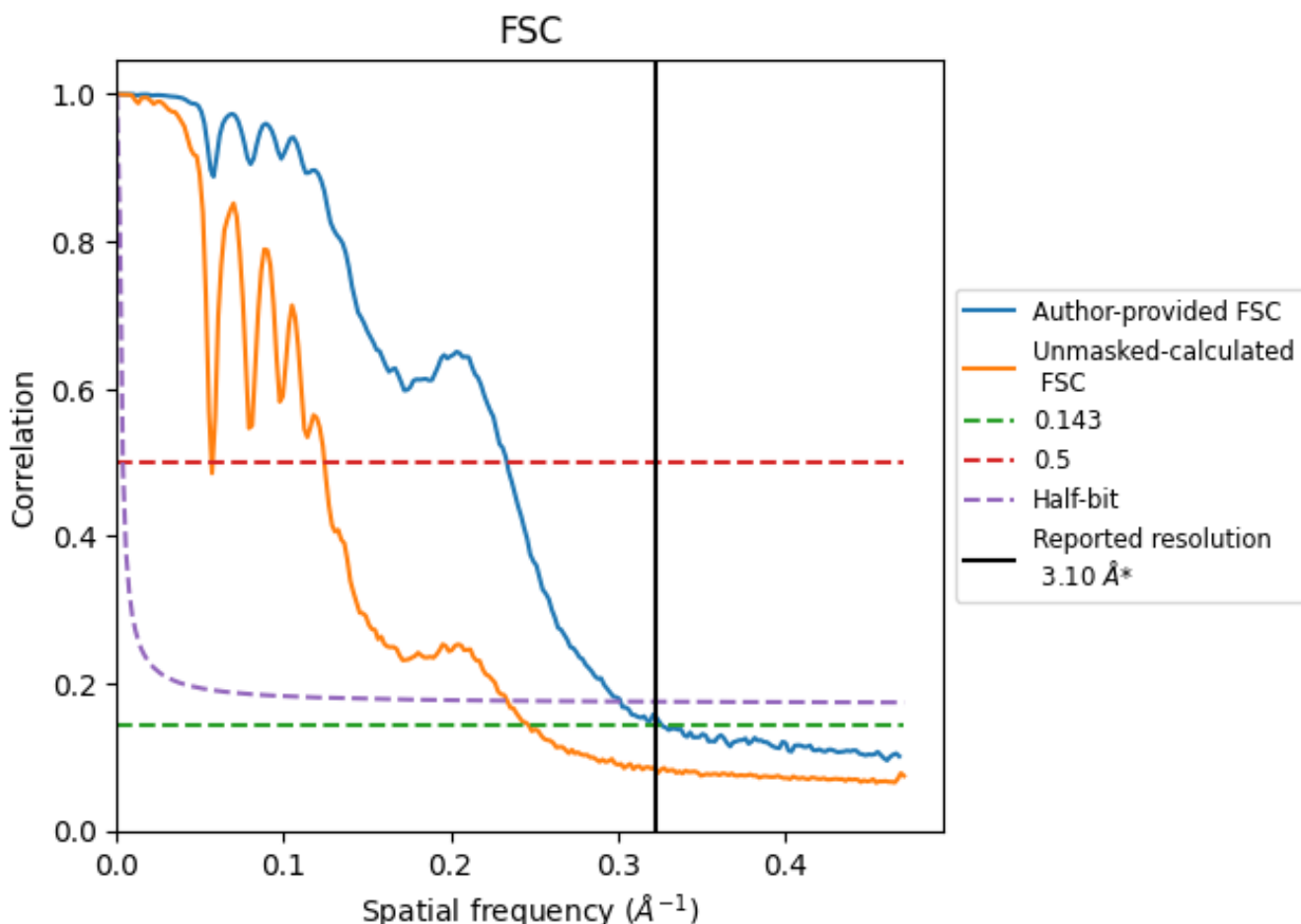


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

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 0.323 Å⁻¹

8.2 Resolution estimates [i](#)

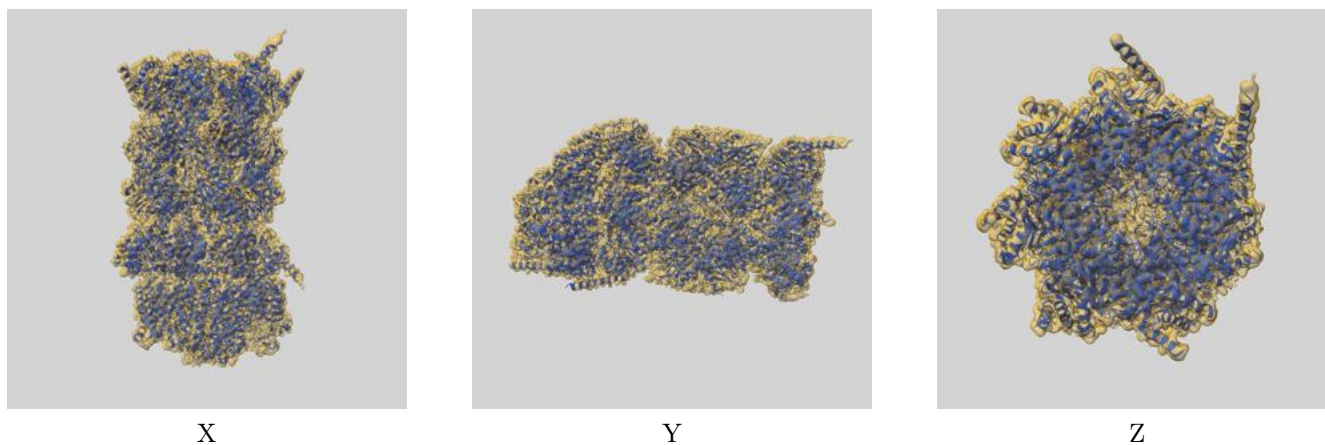
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.06	4.28	3.31
Unmasked-calculated*	4.05	17.61	4.27

*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 4.05 differs from the reported value 3.1 by more than 10 %

9 Map-model fit [i](#)

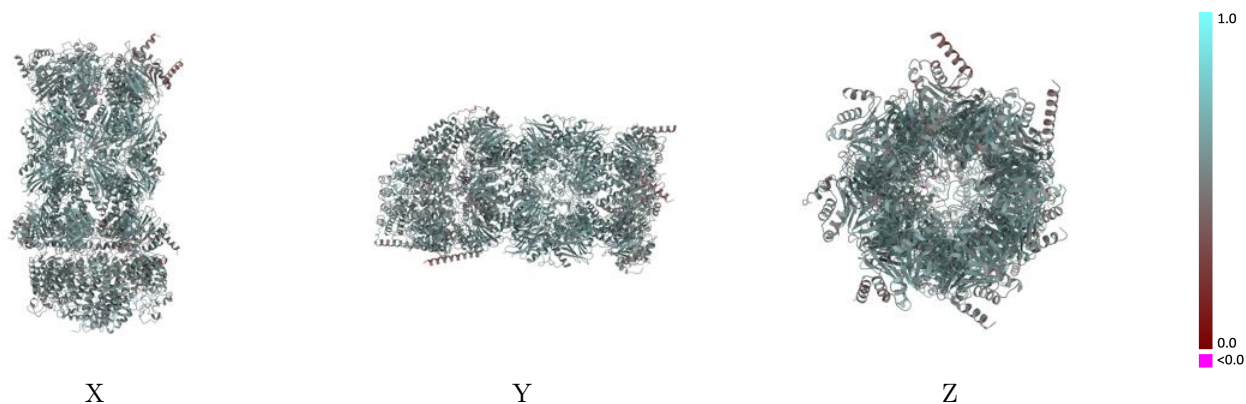
This section contains information regarding the fit between EMDB map EMD-27015 and PDB model 8CVS. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)



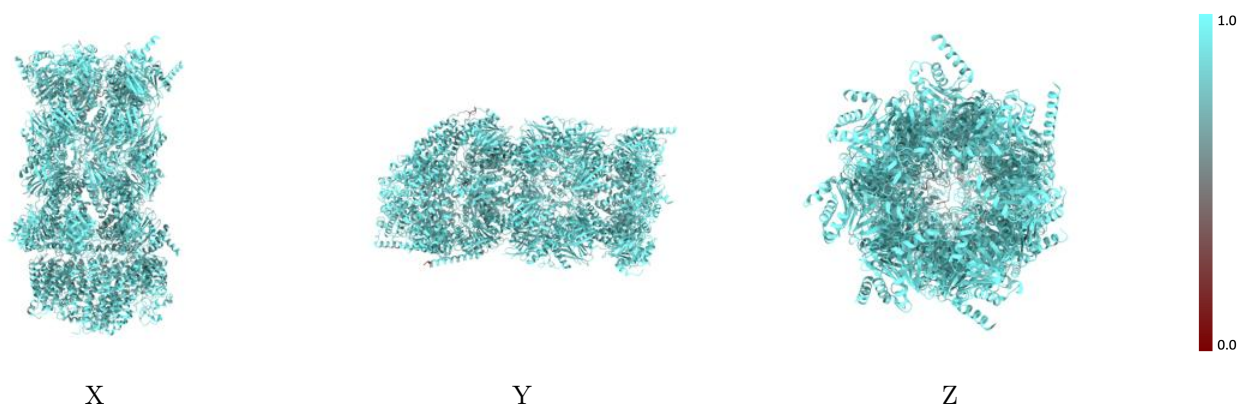
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



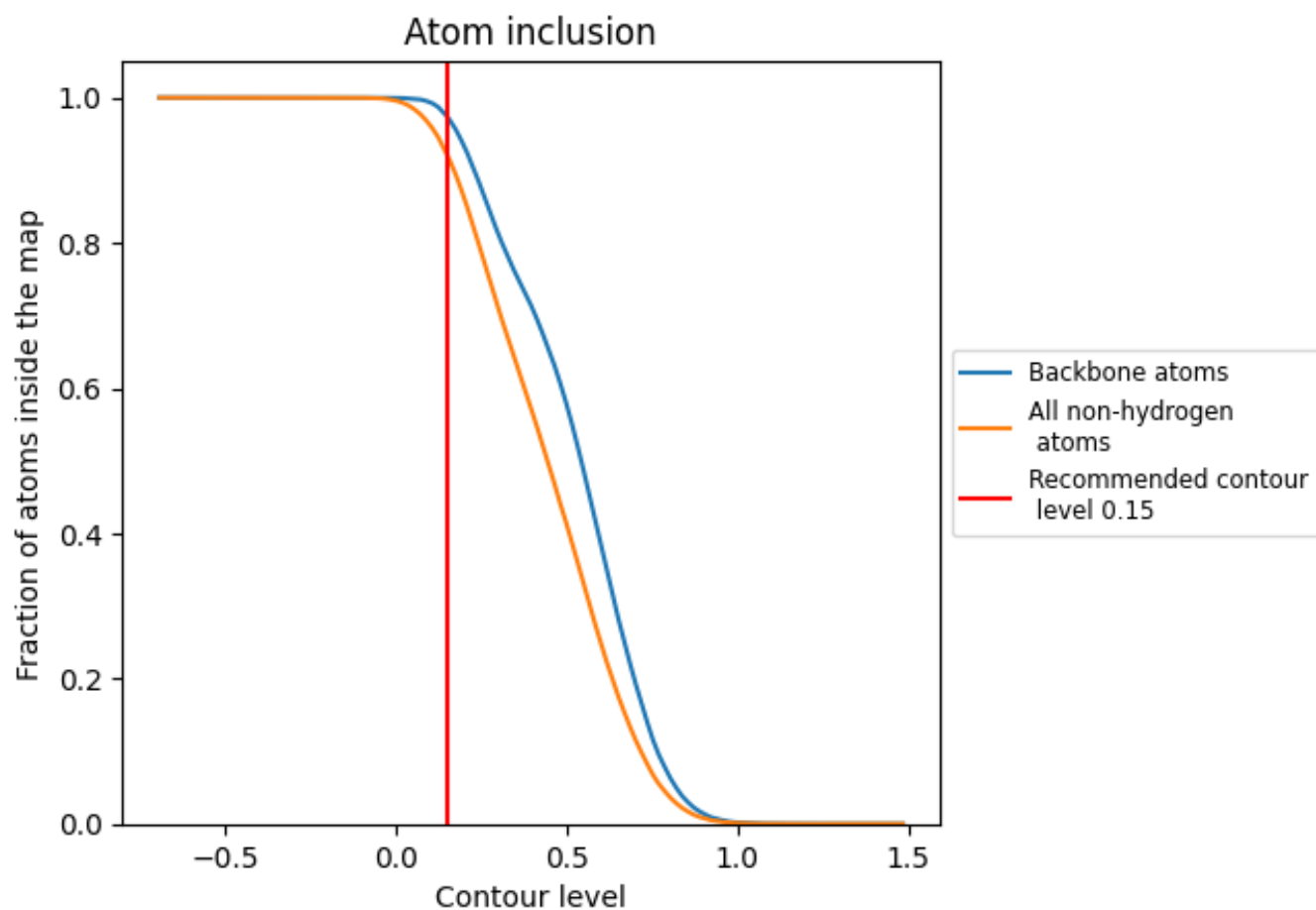
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.15).





























































9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 92% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9224	 0.5590
A	 0.9258	 0.5670
B	 0.8628	 0.5260
C	 0.8661	 0.5230
D	 0.8927	 0.5460
E	 0.9233	 0.5630
F	 0.9261	 0.5620
G	 0.9386	 0.5670
H	 0.9422	 0.5870
I	 0.9491	 0.5860
J	 0.9444	 0.5880
K	 0.9457	 0.5840
L	 0.9528	 0.5860
M	 0.9458	 0.5870
N	 0.9494	 0.5890
O	 0.9402	 0.5590
P	 0.9206	 0.5410
Q	 0.8993	 0.5070
R	 0.9127	 0.5400
S	 0.9397	 0.5430
T	 0.9315	 0.5510
U	 0.9298	 0.5500
V	 0.9497	 0.5780
W	 0.9470	 0.5890
X	 0.9456	 0.5860
Y	 0.9508	 0.5870
Z	 0.9419	 0.5810
a	 0.9510	 0.5880
b	 0.9388	 0.5850
c	 0.8968	 0.5380

