



wwPDB EM Validation Summary Report ⓘ

Apr 2, 2025 – 04:26 am BST

PDB ID : 6TD5 / pdb_00006td5
EMDB ID : EMD-10463
Title : Leishmania tarentolae proteasome 20S subunit complexed with LXE408 and bortezomib
Authors : Srinivas, H.
Deposited on : 2019-11-07
Resolution : 3.20 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:

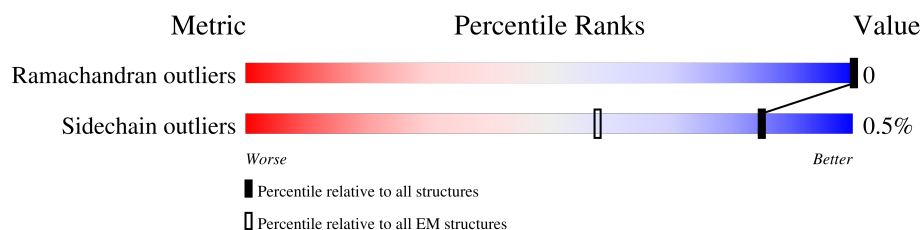
EMDB validation analysis : 0.0.1.dev117
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

1 Overall quality at a glance

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

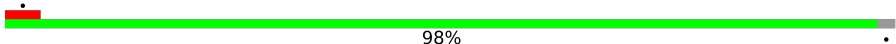

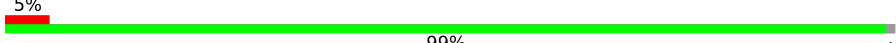
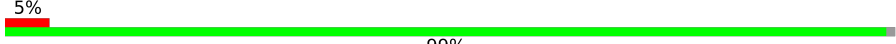
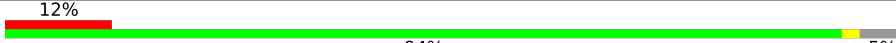




The reported resolution of this entry is 3.20 Å.

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	250	 98% .
1	a	250	 98% .
2	B	231	 5% 99% .
2	b	231	 5% 99% .
3	C	285	 12% 94% . 5%
3	c	285	 12% 94% . 5%
4	D	248	 16% 96% .
4	d	248	 15% 96% .
5	E	344	 5% 68% 32%

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Mol	Chain	Length	Quality of chain
5	e	344	
6	F	428	
6	f	428	
7	G	238	
7	g	238	
8	H	229	
8	h	229	
9	I	225	
9	i	225	
10	J	205	
10	j	205	
11	K	206	
11	k	206	
12	L	203	
12	l	203	
13	M	339	
13	m	339	
14	N	220	
14	n	220	

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 49408 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.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	245	Total	C	N	O	S	0	0
			1861	1171	324	354	12		
1	a	245	Total	C	N	O	S	0	0
			1861	1171	324	354	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	229	Total	C	N	O	S	0	0
			1753	1112	292	341	8		
2	b	229	Total	C	N	O	S	0	0
			1753	1112	292	341	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	272	Total	C	N	O	S	0	0
			2155	1357	371	415	12		
3	c	272	Total	C	N	O	S	0	0
			2155	1357	371	415	12		

- Molecule 4 is a protein called Proteasome endopeptidase complex.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	240	Total	C	N	O	S	0	0
			1882	1186	324	364	8		
4	d	240	Total	C	N	O	S	0	0
			1882	1186	324	364	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	235	Total	C	N	O	S	0	0
			1802	1119	315	356	12		
5	e	235	Total	C	N	O	S	0	0
			1802	1119	315	356	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	238	Total	C	N	O	S	0	0
			1869	1173	325	359	12		
6	f	238	Total	C	N	O	S	0	0
			1869	1173	325	359	12		

- Molecule 7 is a protein called Proteasome endopeptidase complex.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	230	Total	C	N	O	S	0	0
			1741	1085	308	338	10		
7	g	230	Total	C	N	O	S	0	0
			1741	1085	308	338	10		

- Molecule 8 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	229	Total	C	N	O	S	0	0
			1709	1062	295	340	12		
8	h	229	Total	C	N	O	S	0	0
			1709	1062	295	340	12		

- Molecule 9 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	219	Total	C	N	O	S	0	0
			1659	1037	292	318	12		
9	i	219	Total	C	N	O	S	0	0
			1659	1037	292	318	12		

- Molecule 10 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	204	Total	C	N	O	S	0	0
			1557	980	259	302	16		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	j	204	Total	C	N	O	S	0	0
			1557	980	259	302	16		

- Molecule 11 is a protein called Proteasome subunit family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	206	Total	C	N	O	S	0	0
			1612	1012	280	304	16		
11	k	206	Total	C	N	O	S	0	0
			1612	1012	280	304	16		

- Molecule 12 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	201	Total	C	N	O	S	0	0
			1573	995	276	295	7		
12	l	201	Total	C	N	O	S	0	0
			1573	995	276	295	7		

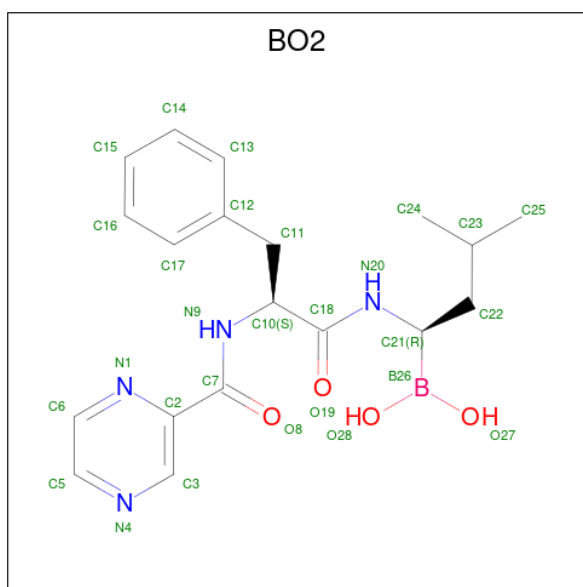
- Molecule 13 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	214	Total	C	N	O	S	0	0
			1702	1079	287	324	12		
13	m	214	Total	C	N	O	S	0	0
			1702	1079	287	324	12		

- Molecule 14 is a protein called Proteasome subunit beta.

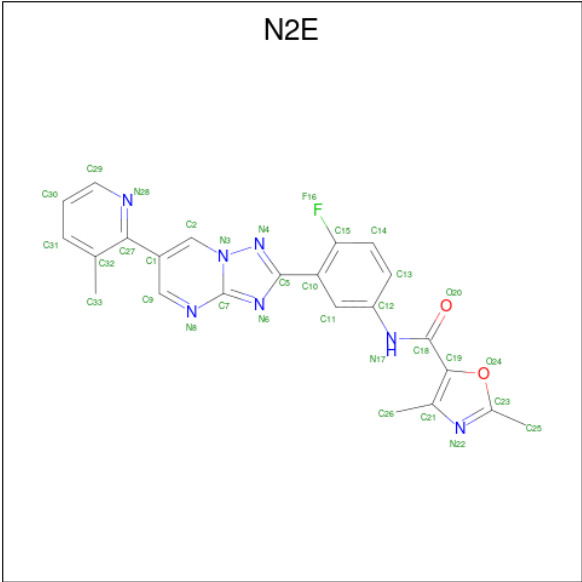
Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	218	Total	C	N	O	S	0	0
			1712	1083	292	323	14		
14	n	218	Total	C	N	O	S	0	0
			1712	1083	292	323	14		

- Molecule 15 is N-[(1R)-1-(DIHYDROXYBORYL)-3-METHYLBUTYL]-N-(PYRAZIN-2-YLCARBONYL)-L-PHENYLALANINAMIDE (CCD ID: BO2) (formula: C₁₉H₂₅BN₄O₄).



Mol	Chain	Residues	Atoms					AltConf
15	H	1	Total	B	C	N	O	0
			28	1	19	4	4	
15	I	1	Total	B	C	N	O	0
			28	1	19	4	4	
15	L	1	Total	B	C	N	O	0
			28	1	19	4	4	
15	h	1	Total	B	C	N	O	0
			28	1	19	4	4	
15	i	1	Total	B	C	N	O	0
			28	1	19	4	4	
15	l	1	Total	B	C	N	O	0
			28	1	19	4	4	

- Molecule 16 is {N}-[4-fluoranyl-3-[6-(3-methylpyridin-2-yl)-[1,2,4]triazolo[1,5-a]pyrimidin-2-yl]phenyl]-2,4-dimethyl-1,3-oxazole-5-carboxamide (CCD ID: N2E) (formula: $C_{23}H_{18}FN_7O_2$).

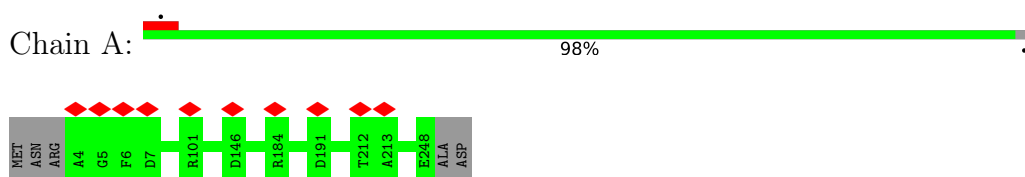


Mol	Chain	Residues	Atoms					AltConf
16	L	1	Total	C	F	N	O	0
			33	23	1	7	2	
16	1	1	Total	C	F	N	O	0
			33	23	1	7	2	

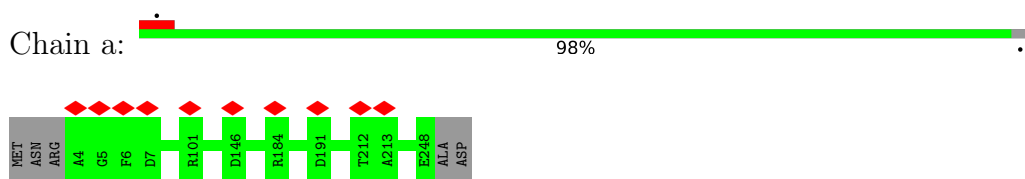
3 Residue-property plots [i](#)

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.

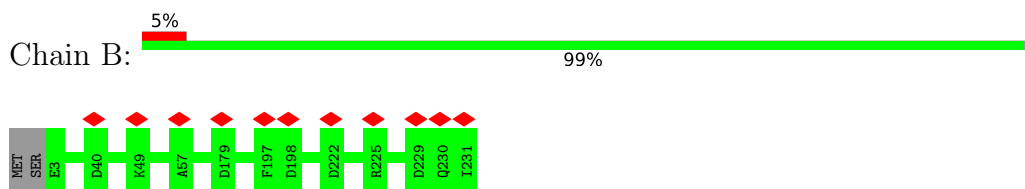
- Molecule 1: Proteasome subunit alpha type



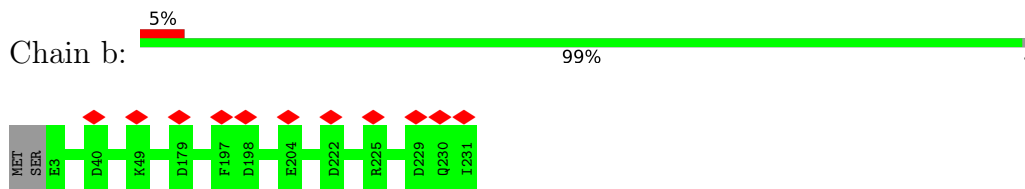
- Molecule 1: Proteasome subunit alpha type



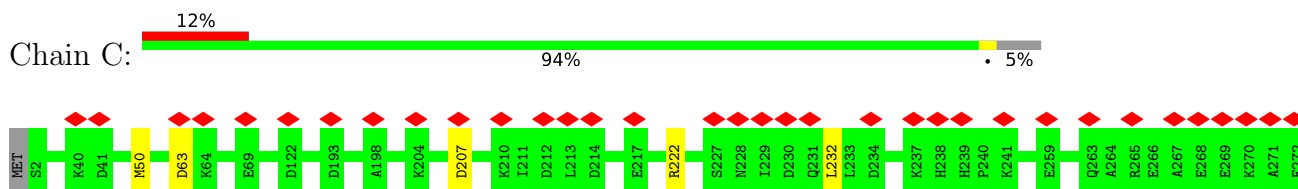
- Molecule 2: Proteasome subunit alpha type

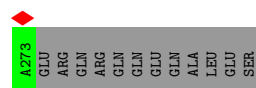


- Molecule 2: Proteasome subunit alpha type

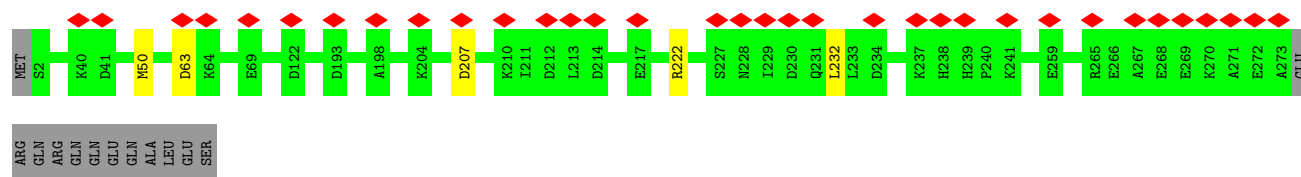


- Molecule 3: Proteasome subunit alpha type

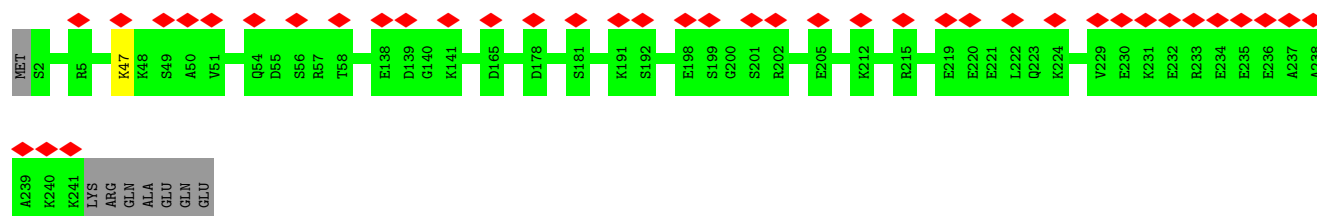




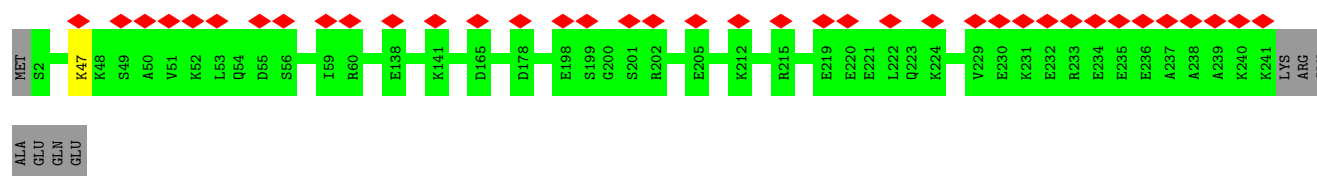
- Molecule 3: Proteasome subunit alpha type



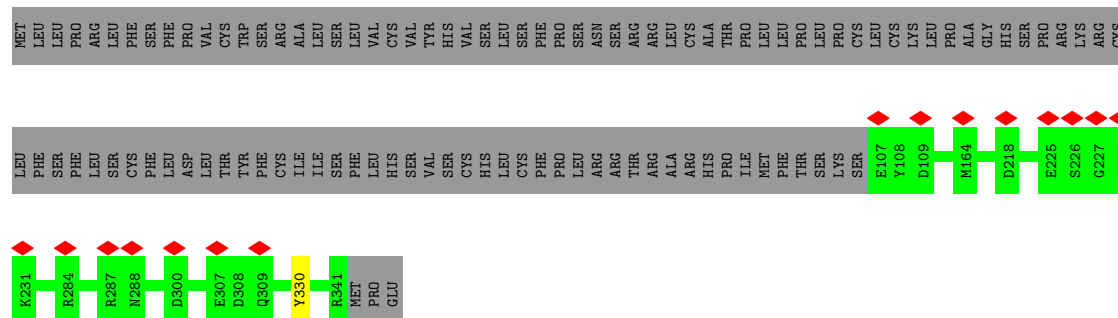
- Molecule 4: Proteasome endopeptidase complex



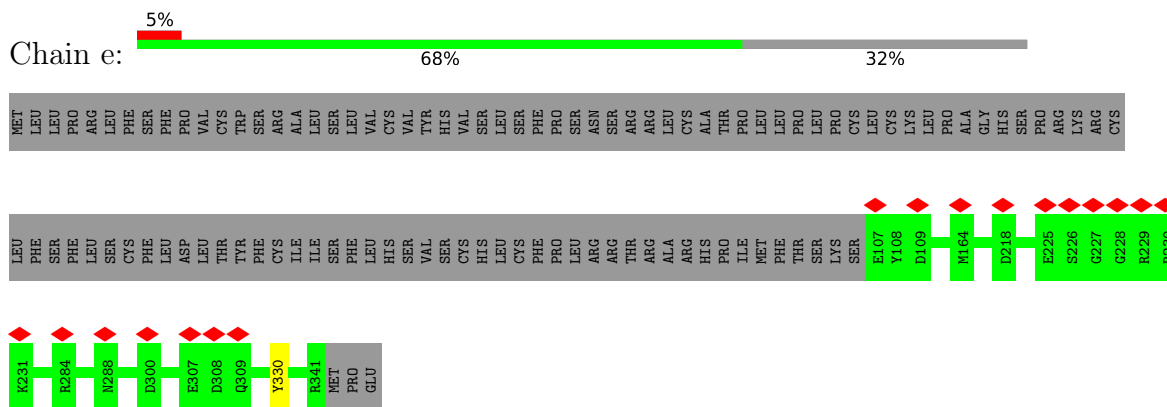
- Molecule 4: Proteasome endopeptidase complex



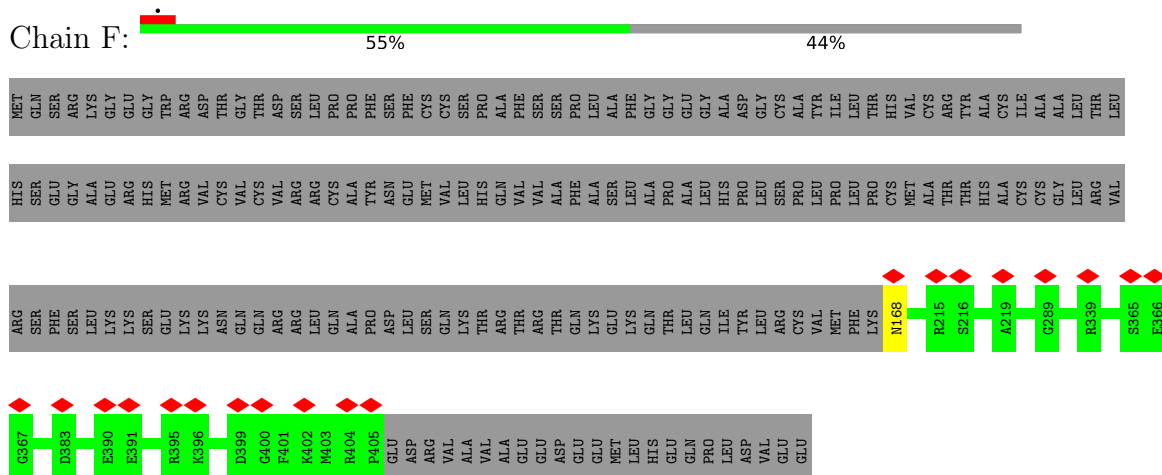
- Molecule 5: Proteasome subunit alpha type



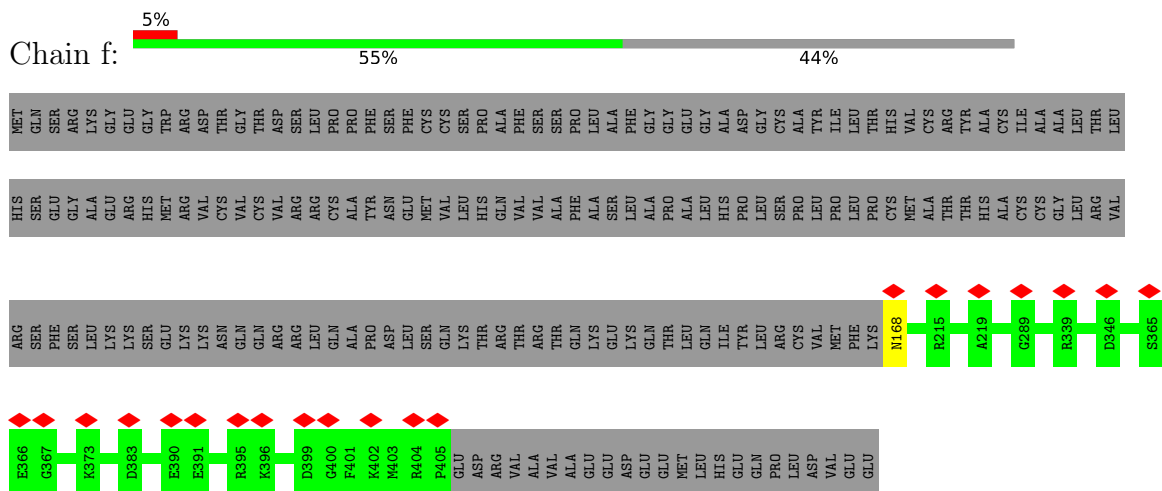
- Molecule 5: Proteasome subunit alpha type



- Molecule 6: Proteasome subunit alpha type

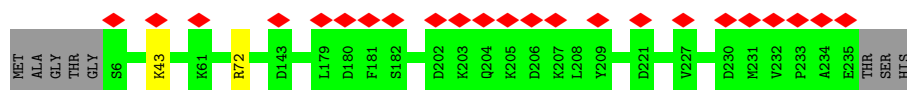


- Molecule 6: Proteasome subunit alpha type



- Molecule 7: Proteasome endopeptidase complex





- Molecule 7: Proteasome endopeptidase complex



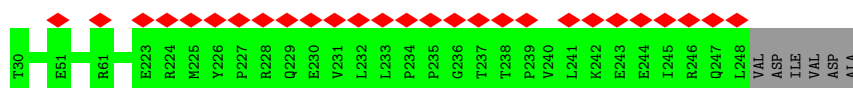
- Molecule 8: Proteasome subunit beta



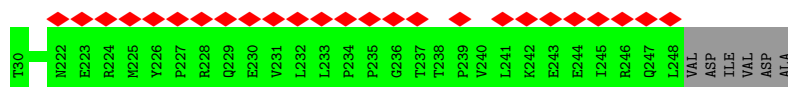
- Molecule 8: Proteasome subunit beta



- Molecule 9: Proteasome subunit beta



- Molecule 9: Proteasome subunit beta



- Molecule 10: Proteasome subunit beta



- Molecule 10: Proteasome subunit beta

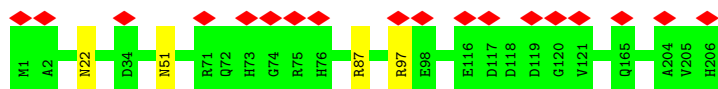




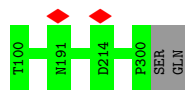
- Molecule 11: Proteasome subunit family protein



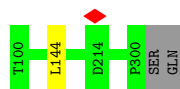
- Molecule 11: Proteasome subunit family protein



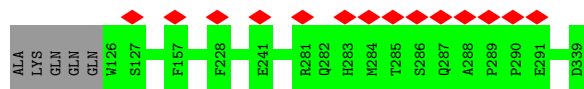
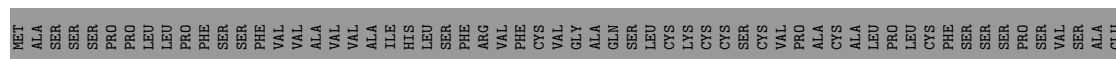
- Molecule 12: Proteasome subunit beta



- Molecule 12: Proteasome subunit beta



- Molecule 13: Proteasome subunit beta



- Molecule 13: Proteasome subunit beta



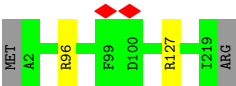
MET	ALA	ASP
ALA	SER	VAL
SER	LEU	ALA
SER	ALA	GLN
PRO	PRO	GLN
LEU	PHE	LEU
LEU	ALA	HIS
LEU	PRO	PRO
PHE	LYS	VAL
SER	VAL	SER
SER	LEU	THR
PHE	PHE	HIS
VAL	VAL	ARG
VAL	VAL	THR
ALA	VAL	PRO
ALA	VAL	THR
ALA	ALA	ALA
ALA	ALA	ARG
ILE	TYR	TYR
HIS	SER	SER
LEU	PRO	PRO
LEU	ILE	ILE
SER	LEU	SER
PHE	ARG	ARG
VAL	VAL	VAL
CYS	CYS	HIS
VAL	GLY	TYR
GLY	ALA	ALA
ALA	GLN	MET
SER	SER	ILE
LEU	GLU	GLU
CYS	ASP	ASP
CYS	LYS	HIS
CYS	CYS	ALA
CYS	CYS	GLU
CYS	TYR	TYR
CYS	GLY	GLY
VAL	HIS	HIS
PRO	ASN	ASN
ALA	TYR	TYR
CYS	TYR	PRO
ALA	ALA	GLN
LEU	LEU	LYS
PRO	LEU	LYS
LEU	ALA	ALA
CYS	SER	SER
PHE	THR	THR
SER	LEU	LEU
SER	THR	THR
PRO	PRO	PRO
VAL	VAL	VAL
ALA	GLN	GLN
ALA	ALA	ALA
GLY	GLY	GLY



• 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	127000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.141	Depositor
Minimum map value	-0.094	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	258.0, 258.0, 258.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.86, 0.86, 0.86	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: N2E, BO2

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	0/1893	0.54	0/2567
1	a	0.29	0/1893	0.54	0/2567
2	B	0.32	0/1786	0.56	0/2421
2	b	0.32	0/1786	0.56	0/2421
3	C	0.28	0/2202	0.56	2/2982 (0.1%)
3	c	0.28	0/2202	0.56	2/2982 (0.1%)
4	D	0.28	0/1911	0.55	0/2573
4	d	0.28	0/1911	0.55	0/2573
5	E	0.27	0/1831	0.51	1/2476 (0.0%)
5	e	0.27	0/1831	0.51	1/2476 (0.0%)
6	F	0.28	0/1907	0.49	0/2575
6	f	0.28	0/1907	0.49	0/2575
7	G	0.31	0/1773	0.51	0/2398
7	g	0.31	0/1773	0.51	0/2398
8	H	0.32	0/1741	0.52	0/2359
8	h	0.32	0/1741	0.52	0/2359
9	I	0.29	0/1685	0.55	0/2284
9	i	0.29	0/1685	0.55	0/2284
10	J	0.29	0/1583	0.51	0/2135
10	j	0.29	0/1583	0.51	0/2135
11	K	0.28	0/1643	0.51	0/2222
11	k	0.28	0/1643	0.51	0/2222
12	L	0.32	0/1607	0.55	0/2175
12	l	0.30	0/1607	0.57	1/2175 (0.0%)
13	M	0.30	0/1743	0.54	0/2354
13	m	0.30	0/1743	0.54	0/2354
14	N	0.30	0/1748	0.52	0/2363
14	n	0.30	0/1748	0.52	0/2363
All	All	0.29	0/50106	0.53	7/67768 (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
4	D	0	1
4	d	0	1
10	J	0	1
10	j	0	1
All	All	0	4

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	330	TYR	C-N-CA	5.90	136.45	121.70
5	e	330	TYR	C-N-CA	5.90	136.46	121.70
12	l	144	LEU	CA-CB-CG	5.50	127.94	115.30
3	C	63	ASP	CB-CG-OD1	5.38	123.14	118.30
3	c	63	ASP	CB-CG-OD1	5.35	123.11	118.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	47	LYS	Peptide
10	J	101	GLY	Peptide
4	d	47	LYS	Peptide
10	j	101	GLY	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	243/250 (97%)	233 (96%)	10 (4%)	0	100	100
1	a	243/250 (97%)	233 (96%)	10 (4%)	0	100	100
2	B	227/231 (98%)	215 (95%)	12 (5%)	0	100	100
2	b	227/231 (98%)	215 (95%)	12 (5%)	0	100	100
3	C	270/285 (95%)	258 (96%)	12 (4%)	0	100	100
3	c	270/285 (95%)	258 (96%)	12 (4%)	0	100	100
4	D	238/248 (96%)	229 (96%)	9 (4%)	0	100	100
4	d	238/248 (96%)	229 (96%)	9 (4%)	0	100	100
5	E	233/344 (68%)	228 (98%)	5 (2%)	0	100	100
5	e	233/344 (68%)	228 (98%)	5 (2%)	0	100	100
6	F	236/428 (55%)	228 (97%)	8 (3%)	0	100	100
6	f	236/428 (55%)	228 (97%)	8 (3%)	0	100	100
7	G	228/238 (96%)	220 (96%)	8 (4%)	0	100	100
7	g	228/238 (96%)	220 (96%)	8 (4%)	0	100	100
8	H	227/229 (99%)	219 (96%)	8 (4%)	0	100	100
8	h	227/229 (99%)	219 (96%)	8 (4%)	0	100	100
9	I	217/225 (96%)	205 (94%)	12 (6%)	0	100	100
9	i	217/225 (96%)	205 (94%)	12 (6%)	0	100	100
10	J	202/205 (98%)	189 (94%)	13 (6%)	0	100	100
10	j	202/205 (98%)	189 (94%)	13 (6%)	0	100	100
11	K	204/206 (99%)	196 (96%)	8 (4%)	0	100	100
11	k	204/206 (99%)	196 (96%)	8 (4%)	0	100	100
12	L	199/203 (98%)	186 (94%)	13 (6%)	0	100	100
12	l	199/203 (98%)	186 (94%)	13 (6%)	0	100	100
13	M	212/339 (62%)	202 (95%)	10 (5%)	0	100	100
13	m	212/339 (62%)	201 (95%)	11 (5%)	0	100	100
14	N	216/220 (98%)	207 (96%)	9 (4%)	0	100	100
14	n	216/220 (98%)	207 (96%)	9 (4%)	0	100	100
All	All	6304/7302 (86%)	6029 (96%)	275 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	193/197 (98%)	193 (100%)	0	100	100
1	a	193/197 (98%)	193 (100%)	0	100	100
2	B	188/190 (99%)	188 (100%)	0	100	100
2	b	188/190 (99%)	188 (100%)	0	100	100
3	C	229/241 (95%)	226 (99%)	3 (1%)	65	83
3	c	229/241 (95%)	226 (99%)	3 (1%)	65	83
4	D	201/208 (97%)	201 (100%)	0	100	100
4	d	201/208 (97%)	201 (100%)	0	100	100
5	E	197/301 (65%)	197 (100%)	0	100	100
5	e	197/301 (65%)	197 (100%)	0	100	100
6	F	200/363 (55%)	199 (100%)	1 (0%)	86	93
6	f	200/363 (55%)	199 (100%)	1 (0%)	86	93
7	G	185/190 (97%)	183 (99%)	2 (1%)	70	86
7	g	185/190 (97%)	183 (99%)	2 (1%)	70	86
8	H	184/184 (100%)	183 (100%)	1 (0%)	86	93
8	h	184/184 (100%)	183 (100%)	1 (0%)	86	93
9	I	180/185 (97%)	180 (100%)	0	100	100
9	i	180/185 (97%)	180 (100%)	0	100	100
10	J	167/168 (99%)	166 (99%)	1 (1%)	84	92
10	j	167/168 (99%)	166 (99%)	1 (1%)	84	92
11	K	172/172 (100%)	168 (98%)	4 (2%)	45	72
11	k	172/172 (100%)	168 (98%)	4 (2%)	45	72
12	L	162/164 (99%)	162 (100%)	0	100	100
12	l	162/164 (99%)	162 (100%)	0	100	100
13	M	181/288 (63%)	181 (100%)	0	100	100
13	m	181/288 (63%)	181 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	N	181/183 (99%)	179 (99%)	2 (1%)	70	86
14	n	181/183 (99%)	179 (99%)	2 (1%)	70	86
All	All	5240/6068 (86%)	5212 (100%)	28 (0%)	85	93

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	c	50	MET
14	n	127	ARG
6	f	168	ASN
11	k	87	ARG
3	c	232	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 42 such sidechains are listed below:

Mol	Chain	Res	Type
6	f	168	ASN
11	k	125	GLN
6	f	271	ASN
11	k	22	ASN
12	l	184	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](#)

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
15	BO2	i	301	9	25,29,29	0.42	0	32,38,38	1.19	5 (15%)
15	BO2	L	401	12	25,29,29	0.40	0	32,38,38	1.24	6 (18%)
16	N2E	l	402	-	30,37,37	2.31	8 (26%)	34,54,54	3.93	16 (47%)
15	BO2	l	401	12	25,29,29	0.46	0	32,38,38	1.15	5 (15%)
15	BO2	h	301	8	25,29,29	0.44	0	32,38,38	1.21	6 (18%)
15	BO2	I	301	9	25,29,29	0.41	0	32,38,38	1.20	5 (15%)
15	BO2	H	301	8	25,29,29	0.43	0	32,38,38	1.21	6 (18%)
16	N2E	L	402	-	30,37,37	2.32	8 (26%)	34,54,54	3.93	16 (47%)

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	BO2	i	301	9	-	9/22/28/28	0/2/2/2
15	BO2	L	401	12	-	10/22/28/28	0/2/2/2
16	N2E	l	402	-	-	3/12/16/16	0/5/5/5
15	BO2	l	401	12	-	6/22/28/28	0/2/2/2
15	BO2	h	301	8	-	4/22/28/28	0/2/2/2
15	BO2	I	301	9	-	9/22/28/28	0/2/2/2
15	BO2	H	301	8	-	4/22/28/28	0/2/2/2
16	N2E	L	402	-	-	3/12/16/16	0/5/5/5

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	l	402	N2E	C7-N6	-7.18	1.25	1.35
16	L	402	N2E	C7-N6	-7.18	1.25	1.35
16	L	402	N2E	C5-N6	6.00	1.43	1.35
16	l	402	N2E	C5-N6	5.97	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	L	402	N2E	C9-C1	5.21	1.48	1.39

The worst 5 of 65 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	l	402	N2E	N4-C5-N6	-17.49	102.98	114.56
16	L	402	N2E	N4-C5-N6	-17.49	102.99	114.56
16	L	402	N2E	C1-C9-N8	-8.25	117.92	125.55
16	l	402	N2E	C1-C9-N8	-8.22	117.94	125.55
16	L	402	N2E	C32-C27-N28	-4.47	119.17	123.05

There are no chirality outliers.

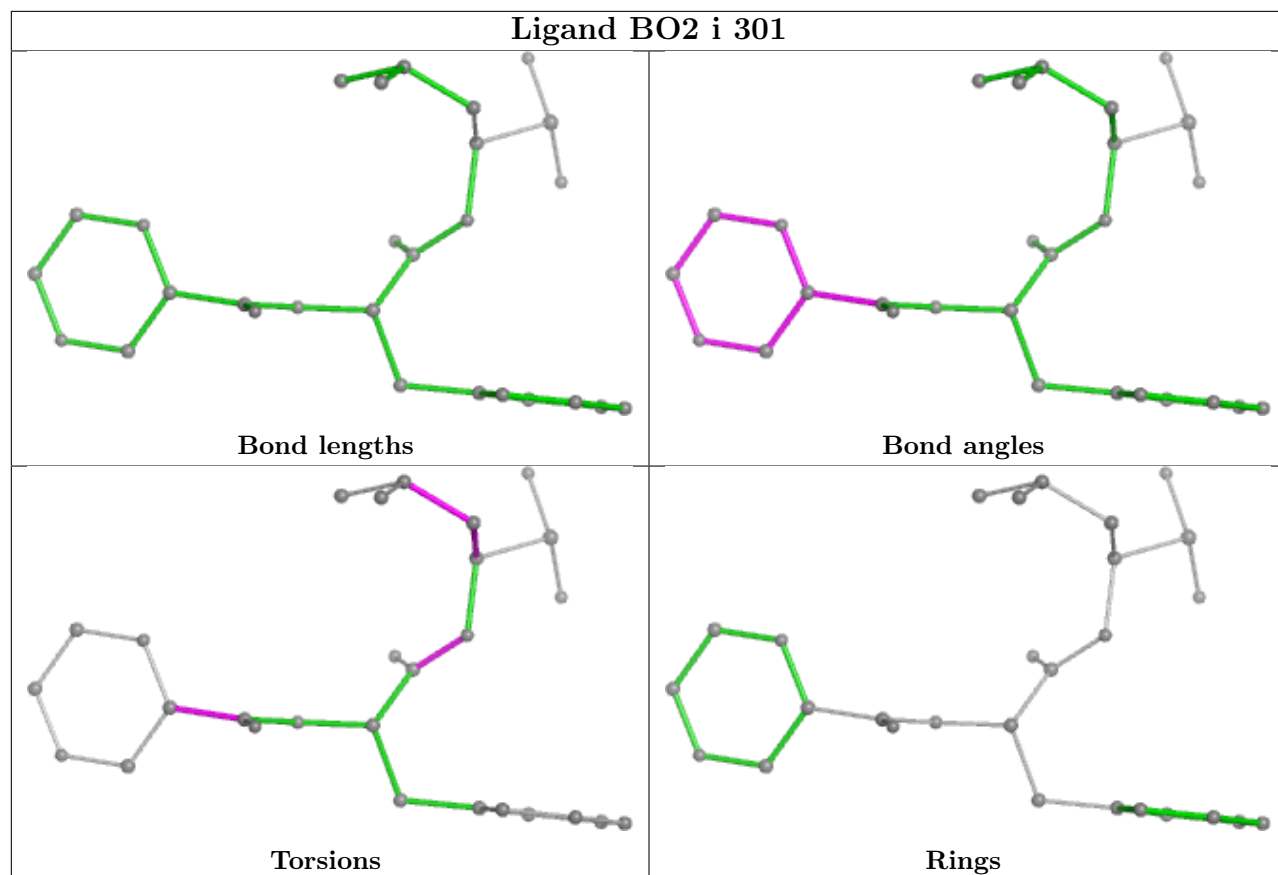
5 of 48 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	H	301	BO2	C3-C2-C7-O8
15	H	301	BO2	C3-C2-C7-N9
15	I	301	BO2	N1-C2-C7-O8
15	I	301	BO2	N1-C2-C7-N9
15	I	301	BO2	C3-C2-C7-O8

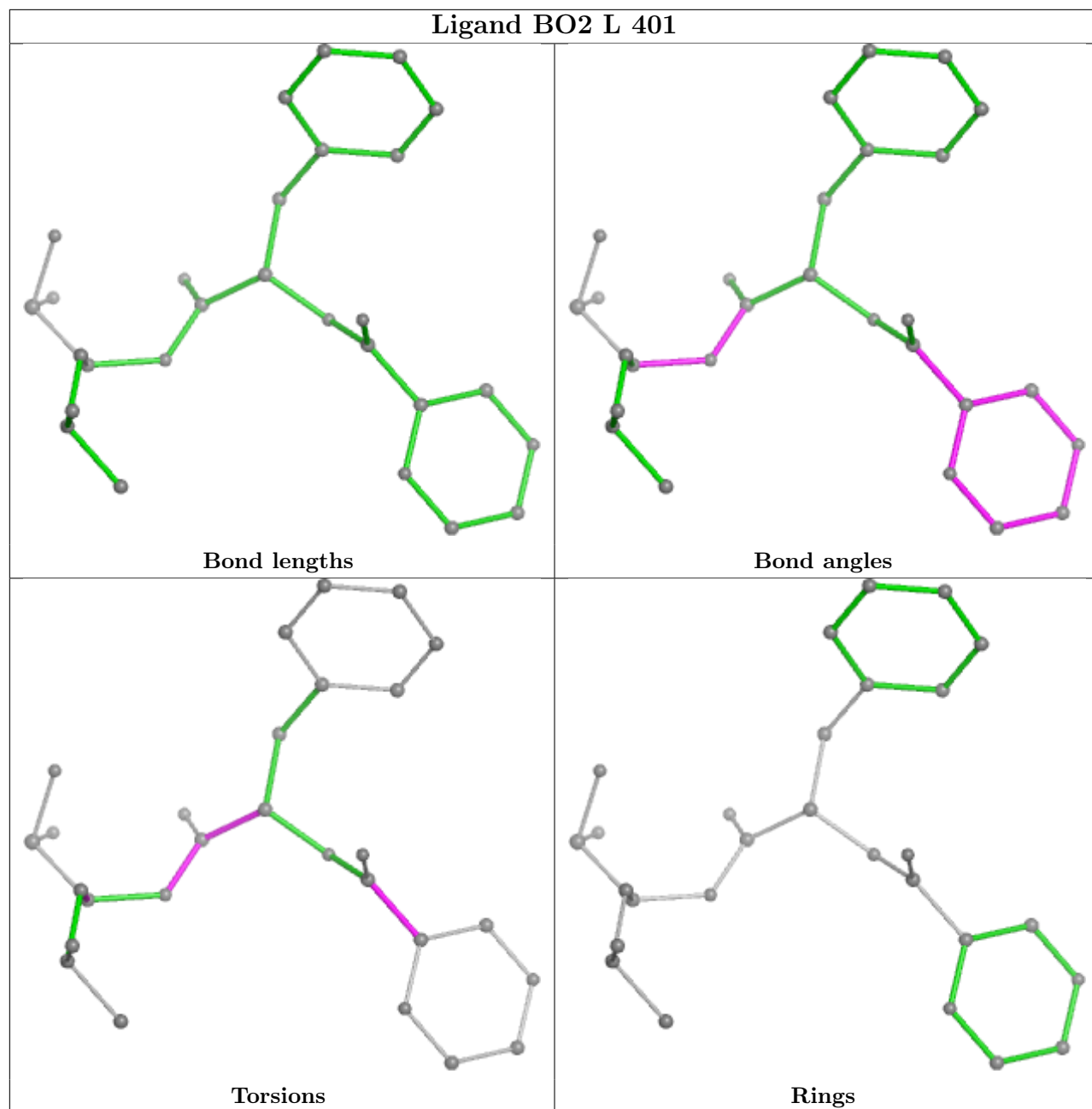
There are no ring outliers.

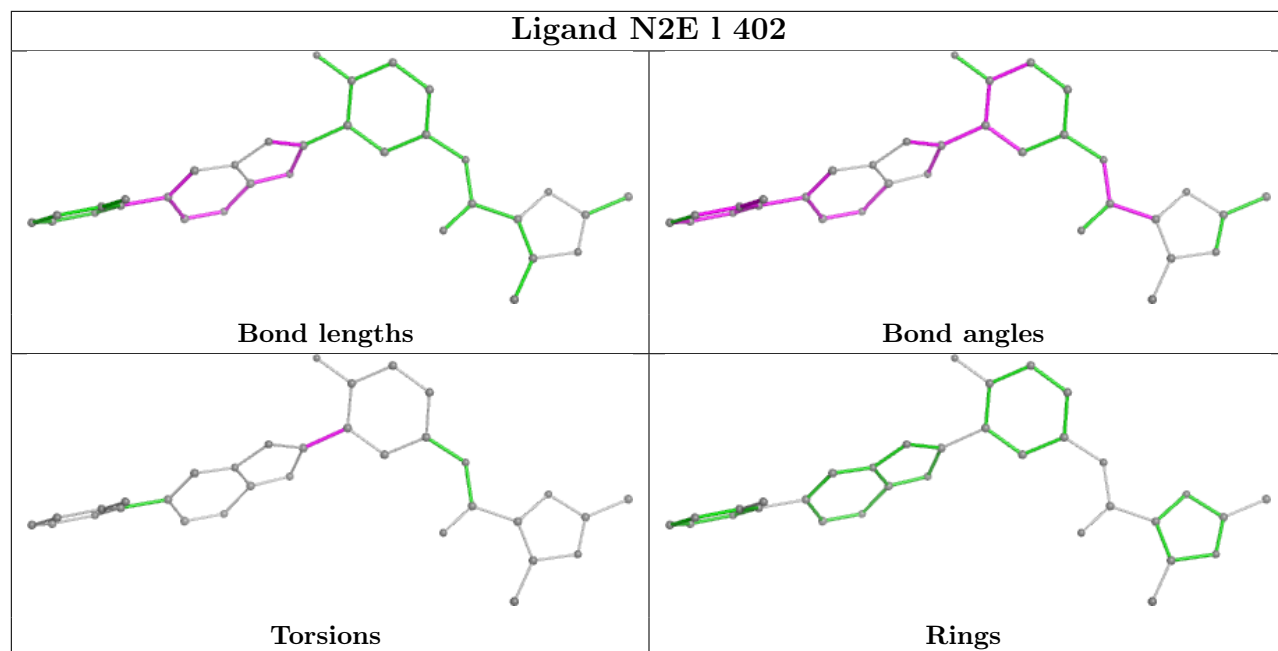
No monomer is involved in short contacts.

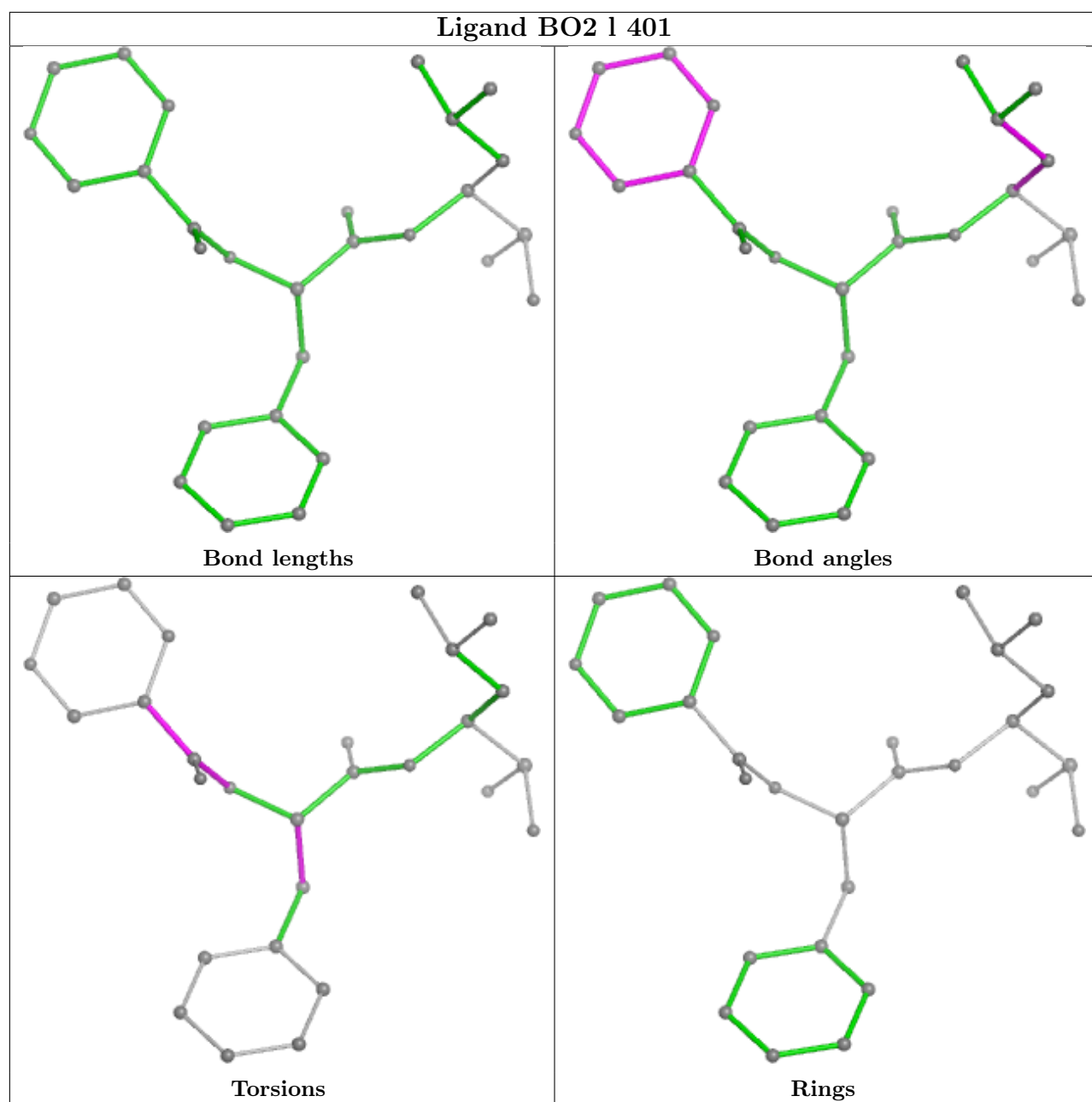
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



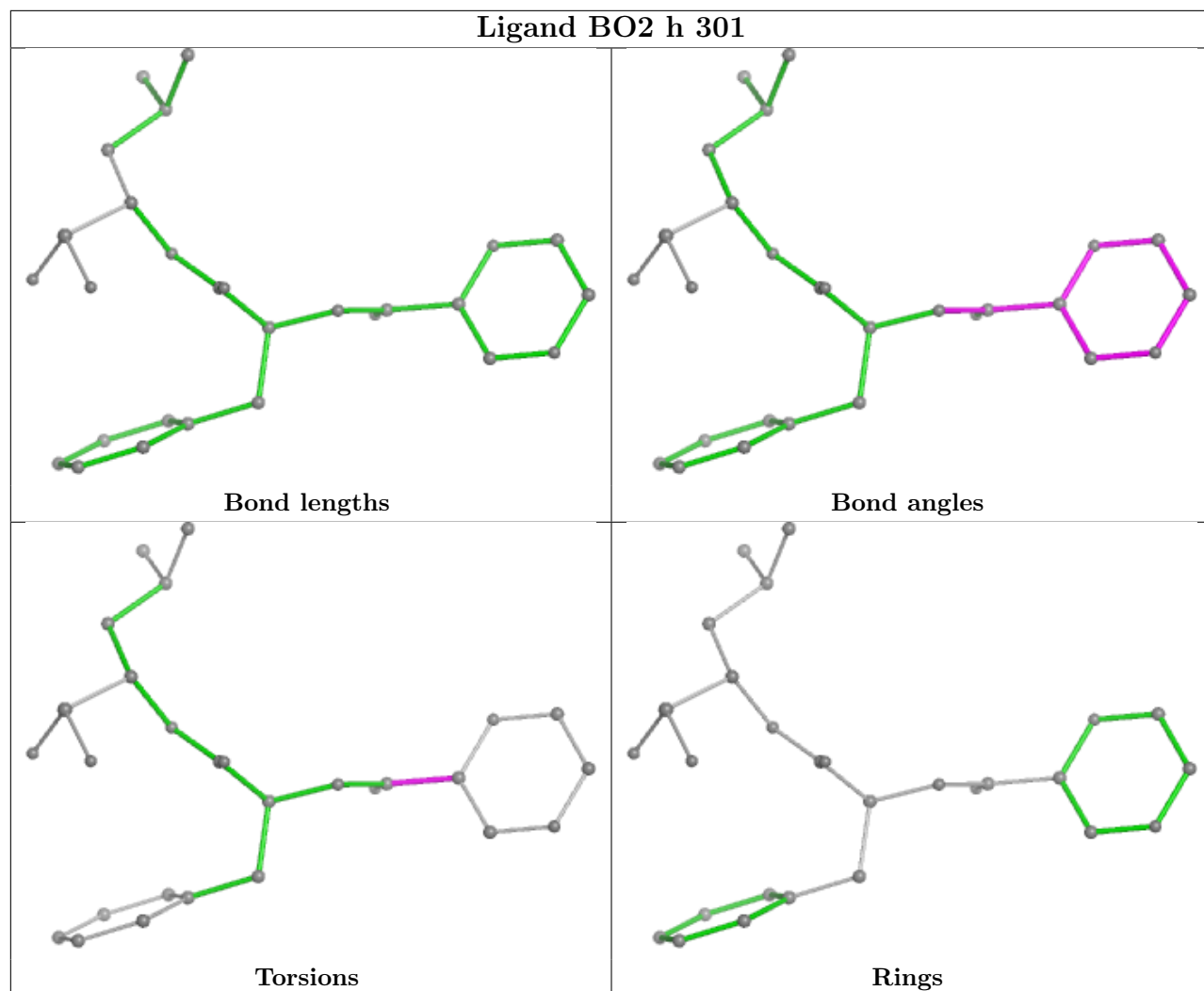
Ligand BO2 L 401

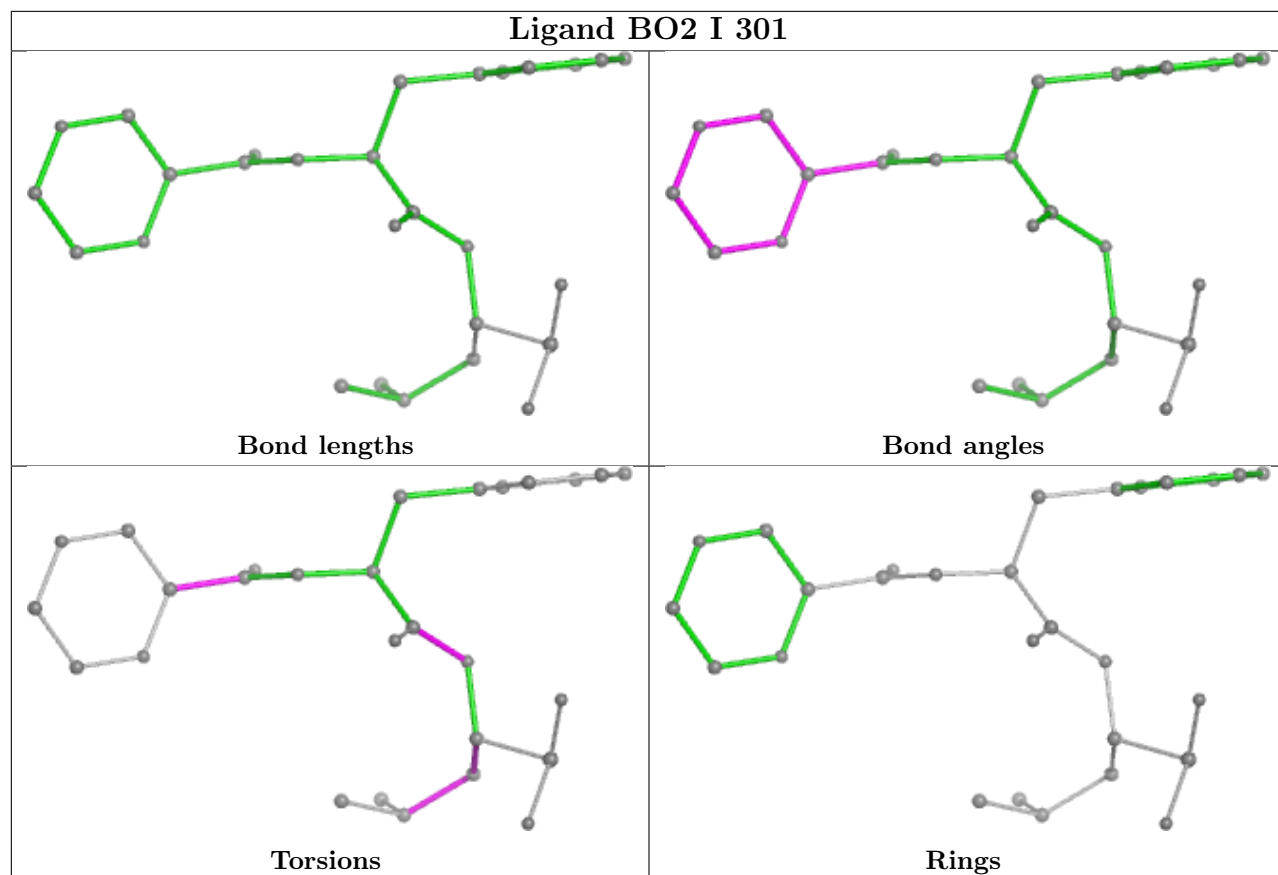




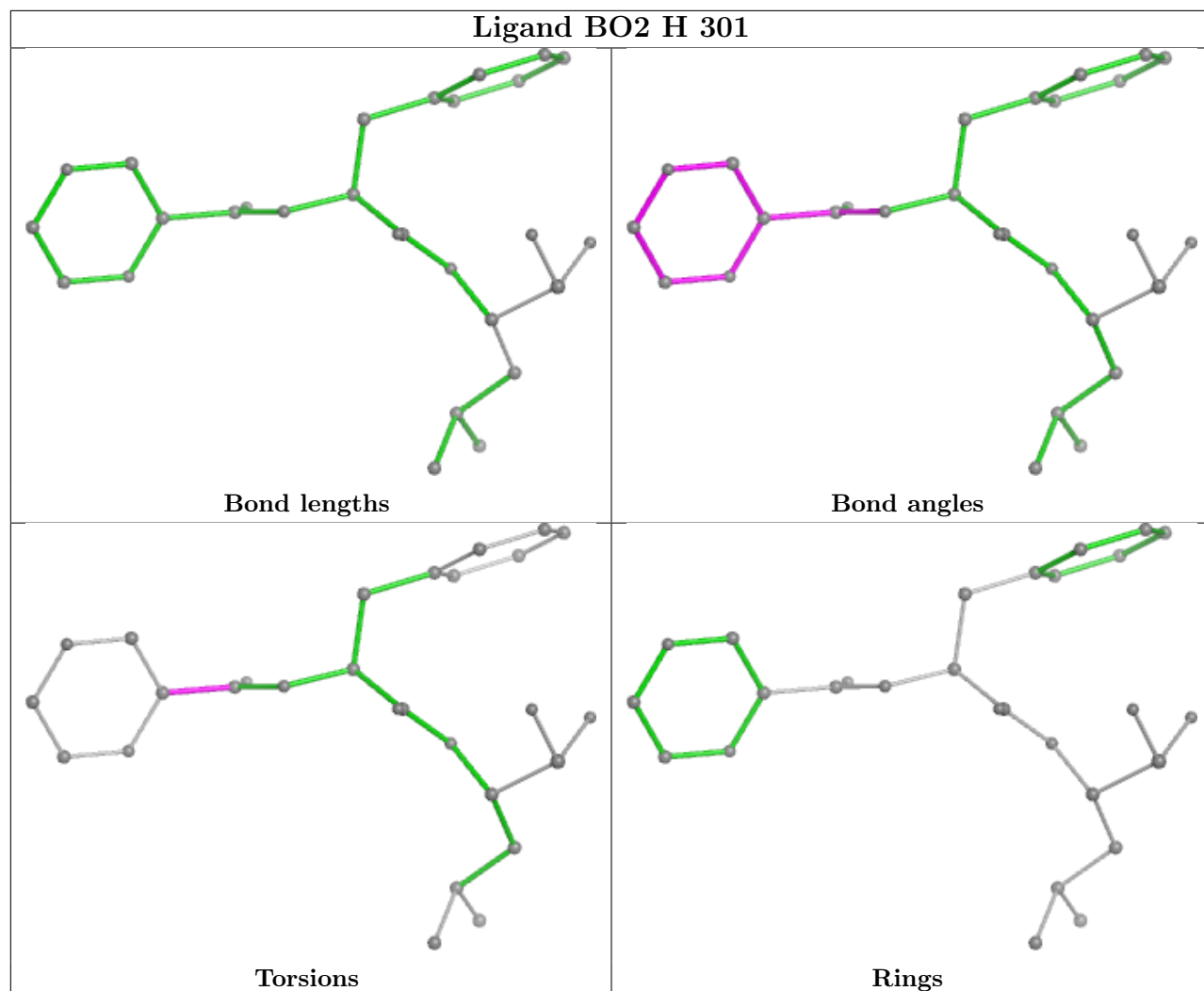


Ligand BO2 h 301

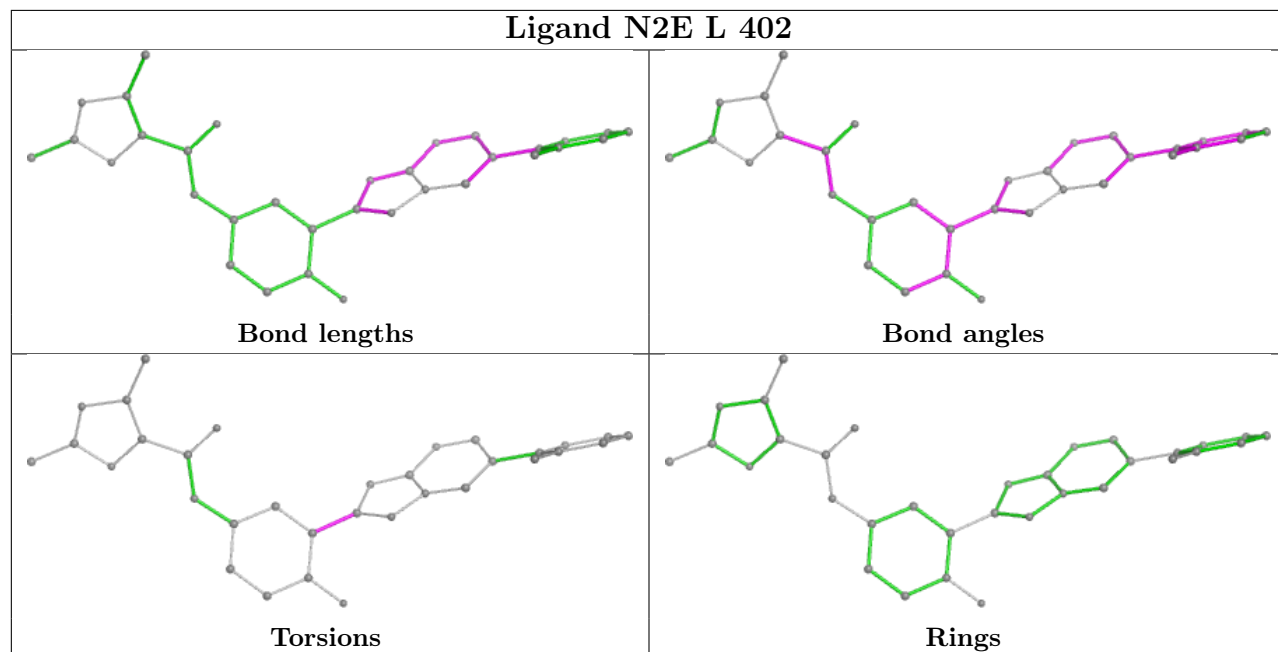




Ligand BO2 H 301



Ligand N2E L 402



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.

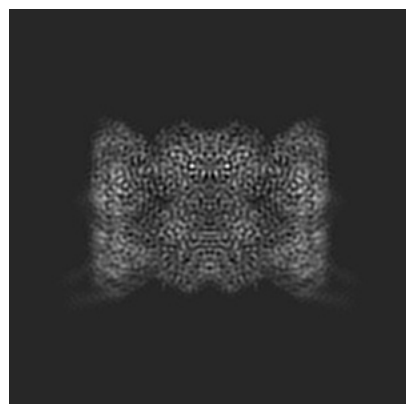
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10463. These allow visual inspection of the internal detail of the map and identification of artifacts.

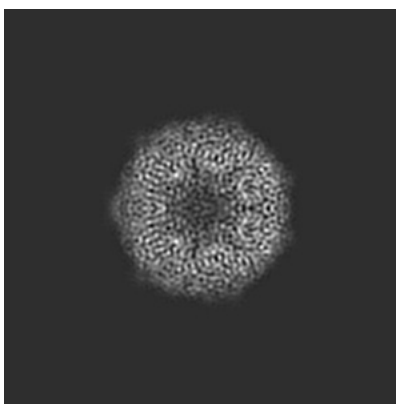
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

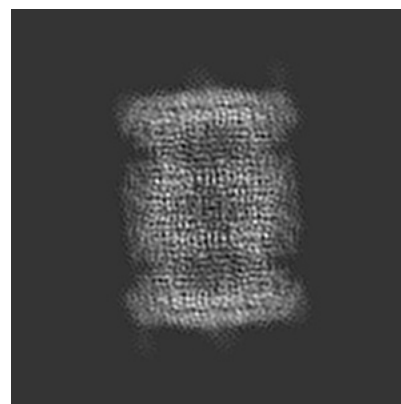
6.1.1 Primary map



X

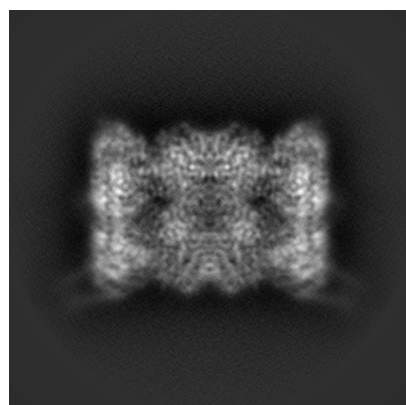


Y

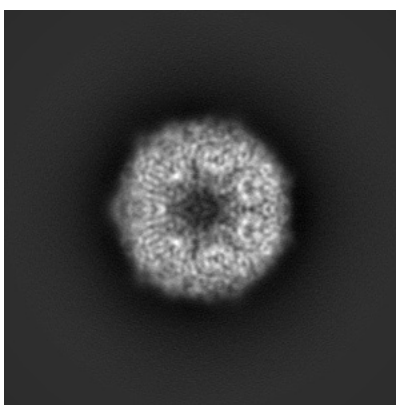


Z

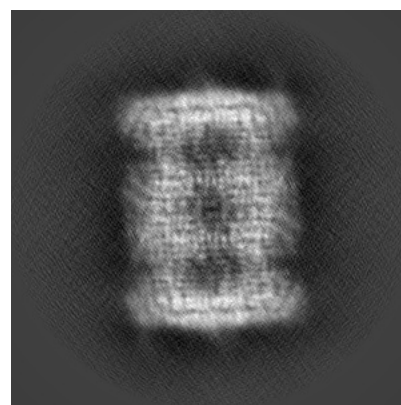
6.1.2 Raw map



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

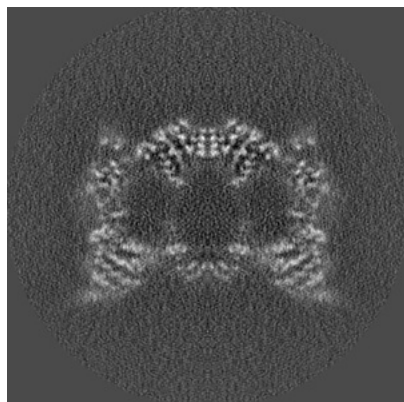


Y Index: 150

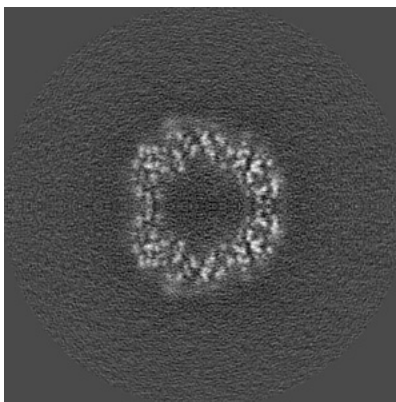


Z Index: 150

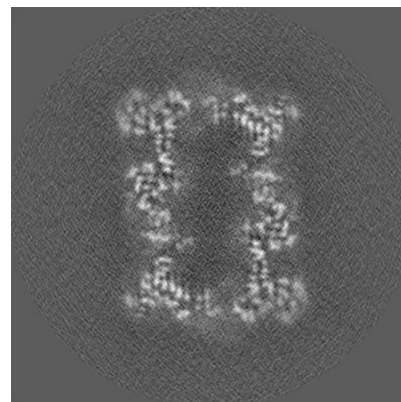
6.2.2 Raw map



X Index: 150



Y Index: 150

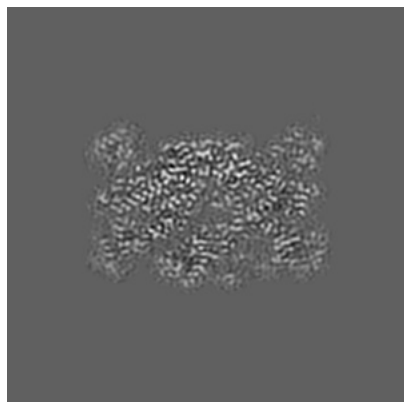


Z Index: 150

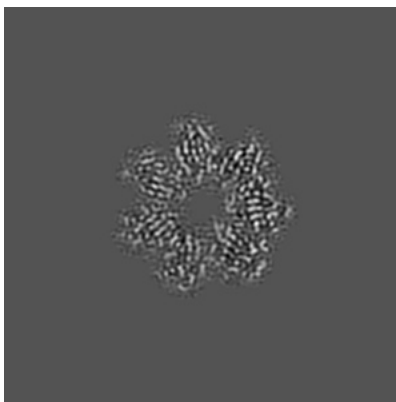
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

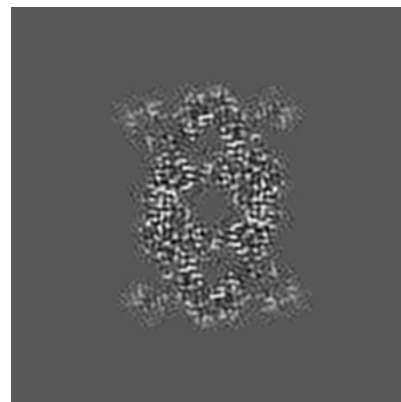
6.3.1 Primary map



X Index: 183

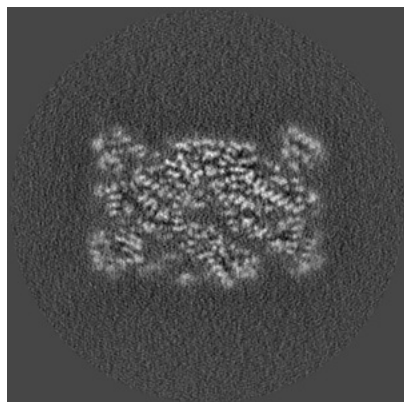


Y Index: 129

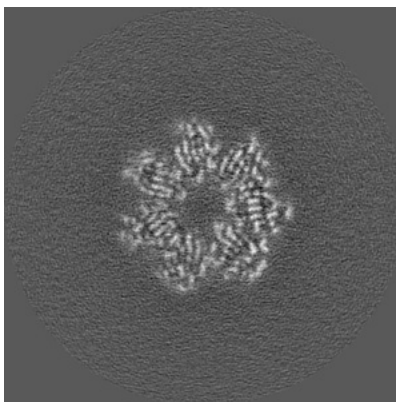


Z Index: 176

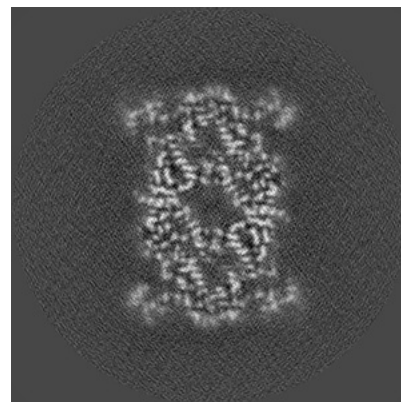
6.3.2 Raw map



X Index: 117



Y Index: 129

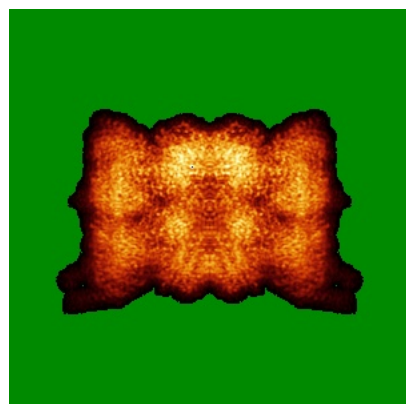


Z Index: 177

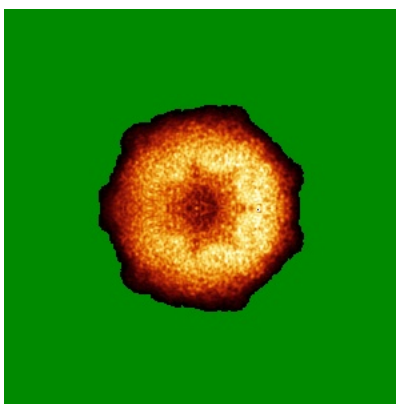
The images above show the largest variance slices of the map in three orthogonal directions.

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

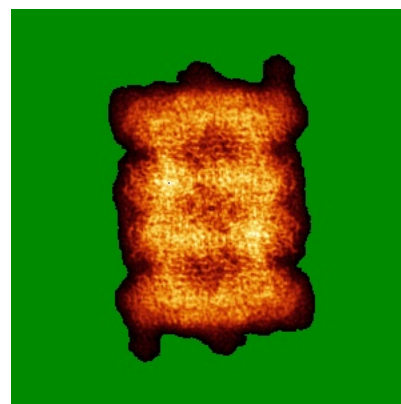
6.4.1 Primary map



X

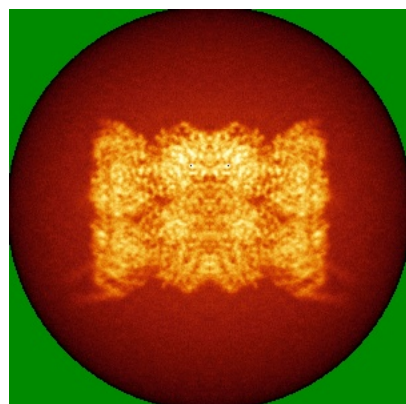


Y

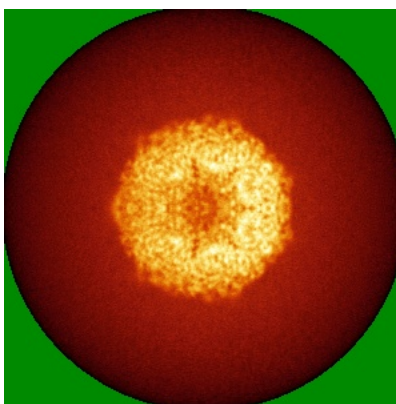


Z

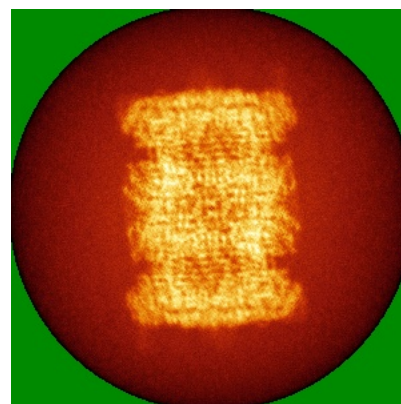
6.4.2 Raw map



X



Y

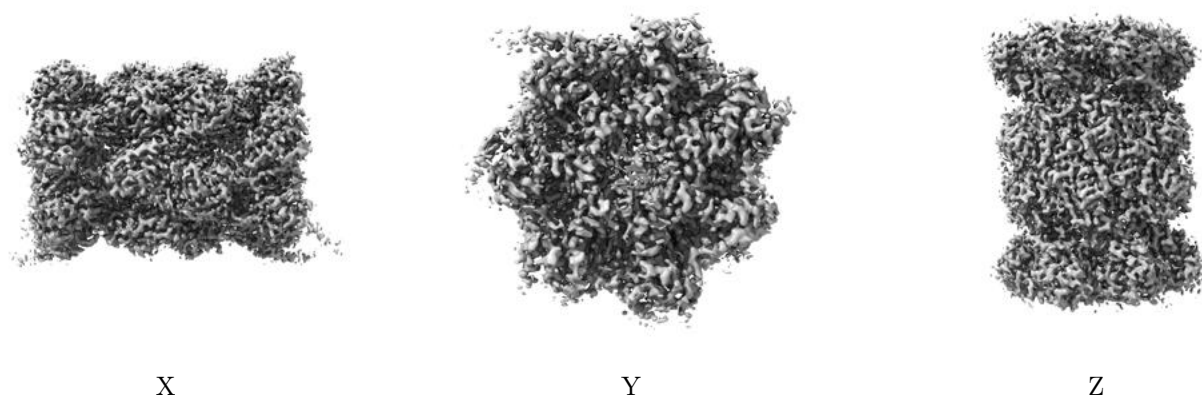


Z

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.

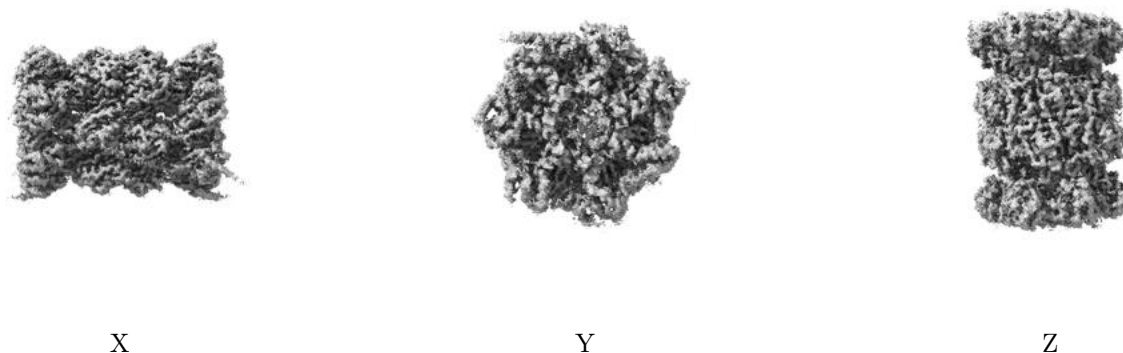
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. 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.

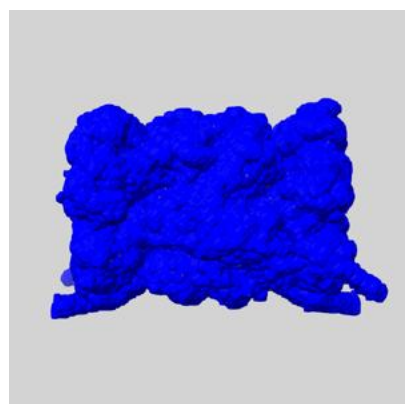
6.6 Mask visualisation [i](#)

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

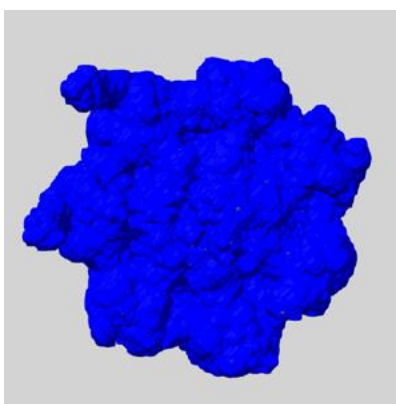
A mask typically either:

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

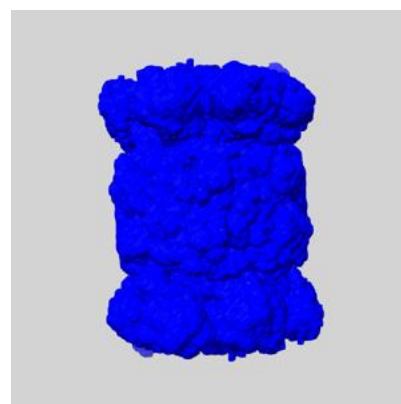
6.6.1 emd_10463_msk_1.map [i](#)



X



Y

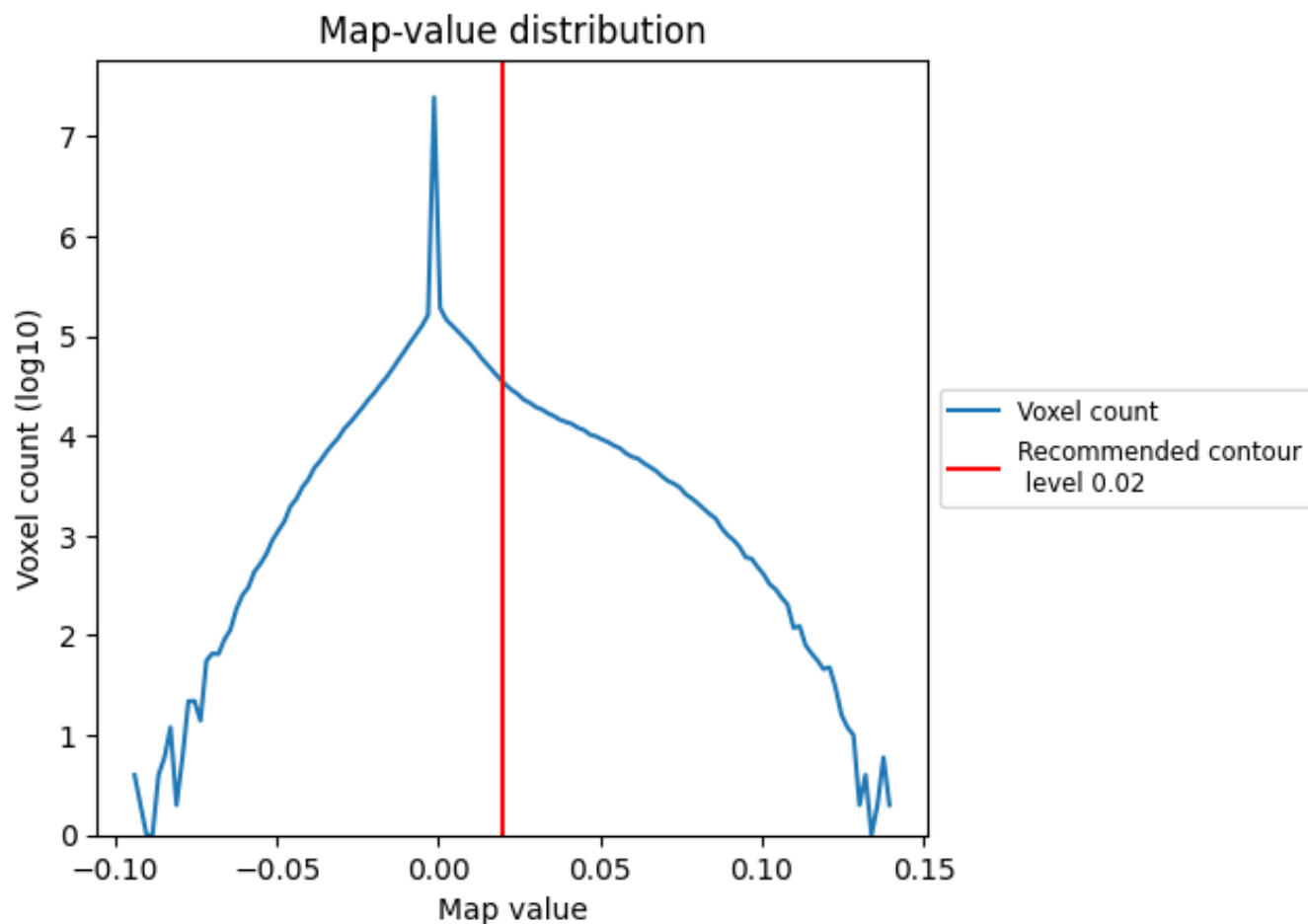


Z

7 Map analysis [i](#)

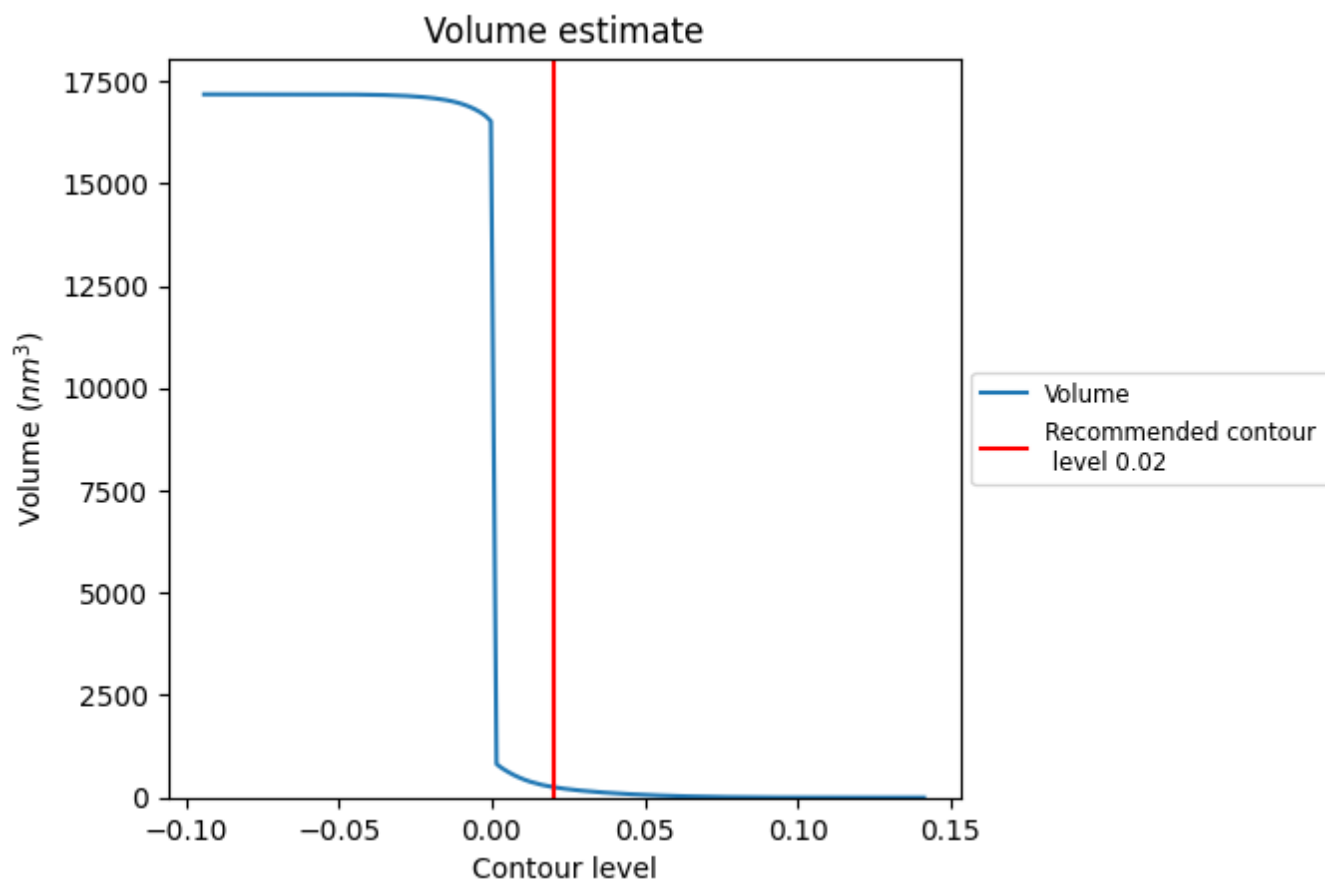
This section contains the results of statistical analysis of the map.

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.

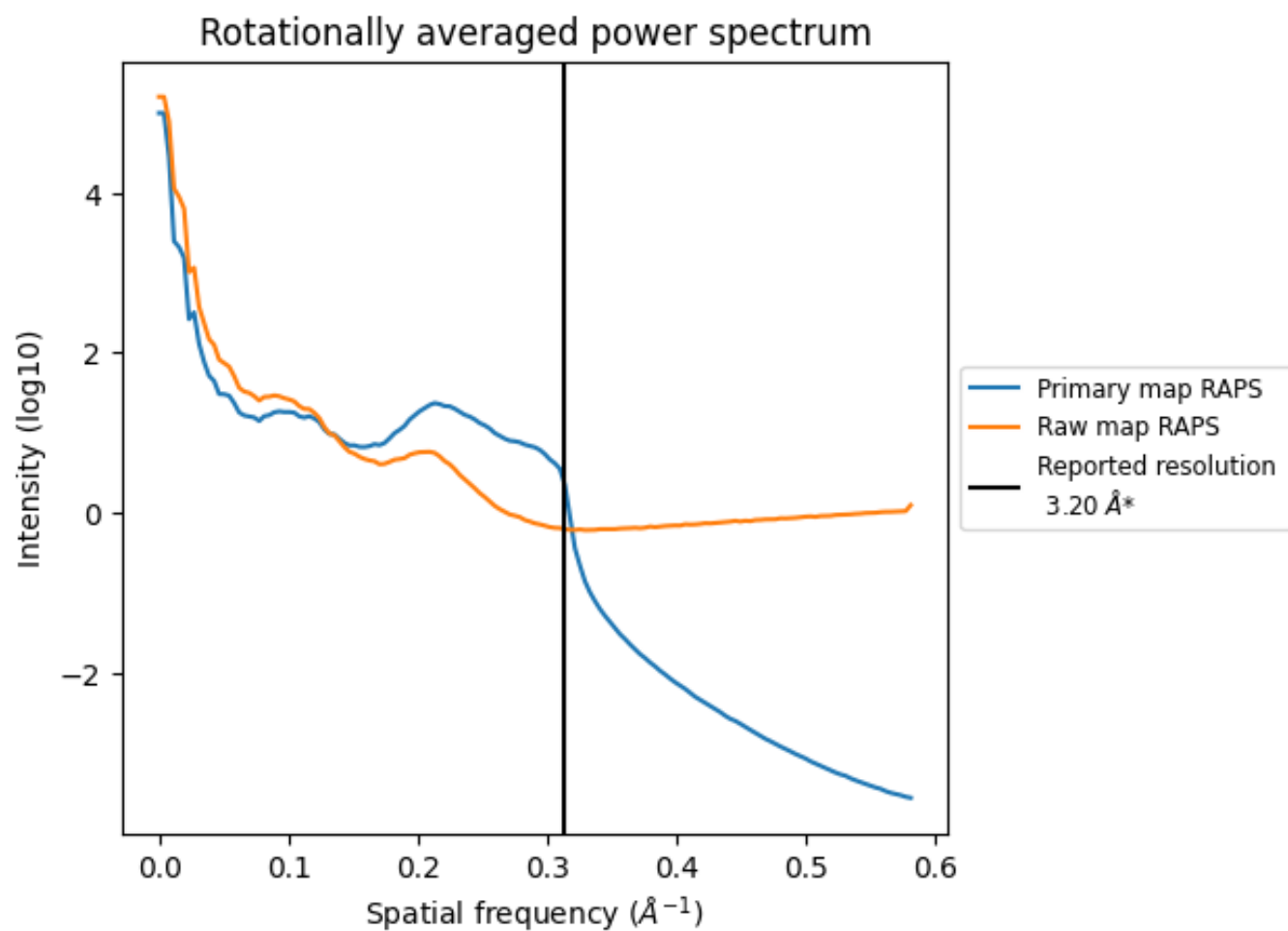
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 257 nm³; this corresponds to an approximate mass of 232 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 ⓘ

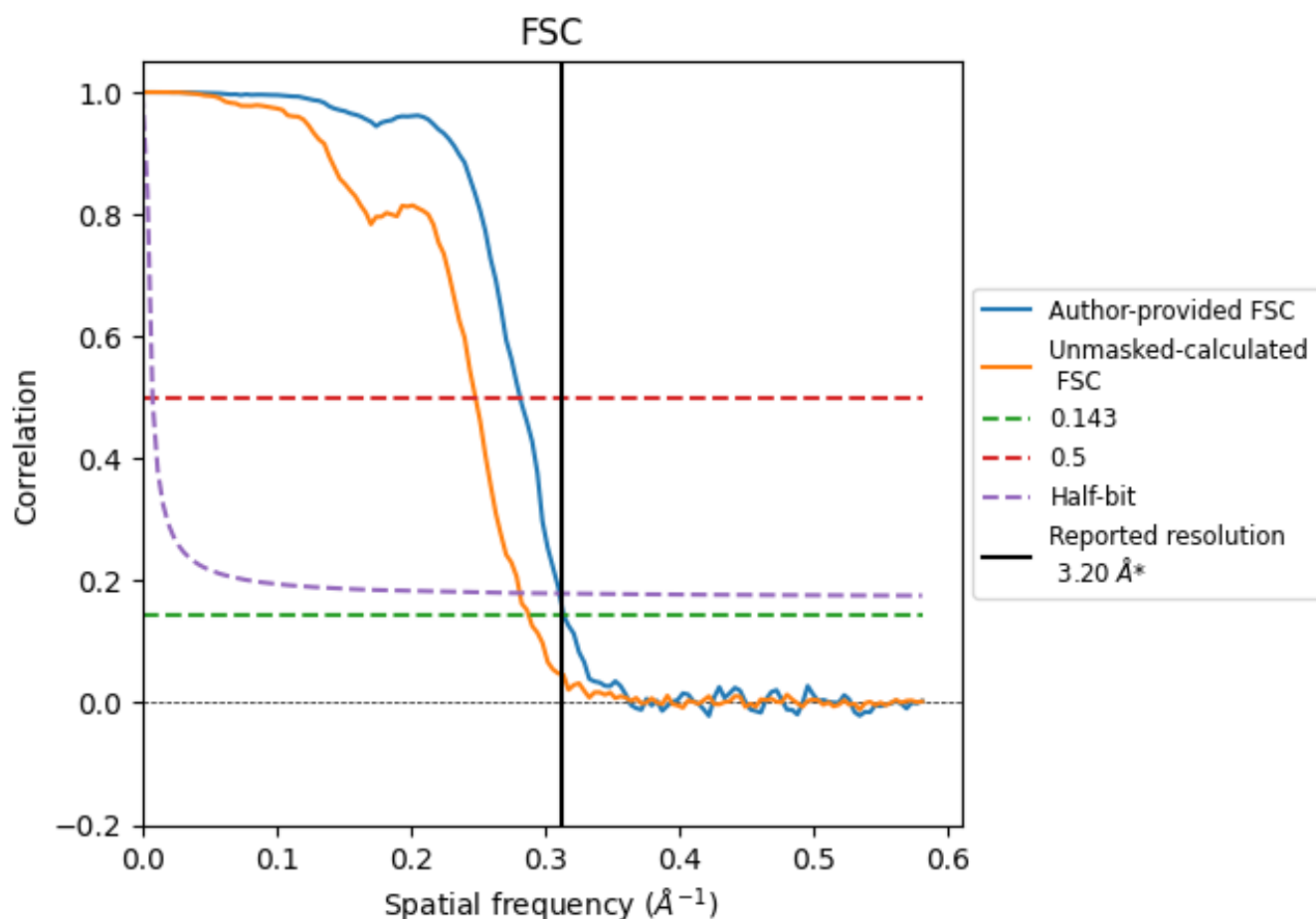


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

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 0.312 \AA^{-1}

8.2 Resolution estimates [i](#)

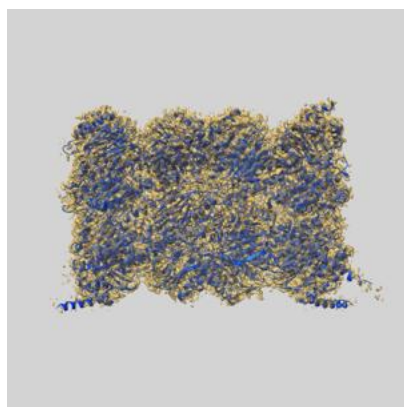
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.18	3.55	3.22
Unmasked-calculated*	3.47	4.03	3.55

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

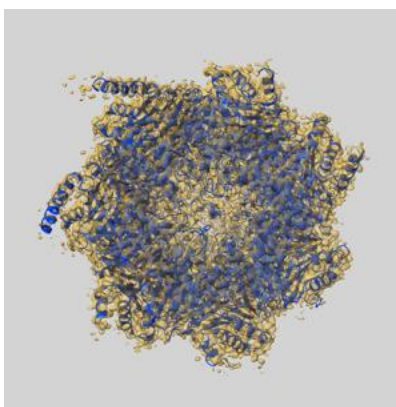
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-10463 and PDB model 6TD5. Per-residue inclusion information can be found in section [3](#) on page [9](#).

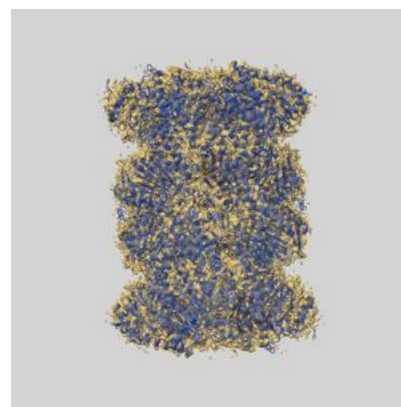
9.1 Map-model overlay [i](#)



X



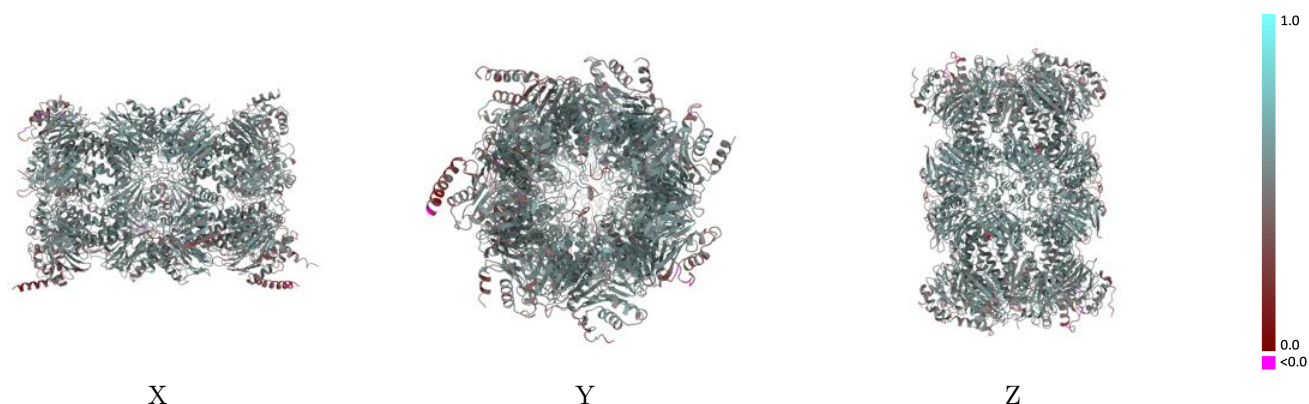
Y



Z

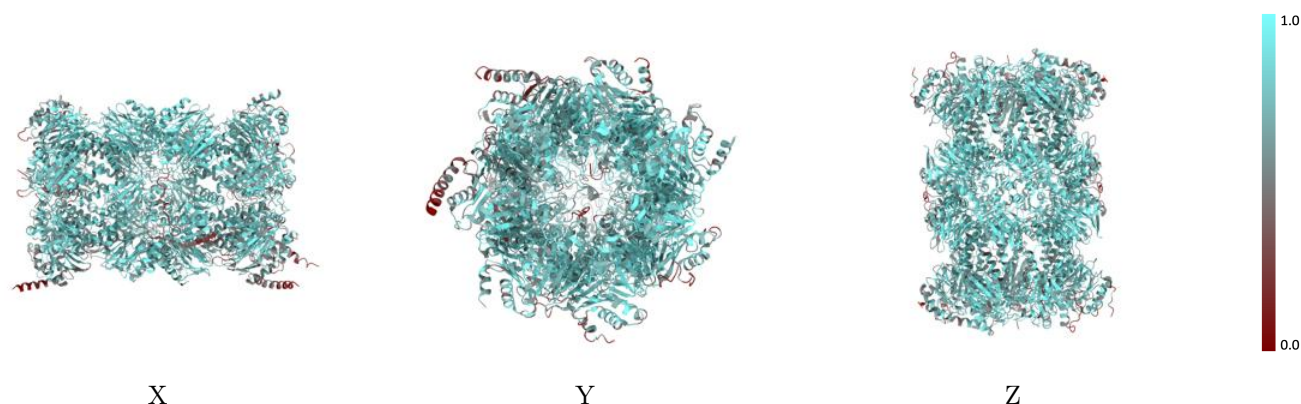
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



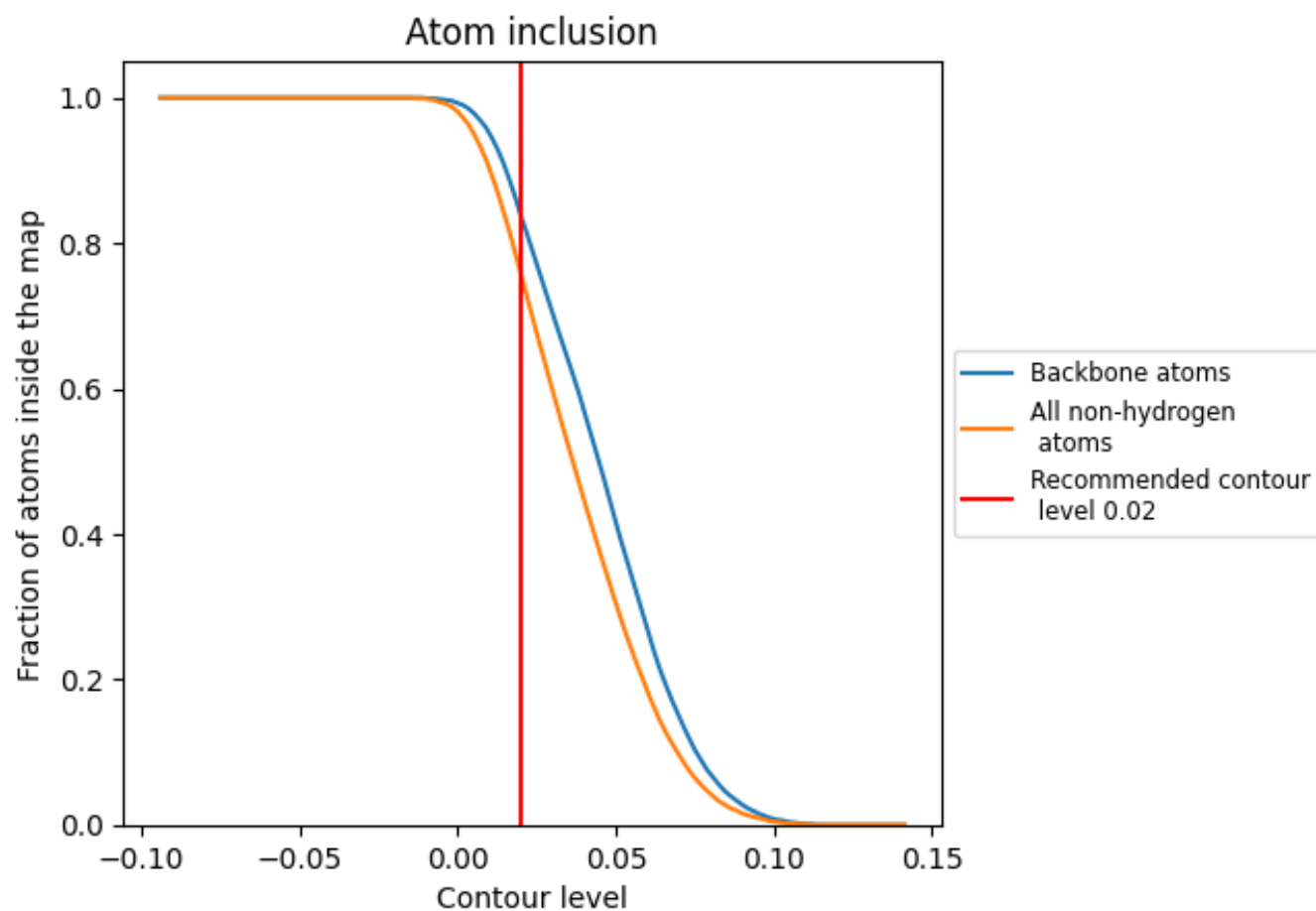
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).



























































9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 76% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7560	 0.5120
A	 0.7690	 0.5110
B	 0.7510	 0.5140
C	 0.6890	 0.4860
D	 0.6370	 0.4490
E	 0.7220	 0.5000
F	 0.7530	 0.5130
G	 0.7310	 0.4910
H	 0.8650	 0.5640
I	 0.7540	 0.5150
J	 0.7980	 0.5310
K	 0.7170	 0.5060
L	 0.8030	 0.5280
M	 0.7860	 0.5190
N	 0.8370	 0.5490
a	 0.7680	 0.5110
b	 0.7550	 0.5160
c	 0.6900	 0.4850
d	 0.6420	 0.4500
e	 0.7220	 0.4960
f	 0.7540	 0.5150
g	 0.7300	 0.4920
h	 0.8670	 0.5670
i	 0.7550	 0.5130
j	 0.7980	 0.5310
k	 0.7230	 0.5060
l	 0.8020	 0.5240
m	 0.7800	 0.5180
n	 0.8350	 0.5510

