wwPDB EM Validation Summary Report

Oct 26, 2026 – 12:37 pm GMT

PDB ID	:	9SDR / pdb_00009sdr
EMDB ID	:	EMD-54791
Title	:	CryoEM structure of human 20S proteasome in complex with proteasome inhibitor Carmaphycin B
Authors	:	Havlikova, J.; Sulzen, H.; Boura, E.; Fajtova, P.; Silhan, J.
Deposited on	:	2025-08-14
Resolution	:	2.78 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:

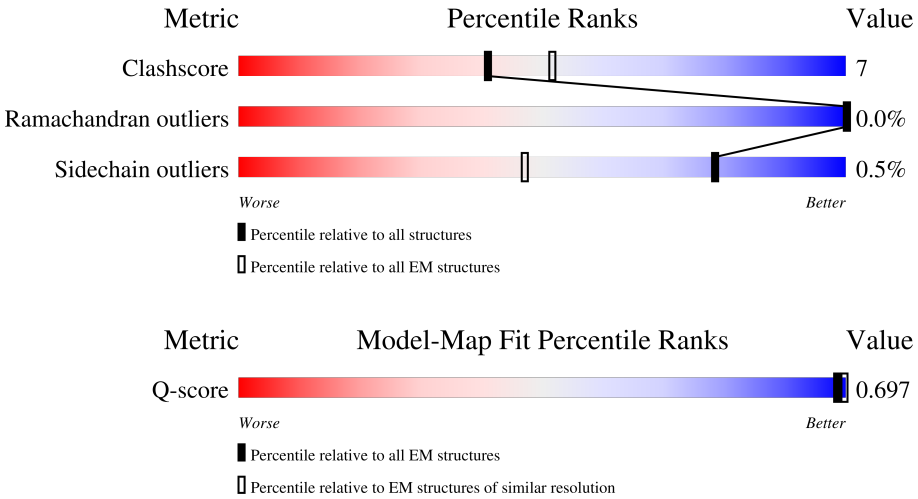
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.2
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.78 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10754 (2.28 - 3.28)

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 <=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	79% 20%
1	O	246	80% 18%
2	B	234	86% 12%
2	P	234	85% 13%

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Mol	Chain	Length	Quality of chain
3	C	261	83% 14%
3	Q	261	84% 14%
4	E	241	86% 12%
4	R	241	86% 12%
5	F	263	70% 20% 10%
5	S	263	70% 20% 10%
6	G	255	82% 12% 6%
6	T	255	83% 11% 6%
7	J	204	87% 13%
7	V	204	88% 12%
8	K	201	85% 13%
8	W	201	86% 12%
9	M	213	86% 13%
9	X	213	85% 15%
10	N	219	81% 17%
10	Y	219	84% 15%
11	D	248	87% 9%
11	Z	248	88% 8%
12	H	205	86% 12%
12	a	205	86% 13%
13	I	234	77% 17% 6%
13	b	234	77% 17% 6%
14	L	200	86% 14%
14	c	200	86% 13%
15	U	3	100% 33% 67%

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Mol	Chain	Length	Quality of chain
15	d	3	33% 33% 33% 33%
15	e	3	100%
15	f	3	100% 33% 67%
15	g	3	33% 33% 33% 33%
15	h	3	67% 33%

2 Entry composition (i)

There are 16 unique types of molecules in this entry. The entry contains 48958 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	242	Total	C	N	O	S	0	0
			1886	1197	315	361	13		
1	O	242	Total	C	N	O	S	0	0
			1886	1197	315	361	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	230	Total	C	N	O	S	0	0
			1792	1147	302	337	6		
2	P	230	Total	C	N	O	S	0	0
			1792	1147	302	337	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	255	Total	C	N	O	S	0	0
			2016	1272	347	387	10		
3	Q	255	Total	C	N	O	S	0	0
			2016	1272	347	387	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	236	Total	C	N	O	S	0	0
			1804	1133	297	363	11		
4	R	236	Total	C	N	O	S	0	0
			1804	1133	297	363	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	237	Total	C	N	O	S	0	0
			1864	1167	335	351	11		
5	S	237	Total	C	N	O	S	0	0
			1864	1167	335	351	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	240	Total	C	N	O	S	0	0
			1881	1193	321	356	11		
6	T	240	Total	C	N	O	S	0	0
			1881	1193	321	356	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	J	204	Total	C	N	O	S	0	0
			1590	1013	265	293	19		
7	V	204	Total	C	N	O	S	0	0
			1590	1013	265	293	19		

- Molecule 8 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	K	197	Total	C	N	O	S	0	0
			1578	1011	268	290	9		
8	W	197	Total	C	N	O	S	0	0
			1578	1011	268	290	9		

- Molecule 9 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	M	212	Total	C	N	O	S	0	0
			1642	1041	280	311	10		
9	X	212	Total	C	N	O	S	0	0
			1642	1041	280	311	10		

- Molecule 10 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	N	216	Total	C	N	O	S	1	0
			1695	1068	292	323	12		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	Y	216	Total	C	N	O	S	1	0
			1695	1068	292	323	12		

- Molecule 11 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	D	239	Total	C	N	O	S	0	0
			1887	1183	334	365	5		
11	Z	239	Total	C	N	O	S	0	0
			1887	1183	334	365	5		

- Molecule 12 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	H	202	Total	C	N	O	S	0	0
			1514	949	258	295	12		
12	a	202	Total	C	N	O	S	0	0
			1514	949	258	295	12		

- Molecule 13 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	I	221	Total	C	N	O	S	0	0
			1667	1050	284	321	12		
13	b	221	Total	C	N	O	S	0	0
			1667	1050	284	321	12		

- Molecule 14 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	L	200	Total	C	N	O	S	0	0
			1555	980	273	293	9		
14	c	200	Total	C	N	O	S	0	0
			1555	980	273	293	9		

- Molecule 15 is a protein called Carmaphycin B, bound form.

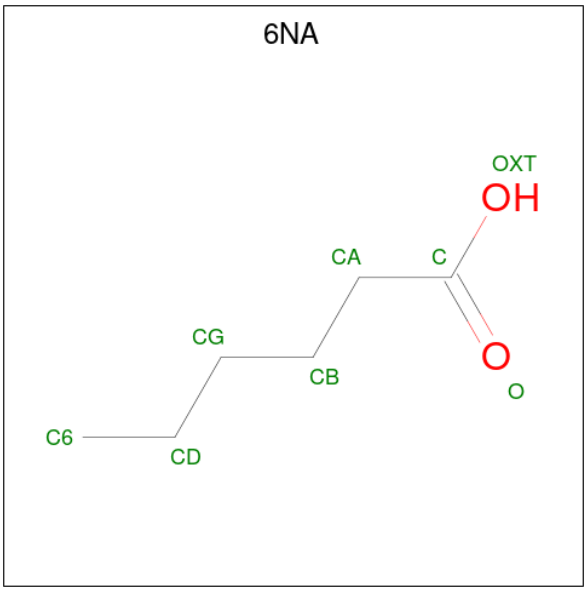
Mol	Chain	Residues	Atoms					AltConf	Trace
15	U	3	Total	C	N	O	S	0	0
			29	19	3	6	1		
15	d	3	Total	C	N	O	S	0	0
			29	19	3	6	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
15	e	3	Total	C	N	O	S	0	0
			29	19	3	6	1		
15	f	3	Total	C	N	O	S	0	0
			29	19	3	6	1		
15	g	3	Total	C	N	O	S	0	0
			29	19	3	6	1		
15	h	3	Total	C	N	O	S	0	0
			29	19	3	6	1		

- Molecule 16 is HEXANOIC ACID (CCD ID: 6NA) (formula: $C_6H_{12}O_2$) (labeled as "Ligand of Interest" by depositor).



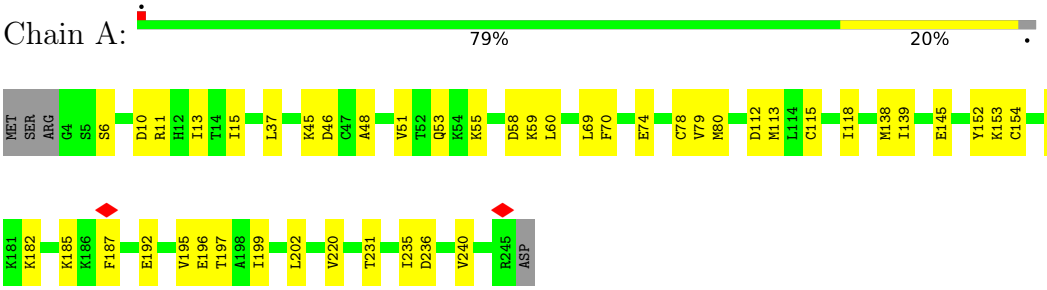
Mol	Chain	Residues	Atoms				AltConf
16	U	1	Total	C	O		0
			7	6	1		
16	d	1	Total	C	O		0
			7	6	1		
16	e	1	Total	C	O		0
			7	6	1		
16	f	1	Total	C	O		0
			7	6	1		
16	g	1	Total	C	O		0
			7	6	1		
16	h	1	Total	C	O		0
			7	6	1		

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.

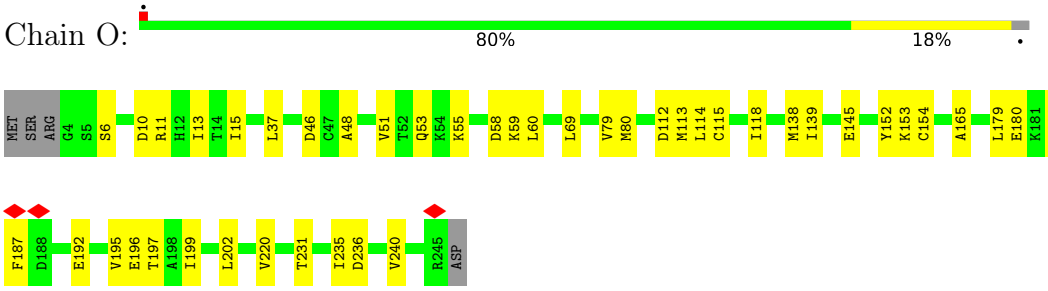
• Molecule 1: Proteasome subunit alpha type-6

Chain A:



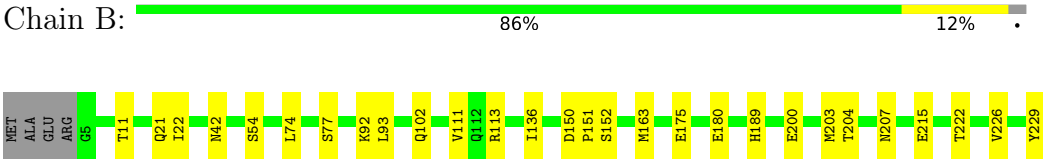
• Molecule 1: Proteasome subunit alpha type-6

Chain O:



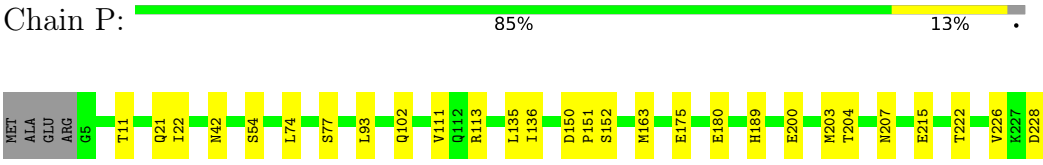
• Molecule 2: Proteasome subunit alpha type-2

Chain B:



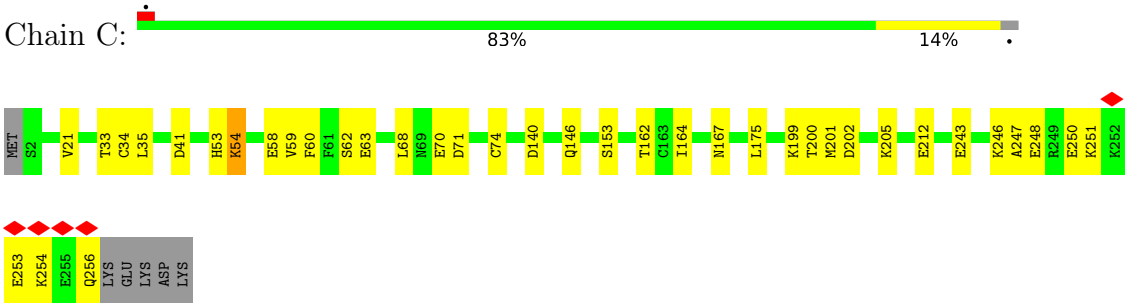
• Molecule 2: Proteasome subunit alpha type-2

Chain P:



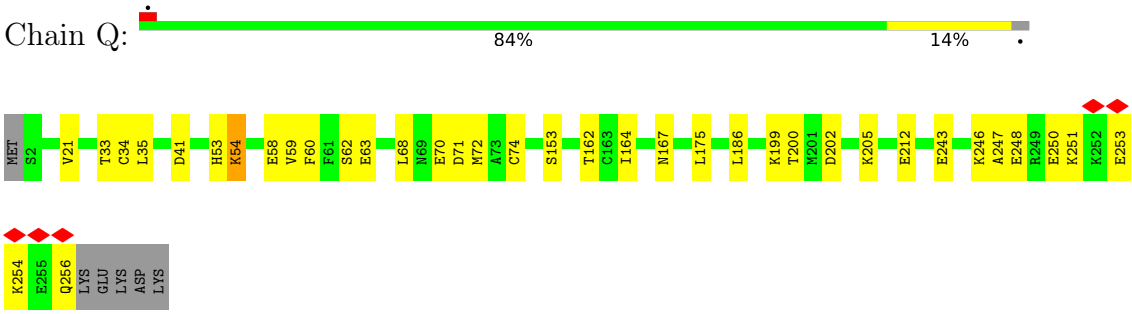
• Molecule 3: Proteasome subunit alpha type-4

Chain C:



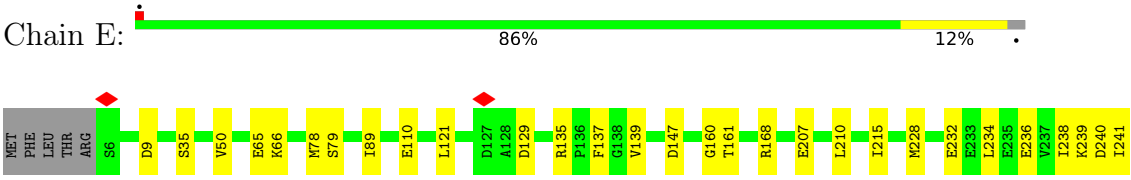
• Molecule 3: Proteasome subunit alpha type-4

Chain Q:



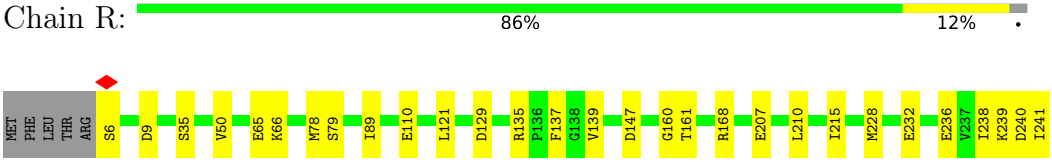
• Molecule 4: Proteasome subunit alpha type-5

Chain E:



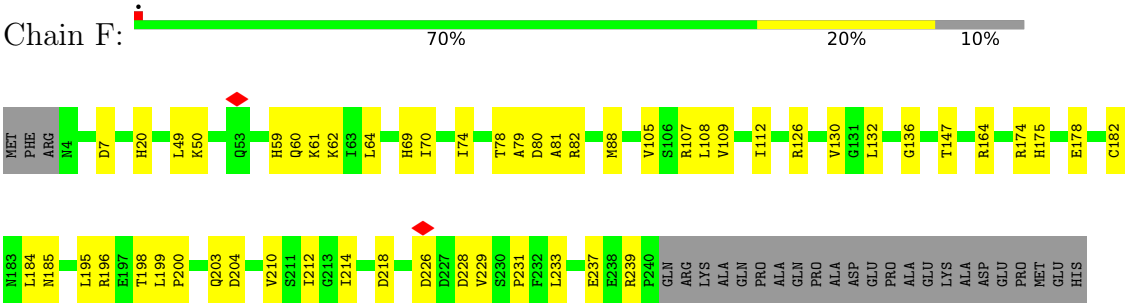
• Molecule 4: Proteasome subunit alpha type-5

Chain R:



• Molecule 5: Proteasome subunit alpha type-1

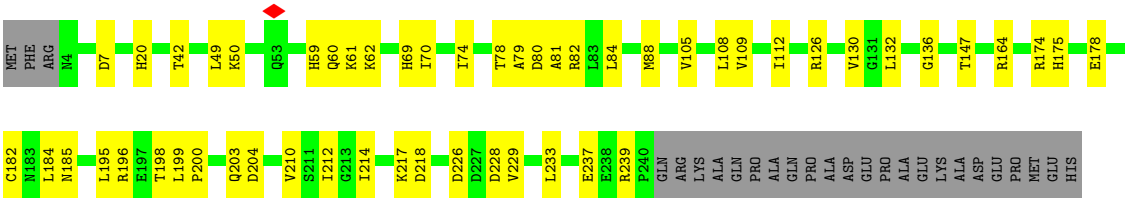
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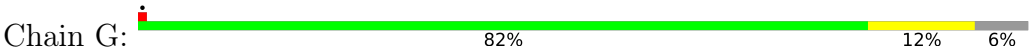
• Molecule 5: Proteasome subunit alpha type-1

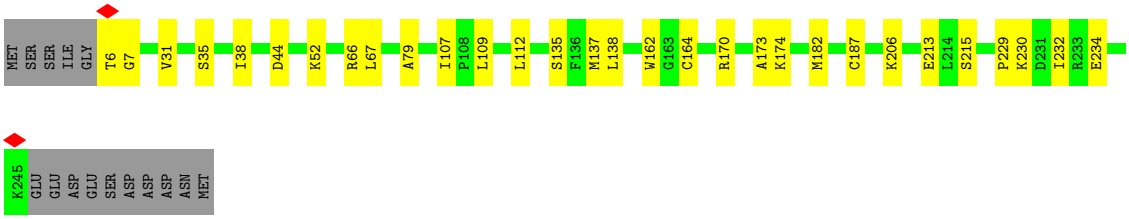
Chain S:



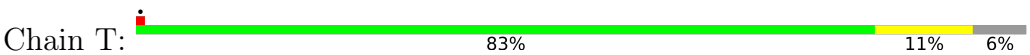


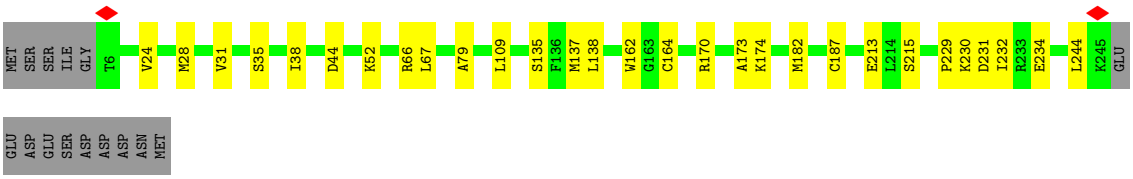
• Molecule 6: Proteasome subunit alpha type-3



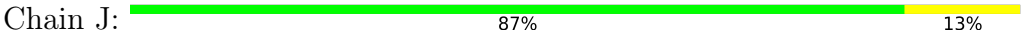


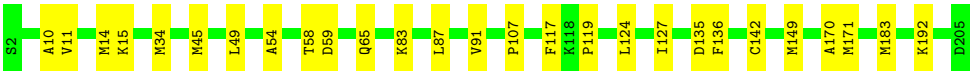
• Molecule 6: Proteasome subunit alpha type-3



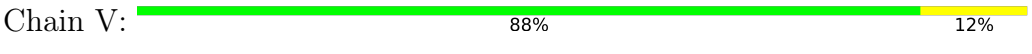


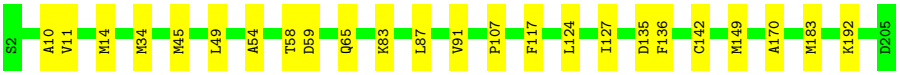
• Molecule 7: Proteasome subunit beta type-3



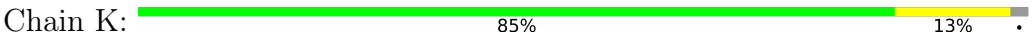


• Molecule 7: Proteasome subunit beta type-3





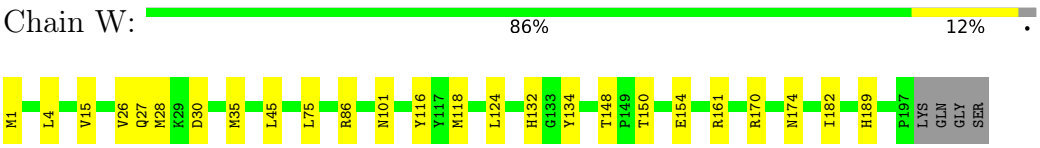
• Molecule 8: Proteasome subunit beta type-2





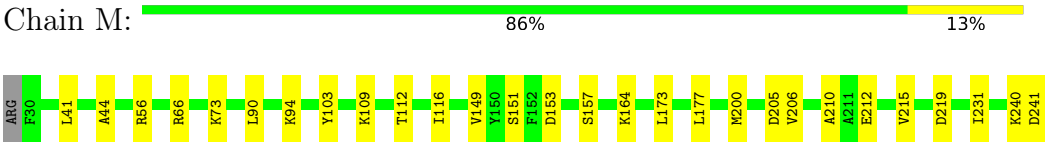
• Molecule 8: Proteasome subunit beta type-2

Chain W:



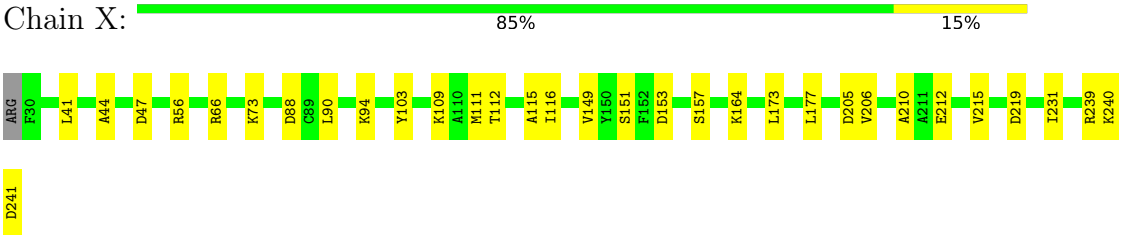
• Molecule 9: Proteasome subunit beta type-1

Chain M:



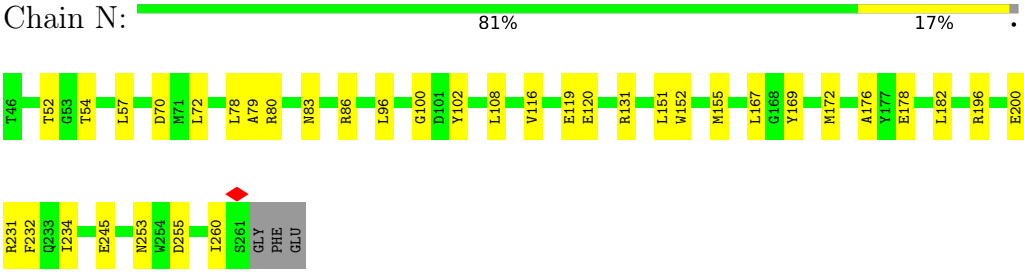
• Molecule 9: Proteasome subunit beta type-1

Chain X:



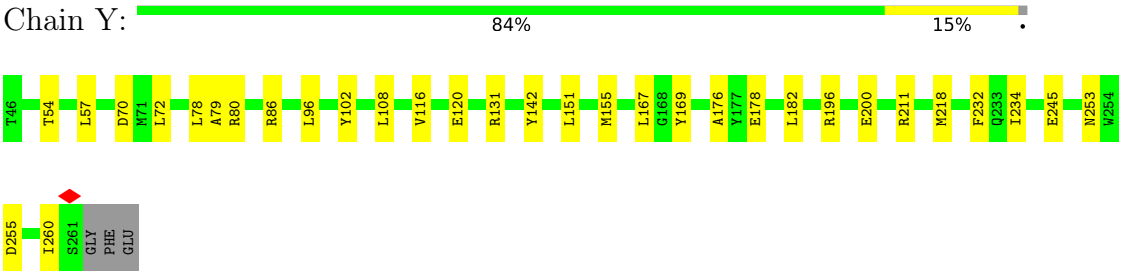
• Molecule 10: Proteasome subunit beta type-4

Chain N:



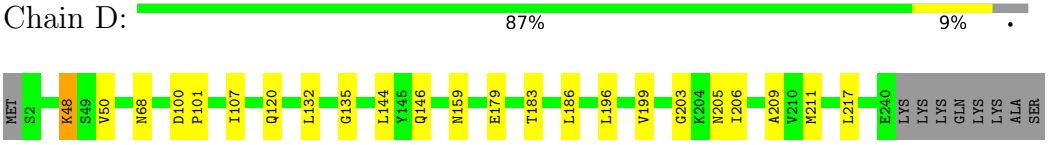
• Molecule 10: Proteasome subunit beta type-4

Chain Y:



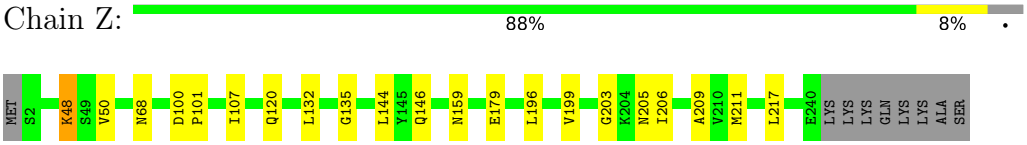
• Molecule 11: Proteasome subunit alpha type-7

Chain D:



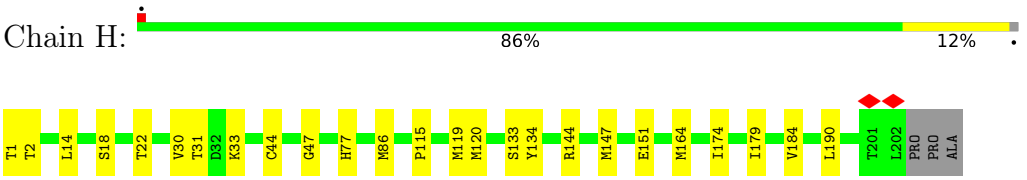
• Molecule 11: Proteasome subunit alpha type-7

Chain Z:



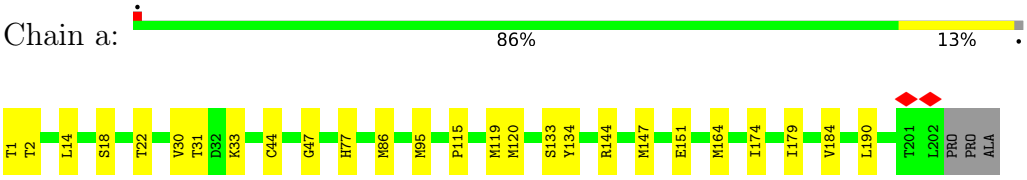
• Molecule 12: Proteasome subunit beta type-6

Chain H:



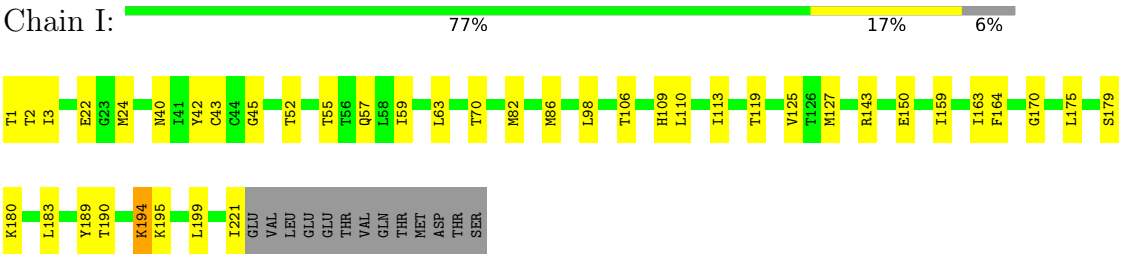
• Molecule 12: Proteasome subunit beta type-6

Chain a:



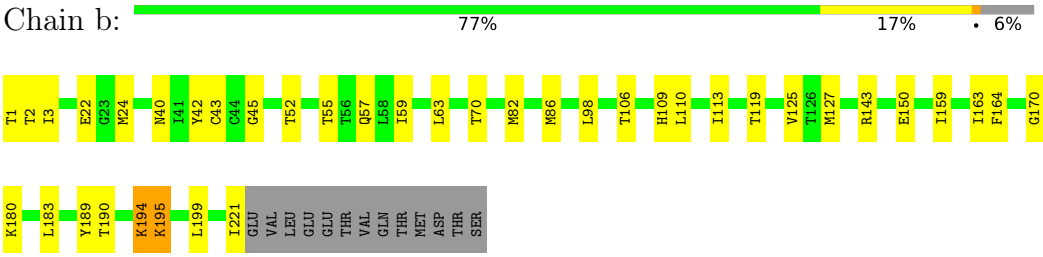
• Molecule 13: Proteasome subunit beta type-7

Chain I:



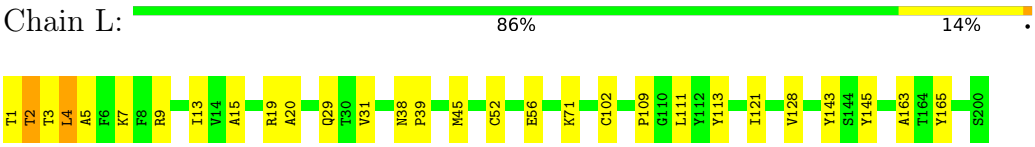
• Molecule 13: Proteasome subunit beta type-7

Chain b:



• Molecule 14: Proteasome subunit beta type-5

Chain L:



• Molecule 14: Proteasome subunit beta type-5

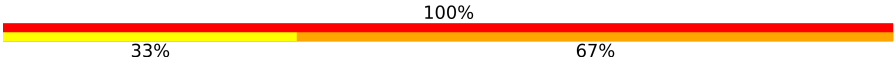
Chain c:





• Molecule 15: Carmaphycin B, bound form

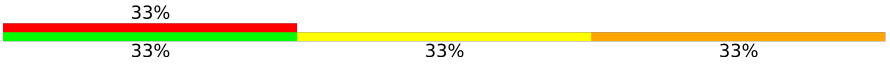
Chain U:





• Molecule 15: Carmaphycin B, bound form

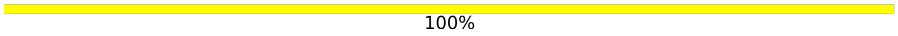
Chain d:





• Molecule 15: Carmaphycin B, bound form

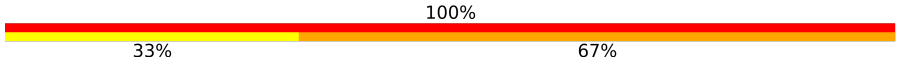
Chain e:





• Molecule 15: Carmaphycin B, bound form

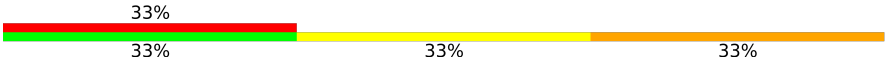
Chain f:





• Molecule 15: Carmaphycin B, bound form

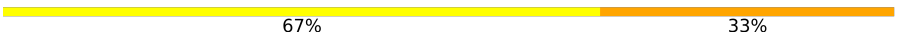
Chain g:





• Molecule 15: Carmaphycin B, bound form

Chain h:




V2
M3
A1KN44

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	15494	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	22.269	Depositor
Minimum map value	-0.258	Depositor
Average map value	0.055	Depositor
Map value standard deviation	0.859	Depositor
Recommended contour level	3.85	Depositor
Map size (Å)	333.44, 333.44, 333.44	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8336, 0.8336, 0.8336	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: A1KN4, OMT, 6NA

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	0.15	0/1920	0.40	0/2595
1	O	0.15	0/1920	0.40	0/2595
2	B	0.13	0/1831	0.32	0/2481
2	P	0.13	0/1831	0.32	0/2481
3	C	0.12	0/2046	0.34	0/2752
3	Q	0.12	0/2046	0.34	0/2752
4	E	0.13	0/1832	0.31	0/2475
4	R	0.13	0/1832	0.31	0/2475
5	F	0.12	0/1899	0.33	0/2567
5	S	0.12	0/1899	0.33	0/2567
6	G	0.11	0/1916	0.29	0/2580
6	T	0.11	0/1916	0.29	0/2580
7	J	0.12	0/1619	0.29	0/2184
7	V	0.12	0/1619	0.29	0/2184
8	K	0.12	0/1611	0.30	0/2180
8	W	0.12	0/1611	0.30	0/2180
9	M	0.14	0/1672	0.36	0/2254
9	X	0.16	0/1672	0.38	0/2254
10	N	0.13	0/1728	0.31	0/2339
10	Y	0.13	0/1728	0.31	0/2339
11	D	0.13	0/1913	0.35	0/2581
11	Z	0.13	0/1913	0.35	0/2581
12	H	0.16	0/1540	0.31	0/2085
12	a	0.16	0/1540	0.31	0/2085
13	I	0.20	0/1694	0.38	0/2293
13	b	0.22	0/1694	0.42	1/2293 (0.0%)
14	L	0.15	0/1586	0.34	1/2142 (0.0%)
14	c	0.15	0/1586	0.34	1/2142 (0.0%)
15	U	0.12	0/6	0.29	0/7
15	d	0.10	0/6	0.72	0/7
15	e	0.18	0/6	0.71	0/7
15	f	0.12	0/6	0.29	0/7

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
15	g	0.10	0/6	0.72	0/7
15	h	0.15	0/6	0.66	0/7
All	All	0.14	0/49650	0.34	3/67058 (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
9	X	0	1
15	U	0	2
15	d	0	1
15	e	0	2
15	f	0	2
15	g	0	1
15	h	0	2
All	All	0	11

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	b	195	LYS	CB-CA-C	-6.55	98.46	109.53
14	L	2	THR	N-CA-C	-5.85	98.55	108.26
14	c	2	THR	N-CA-C	-5.85	98.55	108.26

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
15	U	2	VAL	Peptide
15	U	3	OMT	Peptide
9	X	239	ARG	Sidechain
15	d	2	VAL	Peptide
15	e	2	VAL	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1886	0	1891	34	0
1	O	1886	0	1891	35	0
2	B	1792	0	1787	20	0
2	P	1792	0	1787	21	0
3	C	2016	0	2038	30	0
3	Q	2016	0	2038	30	0
4	E	1804	0	1784	26	0
4	R	1804	0	1784	26	0
5	F	1864	0	1852	38	0
5	S	1864	0	1852	38	0
6	G	1881	0	1868	17	0
6	T	1881	0	1868	17	0
7	J	1590	0	1609	22	0
7	V	1590	0	1609	20	0
8	K	1578	0	1580	22	0
8	W	1578	0	1580	22	0
9	M	1642	0	1640	19	0
9	X	1642	0	1640	24	0
10	N	1695	0	1666	31	0
10	Y	1695	0	1666	28	0
11	D	1887	0	1905	18	0
11	Z	1887	0	1905	17	0
12	H	1514	0	1485	32	0
12	a	1514	0	1485	33	0
13	I	1667	0	1690	44	0
13	b	1667	0	1690	40	0
14	L	1555	0	1518	28	0
14	c	1555	0	1518	27	0
15	U	29	0	16	4	0
15	d	29	0	16	0	0
15	e	29	0	16	0	0
15	f	29	0	16	4	0
15	g	29	0	16	0	0
15	h	29	0	16	0	0
16	U	7	0	11	1	0
16	d	7	0	11	1	0
16	e	7	0	11	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	f	7	0	11	1	0
16	g	7	0	11	1	0
16	h	7	0	11	0	0
All	All	48958	0	48788	672	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 672 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Z:50:VAL:HG11	11:Z:205:ASN:OD1	1.30	1.30
11:D:50:VAL:HG11	11:D:205:ASN:OD1	1.30	1.27
11:D:100:ASP:OD1	11:D:101:PRO:CD	1.84	1.24
11:Z:100:ASP:OD1	11:Z:101:PRO:CD	1.84	1.24
13:I:195:LYS:HB2	9:X:212:GLU:OE2	1.39	1.22

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	240/246 (98%)	237 (99%)	3 (1%)	0	100	100
1	O	240/246 (98%)	237 (99%)	3 (1%)	0	100	100
2	B	228/234 (97%)	226 (99%)	2 (1%)	0	100	100
2	P	228/234 (97%)	226 (99%)	2 (1%)	0	100	100
3	C	253/261 (97%)	247 (98%)	5 (2%)	1 (0%)	30	57
3	Q	253/261 (97%)	247 (98%)	5 (2%)	1 (0%)	30	57
4	E	234/241 (97%)	232 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	R	234/241 (97%)	232 (99%)	2 (1%)	0	100	100
5	F	235/263 (89%)	230 (98%)	5 (2%)	0	100	100
5	S	235/263 (89%)	230 (98%)	5 (2%)	0	100	100
6	G	238/255 (93%)	236 (99%)	2 (1%)	0	100	100
6	T	238/255 (93%)	236 (99%)	2 (1%)	0	100	100
7	J	202/204 (99%)	195 (96%)	7 (4%)	0	100	100
7	V	202/204 (99%)	195 (96%)	7 (4%)	0	100	100
8	K	195/201 (97%)	188 (96%)	7 (4%)	0	100	100
8	W	195/201 (97%)	188 (96%)	7 (4%)	0	100	100
9	M	210/213 (99%)	207 (99%)	3 (1%)	0	100	100
9	X	210/213 (99%)	207 (99%)	3 (1%)	0	100	100
10	N	215/219 (98%)	212 (99%)	3 (1%)	0	100	100
10	Y	215/219 (98%)	212 (99%)	3 (1%)	0	100	100
11	D	237/248 (96%)	233 (98%)	4 (2%)	0	100	100
11	Z	237/248 (96%)	233 (98%)	4 (2%)	0	100	100
12	H	200/205 (98%)	197 (98%)	3 (2%)	0	100	100
12	a	200/205 (98%)	197 (98%)	3 (2%)	0	100	100
13	I	219/234 (94%)	214 (98%)	5 (2%)	0	100	100
13	b	219/234 (94%)	214 (98%)	5 (2%)	0	100	100
14	L	198/200 (99%)	196 (99%)	2 (1%)	0	100	100
14	c	198/200 (99%)	196 (99%)	2 (1%)	0	100	100
All	All	6208/6448 (96%)	6100 (98%)	106 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	54	LYS
3	Q	54	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	206/210 (98%)	206 (100%)	0	100 100
1	O	206/210 (98%)	206 (100%)	0	100 100
2	B	188/191 (98%)	187 (100%)	1 (0%)	81 92
2	P	188/191 (98%)	187 (100%)	1 (0%)	81 92
3	C	215/221 (97%)	215 (100%)	0	100 100
3	Q	215/221 (97%)	215 (100%)	0	100 100
4	E	198/203 (98%)	198 (100%)	0	100 100
4	R	198/203 (98%)	198 (100%)	0	100 100
5	F	203/224 (91%)	201 (99%)	2 (1%)	68 86
5	S	203/224 (91%)	201 (99%)	2 (1%)	68 86
6	G	198/212 (93%)	198 (100%)	0	100 100
6	T	198/212 (93%)	198 (100%)	0	100 100
7	J	173/173 (100%)	172 (99%)	1 (1%)	78 91
7	V	173/173 (100%)	172 (99%)	1 (1%)	78 91
8	K	168/171 (98%)	167 (99%)	1 (1%)	78 91
8	W	168/171 (98%)	167 (99%)	1 (1%)	78 91
9	M	177/178 (99%)	175 (99%)	2 (1%)	65 85
9	X	177/178 (99%)	175 (99%)	2 (1%)	65 85
10	N	180/181 (99%)	180 (100%)	0	100 100
10	Y	180/181 (99%)	180 (100%)	0	100 100
11	D	203/211 (96%)	202 (100%)	1 (0%)	81 92
11	Z	203/211 (96%)	202 (100%)	1 (0%)	81 92
12	H	157/159 (99%)	157 (100%)	0	100 100
12	a	157/159 (99%)	157 (100%)	0	100 100
13	I	182/195 (93%)	180 (99%)	2 (1%)	65 85
13	b	182/195 (93%)	180 (99%)	2 (1%)	65 85
14	L	156/156 (100%)	155 (99%)	1 (1%)	78 91
14	c	156/156 (100%)	155 (99%)	1 (1%)	78 91
15	U	1/1 (100%)	1 (100%)	0	100 100
15	d	1/1 (100%)	0	1 (100%)	0 0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
15	e	1/1 (100%)	1 (100%)	0	100 100
15	f	1/1 (100%)	1 (100%)	0	100 100
15	g	1/1 (100%)	0	1 (100%)	0 0
15	h	1/1 (100%)	0	1 (100%)	0 0
All	All	5214/5376 (97%)	5189 (100%)	25 (0%)	78 92

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	V	83	LYS
9	X	241	ASP
15	h	2	VAL
9	X	240	LYS
11	Z	48	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 58 such sidechains are listed below:

Mol	Chain	Res	Type
14	L	175	ASN
13	b	181	ASN
3	Q	198	ASN
12	a	110	GLN
10	Y	126	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

12 non-standard protein/DNA/RNA residues 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	A1KN4	e	4	15,14	9,11,11	2.01	1 (11%)	8,14,14	3.56	3 (37%)
15	OMT	h	3	15	8,9,10	0.59	0	6,12,14	0.65	0
15	A1KN4	d	4	15,13	9,11,11	2.49	1 (11%)	8,14,14	2.74	2 (25%)
15	OMT	e	3	15	8,9,10	0.59	0	6,12,14	0.59	0
15	A1KN4	f	4	12,15	9,11,11	3.95	1 (11%)	8,14,14	2.35	1 (12%)
15	OMT	U	3	15	8,9,10	0.58	0	6,12,14	0.35	0
15	A1KN4	U	4	12,15	9,11,11	3.95	1 (11%)	8,14,14	2.35	1 (12%)
15	A1KN4	g	4	15,13	9,11,11	2.49	1 (11%)	8,14,14	2.74	2 (25%)
15	OMT	d	3	15	8,9,10	0.54	0	6,12,14	0.33	0
15	OMT	f	3	15	8,9,10	0.58	0	6,12,14	0.35	0
15	A1KN4	h	4	15,14	9,11,11	1.98	1 (11%)	8,14,14	3.70	3 (37%)
15	OMT	g	3	15	8,9,10	0.54	0	6,12,14	0.33	0

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	A1KN4	e	4	15,14	-	7/13/14/14	-
15	OMT	h	3	15	-	3/7/8/10	-
15	A1KN4	d	4	15,13	-	6/13/14/14	-
15	OMT	e	3	15	-	3/7/8/10	-
15	A1KN4	f	4	12,15	-	7/13/14/14	-
15	OMT	U	3	15	-	4/7/8/10	-
15	A1KN4	U	4	12,15	-	7/13/14/14	-
15	A1KN4	g	4	15,13	-	6/13/14/14	-
15	OMT	d	3	15	-	2/7/8/10	-
15	OMT	f	3	15	-	4/7/8/10	-
15	A1KN4	h	4	15,14	-	7/13/14/14	-
15	OMT	g	3	15	-	2/7/8/10	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	U	4	A1KN4	O-C	11.82	1.40	1.21
15	f	4	A1KN4	O-C	11.82	1.40	1.21
15	d	4	A1KN4	O-C	7.37	1.33	1.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	g	4	A1KN4	O-C	7.37	1.33	1.21
15	e	4	A1KN4	O-C	5.91	1.31	1.21

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	d	4	A1KN4	O-C-C23	-7.16	107.98	121.26
15	g	4	A1KN4	O-C-C23	-7.16	107.98	121.26
15	h	4	A1KN4	C-CA-N	7.01	125.58	109.07
15	e	4	A1KN4	C-CA-N	6.76	124.98	109.07
15	U	4	A1KN4	O-C-C23	-6.31	109.56	121.26

There are no chirality outliers.

5 of 58 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	U	3	OMT	N-CA-CB-CG
15	U	3	OMT	CA-CB-CG-SD
15	U	3	OMT	CB-CG-SD-OD1
15	e	3	OMT	N-CA-CB-CG
15	e	3	OMT	C-CA-CB-CG

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	U	3	OMT	3	0
15	f	3	OMT	3	0

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	$\#\|Z\| > 2$
16	6NA	g	101	15	6,6,7	0.37	0	5,5,7	0.38	0
16	6NA	U	101	15	6,6,7	0.38	0	5,5,7	0.39	0
16	6NA	f	101	15	6,6,7	0.38	0	5,5,7	0.39	0
16	6NA	e	101	15	6,6,7	0.35	0	5,5,7	0.39	0
16	6NA	h	101	15	6,6,7	0.36	0	5,5,7	0.40	0
16	6NA	d	101	15	6,6,7	0.37	0	5,5,7	0.38	0

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	6NA	g	101	15	-	2/3/4/5	-
16	6NA	U	101	15	-	2/3/4/5	-
16	6NA	f	101	15	-	2/3/4/5	-
16	6NA	e	101	15	-	3/3/4/5	-
16	6NA	h	101	15	-	3/3/4/5	-
16	6NA	d	101	15	-	2/3/4/5	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	e	101	6NA	C-CA-CB-CG
16	h	101	6NA	CA-CB-CG-CD
16	U	101	6NA	CA-CB-CG-CD
16	f	101	6NA	CA-CB-CG-CD
16	e	101	6NA	C6-CD-CG-CB

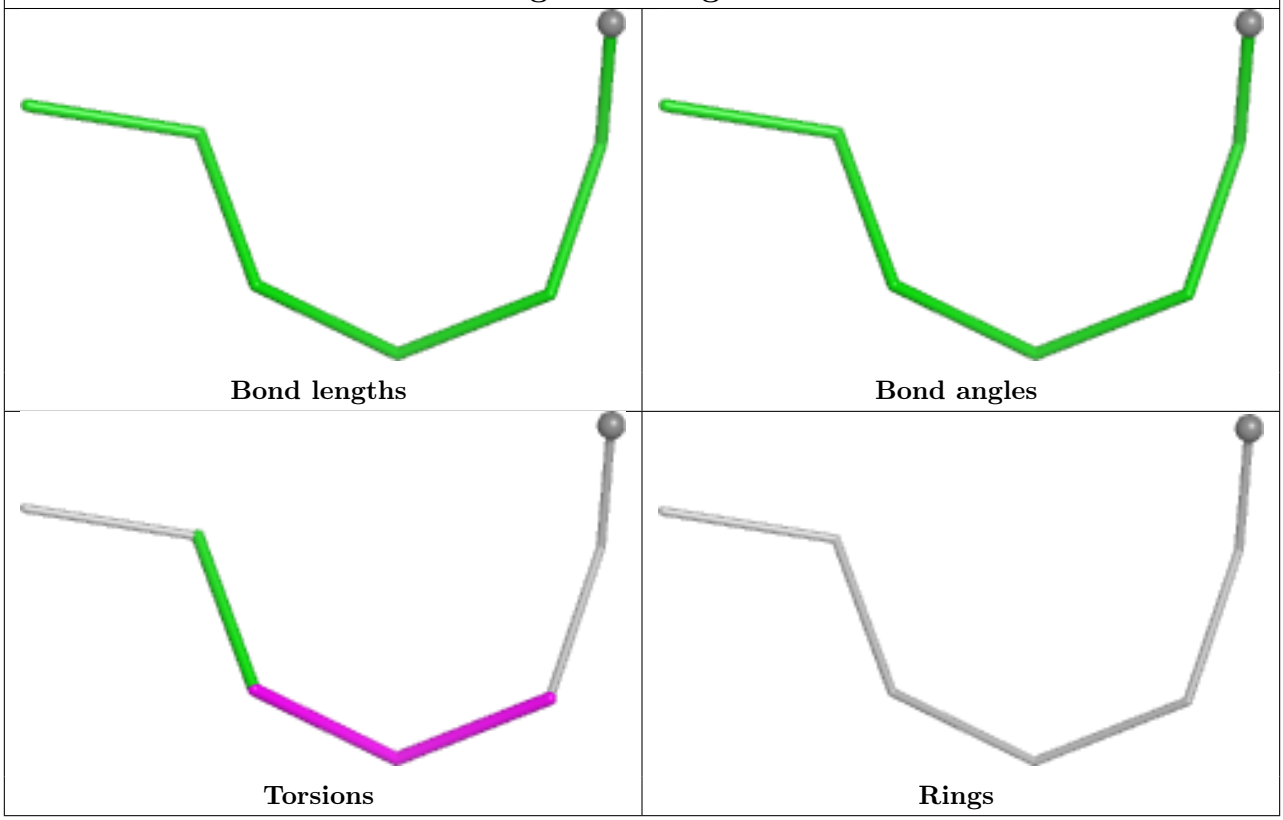
There are no ring outliers.

4 monomers are involved in 4 short contacts:

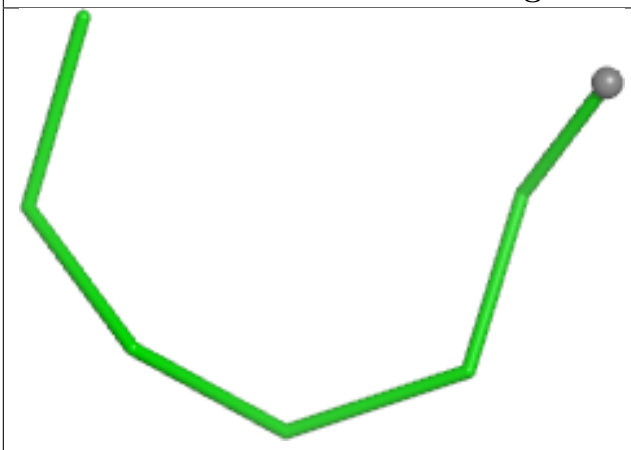
Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	g	101	6NA	1	0
16	U	101	6NA	1	0
16	f	101	6NA	1	0
16	d	101	6NA	1	0

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

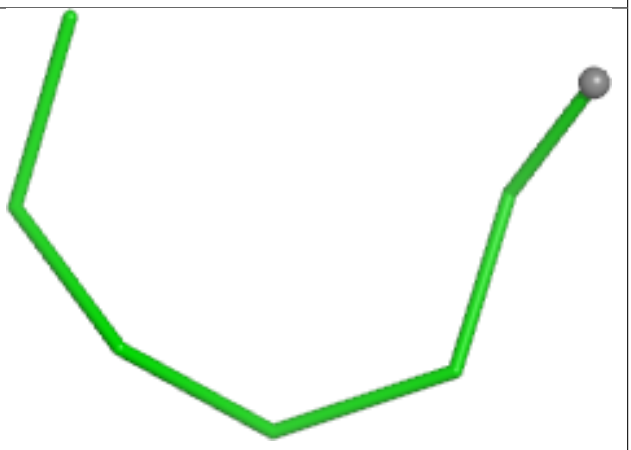
Ligand 6NA g 101



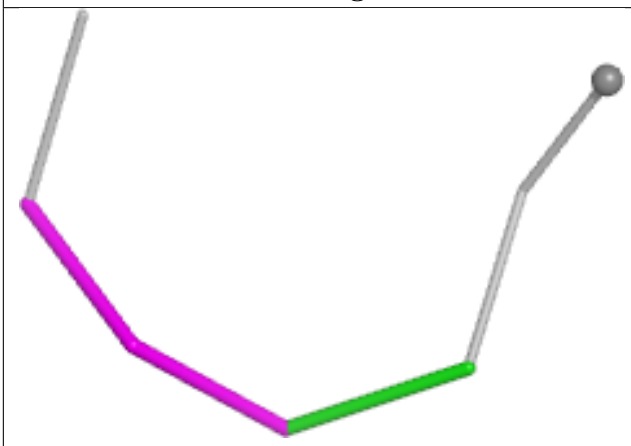
Ligand 6NA U 101



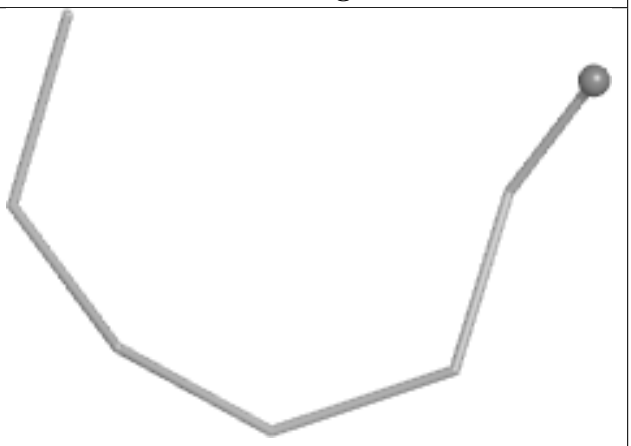
Bond lengths



Bond angles

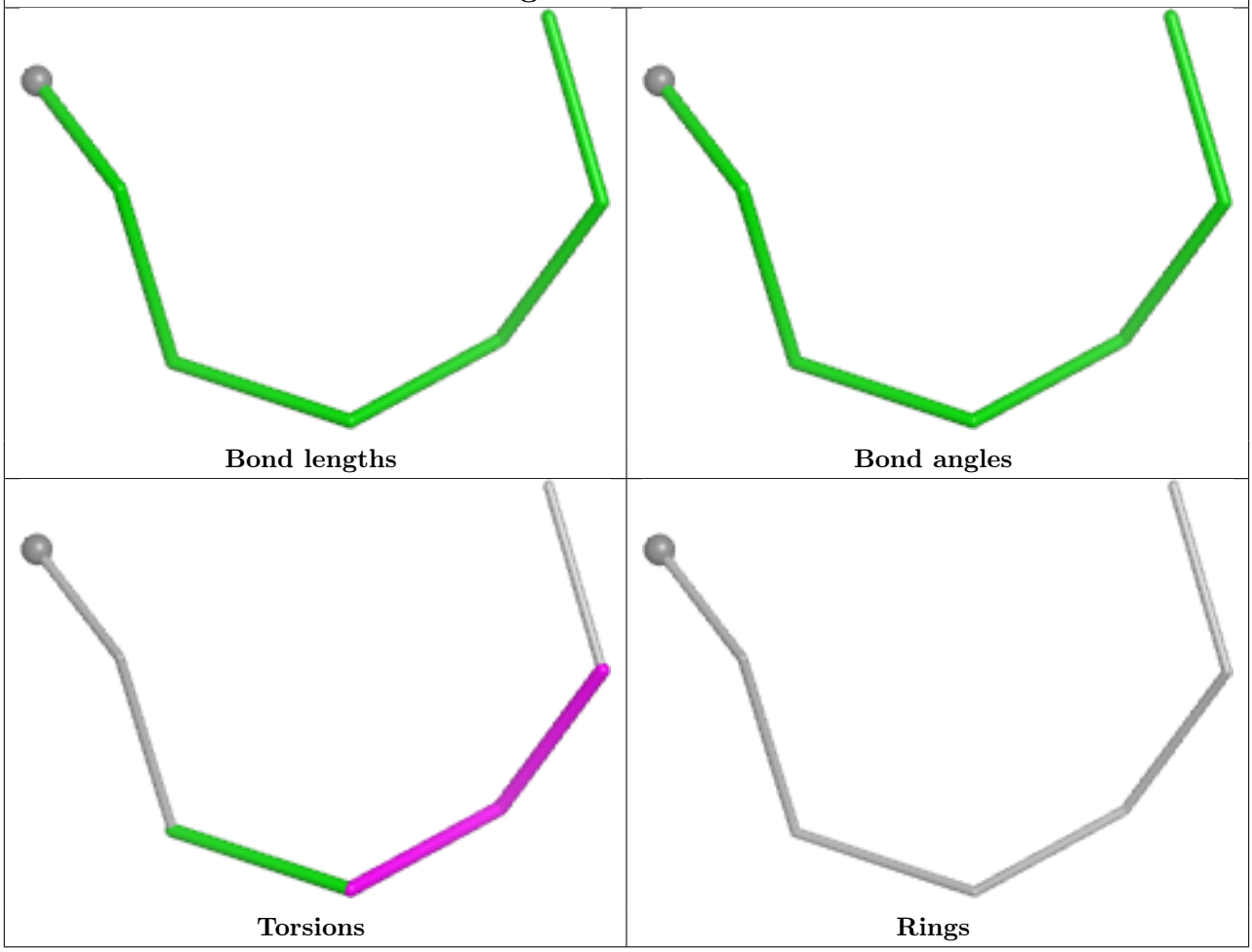


Torsions

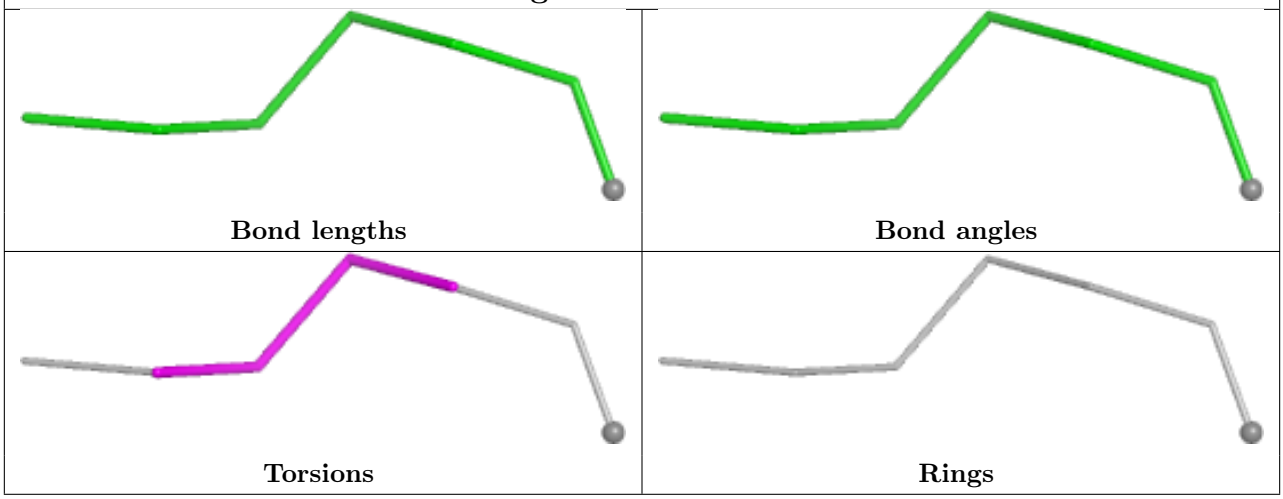


Rings

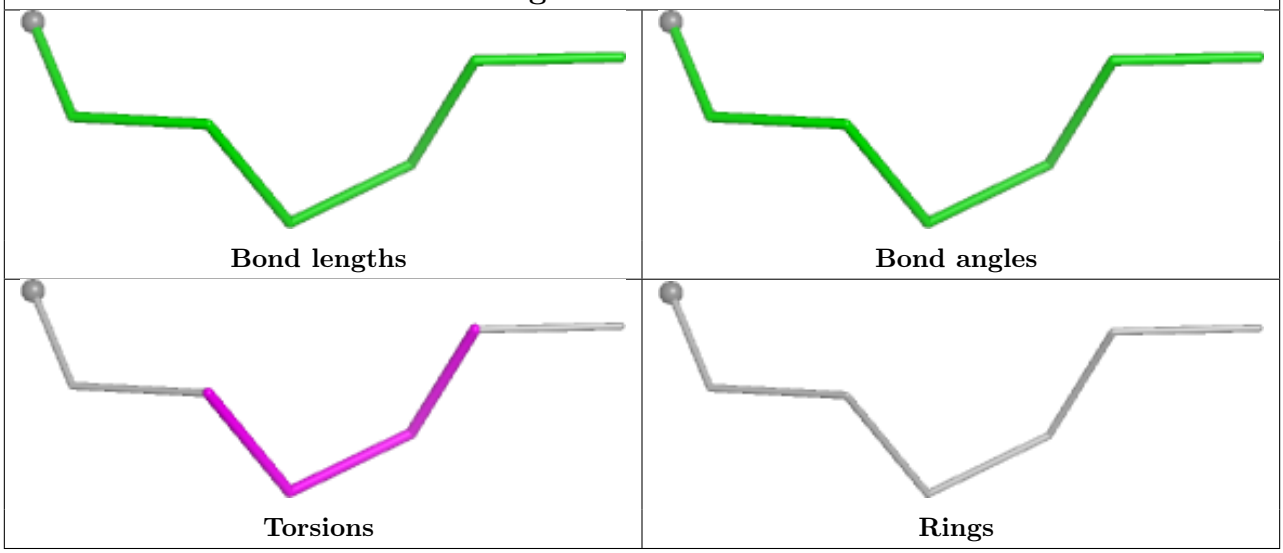
Ligand 6NA f 101



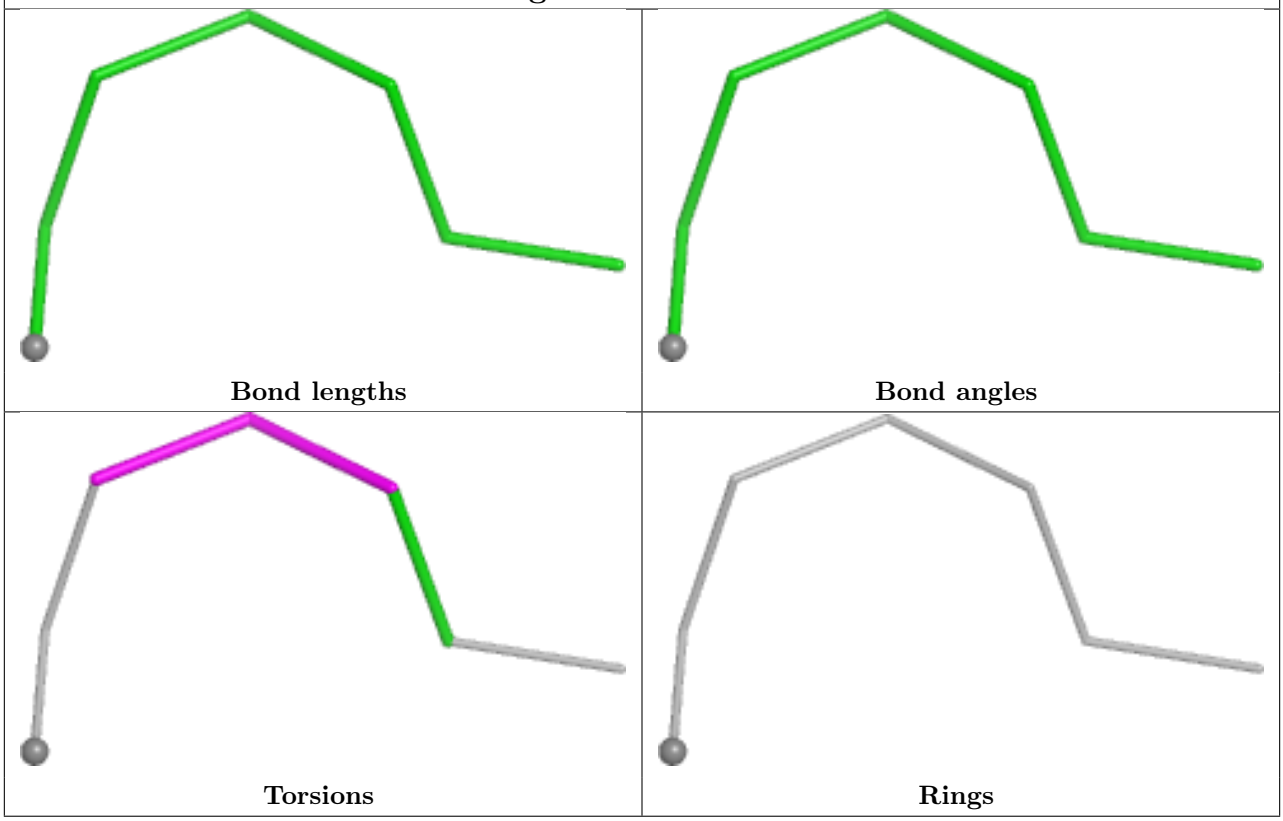
Ligand 6NA e 101



Ligand 6NA h 101



Ligand 6NA d 101



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.

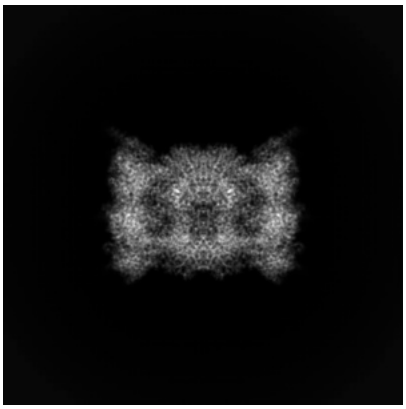
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-54791. These allow visual inspection of the internal detail of the map and identification of artifacts.

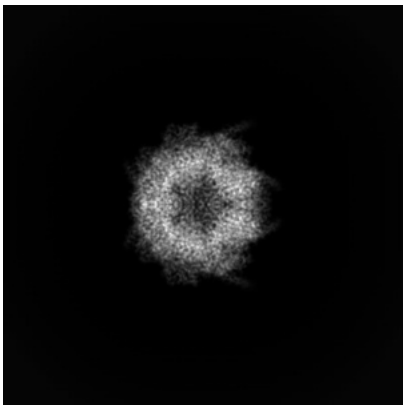
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

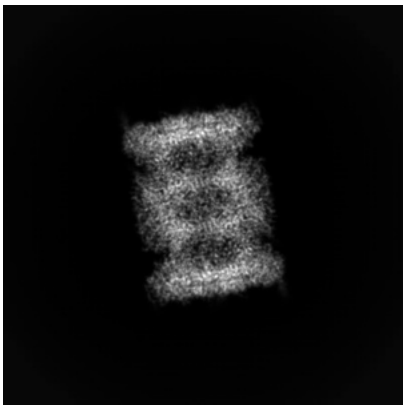
6.1.1 Primary map



X

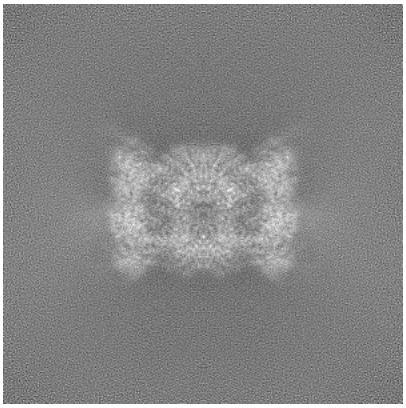


Y

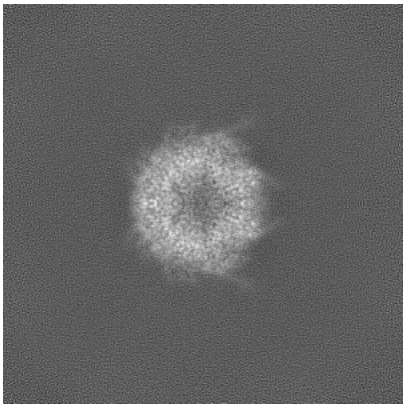


Z

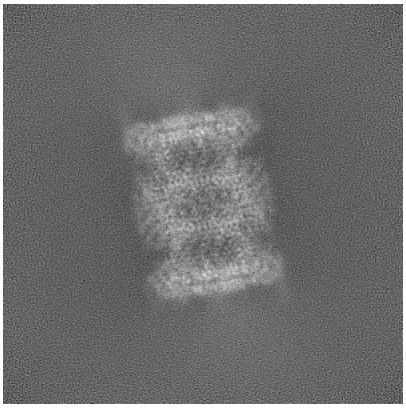
6.1.2 Raw map



X



Y

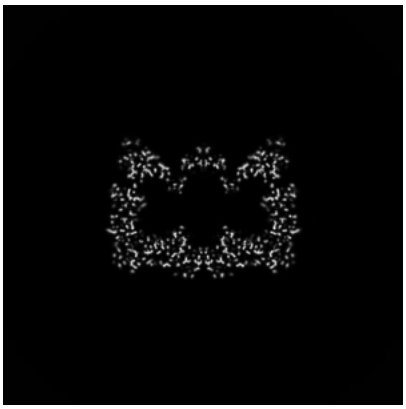


Z

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

6.2 Central slices (i)

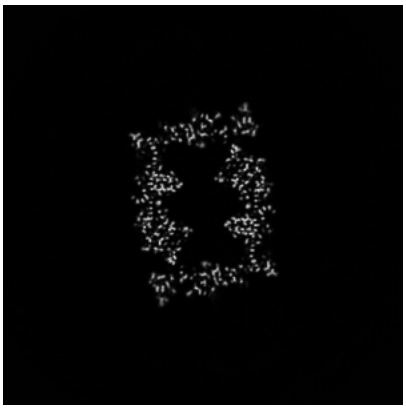
6.2.1 Primary map



X Index: 200

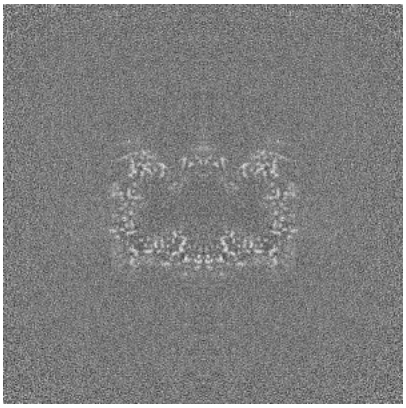


Y Index: 200

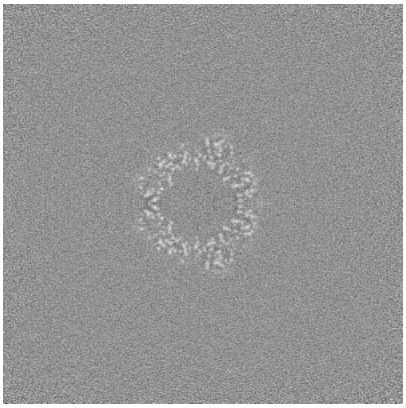


Z Index: 200

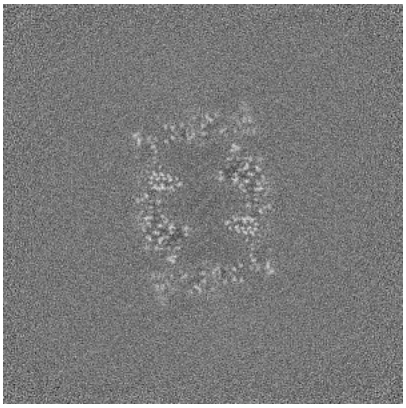
6.2.2 Raw map



X Index: 200



Y Index: 200

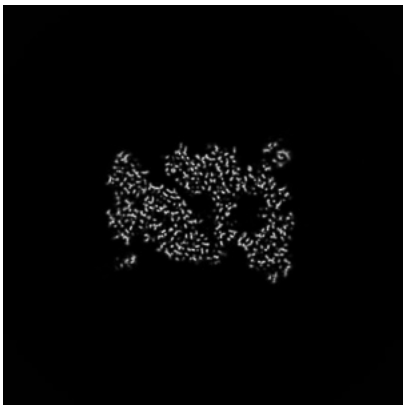


Z Index: 200

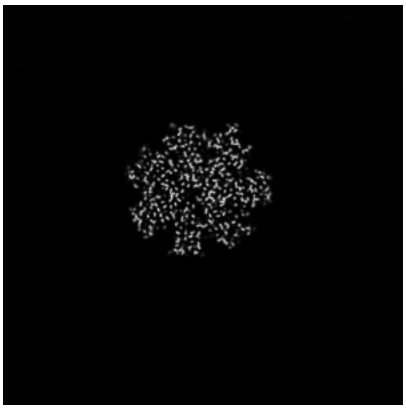
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 169

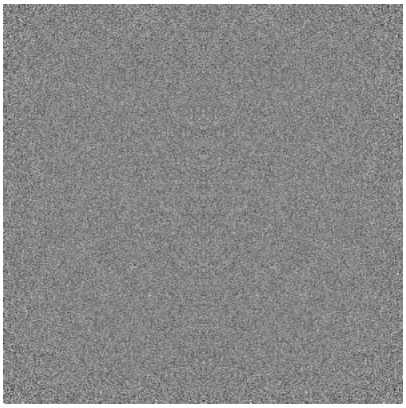


Y Index: 132

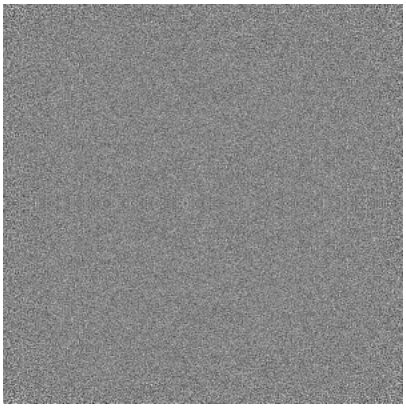


Z Index: 163

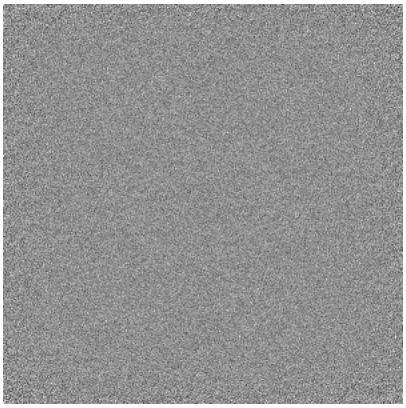
6.3.2 Raw map



X Index: 0



Y Index: 0

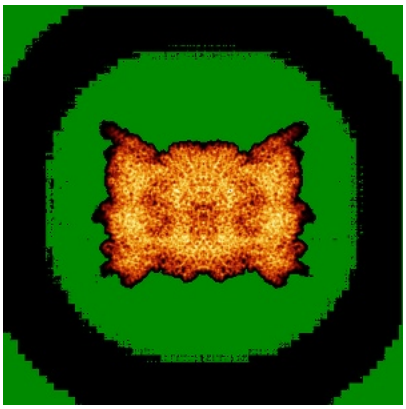


Z Index: 0

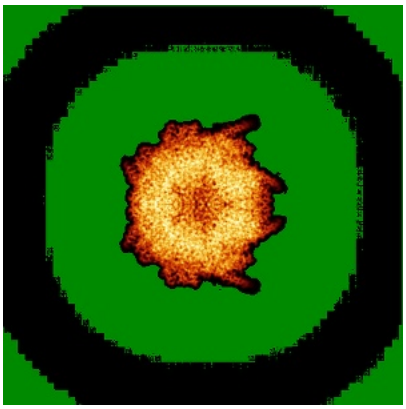
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

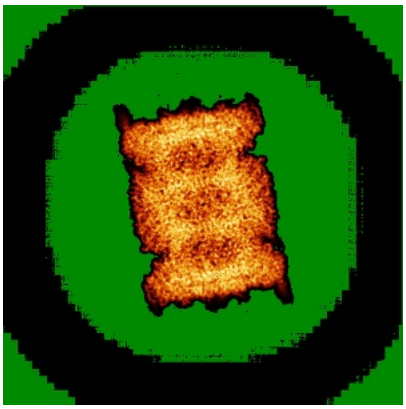
6.4.1 Primary map



X

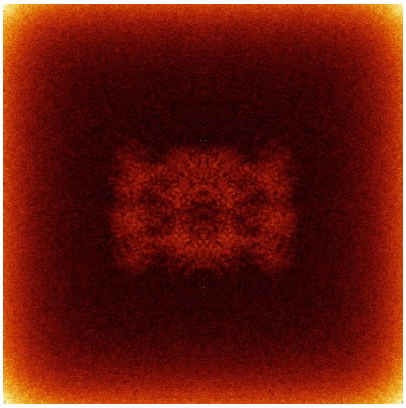


Y

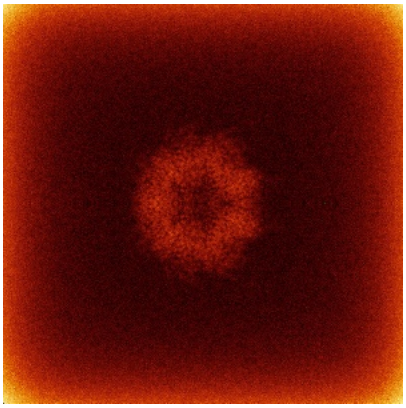


Z

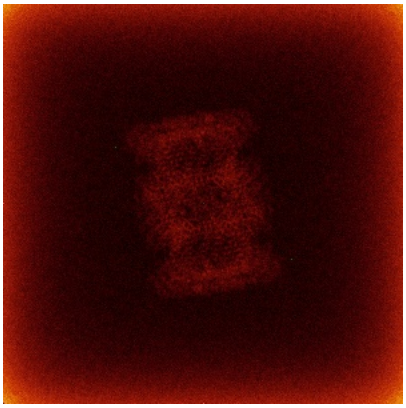
6.4.2 Raw map



X



Y

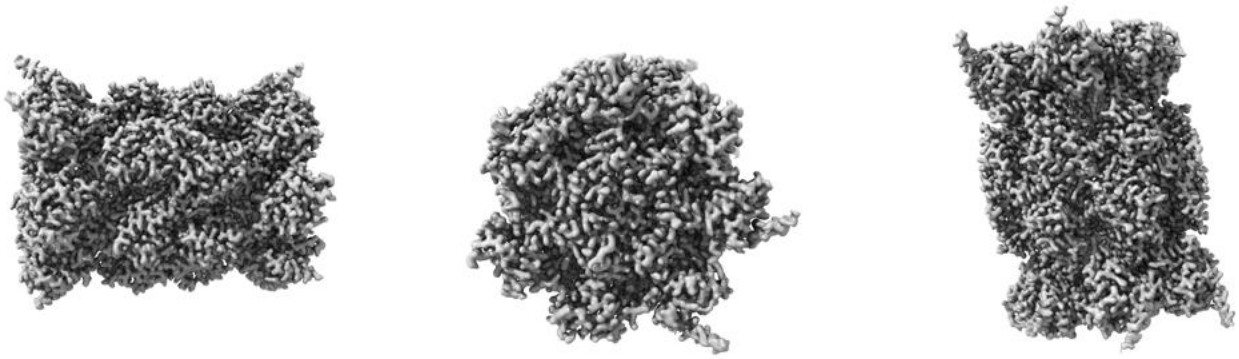


Z

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)

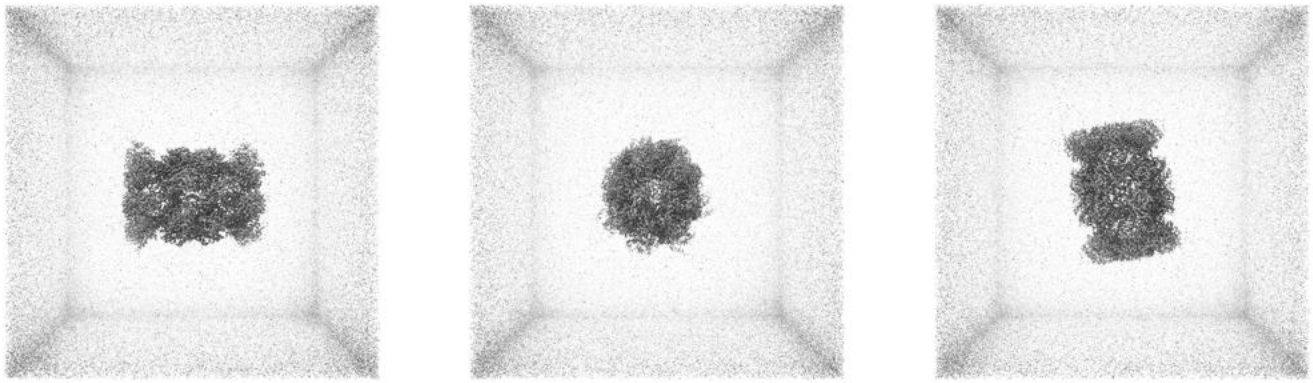
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 3.85. 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



X Y Z

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.

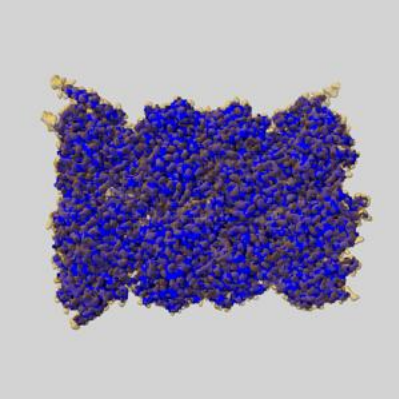
6.6 Mask visualisation

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

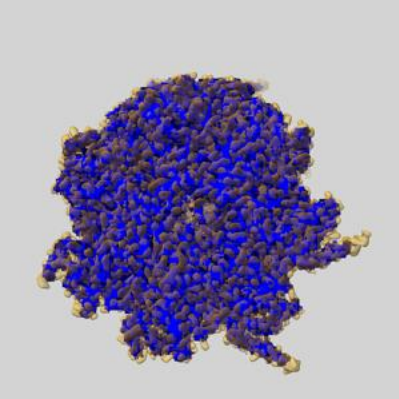
A mask typically either:

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

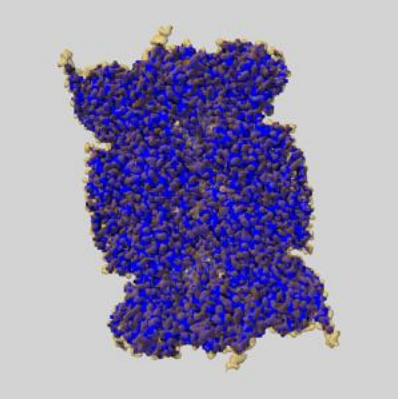
6.6.1 emd_54791_msk_1.map



X



Y

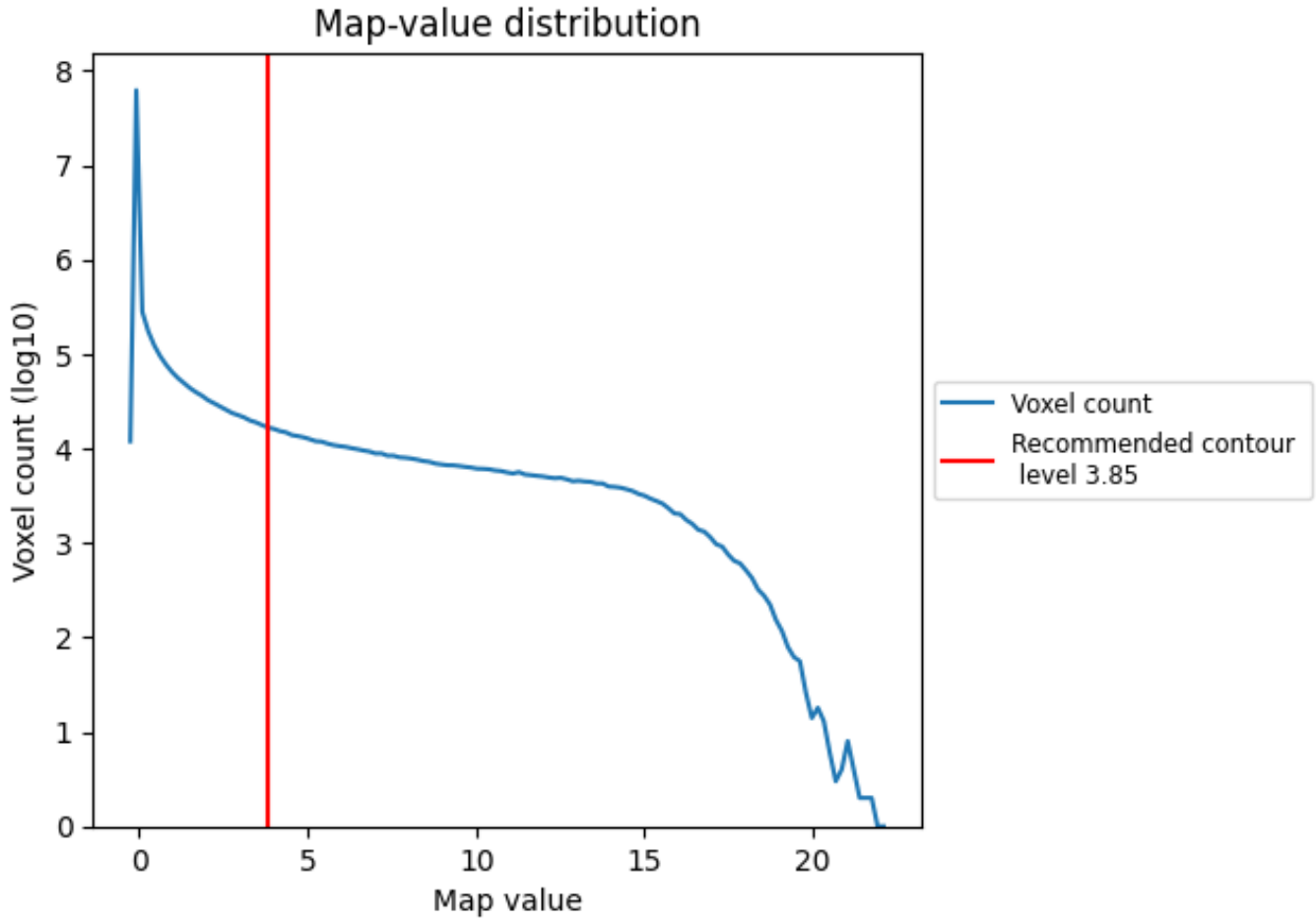


Z

7 Map analysis

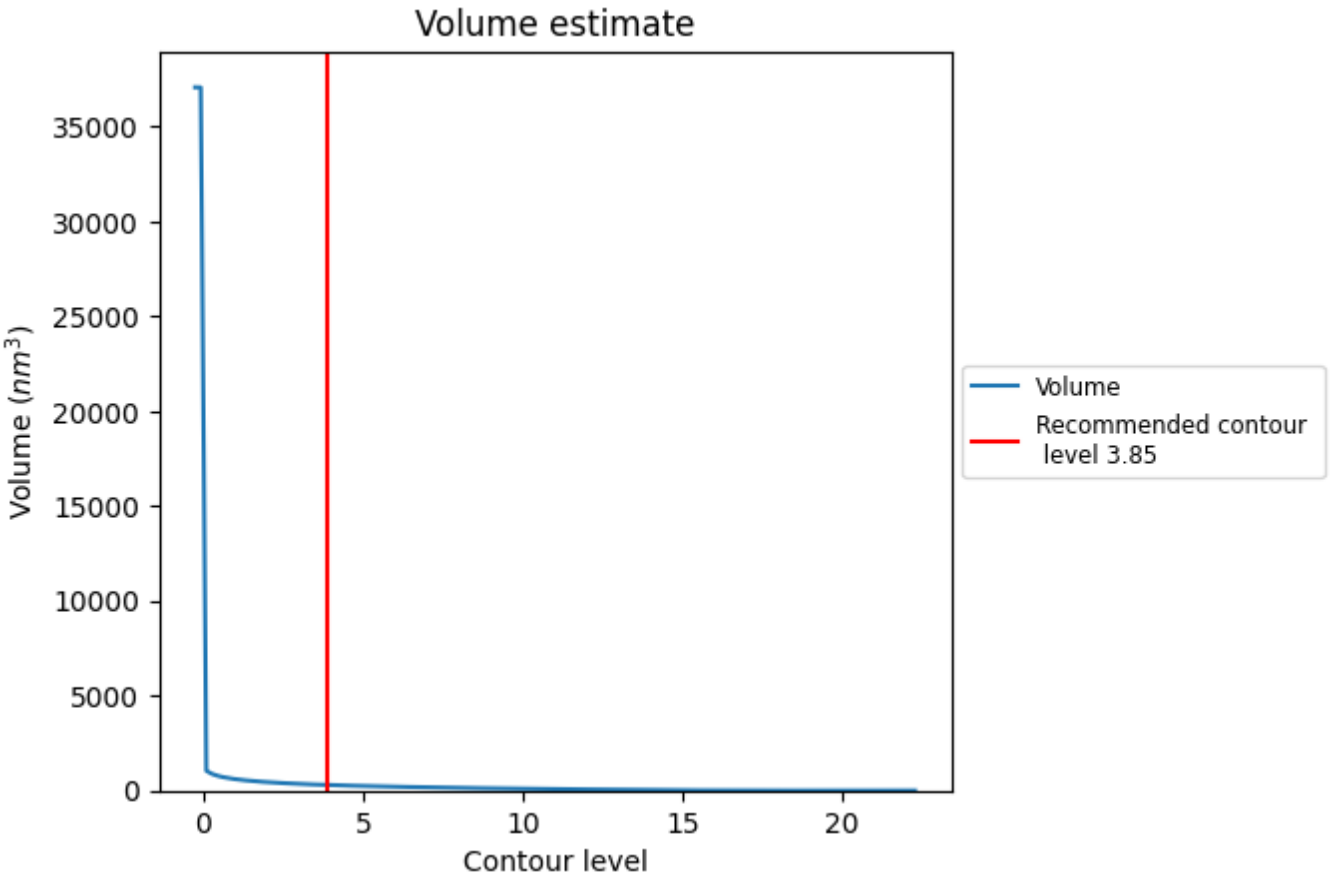
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

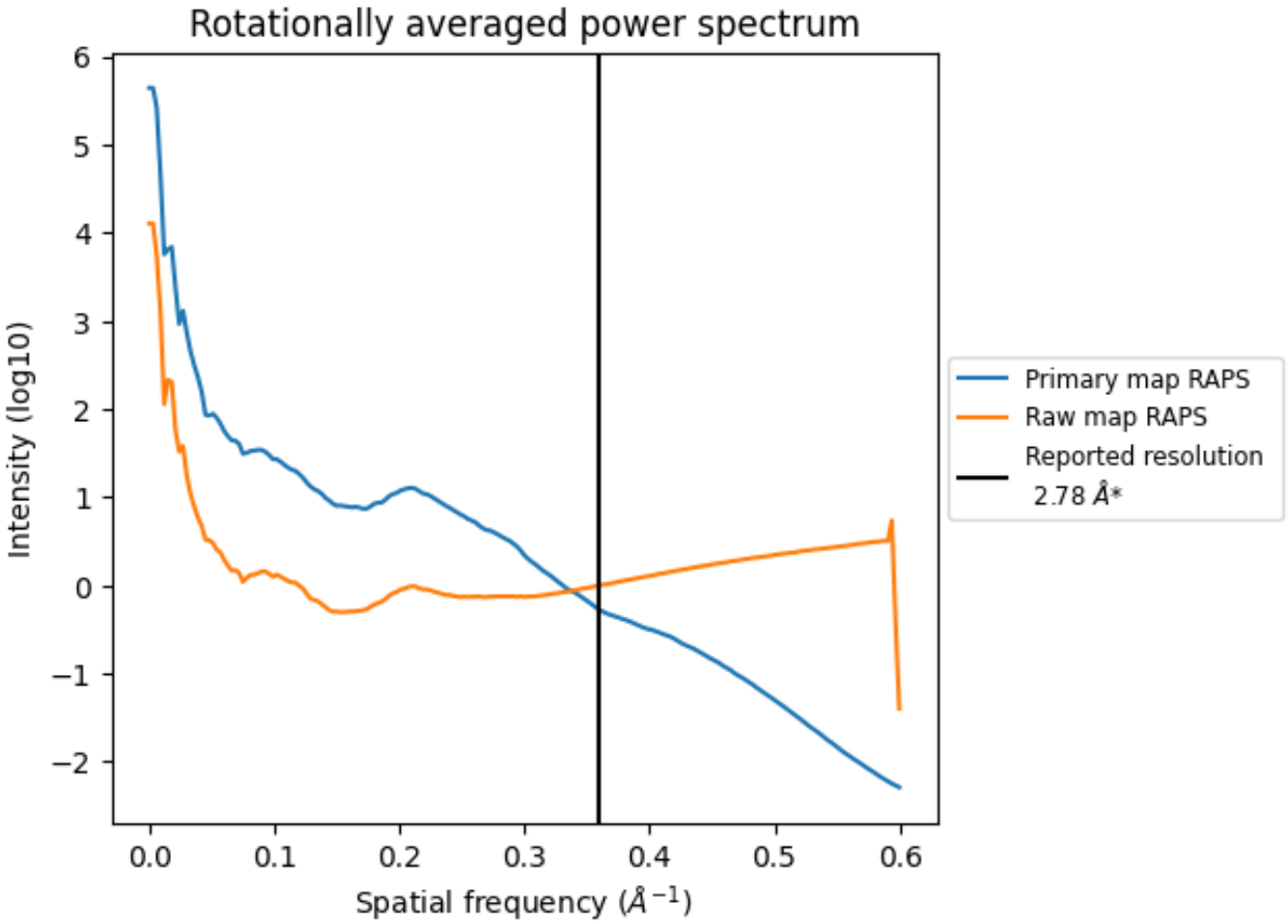
7.2 Volume estimate (i)



The volume at the recommended contour level is 297 nm^3; this corresponds to an approximate mass of 268 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)

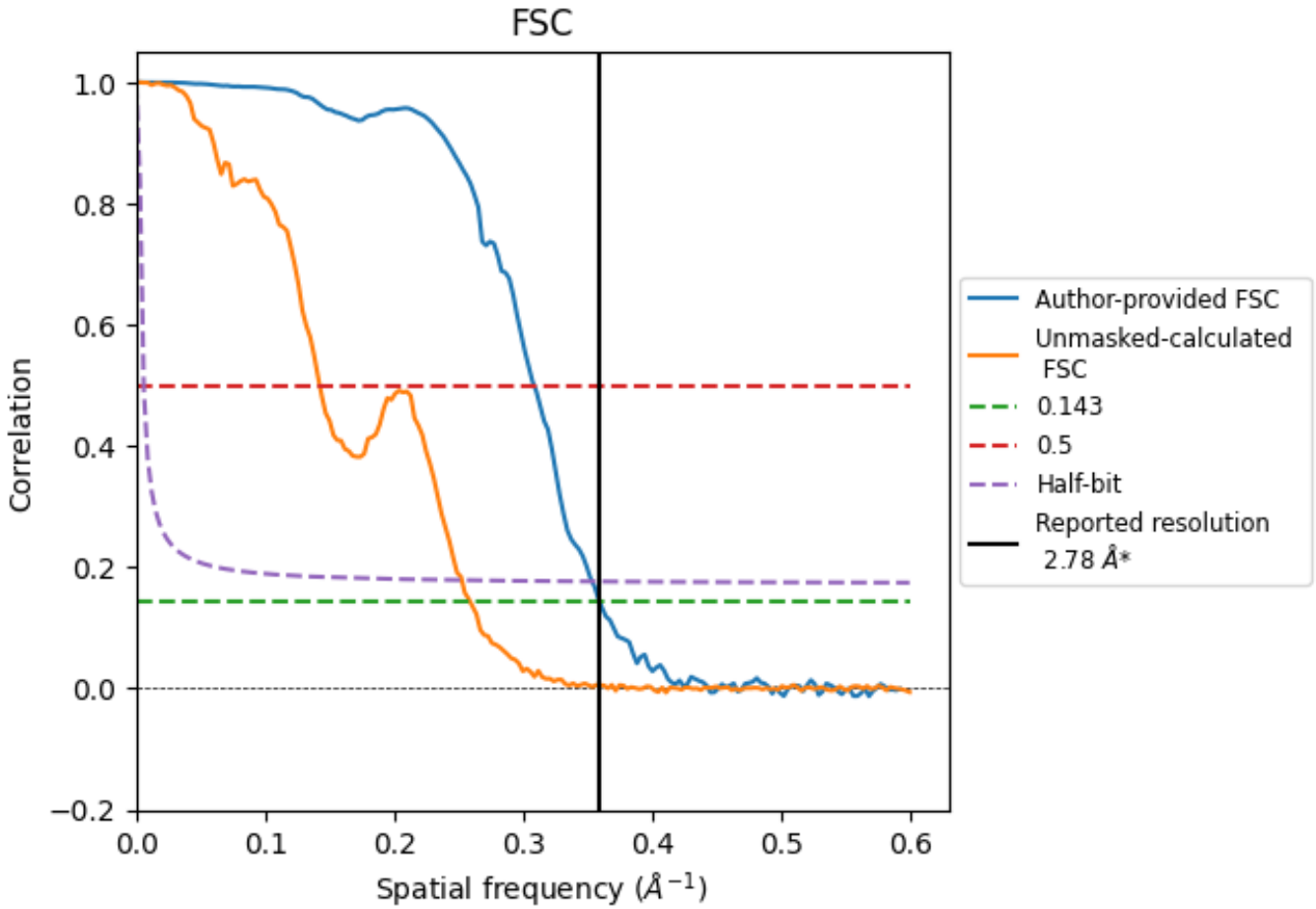


*Reported resolution corresponds to spatial frequency of 0.360 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.360 Å^{-1}

8.2 Resolution estimates (i)

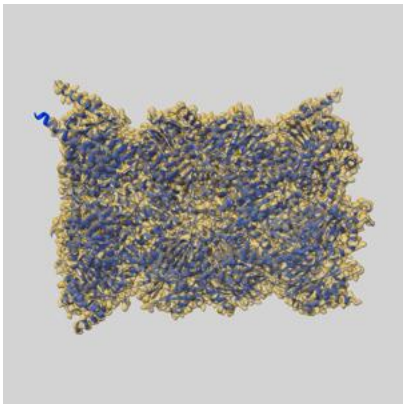
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.78	-	-
Author-provided FSC curve	2.78	3.24	2.83
Unmasked-calculated*	3.86	7.03	3.96

*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 3.86 differs from the reported value 2.78 by more than 10 %

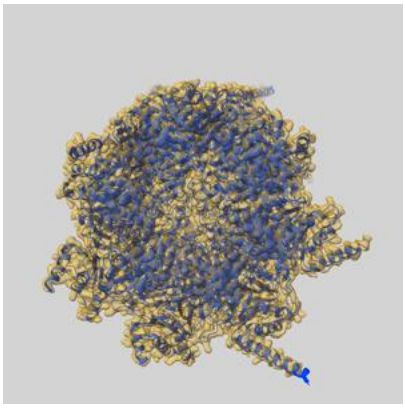
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-54791 and PDB model 9SDR. Per-residue inclusion information can be found in section 3 on page 9.

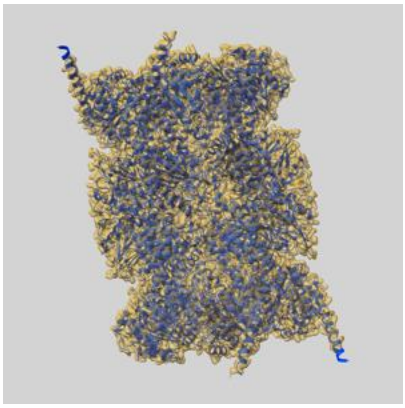
9.1 Map-model overlay



X



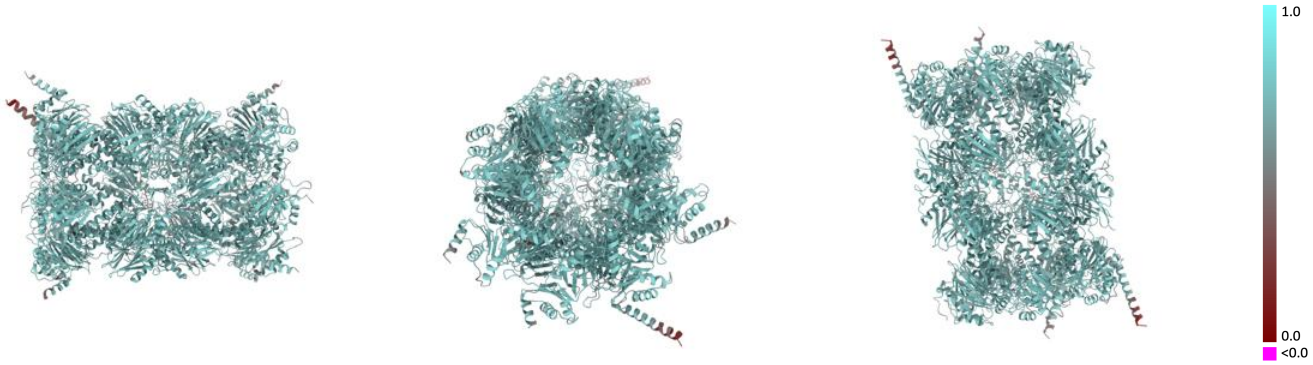
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.85 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.

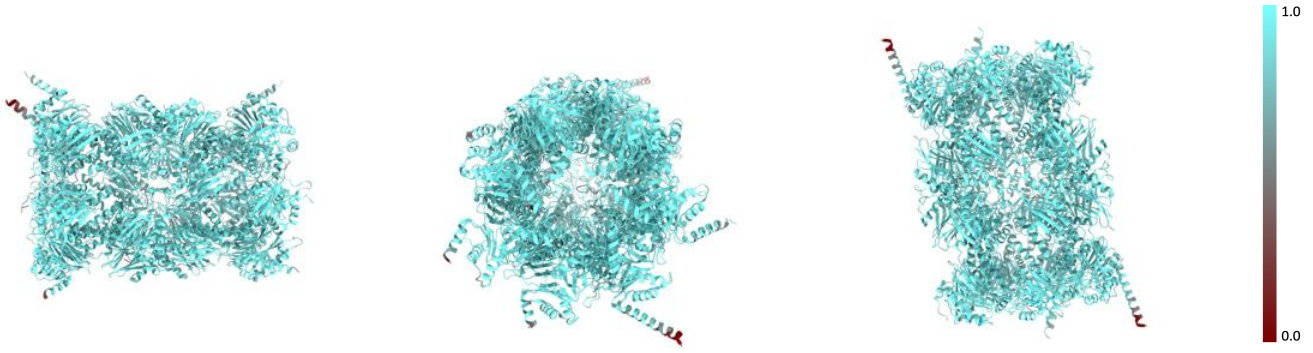
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according 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.

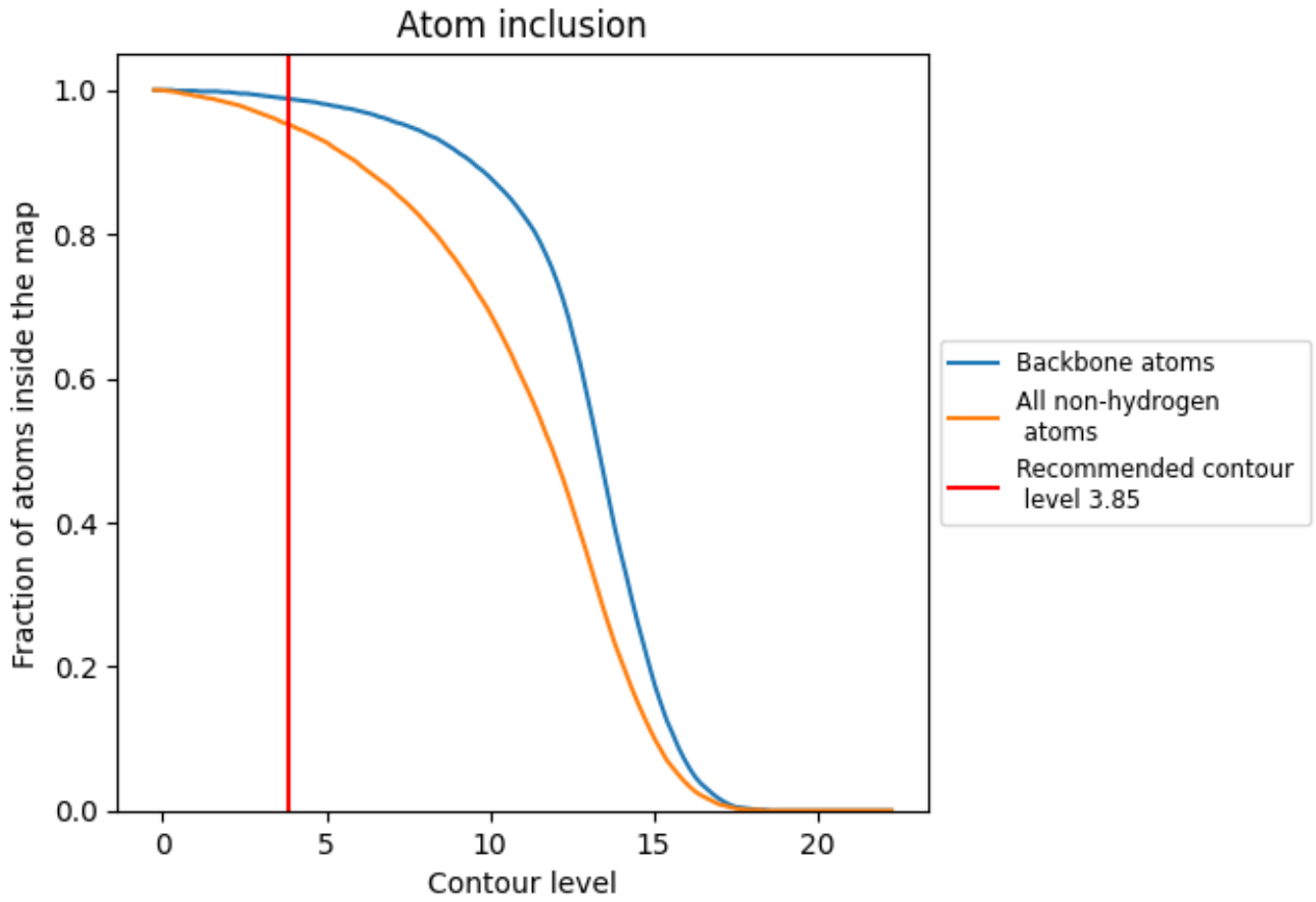
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (3.85).

9.4 Atom inclusion (i)



At the recommended contour level, 99% of all backbone atoms, 95% 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 (3.85) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9520	0.6970
A	0.9470	0.6850
B	0.9580	0.6990
C	0.9150	0.6740
D	0.9320	0.6830
E	0.9440	0.6870
F	0.9420	0.6830
G	0.9500	0.6970
H	0.9640	0.7150
I	0.9710	0.7090
J	0.9760	0.7170
K	0.9760	0.7170
L	0.9750	0.7150
M	0.9710	0.7130
N	0.9690	0.7120
O	0.9440	0.6810
P	0.9580	0.6990
Q	0.9150	0.6700
R	0.9420	0.6870
S	0.9410	0.6840
T	0.9460	0.6940
U	0.0560	0.2550
V	0.9740	0.7160
W	0.9780	0.7170
X	0.9700	0.7130
Y	0.9710	0.7110
Z	0.9290	0.6810
a	0.9640	0.7160
b	0.9710	0.7080
c	0.9750	0.7150
d	0.5000	0.3800
e	0.5830	0.4650
f	0.0560	0.2260
g	0.5000	0.3980
h	0.5830	0.5010

