



wwPDB EM Validation Summary Report ⓘ

Mar 10, 2026 – 12:48 PM UTC

PDB ID : 8CVR / pdb_00008cvr
EMDB ID : EMD-27013
Title : Human 20S proteasome with MG-132
Authors : Zhao, J.
Deposited on : 2022-05-18
Resolution : 2.70 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

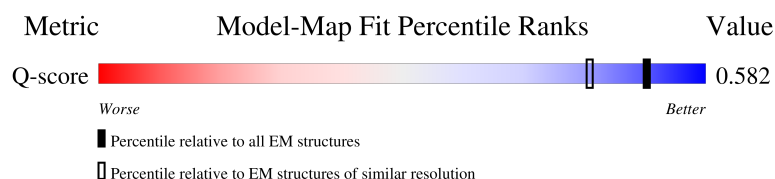
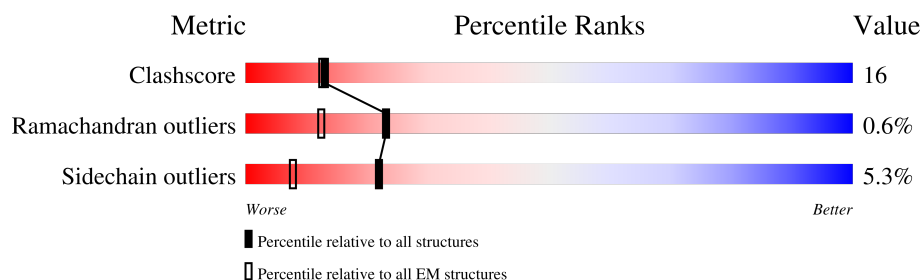
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 2.70 Å.

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



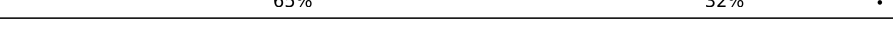
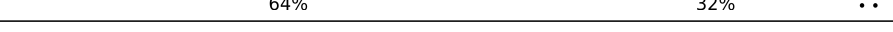
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10327 (2.20 - 3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	246	
1	O	246	
2	B	234	
2	P	234	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	C	261	
3	Q	261	
4	D	248	
4	R	248	
5	E	241	
5	S	241	
6	F	263	
6	T	263	
7	G	255	
7	U	255	
8	H	205	
8	V	205	
9	I	234	
9	W	234	
10	J	205	
10	X	205	
11	K	201	
11	Y	201	
12	L	204	
12	Z	204	
13	M	241	
13	a	241	
14	N	264	
14	b	264	

2 Entry composition [i](#)

There are 15 unique types of molecules in this entry. The entry contains 45586 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	240	Total	C	N	O	S	0	0
			1738	1106	304	316	12		
1	O	240	Total	C	N	O	S	0	0
			1734	1104	304	314	12		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

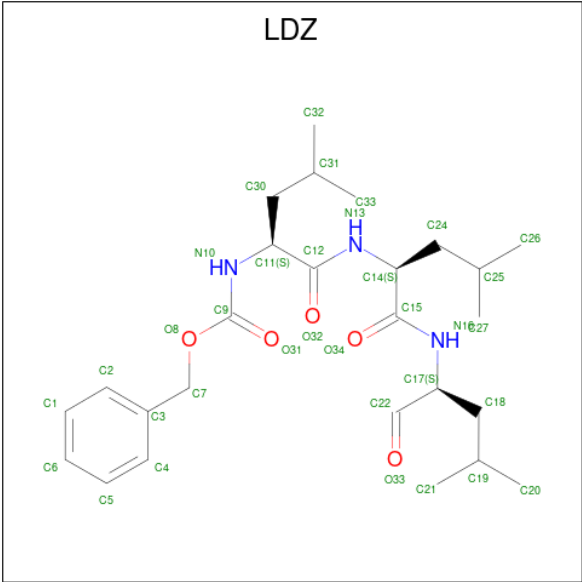
- Molecule 13 is a protein called Proteasome subunit beta type-1.

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

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

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

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

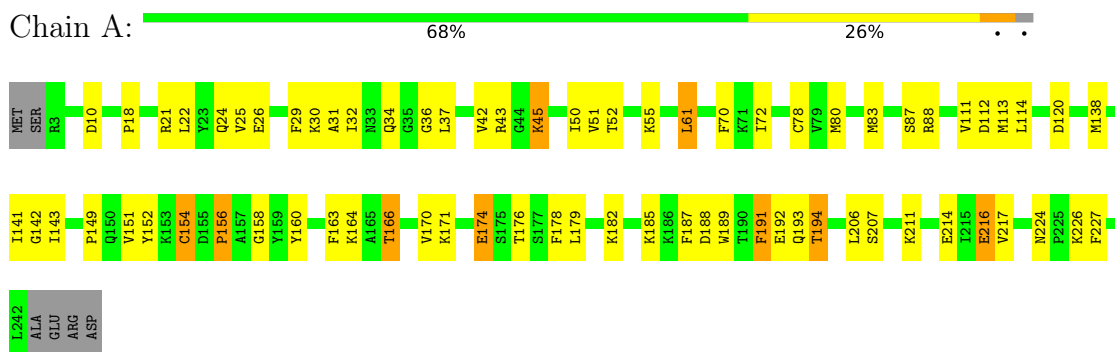


Mol	Chain	Residues	Atoms				AltConf
15	H	1	Total	C	N	O	0
			34	26	3	5	
15	I	1	Total	C	N	O	0
			34	26	3	5	
15	L	1	Total	C	N	O	0
			34	26	3	5	
15	V	1	Total	C	N	O	0
			34	26	3	5	
15	W	1	Total	C	N	O	0
			34	26	3	5	
15	Z	1	Total	C	N	O	0
			34	26	3	5	

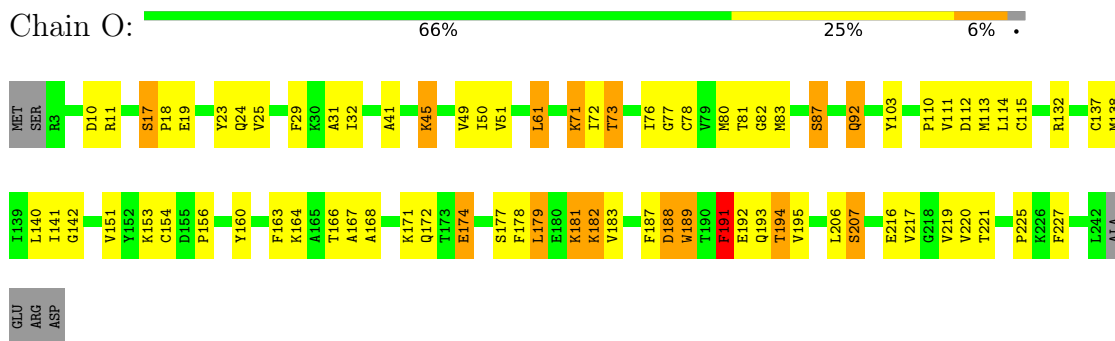
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

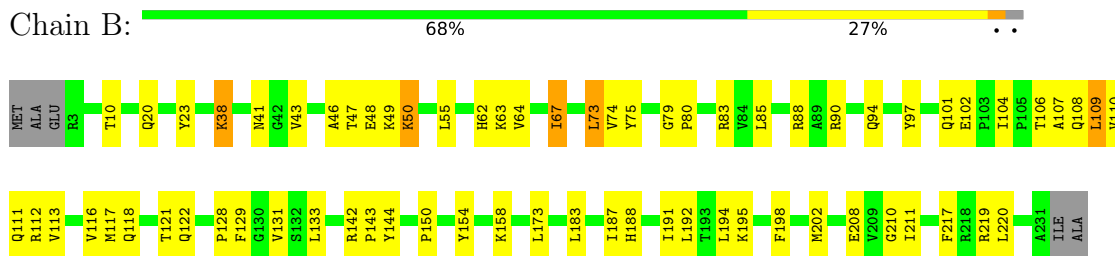
• Molecule 1: Proteasome subunit alpha type-6



• Molecule 1: Proteasome subunit alpha type-6



• Molecule 2: Proteasome subunit alpha type-2



• Molecule 2: Proteasome subunit alpha type-2

C136	G137	P143	P150	S151	Y154	K158	M162	L173	L183	I187	H188	I191	L192	M202	I207	E208	I211	C212	R219	L220	T223	K226	A231	I234	ALA																	
Met	Ala	GLU	R3	P144	I21	Y23	L24	L25	V28	K38	N41	E48	K49	K50	K69	H70	L73	V74	M78	G79	P80	R83	R88	K91	L92	Q95	P105	T106	A107	Q108	L109	V110	Q111	R112	V116	F129	G130	V131	S132	L133	L134	T135

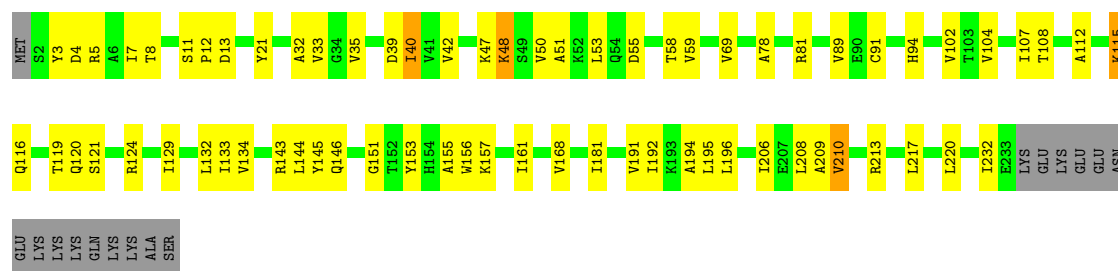
A208	A94	ME1
T215	Q95	S2
L216	Q100	R3
V224	Q109	D6
K229	T112	S7
V233	A113	R8
I237	L114	P14
E248	R128	V21
ARG	L135	A24
GLU	G138	M25
LYS	Y143	E26
GLU	Q146	A27
GLY	L147	I28
GLN	P152	T33
LYS	G158	C34
GLU	W159	L35
ASP	K160	D41
LYS	G162	G42
GLU	A161	V43
ASP	T162	L44
LYS	C163	L45
	I164	A46
	S168	A47
	A171	H53
	V172	L56
	S173	D57
	M174	E58
	L175	Y59
	K176	F60
	K180	F61
	M184	K64
	T185	I65
	L186	Y66
	K187	K67
	L190	L68
	V196	N69
	K199	M72
	T200	A73
	M201	C74
	D202	S75
	S204	V76
	S207	S81
		D82
		A83
		L90
		R91
		L92
		I93

V224	Q119	ME1
I225	G131	S2
V233	V132	R3
I237	S133	T9
E248	L134	P14
ARG	Y136	Q20
GLU	I137	Y23
LYS	G138	A24
LYS	K141	M25
GLU	F145	E26
LYS	Q146	A27
GLN	L147	I28
LYS	Y156	T33
GLU	G157	C34
ASP	G158	L35
LYS	M159	V43
	K160	L44
	A161	L45
	T162	A46
	C163	A47
	I164	E48
	A171	F61
	M174	K64
	L175	L68
	K176	
	Q177	D71
	K180	M72
	M184	A73
	K187	C74
	S188	S75
	A189	V76
	L190	E89
	L194	R91
LYS	K195	L92
LYS	V196	L93
ASP	L197	R96
LYS	N198	T97
	K199	L98
	T200	Y101
	V203	Q102
	L206	Q109
	S207	T112
	A208	A113
	L216	L114
		C115

L208	T108	Met
A209	R109	S2
V210		
M211	K115	R5
R212		
R213		
	T119	S11
L217	Q120	P12
K218	S121	D13
I219		G14
L220	R124	H15
E233	I129	Y21
LYS		
GLU	L132	E24
LYS	I133	
LYS	V134	K27
GLU	G135	
GLU	F136	A32
ASN		V33
GLU	G140	
GLU	T141	R36
LYS	P142	
LYS	R143	V41
LYS	L144	V42
GLN	Y145	
LYS		K47
ALA	Y153	K48
SER	H154	
	A155	L53
	H156	Q54
	K157	D55
	I161	T58
	G162	V59
	R163	
	V168	C63
	L172	V69
		C70
	I181	A80
		R81
	D184	
		I84
	T187	V89
	I188	F90
		C91
	I192	
	K193	
	A194	H94
	L195	R95
	L196	L96
		T97
	V199	V98
	G202	V102
	C203	T103
		V104
	E206	T107

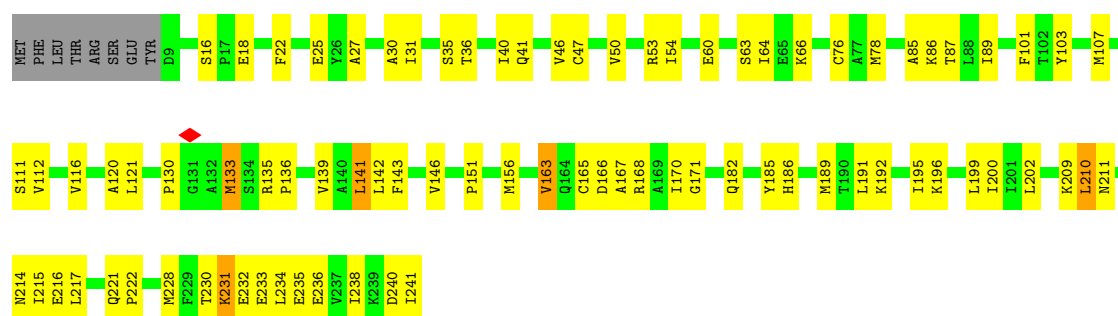
WORLDWIDE
PDB
PROTEIN DATA BANK

Chain R: 



• Molecule 5: Proteasome subunit alpha type-5

Chain E: 



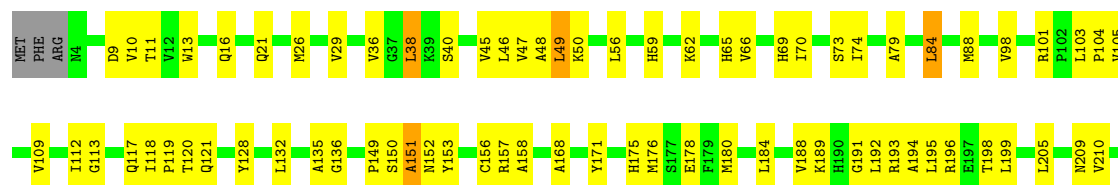
• Molecule 5: Proteasome subunit alpha type-5

Chain S: 

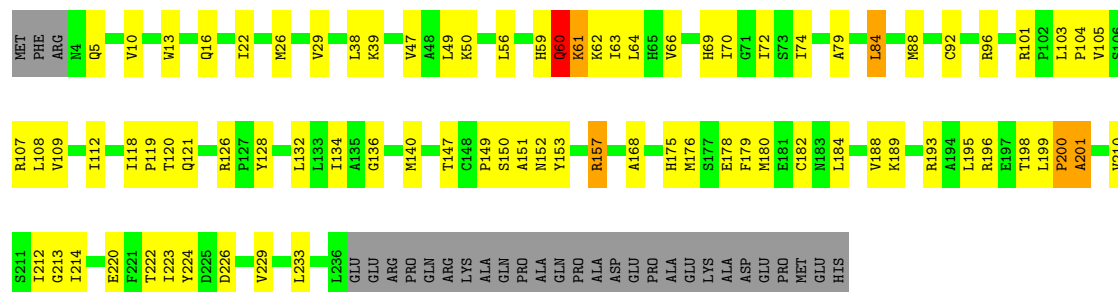


• Molecule 6: Proteasome subunit alpha type-1

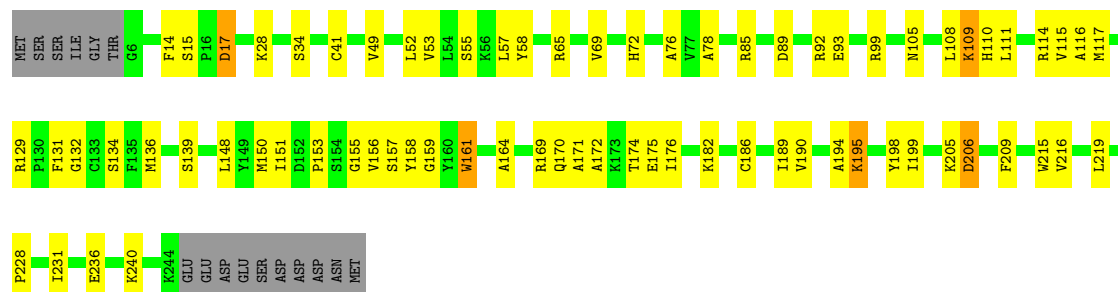
Chain F: 



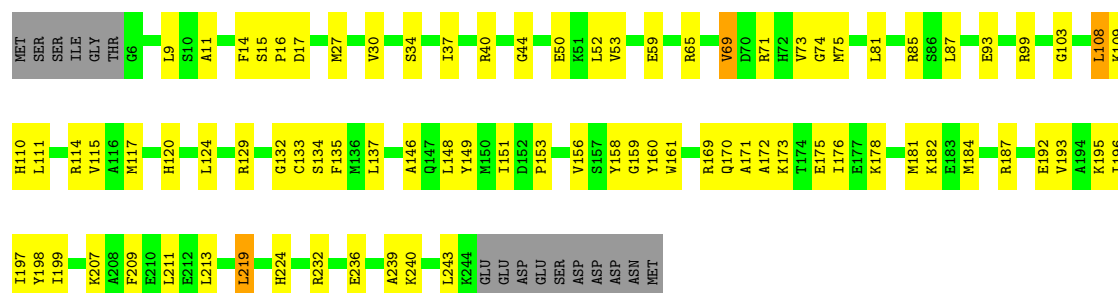
- Molecule 6: Proteasome subunit alpha type-1



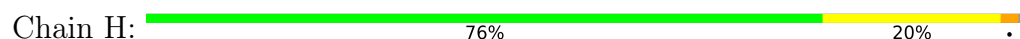
- Molecule 7: Proteasome subunit alpha type-3



- Molecule 7: Proteasome subunit alpha type-3



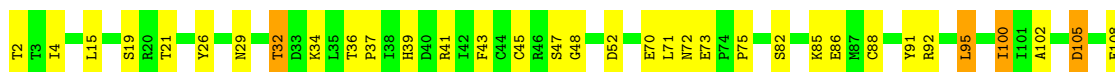
- Molecule 8: Proteasome subunit beta type-6





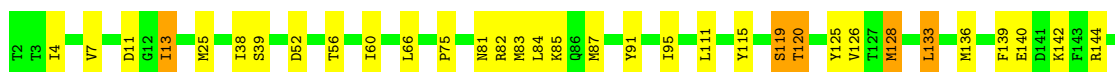
• Molecule 8: Proteasome subunit beta type-6

Chain V: 70% 27% ..



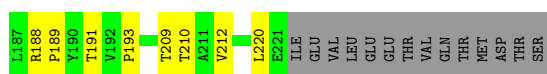
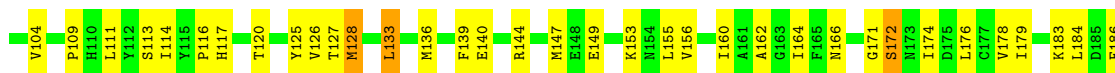
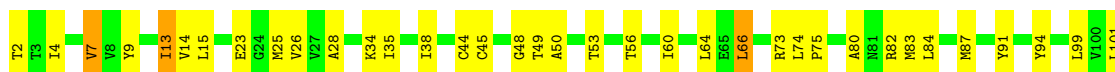
• Molecule 9: Proteasome subunit beta type-7

Chain I: 70% 20% 6%



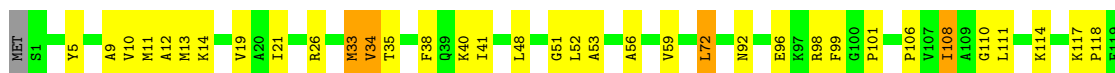
• Molecule 9: Proteasome subunit beta type-7

Chain W: 60% 31% 6%



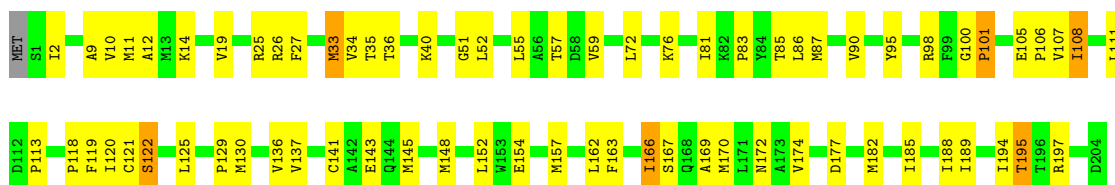
• Molecule 10: Proteasome subunit beta type-3

Chain J: 68% 29%



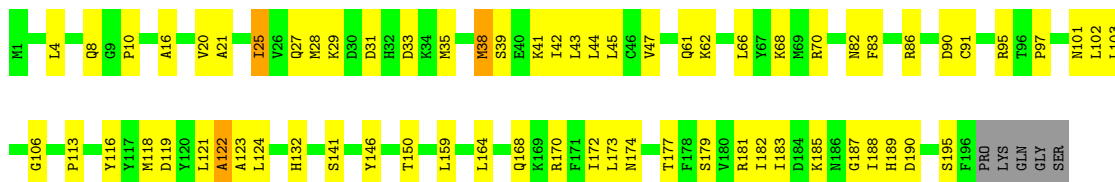
• Molecule 10: Proteasome subunit beta type-3

Chain X: 65% 32%



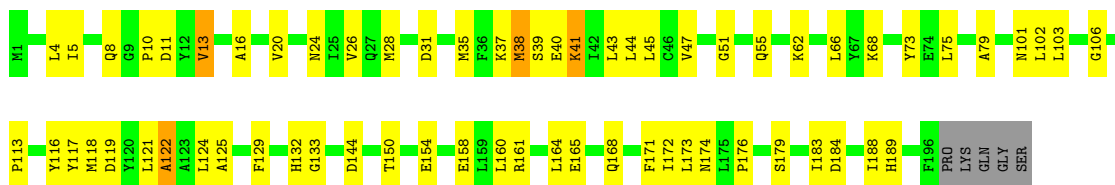
• Molecule 11: Proteasome subunit beta type-2

Chain K: 64% 32% ..



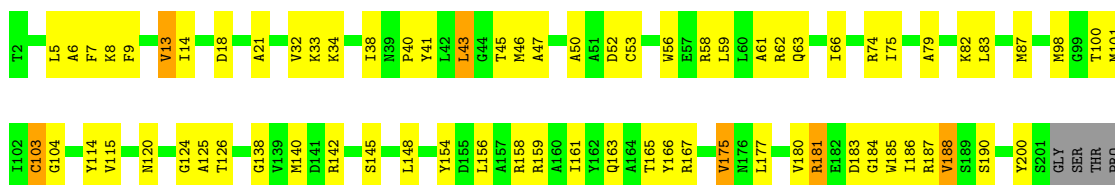
• Molecule 11: Proteasome subunit beta type-2

Chain Y: 65% 30% ..



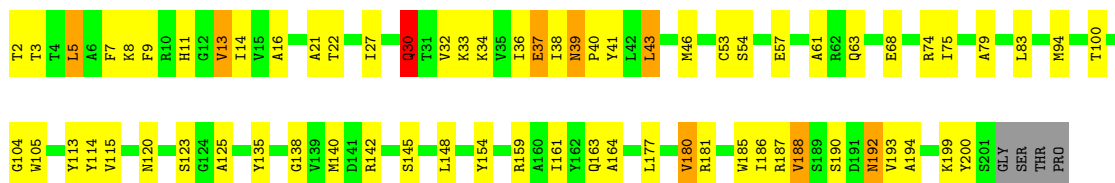
• Molecule 12: Proteasome subunit beta type-5

Chain L: 63% 32% ..



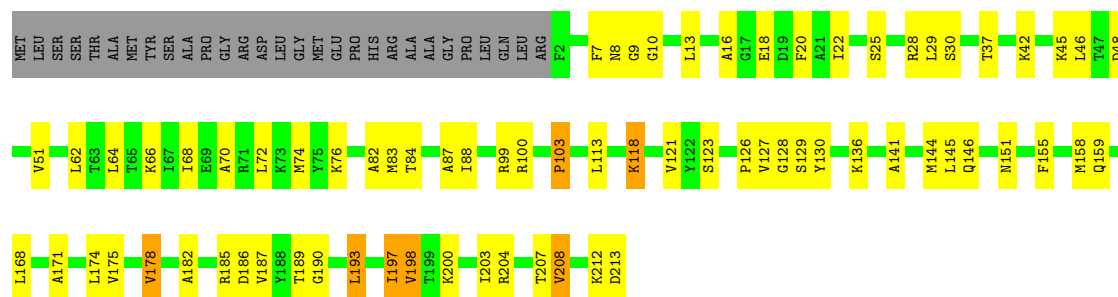
• Molecule 12: Proteasome subunit beta type-5

Chain Z: 64% 29% ..



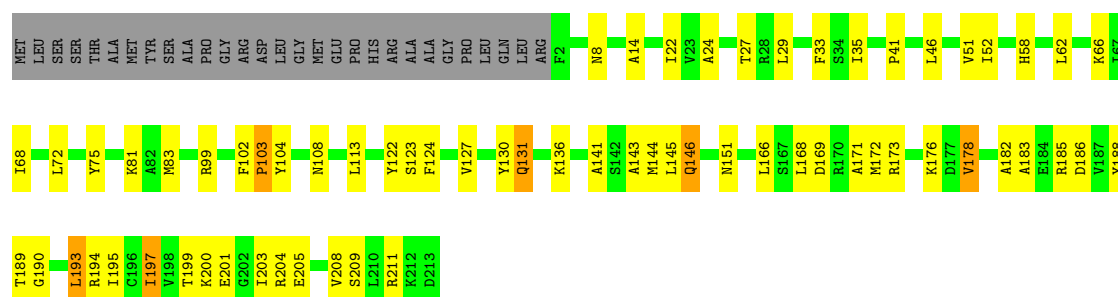
• Molecule 13: Proteasome subunit beta type-1

Chain M: 57% 28% 12%



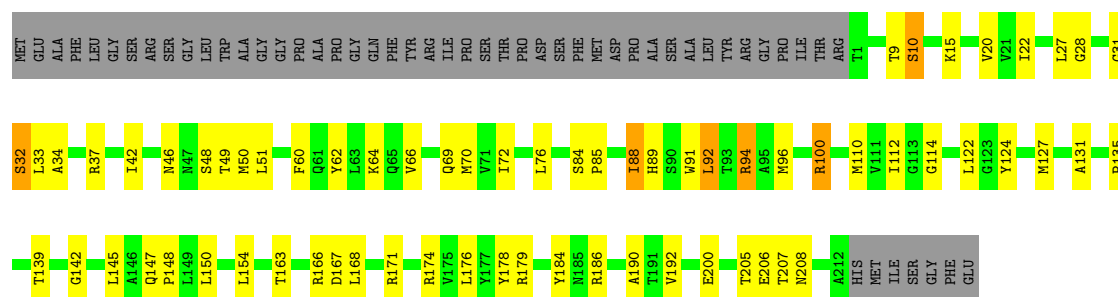
• Molecule 13: Proteasome subunit beta type-1

Chain a: 60% 25% 12%



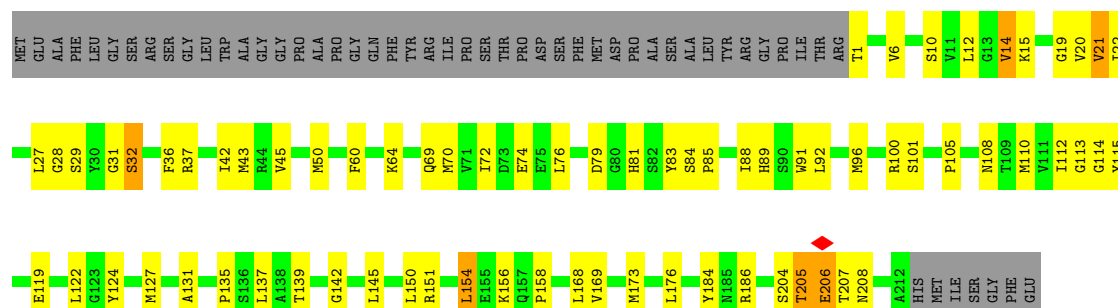
• Molecule 14: Proteasome subunit beta type-4

Chain N: 55% 23% 20%



• Molecule 14: Proteasome subunit beta type-4

Chain b: 53% 25% 20%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	214790	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.788	Depositor
Minimum map value	-0.318	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.035	Depositor
Recommended contour level	0.1	Depositor
Map size ($\text{\AA}$)	339.19998, 339.19998, 339.19998	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.06, 1.06, 1.06	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.93	0/1767	1.21	1/2398 (0.0%)
1	O	0.93	0/1763	1.19	2/2393 (0.1%)
2	B	0.92	0/1701	1.18	2/2318 (0.1%)
2	P	0.92	0/1701	1.18	2/2318 (0.1%)
3	C	0.93	0/1815	1.19	1/2466 (0.0%)
3	Q	0.93	0/1815	1.18	1/2466 (0.0%)
4	D	0.95	0/1657	1.20	2/2261 (0.1%)
4	R	0.95	0/1657	1.19	1/2261 (0.0%)
5	E	0.95	0/1686	1.17	0/2290
5	S	0.94	0/1686	1.16	1/2290 (0.0%)
6	F	0.93	0/1738	1.17	1/2364 (0.0%)
6	T	0.93	0/1741	1.18	2/2367 (0.1%)
7	G	0.92	0/1795	1.17	1/2434 (0.0%)
7	U	0.92	0/1795	1.17	1/2434 (0.0%)
8	H	0.91	0/1495	1.17	0/2026
8	V	0.90	0/1491	1.20	0/2021
9	I	0.91	0/1607	1.21	1/2185 (0.0%)
9	W	0.92	0/1603	1.20	1/2180 (0.0%)
10	J	0.89	0/1575	1.20	4/2128 (0.2%)
10	X	0.89	0/1563	1.21	4/2113 (0.2%)
11	K	0.88	0/1541	1.14	0/2092
11	Y	0.89	0/1538	1.15	1/2088 (0.0%)
12	L	0.88	0/1535	1.14	0/2080
12	Z	0.88	0/1531	1.15	1/2076 (0.0%)
13	M	0.89	0/1614	1.19	1/2178 (0.0%)
13	a	0.90	0/1614	1.18	2/2178 (0.1%)
14	N	0.89	0/1598	1.17	0/2170
14	b	0.90	0/1602	1.18	1/2175 (0.0%)
All	All	0.91	0/46224	1.18	34/62750 (0.1%)

There are no bond length outliers.

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	38	ILE	N-CA-C	-7.93	105.47	111.90
9	W	38	ILE	N-CA-C	-7.55	105.32	111.81
2	B	158	LYS	N-CA-C	-7.14	104.69	113.41
2	P	158	LYS	N-CA-C	-7.08	104.77	113.41
3	C	160	LYS	N-CA-C	-6.69	105.24	113.41

There are no chirality outliers.

There are no planarity outliers.

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	1738	0	1656	58	0
1	O	1734	0	1652	63	0
2	B	1662	0	1590	52	0
2	P	1662	0	1590	49	0
3	C	1786	0	1717	66	0
3	Q	1786	0	1717	52	0
4	D	1633	0	1518	58	0
4	R	1633	0	1518	54	0
5	E	1660	0	1589	59	0
5	S	1660	0	1589	58	0
6	F	1704	0	1638	71	0
6	T	1707	0	1645	64	0
7	G	1760	0	1680	59	0
7	U	1760	0	1680	58	0
8	H	1469	0	1422	42	0
8	V	1465	0	1416	54	0
9	I	1580	0	1559	54	0
9	W	1576	0	1555	70	0
10	J	1546	0	1552	59	0
10	X	1534	0	1539	56	0
11	K	1509	0	1477	49	0
11	Y	1506	0	1475	48	0
12	L	1504	0	1449	57	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	Z	1500	0	1438	65	0
13	M	1584	0	1579	57	0
13	a	1584	0	1579	58	0
14	N	1568	0	1513	53	0
14	b	1572	0	1517	58	0
15	H	34	0	41	3	0
15	I	34	0	41	3	0
15	L	34	0	41	12	0
15	V	34	0	41	9	0
15	W	34	0	41	9	0
15	Z	34	0	41	11	0
All	All	45586	0	44095	1466	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 16.

The worst 5 of 1466 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)
15:Z:301:LDZ:C6	13:a:131:GLN:HB2	1.81	1.11
3:Q:158:GLY:H	4:R:58:THR:HG21	1.16	1.09
3:C:158:GLY:H	4:D:58:THR:HG21	1.03	1.07
8:V:45:CYS:HB2	8:V:100:ILE:HG23	1.43	1.00
9:I:188:ARG:HB3	9:I:189:PRO:HD3	1.46	0.96

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	238/246 (97%)	223 (94%)	12 (5%)	3 (1%)	9 25

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	O	238/246 (97%)	221 (93%)	13 (6%)	4 (2%)	7	19
2	B	227/234 (97%)	222 (98%)	5 (2%)	0	100	100
2	P	227/234 (97%)	224 (99%)	3 (1%)	0	100	100
3	C	245/261 (94%)	231 (94%)	9 (4%)	5 (2%)	6	16
3	Q	245/261 (94%)	240 (98%)	4 (2%)	1 (0%)	30	54
4	D	230/248 (93%)	219 (95%)	9 (4%)	2 (1%)	14	35
4	R	230/248 (93%)	220 (96%)	7 (3%)	3 (1%)	9	25
5	E	231/241 (96%)	219 (95%)	11 (5%)	1 (0%)	30	54
5	S	231/241 (96%)	221 (96%)	9 (4%)	1 (0%)	30	54
6	F	231/263 (88%)	217 (94%)	13 (6%)	1 (0%)	30	54
6	T	231/263 (88%)	220 (95%)	7 (3%)	4 (2%)	7	19
7	G	237/255 (93%)	228 (96%)	9 (4%)	0	100	100
7	U	237/255 (93%)	230 (97%)	5 (2%)	2 (1%)	16	37
8	H	200/205 (98%)	195 (98%)	5 (2%)	0	100	100
8	V	200/205 (98%)	191 (96%)	8 (4%)	1 (0%)	24	48
9	I	218/234 (93%)	211 (97%)	5 (2%)	2 (1%)	14	35
9	W	218/234 (93%)	210 (96%)	7 (3%)	1 (0%)	24	48
10	J	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
10	X	202/205 (98%)	197 (98%)	5 (2%)	0	100	100
11	K	194/201 (96%)	187 (96%)	5 (3%)	2 (1%)	12	32
11	Y	194/201 (96%)	187 (96%)	6 (3%)	1 (0%)	24	48
12	L	198/204 (97%)	190 (96%)	8 (4%)	0	100	100
12	Z	198/204 (97%)	192 (97%)	6 (3%)	0	100	100
13	M	210/241 (87%)	200 (95%)	9 (4%)	1 (0%)	24	48
13	a	210/241 (87%)	202 (96%)	7 (3%)	1 (0%)	24	48
14	N	210/264 (80%)	194 (92%)	15 (7%)	1 (0%)	24	48
14	b	210/264 (80%)	197 (94%)	11 (5%)	2 (1%)	12	32
All	All	6142/6604 (93%)	5883 (96%)	220 (4%)	39 (1%)	23	44

5 of 39 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	203	VAL

Continued on next page...

Continued from previous page...

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	164/210 (78%)	155 (94%)	9 (6%)	19	45
1	O	163/210 (78%)	148 (91%)	15 (9%)	8	22
2	B	150/191 (78%)	143 (95%)	7 (5%)	23	51
2	P	150/191 (78%)	145 (97%)	5 (3%)	33	63
3	C	160/221 (72%)	154 (96%)	6 (4%)	29	58
3	Q	160/221 (72%)	151 (94%)	9 (6%)	19	44
4	D	136/211 (64%)	130 (96%)	6 (4%)	25	53
4	R	136/211 (64%)	132 (97%)	4 (3%)	37	67
5	E	158/203 (78%)	145 (92%)	13 (8%)	10	27
5	S	158/203 (78%)	148 (94%)	10 (6%)	16	39
6	F	160/224 (71%)	151 (94%)	9 (6%)	19	44
6	T	161/224 (72%)	157 (98%)	4 (2%)	42	71
7	G	162/212 (76%)	154 (95%)	8 (5%)	22	49
7	U	162/212 (76%)	153 (94%)	9 (6%)	19	44
8	H	141/159 (89%)	135 (96%)	6 (4%)	26	54
8	V	140/159 (88%)	133 (95%)	7 (5%)	22	48
9	I	158/195 (81%)	145 (92%)	13 (8%)	10	27
9	W	157/195 (80%)	150 (96%)	7 (4%)	24	52
10	J	159/174 (91%)	152 (96%)	7 (4%)	25	53
10	X	155/174 (89%)	148 (96%)	7 (4%)	24	52

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	K	149/171 (87%)	143 (96%)	6 (4%)	28	56
11	Y	148/171 (86%)	142 (96%)	6 (4%)	27	56
12	L	139/159 (87%)	129 (93%)	10 (7%)	13	32
12	Z	138/159 (87%)	124 (90%)	14 (10%)	7	18
13	M	158/199 (79%)	149 (94%)	9 (6%)	18	43
13	a	158/199 (79%)	151 (96%)	7 (4%)	25	53
14	N	149/215 (69%)	142 (95%)	7 (5%)	23	51
14	b	150/215 (70%)	144 (96%)	6 (4%)	28	56
All	All	4279/5488 (78%)	4053 (95%)	226 (5%)	22	46

5 of 226 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
14	N	163	THR
14	b	21	VAL
3	Q	199	LYS
13	a	197	ILE
12	Z	2	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 85 such sidechains are listed below:

Mol	Chain	Res	Type
5	S	152	GLN
11	Y	8	GLN
5	S	164	GLN
7	U	110	HIS
11	Y	101	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	LDZ	Z	301	-	33,34,34	1.73	7 (21%)	42,44,44	1.16	5 (11%)
15	LDZ	V	301	-	33,34,34	1.80	7 (21%)	42,44,44	1.39	4 (9%)
15	LDZ	I	301	-	33,34,34	1.81	7 (21%)	42,44,44	1.34	6 (14%)
15	LDZ	L	301	-	33,34,34	1.85	7 (21%)	42,44,44	1.53	8 (19%)
15	LDZ	W	301	-	33,34,34	1.76	7 (21%)	42,44,44	1.17	2 (4%)
15	LDZ	H	301	-	33,34,34	1.76	7 (21%)	42,44,44	1.22	4 (9%)

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

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

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	V	301	LDZ	C15-N16	5.55	1.45	1.34

Continued on next page...

Continued from previous page...

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

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

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

There are no chirality outliers.

5 of 87 torsion outliers are listed below:

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

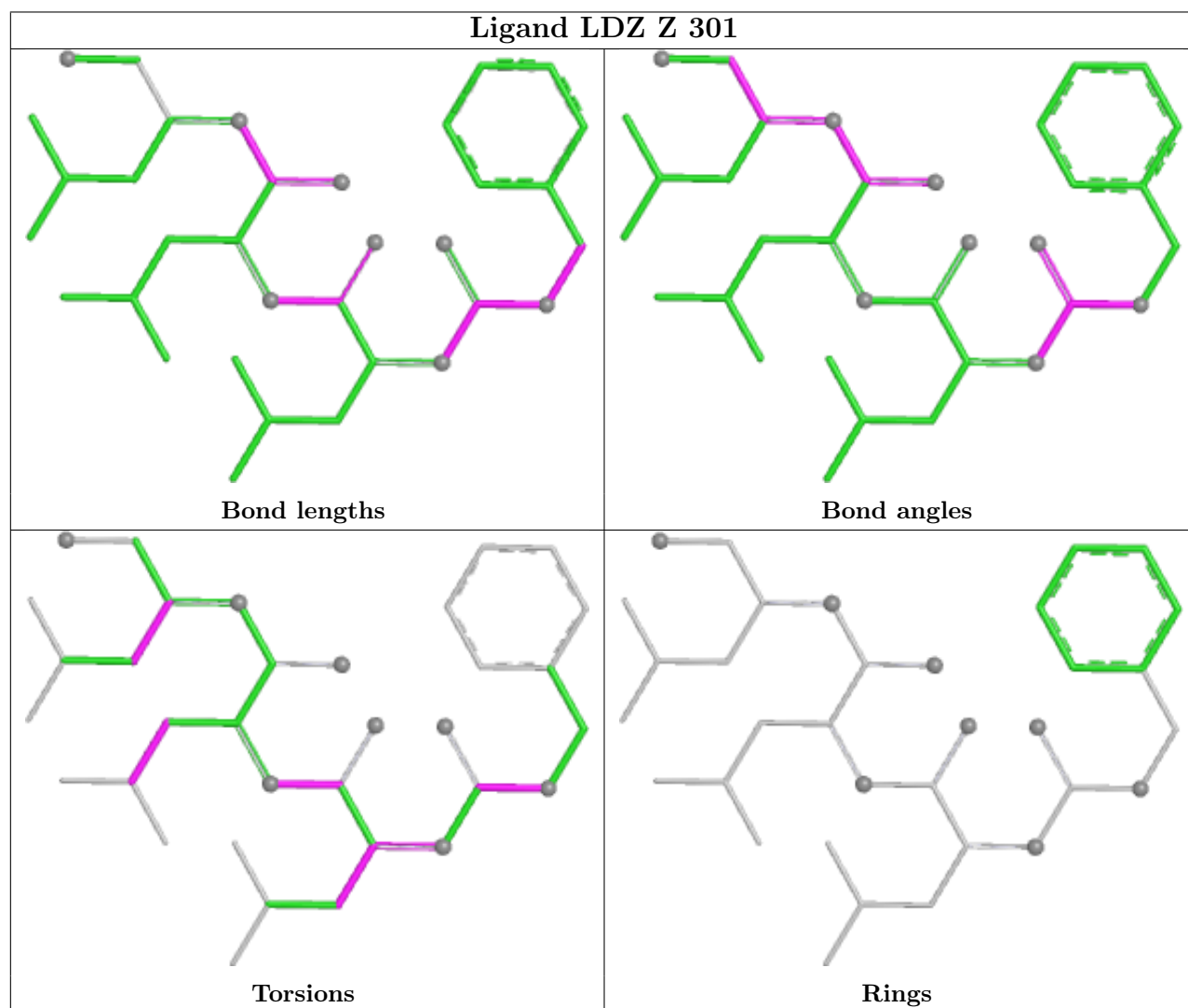
There are no ring outliers.

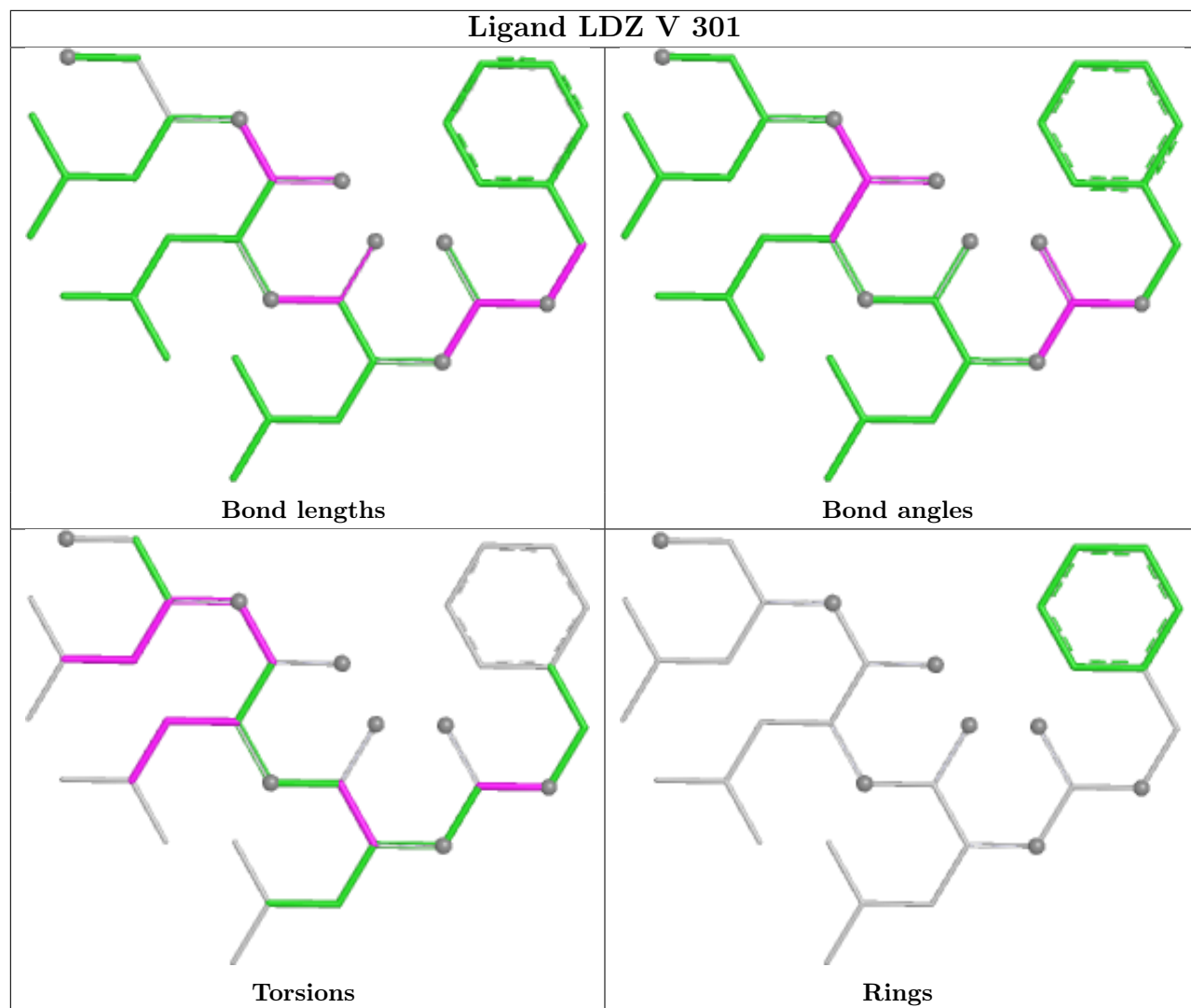
6 monomers are involved in 47 short contacts:

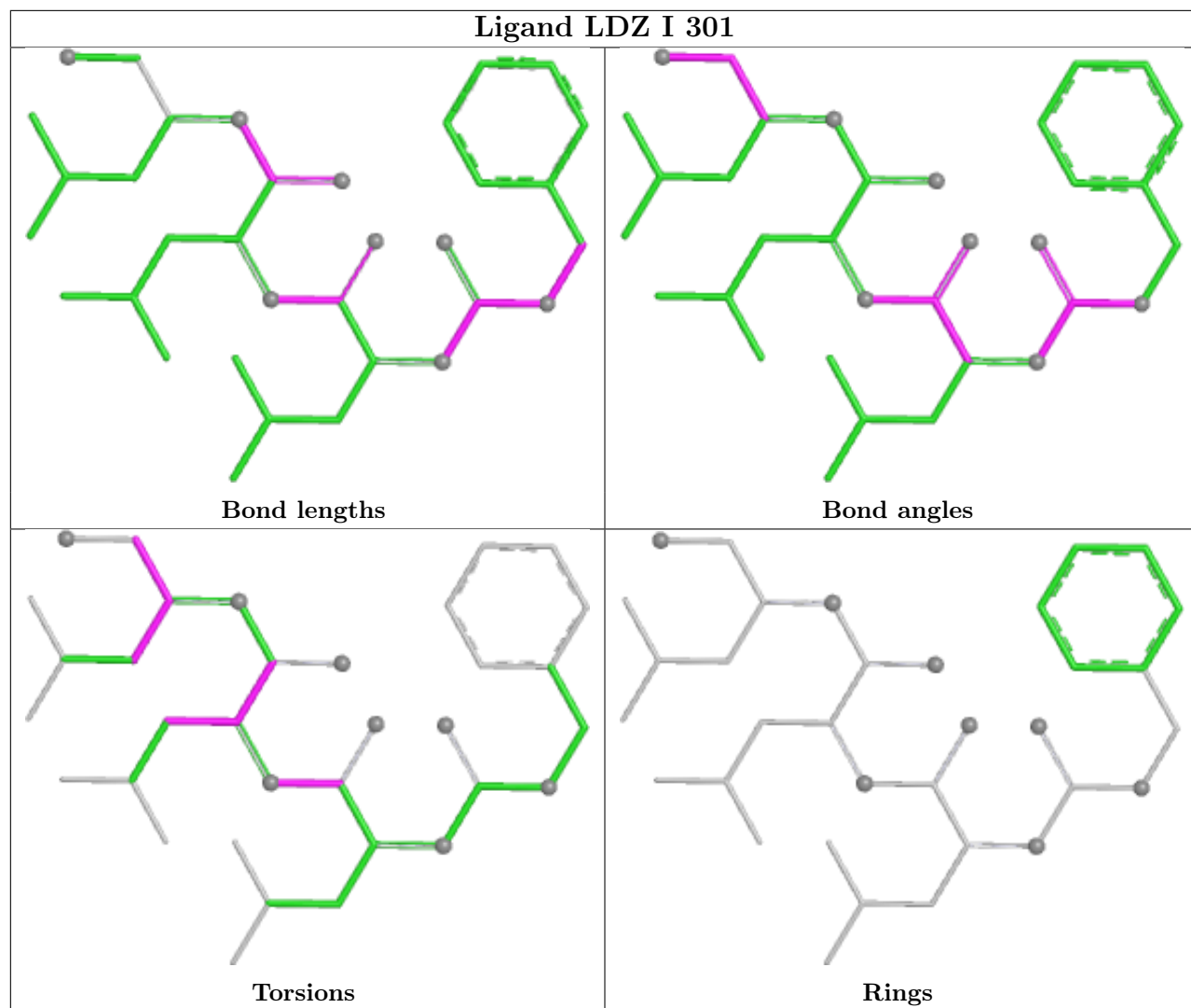
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	Z	301	LDZ	11	0
15	V	301	LDZ	9	0
15	I	301	LDZ	3	0
15	L	301	LDZ	12	0
15	W	301	LDZ	9	0
15	H	301	LDZ	3	0

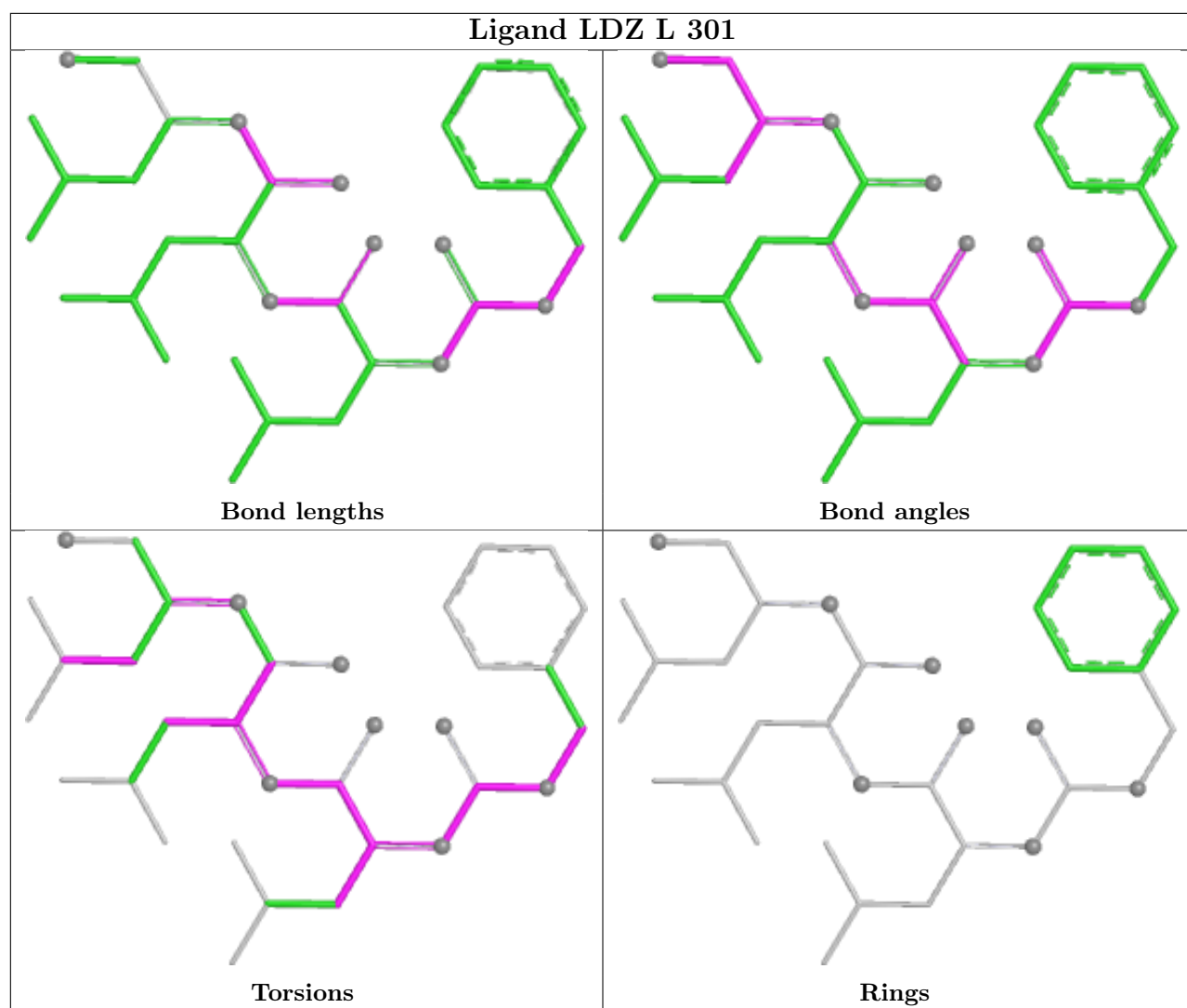
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

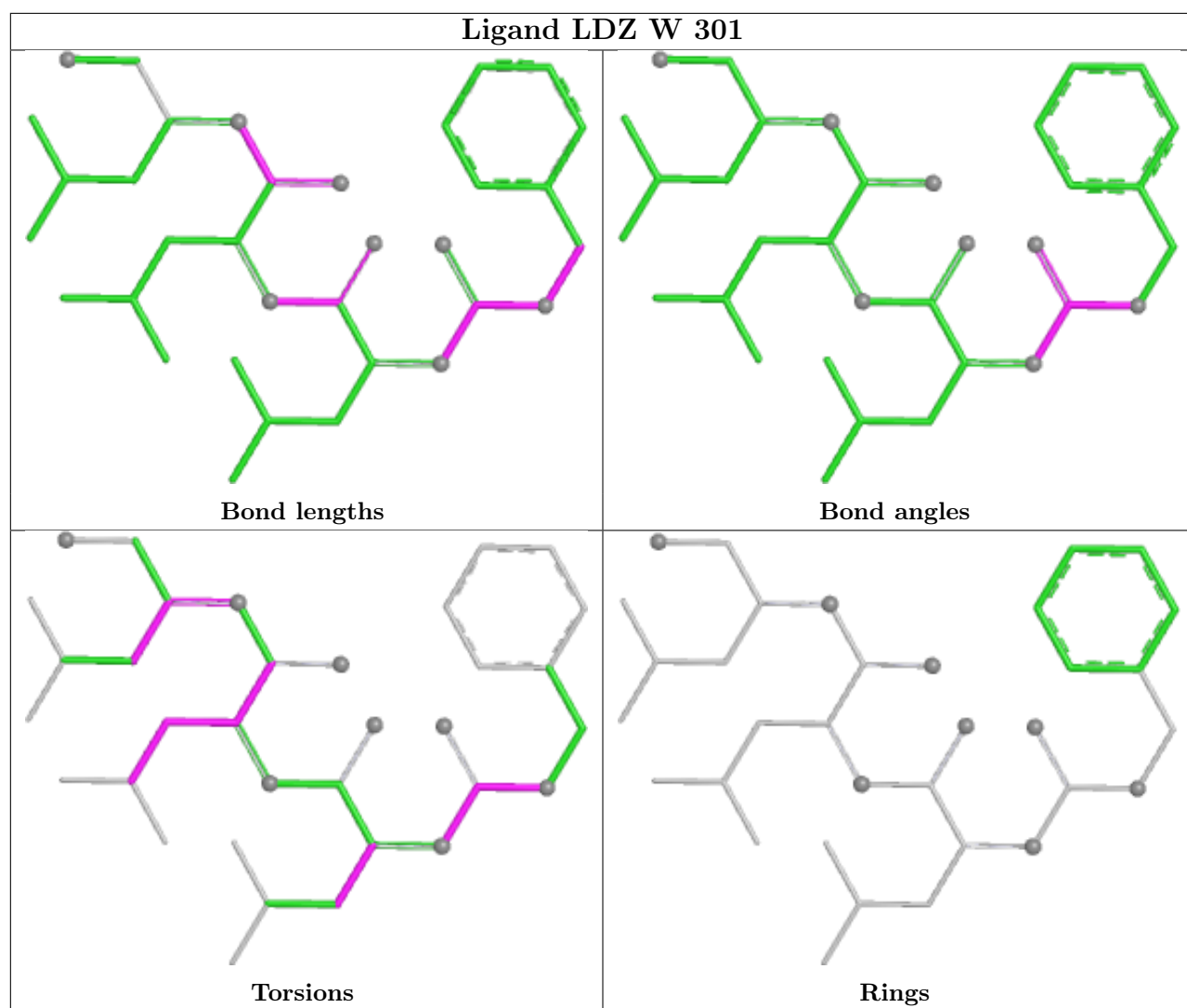
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

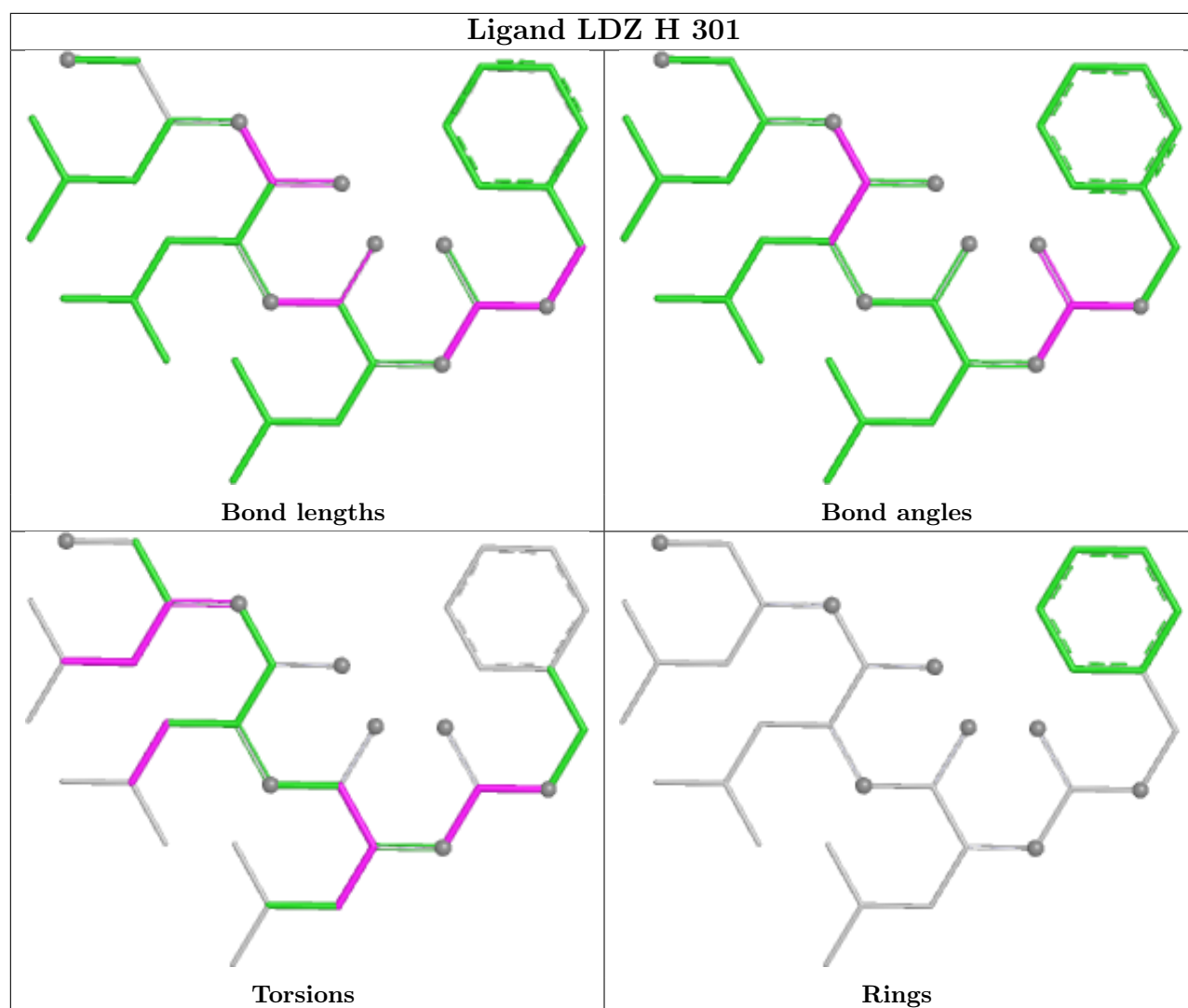












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

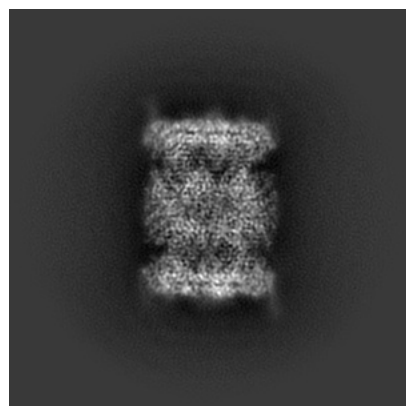
6 Map visualisation [i](#)

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

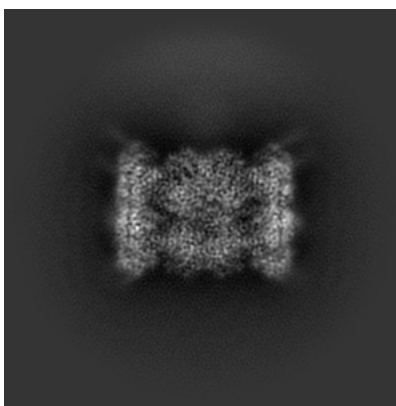
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

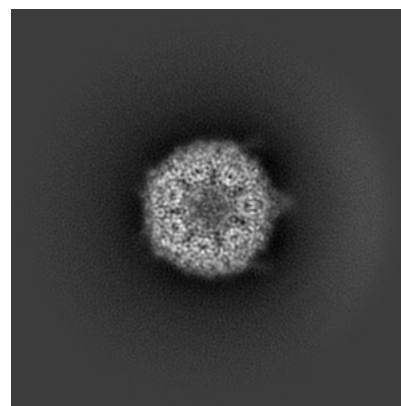
6.1.1 Primary map



X

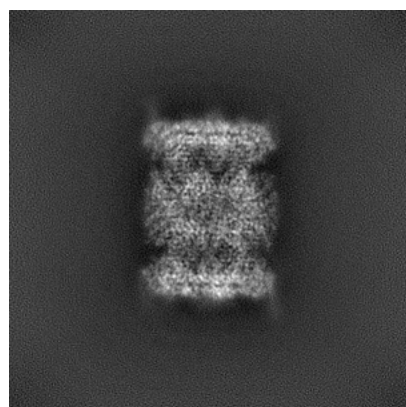


Y

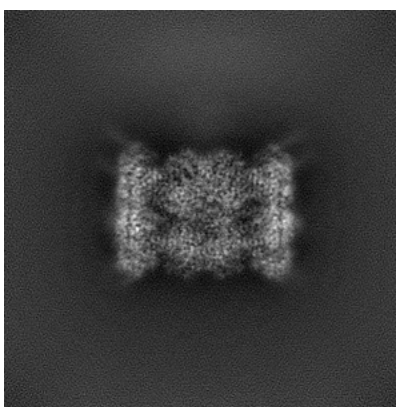


Z

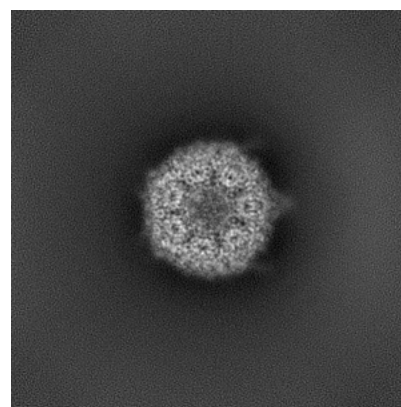
6.1.2 Raw map



X



Y

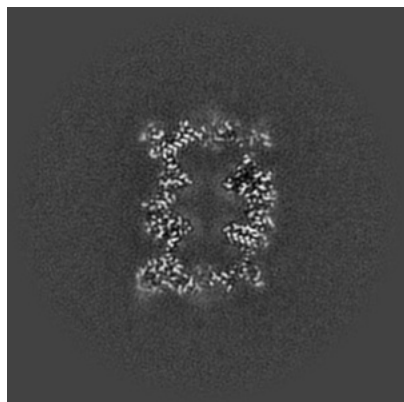


Z

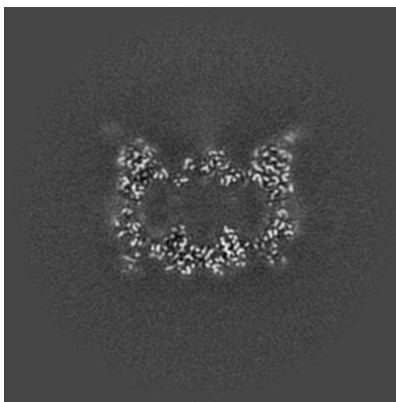
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

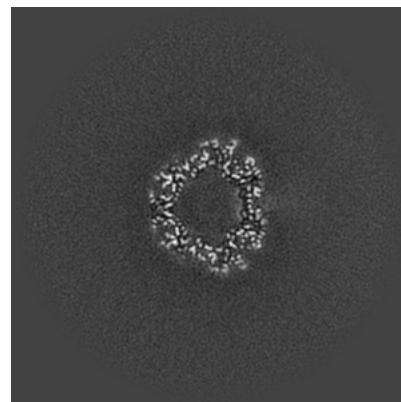
6.2.1 Primary map



X Index: 160

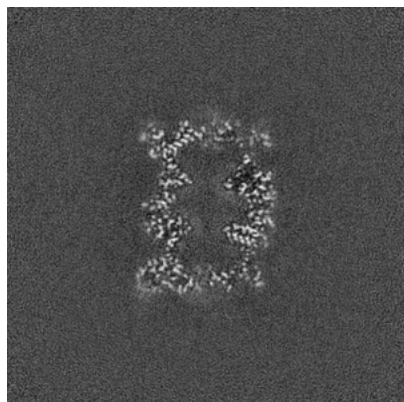


Y Index: 160

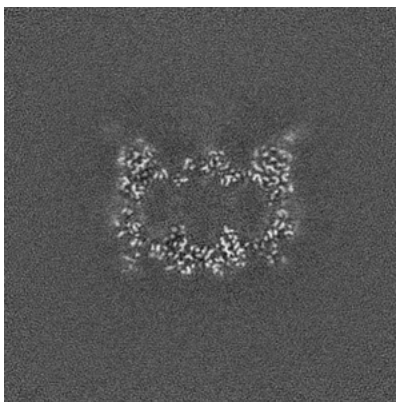


Z Index: 160

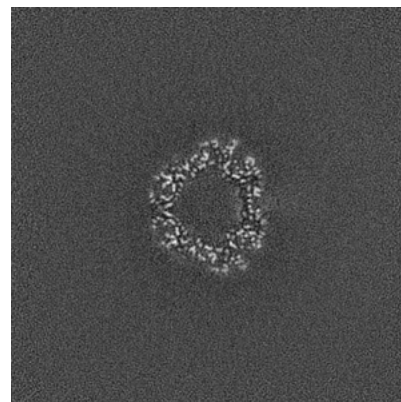
6.2.2 Raw map



X Index: 160



Y Index: 160

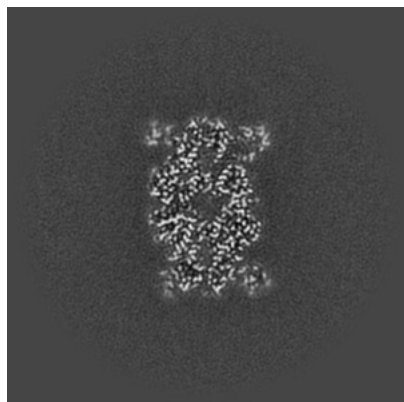


Z Index: 160

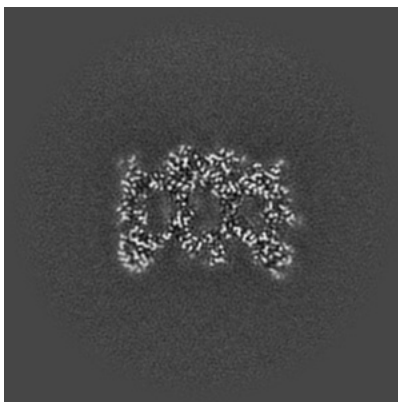
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

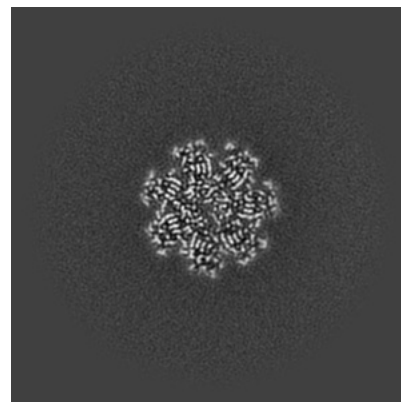
6.3.1 Primary map



X Index: 135

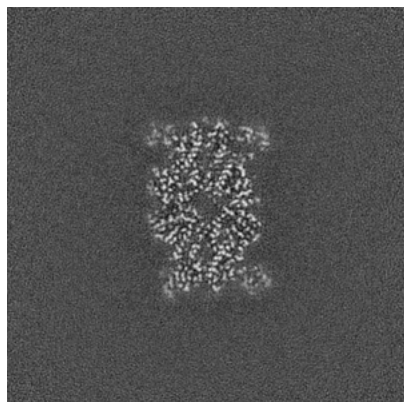


Y Index: 140

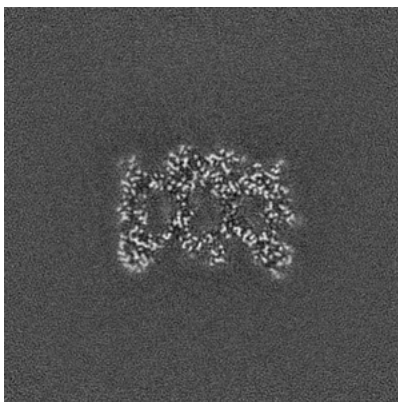


Z Index: 106

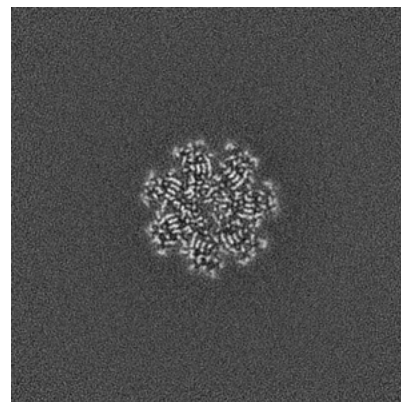
6.3.2 Raw map



X Index: 134



Y Index: 140

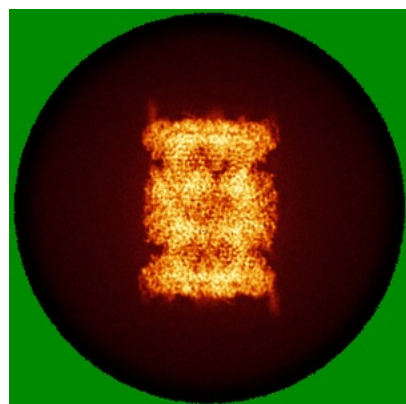


Z Index: 106

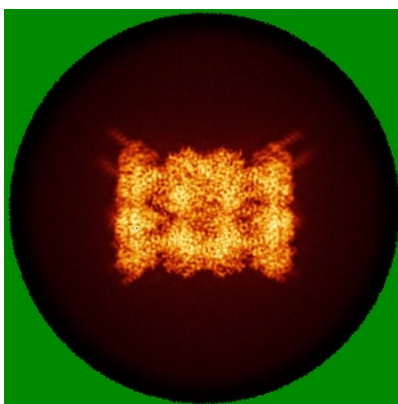
The images above show the largest variance slices of the map in three orthogonal directions.

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

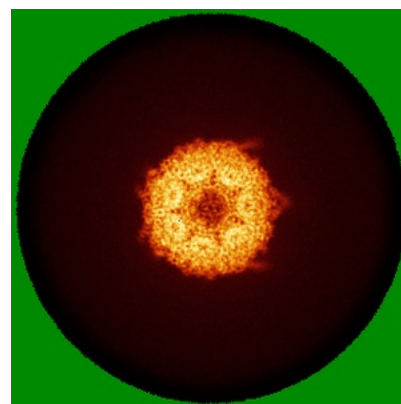
6.4.1 Primary map



X

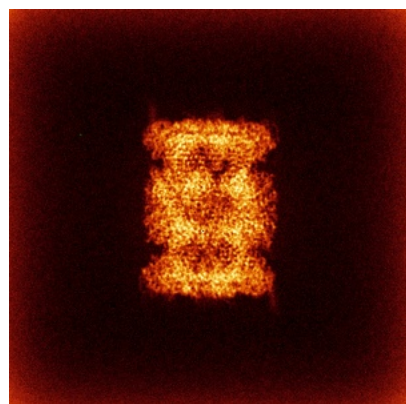


Y

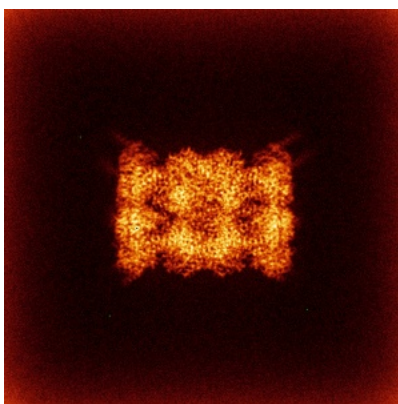


Z

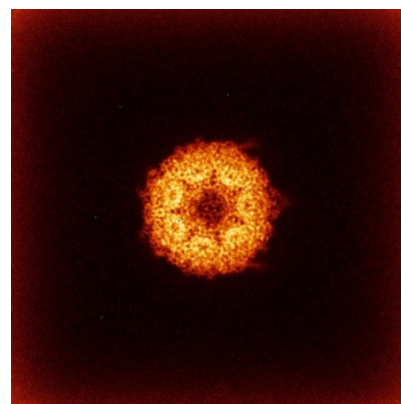
6.4.2 Raw map



X



Y

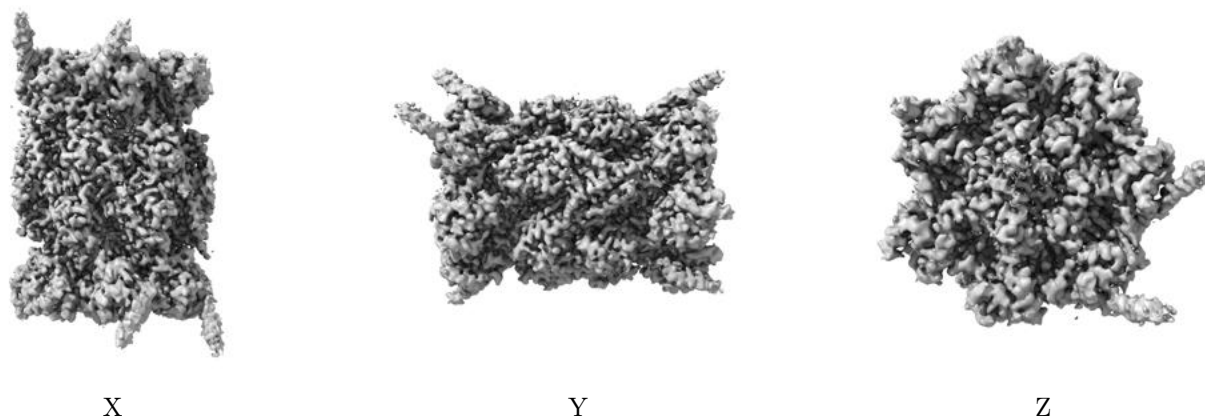


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

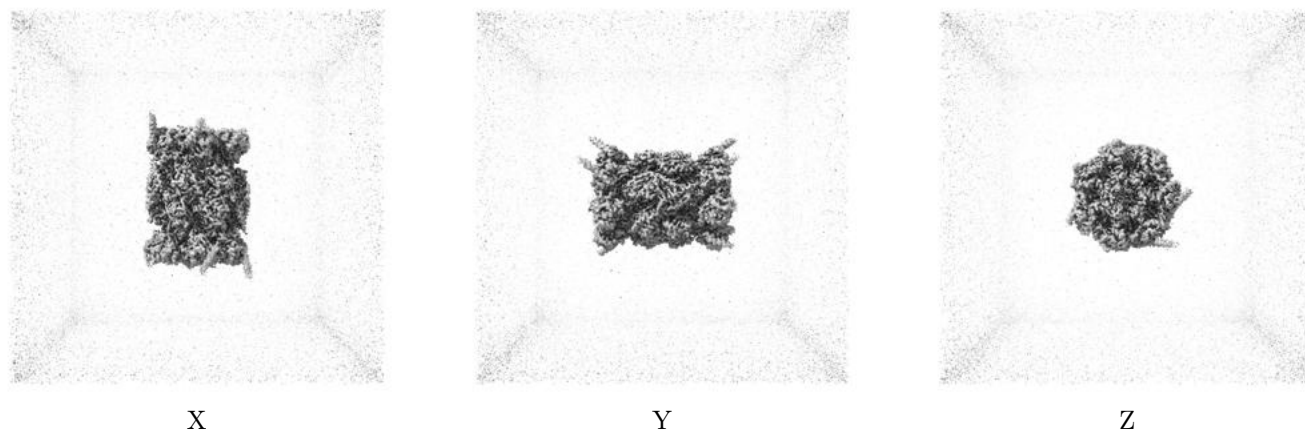
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

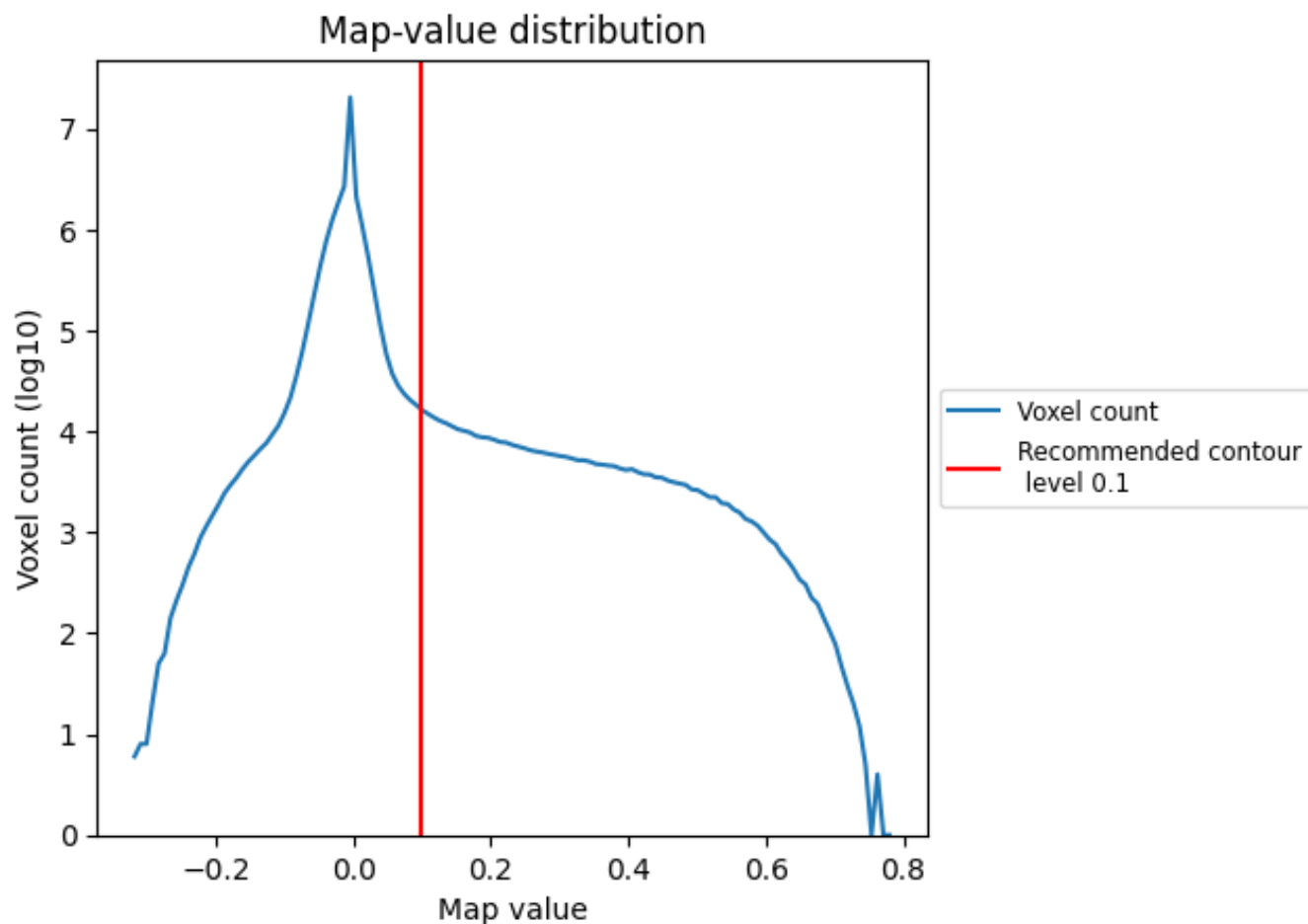
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

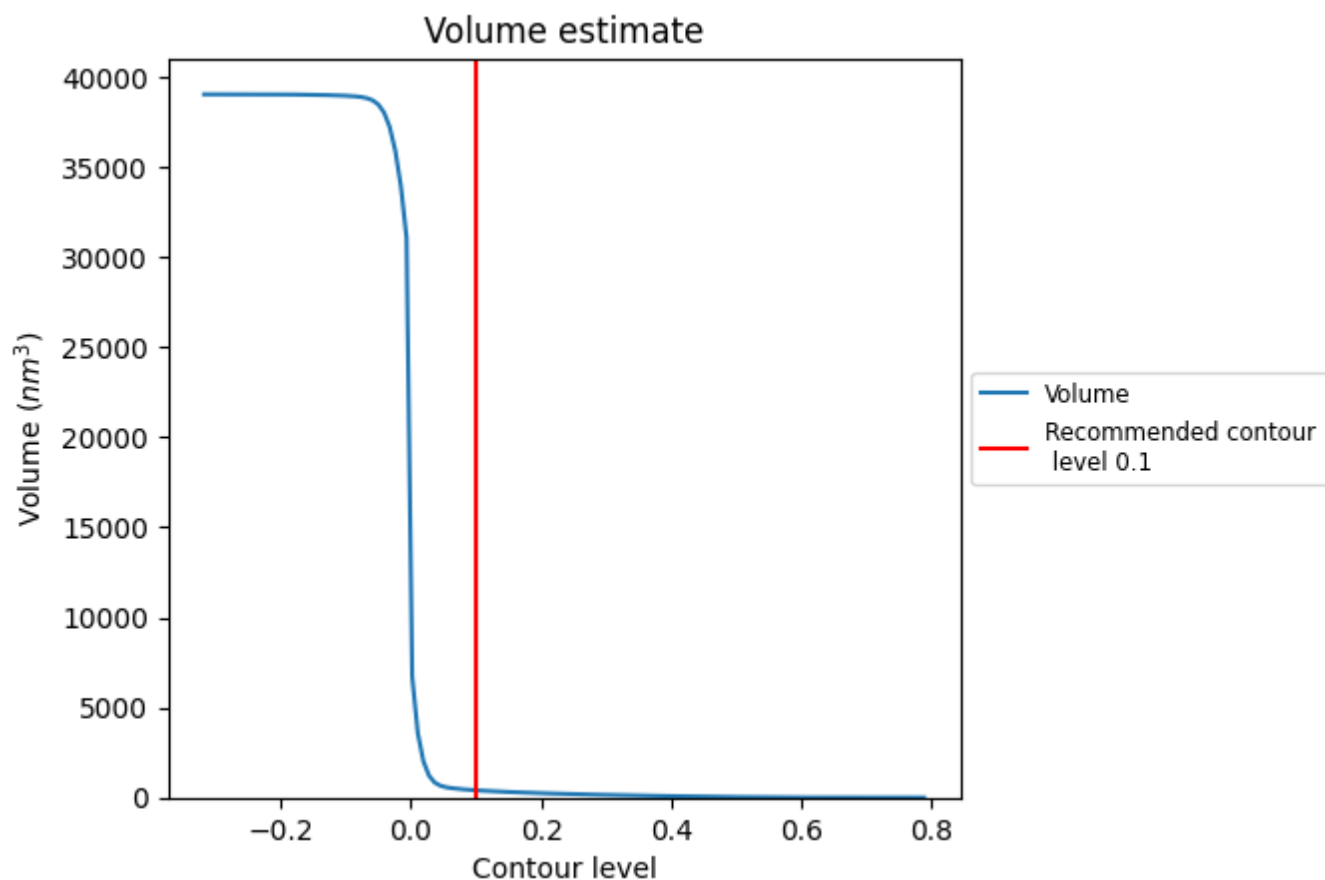
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

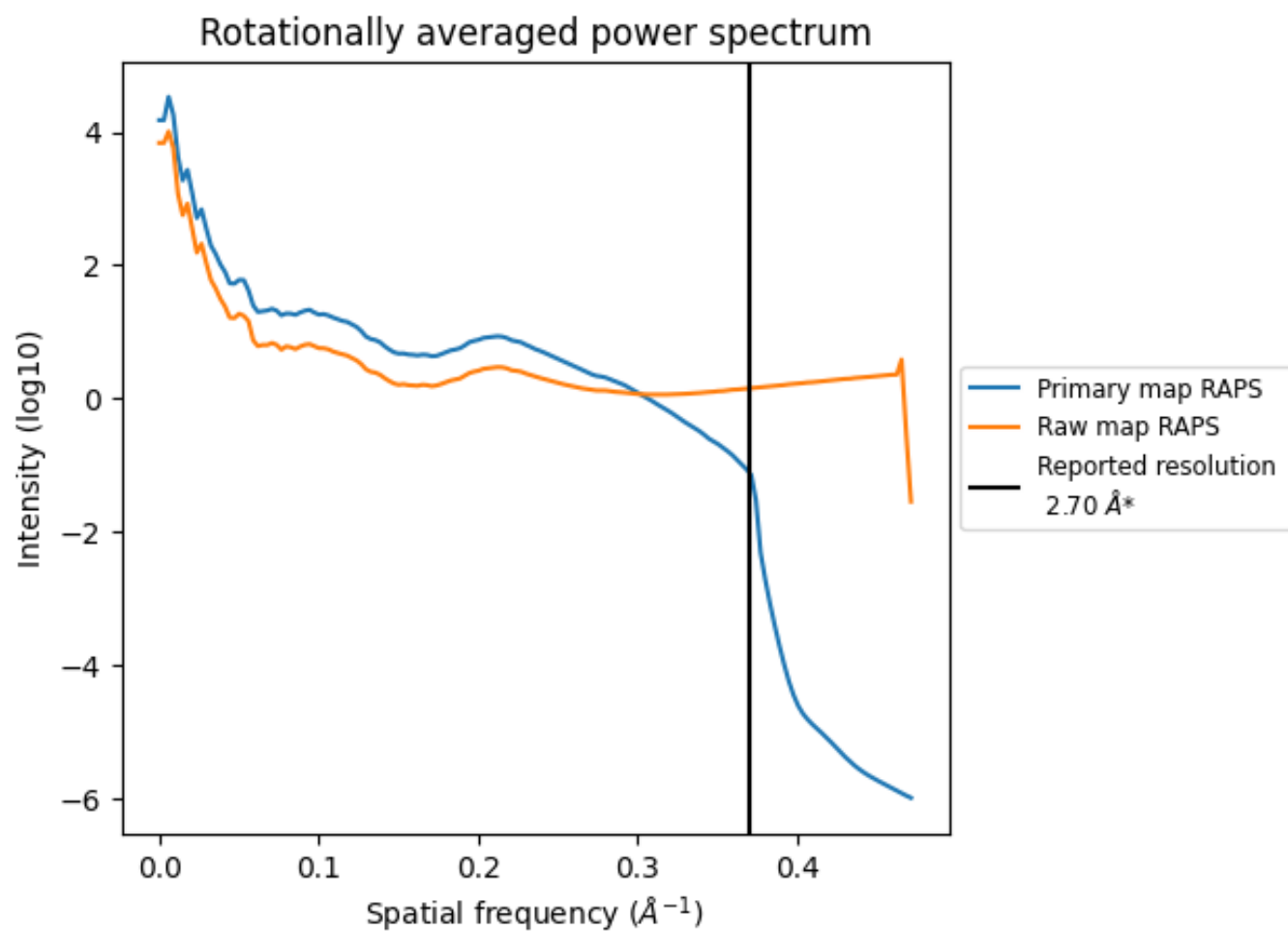
7.2 Volume estimate [i](#)



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

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

7.3 Rotationally averaged power spectrum ⓘ

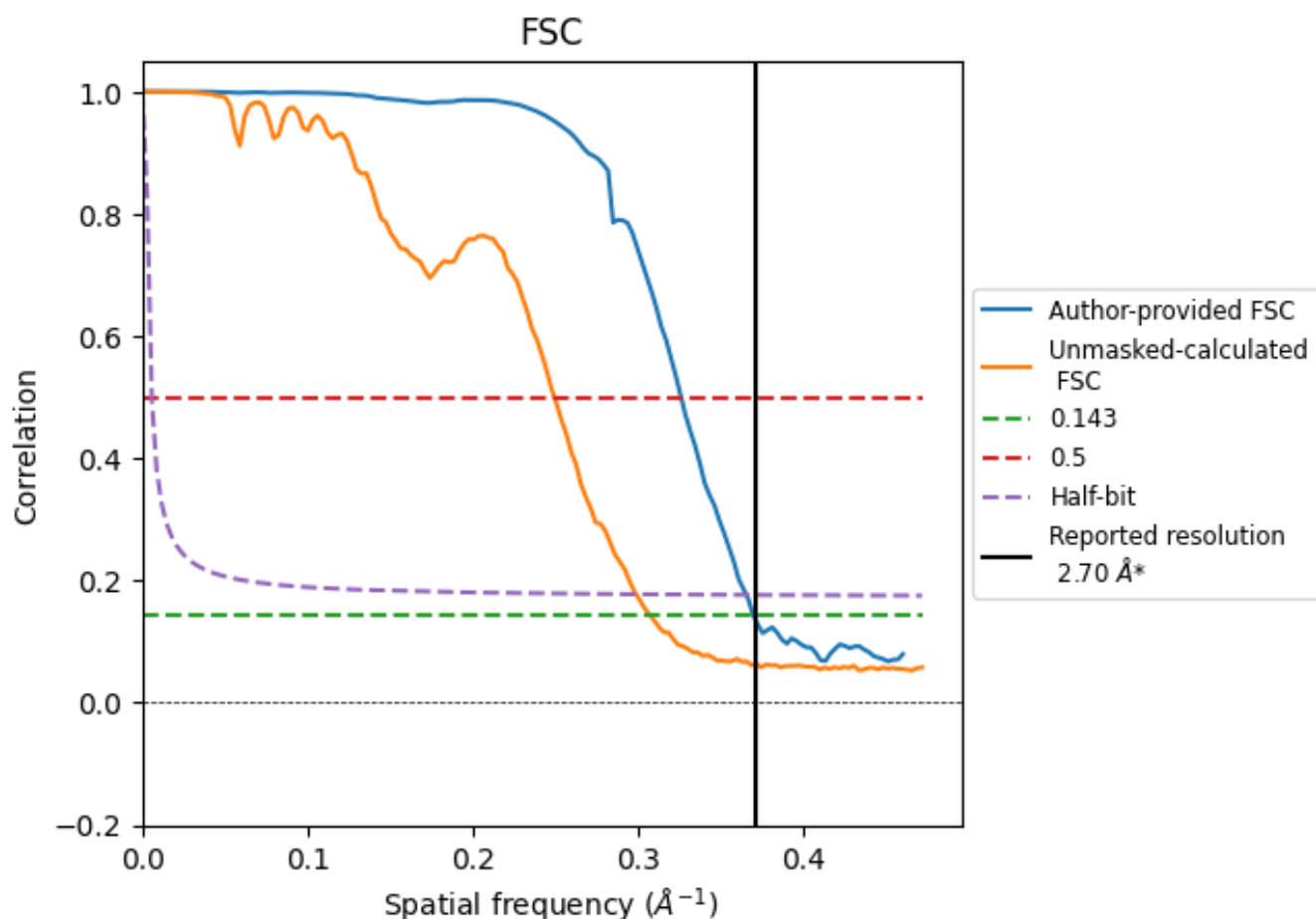


*Reported resolution corresponds to spatial frequency of 0.370 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.370 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

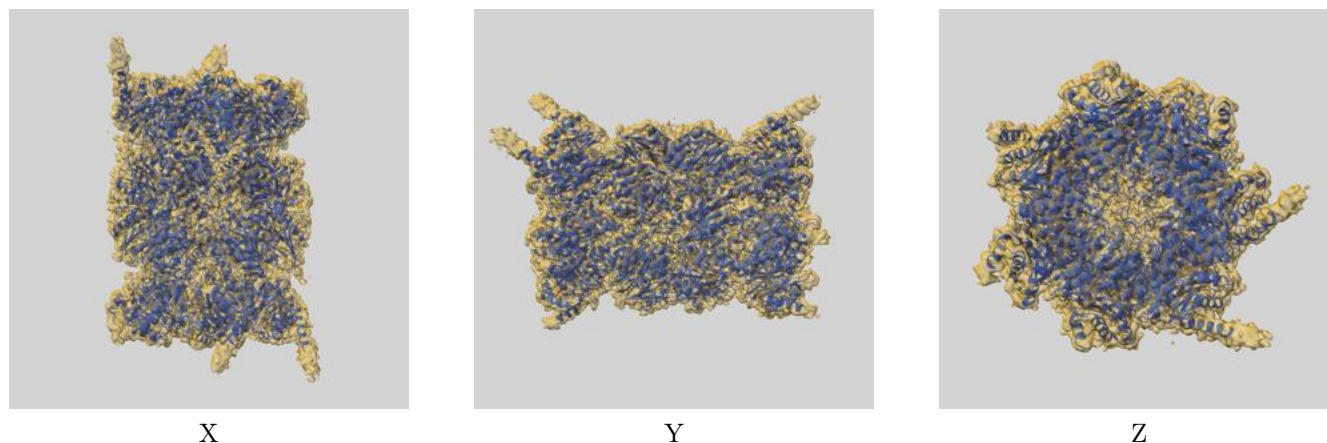
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.71	3.07	2.74
Unmasked-calculated*	3.26	4.01	3.35

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

9 Map-model fit [i](#)

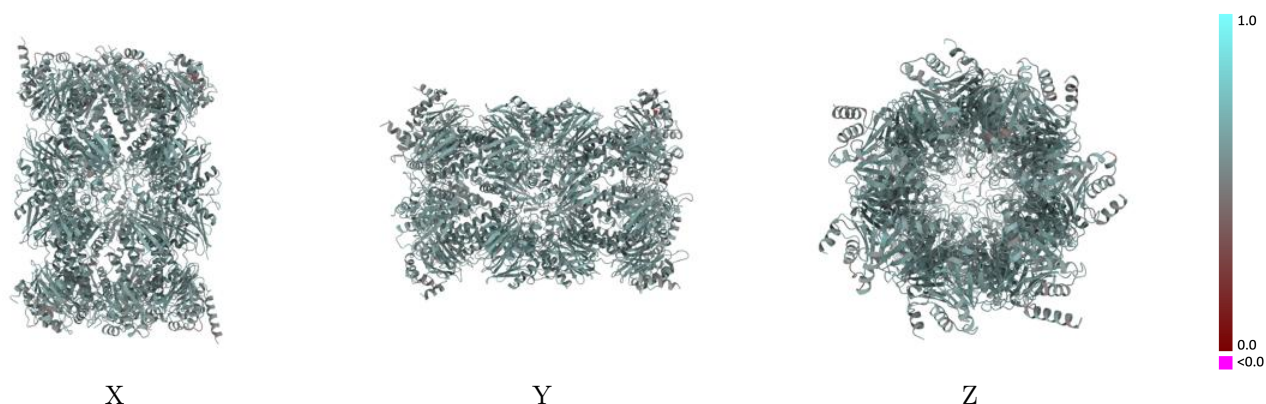
This section contains information regarding the fit between EMDB map EMD-27013 and PDB model 8CVR. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



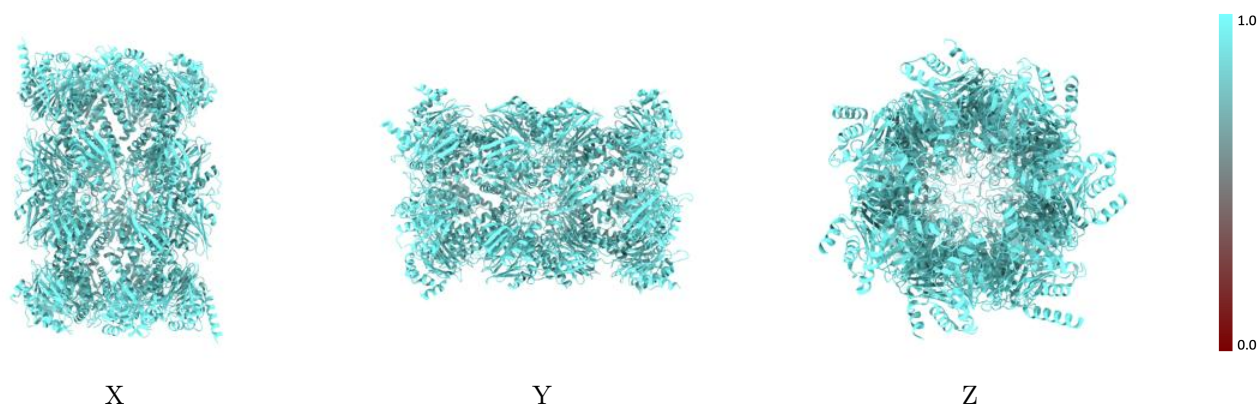
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



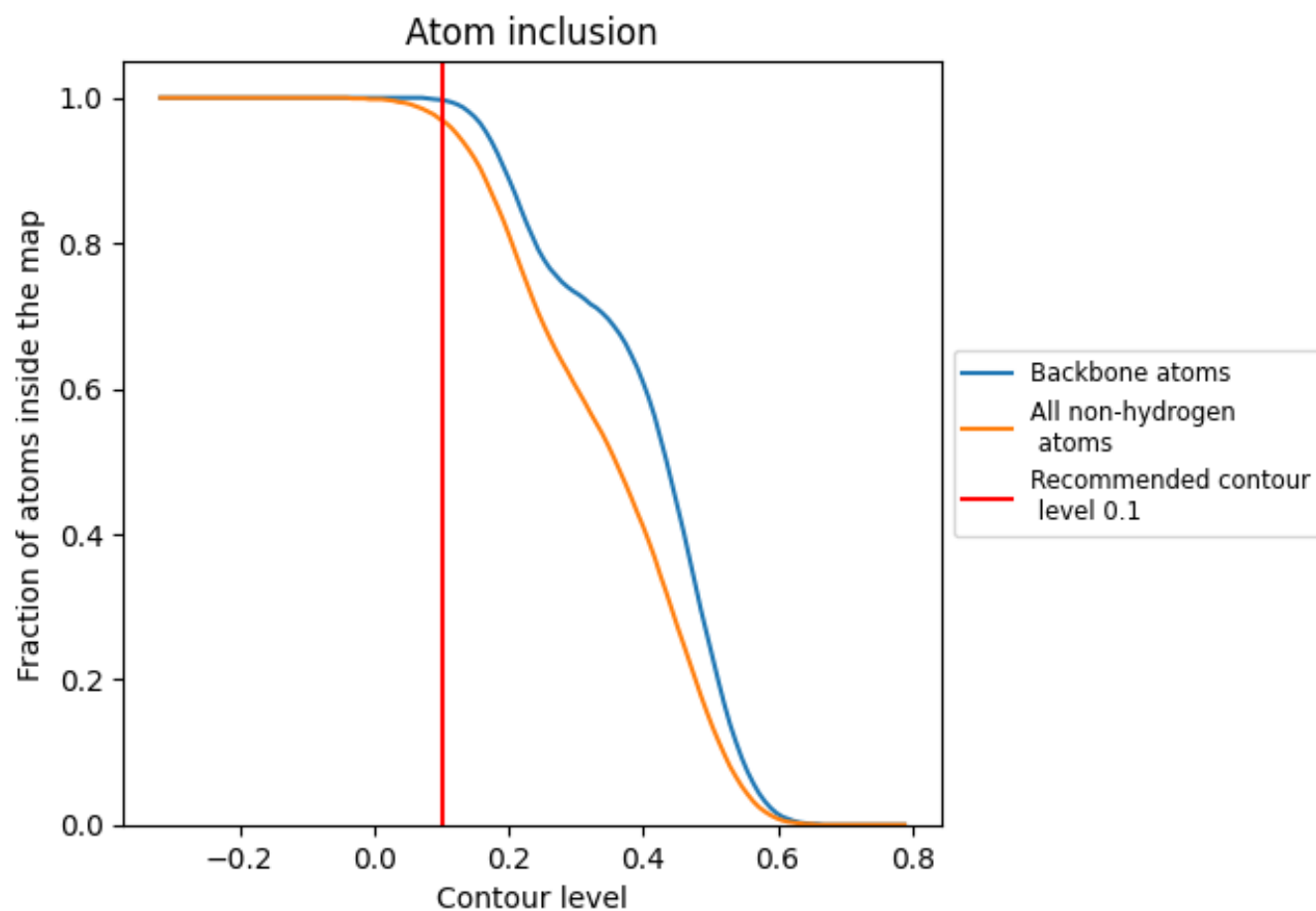
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 97% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.1) and Q-score for the entire model and for each chain.

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

