



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 04:39 PM UTC

PDB ID : 5MP9 / pdb_00005mp9
EMDB ID : EMD-3534
Title : 26S proteasome in presence of ATP (s1)
Authors : Wehmer, M.; Rudack, T.; Beck, F.; Aufderheide, A.; Pfeifer, G.; Plitzko, J.M.;
Foerster, F.; Schulten, K.; Baumeister, W.; Sakata, E.
Deposited on : 2016-12-16
Resolution : 4.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

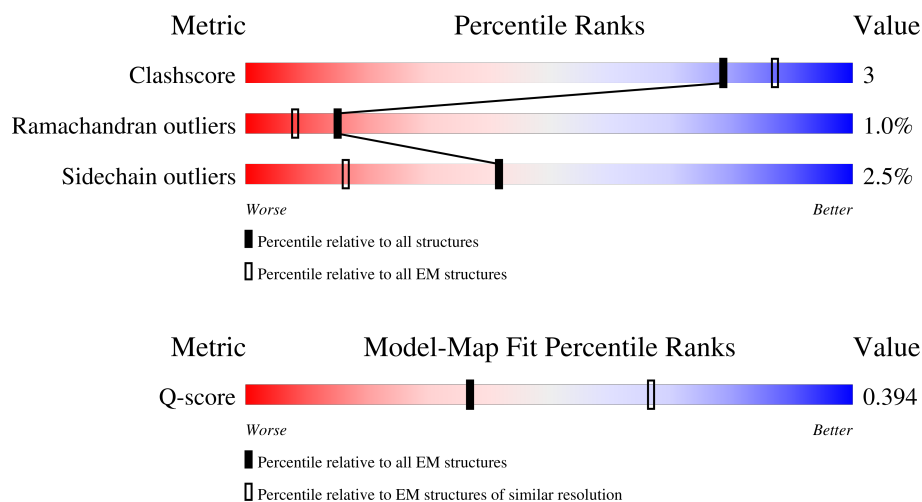
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 4.10 Å.

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



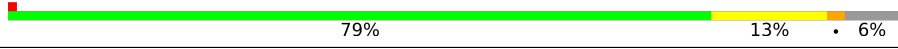
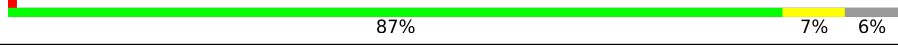
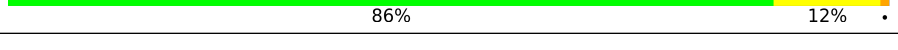
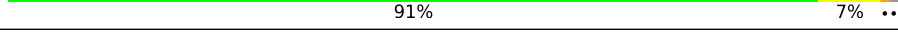
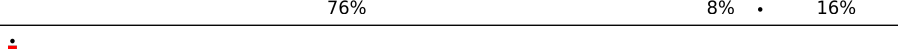
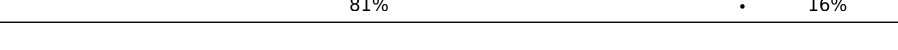
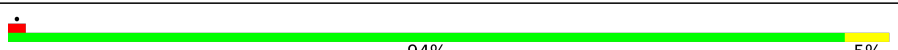
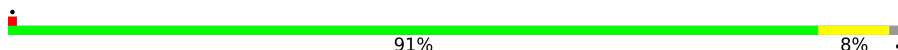
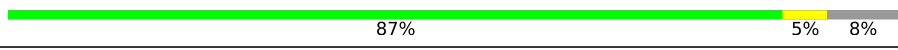
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	6458 (3.60 - 4.60)

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	252	 87% 7% . .
1	a	252	 85% 10% . .
2	B	250	 88% 12% .
2	b	250	 89% 10%

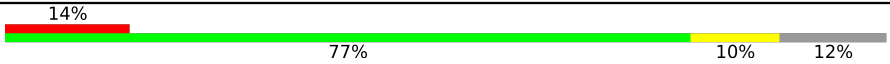
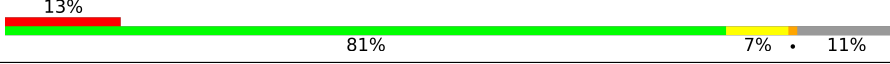
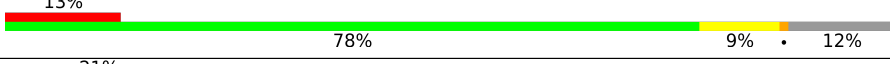
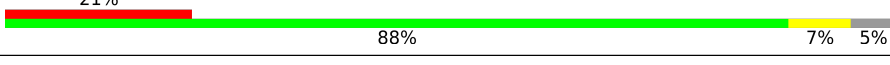
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Mol	Chain	Length	Quality of chain
3	C	258	
3	c	258	
4	D	254	
4	d	254	
5	E	260	
5	e	260	
6	F	234	
6	f	234	
7	G	288	
7	g	288	
8	l	215	
8	h	215	
9	2	261	
9	i	261	
10	3	205	
10	j	205	
11	4	198	
11	k	198	
12	5	287	
12	l	287	
13	6	241	
13	m	241	
14	7	266	
14	n	266	
15	H	467	

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Mol	Chain	Length	Quality of chain
16	I	437	
17	K	428	
18	L	437	
19	M	434	
20	J	405	

2 Entry composition

There are 23 unique types of molecules in this entry. The entry contains 67883 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-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	241	Total	C	N	O	S	0	0
			1907	1214	320	365	8		
1	A	241	Total	C	N	O	S	0	0
			1907	1214	320	365	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	b	250	Total	C	N	O	S	0	0
			1915	1219	315	377	4		
2	B	250	Total	C	N	O	S	0	0
			1915	1219	315	377	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	c	244	Total	C	N	O	S	0	0
			1904	1201	321	379	3		
3	C	244	Total	C	N	O	S	0	0
			1904	1201	321	379	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	d	240	Total	C	N	O	S	0	0
			1881	1176	329	372	4		
4	D	240	Total	C	N	O	S	0	0
			1881	1176	329	372	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	e	242	Total	C	N	O	S	0	0
			1861	1162	314	378	7		
5	E	242	Total	C	N	O	S	0	0
			1861	1162	314	378	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	f	231	Total	C	N	O	S	0	0
			1773	1114	307	348	4		
6	F	233	Total	C	N	O	S	0	0
			1795	1129	312	350	4		

- Molecule 7 is a protein called Probable proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	g	243	Total	C	N	O	S	0	0
			1892	1203	329	356	4		
7	G	243	Total	C	N	O	S	0	0
			1892	1203	329	356	4		

- Molecule 8 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	h	196	Total	C	N	O	S	0	0
			1512	955	250	300	7		
8	1	196	Total	C	N	O	S	0	0
			1512	955	250	300	7		

- Molecule 9 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	i	226	Total	C	N	O	S	0	0
			1719	1082	298	332	7		
9	2	226	Total	C	N	O	S	0	0
			1719	1082	298	332	7		

- 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
			1581	1010	258	305	8		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	3	204	Total	C	N	O	S	0	0
			1581	1010	258	305	8		

- Molecule 11 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	k	195	Total	C	N	O	S	0	0
			1561	992	264	299	6		
11	4	195	Total	C	N	O	S	0	0
			1561	992	264	299	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	l	212	Total	C	N	O	S	0	0
			1644	1045	280	312	7		
12	5	212	Total	C	N	O	S	0	0
			1644	1045	280	312	7		

- Molecule 13 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	m	222	Total	C	N	O	S	0	0
			1757	1115	303	335	4		
13	6	222	Total	C	N	O	S	0	0
			1757	1115	303	335	4		

- Molecule 14 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	n	232	Total	C	N	O	S	0	0
			1815	1148	311	349	7		
14	7	229	Total	C	N	O	S	0	0
			1790	1133	306	344	7		

- Molecule 15 is a protein called 26S protease regulatory subunit 7 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	H	390	Total	C	N	O	S	0	0
			3053	1920	546	570	17		

- Molecule 16 is a protein called 26S protease regulatory subunit 4 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	I	385	Total	C	N	O	S	0	0
			3022	1899	508	598	17		

- Molecule 17 is a protein called 26S protease regulatory subunit 6B homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	K	389	Total	C	N	O	S	0	0
			3078	1933	540	595	10		

- Molecule 18 is a protein called 26S protease subunit RPT4.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	L	388	Total	C	N	O	S	0	0
			3082	1942	548	580	12		

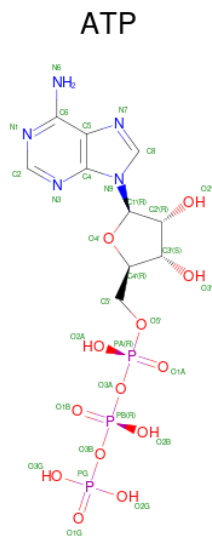
- Molecule 19 is a protein called 26S protease regulatory subunit 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	M	381	Total	C	N	O	S	0	0
			2986	1870	524	580	12		

- Molecule 20 is a protein called 26S protease regulatory subunit 8 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	J	386	Total	C	N	O	S	0	0
			3033	1906	543	567	17		

- Molecule 21 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					AltConf
21	H	1	Total 31	C 10	N 5	O 13	P 3	0
21	I	1	Total 31	C 10	N 5	O 13	P 3	0
21	K	1	Total 31	C 10	N 5	O 13	P 3	0
21	L	1	Total 31	C 10	N 5	O 13	P 3	0
21	M	1	Total 31	C 10	N 5	O 13	P 3	0

- Molecule 22 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
22	H	1	Total 1	Mg 1	0
22	I	1	Total 1	Mg 1	0
22	K	1	Total 1	Mg 1	0
22	L	1	Total 1	Mg 1	0
22	M	1	Total 1	Mg 1	0
22	J	1	Total 1	Mg 1	0

- Molecule 23 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

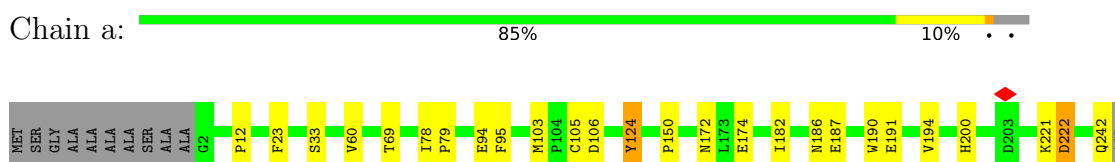


Mol	Chain	Residues	Atoms					AltConf
23	J	1	Total	C	N	O	P	0
			27	10	5	10	2	

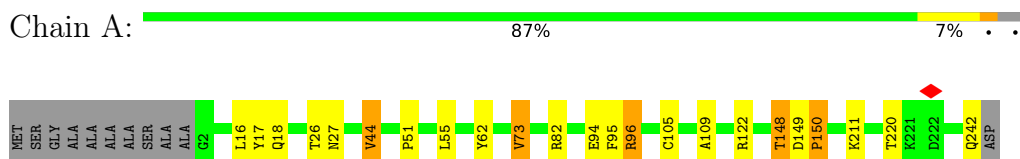
3 Residue-property plots

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.

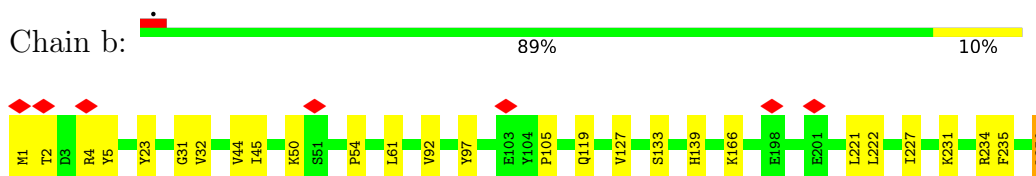
- Molecule 1: Proteasome subunit alpha type-1



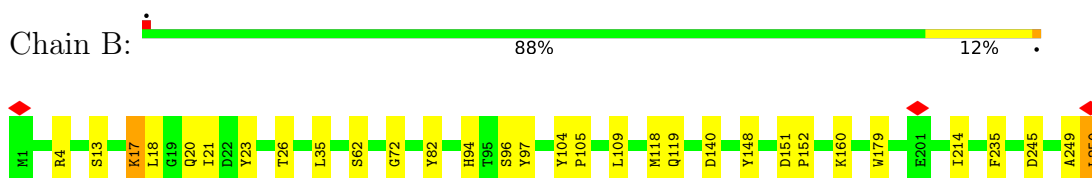
- Molecule 1: Proteasome subunit alpha type-1



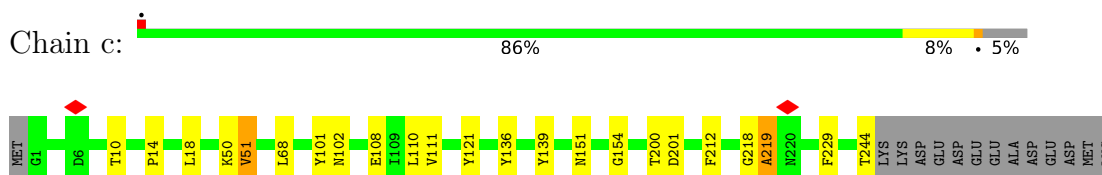
- Molecule 2: Proteasome subunit alpha type-2



- Molecule 2: Proteasome subunit alpha type-2

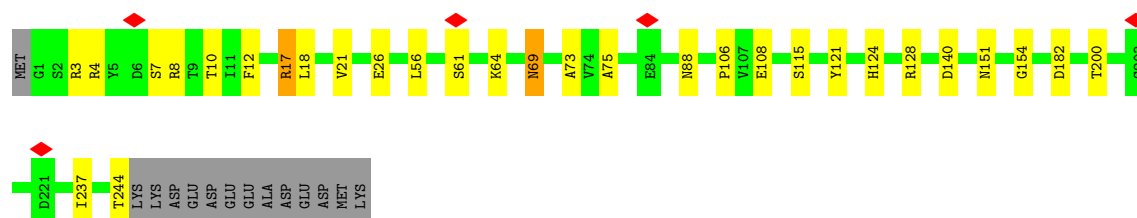


- Molecule 3: Proteasome subunit alpha type-3



- Molecule 3: Proteasome subunit alpha type-3

Chain C: 



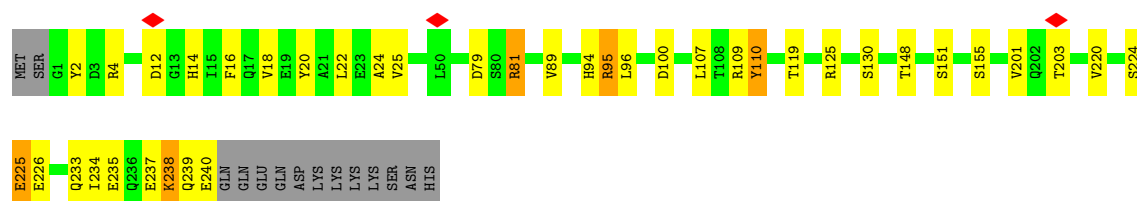
- Molecule 4: Proteasome subunit alpha type-4

Chain d: 



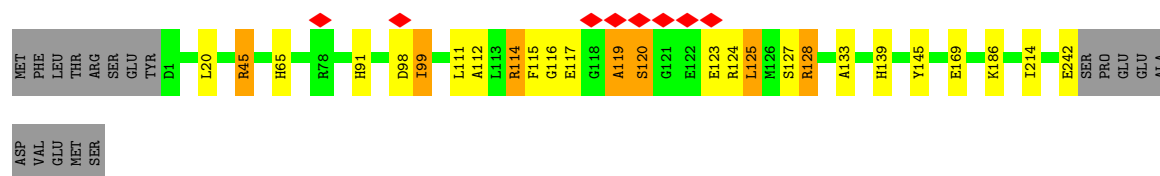
- Molecule 4: Proteasome subunit alpha type-4

Chain D: 



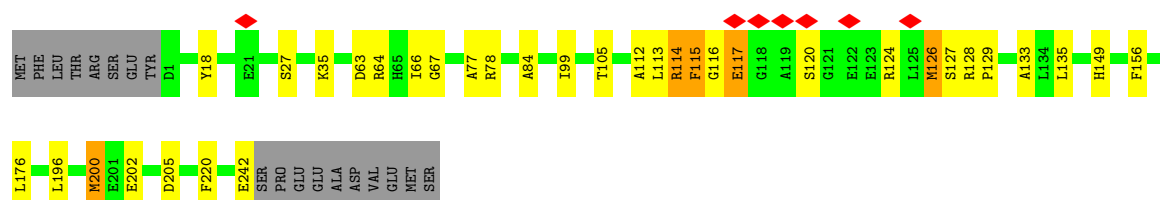
- Molecule 5: Proteasome subunit alpha type-5

Chain e: 



- Molecule 5: Proteasome subunit alpha type-5

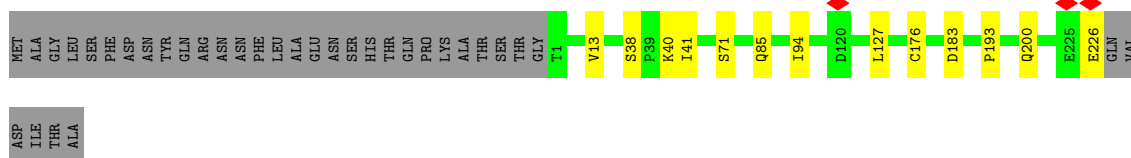
Chain E: 





• Molecule 9: Proteasome subunit beta type-2

Chain i:  82% 5% 13%

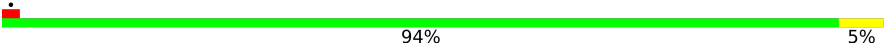


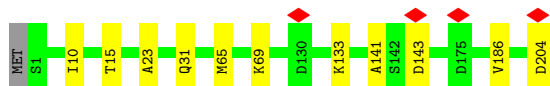
• Molecule 9: Proteasome subunit beta type-2

Chain 2:  78% 8% 13%



• Molecule 10: Proteasome subunit beta type-3

Chain j:  94% 5%



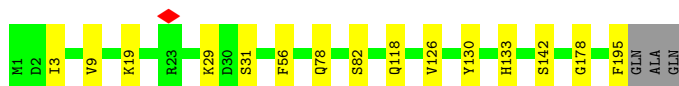
• Molecule 10: Proteasome subunit beta type-3

Chain 3:  88% 12%



• Molecule 11: Proteasome subunit beta type-4

Chain k:  91% 8%



• Molecule 11: Proteasome subunit beta type-4

Chain 4:  91% 7%



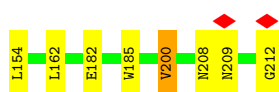
- Molecule 12: Proteasome subunit beta type-5

Chain 1: 68% 6% 26%



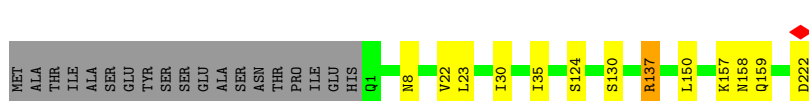
- Molecule 12: Proteasome subunit beta type-5

Chain 5: 63% 11% 26%



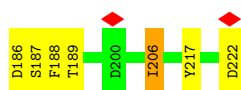
- Molecule 13: Proteasome subunit beta type-6

Chain m: 87% 5% 8%



- Molecule 13: Proteasome subunit beta type-6

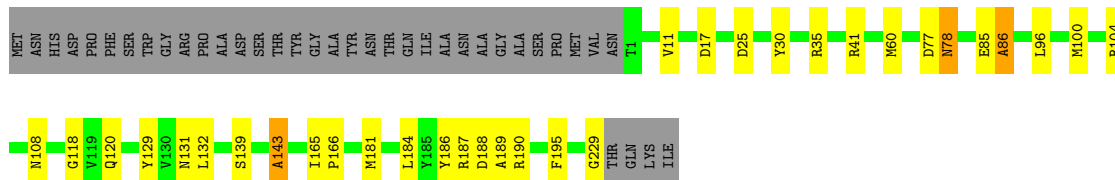
Chain 6: 80% 12% 8%



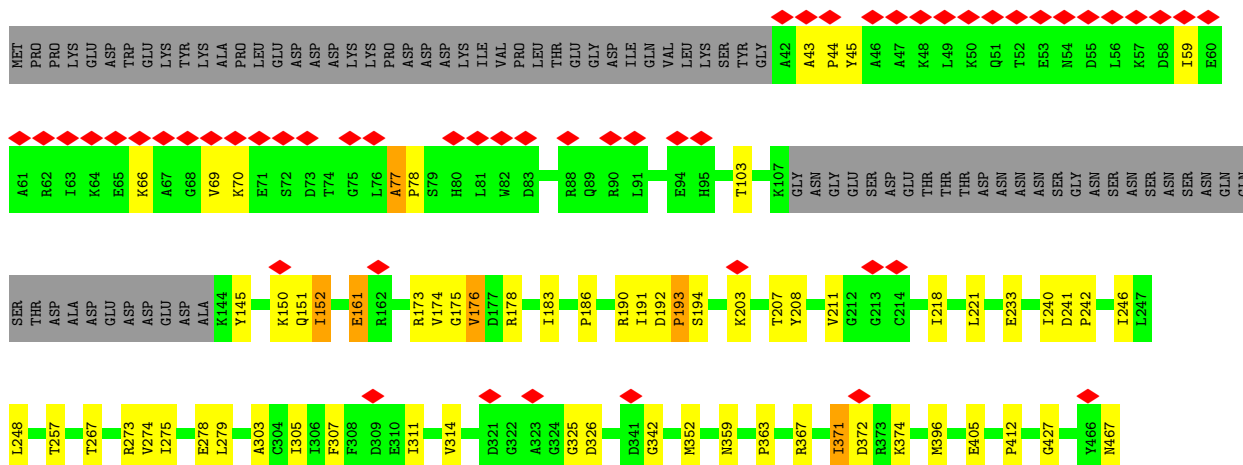
- Molecule 14: Proteasome subunit beta type-7

Chain n: 78% 8% 13%

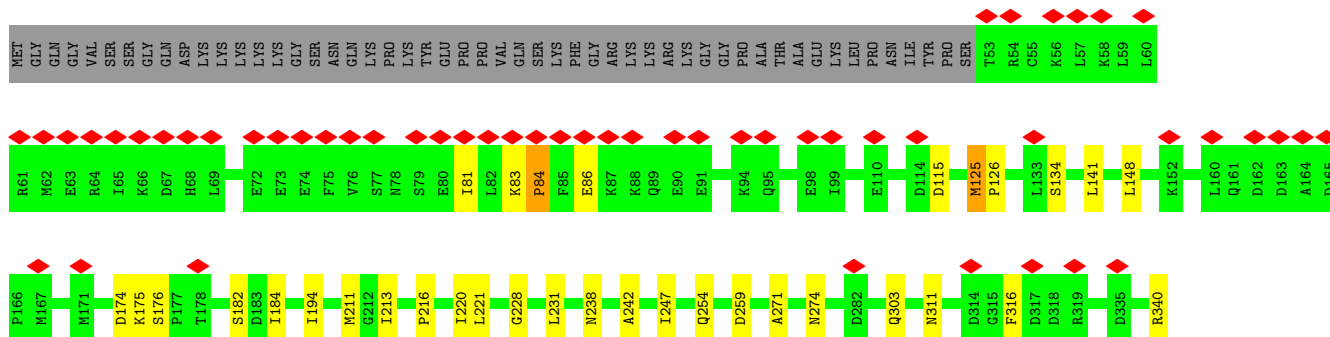
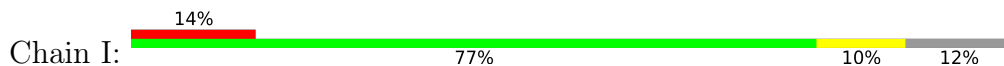
- Molecule 14: Proteasome subunit beta type-7

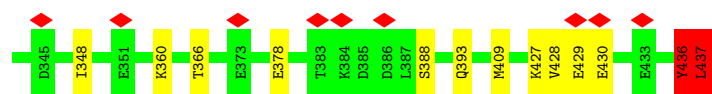


- Molecule 15: 26S protease regulatory subunit 7 homolog



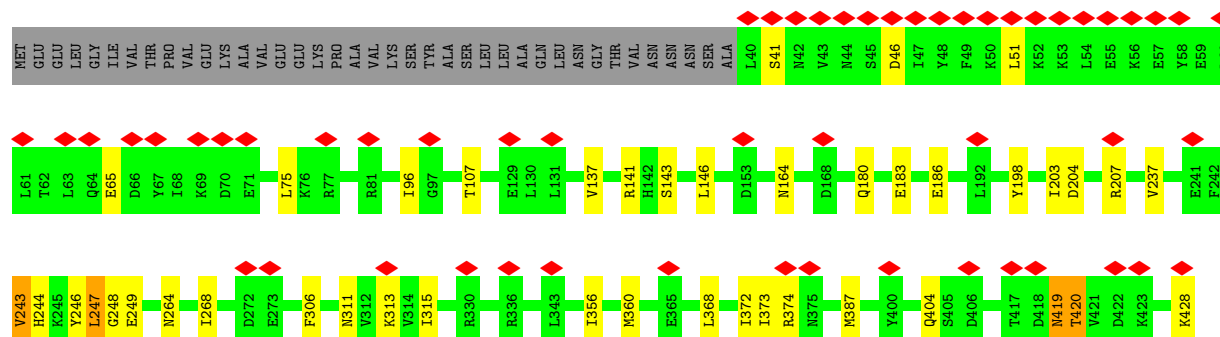
- Molecule 16: 26S protease regulatory subunit 4 homolog





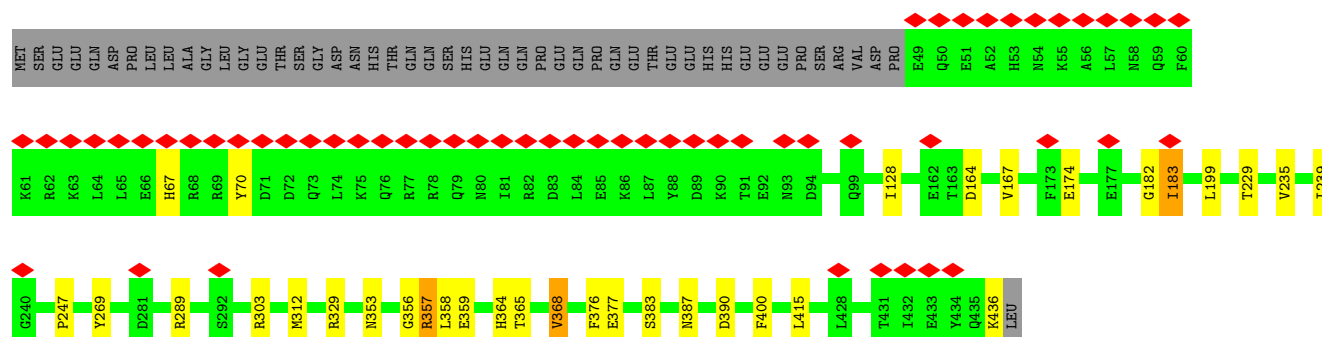
• Molecule 17: 26S protease regulatory subunit 6B homolog

Chain K: 13% 81% 9% 9%



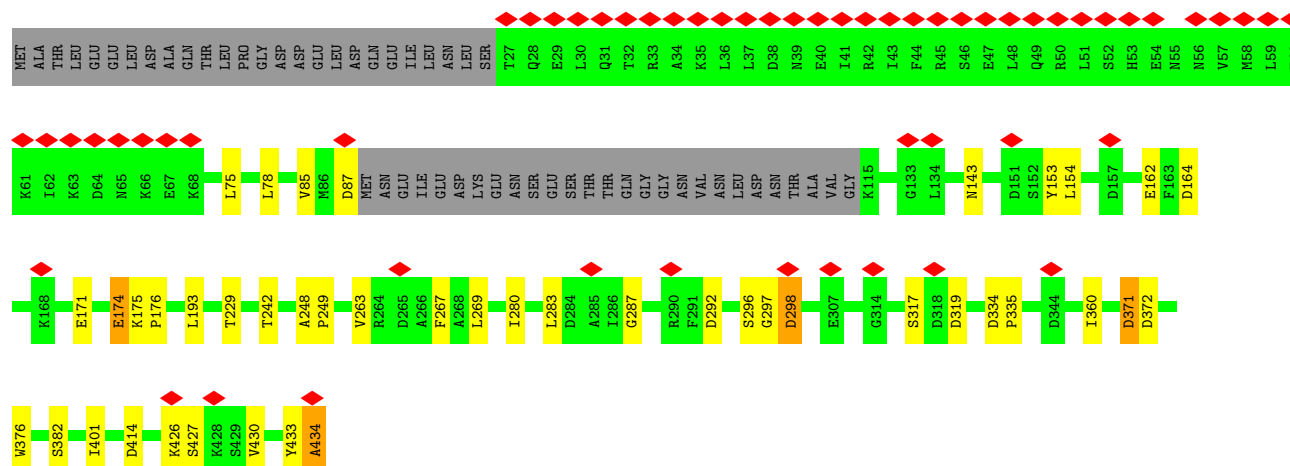
• Molecule 18: 26S protease subunit RPT4

Chain L: 13% 81% 7% 11%

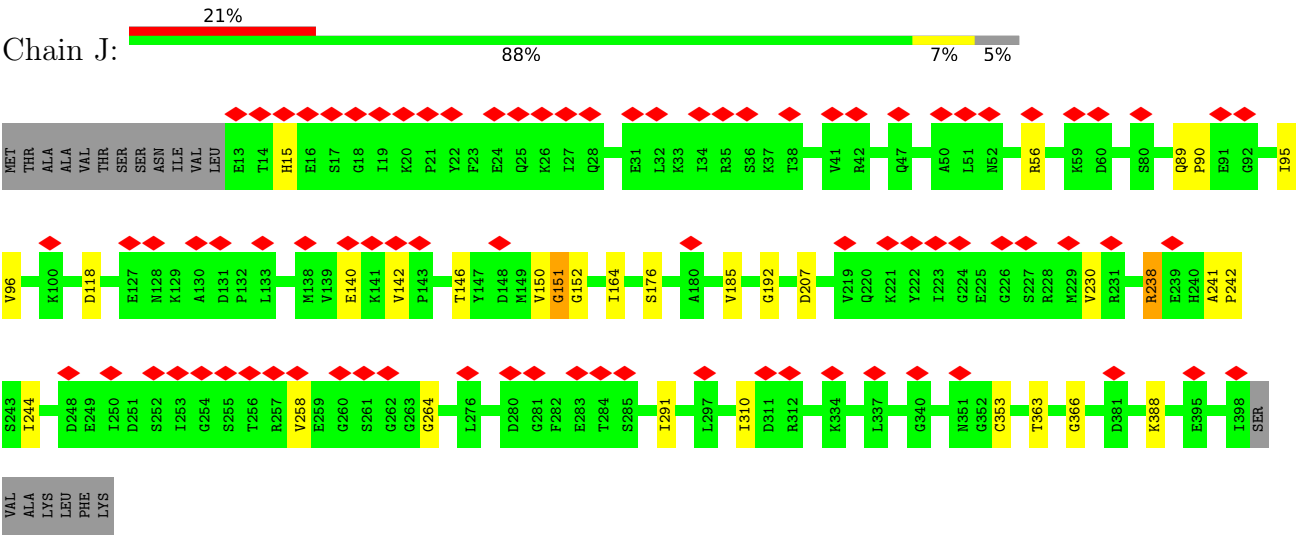


• Molecule 19: 26S protease regulatory subunit 6A

Chain M: 13% 78% 9% 12%



● Molecule 20: 26S protease regulatory subunit 8 homolog



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	286500	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 ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.211	Depositor
Minimum map value	-0.133	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	529.92, 529.92, 529.92	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.38, 1.38, 1.38	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, ADP, MG

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	1.01	14/1945 (0.7%)	1.03	9/2634 (0.3%)
1	a	0.38	1/1945 (0.1%)	0.49	1/2634 (0.0%)
2	B	1.03	7/1952 (0.4%)	1.10	16/2642 (0.6%)
2	b	0.46	2/1952 (0.1%)	0.47	0/2642
3	C	1.01	5/1934 (0.3%)	1.07	12/2618 (0.5%)
3	c	0.38	1/1934 (0.1%)	0.49	1/2618 (0.0%)
4	D	1.02	12/1910 (0.6%)	1.07	11/2586 (0.4%)
4	d	0.38	1/1910 (0.1%)	0.48	1/2586 (0.0%)
5	E	1.26	18/1886 (1.0%)	1.24	14/2541 (0.6%)
5	e	0.90	12/1886 (0.6%)	0.86	6/2541 (0.2%)
6	F	1.12	11/1823 (0.6%)	1.04	7/2463 (0.3%)
6	f	0.47	2/1800 (0.1%)	0.46	0/2433
7	G	1.03	14/1932 (0.7%)	1.00	9/2609 (0.3%)
7	g	0.37	1/1932 (0.1%)	0.46	1/2609 (0.0%)
8	1	0.99	8/1541 (0.5%)	0.97	4/2087 (0.2%)
8	h	0.51	2/1541 (0.1%)	0.48	0/2087
9	2	0.95	7/1750 (0.4%)	1.02	8/2373 (0.3%)
9	i	0.42	1/1750 (0.1%)	0.52	1/2373 (0.0%)
10	3	0.96	5/1611 (0.3%)	0.99	9/2174 (0.4%)
10	j	0.50	2/1611 (0.1%)	0.49	0/2174
11	4	0.95	5/1589 (0.3%)	0.96	3/2142 (0.1%)
11	k	0.42	1/1589 (0.1%)	0.48	1/2142 (0.0%)
12	5	1.05	9/1681 (0.5%)	0.98	5/2274 (0.2%)
12	l	0.50	2/1681 (0.1%)	0.49	0/2274
13	6	1.00	10/1795 (0.6%)	1.05	8/2420 (0.3%)
13	m	0.49	2/1795 (0.1%)	0.52	0/2420
14	7	1.03	8/1821 (0.4%)	1.03	10/2470 (0.4%)
14	n	0.42	1/1846 (0.1%)	0.56	2/2503 (0.1%)
15	H	0.75	12/3102 (0.4%)	0.84	8/4175 (0.2%)
16	I	0.69	7/3061 (0.2%)	0.71	5/4121 (0.1%)
17	K	0.71	11/3121 (0.4%)	0.69	5/4213 (0.1%)
18	L	0.69	4/3128 (0.1%)	0.77	10/4204 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
19	M	0.75	5/3023 (0.2%)	0.77	6/4070 (0.1%)
20	J	0.55	1/3073 (0.0%)	0.66	4/4129 (0.1%)
All	All	0.78	204/68850 (0.3%)	0.81	177/92981 (0.2%)

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
1	A	0	1
2	B	0	1
3	C	0	1
4	D	0	3
5	e	0	2
6	F	0	2
7	G	0	2
8	1	0	1
13	6	0	2
14	7	0	1
14	n	0	1
15	H	0	1
16	I	0	1
18	L	0	1
19	M	0	1
All	All	0	21

The worst 5 of 204 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	2	226	GLU	C-O	-11.62	1.00	1.23
7	g	244	ASN	C-O	-11.59	1.00	1.23
3	C	244	THR	C-O	-11.59	1.00	1.23
16	I	437	LEU	C-OXT	-11.59	1.00	1.23
19	M	434	ALA	C-OXT	-11.58	1.00	1.23

The worst 5 of 177 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	M	267	PHE	CA-CB-CG	-11.17	102.63	113.80
15	H	242	PRO	N-CA-CB	10.10	108.47	103.22
15	H	241	ASP	CA-C-N	9.42	126.44	119.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	H	241	ASP	C-N-CA	9.42	126.44	119.66
4	D	79	ASP	CA-CB-CG	-9.17	103.43	112.60

There are no chirality outliers.

5 of 21 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	96	ARG	Sidechain
2	B	82	TYR	Sidechain
5	e	124	ARG	Sidechain
5	e	128	ARG	Sidechain
14	n	77	ASP	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	1907	0	1901	1	0
1	a	1907	0	1901	17	0
2	B	1915	0	1929	11	0
2	b	1915	0	1929	25	0
3	C	1904	0	1904	12	0
3	c	1904	0	1904	12	0
4	D	1881	0	1895	8	0
4	d	1881	0	1895	6	0
5	E	1861	0	1839	11	0
5	e	1861	0	1839	19	0
6	F	1795	0	1800	11	0
6	f	1773	0	1775	5	0
7	G	1892	0	1883	5	0
7	g	1892	0	1883	3	0
8	1	1512	0	1479	9	0
8	h	1512	0	1481	7	0
9	2	1719	0	1719	37	0
9	i	1719	0	1719	5	0
10	3	1581	0	1574	10	0
10	j	1581	0	1574	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	4	1561	0	1569	4	0
11	k	1561	0	1569	7	0
12	5	1644	0	1595	15	0
12	l	1644	0	1595	5	0
13	6	1757	0	1711	11	0
13	m	1757	0	1711	9	0
14	7	1790	0	1793	15	0
14	n	1815	0	1821	45	0
15	H	3053	0	3127	31	0
16	I	3022	0	3092	36	0
17	K	3078	0	3140	16	0
18	L	3082	0	3157	20	0
19	M	2986	0	3055	18	0
20	J	3033	0	3155	13	0
21	H	31	0	12	2	0
21	I	31	0	12	7	0
21	K	31	0	12	0	0
21	L	31	0	12	2	0
21	M	31	0	12	2	0
22	H	1	0	0	0	0
22	I	1	0	0	0	0
22	J	1	0	0	0	0
22	K	1	0	0	0	0
22	L	1	0	0	0	0
22	M	1	0	0	0	0
23	J	27	0	12	1	0
All	All	67883	0	67985	383	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 3.

The worst 5 of 383 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)
14:n:150:MET:SD	9:2:132:LEU:HD11	1.49	1.52
14:n:150:MET:SD	9:2:132:LEU:CD1	2.10	1.40
14:n:149:HIS:CB	9:2:132:LEU:HD23	1.69	1.23
16:I:184:ILE:HD11	16:I:231:LEU:HG	1.30	1.12
14:n:149:HIS:HB3	9:2:132:LEU:HD23	1.32	1.11

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	239/252 (95%)	228 (95%)	9 (4%)	2 (1%)	16	52
1	a	239/252 (95%)	224 (94%)	14 (6%)	1 (0%)	30	65
2	B	248/250 (99%)	235 (95%)	12 (5%)	1 (0%)	30	65
2	b	248/250 (99%)	232 (94%)	16 (6%)	0	100	100
3	C	242/258 (94%)	232 (96%)	9 (4%)	1 (0%)	30	65
3	c	242/258 (94%)	227 (94%)	13 (5%)	2 (1%)	16	52
4	D	238/254 (94%)	223 (94%)	12 (5%)	3 (1%)	9	41
4	d	238/254 (94%)	224 (94%)	12 (5%)	2 (1%)	16	52
5	E	240/260 (92%)	228 (95%)	9 (4%)	3 (1%)	9	41
5	e	240/260 (92%)	225 (94%)	12 (5%)	3 (1%)	9	41
6	F	231/234 (99%)	214 (93%)	14 (6%)	3 (1%)	9	41
6	f	229/234 (98%)	216 (94%)	11 (5%)	2 (1%)	14	49
7	G	241/288 (84%)	228 (95%)	11 (5%)	2 (1%)	16	52
7	g	241/288 (84%)	229 (95%)	11 (5%)	1 (0%)	30	65
8	1	194/215 (90%)	181 (93%)	12 (6%)	1 (0%)	24	61
8	h	194/215 (90%)	178 (92%)	15 (8%)	1 (0%)	24	61
9	2	224/261 (86%)	214 (96%)	9 (4%)	1 (0%)	30	65
9	i	224/261 (86%)	205 (92%)	17 (8%)	2 (1%)	14	49
10	3	202/205 (98%)	184 (91%)	14 (7%)	4 (2%)	6	33
10	j	202/205 (98%)	181 (90%)	21 (10%)	0	100	100
11	4	193/198 (98%)	184 (95%)	8 (4%)	1 (0%)	24	61
11	k	193/198 (98%)	186 (96%)	5 (3%)	2 (1%)	12	46
12	5	210/287 (73%)	195 (93%)	13 (6%)	2 (1%)	12	46
12	l	210/287 (73%)	196 (93%)	12 (6%)	2 (1%)	12	46
13	6	220/241 (91%)	207 (94%)	13 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	m	220/241 (91%)	202 (92%)	18 (8%)	0	100	100
14	7	227/266 (85%)	209 (92%)	15 (7%)	3 (1%)	9	41
14	n	230/266 (86%)	211 (92%)	19 (8%)	0	100	100
15	H	386/467 (83%)	348 (90%)	26 (7%)	12 (3%)	3	25
16	I	383/437 (88%)	353 (92%)	22 (6%)	8 (2%)	5	32
17	K	387/428 (90%)	357 (92%)	24 (6%)	6 (2%)	7	37
18	L	386/437 (88%)	361 (94%)	23 (6%)	2 (0%)	24	61
19	M	377/434 (87%)	342 (91%)	26 (7%)	9 (2%)	4	30
20	J	384/405 (95%)	356 (93%)	22 (6%)	6 (2%)	7	37
All	All	8602/9546 (90%)	8015 (93%)	499 (6%)	88 (1%)	15	46

5 of 88 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	c	219	ALA
4	d	184	ALA
8	h	72	THR
4	D	203	THR
16	I	84	PRO

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	206/210 (98%)	199 (97%)	7 (3%)	32	55
1	a	206/210 (98%)	200 (97%)	6 (3%)	37	58
2	B	209/209 (100%)	206 (99%)	3 (1%)	59	71
2	b	209/209 (100%)	198 (95%)	11 (5%)	20	44
3	C	203/216 (94%)	197 (97%)	6 (3%)	36	57
3	c	203/216 (94%)	199 (98%)	4 (2%)	48	66
4	D	212/226 (94%)	203 (96%)	9 (4%)	26	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	d	212/226 (94%)	204 (96%)	8 (4%)	29	51
5	E	198/215 (92%)	195 (98%)	3 (2%)	57	70
5	e	198/215 (92%)	193 (98%)	5 (2%)	42	62
6	F	192/193 (100%)	187 (97%)	5 (3%)	40	61
6	f	190/193 (98%)	181 (95%)	9 (5%)	23	47
7	G	201/239 (84%)	198 (98%)	3 (2%)	57	70
7	g	201/239 (84%)	198 (98%)	3 (2%)	57	70
8	1	162/178 (91%)	159 (98%)	3 (2%)	50	67
8	h	162/178 (91%)	160 (99%)	2 (1%)	63	73
9	2	185/214 (86%)	184 (100%)	1 (0%)	81	82
9	i	185/214 (86%)	178 (96%)	7 (4%)	29	51
10	3	172/173 (99%)	170 (99%)	2 (1%)	63	73
10	j	172/173 (99%)	170 (99%)	2 (1%)	63	73
11	4	173/175 (99%)	171 (99%)	2 (1%)	63	73
11	k	173/175 (99%)	170 (98%)	3 (2%)	53	68
12	5	169/235 (72%)	166 (98%)	3 (2%)	51	67
12	l	169/235 (72%)	162 (96%)	7 (4%)	27	50
13	6	185/201 (92%)	179 (97%)	6 (3%)	34	56
13	m	185/201 (92%)	182 (98%)	3 (2%)	55	69
14	7	195/224 (87%)	194 (100%)	1 (0%)	81	82
14	n	198/224 (88%)	191 (96%)	7 (4%)	32	54
15	H	330/399 (83%)	320 (97%)	10 (3%)	36	57
16	I	342/385 (89%)	332 (97%)	10 (3%)	37	58
17	K	342/374 (91%)	331 (97%)	11 (3%)	34	56
18	L	332/377 (88%)	327 (98%)	5 (2%)	57	70
19	M	329/375 (88%)	320 (97%)	9 (3%)	39	60
20	J	336/352 (96%)	329 (98%)	7 (2%)	47	65
All	All	7336/8078 (91%)	7153 (98%)	183 (2%)	42	62

5 of 183 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	1	126	ILE

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Mol	Chain	Res	Type
16	I	259	ASP
11	4	3	ILE
14	7	104	ARG
16	I	437	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 117 such sidechains are listed below:

Mol	Chain	Res	Type
4	D	94	HIS
18	L	393	ASN
8	1	120	HIS
18	L	320	GLN
16	I	418	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 for Mogul analysis.

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
21	ATP	H	501	22	32,33,33	1.37	4 (12%)	48,52,52	1.74	8 (16%)
21	ATP	K	501	22	32,33,33	1.56	8 (25%)	48,52,52	1.67	9 (18%)
23	ADP	J	501	22	28,29,29	1.47	6 (21%)	43,45,45	1.73	8 (18%)
21	ATP	L	501	22	32,33,33	1.40	7 (21%)	48,52,52	1.71	9 (18%)
21	ATP	M	501	22	32,33,33	1.56	6 (18%)	48,52,52	1.60	8 (16%)
21	ATP	I	501	22	32,33,33	1.48	8 (25%)	48,52,52	1.64	8 (16%)

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
21	ATP	H	501	22	-	4/22/38/38	0/3/3/3
21	ATP	K	501	22	-	7/22/38/38	0/3/3/3
23	ADP	J	501	22	-	5/16/32/32	0/3/3/3
21	ATP	L	501	22	-	6/22/38/38	0/3/3/3
21	ATP	M	501	22	-	8/22/38/38	0/3/3/3
21	ATP	I	501	22	-	5/22/38/38	0/3/3/3

The worst 5 of 39 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	K	501	ATP	C5-C4	4.51	1.47	1.39
23	J	501	ADP	C5-C4	4.45	1.47	1.39
21	H	501	ATP	C5-C4	4.37	1.46	1.39
21	I	501	ATP	C5-C4	4.29	1.46	1.39
21	M	501	ATP	C5-C4	4.27	1.46	1.39

The worst 5 of 50 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	H	501	ATP	C5-C4-N3	-6.05	118.39	126.72
21	L	501	ATP	C5-C4-N3	-5.86	118.64	126.72
21	M	501	ATP	C5-C4-N3	-5.80	118.74	126.72
21	I	501	ATP	C5-C4-N3	-5.39	119.30	126.72
23	J	501	ADP	C5-C4-N3	-5.37	119.32	126.72

There are no chirality outliers.

5 of 35 torsion outliers are listed below:

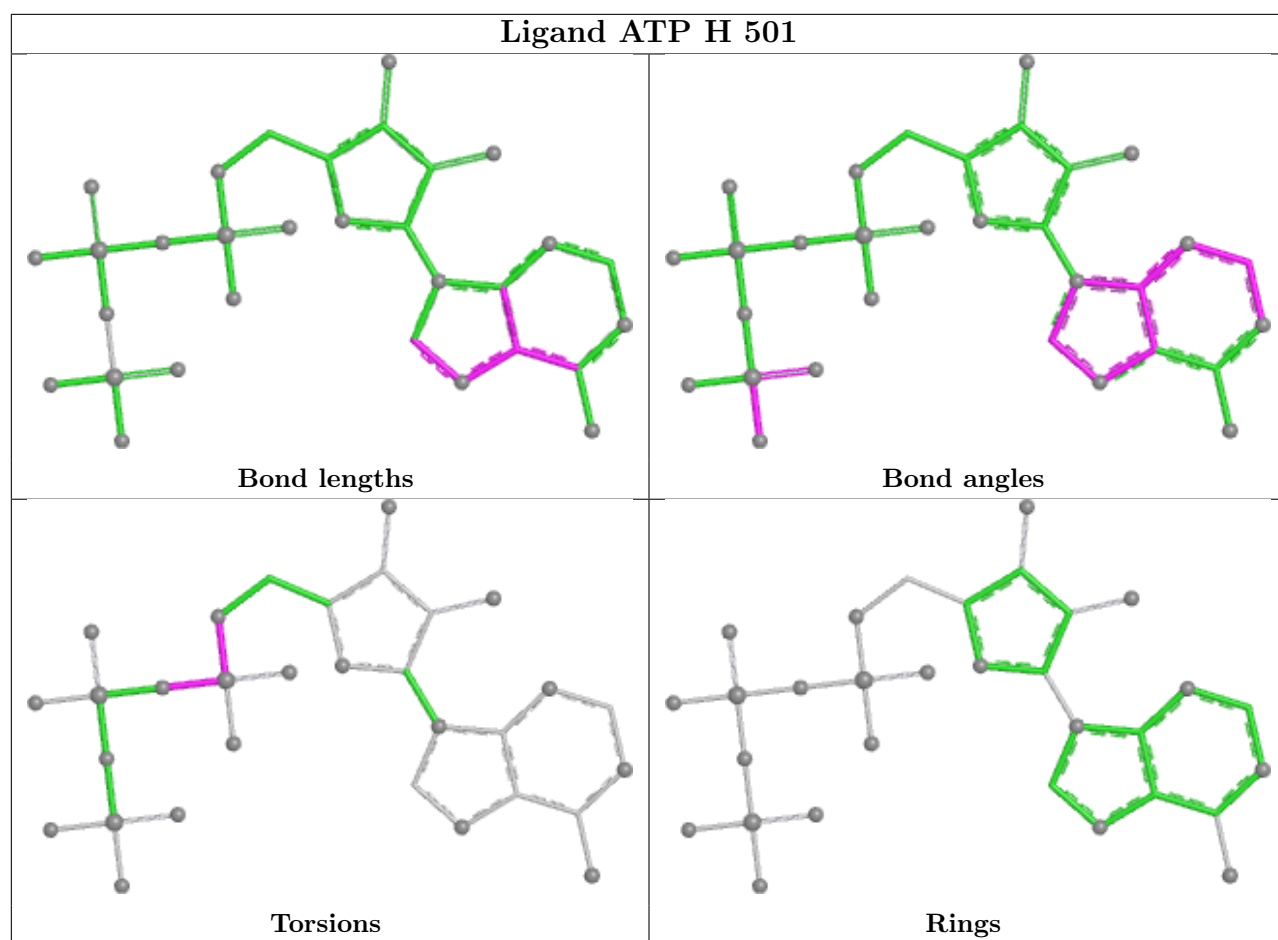
Mol	Chain	Res	Type	Atoms
21	H	501	ATP	C5'-O5'-PA-O1A
21	I	501	ATP	C5'-O5'-PA-O2A
21	I	501	ATP	C5'-O5'-PA-O3A
21	K	501	ATP	PB-O3B-PG-O2G
21	L	501	ATP	C5'-O5'-PA-O2A

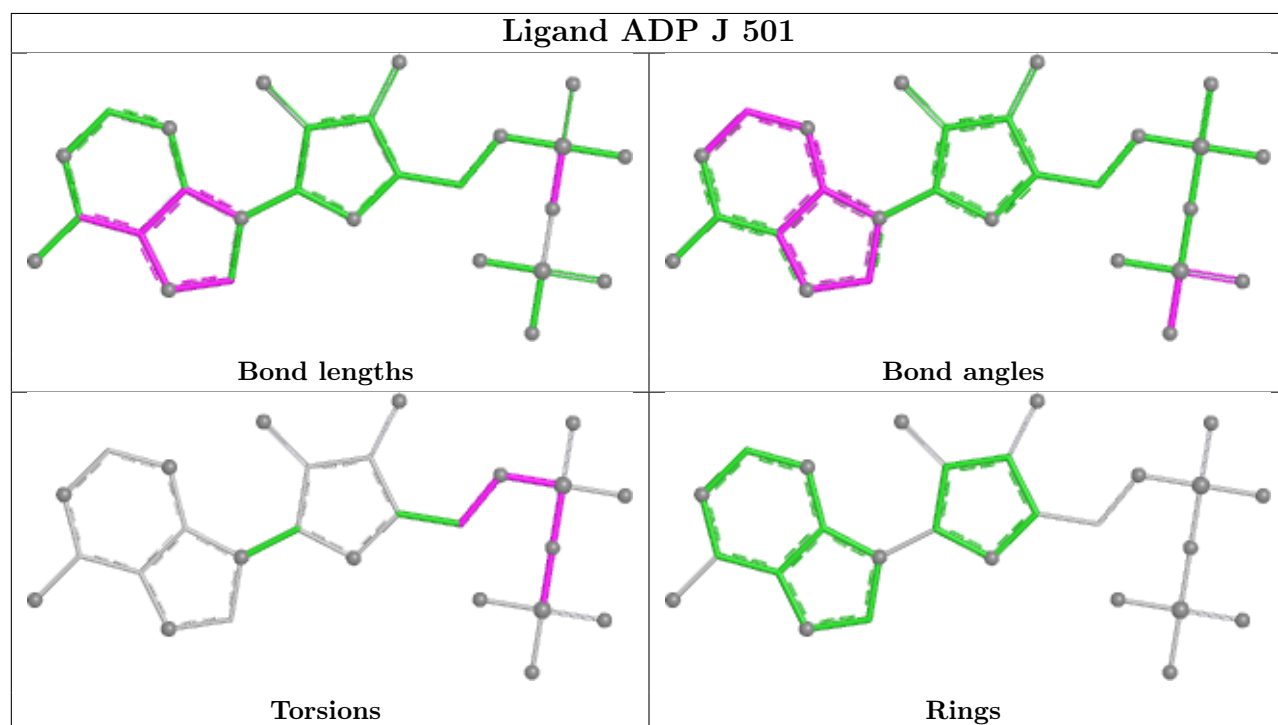
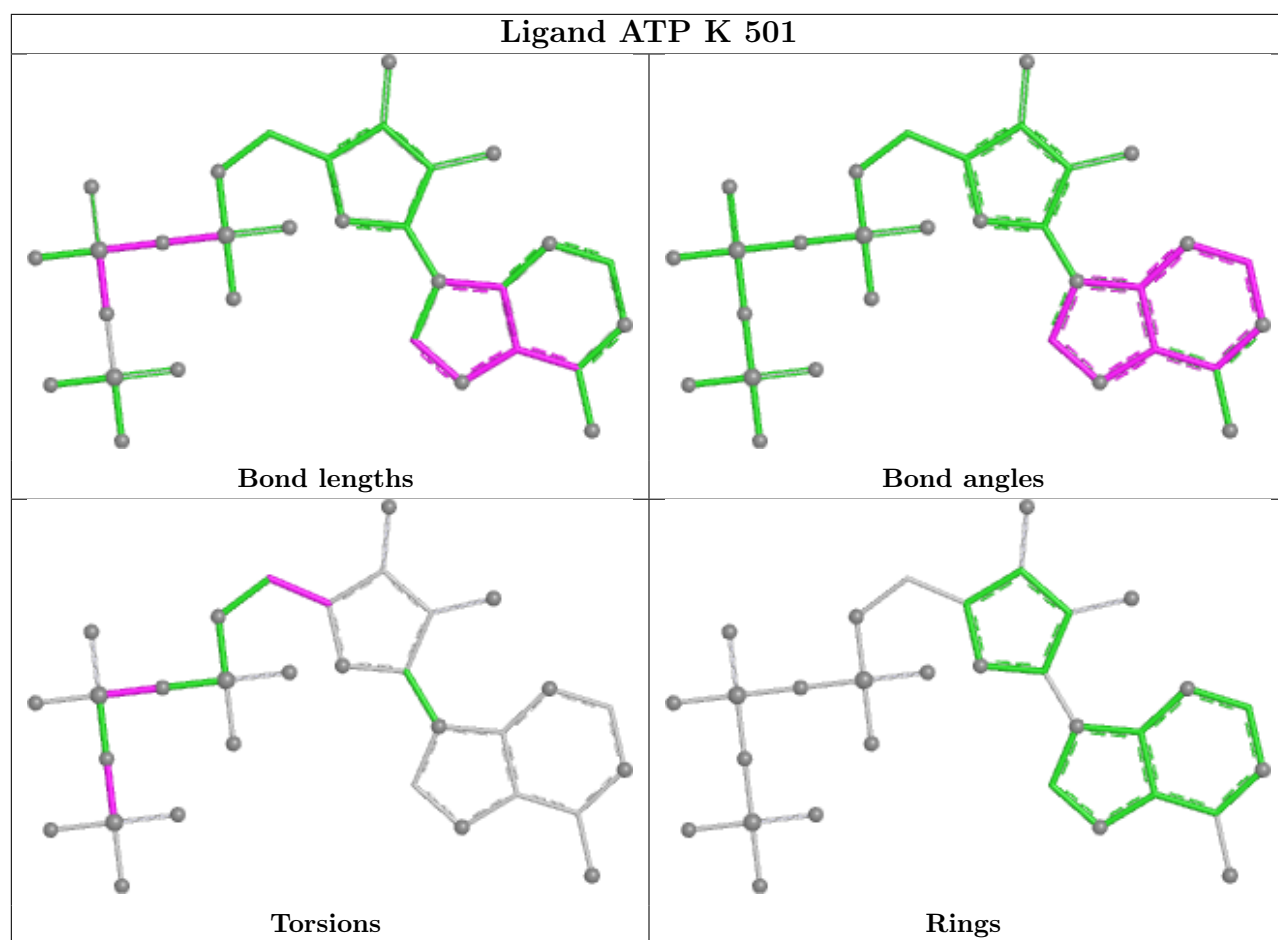
There are no ring outliers.

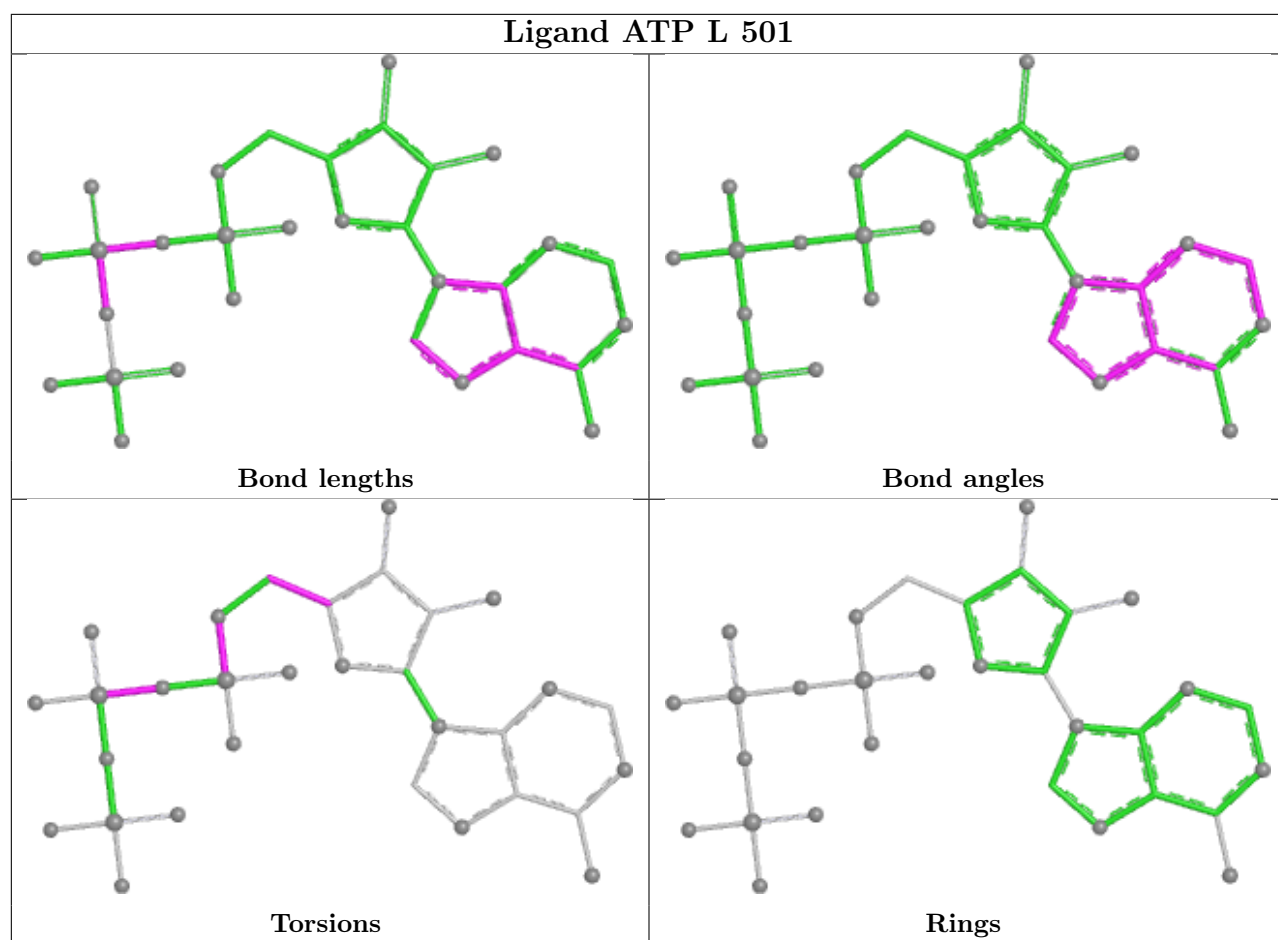
5 monomers are involved in 14 short contacts:

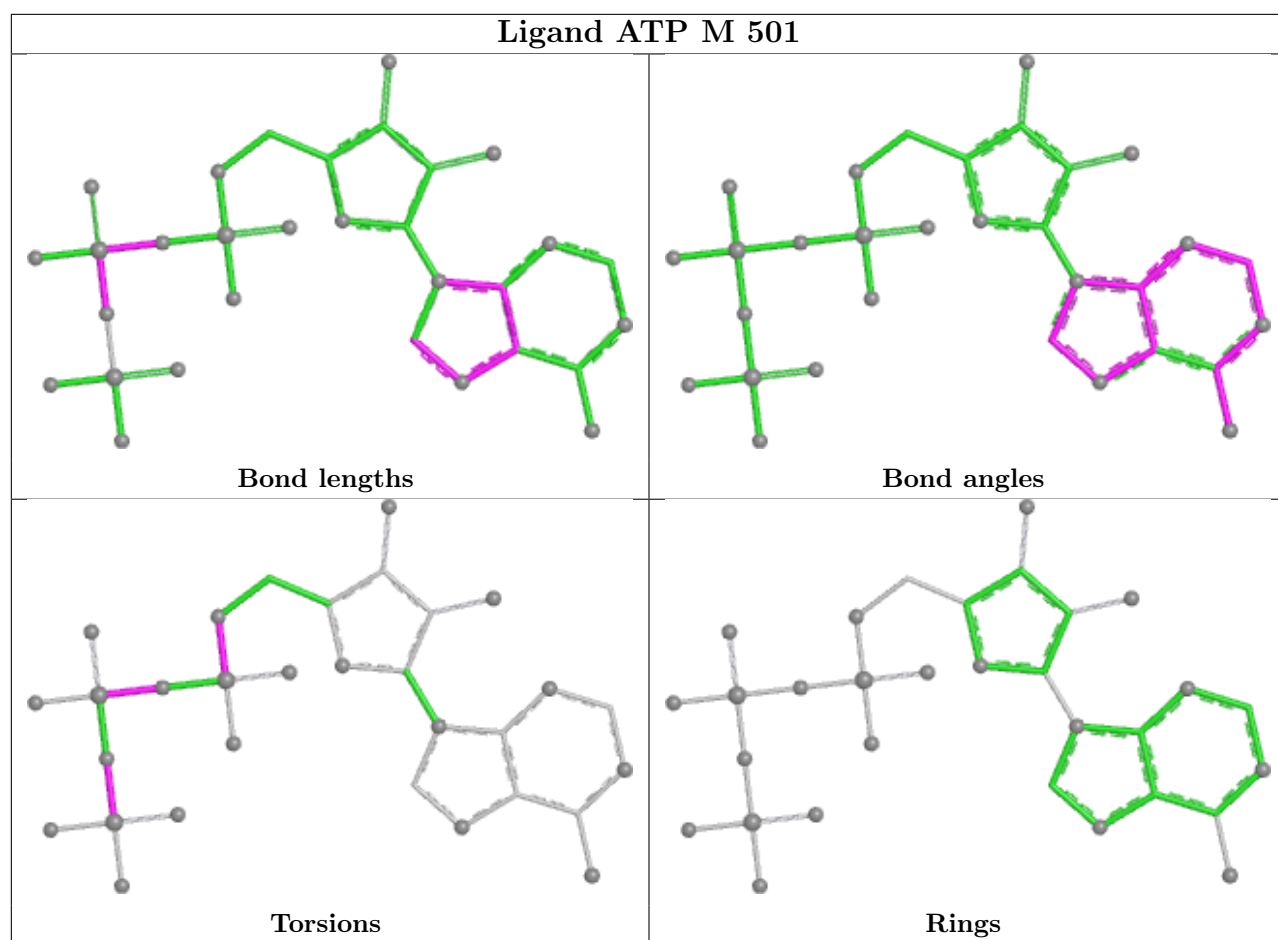
Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	H	501	ATP	2	0
23	J	501	ADP	1	0
21	L	501	ATP	2	0
21	M	501	ATP	2	0
21	I	501	ATP	7	0

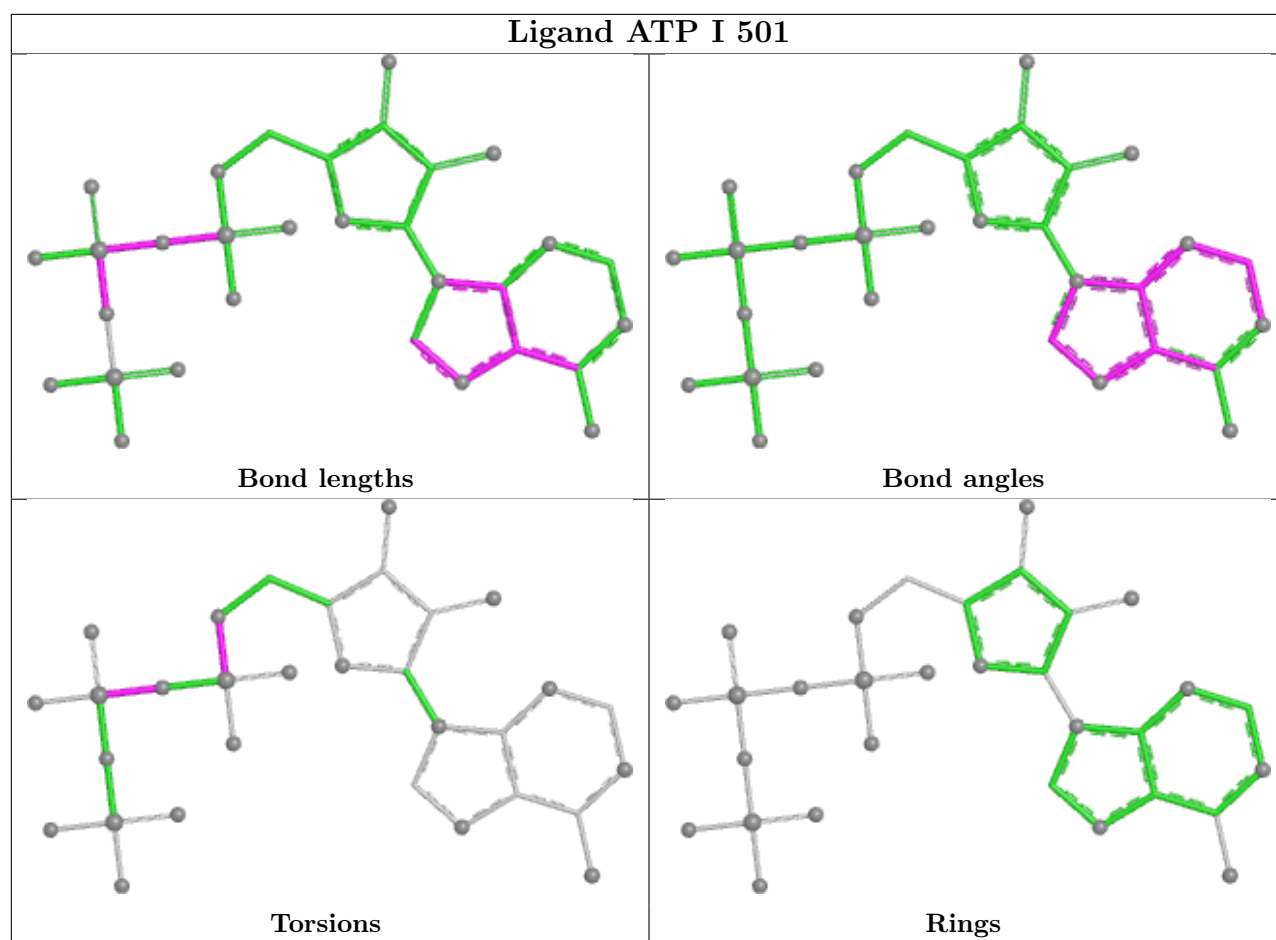
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

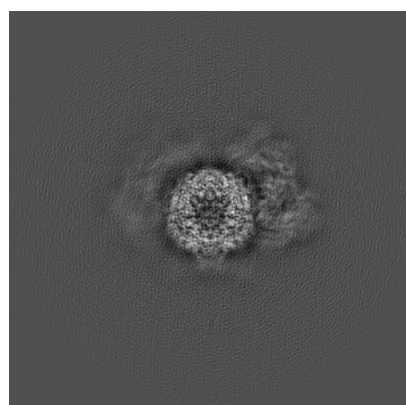
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3534. These allow visual inspection of the internal detail of the map and identification of artifacts.

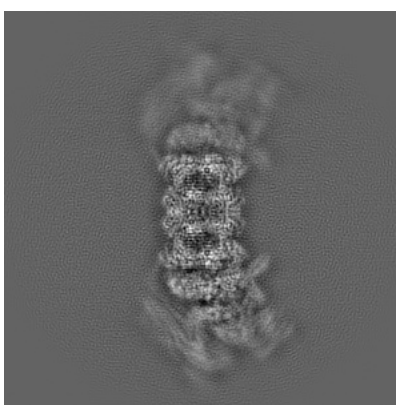
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

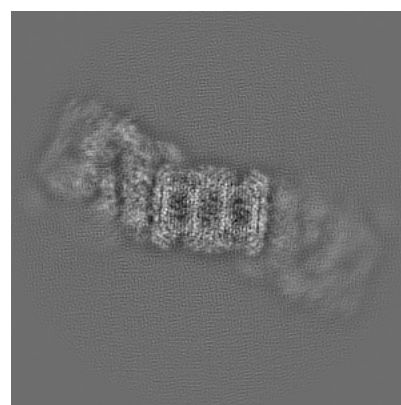
6.1.1 Primary map



X



Y

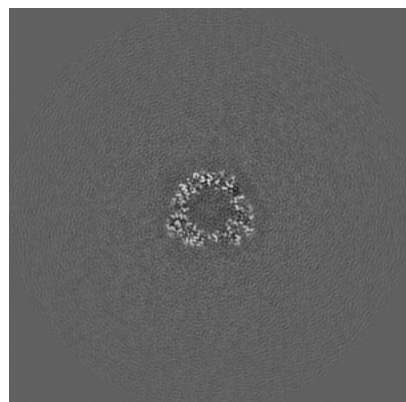


Z

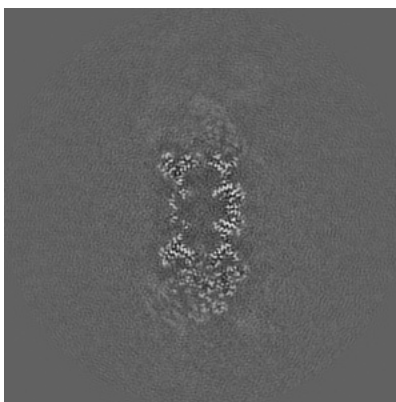
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

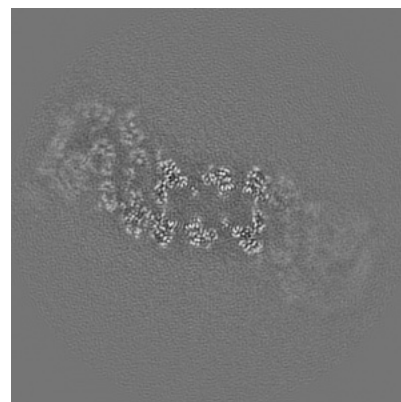
6.2.1 Primary map



X Index: 192



Y Index: 192

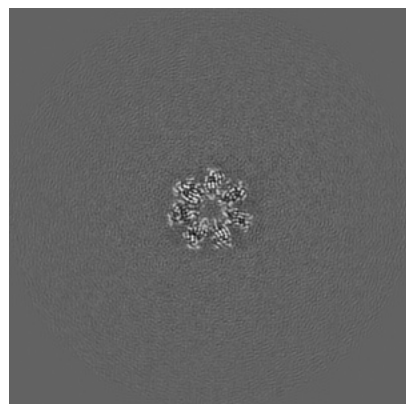


Z Index: 192

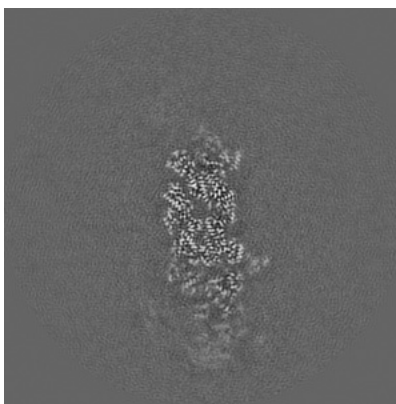
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

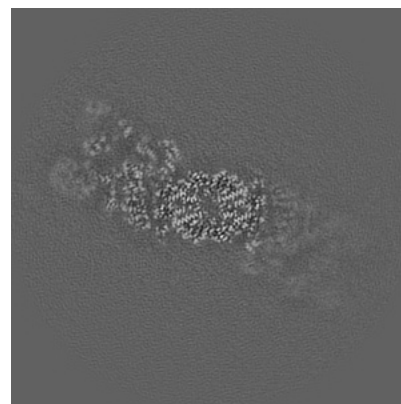
6.3.1 Primary map



X Index: 177



Y Index: 212

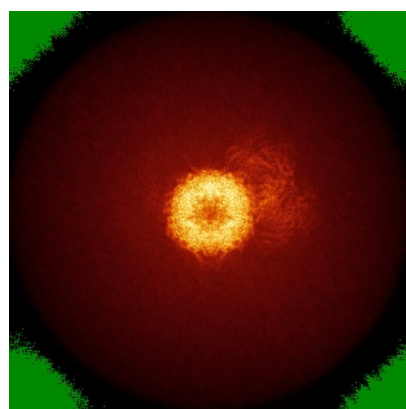


Z Index: 208

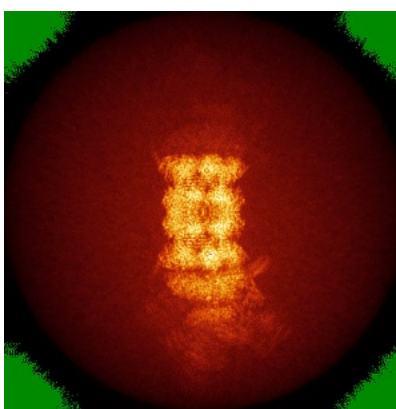
The images above show the largest variance slices of the map in three orthogonal directions.

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

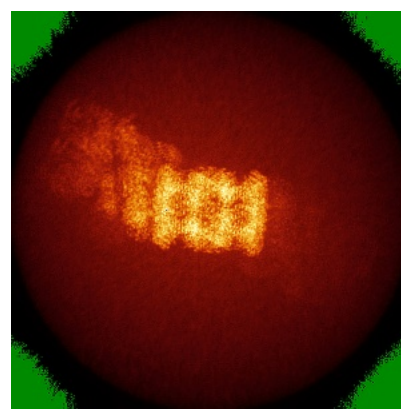
6.4.1 Primary map



X



Y

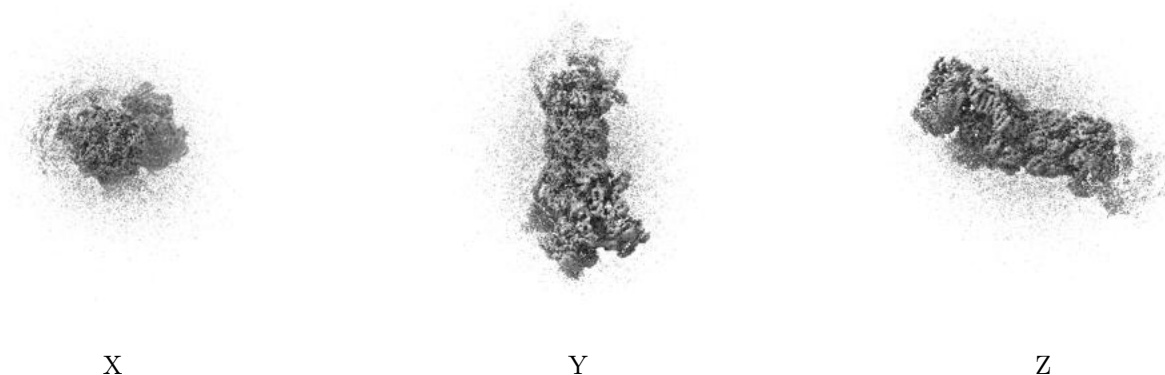


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

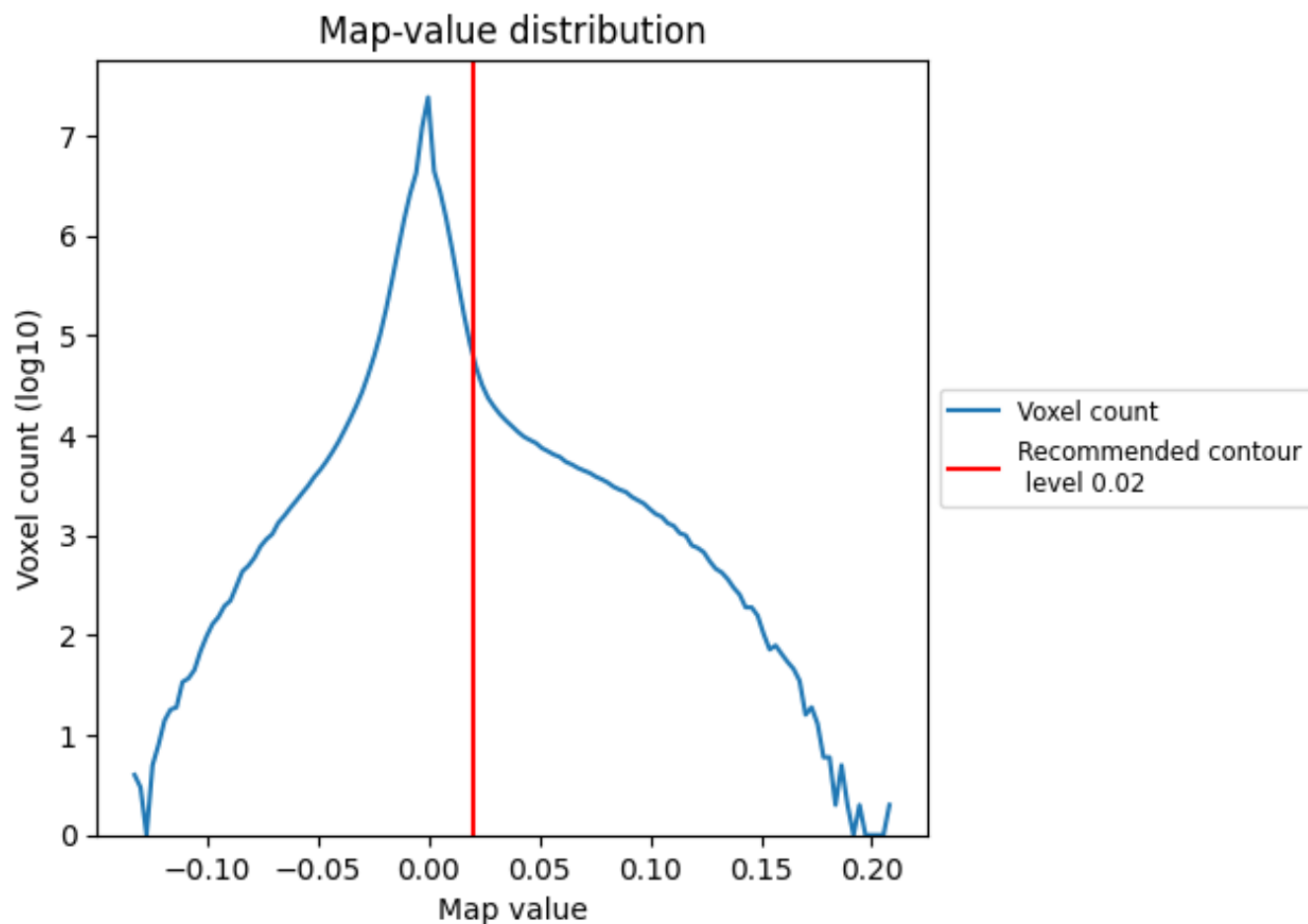
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

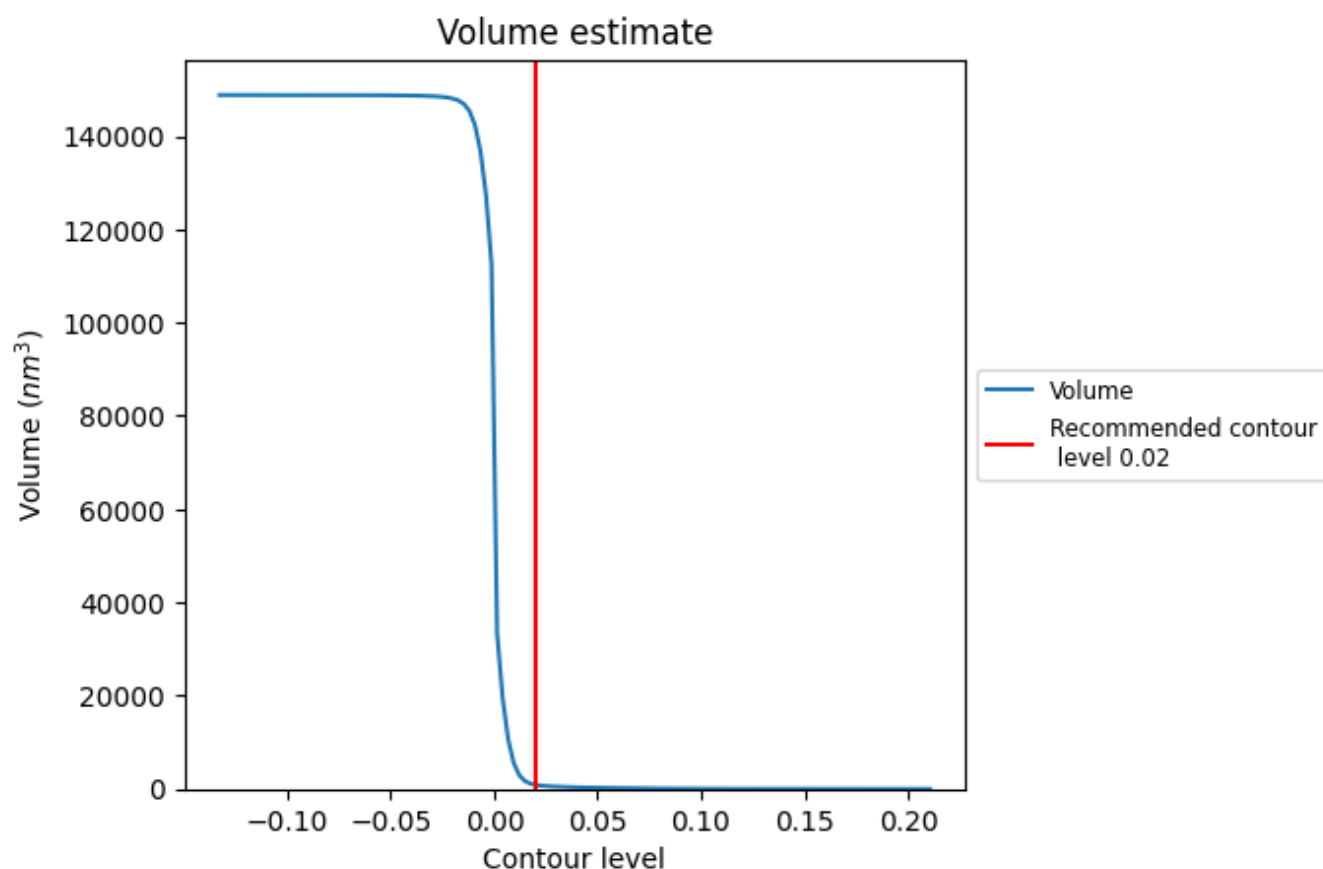
This section contains the results of statistical analysis of the map.

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.

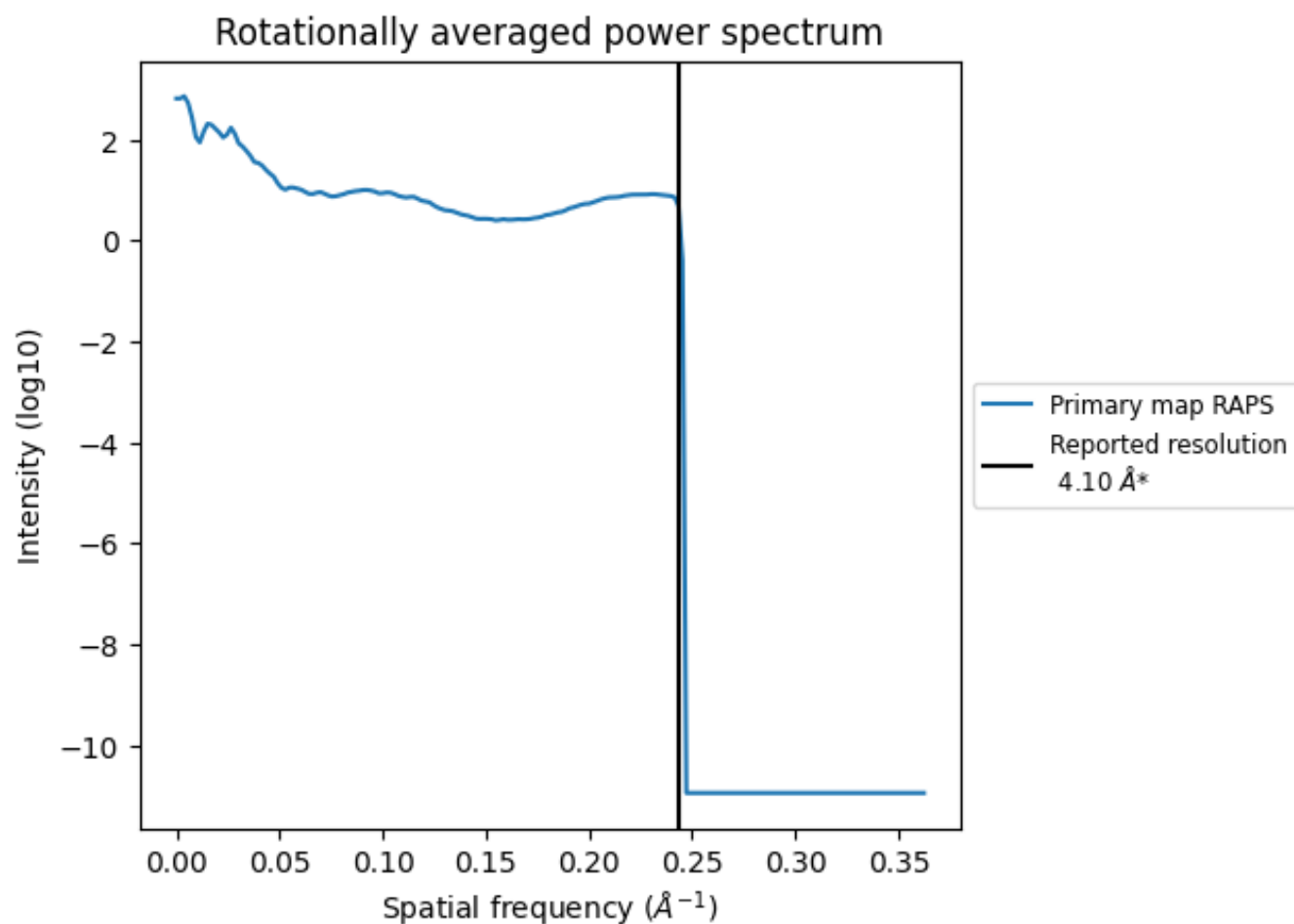
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 881 nm^3 ; this corresponds to an approximate mass of 796 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 0.244 Å⁻¹

8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

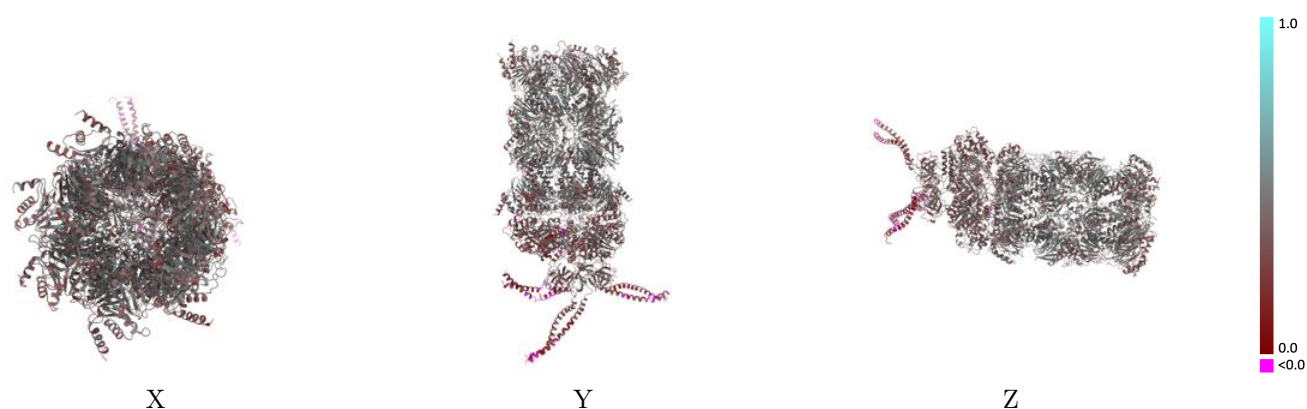
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-3534 and PDB model 5MP9. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)

This section was not generated.

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

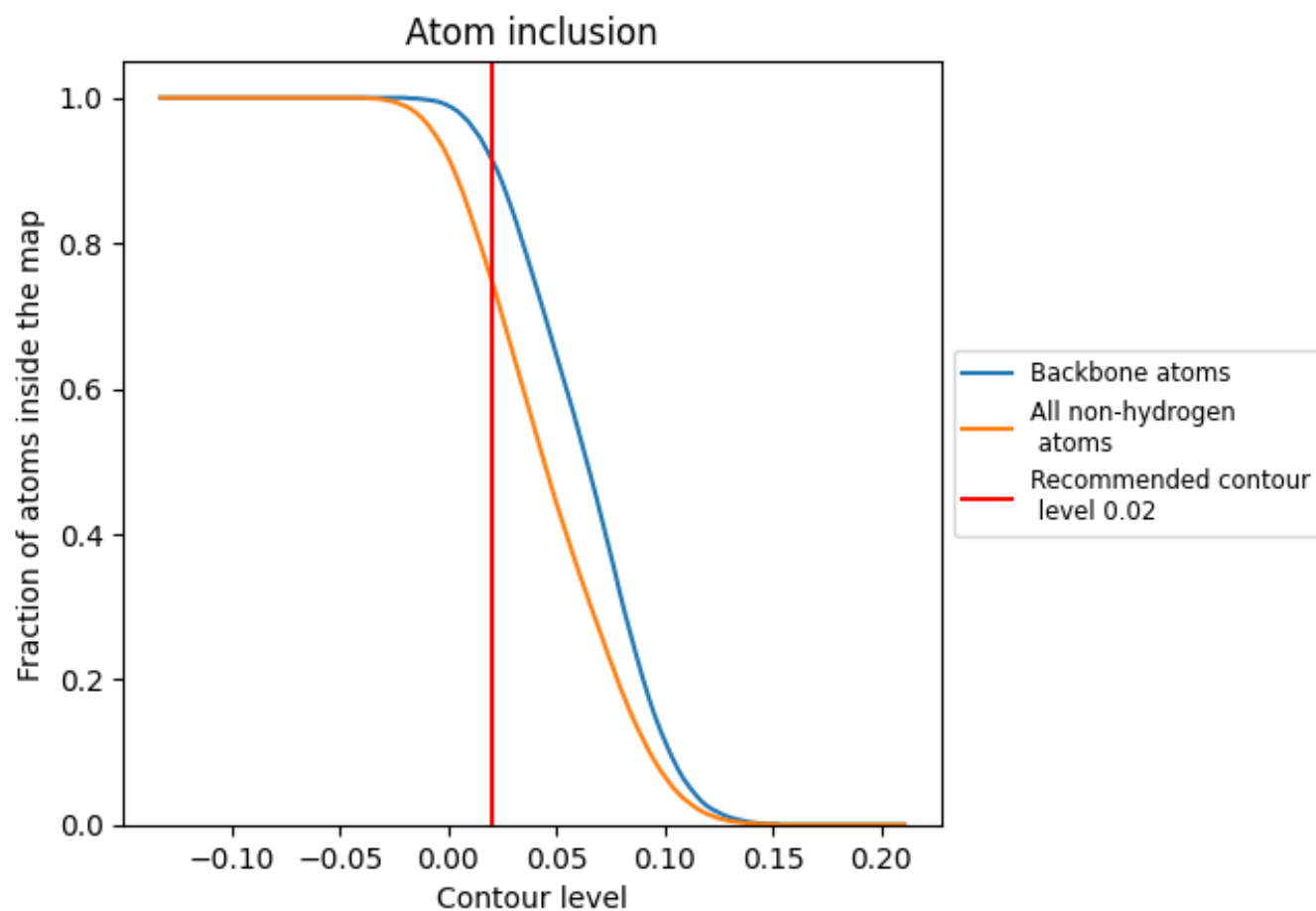


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 75% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7500	 0.3940
1	 0.8160	 0.4380
2	 0.8020	 0.4330
3	 0.7960	 0.4410
4	 0.7970	 0.4300
5	 0.8250	 0.4320
6	 0.8240	 0.4400
7	 0.8260	 0.4380
A	 0.7880	 0.4190
B	 0.7740	 0.4130
C	 0.7760	 0.4060
D	 0.7870	 0.4100
E	 0.7570	 0.4040
F	 0.8040	 0.4290
G	 0.8040	 0.4240
H	 0.6540	 0.3470
I	 0.6090	 0.2990
J	 0.5720	 0.2810
K	 0.6300	 0.3180
L	 0.6280	 0.3290
M	 0.6380	 0.3460
a	 0.7890	 0.4070
b	 0.7740	 0.4040
c	 0.7790	 0.3940
d	 0.7790	 0.4080
e	 0.7560	 0.3920
f	 0.7980	 0.4080
g	 0.7990	 0.4090
h	 0.8230	 0.4400
i	 0.8090	 0.4360
j	 0.8000	 0.4370
k	 0.8040	 0.4340
l	 0.8230	 0.4360
m	 0.8290	 0.4380
n	 0.8250	 0.4370

