



wwPDB EM Validation Summary Report ⓘ

Mar 25, 2026 – 07:08 PM UTC

PDB ID : 5L4G / pdb_00005l4g
EMDB ID : EMD-4002
Title : The human 26S proteasome at 3.9 Å
Authors : Schweitzer, A.; Aufderheide, A.; Rudack, T.; Beck, F.
Deposited on : 2016-05-25
Resolution : 3.90 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:

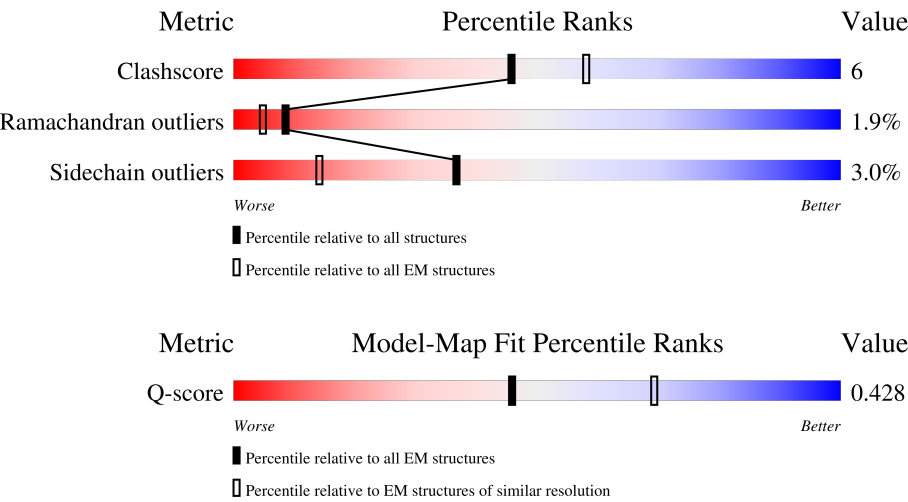
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

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

The reported resolution of this entry is 3.90 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.



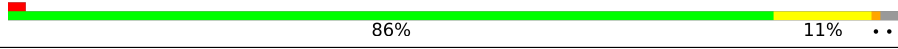
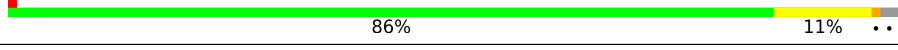
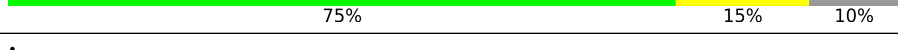
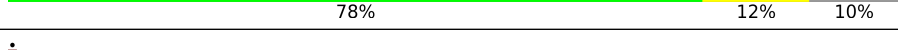
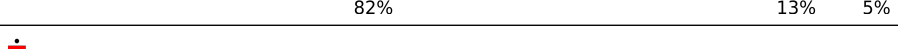
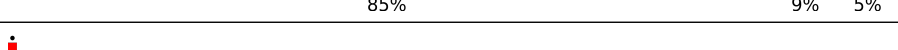
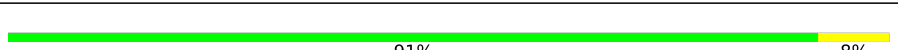
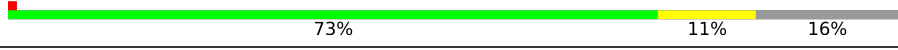
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8855 (3.40 - 4.40)

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	N	246	
2	B	234	
2	O	234	

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Mol	Chain	Length	Quality of chain
3	C	261	
3	P	261	
4	D	248	
4	Q	248	
5	E	241	
5	R	241	
6	F	263	
6	S	263	
7	G	255	
7	T	255	
8	1	241	
8	U	241	
9	2	201	
9	V	201	
10	3	205	
10	W	205	
11	4	264	
11	X	264	
12	5	263	
12	Y	263	
13	6	239	
13	Z	239	
14	7	277	
14	8	277	
15	H	433	

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Mol	Chain	Length	Quality of chain
16	I	440	
17	K	418	
18	L	389	
19	M	439	
20	J	406	

2 Entry composition

There are 23 unique types of molecules in this entry. The entry contains 135560 atoms, of which 67868 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	N	244	Total	C	H	N	O	S	0	0
			3814	1206	1911	320	364	13		
1	A	244	Total	C	H	N	O	S	0	0
			3814	1206	1911	320	364	13		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
2	O	233	Total	C	H	N	O	S	0	0
			3630	1161	1812	308	343	6		
2	B	233	Total	C	H	N	O	S	0	0
			3630	1161	1812	308	343	6		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
3	P	250	Total	C	H	N	O	S	0	0
			3963	1245	1992	339	377	10		
3	C	250	Total	C	H	N	O	S	0	0
			3963	1245	1992	339	377	10		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
4	Q	243	Total	C	H	N	O	S	0	0
			3875	1206	1952	342	370	5		
4	D	243	Total	C	H	N	O	S	0	0
			3875	1206	1952	342	370	5		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
5	R	234	Total	C	H	N	O	S	0	0
			3563	1125	1773	295	359	11		
5	E	234	Total	C	H	N	O	S	0	0
			3563	1125	1773	295	359	11		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
6	S	238	Total	C	H	N	O	S	0	0
			3733	1172	1860	337	353	11		
6	F	238	Total	C	H	N	O	S	0	0
			3733	1172	1860	337	353	11		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
7	T	242	Total	C	H	N	O	S	0	0
			3771	1200	1877	323	360	11		
7	G	241	Total	C	H	N	O	S	0	0
			3764	1198	1874	322	359	11		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
8	U	213	Total	C	H	N	O	S	0	0
			3308	1047	1654	284	313	10		
8	1	213	Total	C	H	N	O	S	0	0
			3308	1047	1654	284	313	10		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
9	V	199	Total	C	H	N	O	S	0	0
			3197	1022	1601	272	293	9		
9	2	199	Total	C	H	N	O	S	0	0
			3197	1022	1601	272	293	9		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
10	W	204	Total	C	H	N	O	S	0	0
			3200	1013	1609	265	294	19		

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Mol	Chain	Residues	Atoms						AltConf	Trace
10	3	204	Total	C	H	N	O	S	0	0
			3200	1013	1609	265	294	19		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
11	X	217	Total	C	H	N	O	S	0	0
			3358	1066	1667	292	321	12		
11	4	217	Total	C	H	N	O	S	0	0
			3358	1066	1667	292	321	12		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
12	Y	201	Total	C	H	N	O	S	0	0
			3080	982	1521	274	294	9		
12	5	201	Total	C	H	N	O	S	0	0
			3080	982	1521	274	294	9		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
13	Z	200	Total	C	H	N	O	S	0	0
			2966	939	1467	256	292	12		
13	6	199	Total	C	H	N	O	S	0	0
			2956	936	1462	255	291	12		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
14	8	220	Total	C	H	N	O	S	0	0
			3338	1044	1679	283	320	12		
14	7	220	Total	C	H	N	O	S	0	0
			3338	1044	1679	283	320	12		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
15	H	396	Total	C	H	N	O	S	0	0
			6283	1961	3167	549	588	18		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
16	I	379	Total	C	H	N	O	S	0	0
			6043	1880	3050	510	588	15		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
17	K	393	Total	C	H	N	O	S	0	0
			6302	1986	3164	537	602	13		

- Molecule 18 is a protein called 26S protease regulatory subunit 10B.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	L	389	Total	C	H	N	O	S	0	0
			6271	1947	3173	552	582	17		

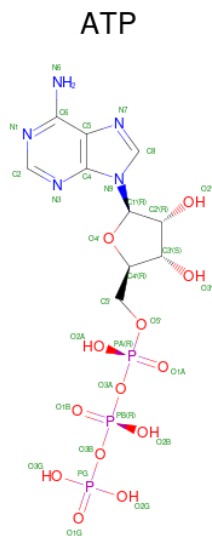
- Molecule 19 is a protein called 26S protease regulatory subunit 6A.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	M	415	Total	C	H	N	O	S	0	0
			6575	2039	3322	561	635	18		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
20	J	391	Total	C	H	N	O	S	0	0
			6252	1928	3178	549	579	18		

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

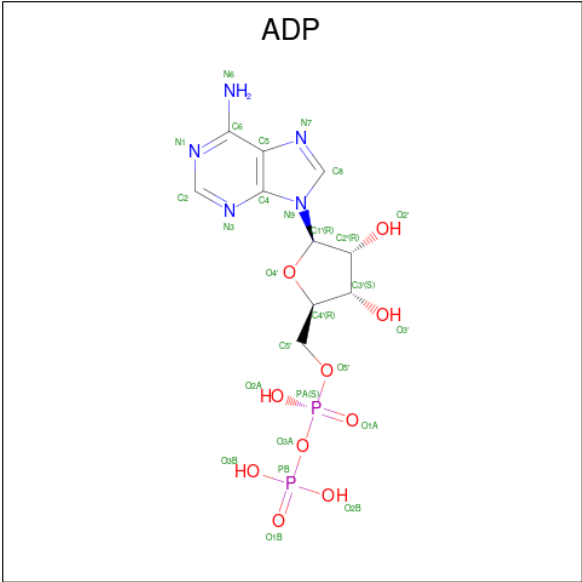


Mol	Chain	Residues	Atoms						AltConf
21	H	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
21	I	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
21	K	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
21	L	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
21	M	1	Total 43	C 10	H 12	N 5	O 13	P 3	0

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

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

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

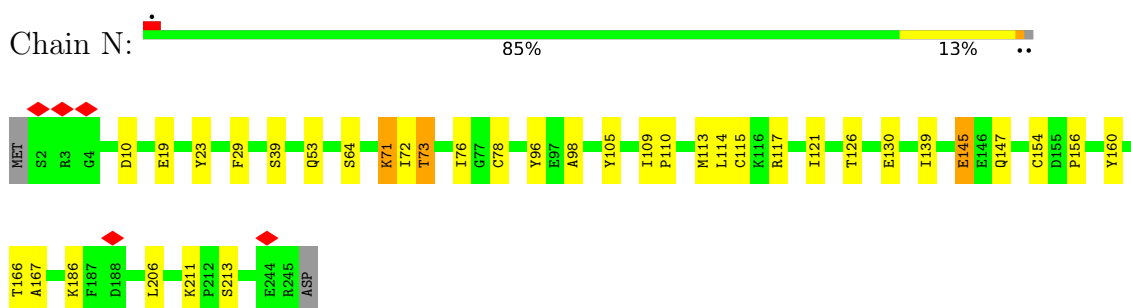


Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
23	J	1	39	10	12	5	10	2	0

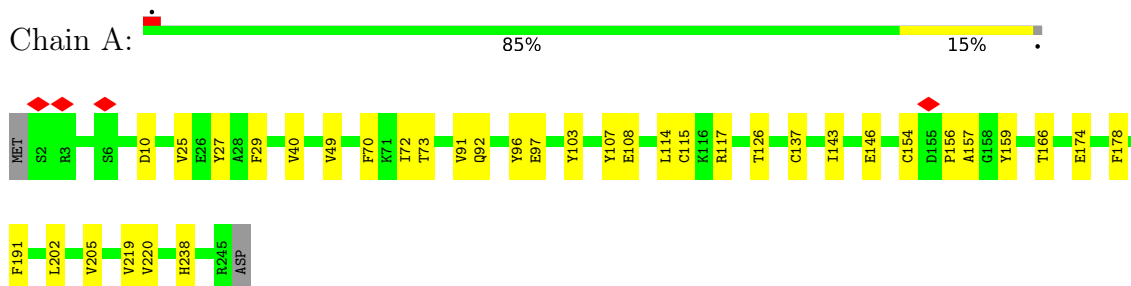
3 Residue-property plots

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.

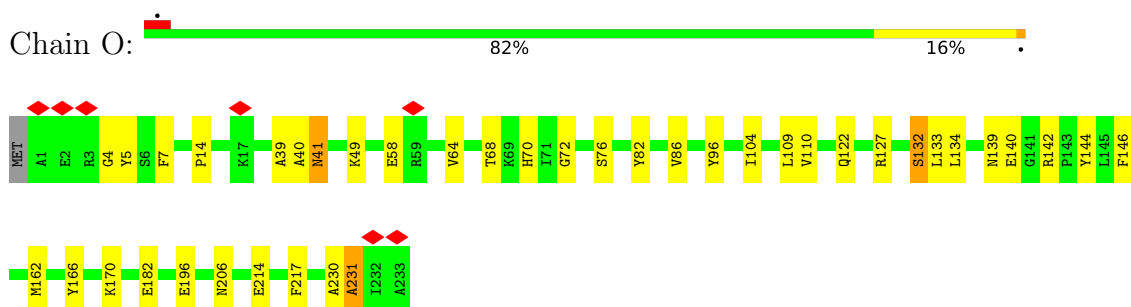
- Molecule 1: Proteasome subunit alpha type-6



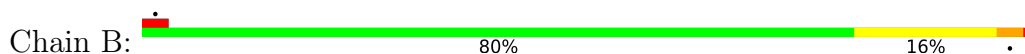
- Molecule 1: Proteasome subunit alpha type-6

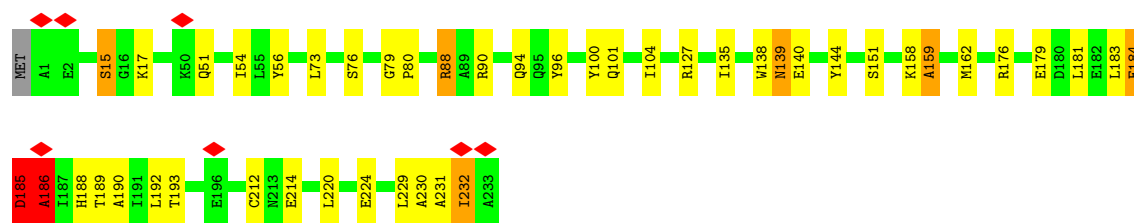


- Molecule 2: Proteasome subunit alpha type-2

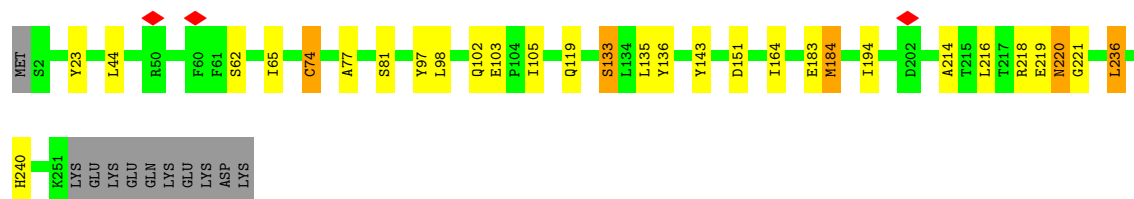
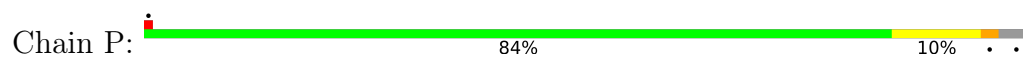


- Molecule 2: Proteasome subunit alpha type-2

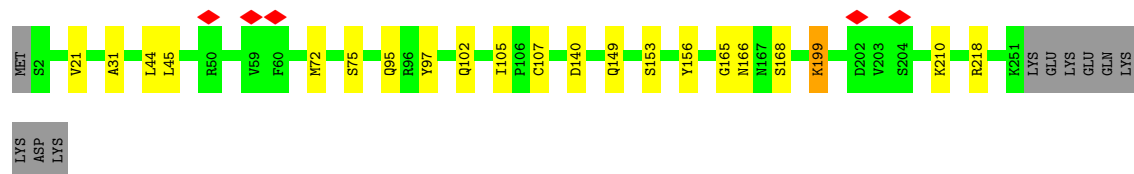
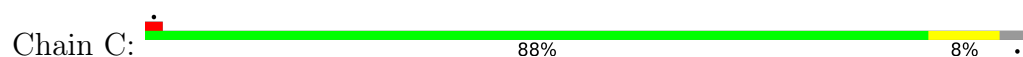




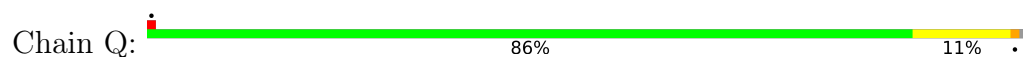
- Molecule 3: Proteasome subunit alpha type-4



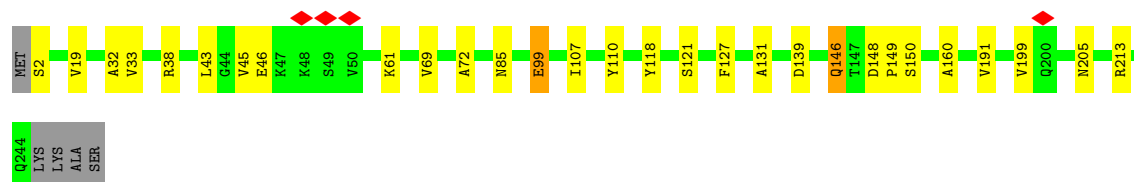
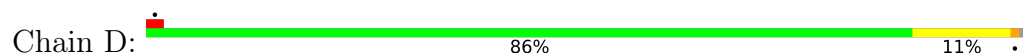
- Molecule 3: Proteasome subunit alpha type-4



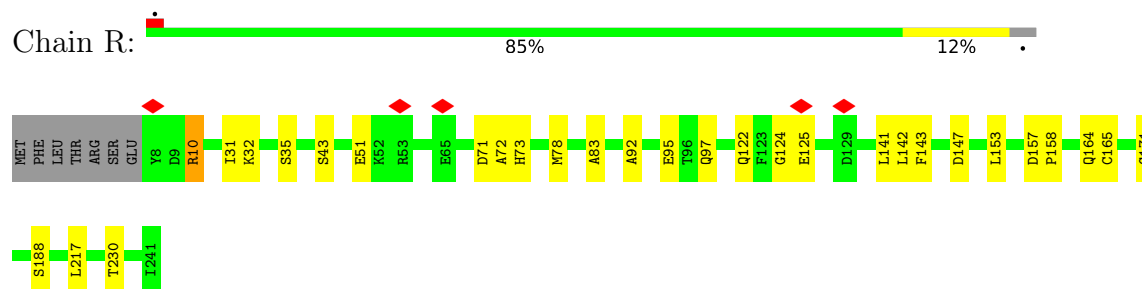
- Molecule 4: Proteasome subunit alpha type-7



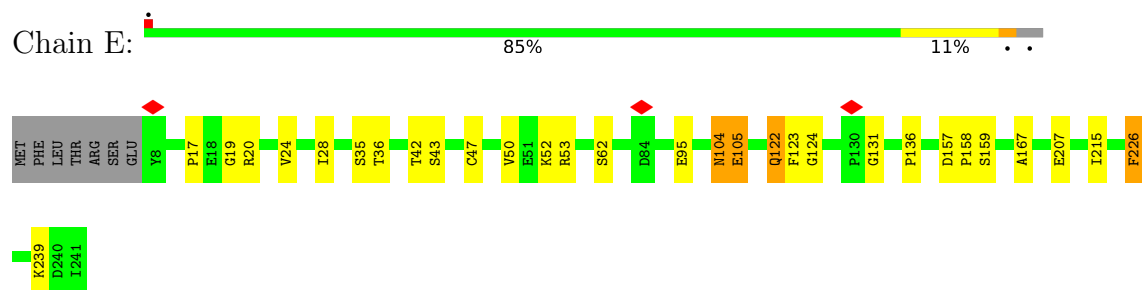
- Molecule 4: Proteasome subunit alpha type-7



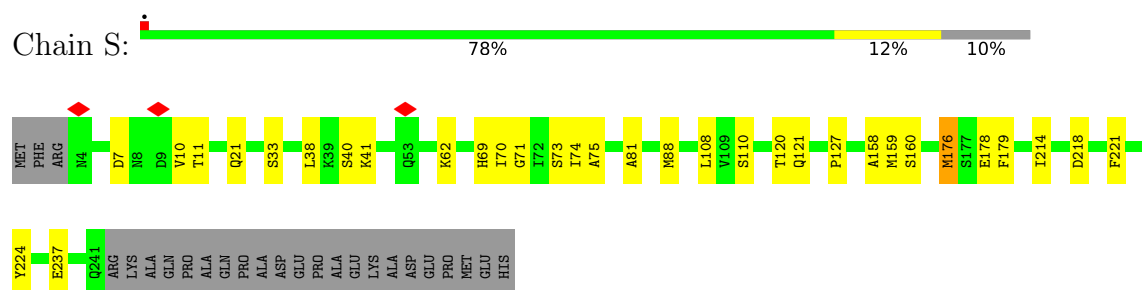
- Molecule 5: Proteasome subunit alpha type-5



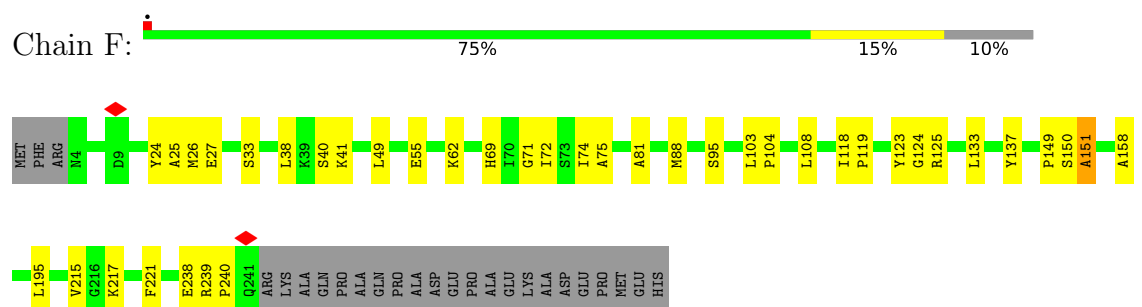
- Molecule 5: Proteasome subunit alpha type-5



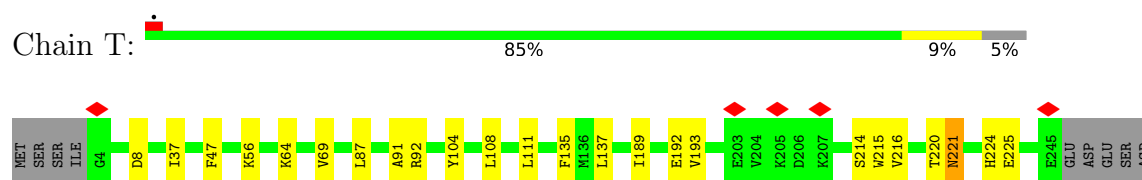
- Molecule 6: Proteasome subunit alpha type-1



- Molecule 6: Proteasome subunit alpha type-1



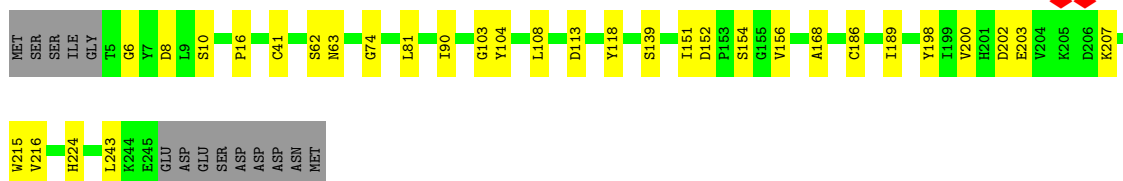
- Molecule 7: Proteasome subunit alpha type-3



ASP
ASP
ASN
MET

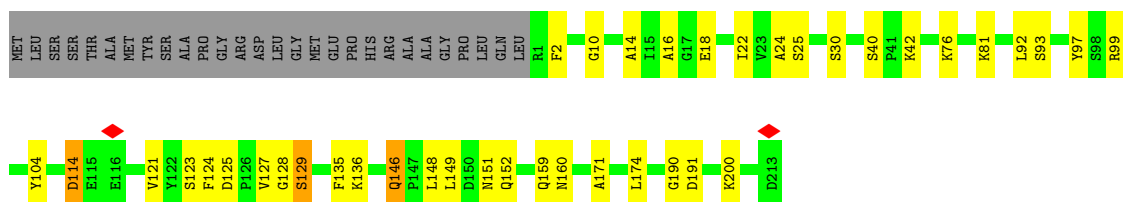
• Molecule 7: Proteasome subunit alpha type-3

Chain G:  82% 13% 5%



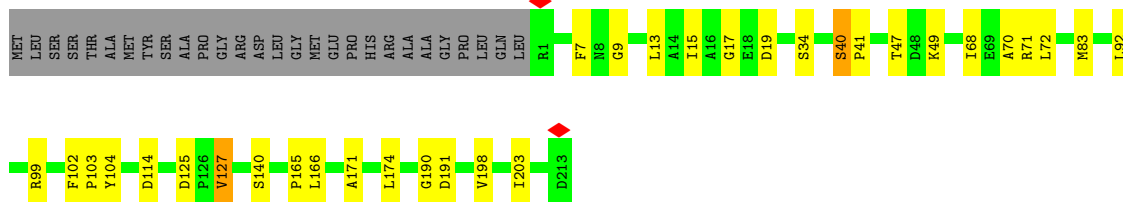
• Molecule 8: Proteasome subunit beta type-1

Chain U:  72% 15% 12%



• Molecule 8: Proteasome subunit beta type-1

Chain 1:  75% 13% 12%



• Molecule 9: Proteasome subunit beta type-2

Chain V:  87% 10% 3%



• Molecule 9: Proteasome subunit beta type-2

Chain 2:  89% 8% 3%



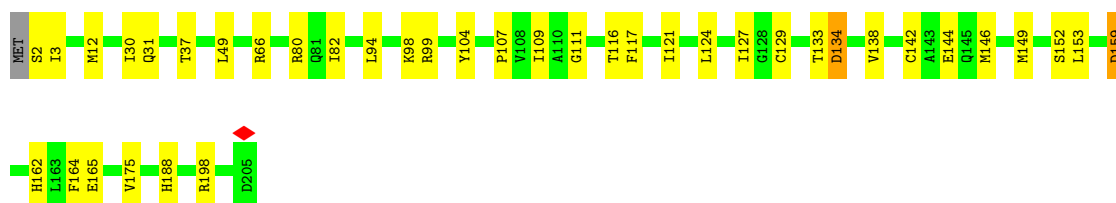
- Molecule 10: Proteasome subunit beta type-3

Chain W:  91% 8%



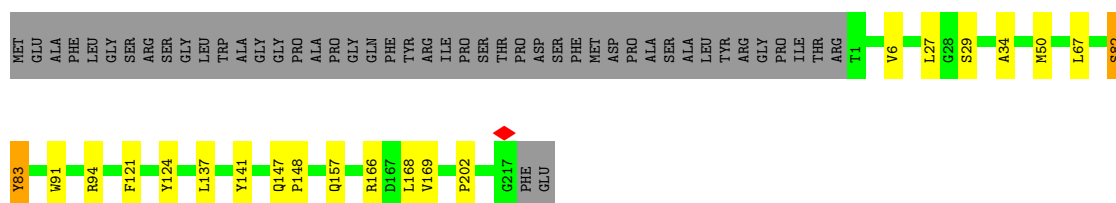
- Molecule 10: Proteasome subunit beta type-3

Chain 3:  80% 18%



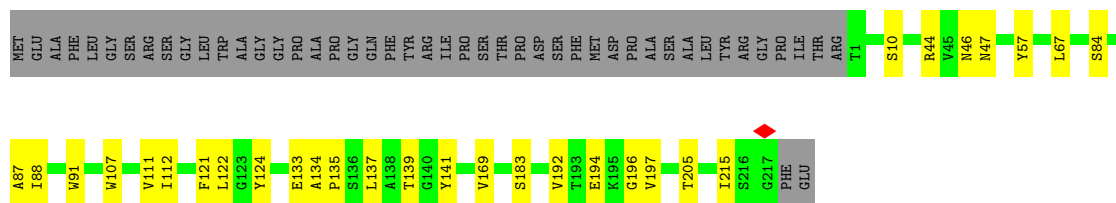
- Molecule 11: Proteasome subunit beta type-4

Chain X:  74% 7% 18%



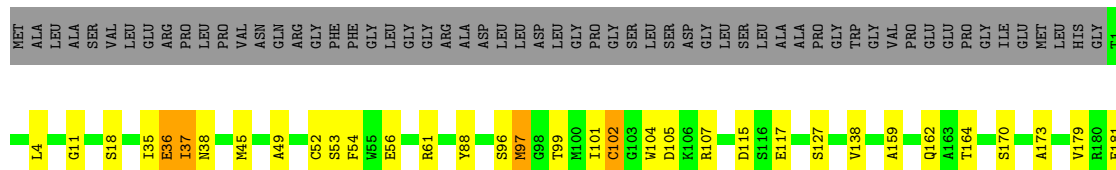
- Molecule 11: Proteasome subunit beta type-4

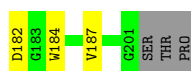
Chain 4:  71% 11% 18%



- Molecule 12: Proteasome subunit beta type-5

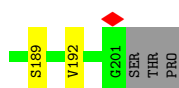
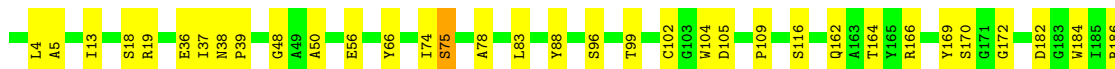
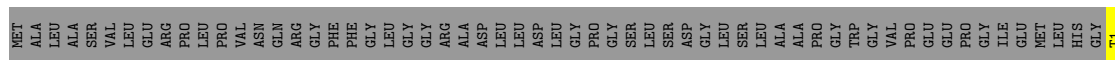
Chain Y:  62% 13% 24%





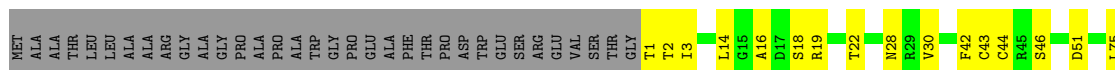
• Molecule 12: Proteasome subunit beta type-5

Chain 5: 62% 14% 24%



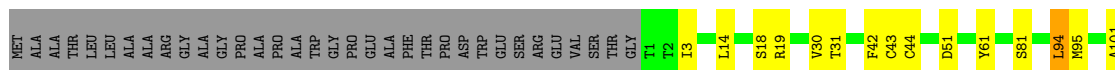
• Molecule 13: Proteasome subunit beta type-6

Chain Z: 73% 11% 16%



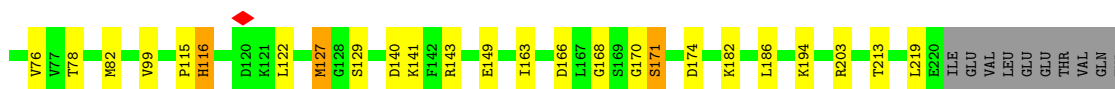
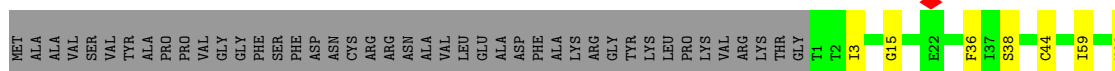
• Molecule 13: Proteasome subunit beta type-6

Chain 6: 74% 9% 17%



• Molecule 14: Proteasome subunit beta type-7

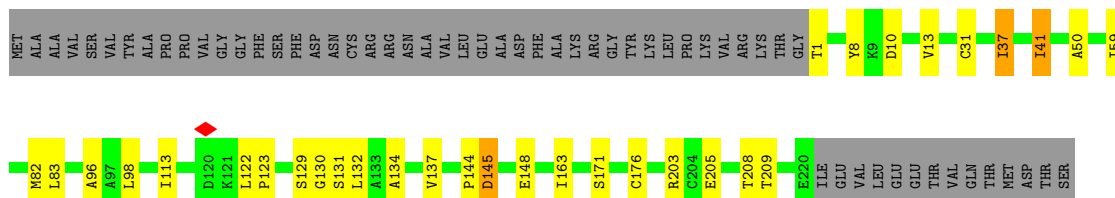
Chain 8: 68% 10% 21%



MET
ASP
THR
SER

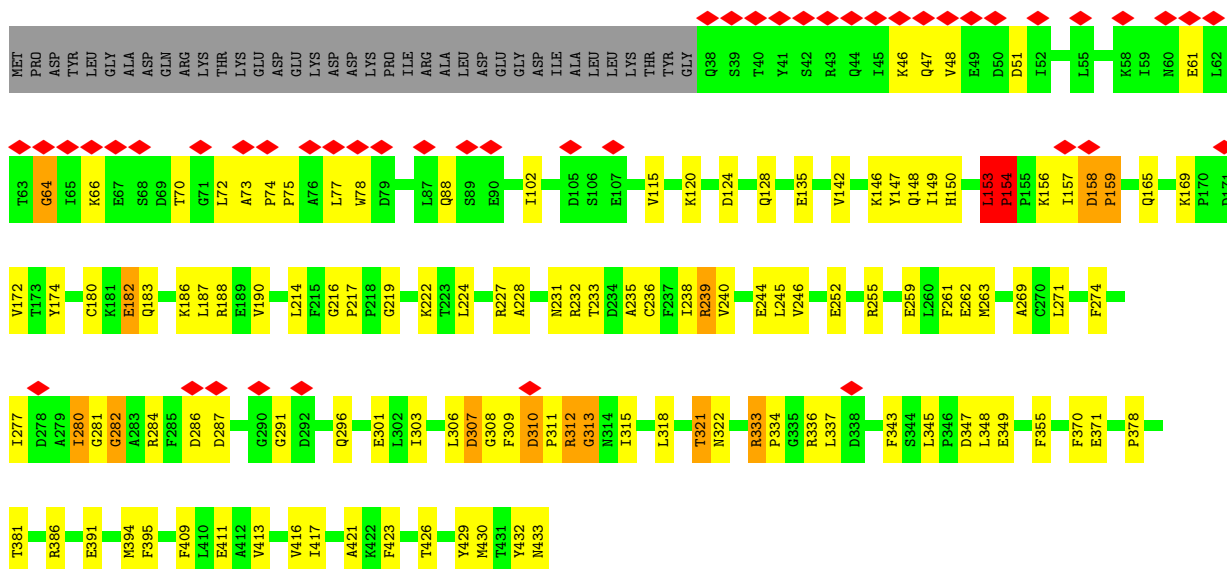
• Molecule 14: Proteasome subunit beta type-7

Chain 7:  68% 10% 21%



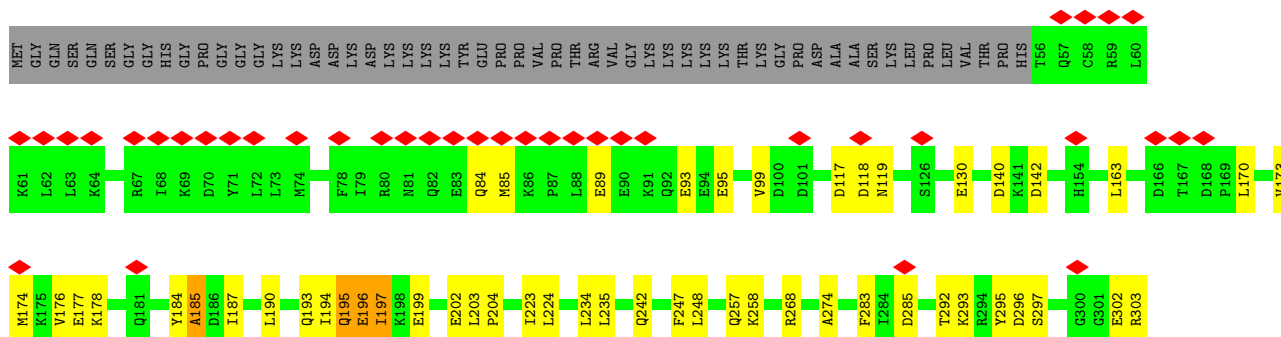
• Molecule 15: 26S protease regulatory subunit 7

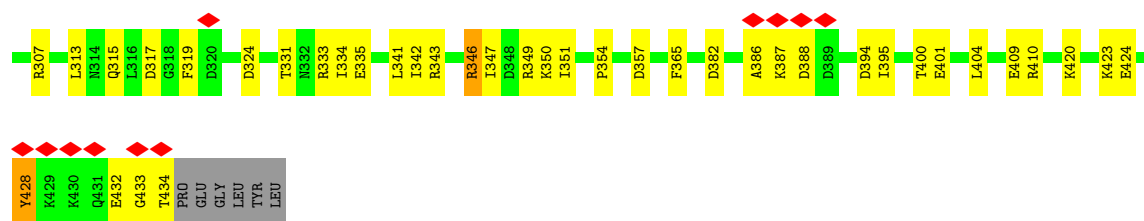
Chain H:  11% 63% 25% 9%



• Molecule 16: 26S protease regulatory subunit 4

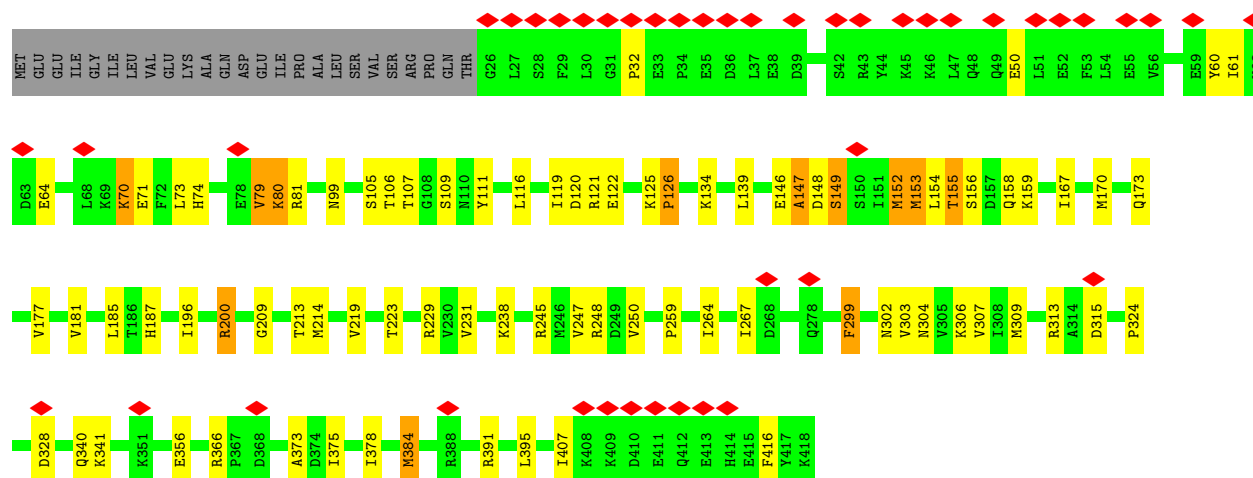
Chain I:  11% 65% 19% 14%





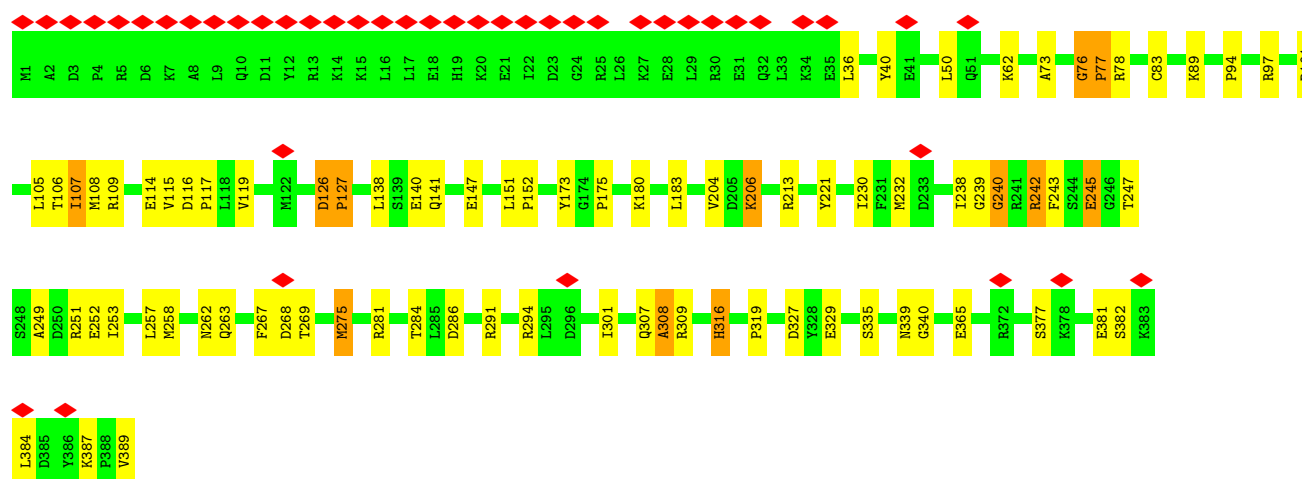
• Molecule 17: 26S protease regulatory subunit 6B

Chain K: 11% 74% 17% 6%



• Molecule 18: 26S protease regulatory subunit 10B

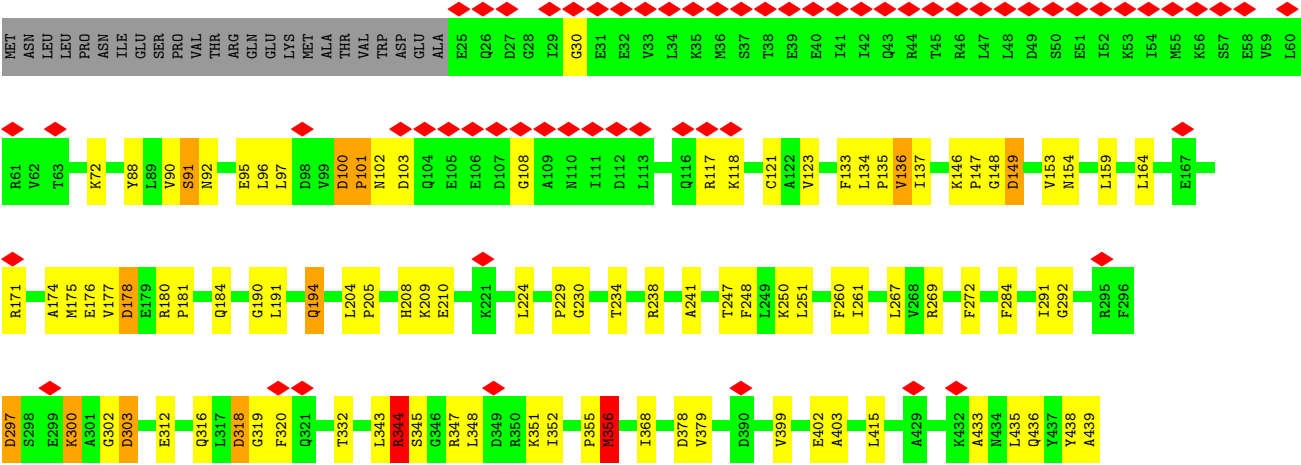
Chain L: 11% 79% 18% 5%



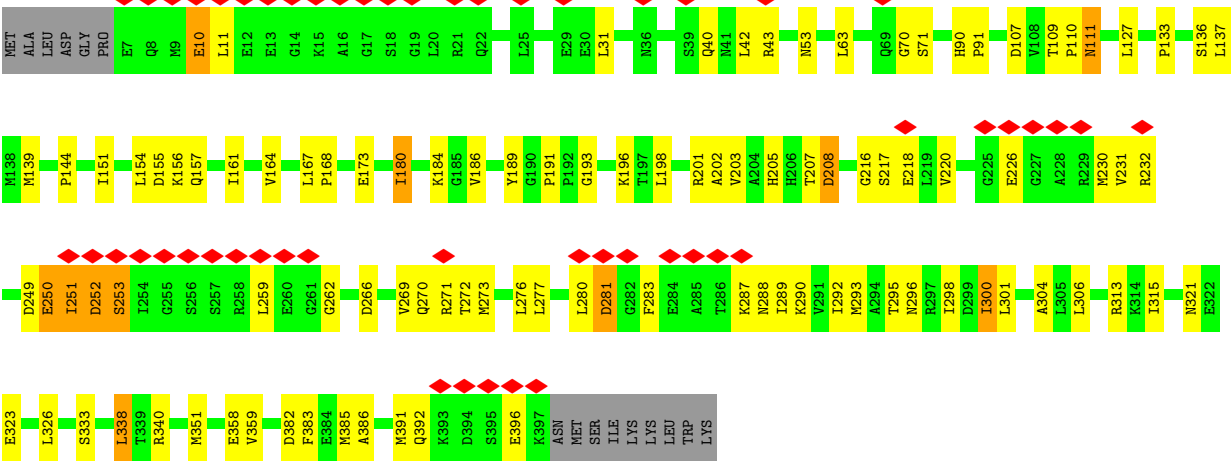
• Molecule 19: 26S protease regulatory subunit 6A

Chain M: 14% 72% 19% 5%





• Molecule 20: 26S protease regulatory subunit 8



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	461402	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)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	OTHER	Depositor
Maximum map value	0.307	Depositor
Minimum map value	-0.195	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.035	Depositor
Map size (Å)	518.4, 518.4, 518.4	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.35, 1.35, 1.35	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, ATP, 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	0.38	1/1937 (0.1%)	0.51	2/2617 (0.1%)
1	N	0.28	0/1937	0.49	0/2617
2	B	0.94	7/1857 (0.4%)	0.90	9/2514 (0.4%)
2	O	0.32	0/1857	0.48	0/2514
3	C	0.30	0/2001	0.47	0/2694
3	P	0.33	1/2001 (0.0%)	0.50	2/2694 (0.1%)
4	D	0.31	0/1949	0.50	0/2626
4	Q	0.27	0/1949	0.48	1/2626 (0.0%)
5	E	0.31	0/1818	0.49	0/2455
5	R	0.33	1/1818 (0.1%)	0.47	2/2455 (0.1%)
6	F	0.30	0/1908	0.52	0/2579
6	S	0.27	0/1908	0.46	0/2579
7	G	0.30	0/1925	0.49	0/2592
7	T	0.27	0/1929	0.46	0/2597
8	1	0.35	1/1684 (0.1%)	0.53	0/2268
8	U	0.31	0/1684	0.53	0/2268
9	2	0.34	0/1629	0.51	0/2203
9	V	0.34	0/1629	0.54	0/2203
10	3	0.37	1/1620 (0.1%)	0.54	1/2184 (0.0%)
10	W	0.33	0/1620	0.53	0/2184
11	4	0.36	0/1724	0.55	0/2333
11	X	0.32	0/1724	0.51	0/2333
12	5	0.34	0/1590	0.53	0/2147
12	Y	0.33	0/1590	0.52	0/2147
13	6	0.33	0/1520	0.49	0/2057
13	Z	0.32	0/1525	0.51	0/2064
14	7	0.29	0/1686	0.49	0/2282
14	8	0.28	0/1686	0.49	0/2282
15	H	0.35	1/3168 (0.0%)	0.62	5/4277 (0.1%)
16	I	0.31	0/3034	0.57	2/4089 (0.0%)
17	K	0.31	0/3191	0.52	0/4306
18	L	0.33	1/3146 (0.0%)	0.52	2/4233 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
19	M	0.30	0/3294	0.49	0/4437
20	J	0.34	1/3113 (0.0%)	0.54	1/4184 (0.0%)
All	All	0.35	15/68651 (0.0%)	0.53	27/92640 (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
2	B	0	1
7	G	0	1
7	T	0	1
15	H	0	2
16	I	0	1
17	K	0	2
20	J	0	1
All	All	0	9

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	185	ASP	CA-CB	22.95	1.92	1.53
2	B	185	ASP	CB-CG	17.27	1.95	1.52
2	B	184	GLU	C-N	14.06	1.53	1.33
2	B	185	ASP	N-CA	11.32	1.60	1.46
2	B	184	GLU	CA-C	10.77	1.67	1.52

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	184	GLU	CA-C-N	15.68	151.50	121.54
2	B	184	GLU	C-N-CA	15.68	151.50	121.54
2	B	185	ASP	N-CA-CB	13.18	132.76	110.49
2	B	185	ASP	CA-CB-CG	12.67	125.27	112.60
15	H	153	LEU	C-N-CD	-11.44	95.42	120.60

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	186	ALA	Peptide
7	G	215	TRP	Peptide
15	H	153	LEU	Peptide
15	H	321	THR	Peptide
7	T	215	TRP	Peptide

5.2 Too-close contacts

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	1903	1911	1911	21	0
1	N	1903	1911	1911	20	0
2	B	1818	1812	1814	48	0
2	O	1818	1812	1814	22	0
3	C	1971	1992	1992	9	0
3	P	1971	1992	1992	17	0
4	D	1923	1952	1952	16	0
4	Q	1923	1952	1952	13	0
5	E	1790	1773	1773	14	0
5	R	1790	1773	1773	14	0
6	F	1873	1860	1860	21	0
6	S	1873	1860	1860	13	0
7	G	1890	1874	1874	11	0
7	T	1894	1877	1877	11	0
8	1	1654	1654	1656	16	0
8	U	1654	1654	1656	24	0
9	2	1596	1601	1601	15	0
9	V	1596	1601	1601	14	0
10	3	1591	1609	1609	23	0
10	W	1591	1609	1609	9	0
11	4	1691	1667	1669	17	0
11	X	1691	1667	1669	10	0
12	5	1559	1521	1523	16	0
12	Y	1559	1521	1523	24	0
13	6	1494	1462	1464	11	0
13	Z	1499	1467	1469	15	0
14	7	1659	1679	1681	21	0
14	8	1659	1679	1681	14	0
15	H	3116	3167	3167	98	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	I	2993	3050	3050	67	0
17	K	3138	3164	3164	59	0
18	L	3098	3173	3173	60	0
19	M	3253	3322	3322	76	0
20	J	3074	3178	3178	80	0
21	H	31	12	12	2	0
21	I	31	12	12	0	0
21	K	31	12	12	5	0
21	L	31	12	12	1	0
21	M	31	12	12	4	0
22	H	1	0	0	0	0
22	I	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	12	12	2	0
All	All	67692	67868	67892	834	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 6.

The worst 5 of 834 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)
2:B:184:GLU:CB	2:B:184:GLU:CG	1.77	1.54
2:B:185:ASP:CB	2:B:185:ASP:CA	1.92	1.45
2:B:185:ASP:CB	2:B:185:ASP:CG	1.95	1.40
2:B:185:ASP:O	2:B:189:THR:N	1.81	1.14
17:K:70:LYS:O	17:K:73:LEU:N	1.97	0.96

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	242/246 (98%)	217 (90%)	23 (10%)	2 (1%)	16	50
1	N	242/246 (98%)	215 (89%)	25 (10%)	2 (1%)	16	50
2	B	231/234 (99%)	208 (90%)	20 (9%)	3 (1%)	9	40
2	O	231/234 (99%)	206 (89%)	21 (9%)	4 (2%)	7	35
3	C	248/261 (95%)	235 (95%)	13 (5%)	0	100	100
3	P	248/261 (95%)	230 (93%)	15 (6%)	3 (1%)	10	41
4	D	241/248 (97%)	221 (92%)	18 (8%)	2 (1%)	16	50
4	Q	241/248 (97%)	217 (90%)	20 (8%)	4 (2%)	7	35
5	E	232/241 (96%)	207 (89%)	17 (7%)	8 (3%)	3	24
5	R	232/241 (96%)	207 (89%)	22 (10%)	3 (1%)	9	40
6	F	236/263 (90%)	214 (91%)	17 (7%)	5 (2%)	5	31
6	S	236/263 (90%)	218 (92%)	14 (6%)	4 (2%)	7	35
7	G	239/255 (94%)	212 (89%)	24 (10%)	3 (1%)	9	40
7	T	240/255 (94%)	224 (93%)	13 (5%)	3 (1%)	9	40
8	1	211/241 (88%)	189 (90%)	17 (8%)	5 (2%)	4	29
8	U	211/241 (88%)	186 (88%)	22 (10%)	3 (1%)	9	38
9	2	197/201 (98%)	176 (89%)	18 (9%)	3 (2%)	8	37
9	V	197/201 (98%)	177 (90%)	17 (9%)	3 (2%)	8	37
10	3	202/205 (98%)	180 (89%)	21 (10%)	1 (0%)	24	59
10	W	202/205 (98%)	180 (89%)	20 (10%)	2 (1%)	12	45
11	4	215/264 (81%)	193 (90%)	21 (10%)	1 (0%)	24	59
11	X	215/264 (81%)	196 (91%)	15 (7%)	4 (2%)	6	33
12	5	199/263 (76%)	176 (88%)	19 (10%)	4 (2%)	6	32
12	Y	199/263 (76%)	178 (89%)	16 (8%)	5 (2%)	4	29
13	6	197/239 (82%)	177 (90%)	17 (9%)	3 (2%)	8	37
13	Z	198/239 (83%)	177 (89%)	19 (10%)	2 (1%)	12	45
14	7	218/277 (79%)	195 (89%)	21 (10%)	2 (1%)	14	47
14	8	218/277 (79%)	192 (88%)	24 (11%)	2 (1%)	14	47
15	H	394/433 (91%)	323 (82%)	51 (13%)	20 (5%)	1	17
16	I	377/440 (86%)	332 (88%)	41 (11%)	4 (1%)	11	43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	K	391/418 (94%)	323 (83%)	53 (14%)	15 (4%)	2	21
18	L	387/389 (100%)	326 (84%)	45 (12%)	16 (4%)	2	20
19	M	413/439 (94%)	348 (84%)	50 (12%)	15 (4%)	2	23
20	J	389/406 (96%)	326 (84%)	52 (13%)	11 (3%)	4	27
All	All	8569/9401 (91%)	7581 (88%)	821 (10%)	167 (2%)	8	33

5 of 167 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	O	41	ASN
2	O	70	HIS
4	Q	120	GLN
7	T	64	LYS
8	U	2	PHE

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	208/210 (99%)	204 (98%)	4 (2%)	50	66
1	N	208/210 (99%)	200 (96%)	8 (4%)	29	52
2	B	190/191 (100%)	181 (95%)	9 (5%)	23	48
2	O	190/191 (100%)	185 (97%)	5 (3%)	40	60
3	C	210/221 (95%)	203 (97%)	7 (3%)	33	56
3	P	210/221 (95%)	204 (97%)	6 (3%)	37	58
4	D	207/211 (98%)	201 (97%)	6 (3%)	37	58
4	Q	207/211 (98%)	201 (97%)	6 (3%)	37	58
5	E	196/203 (97%)	189 (96%)	7 (4%)	31	54
5	R	196/203 (97%)	191 (97%)	5 (3%)	40	60
6	F	204/224 (91%)	200 (98%)	4 (2%)	48	65
6	S	204/224 (91%)	196 (96%)	8 (4%)	28	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	G	199/212 (94%)	192 (96%)	7 (4%)	32	54
7	T	199/212 (94%)	198 (100%)	1 (0%)	81	82
8	1	178/199 (89%)	172 (97%)	6 (3%)	32	55
8	U	178/199 (89%)	171 (96%)	7 (4%)	28	52
9	2	170/171 (99%)	170 (100%)	0	100	100
9	V	170/171 (99%)	166 (98%)	4 (2%)	43	63
10	3	173/174 (99%)	165 (95%)	8 (5%)	24	48
10	W	173/174 (99%)	169 (98%)	4 (2%)	44	63
11	4	179/215 (83%)	172 (96%)	7 (4%)	28	52
11	X	179/215 (83%)	174 (97%)	5 (3%)	38	59
12	5	156/202 (77%)	149 (96%)	7 (4%)	24	49
12	Y	156/202 (77%)	152 (97%)	4 (3%)	40	60
13	6	155/181 (86%)	151 (97%)	4 (3%)	40	60
13	Z	155/181 (86%)	151 (97%)	4 (3%)	40	60
14	7	181/228 (79%)	177 (98%)	4 (2%)	45	64
14	8	181/228 (79%)	169 (93%)	12 (7%)	15	41
15	H	341/372 (92%)	328 (96%)	13 (4%)	29	52
16	I	336/385 (87%)	327 (97%)	9 (3%)	39	60
17	K	344/366 (94%)	334 (97%)	10 (3%)	37	58
18	L	341/341 (100%)	338 (99%)	3 (1%)	70	75
19	M	357/379 (94%)	349 (98%)	8 (2%)	45	64
20	J	339/352 (96%)	323 (95%)	16 (5%)	23	48
All	All	7270/7879 (92%)	7052 (97%)	218 (3%)	37	57

5 of 218 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	F	239	ARG
11	4	205	THR
19	M	344	ARG
7	G	113	ASP
10	3	49	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 75 such sidechains are listed below:

Mol	Chain	Res	Type
11	4	185	ASN
18	L	359	HIS
12	5	119	ASN
16	I	314	ASN
9	V	55	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 11 ligands modelled in this entry, 5 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	I	501	22	32,33,33	1.39	5 (15%)	48,52,52	2.02	10 (20%)
23	ADP	J	501	-	28,29,29	1.53	6 (21%)	43,45,45	1.70	9 (20%)
21	ATP	K	501	22	32,33,33	1.93	7 (21%)	48,52,52	2.02	18 (37%)
21	ATP	H	501	22	32,33,33	1.28	6 (18%)	48,52,52	1.95	11 (22%)
21	ATP	M	501	22	32,33,33	2.04	6 (18%)	48,52,52	2.11	14 (29%)
21	ATP	L	401	22	32,33,33	1.43	7 (21%)	48,52,52	1.99	10 (20%)

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	I	501	22	-	3/22/38/38	0/3/3/3
23	ADP	J	501	-	-	4/16/32/32	0/3/3/3
21	ATP	K	501	22	-	4/22/38/38	0/3/3/3
21	ATP	H	501	22	-	5/22/38/38	0/3/3/3
21	ATP	M	501	22	-	5/22/38/38	0/3/3/3
21	ATP	L	401	22	-	5/22/38/38	0/3/3/3

The worst 5 of 37 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	M	501	ATP	PB-O3B	8.05	1.68	1.59
21	K	501	ATP	PB-O3B	5.26	1.65	1.59
23	J	501	ADP	C5-C4	4.57	1.47	1.39
21	K	501	ATP	C5-C4	4.41	1.46	1.39
21	K	501	ATP	PA-O3A	4.39	1.64	1.59

The worst 5 of 72 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	I	501	ATP	C5-C4-N3	-6.39	117.92	126.72
21	L	401	ATP	C5-C4-N3	-5.70	118.87	126.72
23	J	501	ADP	C5-C4-N3	-5.45	119.21	126.72
21	M	501	ATP	N3-C4-N9	5.44	136.42	127.17
21	M	501	ATP	C4-N9-C8	5.37	111.38	105.74

There are no chirality outliers.

5 of 26 torsion outliers are listed below:

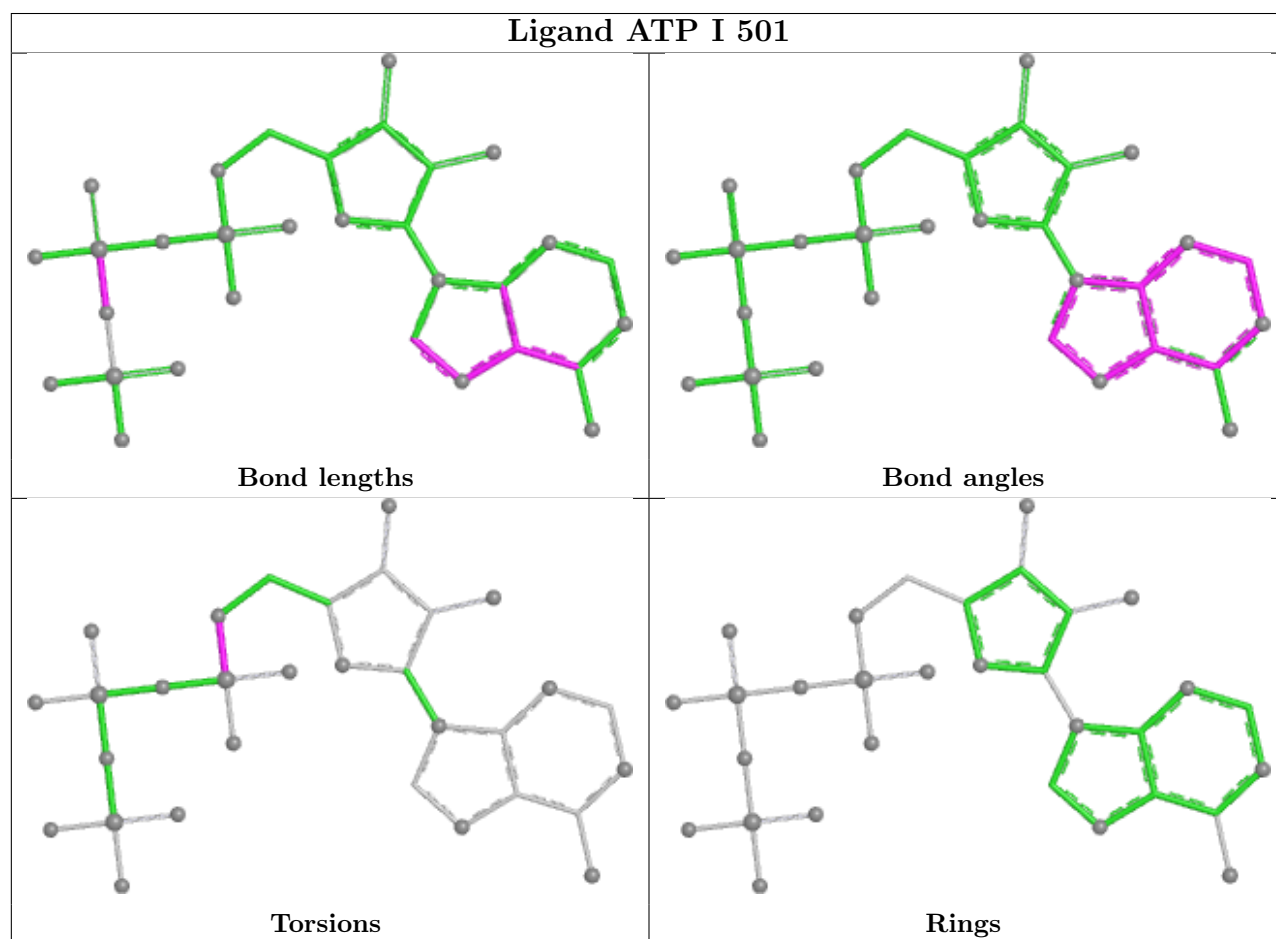
Mol	Chain	Res	Type	Atoms
21	H	501	ATP	C5'-O5'-PA-O1A
21	H	501	ATP	C5'-O5'-PA-O2A
21	H	501	ATP	C5'-O5'-PA-O3A
21	I	501	ATP	C5'-O5'-PA-O1A
21	I	501	ATP	C5'-O5'-PA-O2A

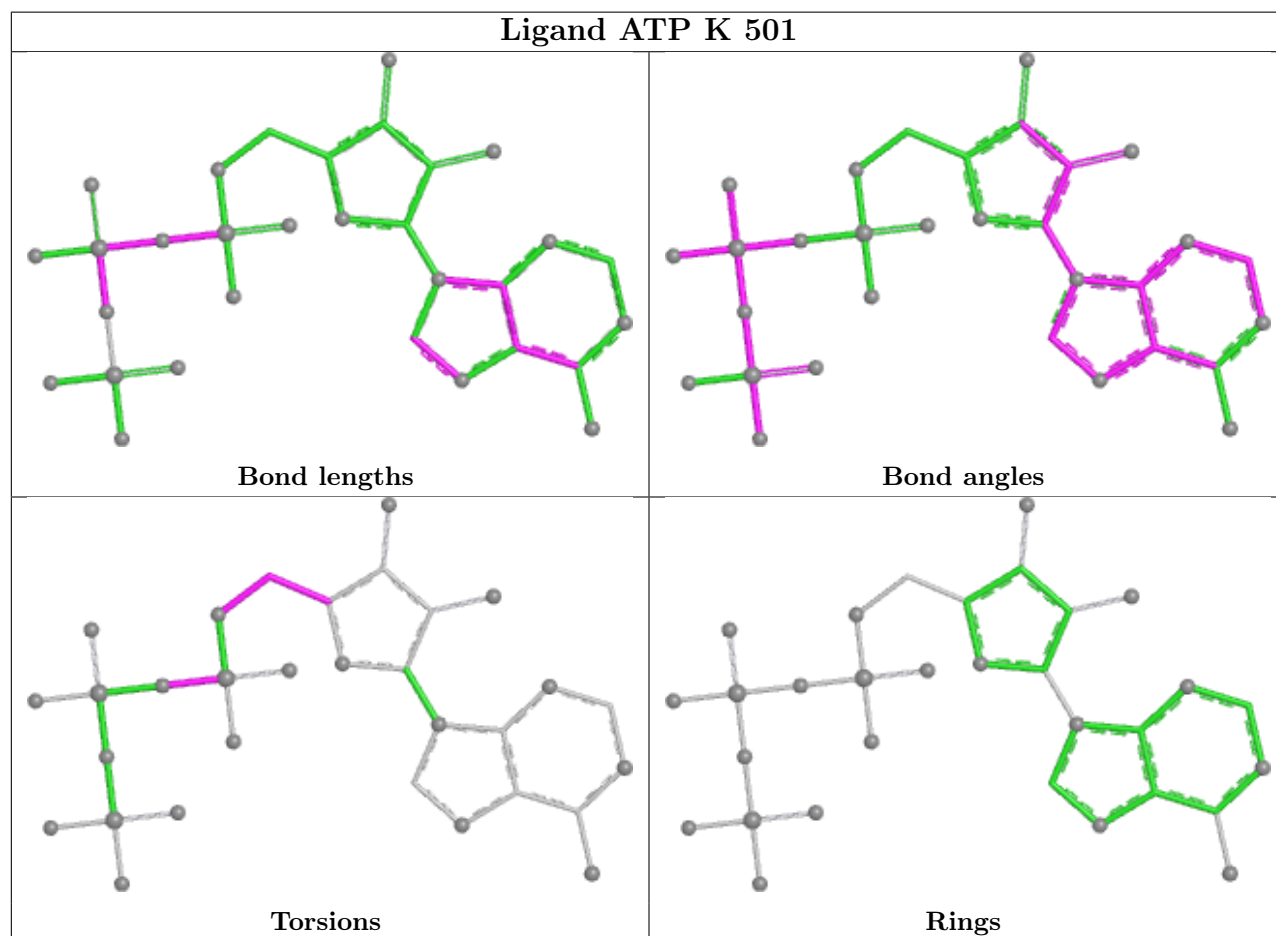
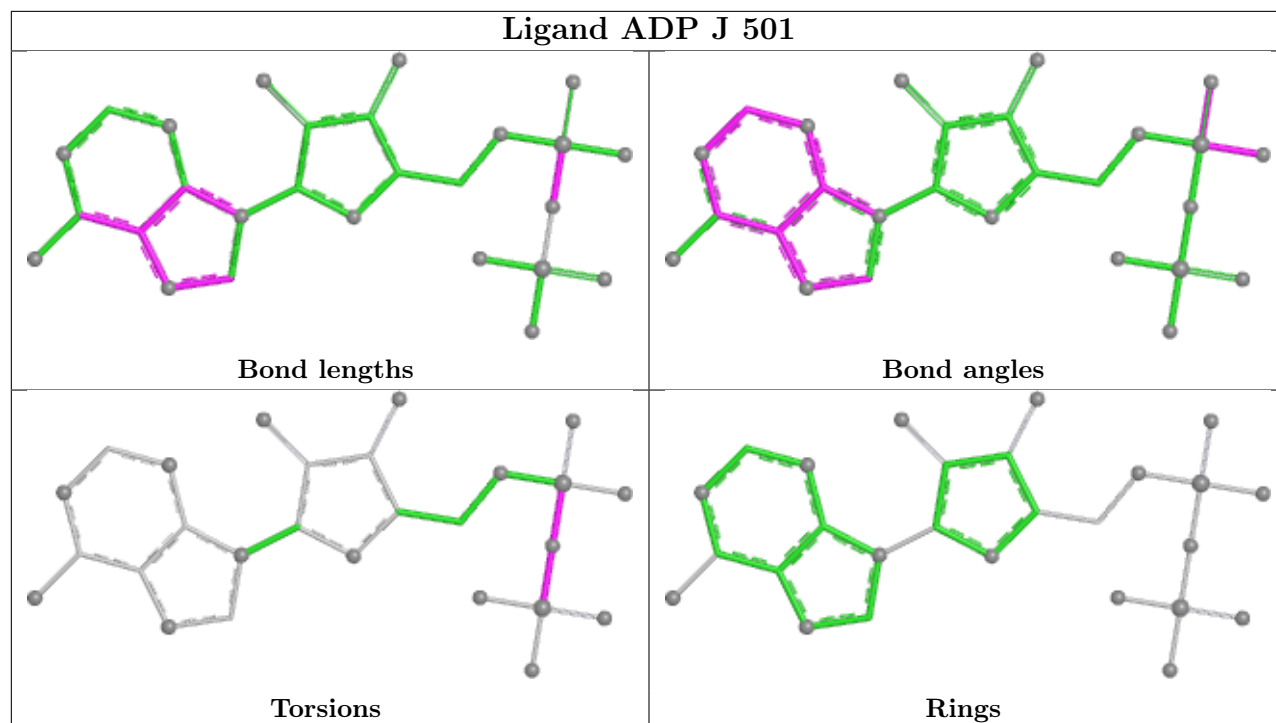
There are no ring outliers.

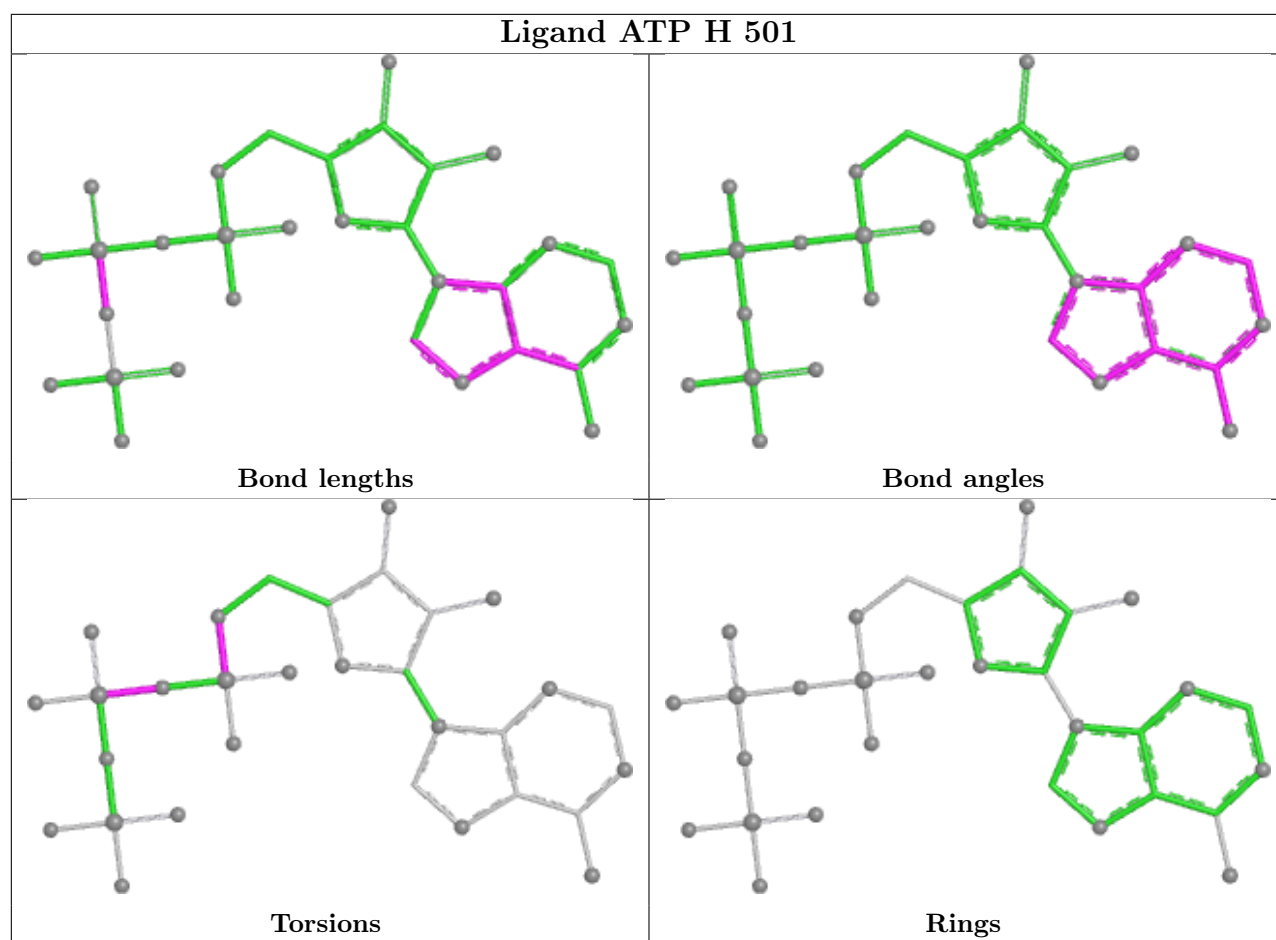
5 monomers are involved in 14 short contacts:

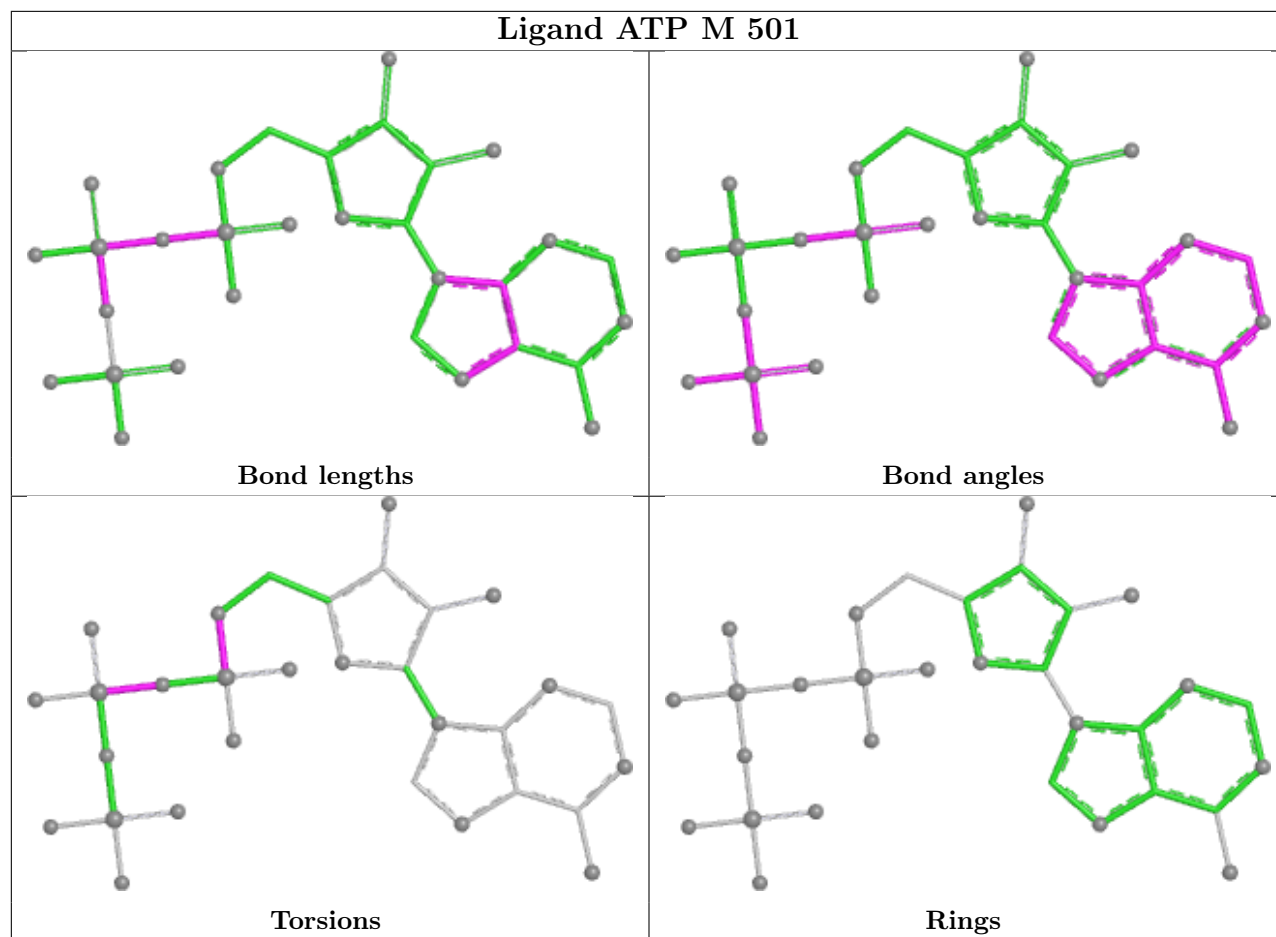
Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	J	501	ADP	2	0
21	K	501	ATP	5	0
21	H	501	ATP	2	0
21	M	501	ATP	4	0
21	L	401	ATP	1	0

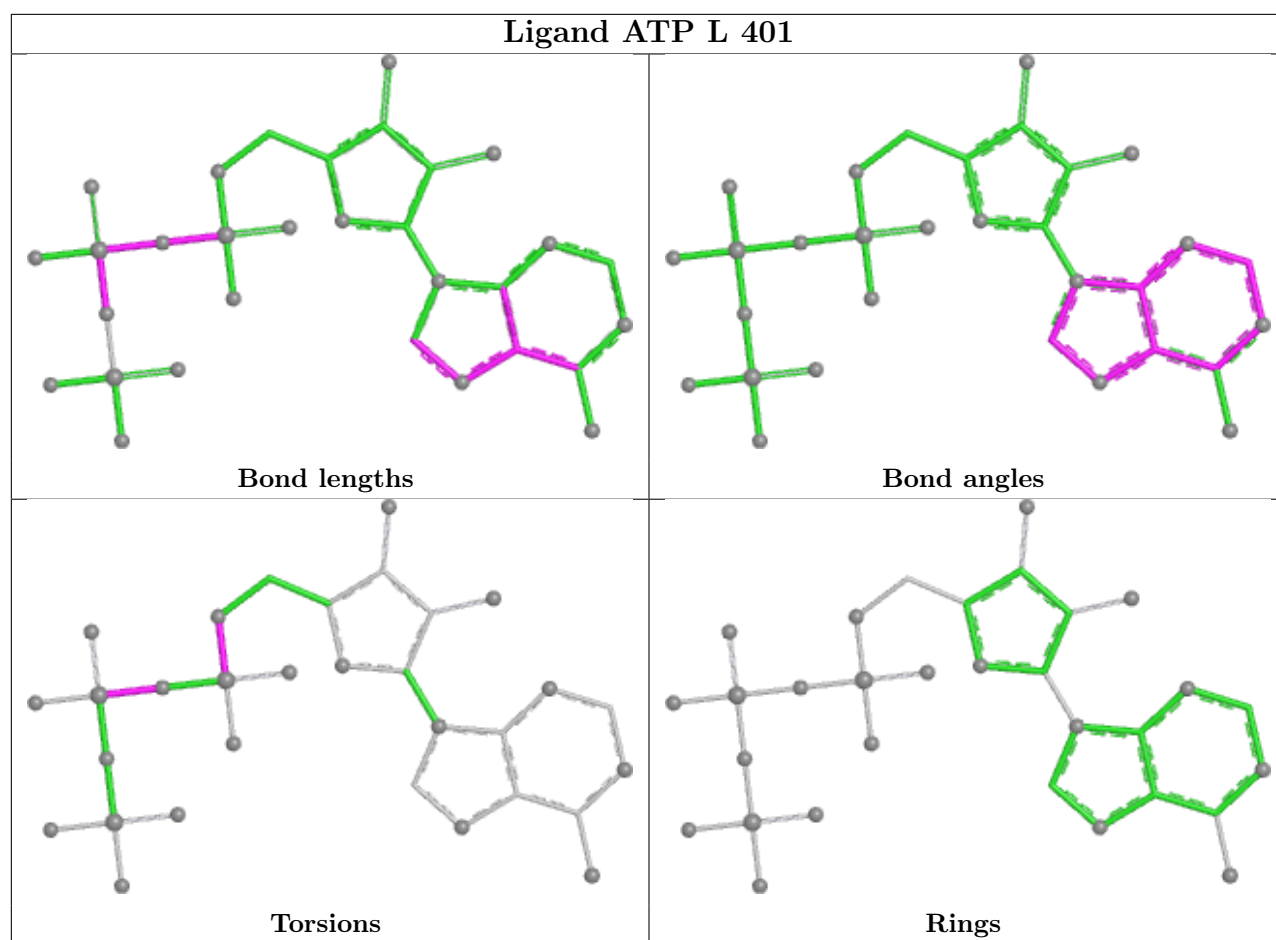
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

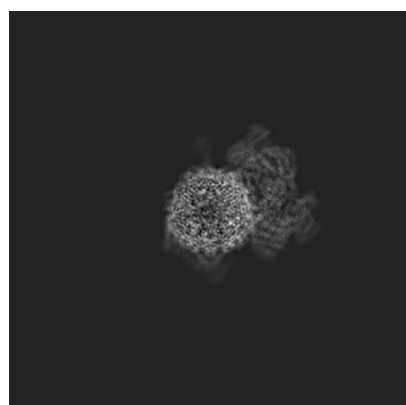
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4002. These allow visual inspection of the internal detail of the map and identification of artifacts.

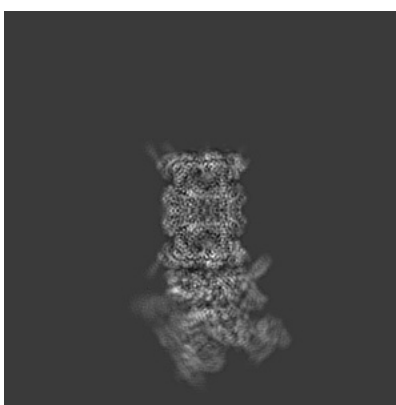
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X



Y

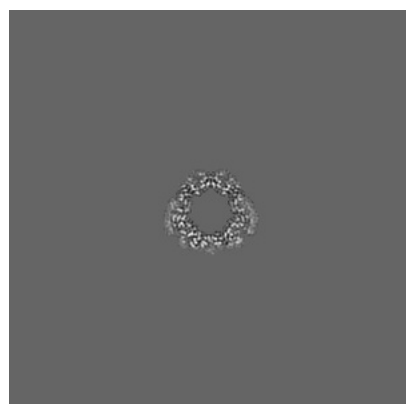


Z

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

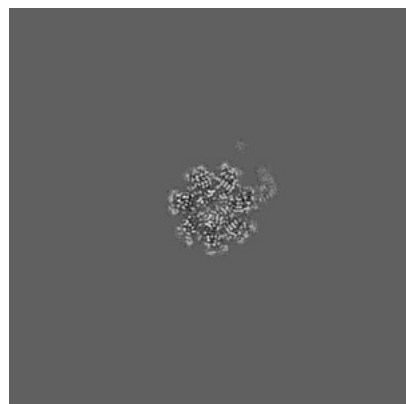


Z Index: 192

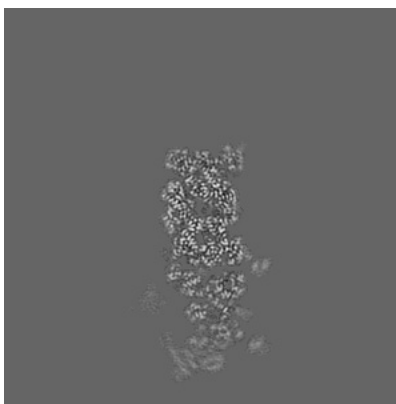
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

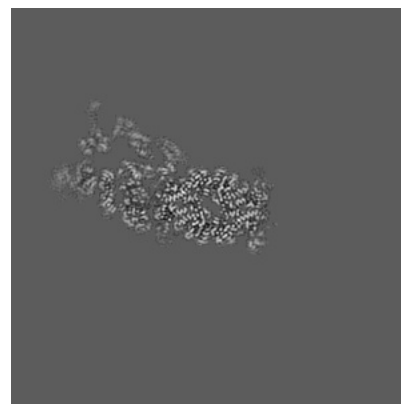
6.3.1 Primary map



X Index: 150



Y Index: 212

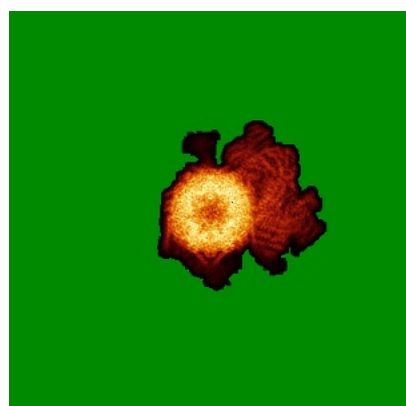


Z Index: 210

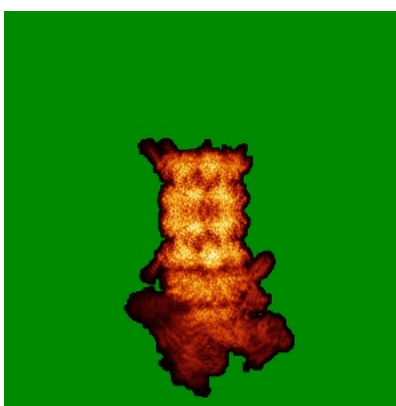
The images above show the largest variance slices of the map in three orthogonal directions.

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

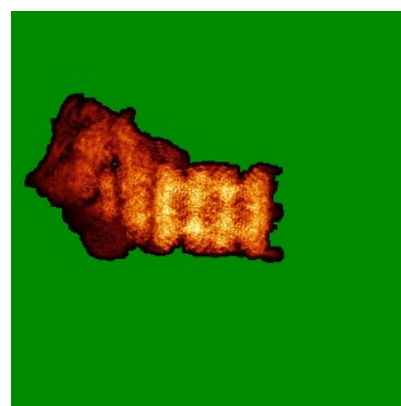
6.4.1 Primary map



X



Y

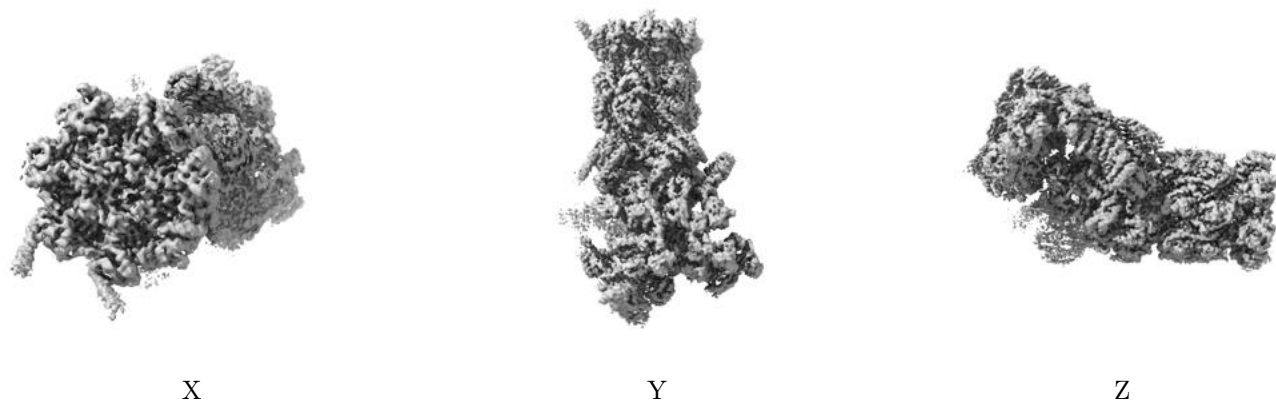


Z

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 0.035. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

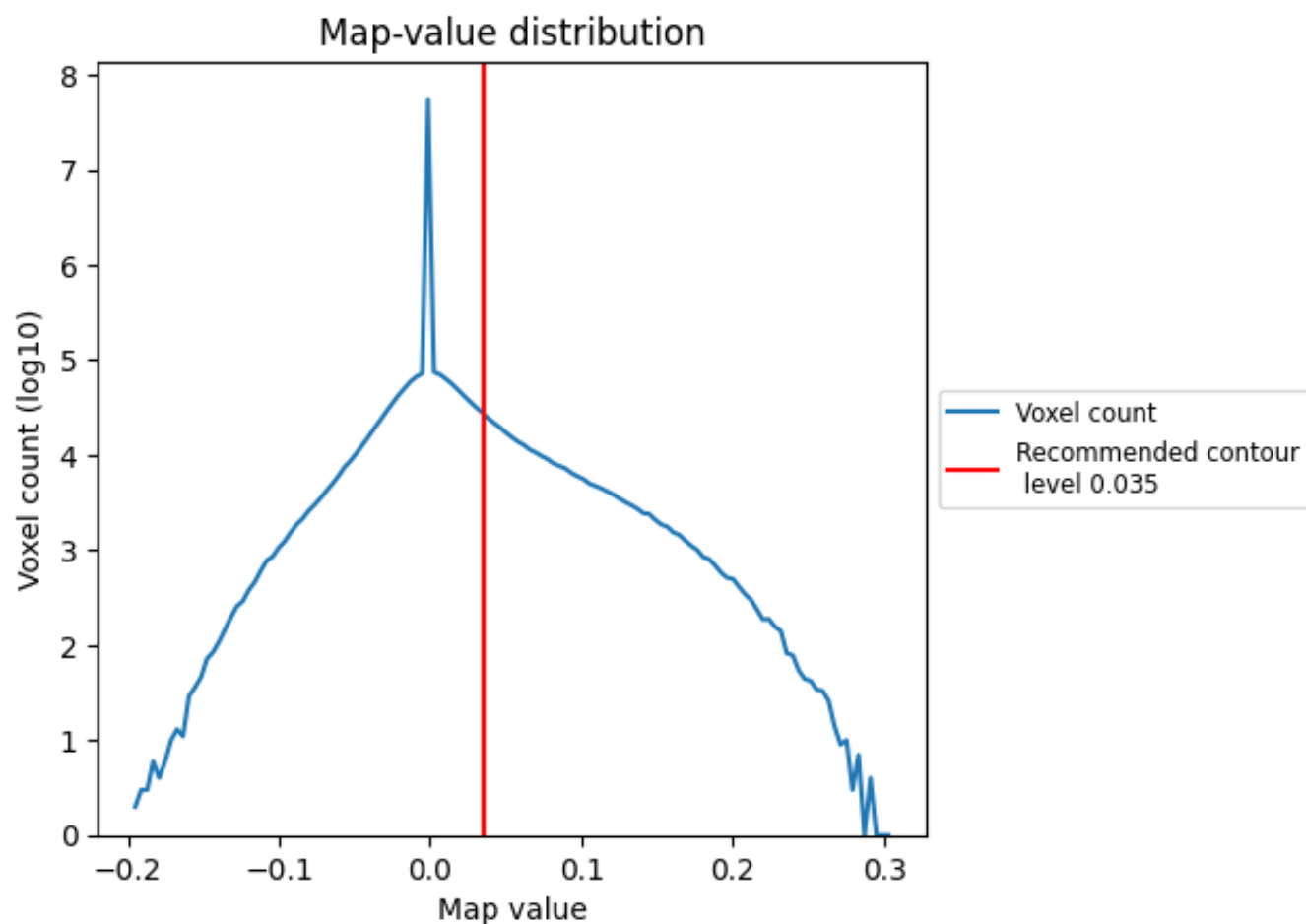
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

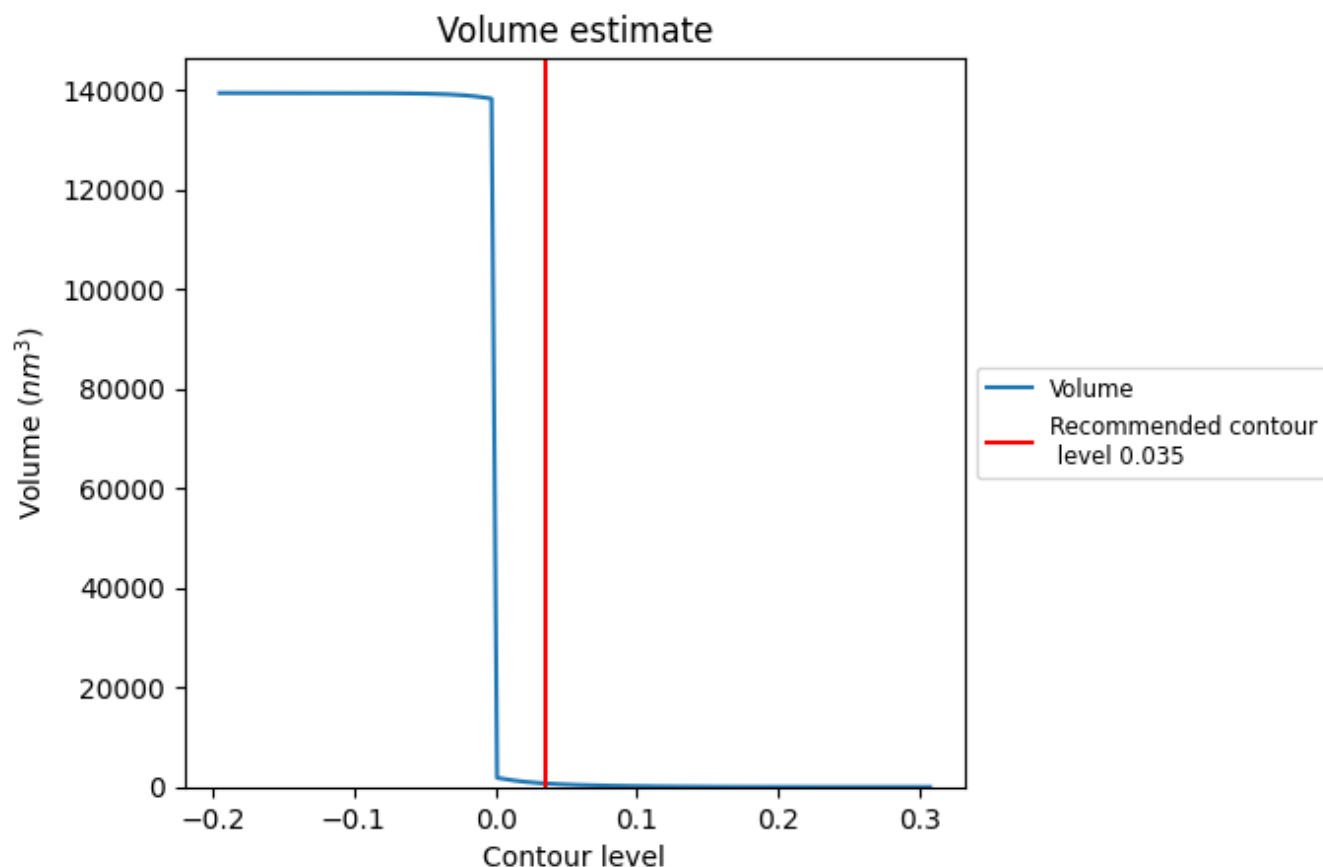
This section contains the results of statistical analysis of the map.

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.

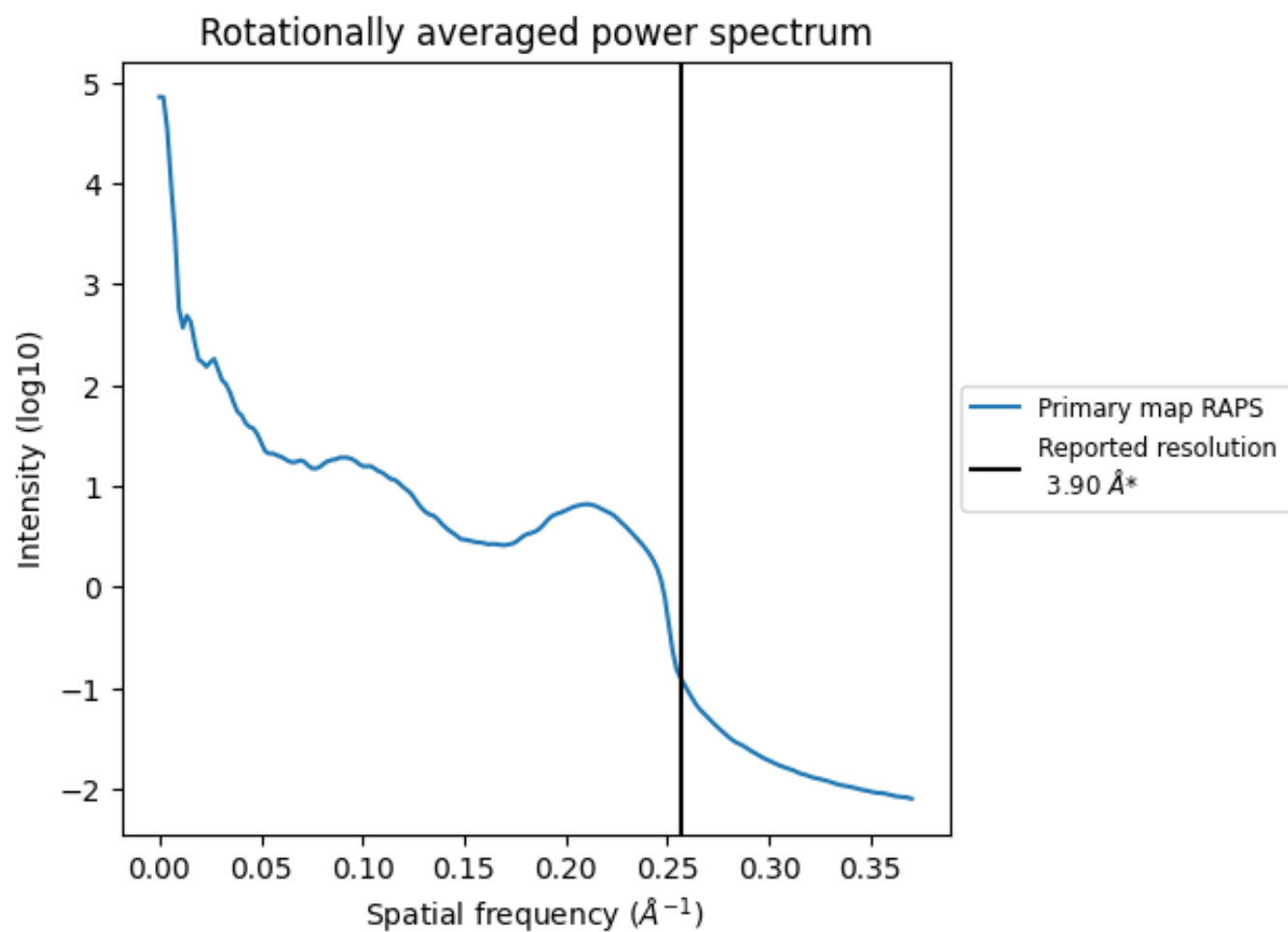
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 708 nm^3 ; this corresponds to an approximate mass of 639 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 0.256 Å⁻¹

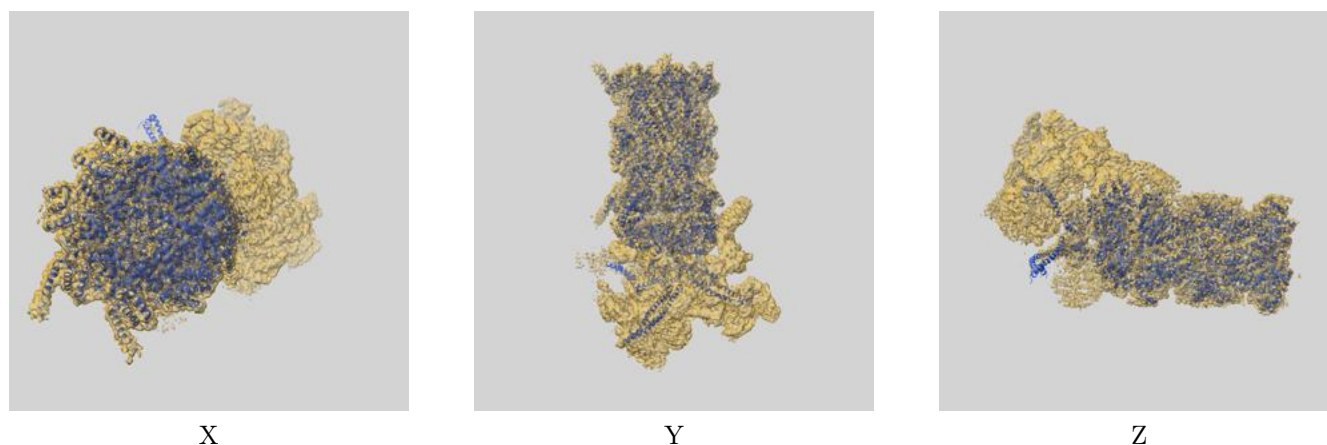
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

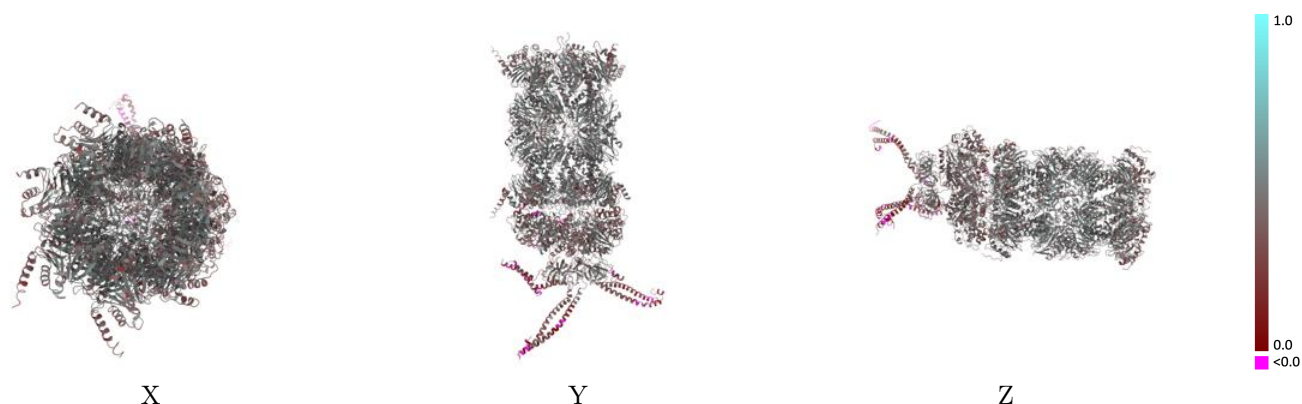
This section contains information regarding the fit between EMDB map EMD-4002 and PDB model 5L4G. Per-residue inclusion information can be found in section [3](#) on page [11](#).

9.1 Map-model overlay [i](#)



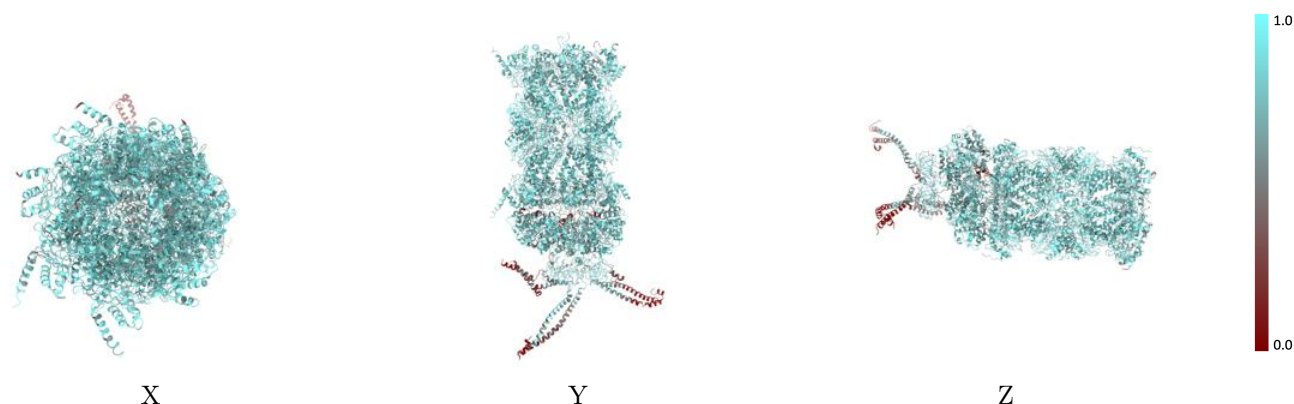
The images above show the 3D surface view of the map at the recommended contour level 0.035 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



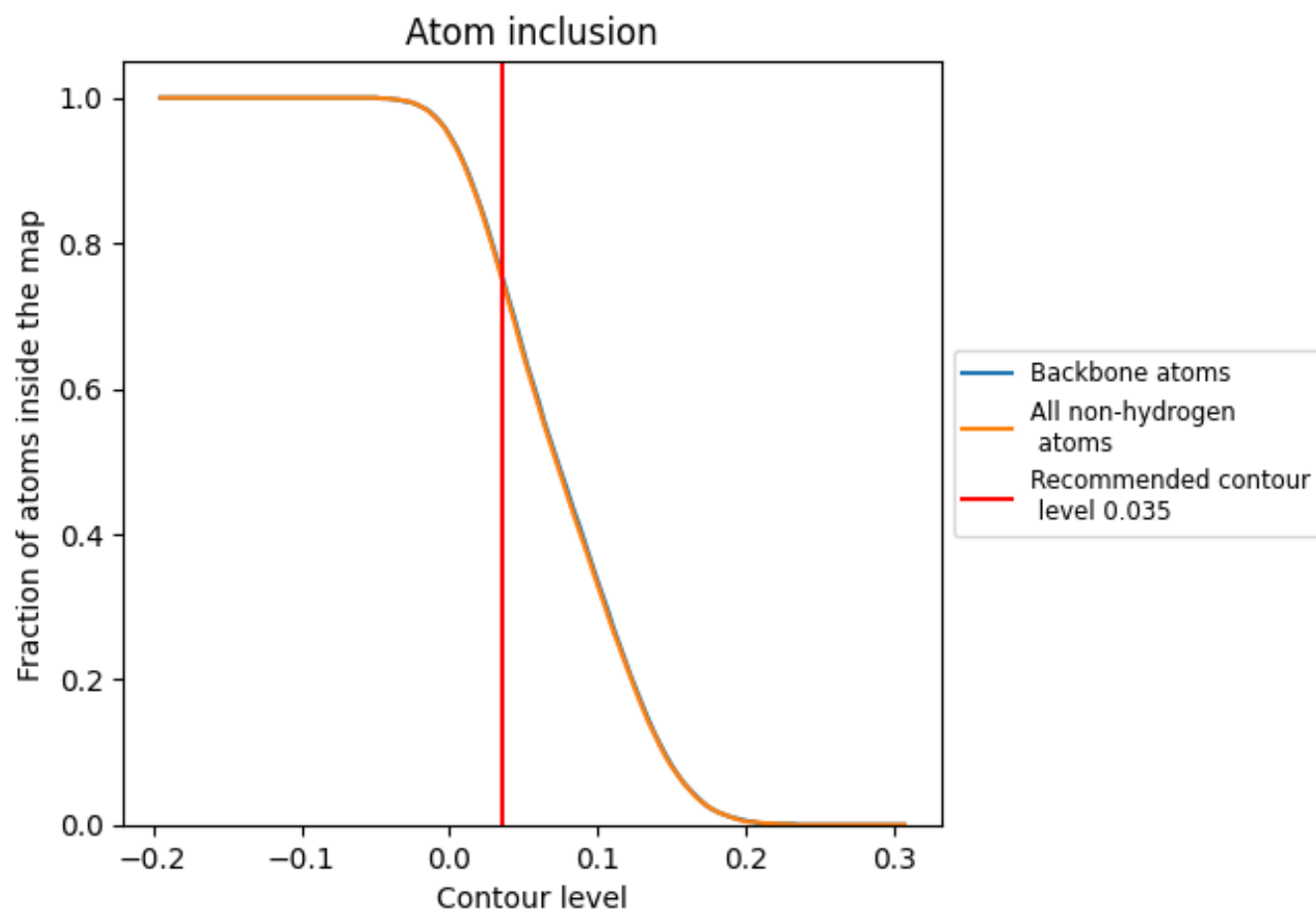
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.035).

9.4 Atom inclusion [i](#)



At the recommended contour level, 76% 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 (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7540	 0.4280
1	 0.8250	 0.4670
2	 0.8250	 0.4610
3	 0.8100	 0.4630
4	 0.8540	 0.4740
5	 0.8500	 0.4690
6	 0.8290	 0.4660
7	 0.8100	 0.4540
8	 0.8330	 0.4580
A	 0.7940	 0.4470
B	 0.7860	 0.4420
C	 0.8010	 0.4430
D	 0.7930	 0.4420
E	 0.7970	 0.4570
F	 0.8170	 0.4560
G	 0.8080	 0.4480
H	 0.6880	 0.3810
I	 0.6440	 0.3490
J	 0.6680	 0.3620
K	 0.6610	 0.3600
L	 0.6690	 0.3700
M	 0.6540	 0.3800
N	 0.7690	 0.4300
O	 0.7830	 0.4370
P	 0.7810	 0.4340
Q	 0.7770	 0.4240
R	 0.7640	 0.4320
S	 0.7880	 0.4380
T	 0.7770	 0.4290
U	 0.8130	 0.4580
V	 0.8190	 0.4560
W	 0.8120	 0.4660
X	 0.8470	 0.4690
Y	 0.8430	 0.4690
Z	 0.8180	 0.4690

