



wwPDB EM Validation Summary Report ⓘ

Apr 20, 2026 – 10:25 PM JST

PDB ID : 9K5E / pdb_00009k5e
EMDB ID : EMD-62090
Title : Structure of substrate-engaged double-cap human proteasome in state EA1-EA1
Authors : Wu, Z.; Chen, E.; Mao, Y.
Deposited on : 2024-10-21
Resolution : 3.80 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 : 1.8.5 (274361), CSD as541be (2020)
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

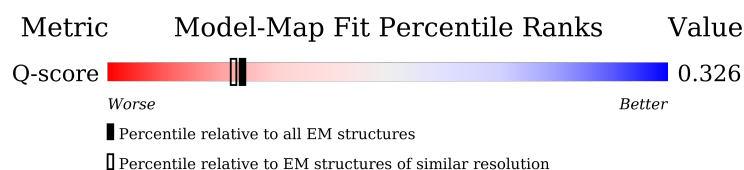
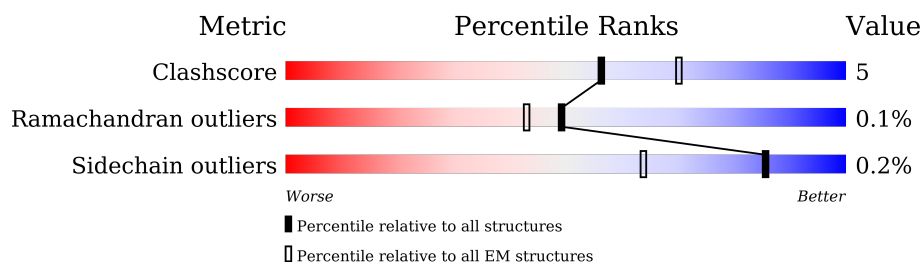
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 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.





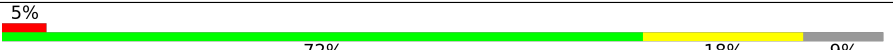
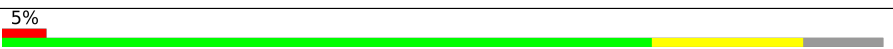

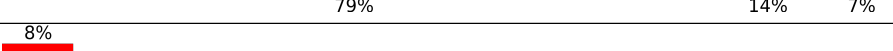
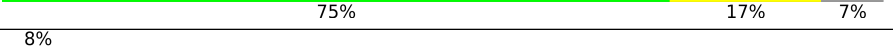


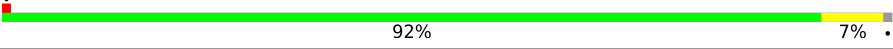


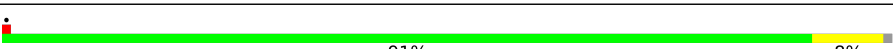


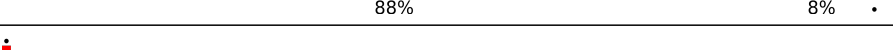








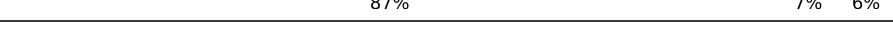
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10198 (3.30 - 4.30)

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	AA	433	
1	BA	433	
2	AB	440	
2	BB	440	

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Mol	Chain	Length	Quality of chain
3	AC	398	
3	BC	398	
4	AD	418	
4	BD	418	
5	AE	403	
5	BE	403	
6	AF	439	
6	BF	439	
7	AG	246	
7	BG	246	
8	AH	234	
8	BH	234	
9	AI	261	
9	BI	261	
10	AJ	248	
10	BJ	248	
11	AK	241	
11	BK	241	
12	AL	263	
12	BL	263	
13	AM	255	
13	BM	255	
14	AN	239	
14	BN	239	
15	AO	277	

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Mol	Chain	Length	Quality of chain
15	BO	277	
16	AP	205	
16	BP	205	
17	AQ	201	
17	BQ	201	
18	AR	263	
18	BR	263	
19	AS	241	
19	BS	241	
20	AT	264	
20	BT	264	
21	AU	953	
21	BU	953	
22	AV	534	
22	BV	534	
23	AW	456	
23	BW	456	
24	AX	422	
24	BX	422	
25	AY	389	
25	BY	389	
26	AZ	324	
26	BZ	324	
27	Aa	376	
27	Ba	376	

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Mol	Chain	Length	Quality of chain
28	Ab	377	
28	Bb	377	
29	Ac	310	
29	Bc	310	
30	Ad	350	
30	Bd	350	
31	Ae	70	
31	Be	70	
32	Af	908	
32	Bf	908	
33	Au	76	
33	Aw	76	
33	Bu	76	
33	Bw	76	

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 164552 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 26S proteasome regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AA	413	Total	C	N	O	S	0	0
			3240	2042	567	613	18		
1	BA	413	Total	C	N	O	S	0	0
			3240	2042	567	613	18		

- Molecule 2 is a protein called 26S proteasome regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AB	388	Total	C	N	O	S	0	0
			3042	1915	519	593	15		
2	BB	388	Total	C	N	O	S	0	0
			3042	1915	519	593	15		

- Molecule 3 is a protein called 26S proteasome regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	AC	363	Total	C	N	O	S	0	0
			2864	1808	515	525	16		
3	BC	363	Total	C	N	O	S	0	0
			2864	1808	515	525	16		

- Molecule 4 is a protein called 26S proteasome regulatory subunit 6B.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	AD	380	Total	C	N	O	S	0	0
			3039	1923	524	579	13		
4	BD	380	Total	C	N	O	S	0	0
			3039	1923	524	579	13		

- Molecule 5 is a protein called Proteasome 26S subunit, ATPase 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AE	375	Total	C	N	O	S	0	0
			2860	1796	512	536	16		
5	BE	375	Total	C	N	O	S	0	0
			2860	1796	512	536	16		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AF	376	Total	C	N	O	S	0	0
			2858	1802	496	545	15		
6	BF	376	Total	C	N	O	S	0	0
			2858	1802	496	545	15		

- Molecule 7 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AG	244	Total	C	N	O	S	0	0
			1889	1198	316	362	13		
7	BG	244	Total	C	N	O	S	0	0
			1889	1198	316	362	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	AH	232	Total	C	N	O	S	0	0
			1809	1155	306	342	6		
8	BH	232	Total	C	N	O	S	0	0
			1809	1155	306	342	6		

- Molecule 9 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AI	250	Total	C	N	O	S	1	0
			1954	1233	335	376	10		
9	BI	250	Total	C	N	O	S	1	0
			1954	1233	335	376	10		

- Molecule 10 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AJ	239	Total	C	N	O	S	0	0
			1858	1165	327	361	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	BJ	239	Total	C	N	O	S	0	0
			1858	1165	327	361	5		

- Molecule 11 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AK	234	Total	C	N	O	S	0	0
			1773	1115	295	352	11		
11	BK	234	Total	C	N	O	S	0	0
			1773	1115	295	352	11		

- Molecule 12 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AL	238	Total	C	N	O	S	0	0
			1866	1169	336	350	11		
12	BL	238	Total	C	N	O	S	0	0
			1866	1169	336	350	11		

- Molecule 13 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AM	240	Total	C	N	O	S	1	0
			1879	1193	321	353	12		
13	BM	240	Total	C	N	O	S	1	0
			1879	1193	321	353	12		

- Molecule 14 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AN	202	Total	C	N	O	S	0	0
			1514	949	258	295	12		
14	BN	202	Total	C	N	O	S	0	0
			1514	949	258	295	12		

- Molecule 15 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AO	220	Total	C	N	O	S	0	0
			1649	1038	279	320	12		
15	BO	220	Total	C	N	O	S	0	0
			1649	1038	279	320	12		

- Molecule 16 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AP	204	Total	C	N	O	S	0	0
			1587	1010	264	294	19		
16	BP	204	Total	C	N	O	S	0	0
			1587	1010	264	294	19		

- Molecule 17 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	AQ	199	Total	C	N	O	S	0	0
			1588	1017	270	292	9		
17	BQ	199	Total	C	N	O	S	0	0
			1588	1017	270	292	9		

- Molecule 18 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	AR	201	Total	C	N	O	S	0	0
			1559	982	274	294	9		
18	BR	201	Total	C	N	O	S	0	0
			1559	982	274	294	9		

- Molecule 19 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AS	213	Total	C	N	O	S	0	0
			1641	1041	281	309	10		
19	BS	213	Total	C	N	O	S	0	0
			1641	1041	281	309	10		

- Molecule 20 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AT	216	Total	C	N	O	S	0	0
			1683	1062	291	318	12		
20	BT	216	Total	C	N	O	S	0	0
			1683	1062	291	318	12		

- Molecule 21 is a protein called 26S proteasome non-ATPase regulatory subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	AU	868	Total	C	N	O	S	0	0
			6787	4303	1153	1285	46		
21	BU	868	Total	C	N	O	S	0	0
			6787	4303	1153	1285	46		

- Molecule 22 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	AV	472	Total	C	N	O	S	0	0
			3754	2387	673	681	13		
22	BV	472	Total	C	N	O	S	0	0
			3754	2387	673	681	13		

- Molecule 23 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	AW	441	Total	C	N	O	S	0	0
			3596	2277	613	682	24		
23	BW	441	Total	C	N	O	S	0	0
			3596	2277	613	682	24		

- Molecule 24 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	AX	422	Total	C	N	O	S	0	0
			3335	2116	567	639	13		
24	BX	422	Total	C	N	O	S	0	0
			3335	2116	567	639	13		

- Molecule 25 is a protein called 26S proteasome non-ATPase regulatory subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	AY	389	Total	C	N	O	S	0	0
			3202	2041	545	598	18		
25	BY	389	Total	C	N	O	S	0	0
			3202	2041	545	598	18		

- Molecule 26 is a protein called 26S proteasome non-ATPase regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	AZ	286	Total	C	N	O	S	0	0
			2281	1457	392	427	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
26	BZ	286	Total	C	N	O	S	0	0
			2281	1457	392	427	5		

- Molecule 27 is a protein called 26S proteasome non-ATPase regulatory subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Aa	373	Total	C	N	O	S	0	0
			2995	1911	510	559	15		
27	Ba	373	Total	C	N	O	S	0	0
			2995	1911	510	559	15		

- Molecule 28 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Ab	191	Total	C	N	O	S	0	0
			1458	910	261	279	8		
28	Bb	191	Total	C	N	O	S	0	0
			1458	910	261	279	8		

- Molecule 29 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Ac	287	Total	C	N	O	S	0	0
			2260	1430	389	422	19		
29	Bc	287	Total	C	N	O	S	0	0
			2260	1430	389	422	19		

- Molecule 30 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Ad	257	Total	C	N	O	S	0	0
			2116	1371	346	390	9		
30	Bd	257	Total	C	N	O	S	0	0
			2116	1371	346	390	9		

- Molecule 31 is a protein called 26S proteasome complex subunit SEM1.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	Ae	50	Total	C	N	O	0	0
			425	260	65	100		
31	Be	50	Total	C	N	O	0	0
			425	260	65	100		

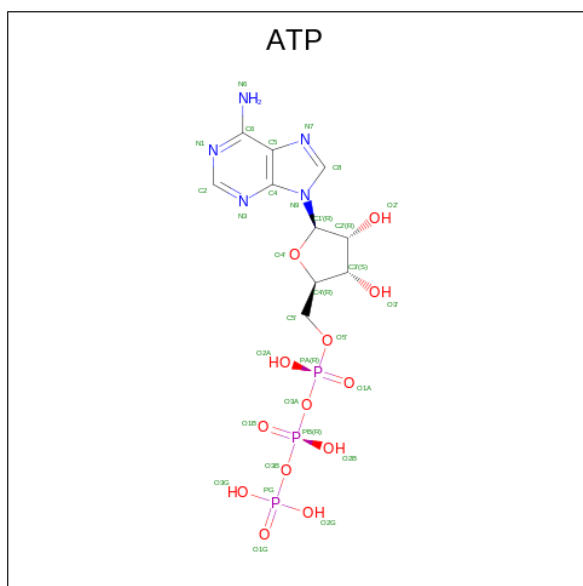
- Molecule 32 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Af	844	Total	C	N	O	S	0	0
			6529	4126	1108	1250	45		
32	Bf	844	Total	C	N	O	S	0	0
			6529	4126	1108	1250	45		

- Molecule 33 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Au	76	Total	C	N	O	S	0	0
			601	378	105	117	1		
33	Aw	76	Total	C	N	O	S	0	0
			601	378	105	117	1		
33	Bu	76	Total	C	N	O	S	0	0
			601	378	105	117	1		
33	Bw	76	Total	C	N	O	S	0	0
			601	378	105	117	1		

- Molecule 34 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
34	AA	1	Total	C	N	O	P	0
			31	10	5	13	3	
34	AB	1	Total	C	N	O	P	0
			31	10	5	13	3	

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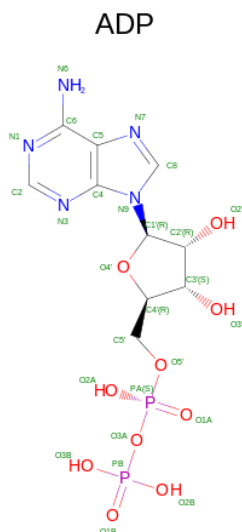
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Mol	Chain	Residues	Atoms					AltConf
34	AD	1	Total	C	N	O	P	0
			31	10	5	13	3	
34	AE	1	Total	C	N	O	P	0
			31	10	5	13	3	
34	BA	1	Total	C	N	O	P	0
			31	10	5	13	3	
34	BB	1	Total	C	N	O	P	0
			31	10	5	13	3	
34	BD	1	Total	C	N	O	P	0
			31	10	5	13	3	
34	BE	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 35 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
35	AA	1	Total	Mg	0
			1	1	
35	AB	1	Total	Mg	0
			1	1	
35	AD	1	Total	Mg	0
			1	1	
35	AE	1	Total	Mg	0
			1	1	
35	AF	1	Total	Mg	0
			1	1	
35	BA	1	Total	Mg	0
			1	1	
35	BB	1	Total	Mg	0
			1	1	
35	BD	1	Total	Mg	0
			1	1	
35	BE	1	Total	Mg	0
			1	1	
35	BF	1	Total	Mg	0
			1	1	

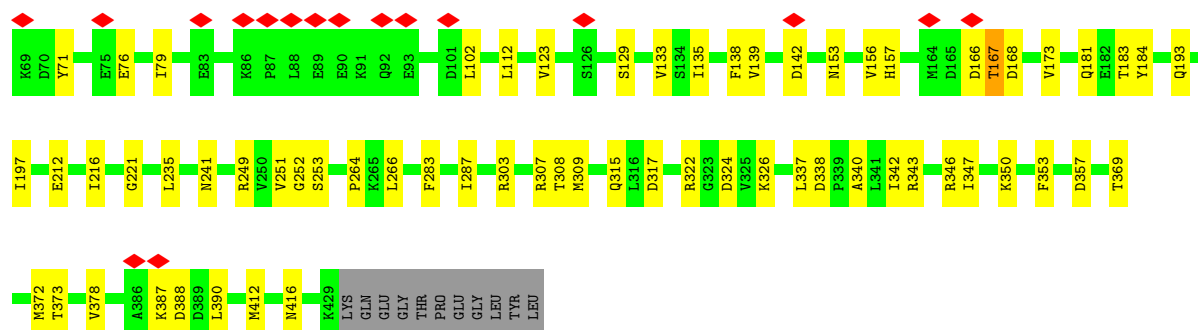
- Molecule 36 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).



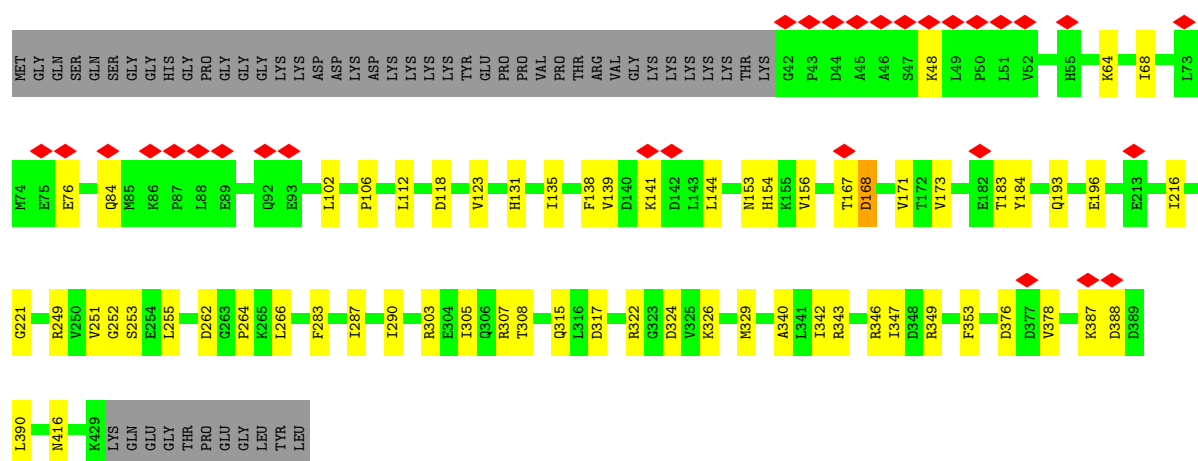
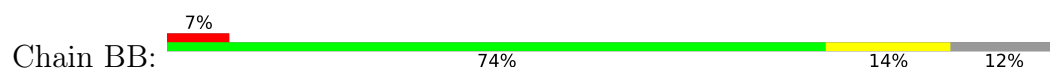
Mol	Chain	Residues	Atoms					AltConf
36	AC	1	Total 27	C 10	N 5	O 10	P 2	0
36	AF	1	Total 27	C 10	N 5	O 10	P 2	0
36	BC	1	Total 27	C 10	N 5	O 10	P 2	0
36	BF	1	Total 27	C 10	N 5	O 10	P 2	0

- Molecule 37 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

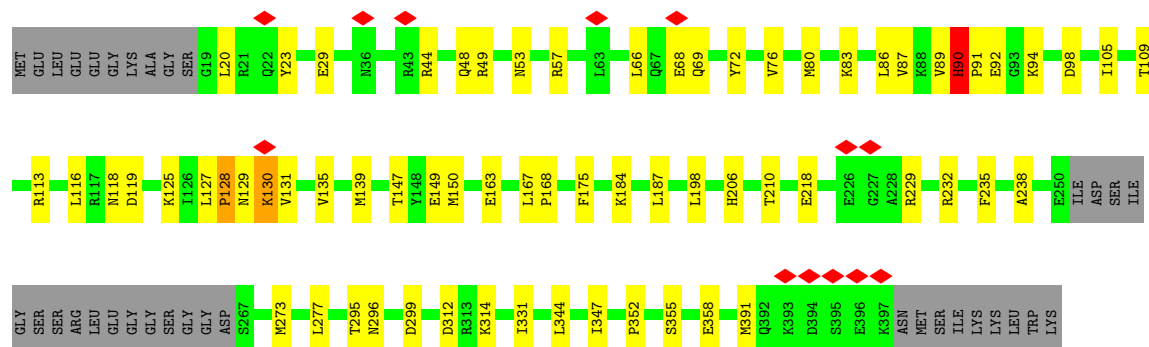
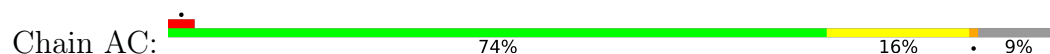
Mol	Chain	Residues	Atoms	AltConf
37	Ac	1	Total Zn 1 1	0
37	Bc	1	Total Zn 1 1	0



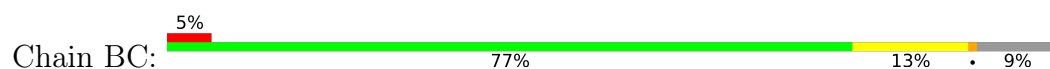
• Molecule 2: 26S proteasome regulatory subunit 4

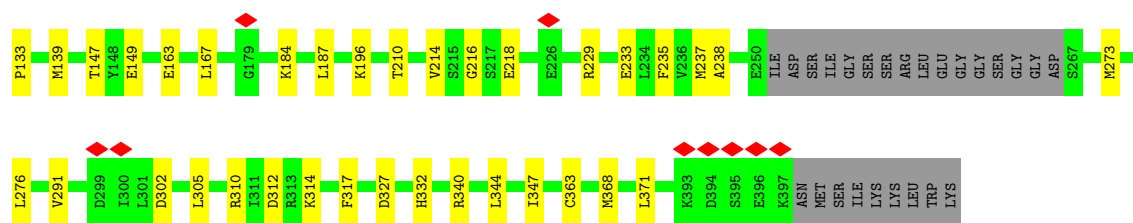


• Molecule 3: 26S proteasome regulatory subunit 8

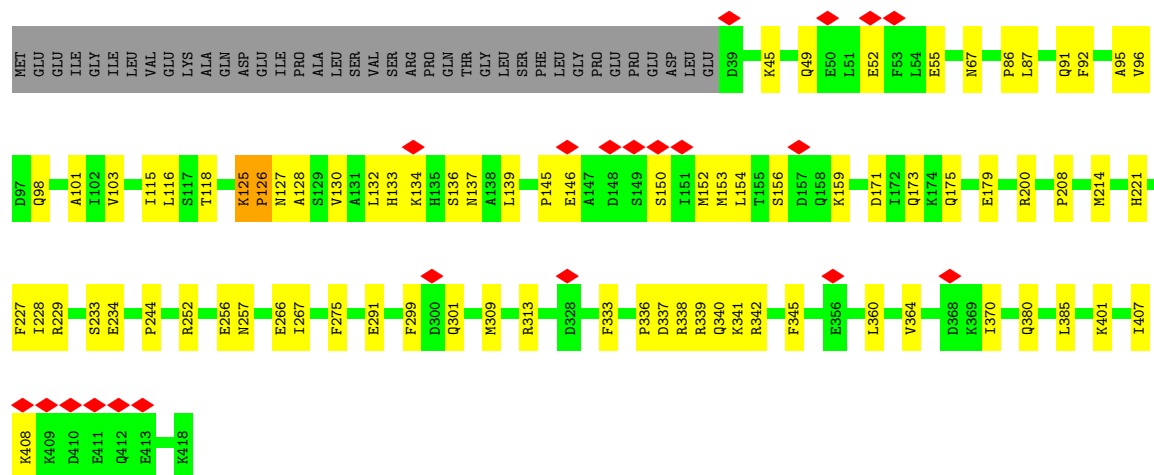
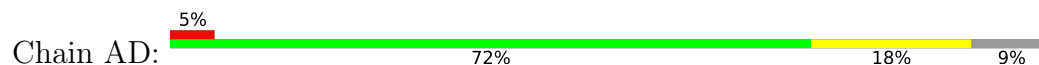


• Molecule 3: 26S proteasome regulatory subunit 8

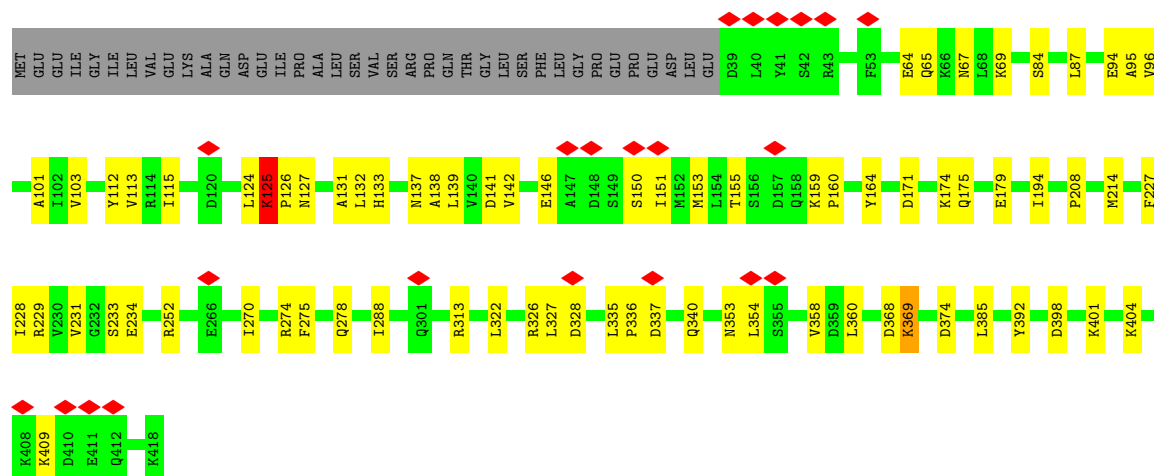
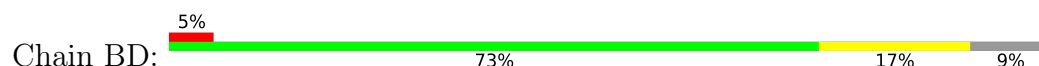




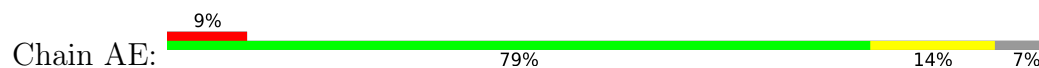
• Molecule 4: 26S proteasome regulatory subunit 6B

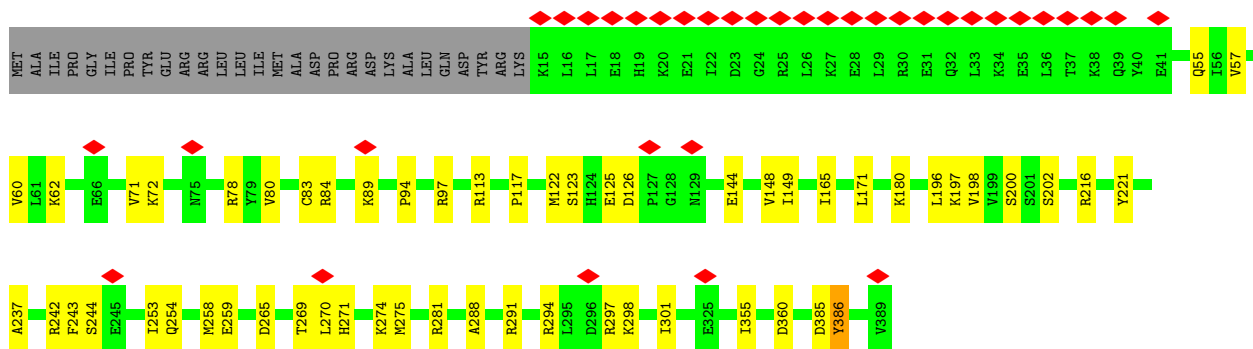


• Molecule 4: 26S proteasome regulatory subunit 6B

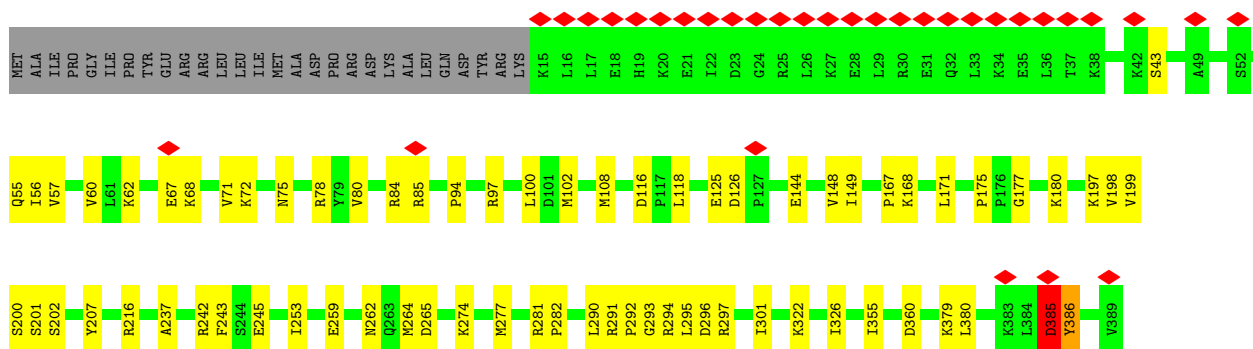
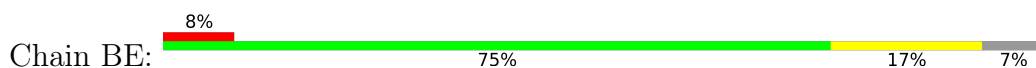


• Molecule 5: Proteasome 26S subunit, ATPase 6

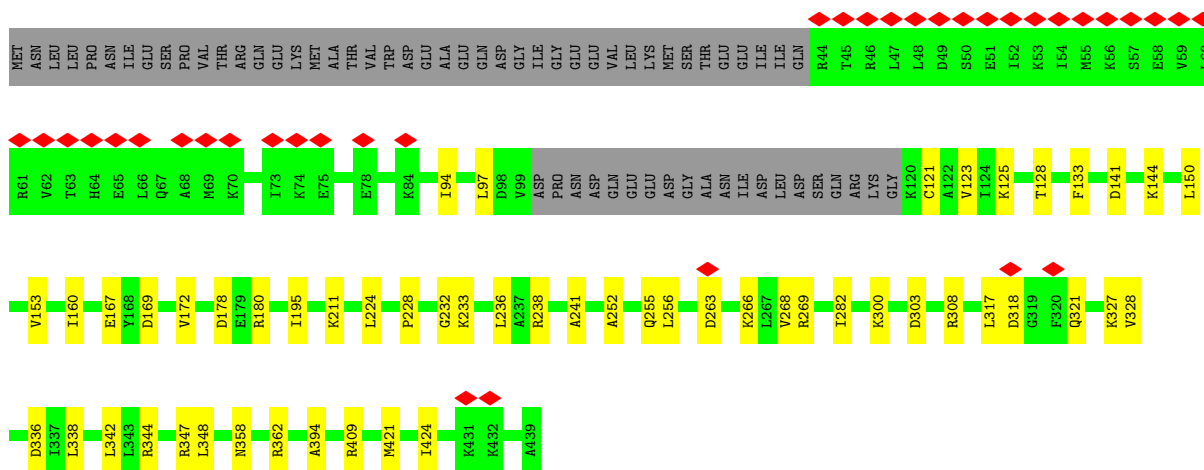
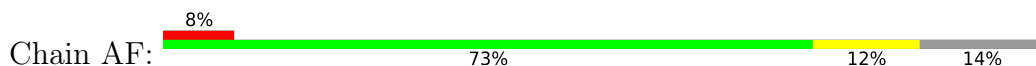




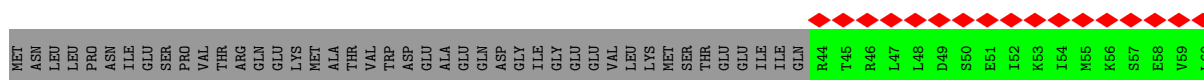
• Molecule 5: Proteasome 26S subunit, ATPase 6

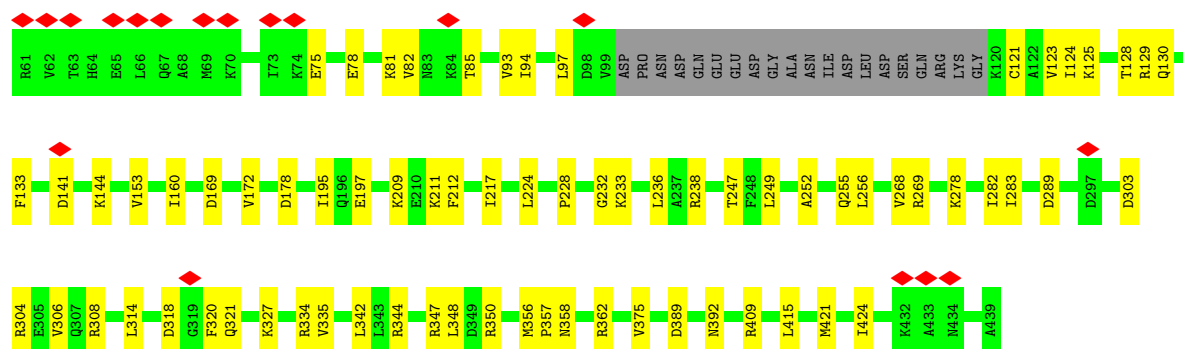


• Molecule 6: 26S proteasome regulatory subunit 6A

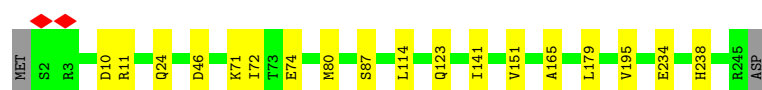


• Molecule 6: 26S proteasome regulatory subunit 6A





- Molecule 7: Proteasome subunit alpha type-6



- Molecule 7: Proteasome subunit alpha type-6



- Molecule 8: Proteasome subunit alpha type-2




- Molecule 8: Proteasome subunit alpha type-2

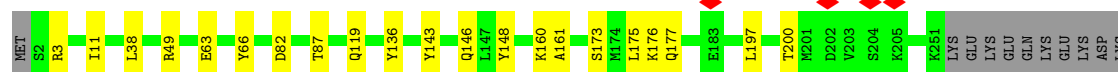


- Molecule 9: Proteasome subunit alpha type-4



- Molecule 9: Proteasome subunit alpha type-4

Chain BI:  88% 8%




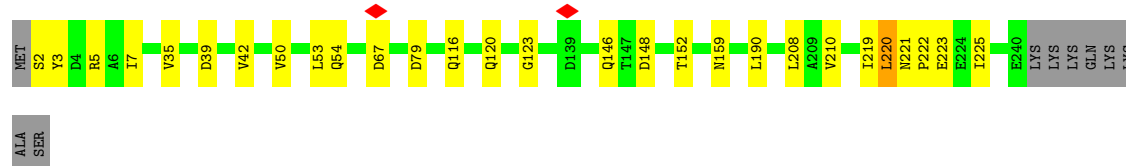
- Molecule 10: Proteasome subunit alpha type-7

Chain AJ:  88% 8%




- Molecule 10: Proteasome subunit alpha type-7

Chain BJ:  85% 11%



- Molecule 11: Proteasome subunit alpha type-5

Chain AK:  88% 9%



- Molecule 11: Proteasome subunit alpha type-5

Chain BK:  89% 8%




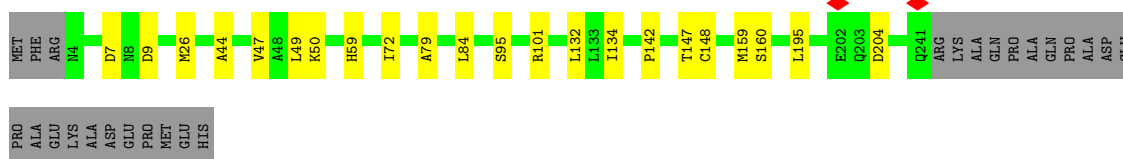
- Molecule 12: Proteasome subunit alpha type-1

Chain AL:  86% 5% 10%



- Molecule 12: Proteasome subunit alpha type-1

Chain BL:  82% 8% 10%



- Molecule 13: Proteasome subunit alpha type-3

Chain AM: 86% 8% 6%



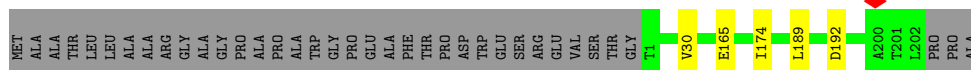
- Molecule 13: Proteasome subunit alpha type-3

Chain BM: 87% 7% 6%



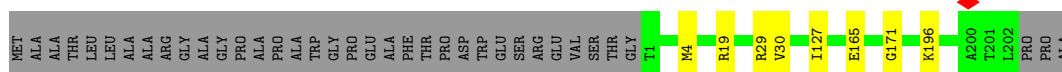
- Molecule 14: Proteasome subunit beta type-6

Chain AN: 82% 15%



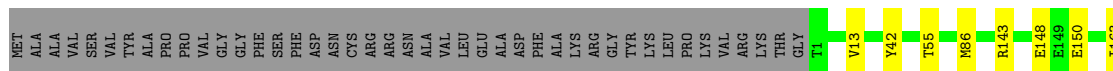
- Molecule 14: Proteasome subunit beta type-6

Chain BN: 81% 15%



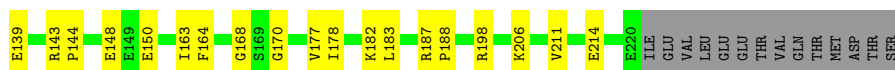
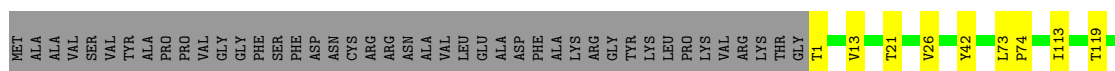
- Molecule 15: Proteasome subunit beta type-7

Chain AO: 74% 5% 21%



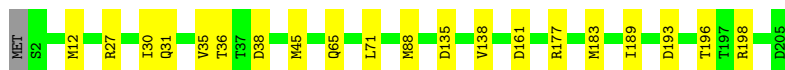
- Molecule 15: Proteasome subunit beta type-7

Chain BO: 69% 10% 21%



• Molecule 16: Proteasome subunit beta type-3

Chain AP: 90% 10%



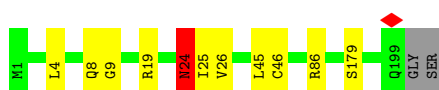
• Molecule 16: Proteasome subunit beta type-3

Chain BP: 90% 9%



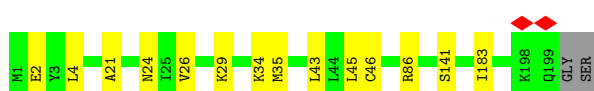
• Molecule 17: Proteasome subunit beta type-2

Chain AQ: 94% 5%



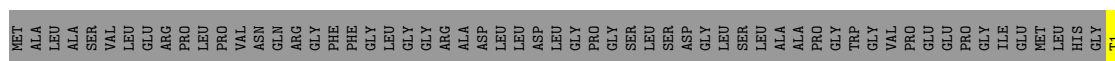
• Molecule 17: Proteasome subunit beta type-2

Chain BQ: 92% 7%



• Molecule 18: Proteasome subunit beta type-5

Chain AR: 72% 24%



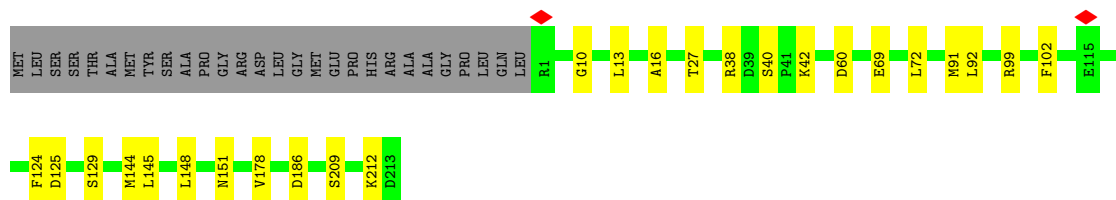
• Molecule 18: Proteasome subunit beta type-5

Chain BR: 71% 5% 24%



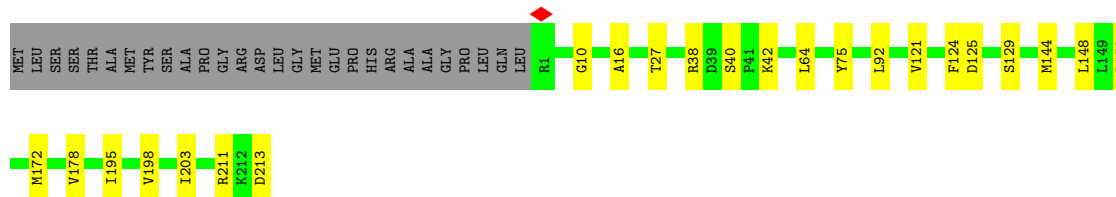
- Molecule 19: Proteasome subunit beta type-1

Chain AS: 78% 11% 12%



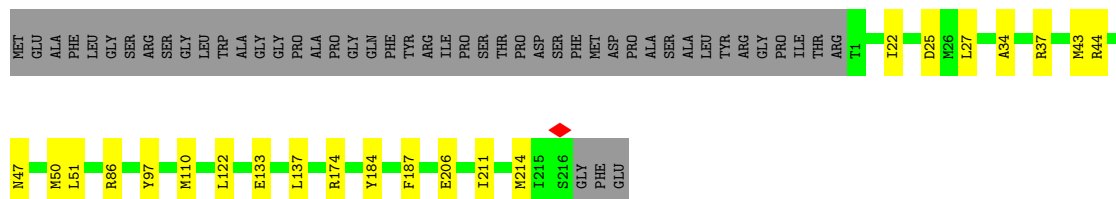
- Molecule 19: Proteasome subunit beta type-1

Chain BS: 79% 10% 12%



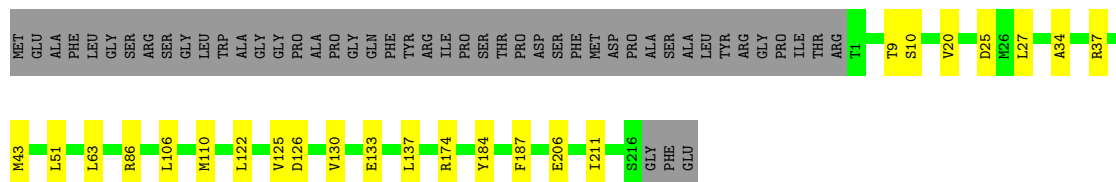
- Molecule 20: Proteasome subunit beta type-4

Chain AT: 73% 8% 18%

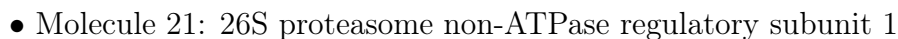


- Molecule 20: Proteasome subunit beta type-4

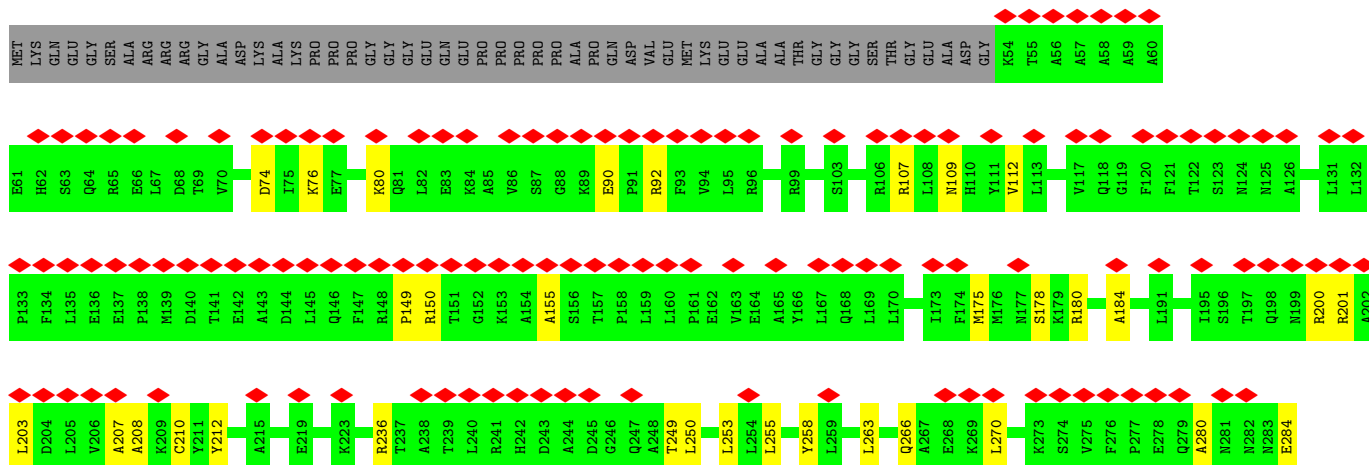
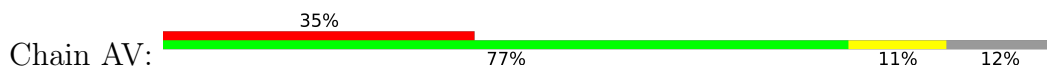
Chain BT: 73% 9% 18%

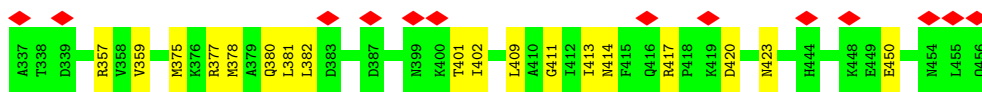


- Molecule 21: 26S proteasome non-ATPase regulatory subunit 1



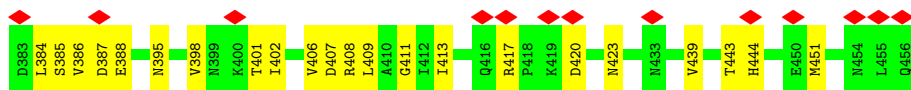
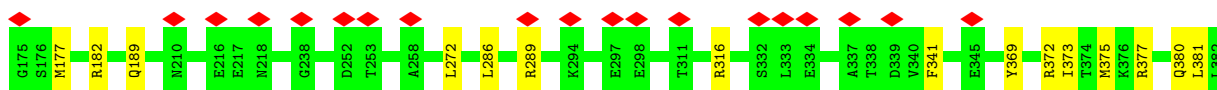
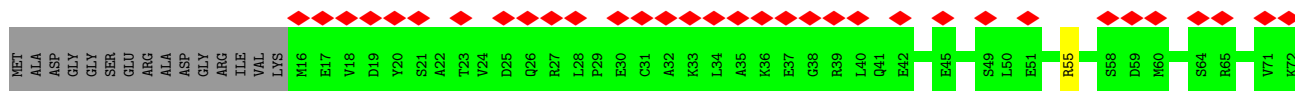
- Molecule 22: 26S proteasome non-ATPase regulatory subunit 3





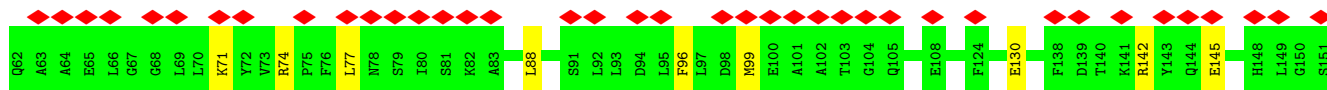
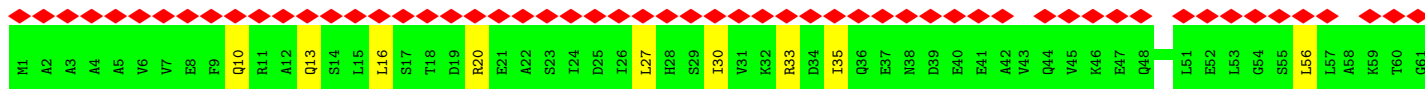
- Molecule 23: 26S proteasome non-ATPase regulatory subunit 12

Chain BW: 21% 87% 10%



- Molecule 24: 26S proteasome non-ATPase regulatory subunit 11

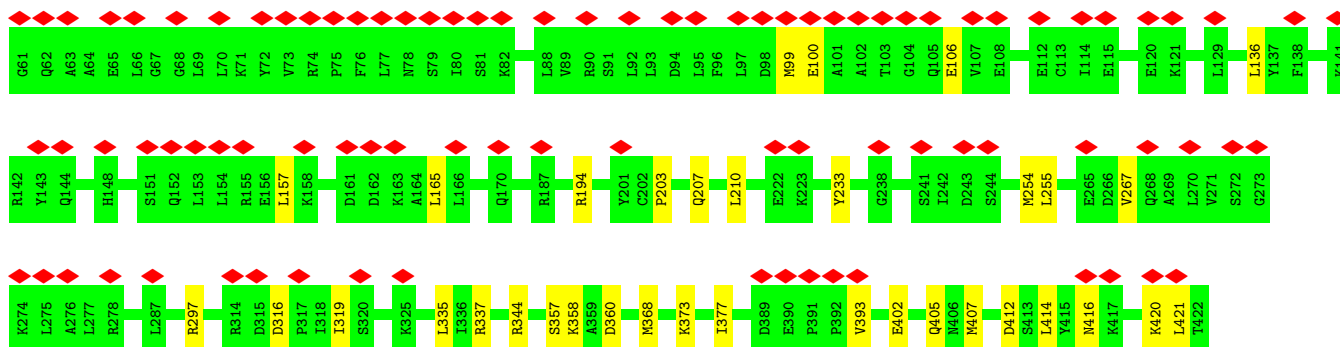
Chain AX: 36% 89% 11%



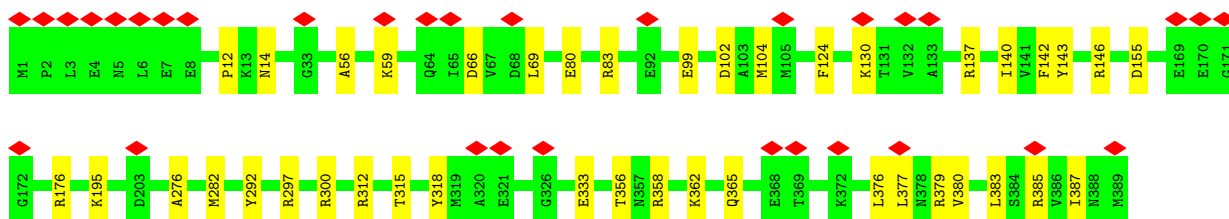
- Molecule 24: 26S proteasome non-ATPase regulatory subunit 11

Chain BX: 35% 90% 10%

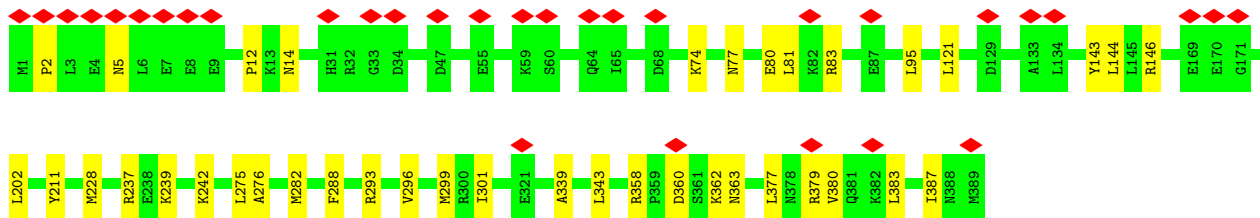
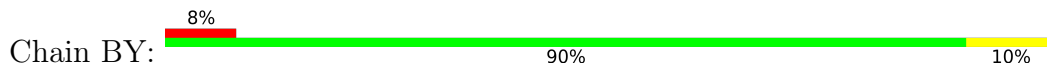




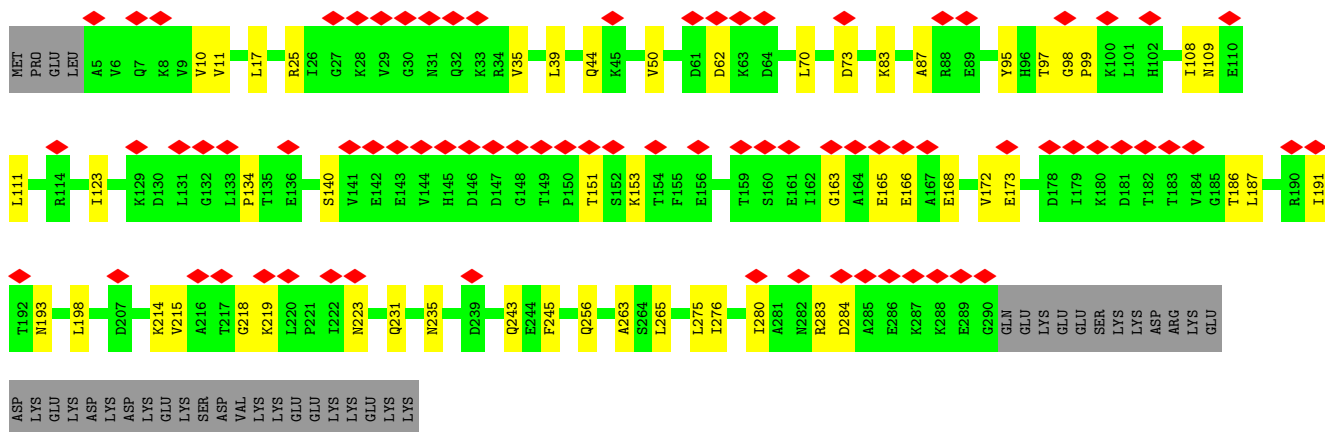
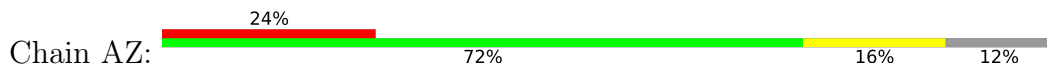
- Molecule 25: 26S proteasome non-ATPase regulatory subunit 6



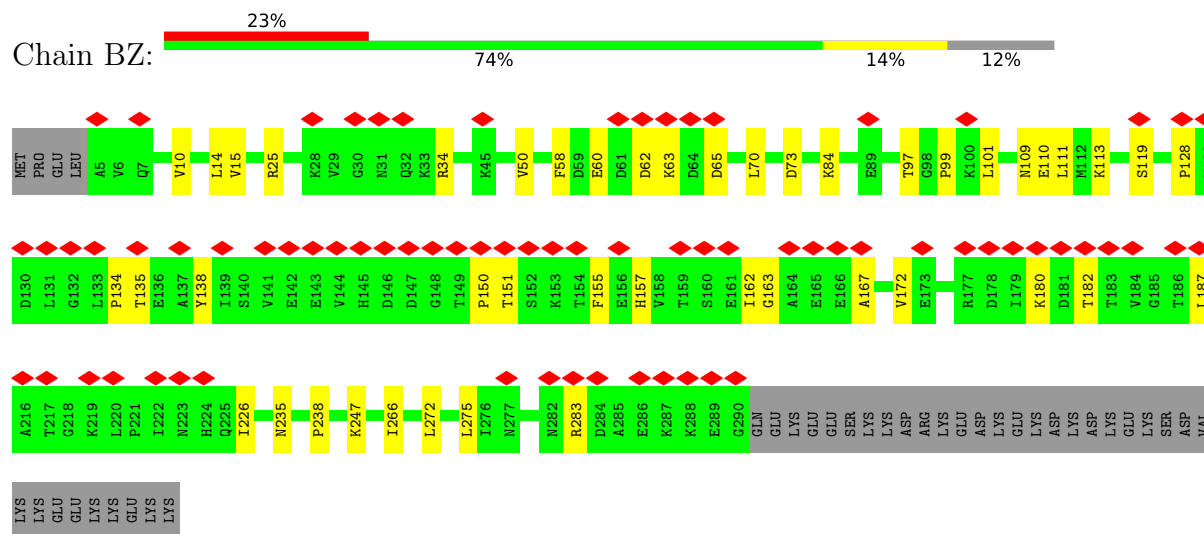
- Molecule 25: 26S proteasome non-ATPase regulatory subunit 6



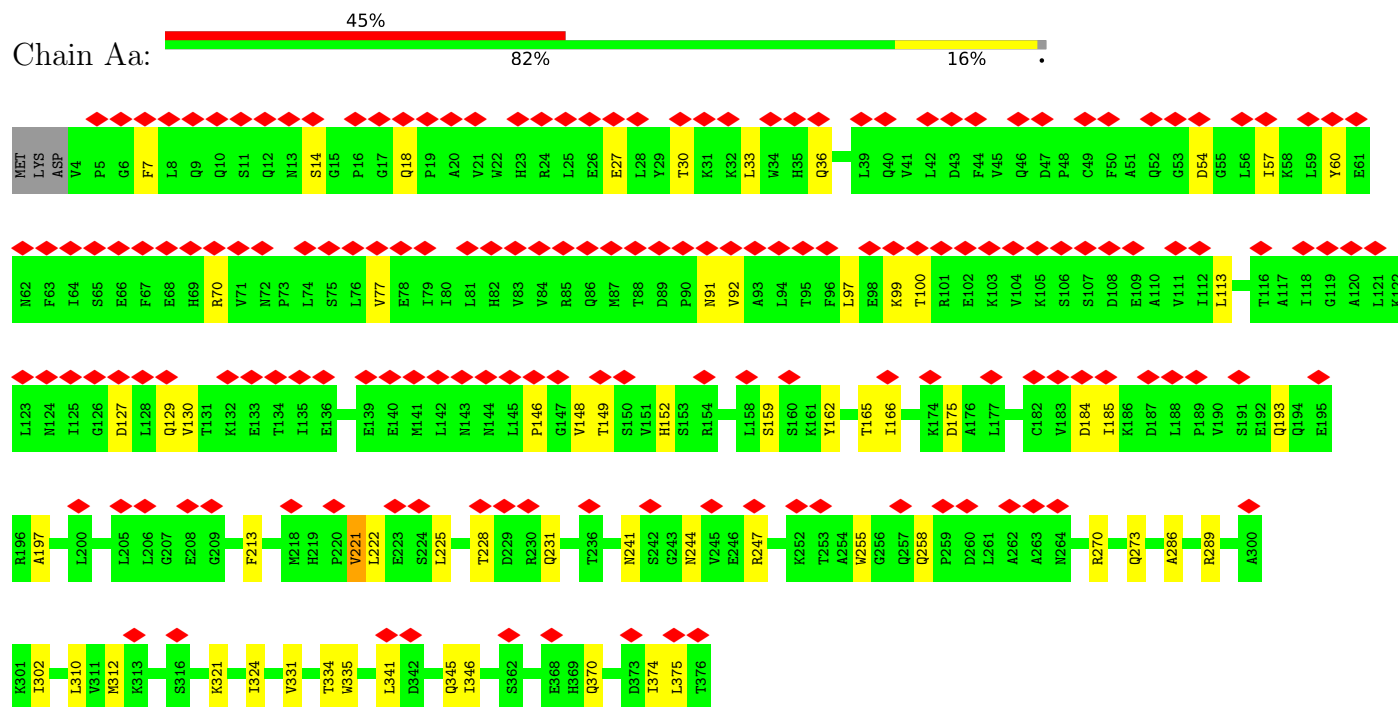
- Molecule 26: 26S proteasome non-ATPase regulatory subunit 7



Chain BZ:

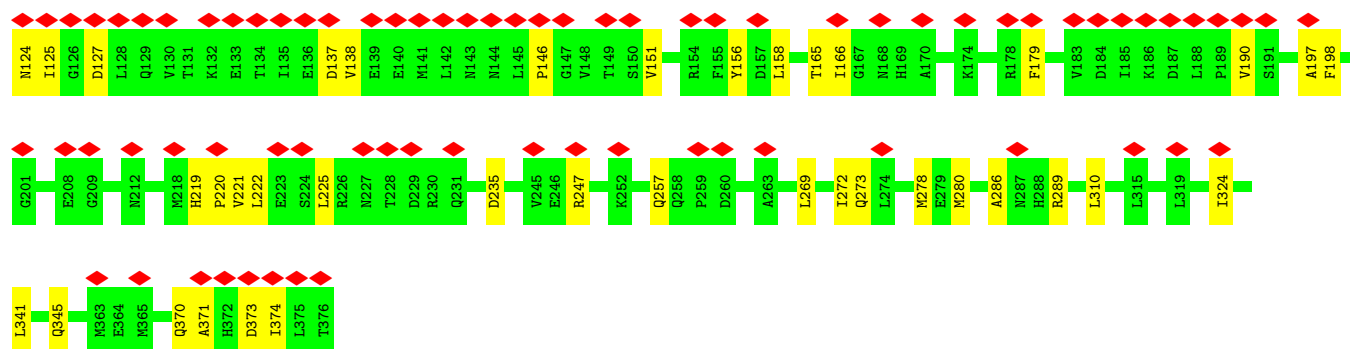


Chain Aa:



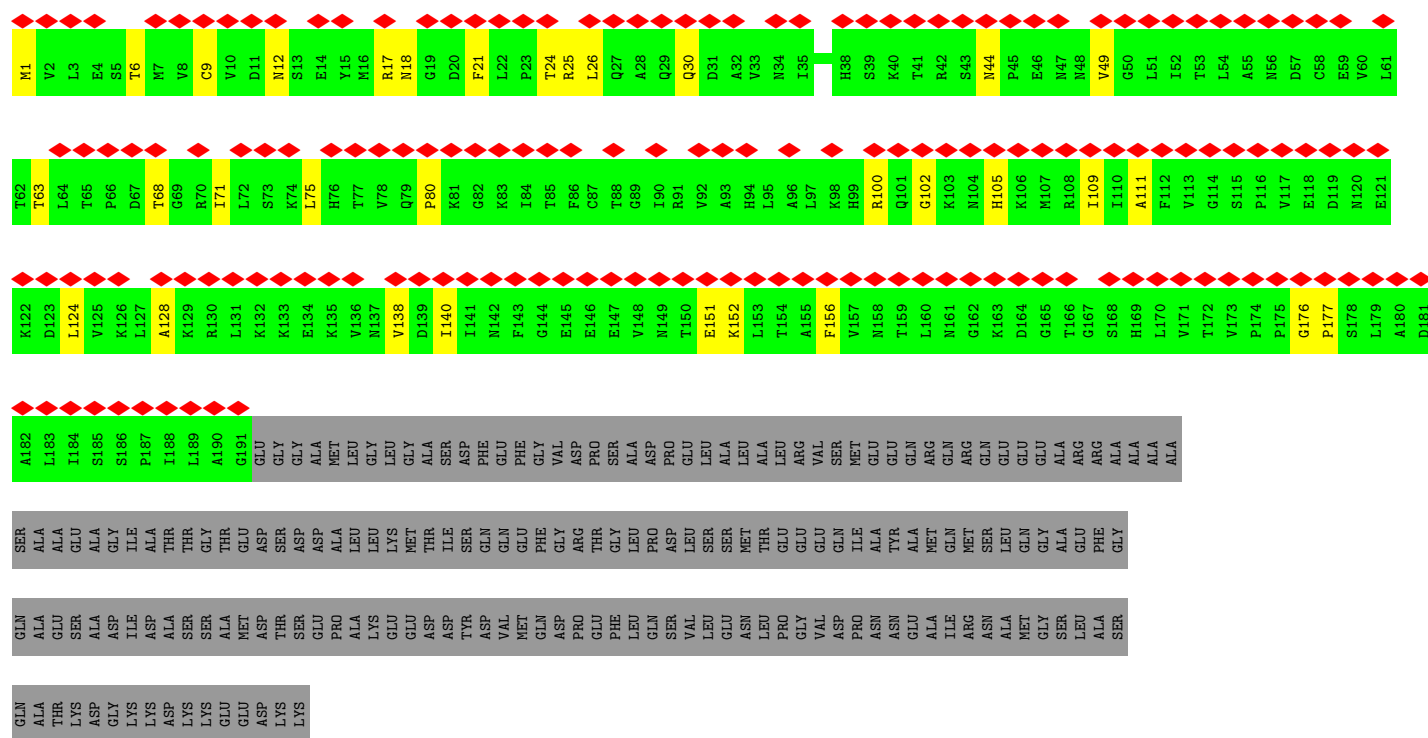
Chain Ba:





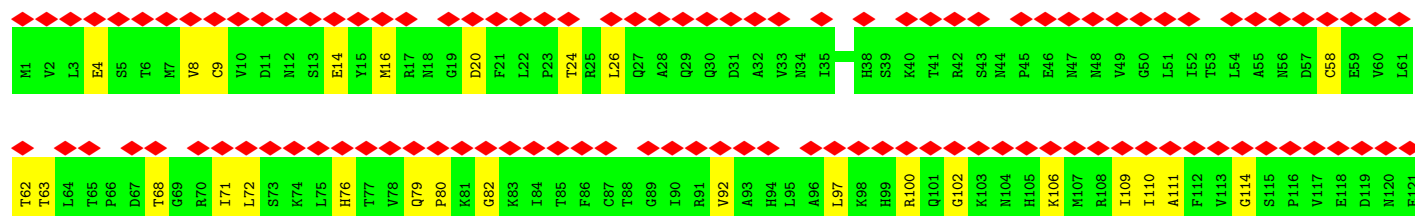
• Molecule 28: 26S proteasome non-ATPase regulatory subunit 4

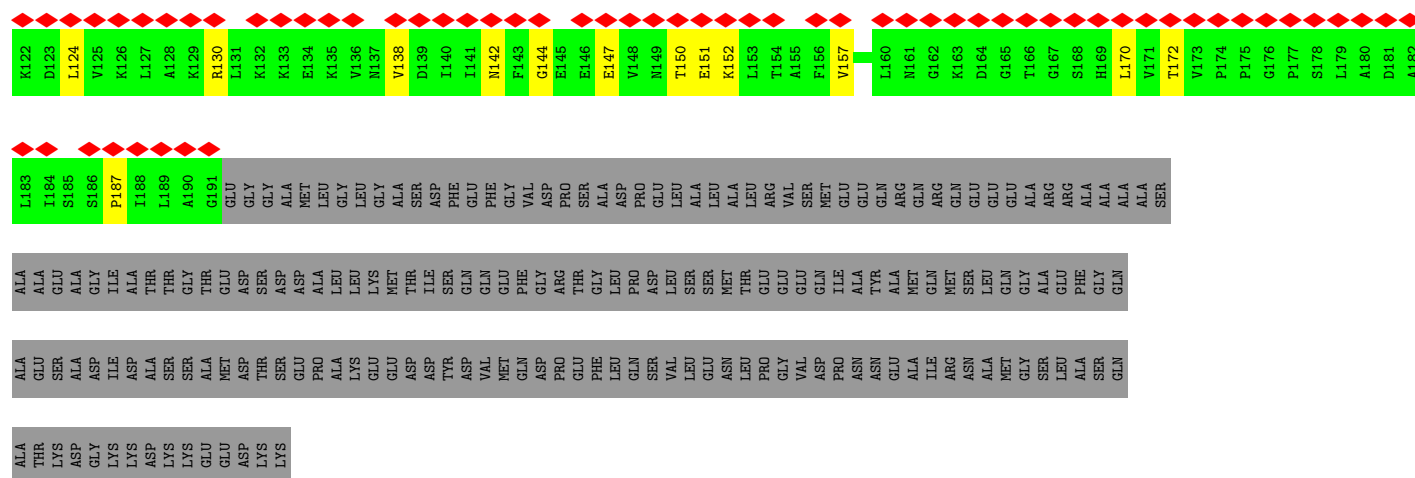
Chain Ab: 44% 42% 8% 49%



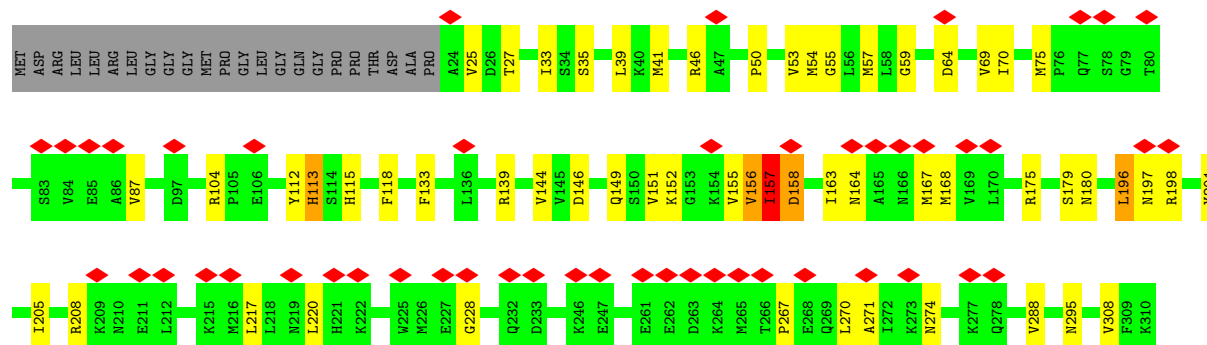
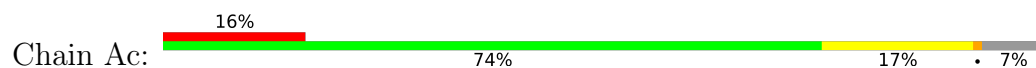
• Molecule 28: 26S proteasome non-ATPase regulatory subunit 4

Chain Bb: 45% 40% 11% 49%

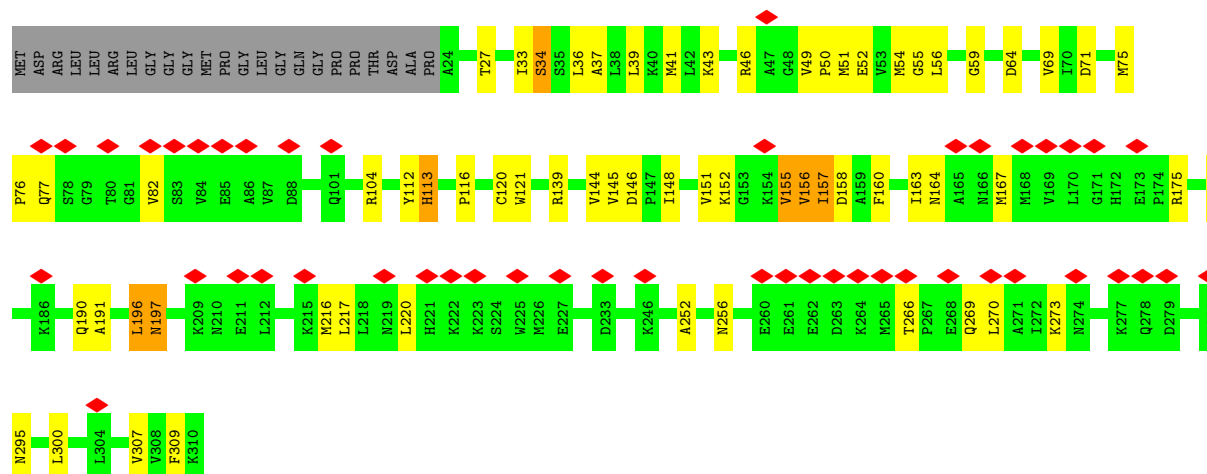
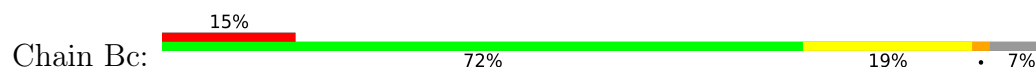




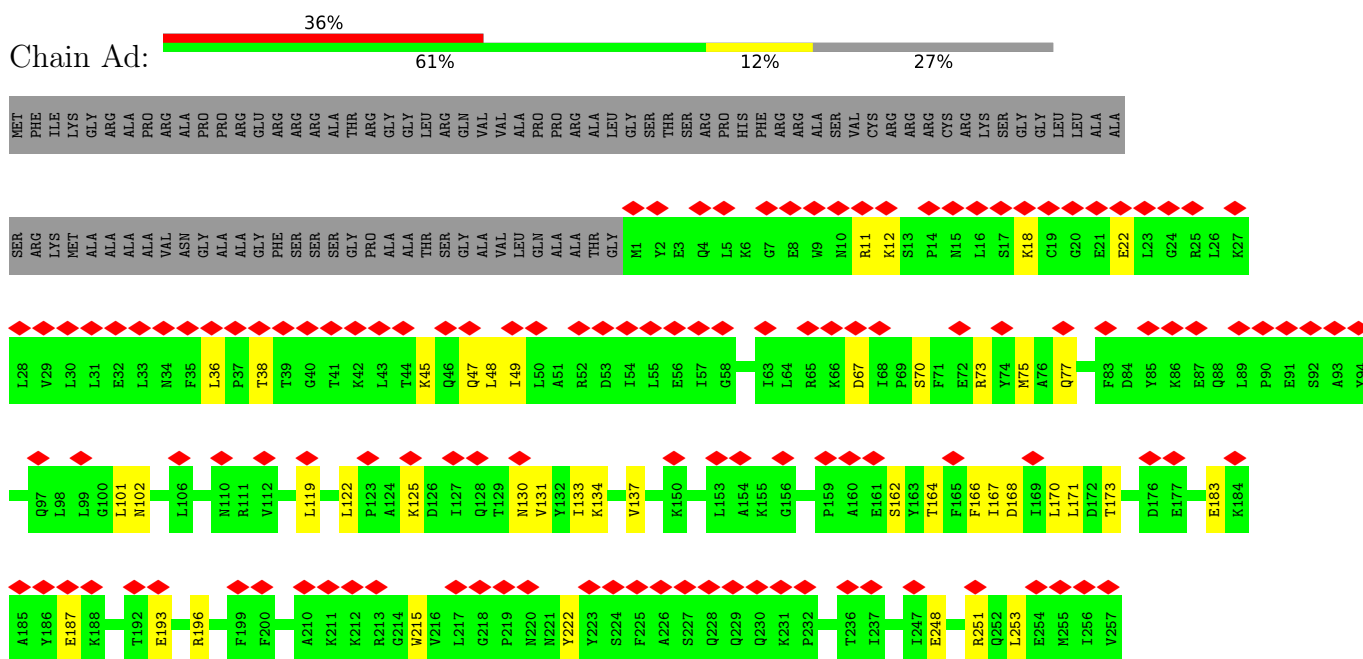
- Molecule 29: 26S proteasome non-ATPase regulatory subunit 14



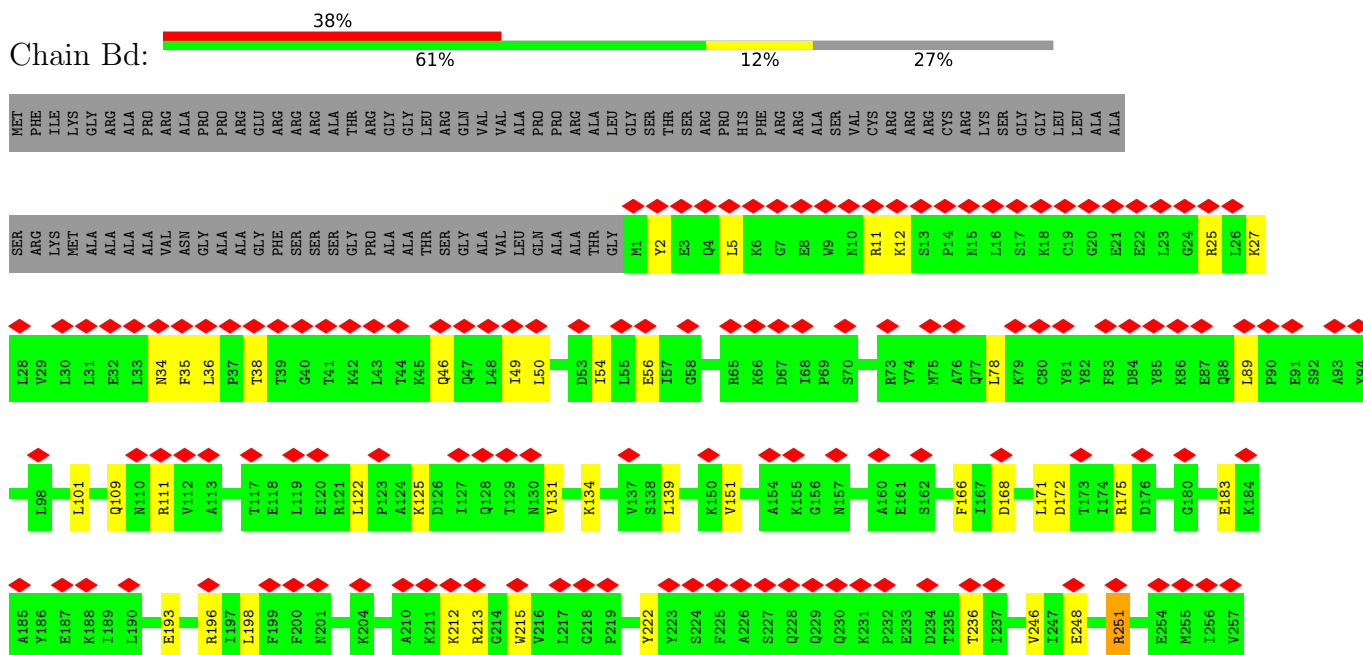
- Molecule 29: 26S proteasome non-ATPase regulatory subunit 14



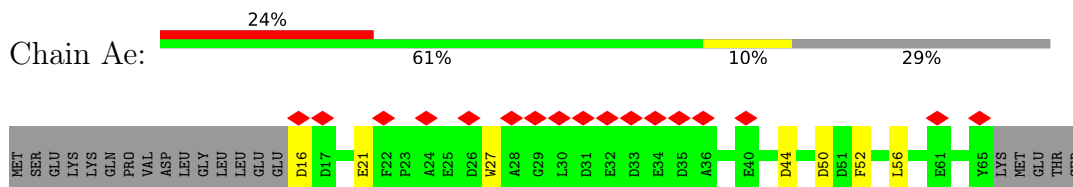
- Molecule 30: 26S proteasome non-ATPase regulatory subunit 8



- Molecule 30: 26S proteasome non-ATPase regulatory subunit 8

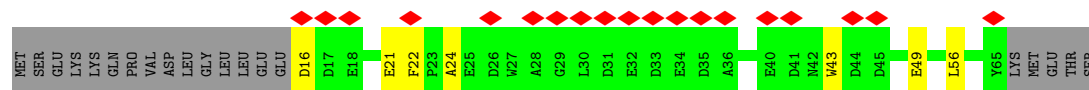


- Molecule 31: 26S proteasome complex subunit SEM1

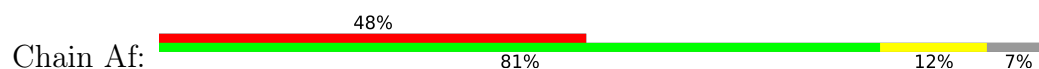


- Molecule 31: 26S proteasome complex subunit SEM1





• Molecule 32: 26S proteasome non-ATPase regulatory subunit 2



• Molecule 32: 26S proteasome non-ATPase regulatory subunit 2

Chain Bf:



[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	14284	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	44	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.025	Depositor
Minimum map value	-0.004	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.006	Depositor
Map size (Å)	548.0, 548.0, 548.0	wwPDB
Map dimensions	800, 800, 800	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.685, 0.685, 0.685	Depositor

5 Model quality

5.1 Standard geometry

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

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	AA	0.18	0/3294	0.53	2/4447 (0.0%)
1	BA	0.20	0/3294	0.53	0/4447
2	AB	0.18	0/3086	0.48	1/4164 (0.0%)
2	BB	0.18	0/3086	0.47	0/4164
3	AC	0.22	0/2902	0.48	0/3904
3	BC	0.19	0/2902	0.46	0/3904
4	AD	0.21	0/3089	0.51	0/4168
4	BD	0.23	0/3089	0.54	0/4168
5	AE	0.18	0/2904	0.48	0/3924
5	BE	0.18	0/2904	0.48	1/3924 (0.0%)
6	AF	0.15	0/2896	0.42	0/3912
6	BF	0.15	0/2896	0.42	0/3912
7	AG	0.13	0/1923	0.41	0/2601
7	BG	0.12	0/1923	0.38	0/2601
8	AH	0.15	0/1848	0.38	0/2503
8	BH	0.13	0/1848	0.38	0/2503
9	AI	0.12	0/1987	0.36	0/2681
9	BI	0.12	0/1987	0.38	0/2681
10	AJ	0.17	0/1884	0.40	0/2549
10	BJ	0.19	0/1884	0.44	0/2549
11	AK	0.13	0/1800	0.38	0/2431
11	BK	0.13	0/1800	0.37	0/2431
12	AL	0.12	0/1901	0.33	0/2570
12	BL	0.13	0/1901	0.36	0/2570
13	AM	0.14	0/1917	0.37	0/2581
13	BM	0.15	0/1917	0.39	0/2581
14	AN	0.10	0/1540	0.29	0/2085
14	BN	0.11	0/1540	0.33	0/2085
15	AO	0.14	0/1676	0.41	0/2271
15	BO	0.13	0/1676	0.37	0/2271
16	AP	0.13	0/1616	0.39	0/2180
16	BP	0.14	0/1616	0.41	0/2180

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.17	0/1621	0.35	0/2194
17	BQ	0.14	0/1621	0.37	0/2194
18	AR	0.11	0/1590	0.30	0/2147
18	BR	0.12	0/1590	0.34	0/2147
19	AS	0.14	0/1671	0.40	0/2252
19	BS	0.13	0/1671	0.41	0/2252
20	AT	0.11	0/1716	0.33	0/2323
20	BT	0.13	0/1716	0.37	0/2323
21	AU	0.16	0/6903	0.44	0/9324
21	BU	0.15	0/6903	0.44	0/9324
22	AV	0.15	0/3824	0.41	0/5170
22	BV	0.15	0/3824	0.39	0/5170
23	AW	0.13	0/3644	0.37	0/4901
23	BW	0.13	0/3644	0.38	0/4901
24	AX	0.14	0/3381	0.40	0/4558
24	BX	0.14	0/3381	0.38	0/4558
25	AY	0.13	0/3261	0.41	0/4393
25	BY	0.14	0/3261	0.41	0/4393
26	AZ	0.17	0/2324	0.48	0/3150
26	BZ	0.20	0/2324	0.55	1/3150 (0.0%)
27	Aa	0.17	0/3053	0.51	1/4133 (0.0%)
27	Ba	0.18	0/3053	0.50	1/4133 (0.0%)
28	Ab	0.19	0/1478	0.53	0/2001
28	Bb	0.22	0/1478	0.55	1/2001 (0.0%)
29	Ac	0.28	0/2302	0.61	1/3110 (0.0%)
29	Bc	0.29	0/2302	0.64	0/3110
30	Ad	0.21	0/2162	0.53	2/2919 (0.1%)
30	Bd	0.19	0/2162	0.50	0/2919
31	Ae	0.20	0/437	0.55	0/595
31	Be	0.17	0/437	0.53	0/595
32	Af	0.15	0/6640	0.41	0/8988
32	Bf	0.14	0/6640	0.40	2/8988 (0.0%)
33	Au	0.11	0/607	0.30	0/816
33	Aw	0.12	0/607	0.38	0/816
33	Bu	0.12	0/607	0.32	0/816
33	Bw	0.15	0/607	0.38	0/816
All	All	0.16	0/166968	0.44	13/225522 (0.0%)

There are no bond length outliers.

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	Ac	155	VAL	N-CA-C	-7.62	106.47	113.71
27	Aa	221	VAL	N-CA-C	-6.16	107.86	113.71
1	AA	327	LEU	CA-C-N	5.91	128.89	120.49
1	AA	327	LEU	C-N-CA	5.91	128.89	120.49
27	Ba	220	PRO	CA-N-CD	-5.72	103.99	112.00

There are no chirality outliers.

There are no planarity outliers.

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	AA	3240	0	3286	35	0
1	BA	3240	0	3287	46	0
2	AB	3042	0	3100	43	0
2	BB	3042	0	3100	45	0
3	AC	2864	0	2971	54	0
3	BC	2864	0	2971	47	0
4	AD	3039	0	3076	57	0
4	BD	3039	0	3076	55	0
5	AE	2860	0	2827	43	0
5	BE	2860	0	2827	58	0
6	AF	2858	0	2853	38	0
6	BF	2858	0	2853	54	0
7	AG	1889	0	1885	12	0
7	BG	1889	0	1885	13	0
8	AH	1809	0	1795	17	0
8	BH	1809	0	1795	13	0
9	AI	1954	0	1949	11	0
9	BI	1954	0	1949	13	0
10	AJ	1858	0	1844	17	0
10	BJ	1858	0	1844	18	0
11	AK	1773	0	1758	13	0
11	BK	1773	0	1758	13	0
12	AL	1866	0	1852	8	0
12	BL	1866	0	1852	14	0
13	AM	1879	0	1866	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	BM	1879	0	1866	9	0
14	AN	1514	0	1487	4	0
14	BN	1514	0	1487	6	0
15	AO	1649	0	1659	10	0
15	BO	1649	0	1659	18	0
16	AP	1587	0	1598	14	0
16	BP	1587	0	1598	15	0
17	AQ	1588	0	1584	6	0
17	BQ	1588	0	1584	10	0
18	AR	1559	0	1523	7	0
18	BR	1559	0	1523	8	0
19	AS	1641	0	1639	15	0
19	BS	1641	0	1639	14	0
20	AT	1683	0	1662	14	0
20	BT	1683	0	1662	16	0
21	AU	6787	0	6858	95	0
21	BU	6787	0	6858	88	0
22	AV	3754	0	3749	39	0
22	BV	3754	0	3749	39	0
23	AW	3596	0	3713	28	0
23	BW	3596	0	3713	27	0
24	AX	3335	0	3435	35	0
24	BX	3335	0	3435	25	0
25	AY	3202	0	3204	29	0
25	BY	3202	0	3204	26	0
26	AZ	2281	0	2312	40	0
26	BZ	2281	0	2312	37	0
27	Aa	2995	0	3012	44	0
27	Ba	2995	0	3012	35	0
28	Ab	1458	0	1505	21	0
28	Bb	1458	0	1505	24	0
29	Ac	2260	0	2276	45	0
29	Bc	2260	0	2276	54	0
30	Ad	2116	0	2146	27	0
30	Bd	2116	0	2146	29	0
31	Ae	425	0	328	8	0
31	Be	425	0	328	7	0
32	Af	6529	0	6541	62	0
32	Bf	6529	0	6541	76	0
33	Au	601	0	629	7	0
33	Aw	601	0	629	10	0
33	Bu	601	0	629	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	Bw	601	0	629	10	0
34	AA	31	0	12	2	0
34	AB	31	0	12	0	0
34	AD	31	0	12	2	0
34	AE	31	0	12	1	0
34	BA	31	0	12	2	0
34	BB	31	0	12	0	0
34	BD	31	0	12	2	0
34	BE	31	0	12	0	0
35	AA	1	0	0	0	0
35	AB	1	0	0	0	0
35	AD	1	0	0	0	0
35	AE	1	0	0	0	0
35	AF	1	0	0	0	0
35	BA	1	0	0	0	0
35	BB	1	0	0	0	0
35	BD	1	0	0	0	0
35	BE	1	0	0	0	0
35	BF	1	0	0	0	0
36	AC	27	0	12	1	0
36	AF	27	0	12	1	0
36	BC	27	0	12	0	0
36	BF	27	0	12	1	0
37	Ac	1	0	0	0	0
37	Bc	1	0	0	0	0
All	All	164552	0	165247	1615	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 5.

The worst 5 of 1615 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)
3:AC:89:VAL:HB	3:AC:92:GLU:HB3	1.43	0.98
29:Ac:113:HIS:HE1	29:Ac:144:VAL:HG22	1.34	0.92
10:BJ:208:LEU:HD22	10:BJ:220:LEU:HG	1.54	0.90
3:BC:90:HIS:HB2	3:BC:91:PRO:HD2	1.54	0.87
29:Bc:113:HIS:HE1	29:Bc:144:VAL:HG22	1.39	0.86

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	AA	411/433 (95%)	373 (91%)	38 (9%)	0	100	100
1	BA	411/433 (95%)	368 (90%)	42 (10%)	1 (0%)	43	73
2	AB	386/440 (88%)	360 (93%)	25 (6%)	1 (0%)	36	67
2	BB	386/440 (88%)	361 (94%)	24 (6%)	1 (0%)	36	67
3	AC	359/398 (90%)	331 (92%)	26 (7%)	2 (1%)	21	54
3	BC	359/398 (90%)	337 (94%)	20 (6%)	2 (1%)	21	54
4	AD	378/418 (90%)	333 (88%)	43 (11%)	2 (0%)	24	57
4	BD	378/418 (90%)	336 (89%)	41 (11%)	1 (0%)	36	67
5	AE	373/403 (93%)	348 (93%)	23 (6%)	2 (0%)	24	57
5	BE	373/403 (93%)	348 (93%)	24 (6%)	1 (0%)	36	67
6	AF	372/439 (85%)	347 (93%)	25 (7%)	0	100	100
6	BF	372/439 (85%)	347 (93%)	25 (7%)	0	100	100
7	AG	242/246 (98%)	234 (97%)	8 (3%)	0	100	100
7	BG	242/246 (98%)	234 (97%)	8 (3%)	0	100	100
8	AH	230/234 (98%)	220 (96%)	10 (4%)	0	100	100
8	BH	230/234 (98%)	222 (96%)	8 (4%)	0	100	100
9	AI	249/261 (95%)	241 (97%)	8 (3%)	0	100	100
9	BI	249/261 (95%)	242 (97%)	7 (3%)	0	100	100
10	AJ	237/248 (96%)	231 (98%)	6 (2%)	0	100	100
10	BJ	237/248 (96%)	227 (96%)	10 (4%)	0	100	100
11	AK	232/241 (96%)	221 (95%)	10 (4%)	1 (0%)	30	62
11	BK	232/241 (96%)	224 (97%)	8 (3%)	0	100	100
12	AL	236/263 (90%)	233 (99%)	3 (1%)	0	100	100
12	BL	236/263 (90%)	233 (99%)	3 (1%)	0	100	100
13	AM	239/255 (94%)	233 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	BM	239/255 (94%)	232 (97%)	7 (3%)	0	100	100
14	AN	200/239 (84%)	192 (96%)	8 (4%)	0	100	100
14	BN	200/239 (84%)	198 (99%)	2 (1%)	0	100	100
15	AO	218/277 (79%)	211 (97%)	7 (3%)	0	100	100
15	BO	218/277 (79%)	211 (97%)	7 (3%)	0	100	100
16	AP	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
16	BP	202/205 (98%)	197 (98%)	5 (2%)	0	100	100
17	AQ	197/201 (98%)	189 (96%)	7 (4%)	1 (0%)	24	57
17	BQ	197/201 (98%)	190 (96%)	7 (4%)	0	100	100
18	AR	199/263 (76%)	195 (98%)	4 (2%)	0	100	100
18	BR	199/263 (76%)	194 (98%)	5 (2%)	0	100	100
19	AS	211/241 (88%)	204 (97%)	7 (3%)	0	100	100
19	BS	211/241 (88%)	206 (98%)	5 (2%)	0	100	100
20	AT	214/264 (81%)	210 (98%)	4 (2%)	0	100	100
20	BT	214/264 (81%)	206 (96%)	8 (4%)	0	100	100
21	AU	864/953 (91%)	816 (94%)	48 (6%)	0	100	100
21	BU	864/953 (91%)	824 (95%)	40 (5%)	0	100	100
22	AV	470/534 (88%)	450 (96%)	20 (4%)	0	100	100
22	BV	470/534 (88%)	451 (96%)	19 (4%)	0	100	100
23	AW	439/456 (96%)	433 (99%)	6 (1%)	0	100	100
23	BW	439/456 (96%)	433 (99%)	6 (1%)	0	100	100
24	AX	420/422 (100%)	400 (95%)	20 (5%)	0	100	100
24	BX	420/422 (100%)	405 (96%)	15 (4%)	0	100	100
25	AY	387/389 (100%)	369 (95%)	18 (5%)	0	100	100
25	BY	387/389 (100%)	371 (96%)	16 (4%)	0	100	100
26	AZ	284/324 (88%)	252 (89%)	32 (11%)	0	100	100
26	BZ	284/324 (88%)	251 (88%)	33 (12%)	0	100	100
27	Aa	371/376 (99%)	342 (92%)	29 (8%)	0	100	100
27	Ba	371/376 (99%)	346 (93%)	25 (7%)	0	100	100
28	Ab	189/377 (50%)	176 (93%)	13 (7%)	0	100	100
28	Bb	189/377 (50%)	173 (92%)	16 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	Ac	285/310 (92%)	250 (88%)	32 (11%)	3 (1%)	11	41
29	Bc	285/310 (92%)	246 (86%)	34 (12%)	5 (2%)	6	33
30	Ad	255/350 (73%)	223 (88%)	32 (12%)	0	100	100
30	Bd	255/350 (73%)	223 (88%)	32 (12%)	0	100	100
31	Ae	48/70 (69%)	40 (83%)	8 (17%)	0	100	100
31	Be	48/70 (69%)	38 (79%)	10 (21%)	0	100	100
32	Af	840/908 (92%)	805 (96%)	34 (4%)	1 (0%)	48	79
32	Bf	840/908 (92%)	808 (96%)	31 (4%)	1 (0%)	48	79
33	Au	74/76 (97%)	73 (99%)	1 (1%)	0	100	100
33	Aw	74/76 (97%)	70 (95%)	4 (5%)	0	100	100
33	Bu	74/76 (97%)	72 (97%)	2 (3%)	0	100	100
33	Bw	74/76 (97%)	73 (99%)	1 (1%)	0	100	100
All	All	20770/23180 (90%)	19627 (94%)	1118 (5%)	25 (0%)	49	79

5 of 25 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	AD	125	LYS
5	AE	385	ASP
5	AE	386	TYR
2	BB	167	THR
4	BD	125	LYS

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	AA	352/372 (95%)	350 (99%)	2 (1%)	78	79
1	BA	352/372 (95%)	349 (99%)	3 (1%)	70	74
2	AB	341/385 (89%)	340 (100%)	1 (0%)	86	84
2	BB	341/385 (89%)	340 (100%)	1 (0%)	86	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	AC	314/346 (91%)	309 (98%)	5 (2%)	55	68
3	BC	314/346 (91%)	313 (100%)	1 (0%)	86	84
4	AD	333/366 (91%)	332 (100%)	1 (0%)	86	84
4	BD	333/366 (91%)	331 (99%)	2 (1%)	78	79
5	AE	298/353 (84%)	297 (100%)	1 (0%)	86	84
5	BE	298/353 (84%)	297 (100%)	1 (0%)	86	84
6	AF	296/379 (78%)	296 (100%)	0	100	100
6	BF	296/379 (78%)	296 (100%)	0	100	100
7	AG	205/210 (98%)	205 (100%)	0	100	100
7	BG	205/210 (98%)	205 (100%)	0	100	100
8	AH	189/191 (99%)	188 (100%)	1 (0%)	81	81
8	BH	189/191 (99%)	189 (100%)	0	100	100
9	AI	206/221 (93%)	206 (100%)	0	100	100
9	BI	206/221 (93%)	206 (100%)	0	100	100
10	AJ	196/211 (93%)	194 (99%)	2 (1%)	68	74
10	BJ	196/211 (93%)	194 (99%)	2 (1%)	68	74
11	AK	192/203 (95%)	192 (100%)	0	100	100
11	BK	192/203 (95%)	192 (100%)	0	100	100
12	AL	202/224 (90%)	202 (100%)	0	100	100
12	BL	202/224 (90%)	202 (100%)	0	100	100
13	AM	197/212 (93%)	197 (100%)	0	100	100
13	BM	197/212 (93%)	196 (100%)	1 (0%)	81	81
14	AN	157/181 (87%)	157 (100%)	0	100	100
14	BN	157/181 (87%)	157 (100%)	0	100	100
15	AO	179/228 (78%)	179 (100%)	0	100	100
15	BO	179/228 (78%)	179 (100%)	0	100	100
16	AP	172/174 (99%)	172 (100%)	0	100	100
16	BP	172/174 (99%)	172 (100%)	0	100	100
17	AQ	168/171 (98%)	166 (99%)	2 (1%)	63	72
17	BQ	168/171 (98%)	167 (99%)	1 (1%)	78	79
18	AR	156/202 (77%)	156 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	BR	156/202 (77%)	156 (100%)	0	100	100
19	AS	175/199 (88%)	175 (100%)	0	100	100
19	BS	175/199 (88%)	175 (100%)	0	100	100
20	AT	178/215 (83%)	178 (100%)	0	100	100
20	BT	178/215 (83%)	178 (100%)	0	100	100
21	AU	742/816 (91%)	741 (100%)	1 (0%)	88	89
21	BU	742/816 (91%)	742 (100%)	0	100	100
22	AV	391/460 (85%)	390 (100%)	1 (0%)	86	84
22	BV	391/460 (85%)	391 (100%)	0	100	100
23	AW	406/416 (98%)	406 (100%)	0	100	100
23	BW	406/416 (98%)	406 (100%)	0	100	100
24	AX	362/362 (100%)	362 (100%)	0	100	100
24	BX	362/362 (100%)	362 (100%)	0	100	100
25	AY	344/344 (100%)	344 (100%)	0	100	100
25	BY	344/344 (100%)	344 (100%)	0	100	100
26	AZ	257/295 (87%)	256 (100%)	1 (0%)	84	83
26	BZ	257/295 (87%)	257 (100%)	0	100	100
27	Aa	333/336 (99%)	333 (100%)	0	100	100
27	Ba	333/336 (99%)	333 (100%)	0	100	100
28	Ab	167/312 (54%)	167 (100%)	0	100	100
28	Bb	167/312 (54%)	167 (100%)	0	100	100
29	Ac	252/268 (94%)	249 (99%)	3 (1%)	63	72
29	Bc	252/268 (94%)	249 (99%)	3 (1%)	63	72
30	Ad	231/294 (79%)	231 (100%)	0	100	100
30	Bd	231/294 (79%)	230 (100%)	1 (0%)	84	83
31	Ae	44/63 (70%)	44 (100%)	0	100	100
31	Be	44/63 (70%)	44 (100%)	0	100	100
32	Af	711/763 (93%)	711 (100%)	0	100	100
32	Bf	711/763 (93%)	711 (100%)	0	100	100
33	Au	68/68 (100%)	68 (100%)	0	100	100
33	Aw	68/68 (100%)	68 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	Bu	68/68 (100%)	68 (100%)	0	100	100
33	Bw	68/68 (100%)	68 (100%)	0	100	100
All	All	17764/19816 (90%)	17727 (100%)	37 (0%)	85	87

5 of 37 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	BE	385	ASP
29	Bc	196	LEU
10	BJ	219	ILE
17	BQ	46	CYS
10	AJ	221	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 187 such sidechains are listed below:

Mol	Chain	Res	Type
4	BD	414	HIS
17	BQ	87	ASN
7	BG	75	ASN
9	BI	109	GLN
21	BU	247	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 24 ligands modelled in this entry, 12 are monoatomic - leaving 12 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
34	ATP	BD	501	35	29,33,33	0.28	0	44,52,52	0.46	1 (2%)
34	ATP	BB	502	35	29,33,33	0.28	0	44,52,52	0.45	1 (2%)
34	ATP	AD	501	35	29,33,33	0.29	0	44,52,52	0.52	1 (2%)
34	ATP	AE	402	35	29,33,33	0.27	0	44,52,52	0.45	1 (2%)
36	ADP	BF	501	35	27,29,29	1.36	4 (14%)	42,45,45	1.96	11 (26%)
36	ADP	AF	501	35	27,29,29	1.36	4 (14%)	42,45,45	1.97	10 (23%)
34	ATP	BA	501	35	29,33,33	0.28	0	44,52,52	0.47	1 (2%)
34	ATP	BE	401	35	29,33,33	0.27	0	44,52,52	0.45	1 (2%)
36	ADP	AC	501	-	27,29,29	1.37	4 (14%)	42,45,45	2.05	9 (21%)
34	ATP	AA	501	35	29,33,33	0.28	0	44,52,52	0.45	1 (2%)
36	ADP	BC	501	-	27,29,29	1.36	4 (14%)	42,45,45	2.01	9 (21%)
34	ATP	AB	501	35	29,33,33	0.28	0	44,52,52	0.45	1 (2%)

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
34	ATP	BD	501	35	-	11/22/38/38	0/3/3/3
34	ATP	BB	502	35	-	6/22/38/38	0/3/3/3
34	ATP	AD	501	35	-	10/22/38/38	0/3/3/3
34	ATP	AE	402	35	-	5/22/38/38	0/3/3/3
36	ADP	BF	501	35	-	7/16/32/32	0/3/3/3
36	ADP	AF	501	35	-	7/16/32/32	0/3/3/3
34	ATP	BA	501	35	-	6/22/38/38	0/3/3/3
34	ATP	BE	401	35	-	3/22/38/38	0/3/3/3
36	ADP	AC	501	-	-	2/16/32/32	0/3/3/3
34	ATP	AA	501	35	-	4/22/38/38	0/3/3/3
36	ADP	BC	501	-	-	5/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	ATP	AB	501	35	-	6/22/38/38	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	BC	501	ADP	C5-C4	4.64	1.47	1.39
36	AC	501	ADP	C5-C4	4.63	1.47	1.39
36	AF	501	ADP	C5-C4	4.55	1.47	1.39
36	BF	501	ADP	C5-C4	4.52	1.47	1.39
36	BC	501	ADP	C5-C6	2.69	1.48	1.41

The worst 5 of 47 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	AC	501	ADP	C5-C4-N3	-6.73	117.97	126.75
36	BC	501	ADP	C5-C4-N3	-6.66	118.06	126.75
36	AF	501	ADP	C5-C4-N3	-6.22	118.63	126.75
36	BF	501	ADP	C5-C4-N3	-6.20	118.67	126.75
36	AC	501	ADP	N3-C4-N9	5.28	135.77	127.08

There are no chirality outliers.

5 of 72 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
34	AB	501	ATP	PB-O3B-PG-O3G
34	AB	501	ATP	C5'-O5'-PA-O1A
34	AD	501	ATP	C5'-O5'-PA-O1A
34	AD	501	ATP	C5'-O5'-PA-O2A
34	AD	501	ATP	C5'-O5'-PA-O3A

There are no ring outliers.

8 monomers are involved in 12 short contacts:

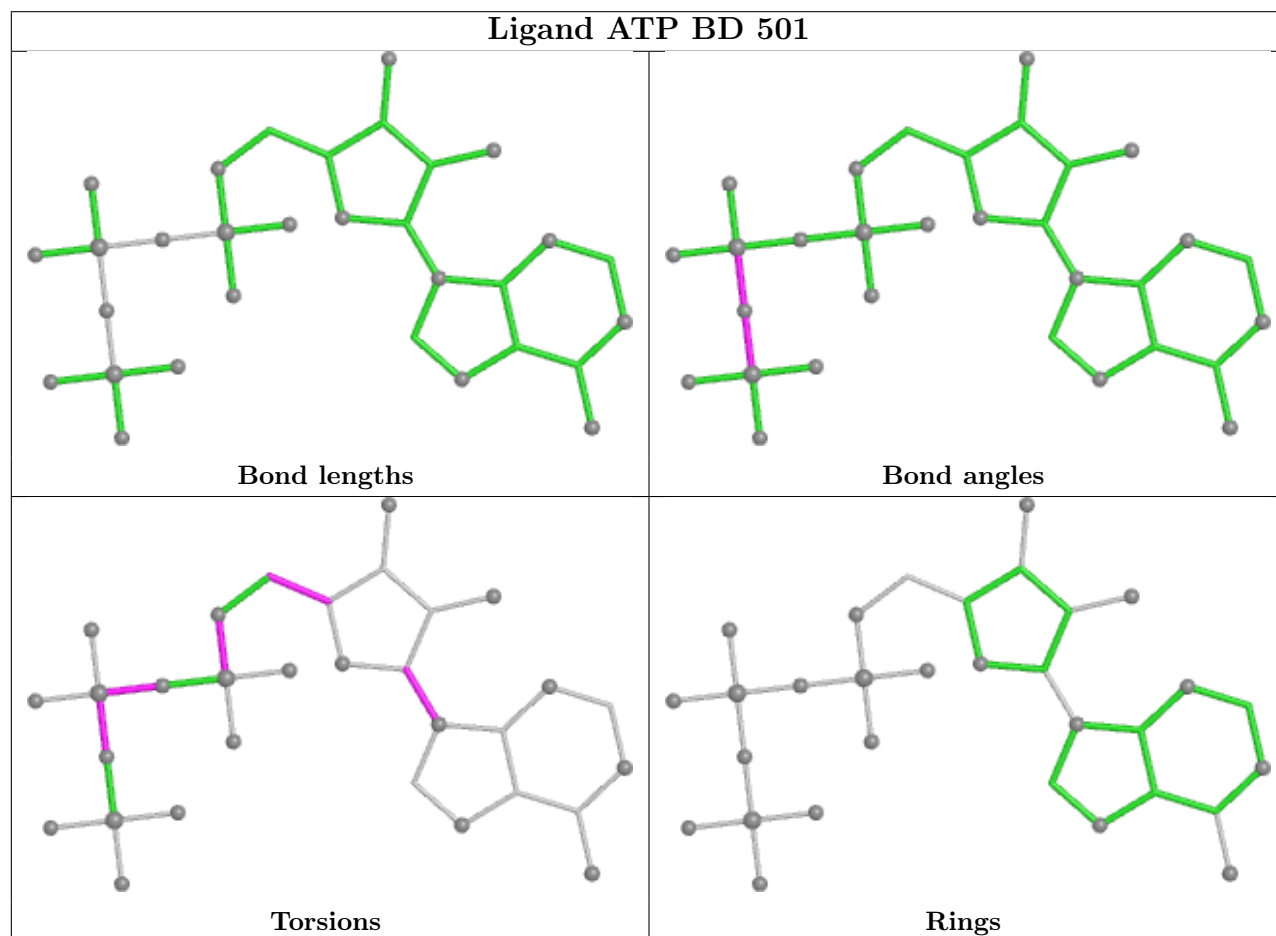
Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	BD	501	ATP	2	0
34	AD	501	ATP	2	0
34	AE	402	ATP	1	0
36	BF	501	ADP	1	0
36	AF	501	ADP	1	0
34	BA	501	ATP	2	0
36	AC	501	ADP	1	0

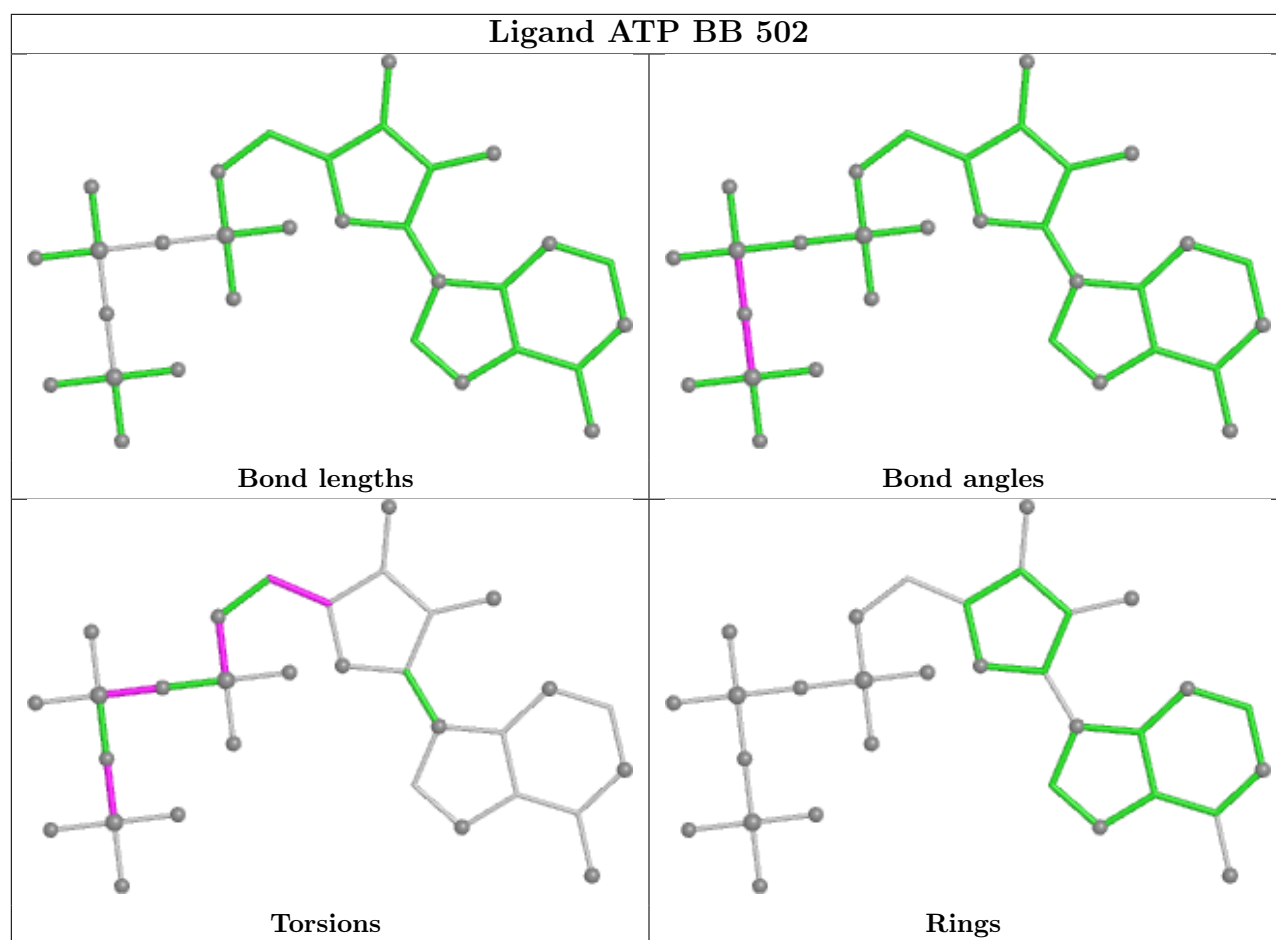
Continued on next page...

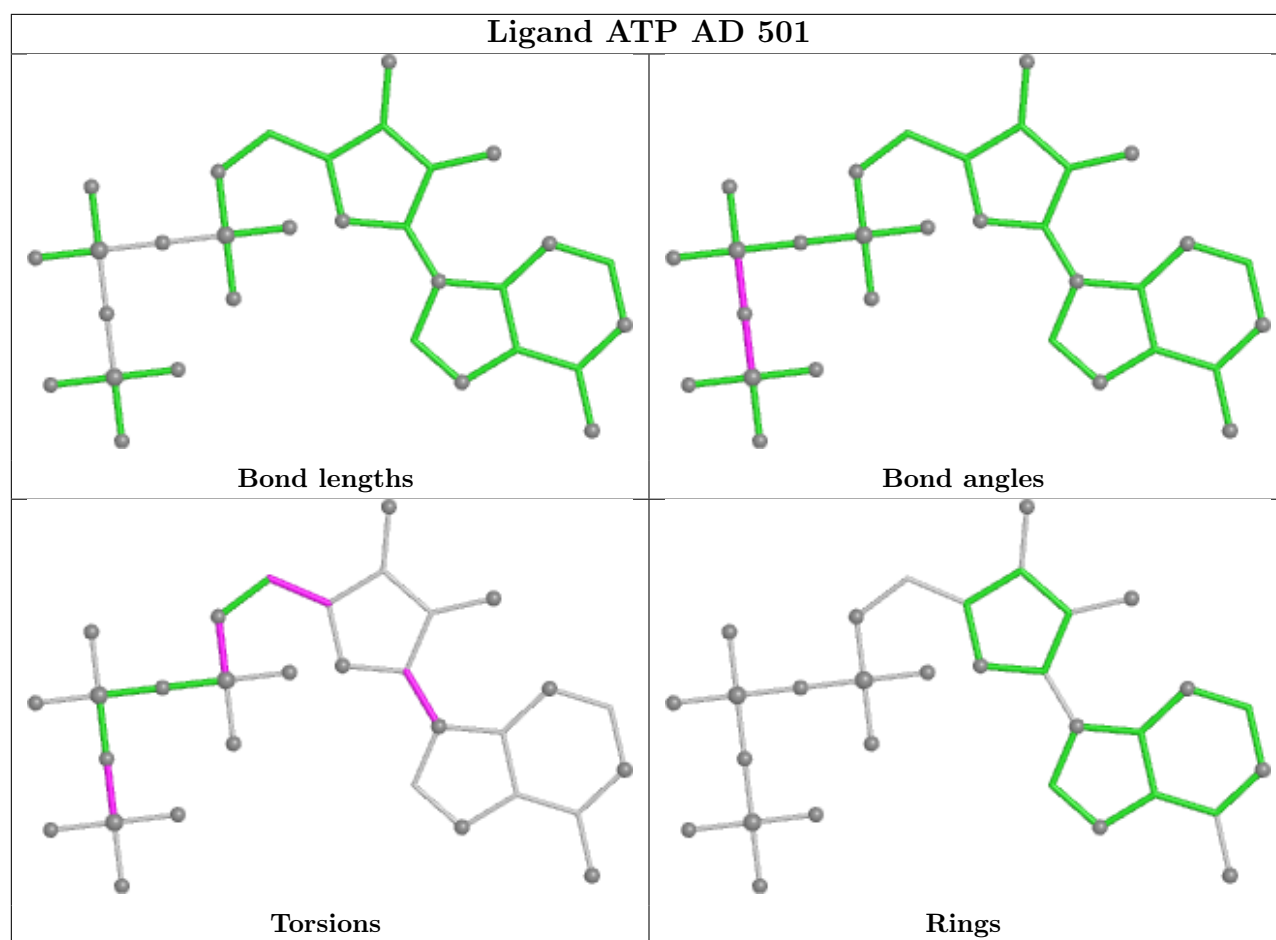
Continued from previous page...

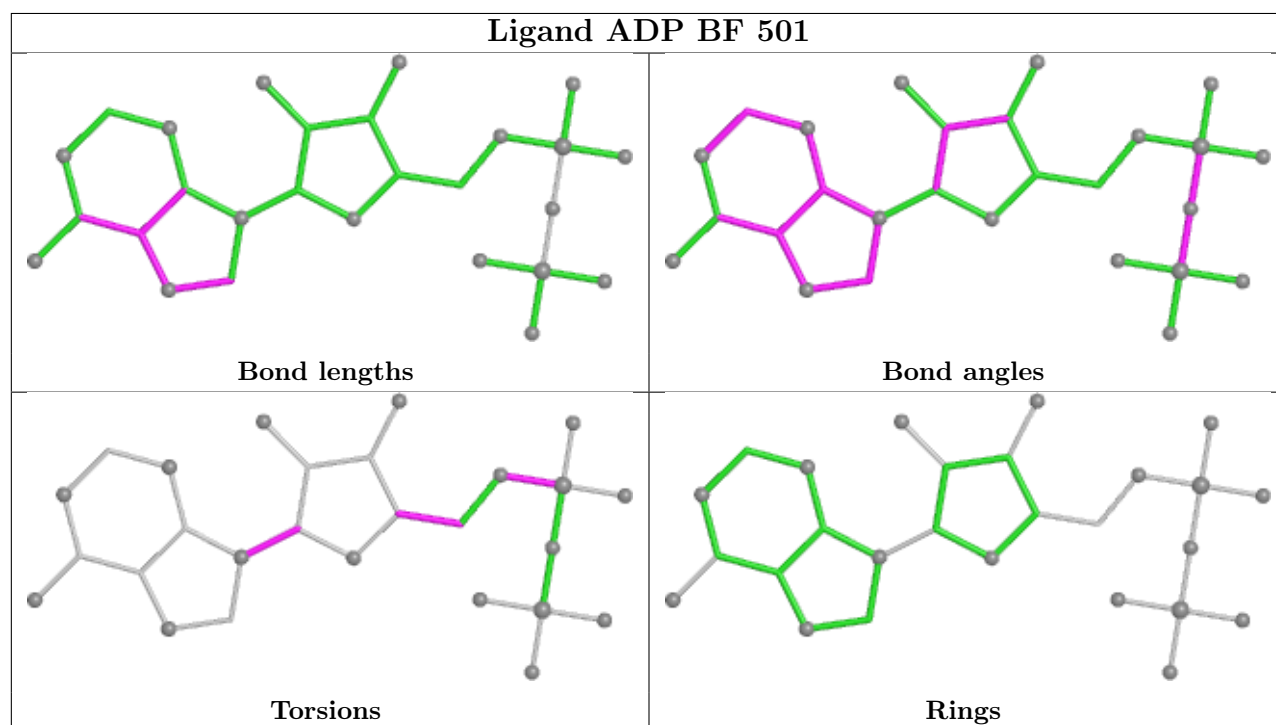
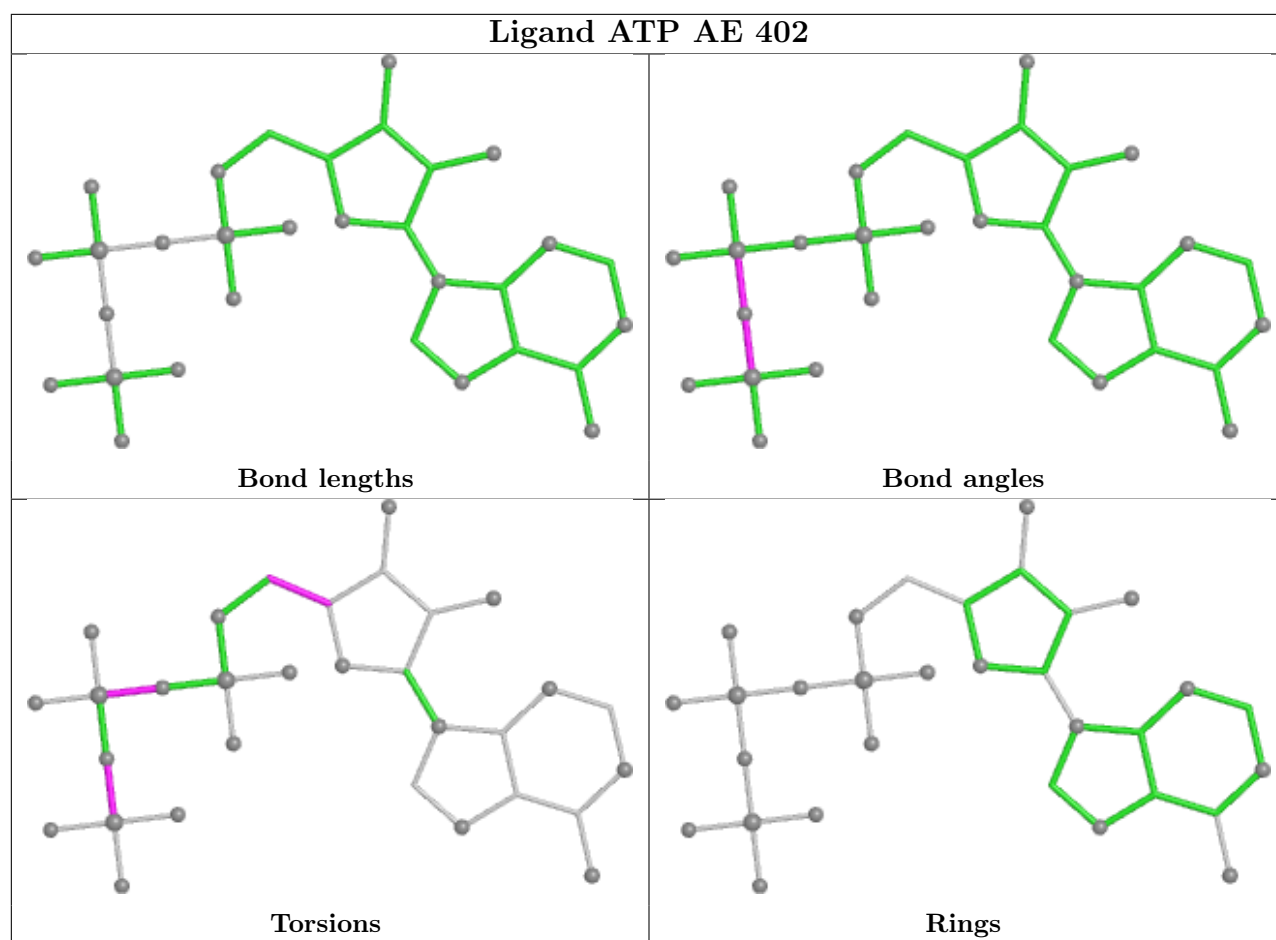
Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	AA	501	ATP	2	0

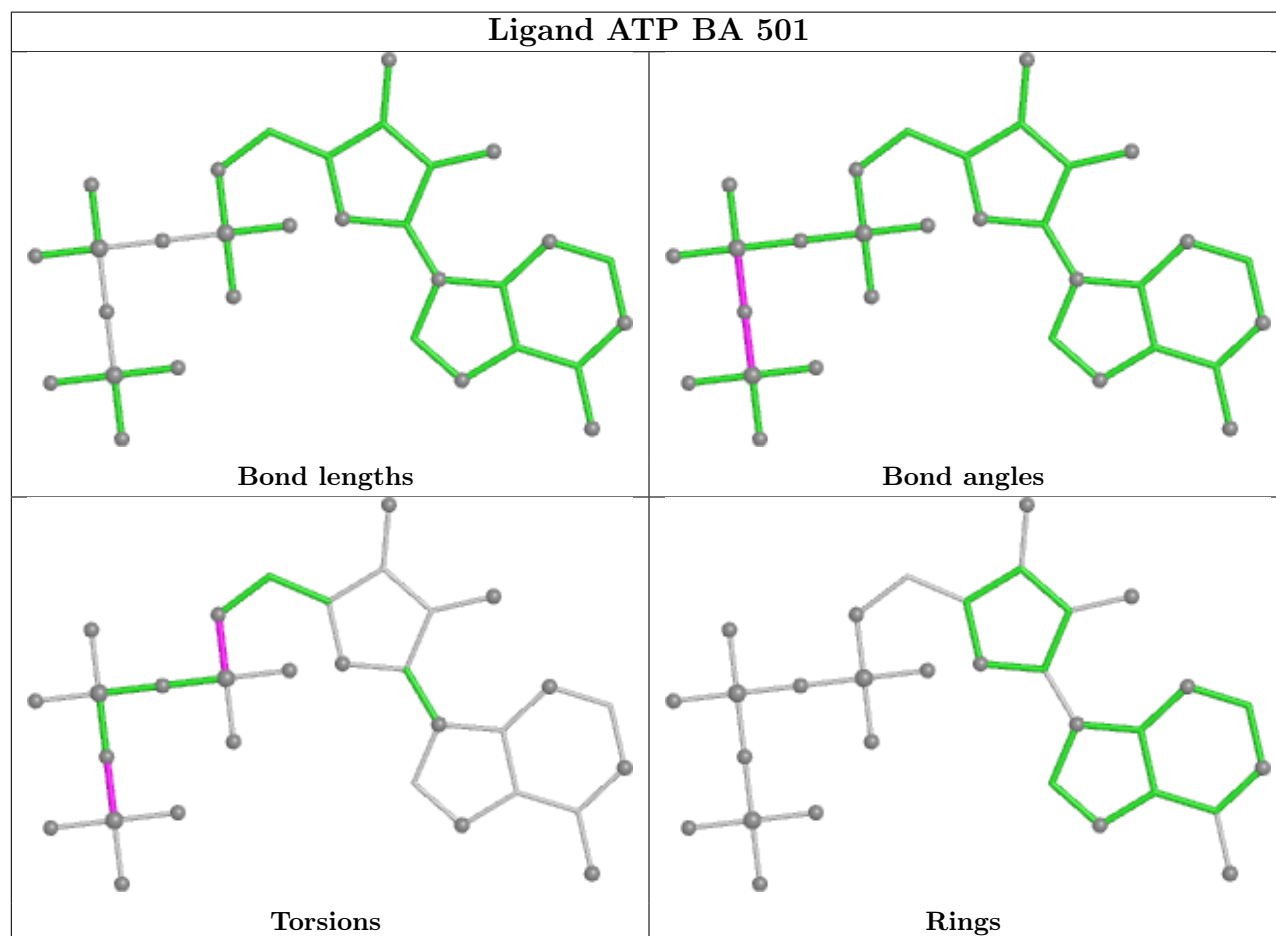
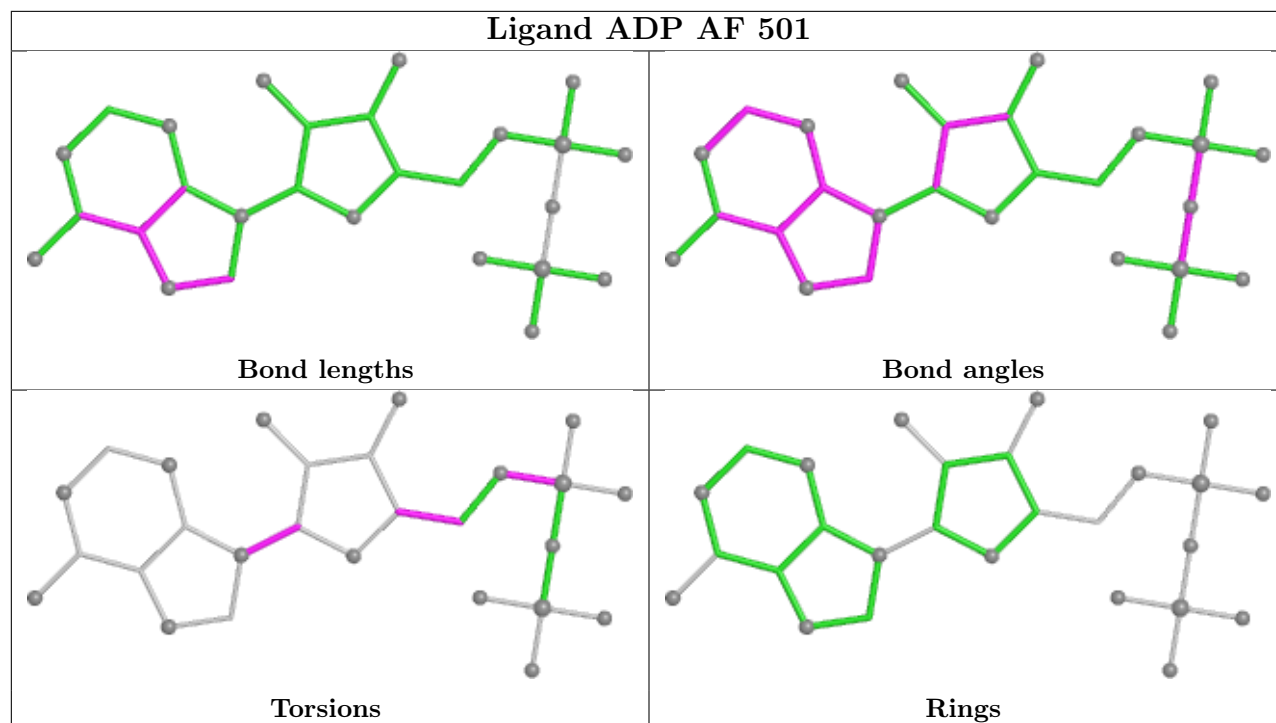
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



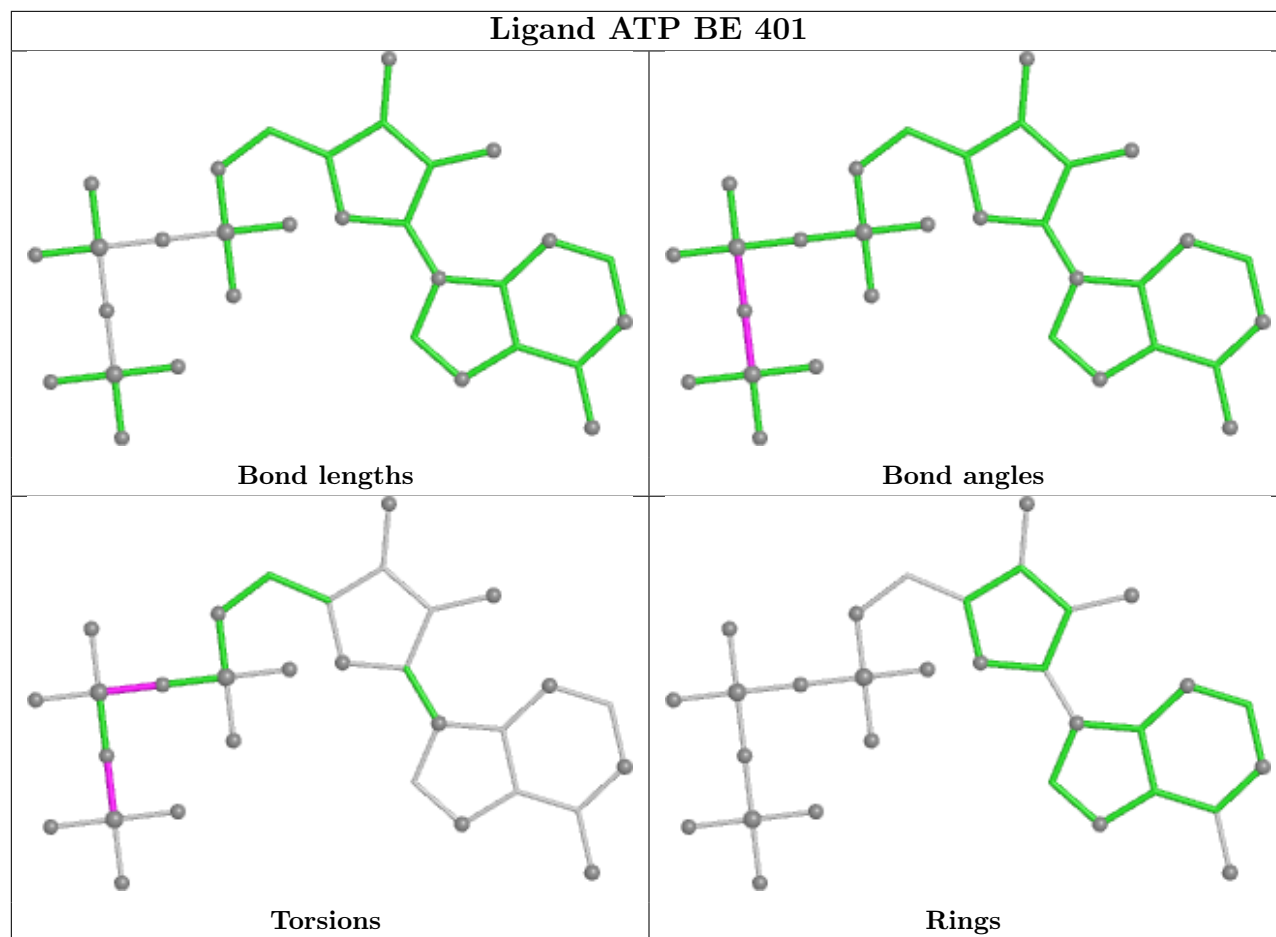




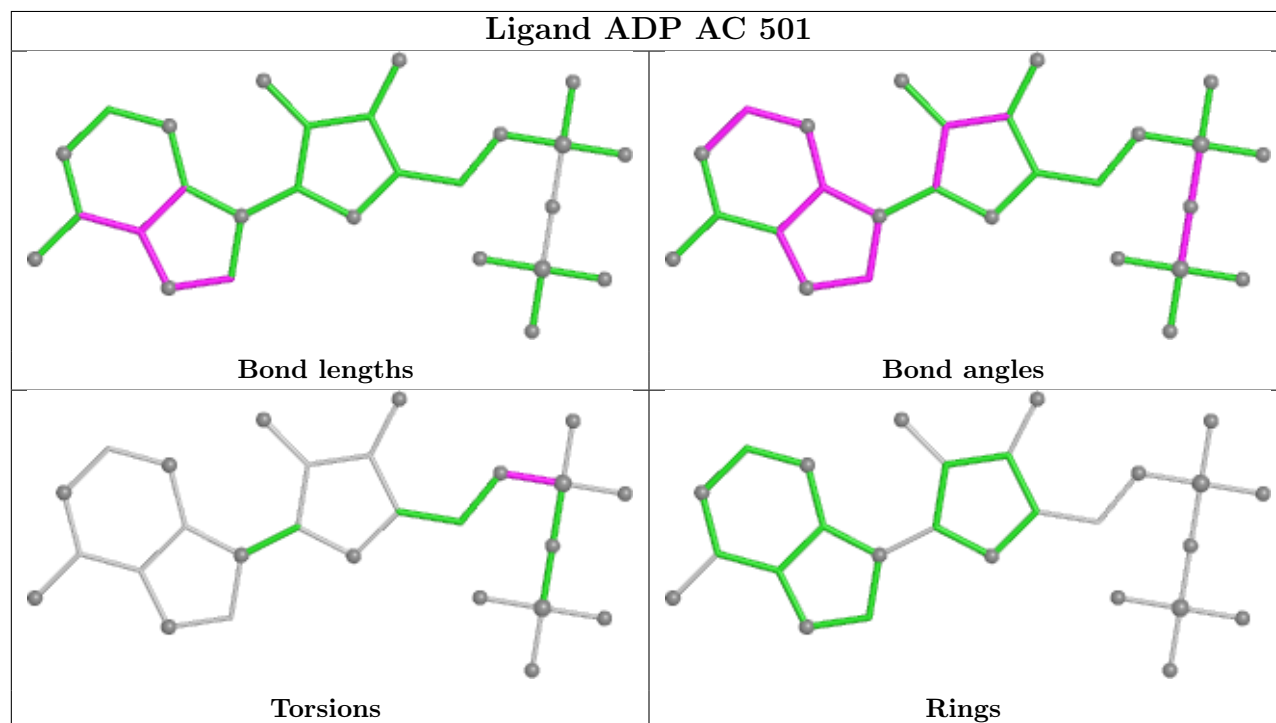




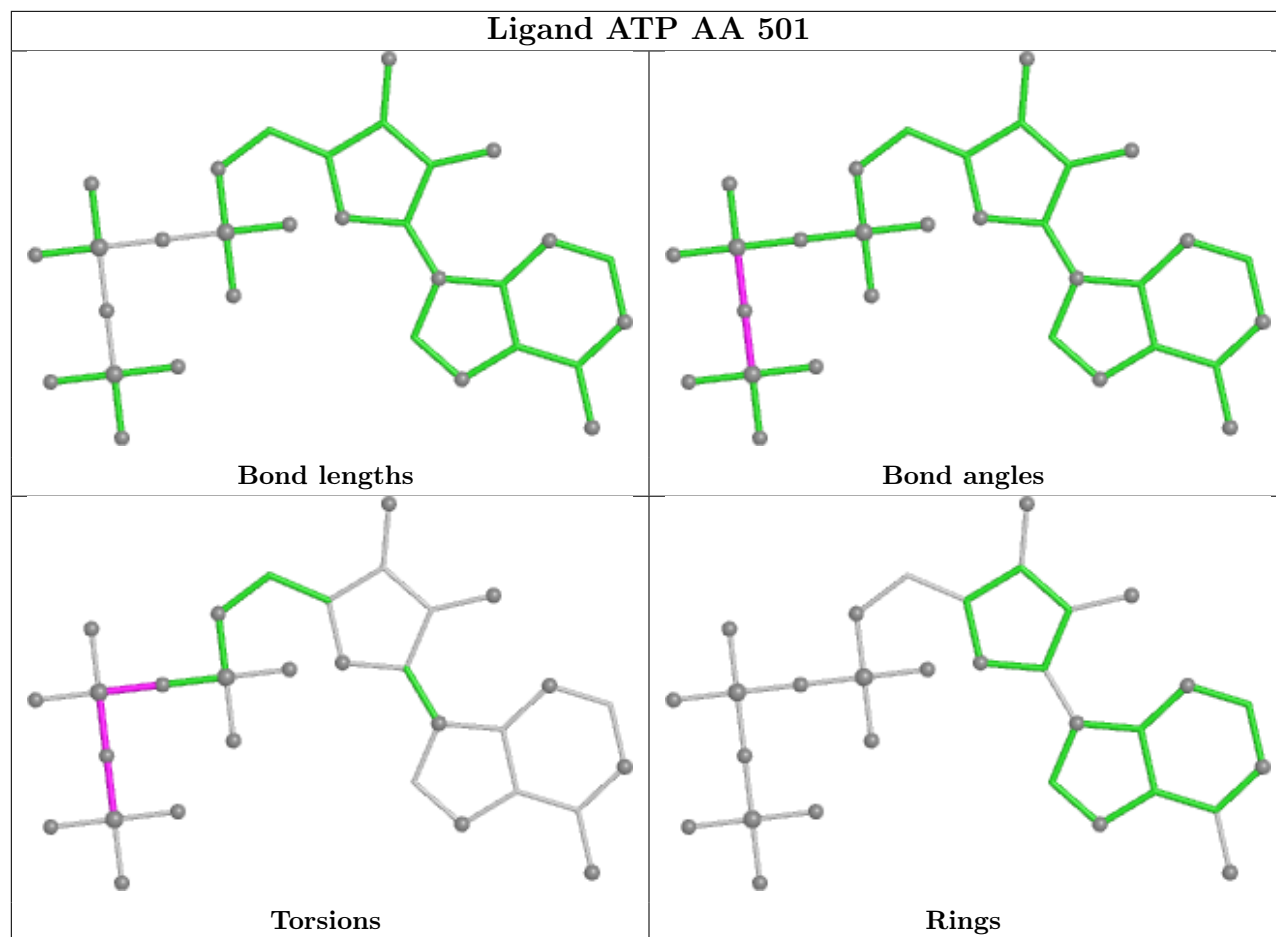
Ligand ATP BE 401



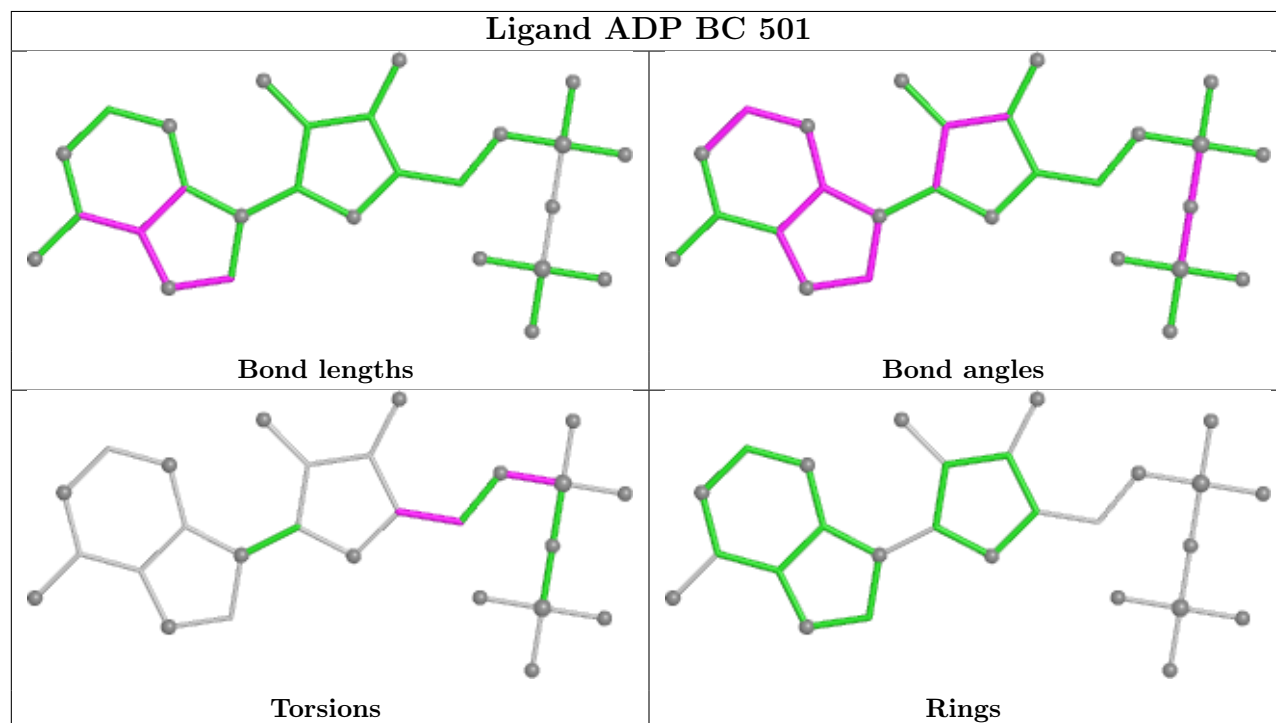
Ligand ADP AC 501

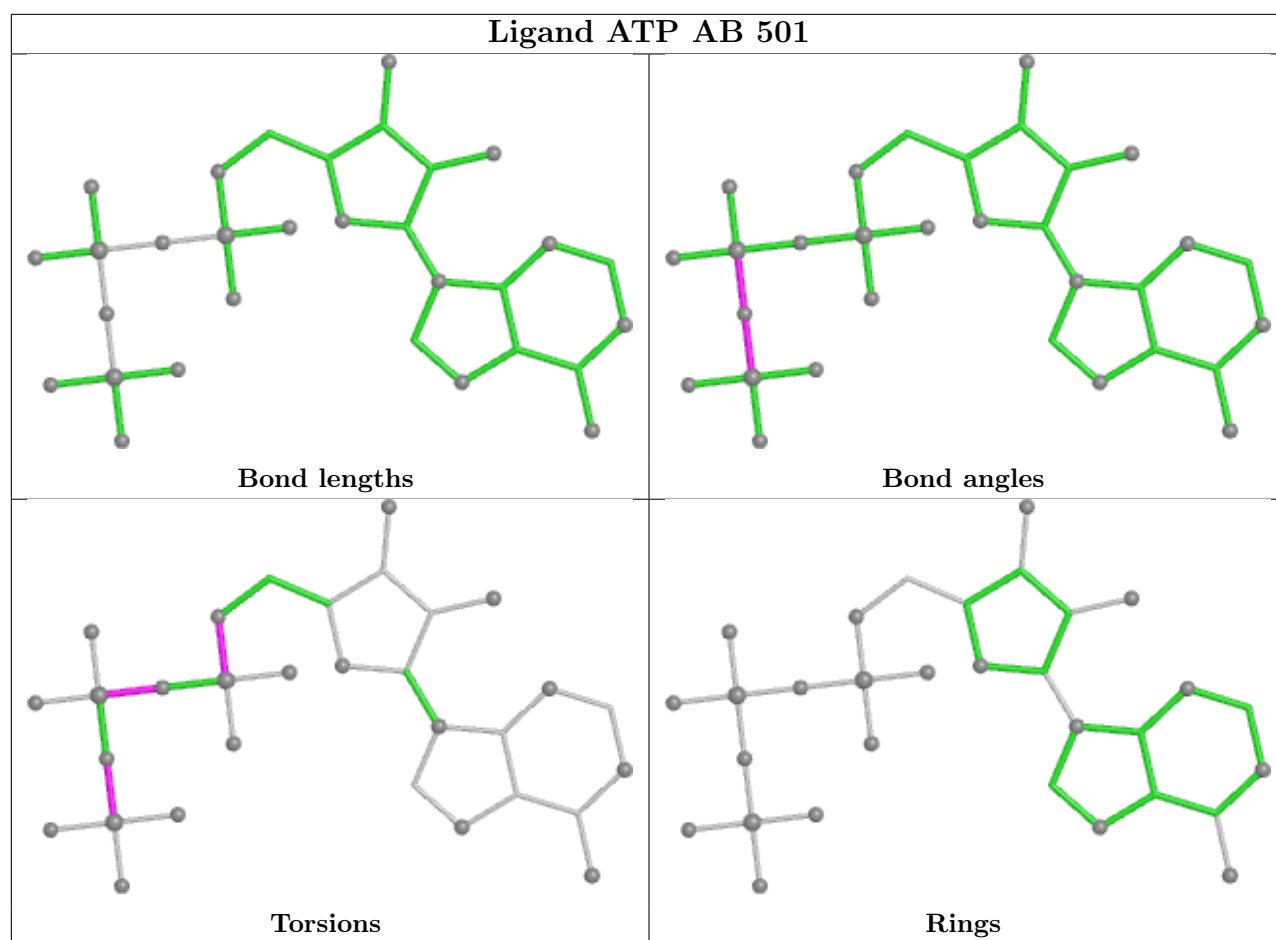


Ligand ATP AA 501



Ligand ADP BC 501





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.

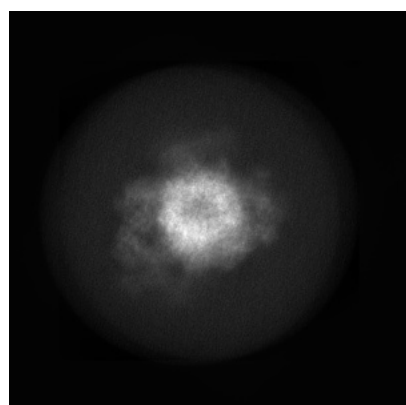
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62090. These allow visual inspection of the internal detail of the map and identification of artifacts.

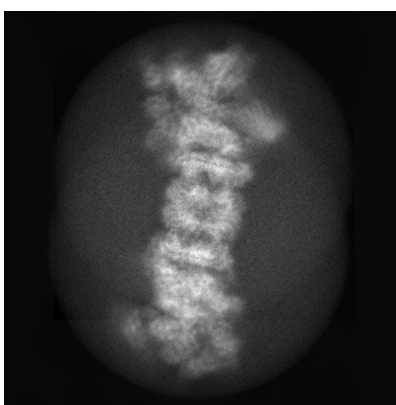
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

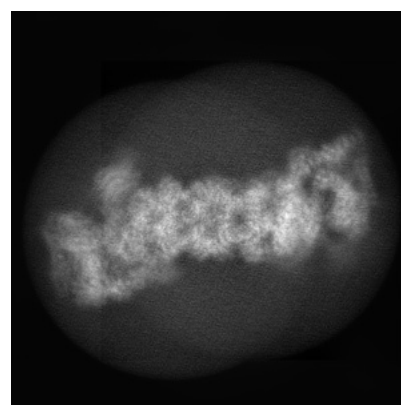
6.1.1 Primary map



X



Y

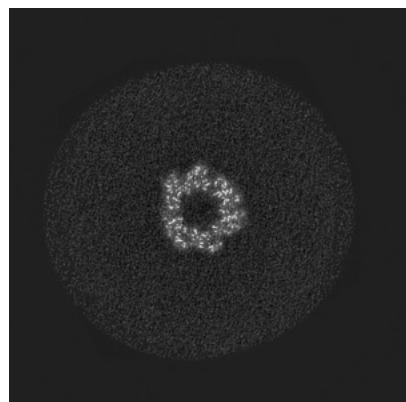


Z

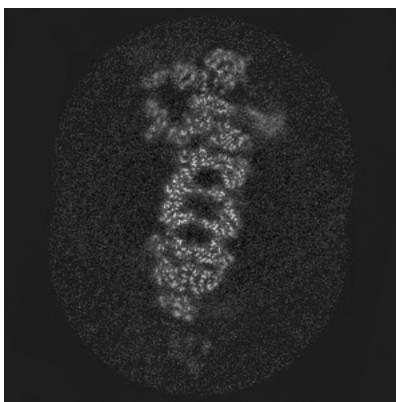
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

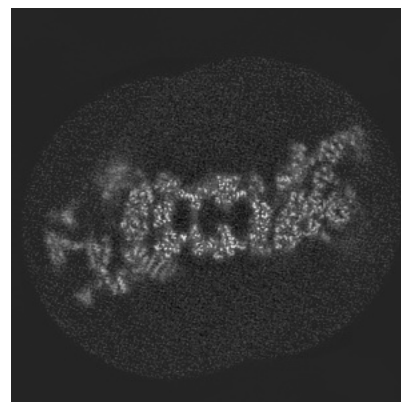
6.2.1 Primary map



X Index: 400



Y Index: 400

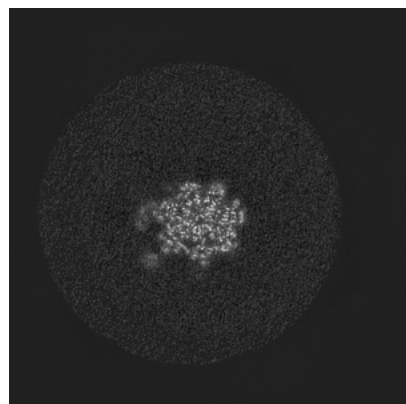


Z Index: 400

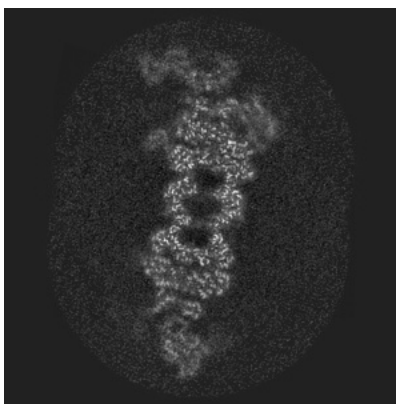
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

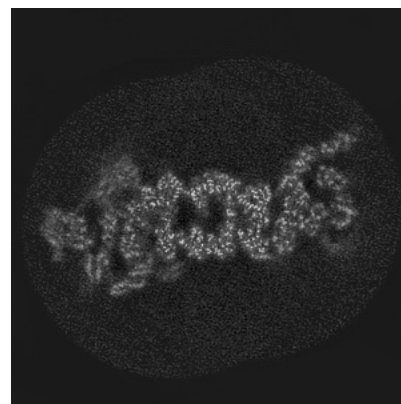
6.3.1 Primary map



X Index: 318



Y Index: 369

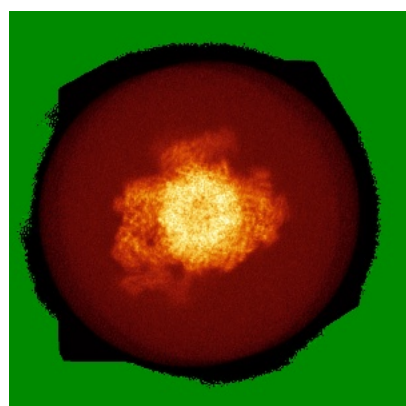


Z Index: 379

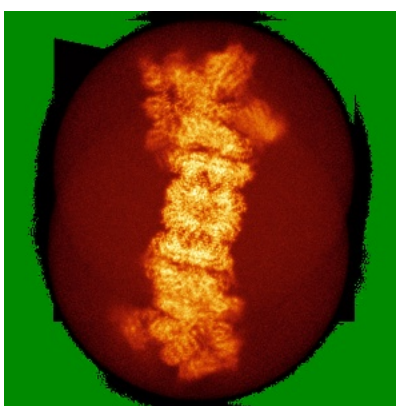
The images above show the largest variance slices of the map in three orthogonal directions.

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

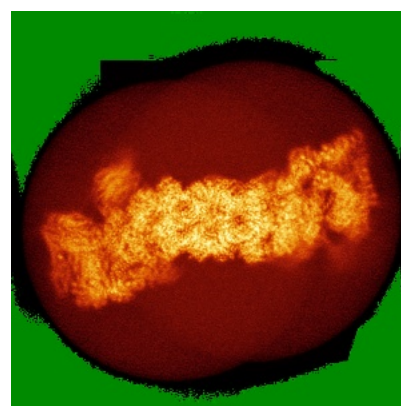
6.4.1 Primary map



X



Y

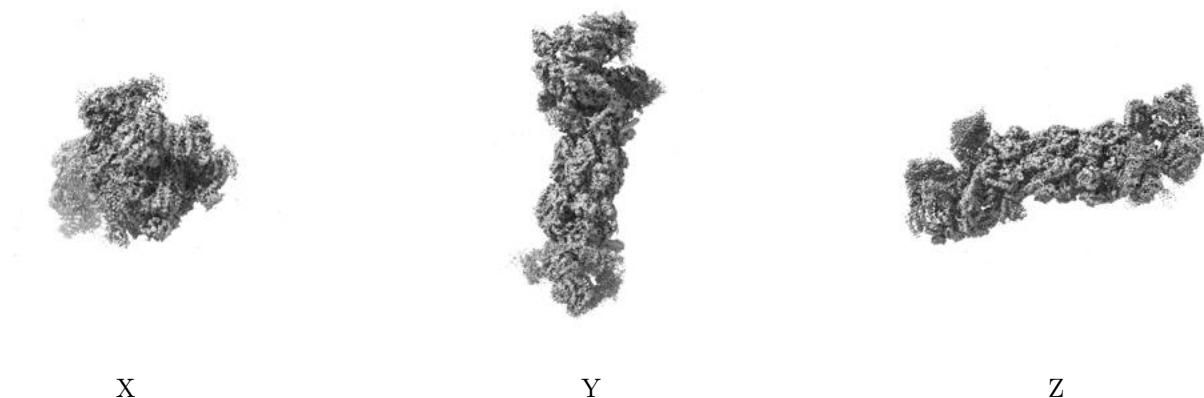


Z

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

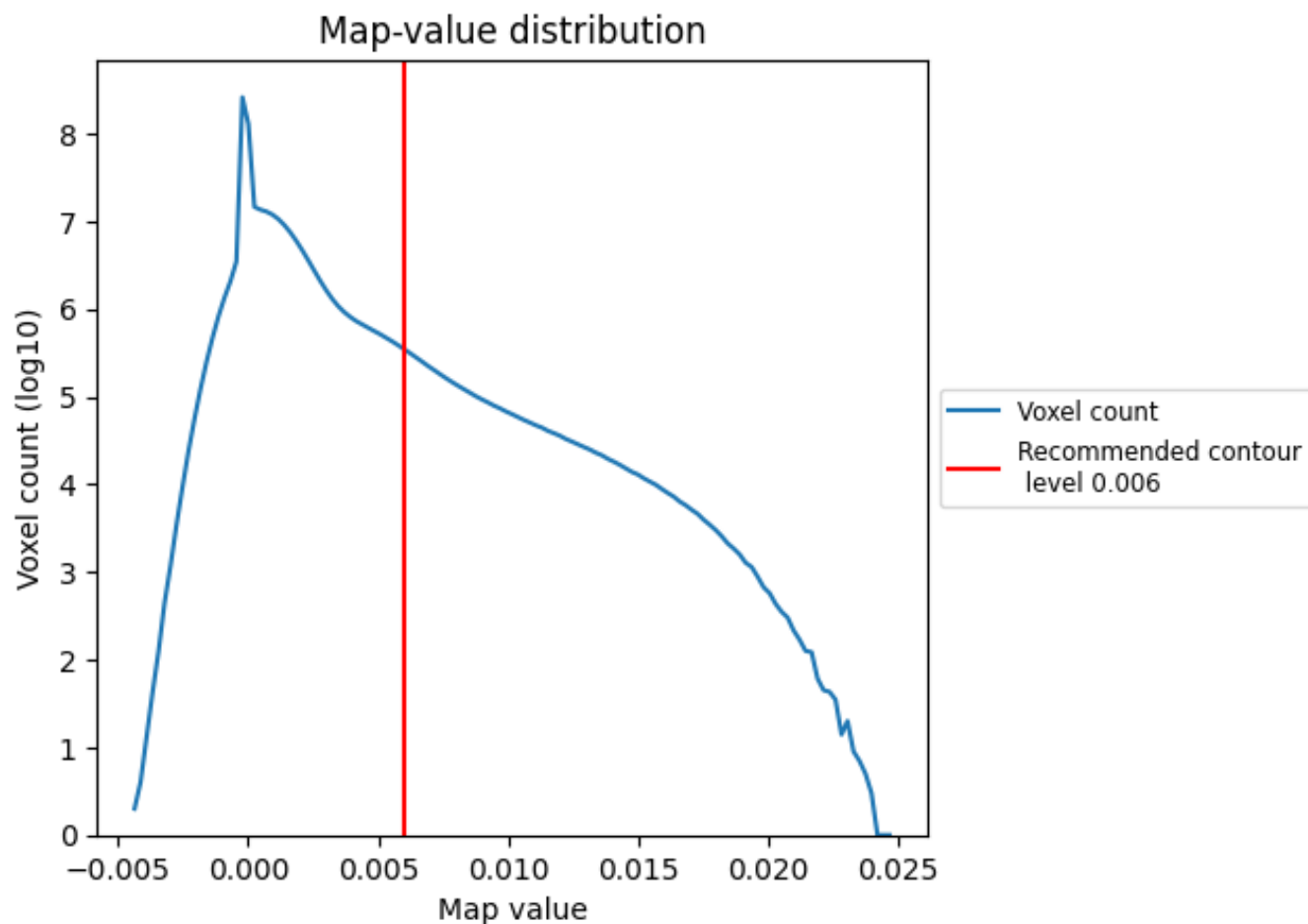
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

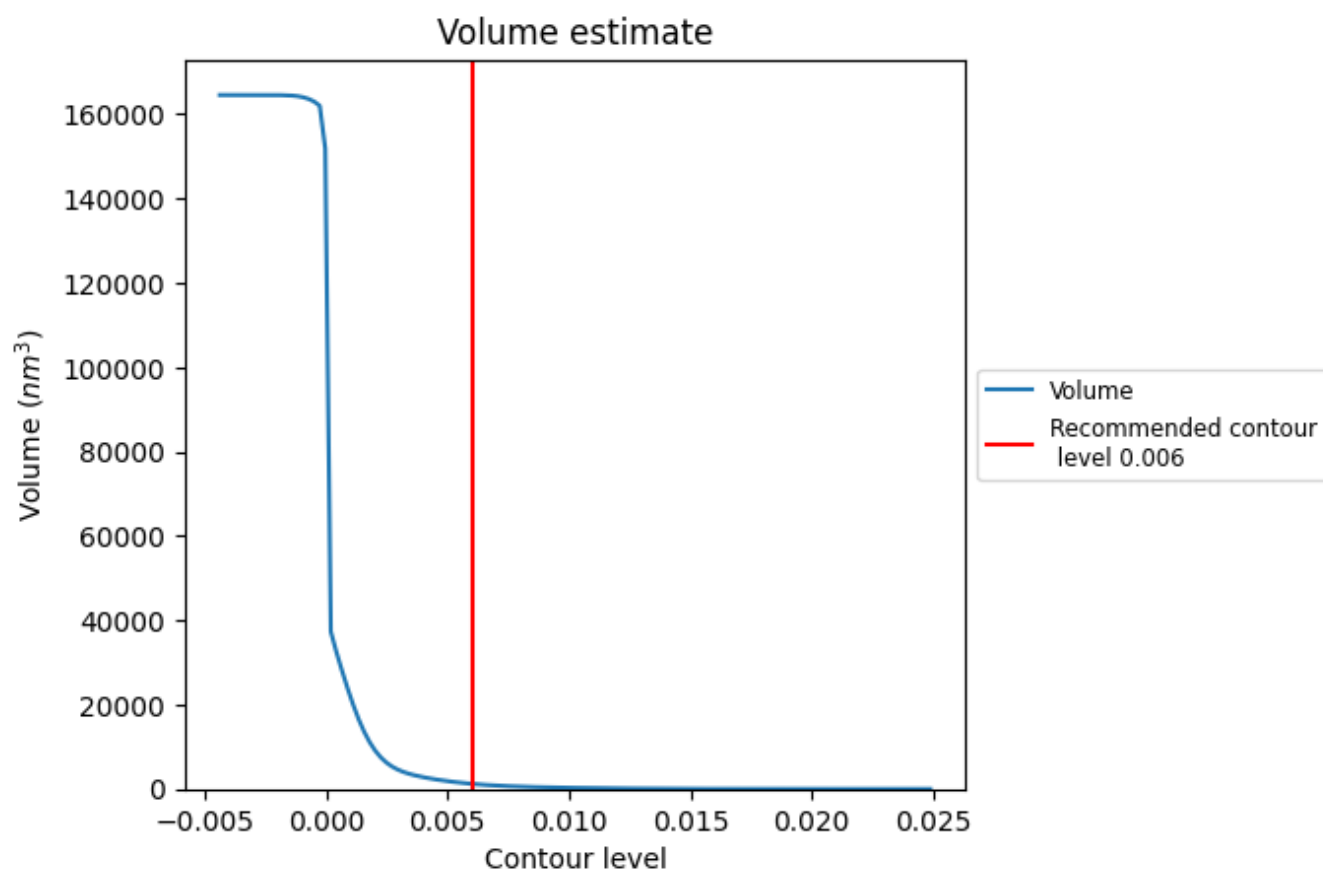
This section contains the results of statistical analysis of the map.

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.

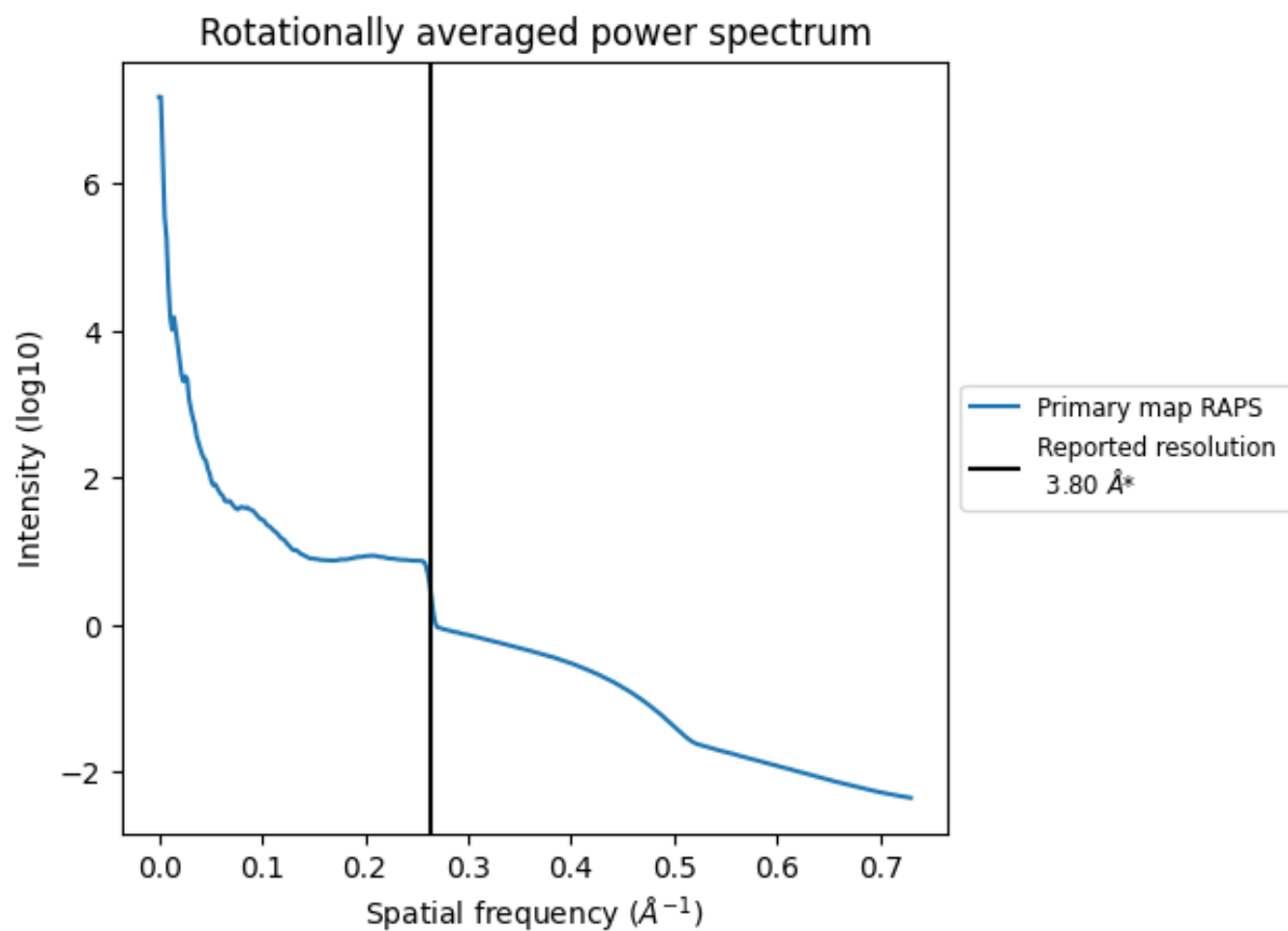
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1220 nm^3 ; this corresponds to an approximate mass of 1102 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)



*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

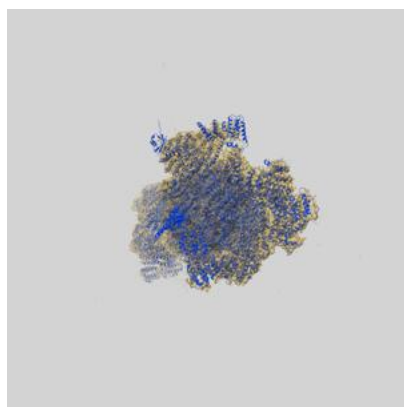
8 Fourier-Shell correlation

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

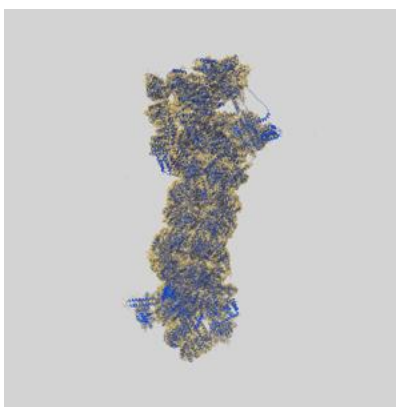
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-62090 and PDB model 9K5E. Per-residue inclusion information can be found in [section 3](#) on [page 15](#).

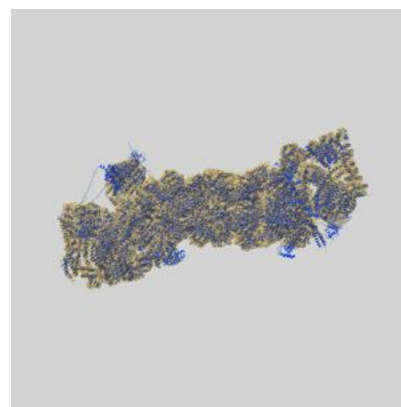
9.1 Map-model overlay [i](#)



X



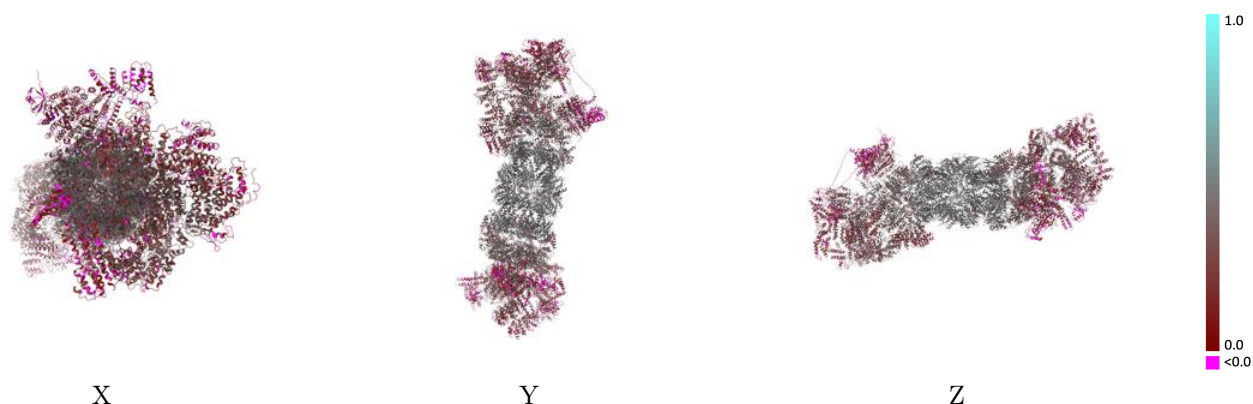
Y



Z

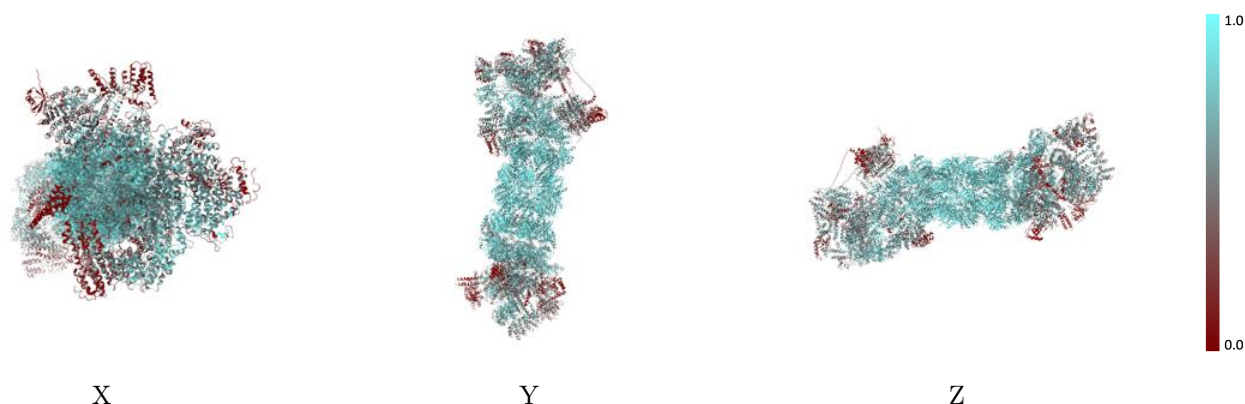
The images above show the 3D surface view of the map at the recommended contour level 0.006 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



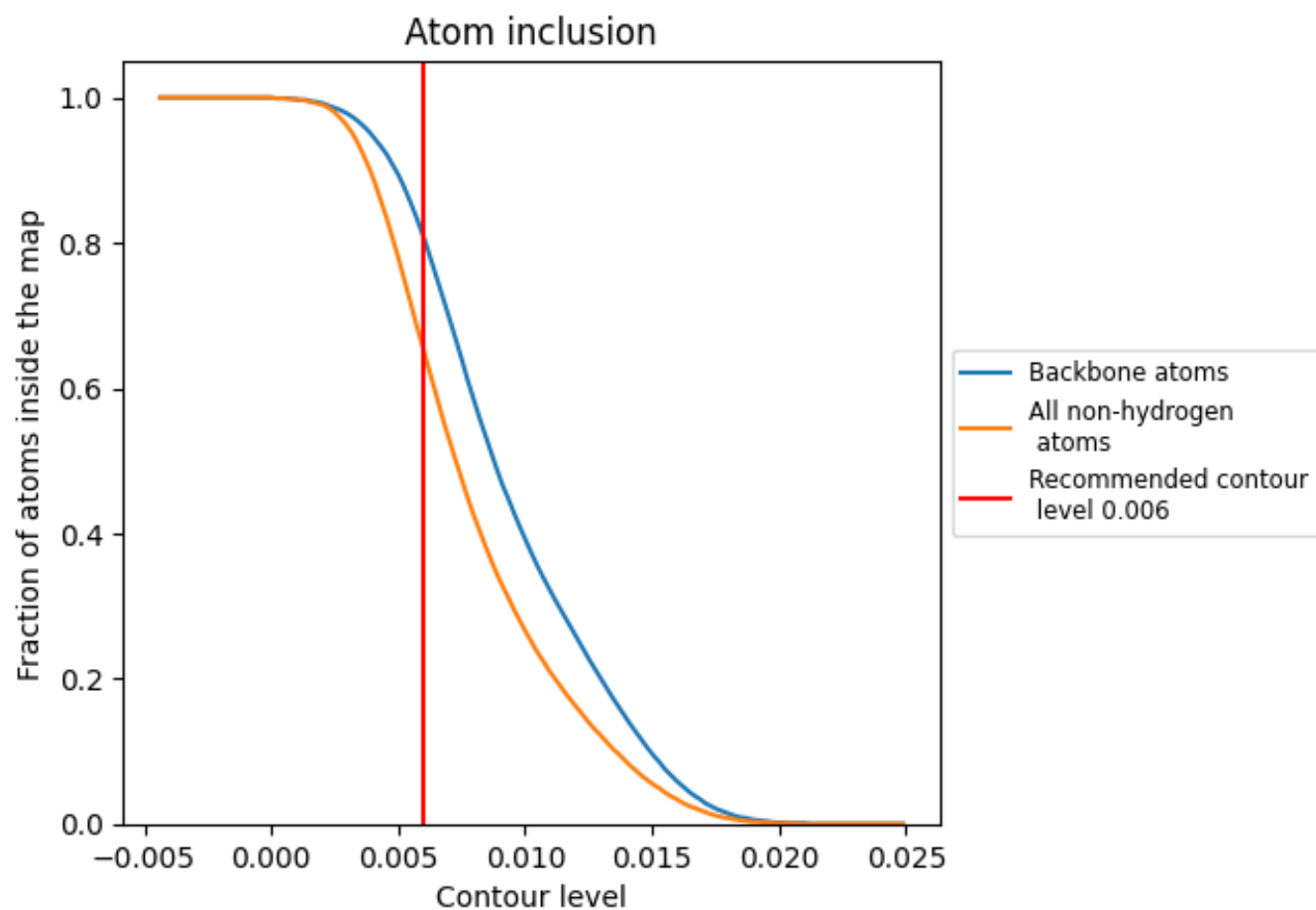
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.006).







































































9.4 Atom inclusion ⓘ



At the recommended contour level, 81% of all backbone atoms, 65% 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 (0.006) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6520	 0.3260
AA	 0.7320	 0.3500
AB	 0.7240	 0.3530
AC	 0.7510	 0.3710
AD	 0.7320	 0.3610
AE	 0.7400	 0.3610
AF	 0.7410	 0.3720
AG	 0.8700	 0.4430
AH	 0.8690	 0.4540
AI	 0.8460	 0.4350
AJ	 0.8370	 0.4210
AK	 0.8530	 0.4460
AL	 0.8890	 0.4590
AM	 0.8560	 0.4370
AN	 0.9030	 0.4630
AO	 0.9160	 0.4690
AP	 0.9030	 0.4610
AQ	 0.8870	 0.4620
AR	 0.9240	 0.4720
AS	 0.8910	 0.4600
AT	 0.8930	 0.4620
AU	 0.5340	 0.2320
AV	 0.4860	 0.2480
AW	 0.5730	 0.2760
AX	 0.4900	 0.2710
AY	 0.7270	 0.3140
AZ	 0.5390	 0.2720
Aa	 0.4310	 0.2070
Ab	 0.1880	 0.1460
Ac	 0.6150	 0.3230
Ad	 0.4070	 0.1900
Ae	 0.5270	 0.2850
Af	 0.3860	 0.1700
Au	 0.0030	 0.0460
Aw	 0.0070	 0.0790



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Chain	Atom inclusion	Q-score
BA	 0.7430	 0.3510
BB	 0.7260	 0.3540
BC	 0.7410	 0.3710
BD	 0.7220	 0.3610
BE	 0.7410	 0.3610
BF	 0.7580	 0.3740
BG	 0.8610	 0.4380
BH	 0.8660	 0.4470
BI	 0.8360	 0.4330
BJ	 0.8300	 0.4210
BK	 0.8390	 0.4410
BL	 0.8880	 0.4530
BM	 0.8590	 0.4490
BN	 0.8950	 0.4650
BO	 0.9060	 0.4630
BP	 0.8990	 0.4660
BQ	 0.8990	 0.4630
BR	 0.9070	 0.4680
BS	 0.9020	 0.4680
BT	 0.8950	 0.4690
BU	 0.5260	 0.2310
BV	 0.4660	 0.2290
BW	 0.5720	 0.2860
BX	 0.4920	 0.2750
BY	 0.7130	 0.3060
BZ	 0.5400	 0.2780
Ba	 0.4350	 0.2210
Bb	 0.1830	 0.1610
Bc	 0.6170	 0.3250
Bd	 0.3980	 0.1900
Be	 0.4650	 0.2530
Bf	 0.3600	 0.1780
Bu	 0.0030	 0.0970
Bw	 0.0080	 0.0740