



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 12:10 PM UTC

PDB ID : 9RAI / pdb_00009rai
EMDB ID : EMD-53879
Title : Structure of the S.aureus MecA/ClpC/ClpP degradation system
Authors : Azinas, S.; Wallden, K.; Katikaridis, P.; Schahl, A.; Mogk, A.; Carroni, M.
Deposited on : 2025-05-20
Resolution : 3.00 Å(reported)
Based on initial model : .

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

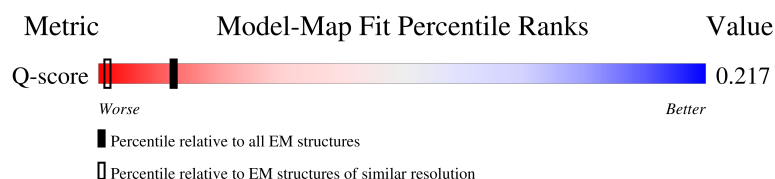
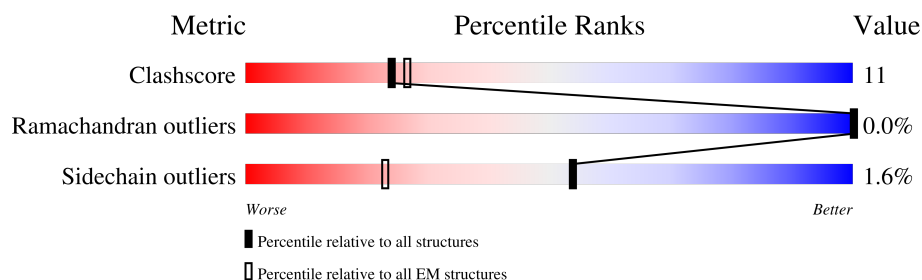
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 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	14081 (2.50 - 3.50)

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	239	25% 23% 18% 59%
1	B	239	31% 26% 15% 59%
1	C	239	10% 28% 13% 59%
1	D	239	9% 31% 10% 59%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	E	239	
1	F	239	
2	S	18	
3	a	818	
3	b	818	
3	c	818	
3	d	818	
3	e	818	
3	f	818	
4	G	195	
4	H	195	
4	I	195	
4	J	195	
4	K	195	
4	L	195	
4	M	195	
4	N	195	
4	O	195	
4	P	195	
4	Q	195	
4	R	195	
4	T	195	
4	U	195	

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 60975 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 Adapter protein MecA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	98	Total	C	N	O	S	0	0
			827	533	127	165	2		
1	B	98	Total	C	N	O	S	0	0
			827	533	127	165	2		
1	C	98	Total	C	N	O	S	0	0
			827	533	127	165	2		
1	D	98	Total	C	N	O	S	0	0
			827	533	127	165	2		
1	E	98	Total	C	N	O	S	0	0
			827	533	127	165	2		
1	F	98	Total	C	N	O	S	0	0
			827	533	127	165	2		

- Molecule 2 is a protein called unknown substrate.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	S	16	Total	C	N	O	0	0
			80	48	16	16		

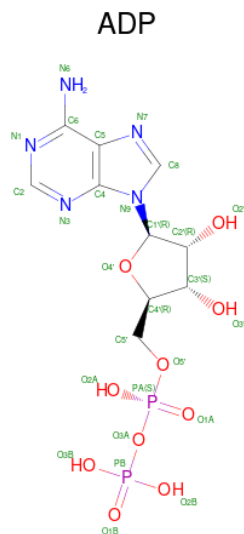
- Molecule 3 is a protein called ATP-dependent Clp protease ATP-binding subunit ClpC.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	a	710	Total	C	N	O	S	0	0
			5593	3508	989	1081	15		
3	b	767	Total	C	N	O	S	0	0
			6022	3769	1066	1172	15		
3	c	774	Total	C	N	O	S	0	0
			6081	3803	1076	1186	16		
3	d	762	Total	C	N	O	S	0	0
			5990	3751	1058	1166	15		
3	e	768	Total	C	N	O	S	0	0
			6036	3777	1067	1177	15		
3	f	752	Total	C	N	O	S	0	0
			5927	3711	1049	1152	15		

- Molecule 4 is a protein called ATP-dependent Clp protease proteolytic subunit.

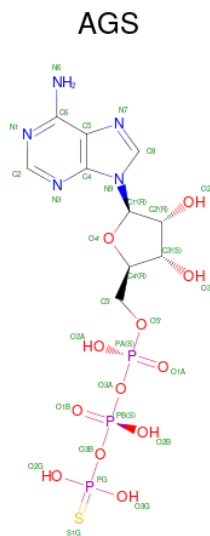
Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	190	Total	C	N	O	S	0	0
			1468	921	252	289	6		
4	H	190	Total	C	N	O	S	0	0
			1468	921	252	289	6		
4	I	189	Total	C	N	O	S	0	0
			1459	916	251	286	6		
4	J	190	Total	C	N	O	S	0	0
			1468	921	252	289	6		
4	K	188	Total	C	N	O	S	0	0
			1445	908	245	286	6		
4	L	190	Total	C	N	O	S	0	0
			1468	921	252	289	6		
4	M	182	Total	C	N	O	S	0	0
			1403	884	237	276	6		
4	N	183	Total	C	N	O	S	0	0
			1411	890	238	277	6		
4	O	182	Total	C	N	O	S	0	0
			1402	885	237	274	6		
4	P	182	Total	C	N	O	S	0	0
			1402	885	237	274	6		
4	Q	184	Total	C	N	O	S	0	0
			1422	896	242	278	6		
4	R	183	Total	C	N	O	S	0	0
			1413	891	241	275	6		
4	T	179	Total	C	N	O	S	0	0
			1377	867	234	270	6		
4	U	179	Total	C	N	O	S	0	0
			1377	867	234	270	6		

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



Mol	Chain	Residues	Atoms					AltConf
5	a	1	Total 27	C 10	N 5	O 10	P 2	0
5	b	1	Total 27	C 10	N 5	O 10	P 2	0
5	e	1	Total 27	C 10	N 5	O 10	P 2	0
5	f	1	Total 27	C 10	N 5	O 10	P 2	0

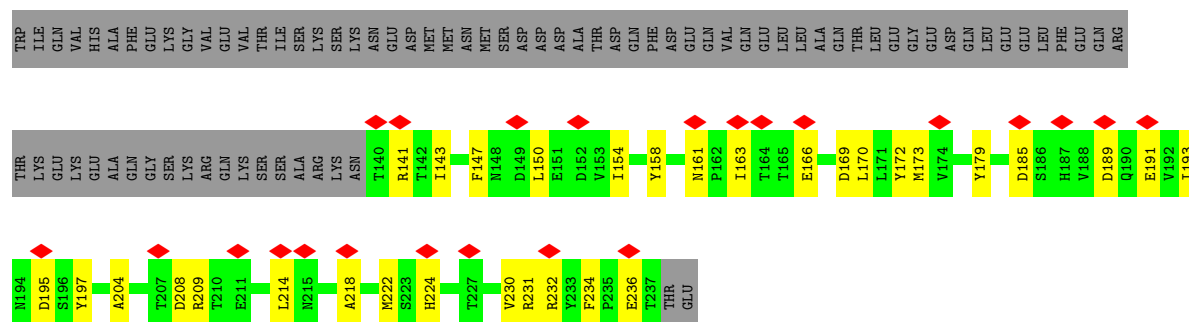
- Molecule 6 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: $\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{12}\text{P}_3\text{S}$) (labeled as "Ligand of Interest" by depositor).



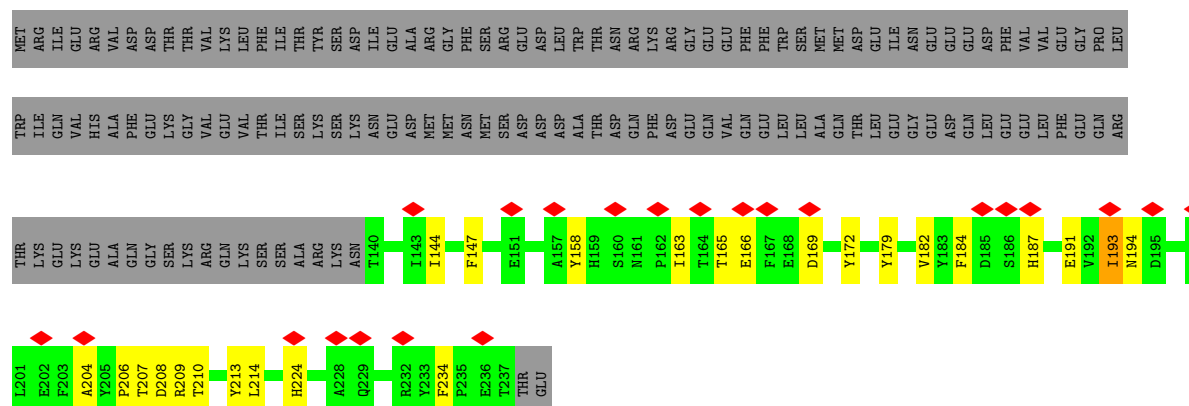
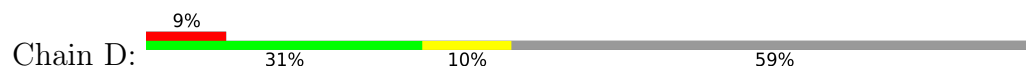
Mol	Chain	Residues	Atoms						AltConf
6	b	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
6	c	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
6	c	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
6	c	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
6	d	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
6	e	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

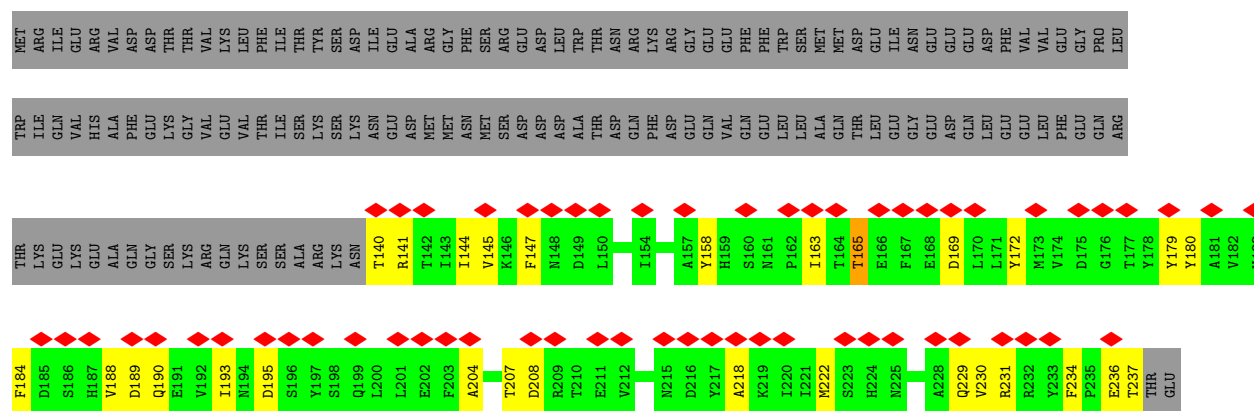
Mol	Chain	Residues	Atoms		AltConf
7	b	1	Total	Mg	0
			1	1	
7	c	2	Total	Mg	0
			2	2	
7	d	2	Total	Mg	0
			2	2	
7	e	2	Total	Mg	0
			2	2	



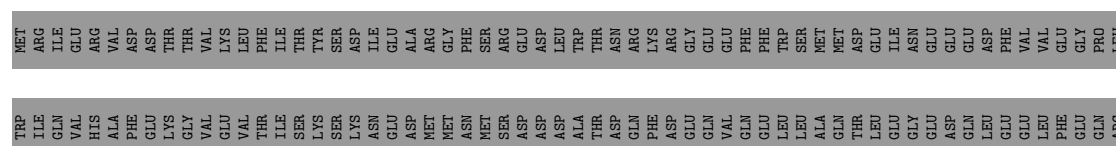
• Molecule 1: Adapter protein MecA

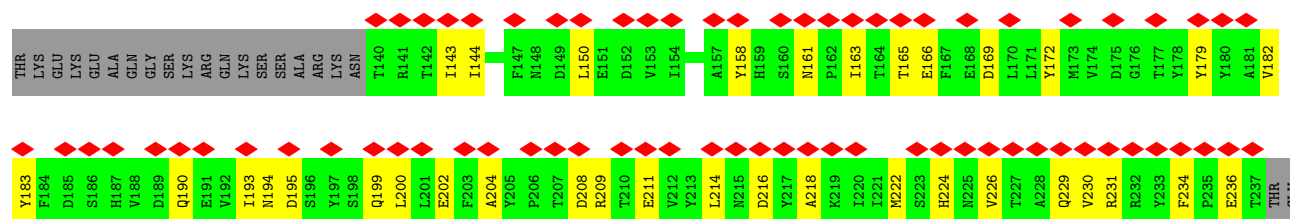


• Molecule 1: Adapter protein MecA

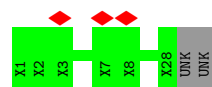
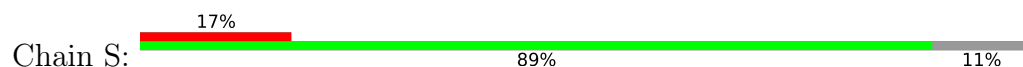


• Molecule 1: Adapter protein MecA

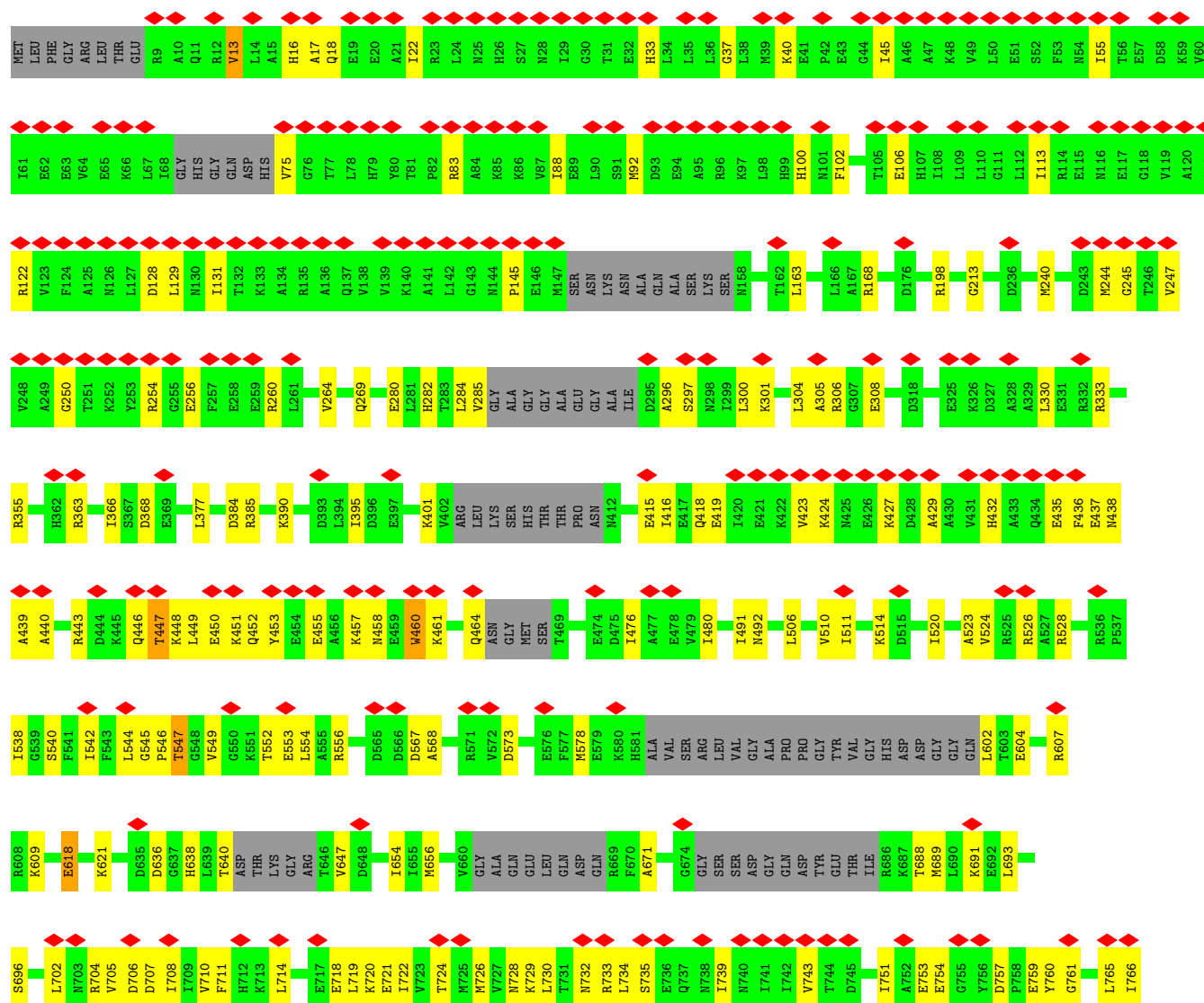


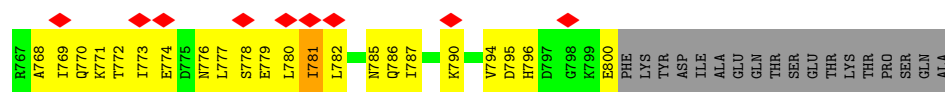


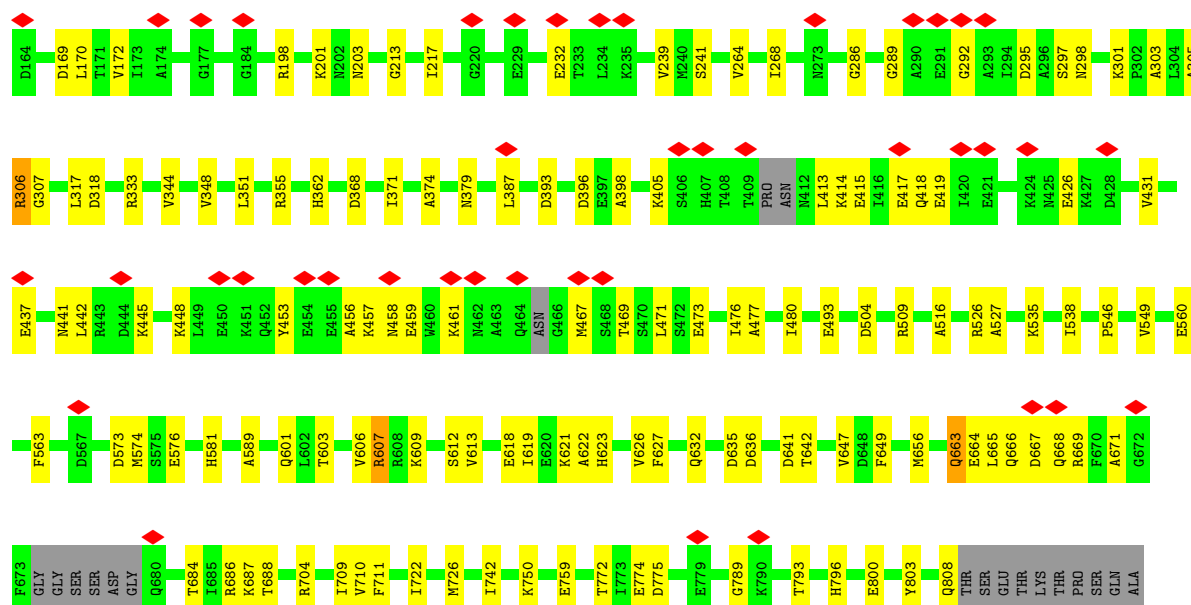
- Molecule 2: unknown substrate



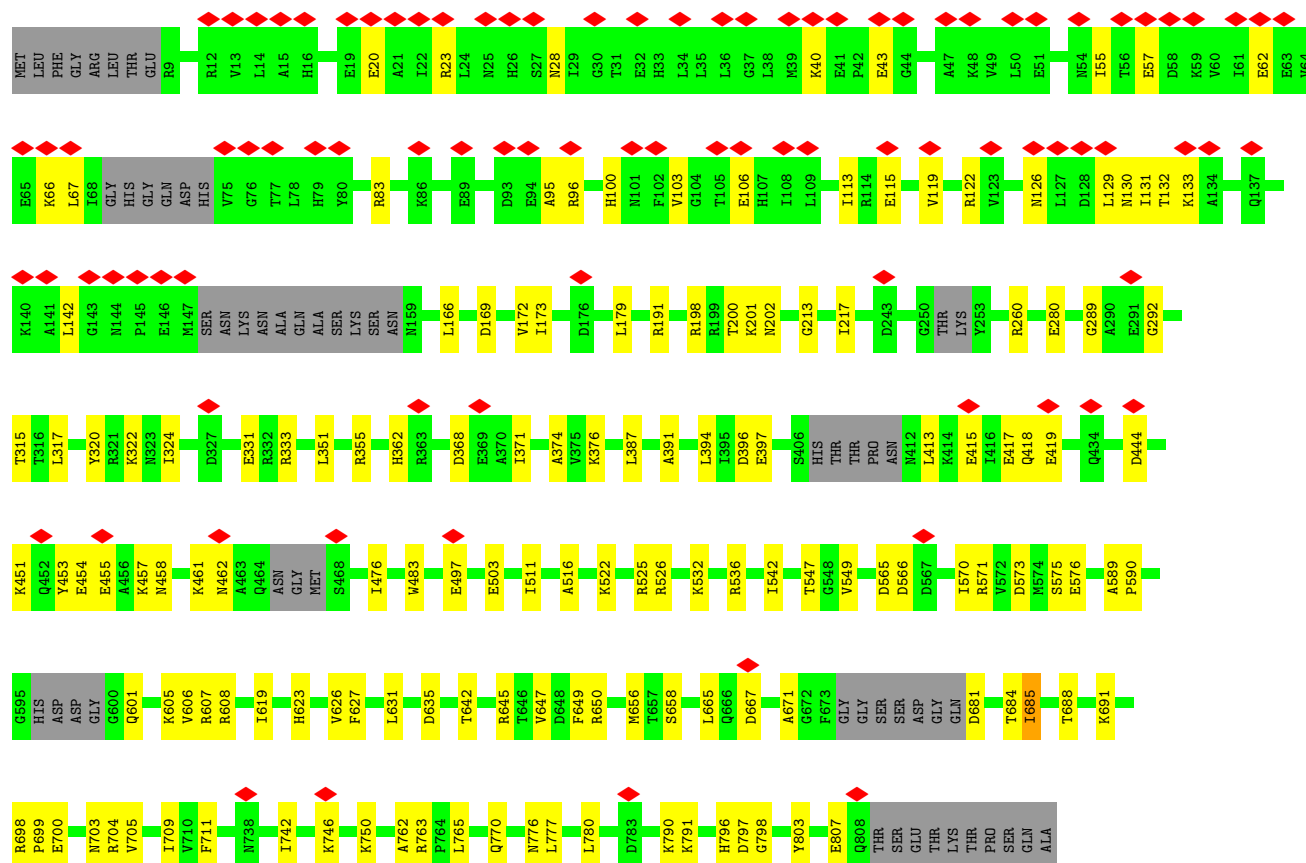
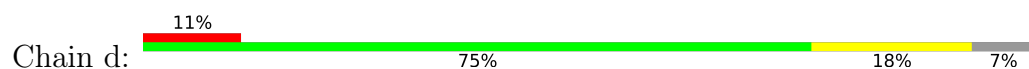
- Molecule 3: ATP-dependent Clp protease ATP-binding subunit ClpC



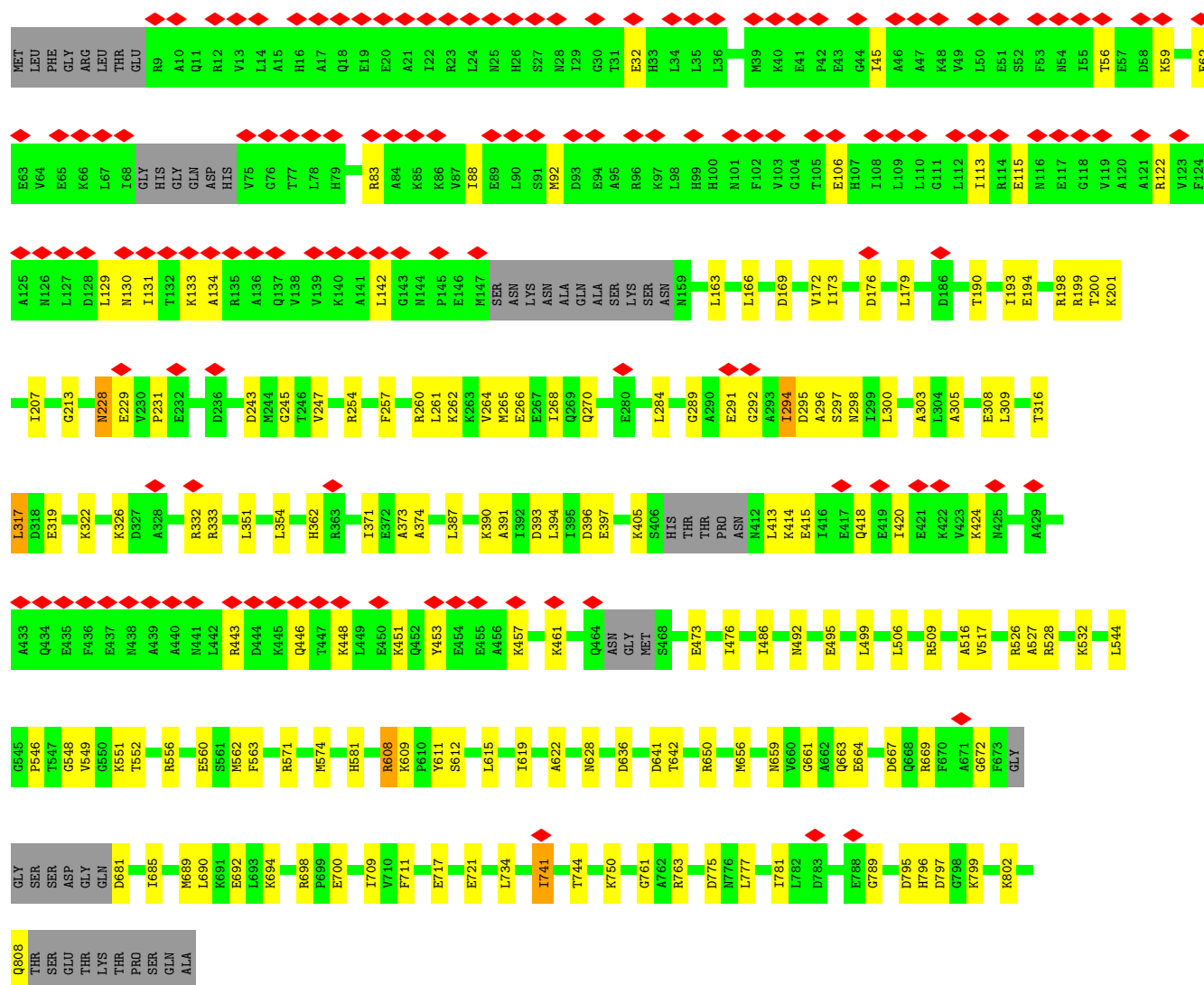




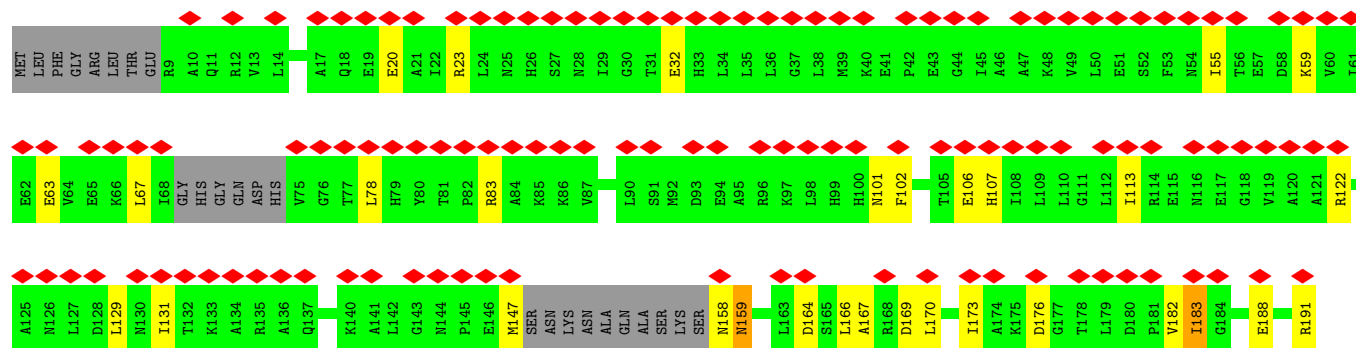
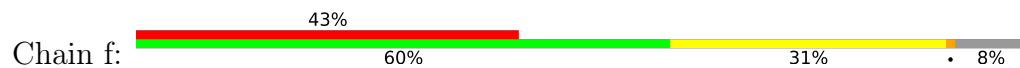
• Molecule 3: ATP-dependent Clp protease ATP-binding subunit ClpC

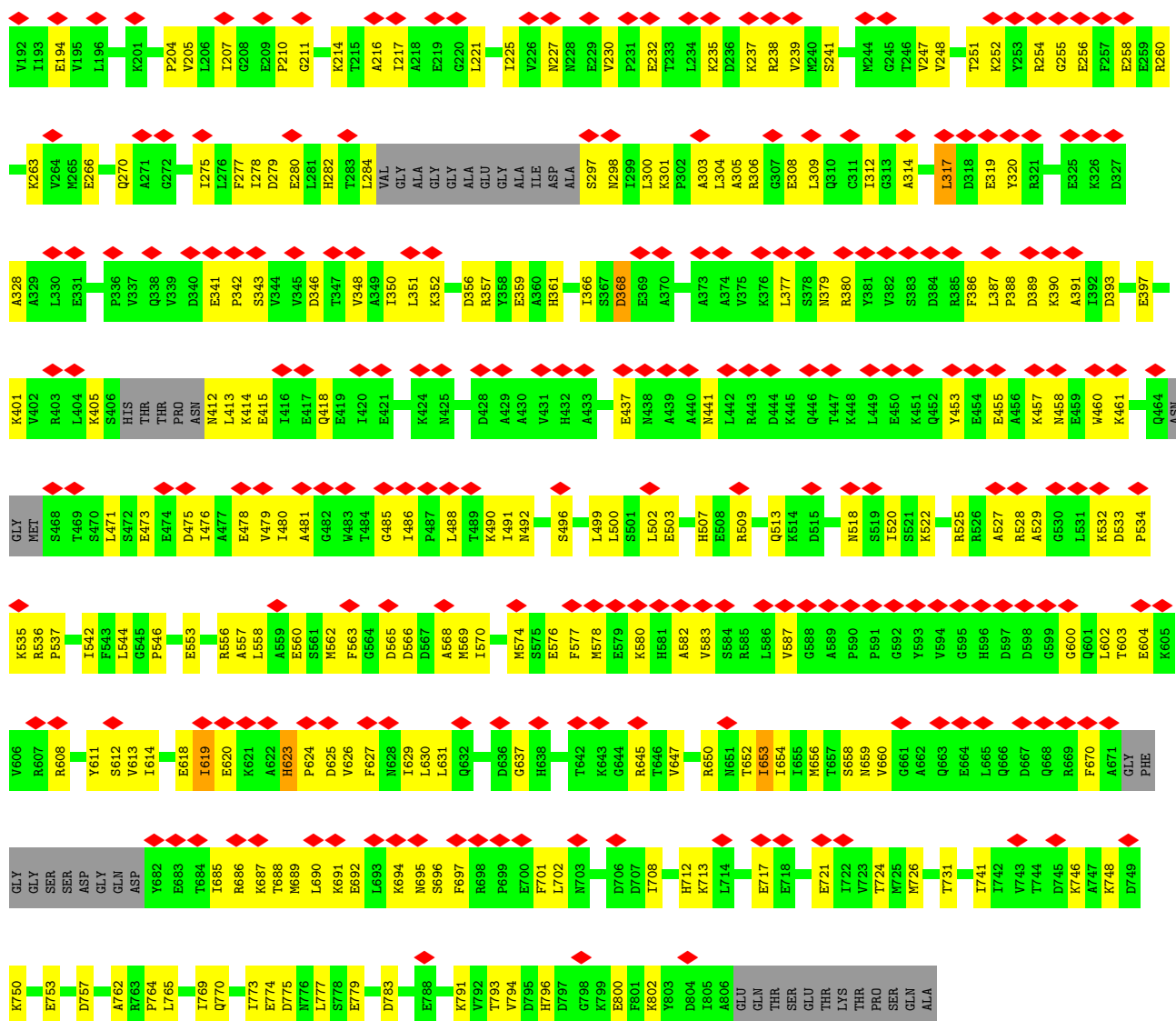


• Molecule 3: ATP-dependent Clp protease ATP-binding subunit ClpC

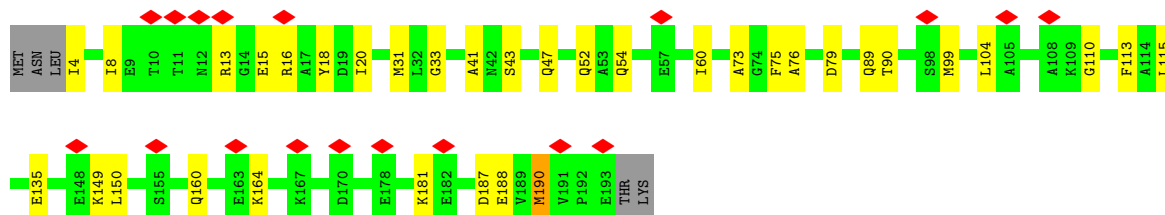
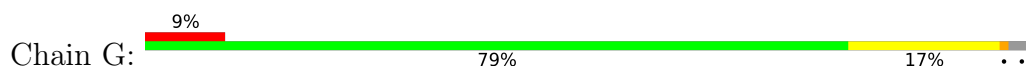


• Molecule 3: ATP-dependent Clp protease ATP-binding subunit ClpC



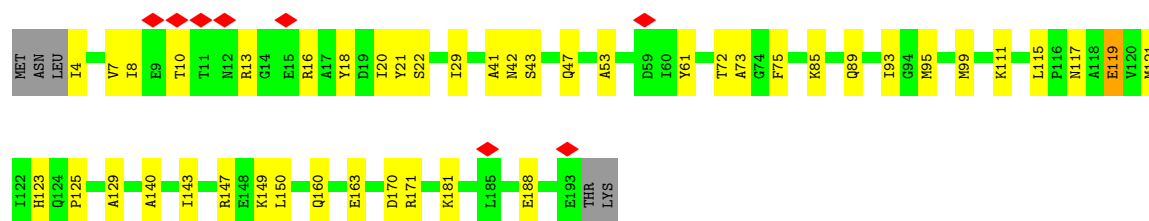


• Molecule 4: ATP-dependent Clp protease proteolytic subunit

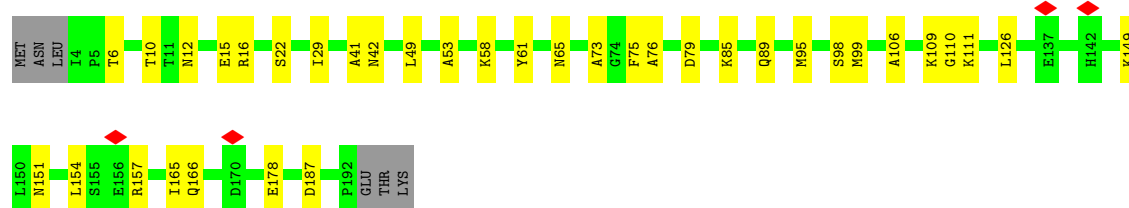
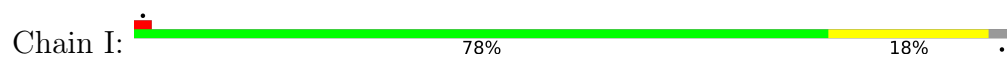


• Molecule 4: ATP-dependent Clp protease proteolytic subunit

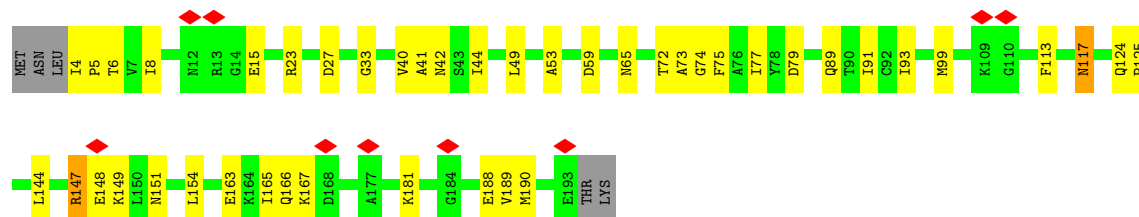
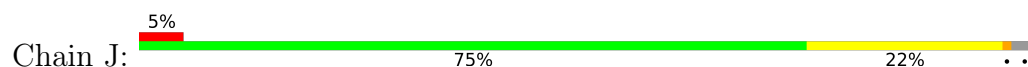




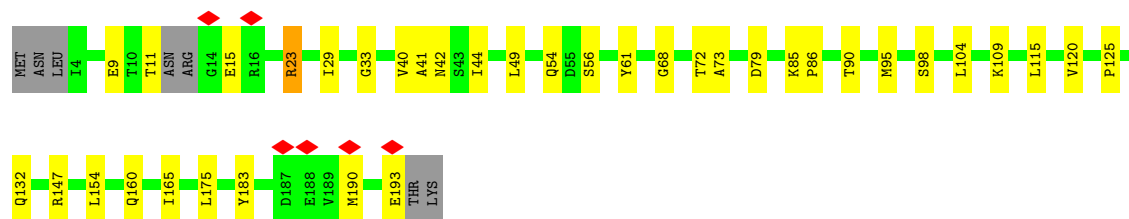
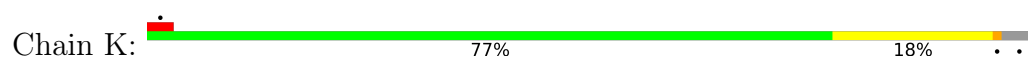
- Molecule 4: ATP-dependent Clp protease proteolytic subunit



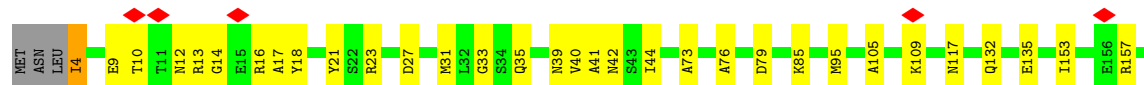
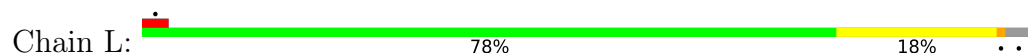
- Molecule 4: ATP-dependent Clp protease proteolytic subunit



- Molecule 4: ATP-dependent Clp protease proteolytic subunit

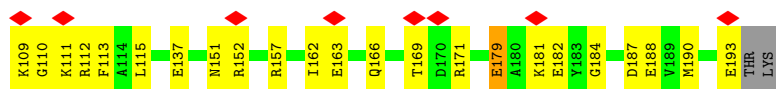


- Molecule 4: ATP-dependent Clp protease proteolytic subunit

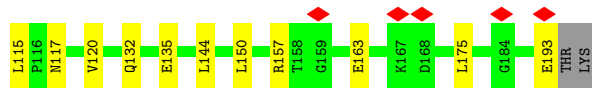
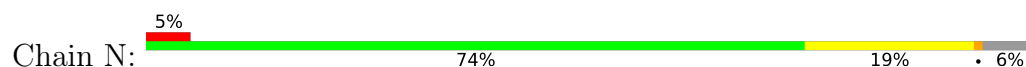




- Molecule 4: ATP-dependent Clp protease proteolytic subunit



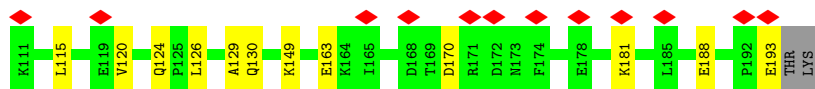
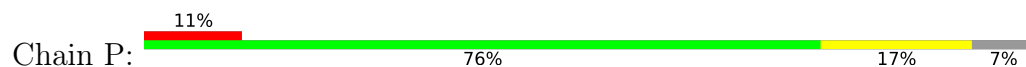
- Molecule 4: ATP-dependent Clp protease proteolytic subunit



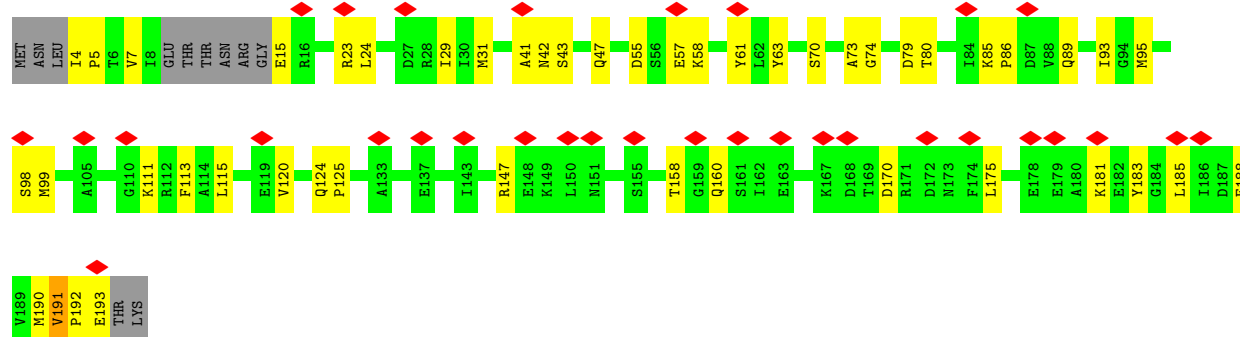
- Molecule 4: ATP-dependent Clp protease proteolytic subunit



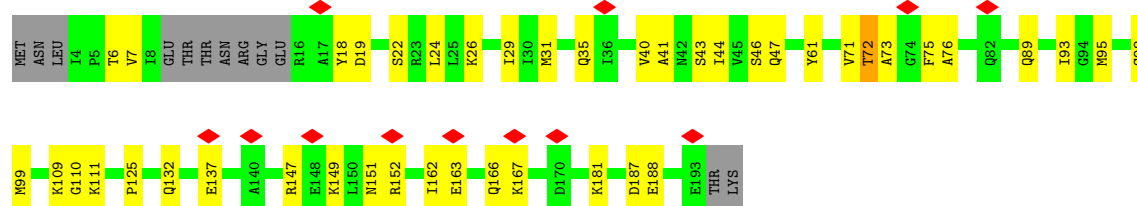
- Molecule 4: ATP-dependent Clp protease proteolytic subunit



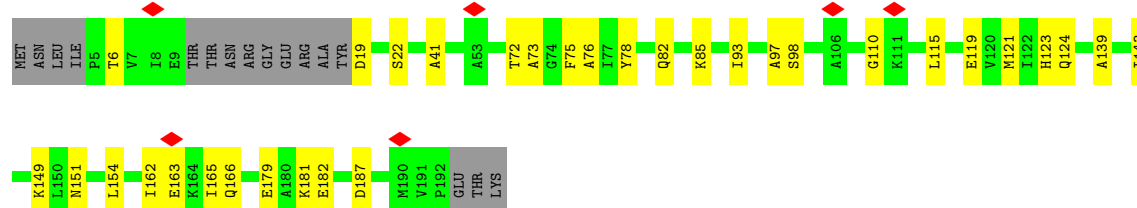
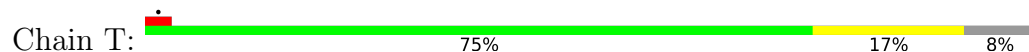
- Molecule 4: ATP-dependent Clp protease proteolytic subunit



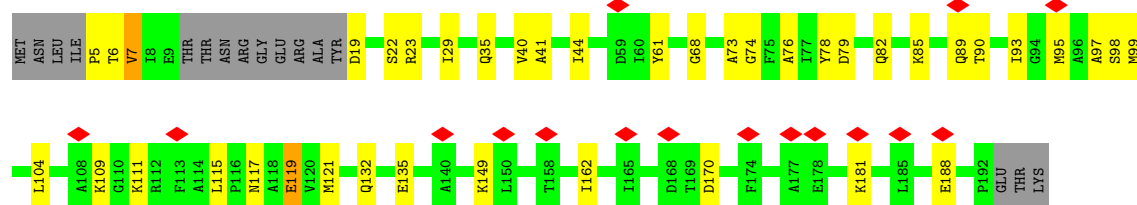
- Molecule 4: ATP-dependent Clp protease proteolytic subunit



- Molecule 4: ATP-dependent Clp protease proteolytic subunit



- Molecule 4: ATP-dependent Clp protease proteolytic subunit



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	82854	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.366	Depositor
Minimum map value	-0.004	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.031	Depositor
Recommended contour level	0.08	Depositor
Map size (Å)	397.6, 397.6, 397.6	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.994, 0.994, 0.994	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.19	0/849	0.49	0/1160
1	B	0.15	0/849	0.38	0/1160
1	C	0.16	0/849	0.38	0/1160
1	D	0.15	0/849	0.37	0/1160
1	E	0.16	0/849	0.40	0/1160
1	F	0.17	0/849	0.40	0/1160
3	a	0.16	0/5654	0.43	1/7609 (0.0%)
3	b	0.15	0/6094	0.35	0/8207
3	c	0.16	0/6154	0.42	4/8288 (0.0%)
3	d	0.15	0/6059	0.37	0/8157
3	e	0.16	0/6108	0.39	0/8226
3	f	0.17	0/5997	0.46	0/8077
4	G	0.15	0/1487	0.35	0/2008
4	H	0.14	0/1487	0.31	0/2008
4	I	0.14	0/1478	0.34	0/1996
4	J	0.13	0/1487	0.31	0/2008
4	K	0.15	0/1464	0.35	0/1979
4	L	0.14	0/1487	0.34	0/2008
4	M	0.17	0/1421	0.42	0/1917
4	N	0.14	0/1429	0.32	0/1929
4	O	0.15	0/1420	0.33	0/1917
4	P	0.14	0/1420	0.33	0/1917
4	Q	0.15	0/1440	0.34	0/1943
4	R	0.15	0/1431	0.37	0/1931
4	T	0.15	0/1394	0.33	0/1880
4	U	0.15	0/1394	0.33	0/1880
All	All	0.16	0/61399	0.38	5/82845 (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
3	c	0	2

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	c	306	ARG	CG-CD-NE	-9.08	92.02	112.00
3	c	306	ARG	CB-CG-CD	6.66	126.61	111.30
3	a	618	GLU	CA-CB-CG	5.91	125.93	114.10
3	c	306	ARG	N-CA-C	5.81	117.36	109.11
3	c	306	ARG	CA-CB-CG	5.81	125.72	114.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	c	306	ARG	Peptide,Sidechain

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	827	0	768	39	0
1	B	827	0	768	28	0
1	C	827	0	768	28	0
1	D	827	0	768	14	0
1	E	827	0	768	24	0
1	F	827	0	768	29	0
2	S	80	0	20	0	0
3	a	5593	0	5709	150	0
3	b	6022	0	6125	116	0
3	c	6081	0	6173	135	0
3	d	5990	0	6092	118	0
3	e	6036	0	6133	130	0
3	f	5927	0	6031	218	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	G	1468	0	1480	23	0
4	H	1468	0	1480	31	0
4	I	1459	0	1474	28	0
4	J	1468	0	1480	32	0
4	K	1445	0	1450	30	0
4	L	1468	0	1480	29	0
4	M	1403	0	1414	40	0
4	N	1411	0	1424	29	0
4	O	1402	0	1418	34	0
4	P	1402	0	1418	22	0
4	Q	1422	0	1437	35	0
4	R	1413	0	1431	28	0
4	T	1377	0	1394	22	0
4	U	1377	0	1394	29	0
5	a	27	0	12	1	0
5	b	27	0	11	1	0
5	e	27	0	12	2	0
5	f	27	0	12	1	0
6	b	31	0	12	2	0
6	c	93	0	35	9	0
6	d	31	0	12	8	0
6	e	31	0	12	2	0
7	b	1	0	0	0	0
7	c	2	0	0	0	0
7	d	2	0	0	0	0
7	e	2	0	0	0	0
All	All	60975	0	61183	1313	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 11.

The worst 5 of 1313 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:a:13:VAL:O	3:a:16:HIS:ND1	2.04	0.91
3:f:414:LYS:HD2	3:f:414:LYS:H	1.39	0.88
3:e:228:ASN:ND2	3:e:228:ASN:O	2.10	0.85
3:b:13:VAL:O	3:b:16:HIS:ND1	2.11	0.84
4:O:95:MET:HB2	4:P:72:THR:HG21	1.60	0.83

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	96/239 (40%)	91 (95%)	5 (5%)	0	100	100
1	B	96/239 (40%)	90 (94%)	6 (6%)	0	100	100
1	C	96/239 (40%)	91 (95%)	5 (5%)	0	100	100
1	D	96/239 (40%)	93 (97%)	3 (3%)	0	100	100
1	E	96/239 (40%)	91 (95%)	5 (5%)	0	100	100
1	F	96/239 (40%)	91 (95%)	5 (5%)	0	100	100
3	a	690/818 (84%)	665 (96%)	23 (3%)	2 (0%)	36	70
3	b	755/818 (92%)	735 (97%)	20 (3%)	0	100	100
3	c	762/818 (93%)	731 (96%)	30 (4%)	1 (0%)	48	80
3	d	746/818 (91%)	728 (98%)	18 (2%)	0	100	100
3	e	756/818 (92%)	738 (98%)	18 (2%)	0	100	100
3	f	738/818 (90%)	713 (97%)	25 (3%)	0	100	100
4	G	188/195 (96%)	186 (99%)	2 (1%)	0	100	100
4	H	188/195 (96%)	183 (97%)	5 (3%)	0	100	100
4	I	187/195 (96%)	182 (97%)	5 (3%)	0	100	100
4	J	188/195 (96%)	183 (97%)	5 (3%)	0	100	100
4	K	186/195 (95%)	179 (96%)	7 (4%)	0	100	100
4	L	188/195 (96%)	183 (97%)	5 (3%)	0	100	100
4	M	178/195 (91%)	174 (98%)	4 (2%)	0	100	100
4	N	179/195 (92%)	172 (96%)	7 (4%)	0	100	100
4	O	178/195 (91%)	173 (97%)	5 (3%)	0	100	100
4	P	178/195 (91%)	173 (97%)	5 (3%)	0	100	100
4	Q	180/195 (92%)	175 (97%)	5 (3%)	0	100	100
4	R	179/195 (92%)	174 (97%)	5 (3%)	0	100	100
4	T	175/195 (90%)	174 (99%)	1 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	U	175/195 (90%)	173 (99%)	2 (1%)	0	100	100
All	All	7570/9072 (83%)	7341 (97%)	226 (3%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	a	511	ILE
3	c	101	ASN
3	a	547	THR

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	92/221 (42%)	91 (99%)	1 (1%)	65	83
1	B	92/221 (42%)	90 (98%)	2 (2%)	45	74
1	C	92/221 (42%)	88 (96%)	4 (4%)	26	60
1	D	92/221 (42%)	87 (95%)	5 (5%)	20	53
1	E	92/221 (42%)	89 (97%)	3 (3%)	33	67
1	F	92/221 (42%)	91 (99%)	1 (1%)	65	83
3	a	610/695 (88%)	600 (98%)	10 (2%)	55	79
3	b	653/695 (94%)	645 (99%)	8 (1%)	63	82
3	c	660/695 (95%)	652 (99%)	8 (1%)	63	82
3	d	650/695 (94%)	644 (99%)	6 (1%)	70	85
3	e	655/695 (94%)	649 (99%)	6 (1%)	70	85
3	f	646/695 (93%)	632 (98%)	14 (2%)	45	74
4	G	158/163 (97%)	155 (98%)	3 (2%)	50	76
4	H	158/163 (97%)	155 (98%)	3 (2%)	50	76
4	I	157/163 (96%)	155 (99%)	2 (1%)	61	81
4	J	158/163 (97%)	155 (98%)	3 (2%)	50	76

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	K	155/163 (95%)	154 (99%)	1 (1%)	78	88
4	L	158/163 (97%)	155 (98%)	3 (2%)	50	76
4	M	151/163 (93%)	148 (98%)	3 (2%)	48	76
4	N	152/163 (93%)	151 (99%)	1 (1%)	76	86
4	O	151/163 (93%)	147 (97%)	4 (3%)	40	72
4	P	151/163 (93%)	148 (98%)	3 (2%)	48	76
4	Q	153/163 (94%)	150 (98%)	3 (2%)	48	76
4	R	152/163 (93%)	149 (98%)	3 (2%)	48	76
4	T	149/163 (91%)	148 (99%)	1 (1%)	76	86
4	U	149/163 (91%)	144 (97%)	5 (3%)	32	66
All	All	6578/7778 (85%)	6472 (98%)	106 (2%)	54	79

5 of 106 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	f	278	ILE
4	H	117	ASN
4	R	109	LYS
3	f	317	LEU
3	f	623	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 67 such sidechains are listed below:

Mol	Chain	Res	Type
4	O	151	ASN
4	P	124	GLN
4	T	124	GLN
3	c	796	HIS
3	c	703	ASN

5.3.3 RNA ⓘ

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 17 ligands modelled in this entry, 7 are monoatomic - leaving 10 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$
6	AGS	b	901	7	32,33,33	0.50	1 (3%)	45,52,52	0.65	1 (2%)
6	AGS	c	901	-	32,33,33	0.49	1 (3%)	45,52,52	0.62	1 (2%)
6	AGS	c	902	-	32,33,33	0.51	1 (3%)	45,52,52	0.64	1 (2%)
5	ADP	e	901	7	28,29,29	1.42	4 (14%)	43,45,45	1.85	8 (18%)
6	AGS	c	905	-	32,33,33	0.63	1 (3%)	45,52,52	0.93	3 (6%)
5	ADP	f	901	-	28,29,29	1.41	4 (14%)	43,45,45	1.88	8 (18%)
5	ADP	b	902	-	28,29,29	1.49	4 (14%)	43,45,45	1.85	10 (23%)
6	AGS	e	902	7	32,33,33	0.55	1 (3%)	45,52,52	0.77	1 (2%)
5	ADP	a	901	-	28,29,29	1.41	4 (14%)	43,45,45	1.86	8 (18%)
6	AGS	d	901	7	32,33,33	0.48	1 (3%)	45,52,52	0.72	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
6	AGS	b	901	7	-	5/21/38/38	0/3/3/3
6	AGS	c	901	-	-	2/21/38/38	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	AGS	c	902	-	-	5/21/38/38	0/3/3/3
5	ADP	e	901	7	-	4/16/32/32	0/3/3/3
6	AGS	c	905	-	-	9/21/38/38	0/3/3/3
5	ADP	f	901	-	-	2/16/32/32	0/3/3/3
5	ADP	b	902	-	-	3/16/32/32	0/3/3/3
6	AGS	e	902	7	-	7/21/38/38	0/3/3/3
5	ADP	a	901	-	-	3/16/32/32	0/3/3/3
6	AGS	d	901	7	-	8/21/38/38	0/3/3/3

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	b	902	ADP	C5-C4	4.96	1.47	1.39
5	e	901	ADP	C5-C4	4.75	1.47	1.39
5	f	901	ADP	C5-C4	4.70	1.47	1.39
5	a	901	ADP	C5-C4	4.69	1.47	1.39
5	b	902	ADP	C5-C6	2.92	1.49	1.41

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	e	901	ADP	C5-C4-N3	-6.16	118.24	126.72
5	f	901	ADP	C5-C4-N3	-6.15	118.25	126.72
5	a	901	ADP	C5-C4-N3	-5.86	118.65	126.72
5	b	902	ADP	C5-C4-N3	-5.47	119.18	126.72
5	f	901	ADP	N3-C4-N9	4.96	135.60	127.17

There are no chirality outliers.

5 of 48 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	a	901	ADP	C5'-O5'-PA-O2A
5	a	901	ADP	C5'-O5'-PA-O3A
5	b	902	ADP	C5'-O5'-PA-O1A
5	b	902	ADP	C5'-O5'-PA-O3A
5	e	901	ADP	C5'-O5'-PA-O3A

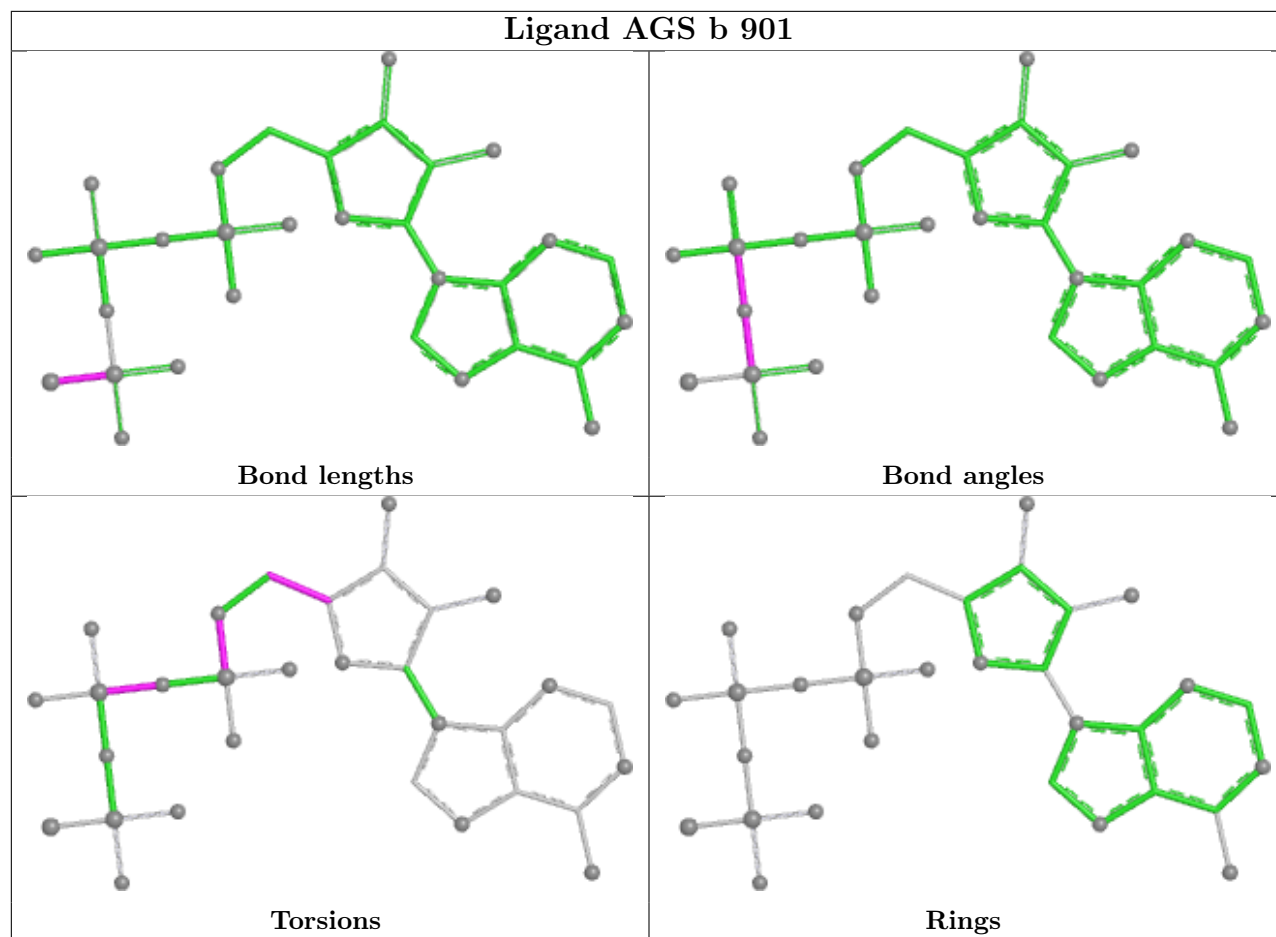
There are no ring outliers.

10 monomers are involved in 26 short contacts:

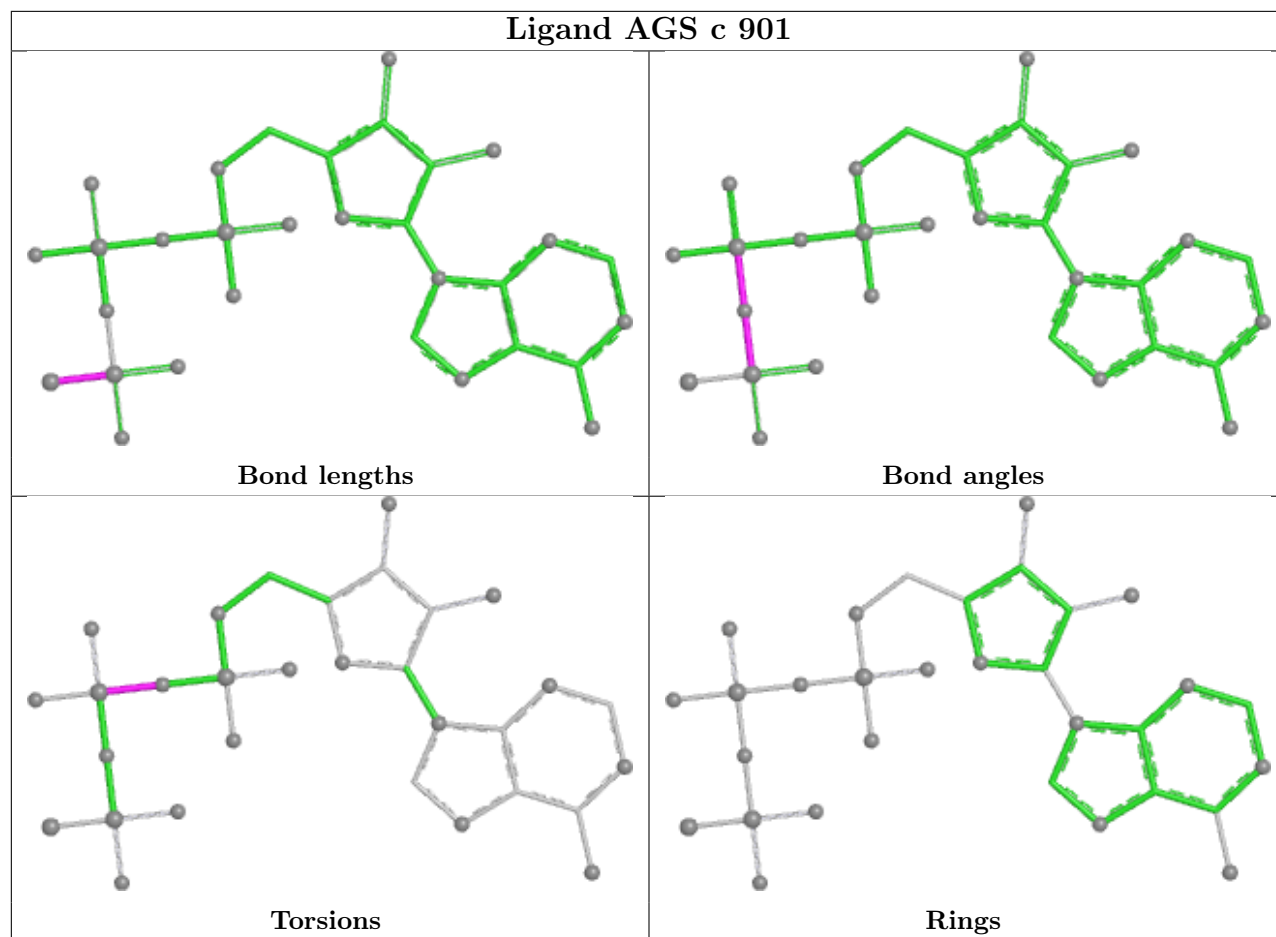
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	b	901	AGS	2	0
6	c	901	AGS	1	0
6	c	902	AGS	2	0
5	e	901	ADP	2	0
6	c	905	AGS	6	0
5	f	901	ADP	1	0
5	b	902	ADP	1	0
6	e	902	AGS	2	0
5	a	901	ADP	1	0
6	d	901	AGS	8	0

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.

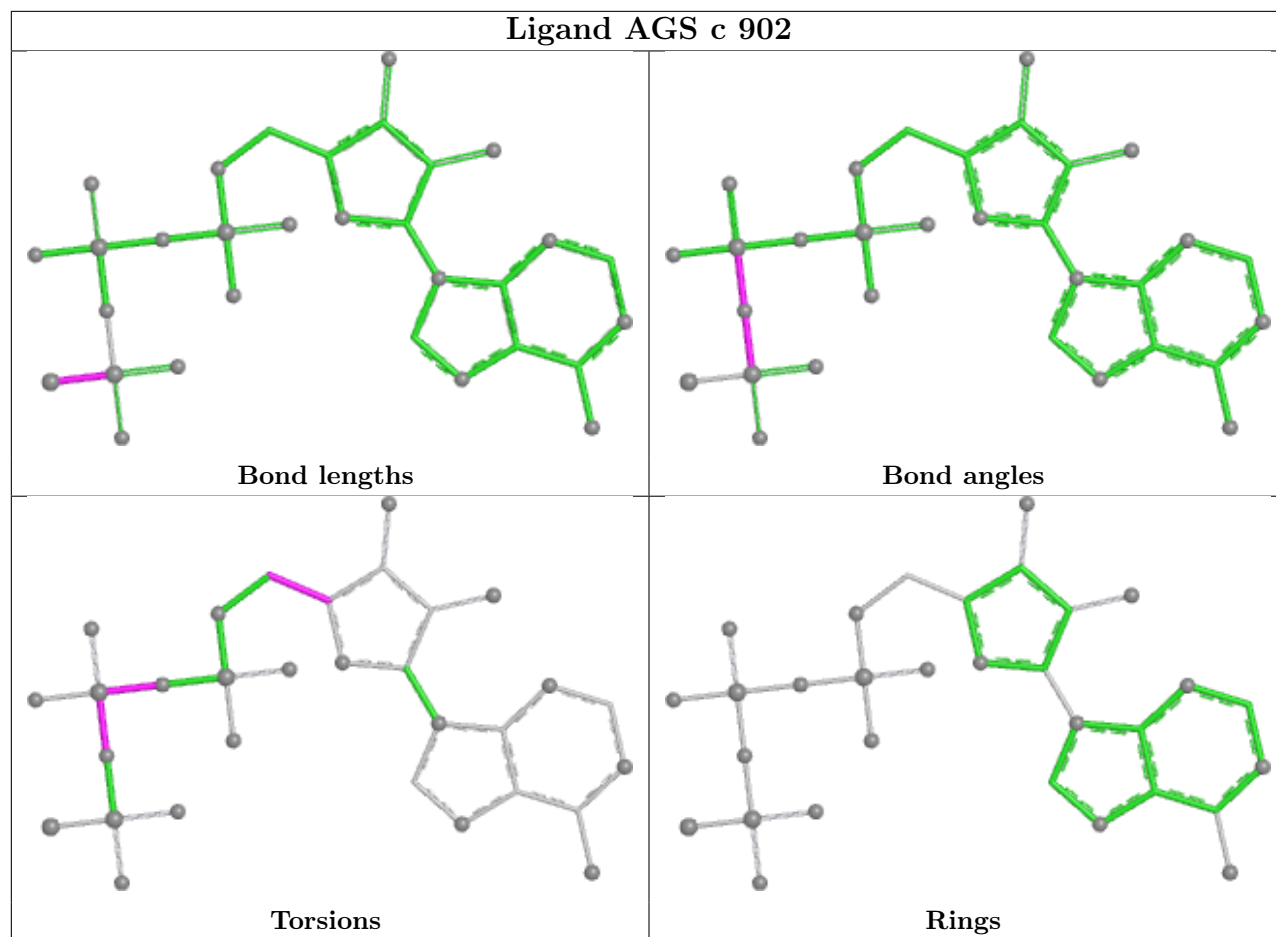
Ligand AGS b 901



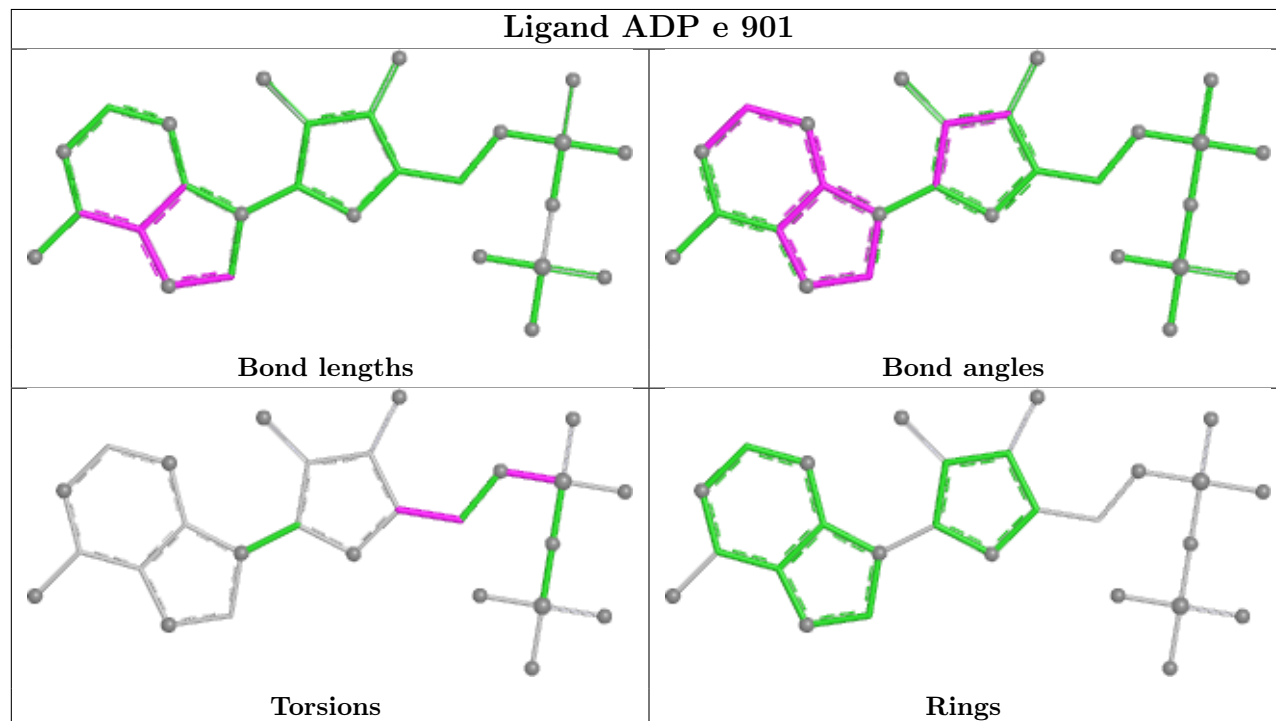
Ligand AGS c 901



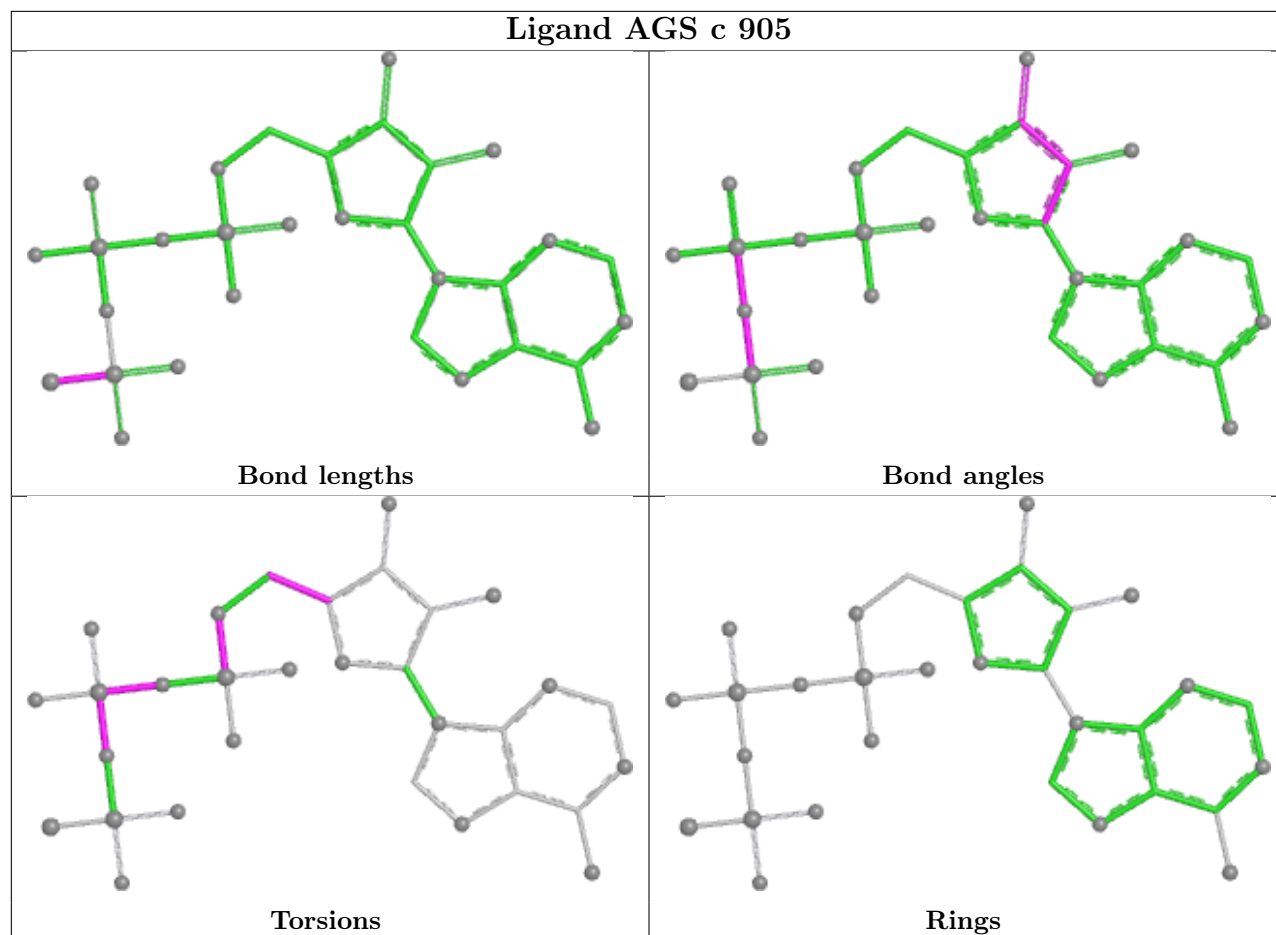
Ligand AGS c 902



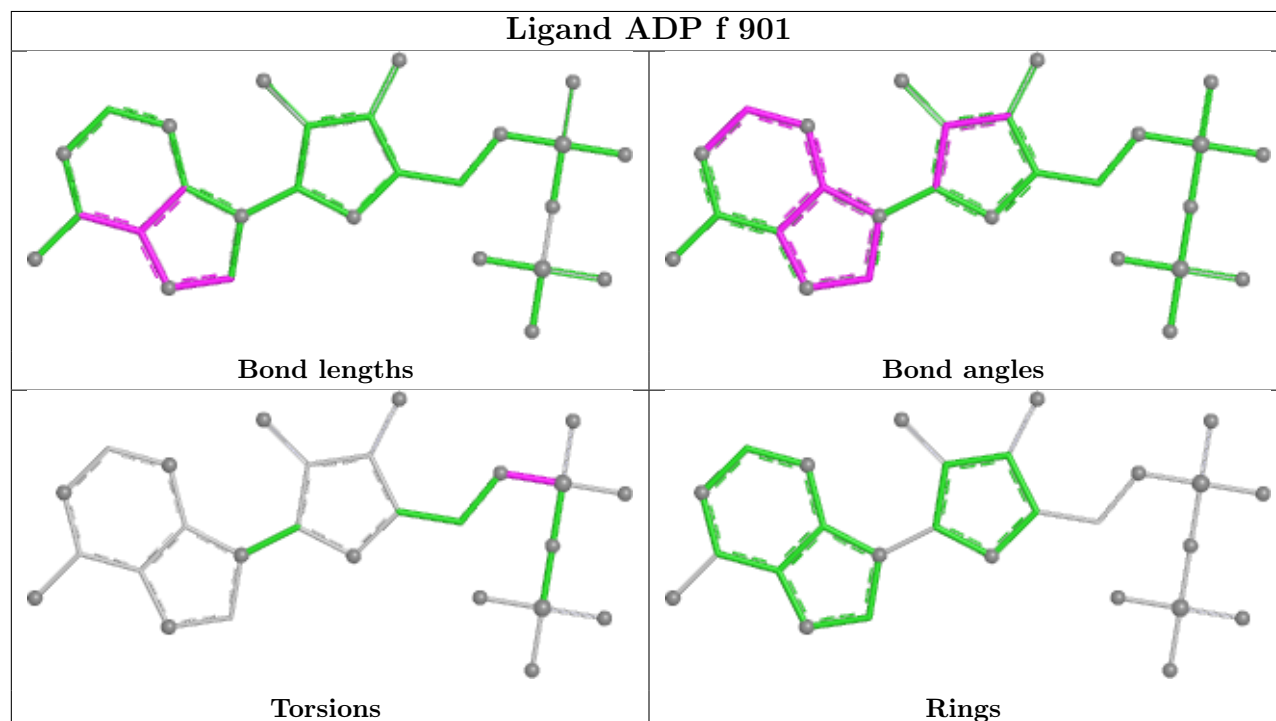
Ligand ADP e 901

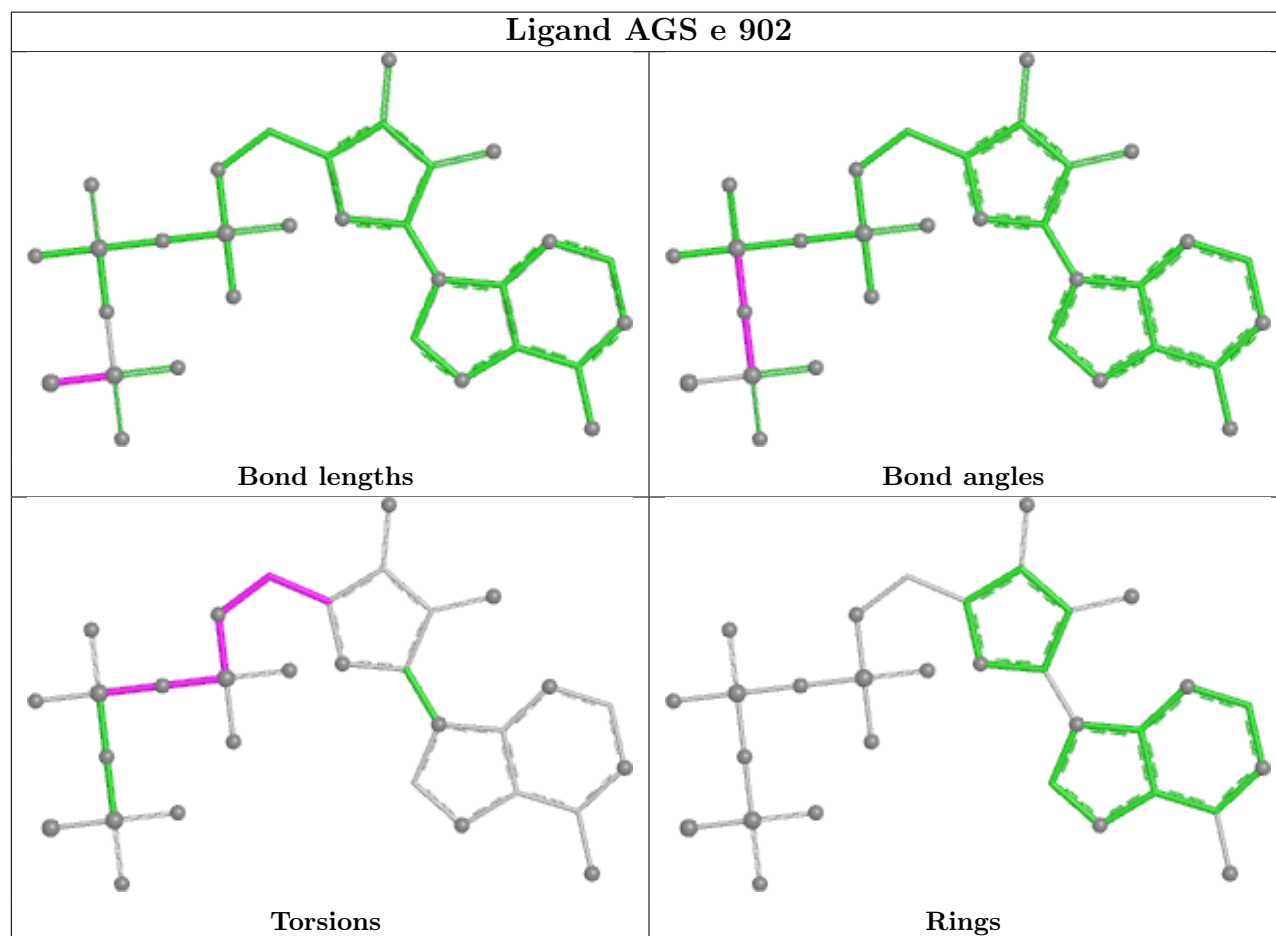
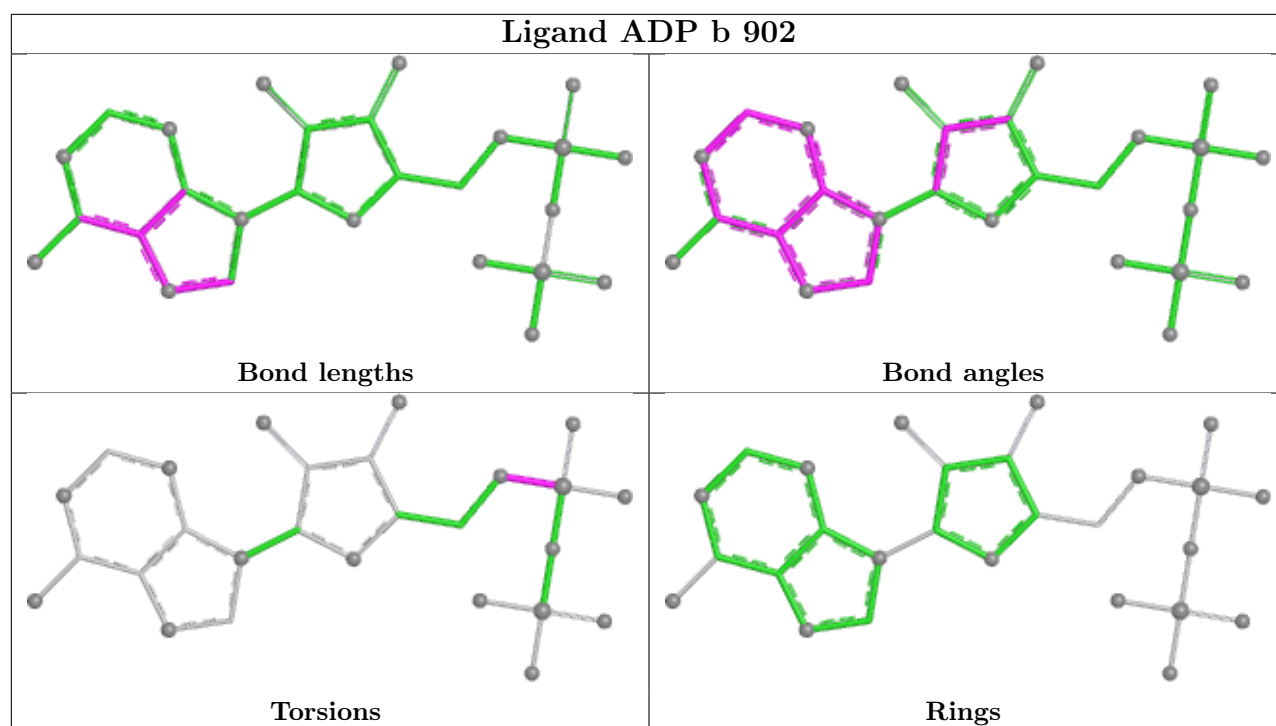


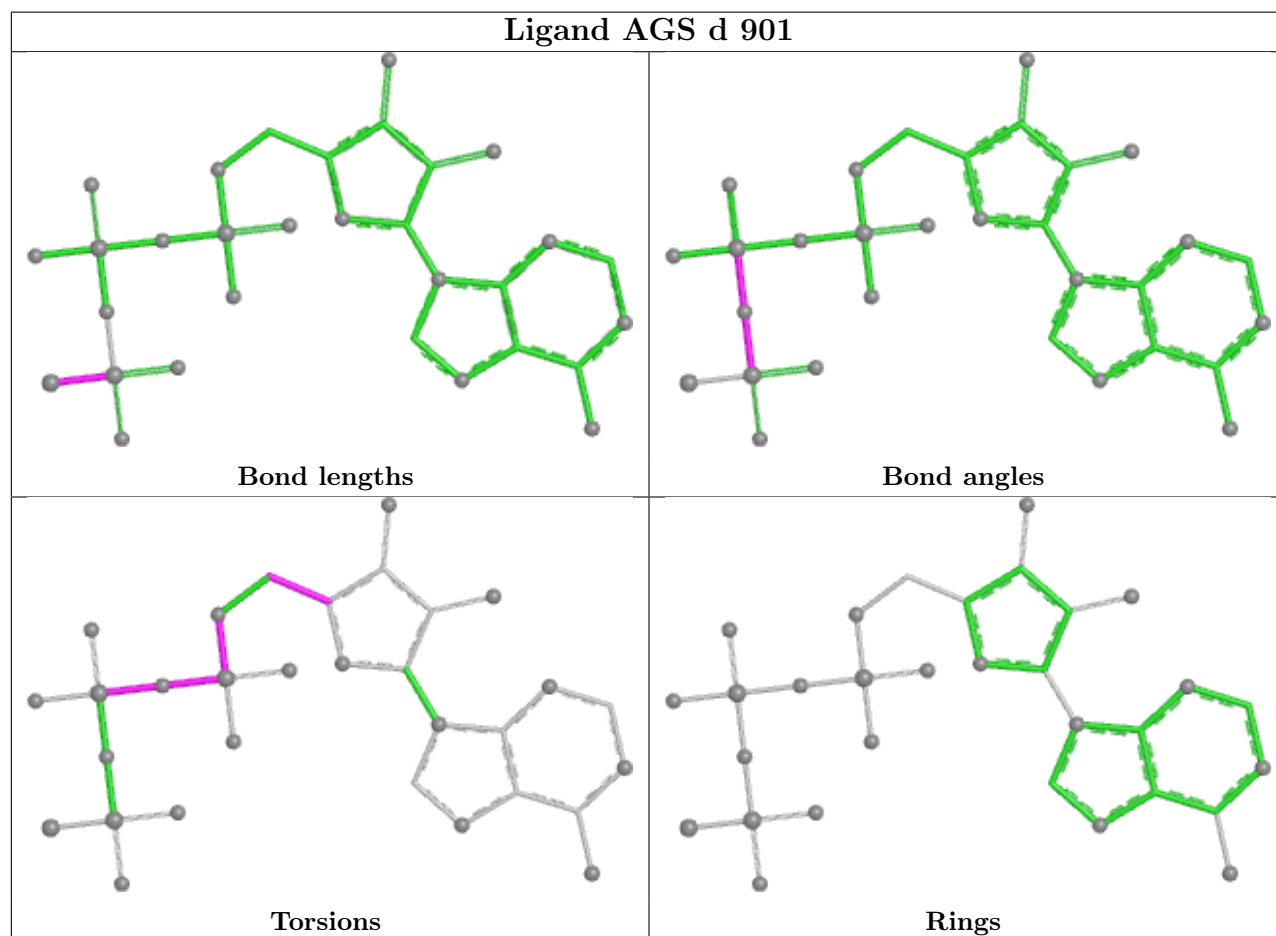
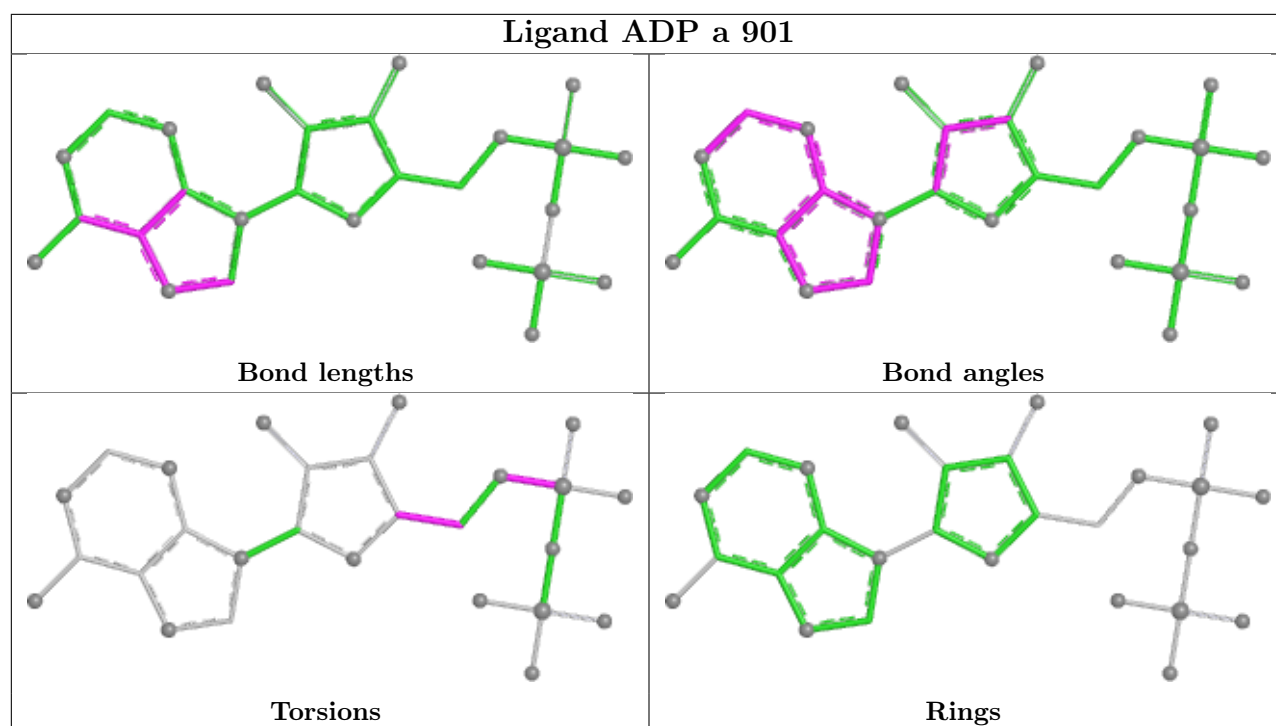
Ligand AGS c 905



Ligand ADP f 901







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	S	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	S	8:UNK	C	21:UNK	N	19.12

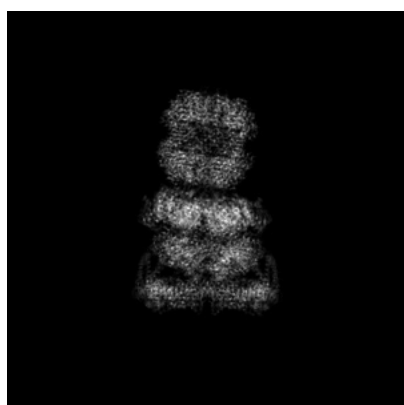
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53879. These allow visual inspection of the internal detail of the map and identification of artifacts.

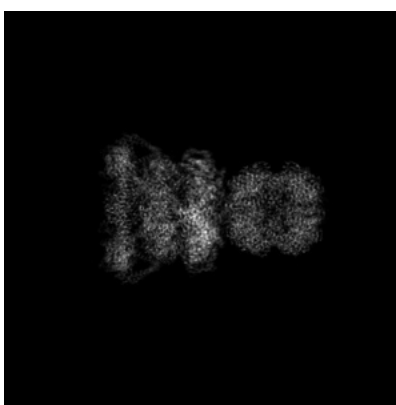
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

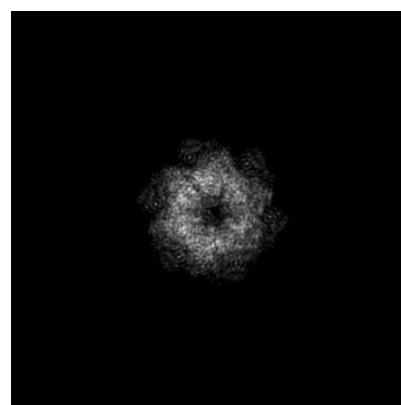
6.1.1 Primary map



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: 200



Y Index: 200



Z Index: 200

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

6.3 Largest variance slices [i](#)

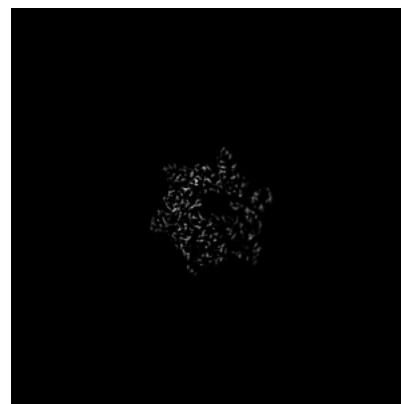
6.3.1 Primary map



X Index: 178



Y Index: 183

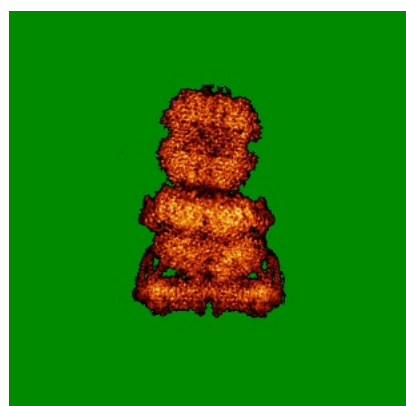


Z Index: 198

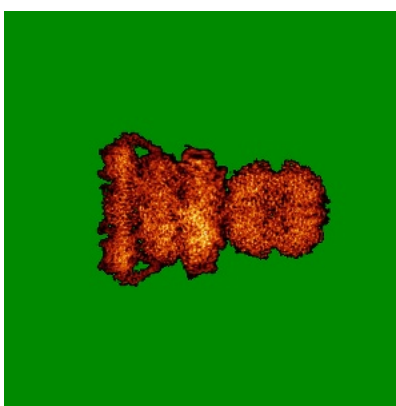
The images above show the largest variance slices of the map in three orthogonal directions.

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

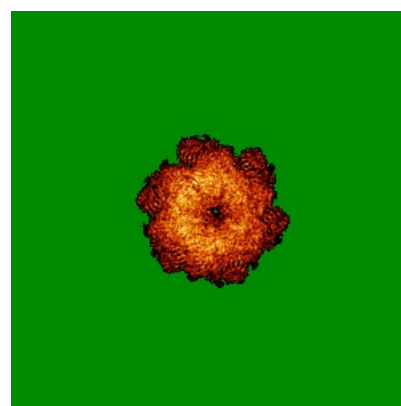
6.4.1 Primary map



X



Y

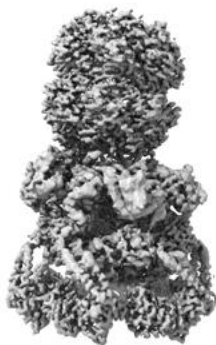


Z

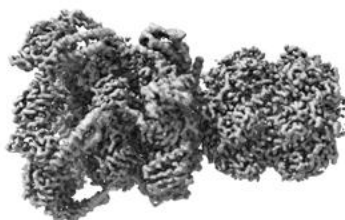
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

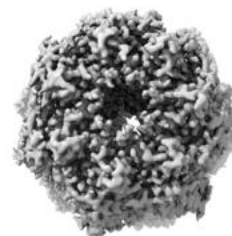
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.08. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

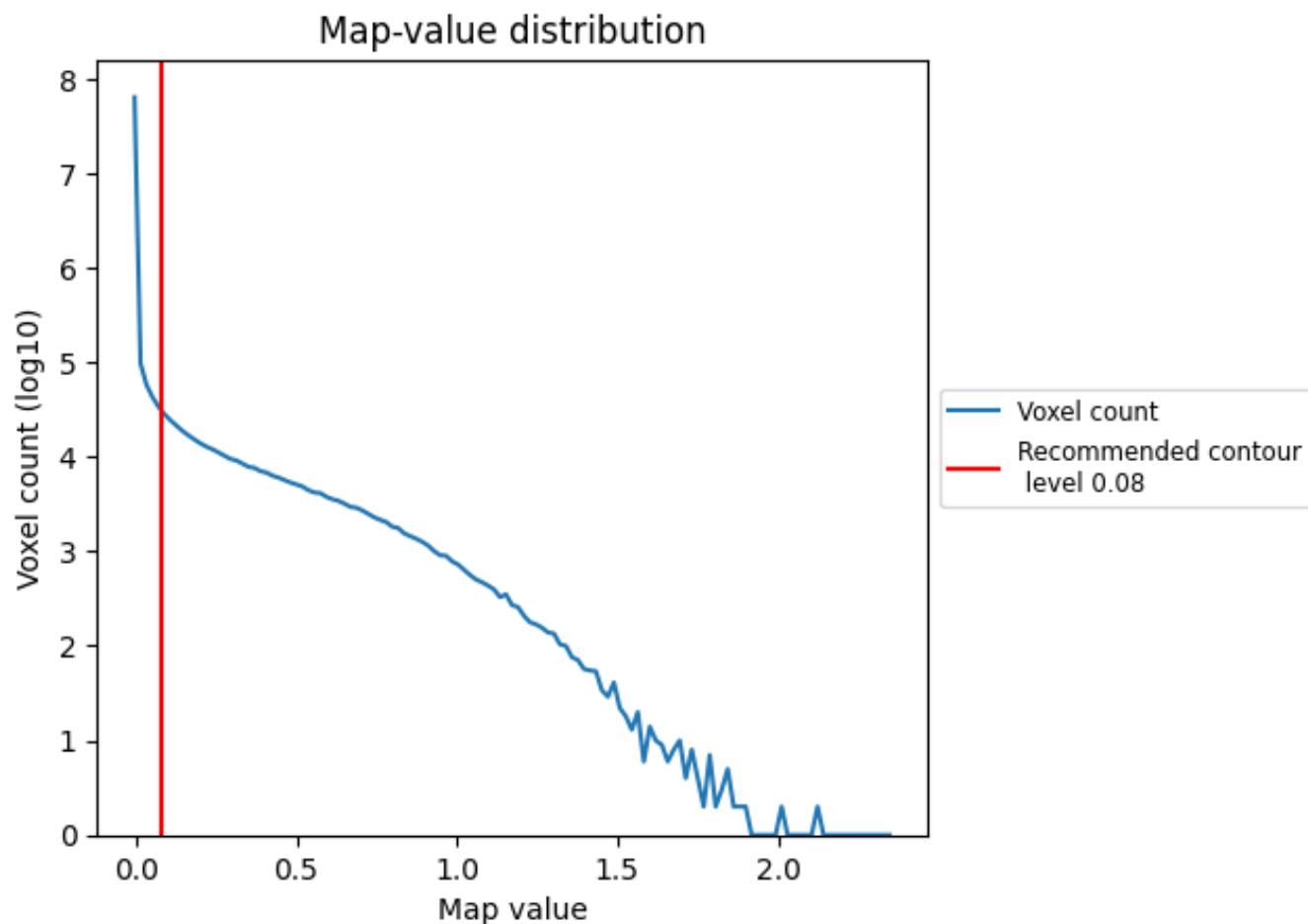
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

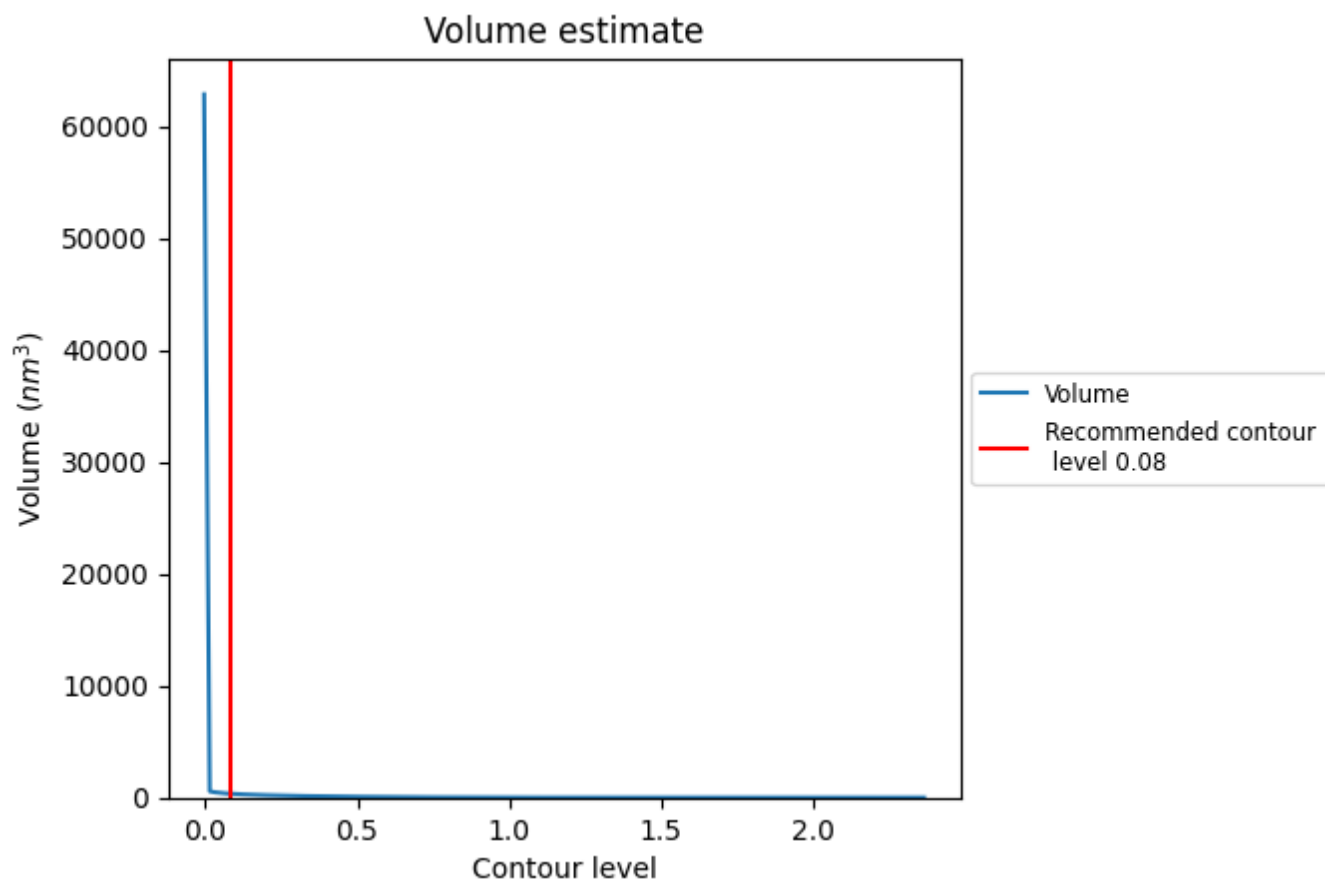
This section contains the results of statistical analysis of the map.

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.

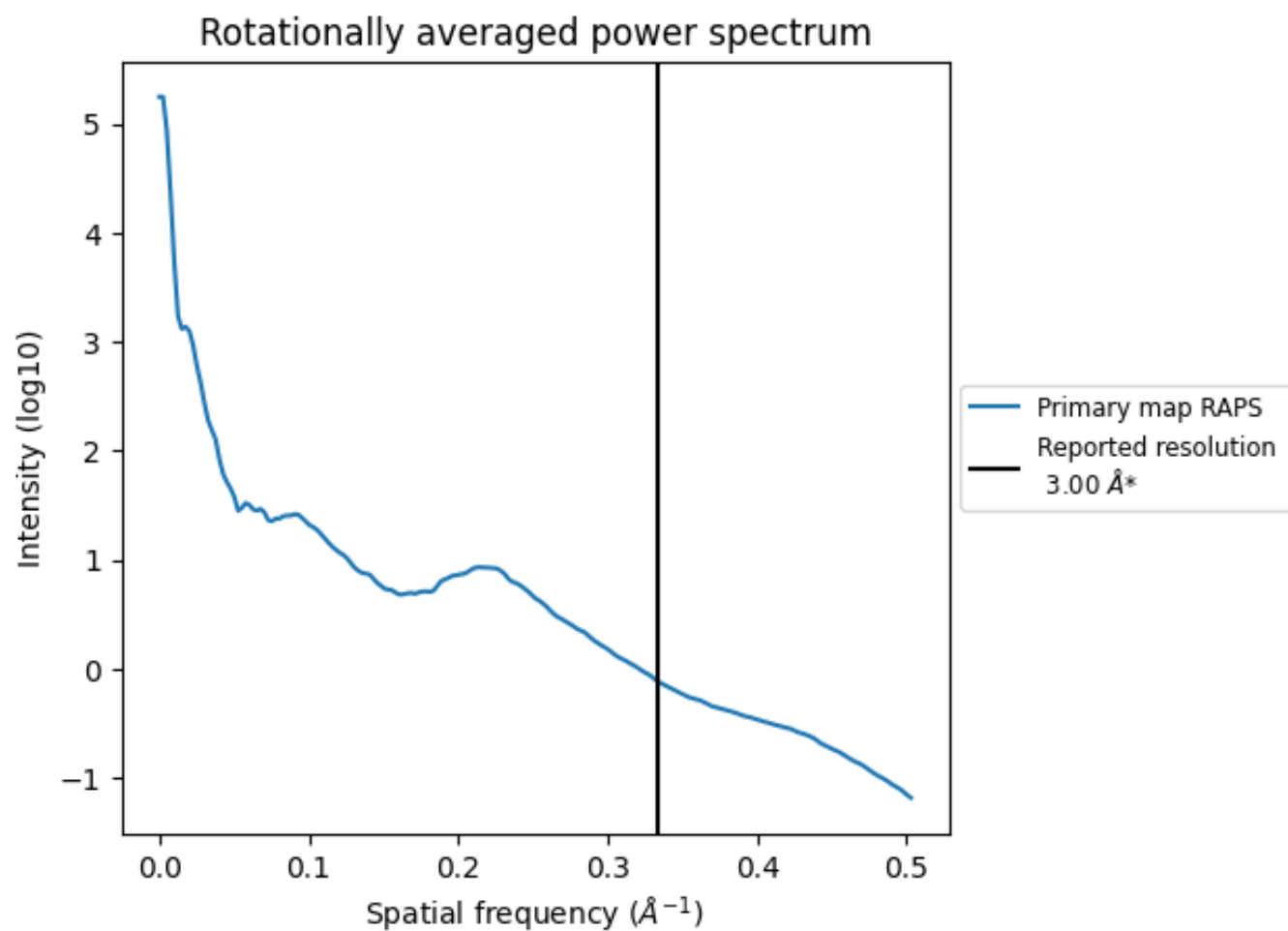
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 350 nm^3 ; this corresponds to an approximate mass of 316 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 0.333 Å⁻¹

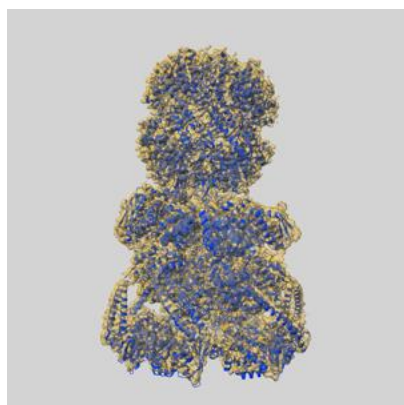
8 Fourier-Shell correlation

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

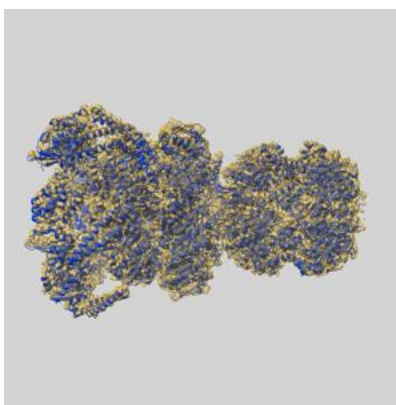
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-53879 and PDB model 9RAI. Per-residue inclusion information can be found in section [3](#) on page [8](#).

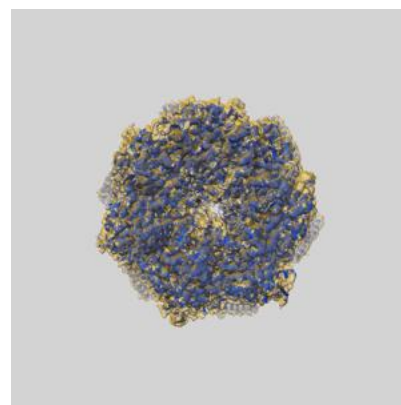
9.1 Map-model overlay [i](#)



X



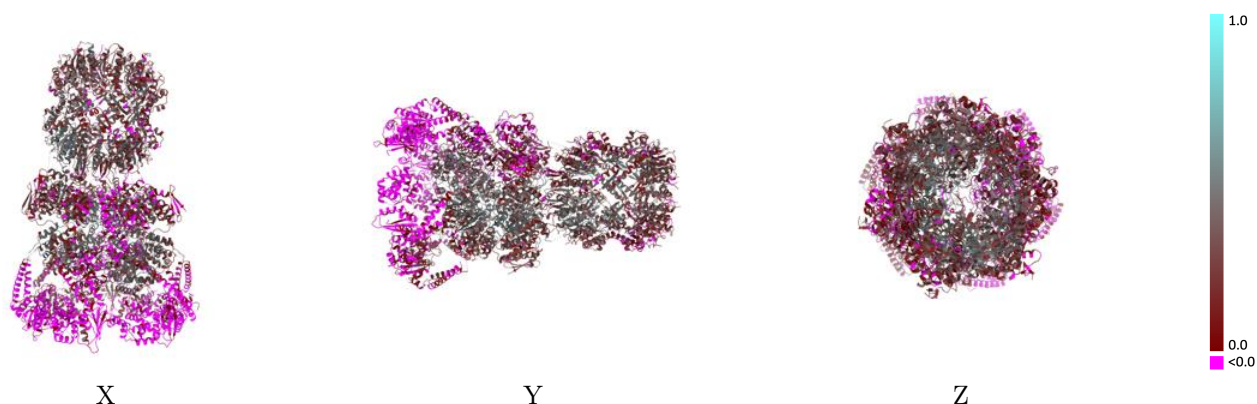
Y



Z

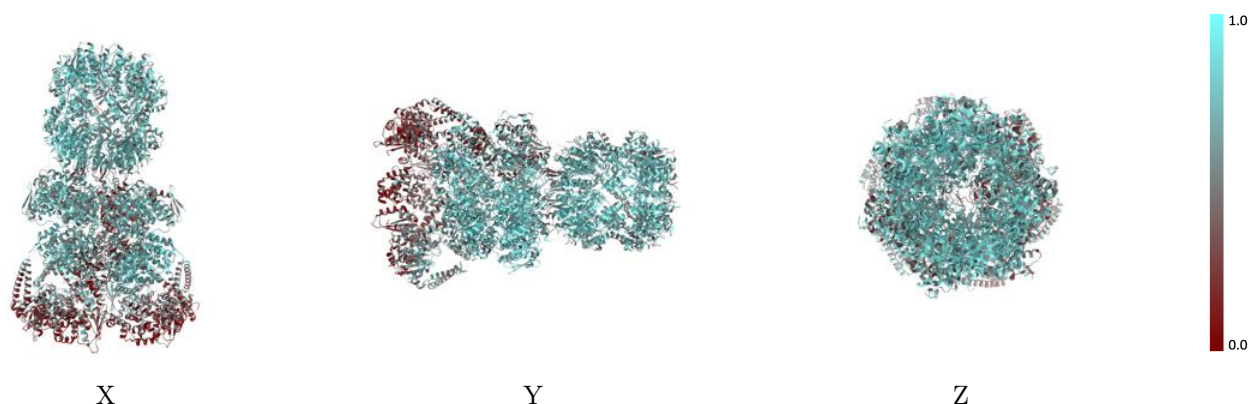
The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



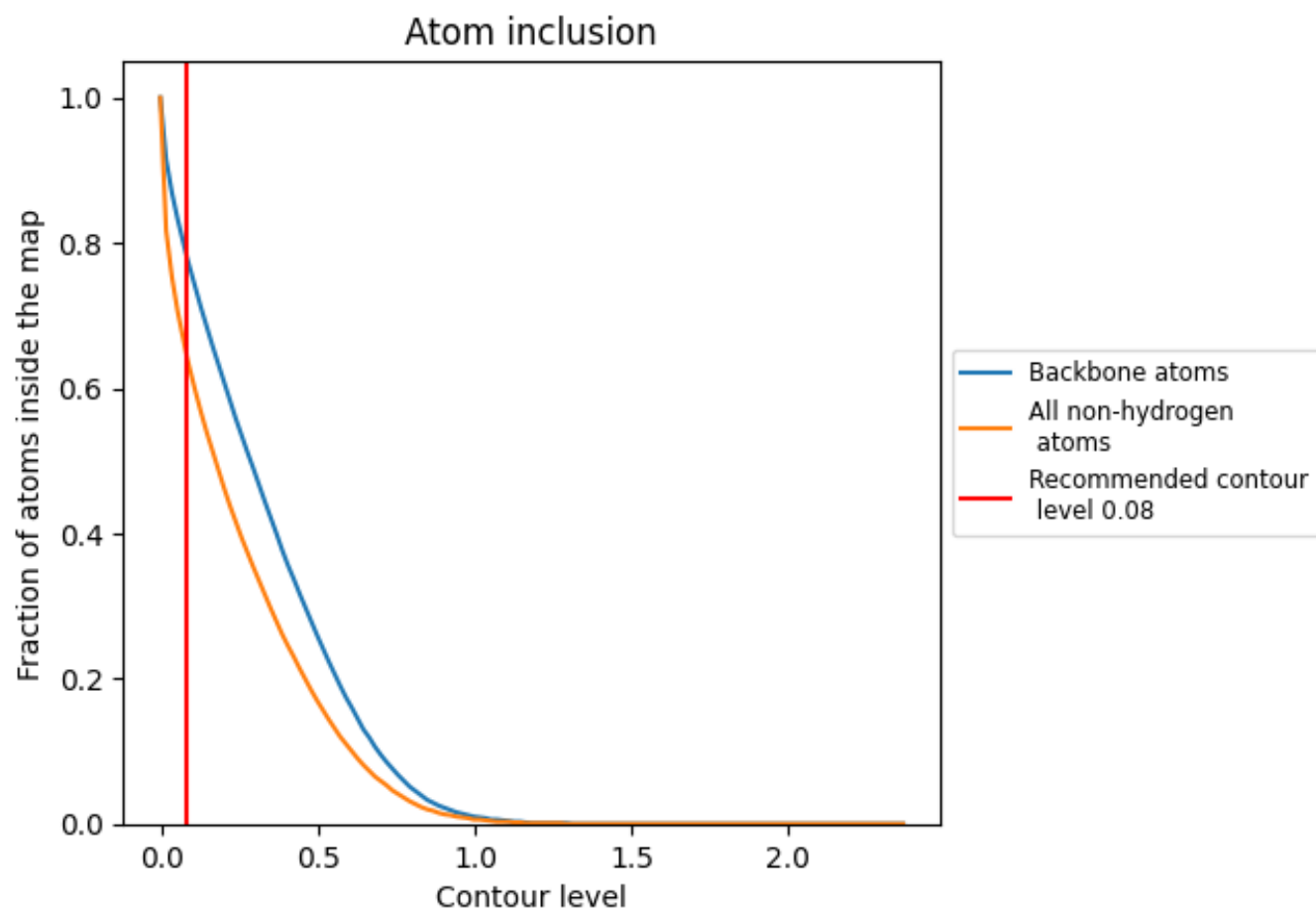
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.08).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 64% 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 (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6440	 0.2170
A	 0.3330	 -0.0690
B	 0.2960	 -0.1000
C	 0.5700	 0.1340
D	 0.5660	 0.0960
E	 0.3510	 -0.0780
F	 0.2900	 -0.0840
G	 0.7080	 0.2640
H	 0.7940	 0.4190
I	 0.7870	 0.3660
J	 0.7450	 0.3000
K	 0.7830	 0.3730
L	 0.7550	 0.3240
M	 0.7140	 0.2410
N	 0.7220	 0.2970
O	 0.7420	 0.3320
P	 0.6600	 0.1960
Q	 0.6150	 0.1330
R	 0.7190	 0.2430
S	 0.7130	 0.3140
T	 0.7690	 0.3320
U	 0.7140	 0.2600
a	 0.5250	 0.1070
b	 0.6780	 0.2690
c	 0.7180	 0.2980
d	 0.7270	 0.2980
e	 0.6670	 0.2370
f	 0.4450	 0.0270

