



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 10:56 AM UTC

PDB ID : 9IF4 / pdb_00009if4
EMDB ID : EMD-52840
Title : Structure of the Mycobacterium Tuberculosis ClpC1P1P2 complex bound to the activator Bz-Leu-Leu
Authors : Weinhaeupl, K.; Semchonok, D.; Gragera, M.; Arranz, R.; Bueno Carrasco, M.T.; Fraga, H.
Deposited on : 2025-02-17
Resolution : 3.09 Å(reported)

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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

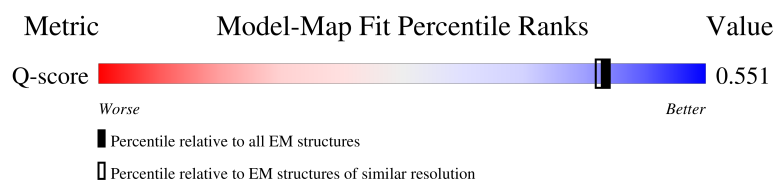
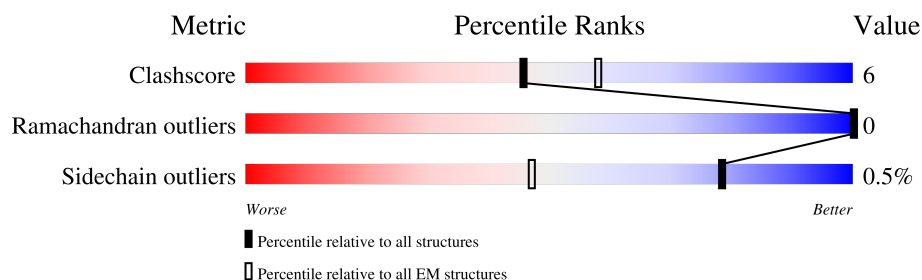
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.09 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	14003 (2.59 - 3.59)

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	658	
1	B	658	
1	C	658	
1	D	658	

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Mol	Chain	Length	Quality of chain
1	E	658	
1	F	658	
2	G	200	
2	H	200	
2	I	200	
2	J	200	
2	K	200	
2	L	200	
2	M	200	
3	N	179	
3	O	179	
3	P	179	
3	Q	179	
3	R	179	
3	S	179	
3	T	179	
4	U	2	
4	V	2	
4	W	2	
4	Y	2	
4	Z	2	
4	a	2	
4	b	2	
5	X	26	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 90720 atoms, of which 45538 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 ATP-dependent Clp protease ATP-binding subunit ClpC1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	461	Total	C	H	N	O	S	0	0
			7370	2310	3714	647	691	8		
1	B	548	Total	C	H	N	O	S	0	0
			8749	2728	4432	772	808	9		
1	C	581	Total	C	H	N	O	S	0	0
			9224	2880	4654	816	864	10		
1	D	580	Total	C	H	N	O	S	0	0
			9197	2875	4632	814	866	10		
1	E	563	Total	C	H	N	O	S	0	0
			8977	2807	4528	792	840	10		
1	F	408	Total	C	H	N	O	S	0	0
			6532	2038	3313	569	604	8		

- Molecule 2 is a protein called ATP-dependent Clp protease proteolytic subunit 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	G	190	Total	C	H	N	O	S	0	0
			2937	917	1477	249	286	8		
2	H	192	Total	C	H	N	O	S	0	0
			2964	924	1491	252	289	8		
2	I	190	Total	C	H	N	O	S	0	0
			2932	917	1472	249	286	8		
2	J	187	Total	C	H	N	O	S	0	0
			2895	904	1458	245	280	8		
2	L	192	Total	C	H	N	O	S	0	0
			2961	924	1489	251	289	8		
2	M	190	Total	C	H	N	O	S	0	0
			2935	917	1474	250	286	8		
2	K	190	Total	C	H	N	O	S	0	0
			2937	917	1477	249	286	8		

- Molecule 3 is a protein called ATP-dependent Clp protease proteolytic subunit 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	N	179	Total	C	H	N	O	S	0	0
			2726	864	1361	230	262	9		
3	O	179	Total	C	H	N	O	S	0	0
			2726	864	1361	230	262	9		
3	P	179	Total	C	H	N	O	S	0	0
			2726	864	1361	230	262	9		
3	Q	178	Total	C	H	N	O	S	0	0
			2702	858	1348	226	261	9		
3	R	178	Total	C	H	N	O	S	0	0
			2702	858	1348	226	261	9		
3	S	178	Total	C	H	N	O	S	0	0
			2702	858	1348	226	261	9		
3	T	179	Total	C	H	N	O	S	0	0
			2726	864	1361	230	262	9		

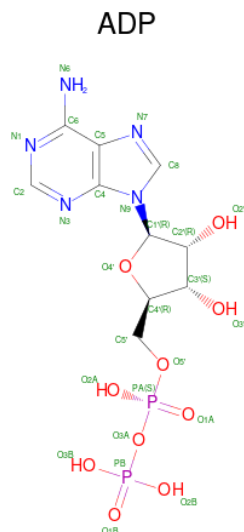
- Molecule 4 is a protein called activator Bz-Leu-Leu.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	U	2	Total	C	H	N	O		0	0
			52	19	27	2	4			
4	V	2	Total	C	H	N	O		0	0
			52	19	27	2	4			
4	W	2	Total	C	H	N	O		0	0
			52	19	27	2	4			
4	Y	2	Total	C	H	N	O		0	0
			52	19	27	2	4			
4	Z	2	Total	C	H	N	O		0	0
			52	19	27	2	4			
4	a	2	Total	C	H	N	O		0	0
			52	19	27	2	4			
4	b	2	Total	C	H	N	O		0	0
			52	19	27	2	4			

- Molecule 5 is a protein called Unknown peptide.

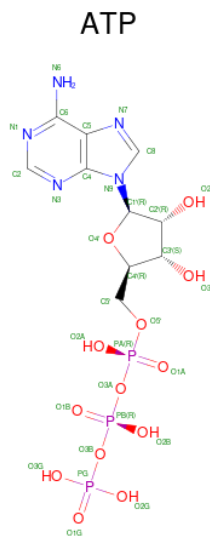
Mol	Chain	Residues	Atoms						AltConf	Trace
5	X	26	Total	C	H	N	O		0	0
			236	78	106	26	26			

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).

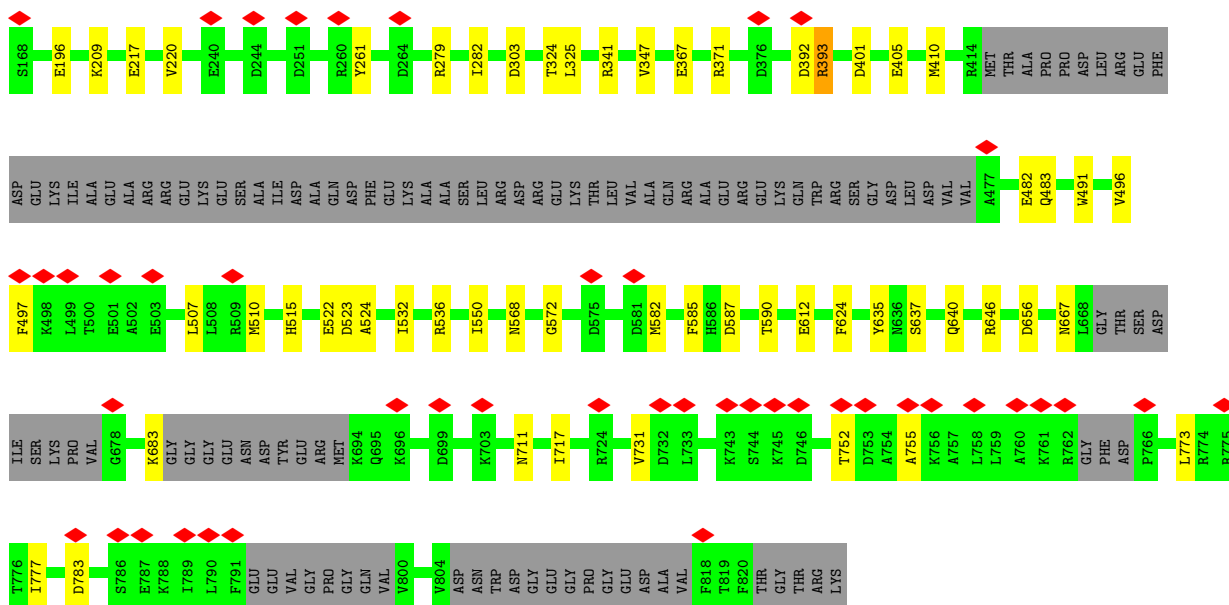


Id	Chain	Residues	Atoms						AltC
6	A	1	Total 39	C 10	H 12	N 5	O 10	P 2	0
6	A	1	Total 39	C 10	H 12	N 5	O 10	P 2	0
6	F	1	Total 39	C 10	H 12	N 5	O 10	P 2	0
6	F	1	Total 39	C 10	H 12	N 5	O 10	P 2	0

- Molecule 7 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{13}\text{P}_3$) (labeled as "Ligand of Interest" by depositor).

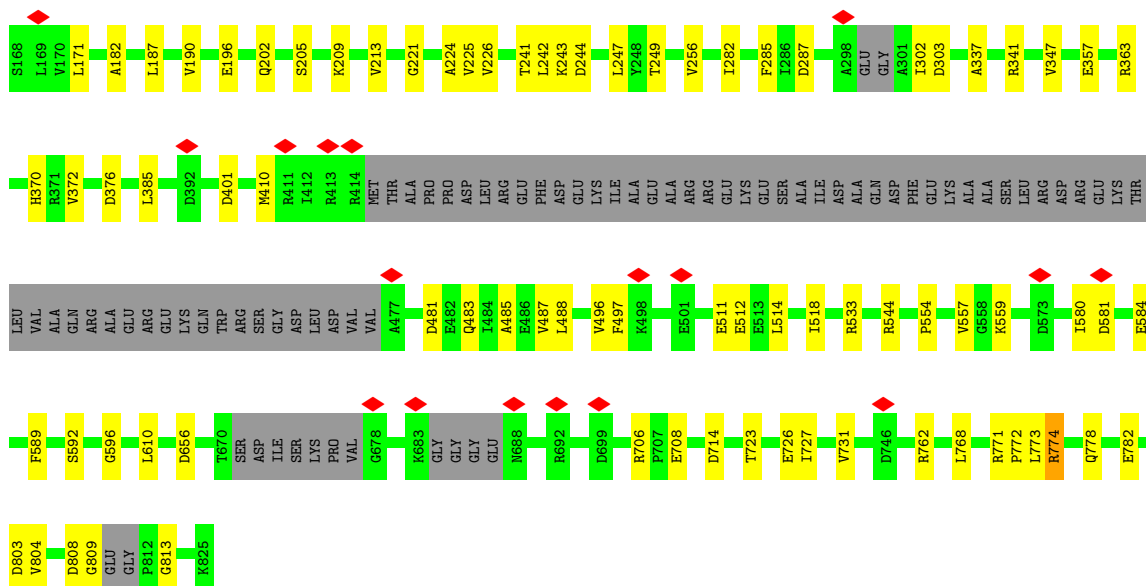


Mol	Chain	Residues	Atoms						AltConf
7	B	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
7	B	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
7	C	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
7	C	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
7	D	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
7	D	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
7	E	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
7	E	1	Total 43	C 10	H 12	N 5	O 13	P 3	0



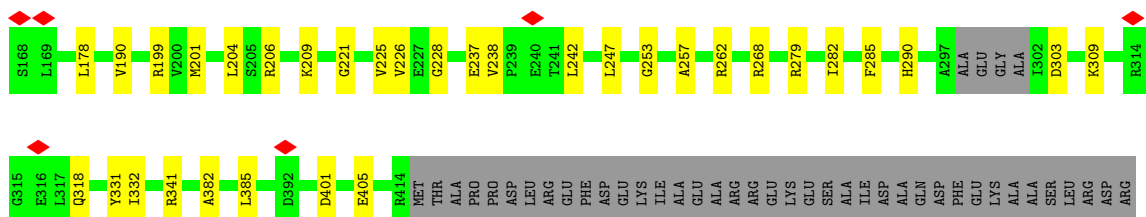
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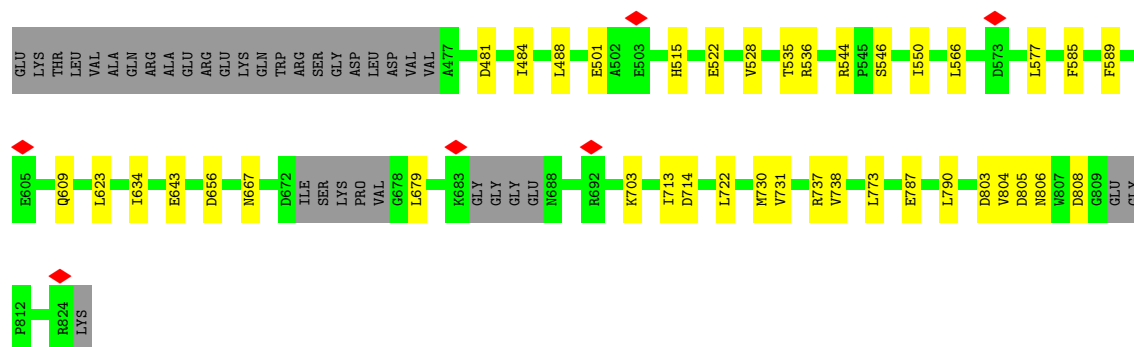
Chain C: 76% 12% 12%



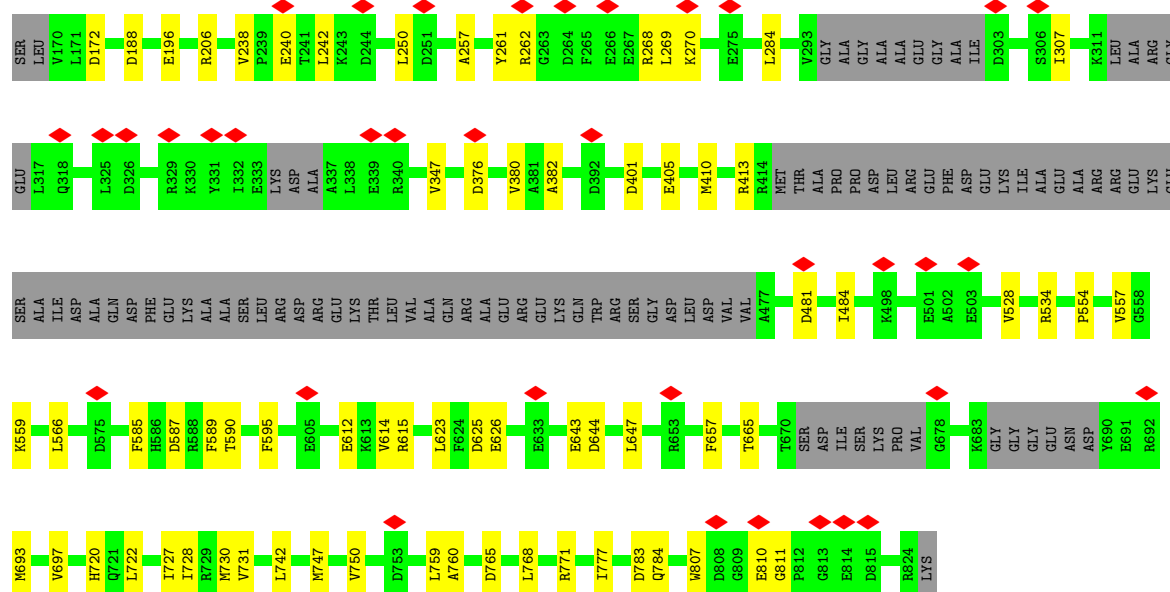
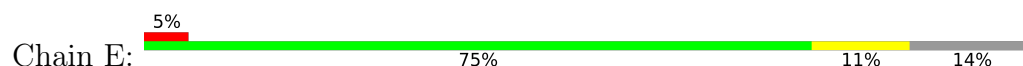
• Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpC1

Chain D: 77% 11% 12%

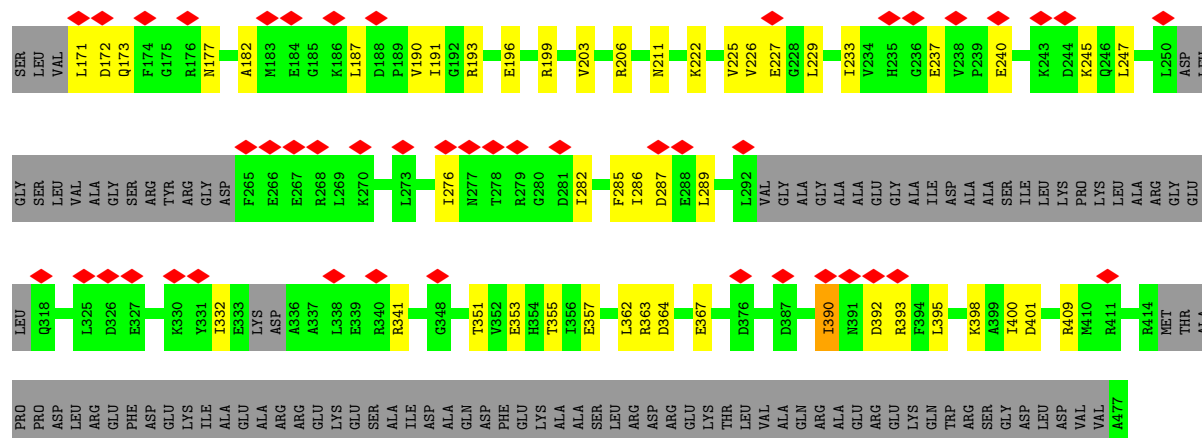


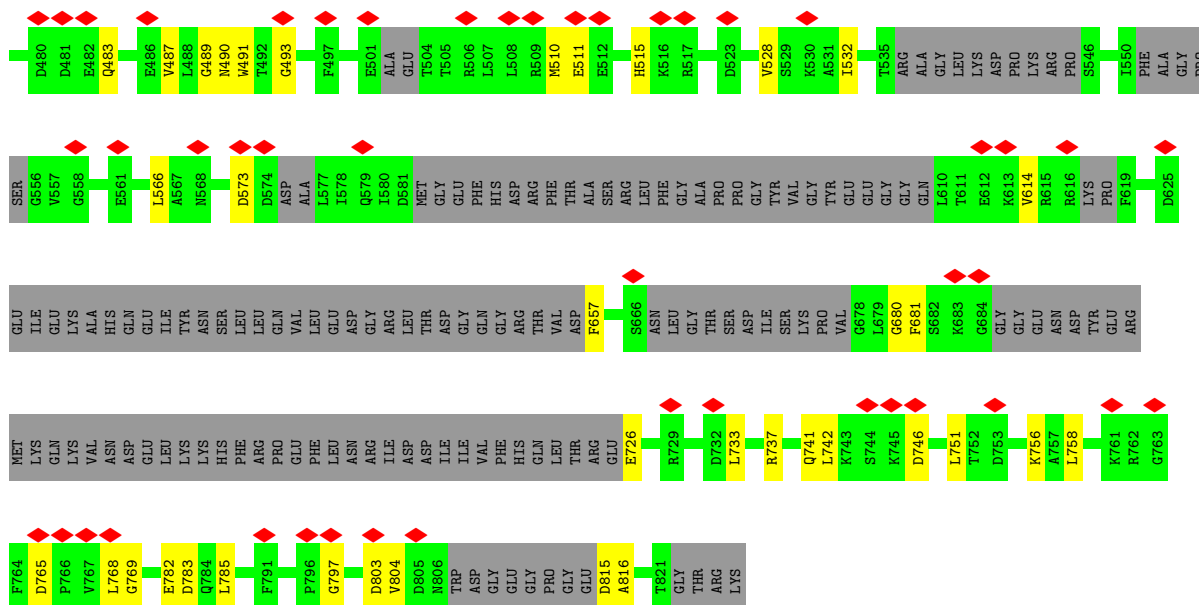


- Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpC1

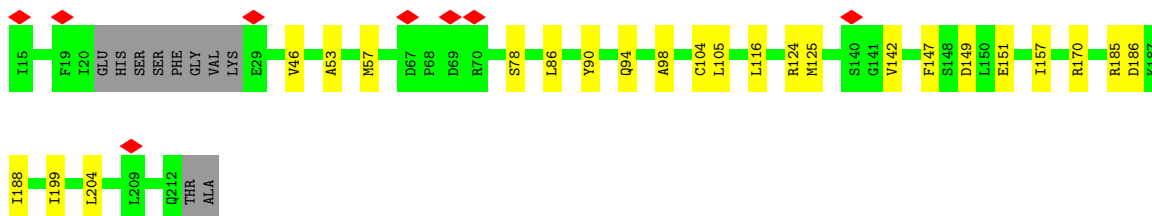
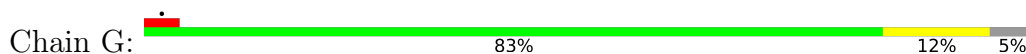


- Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpC1

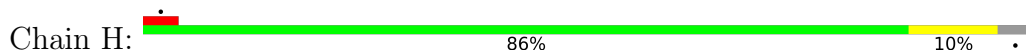




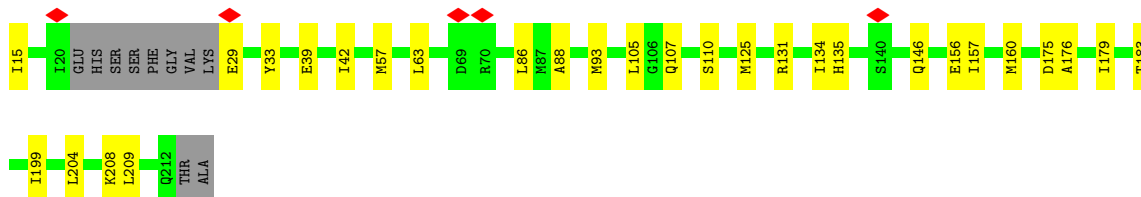
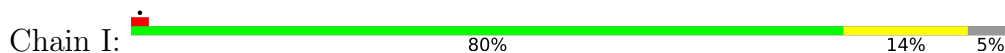
- Molecule 2: ATP-dependent Clp protease proteolytic subunit 2




- Molecule 2: ATP-dependent Clp protease proteolytic subunit 2

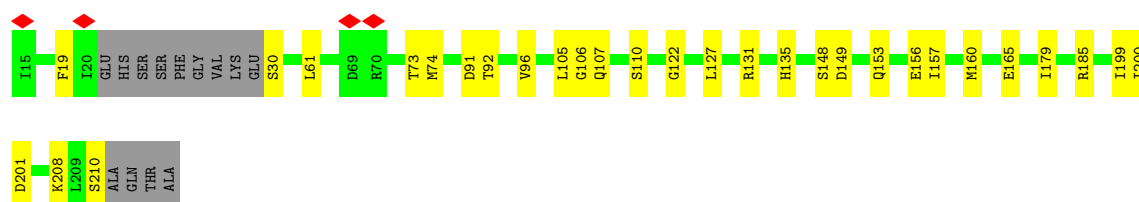


- Molecule 2: ATP-dependent Clp protease proteolytic subunit 2




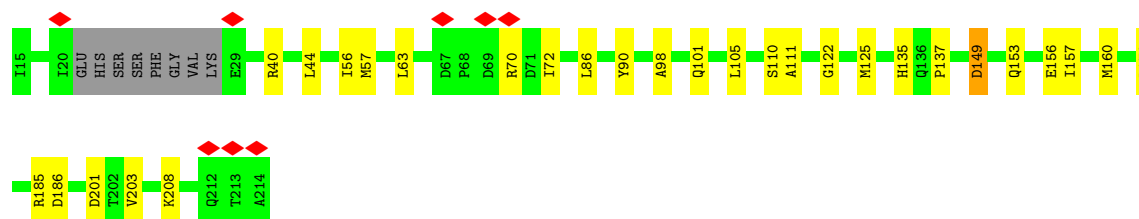
- Molecule 2: ATP-dependent Clp protease proteolytic subunit 2

Chain J: 




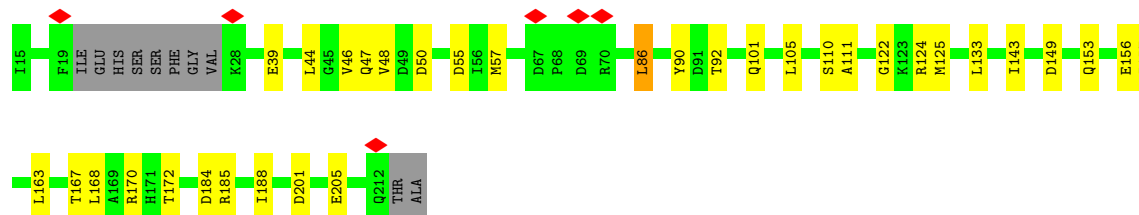
- Molecule 2: ATP-dependent Clp protease proteolytic subunit 2

Chain L: 




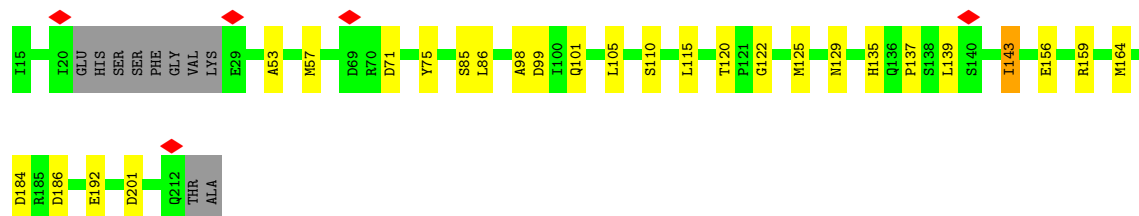
- Molecule 2: ATP-dependent Clp protease proteolytic subunit 2

Chain M: 




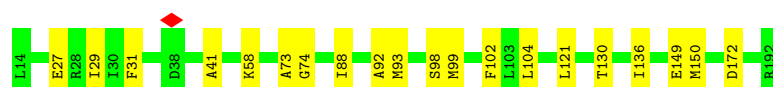
- Molecule 2: ATP-dependent Clp protease proteolytic subunit 2

Chain K: 

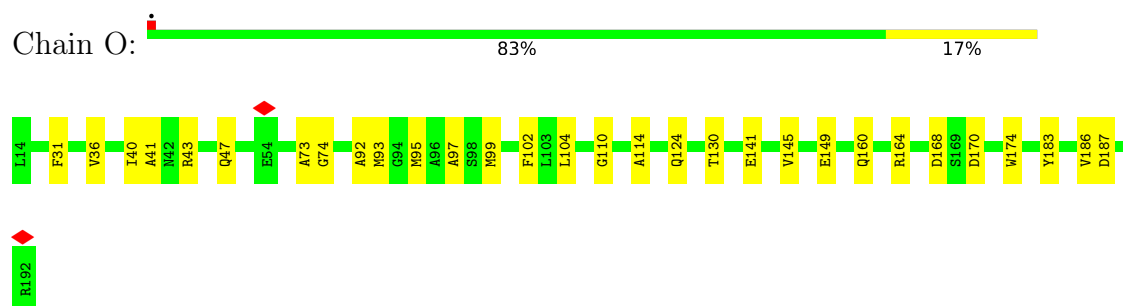


- Molecule 3: ATP-dependent Clp protease proteolytic subunit 1

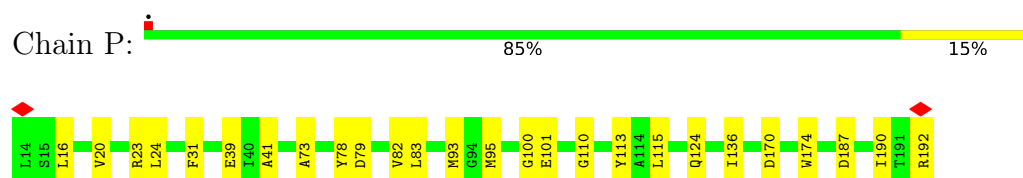
Chain N: 



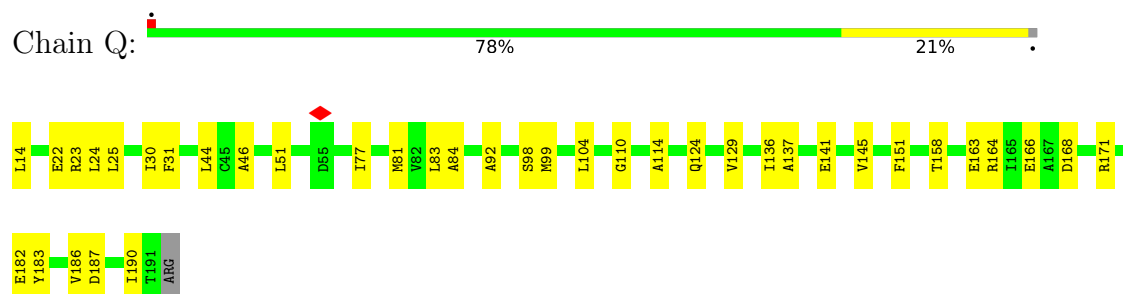
- Molecule 3: ATP-dependent Clp protease proteolytic subunit 1



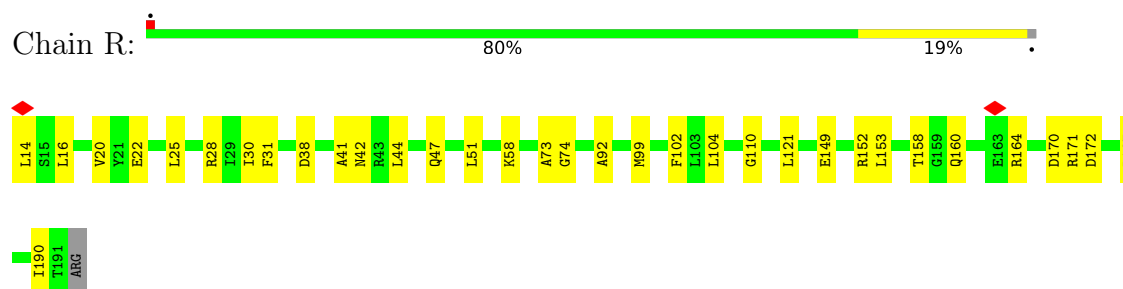
- Molecule 3: ATP-dependent Clp protease proteolytic subunit 1



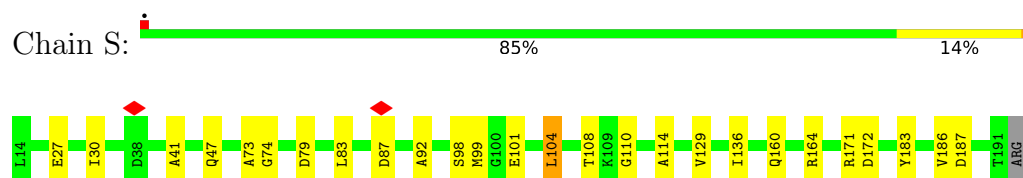
- Molecule 3: ATP-dependent Clp protease proteolytic subunit 1



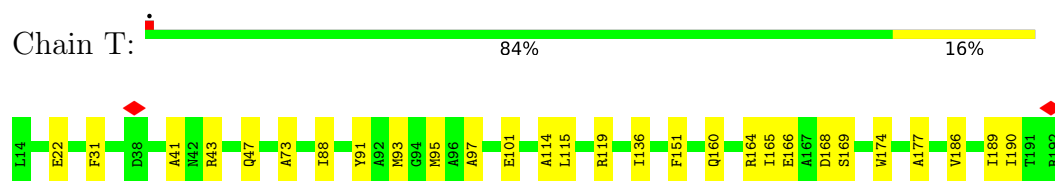
- Molecule 3: ATP-dependent Clp protease proteolytic subunit 1



- Molecule 3: ATP-dependent Clp protease proteolytic subunit 1



- Molecule 3: ATP-dependent Clp protease proteolytic subunit 1



- Molecule 4: activator Bz-Leu-Leu



L1
L2

- Molecule 4: activator Bz-Leu-Leu



L1
L2

- Molecule 4: activator Bz-Leu-Leu



L1
L2

- Molecule 4: activator Bz-Leu-Leu



L1
L2

- Molecule 4: activator Bz-Leu-Leu



L1
L2

- Molecule 4: activator Bz-Leu-Leu



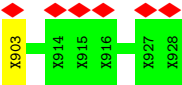
L1
L2

- Molecule 4: activator Bz-Leu-Leu



L1
L2

- Molecule 5: Unknown peptide



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	71218	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	46	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	0.339	Depositor
Minimum map value	-0.076	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	315.0, 315.0, 315.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.525, 0.525, 0.525	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, ADP, S0R

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	0.12	0/3695	0.23	0/4960
1	B	0.16	0/4373	0.25	0/5879
1	C	0.17	0/4633	0.26	0/6234
1	D	0.17	0/4628	0.24	0/6228
1	E	0.14	0/4511	0.24	0/6070
1	F	0.12	0/3246	0.26	1/4353 (0.0%)
2	G	0.34	0/1478	0.30	0/1999
2	H	0.35	0/1491	0.28	0/2016
2	I	0.36	0/1478	0.30	0/1999
2	J	0.35	0/1455	0.30	0/1968
2	K	0.34	0/1478	0.27	0/1999
2	L	0.32	0/1490	0.28	0/2016
2	M	0.33	0/1479	0.29	0/1999
3	N	0.32	0/1387	0.29	0/1875
3	O	0.33	0/1387	0.29	0/1875
3	P	0.32	0/1387	0.30	0/1875
3	Q	0.33	0/1376	0.32	0/1861
3	R	0.32	0/1376	0.28	0/1861
3	S	0.31	0/1376	0.29	0/1861
3	T	0.33	0/1387	0.27	0/1875
4	U	0.84	0/8	1.17	0/8
4	V	0.81	0/8	1.02	0/8
4	W	0.82	0/8	0.84	0/8
4	Y	0.77	0/8	0.66	0/8
4	Z	0.79	0/8	0.56	0/8
4	a	0.77	0/8	0.60	0/8
4	b	0.76	0/8	0.52	0/8
All	All	0.25	0/45167	0.27	1/60859 (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
1	B	0	1
1	C	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	390	ILE	N-CA-C	-5.01	107.45	111.91

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	393	ARG	Sidechain
1	C	774	ARG	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	3656	3714	3724	50	0
1	B	4317	4432	4429	42	0
1	C	4570	4654	4649	63	0
1	D	4565	4632	4635	51	0
1	E	4449	4528	4520	49	0
1	F	3219	3313	3315	63	0
2	G	1460	1477	1475	26	0
2	H	1473	1491	1489	23	0
2	I	1460	1472	1475	25	0
2	J	1437	1458	1456	20	0
2	K	1460	1477	1475	19	0
2	L	1472	1489	1487	29	0
2	M	1461	1474	1477	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	N	1365	1361	1360	17	0
3	O	1365	1361	1360	18	0
3	P	1365	1361	1360	21	0
3	Q	1354	1348	1347	31	0
3	R	1354	1348	1347	25	0
3	S	1354	1348	1347	17	0
3	T	1365	1361	1360	20	0
4	U	25	27	10	0	0
4	V	25	27	10	3	0
4	W	25	27	10	1	0
4	Y	25	27	10	0	0
4	Z	25	27	10	5	0
4	a	25	27	10	1	0
4	b	25	27	10	1	0
5	X	130	106	29	1	0
6	A	54	24	22	1	0
6	F	54	24	22	1	0
7	B	62	24	21	2	0
7	C	62	24	21	1	0
7	D	62	24	22	0	0
7	E	62	24	23	0	0
All	All	45182	45538	45317	563	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 563 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:110:SER:HG	2:H:135:HIS:HE2	1.17	0.88
1:E:250:LEU:HD13	1:E:284:LEU:HD11	1.55	0.87
2:I:57:MET:CE	2:I:88:ALA:HB1	2.06	0.86
2:L:57:MET:HE3	2:M:105:LEU:HD13	1.59	0.84
2:L:105:LEU:HD13	2:K:57:MET:HE1	1.61	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	433/658 (66%)	423 (98%)	10 (2%)	0	100	100
1	B	534/658 (81%)	517 (97%)	17 (3%)	0	100	100
1	C	569/658 (86%)	554 (97%)	15 (3%)	0	100	100
1	D	568/658 (86%)	554 (98%)	14 (2%)	0	100	100
1	E	549/658 (83%)	535 (97%)	14 (3%)	0	100	100
1	F	378/658 (57%)	368 (97%)	10 (3%)	0	100	100
2	G	186/200 (93%)	177 (95%)	9 (5%)	0	100	100
2	H	188/200 (94%)	181 (96%)	7 (4%)	0	100	100
2	I	186/200 (93%)	178 (96%)	8 (4%)	0	100	100
2	J	183/200 (92%)	178 (97%)	5 (3%)	0	100	100
2	K	186/200 (93%)	175 (94%)	11 (6%)	0	100	100
2	L	188/200 (94%)	181 (96%)	7 (4%)	0	100	100
2	M	186/200 (93%)	178 (96%)	8 (4%)	0	100	100
3	N	177/179 (99%)	173 (98%)	4 (2%)	0	100	100
3	O	177/179 (99%)	167 (94%)	10 (6%)	0	100	100
3	P	177/179 (99%)	173 (98%)	4 (2%)	0	100	100
3	Q	176/179 (98%)	169 (96%)	7 (4%)	0	100	100
3	R	176/179 (98%)	169 (96%)	7 (4%)	0	100	100
3	S	176/179 (98%)	169 (96%)	7 (4%)	0	100	100
3	T	177/179 (99%)	172 (97%)	5 (3%)	0	100	100
All	All	5570/6601 (84%)	5391 (97%)	179 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	391/546 (72%)	391 (100%)	0	100	100
1	B	458/546 (84%)	457 (100%)	1 (0%)	87	89
1	C	484/546 (89%)	483 (100%)	1 (0%)	87	89
1	D	485/546 (89%)	483 (100%)	2 (0%)	84	86
1	E	474/546 (87%)	473 (100%)	1 (0%)	87	89
1	F	346/546 (63%)	346 (100%)	0	100	100
2	G	157/165 (95%)	157 (100%)	0	100	100
2	H	158/165 (96%)	158 (100%)	0	100	100
2	I	157/165 (95%)	157 (100%)	0	100	100
2	J	155/165 (94%)	154 (99%)	1 (1%)	78	83
2	K	157/165 (95%)	153 (98%)	4 (2%)	42	69
2	L	158/165 (96%)	157 (99%)	1 (1%)	78	83
2	M	157/165 (95%)	155 (99%)	2 (1%)	61	77
3	N	140/140 (100%)	140 (100%)	0	100	100
3	O	140/140 (100%)	140 (100%)	0	100	100
3	P	140/140 (100%)	140 (100%)	0	100	100
3	Q	139/140 (99%)	137 (99%)	2 (1%)	59	76
3	R	139/140 (99%)	138 (99%)	1 (1%)	76	82
3	S	139/140 (99%)	137 (99%)	2 (1%)	59	76
3	T	140/140 (100%)	139 (99%)	1 (1%)	76	82
4	U	1/1 (100%)	1 (100%)	0	100	100
4	V	1/1 (100%)	0	1 (100%)	0	0
4	W	1/1 (100%)	0	1 (100%)	0	0
4	Y	1/1 (100%)	0	1 (100%)	0	0
4	Z	1/1 (100%)	0	1 (100%)	0	0
4	a	1/1 (100%)	1 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	b	1/1 (100%)	1 (100%)	0	100	100
All	All	4721/5418 (87%)	4698 (100%)	23 (0%)	78	85

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	T	101	GLU
2	K	143	ILE
2	K	85	SER
2	K	164	MET
2	L	149	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
2	I	153	GLN
3	O	42	ASN
2	J	34	ASN
2	L	94	GLN
3	Q	37	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

7 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	S0R	Y	1	4	15,16,17	1.49	2 (13%)	19,20,22	1.09	2 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	S0R	a	1	4	15,16,17	1.44	2 (13%)	19,20,22	0.82	0
4	S0R	b	1	4	15,16,17	1.45	2 (13%)	19,20,22	0.91	2 (10%)
4	S0R	U	1	4	15,16,17	1.42	2 (13%)	19,20,22	0.95	1 (5%)
4	S0R	Z	1	4	15,16,17	1.46	2 (13%)	19,20,22	1.00	2 (10%)
4	S0R	V	1	4	15,16,17	1.49	2 (13%)	19,20,22	1.40	3 (15%)
4	S0R	W	1	4	15,16,17	1.43	2 (13%)	19,20,22	0.86	0

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
4	S0R	Y	1	4	-	3/13/14/16	0/1/1/1
4	S0R	a	1	4	-	2/13/14/16	0/1/1/1
4	S0R	b	1	4	-	2/13/14/16	0/1/1/1
4	S0R	U	1	4	-	0/13/14/16	0/1/1/1
4	S0R	Z	1	4	-	1/13/14/16	0/1/1/1
4	S0R	V	1	4	-	4/13/14/16	0/1/1/1
4	S0R	W	1	4	-	2/13/14/16	0/1/1/1

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	Y	1	S0R	C-N	4.78	1.45	1.34
4	V	1	S0R	C-N	4.62	1.44	1.34
4	a	1	S0R	C-N	4.61	1.44	1.34
4	Z	1	S0R	C-N	4.54	1.44	1.34
4	b	1	S0R	C-N	4.50	1.44	1.34

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	V	1	S0R	C1-C-N	3.14	122.87	117.04
4	V	1	S0R	C7-CA-N	-2.90	103.89	109.50
4	Z	1	S0R	C7-CA-N	-2.69	104.31	109.50
4	U	1	S0R	C7-CA-N	-2.37	104.92	109.50
4	Z	1	S0R	O-C7-CA	-2.27	118.93	124.77

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	V	1	S0R	O-C7-CA-CB
4	W	1	S0R	O-C7-CA-CB
4	Y	1	S0R	O-C7-CA-CB
4	a	1	S0R	O-C7-CA-CB
4	b	1	S0R	C7-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	ATP	D	902	-	32,33,33	3.50	14 (43%)	48,52,52	2.13	15 (31%)
7	ATP	C	901	-	32,33,33	3.52	15 (46%)	48,52,52	2.08	15 (31%)
7	ATP	E	901	-	32,33,33	3.50	14 (43%)	48,52,52	2.11	15 (31%)
7	ATP	E	902	-	32,33,33	3.52	15 (46%)	48,52,52	2.06	14 (29%)
6	ADP	A	901	-	28,29,29	3.01	11 (39%)	43,45,45	2.70	10 (23%)
6	ADP	A	902	-	28,29,29	3.02	11 (39%)	43,45,45	2.87	11 (25%)
7	ATP	B	902	-	32,33,33	3.54	15 (46%)	48,52,52	2.11	16 (33%)
7	ATP	B	901	-	32,33,33	3.54	14 (43%)	48,52,52	2.06	13 (27%)
7	ATP	C	902	-	32,33,33	3.52	15 (46%)	48,52,52	2.14	15 (31%)
7	ATP	D	901	-	32,33,33	3.54	14 (43%)	48,52,52	2.08	15 (31%)
6	ADP	F	1001	-	28,29,29	3.05	11 (39%)	43,45,45	2.84	9 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	ADP	F	1000	-	28,29,29	3.01	11 (39%)	43,45,45	2.80	11 (25%)

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
7	ATP	D	902	-	-	8/22/38/38	0/3/3/3
7	ATP	C	901	-	-	5/22/38/38	0/3/3/3
7	ATP	E	901	-	-	6/22/38/38	0/3/3/3
7	ATP	E	902	-	-	10/22/38/38	0/3/3/3
6	ADP	A	901	-	-	4/16/32/32	0/3/3/3
6	ADP	A	902	-	-	3/16/32/32	0/3/3/3
7	ATP	B	902	-	-	4/22/38/38	0/3/3/3
7	ATP	B	901	-	-	4/22/38/38	0/3/3/3
7	ATP	C	902	-	-	9/22/38/38	0/3/3/3
7	ATP	D	901	-	-	11/22/38/38	0/3/3/3
6	ADP	F	1001	-	-	4/16/32/32	0/3/3/3
6	ADP	F	1000	-	-	1/16/32/32	0/3/3/3

The worst 5 of 160 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	E	902	ATP	C2'-C3'	-10.88	1.23	1.53
7	E	901	ATP	C2'-C3'	-10.85	1.24	1.53
7	B	901	ATP	C2'-C3'	-10.82	1.24	1.53
7	C	901	ATP	C2'-C3'	-10.81	1.24	1.53
7	C	902	ATP	C2'-C3'	-10.80	1.24	1.53

The worst 5 of 159 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	1001	ADP	C1'-N9-C8	-10.06	104.77	127.09
6	A	902	ADP	C1'-N9-C8	-10.03	104.84	127.09
6	F	1000	ADP	C1'-N9-C8	-9.38	106.28	127.09
6	A	901	ADP	C1'-N9-C8	-9.14	106.81	127.09
6	F	1001	ADP	C4-N9-C8	6.90	112.98	105.74

There are no chirality outliers.

5 of 69 torsion outliers are listed below:

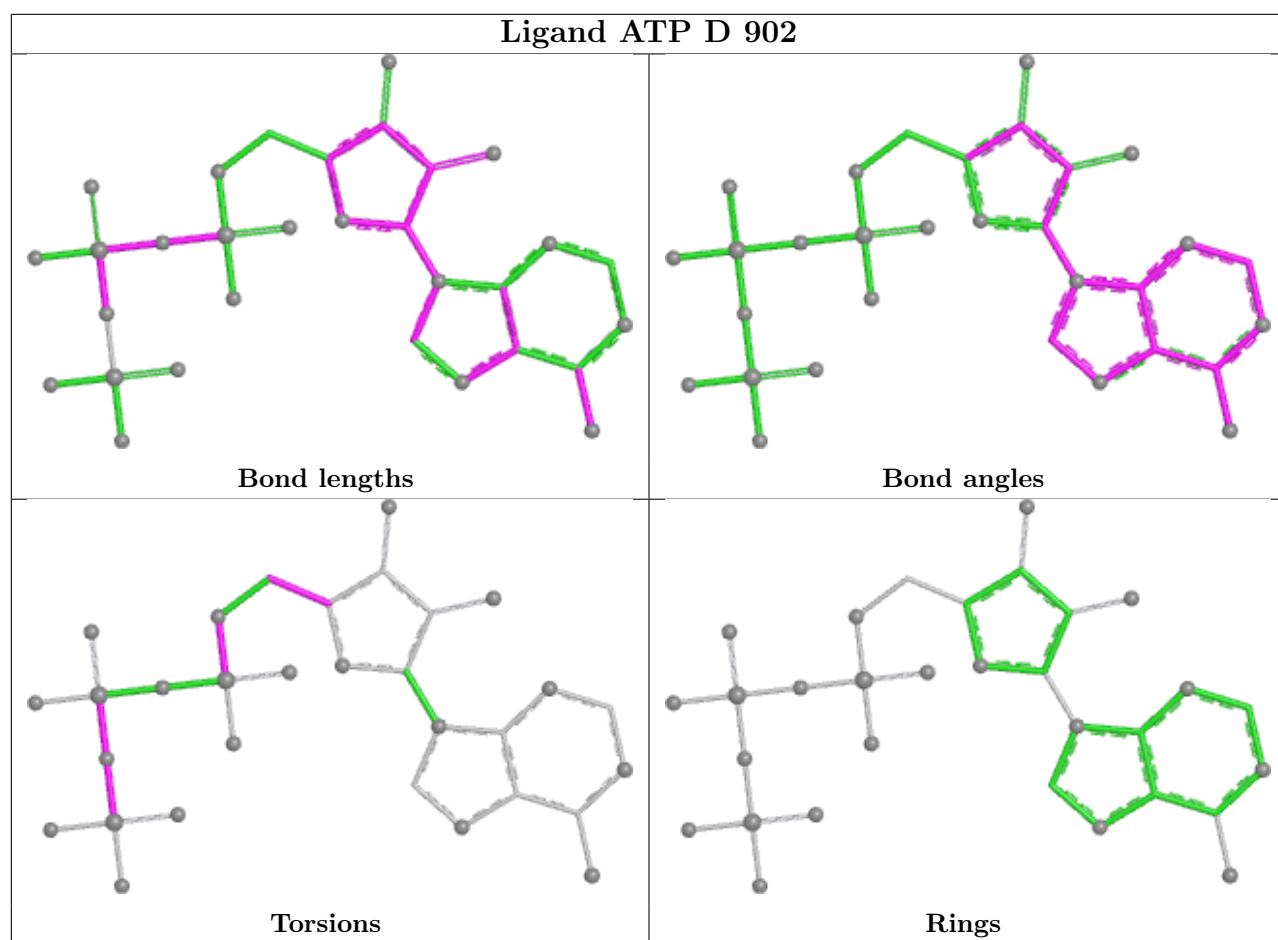
Mol	Chain	Res	Type	Atoms
6	A	901	ADP	PA-O3A-PB-O2B
6	F	1000	ADP	PA-O3A-PB-O3B
6	F	1001	ADP	C5'-O5'-PA-O2A
6	F	1001	ADP	C5'-O5'-PA-O3A
6	F	1001	ADP	O4'-C1'-N9-C8

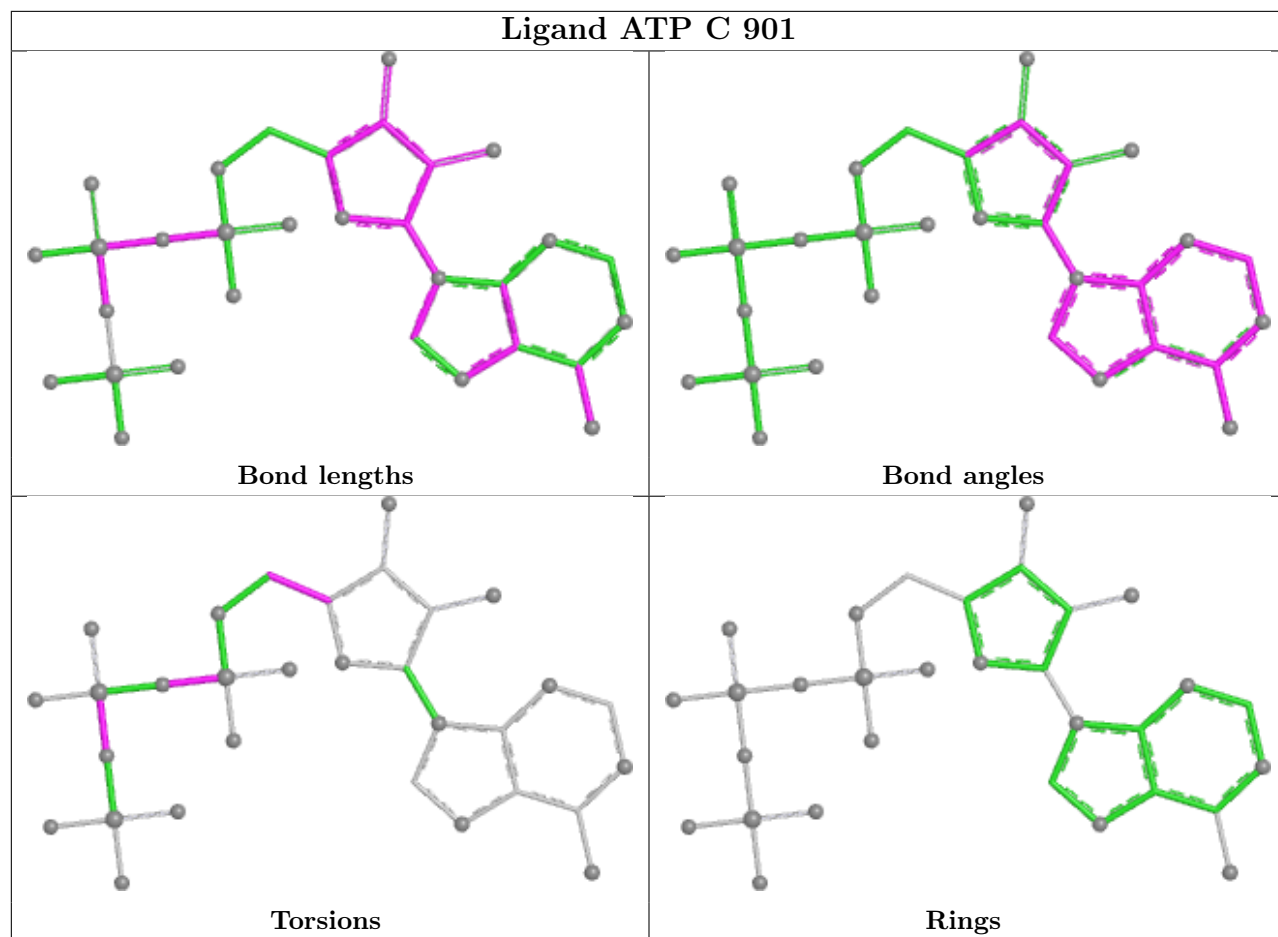
There are no ring outliers.

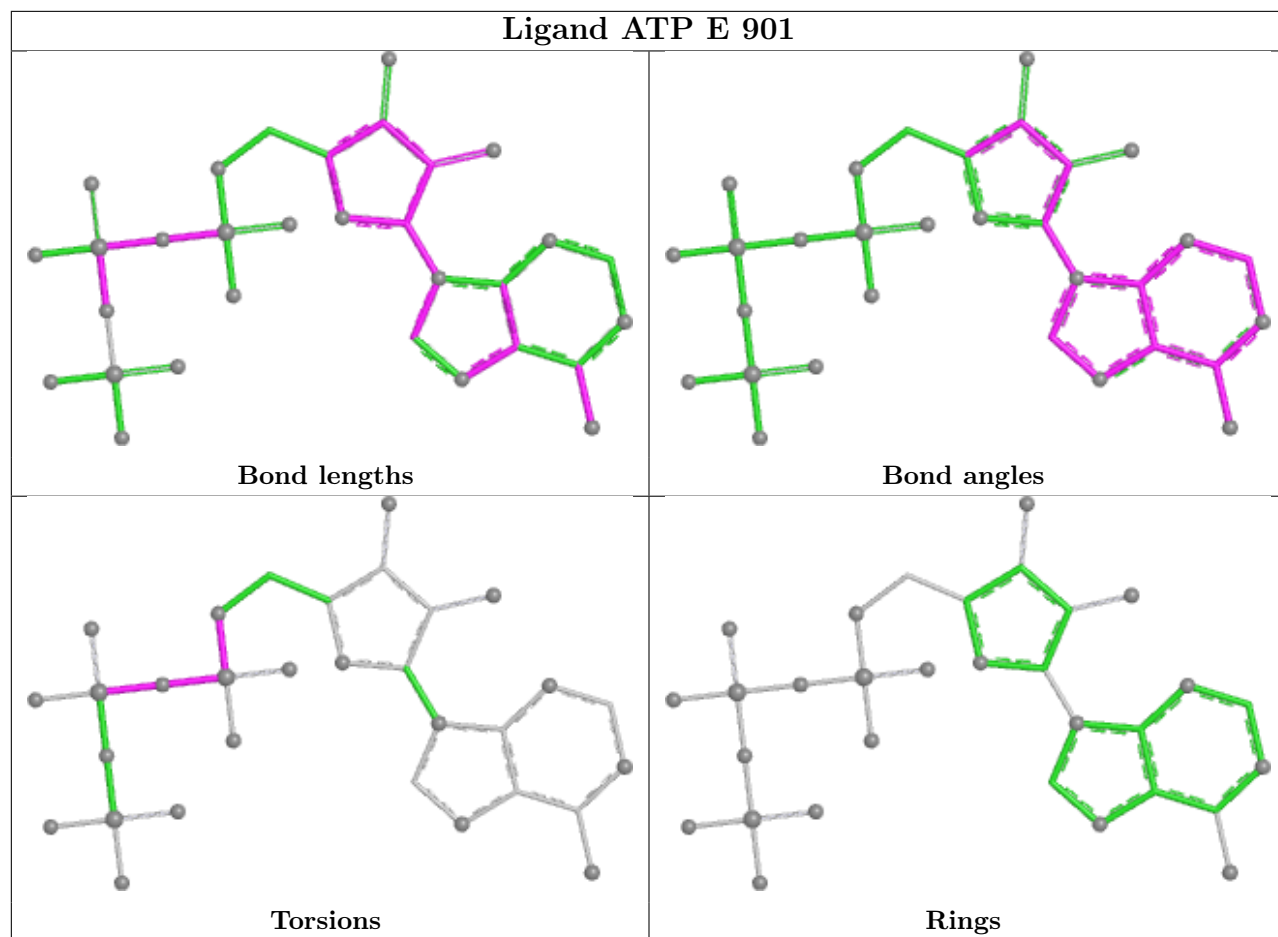
5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	901	ATP	1	0
6	A	901	ADP	1	0
7	B	902	ATP	1	0
7	B	901	ATP	1	0
6	F	1000	ADP	1	0

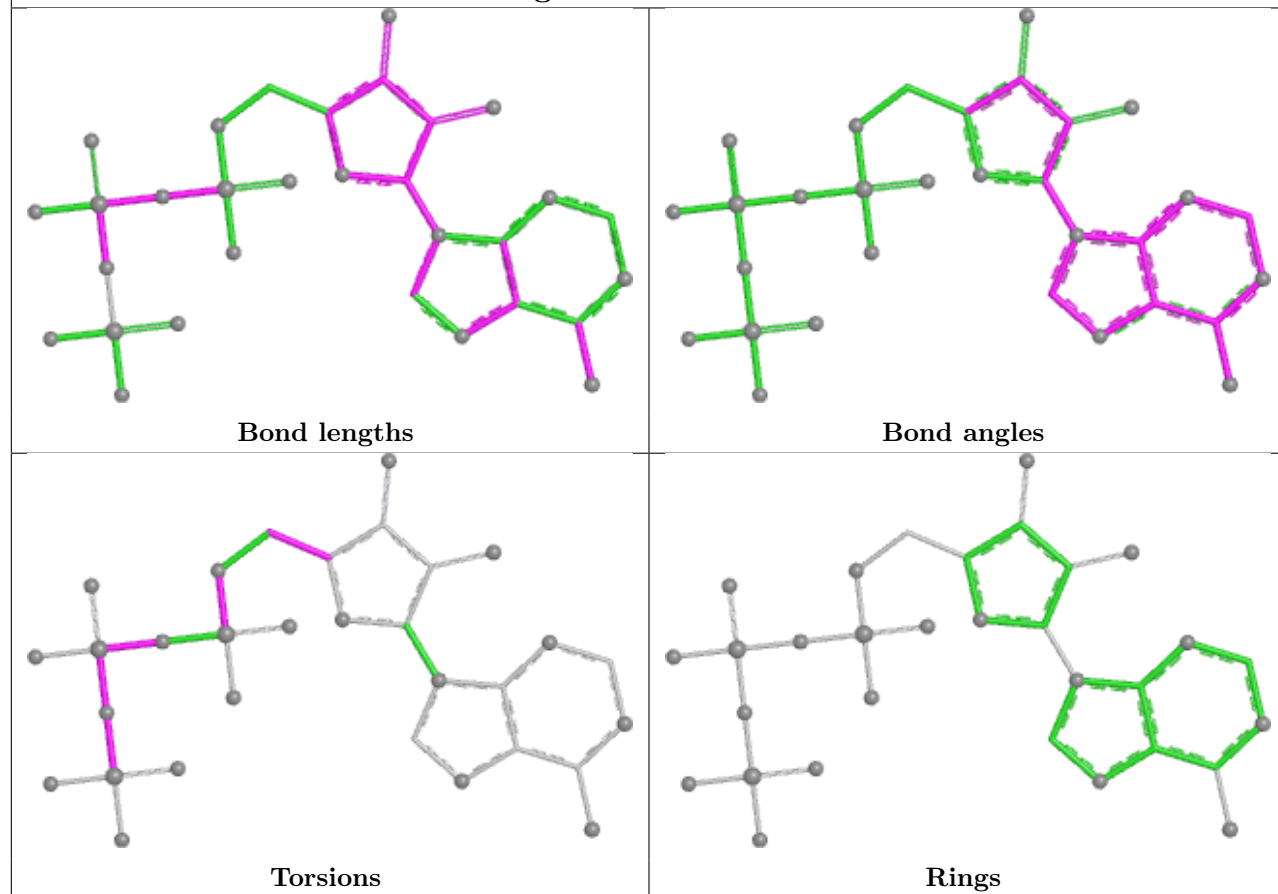
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



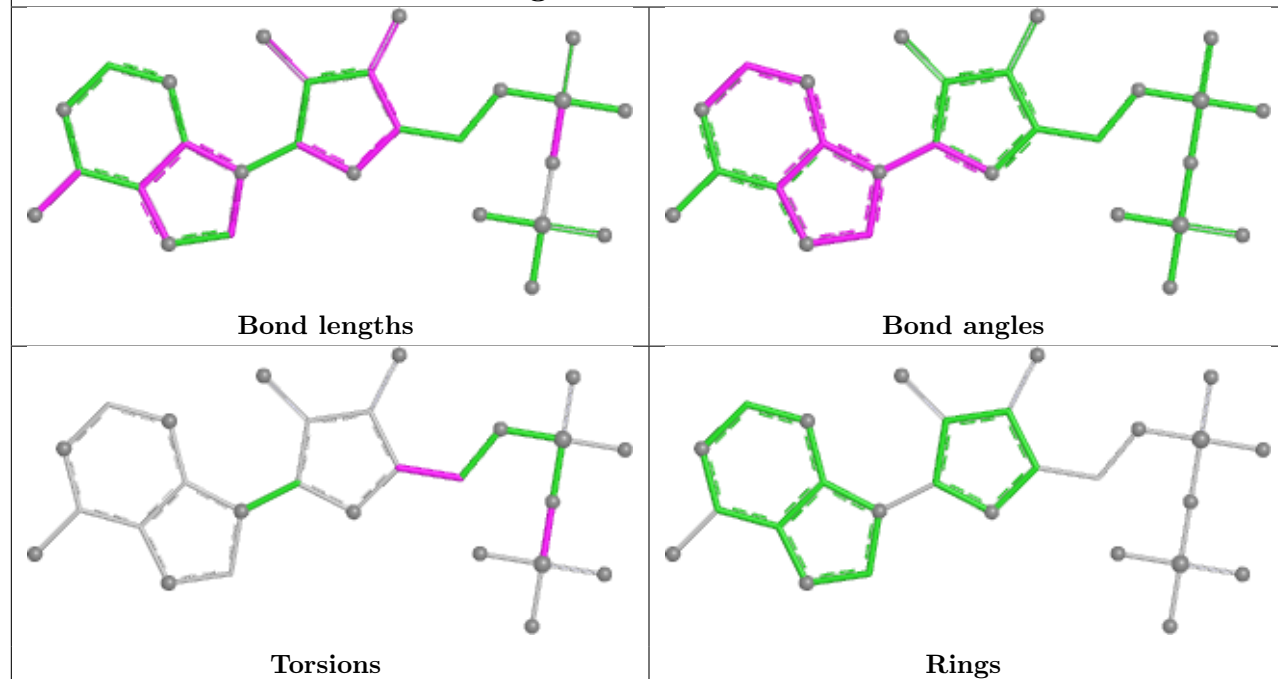


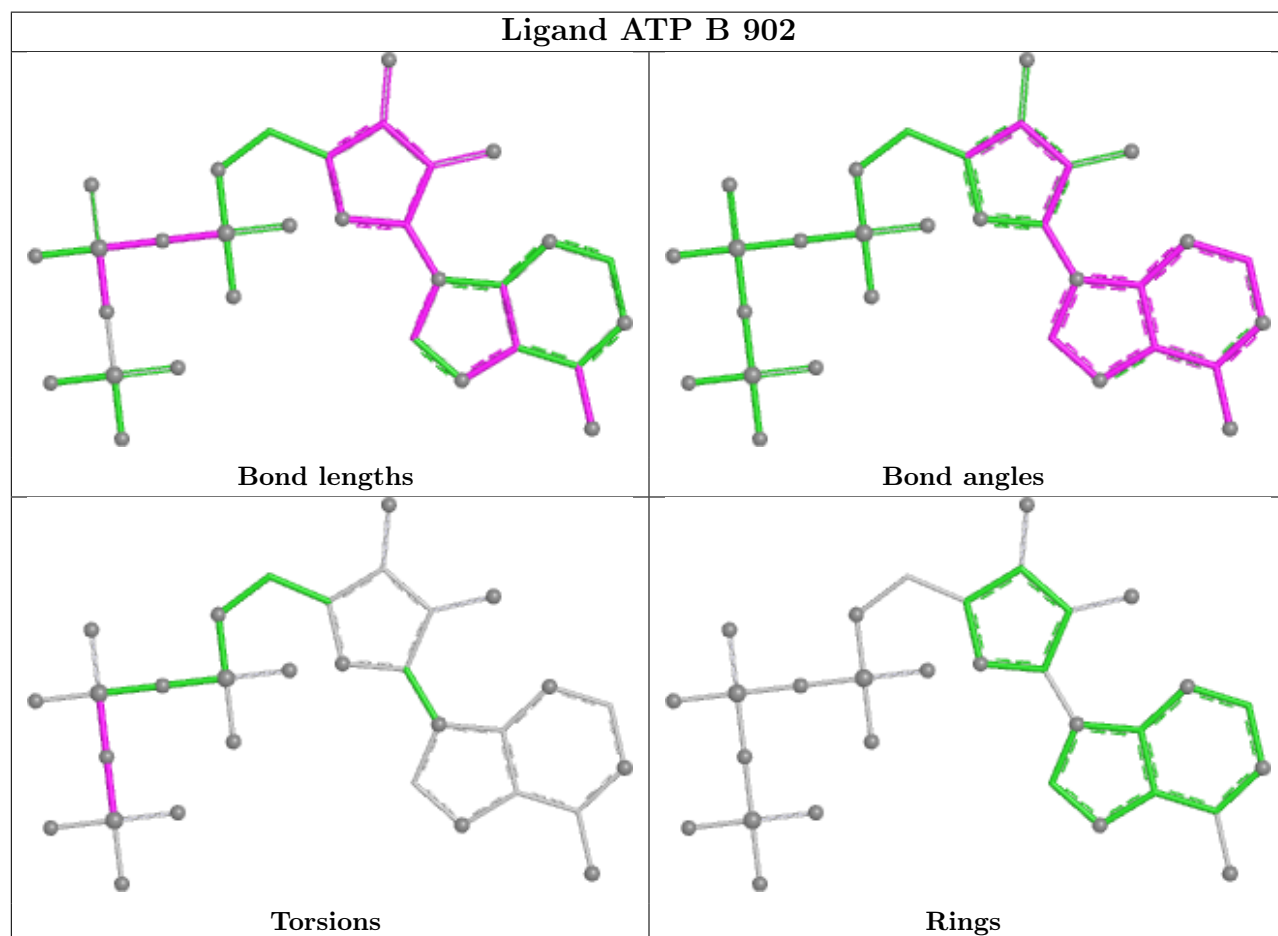
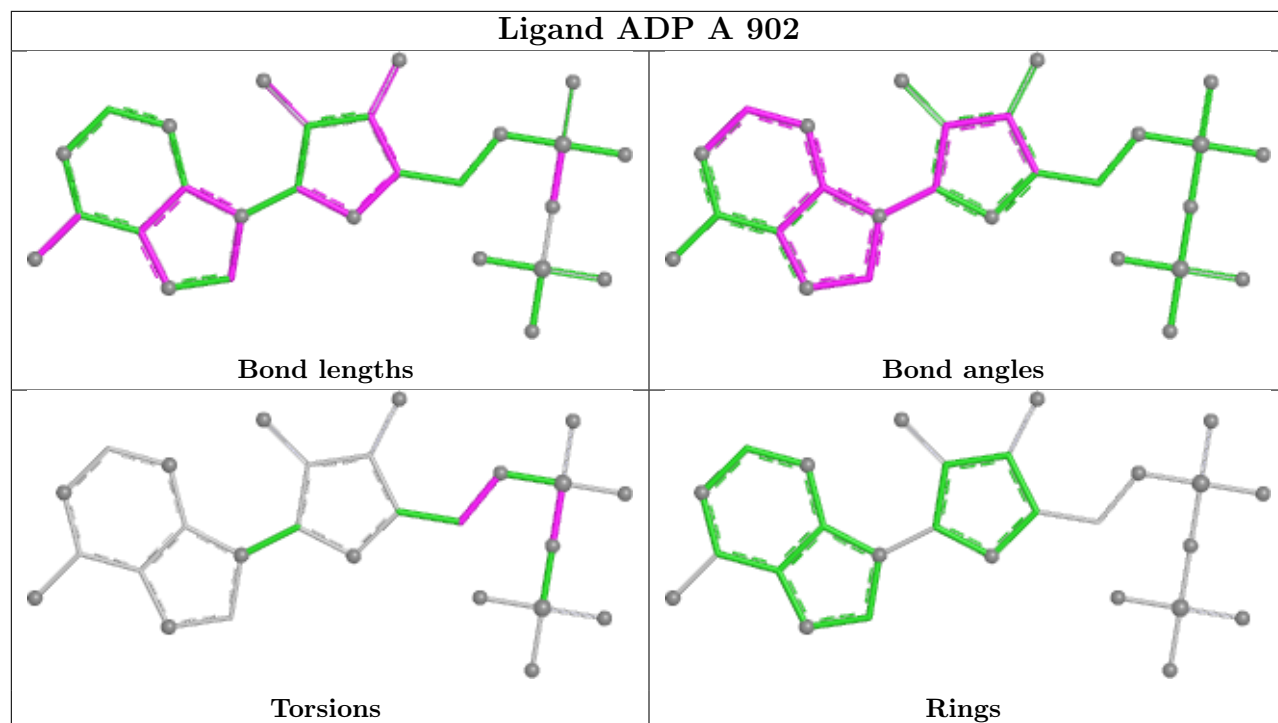


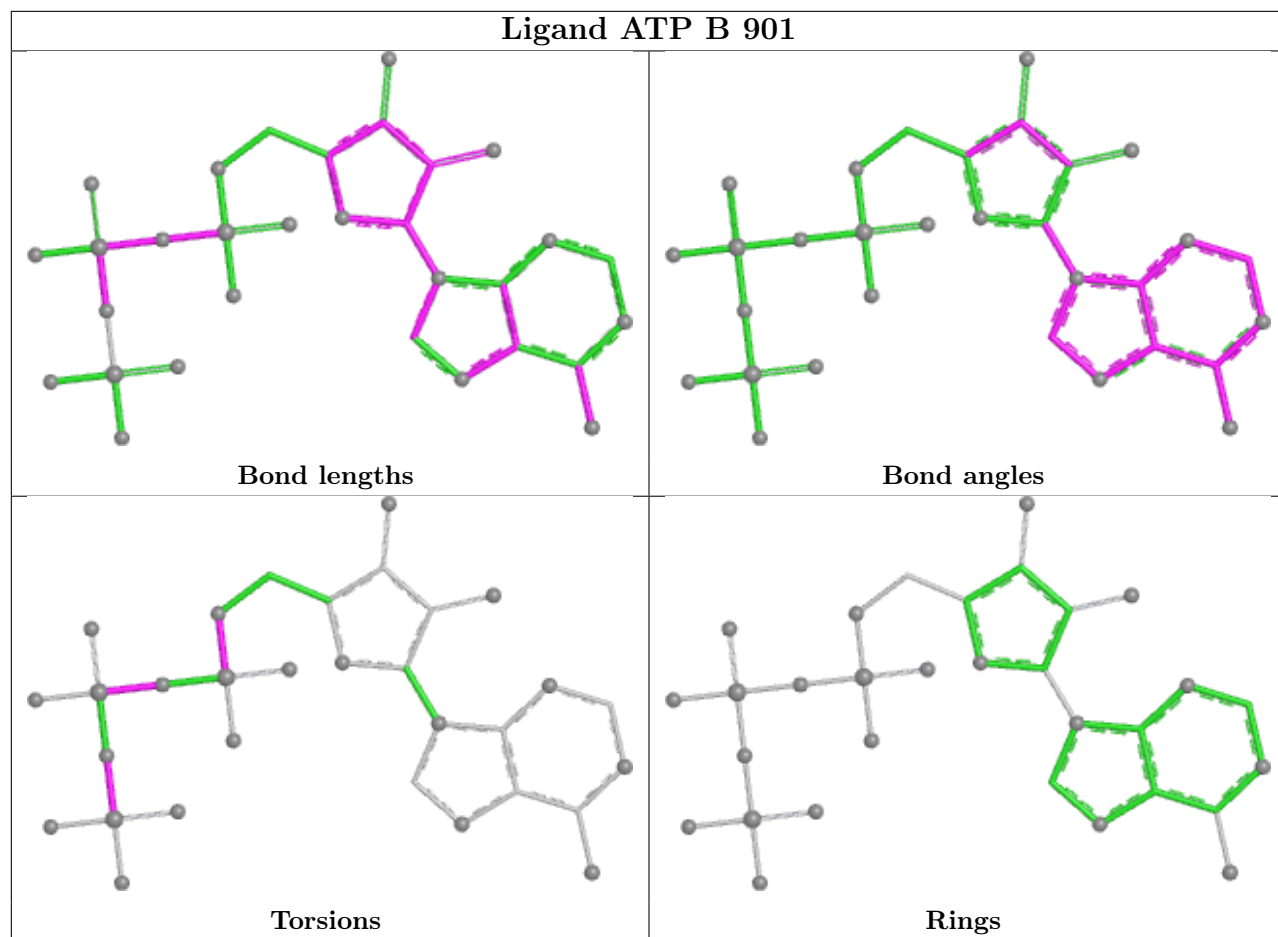
Ligand ATP E 902

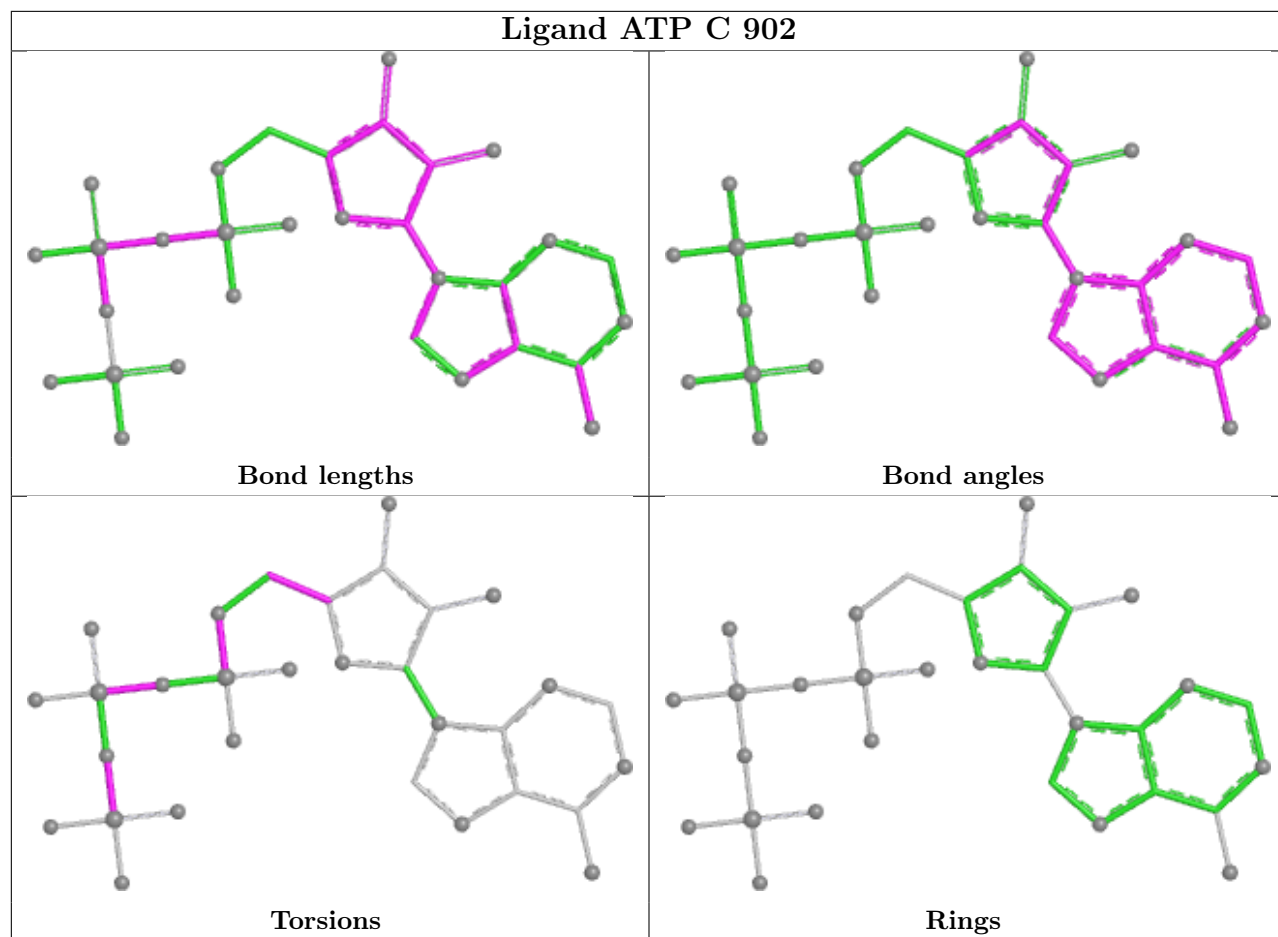


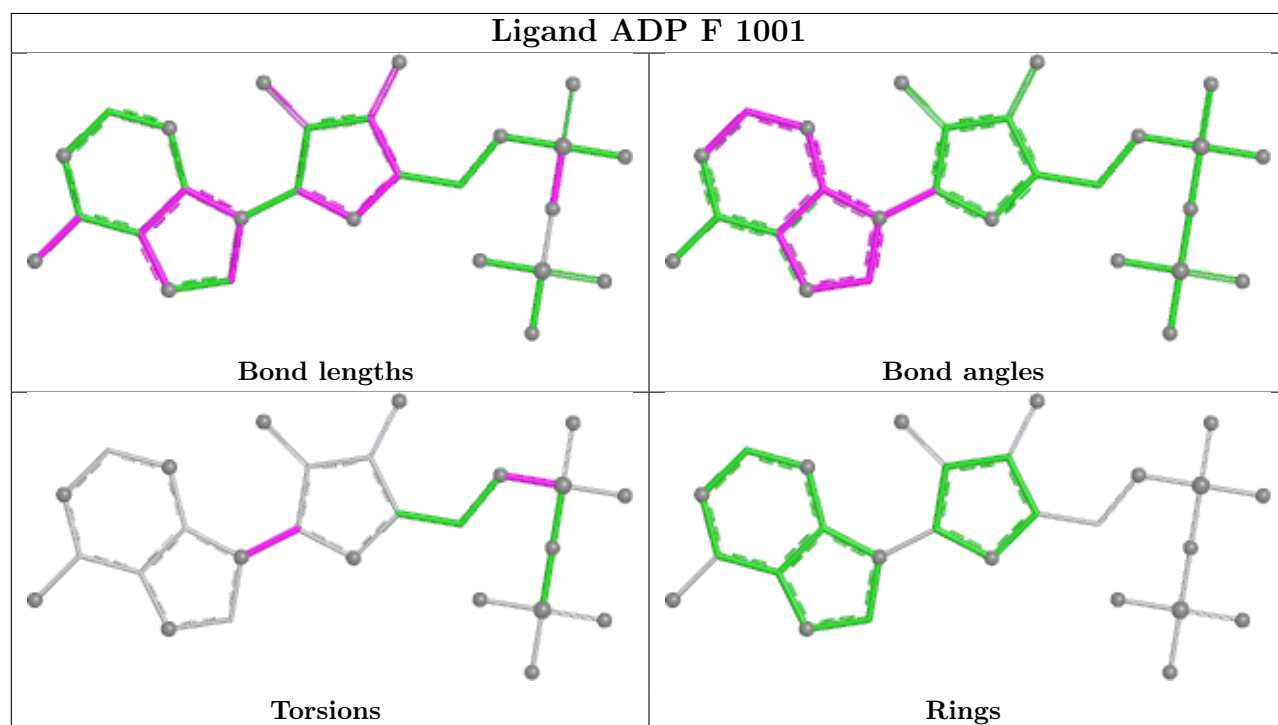
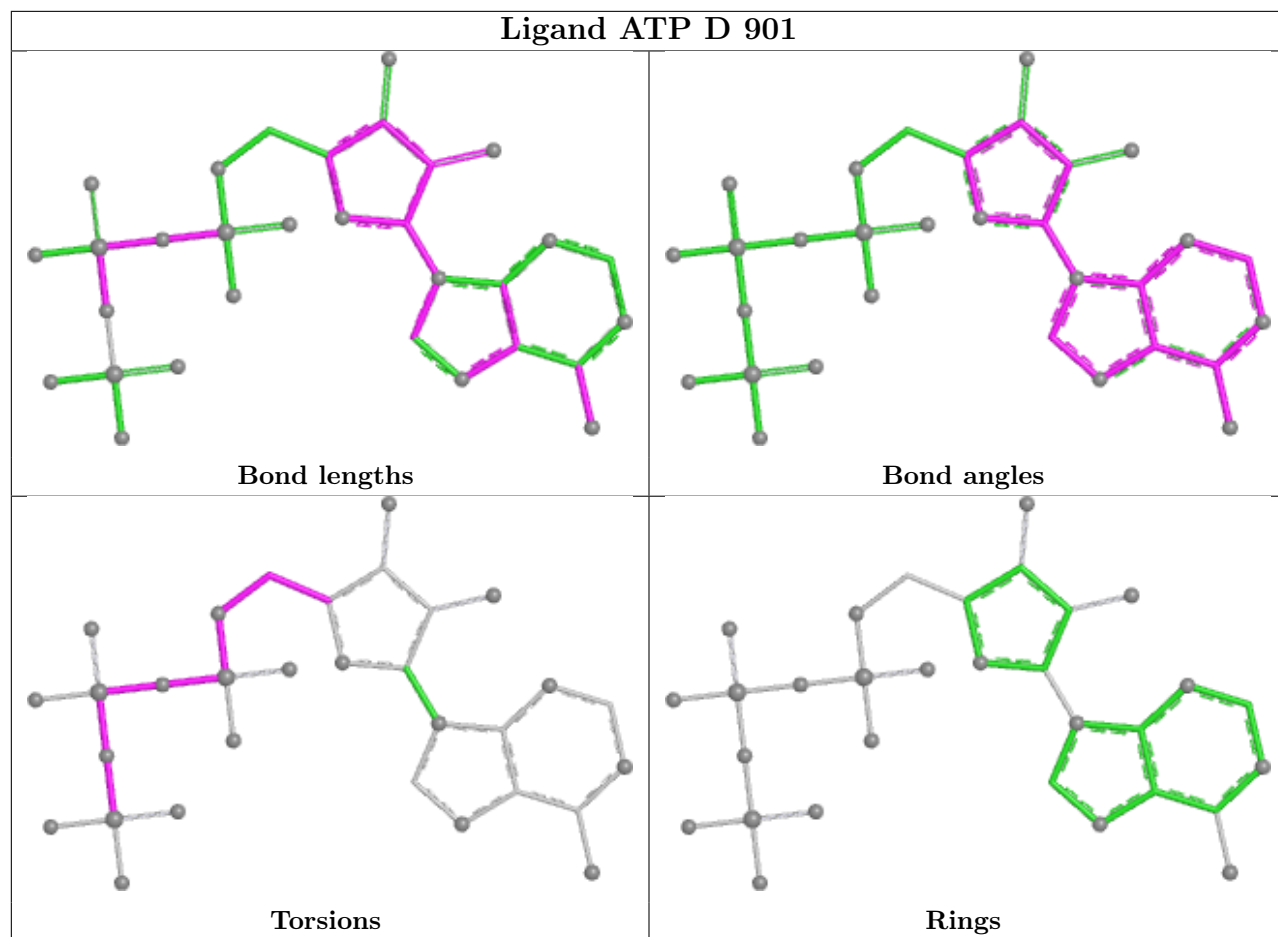
Ligand ADP A 901

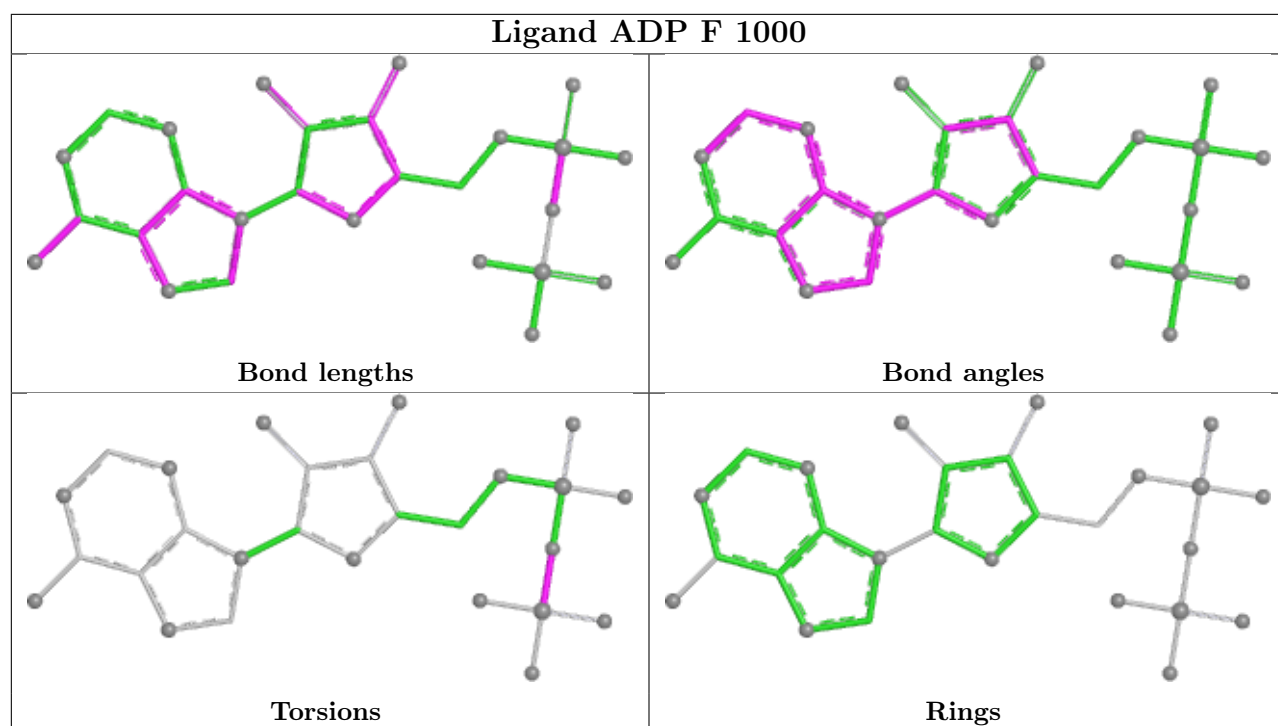












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

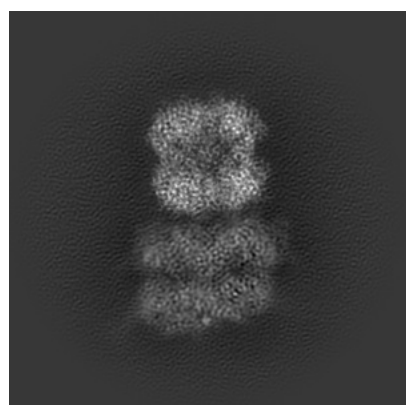
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52840. These allow visual inspection of the internal detail of the map and identification of artifacts.

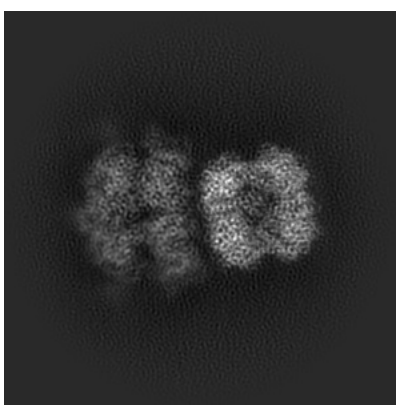
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

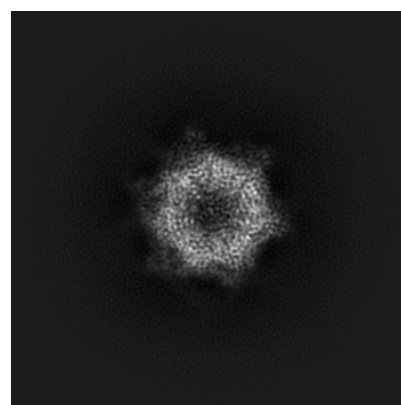
6.1.1 Primary map



X



Y



Z

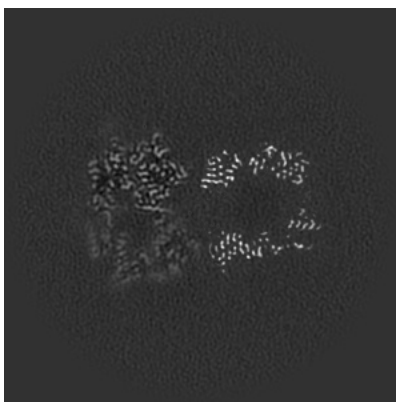
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

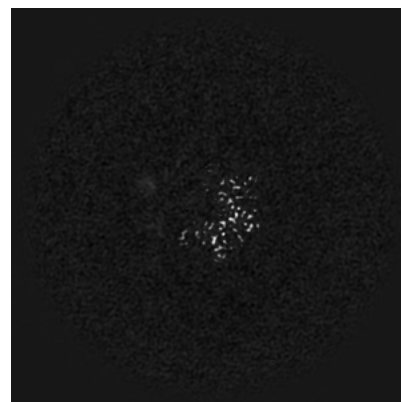
6.2.1 Primary map



X Index: 300



Y Index: 300

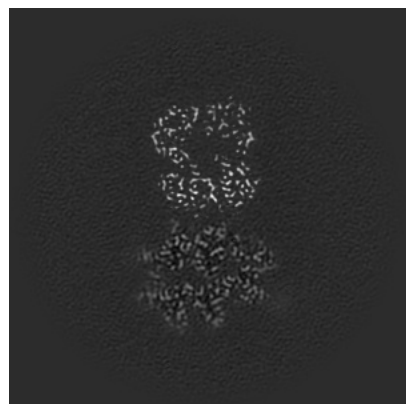


Z Index: 300

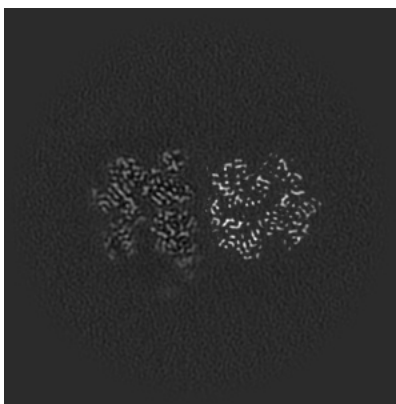
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

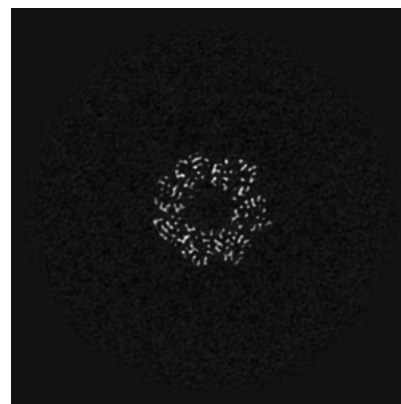
6.3.1 Primary map



X Index: 346



Y Index: 352

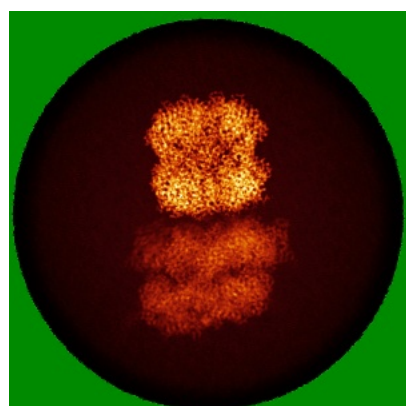


Z Index: 337

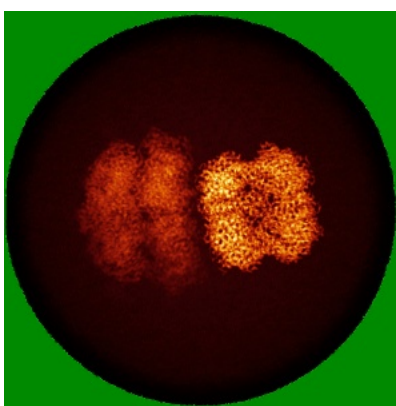
The images above show the largest variance slices of the map in three orthogonal directions.

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

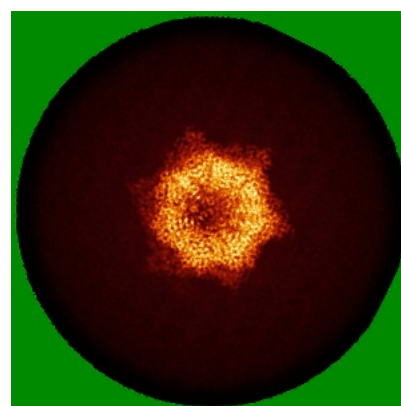
6.4.1 Primary map



X



Y

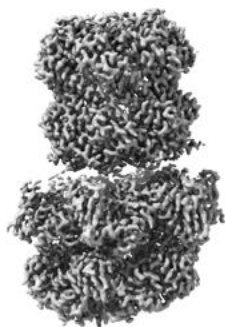


Z

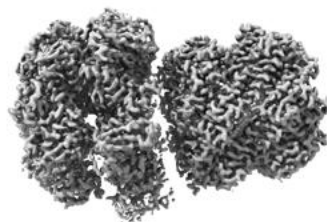
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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

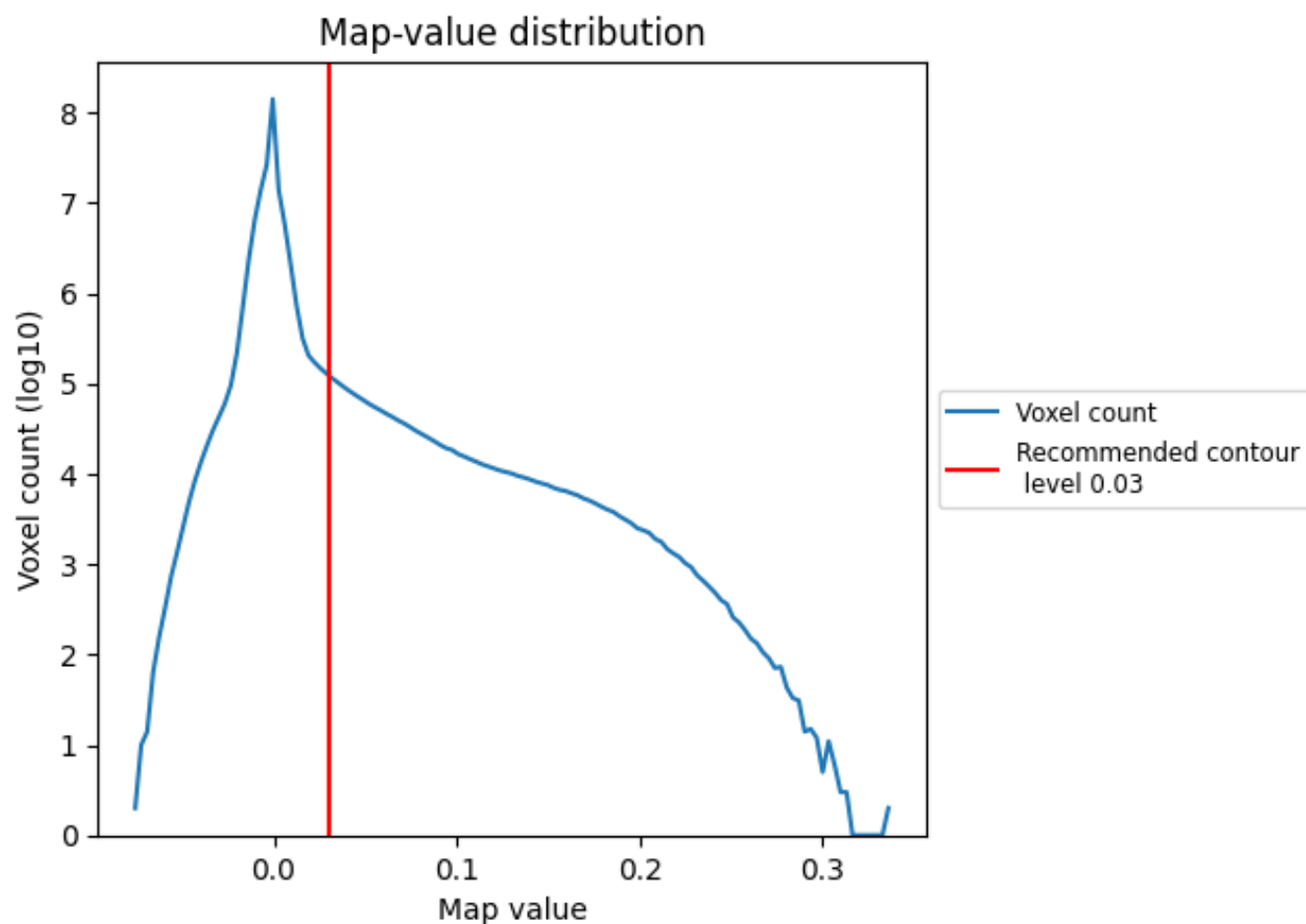
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

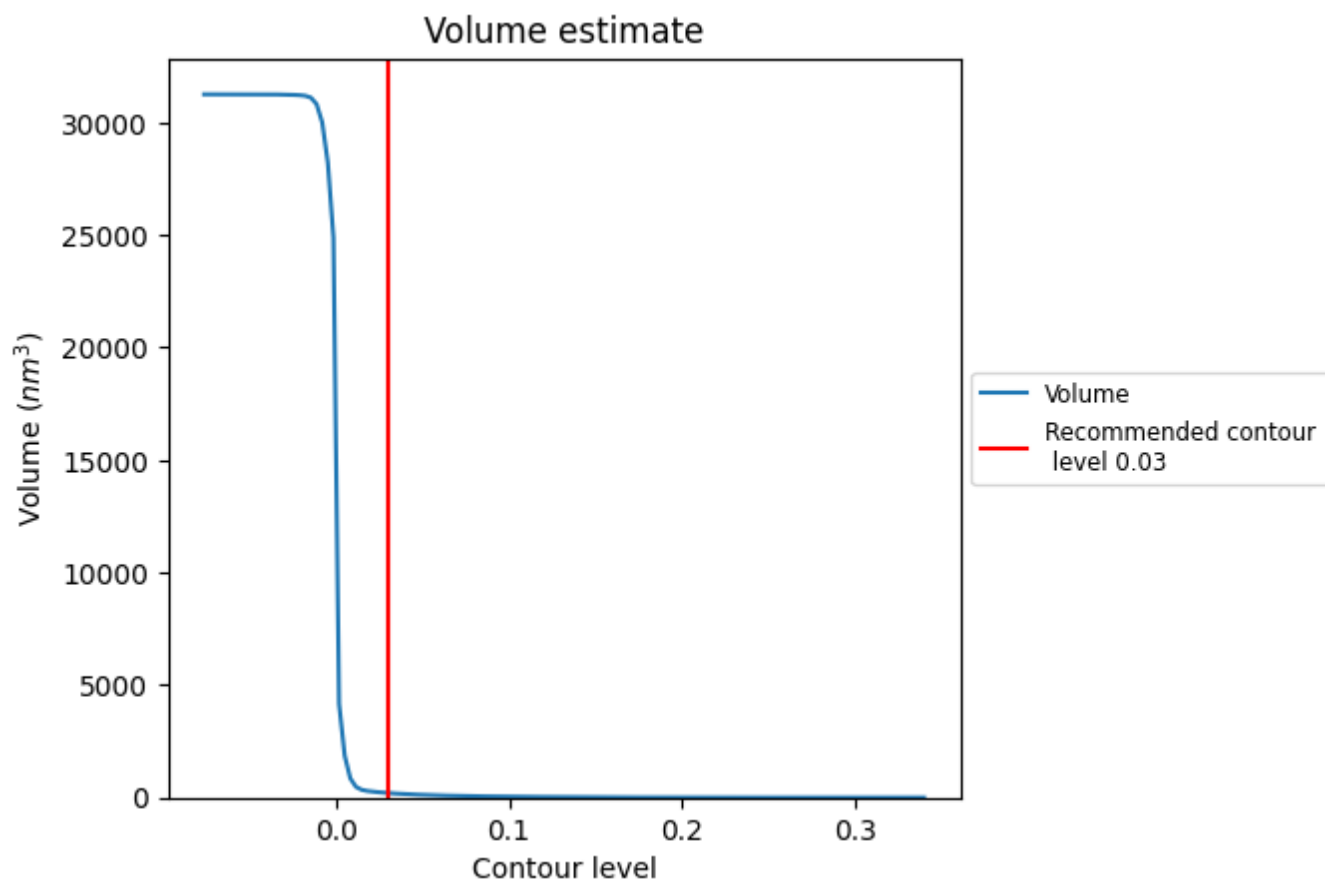
This section contains the results of statistical analysis of the map.

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.

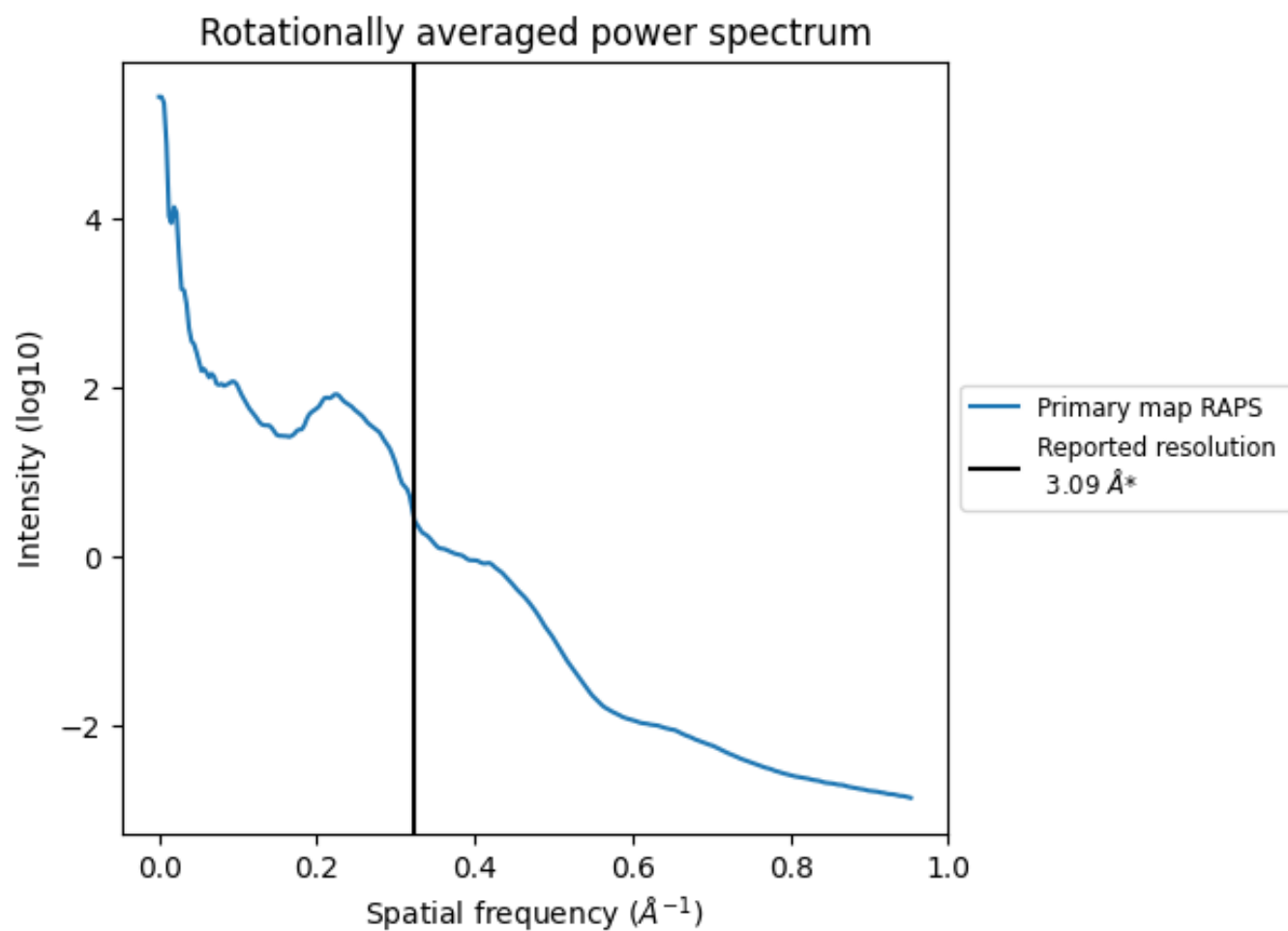
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 204 nm^3 ; this corresponds to an approximate mass of 184 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 0.324 Å⁻¹

8 Fourier-Shell correlation

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

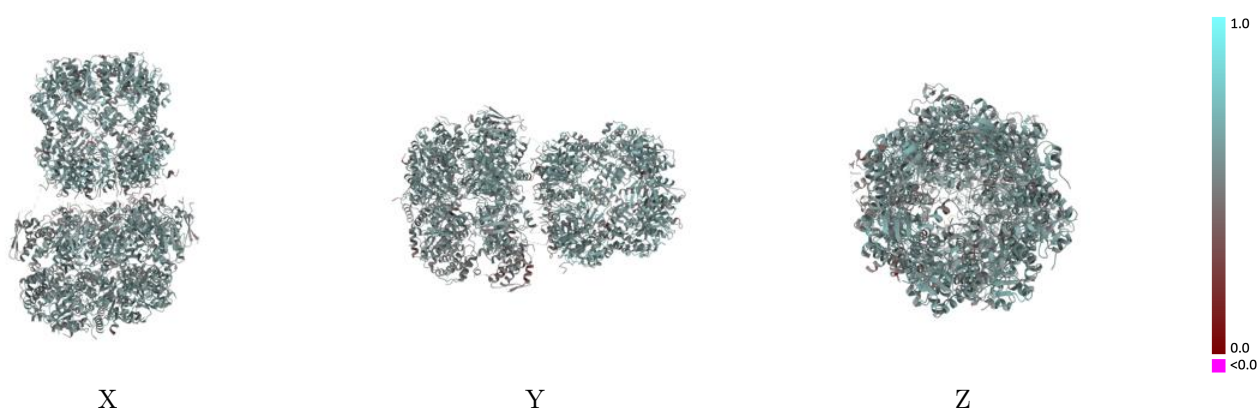
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-52840 and PDB model 9IF4. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)

This section was not generated.

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

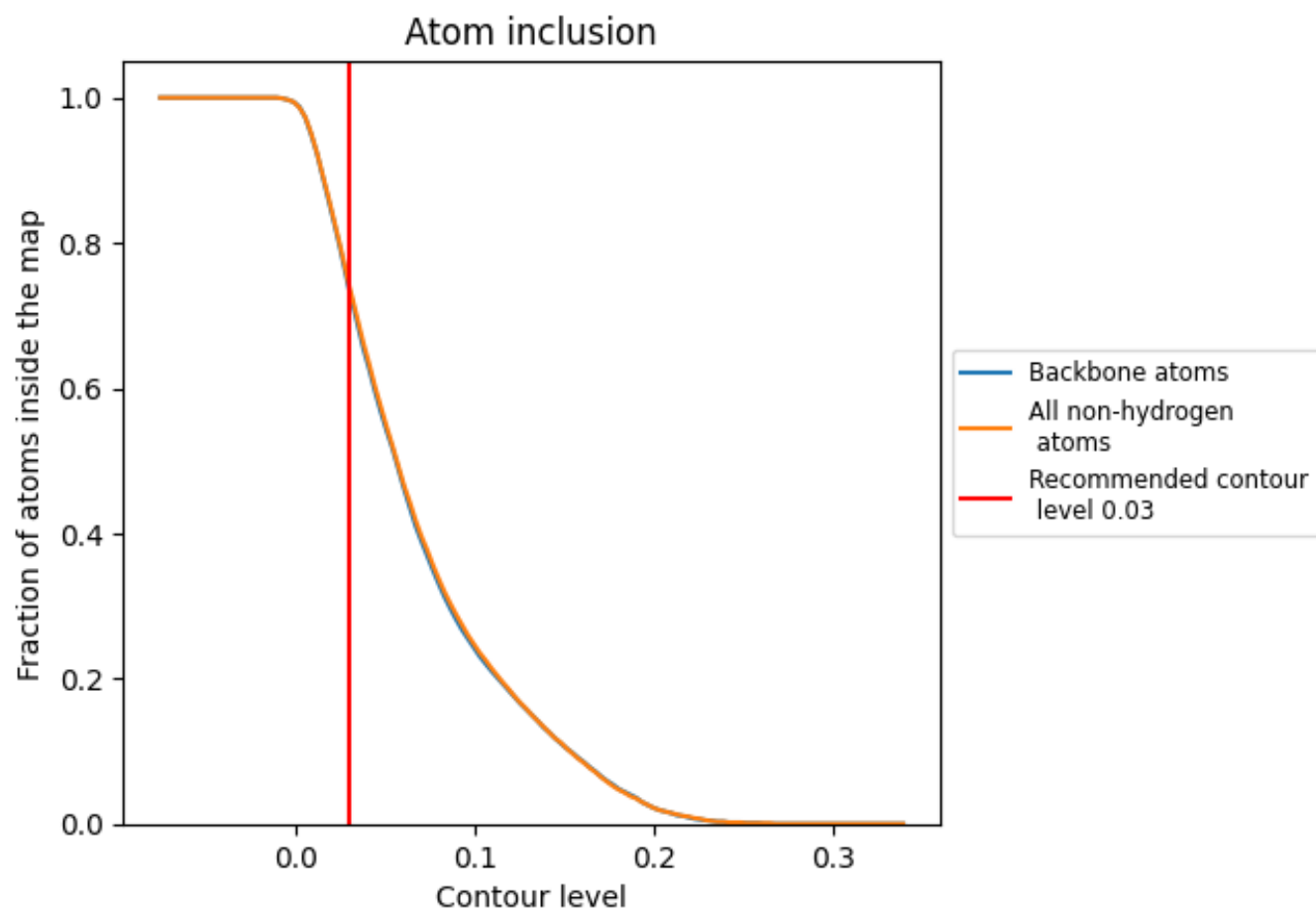


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.



























































9.4 Atom inclusion ⓘ



At the recommended contour level, 73% of all backbone atoms, 74% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7390	 0.5510
A	 0.5740	 0.5050
B	 0.7110	 0.5460
C	 0.7740	 0.5650
D	 0.7710	 0.5650
E	 0.7130	 0.5460
F	 0.5470	 0.4950
G	 0.8040	 0.5590
H	 0.8170	 0.5680
I	 0.8090	 0.5680
J	 0.8180	 0.5660
K	 0.8140	 0.5640
L	 0.7980	 0.5570
M	 0.7940	 0.5550
N	 0.8210	 0.5690
O	 0.8150	 0.5710
P	 0.8200	 0.5670
Q	 0.8160	 0.5690
R	 0.8210	 0.5670
S	 0.8160	 0.5680
T	 0.8290	 0.5730
U	 0.7200	 0.4730
V	 0.7200	 0.4550
W	 0.7200	 0.4870
X	 0.6770	 0.5500
Y	 0.7600	 0.5240
Z	 0.8000	 0.5230
a	 0.6800	 0.4370
b	 0.7600	 0.4810

