



## wwPDB EM Validation Summary Report ⓘ

Nov 13, 2022 – 08:31 AM EST

PDB ID : 6VFX  
EMDB ID : EMD-21194  
Title : ClpXP from Neisseria meningitidis - Conformation B  
Authors : Ripstein, Z.A.; Vahidi, S.; Houry, W.A.; Rubinstein, J.L.; Kay, L.E.  
Deposited on : 2020-01-06  
Resolution : 2.90 Å (reported)  
Based on initial model : 3HWS

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

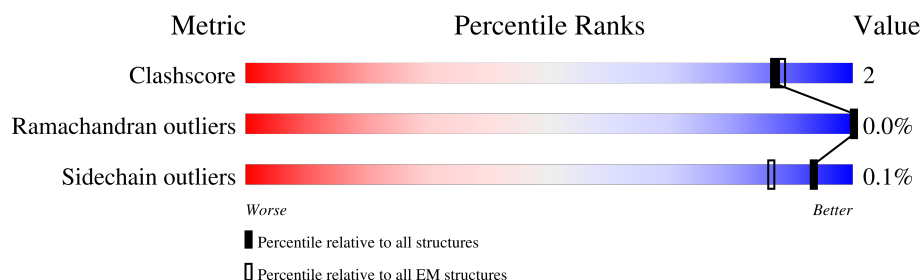
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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  $\geq 3$ , 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	414	<div> <div>12%</div> <div>71%</div> <div>10%</div> <div>18%</div> </div>
1	B	414	<div> <div>75%</div> <div>7%</div> <div>19%</div> </div>
1	C	414	<div> <div>78%</div> <div>•</div> <div>20%</div> </div>
1	D	414	<div> <div>78%</div> <div>•</div> <div>18%</div> </div>
1	E	414	<div> <div>76%</div> <div>6%</div> <div>18%</div> </div>
1	F	414	<div> <div>12%</div> <div>72%</div> <div>5%</div> <div>22%</div> </div>
2	G	7	<div> <div>43%</div> <div>57%</div> <div>43%</div> </div>
3	H	204	<div> <div>34%</div> <div>91%</div> <div>•</div> <div>7%</div> </div>

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Mol	Chain	Length	Quality of chain
3	I	204	<div> <div>27%</div> <div>90%</div> <div>6%</div> </div>
3	J	204	<div> <div>23%</div> <div>90%</div> <div>6%</div> </div>
3	K	204	<div> <div>25%</div> <div>91%</div> <div>5%</div> </div>
3	L	204	<div> <div>92%</div> <div>92%</div> <div>6%</div> </div>
3	M	204	<div> <div>39%</div> <div>87%</div> <div>9%</div> </div>
3	N	204	<div> <div>47%</div> <div>91%</div> <div>6%</div> </div>
3	O	204	<div> <div>92%</div> <div>92%</div> <div>6%</div> </div>
3	P	204	<div> <div>91%</div> <div>92%</div> <div>6%</div> </div>
3	Q	204	<div> <div>92%</div> <div>92%</div> <div>6%</div> </div>
3	R	204	<div> <div>90%</div> <div>92%</div> <div>6%</div> </div>
3	S	204	<div> <div>91%</div> <div>92%</div> <div>6%</div> </div>
3	T	204	<div> <div>94%</div> <div>92%</div> <div>6%</div> </div>
3	U	204	<div> <div>45%</div> <div>90%</div> <div>6%</div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 73452 atoms, of which 37000 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 ClpX.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	C	333	Total	C	H	N	O	S	0	0
			5207	1624	2655	440	481	7		
1	B	337	Total	C	H	N	O	S	0	0
			5283	1647	2695	445	489	7		
1	E	341	Total	C	H	N	O	S	0	0
			5357	1667	2735	457	491	7		
1	F	321	Total	C	H	N	O	S	0	0
			5038	1575	2573	421	462	7		
1	D	339	Total	C	H	N	O	S	0	0
			5314	1654	2710	451	492	7		
1	A	340	Total	C	H	N	O	S	0	0
			5311	1655	2707	449	493	7		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	185	GLN	GLU	conflict	UNP A0A0Y4ZJG4
C	315	ILE	GLU	conflict	UNP A0A0Y4ZJG4
B	185	GLN	GLU	conflict	UNP A0A0Y4ZJG4
B	315	ILE	GLU	conflict	UNP A0A0Y4ZJG4
E	185	GLN	GLU	conflict	UNP A0A0Y4ZJG4
E	315	ILE	GLU	conflict	UNP A0A0Y4ZJG4
F	185	GLN	GLU	conflict	UNP A0A0Y4ZJG4
F	315	ILE	GLU	conflict	UNP A0A0Y4ZJG4
D	185	GLN	GLU	conflict	UNP A0A0Y4ZJG4
D	315	ILE	GLU	conflict	UNP A0A0Y4ZJG4
A	185	GLN	GLU	conflict	UNP A0A0Y4ZJG4
A	315	ILE	GLU	conflict	UNP A0A0Y4ZJG4

- Molecule 2 is a protein called Unidentified peptide substrate.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	7	Total	C	H	N	O	0	0
			66	20	32	7	7		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
3	L	191	Total 2975	C 940	H 1488	N 251	O 288	S 8	0	0
3	O	191	Total 2975	C 940	H 1488	N 251	O 288	S 8	0	0
3	P	191	Total 2975	C 940	H 1488	N 251	O 288	S 8	0	0
3	Q	191	Total 2975	C 940	H 1488	N 251	O 288	S 8	0	0
3	R	191	Total 2975	C 940	H 1488	N 251	O 288	S 8	0	0
3	S	191	Total 2975	C 940	H 1488	N 251	O 288	S 8	0	0
3	T	191	Total 2975	C 940	H 1488	N 251	O 288	S 8	0	0
3	U	191	Total 2975	C 940	H 1488	N 251	O 288	S 8	0	0
3	H	190	Total 2968	C 938	H 1485	N 250	O 287	S 8	0	0
3	I	192	Total 2982	C 942	H 1491	N 252	O 289	S 8	0	0
3	J	191	Total 2975	C 940	H 1488	N 251	O 288	S 8	0	0
3	K	193	Total 3007	C 948	H 1505	N 256	O 290	S 8	0	0
3	M	186	Total 2910	C 920	H 1460	N 245	O 277	S 8	0	0
3	N	191	Total 2975	C 940	H 1488	N 251	O 288	S 8	0	0

There are 14 discrepancies between the modelled and reference sequences:

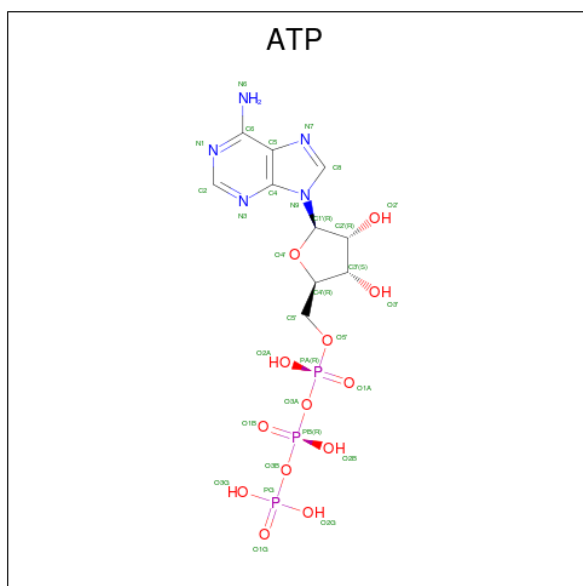
Chain	Residue	Modelled	Actual	Comment	Reference
L	165	ASP	GLY	conflict	UNP A0A0Y5K536
O	165	ASP	GLY	conflict	UNP A0A0Y5K536
P	165	ASP	GLY	conflict	UNP A0A0Y5K536
Q	165	ASP	GLY	conflict	UNP A0A0Y5K536
R	165	ASP	GLY	conflict	UNP A0A0Y5K536

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Chain	Residue	Modelled	Actual	Comment	Reference
S	165	ASP	GLY	conflict	UNP A0A0Y5K536
T	165	ASP	GLY	conflict	UNP A0A0Y5K536
U	165	ASP	GLY	conflict	UNP A0A0Y5K536
H	165	ASP	GLY	conflict	UNP A0A0Y5K536
I	165	ASP	GLY	conflict	UNP A0A0Y5K536
J	165	ASP	GLY	conflict	UNP A0A0Y5K536
K	165	ASP	GLY	conflict	UNP A0A0Y5K536
M	165	ASP	GLY	conflict	UNP A0A0Y5K536
N	165	ASP	GLY	conflict	UNP A0A0Y5K536

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ) (labeled as "Ligand of Interest" by depositor).

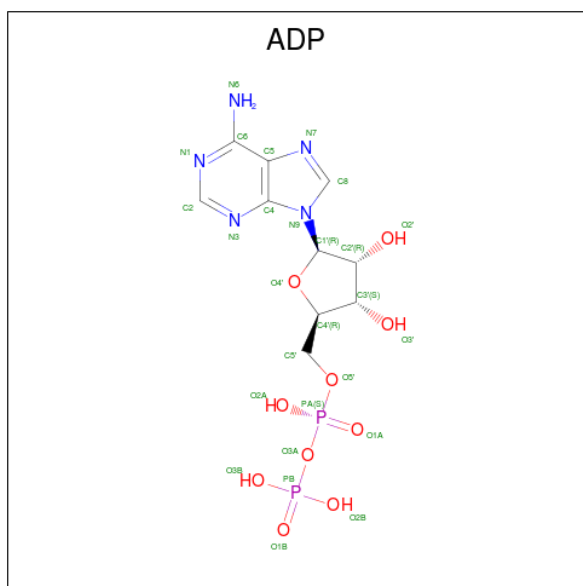


Mol	Chain	Residues	Atoms						AltConf
4	C	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
4	B	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
4	E	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
4	D	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
4	A	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
5	C	1	Total	Mg	0
			1	1	
5	B	1	Total	Mg	0
			1	1	
5	E	1	Total	Mg	0
			1	1	
5	D	1	Total	Mg	0
			1	1	
5	A	1	Total	Mg	0
			1	1	

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ) (labeled as "Ligand of Interest" by depositor).

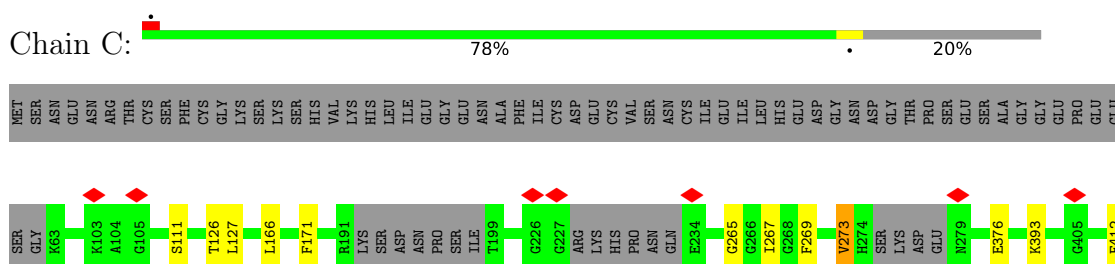


Mol	Chain	Residues	Atoms						AltConf
6	F	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	

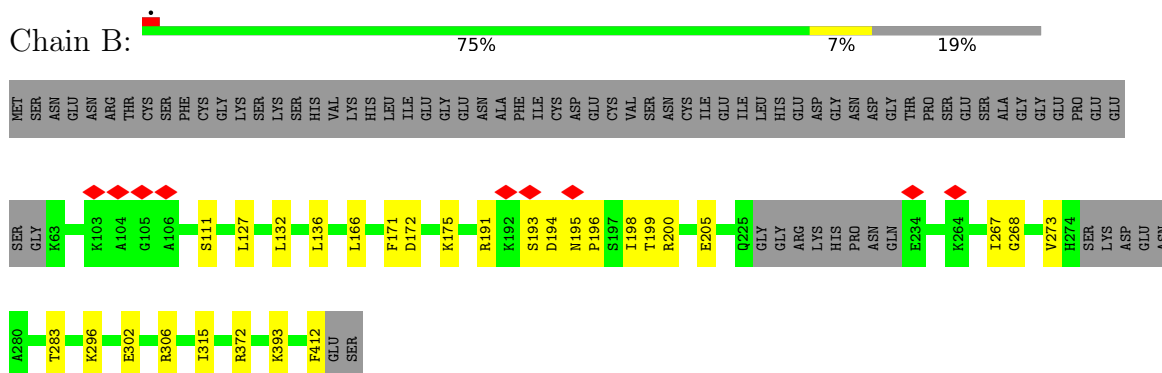
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

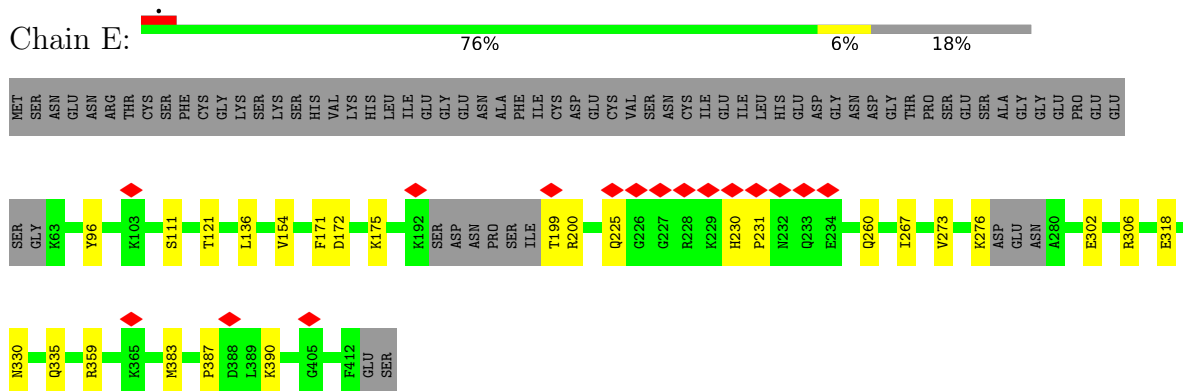
- Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpX



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

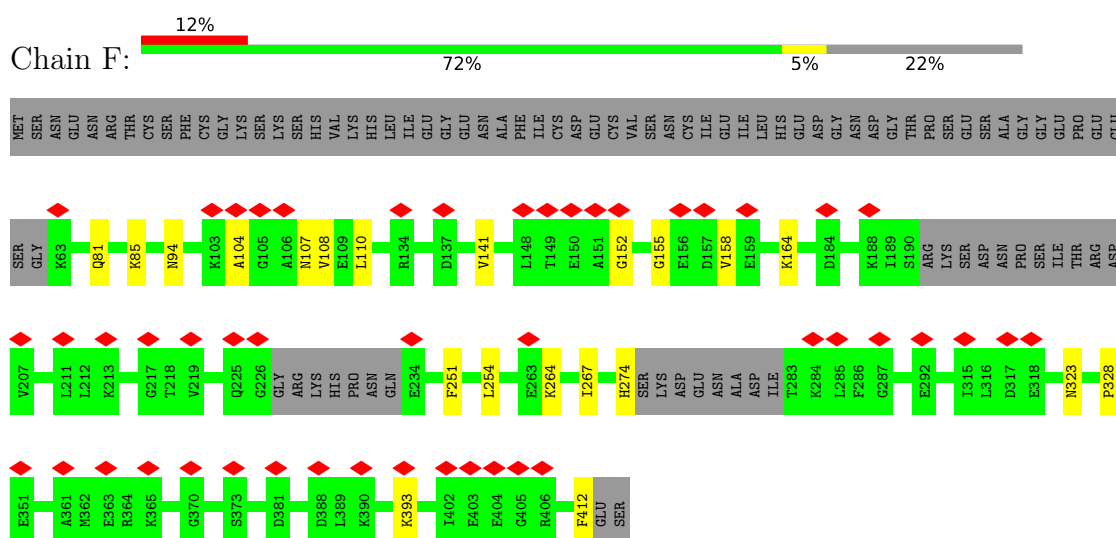


- Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpX

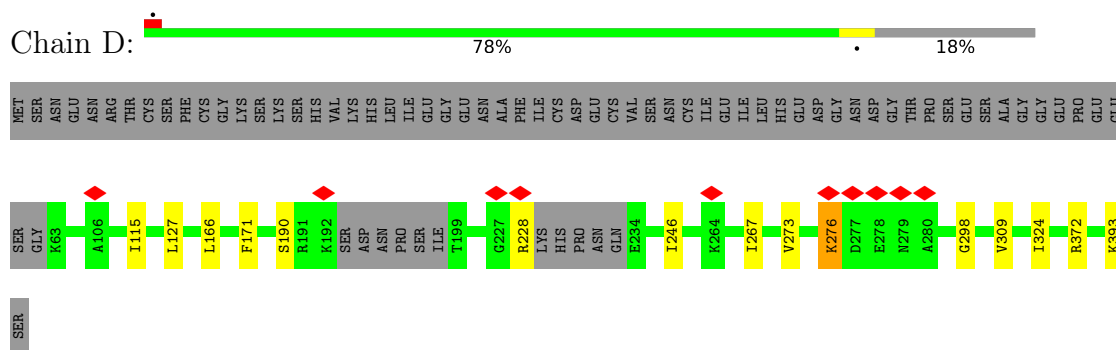


- Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpX

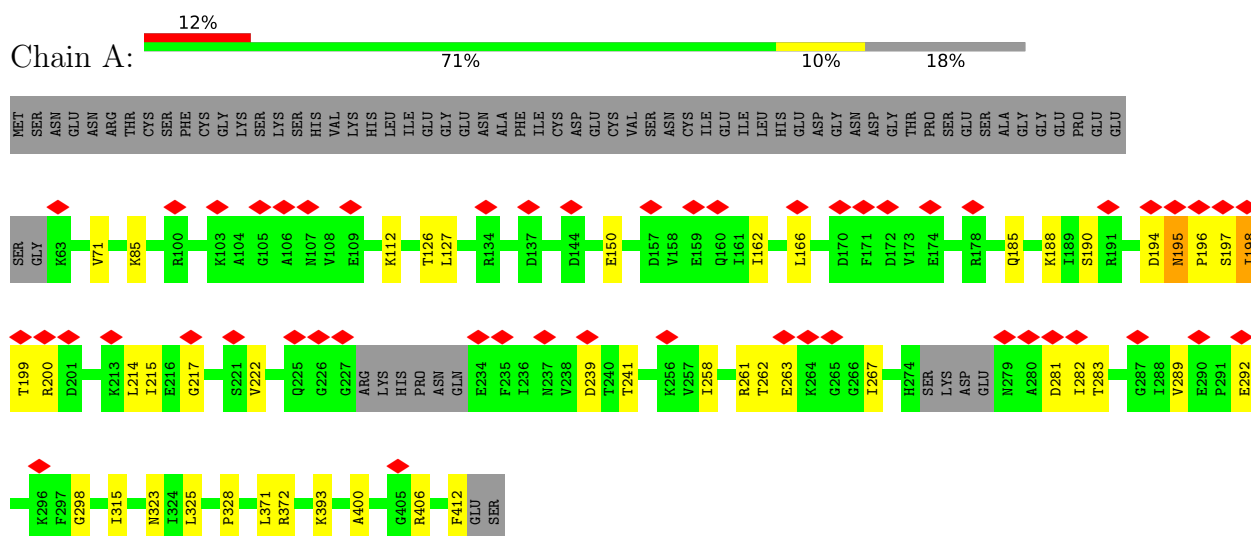




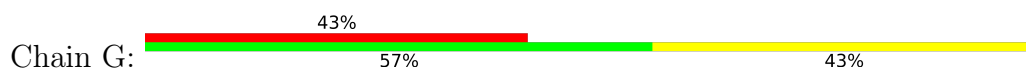
- Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpX

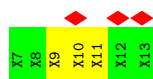


- Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpX



- Molecule 2: Unidentified peptide substrate

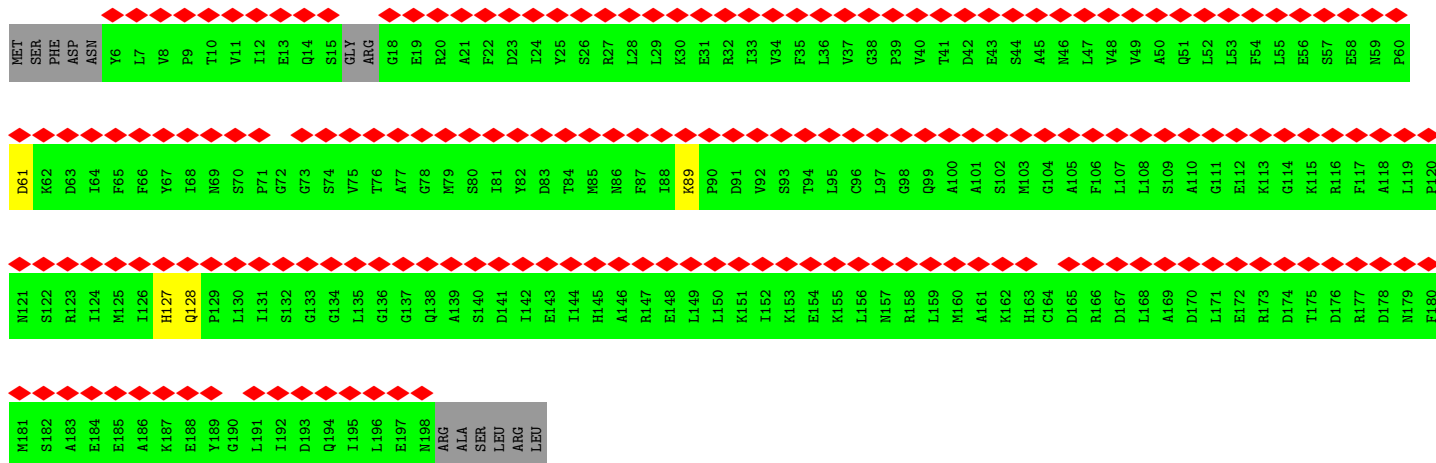




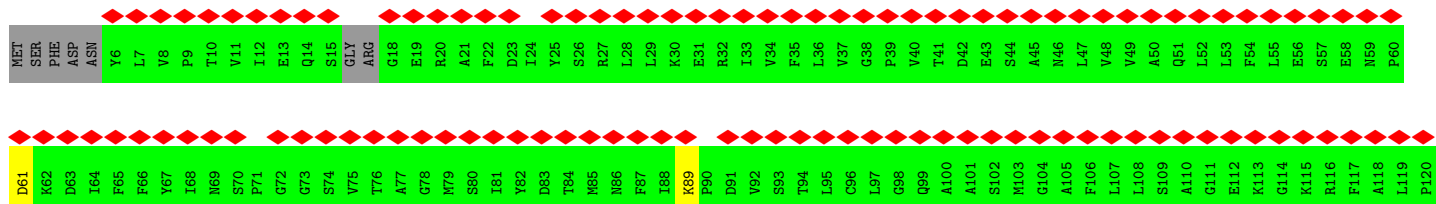
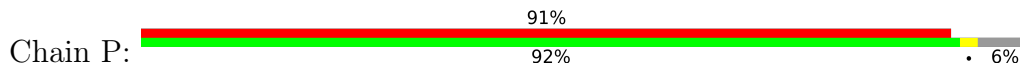
• Molecule 3: ATP-dependent Clp protease proteolytic subunit



• Molecule 3: ATP-dependent Clp protease proteolytic subunit

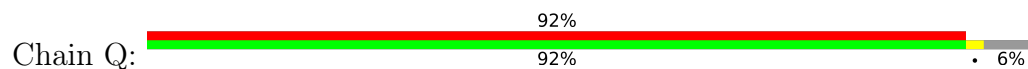


• Molecule 3: ATP-dependent Clp protease proteolytic subunit

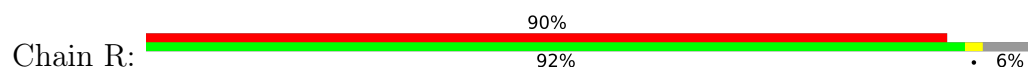




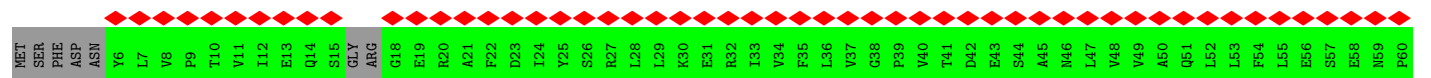
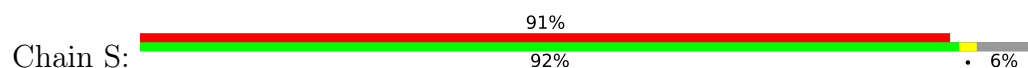
• Molecule 3: ATP-dependent Clp protease proteolytic subunit

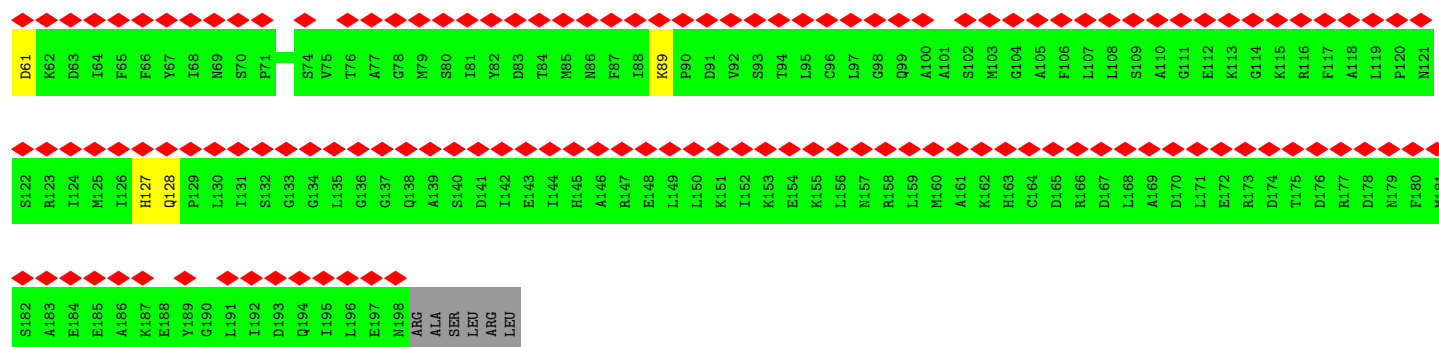


• Molecule 3: ATP-dependent Clp protease proteolytic subunit



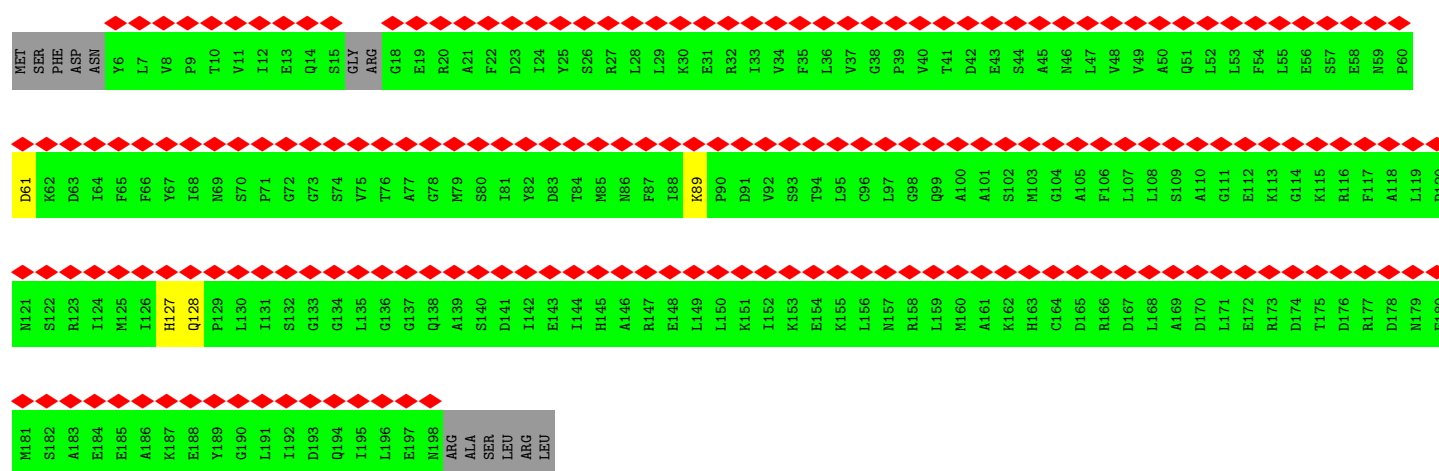
• Molecule 3: ATP-dependent Clp protease proteolytic subunit





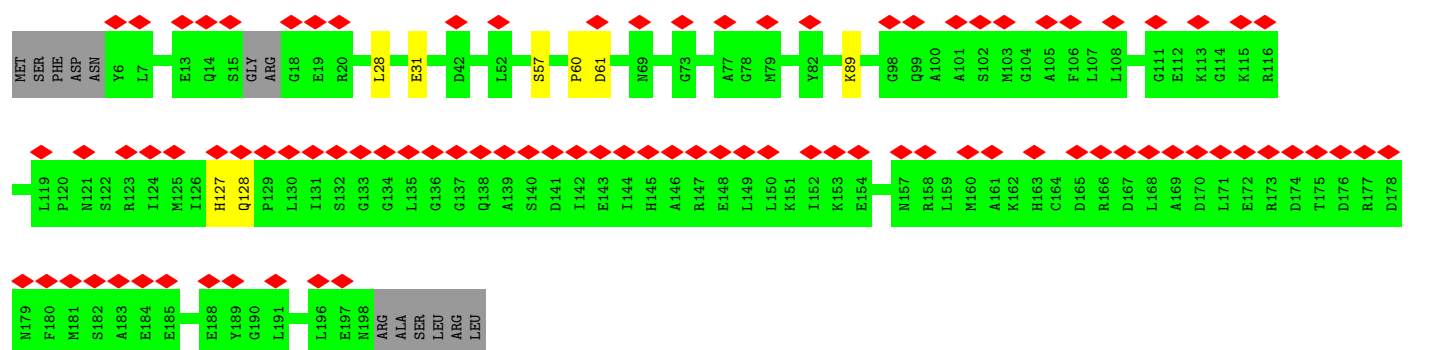
• Molecule 3: ATP-dependent Clp protease proteolytic subunit

Chain T: 94% (red bar), 92% (green bar), 6% (yellow bar)



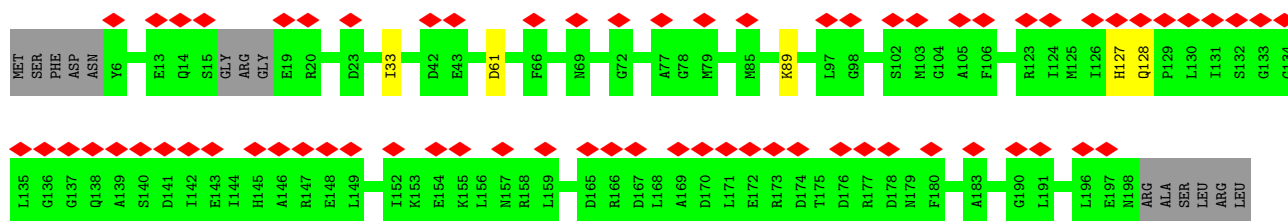
• Molecule 3: ATP-dependent Clp protease proteolytic subunit

Chain U: 45% (red bar), 90% (green bar), 6% (yellow bar)

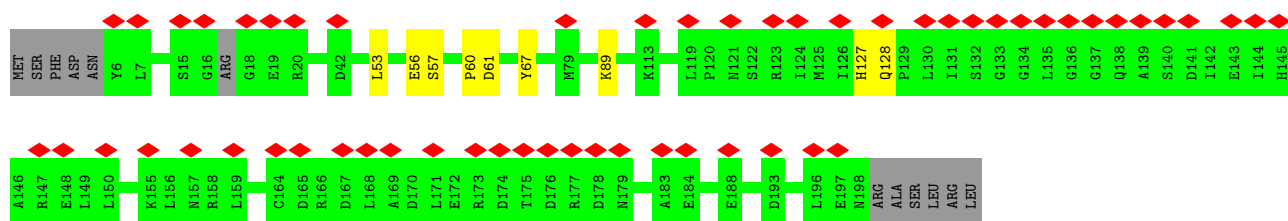
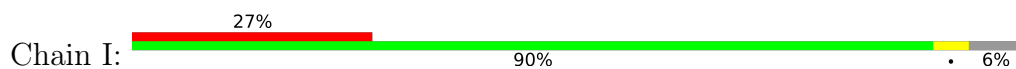


• Molecule 3: ATP-dependent Clp protease proteolytic subunit

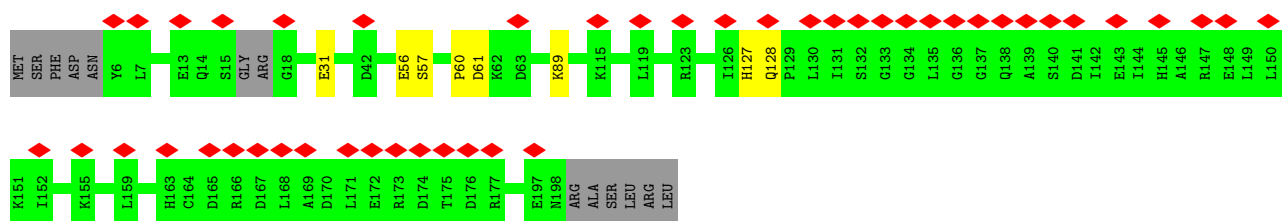
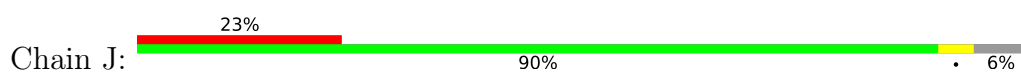
Chain H: 34% (red bar), 91% (green bar), 7% (yellow bar)



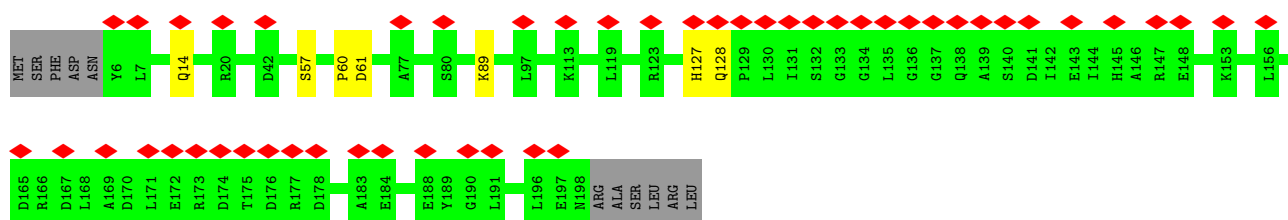
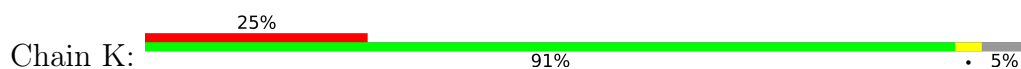
• Molecule 3: ATP-dependent Clp protease proteolytic subunit



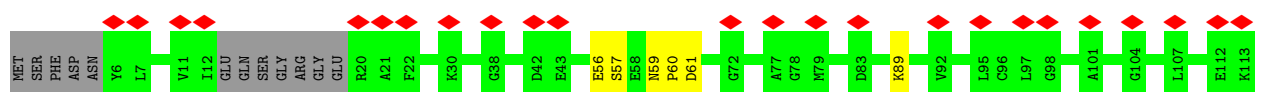
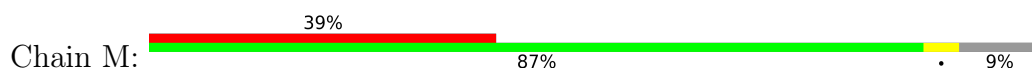
• Molecule 3: ATP-dependent Clp protease proteolytic subunit

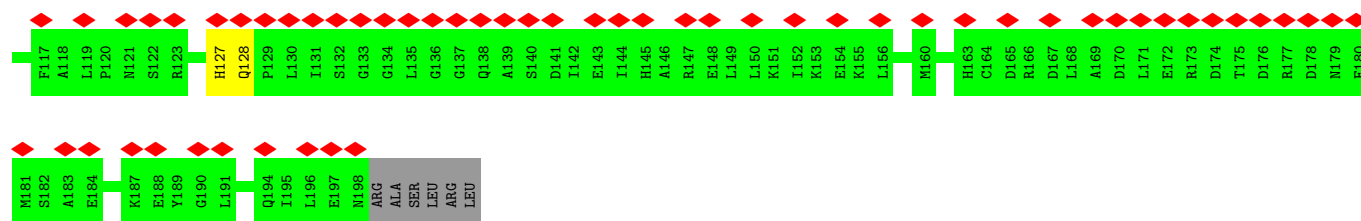


• Molecule 3: ATP-dependent Clp protease proteolytic subunit

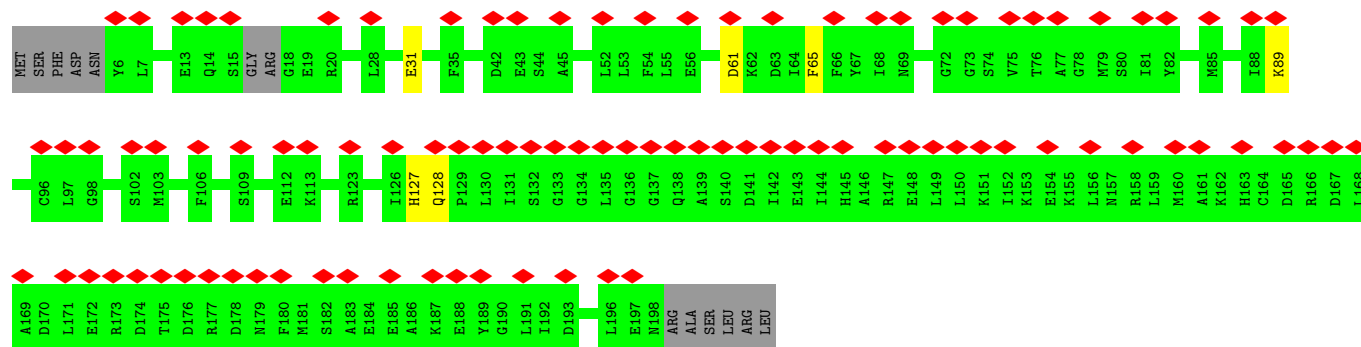
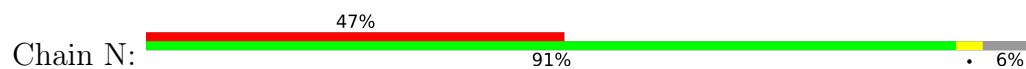


• Molecule 3: ATP-dependent Clp protease proteolytic subunit





• Molecule 3: ATP-dependent Clp protease proteolytic subunit



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	178448	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 ( $e^-/\text{\AA}^2$ )	43	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	1700	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	5.699	Depositor
Minimum map value	-2.085	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.120	Depositor
Recommended contour level	0.6	Depositor
Map size (Å)	317.99997, 317.99997, 317.99997	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	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, 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	A	0.24	0/2636	0.41	0/3556
1	B	0.24	0/2620	0.40	0/3535
1	C	0.24	0/2582	0.40	0/3481
1	D	0.24	0/2635	0.40	0/3551
1	E	0.24	0/2655	0.40	0/3578
1	F	0.24	0/2495	0.40	0/3364
3	H	0.26	0/1505	0.42	0/2027
3	I	0.27	0/1513	0.43	0/2037
3	J	0.27	0/1509	0.42	0/2032
3	K	0.27	0/1525	0.43	0/2054
3	L	0.26	0/1509	0.42	0/2032
3	M	0.27	0/1472	0.42	0/1983
3	N	0.27	0/1509	0.42	0/2032
3	O	0.26	0/1509	0.42	0/2032
3	P	0.26	0/1509	0.42	0/2032
3	Q	0.26	0/1509	0.42	0/2032
3	R	0.26	0/1509	0.42	0/2032
3	S	0.26	0/1509	0.42	0/2032
3	T	0.26	0/1509	0.42	0/2032
3	U	0.27	0/1509	0.42	0/2032
All	All	0.25	0/36728	0.41	0/49486

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3

There are no bond length outliers.



There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	194	ASP	Peptide
1	A	195	ASN	Peptide
1	A	198	ILE	Peptide

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2604	2707	2707	39	0
1	B	2588	2695	2695	25	0
1	C	2552	2655	2655	10	0
1	D	2604	2710	2710	19	0
1	E	2622	2735	2735	28	0
1	F	2465	2573	2573	18	0
2	G	34	32	12	3	0
3	H	1483	1485	1485	3	0
3	I	1491	1491	1491	7	0
3	J	1487	1488	1488	6	0
3	K	1502	1505	1505	14	0
3	L	1487	1488	1488	2	0
3	M	1450	1460	1460	8	0
3	N	1487	1488	1488	6	0
3	O	1487	1488	1488	2	0
3	P	1487	1488	1488	2	0
3	Q	1487	1488	1488	2	0
3	R	1487	1488	1488	2	0
3	S	1487	1488	1488	2	0
3	T	1487	1488	1488	2	0
3	U	1487	1488	1488	10	0
4	A	31	12	12	2	0
4	B	31	12	12	1	0
4	C	31	12	12	2	0
4	D	31	12	12	2	0
4	E	31	12	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
6	F	27	12	12	0	0
All	All	36452	37000	36980	150	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 2.

The worst 5 of 150 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)
1:B:273:VAL:HG12	3:I:60:PRO:HG3	1.53	0.91
1:C:273:VAL:HG12	3:J:60:PRO:HG3	1.60	0.81
1:E:154:VAL:HG22	1:F:152:GLY:HA2	1.63	0.81
1:E:273:VAL:HB	3:M:60:PRO:HG3	1.67	0.76
1:A:127:LEU:HD11	4:A:501:ATP:H2'	1.69	0.75

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	334/414 (81%)	320 (96%)	14 (4%)	0	100	100
1	B	331/414 (80%)	322 (97%)	9 (3%)	0	100	100
1	C	325/414 (78%)	317 (98%)	7 (2%)	1 (0%)	41	71
1	D	333/414 (80%)	326 (98%)	7 (2%)	0	100	100
1	E	335/414 (81%)	328 (98%)	7 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	313/414 (76%)	305 (97%)	8 (3%)	0	100	100
3	H	186/204 (91%)	178 (96%)	8 (4%)	0	100	100
3	I	188/204 (92%)	179 (95%)	9 (5%)	0	100	100
3	J	187/204 (92%)	180 (96%)	7 (4%)	0	100	100
3	K	191/204 (94%)	182 (95%)	9 (5%)	0	100	100
3	L	187/204 (92%)	179 (96%)	8 (4%)	0	100	100
3	M	182/204 (89%)	174 (96%)	8 (4%)	0	100	100
3	N	187/204 (92%)	179 (96%)	8 (4%)	0	100	100
3	O	187/204 (92%)	179 (96%)	8 (4%)	0	100	100
3	P	187/204 (92%)	179 (96%)	8 (4%)	0	100	100
3	Q	187/204 (92%)	179 (96%)	8 (4%)	0	100	100
3	R	187/204 (92%)	179 (96%)	8 (4%)	0	100	100
3	S	187/204 (92%)	179 (96%)	8 (4%)	0	100	100
3	T	187/204 (92%)	179 (96%)	8 (4%)	0	100	100
3	U	187/204 (92%)	179 (96%)	8 (4%)	0	100	100
All	All	4588/5340 (86%)	4422 (96%)	165 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	265	GLY

### 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	281/346 (81%)	281 (100%)	0	100	100
1	B	280/346 (81%)	280 (100%)	0	100	100
1	C	274/346 (79%)	273 (100%)	1 (0%)	91	97

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	280/346 (81%)	279 (100%)	1 (0%)	91	97
1	E	282/346 (82%)	282 (100%)	0	100	100
1	F	265/346 (77%)	265 (100%)	0	100	100
3	H	162/173 (94%)	162 (100%)	0	100	100
3	I	162/173 (94%)	162 (100%)	0	100	100
3	J	162/173 (94%)	162 (100%)	0	100	100
3	K	163/173 (94%)	163 (100%)	0	100	100
3	L	162/173 (94%)	162 (100%)	0	100	100
3	M	158/173 (91%)	158 (100%)	0	100	100
3	N	162/173 (94%)	162 (100%)	0	100	100
3	O	162/173 (94%)	162 (100%)	0	100	100
3	P	162/173 (94%)	162 (100%)	0	100	100
3	Q	162/173 (94%)	162 (100%)	0	100	100
3	R	162/173 (94%)	162 (100%)	0	100	100
3	S	162/173 (94%)	162 (100%)	0	100	100
3	T	162/173 (94%)	162 (100%)	0	100	100
3	U	162/173 (94%)	162 (100%)	0	100	100
All	All	3927/4498 (87%)	3925 (100%)	2 (0%)	93	98

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	273	VAL
1	D	276	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 5 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	ATP	C	501	5	26,33,33	0.94	1 (3%)	31,52,52	1.55	5 (16%)
6	ADP	F	501	-	24,29,29	0.96	1 (4%)	29,45,45	1.47	4 (13%)
4	ATP	A	501	5	26,33,33	0.94	1 (3%)	31,52,52	1.56	5 (16%)
4	ATP	E	501	5	26,33,33	0.94	1 (3%)	31,52,52	1.56	5 (16%)
4	ATP	D	501	5	26,33,33	0.94	1 (3%)	31,52,52	1.55	5 (16%)
4	ATP	B	501	5	26,33,33	0.94	1 (3%)	31,52,52	1.55	5 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ATP	C	501	5	-	6/18/38/38	0/3/3/3
6	ADP	F	501	-	-	4/12/32/32	0/3/3/3
4	ATP	A	501	5	-	5/18/38/38	0/3/3/3
4	ATP	E	501	5	-	5/18/38/38	0/3/3/3
4	ATP	D	501	5	-	6/18/38/38	0/3/3/3
4	ATP	B	501	5	-	5/18/38/38	0/3/3/3

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	501	ATP	C5-C4	2.54	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	501	ATP	C5-C4	2.52	1.47	1.40
4	C	501	ATP	C5-C4	2.52	1.47	1.40
4	B	501	ATP	C5-C4	2.51	1.47	1.40
6	F	501	ADP	C5-C4	2.51	1.47	1.40

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	501	ATP	C3'-C2'-C1'	3.74	106.61	100.98
6	F	501	ADP	PA-O3A-PB	-3.66	120.28	132.83
4	C	501	ATP	C3'-C2'-C1'	3.65	106.48	100.98
4	B	501	ATP	C3'-C2'-C1'	3.65	106.47	100.98
4	E	501	ATP	C3'-C2'-C1'	3.59	106.38	100.98

There are no chirality outliers.

5 of 31 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	501	ATP	C5'-O5'-PA-O1A
4	C	501	ATP	C5'-O5'-PA-O2A
4	B	501	ATP	C5'-O5'-PA-O1A
4	B	501	ATP	C5'-O5'-PA-O2A
4	E	501	ATP	C5'-O5'-PA-O1A

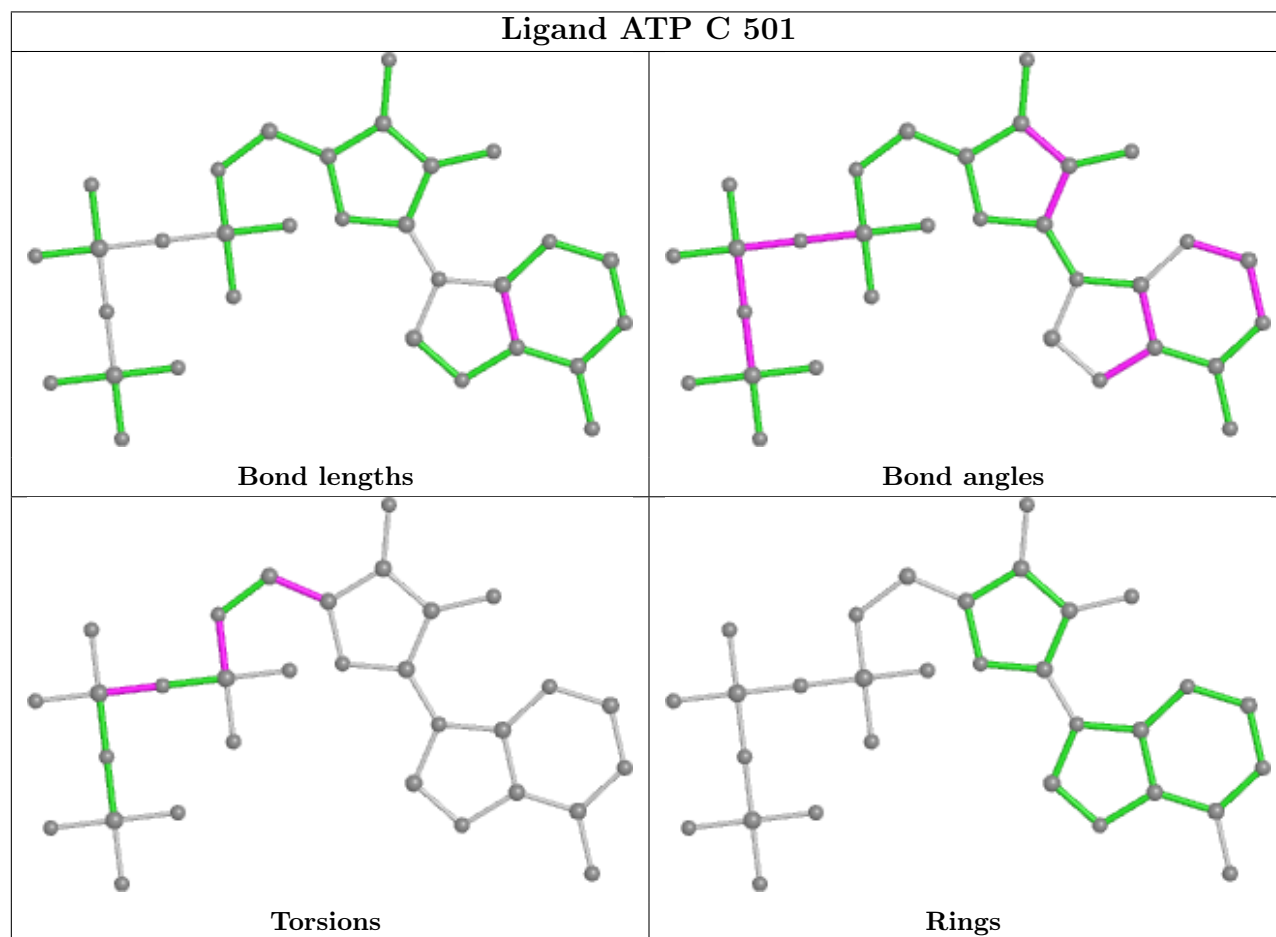
There are no ring outliers.

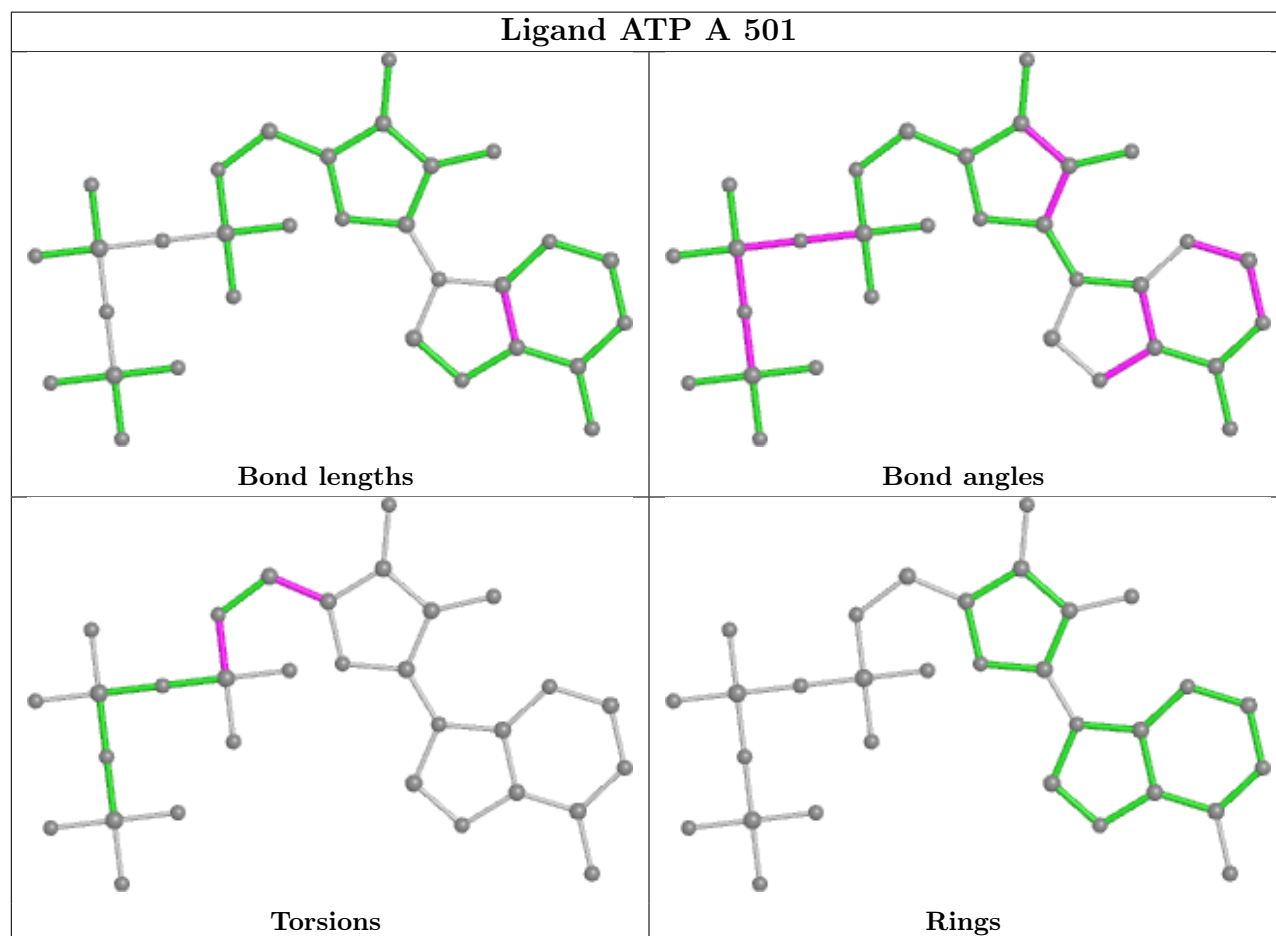
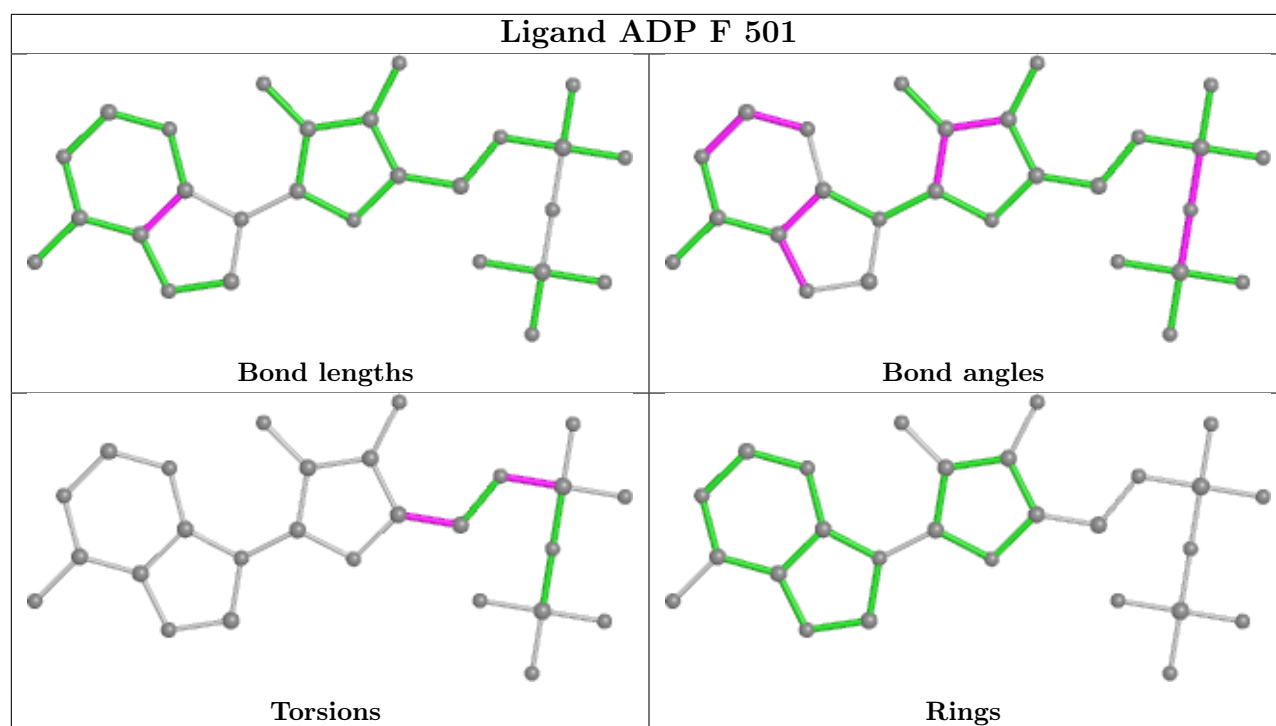
5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	501	ATP	2	0
4	A	501	ATP	2	0
4	E	501	ATP	1	0
4	D	501	ATP	2	0
4	B	501	ATP	1	0

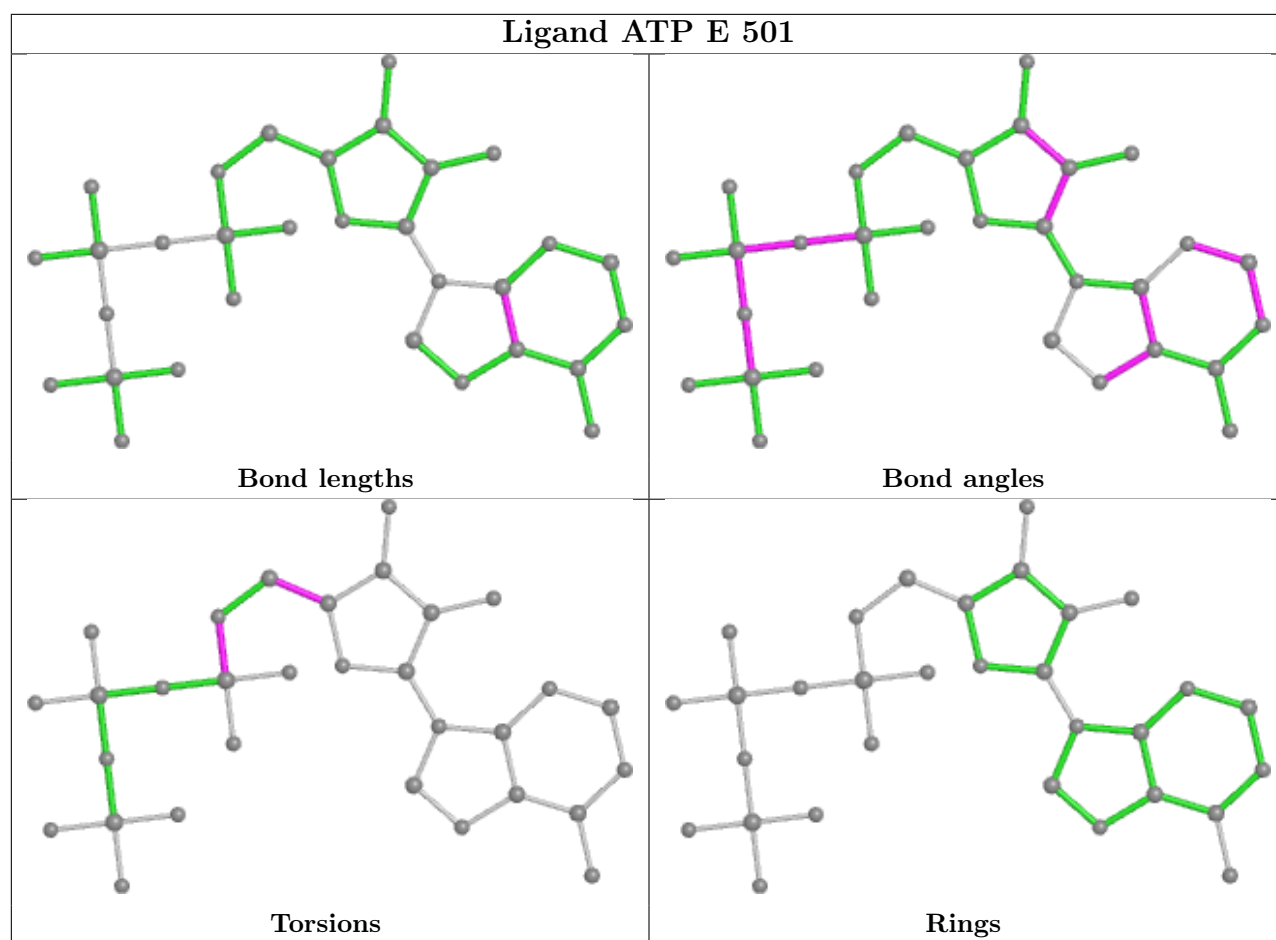
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

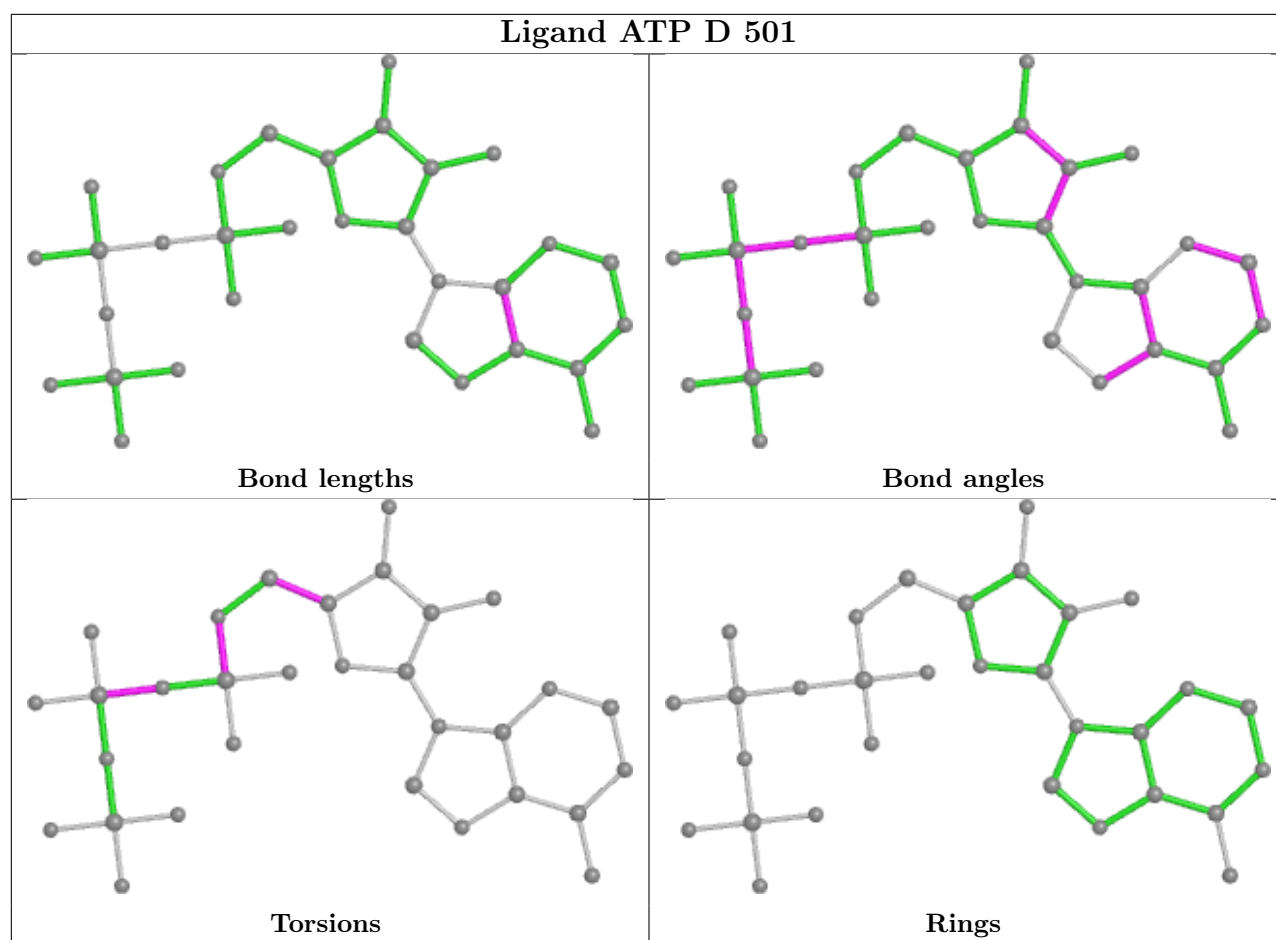
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

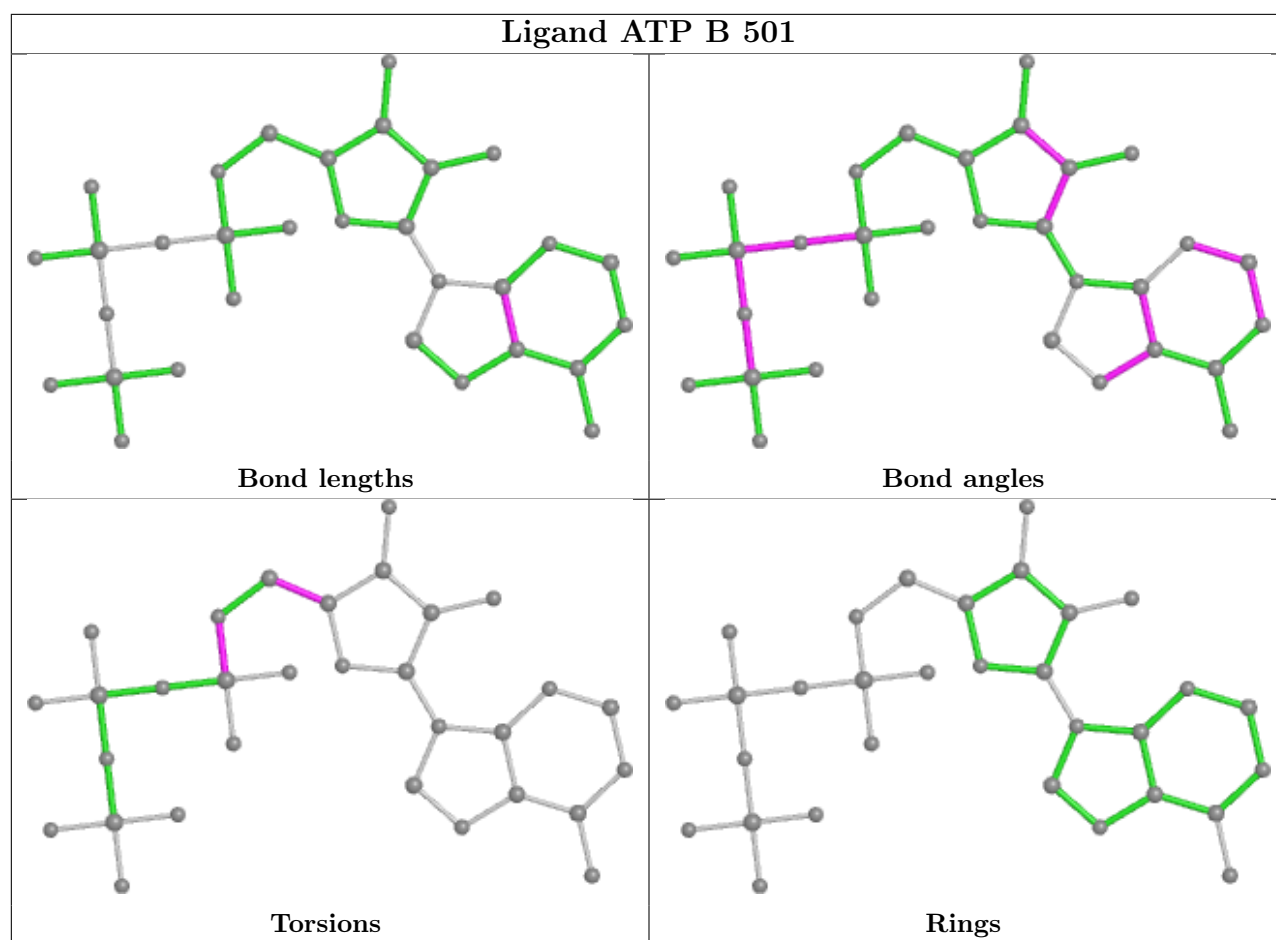












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

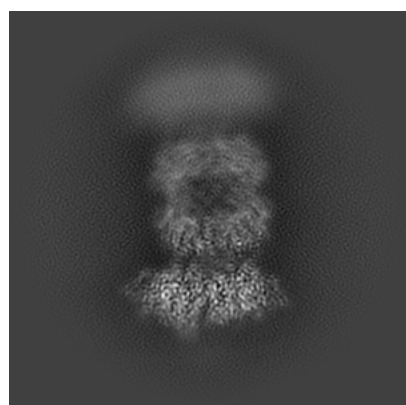
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21194. These allow visual inspection of the internal detail of the map and identification of artifacts.

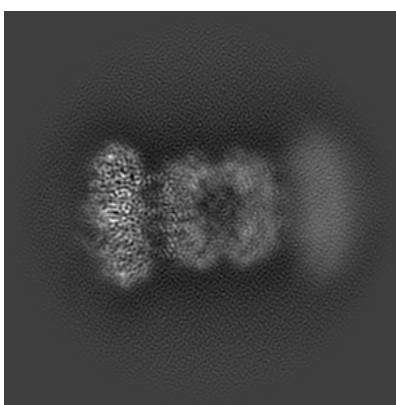
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

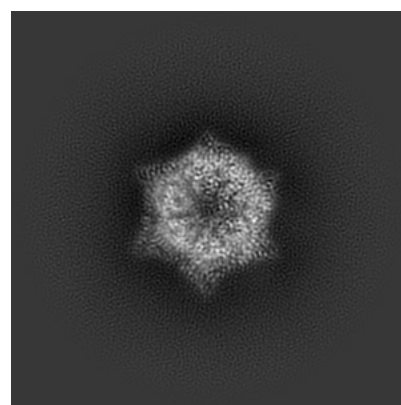
#### 6.1.1 Primary map



X



Y

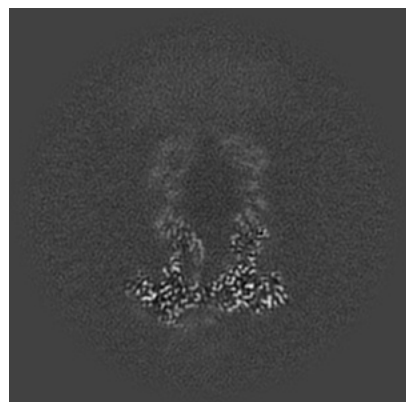


Z

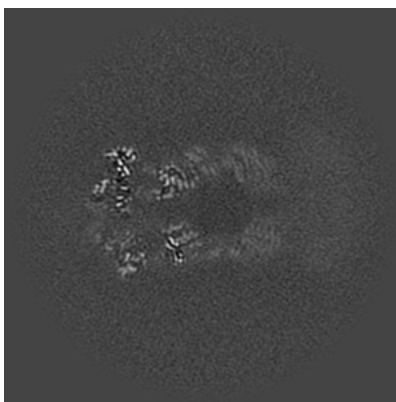
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

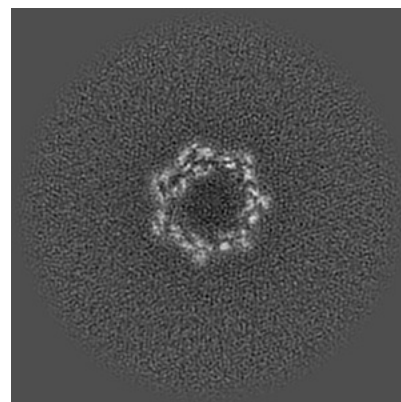
#### 6.2.1 Primary map



X Index: 150



Y Index: 150

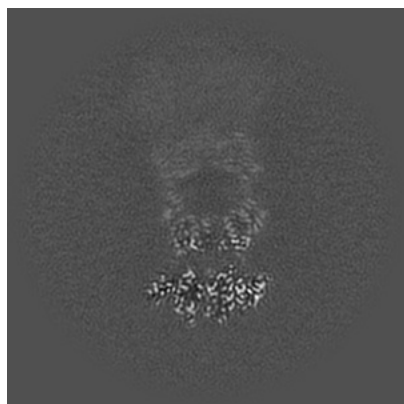


Z Index: 150

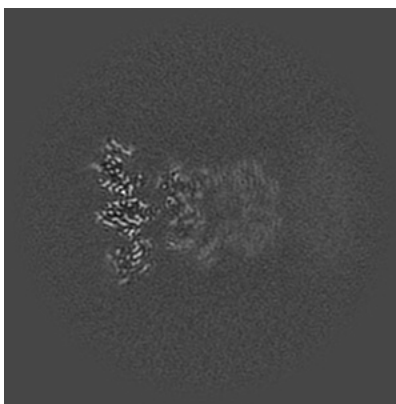
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

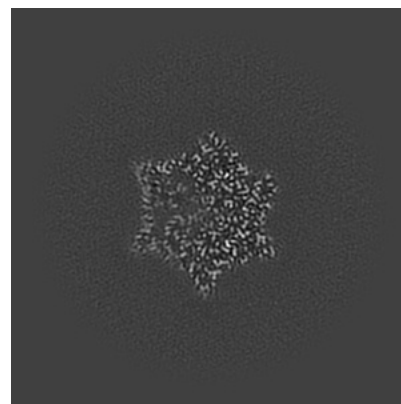
### 6.3.1 Primary map



X Index: 165



Y Index: 174



Z Index: 89

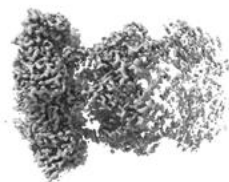
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views [i](#)

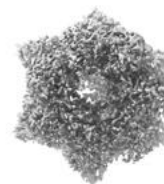
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.6. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

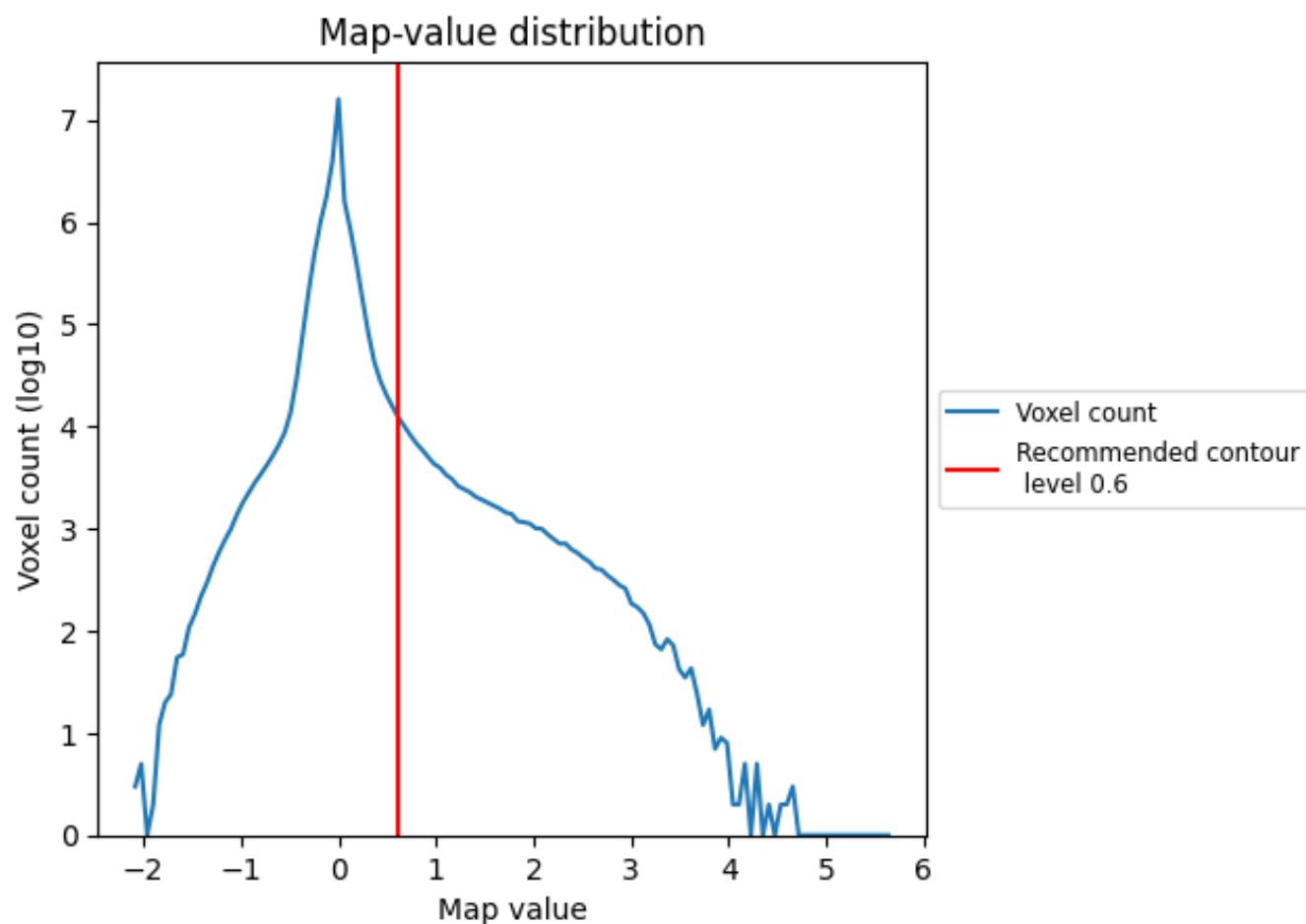
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

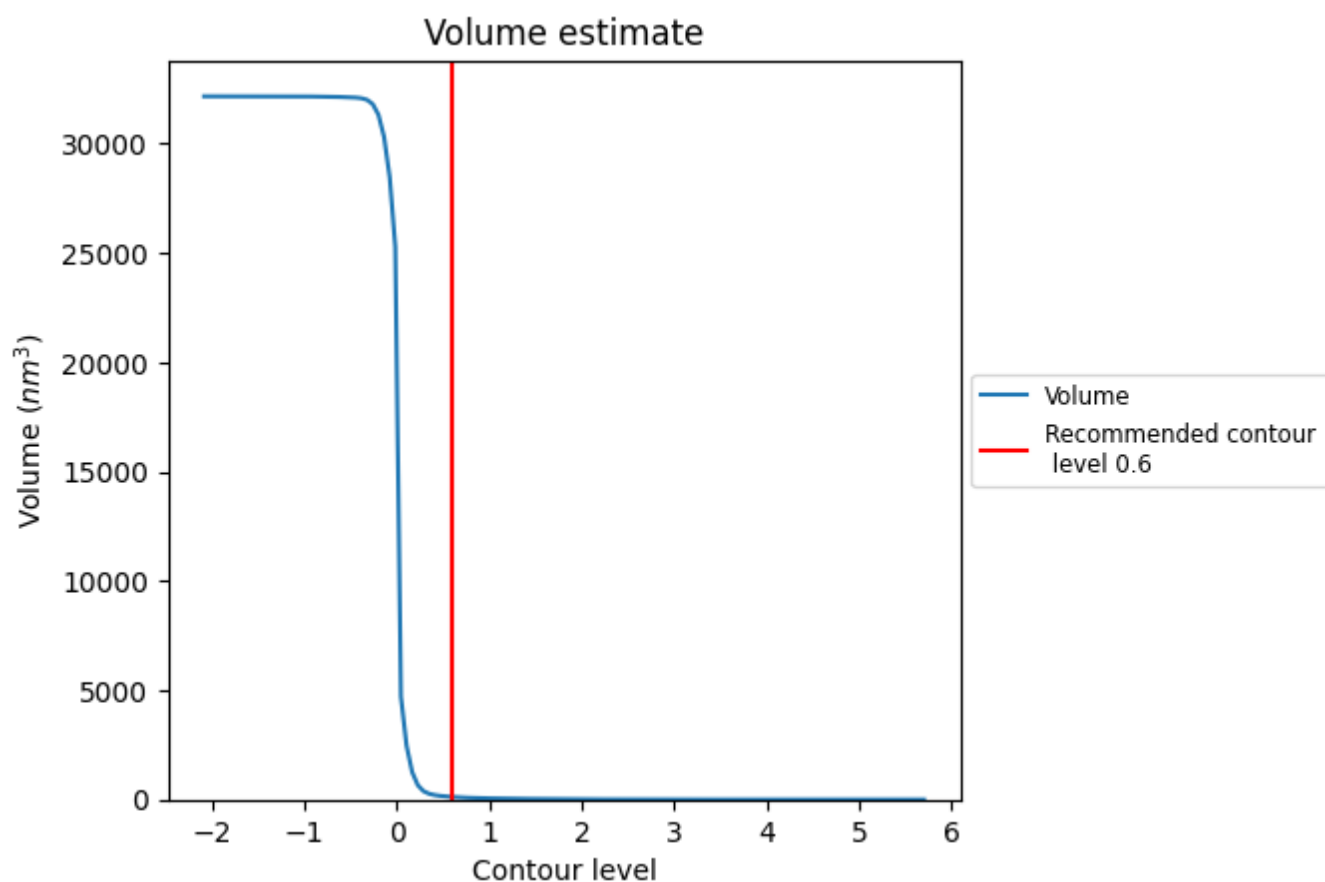
This section contains the results of statistical analysis of the map.

### 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](#)

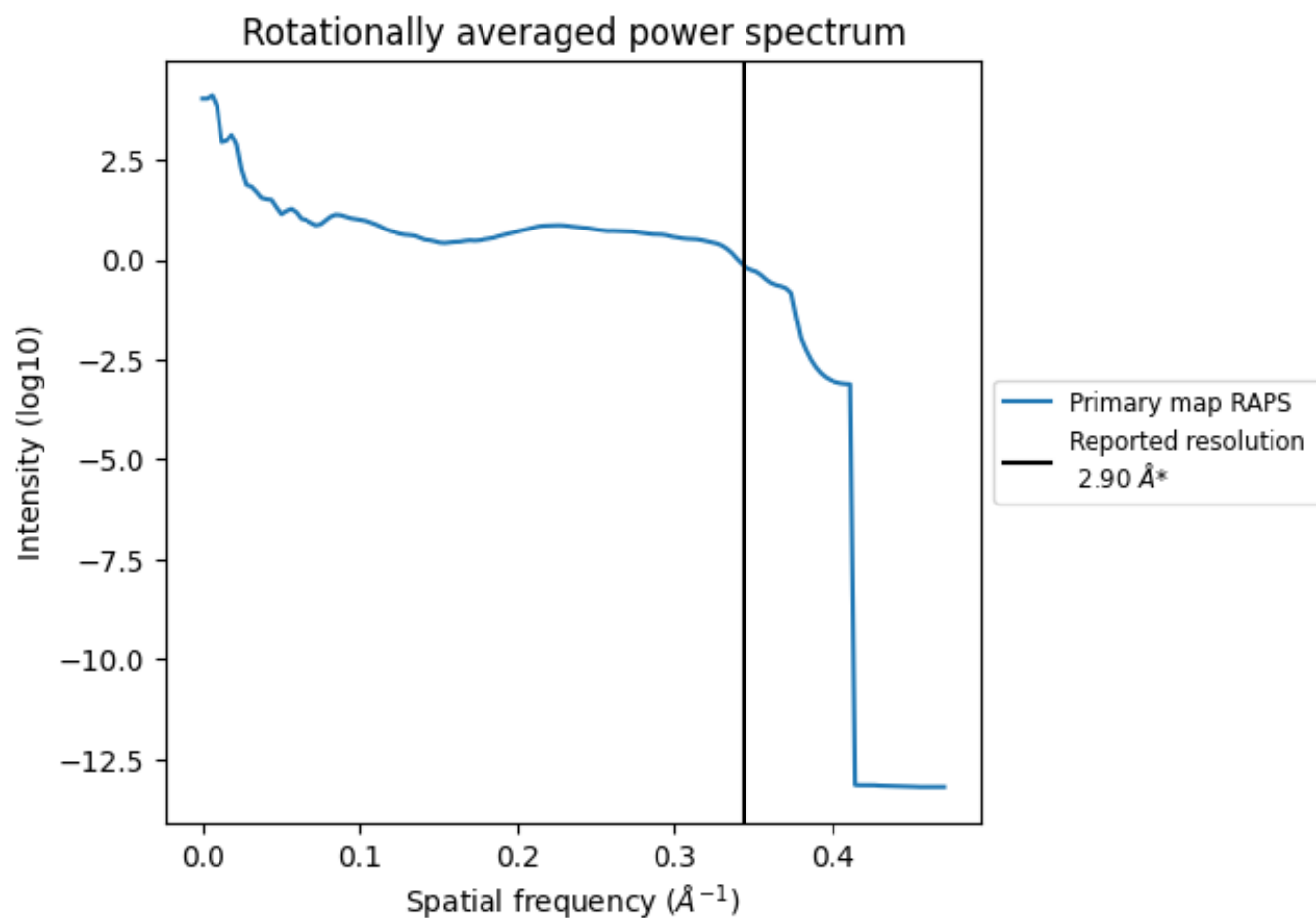


The volume at the recommended contour level is 118  $\text{nm}^3$ ; this corresponds to an approximate mass of 107 kDa.

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 0.345 Å<sup>-1</sup>

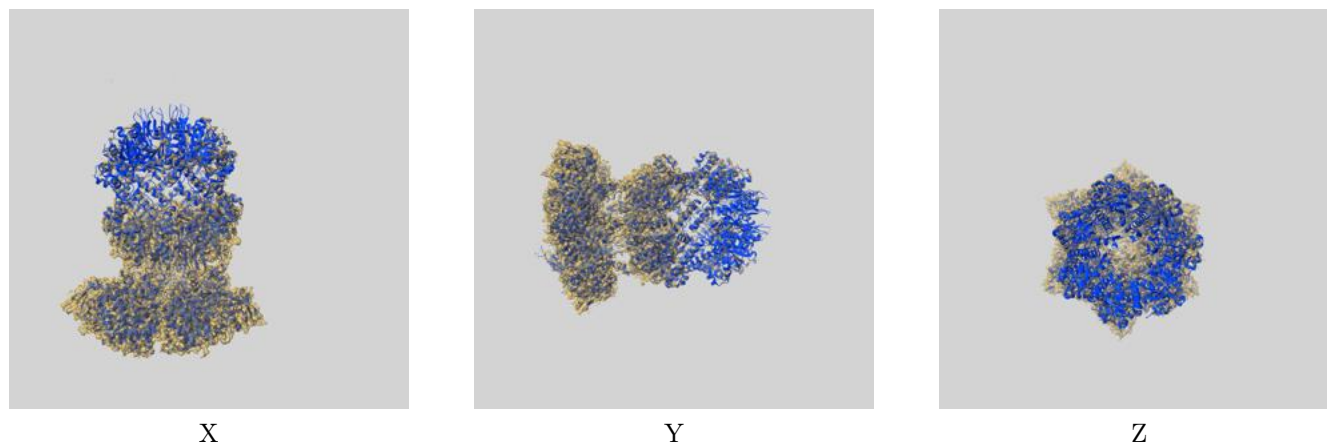
## 8 Fourier-Shell correlation

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

## 9 Map-model fit [i](#)

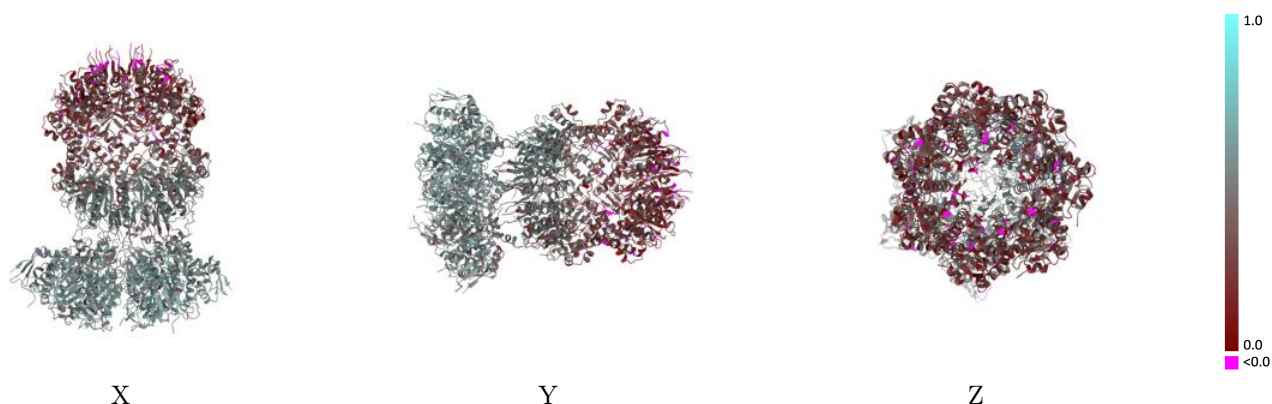
This section contains information regarding the fit between EMDB map EMD-21194 and PDB model 6VFX. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

### 9.1 Map-model overlay [i](#)



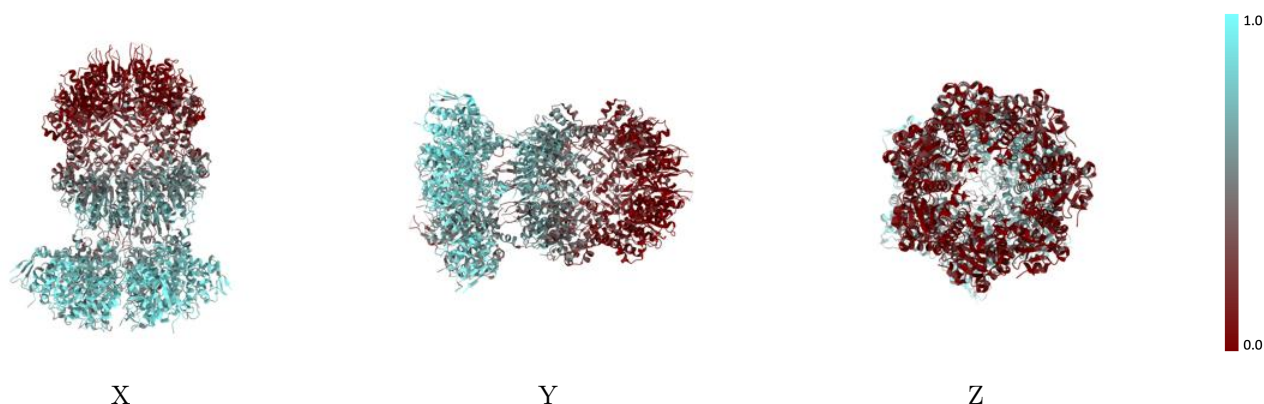
The images above show the 3D surface view of the map at the recommended contour level 0.6 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



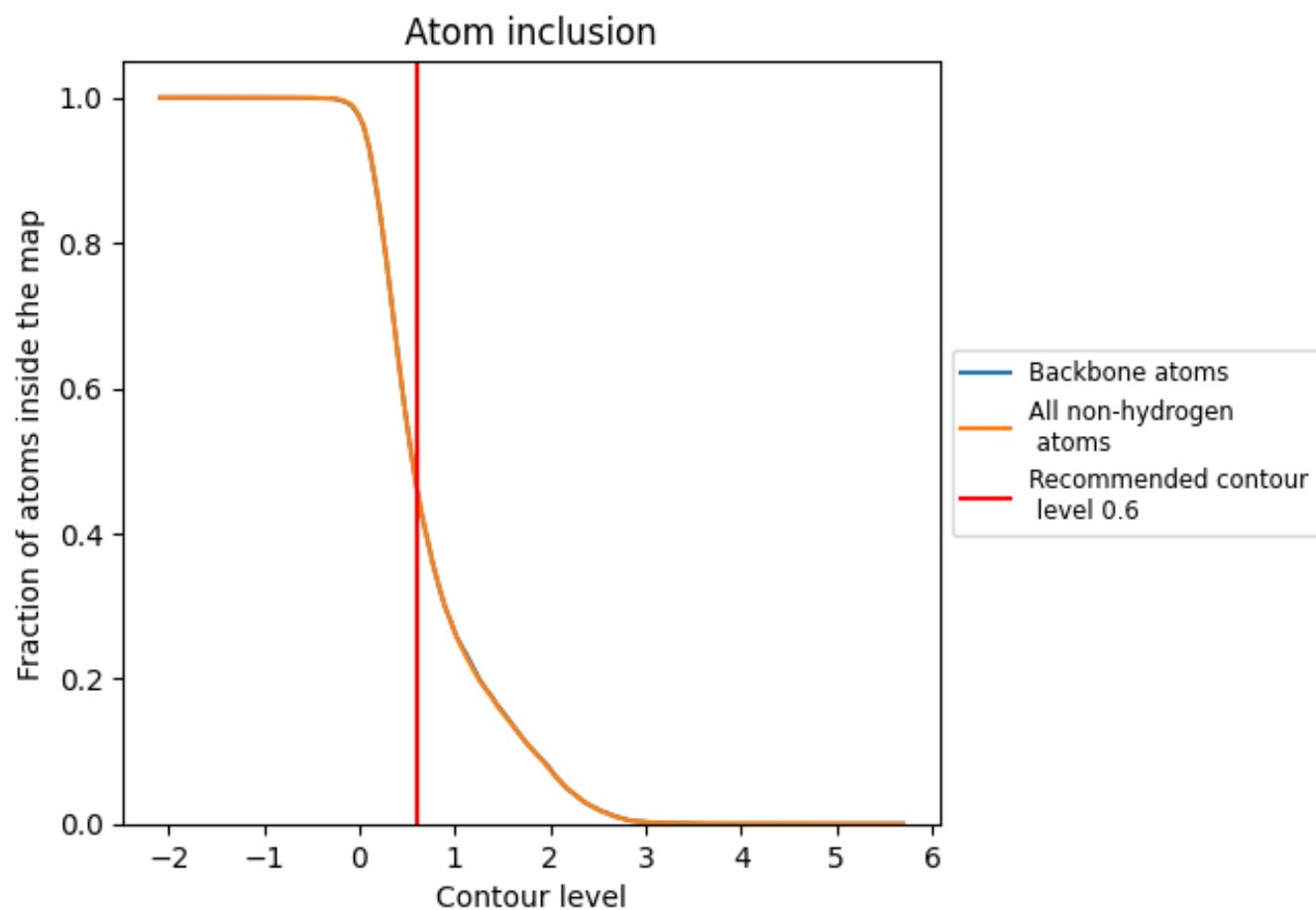
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.6).













































## 9.4 Atom inclusion ⓘ



At the recommended contour level, 46% of all backbone atoms, 46% 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 (0.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4646	 0.4130
A	 0.6198	 0.4770
B	 0.7597	 0.5390
C	 0.7936	 0.5530
D	 0.7826	 0.5490
E	 0.7431	 0.5360
F	 0.6091	 0.4600
G	 0.4706	 0.4560
H	 0.4733	 0.4380
I	 0.5184	 0.4440
J	 0.5363	 0.4510
K	 0.5376	 0.4540
L	 0.0568	 0.2200
M	 0.4330	 0.3950
N	 0.3892	 0.3740
O	 0.0568	 0.2280
P	 0.0800	 0.2400
Q	 0.0821	 0.2520
R	 0.1231	 0.2620
S	 0.1094	 0.2570
T	 0.0561	 0.2310
U	 0.4227	 0.4070

