



wwPDB EM Validation Summary Report ⓘ

Apr 22, 2025 – 02:26 PM EDT

PDB ID : 9C87 / pdb_00009c87
EMDB ID : EMD-45299
Title : Cryo-EM Structure of a Proteolytic ClpXP AAA+ Machine Poised to Unfold a Linear-Degron DHFR-ssrA Substrate Bound with MTX
Authors : Ghanbarpour, A.; Sauer, R.T.; Davis, J.H.
Deposited on : 2024-06-12
Resolution : 3.70 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev117
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

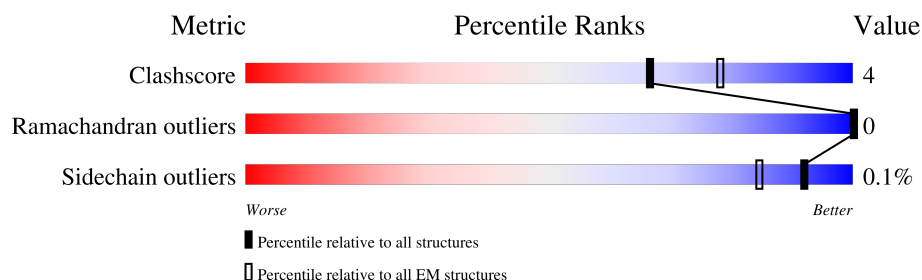
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	389	
1	B	389	
1	C	389	
1	D	389	
1	E	389	
1	F	389	
2	S	210	
3	h	207	

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Mol	Chain	Length	Quality of chain
3	i	207	
3	j	207	
3	k	207	
3	l	207	
3	m	207	
3	n	207	
3	p	207	
3	q	207	
3	r	207	
3	s	207	
3	t	207	
3	u	207	
3	v	207	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 77196 atoms, of which 38760 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	A	353	Total	C	H	N	O	S	0	0
			5451	1704	2753	457	532	5		
1	B	352	Total	C	H	N	O	S	0	0
			5441	1701	2749	456	530	5		
1	C	352	Total	C	H	N	O	S	0	0
			5441	1701	2749	456	530	5		
1	D	352	Total	C	H	N	O	S	0	0
			5441	1701	2749	456	530	5		
1	E	341	Total	C	H	N	O	S	0	0
			5286	1655	2674	441	511	5		
1	F	322	Total	C	H	N	O	S	0	0
			5010	1570	2536	413	486	5		

There are 168 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	37	MET	-	initiating methionine	UNP P0A6H1
A	38	GLY	-	expression tag	UNP P0A6H1
A	39	SER	-	expression tag	UNP P0A6H1
A	40	SER	-	expression tag	UNP P0A6H1
A	41	HIS	-	expression tag	UNP P0A6H1
A	42	HIS	-	expression tag	UNP P0A6H1
A	43	HIS	-	expression tag	UNP P0A6H1
A	44	HIS	-	expression tag	UNP P0A6H1
A	45	HIS	-	expression tag	UNP P0A6H1
A	46	HIS	-	expression tag	UNP P0A6H1
A	47	ASP	-	expression tag	UNP P0A6H1
A	48	TYR	-	expression tag	UNP P0A6H1
A	49	ASP	-	expression tag	UNP P0A6H1
A	50	ILE	-	expression tag	UNP P0A6H1
A	51	PRO	-	expression tag	UNP P0A6H1
A	52	THR	-	expression tag	UNP P0A6H1
A	53	THR	-	expression tag	UNP P0A6H1
A	54	GLU	-	expression tag	UNP P0A6H1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	55	ASN	-	expression tag	UNP P0A6H1
A	56	LEU	-	expression tag	UNP P0A6H1
A	57	TYR	-	expression tag	UNP P0A6H1
A	58	PHE	-	expression tag	UNP P0A6H1
A	59	GLN	-	expression tag	UNP P0A6H1
A	60	GLY	-	expression tag	UNP P0A6H1
A	61	SER	-	expression tag	UNP P0A6H1
A	169	SER	CYS	conflict	UNP P0A6H1
A	408	GLU	LYS	conflict	UNP P0A6H1
A	436	GLY	-	expression tag	UNP P0A6H1
B	37	MET	-	initiating methionine	UNP P0A6H1
B	38	GLY	-	expression tag	UNP P0A6H1
B	39	SER	-	expression tag	UNP P0A6H1
B	40	SER	-	expression tag	UNP P0A6H1
B	41	HIS	-	expression tag	UNP P0A6H1
B	42	HIS	-	expression tag	UNP P0A6H1
B	43	HIS	-	expression tag	UNP P0A6H1
B	44	HIS	-	expression tag	UNP P0A6H1
B	45	HIS	-	expression tag	UNP P0A6H1
B	46	HIS	-	expression tag	UNP P0A6H1
B	47	ASP	-	expression tag	UNP P0A6H1
B	48	TYR	-	expression tag	UNP P0A6H1
B	49	ASP	-	expression tag	UNP P0A6H1
B	50	ILE	-	expression tag	UNP P0A6H1
B	51	PRO	-	expression tag	UNP P0A6H1
B	52	THR	-	expression tag	UNP P0A6H1
B	53	THR	-	expression tag	UNP P0A6H1
B	54	GLU	-	expression tag	UNP P0A6H1
B	55	ASN	-	expression tag	UNP P0A6H1
B	56	LEU	-	expression tag	UNP P0A6H1
B	57	TYR	-	expression tag	UNP P0A6H1
B	58	PHE	-	expression tag	UNP P0A6H1
B	59	GLN	-	expression tag	UNP P0A6H1
B	60	GLY	-	expression tag	UNP P0A6H1
B	61	SER	-	expression tag	UNP P0A6H1
B	169	SER	CYS	conflict	UNP P0A6H1
B	408	GLU	LYS	conflict	UNP P0A6H1
B	436	GLY	-	expression tag	UNP P0A6H1
C	37	MET	-	initiating methionine	UNP P0A6H1
C	38	GLY	-	expression tag	UNP P0A6H1
C	39	SER	-	expression tag	UNP P0A6H1
C	40	SER	-	expression tag	UNP P0A6H1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	41	HIS	-	expression tag	UNP P0A6H1
C	42	HIS	-	expression tag	UNP P0A6H1
C	43	HIS	-	expression tag	UNP P0A6H1
C	44	HIS	-	expression tag	UNP P0A6H1
C	45	HIS	-	expression tag	UNP P0A6H1
C	46	HIS	-	expression tag	UNP P0A6H1
C	47	ASP	-	expression tag	UNP P0A6H1
C	48	TYR	-	expression tag	UNP P0A6H1
C	49	ASP	-	expression tag	UNP P0A6H1
C	50	ILE	-	expression tag	UNP P0A6H1
C	51	PRO	-	expression tag	UNP P0A6H1
C	52	THR	-	expression tag	UNP P0A6H1
C	53	THR	-	expression tag	UNP P0A6H1
C	54	GLU	-	expression tag	UNP P0A6H1
C	55	ASN	-	expression tag	UNP P0A6H1
C	56	LEU	-	expression tag	UNP P0A6H1
C	57	TYR	-	expression tag	UNP P0A6H1
C	58	PHE	-	expression tag	UNP P0A6H1
C	59	GLN	-	expression tag	UNP P0A6H1
C	60	GLY	-	expression tag	UNP P0A6H1
C	61	SER	-	expression tag	UNP P0A6H1
C	169	SER	CYS	conflict	UNP P0A6H1
C	408	GLU	LYS	conflict	UNP P0A6H1
C	436	GLY	-	expression tag	UNP P0A6H1
D	37	MET	-	initiating methionine	UNP P0A6H1
D	38	GLY	-	expression tag	UNP P0A6H1
D	39	SER	-	expression tag	UNP P0A6H1
D	40	SER	-	expression tag	UNP P0A6H1
D	41	HIS	-	expression tag	UNP P0A6H1
D	42	HIS	-	expression tag	UNP P0A6H1
D	43	HIS	-	expression tag	UNP P0A6H1
D	44	HIS	-	expression tag	UNP P0A6H1
D	45	HIS	-	expression tag	UNP P0A6H1
D	46	HIS	-	expression tag	UNP P0A6H1
D	47	ASP	-	expression tag	UNP P0A6H1
D	48	TYR	-	expression tag	UNP P0A6H1
D	49	ASP	-	expression tag	UNP P0A6H1
D	50	ILE	-	expression tag	UNP P0A6H1
D	51	PRO	-	expression tag	UNP P0A6H1
D	52	THR	-	expression tag	UNP P0A6H1
D	53	THR	-	expression tag	UNP P0A6H1
D	54	GLU	-	expression tag	UNP P0A6H1

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Chain	Residue	Modelled	Actual	Comment	Reference
D	55	ASN	-	expression tag	UNP P0A6H1
D	56	LEU	-	expression tag	UNP P0A6H1
D	57	TYR	-	expression tag	UNP P0A6H1
D	58	PHE	-	expression tag	UNP P0A6H1
D	59	GLN	-	expression tag	UNP P0A6H1
D	60	GLY	-	expression tag	UNP P0A6H1
D	61	SER	-	expression tag	UNP P0A6H1
D	169	SER	CYS	conflict	UNP P0A6H1
D	408	GLU	LYS	conflict	UNP P0A6H1
D	436	GLY	-	expression tag	UNP P0A6H1
E	37	MET	-	initiating methionine	UNP P0A6H1
E	38	GLY	-	expression tag	UNP P0A6H1
E	39	SER	-	expression tag	UNP P0A6H1
E	40	SER	-	expression tag	UNP P0A6H1
E	41	HIS	-	expression tag	UNP P0A6H1
E	42	HIS	-	expression tag	UNP P0A6H1
E	43	HIS	-	expression tag	UNP P0A6H1
E	44	HIS	-	expression tag	UNP P0A6H1
E	45	HIS	-	expression tag	UNP P0A6H1
E	46	HIS	-	expression tag	UNP P0A6H1
E	47	ASP	-	expression tag	UNP P0A6H1
E	48	TYR	-	expression tag	UNP P0A6H1
E	49	ASP	-	expression tag	UNP P0A6H1
E	50	ILE	-	expression tag	UNP P0A6H1
E	51	PRO	-	expression tag	UNP P0A6H1
E	52	THR	-	expression tag	UNP P0A6H1
E	53	THR	-	expression tag	UNP P0A6H1
E	54	GLU	-	expression tag	UNP P0A6H1
E	55	ASN	-	expression tag	UNP P0A6H1
E	56	LEU	-	expression tag	UNP P0A6H1
E	57	TYR	-	expression tag	UNP P0A6H1
E	58	PHE	-	expression tag	UNP P0A6H1
E	59	GLN	-	expression tag	UNP P0A6H1
E	60	GLY	-	expression tag	UNP P0A6H1
E	61	SER	-	expression tag	UNP P0A6H1
E	169	SER	CYS	conflict	UNP P0A6H1
E	408	GLU	LYS	conflict	UNP P0A6H1
E	425	GLY	-	expression tag	UNP P0A6H1
F	37	MET	-	initiating methionine	UNP P0A6H1
F	38	GLY	-	expression tag	UNP P0A6H1
F	39	SER	-	expression tag	UNP P0A6H1
F	40	SER	-	expression tag	UNP P0A6H1

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Chain	Residue	Modelled	Actual	Comment	Reference
F	41	HIS	-	expression tag	UNP P0A6H1
F	42	HIS	-	expression tag	UNP P0A6H1
F	43	HIS	-	expression tag	UNP P0A6H1
F	44	HIS	-	expression tag	UNP P0A6H1
F	45	HIS	-	expression tag	UNP P0A6H1
F	46	HIS	-	expression tag	UNP P0A6H1
F	47	ASP	-	expression tag	UNP P0A6H1
F	48	TYR	-	expression tag	UNP P0A6H1
F	49	ASP	-	expression tag	UNP P0A6H1
F	50	ILE	-	expression tag	UNP P0A6H1
F	51	PRO	-	expression tag	UNP P0A6H1
F	52	THR	-	expression tag	UNP P0A6H1
F	53	THR	-	expression tag	UNP P0A6H1
F	54	GLU	-	expression tag	UNP P0A6H1
F	55	ASN	-	expression tag	UNP P0A6H1
F	56	LEU	-	expression tag	UNP P0A6H1
F	57	TYR	-	expression tag	UNP P0A6H1
F	58	PHE	-	expression tag	UNP P0A6H1
F	59	GLN	-	expression tag	UNP P0A6H1
F	60	GLY	-	expression tag	UNP P0A6H1
F	61	SER	-	expression tag	UNP P0A6H1
F	169	SER	CYS	conflict	UNP P0A6H1
F	408	GLU	LYS	conflict	UNP P0A6H1
F	425	GLY	-	expression tag	UNP P0A6H1

- Molecule 2 is a protein called Dihydrofolate reductase.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	S	167	Total	C	H	N	O	S	
			2599	841	1276	226	250	6	
								0	0

There are 53 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	-12	MET	-	initiating methionine	UNP A0A4C7B7M9
S	-11	HIS	-	expression tag	UNP A0A4C7B7M9
S	-10	HIS	-	expression tag	UNP A0A4C7B7M9
S	-9	HIS	-	expression tag	UNP A0A4C7B7M9
S	-8	HIS	-	expression tag	UNP A0A4C7B7M9
S	-7	HIS	-	expression tag	UNP A0A4C7B7M9
S	-6	HIS	-	expression tag	UNP A0A4C7B7M9
S	-5	GLU	-	expression tag	UNP A0A4C7B7M9

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Chain	Residue	Modelled	Actual	Comment	Reference
S	-4	ASN	-	expression tag	UNP A0A4C7B7M9
S	-3	LEU	-	expression tag	UNP A0A4C7B7M9
S	-2	TYR	-	expression tag	UNP A0A4C7B7M9
S	-1	PHE	-	expression tag	UNP A0A4C7B7M9
S	0	GLN	-	expression tag	UNP A0A4C7B7M9
S	1	GLY	-	expression tag	UNP A0A4C7B7M9
S	37	ASP	ASN	conflict	UNP A0A4C7B7M9
S	160	GLY	-	expression tag	UNP A0A4C7B7M9
S	161	SER	-	expression tag	UNP A0A4C7B7M9
S	162	HIS	-	expression tag	UNP A0A4C7B7M9
S	163	LEU	-	expression tag	UNP A0A4C7B7M9
S	164	GLY	-	expression tag	UNP A0A4C7B7M9
S	165	LEU	-	expression tag	UNP A0A4C7B7M9
S	166	ILE	-	expression tag	UNP A0A4C7B7M9
S	167	GLU	-	expression tag	UNP A0A4C7B7M9
S	168	VAL	-	expression tag	UNP A0A4C7B7M9
S	169	GLU	-	expression tag	UNP A0A4C7B7M9
S	170	LYS	-	expression tag	UNP A0A4C7B7M9
S	171	PRO	-	expression tag	UNP A0A4C7B7M9
S	172	LEU	-	expression tag	UNP A0A4C7B7M9
S	173	TYR	-	expression tag	UNP A0A4C7B7M9
S	174	CYS	-	expression tag	UNP A0A4C7B7M9
S	175	GLY	-	expression tag	UNP A0A4C7B7M9
S	176	SER	-	expression tag	UNP A0A4C7B7M9
S	177	GLY	-	expression tag	UNP A0A4C7B7M9
S	178	SER	-	expression tag	UNP A0A4C7B7M9
S	179	TRP	-	expression tag	UNP A0A4C7B7M9
S	180	SER	-	expression tag	UNP A0A4C7B7M9
S	181	HIS	-	expression tag	UNP A0A4C7B7M9
S	182	PRO	-	expression tag	UNP A0A4C7B7M9
S	183	GLN	-	expression tag	UNP A0A4C7B7M9
S	184	PHE	-	expression tag	UNP A0A4C7B7M9
S	185	GLU	-	expression tag	UNP A0A4C7B7M9
S	186	LYS	-	expression tag	UNP A0A4C7B7M9
S	187	ALA	-	expression tag	UNP A0A4C7B7M9
S	188	ALA	-	expression tag	UNP A0A4C7B7M9
S	189	ASN	-	expression tag	UNP A0A4C7B7M9
S	190	ASP	-	expression tag	UNP A0A4C7B7M9
S	191	GLU	-	expression tag	UNP A0A4C7B7M9
S	192	ASN	-	expression tag	UNP A0A4C7B7M9
S	193	TYR	-	expression tag	UNP A0A4C7B7M9
S	194	ALA	-	expression tag	UNP A0A4C7B7M9

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Chain	Residue	Modelled	Actual	Comment	Reference
S	195	LEU	-	expression tag	UNP A0A4C7B7M9
S	196	ALA	-	expression tag	UNP A0A4C7B7M9
S	197	ALA	-	expression tag	UNP A0A4C7B7M9

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

Mol	Chain	Residues	Atoms						AltConf	Trace
3	h	192	Total 3016	C 947	H 1513	N 261	O 283	S 12	0	0
3	i	192	Total 3016	C 947	H 1513	N 261	O 283	S 12	0	0
3	j	192	Total 3016	C 947	H 1513	N 261	O 283	S 12	0	0
3	k	192	Total 3016	C 947	H 1513	N 261	O 283	S 12	0	0
3	l	192	Total 3016	C 947	H 1513	N 261	O 283	S 12	0	0
3	m	192	Total 3016	C 947	H 1513	N 261	O 283	S 12	0	0
3	n	192	Total 3016	C 947	H 1513	N 261	O 283	S 12	0	0
3	p	192	Total 3016	C 947	H 1513	N 261	O 283	S 12	0	0
3	q	192	Total 3016	C 947	H 1513	N 261	O 283	S 12	0	0
3	r	192	Total 3016	C 947	H 1513	N 261	O 283	S 12	0	0
3	s	192	Total 3016	C 947	H 1513	N 261	O 283	S 12	0	0
3	t	192	Total 3016	C 947	H 1513	N 261	O 283	S 12	0	0
3	u	192	Total 3016	C 947	H 1513	N 261	O 283	S 12	0	0
3	v	192	Total 3016	C 947	H 1513	N 261	O 283	S 12	0	0

There are 210 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
h	194	GLU	-	expression tag	UNP P0A6G7
h	195	ASN	-	expression tag	UNP P0A6G7
h	196	LEU	-	expression tag	UNP P0A6G7

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Chain	Residue	Modelled	Actual	Comment	Reference
h	197	TYR	-	expression tag	UNP P0A6G7
h	198	PHE	-	expression tag	UNP P0A6G7
h	199	GLN	-	expression tag	UNP P0A6G7
h	200	SER	-	expression tag	UNP P0A6G7
h	201	LEU	-	expression tag	UNP P0A6G7
h	202	GLU	-	expression tag	UNP P0A6G7
h	203	HIS	-	expression tag	UNP P0A6G7
h	204	HIS	-	expression tag	UNP P0A6G7
h	205	HIS	-	expression tag	UNP P0A6G7
h	206	HIS	-	expression tag	UNP P0A6G7
h	207	HIS	-	expression tag	UNP P0A6G7
h	208	HIS	-	expression tag	UNP P0A6G7
i	194	GLU	-	expression tag	UNP P0A6G7
i	195	ASN	-	expression tag	UNP P0A6G7
i	196	LEU	-	expression tag	UNP P0A6G7
i	197	TYR	-	expression tag	UNP P0A6G7
i	198	PHE	-	expression tag	UNP P0A6G7
i	199	GLN	-	expression tag	UNP P0A6G7
i	200	SER	-	expression tag	UNP P0A6G7
i	201	LEU	-	expression tag	UNP P0A6G7
i	202	GLU	-	expression tag	UNP P0A6G7
i	203	HIS	-	expression tag	UNP P0A6G7
i	204	HIS	-	expression tag	UNP P0A6G7
i	205	HIS	-	expression tag	UNP P0A6G7
i	206	HIS	-	expression tag	UNP P0A6G7
i	207	HIS	-	expression tag	UNP P0A6G7
i	208	HIS	-	expression tag	UNP P0A6G7
j	194	GLU	-	expression tag	UNP P0A6G7
j	195	ASN	-	expression tag	UNP P0A6G7
j	196	LEU	-	expression tag	UNP P0A6G7
j	197	TYR	-	expression tag	UNP P0A6G7
j	198	PHE	-	expression tag	UNP P0A6G7
j	199	GLN	-	expression tag	UNP P0A6G7
j	200	SER	-	expression tag	UNP P0A6G7
j	201	LEU	-	expression tag	UNP P0A6G7
j	202	GLU	-	expression tag	UNP P0A6G7
j	203	HIS	-	expression tag	UNP P0A6G7
j	204	HIS	-	expression tag	UNP P0A6G7
j	205	HIS	-	expression tag	UNP P0A6G7
j	206	HIS	-	expression tag	UNP P0A6G7
j	207	HIS	-	expression tag	UNP P0A6G7
j	208	HIS	-	expression tag	UNP P0A6G7

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Chain	Residue	Modelled	Actual	Comment	Reference
k	194	GLU	-	expression tag	UNP P0A6G7
k	195	ASN	-	expression tag	UNP P0A6G7
k	196	LEU	-	expression tag	UNP P0A6G7
k	197	TYR	-	expression tag	UNP P0A6G7
k	198	PHE	-	expression tag	UNP P0A6G7
k	199	GLN	-	expression tag	UNP P0A6G7
k	200	SER	-	expression tag	UNP P0A6G7
k	201	LEU	-	expression tag	UNP P0A6G7
k	202	GLU	-	expression tag	UNP P0A6G7
k	203	HIS	-	expression tag	UNP P0A6G7
k	204	HIS	-	expression tag	UNP P0A6G7
k	205	HIS	-	expression tag	UNP P0A6G7
k	206	HIS	-	expression tag	UNP P0A6G7
k	207	HIS	-	expression tag	UNP P0A6G7
k	208	HIS	-	expression tag	UNP P0A6G7
l	194	GLU	-	expression tag	UNP P0A6G7
l	195	ASN	-	expression tag	UNP P0A6G7
l	196	LEU	-	expression tag	UNP P0A6G7
l	197	TYR	-	expression tag	UNP P0A6G7
l	198	PHE	-	expression tag	UNP P0A6G7
l	199	GLN	-	expression tag	UNP P0A6G7
l	200	SER	-	expression tag	UNP P0A6G7
l	201	LEU	-	expression tag	UNP P0A6G7
l	202	GLU	-	expression tag	UNP P0A6G7
l	203	HIS	-	expression tag	UNP P0A6G7
l	204	HIS	-	expression tag	UNP P0A6G7
l	205	HIS	-	expression tag	UNP P0A6G7
l	206	HIS	-	expression tag	UNP P0A6G7
l	207	HIS	-	expression tag	UNP P0A6G7
l	208	HIS	-	expression tag	UNP P0A6G7
m	194	GLU	-	expression tag	UNP P0A6G7
m	195	ASN	-	expression tag	UNP P0A6G7
m	196	LEU	-	expression tag	UNP P0A6G7
m	197	TYR	-	expression tag	UNP P0A6G7
m	198	PHE	-	expression tag	UNP P0A6G7
m	199	GLN	-	expression tag	UNP P0A6G7
m	200	SER	-	expression tag	UNP P0A6G7
m	201	LEU	-	expression tag	UNP P0A6G7
m	202	GLU	-	expression tag	UNP P0A6G7
m	203	HIS	-	expression tag	UNP P0A6G7
m	204	HIS	-	expression tag	UNP P0A6G7
m	205	HIS	-	expression tag	UNP P0A6G7

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Chain	Residue	Modelled	Actual	Comment	Reference
m	206	HIS	-	expression tag	UNP P0A6G7
m	207	HIS	-	expression tag	UNP P0A6G7
m	208	HIS	-	expression tag	UNP P0A6G7
n	194	GLU	-	expression tag	UNP P0A6G7
n	195	ASN	-	expression tag	UNP P0A6G7
n	196	LEU	-	expression tag	UNP P0A6G7
n	197	TYR	-	expression tag	UNP P0A6G7
n	198	PHE	-	expression tag	UNP P0A6G7
n	199	GLN	-	expression tag	UNP P0A6G7
n	200	SER	-	expression tag	UNP P0A6G7
n	201	LEU	-	expression tag	UNP P0A6G7
n	202	GLU	-	expression tag	UNP P0A6G7
n	203	HIS	-	expression tag	UNP P0A6G7
n	204	HIS	-	expression tag	UNP P0A6G7
n	205	HIS	-	expression tag	UNP P0A6G7
n	206	HIS	-	expression tag	UNP P0A6G7
n	207	HIS	-	expression tag	UNP P0A6G7
n	208	HIS	-	expression tag	UNP P0A6G7
p	194	GLU	-	expression tag	UNP P0A6G7
p	195	ASN	-	expression tag	UNP P0A6G7
p	196	LEU	-	expression tag	UNP P0A6G7
p	197	TYR	-	expression tag	UNP P0A6G7
p	198	PHE	-	expression tag	UNP P0A6G7
p	199	GLN	-	expression tag	UNP P0A6G7
p	200	SER	-	expression tag	UNP P0A6G7
p	201	LEU	-	expression tag	UNP P0A6G7
p	202	GLU	-	expression tag	UNP P0A6G7
p	203	HIS	-	expression tag	UNP P0A6G7
p	204	HIS	-	expression tag	UNP P0A6G7
p	205	HIS	-	expression tag	UNP P0A6G7
p	206	HIS	-	expression tag	UNP P0A6G7
p	207	HIS	-	expression tag	UNP P0A6G7
p	208	HIS	-	expression tag	UNP P0A6G7
q	194	GLU	-	expression tag	UNP P0A6G7
q	195	ASN	-	expression tag	UNP P0A6G7
q	196	LEU	-	expression tag	UNP P0A6G7
q	197	TYR	-	expression tag	UNP P0A6G7
q	198	PHE	-	expression tag	UNP P0A6G7
q	199	GLN	-	expression tag	UNP P0A6G7
q	200	SER	-	expression tag	UNP P0A6G7
q	201	LEU	-	expression tag	UNP P0A6G7
q	202	GLU	-	expression tag	UNP P0A6G7

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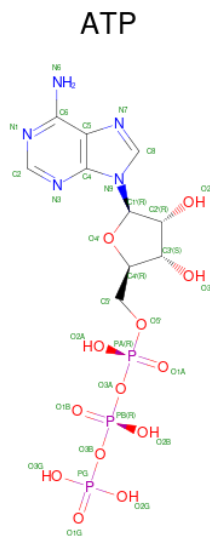
Chain	Residue	Modelled	Actual	Comment	Reference
q	203	HIS	-	expression tag	UNP P0A6G7
q	204	HIS	-	expression tag	UNP P0A6G7
q	205	HIS	-	expression tag	UNP P0A6G7
q	206	HIS	-	expression tag	UNP P0A6G7
q	207	HIS	-	expression tag	UNP P0A6G7
q	208	HIS	-	expression tag	UNP P0A6G7
r	194	GLU	-	expression tag	UNP P0A6G7
r	195	ASN	-	expression tag	UNP P0A6G7
r	196	LEU	-	expression tag	UNP P0A6G7
r	197	TYR	-	expression tag	UNP P0A6G7
r	198	PHE	-	expression tag	UNP P0A6G7
r	199	GLN	-	expression tag	UNP P0A6G7
r	200	SER	-	expression tag	UNP P0A6G7
r	201	LEU	-	expression tag	UNP P0A6G7
r	202	GLU	-	expression tag	UNP P0A6G7
r	203	HIS	-	expression tag	UNP P0A6G7
r	204	HIS	-	expression tag	UNP P0A6G7
r	205	HIS	-	expression tag	UNP P0A6G7
r	206	HIS	-	expression tag	UNP P0A6G7
r	207	HIS	-	expression tag	UNP P0A6G7
r	208	HIS	-	expression tag	UNP P0A6G7
s	194	GLU	-	expression tag	UNP P0A6G7
s	195	ASN	-	expression tag	UNP P0A6G7
s	196	LEU	-	expression tag	UNP P0A6G7
s	197	TYR	-	expression tag	UNP P0A6G7
s	198	PHE	-	expression tag	UNP P0A6G7
s	199	GLN	-	expression tag	UNP P0A6G7
s	200	SER	-	expression tag	UNP P0A6G7
s	201	LEU	-	expression tag	UNP P0A6G7
s	202	GLU	-	expression tag	UNP P0A6G7
s	203	HIS	-	expression tag	UNP P0A6G7
s	204	HIS	-	expression tag	UNP P0A6G7
s	205	HIS	-	expression tag	UNP P0A6G7
s	206	HIS	-	expression tag	UNP P0A6G7
s	207	HIS	-	expression tag	UNP P0A6G7
s	208	HIS	-	expression tag	UNP P0A6G7
t	194	GLU	-	expression tag	UNP P0A6G7
t	195	ASN	-	expression tag	UNP P0A6G7
t	196	LEU	-	expression tag	UNP P0A6G7
t	197	TYR	-	expression tag	UNP P0A6G7
t	198	PHE	-	expression tag	UNP P0A6G7
t	199	GLN	-	expression tag	UNP P0A6G7

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Chain	Residue	Modelled	Actual	Comment	Reference
t	200	SER	-	expression tag	UNP P0A6G7
t	201	LEU	-	expression tag	UNP P0A6G7
t	202	GLU	-	expression tag	UNP P0A6G7
t	203	HIS	-	expression tag	UNP P0A6G7
t	204	HIS	-	expression tag	UNP P0A6G7
t	205	HIS	-	expression tag	UNP P0A6G7
t	206	HIS	-	expression tag	UNP P0A6G7
t	207	HIS	-	expression tag	UNP P0A6G7
t	208	HIS	-	expression tag	UNP P0A6G7
u	194	GLU	-	expression tag	UNP P0A6G7
u	195	ASN	-	expression tag	UNP P0A6G7
u	196	LEU	-	expression tag	UNP P0A6G7
u	197	TYR	-	expression tag	UNP P0A6G7
u	198	PHE	-	expression tag	UNP P0A6G7
u	199	GLN	-	expression tag	UNP P0A6G7
u	200	SER	-	expression tag	UNP P0A6G7
u	201	LEU	-	expression tag	UNP P0A6G7
u	202	GLU	-	expression tag	UNP P0A6G7
u	203	HIS	-	expression tag	UNP P0A6G7
u	204	HIS	-	expression tag	UNP P0A6G7
u	205	HIS	-	expression tag	UNP P0A6G7
u	206	HIS	-	expression tag	UNP P0A6G7
u	207	HIS	-	expression tag	UNP P0A6G7
u	208	HIS	-	expression tag	UNP P0A6G7
v	194	GLU	-	expression tag	UNP P0A6G7
v	195	ASN	-	expression tag	UNP P0A6G7
v	196	LEU	-	expression tag	UNP P0A6G7
v	197	TYR	-	expression tag	UNP P0A6G7
v	198	PHE	-	expression tag	UNP P0A6G7
v	199	GLN	-	expression tag	UNP P0A6G7
v	200	SER	-	expression tag	UNP P0A6G7
v	201	LEU	-	expression tag	UNP P0A6G7
v	202	GLU	-	expression tag	UNP P0A6G7
v	203	HIS	-	expression tag	UNP P0A6G7
v	204	HIS	-	expression tag	UNP P0A6G7
v	205	HIS	-	expression tag	UNP P0A6G7
v	206	HIS	-	expression tag	UNP P0A6G7
v	207	HIS	-	expression tag	UNP P0A6G7
v	208	HIS	-	expression tag	UNP P0A6G7

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).



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

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

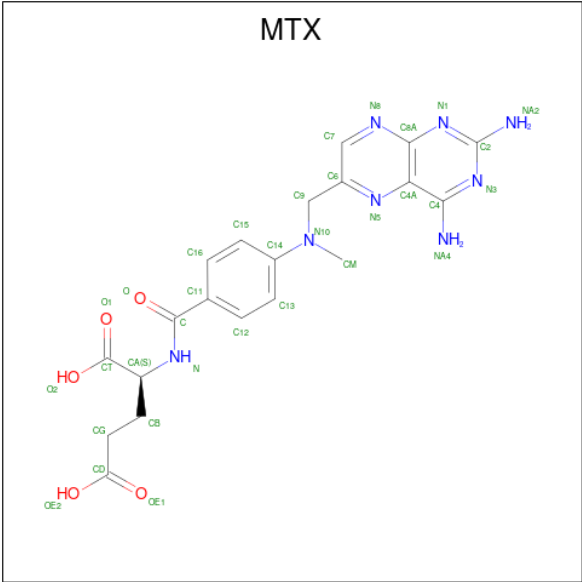
Mol	Chain	Residues	Atoms	AltConf
5	A	1	Total Mg 1 1	0
5	B	1	Total Mg 1 1	0
5	C	1	Total Mg 1 1	0
5	D	1	Total Mg 1 1	0

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$) (labeled as "Ligand of Interest" by depositor).




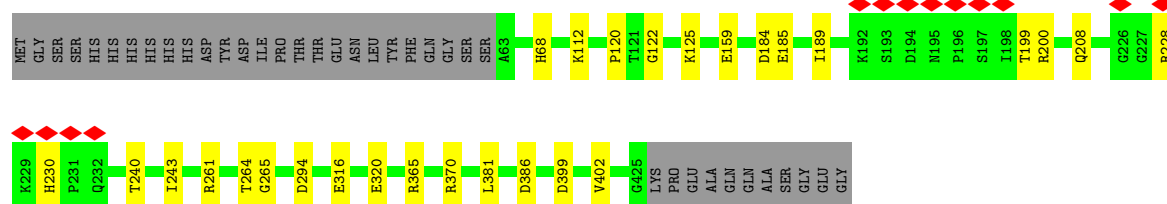
Mol	Chain	Residues	Atoms						AltConf
6	D	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	
6	E	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	
6	F	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	

- Molecule 7 is METHOTREXATE (CCD ID: MTX) (formula: C₂₀H₂₂N₈O₅) (labeled as "Ligand of Interest" by depositor).




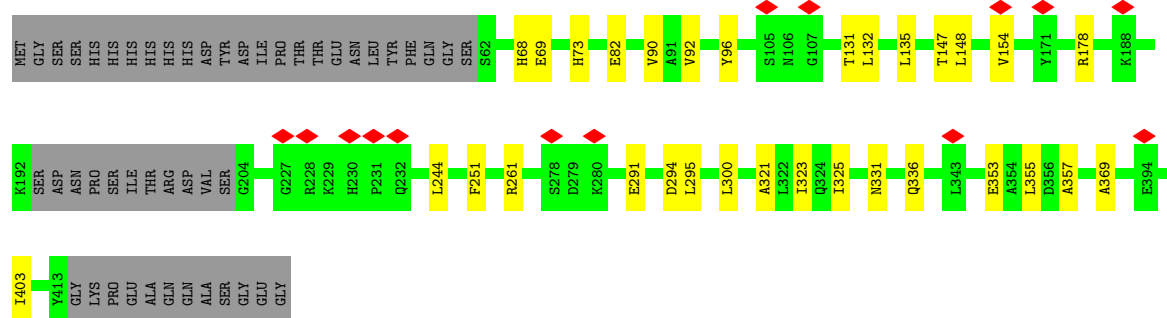
Mol	Chain	Residues	Atoms					AltConf
			Total	C	H	N	O	
7	S	1	53	20	20	8	5	0

Chain D: 




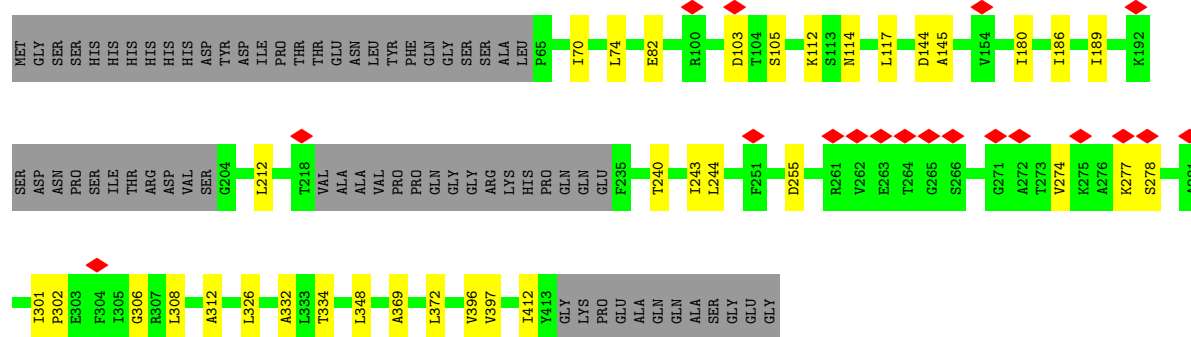
- Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpX

Chain E: 



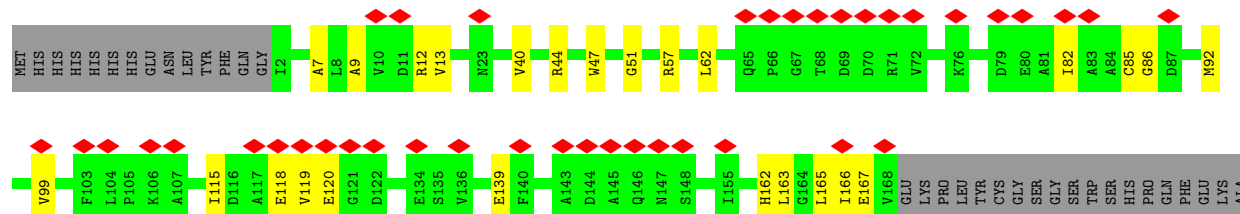
- Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpX

Chain F: 



- Molecule 2: Dihydrofolate reductase

Chain S: 



ALA
ASN
ASP
GLU
ASN
TYR
ALA
LEU
ALA
ALA

- Molecule 3: ATP-dependent Clp protease proteolytic subunit

Chain h:  93% 7%

L2 S11 R12 N193
GLU ASN
LEU TYR
PHE GLN
SER SER
LEU LEU
GLU HIS
HIS HIS
HIS HIS
HIS HIS

- Molecule 3: ATP-dependent Clp protease proteolytic subunit

Chain i:  93% 7%

L2 S11 R12 N193
GLU ASN
LEU TYR
PHE GLN
SER SER
LEU LEU
GLU HIS
HIS HIS
HIS HIS
HIS HIS

- Molecule 3: ATP-dependent Clp protease proteolytic subunit

Chain j:  93% 7%

L2 N193
GLU ASN
LEU TYR
PHE SER
LEU GLU
HIS HIS
HIS HIS
HIS HIS

- Molecule 3: ATP-dependent Clp protease proteolytic subunit

Chain k:  93% 7%

L2 S11 R12 R15 N193
GLU ASN
LEU TYR
PHE GLN
SER SER
LEU LEU
GLU HIS
HIS HIS
HIS HIS
HIS HIS

- Molecule 3: ATP-dependent Clp protease proteolytic subunit

Chain l:  93% 7%

L2 R12 N193
GLU ASN
LEU TYR
PHE GLN
SER SER
LEU LEU
GLU HIS
HIS HIS
HIS HIS
HIS HIS

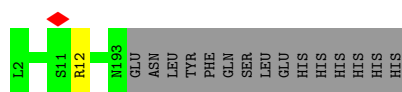
- Molecule 3: ATP-dependent Clp protease proteolytic subunit

Chain m:  93% 7%


L2 R12 N193
GLU ASN
LEU TYR
PHE GLN
SER SER
LEU LEU
GLU HIS
HIS HIS
HIS HIS
HIS HIS

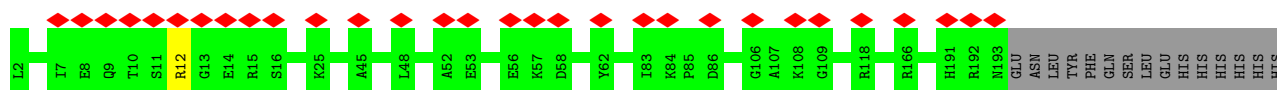
- Molecule 3: ATP-dependent Clp protease proteolytic subunit

Chain n:  92% 7%



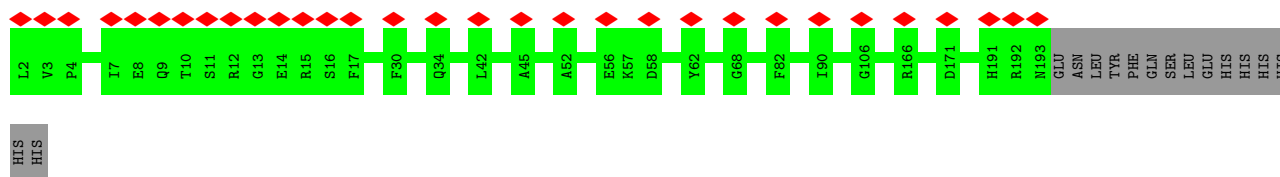
- Molecule 3: ATP-dependent Clp protease proteolytic subunit

Chain p:  14% 92% 7%




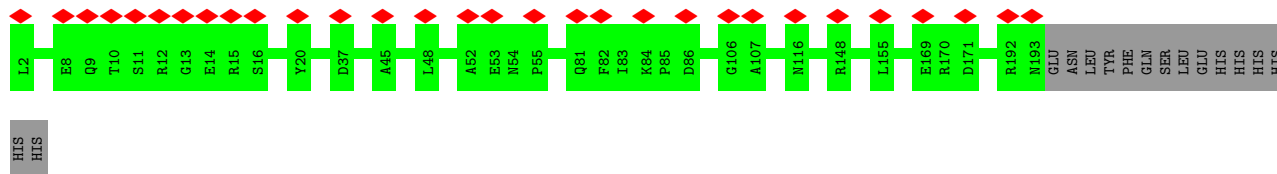
- Molecule 3: ATP-dependent Clp protease proteolytic subunit

Chain q:  15% 93% 7%




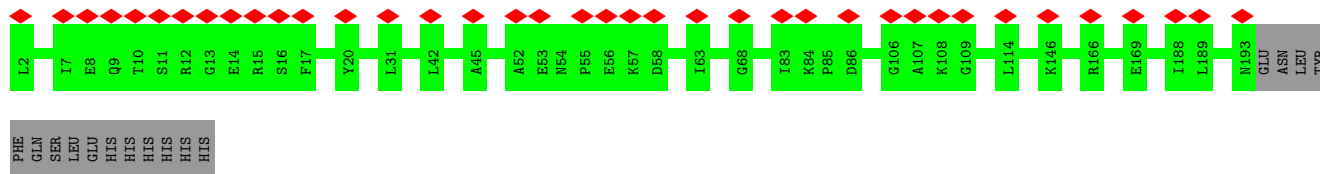
- Molecule 3: ATP-dependent Clp protease proteolytic subunit

Chain r:  14% 93% 7%




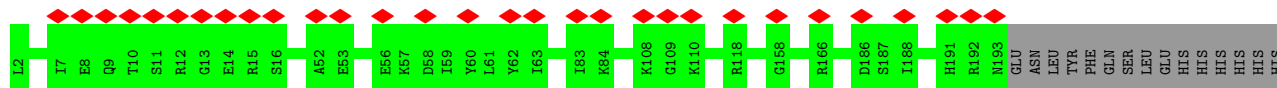
- Molecule 3: ATP-dependent Clp protease proteolytic subunit

Chain s:  18% 93% 7%

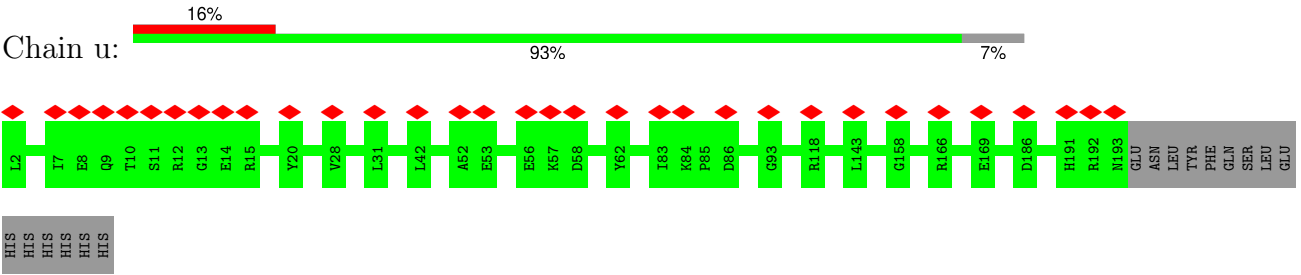


- Molecule 3: ATP-dependent Clp protease proteolytic subunit

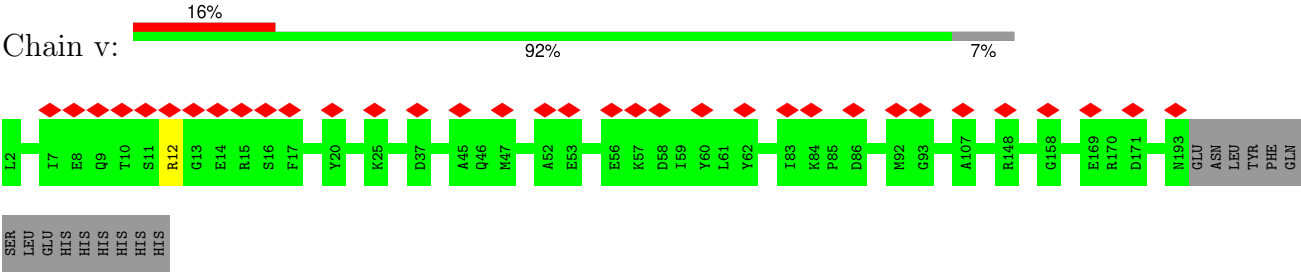
Chain t:  14% 93% 7%



● 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	71203	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE; Patch CTF estimation, cryoSPARC	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	47.54	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1750	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.417	Depositor
Minimum map value	-0.185	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.0676	Depositor
Map size (\AA)	286.0032, 286.0032, 286.0032	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.1172, 1.1172, 1.1172	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.25	0/2734	0.48	0/3697
1	B	0.25	0/2728	0.49	0/3689
1	C	0.25	0/2728	0.48	0/3689
1	D	0.25	0/2728	0.47	0/3689
1	E	0.26	0/2646	0.51	0/3575
1	F	0.27	0/2503	0.50	0/3377
2	S	0.28	0/1358	0.55	0/1848
3	h	0.26	0/1527	0.49	0/2058
3	i	0.25	0/1527	0.48	0/2058
3	j	0.25	0/1527	0.49	0/2058
3	k	0.25	0/1527	0.48	0/2058
3	l	0.25	0/1527	0.49	0/2058
3	m	0.25	0/1527	0.49	0/2058
3	n	0.25	0/1527	0.47	0/2058
3	p	0.26	0/1527	0.49	0/2058
3	q	0.25	0/1527	0.48	0/2058
3	r	0.26	0/1527	0.48	0/2058
3	s	0.25	0/1527	0.48	0/2058
3	t	0.26	0/1527	0.49	0/2058
3	u	0.25	0/1527	0.47	0/2058
3	v	0.26	0/1527	0.48	0/2058
All	All	0.26	0/38803	0.49	0/52376

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2698	2753	2754	24	0
1	B	2692	2749	2749	18	0
1	C	2692	2749	2749	19	0
1	D	2692	2749	2749	20	0
1	E	2612	2674	2674	22	0
1	F	2474	2536	2535	21	0
2	S	1323	1276	1275	19	0
3	h	1503	1513	1513	0	0
3	i	1503	1513	1513	0	0
3	j	1503	1513	1513	0	0
3	k	1503	1513	1513	0	0
3	l	1503	1513	1513	0	0
3	m	1503	1513	1513	0	0
3	n	1503	1513	1513	0	0
3	p	1503	1513	1513	0	0
3	q	1503	1513	1513	0	0
3	r	1503	1513	1513	0	0
3	s	1503	1513	1513	0	0
3	t	1503	1513	1513	0	0
3	u	1503	1513	1513	0	0
3	v	1503	1513	1513	0	0
4	A	31	12	12	2	0
4	B	31	12	12	2	0
4	C	31	12	12	2	0
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
6	D	27	12	12	2	0
6	E	27	12	12	1	0
6	F	27	12	12	0	0
7	S	33	20	20	1	0
All	All	38436	38760	38759	128	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 4.

The worst 5 of 128 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:399:ASP:OD1	1:B:401:SER:OG	2.05	0.74
1:A:233:GLN:NE2	2:S:139:GLU:O	2.22	0.73
1:C:338:GLN:O	1:C:342:ASN:ND2	2.24	0.70
1:A:98:ARG:NH2	1:A:111:GLY:O	2.27	0.68
1:A:185:GLU:OE1	1:A:188:LYS:NZ	2.28	0.67

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	351/389 (90%)	351 (100%)	0	0	100	100
1	B	350/389 (90%)	350 (100%)	0	0	100	100
1	C	350/389 (90%)	350 (100%)	0	0	100	100
1	D	350/389 (90%)	350 (100%)	0	0	100	100
1	E	337/389 (87%)	334 (99%)	3 (1%)	0	100	100
1	F	316/389 (81%)	316 (100%)	0	0	100	100
2	S	165/210 (79%)	165 (100%)	0	0	100	100
3	h	190/207 (92%)	190 (100%)	0	0	100	100
3	i	190/207 (92%)	190 (100%)	0	0	100	100
3	j	190/207 (92%)	190 (100%)	0	0	100	100
3	k	190/207 (92%)	190 (100%)	0	0	100	100
3	l	190/207 (92%)	190 (100%)	0	0	100	100
3	m	190/207 (92%)	190 (100%)	0	0	100	100
3	n	190/207 (92%)	190 (100%)	0	0	100	100
3	p	190/207 (92%)	190 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	q	190/207 (92%)	190 (100%)	0	0	100	100
3	r	190/207 (92%)	190 (100%)	0	0	100	100
3	s	190/207 (92%)	190 (100%)	0	0	100	100
3	t	190/207 (92%)	190 (100%)	0	0	100	100
3	u	190/207 (92%)	190 (100%)	0	0	100	100
3	v	190/207 (92%)	190 (100%)	0	0	100	100
All	All	4879/5442 (90%)	4876 (100%)	3 (0%)	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	292/322 (91%)	292 (100%)	0	100	100
1	B	291/322 (90%)	291 (100%)	0	100	100
1	C	291/322 (90%)	291 (100%)	0	100	100
1	D	291/322 (90%)	290 (100%)	1 (0%)	91	94
1	E	281/322 (87%)	281 (100%)	0	100	100
1	F	267/322 (83%)	267 (100%)	0	100	100
2	S	142/177 (80%)	141 (99%)	1 (1%)	81	88
3	h	163/178 (92%)	163 (100%)	0	100	100
3	i	163/178 (92%)	163 (100%)	0	100	100
3	j	163/178 (92%)	163 (100%)	0	100	100
3	k	163/178 (92%)	163 (100%)	0	100	100
3	l	163/178 (92%)	163 (100%)	0	100	100
3	m	163/178 (92%)	163 (100%)	0	100	100
3	n	163/178 (92%)	162 (99%)	1 (1%)	84	90
3	p	163/178 (92%)	162 (99%)	1 (1%)	84	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	q	163/178 (92%)	163 (100%)	0	100	100
3	r	163/178 (92%)	163 (100%)	0	100	100
3	s	163/178 (92%)	163 (100%)	0	100	100
3	t	163/178 (92%)	163 (100%)	0	100	100
3	u	163/178 (92%)	163 (100%)	0	100	100
3	v	163/178 (92%)	162 (99%)	1 (1%)	84	90
All	All	4137/4601 (90%)	4132 (100%)	5 (0%)	92	96

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	228	ARG
2	S	44	ARG
3	n	12	ARG
3	p	12	ARG
3	v	12	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
3	r	193	ASN
3	t	41	ASN
3	t	94	GLN
1	E	342	ASN
1	E	160	ASN

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 11 ligands modelled in this entry, 4 are monoatomic - leaving 7 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	ADP	E	501	-	24,29,29	0.90	1 (4%)	29,45,45	1.25	2 (6%)
7	MTX	S	201	-	35,35,35	1.83	4 (11%)	47,49,49	1.67	9 (19%)
6	ADP	F	500	-	24,29,29	0.92	1 (4%)	29,45,45	1.26	2 (6%)
4	ATP	C	500	5	28,33,33	0.96	0	34,52,52	1.23	2 (5%)
4	ATP	A	500	5	28,33,33	0.97	0	34,52,52	1.23	2 (5%)
4	ATP	B	500	5	28,33,33	0.96	0	34,52,52	1.21	2 (5%)
6	ADP	D	500	5	24,29,29	0.91	0	29,45,45	1.29	2 (6%)

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	ADP	E	501	-	-	2/12/32/32	0/3/3/3
7	MTX	S	201	-	-	7/25/25/25	0/3/3/3
6	ADP	F	500	-	-	1/12/32/32	0/3/3/3
4	ATP	C	500	5	-	2/18/38/38	0/3/3/3
4	ATP	A	500	5	-	2/18/38/38	0/3/3/3
4	ATP	B	500	5	-	2/18/38/38	0/3/3/3
6	ADP	D	500	5	-	0/12/32/32	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)
7	S	201	MTX	O-C	7.77	1.41	1.23
7	S	201	MTX	C7-N8	4.02	1.38	1.31
7	S	201	MTX	C6-N5	3.40	1.38	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	S	201	MTX	C4-N3	2.61	1.38	1.33
6	E	501	ADP	O4'-C1'	2.08	1.43	1.40

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	S	201	MTX	N1-C2-N3	-5.54	120.17	127.21
6	E	501	ADP	N3-C2-N1	-4.27	122.88	128.67
6	F	500	ADP	N3-C2-N1	-4.19	122.98	128.67
4	A	500	ATP	N3-C2-N1	-4.18	122.99	128.67
6	D	500	ADP	N3-C2-N1	-4.15	123.04	128.67

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	500	ATP	C5'-O5'-PA-O2A
4	A	500	ATP	C5'-O5'-PA-O3A
4	B	500	ATP	C5'-O5'-PA-O2A
4	B	500	ATP	C5'-O5'-PA-O3A
4	C	500	ATP	C5'-O5'-PA-O2A

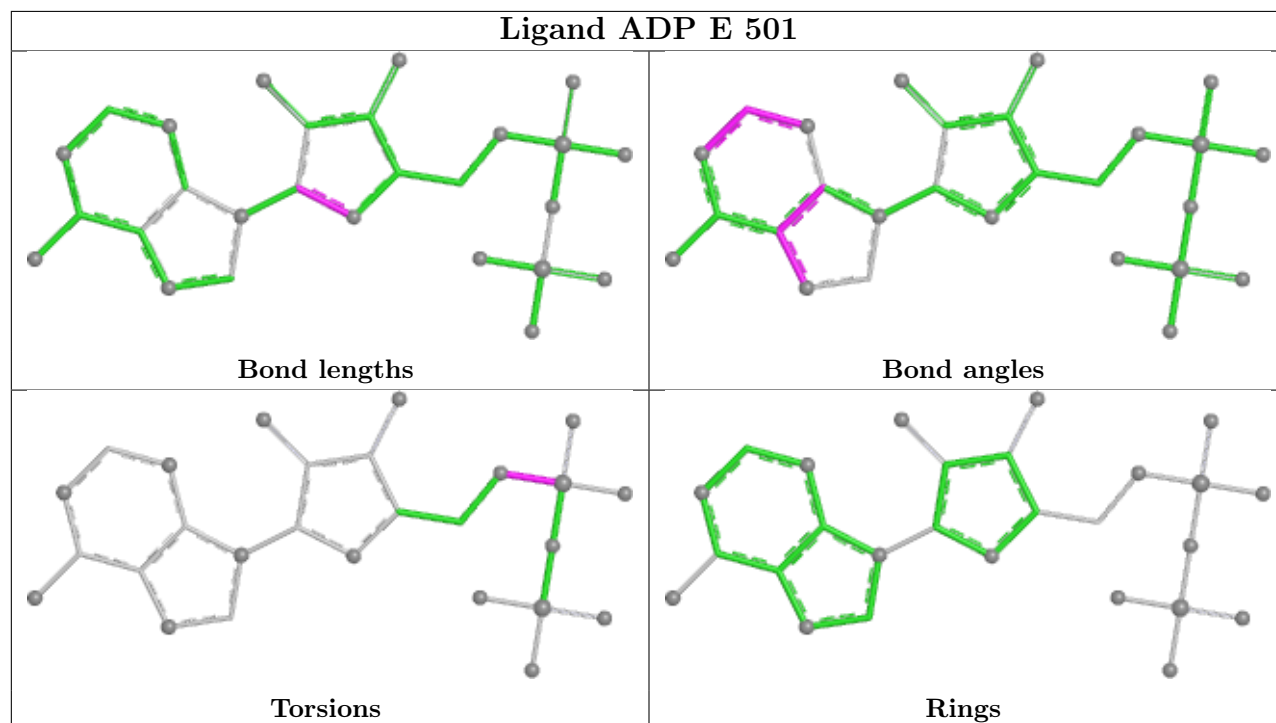
There are no ring outliers.

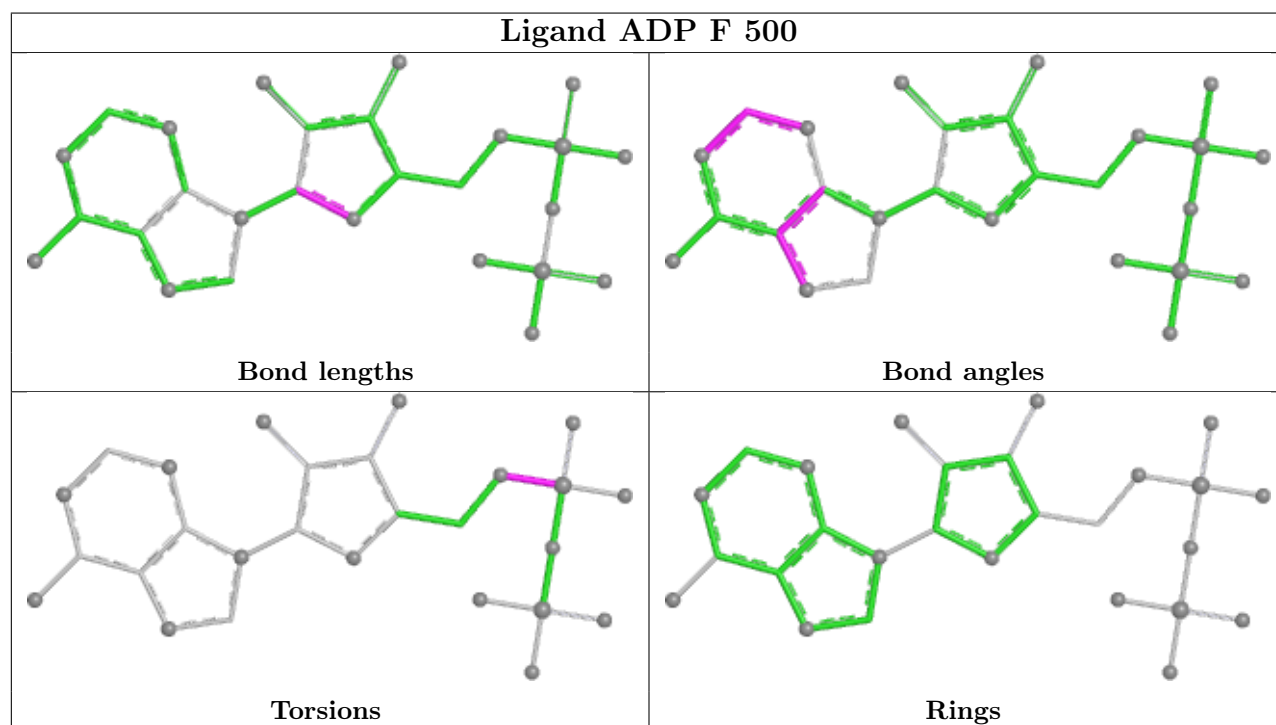
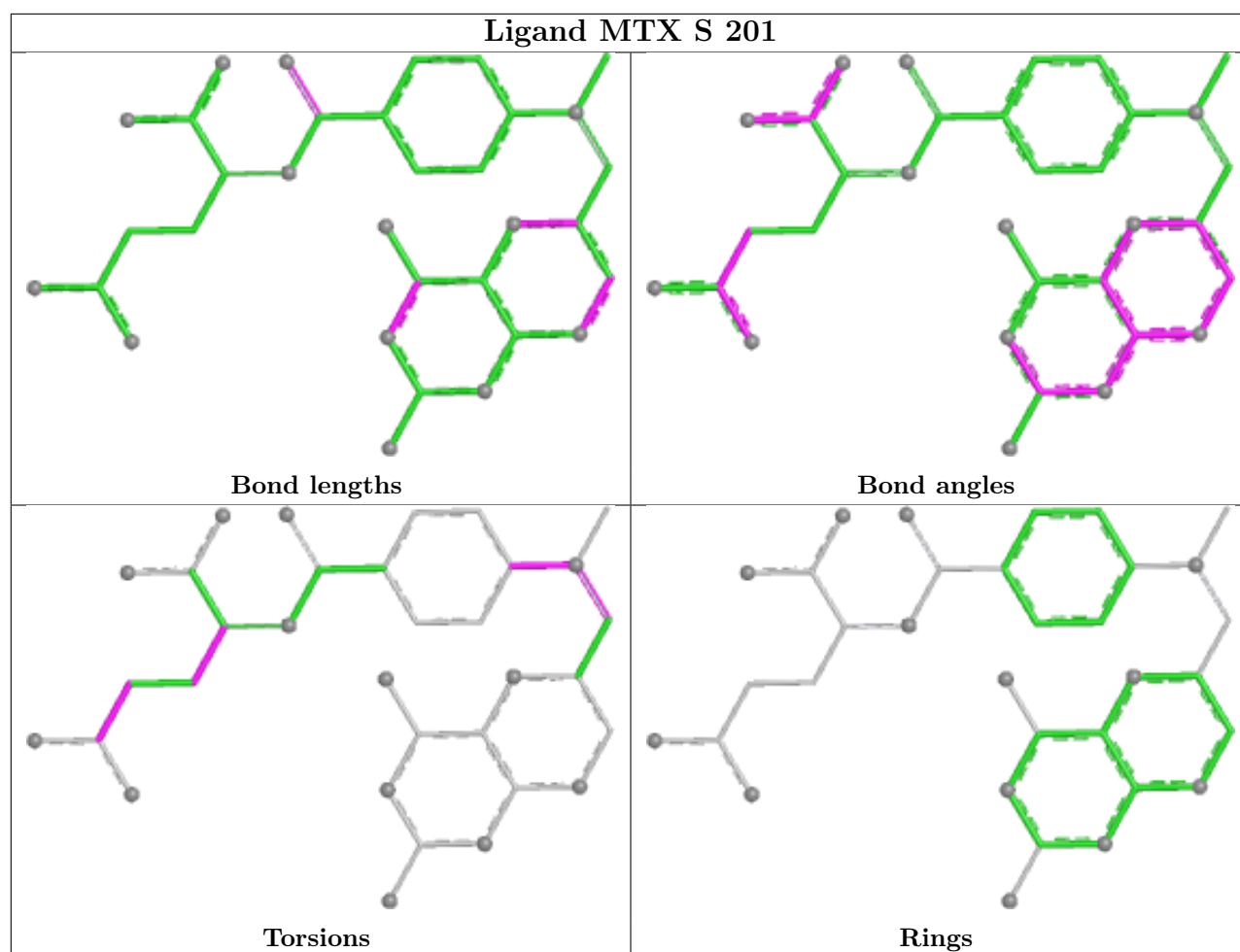
6 monomers are involved in 10 short contacts:

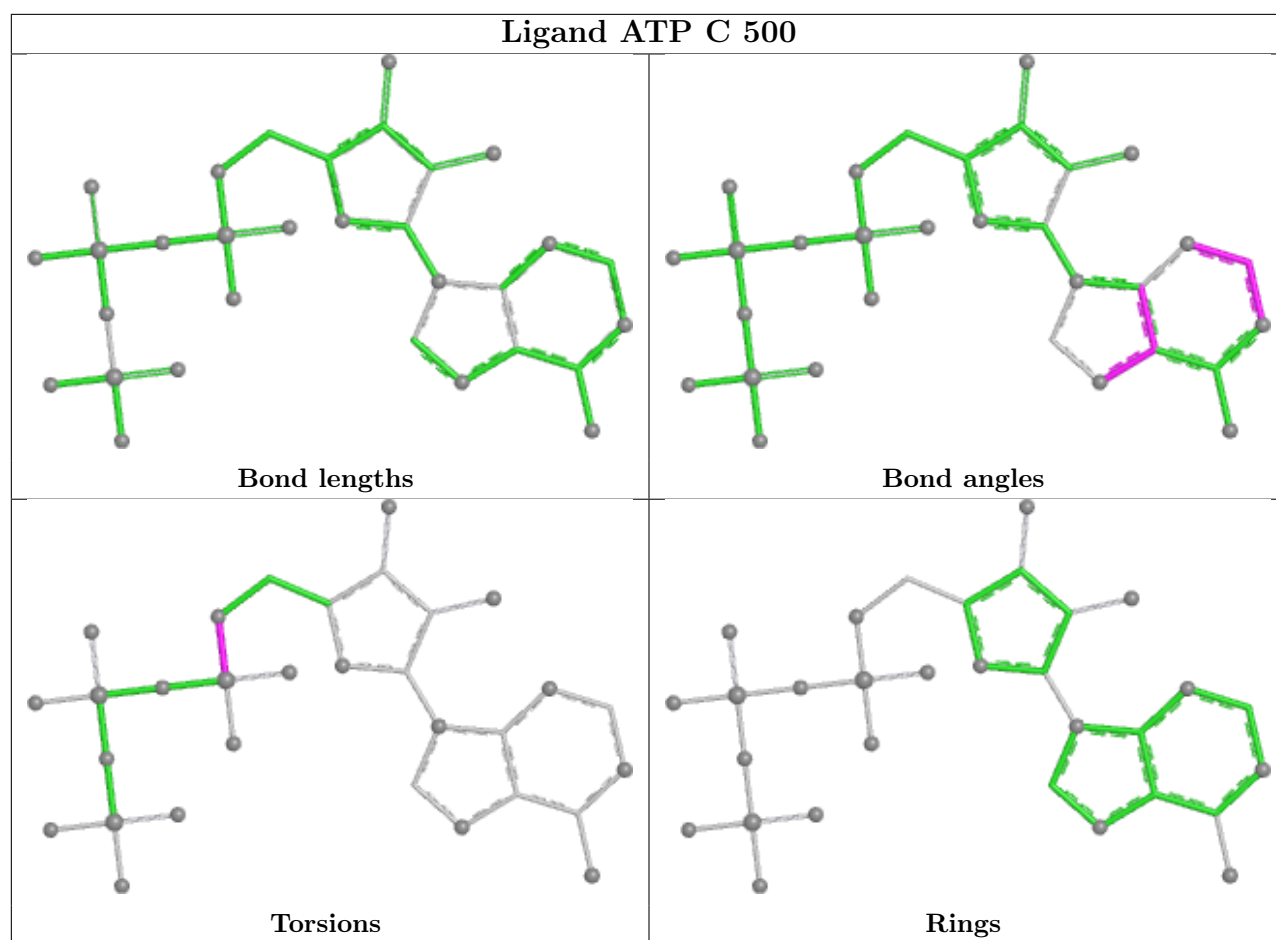
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	501	ADP	1	0
7	S	201	MTX	1	0
4	C	500	ATP	2	0
4	A	500	ATP	2	0
4	B	500	ATP	2	0
6	D	500	ADP	2	0

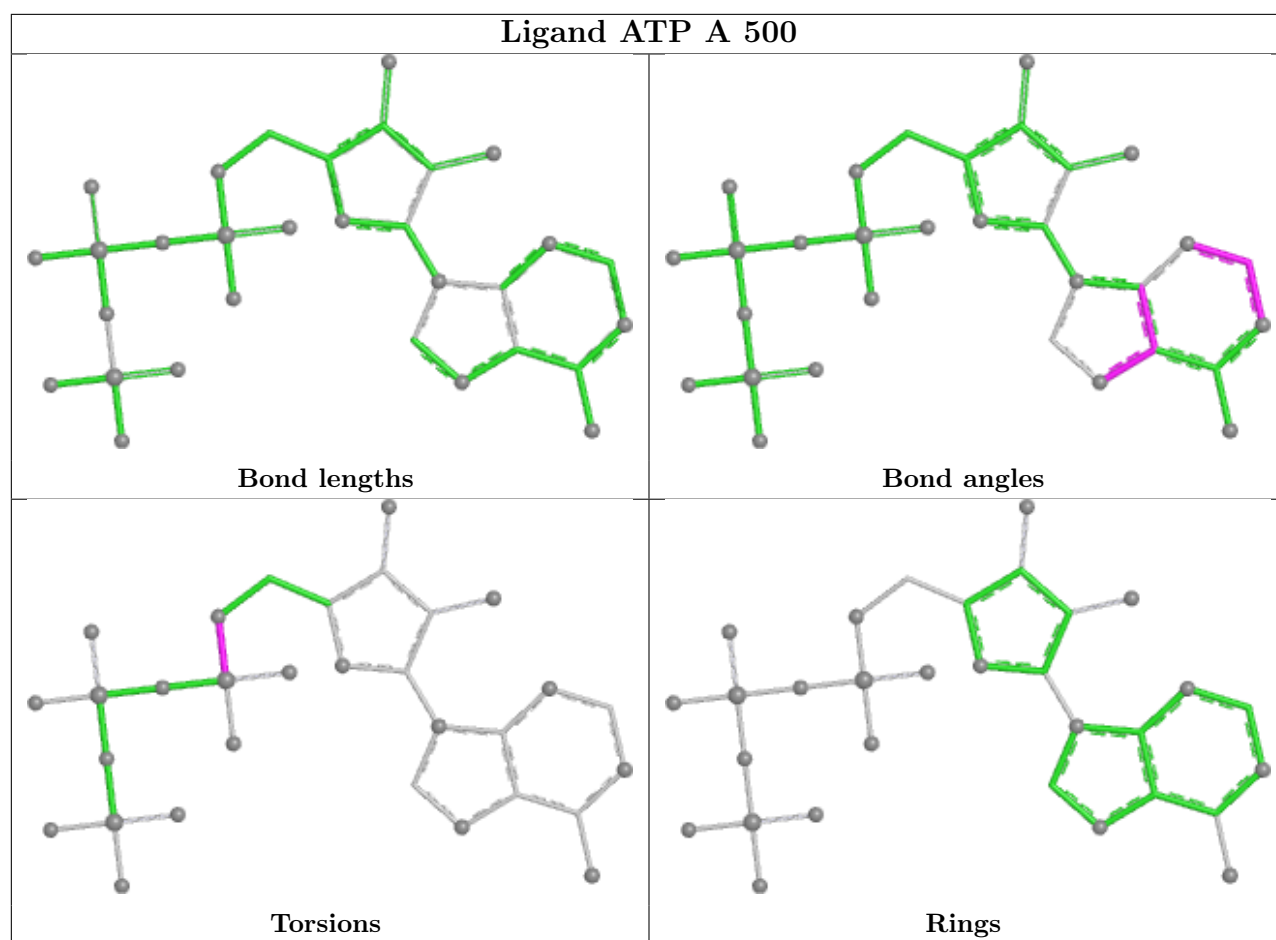
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

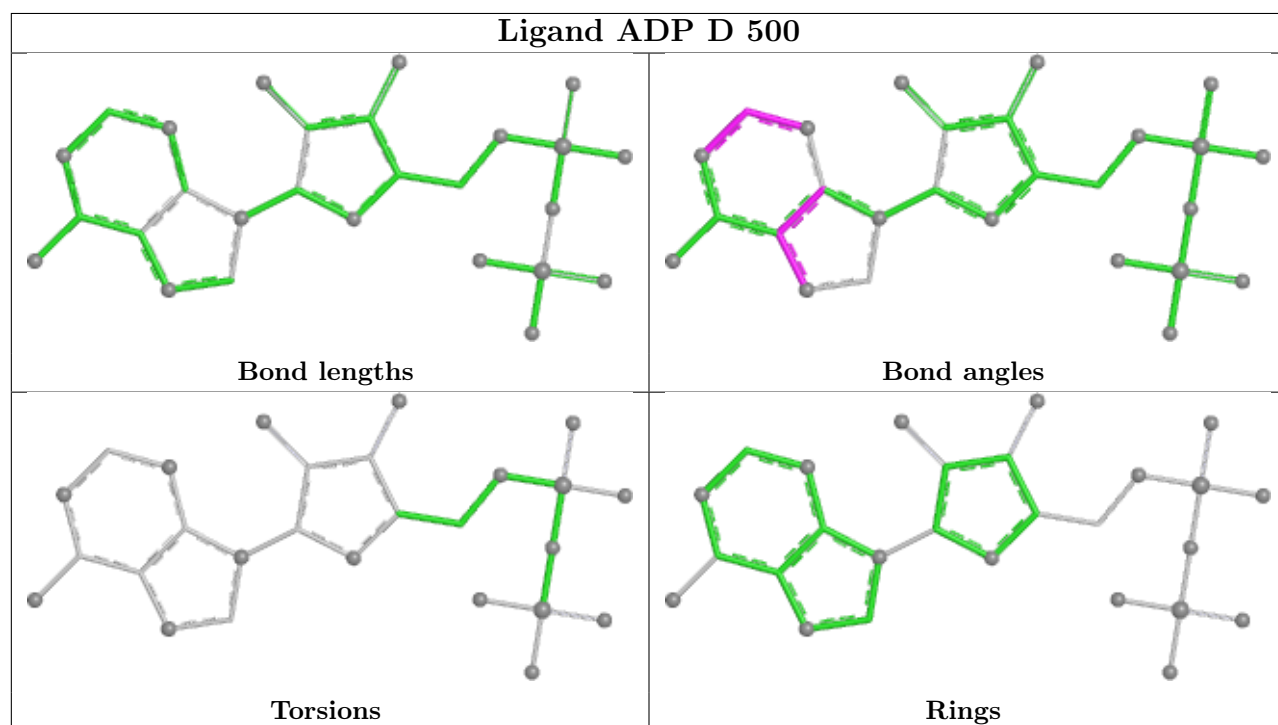
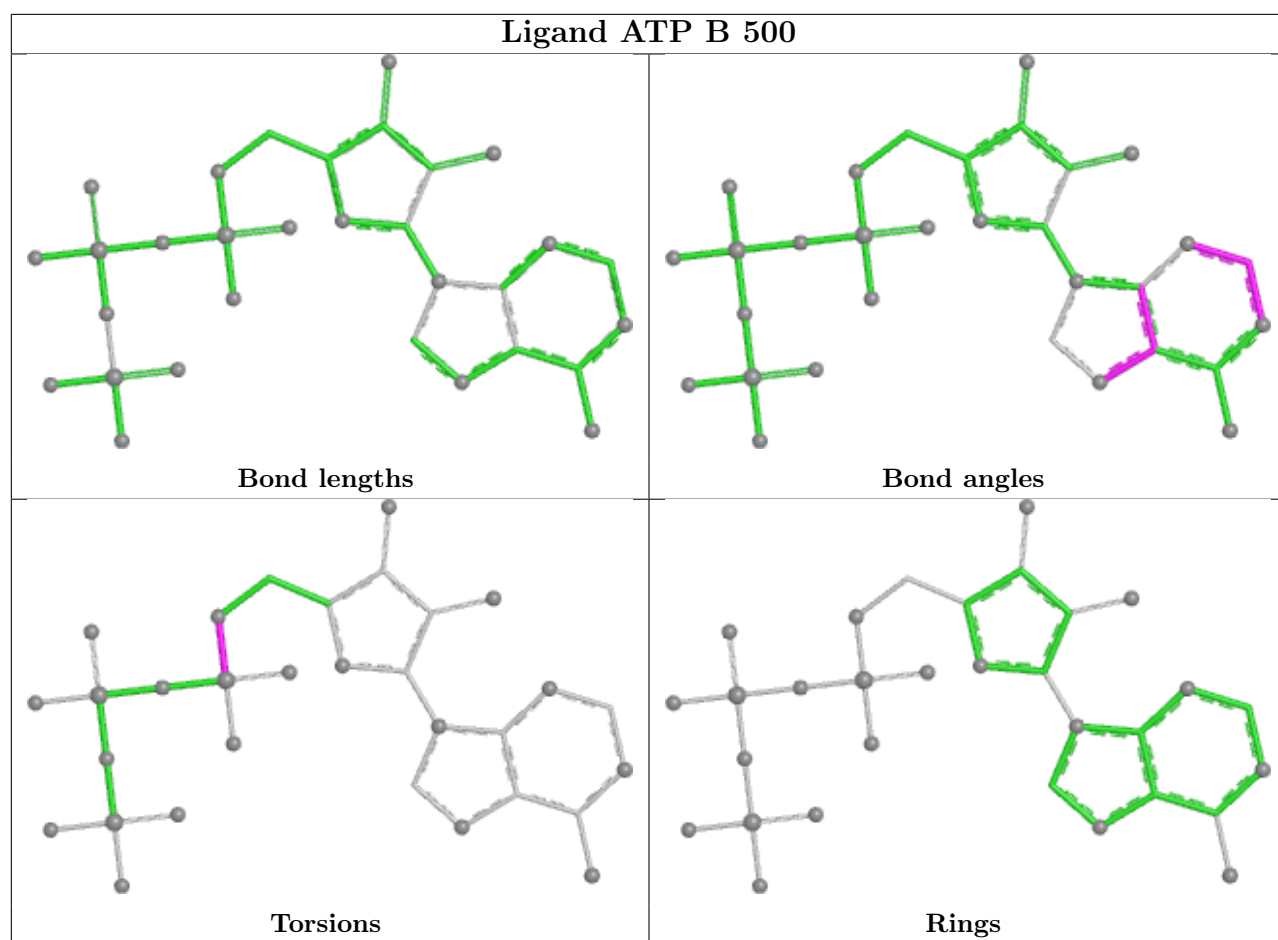
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











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.

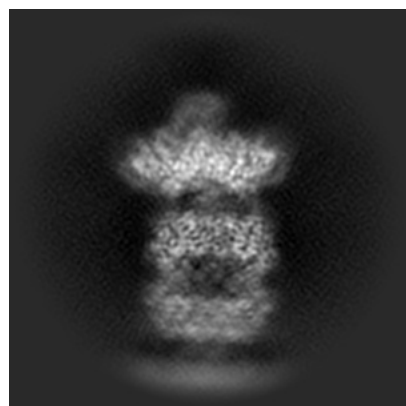
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45299. These allow visual inspection of the internal detail of the map and identification of artifacts.

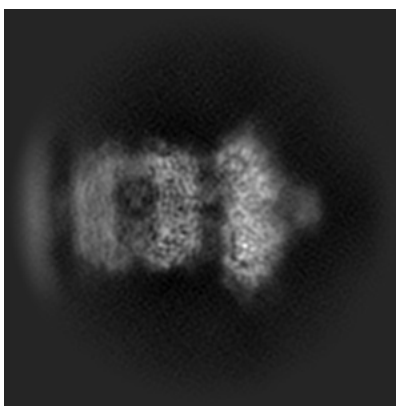
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

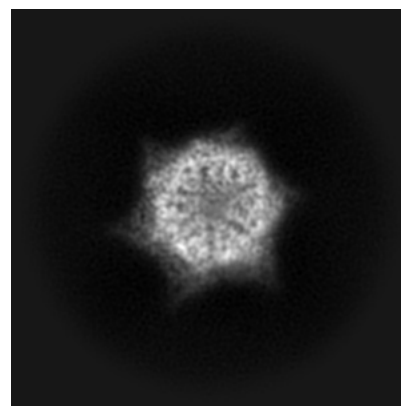
6.1.1 Primary map



X

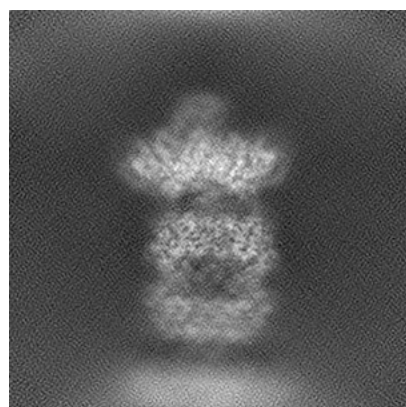


Y

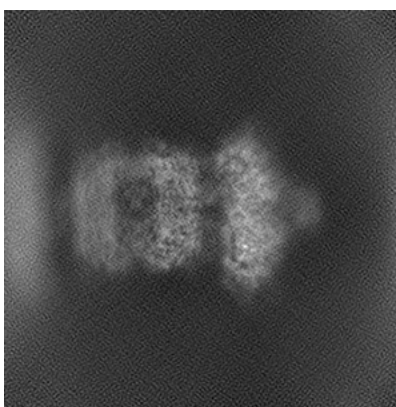


Z

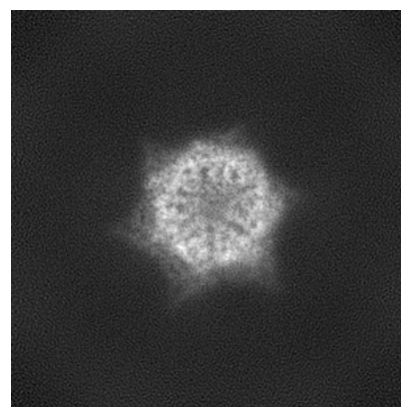
6.1.2 Raw map



X



Y

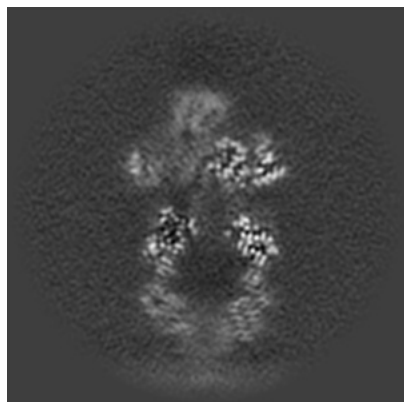


Z

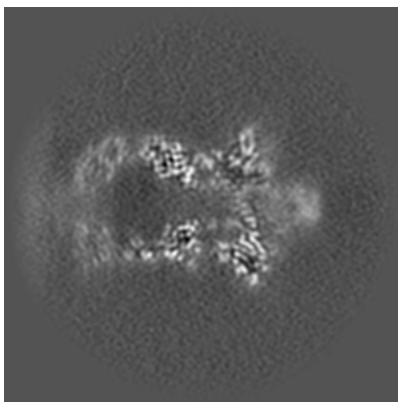
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

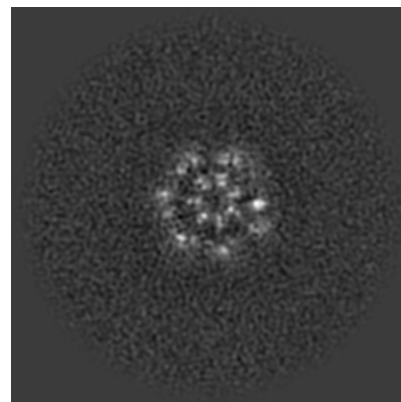
6.2.1 Primary map



X Index: 128

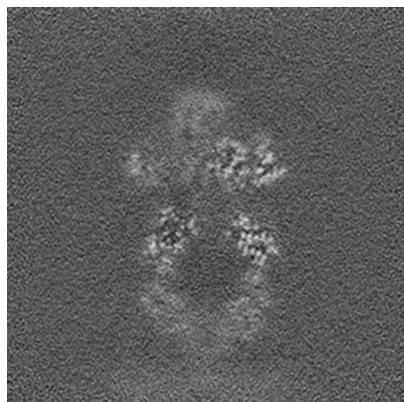


Y Index: 128

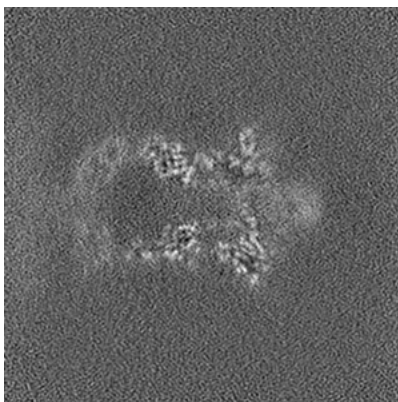


Z Index: 128

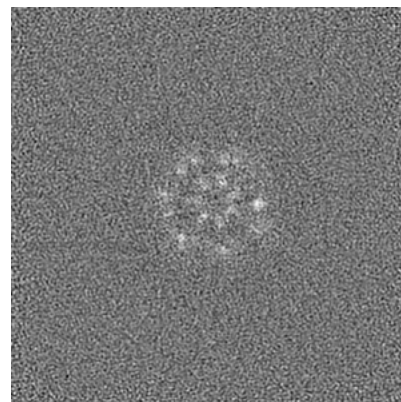
6.2.2 Raw map



X Index: 128



Y Index: 128

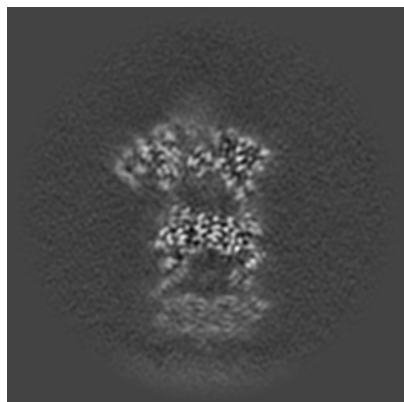


Z Index: 128

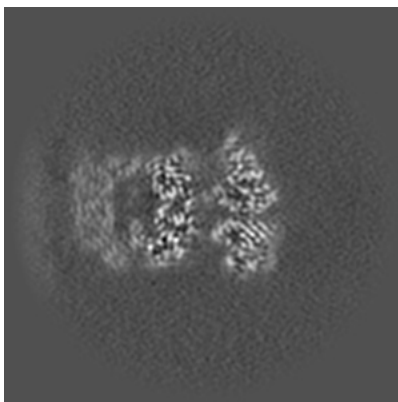
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

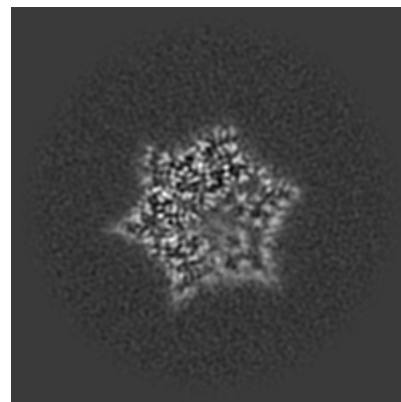
6.3.1 Primary map



X Index: 110

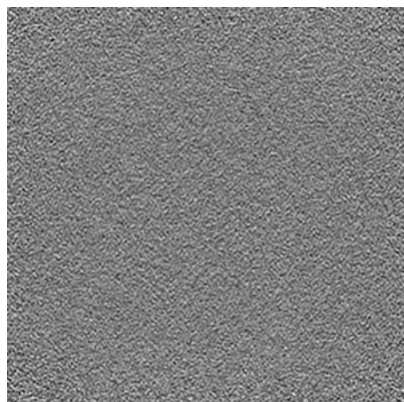


Y Index: 148

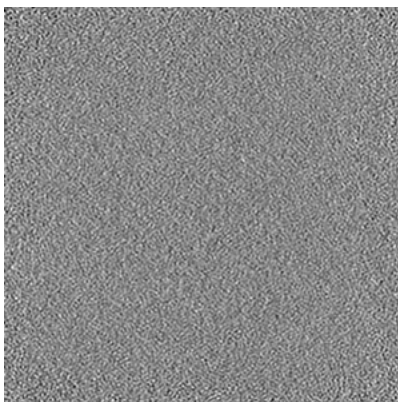


Z Index: 154

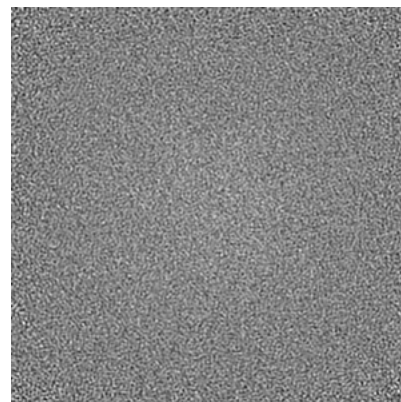
6.3.2 Raw map



X Index: 0



Y Index: 0

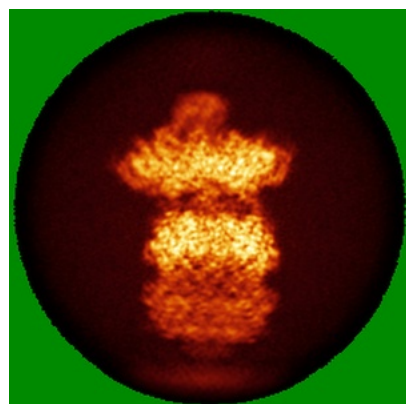


Z Index: 0

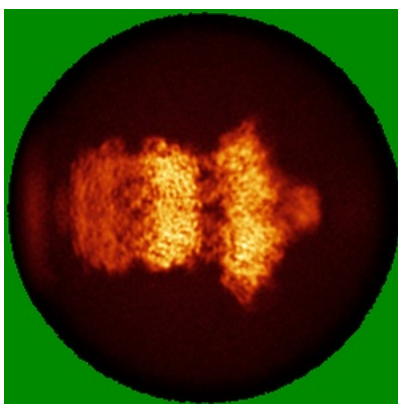
The images above show the largest variance slices of the map in three orthogonal directions.

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

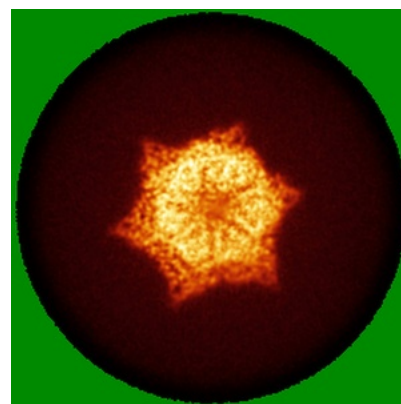
6.4.1 Primary map



X

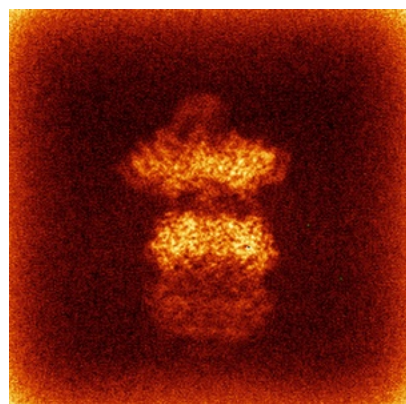


Y

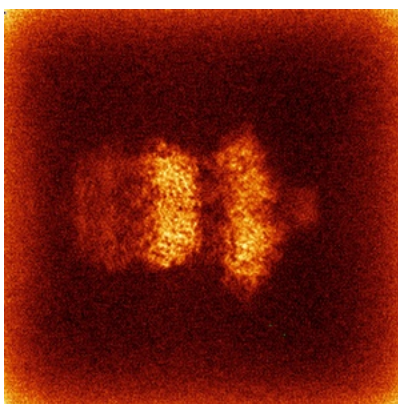


Z

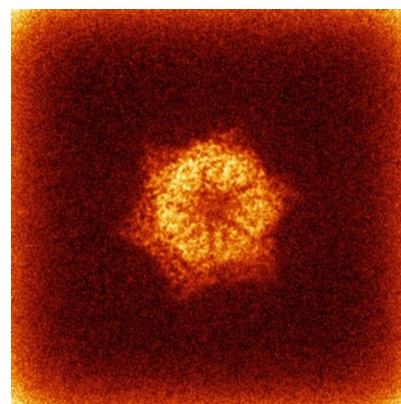
6.4.2 Raw map



X



Y



Z

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

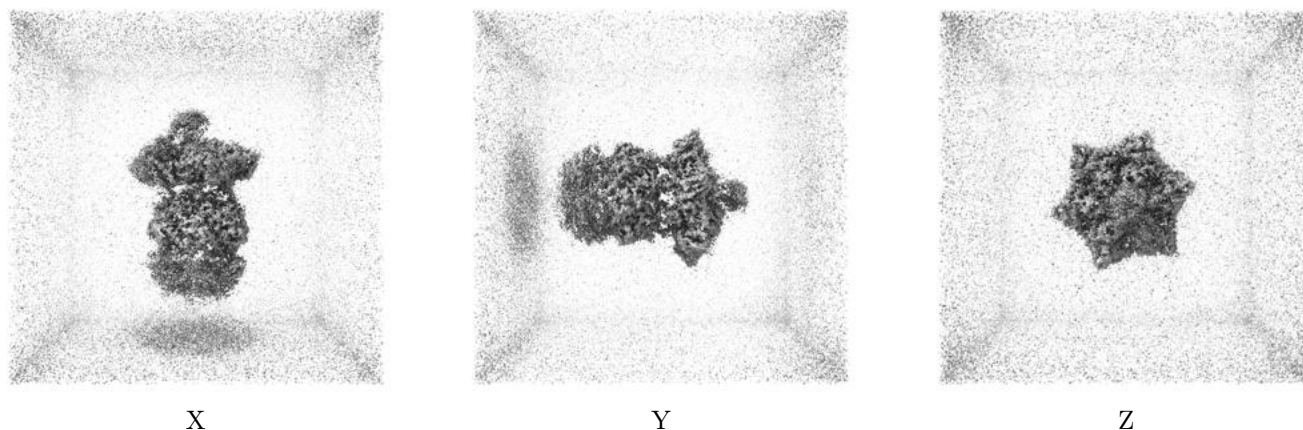
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0676. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

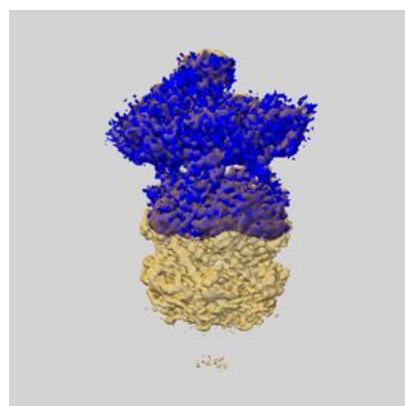
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

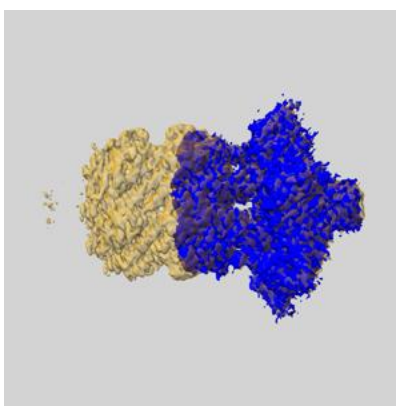
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

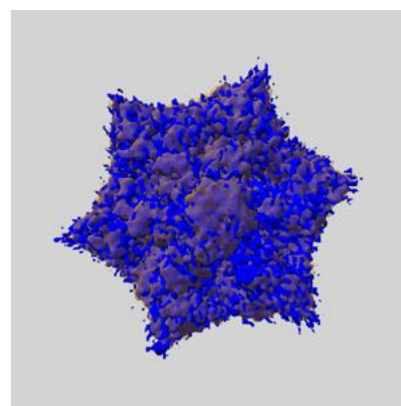
6.6.1 emd_45299_msk_1.map [i](#)



X



Y

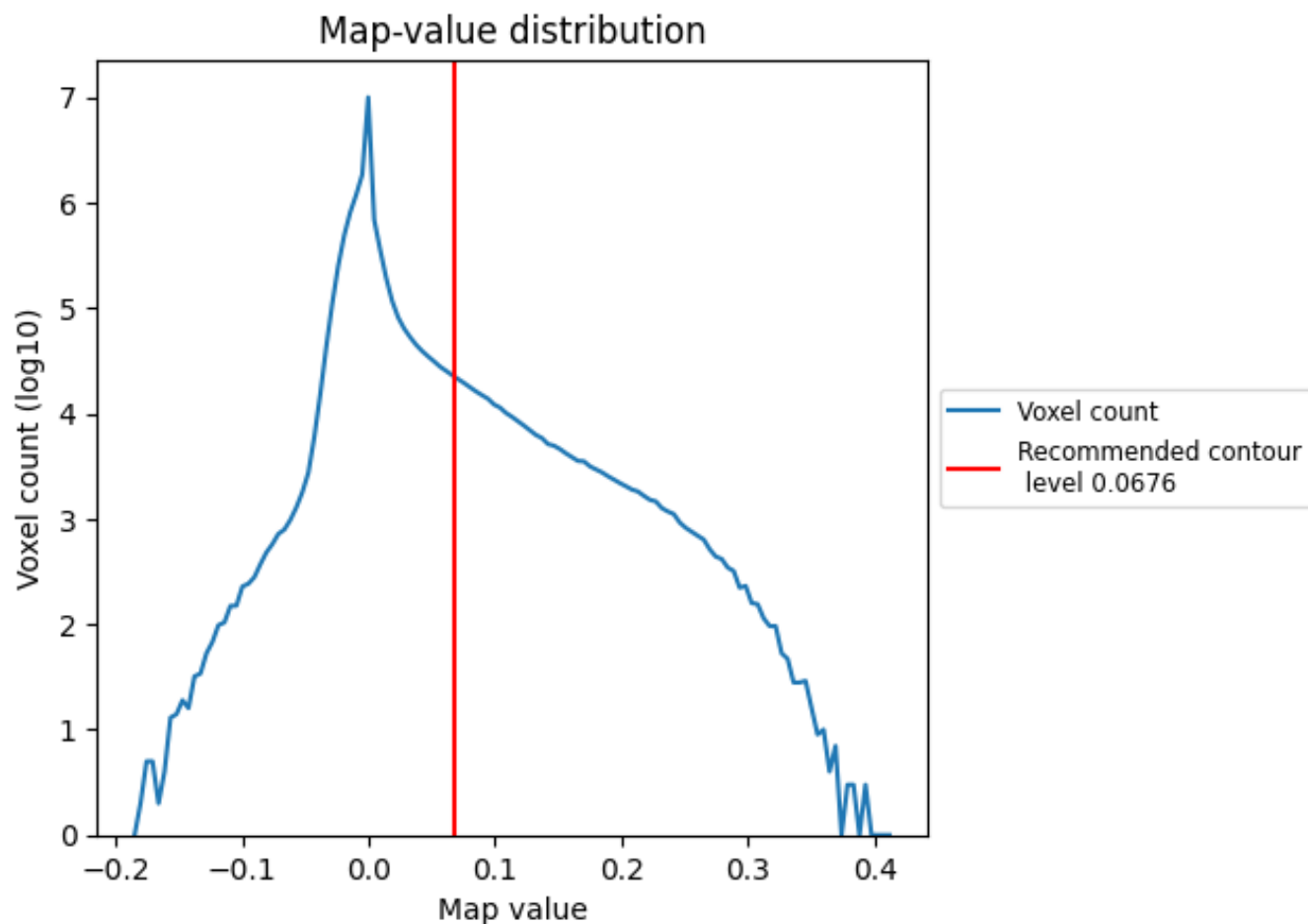


Z

7 Map analysis [i](#)

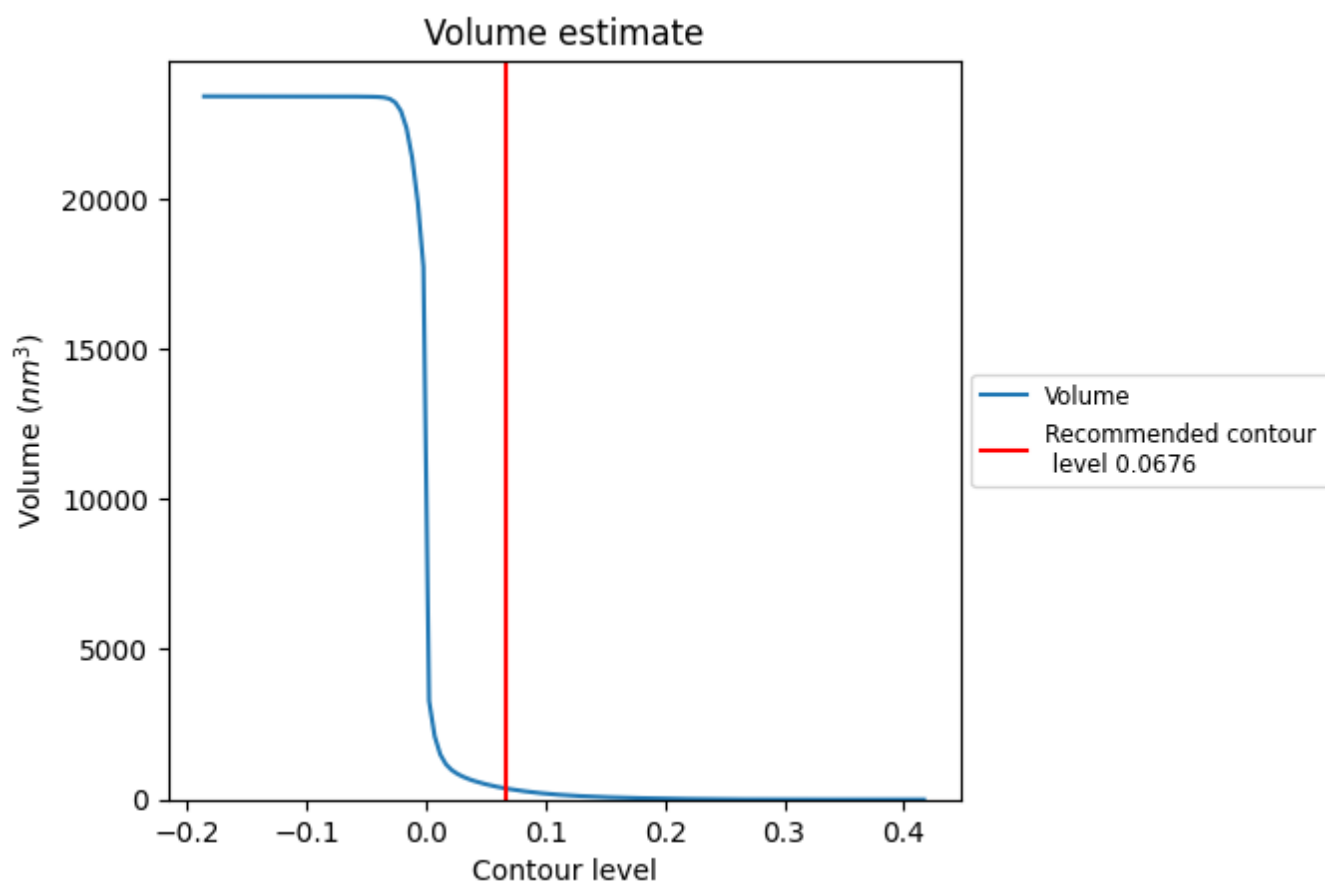
This section contains the results of statistical analysis of the map.

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.

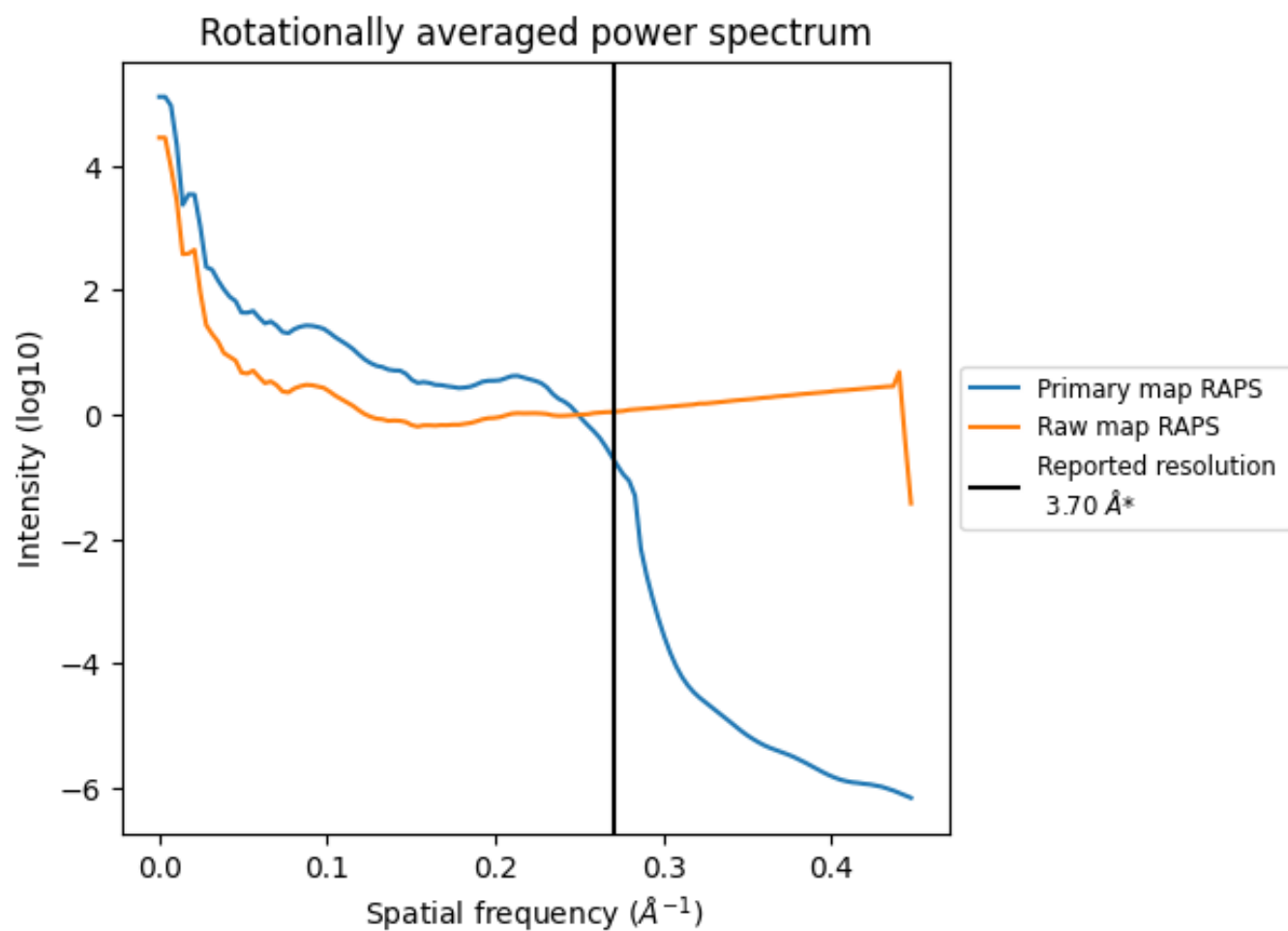
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 366 nm^3 ; this corresponds to an approximate mass of 331 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 ⓘ

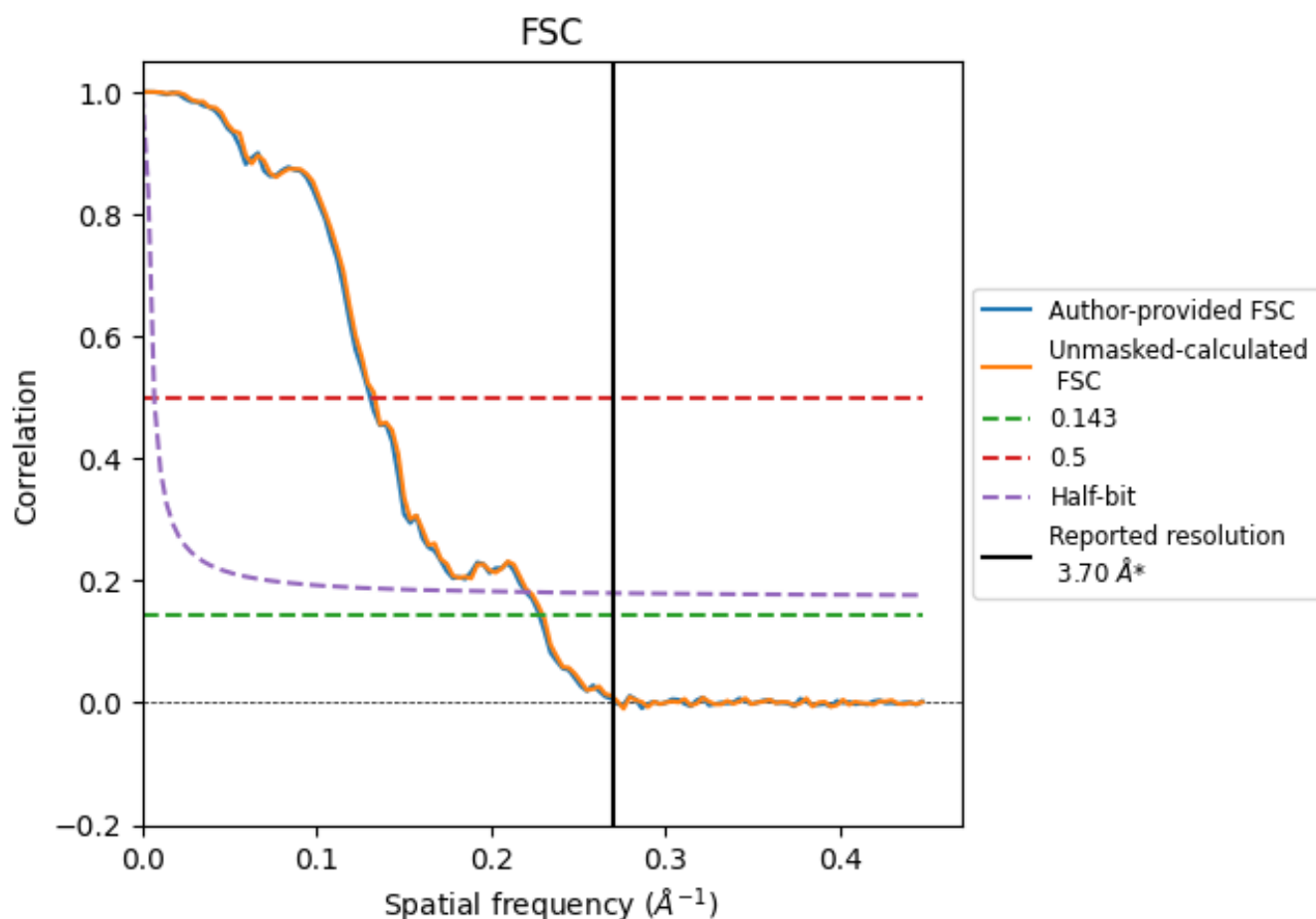


*Reported resolution corresponds to spatial frequency of 0.270 \AA^{-1}

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.270 \AA^{-1}

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	4.39	7.65	4.54
Unmasked-calculated*	4.35	7.50	4.50

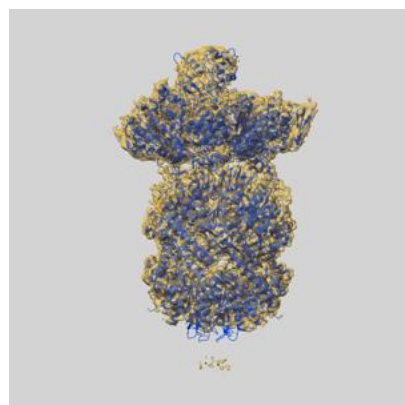
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 4.39 differs from the reported value 3.7 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.35 differs from the reported value 3.7 by more than 10 %

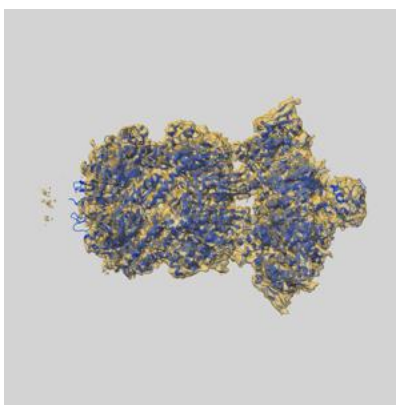
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-45299 and PDB model 9C87. Per-residue inclusion information can be found in [section 3](#) on [page 19](#).

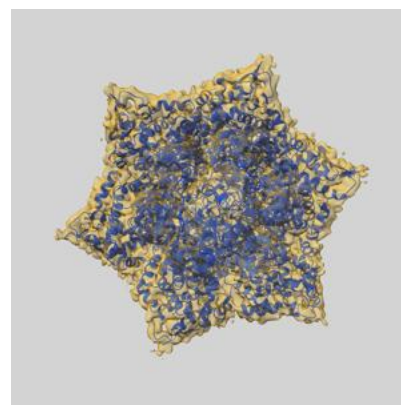
9.1 Map-model overlay [i](#)



X



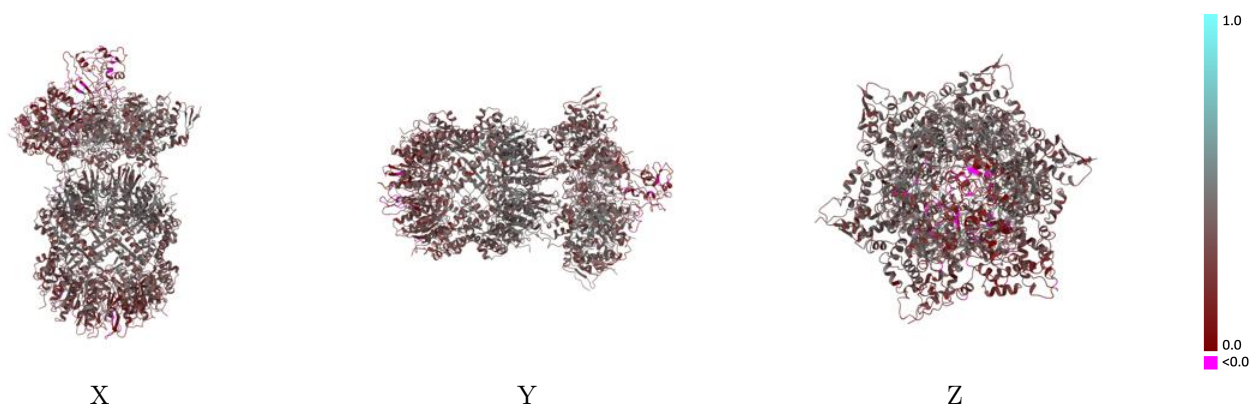
Y



Z

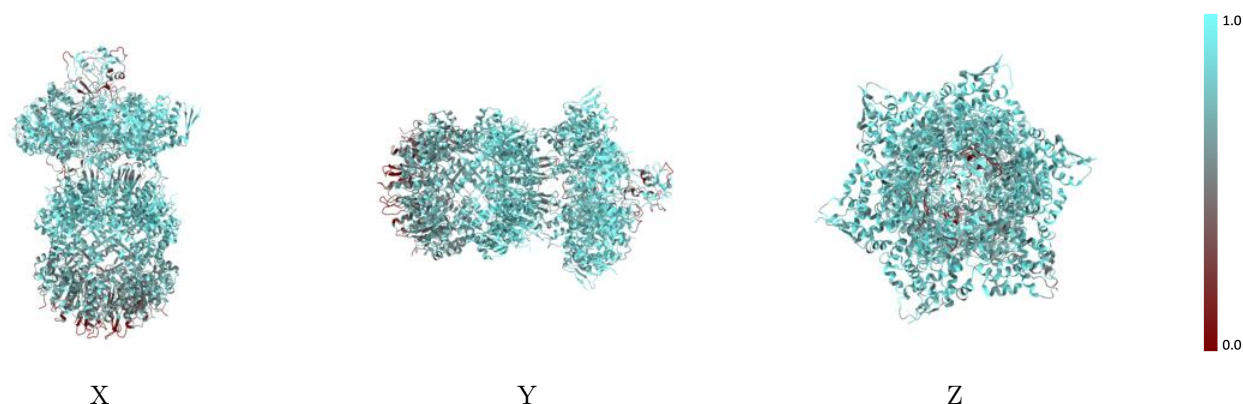
The images above show the 3D surface view of the map at the recommended contour level 0.0676 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



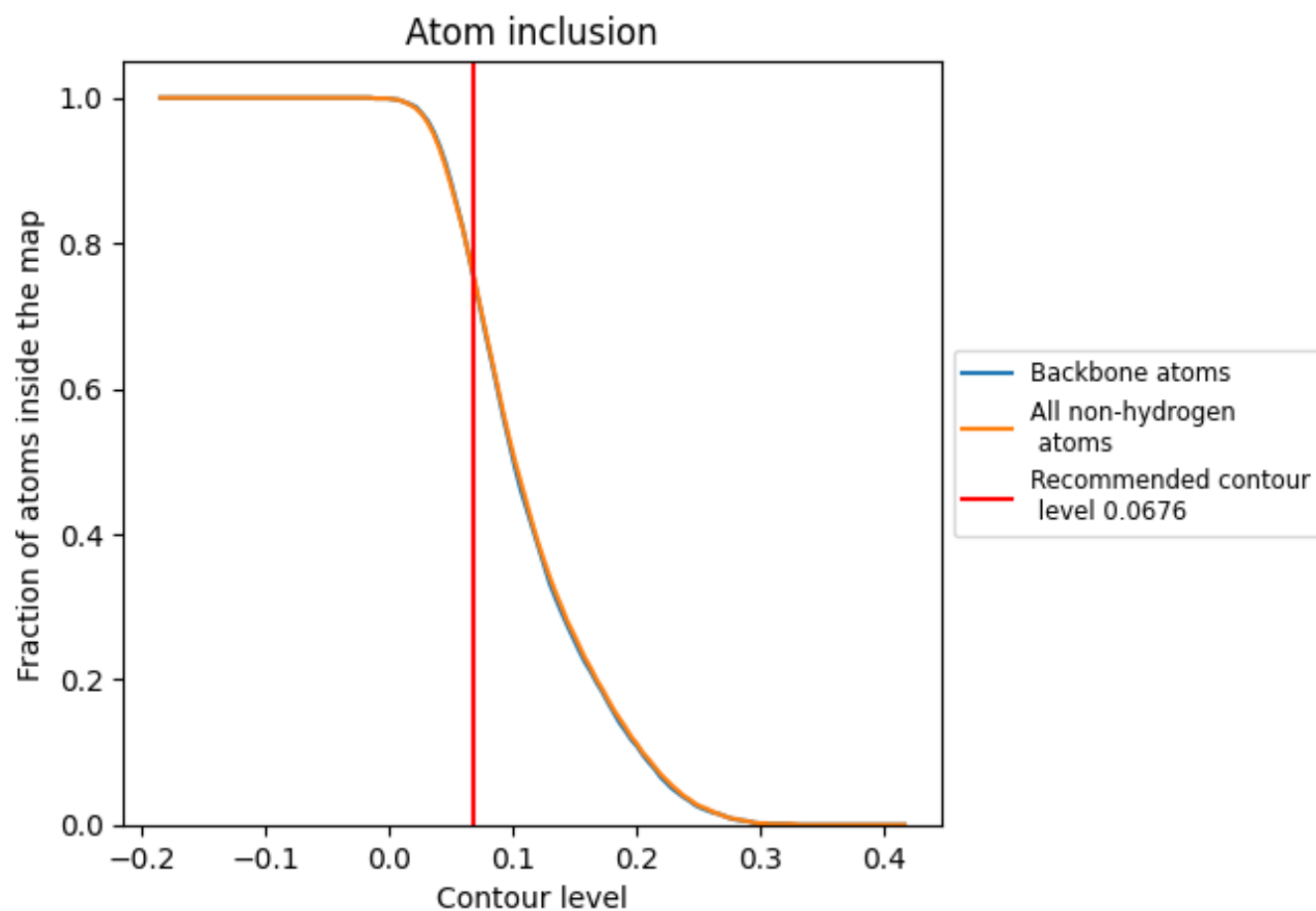
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0676).













































9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 76% 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 (0.0676) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7580	 0.3350
A	 0.8150	 0.3360
B	 0.8350	 0.3710
C	 0.8490	 0.3750
D	 0.8330	 0.3670
E	 0.7920	 0.3130
F	 0.7580	 0.2360
S	 0.6290	 0.1480
h	 0.8690	 0.3980
i	 0.8590	 0.3920
j	 0.8550	 0.3880
k	 0.8590	 0.3860
l	 0.8700	 0.3940
m	 0.8710	 0.3920
n	 0.8670	 0.3990
p	 0.6150	 0.3180
q	 0.6370	 0.2800
r	 0.6080	 0.2930
s	 0.5970	 0.3010
t	 0.6290	 0.3090
u	 0.6250	 0.3100
v	 0.6060	 0.3120

