



wwPDB EM Validation Summary Report ⓘ

Oct 7, 2024 – 02:35 PM EDT

PDB ID : 8V9R
EMDB ID : EMD-43081
Title : Cryo-EM Structure of a Proteolytic ClpXP AAA+ Machine Poised to Unfold a Branched-Degron DHFR-ssrA Substrate Bound with MTX
Authors : Ghanbarpour, A.; Sauer, R.T.; Davis, J.H.
Deposited on : 2023-12-09
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev113
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) : 2.39

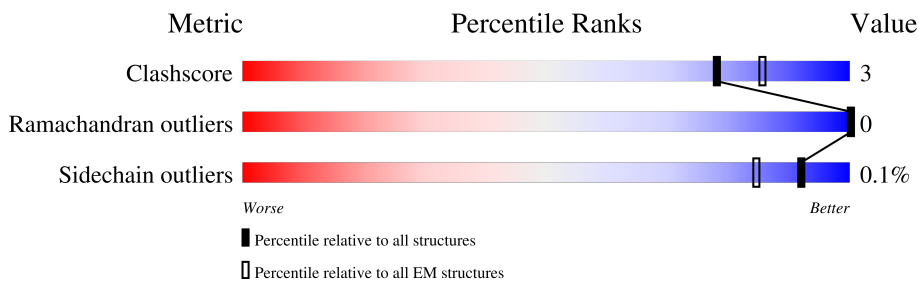
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
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	388	83% 8% 9% 5%
1	B	388	85% 5% 9% 5%
1	C	388	88% 9% 5%
1	D	388	86% 5% 9% 5%
1	E	388	82% 6% 12% 5%
1	F	388	78% 9% 13% 5%
2	S	208	80% 6% 14% 5%
3	h	207	93% 7%

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Mol	Chain	Length	Quality of chain
3	i	207	 93% 7%
3	j	207	 93% 7%
3	k	207	 93% 7%
3	l	207	 93% 7%
3	m	207	 93% 7%
3	n	207	 92% 7%
3	p	207	 92% 7%
3	q	207	 93% 7%
3	r	207	 93% 7%
3	s	207	 93% 7%
3	t	207	 93% 7%
3	u	207	 93% 7%
3	v	207	 92% 7%

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 77629 atoms, of which 38975 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	
			Total	C	H	N	O			S
1	A	353	5452	1704	2754	457	532	5	0	0
1	B	352	5440	1701	2748	456	530	5	0	0
1	C	352	5440	1701	2748	456	530	5	0	0
1	D	352	5441	1701	2749	456	530	5	0	0
1	E	341	5286	1655	2674	441	511	5	0	0
1	F	339	5258	1646	2659	439	509	5	0	0

There are 162 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	37	MET	-	expression tag	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
B	37	MET	-	expression tag	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
C	37	MET	-	expression tag	UNP P0A6H1
C	38	GLY	-	expression tag	UNP P0A6H1
C	39	SER	-	expression tag	UNP P0A6H1
C	40	SER	-	expression tag	UNP P0A6H1
C	41	HIS	-	expression tag	UNP P0A6H1
C	42	HIS	-	expression tag	UNP P0A6H1

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Chain	Residue	Modelled	Actual	Comment	Reference
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
D	37	MET	-	expression tag	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
D	55	ASN	-	expression tag	UNP P0A6H1
D	56	LEU	-	expression tag	UNP P0A6H1
D	57	TYR	-	expression tag	UNP P0A6H1

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Chain	Residue	Modelled	Actual	Comment	Reference
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
E	37	MET	-	expression tag	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
F	37	MET	-	expression tag	UNP P0A6H1
F	38	GLY	-	expression tag	UNP P0A6H1
F	39	SER	-	expression tag	UNP P0A6H1
F	40	SER	-	expression tag	UNP P0A6H1
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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

- Molecule 2 is a protein called Dihydrofolate reductase.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	S	178	2785	904	1369	238	266	8	0	0

There are 50 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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

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Chain	Residue	Modelled	Actual	Comment	Reference
S	173	TYR	-	expression tag	UNP A0A4C7B7M9
S	174	CYS	-	expression tag	UNP A0A4C7B7M9
S	175	VAL	-	expression tag	UNP A0A4C7B7M9
S	176	GLU	-	expression tag	UNP A0A4C7B7M9
S	177	PRO	-	expression tag	UNP A0A4C7B7M9
S	178	PHE	-	expression tag	UNP A0A4C7B7M9
S	179	VAL	-	expression tag	UNP A0A4C7B7M9
S	180	GLY	-	expression tag	UNP A0A4C7B7M9
S	181	GLU	-	expression tag	UNP A0A4C7B7M9
S	182	THR	-	expression tag	UNP A0A4C7B7M9
S	183	ALA	-	expression tag	UNP A0A4C7B7M9
S	184	HIS	-	expression tag	UNP A0A4C7B7M9
S	185	PHE	-	expression tag	UNP A0A4C7B7M9
S	186	GLU	-	expression tag	UNP A0A4C7B7M9
S	187	ILE	-	expression tag	UNP A0A4C7B7M9
S	188	GLU	-	expression tag	UNP A0A4C7B7M9
S	189	LEU	-	expression tag	UNP A0A4C7B7M9
S	190	SER	-	expression tag	UNP A0A4C7B7M9
S	191	GLU	-	expression tag	UNP A0A4C7B7M9
S	192	PRO	-	expression tag	UNP A0A4C7B7M9
S	193	ASP	-	expression tag	UNP A0A4C7B7M9
S	194	VAL	-	expression tag	UNP A0A4C7B7M9
S	195	HIS	-	expression tag	UNP A0A4C7B7M9
S	196	GLY	-	expression tag	UNP A0A4C7B7M9
S	197	GLN	-	expression tag	UNP A0A4C7B7M9
S	198	TRP	-	expression tag	UNP A0A4C7B7M9
S	199	LYS	-	expression tag	UNP A0A4C7B7M9
S	200	LEU	-	expression tag	UNP A0A4C7B7M9
S	201	THR	-	expression tag	UNP A0A4C7B7M9
S	202	SER	-	expression tag	UNP A0A4C7B7M9
S	203	HIS	-	expression tag	UNP A0A4C7B7M9
S	204	HIS	-	expression tag	UNP A0A4C7B7M9
S	205	HIS	-	expression tag	UNP A0A4C7B7M9
S	206	HIS	-	expression tag	UNP A0A4C7B7M9
S	207	HIS	-	expression tag	UNP A0A4C7B7M9
S	208	HIS	-	expression tag	UNP A0A4C7B7M9

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	h	192	3016	947	1513	261	283	12	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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 (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

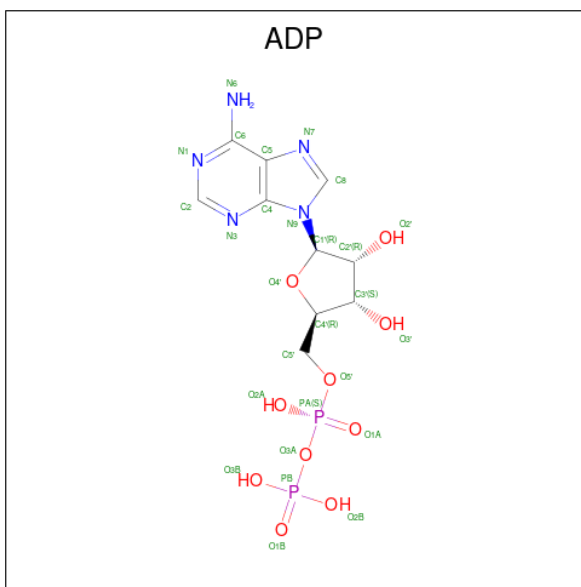


Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	N	O		P
4	A	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
4	B	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
4	C	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

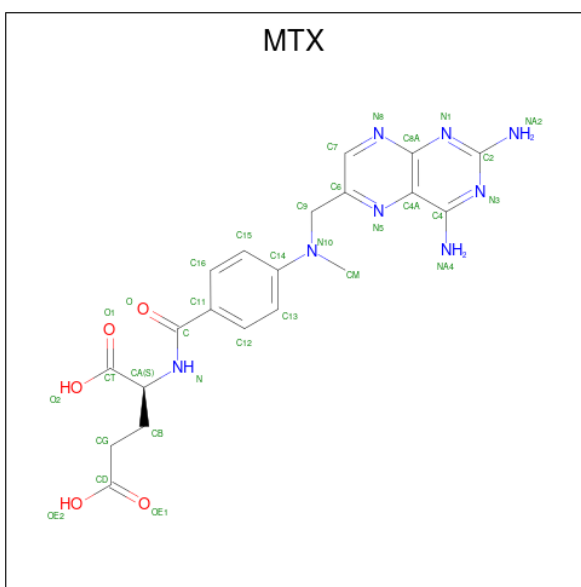
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
5	A	1	Total	Mg	0
			1	1	
5	B	1	Total	Mg	0
			1	1	
5	C	1	Total	Mg	0
			1	1	
5	D	1	Total	Mg	0
			1	1	

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	N	O		P
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 (three-letter code: MTX) (formula: C₂₀H₂₂N₈O₅).

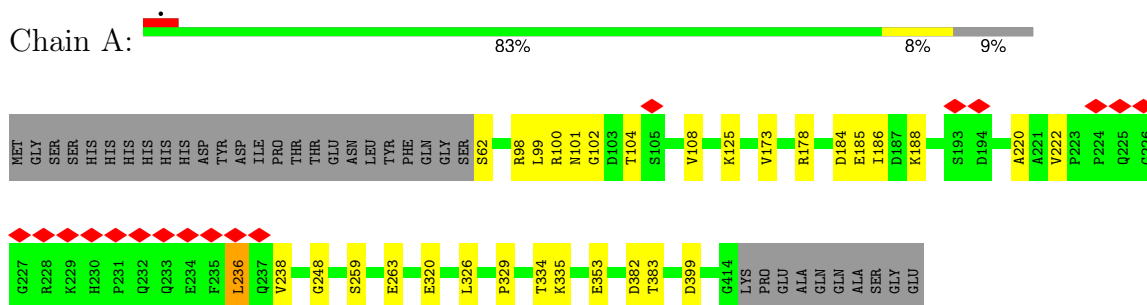


Mol	Chain	Residues	Atoms				AltConf	
			Total	C	H	N		O
7	S	1	Total	C	H	N	O	0
			53	20	20	8	5	

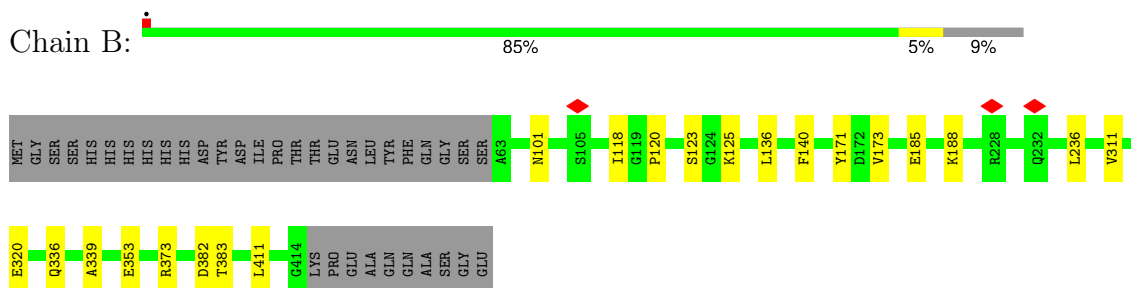
3 Residue-property plots

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.

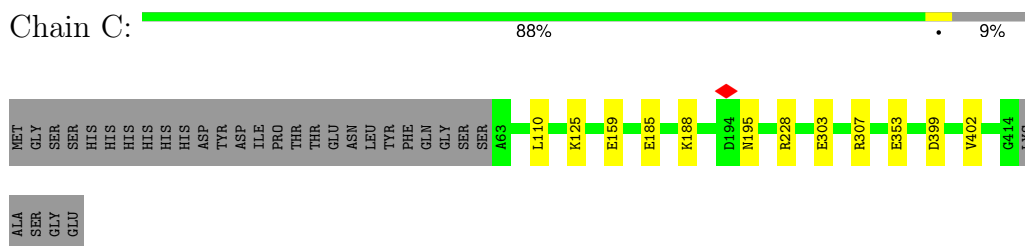
- Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpX



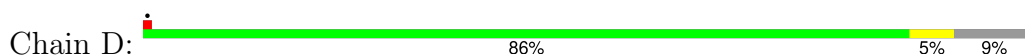
- Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpX

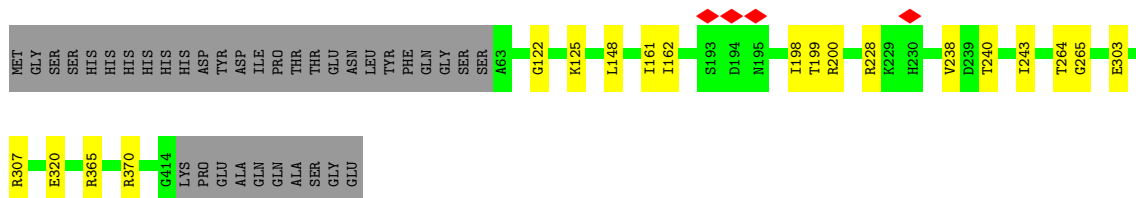


- Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpX

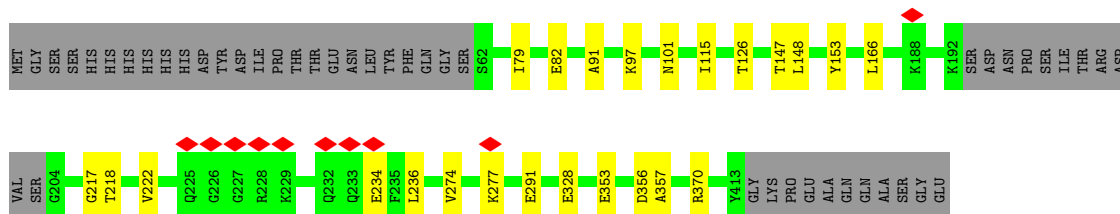
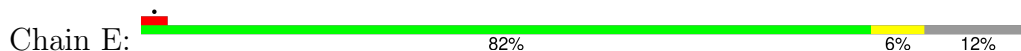


- Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpX

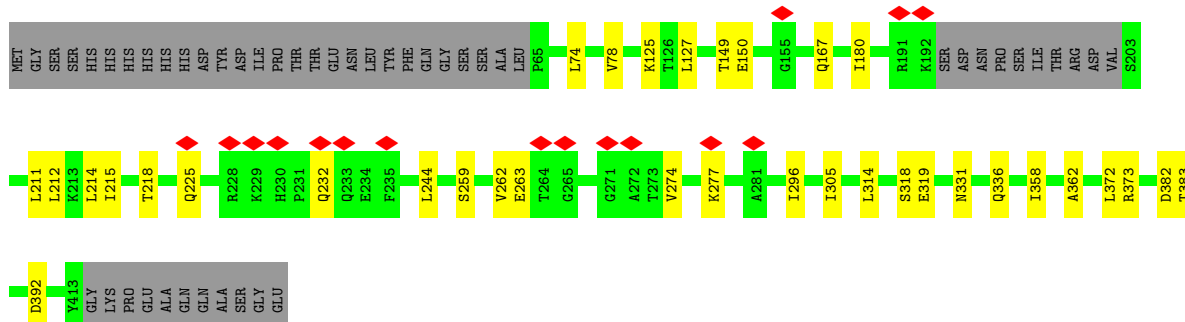
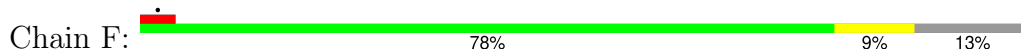




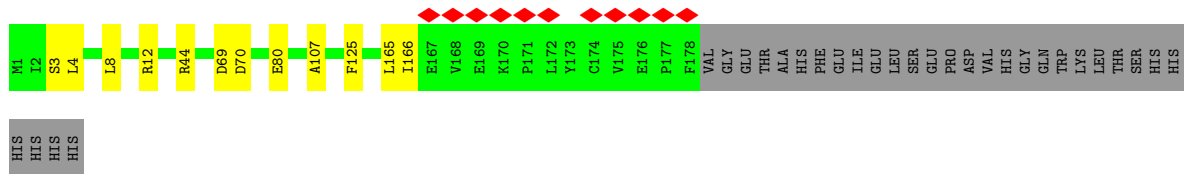
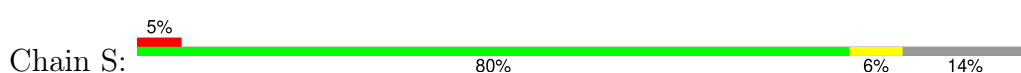
• Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpX



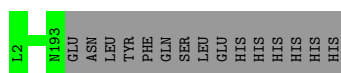
• Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpX



• Molecule 2: Dihydrofolate reductase

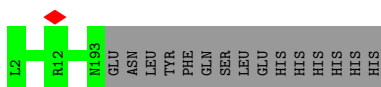


• Molecule 3: ATP-dependent Clp protease proteolytic subunit



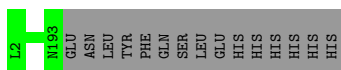
• Molecule 3: ATP-dependent Clp protease proteolytic subunit

Chain i:  93% 7%



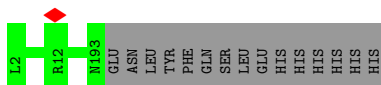
- Molecule 3: ATP-dependent Clp protease proteolytic subunit

Chain j:  93% 7%



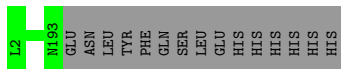
- Molecule 3: ATP-dependent Clp protease proteolytic subunit

Chain k:  93% 7%



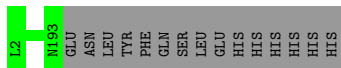
- Molecule 3: ATP-dependent Clp protease proteolytic subunit

Chain l:  93% 7%



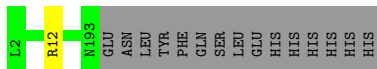
- Molecule 3: ATP-dependent Clp protease proteolytic subunit

Chain m:  93% 7%



- Molecule 3: ATP-dependent Clp protease proteolytic subunit

Chain n:  92% 7%

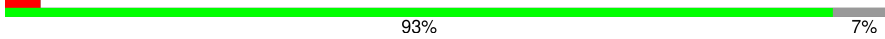


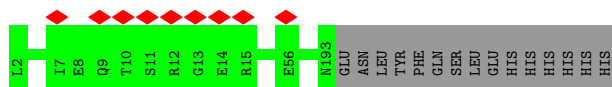
- Molecule 3: ATP-dependent Clp protease proteolytic subunit

Chain p:  92% 7%




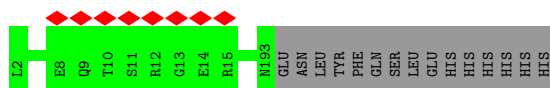
- Molecule 3: ATP-dependent Clp protease proteolytic subunit

Chain q:  93% 7%



- Molecule 3: ATP-dependent Clp protease proteolytic subunit

Chain r:  93% 7%



- Molecule 3: ATP-dependent Clp protease proteolytic subunit

Chain s:  93% 7%



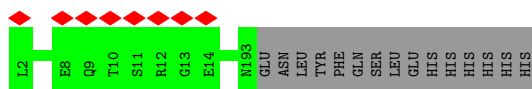
- Molecule 3: ATP-dependent Clp protease proteolytic subunit

Chain t:  93% 7%

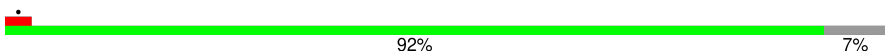


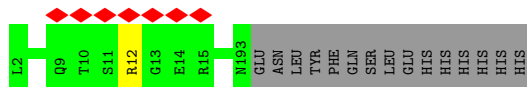
- Molecule 3: ATP-dependent Clp protease proteolytic subunit

Chain u:  93% 7%



- Molecule 3: ATP-dependent Clp protease proteolytic subunit

Chain v:  92% 7%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	449424	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 ($e^-/\text{\AA}^2$)	51.94	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.736	Depositor
Minimum map value	-0.286	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.024	Depositor
Recommended contour level	0.0702	Depositor
Map size (\AA)	287.872, 287.872, 287.872	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.1245, 1.1245, 1.1245	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: ATP, MG, MTX, ADP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.27	0/2734	0.50	1/3697 (0.0%)
1	B	0.28	0/2728	0.51	0/3689
1	C	0.28	0/2728	0.50	0/3689
1	D	0.28	0/2728	0.49	0/3689
1	E	0.27	0/2646	0.51	0/3575
1	F	0.28	0/2633	0.53	1/3556 (0.0%)
2	S	0.26	0/1455	0.53	0/1980
3	h	0.31	0/1527	0.50	0/2058
3	i	0.30	0/1527	0.50	0/2058
3	j	0.31	0/1527	0.50	0/2058
3	k	0.32	0/1527	0.50	0/2058
3	l	0.32	0/1527	0.51	0/2058
3	m	0.31	0/1527	0.50	0/2058
3	n	0.32	0/1527	0.50	0/2058
3	p	0.26	0/1527	0.48	0/2058
3	q	0.25	0/1527	0.48	0/2058
3	r	0.25	0/1527	0.47	0/2058
3	s	0.26	0/1527	0.48	0/2058
3	t	0.26	0/1527	0.48	0/2058
3	u	0.25	0/1527	0.47	0/2058
3	v	0.26	0/1527	0.48	0/2058
All	All	0.28	0/39030	0.50	2/52687 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	392	ASP	CB-CG-OD1	6.98	124.58	118.30
1	A	236	LEU	CA-CB-CG	5.76	128.54	115.30

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	2754	2753	20	0
1	B	2692	2748	2748	14	0
1	C	2692	2748	2748	8	0
1	D	2692	2749	2749	13	0
1	E	2612	2674	2674	17	0
1	F	2599	2659	2659	21	0
2	S	1416	1369	1369	9	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	1	0
4	B	31	12	12	1	0
4	C	31	12	12	1	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	3	0
6	E	27	12	12	2	0
6	F	27	12	12	0	0
7	S	33	20	20	0	0
All	All	38654	38975	38974	96	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 3.

The worst 5 of 96 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:E:166:LEU:HD22	1:E:222:VAL:HG11	1.54	0.89
1:D:162:ILE:HG21	1:D:238:VAL:HG21	1.65	0.79
1:A:173:VAL:HG12	1:A:222:VAL:HG21	1.65	0.78
1:F:167:GLN:OE1	1:F:225:GLN:NE2	2.25	0.70
1:D:228:ARG:NH2	1:E:234:GLU:OE2	2.27	0.68

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	351/388 (90%)	348 (99%)	3 (1%)	0	100	100
1	B	350/388 (90%)	348 (99%)	2 (1%)	0	100	100
1	C	350/388 (90%)	348 (99%)	2 (1%)	0	100	100
1	D	350/388 (90%)	345 (99%)	5 (1%)	0	100	100
1	E	337/388 (87%)	332 (98%)	5 (2%)	0	100	100
1	F	335/388 (86%)	331 (99%)	4 (1%)	0	100	100
2	S	176/208 (85%)	176 (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%)	188 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	m	190/207 (92%)	189 (100%)	1 (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
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	4909/5434 (90%)	4885 (100%)	24 (0%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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%)	290 (100%)	1 (0%)	91	97
1	D	291/322 (90%)	291 (100%)	0	100	100
1	E	281/322 (87%)	281 (100%)	0	100	100
1	F	280/322 (87%)	279 (100%)	1 (0%)	89	96
2	S	153/180 (85%)	152 (99%)	1 (1%)	81	94
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	m	163/178 (92%)	163 (100%)	0	100	100
3	n	163/178 (92%)	162 (99%)	1 (1%)	84	95
3	p	163/178 (92%)	162 (99%)	1 (1%)	84	95
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	95
All	All	4161/4604 (90%)	4155 (100%)	6 (0%)	92	98

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	n	12	ARG
3	p	12	ARG
3	v	12	ARG
1	F	373	ARG
1	C	228	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	230	HIS
3	l	34	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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
4	ATP	A	500	5	28,33,33	0.90	0	34,52,52	1.20	2 (5%)
7	MTX	S	301	-	35,35,35	1.23	3 (8%)	47,49,49	1.65	8 (17%)
6	ADP	D	500	5	24,29,29	0.85	0	29,45,45	1.24	2 (6%)
4	ATP	C	500	5	28,33,33	0.89	0	34,52,52	1.28	3 (8%)
6	ADP	F	500	-	24,29,29	0.91	0	29,45,45	1.27	2 (6%)
6	ADP	E	500	-	24,29,29	0.86	0	29,45,45	1.29	2 (6%)
4	ATP	B	500	5	28,33,33	0.90	0	34,52,52	1.24	3 (8%)

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	A	500	5	-	2/18/38/38	0/3/3/3
7	MTX	S	301	-	-	5/25/25/25	0/3/3/3
6	ADP	D	500	5	-	2/12/32/32	0/3/3/3
4	ATP	C	500	5	-	2/18/38/38	0/3/3/3
6	ADP	F	500	-	-	2/12/32/32	0/3/3/3
6	ADP	E	500	-	-	2/12/32/32	0/3/3/3
4	ATP	B	500	5	-	4/18/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	S	301	MTX	C7-N8	3.82	1.38	1.31
7	S	301	MTX	C6-N5	3.42	1.38	1.32
7	S	301	MTX	C4-N3	2.52	1.38	1.33

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	S	301	MTX	N1-C2-N3	-5.50	120.22	127.21
6	E	500	ADP	N3-C2-N1	-4.35	122.76	128.67
6	F	500	ADP	N3-C2-N1	-4.25	122.91	128.67
7	S	301	MTX	C2-N1-C8A	4.18	119.99	115.48
4	A	500	ATP	N3-C2-N1	-4.08	123.13	128.67

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

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

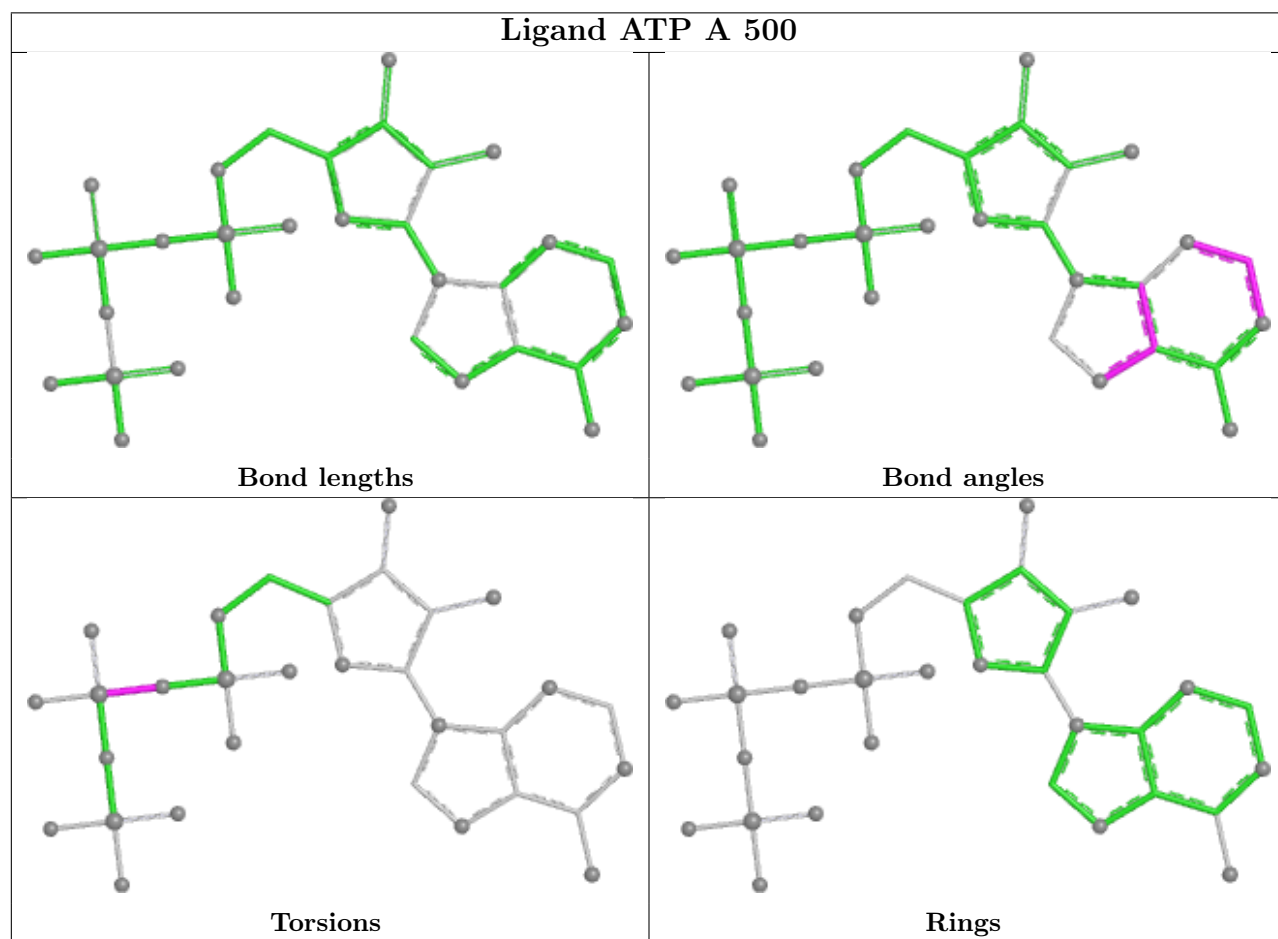
There are no ring outliers.

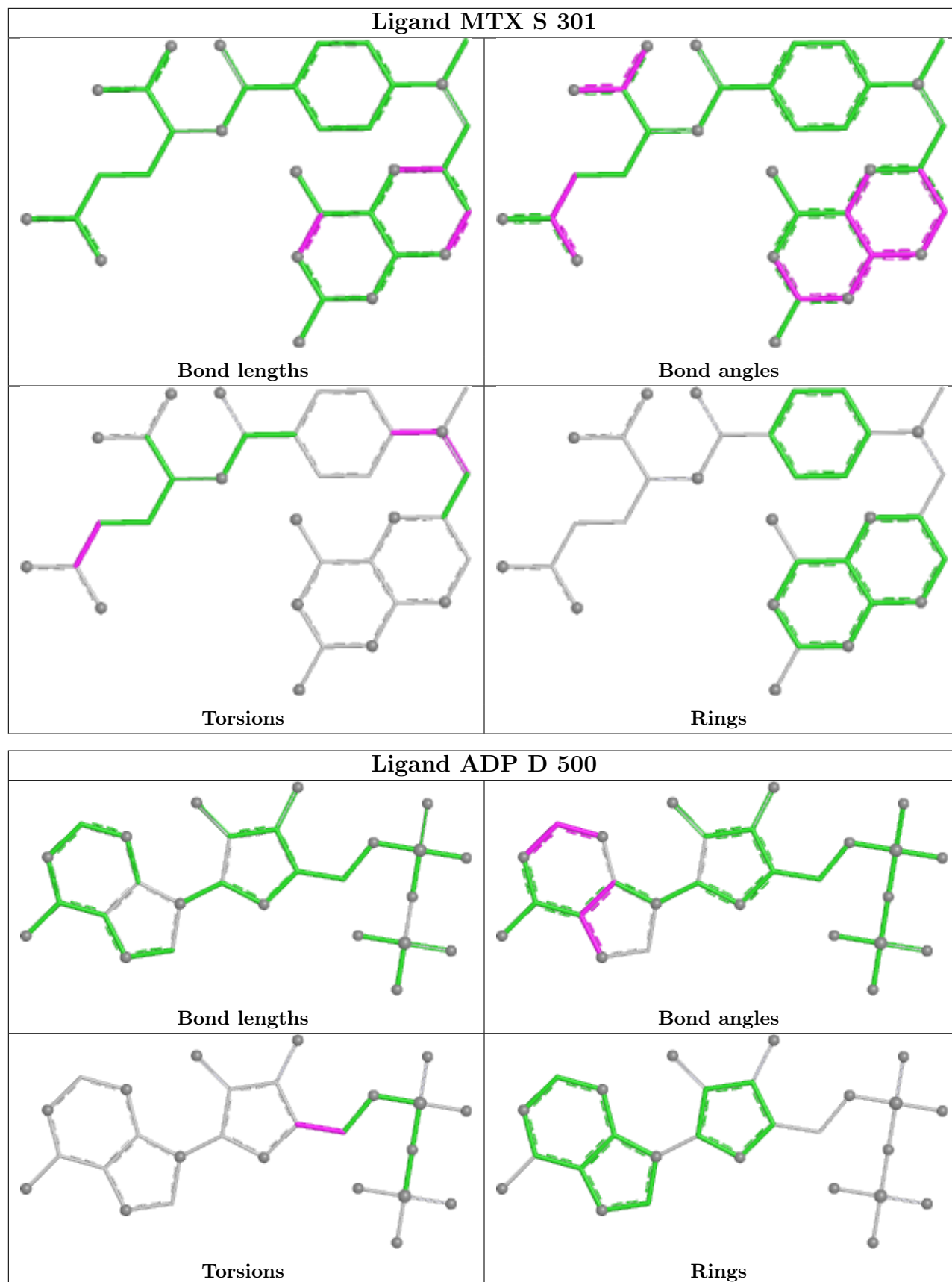
5 monomers are involved in 8 short contacts:

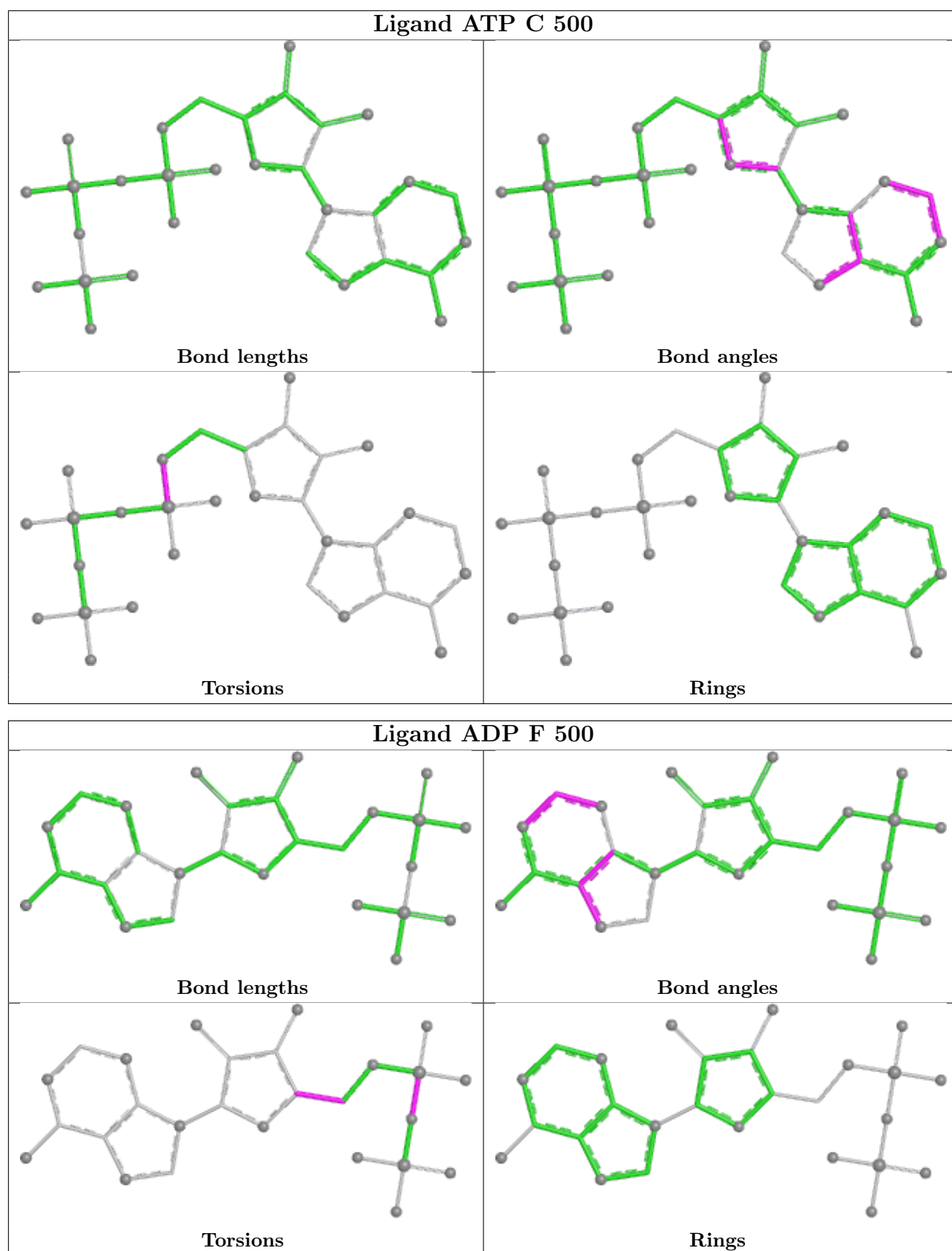
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	500	ATP	1	0
6	D	500	ADP	3	0
4	C	500	ATP	1	0
6	E	500	ADP	2	0
4	B	500	ATP	1	0

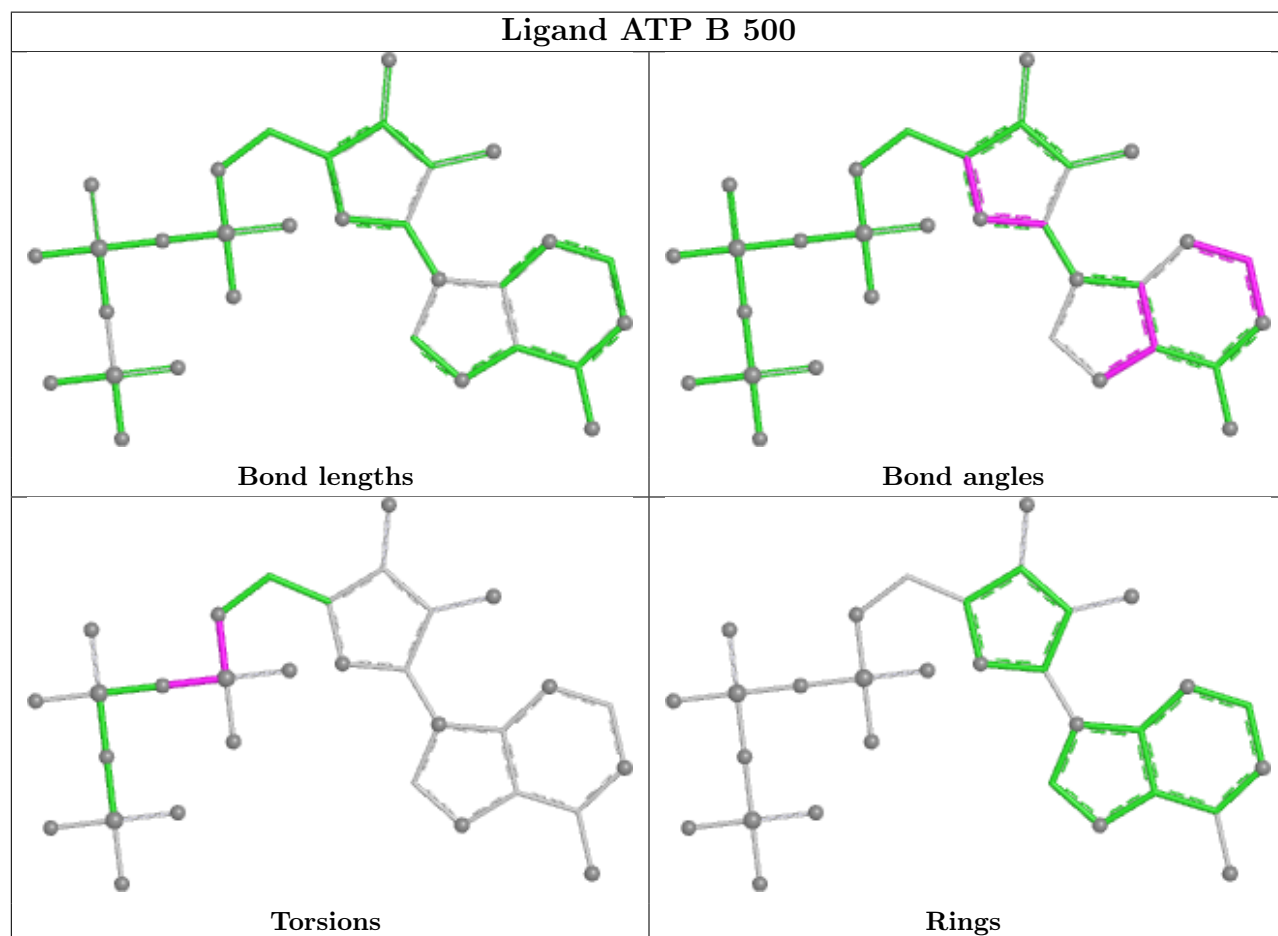
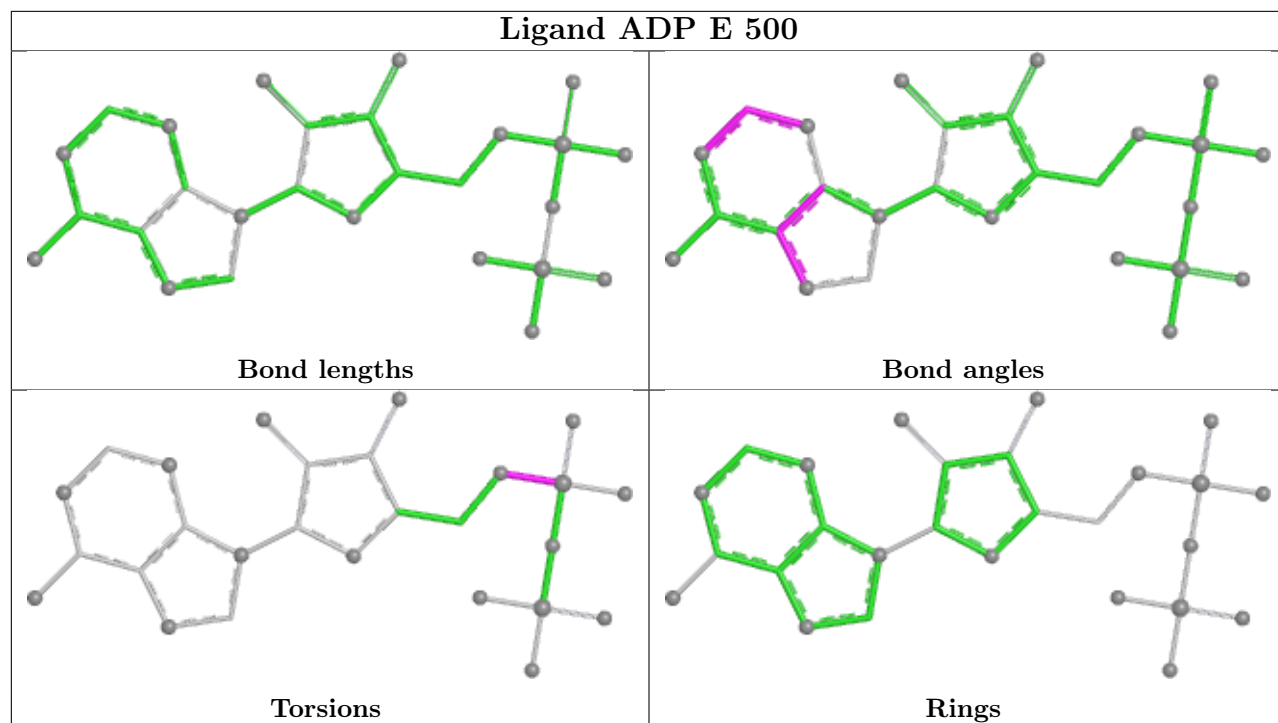
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

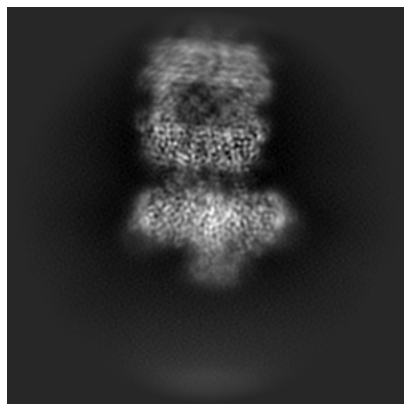
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-43081. These allow visual inspection of the internal detail of the map and identification of artifacts.

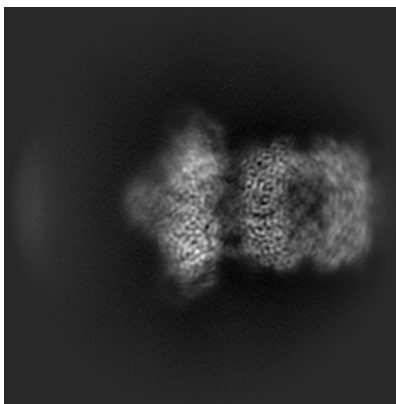
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

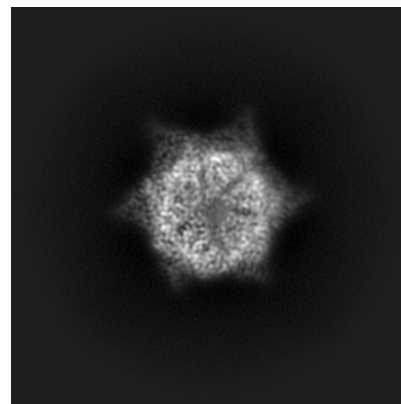
6.1.1 Primary map



X

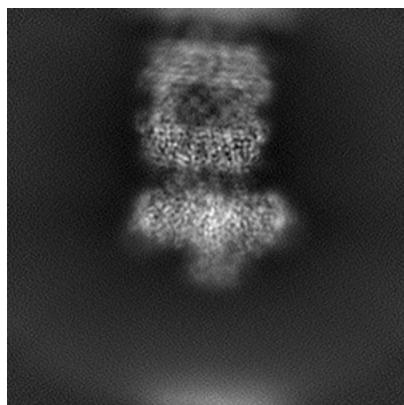


Y

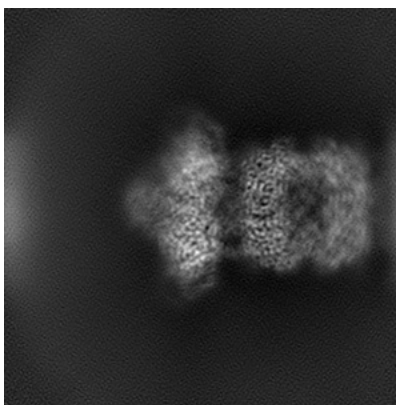


Z

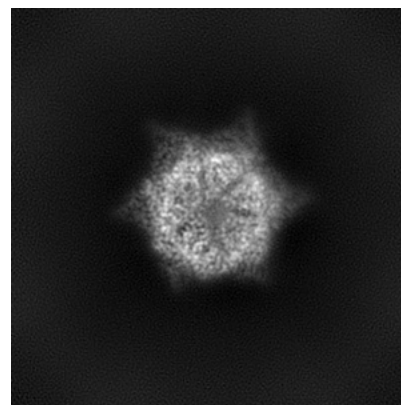
6.1.2 Raw map



X



Y

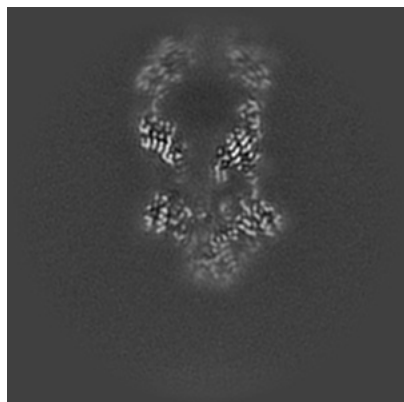


Z

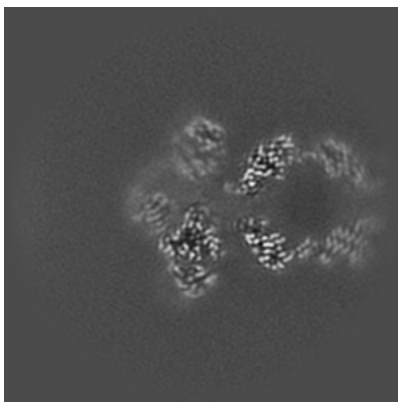
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

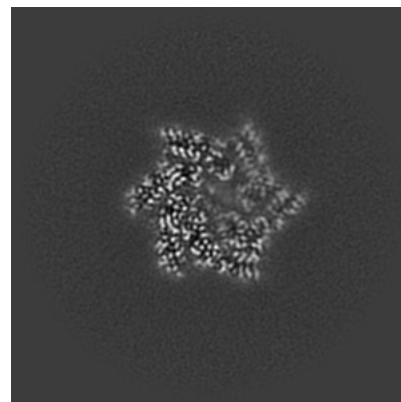
6.2.1 Primary map



X Index: 128

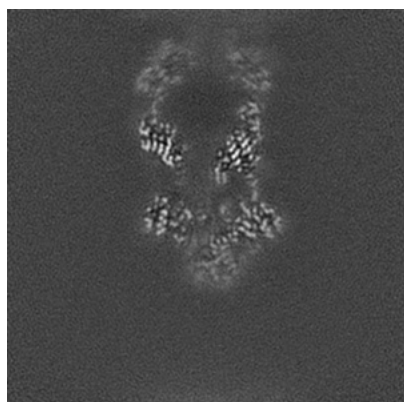


Y Index: 128

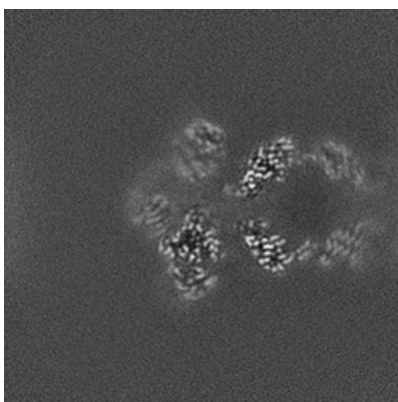


Z Index: 128

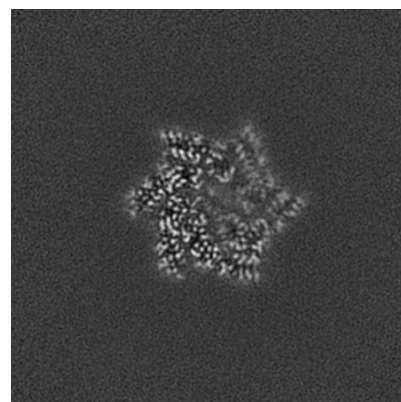
6.2.2 Raw map



X Index: 128



Y Index: 128

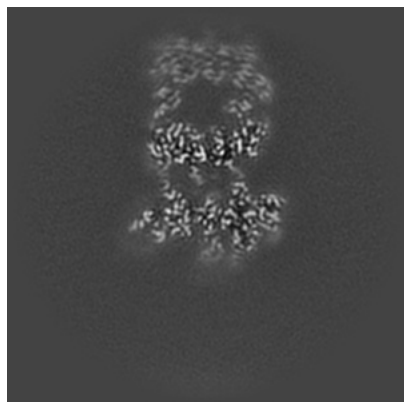


Z Index: 128

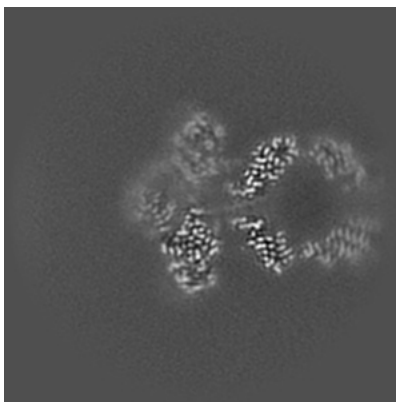
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

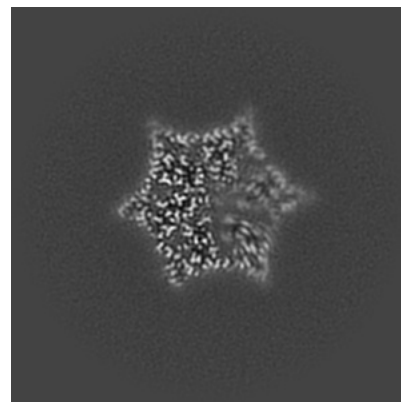
6.3.1 Primary map



X Index: 112

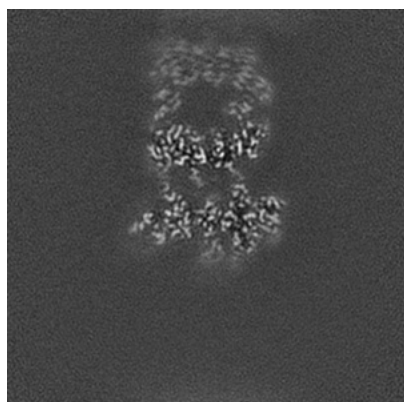


Y Index: 130

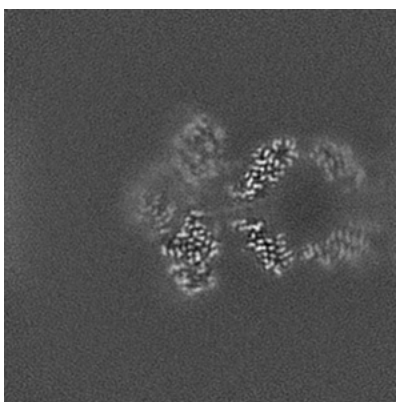


Z Index: 119

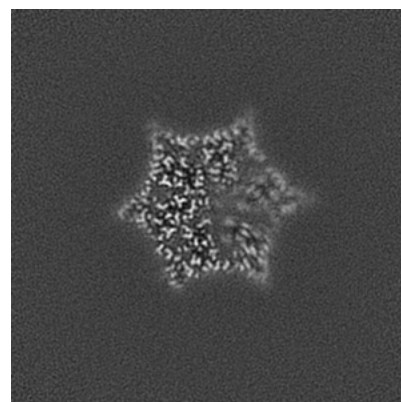
6.3.2 Raw map



X Index: 112



Y Index: 130

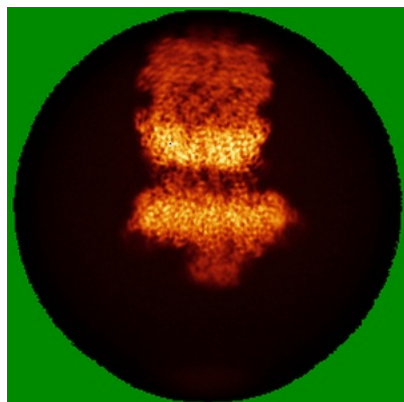


Z Index: 119

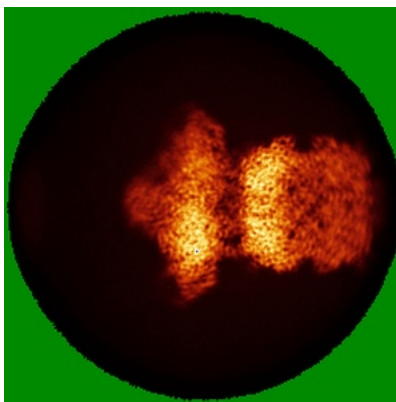
The images above show the largest variance slices of the map in three orthogonal directions.

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

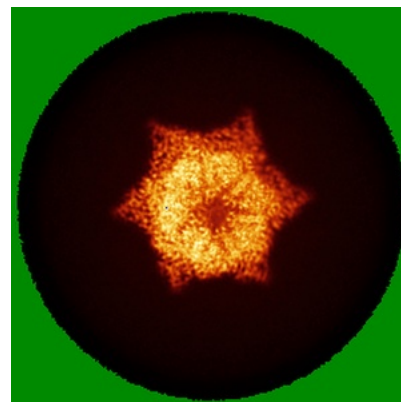
6.4.1 Primary map



X

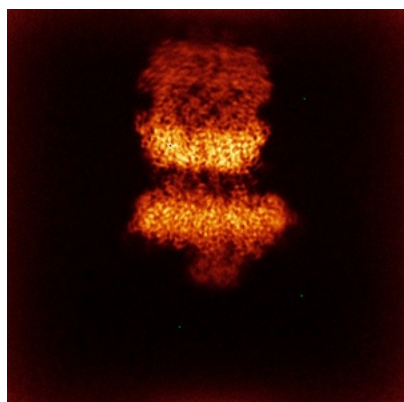


Y

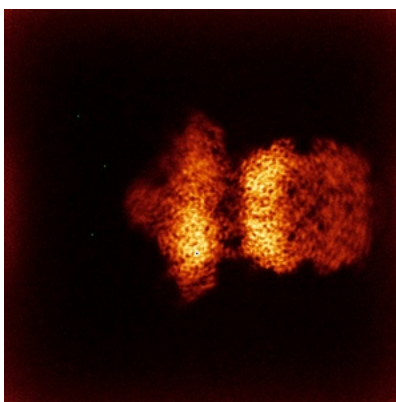


Z

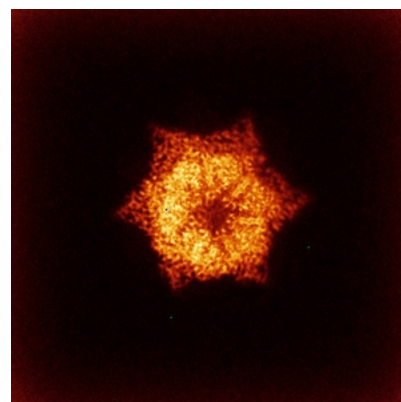
6.4.2 Raw map



X



Y

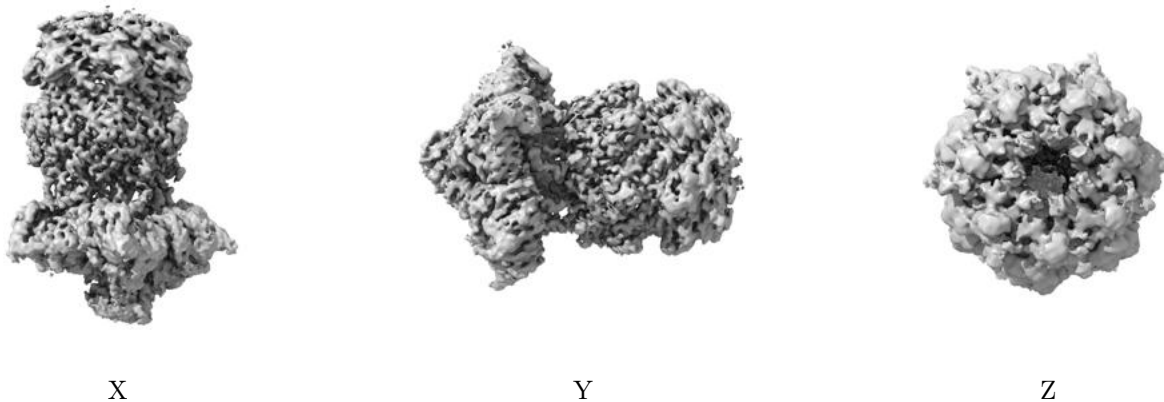


Z

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.

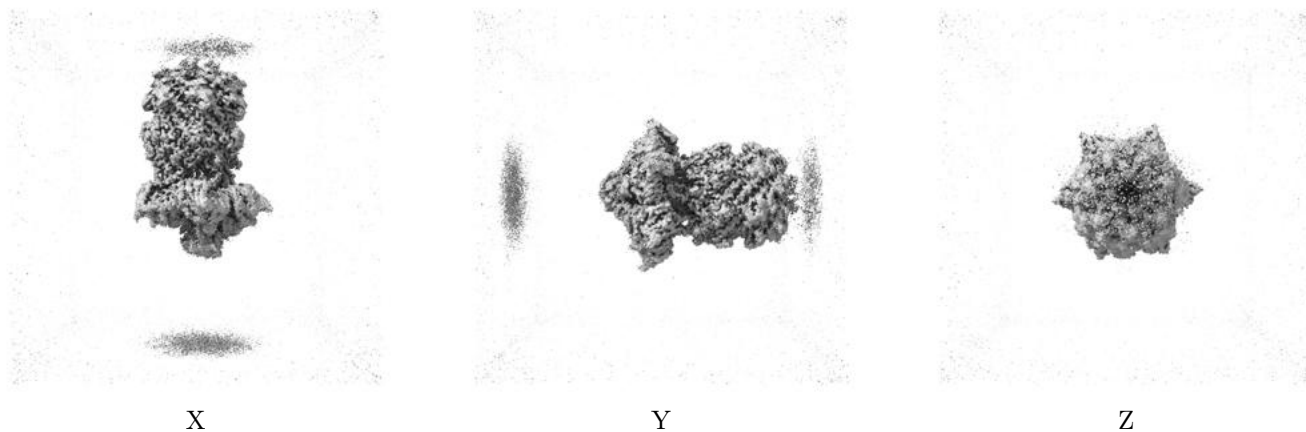
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0702. 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.

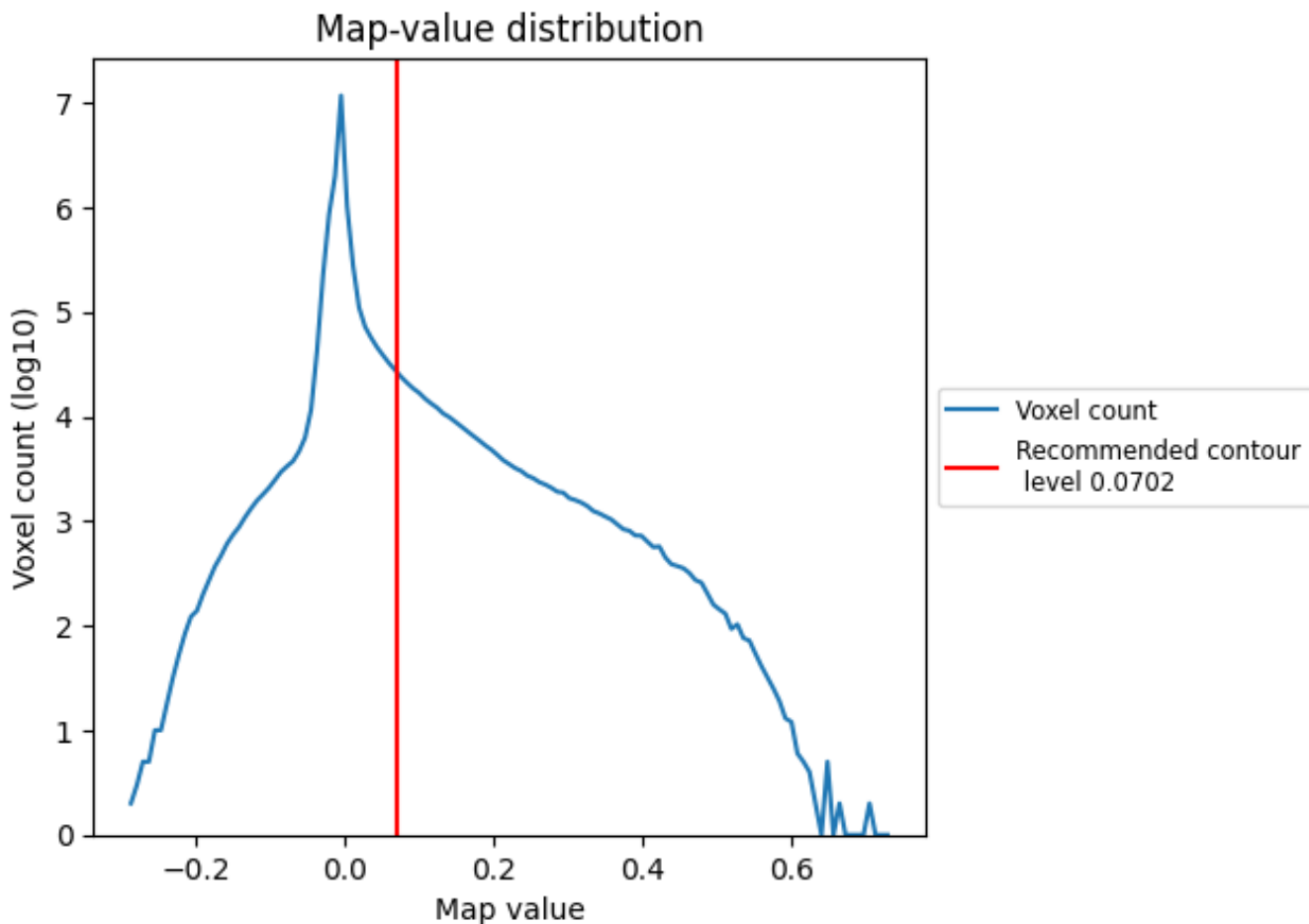
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

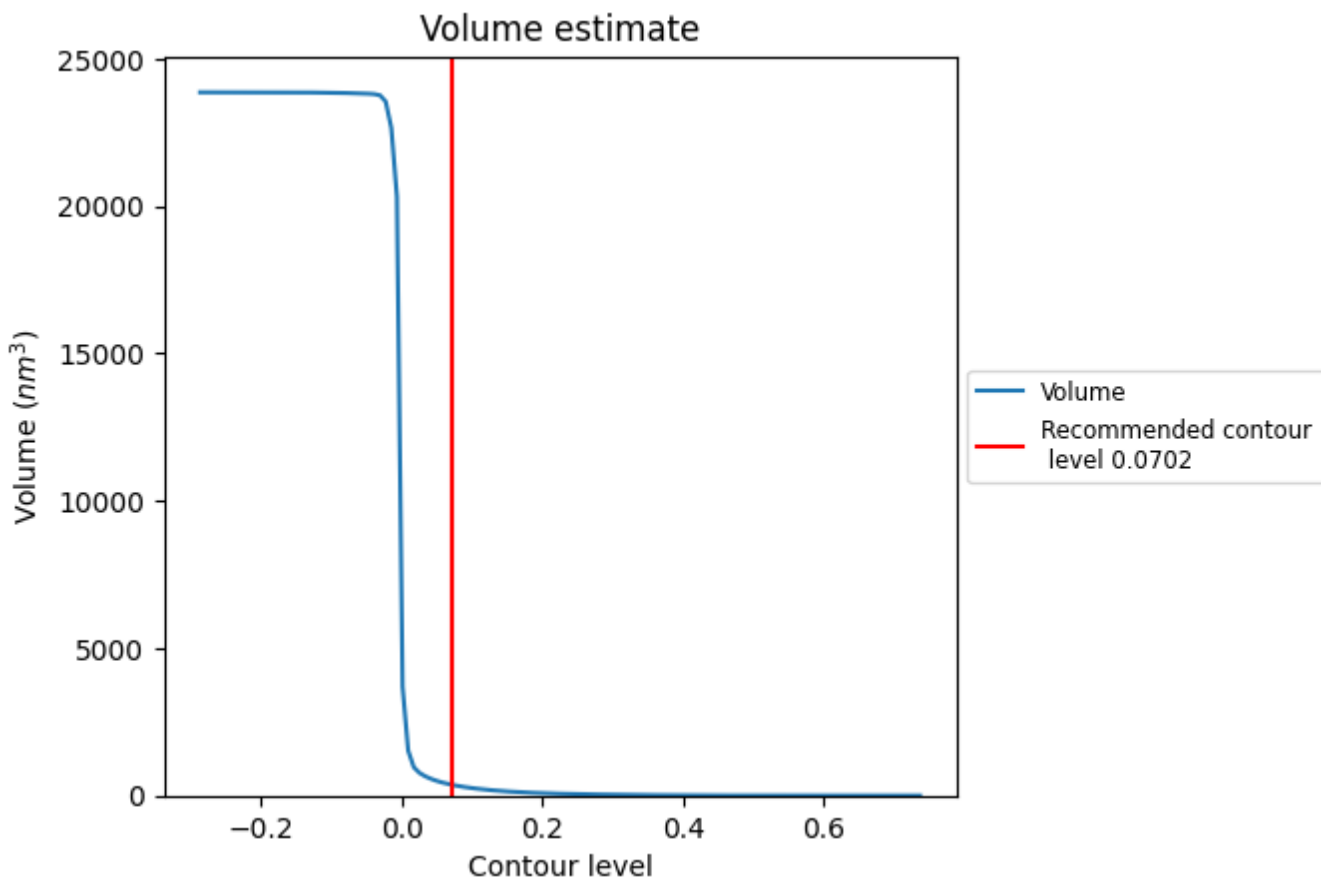
This section contains the results of statistical analysis of the map.

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.

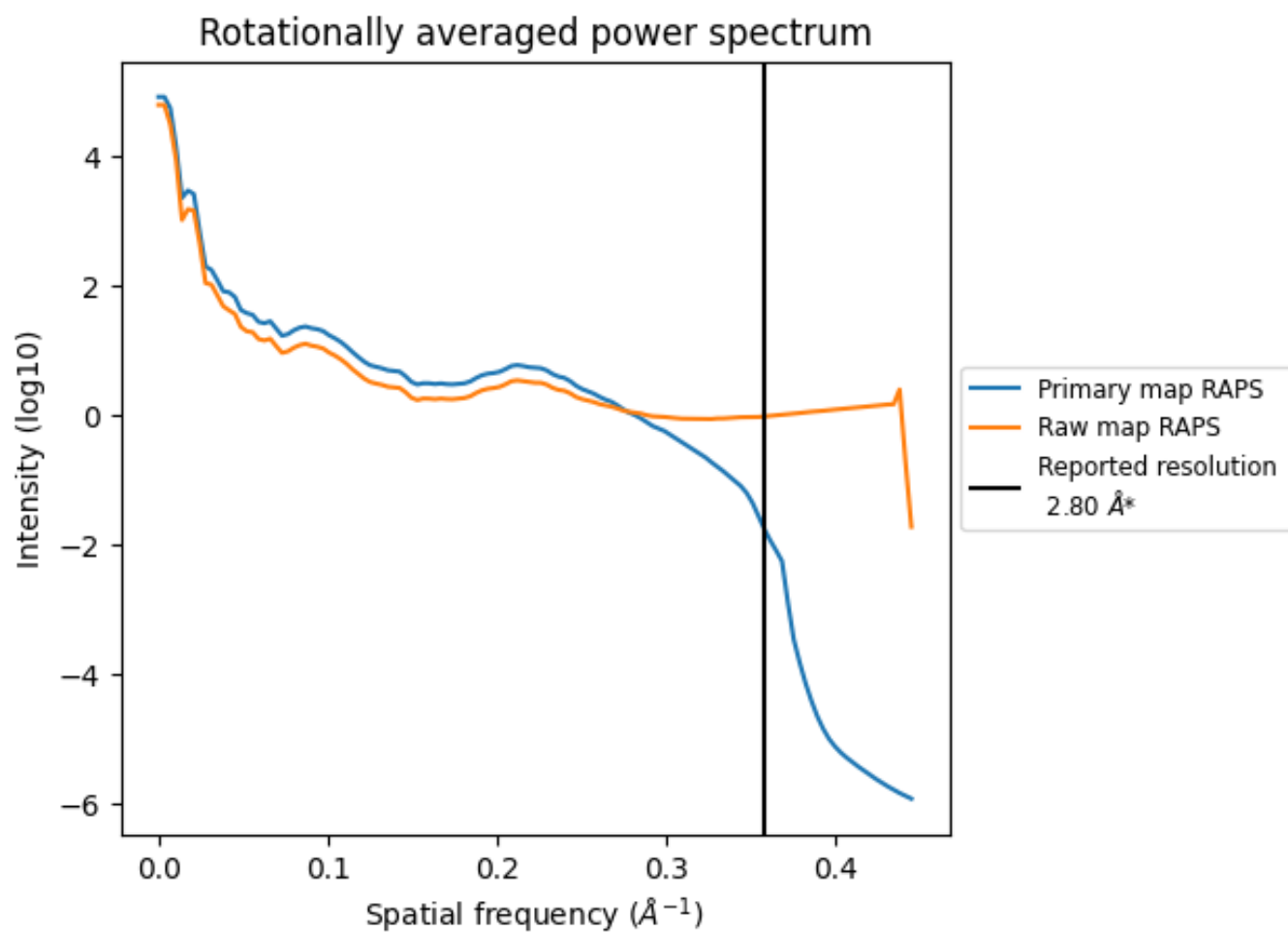
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 372 nm³; this corresponds to an approximate mass of 336 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

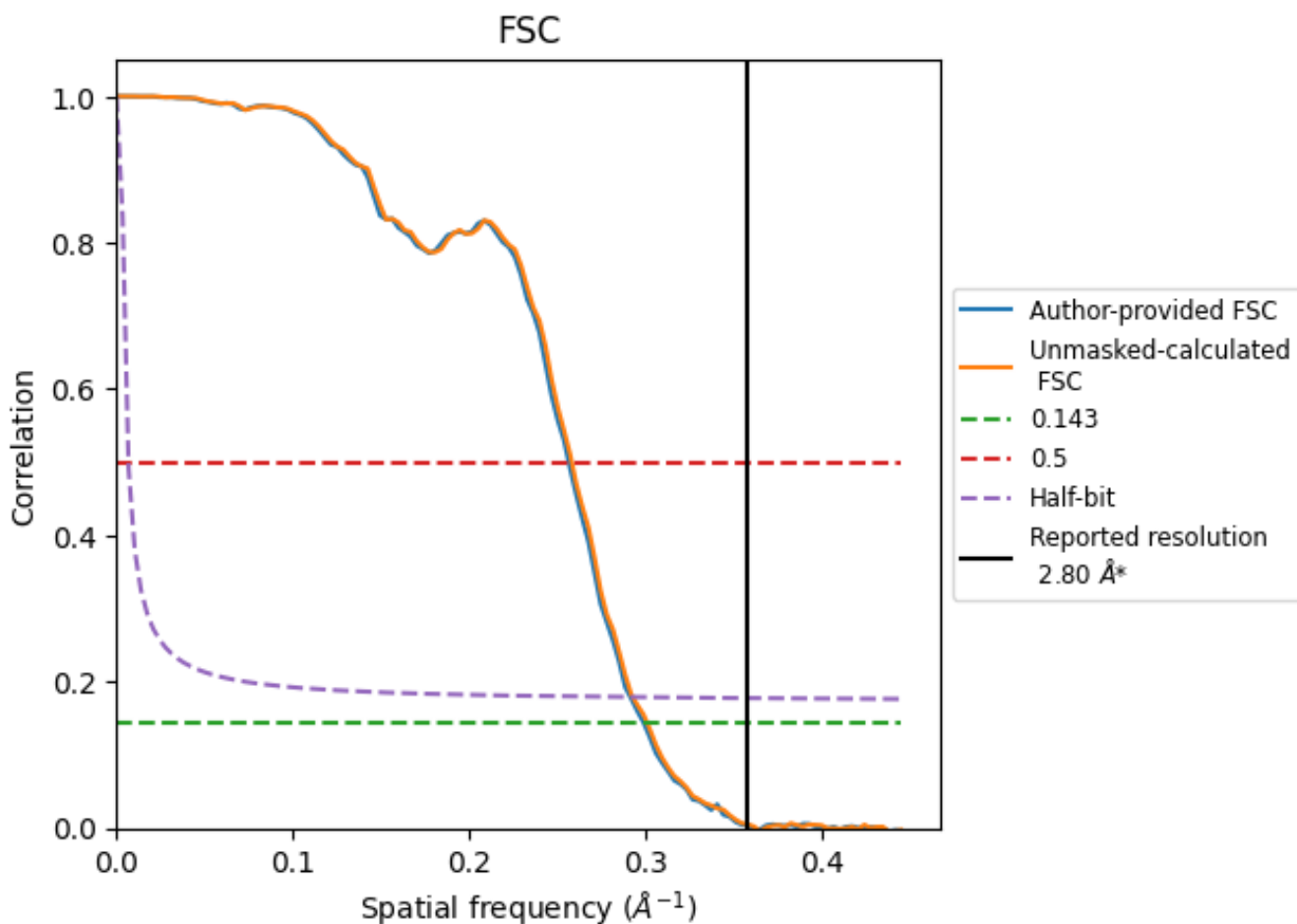


*Reported resolution corresponds to spatial frequency of 0.357 Å⁻¹

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 0.357 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	3.35	3.90	3.43
Unmasked-calculated*	3.32	3.88	3.42

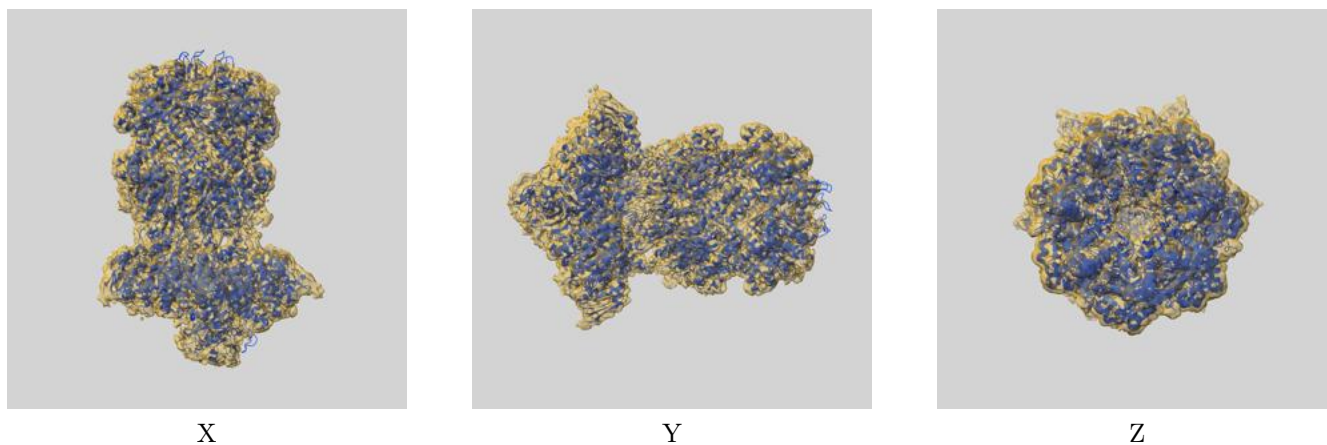
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 3.35 differs from the reported value 2.8 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.32 differs from the reported value 2.8 by more than 10 %

9 Map-model fit [i](#)

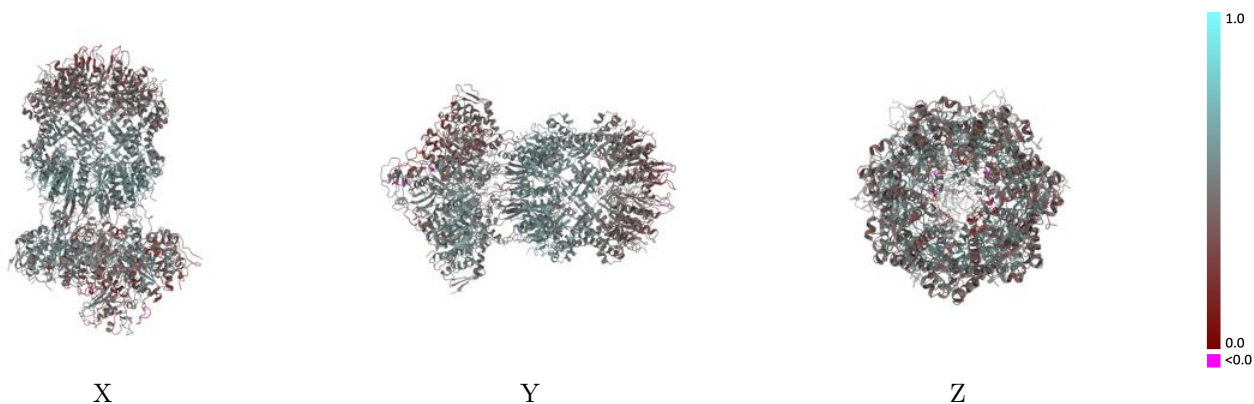
This section contains information regarding the fit between EMDB map EMD-43081 and PDB model 8V9R. Per-residue inclusion information can be found in section 3 on page 18.

9.1 Map-model overlay [i](#)



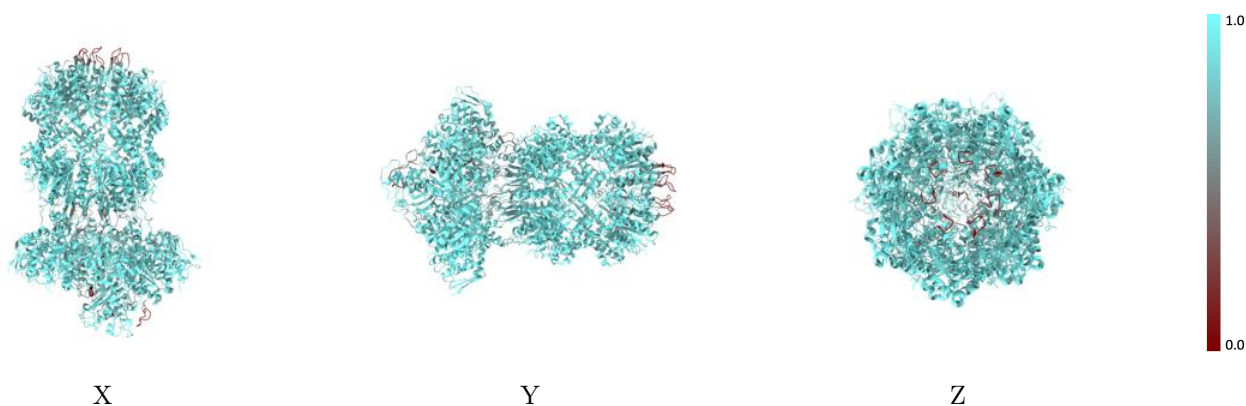
The images above show the 3D surface view of the map at the recommended contour level 0.0702 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



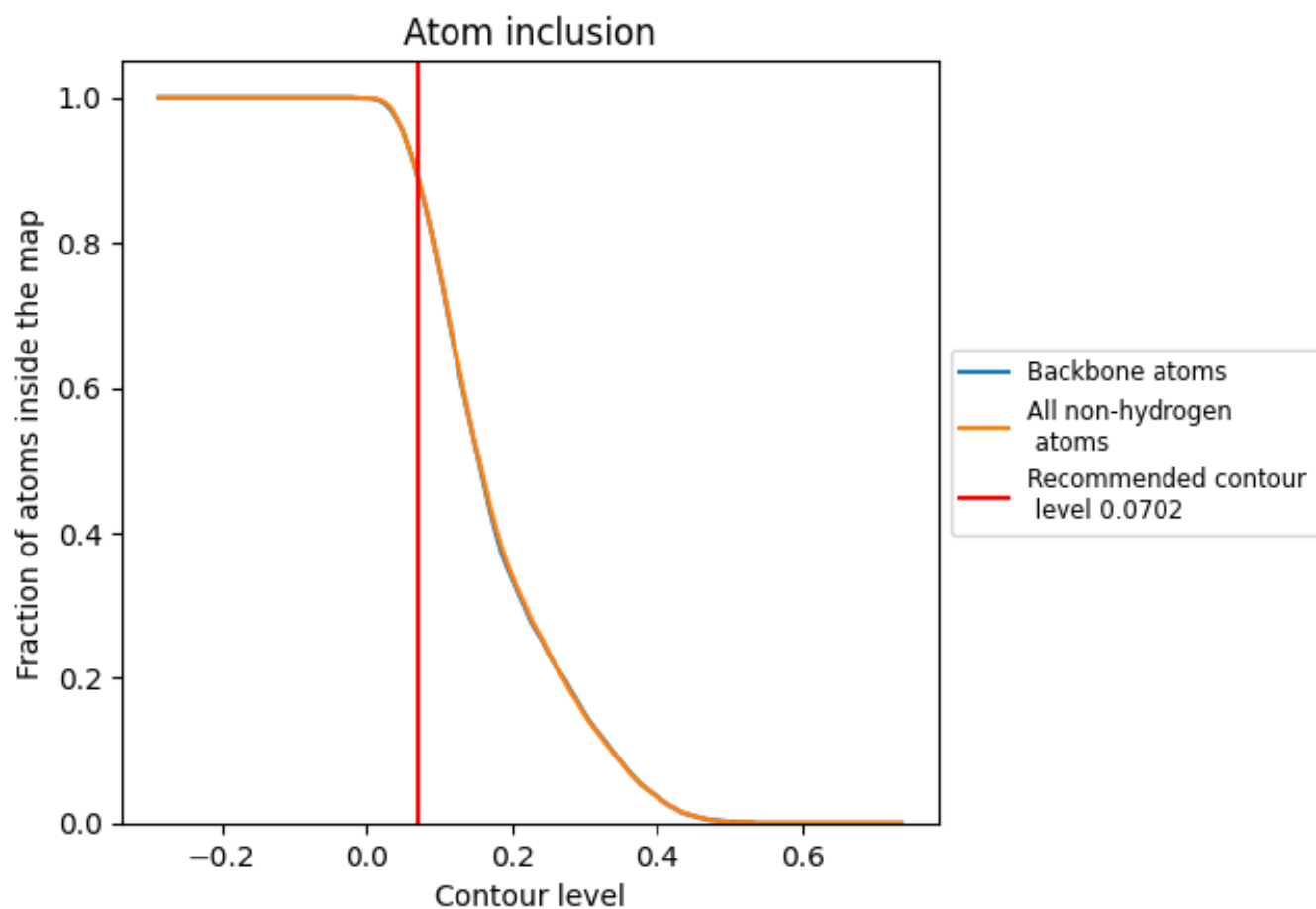
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0702).













































9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 89% 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 (0.0702) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8900	 0.4750
A	 0.8700	 0.4570
B	 0.9280	 0.5040
C	 0.9320	 0.5160
D	 0.9200	 0.5100
E	 0.8480	 0.4250
F	 0.8170	 0.3530
S	 0.8660	 0.4530
h	 0.9550	 0.5480
i	 0.9460	 0.5390
j	 0.9490	 0.5460
k	 0.9530	 0.5550
l	 0.9460	 0.5510
m	 0.9500	 0.5470
n	 0.9550	 0.5490
p	 0.8460	 0.4250
q	 0.8500	 0.4220
r	 0.8450	 0.4200
s	 0.8430	 0.4230
t	 0.8490	 0.4220
u	 0.8600	 0.4360
v	 0.8570	 0.4320

