Full wwPDB EM Validation Report ⓘ

Feb 25, 2024 – 06:09 PM EST

PDB ID	:	6WSG
EMDB ID	:	EMD-21892
Title	:	ClpX-ClpP complex bound to ssrA-tagged GFP, intermediate complex
Authors	:	Fei, X.; Sauer, R.T.
Deposited on	:	2020-04-30
Resolution	:	3.16 Å(reported)
Based on initial model	:	6POD

This is a Full wwPDB EM Validation 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:

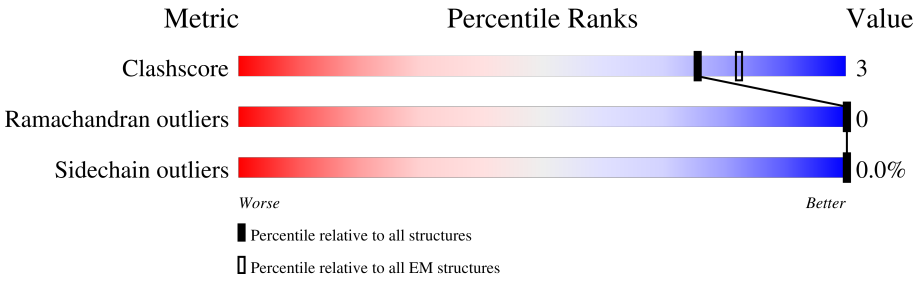
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.16 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=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 <=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	74% · 22%
1	B	388	78% 8% 14%
1	C	388	84% · 13%
1	D	388	81% 6% 13%
1	E	388	80% 7% 12%
1	F	388	78% 7% 15%
2	H	207	53% 86% 7% 7%
2	I	207	44% 85% 8% 7%

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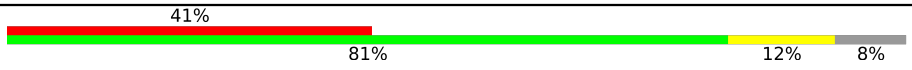
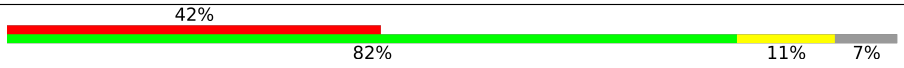
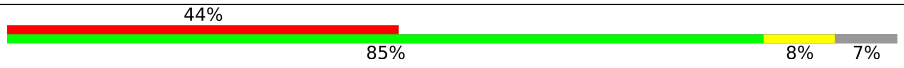
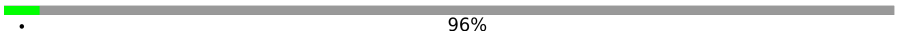
Mol	Chain	Length	Quality of chain
2	J	207	
2	K	207	
2	L	207	
2	M	207	
2	N	207	
3	S	274	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 52147 atoms, of which 26215 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	301	Total	C	H	N	O	S	0	0
			4718	1478	2397	388	450	5		
1	B	334	Total	C	H	N	O	S	0	0
			5175	1623	2618	428	501	5		
1	C	338	Total	C	H	N	O	S	0	0
			5243	1644	2652	433	509	5		
1	D	338	Total	C	H	N	O	S	0	0
			5235	1642	2648	432	508	5		
1	E	341	Total	C	H	N	O	S	0	0
			5224	1654	2614	437	514	5		
1	F	331	Total	C	H	N	O	S	0	0
			5131	1610	2595	424	497	5		

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 ATP-dependent Clp protease proteolytic subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	L	192	Total	C	H	N	O	S	0	0
			3016	947	1513	261	283	12		
2	K	192	Total	C	H	N	O	S	0	0
			3016	947	1513	261	283	12		
2	J	191	Total	C	H	N	O	S	0	0
			3002	943	1507	259	281	12		
2	I	192	Total	C	H	N	O	S	0	0
			3016	947	1513	261	283	12		
2	H	192	Total	C	H	N	O	S	0	0
			3016	947	1513	261	283	12		
2	N	191	Total	C	H	N	O	S	0	0
			3002	943	1507	259	281	12		
2	M	191	Total	C	H	N	O	S	0	0
			3002	943	1507	259	281	12		

There are 105 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	194	GLU	-	expression tag	UNP P0A6G7
L	195	ASN	-	expression tag	UNP P0A6G7

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
J	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
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
H	207	HIS	-	expression tag	UNP P0A6G7
H	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

- Molecule 3 is a protein called Green fluorescent protein, + ssrA tag.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	S	10	Total	C	H	N	O	0	0
			125	40	58	11	16		

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	6	MET	-	expression tag	UNP P42212
S	7	GLY	-	expression tag	UNP P42212
S	8	SER	-	expression tag	UNP P42212
S	9	SER	-	expression tag	UNP P42212
S	10	HIS	-	expression tag	UNP P42212
S	11	HIS	-	expression tag	UNP P42212
S	12	HIS	-	expression tag	UNP P42212
S	13	HIS	-	expression tag	UNP P42212
S	14	HIS	-	expression tag	UNP P42212
S	15	HIS	-	expression tag	UNP P42212
S	16	ASP	-	expression tag	UNP P42212
S	17	TYR	-	expression tag	UNP P42212
S	18	ASP	-	expression tag	UNP P42212

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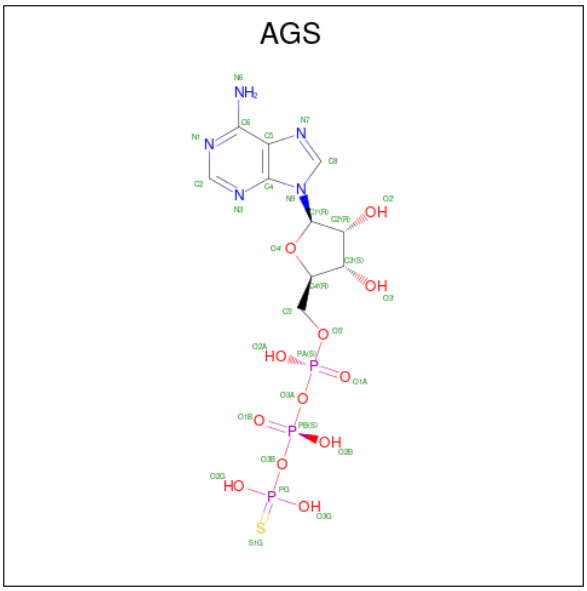
Chain	Residue	Modelled	Actual	Comment	Reference
S	19	ILE	-	expression tag	UNP P42212
S	20	PRO	-	expression tag	UNP P42212
S	21	THR	-	expression tag	UNP P42212
S	22	THR	-	expression tag	UNP P42212
S	23	GLU	-	expression tag	UNP P42212
S	24	ASN	-	expression tag	UNP P42212
S	25	LEU	-	expression tag	UNP P42212
S	26	TYR	-	expression tag	UNP P42212
S	27	PHE	-	expression tag	UNP P42212
S	28	GLN	-	expression tag	UNP P42212
S	29	GLY	-	expression tag	UNP P42212
S	30	SER	-	expression tag	UNP P42212
S	31	ARG	-	expression tag	UNP P42212
S	94	GLY	SER	conflict	UNP P42212
S	101	ALA	SER	conflict	UNP P42212

- Molecule 4 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: $C_{10}H_{16}N_5O_{12}P_3S$).



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

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Mol	Chain	Residues	Atoms							AltConf
4	E	1	Total	C	H	N	O	P	S	0
			43	10	12	5	12	3	1	
4	F	1	Total	C	H	N	O	P	S	0
			43	10	12	5	12	3	1	

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

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

- Molecule 6 is water.

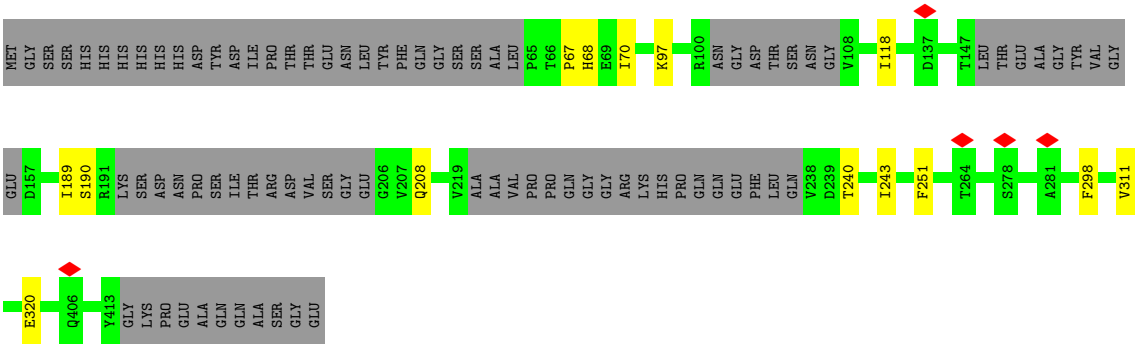
Mol	Chain	Residues	Atoms		AltConf
6	L	1	Total	O	0
			1	1	
6	K	1	Total	O	0
			1	1	
6	J	1	Total	O	0
			1	1	
6	I	1	Total	O	0
			1	1	
6	H	1	Total	O	0
			1	1	
6	N	1	Total	O	0
			1	1	
6	M	1	Total	O	0
			1	1	

3 Residue-property plots (i)

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.

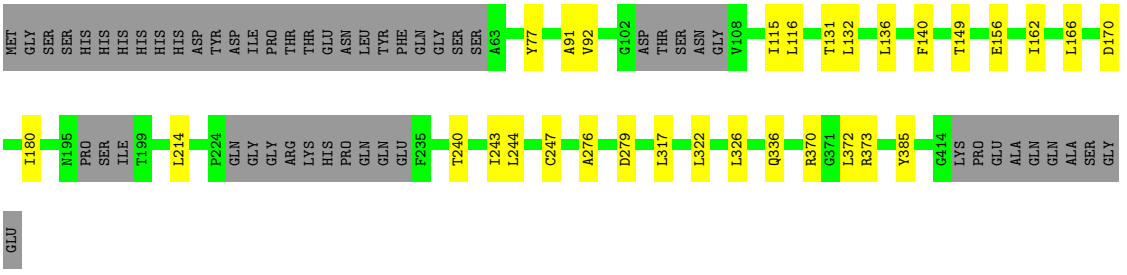
• Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpX

Chain A:



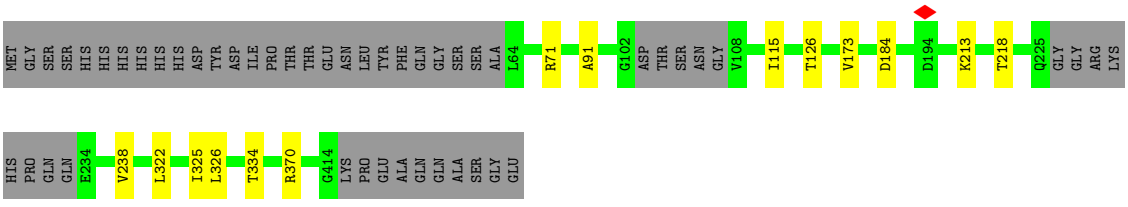
• Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpX

Chain B:



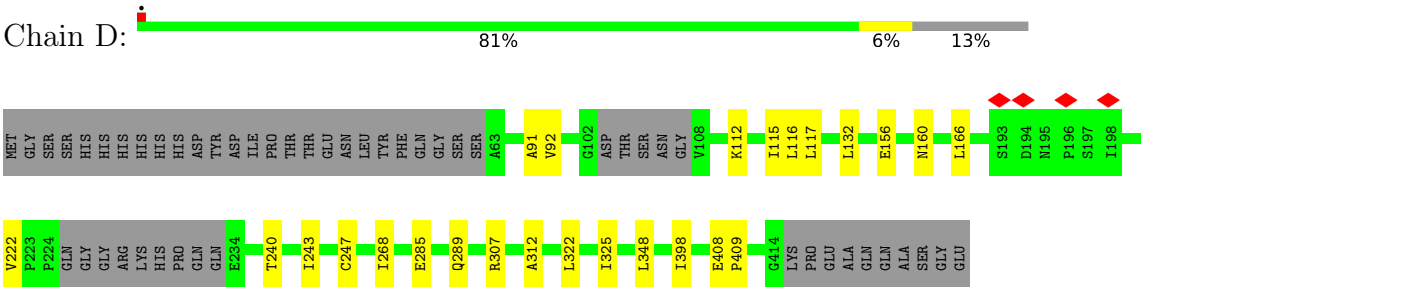
• Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpX

Chain C:



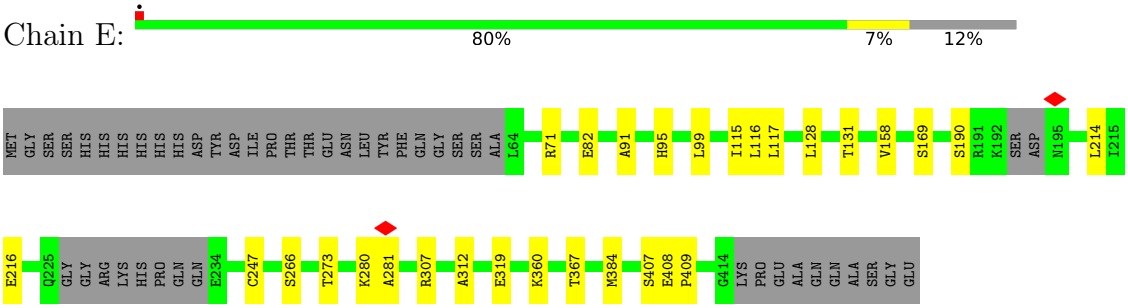
• Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpX

Chain D:



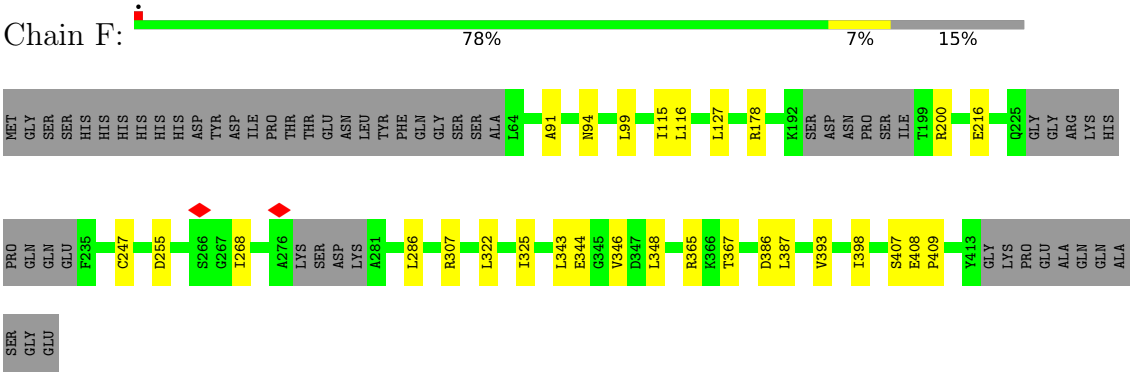
• Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpX

Chain E:



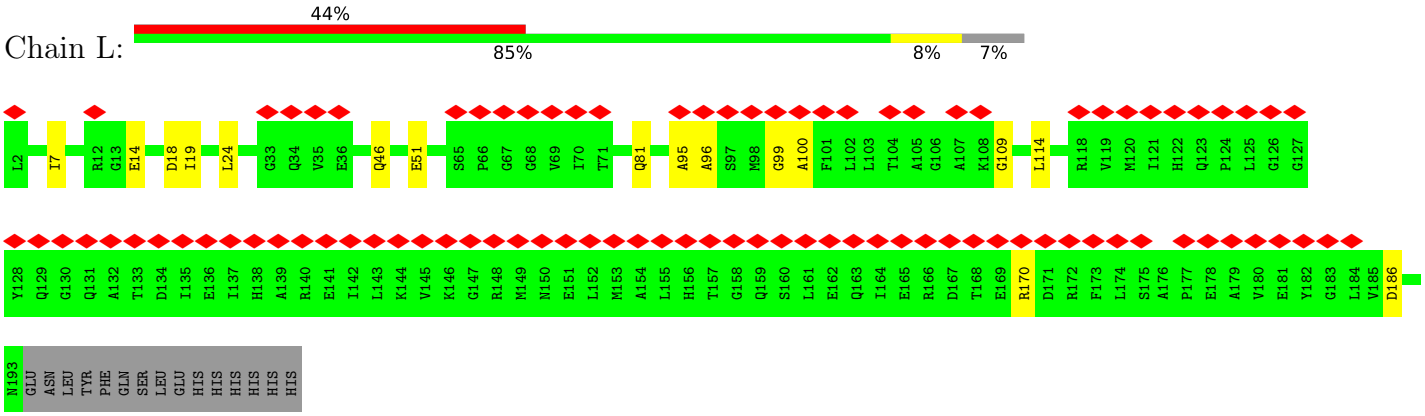
• Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpX

Chain F:



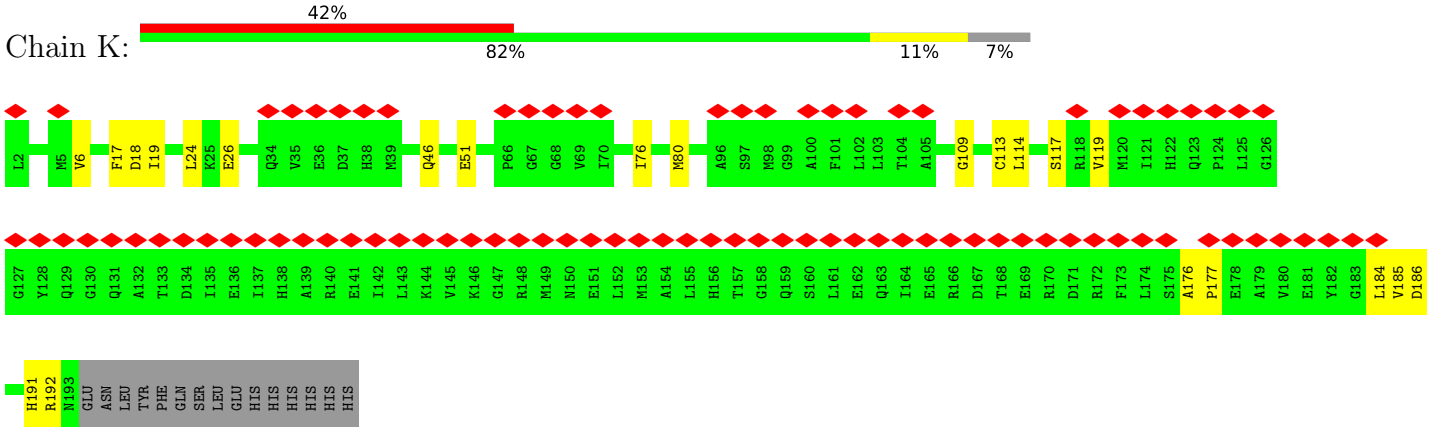
• Molecule 2: ATP-dependent Clp protease proteolytic subunit

Chain L:



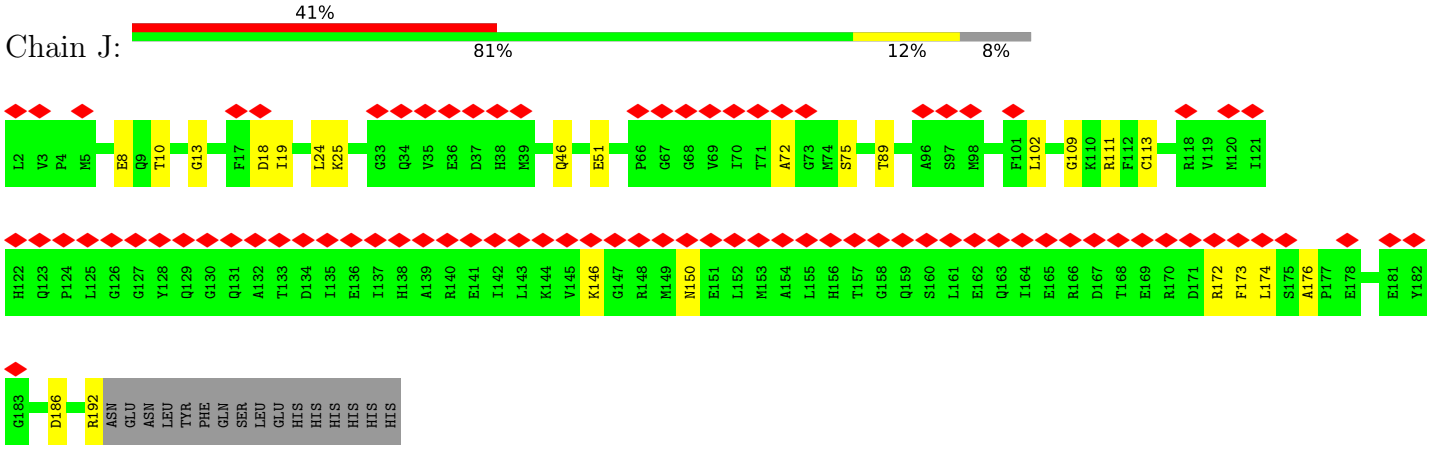
• Molecule 2: ATP-dependent Clp protease proteolytic subunit

Chain K:



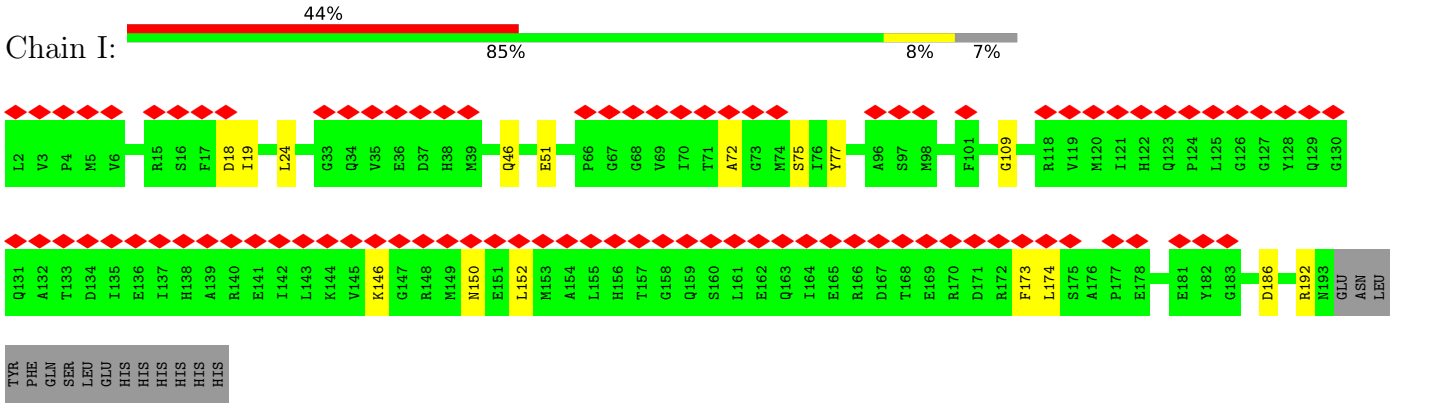
• Molecule 2: ATP-dependent Clp protease proteolytic subunit

Chain J:



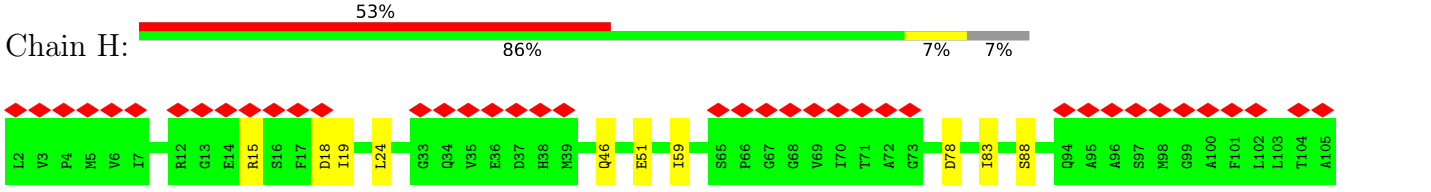
• Molecule 2: ATP-dependent Clp protease proteolytic subunit

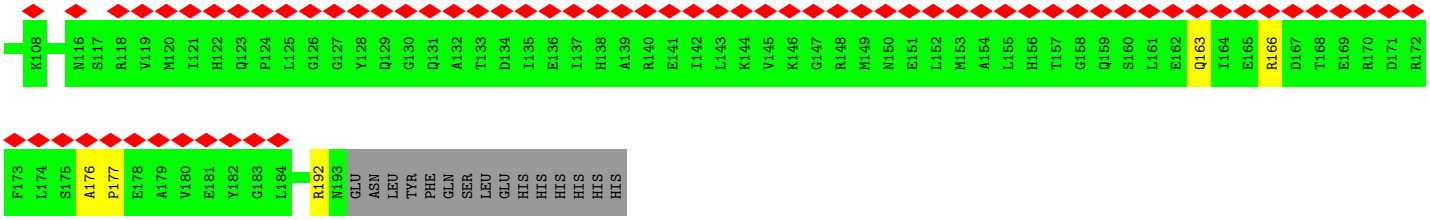
Chain I:



• Molecule 2: ATP-dependent Clp protease proteolytic subunit

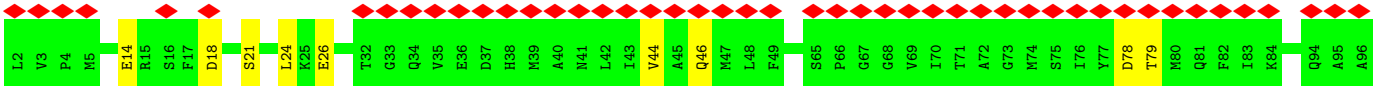
Chain H:





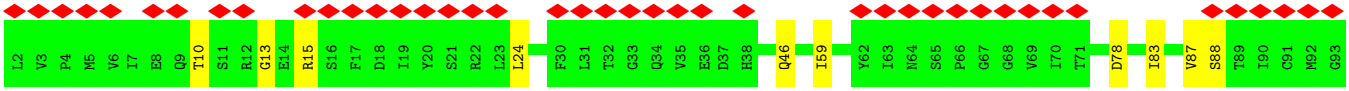
• Molecule 2: ATP-dependent Clp protease proteolytic subunit

Chain N:



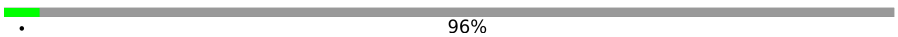
• Molecule 2: ATP-dependent Clp protease proteolytic subunit

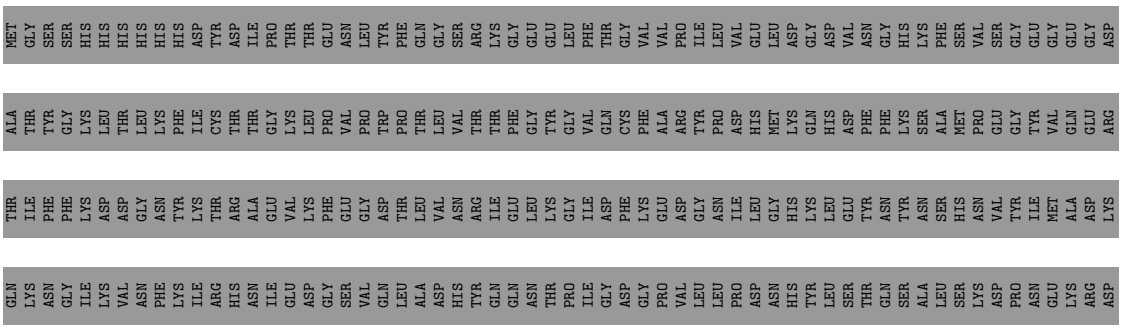
Chain M:

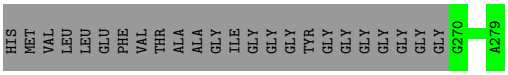


• Molecule 3: Green fluorescent protein, + ssrA tag

Chain S:






HIS
MET
VAL
LEU
LEU
GLU
PHE
VAL
THR
ALA
ALA
GLY
ILE
GLY
GLY
GLY
TYR
GLY
GLY
GLY
GLY
GLY
GLY
GLY
G270
A279

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	130240	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	54	Depositor
Minimum defocus (nm)	-800	Depositor
Maximum defocus (nm)	-2500	Depositor
Magnification	45000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	53.082	Depositor
Minimum map value	-18.793	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	5.6	Depositor
Map size (Å)	348.0, 348.0, 348.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.87, 0.87, 0.87	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.31	0/2346	0.50	0/3163
1	B	0.44	0/2587	0.58	0/3494
1	C	0.52	0/2623	0.60	1/3545 (0.0%)
1	D	0.54	0/2619	0.59	0/3540
1	E	0.53	0/2642	0.59	0/3571
1	F	0.44	0/2566	0.56	0/3468
2	H	0.42	0/1527	0.54	0/2058
2	I	0.44	0/1527	0.55	0/2058
2	J	0.50	0/1519	0.56	0/2047
2	K	0.51	0/1527	0.58	0/2058
2	L	0.46	0/1527	0.56	0/2058
2	M	0.39	0/1519	0.54	0/2047
2	N	0.38	0/1519	0.53	0/2047
3	S	0.38	0/67	0.47	0/88
All	All	0.46	0/26115	0.56	1/35242 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	370	ARG	NE-CZ-NH2	5.02	122.81	120.30

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	2321	2397	2399	9	0
1	B	2557	2618	2621	18	0
1	C	2591	2652	2654	8	0
1	D	2587	2648	2651	19	0
1	E	2610	2614	2670	20	0
1	F	2536	2595	2597	21	0
2	H	1503	1513	1513	9	0
2	I	1503	1513	1513	9	0
2	J	1495	1507	1507	14	0
2	K	1503	1513	1513	14	0
2	L	1503	1513	1513	12	0
2	M	1495	1507	1507	16	0
2	N	1495	1507	1507	14	0
3	S	67	58	57	0	0
4	B	31	12	12	3	0
4	C	31	12	12	2	0
4	D	31	12	12	1	0
4	E	31	12	12	0	0
4	F	31	12	12	1	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
6	H	1	0	0	0	0
6	I	1	0	0	0	0
6	J	1	0	0	0	0
6	K	1	0	0	0	0
6	L	1	0	0	0	0
6	M	1	0	0	0	0
6	N	1	0	0	0	0
All	All	25932	26215	26282	162	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.

All (162) 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:D:408:GLU:HG3	1:D:409:PRO:HD2	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:408:GLU:CD	1:F:409:PRO:HD2	1.99	0.81
1:D:408:GLU:CG	1:D:409:PRO:HD2	2.13	0.78
4:B:501:AGS:O2G	4:B:501:AGS:O2B	2.04	0.76
1:B:326:LEU:HD21	1:B:372:LEU:HD21	1.75	0.69
1:A:190:SER:OG	1:A:298:PHE:O	2.09	0.69
2:J:51:GLU:OE2	2:I:192:ARG:NH1	2.27	0.68
4:C:501:AGS:O2G	4:C:501:AGS:O2B	2.11	0.67
2:K:51:GLU:OE2	2:J:192:ARG:NE	2.29	0.66
1:E:408:GLU:HG3	1:E:409:PRO:HD2	1.77	0.65
1:D:348:LEU:HD11	1:D:398:ILE:HD11	1.78	0.64
1:E:408:GLU:CG	1:E:409:PRO:HD2	2.27	0.64
2:N:78:ASP:CB	2:M:114:LEU:HD23	2.28	0.64
1:F:348:LEU:HD11	1:F:398:ILE:HD11	1.79	0.63
1:F:346:VAL:HG21	1:F:387:LEU:HD11	1.81	0.62
2:N:78:ASP:HB2	2:M:114:LEU:HD23	1.83	0.61
2:J:10:THR:OG1	2:J:13:GLY:O	2.12	0.60
1:D:166:LEU:HD12	1:D:222:VAL:HG11	1.84	0.59
1:E:116:LEU:HD12	1:E:247:CYS:O	2.02	0.59
2:L:114:LEU:HD23	2:M:78:ASP:HB2	1.85	0.58
2:L:81:GLN:O	2:K:191:HIS:ND1	2.37	0.57
1:D:268:ILE:HD12	2:K:26:GLU:HG3	1.88	0.56
2:L:51:GLU:OE2	2:K:192:ARG:NE	2.37	0.56
2:M:83:ILE:HD11	2:M:87:VAL:CG2	2.36	0.55
2:N:24:LEU:HD13	2:N:46:GLN:OE1	2.06	0.55
1:E:266:SER:HB3	1:E:273:THR:O	2.08	0.54
2:K:18:ASP:OD1	2:K:19:ILE:N	2.41	0.54
2:J:111:ARG:NH2	2:J:186:ASP:OD1	2.41	0.53
1:C:322:LEU:HA	1:C:325:ILE:HD12	1.90	0.53
2:J:146:LYS:O	2:J:150:ASN:ND2	2.42	0.53
1:D:116:LEU:HD12	1:D:247:CYS:O	2.10	0.52
2:J:89:THR:HG21	2:J:102:LEU:O	2.09	0.52
2:M:24:LEU:HD13	2:M:46:GLN:OE1	2.09	0.52
1:B:116:LEU:HD12	1:B:247:CYS:O	2.09	0.52
2:L:24:LEU:HD13	2:L:46:GLN:OE1	2.10	0.52
1:C:326:LEU:O	1:C:334:THR:OG1	2.17	0.52
2:L:7:ILE:HD12	2:M:15:ARG:HD3	1.91	0.52
2:K:113:CYS:SG	2:K:185:VAL:HG21	2.50	0.52
2:M:163:GLN:OE1	2:M:166:ARG:NH1	2.43	0.52
1:A:320:GLU:N	1:A:320:GLU:OE2	2.42	0.52
1:B:317:LEU:HD13	1:B:322:LEU:HD21	1.90	0.52
2:N:18:ASP:OD1	2:N:21:SER:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:18:ASP:OD1	2:H:19:ILE:N	2.44	0.51
2:M:10:THR:OG1	2:M:13:GLY:O	2.26	0.51
1:B:149:THR:OG1	1:B:156:GLU:O	2.23	0.51
1:A:189:ILE:HD12	1:A:208:GLN:HG2	1.91	0.51
1:E:384:MET:SD	1:F:94:ASN:ND2	2.81	0.51
2:I:146:LYS:O	2:I:150:ASN:ND2	2.44	0.51
1:B:162:ILE:HD11	1:B:214:LEU:HD11	1.93	0.51
1:D:156:GLU:OE1	1:D:160:ASN:ND2	2.44	0.51
1:F:322:LEU:HA	1:F:325:ILE:HD12	1.93	0.51
2:I:18:ASP:OD1	2:I:19:ILE:N	2.43	0.51
2:N:78:ASP:HB3	2:M:114:LEU:HD23	1.92	0.51
1:B:92:VAL:HG21	1:B:132:LEU:HD11	1.93	0.50
1:E:190:SER:O	1:F:200:ARG:NH1	2.44	0.50
1:F:348:LEU:HD11	1:F:398:ILE:CD1	2.41	0.50
1:D:408:GLU:HG2	1:D:409:PRO:HD2	1.92	0.50
1:F:408:GLU:CG	1:F:409:PRO:HD2	2.42	0.50
1:B:326:LEU:HD21	1:B:372:LEU:CD2	2.41	0.50
1:D:322:LEU:HA	1:D:325:ILE:HD12	1.94	0.50
2:L:14:GLU:OE1	2:M:15:ARG:NH2	2.45	0.50
2:K:176:ALA:HB3	2:K:177:PRO:HD3	1.94	0.50
2:N:111:ARG:NH2	2:N:186:ASP:OD1	2.43	0.49
4:C:501:AGS:O3G	1:D:307:ARG:NH2	2.46	0.49
1:E:117:LEU:HD23	1:E:312:ALA:HB3	1.94	0.48
2:L:114:LEU:HD23	2:M:78:ASP:CB	2.43	0.48
2:H:24:LEU:HD13	2:H:46:GLN:OE1	2.14	0.48
1:A:68:HIS:NE2	1:F:386:ASP:OD1	2.45	0.48
1:F:268:ILE:HD12	2:N:26:GLU:HG3	1.95	0.48
1:D:117:LEU:HD23	1:D:312:ALA:HB3	1.96	0.48
2:N:78:ASP:OD1	2:M:116:ASN:ND2	2.45	0.47
1:B:180:ILE:HD12	1:B:244:LEU:HD23	1.96	0.47
2:L:18:ASP:OD1	2:L:19:ILE:N	2.46	0.47
2:K:6:VAL:HG11	2:K:19:ILE:HD12	1.95	0.47
2:K:109:GLY:N	2:K:186:ASP:OD2	2.45	0.47
1:A:97:LYS:HG3	1:F:343:LEU:HD13	1.96	0.47
1:D:408:GLU:CG	1:D:409:PRO:CD	2.91	0.47
2:J:172:ARG:HD3	2:J:174:LEU:HD11	1.97	0.47
2:J:173:PHE:C	2:J:174:LEU:HD12	2.34	0.47
1:E:71:ARG:NH2	1:E:82:GLU:OE1	2.45	0.46
2:N:109:GLY:N	2:N:186:ASP:OD2	2.48	0.46
1:A:67:PRO:HA	1:A:70:ILE:HG22	1.97	0.46
1:A:311:VAL:O	1:A:311:VAL:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:370:ARG:NH2	4:B:501:AGS:O3G	2.48	0.46
1:E:319:GLU:OE2	1:E:360:LYS:NZ	2.39	0.46
4:B:501:AGS:O2B	4:B:501:AGS:O1A	2.34	0.46
1:C:91:ALA:CB	1:C:115:ILE:HD11	2.46	0.46
2:H:78:ASP:OD1	2:N:116:ASN:ND2	2.43	0.46
2:K:76:ILE:HG22	2:K:80:MET:SD	2.56	0.46
2:J:18:ASP:OD1	2:J:19:ILE:N	2.49	0.46
1:B:336:GLN:OE1	1:B:373:ARG:NH2	2.48	0.46
2:L:95:ALA:O	2:L:100:ALA:HB2	2.16	0.46
2:I:51:GLU:OE2	2:H:192:ARG:NE	2.49	0.46
1:B:385:TYR:OH	1:C:71:ARG:NH1	2.48	0.45
1:F:343:LEU:HD12	1:F:344:GLU:N	2.32	0.45
2:I:109:GLY:N	2:I:186:ASP:OD2	2.47	0.45
1:F:408:GLU:OE2	1:F:409:PRO:HD2	2.16	0.45
1:B:317:LEU:HD13	1:B:322:LEU:CD2	2.47	0.45
1:E:158:VAL:HG12	1:E:214:LEU:HD22	1.97	0.45
1:E:407:SER:OG	1:E:408:GLU:N	2.48	0.45
1:D:240:THR:HA	1:D:243:ILE:HD12	1.99	0.45
1:F:91:ALA:CB	1:F:115:ILE:HD11	2.47	0.45
2:N:131:GLN:OE1	2:M:170:ARG:NH1	2.46	0.45
1:A:240:THR:HA	1:A:243:ILE:HD12	1.98	0.45
1:B:77:TYR:HB2	1:B:131:THR:HG21	1.99	0.45
1:E:91:ALA:HB2	1:E:115:ILE:HD11	1.97	0.45
1:E:95:HIS:O	1:E:99:LEU:HD13	2.17	0.45
1:D:285:GLU:O	1:D:289:GLN:NE2	2.50	0.45
2:H:15:ARG:NH1	2:N:14:GLU:OE1	2.48	0.44
1:A:118:ILE:HG23	1:A:251:PHE:HD2	1.82	0.44
2:I:24:LEU:HD13	2:I:46:GLN:OE1	2.16	0.44
1:F:346:VAL:HG22	1:F:393:VAL:O	2.17	0.44
1:F:127:LEU:HD22	4:F:600:AGS:H2'	1.98	0.44
2:K:24:LEU:HD13	2:K:46:GLN:OE1	2.17	0.44
4:D:501:AGS:S1G	1:E:307:ARG:NH1	2.89	0.44
1:E:128:LEU:O	1:E:131:THR:OG1	2.32	0.44
1:B:276:ALA:O	1:B:279:ASP:N	2.51	0.43
2:H:51:GLU:OE1	2:H:83:ILE:HG22	2.19	0.43
1:B:91:ALA:CB	1:B:115:ILE:HD11	2.48	0.43
1:D:112:LYS:NZ	1:D:243:ILE:O	2.40	0.43
2:N:44:VAL:HG13	2:N:79:THR:HG21	2.01	0.43
1:E:367:THR:HG22	1:E:367:THR:O	2.19	0.43
1:F:116:LEU:HD12	1:F:247:CYS:O	2.19	0.43
1:D:91:ALA:CB	1:D:115:ILE:HD11	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:216:GLU:HB2	1:E:307:ARG:HE	1.84	0.42
1:F:216:GLU:HB2	1:F:307:ARG:HE	1.84	0.42
2:M:59:ILE:O	2:M:88:SER:N	2.50	0.42
1:E:169:SER:O	1:E:169:SER:OG	2.37	0.42
2:I:77:TYR:OH	2:I:152:LEU:HD22	2.19	0.42
1:D:92:VAL:HG21	1:D:132:LEU:HD11	2.02	0.42
2:J:8:GLU:OE2	2:J:25:LYS:NZ	2.44	0.42
1:E:280:LYS:HG3	1:E:281:ALA:H	1.85	0.42
1:F:99:LEU:HD23	1:F:178:ARG:HG3	2.02	0.42
2:M:190:THR:O	2:M:191:HIS:ND1	2.52	0.42
1:B:240:THR:HG22	1:B:243:ILE:HD12	2.02	0.42
2:I:72:ALA:O	2:I:75:SER:OG	2.28	0.42
2:J:109:GLY:N	2:J:186:ASP:OD2	2.47	0.42
2:K:6:VAL:N	2:K:17:PHE:O	2.51	0.42
2:N:190:THR:HG22	2:N:191:HIS:ND1	2.35	0.42
1:C:173:VAL:HG13	1:C:238:VAL:HG22	2.02	0.42
2:H:59:ILE:O	2:H:88:SER:N	2.52	0.42
1:C:126:THR:OG1	1:C:184:ASP:OD2	2.37	0.41
1:F:365:ARG:O	1:F:367:THR:N	2.53	0.41
2:J:72:ALA:O	2:J:75:SER:OG	2.30	0.41
1:F:255:ASP:HB2	1:F:286:LEU:HD23	2.01	0.41
1:B:166:LEU:O	1:B:170:ASP:N	2.54	0.41
2:K:119:VAL:HG11	2:K:184:LEU:HD13	2.02	0.41
2:K:114:LEU:O	2:K:117:SER:OG	2.28	0.41
2:H:176:ALA:HB3	2:H:177:PRO:HD3	2.02	0.41
1:D:166:LEU:CD1	1:D:222:VAL:HG11	2.48	0.41
1:B:136:LEU:HD11	1:B:140:PHE:HB2	2.03	0.41
1:E:91:ALA:CB	1:E:115:ILE:HD11	2.51	0.41
2:J:24:LEU:HD13	2:J:46:GLN:OE1	2.21	0.41
1:C:91:ALA:HB2	1:C:115:ILE:HD11	2.03	0.41
2:L:109:GLY:N	2:L:186:ASP:OD2	2.54	0.41
2:H:163:GLN:OE1	2:H:166:ARG:NH1	2.48	0.41
2:I:173:PHE:C	2:I:174:LEU:HD12	2.41	0.40
1:C:213:LYS:O	1:C:218:THR:HG22	2.21	0.40
1:D:408:GLU:HG2	1:D:409:PRO:CD	2.51	0.40
2:L:96:ALA:O	2:L:99:GLY:N	2.55	0.40
2:J:113:CYS:SG	2:J:176:ALA:HB1	2.61	0.40
2:L:170:ARG:NH1	2:M:131:GLN:OE1	2.50	0.40

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	291/388 (75%)	291 (100%)	0	0	100	100
1	B	326/388 (84%)	320 (98%)	6 (2%)	0	100	100
1	C	332/388 (86%)	331 (100%)	1 (0%)	0	100	100
1	D	332/388 (86%)	325 (98%)	7 (2%)	0	100	100
1	E	335/388 (86%)	335 (100%)	0	0	100	100
1	F	323/388 (83%)	318 (98%)	5 (2%)	0	100	100
2	H	190/207 (92%)	190 (100%)	0	0	100	100
2	I	190/207 (92%)	190 (100%)	0	0	100	100
2	J	189/207 (91%)	188 (100%)	1 (0%)	0	100	100
2	K	190/207 (92%)	189 (100%)	1 (0%)	0	100	100
2	L	190/207 (92%)	188 (99%)	2 (1%)	0	100	100
2	M	189/207 (91%)	189 (100%)	0	0	100	100
2	N	189/207 (91%)	189 (100%)	0	0	100	100
3	S	8/274 (3%)	8 (100%)	0	0	100	100
All	All	3274/4051 (81%)	3251 (99%)	23 (1%)	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	252/322 (78%)	252 (100%)	0	100	100
1	B	276/322 (86%)	276 (100%)	0	100	100
1	C	281/322 (87%)	281 (100%)	0	100	100
1	D	280/322 (87%)	280 (100%)	0	100	100
1	E	283/322 (88%)	283 (100%)	0	100	100
1	F	274/322 (85%)	273 (100%)	1 (0%)	91	96
2	H	163/178 (92%)	163 (100%)	0	100	100
2	I	163/178 (92%)	163 (100%)	0	100	100
2	J	162/178 (91%)	162 (100%)	0	100	100
2	K	163/178 (92%)	163 (100%)	0	100	100
2	L	163/178 (92%)	163 (100%)	0	100	100
2	M	162/178 (91%)	162 (100%)	0	100	100
2	N	162/178 (91%)	162 (100%)	0	100	100
3	S	5/226 (2%)	5 (100%)	0	100	100
All	All	2789/3404 (82%)	2788 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	407	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	167	GLN
1	D	95	HIS
1	F	81	GLN
1	F	208	GLN
2	K	41	ASN
2	J	150	ASN
2	I	41	ASN
2	I	150	ASN
2	N	41	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 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	AGS	F	600	-	26,33,33	0.74	1 (3%)	26,52,52	1.16	2 (7%)
4	AGS	E	501	5	26,33,33	0.76	0	26,52,52	1.15	2 (7%)
4	AGS	C	501	5	26,33,33	0.74	0	26,52,52	1.17	2 (7%)
4	AGS	D	501	5	26,33,33	0.76	0	26,52,52	1.29	2 (7%)
4	AGS	B	501	5	26,33,33	0.75	0	26,52,52	1.34	2 (7%)

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	AGS	F	600	-	-	4/17/38/38	0/3/3/3
4	AGS	E	501	5	-	3/17/38/38	0/3/3/3
4	AGS	C	501	5	-	4/17/38/38	0/3/3/3
4	AGS	D	501	5	-	2/17/38/38	0/3/3/3
4	AGS	B	501	5	-	9/17/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	600	AGS	PG-S1G	2.08	1.95	1.90

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	501	AGS	PA-O3A-PB	-5.29	114.66	132.83
4	D	501	AGS	PA-O3A-PB	-4.98	115.73	132.83
4	C	501	AGS	PA-O3A-PB	-4.52	117.32	132.83
4	E	501	AGS	PA-O3A-PB	-4.40	117.73	132.83
4	F	600	AGS	PA-O3A-PB	-4.35	117.89	132.83
4	F	600	AGS	C5-C6-N6	2.14	123.61	120.35
4	B	501	AGS	C5-C6-N6	2.13	123.58	120.35
4	C	501	AGS	C5-C6-N6	2.10	123.54	120.35
4	D	501	AGS	C5-C6-N6	2.08	123.52	120.35
4	E	501	AGS	C5-C6-N6	2.08	123.51	120.35

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	501	AGS	PB-O3B-PG-O2G
4	B	501	AGS	PB-O3B-PG-O3G
4	B	501	AGS	C5'-O5'-PA-O1A
4	B	501	AGS	C5'-O5'-PA-O2A
4	C	501	AGS	PB-O3B-PG-O2G
4	D	501	AGS	PB-O3B-PG-O2G
4	D	501	AGS	PB-O3B-PG-O3G
4	E	501	AGS	PB-O3B-PG-O2G
4	F	600	AGS	C5'-O5'-PA-O2A
4	F	600	AGS	C5'-O5'-PA-O3A
4	B	501	AGS	O4'-C4'-C5'-O5'
4	B	501	AGS	C3'-C4'-C5'-O5'
4	B	501	AGS	PG-O3B-PB-O2B
4	E	501	AGS	PG-O3B-PB-O2B
4	C	501	AGS	PB-O3B-PG-O3G
4	E	501	AGS	PB-O3B-PG-O3G
4	F	600	AGS	C4'-C5'-O5'-PA
4	B	501	AGS	PG-O3B-PB-O1B
4	C	501	AGS	PG-O3B-PB-O1B
4	C	501	AGS	PG-O3B-PB-O2B
4	B	501	AGS	C5'-O5'-PA-O3A
4	F	600	AGS	PB-O3A-PA-O2A

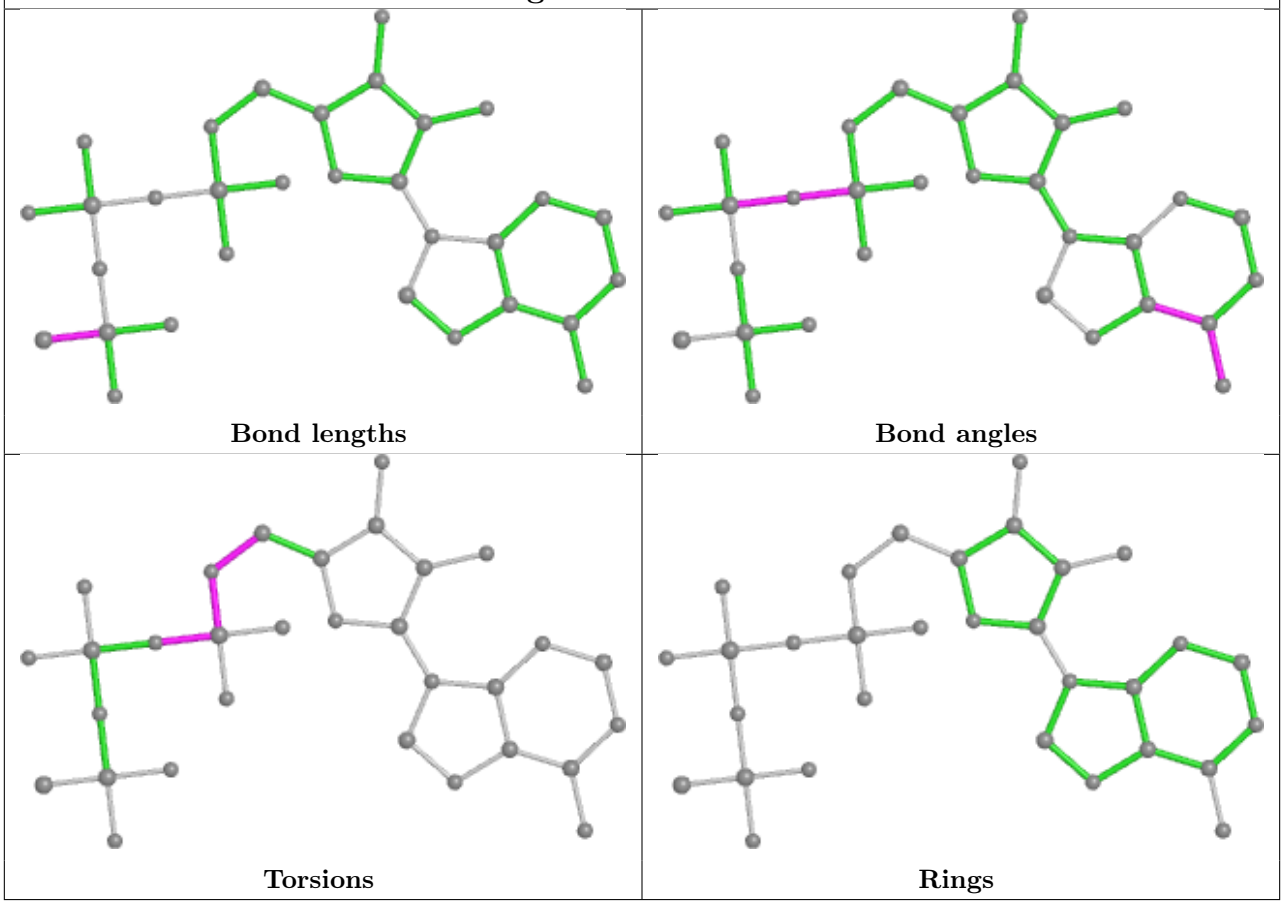
There are no ring outliers.

4 monomers are involved in 7 short contacts:

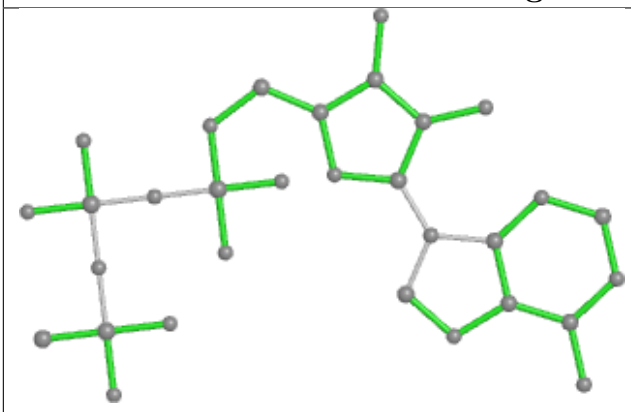
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	600	AGS	1	0
4	C	501	AGS	2	0
4	D	501	AGS	1	0
4	B	501	AGS	3	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

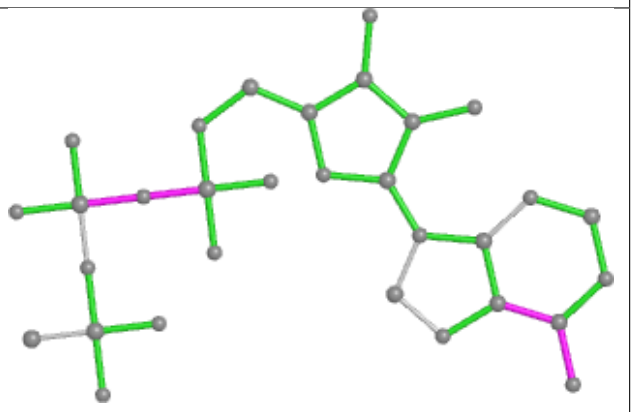
Ligand AGS F 600



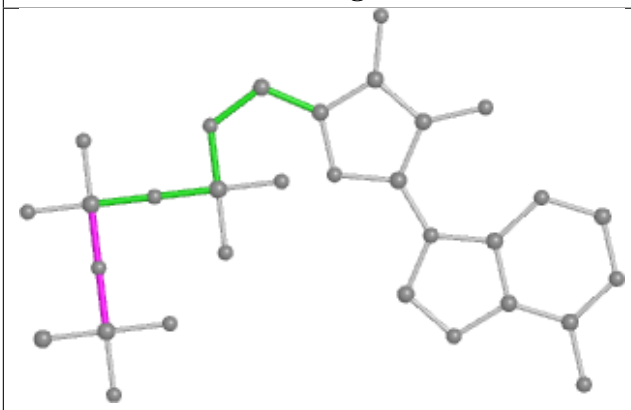
Ligand AGS E 501



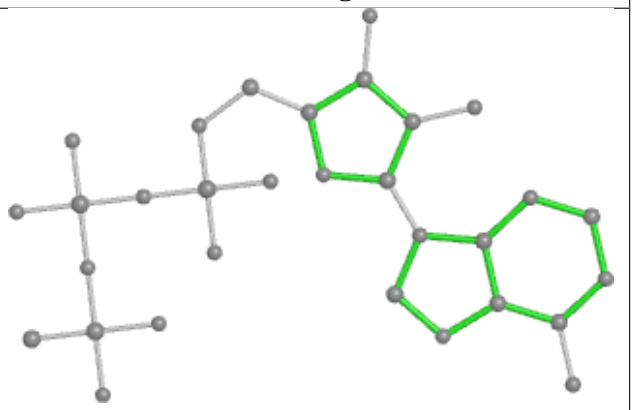
Bond lengths



Bond angles

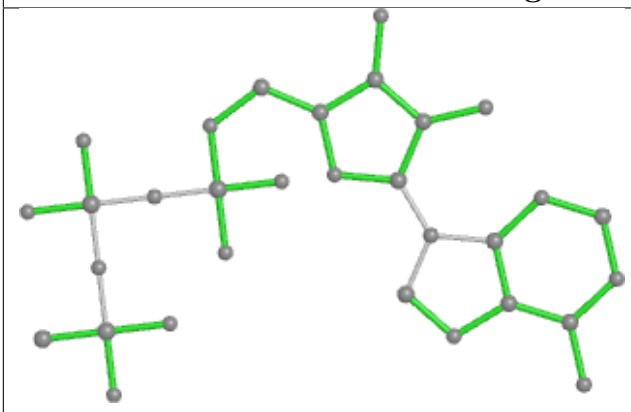


Torsions

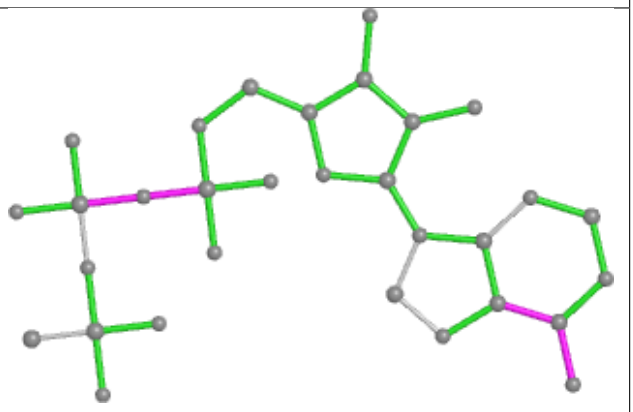


Rings

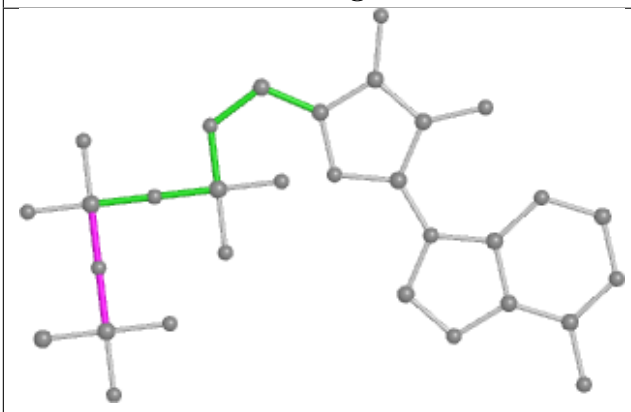
Ligand AGS C 501



Bond lengths



Bond angles



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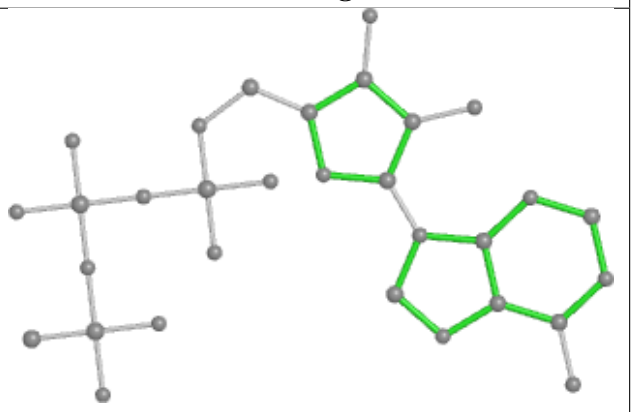

Rings

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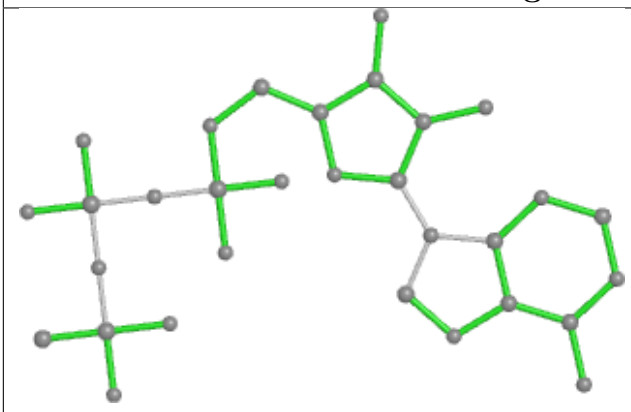
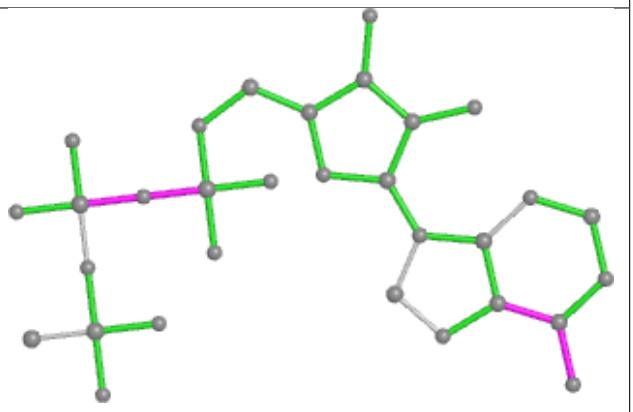
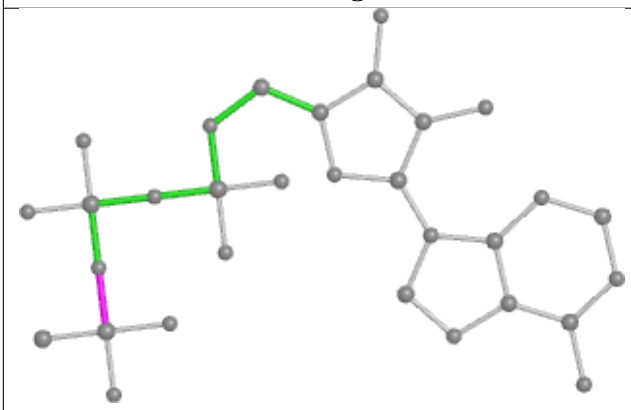


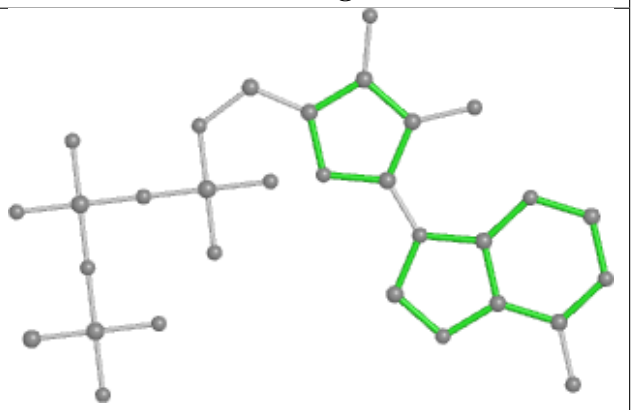
Bond lengths



Bond angles

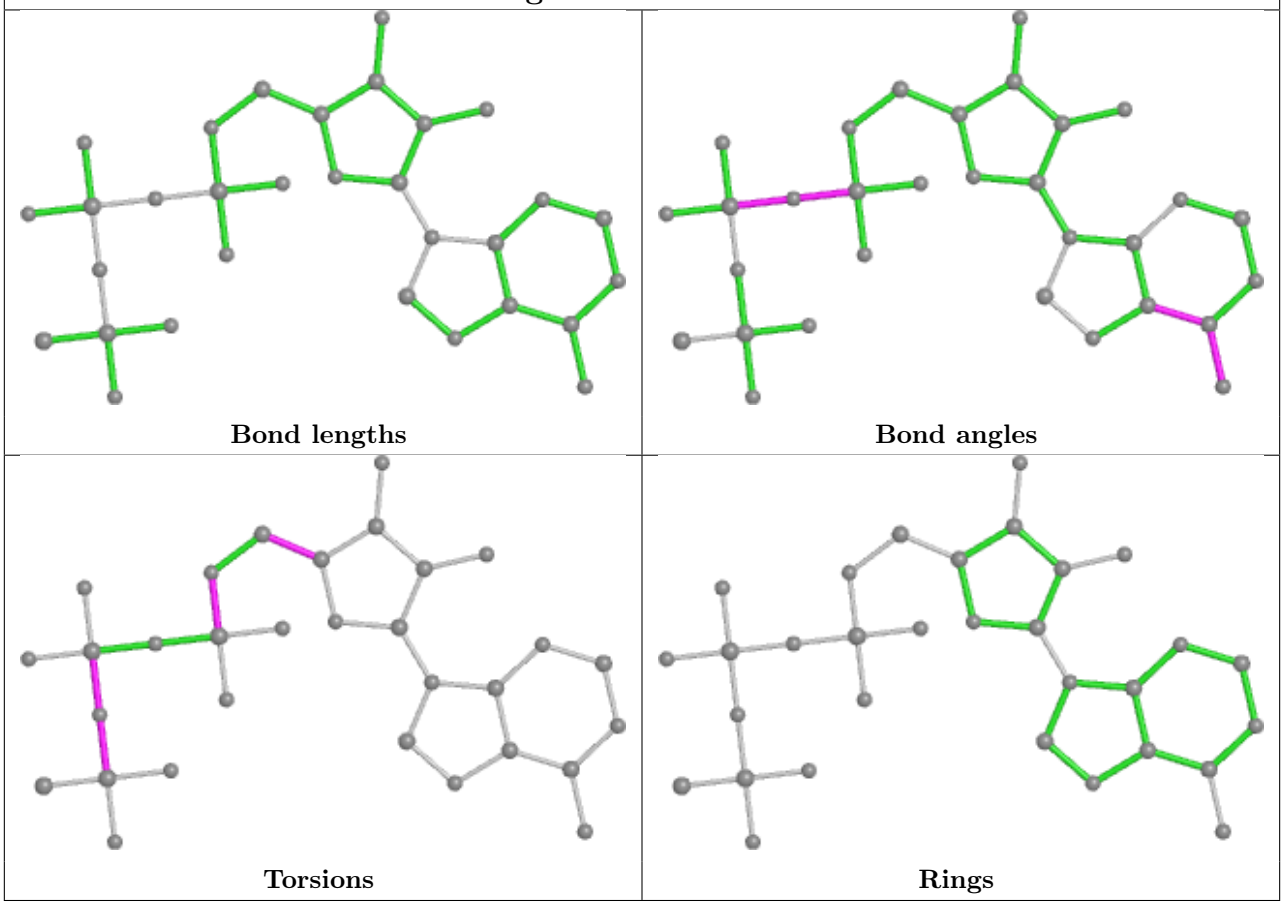


Torsions



Rings

Ligand AGS B 501



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.

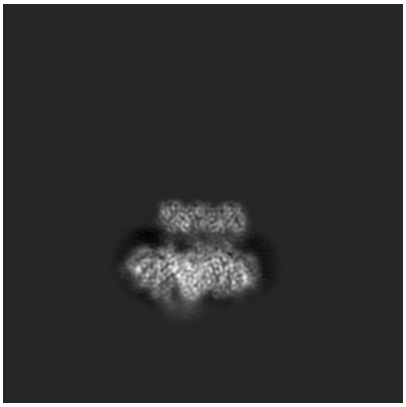
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-21892. These allow visual inspection of the internal detail of the map and identification of artifacts.

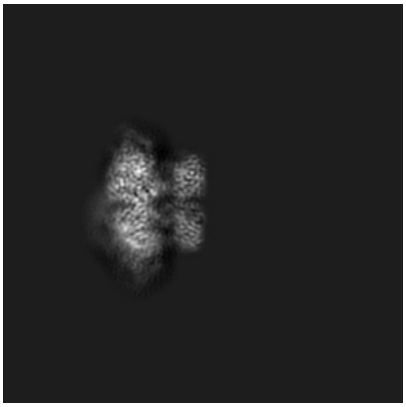
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

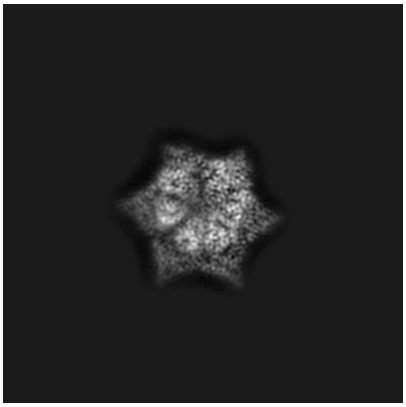
6.1.1 Primary map



X



Y



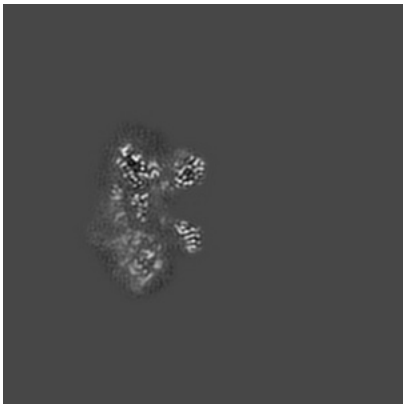
Z

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

6.2 Central slices

6.2.1 Primary map

X Index: 200



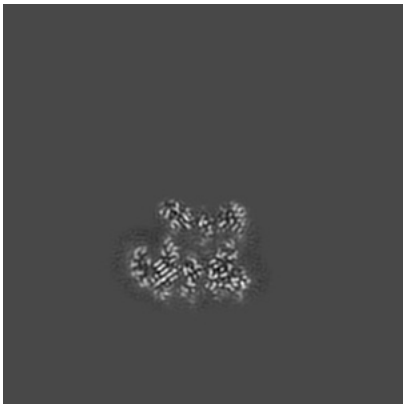
Y Index: 200

Z Index: 200

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

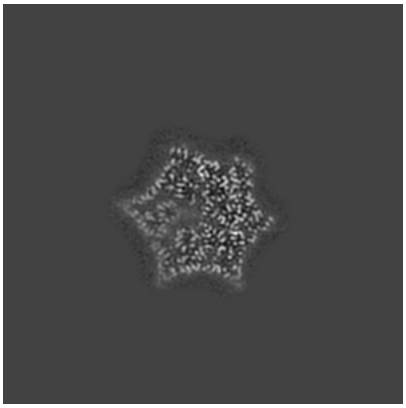
6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 219

Y Index: 217

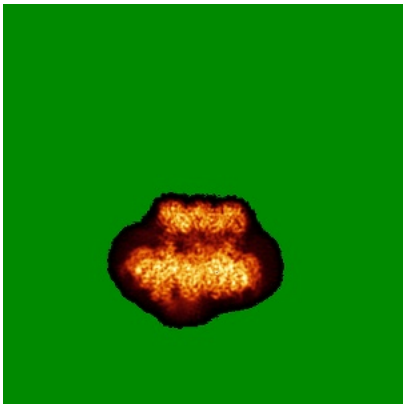


Z Index: 134

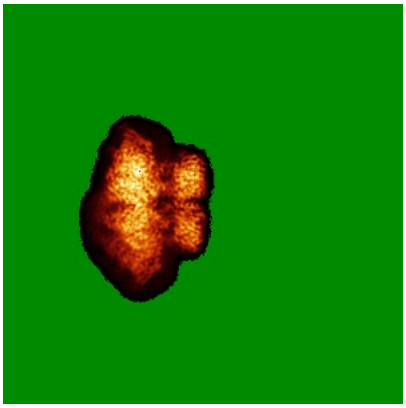
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

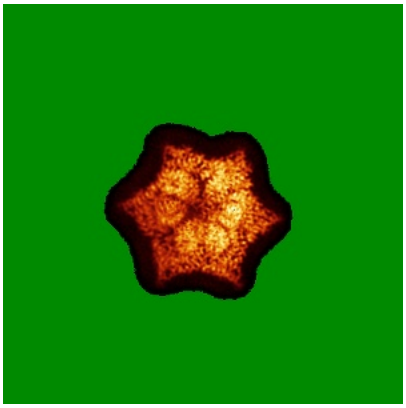
6.4.1 Primary map



X



Y

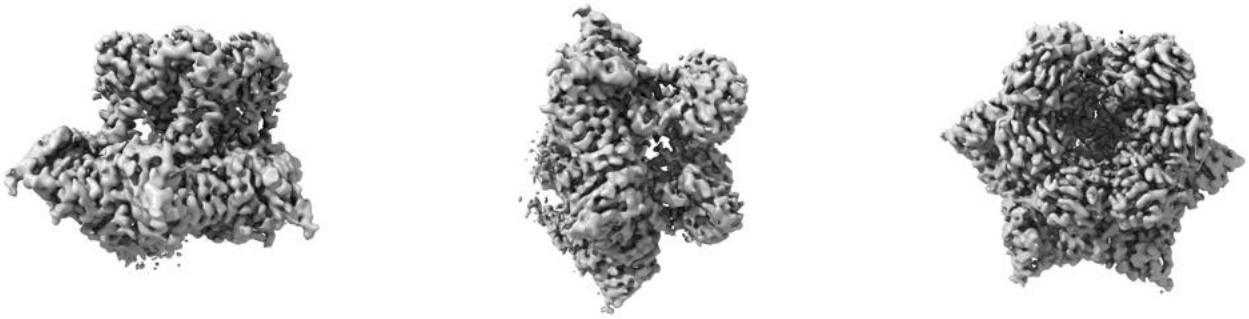


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 5.6. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

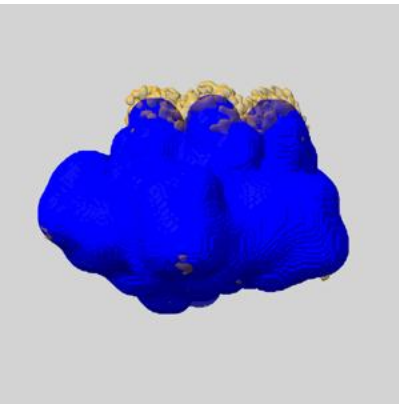
6.6 Mask visualisation (i)

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

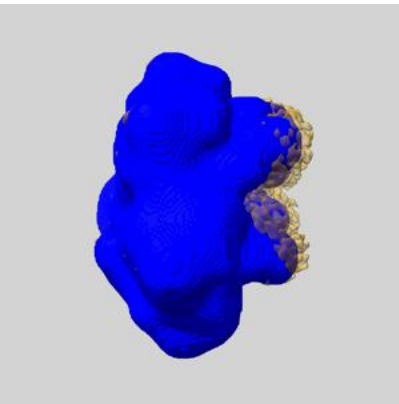
A mask typically either:

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

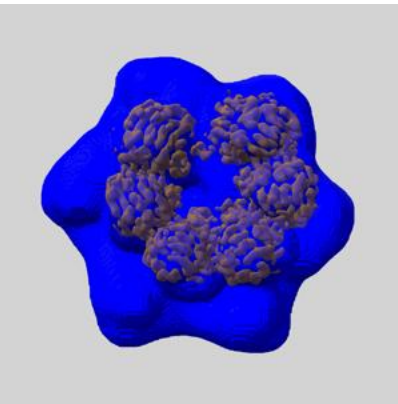
6.6.1 emd_21892_msk_1.map (i)



X



Y

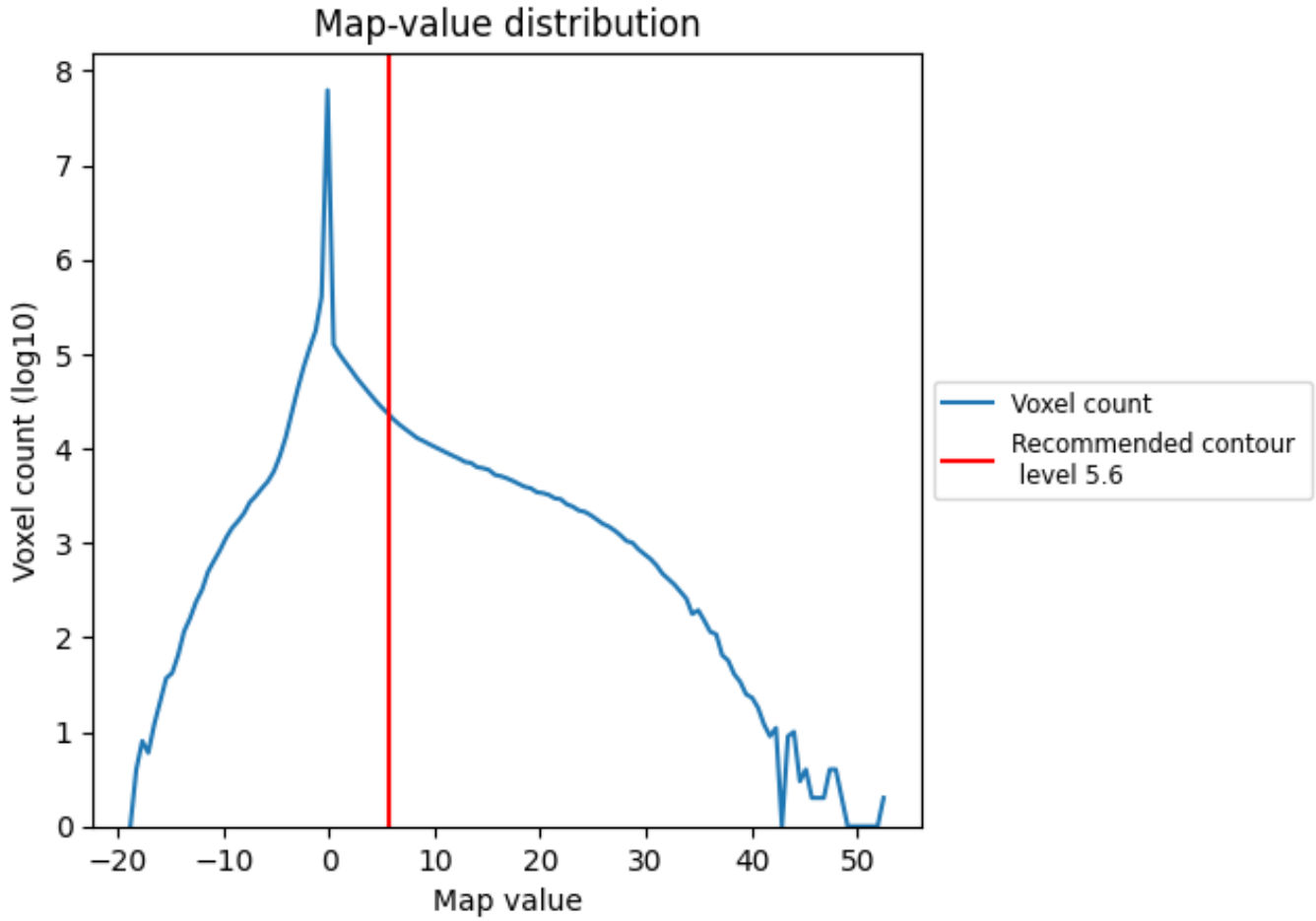


Z

7 Map analysis

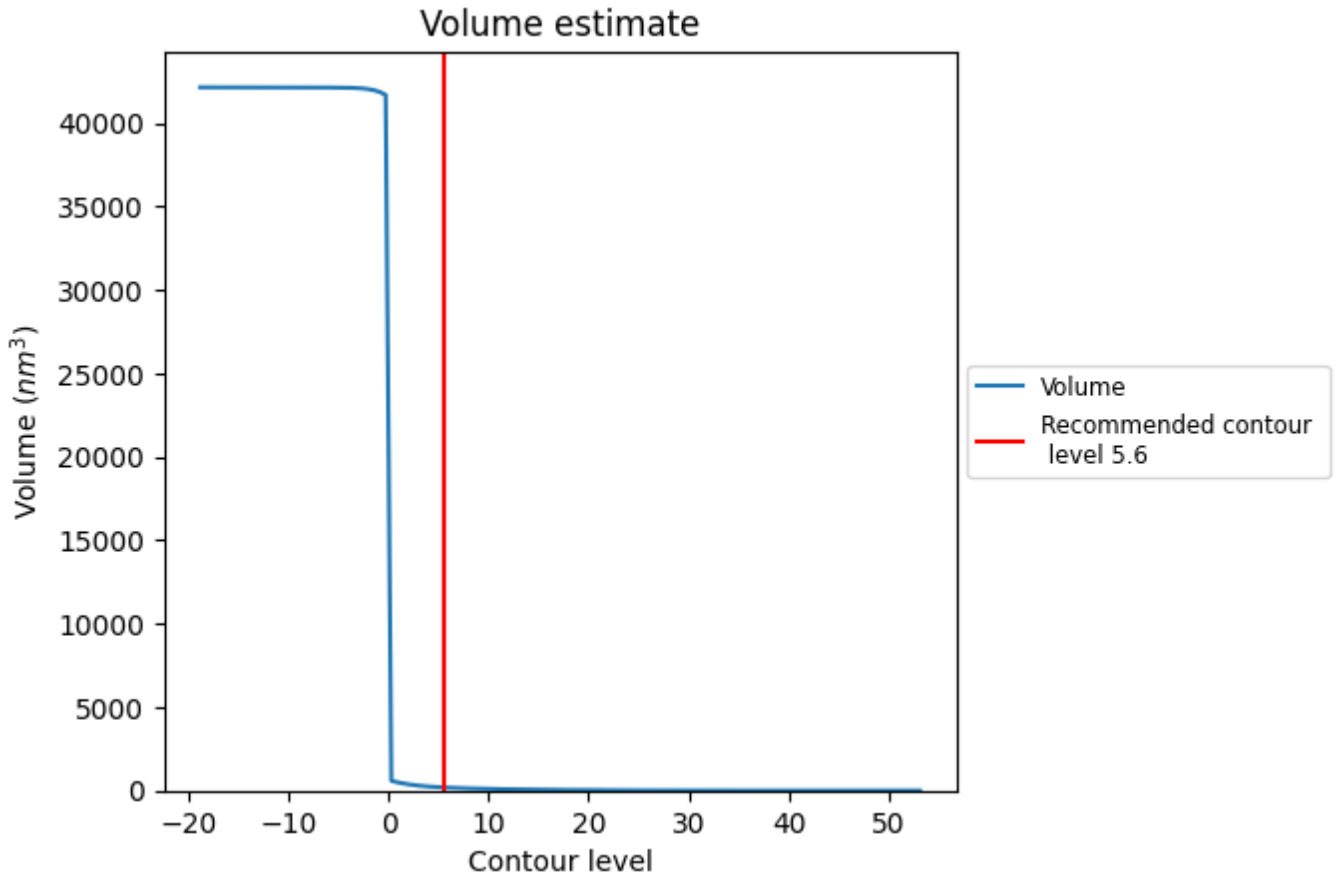
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

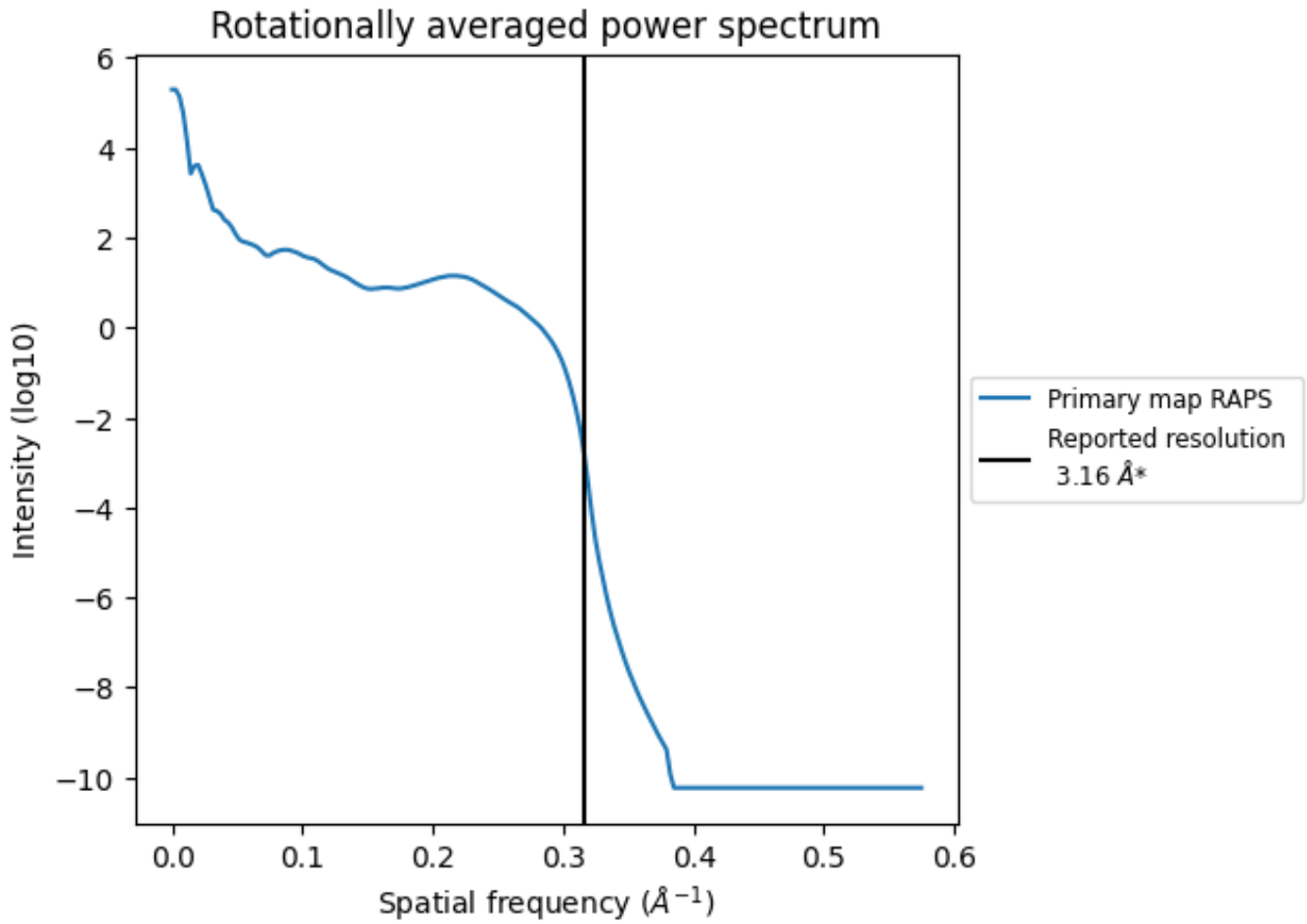
7.2 Volume estimate



The volume at the recommended contour level is 184 nm^3; this corresponds to an approximate mass of 166 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)

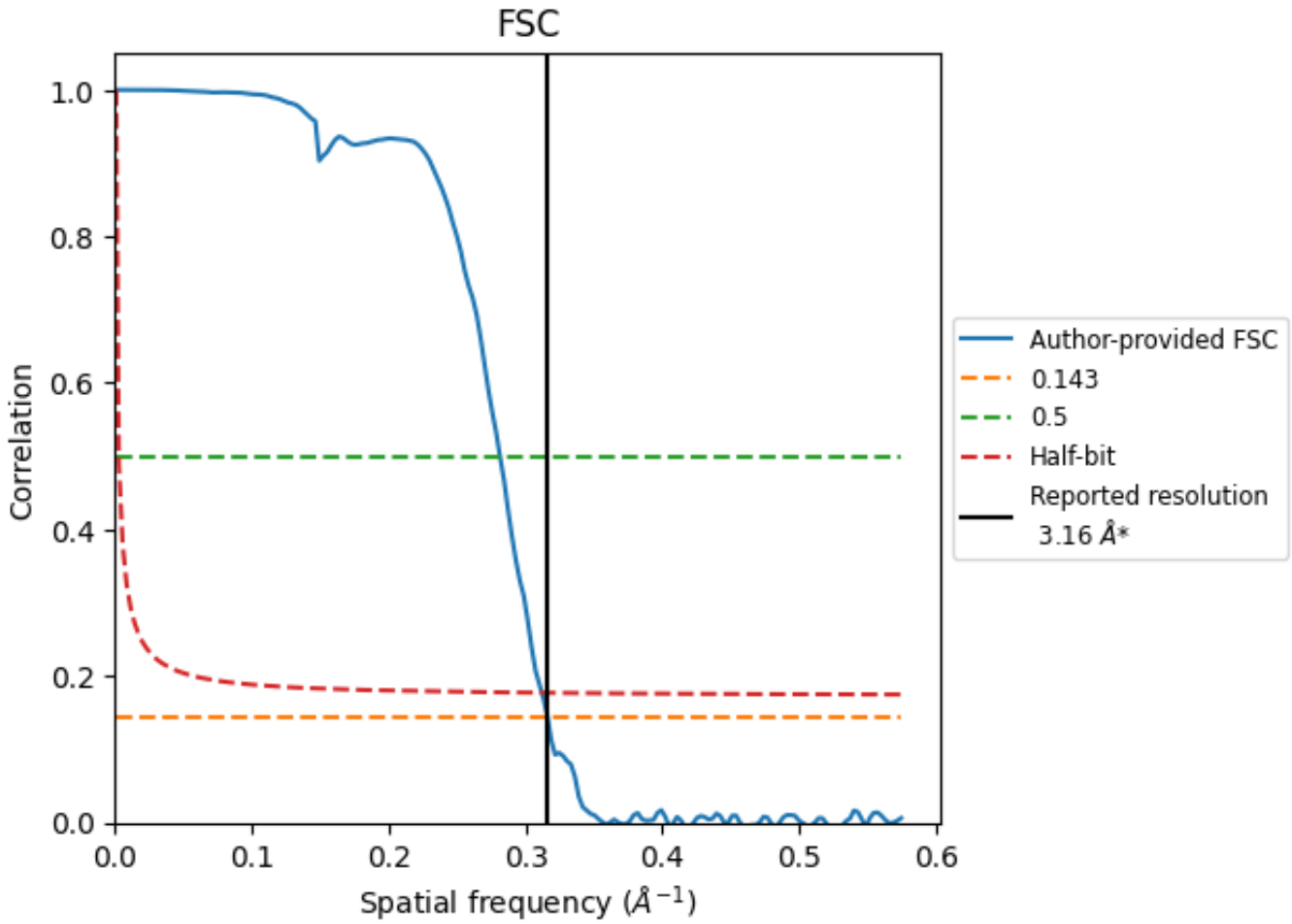


*Reported resolution corresponds to spatial frequency of 0.316 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.316 Å^{-1}

8.2 Resolution estimates (i)

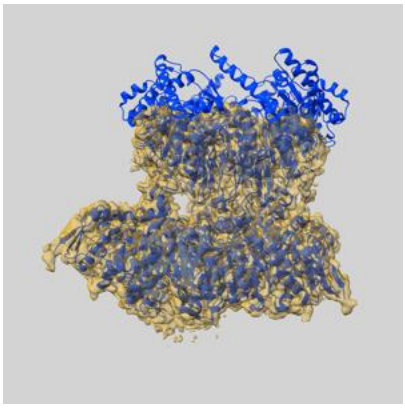
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.16	-	-
Author-provided FSC curve	3.16	3.55	3.20
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

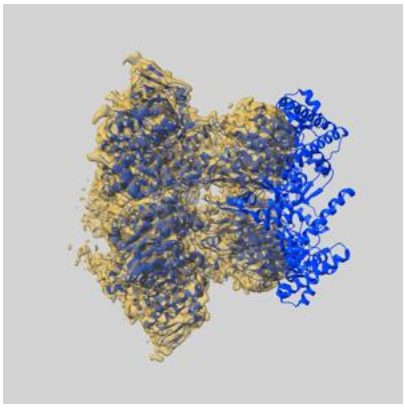
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-21892 and PDB model 6WSG. Per-residue inclusion information can be found in section 3 on page 14.

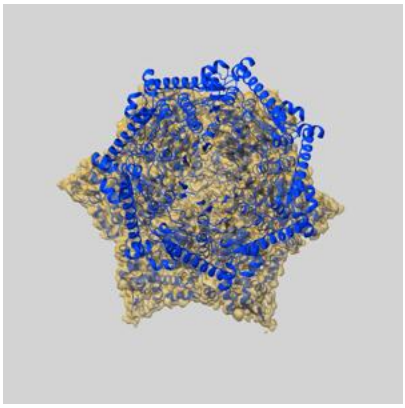
9.1 Map-model overlay



X



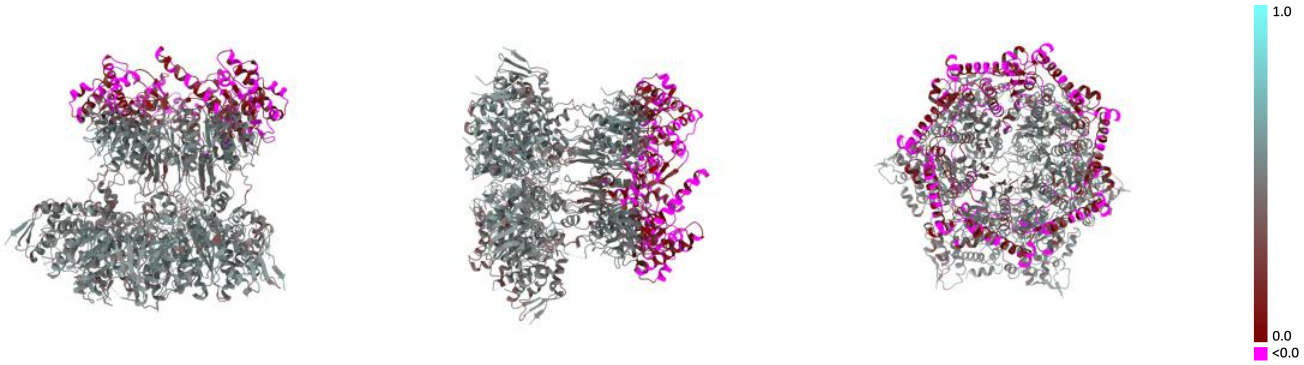
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 5.6 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

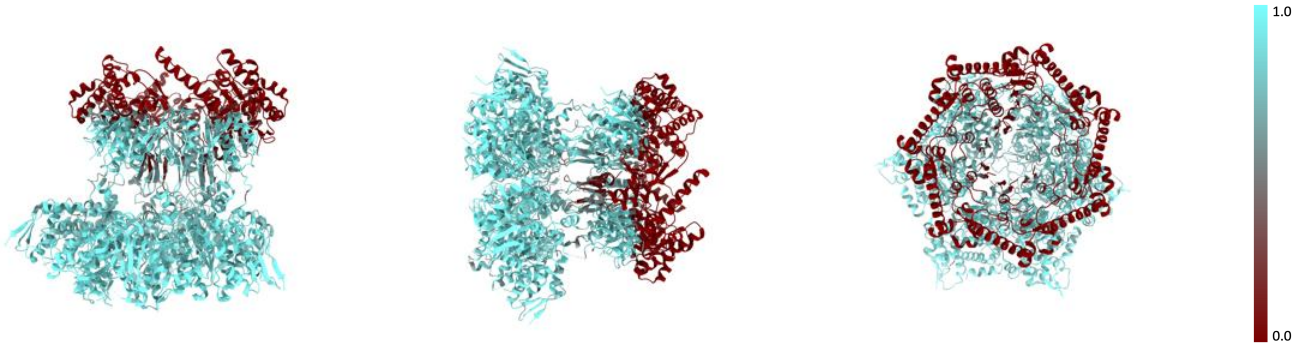
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

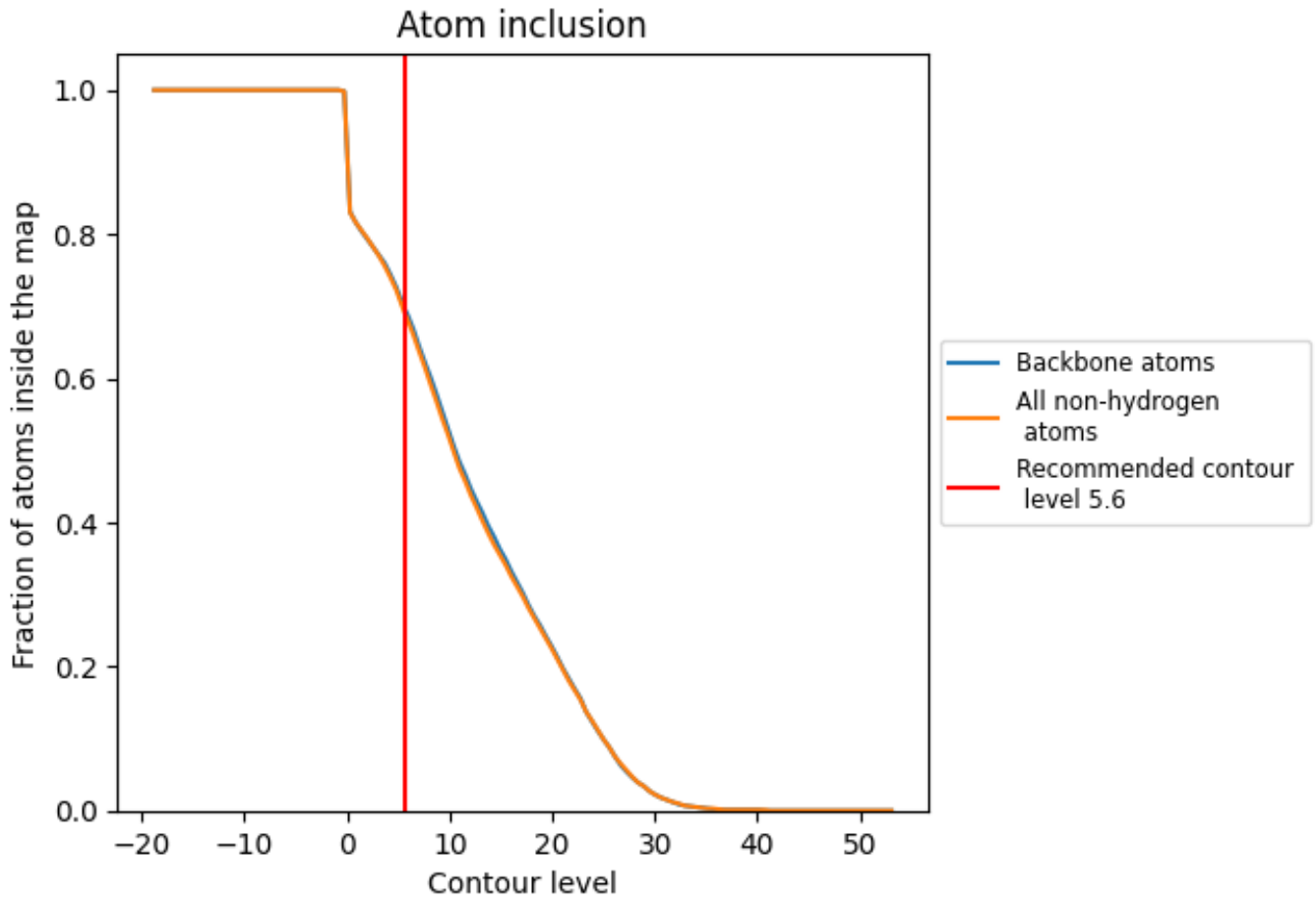
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (5.6).

9.4 Atom inclusion (i)



At the recommended contour level, 70% of all backbone atoms, 69% 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 (5.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6910	0.4060
A	0.8540	0.4380
B	0.8910	0.4920
C	0.9090	0.5080
D	0.9030	0.5080
E	0.9090	0.5110
F	0.8990	0.4990
H	0.3930	0.2720
I	0.4540	0.2940
J	0.4940	0.3220
K	0.4890	0.3260
L	0.4780	0.3200
M	0.2500	0.1920
N	0.3080	0.2160
S	0.7580	0.4980