



Full wwPDB EM Validation Report ⓘ

Nov 4, 2025 – 04:17 PM EST

PDB ID : 9PIO / pdb_00009pio
EMDB ID : EMD-71674
Title : Cryo-EM structure of the ClpXP AAA+ protease bound to lambdaO-tagged Arc in a recognition complex
Authors : Ghanbarpour, A.; Davis, J.H.; Sauer, R.T.
Deposited on : 2025-07-10
Resolution : 2.61 Å(reported)
Based on initial model : 6WRF

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:

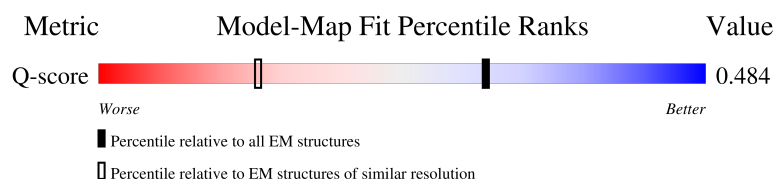
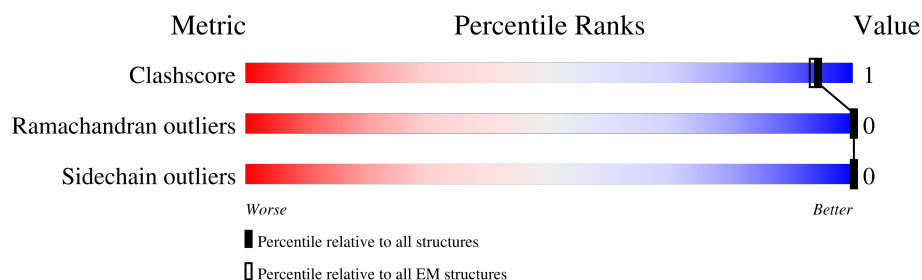
EMDB validation analysis : 0.0.1.dev129
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.46

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 2.61 Å.

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




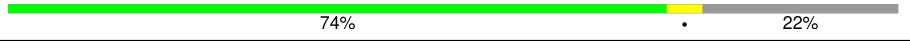
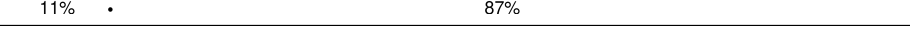
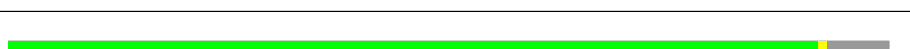



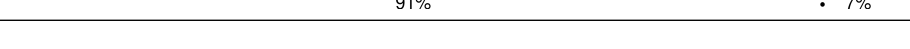
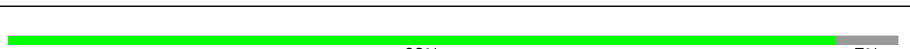

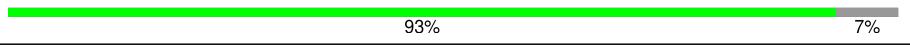
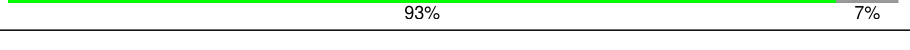
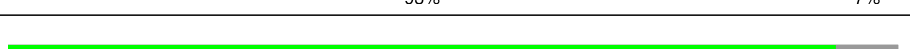
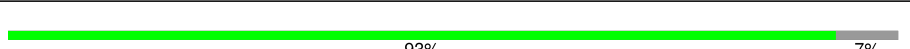



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	8735 (2.11 - 3.11)

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	424	
1	B	424	
1	C	424	
1	D	424	

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Mol	Chain	Length	Quality of chain
1	E	424	
1	F	424	
2	G	79	
3	H	207	
3	I	207	
3	J	207	
3	K	207	
3	L	207	
3	M	207	
3	N	207	
3	O	207	
3	P	207	
3	Q	207	
3	R	207	
3	S	207	
3	T	207	
3	U	207	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 73281 atoms, of which 36845 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	297	Total	C	H	N	O	S	0	0
			4640	1458	2352	381	443	6		
1	B	332	Total	C	H	N	O	S	0	0
			5148	1614	2604	426	498	6		
1	C	338	Total	C	H	N	O	S	0	0
			5243	1644	2652	433	508	6		
1	D	338	Total	C	H	N	O	S	0	0
			5235	1642	2648	432	507	6		
1	E	341	Total	C	H	N	O	S	0	0
			5277	1654	2667	437	513	6		
1	F	331	Total	C	H	N	O	S	0	0
			5130	1610	2594	424	496	6		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	408	GLU	LYS	conflict	UNP C3TLS7
B	408	GLU	LYS	conflict	UNP C3TLS7
C	408	GLU	LYS	conflict	UNP C3TLS7
D	408	GLU	LYS	conflict	UNP C3TLS7
E	408	GLU	LYS	conflict	UNP C3TLS7
F	408	GLU	LYS	conflict	UNP C3TLS7

- Molecule 2 is a protein called Arc family DNA-binding protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	G	10	Total	C	H	N	O	S	0	0
			165	51	86	13	14	1		

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	1	MET	-	initiating methionine	UNP A0A1Y5CGZ0

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Chain	Residue	Modelled	Actual	Comment	Reference
G	2	THR	-	expression tag	UNP A0A1Y5CGZ0
G	3	ASN	-	expression tag	UNP A0A1Y5CGZ0
G	4	THR	-	expression tag	UNP A0A1Y5CGZ0
G	5	ALA	-	expression tag	UNP A0A1Y5CGZ0
G	6	LYS	-	expression tag	UNP A0A1Y5CGZ0
G	7	ILE	-	expression tag	UNP A0A1Y5CGZ0
G	8	LEU	-	expression tag	UNP A0A1Y5CGZ0
G	9	ASN	-	expression tag	UNP A0A1Y5CGZ0
G	10	PHE	-	expression tag	UNP A0A1Y5CGZ0
G	11	GLY	-	expression tag	UNP A0A1Y5CGZ0
G	12	ARG	-	expression tag	UNP A0A1Y5CGZ0
G	13	ALA	-	expression tag	UNP A0A1Y5CGZ0
G	14	SER	-	expression tag	UNP A0A1Y5CGZ0
G	15	MET	-	expression tag	UNP A0A1Y5CGZ0
G	16	GLY	-	expression tag	UNP A0A1Y5CGZ0
G	31	ARG	LYS	conflict	UNP A0A1Y5CGZ0
G	69	HIS	-	expression tag	UNP A0A1Y5CGZ0
G	70	HIS	-	expression tag	UNP A0A1Y5CGZ0
G	71	HIS	-	expression tag	UNP A0A1Y5CGZ0
G	72	HIS	-	expression tag	UNP A0A1Y5CGZ0
G	73	HIS	-	expression tag	UNP A0A1Y5CGZ0
G	74	HIS	-	expression tag	UNP A0A1Y5CGZ0
G	75	LYS	-	expression tag	UNP A0A1Y5CGZ0
G	76	ASN	-	expression tag	UNP A0A1Y5CGZ0
G	77	GLN	-	expression tag	UNP A0A1Y5CGZ0
G	78	HIS	-	expression tag	UNP A0A1Y5CGZ0
G	79	ASP	-	expression tag	UNP A0A1Y5CGZ0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
3	H	192	Total	C	H	N	O	S	0	0
			3016	947	1513	261	283	12		
3	I	192	Total	C	H	N	O	S	0	0
			3016	947	1513	261	283	12		
3	J	192	Total	C	H	N	O	S	0	0
			3016	947	1513	261	283	12		
3	K	192	Total	C	H	N	O	S	0	0
			3016	947	1513	261	283	12		
3	L	192	Total	C	H	N	O	S	0	0
			3016	947	1513	261	283	12		
3	M	192	Total	C	H	N	O	S	0	0
			3016	947	1513	261	283	12		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	N	192	Total	C	H	N	O	S	
			3016	947	1513	261	283	12	0
3	O	192	Total	C	H	N	O	S	
			3016	947	1513	261	283	12	0
3	P	192	Total	C	H	N	O	S	
			3016	947	1513	261	283	12	0
3	Q	192	Total	C	H	N	O	S	
			3016	947	1513	261	283	12	0
3	R	192	Total	C	H	N	O	S	
			3016	947	1513	261	283	12	0
3	S	192	Total	C	H	N	O	S	
			3016	947	1513	261	283	12	0
3	T	192	Total	C	H	N	O	S	
			3016	947	1513	261	283	12	0
3	U	192	Total	C	H	N	O	S	
			3016	947	1513	261	283	12	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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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

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Chain	Residue	Modelled	Actual	Comment	Reference
O	196	LEU	-	expression tag	UNP P0A6G7
O	197	TYR	-	expression tag	UNP P0A6G7
O	198	PHE	-	expression tag	UNP P0A6G7
O	199	GLN	-	expression tag	UNP P0A6G7
O	200	SER	-	expression tag	UNP P0A6G7
O	201	LEU	-	expression tag	UNP P0A6G7
O	202	GLU	-	expression tag	UNP P0A6G7
O	203	HIS	-	expression tag	UNP P0A6G7
O	204	HIS	-	expression tag	UNP P0A6G7
O	205	HIS	-	expression tag	UNP P0A6G7
O	206	HIS	-	expression tag	UNP P0A6G7
O	207	HIS	-	expression tag	UNP P0A6G7
O	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

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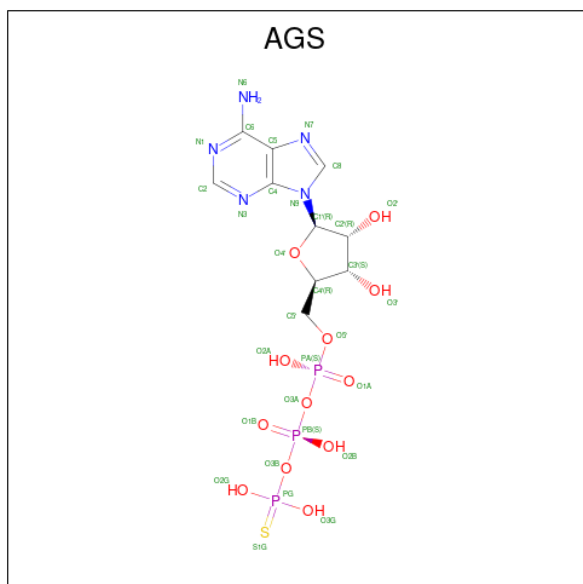
Chain	Residue	Modelled	Actual	Comment	Reference
Q	208	HIS	-	expression tag	UNP P0A6G7
R	194	GLU	-	expression tag	UNP P0A6G7
R	195	ASN	-	expression tag	UNP P0A6G7
R	196	LEU	-	expression tag	UNP P0A6G7
R	197	TYR	-	expression tag	UNP P0A6G7
R	198	PHE	-	expression tag	UNP P0A6G7
R	199	GLN	-	expression tag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

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

- Molecule 4 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S).



Mol	Chain	Residues	Atoms							AltConf
4	B	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	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	
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	

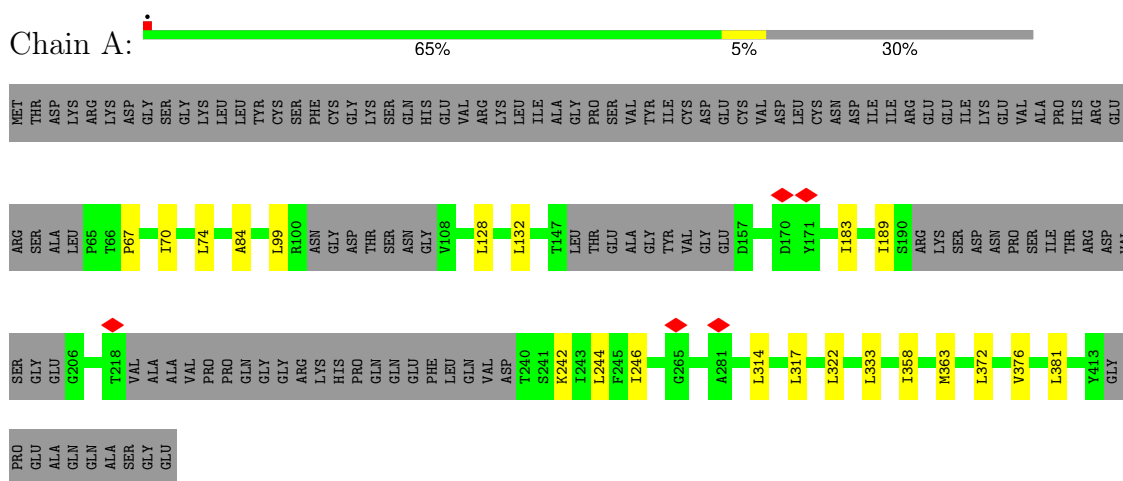
- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
5	B	1	Total	Mg	0
			1	1	
5	D	2	Total	Mg	0
			2	2	
5	E	1	Total	Mg	0
			1	1	

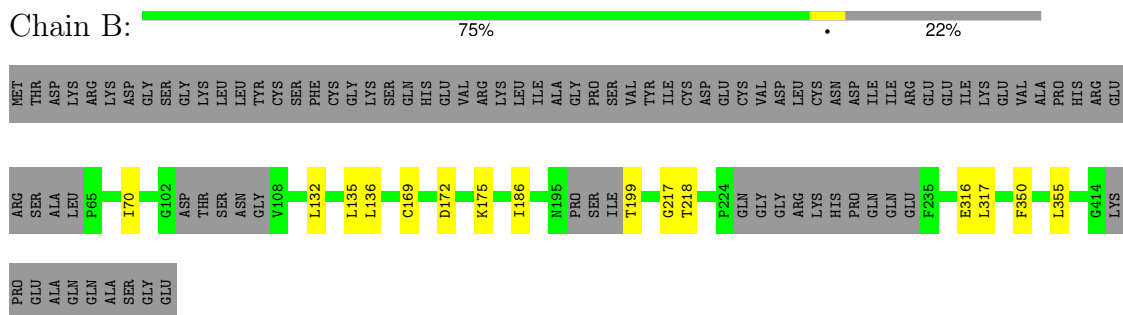
3 Residue-property plots

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.

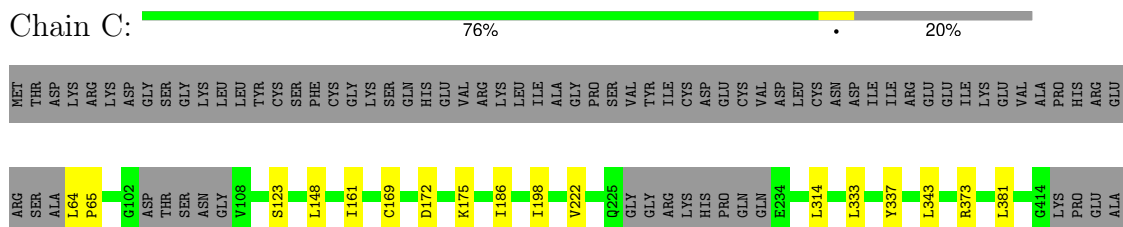
- Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpX



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




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



GLN
GLN
ALA
SER
GLY
GLU


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

Chain D:  78% 20%

MET THR ASP LYS ARG LYS ASP GLY SER GLY LYS LEU LEU TYR CYS SER PHE CYS GLY LYS SER HIS VAL ARG LYS LEU ILE GLY ALA PRO SER VAL TYR ILE CYS ASP GLU CYS VAL ASP LEU CYS ASN ASP ILE ILE ARG GLU ILE ILE LYS VAL VAL PRO HIS ARG GLU

ARG SER A63 W87 K97 G102 THR SER ASN GLY V108 C169 D172 T218 V219 V222 P223 P224 GLN GLY ARG LYS HIS PRO SER VAL TYR ILE E234 A312 T412 V413 G414 LYS PRO GLU ALA ALA GLN ALA SER GLY GLU

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

Chain E:  79% 20%

MET THR ASP LYS ARG LYS ASP GLY SER GLY LYS LEU LEU TYR CYS SER PHE CYS GLY LYS SER HIS VAL ARG LYS LEU ILE GLY ALA PRO SER VAL TYR ILE CYS ASP GLU CYS VAL ASP LEU CYS ASN ASP ILE ILE ARG GLU ILE ILE LYS VAL VAL PRO HIS ARG GLU

ARG SER L64 T141 L165 C169 K175 I183 K192 ASP R195 Q225 GLY ARG LYS HIS PRO SER VAL TYR ILE E234 K280 A281 E391 D392 V393 Q406 C414 LYS PRO GLU ALA GLN ALA SER GLY GLU

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

Chain F:  74% 22%

MET THR ASP LYS ARG LYS ASP GLY SER GLY LYS LEU LEU TYR CYS SER PHE CYS GLY LYS SER HIS VAL ARG LYS LEU ILE GLY ALA PRO SER VAL TYR ILE CYS ASP GLU CYS VAL ASP LEU CYS ASN ASP ILE ILE ARG GLU ILE ILE LYS VAL VAL PRO HIS ARG GLU

ARG SER L64 L88 A91 V92 I115 L132 L148 I161 L166 C169 D172 I189 K192 ASP ASN PRO SER ILE T199 Q225 GLY ARG LYS HIS PRO GLN GLU P235 A276 LYS SER ASP A281 N315 E316 L317 A364

D399 V402 Q406 Y413 GLY LYS PRO GLU ALA GLN ALA SER GLY GLU

• Molecule 2: Arc family DNA-binding protein

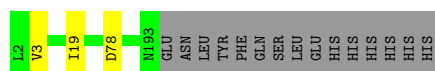
Chain G:  11% 87%

M1 N8 N9 F10 GLY ARG ALA SER MET GLY LYS MET SER LYS MET PRO PHE ASN ARG TRP PRO ARG GLU VAL LEU ASP LEU VAL ARG LYS VAL ALA GLU GLU ASN GLY ARG SER VAL ASN SER GLU ILE TYR GLN ARG VAL MET GLU SER PHE LYS LYS GLU ARG

ILE GLY ALA HIS HIS HIS HIS HIS ASN GLN HIS ASP

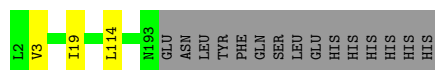
• Molecule 3: ATP-dependent Clp protease proteolytic subunit

Chain H:  91% 7%



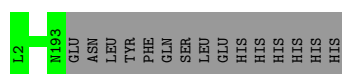
- Molecule 3: ATP-dependent Clp protease proteolytic subunit

Chain I: 91% 7%



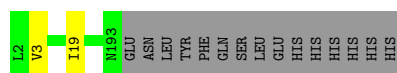
- Molecule 3: ATP-dependent Clp protease proteolytic subunit

Chain J: 93% 7%



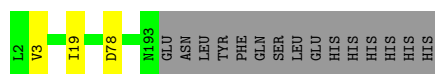
- Molecule 3: ATP-dependent Clp protease proteolytic subunit

Chain K: 92% 7%



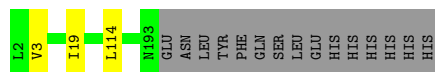
- Molecule 3: ATP-dependent Clp protease proteolytic subunit

Chain L: 91% 7%



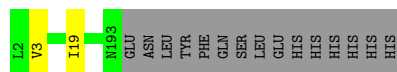
- Molecule 3: ATP-dependent Clp protease proteolytic subunit

Chain M: 91% 7%



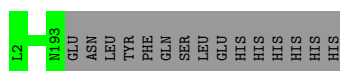
- Molecule 3: ATP-dependent Clp protease proteolytic subunit

Chain N: 92% 7%



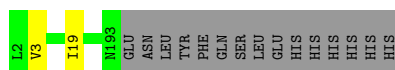
- Molecule 3: ATP-dependent Clp protease proteolytic subunit

Chain O: 93% 7%



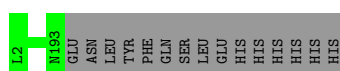
- Molecule 3: ATP-dependent Clp protease proteolytic subunit

Chain P:  92% 7%



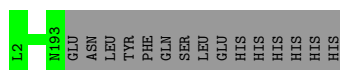
- Molecule 3: ATP-dependent Clp protease proteolytic subunit

Chain Q:  93% 7%



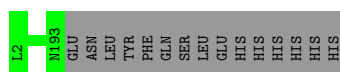
- Molecule 3: ATP-dependent Clp protease proteolytic subunit

Chain R:  93% 7%



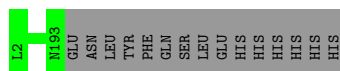
- Molecule 3: ATP-dependent Clp protease proteolytic subunit

Chain S:  93% 7%



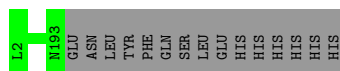
- Molecule 3: ATP-dependent Clp protease proteolytic subunit

Chain T:  93% 7%



- Molecule 3: ATP-dependent Clp protease proteolytic subunit

Chain U:  93% 7%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	217969	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE; Patch CTF estimation, cryoSPARC	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	52.67	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	1750	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.857	Depositor
Minimum map value	-0.392	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.031	Depositor
Recommended contour level	0.0577	Depositor
Map size (\AA)	287.744, 287.744, 287.744	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.124, 1.124, 1.124	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	0.07	0/2313	0.24	0/3118
1	B	0.07	0/2574	0.23	0/3475
1	C	0.07	0/2623	0.22	0/3545
1	D	0.07	0/2619	0.20	0/3540
1	E	0.07	0/2642	0.20	0/3571
1	F	0.07	0/2566	0.22	0/3468
2	G	0.05	0/79	0.19	0/105
3	H	0.06	0/1527	0.18	0/2058
3	I	0.06	0/1527	0.18	0/2058
3	J	0.06	0/1527	0.17	0/2058
3	K	0.06	0/1527	0.17	0/2058
3	L	0.06	0/1527	0.17	0/2058
3	M	0.06	0/1527	0.18	0/2058
3	N	0.06	0/1527	0.17	0/2058
3	O	0.06	0/1527	0.17	0/2058
3	P	0.06	0/1527	0.17	0/2058
3	Q	0.05	0/1527	0.17	0/2058
3	R	0.06	0/1527	0.17	0/2058
3	S	0.05	0/1527	0.17	0/2058
3	T	0.06	0/1527	0.17	0/2058
3	U	0.05	0/1527	0.17	0/2058
All	All	0.06	0/36794	0.19	0/49634

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2288	2352	2364	17	0
1	B	2544	2604	2607	14	0
1	C	2591	2652	2655	18	0
1	D	2587	2648	2651	8	0
1	E	2610	2667	2670	7	0
1	F	2536	2594	2597	11	0
2	G	79	86	86	1	0
3	H	1503	1513	1513	2	0
3	I	1503	1513	1513	2	0
3	J	1503	1513	1513	0	0
3	K	1503	1513	1513	1	0
3	L	1503	1513	1513	2	0
3	M	1503	1513	1513	2	0
3	N	1503	1513	1513	1	0
3	O	1503	1513	1513	0	0
3	P	1503	1513	1513	1	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
4	B	31	12	12	0	0
4	C	31	12	12	0	0
4	D	31	12	12	0	0
4	E	31	12	12	0	0
4	F	31	12	12	0	0
5	B	1	0	0	0	0
5	D	2	0	0	0	0
5	E	1	0	0	0	0
All	All	36436	36845	36872	82	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 1.

All (82) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:CYS:SG	1:B:172:ASP:HB3	2.02	0.99
1:C:169:CYS:SG	1:C:175:LYS:HB3	2.05	0.95
1:C:169:CYS:SG	1:C:172:ASP:HB3	2.08	0.93
1:E:169:CYS:SG	1:E:175:LYS:HB3	2.13	0.88
1:D:169:CYS:SG	1:D:172:ASP:OD1	2.37	0.81
1:B:70:ILE:HD11	1:B:135:LEU:HD13	1.72	0.71
1:F:166:LEU:HA	1:F:169:CYS:SG	2.34	0.68
1:B:132:LEU:HD12	1:B:135:LEU:HD11	1.79	0.64
1:F:92:VAL:HG21	1:F:132:LEU:HD21	1.80	0.63
1:C:169:CYS:SG	1:C:175:LYS:CB	2.85	0.61
1:B:169:CYS:SG	1:B:172:ASP:CB	2.87	0.60
1:B:135:LEU:HD12	1:B:136:LEU:N	2.20	0.57
1:E:169:CYS:SG	1:E:175:LYS:HE2	2.47	0.55
1:C:169:CYS:HG	1:C:172:ASP:HB3	1.69	0.54
1:F:399:ASP:OD1	1:F:402:VAL:HG23	2.09	0.52
1:A:358:ILE:HD11	1:A:376:VAL:HG22	1.92	0.51
1:A:372:LEU:O	1:A:376:VAL:HG23	2.09	0.51
1:A:358:ILE:CD1	1:A:376:VAL:HG22	2.40	0.51
1:C:333:LEU:HD11	1:C:337:TYR:CE2	2.46	0.50
1:E:169:CYS:SG	1:E:175:LYS:CE	3.00	0.50
1:A:322:LEU:HD11	1:A:363:MET:HE2	1.93	0.50
1:A:128:LEU:O	1:A:132:LEU:HD23	2.11	0.50
1:B:350:PHE:HB3	1:B:355:LEU:HD21	1.93	0.49
1:A:317:LEU:O	1:A:363:MET:HE1	2.13	0.49
1:C:381:LEU:HD11	1:D:87:VAL:HG12	1.95	0.48
1:F:317:LEU:H	1:F:317:LEU:HD23	1.79	0.48
1:A:183:ILE:HD12	1:A:183:ILE:N	2.29	0.47
1:D:87:VAL:HG21	1:D:312:ALA:HB2	1.98	0.46
1:B:169:CYS:SG	1:B:175:LYS:HB3	2.56	0.46
1:C:148:LEU:HD11	1:C:161:ILE:HD11	1.99	0.45
1:A:84:ALA:CB	1:A:314:LEU:HD23	2.47	0.45
3:H:78:ASP:HB2	3:I:114:LEU:HD13	1.99	0.45
1:A:322:LEU:CD1	1:A:363:MET:HE2	2.47	0.44
1:A:244:LEU:CD2	1:A:246:ILE:HG23	2.47	0.44
1:A:381:LEU:C	1:A:381:LEU:HD23	2.42	0.44
1:D:169:CYS:SG	1:D:169:CYS:O	2.75	0.44
1:A:67:PRO:HA	1:A:70:ILE:HG22	1.99	0.44
1:C:333:LEU:HD13	1:C:373:ARG:CD	2.47	0.44
1:A:189:ILE:N	1:A:189:ILE:HD12	2.33	0.44
1:C:222:VAL:HG23	1:C:222:VAL:O	2.18	0.44
1:E:169:CYS:SG	1:E:169:CYS:O	2.76	0.43
1:B:199:THR:HG21	2:G:8:LEU:HD13	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:3:VAL:HG13	3:M:19:ILE:HG22	2.00	0.43
1:A:333:LEU:CD1	1:A:376:VAL:HG21	2.48	0.43
1:F:92:VAL:CG2	1:F:132:LEU:HD21	2.47	0.43
1:B:70:ILE:CD1	1:B:135:LEU:HD13	2.44	0.42
1:D:218:THR:HG22	1:D:219:VAL:N	2.35	0.42
1:A:333:LEU:HD13	1:A:376:VAL:HG21	2.02	0.42
1:B:316:GLU:O	1:B:317:LEU:HG	2.19	0.42
3:L:3:VAL:HG13	3:L:19:ILE:HG22	2.02	0.42
3:H:3:VAL:HG13	3:H:19:ILE:HG22	2.02	0.42
1:C:169:CYS:SG	1:C:175:LYS:CG	3.07	0.42
3:L:78:ASP:HB2	3:M:114:LEU:HD13	2.00	0.42
1:C:198:ILE:HD12	1:C:198:ILE:H	1.85	0.42
1:E:141:THR:HG21	1:E:165:LEU:HA	2.01	0.42
1:E:391:GLU:O	1:E:393:VAL:HG23	2.20	0.42
3:N:3:VAL:HG13	3:N:19:ILE:HG22	2.02	0.42
1:B:70:ILE:HD11	1:B:135:LEU:CD1	2.47	0.41
1:B:132:LEU:O	1:B:136:LEU:HD22	2.20	0.41
1:F:189:ILE:O	1:F:189:ILE:HG22	2.20	0.41
1:C:186:ILE:N	1:C:186:ILE:HD12	2.36	0.41
1:F:169:CYS:HB2	1:F:172:ASP:OD1	2.20	0.41
3:K:3:VAL:HG13	3:K:19:ILE:HG22	2.02	0.41
1:C:123:SER:HB3	1:C:314:LEU:HD23	2.03	0.41
1:C:343:LEU:HD11	1:D:97:LYS:HE2	2.01	0.41
1:A:74:LEU:HD11	1:A:132:LEU:HD22	2.03	0.41
1:E:183:ILE:HD12	1:E:183:ILE:N	2.35	0.41
1:D:412:ILE:HD12	1:D:412:ILE:N	2.35	0.41
1:D:222:VAL:O	1:D:222:VAL:HG13	2.19	0.41
1:C:169:CYS:SG	1:C:169:CYS:O	2.79	0.41
1:F:88:LEU:O	1:F:92:VAL:HG23	2.21	0.41
1:F:91:ALA:HB1	1:F:115:ILE:HD11	2.02	0.41
1:A:99:LEU:HD21	1:A:242:LYS:O	2.21	0.41
1:B:186:ILE:HD12	1:B:186:ILE:N	2.36	0.40
1:B:217:GLY:O	1:B:218:THR:HG23	2.21	0.40
1:F:315:ASN:O	1:F:316:GLU:HB2	2.22	0.40
3:P:3:VAL:HG13	3:P:19:ILE:HG22	2.03	0.40
3:I:3:VAL:HG13	3:I:19:ILE:HG22	2.03	0.40
1:C:64:LEU:HB3	1:C:65:PRO:HD3	2.03	0.40
1:C:64:LEU:N	1:C:65:PRO:CD	2.84	0.40
1:C:333:LEU:HD13	1:C:373:ARG:HD2	2.04	0.40
1:F:148:LEU:HD21	1:F:161:ILE:HD11	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	287/424 (68%)	283 (99%)	4 (1%)	0	100	100
1	B	324/424 (76%)	315 (97%)	9 (3%)	0	100	100
1	C	332/424 (78%)	325 (98%)	7 (2%)	0	100	100
1	D	332/424 (78%)	319 (96%)	13 (4%)	0	100	100
1	E	335/424 (79%)	328 (98%)	7 (2%)	0	100	100
1	F	323/424 (76%)	308 (95%)	15 (5%)	0	100	100
2	G	8/79 (10%)	8 (100%)	0	0	100	100
3	H	190/207 (92%)	186 (98%)	4 (2%)	0	100	100
3	I	190/207 (92%)	186 (98%)	4 (2%)	0	100	100
3	J	190/207 (92%)	187 (98%)	3 (2%)	0	100	100
3	K	190/207 (92%)	187 (98%)	3 (2%)	0	100	100
3	L	190/207 (92%)	187 (98%)	3 (2%)	0	100	100
3	M	190/207 (92%)	187 (98%)	3 (2%)	0	100	100
3	N	190/207 (92%)	187 (98%)	3 (2%)	0	100	100
3	O	190/207 (92%)	186 (98%)	4 (2%)	0	100	100
3	P	190/207 (92%)	187 (98%)	3 (2%)	0	100	100
3	Q	190/207 (92%)	186 (98%)	4 (2%)	0	100	100
3	R	190/207 (92%)	187 (98%)	3 (2%)	0	100	100
3	S	190/207 (92%)	187 (98%)	3 (2%)	0	100	100
3	T	190/207 (92%)	186 (98%)	4 (2%)	0	100	100
3	U	190/207 (92%)	187 (98%)	3 (2%)	0	100	100
All	All	4601/5521 (83%)	4499 (98%)	102 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	248/354 (70%)	248 (100%)	0	100	100
1	B	275/354 (78%)	275 (100%)	0	100	100
1	C	281/354 (79%)	281 (100%)	0	100	100
1	D	280/354 (79%)	280 (100%)	0	100	100
1	E	283/354 (80%)	283 (100%)	0	100	100
1	F	274/354 (77%)	274 (100%)	0	100	100
2	G	9/69 (13%)	9 (100%)	0	100	100
3	H	163/178 (92%)	163 (100%)	0	100	100
3	I	163/178 (92%)	163 (100%)	0	100	100
3	J	163/178 (92%)	163 (100%)	0	100	100
3	K	163/178 (92%)	163 (100%)	0	100	100
3	L	163/178 (92%)	163 (100%)	0	100	100
3	M	163/178 (92%)	163 (100%)	0	100	100
3	N	163/178 (92%)	163 (100%)	0	100	100
3	O	163/178 (92%)	163 (100%)	0	100	100
3	P	163/178 (92%)	163 (100%)	0	100	100
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
All	All	3932/4685 (84%)	3932 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	GLN
1	A	289	GLN
1	C	101	ASN
1	E	163	GLN
1	E	167	GLN
1	E	208	GLN
1	F	114	ASN
3	H	156	HIS
3	J	41	ASN
3	K	156	HIS
3	M	9	GLN
3	M	41	ASN
3	M	156	HIS
3	O	156	HIS
3	P	156	HIS
3	Q	156	HIS
3	R	41	ASN
3	R	156	HIS
3	S	156	HIS
3	T	156	HIS
3	U	156	HIS

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 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	D	502	5	28,33,33	0.74	1 (3%)	31,52,52	0.94	2 (6%)
4	AGS	B	501	-	28,33,33	0.74	1 (3%)	31,52,52	0.94	2 (6%)
4	AGS	E	501	5	28,33,33	0.74	1 (3%)	31,52,52	0.96	2 (6%)
4	AGS	C	501	-	28,33,33	0.75	1 (3%)	31,52,52	0.92	2 (6%)
4	AGS	F	600	-	28,33,33	0.73	1 (3%)	31,52,52	0.92	2 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	AGS	D	502	5	-	2/17/38/38	0/3/3/3
4	AGS	B	501	-	-	2/17/38/38	0/3/3/3
4	AGS	E	501	5	-	2/17/38/38	0/3/3/3
4	AGS	C	501	-	-	4/17/38/38	0/3/3/3
4	AGS	F	600	-	-	2/17/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	501	AGS	PG-S1G	2.16	1.95	1.90
4	F	600	AGS	PG-S1G	2.13	1.95	1.90
4	E	501	AGS	PG-S1G	2.12	1.95	1.90
4	D	502	AGS	PG-S1G	2.12	1.95	1.90
4	C	501	AGS	PG-S1G	2.09	1.95	1.90

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	501	AGS	PB-O3B-PG	-3.72	119.57	133.17
4	D	502	AGS	PB-O3B-PG	-3.59	120.02	133.17
4	B	501	AGS	PB-O3B-PG	-3.59	120.04	133.17
4	F	600	AGS	PB-O3B-PG	-3.41	120.70	133.17
4	C	501	AGS	PB-O3B-PG	-3.36	120.87	133.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	501	AGS	C5-C6-N6	2.33	123.86	120.31
4	C	501	AGS	C5-C6-N6	2.32	123.84	120.31
4	F	600	AGS	C5-C6-N6	2.30	123.82	120.31
4	D	502	AGS	C5-C6-N6	2.28	123.78	120.31
4	E	501	AGS	C5-C6-N6	2.27	123.77	120.31

There are no chirality outliers.

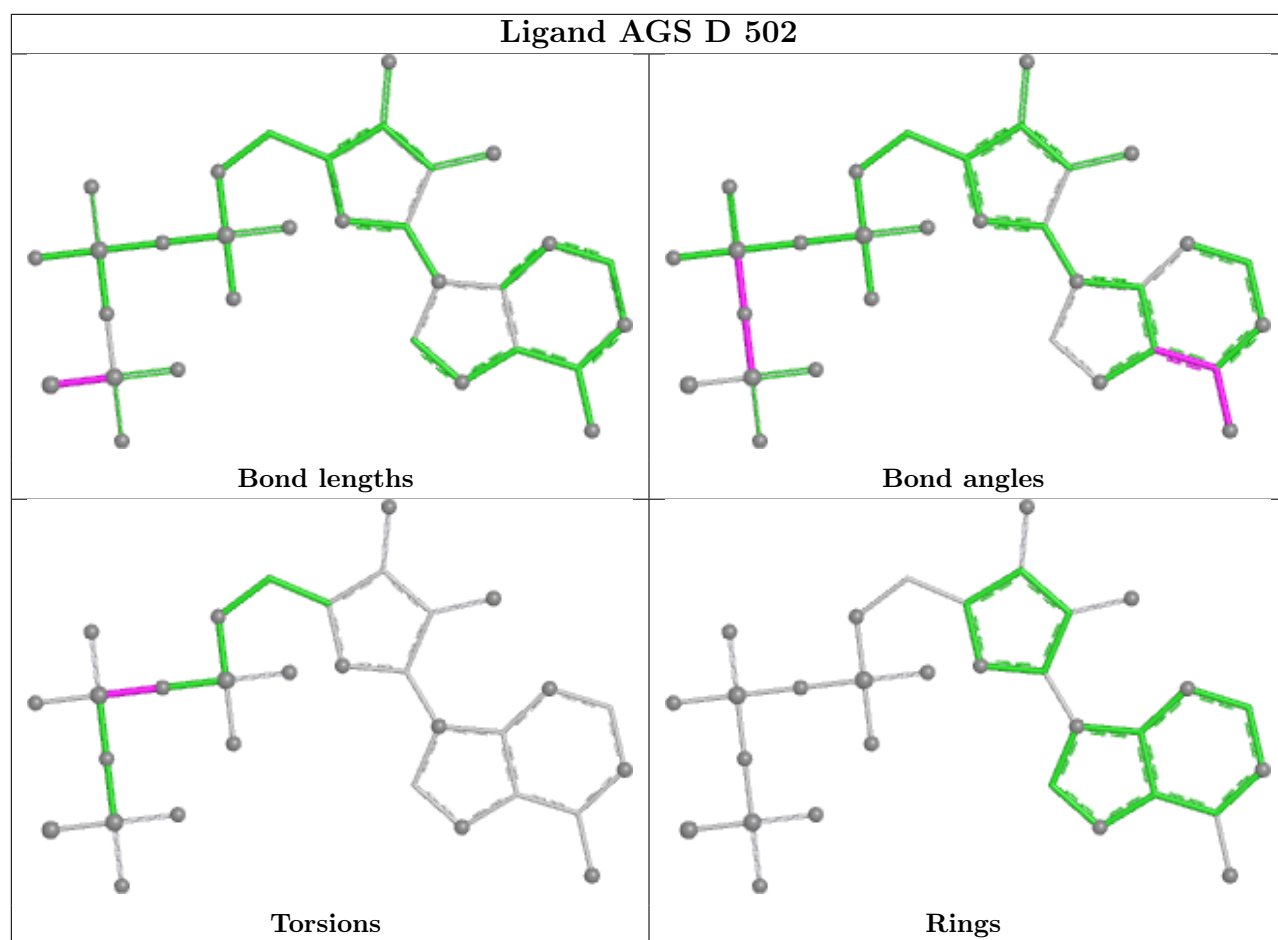
All (12) torsion outliers are listed below:

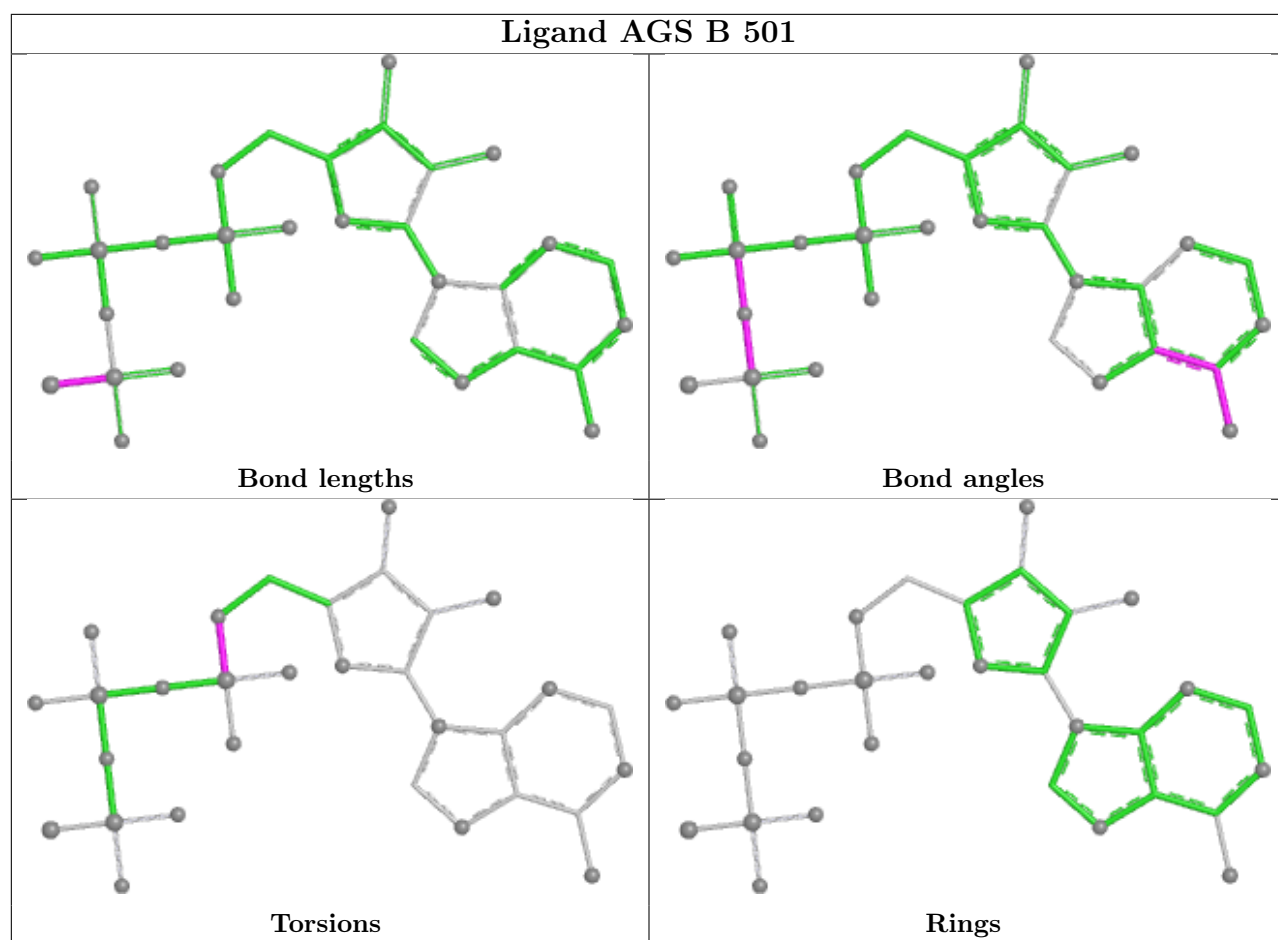
Mol	Chain	Res	Type	Atoms
4	B	501	AGS	C5'-O5'-PA-O2A
4	B	501	AGS	C5'-O5'-PA-O3A
4	C	501	AGS	C5'-O5'-PA-O2A
4	C	501	AGS	C5'-O5'-PA-O3A
4	F	600	AGS	C5'-O5'-PA-O2A
4	F	600	AGS	C5'-O5'-PA-O3A
4	C	501	AGS	O4'-C4'-C5'-O5'
4	C	501	AGS	C3'-C4'-C5'-O5'
4	D	502	AGS	PA-O3A-PB-O2B
4	E	501	AGS	PA-O3A-PB-O1B
4	E	501	AGS	PA-O3A-PB-O2B
4	D	502	AGS	PA-O3A-PB-O1B

There are no ring outliers.

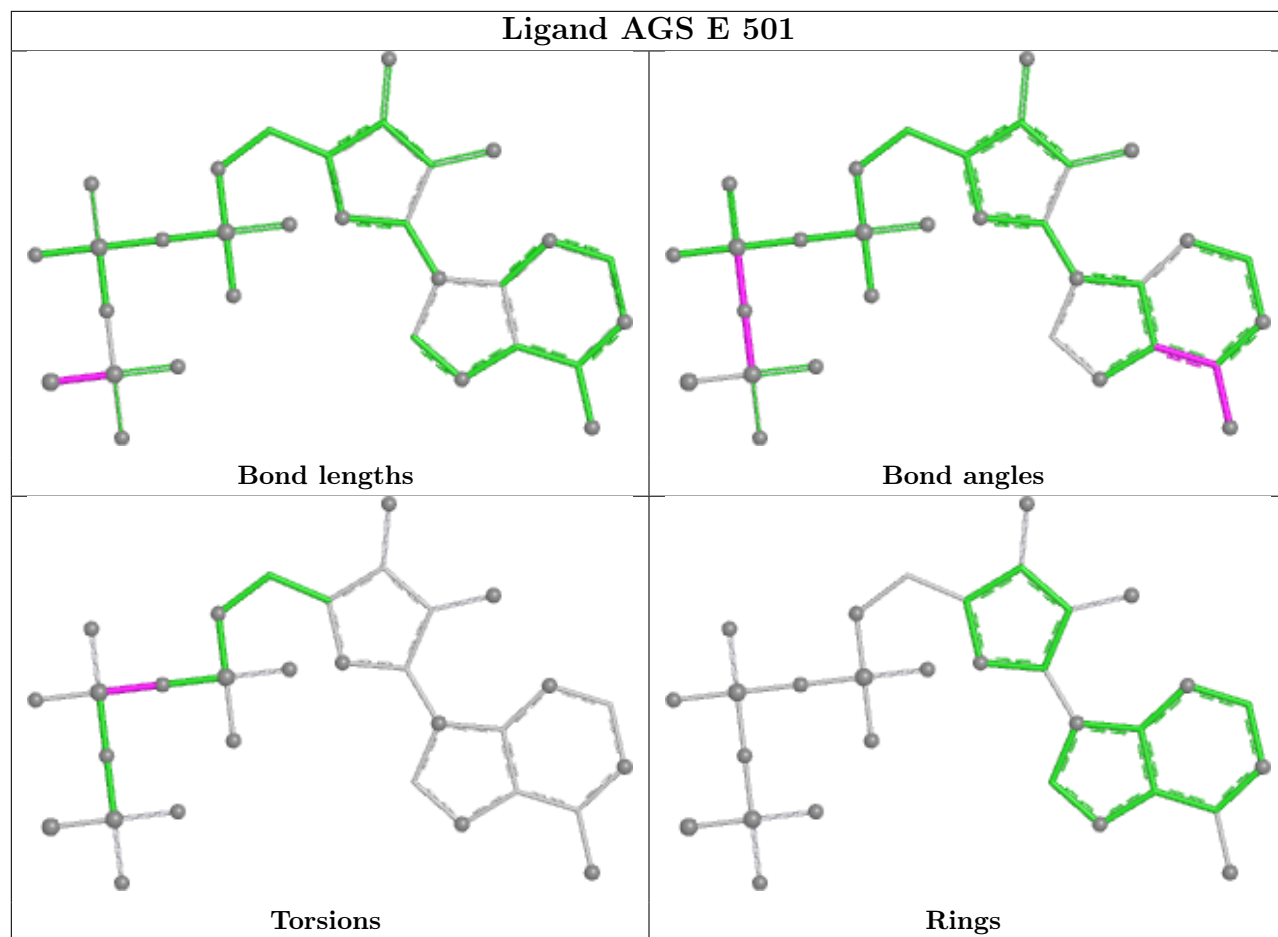
No monomer is involved in short contacts.

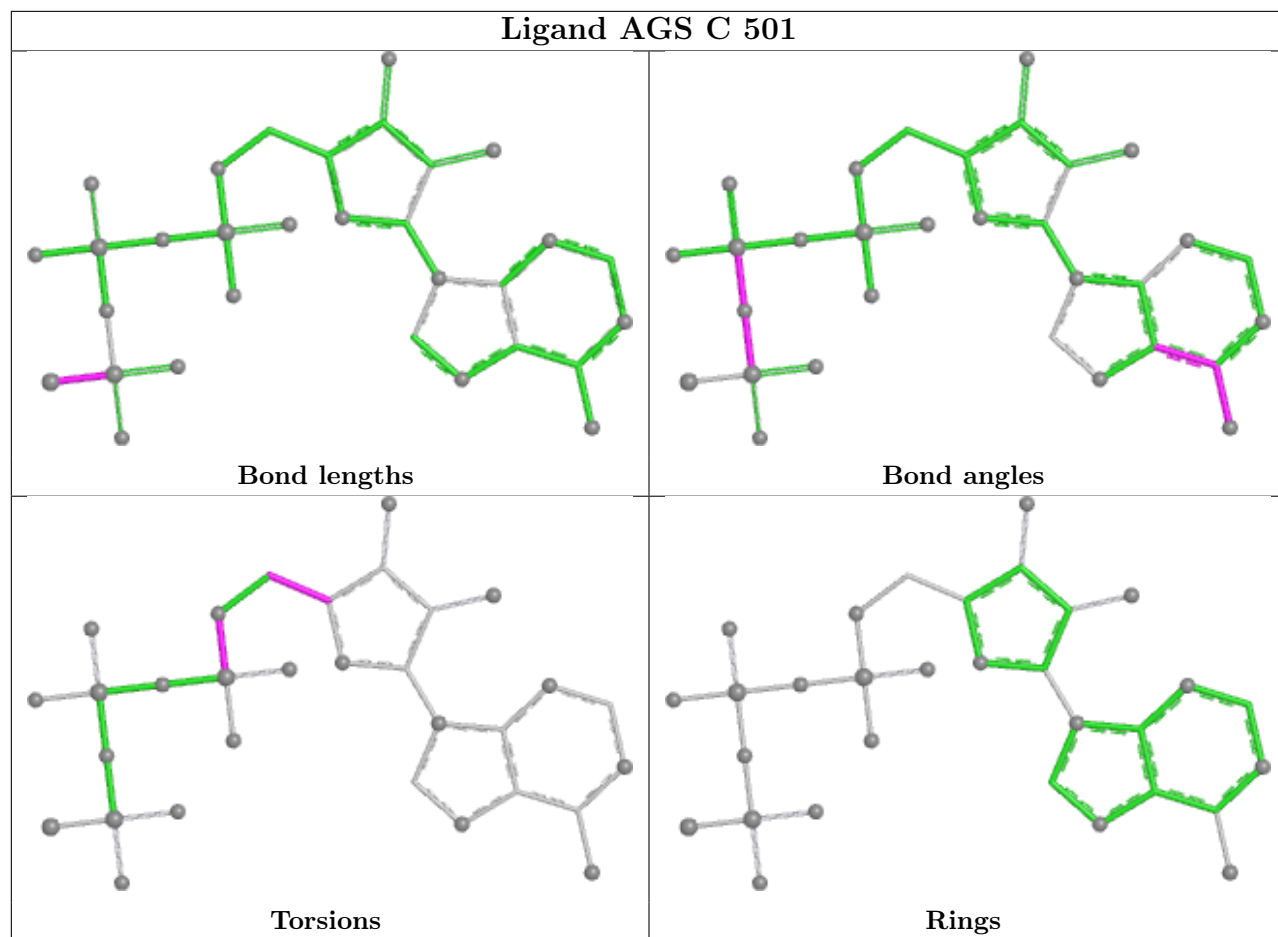
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

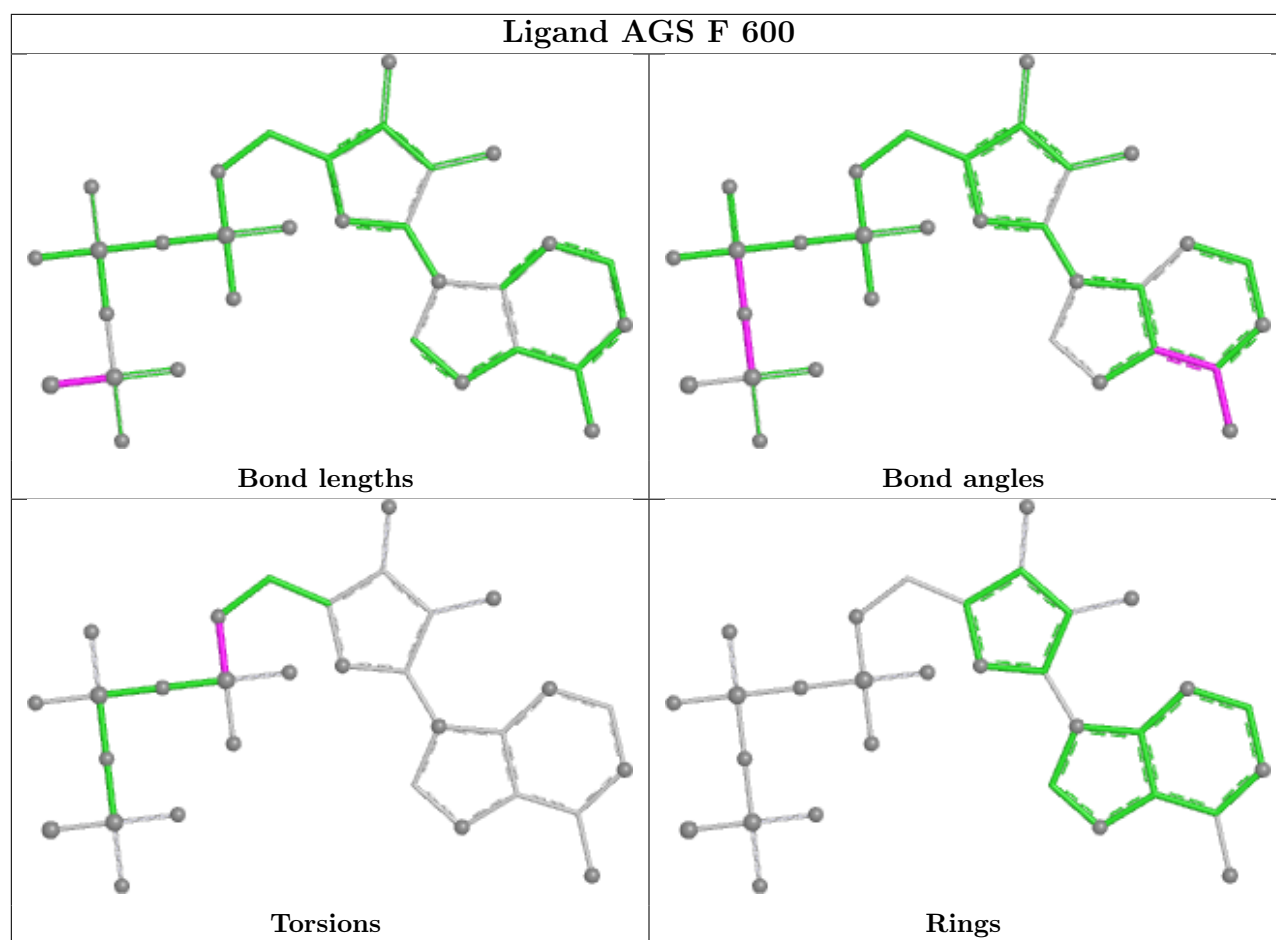




Ligand AGS E 501







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.

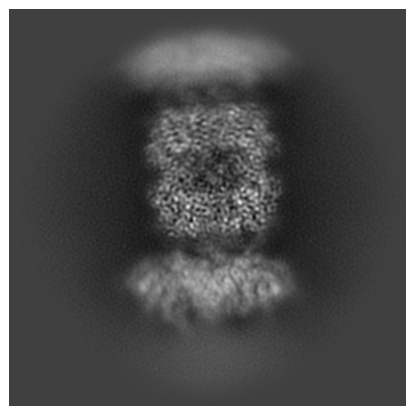
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71674. These allow visual inspection of the internal detail of the map and identification of artifacts.

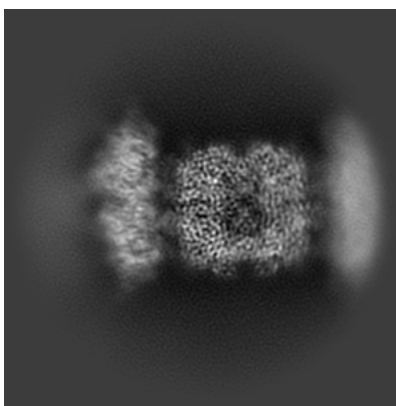
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

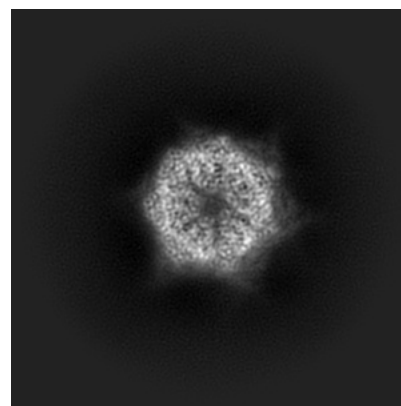
6.1.1 Primary map



X

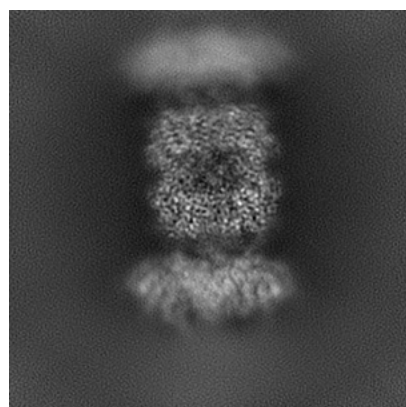


Y

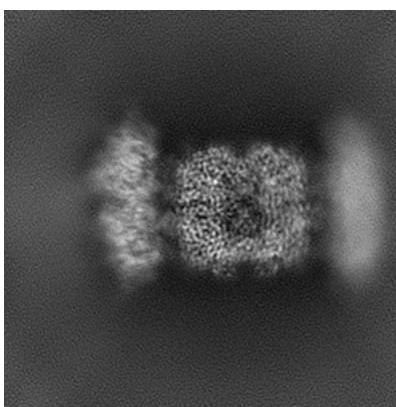


Z

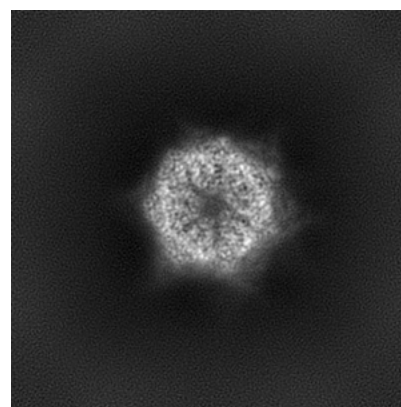
6.1.2 Raw map



X



Y

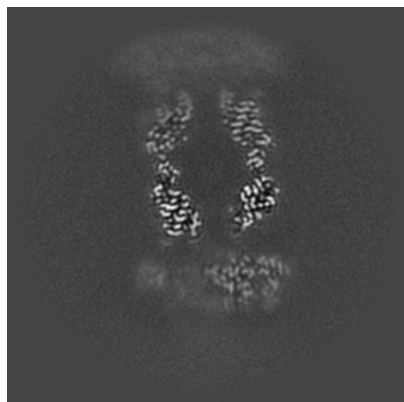


Z

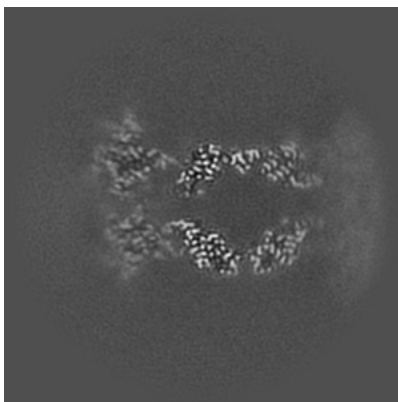
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

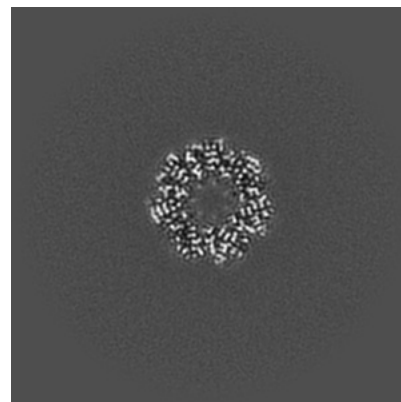
6.2.1 Primary map



X Index: 128

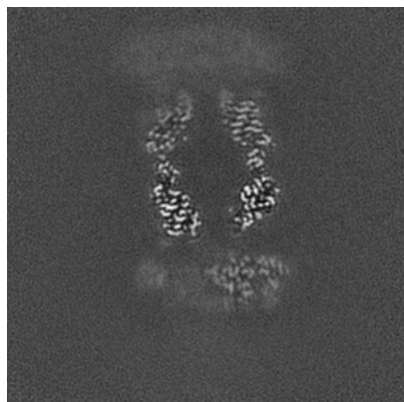


Y Index: 128

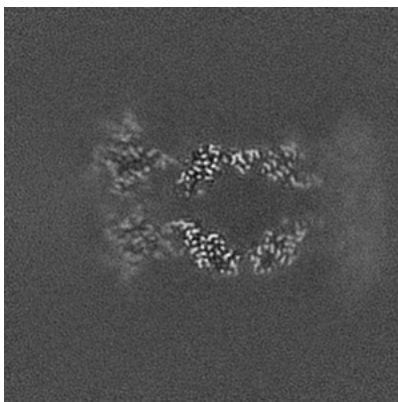


Z Index: 128

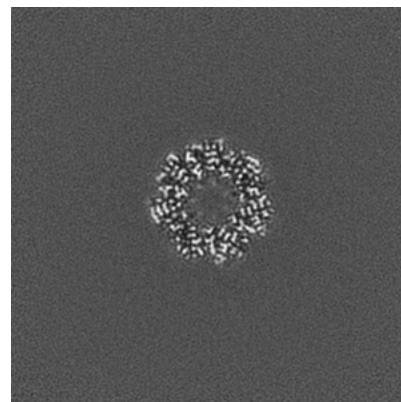
6.2.2 Raw map



X Index: 128



Y Index: 128

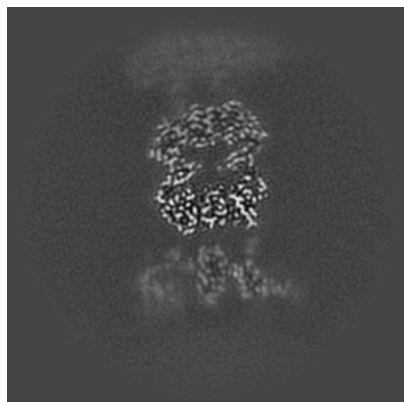


Z Index: 128

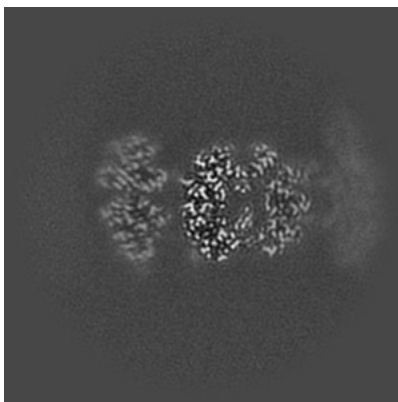
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

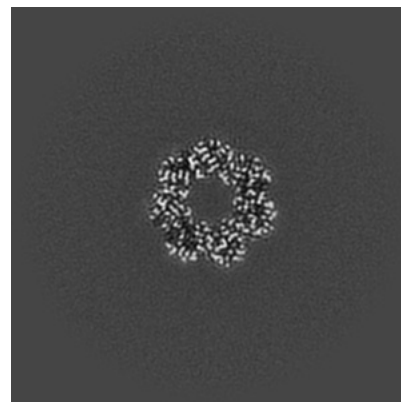
6.3.1 Primary map



X Index: 108

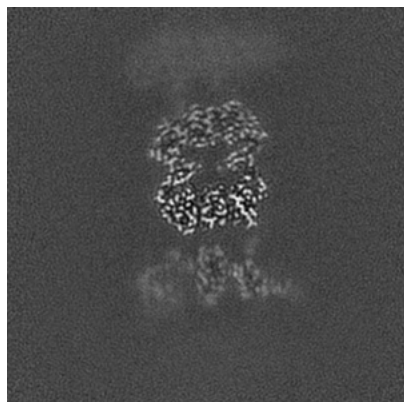


Y Index: 152

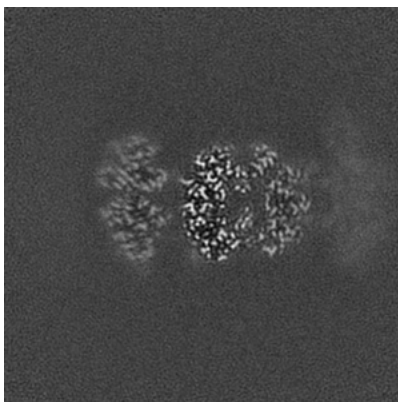


Z Index: 132

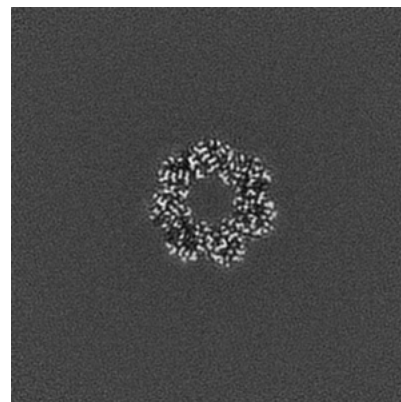
6.3.2 Raw map



X Index: 108



Y Index: 152

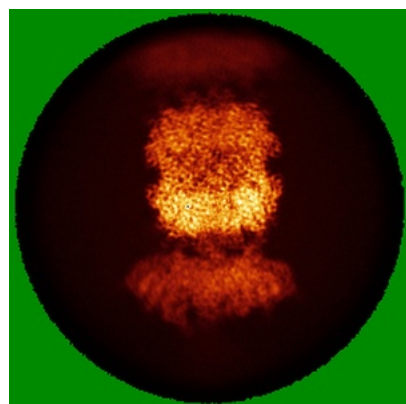


Z Index: 132

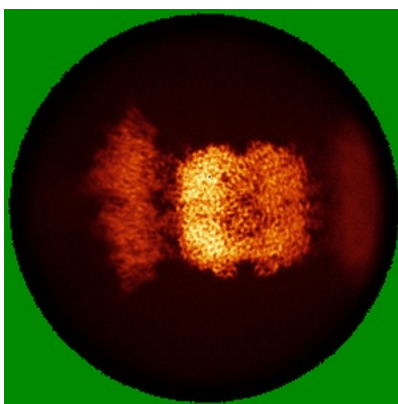
The images above show the largest variance slices of the map in three orthogonal directions.

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

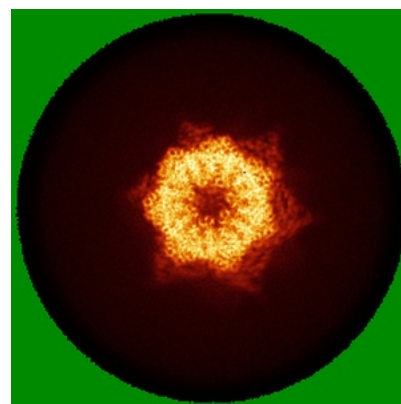
6.4.1 Primary map



X

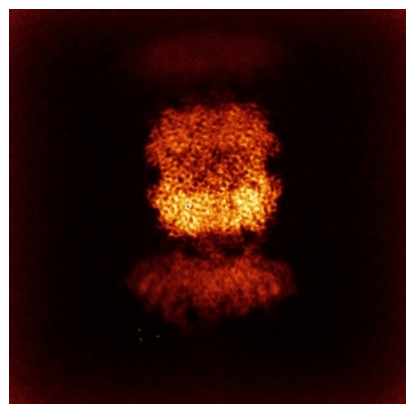


Y

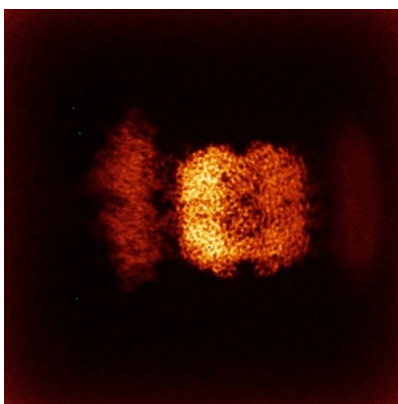


Z

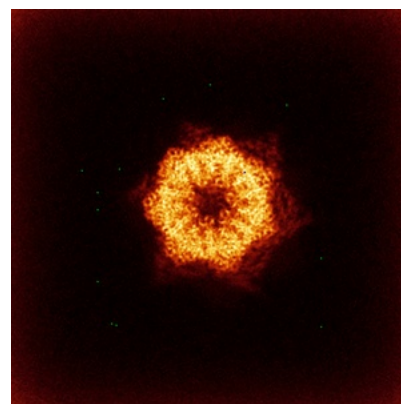
6.4.2 Raw map



X



Y



Z

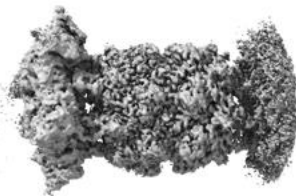
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

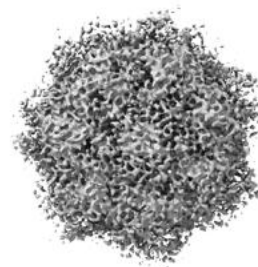
6.5.1 Primary map



X



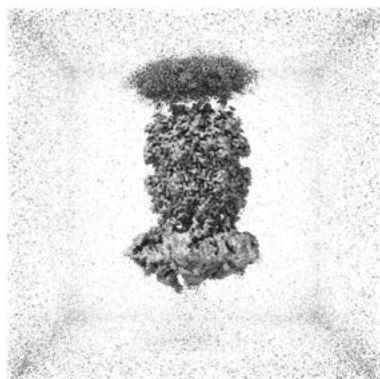
Y



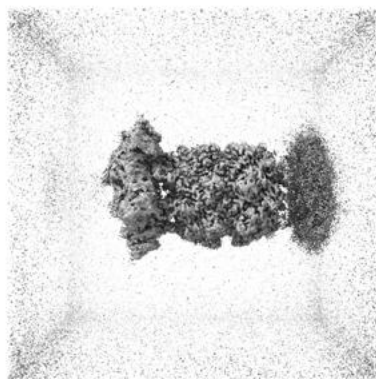
Z

The images above show the 3D surface view of the map at the recommended contour level 0.0577. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

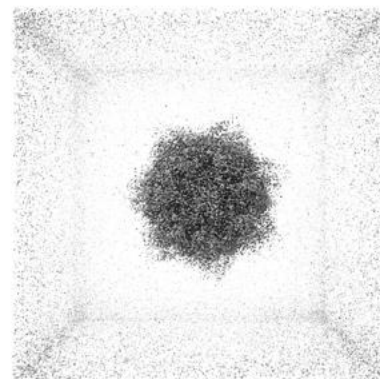
6.5.2 Raw map



X



Y



Z

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

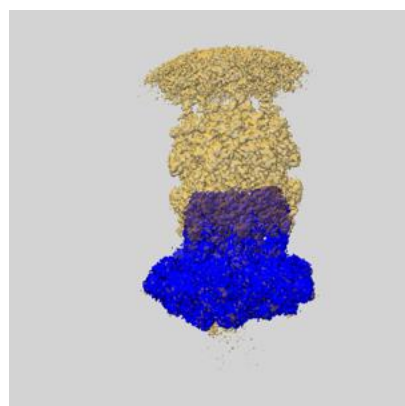
6.6 Mask visualisation [i](#)

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

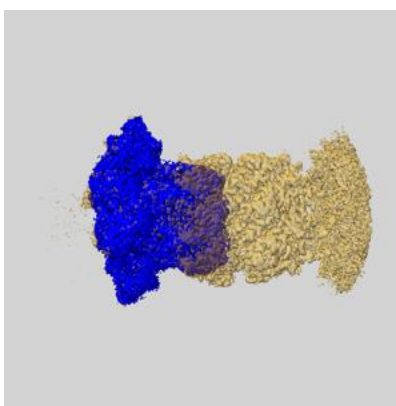
A mask typically either:

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

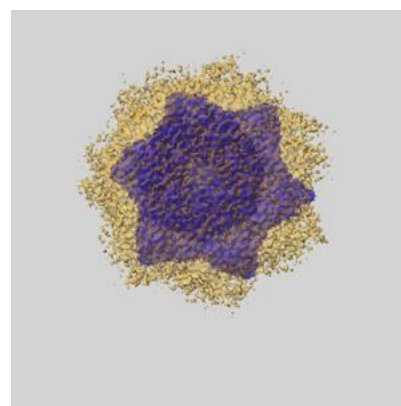
6.6.1 emd_71674_msk_1.map [i](#)



X



Y

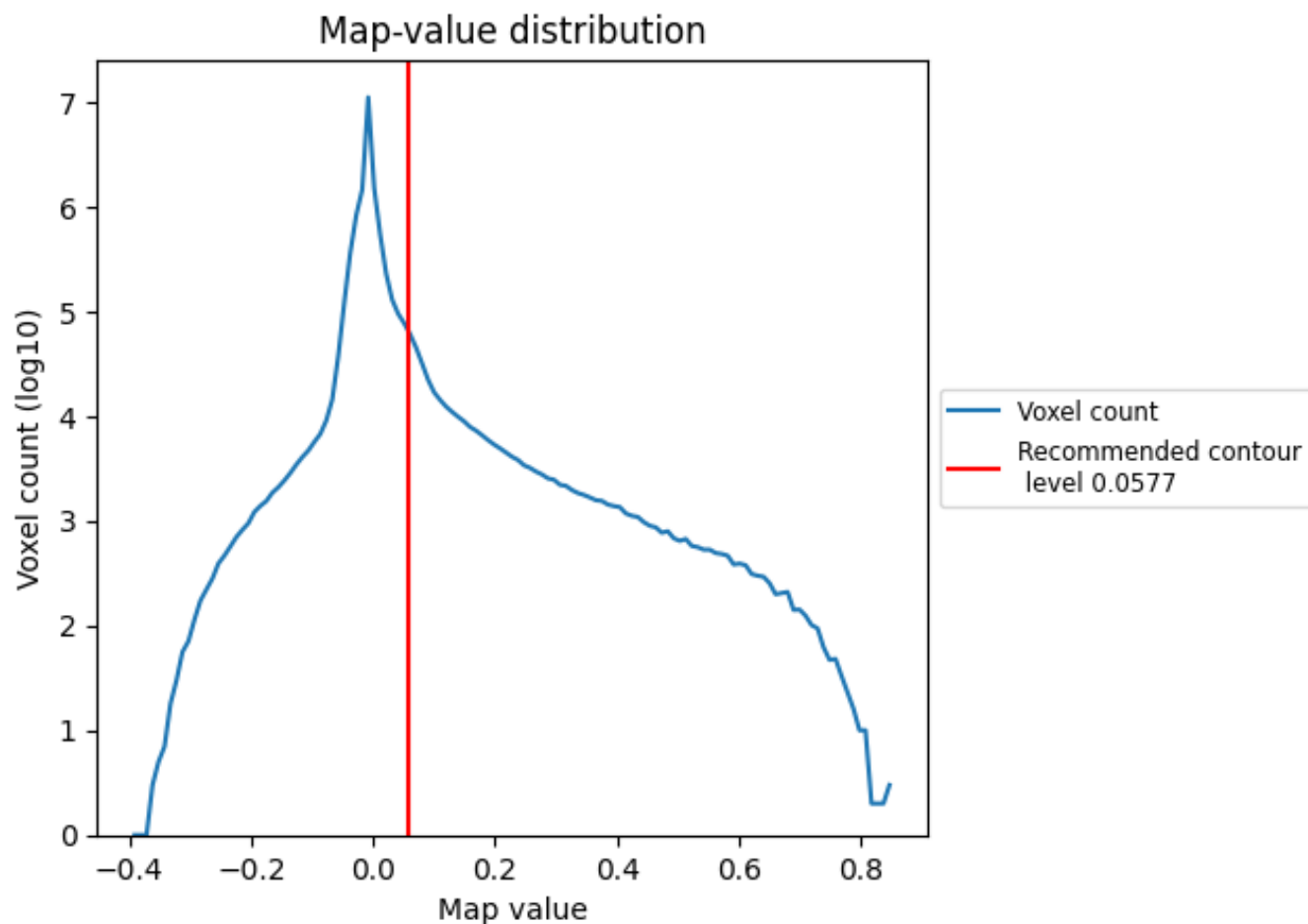


Z

7 Map analysis [i](#)

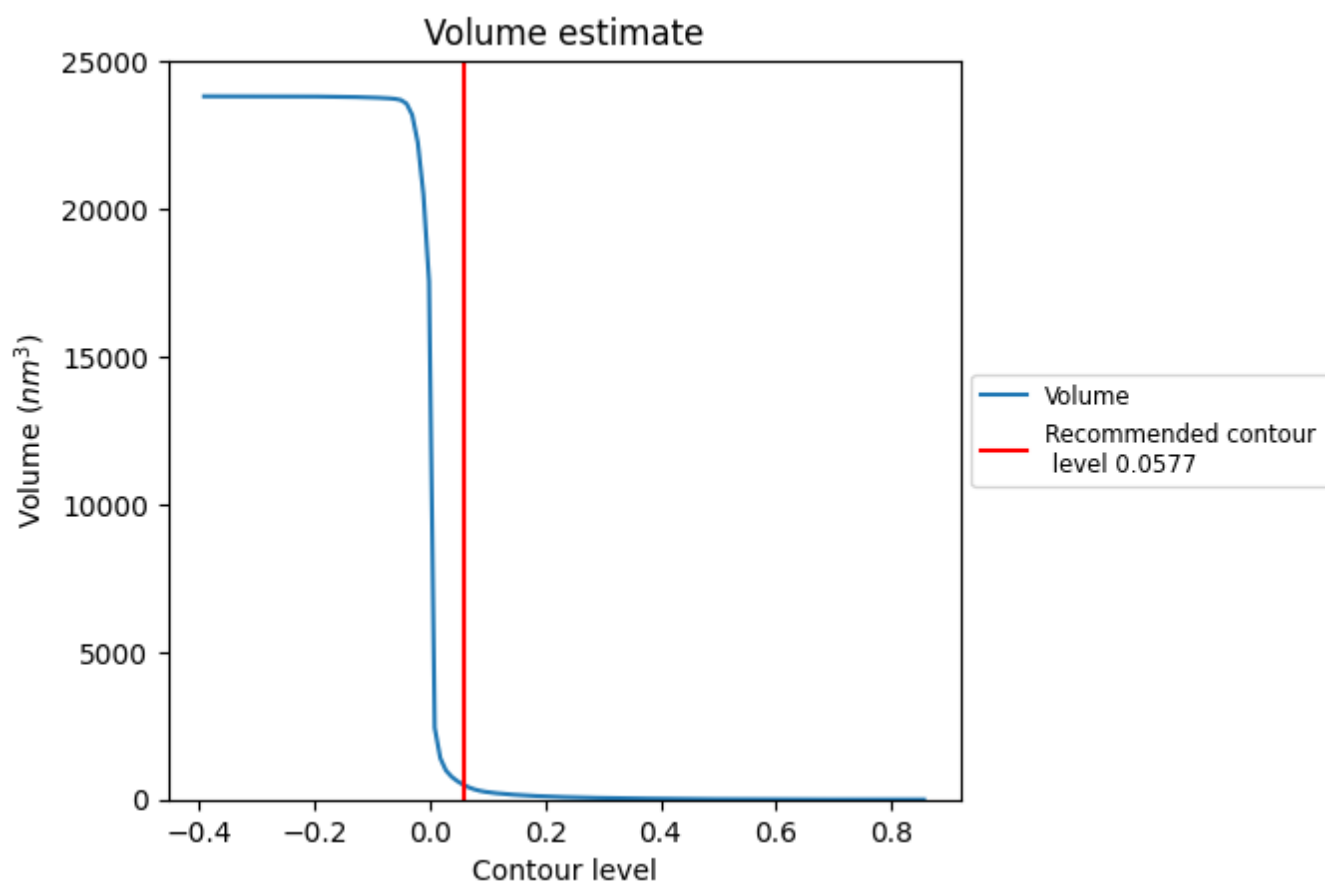
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

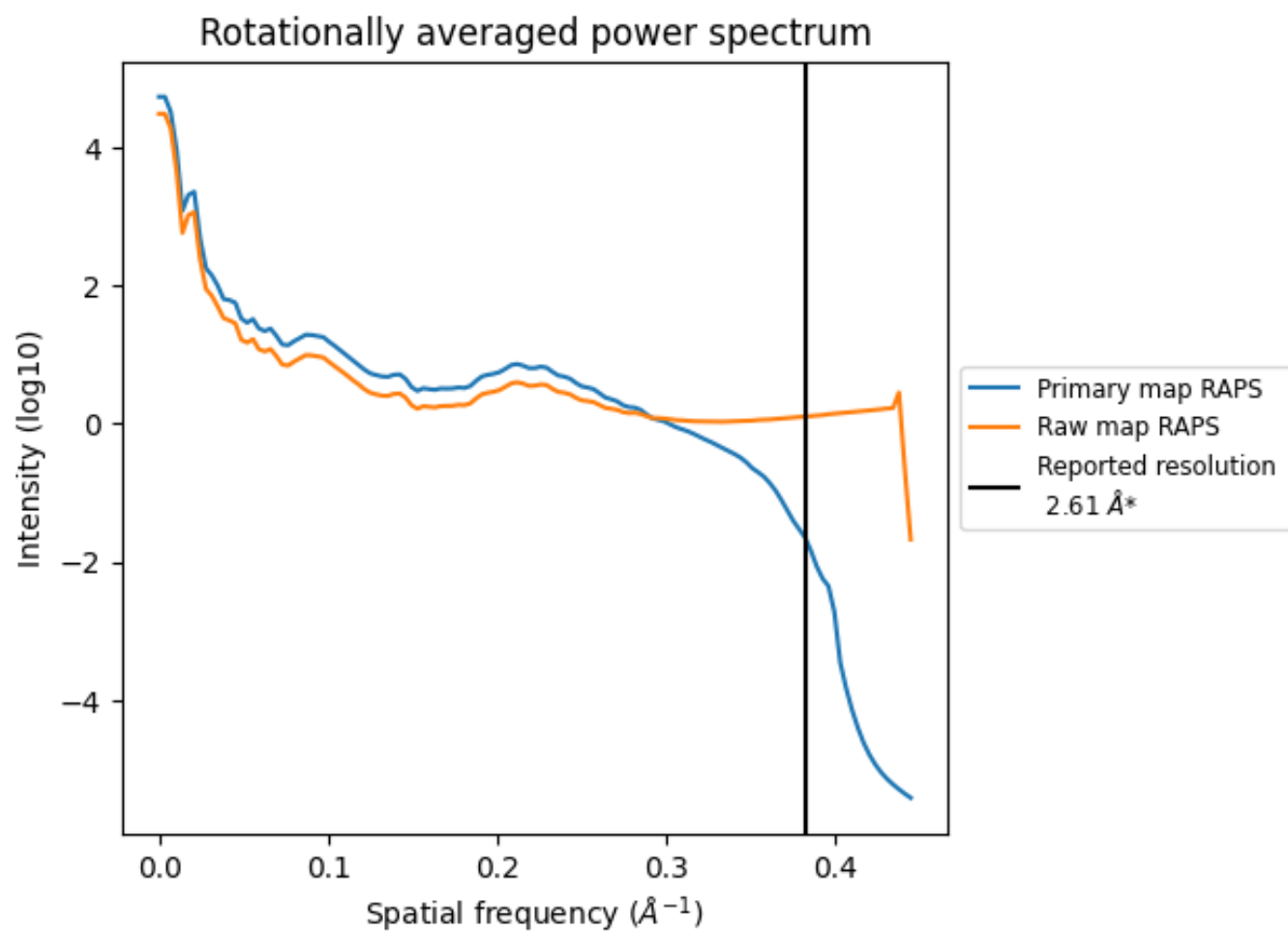
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 507 nm³; this corresponds to an approximate mass of 458 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](#)

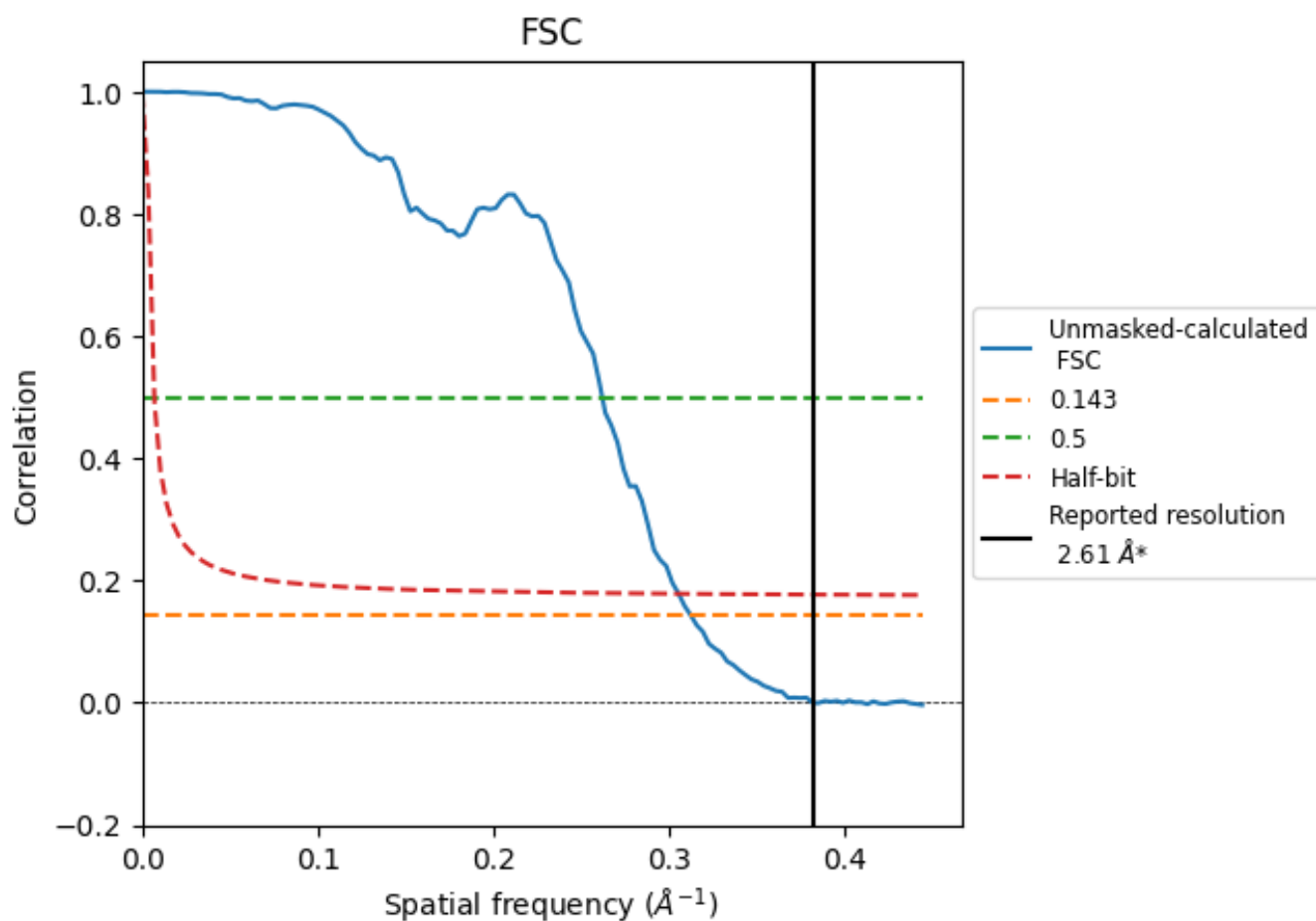


*Reported resolution corresponds to spatial frequency of 0.383 Å⁻¹

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 0.383 \AA^{-1}

8.2 Resolution estimates [i](#)

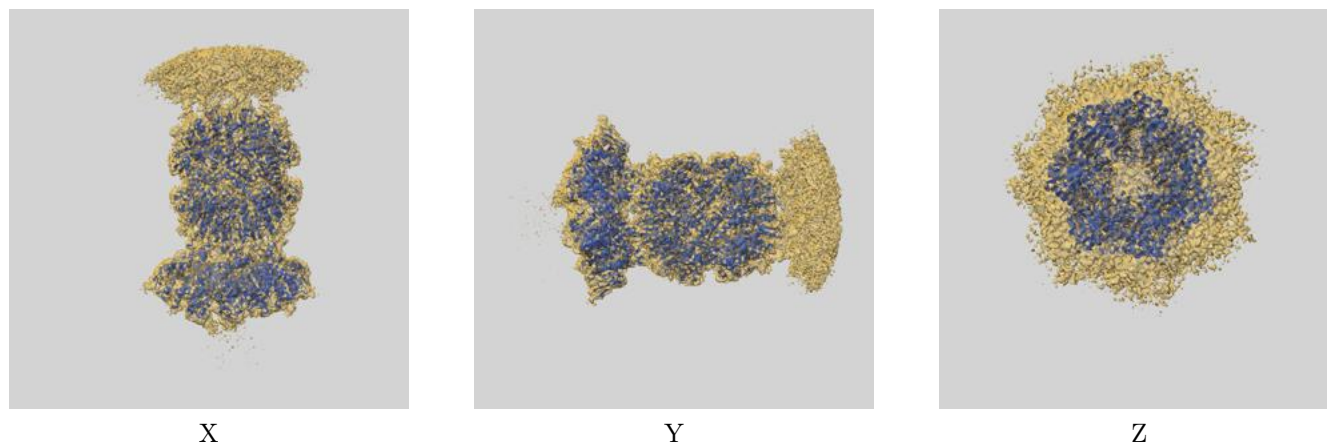
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.61	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.20	3.81	3.27

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.20 differs from the reported value 2.61 by more than 10 %

9 Map-model fit [i](#)

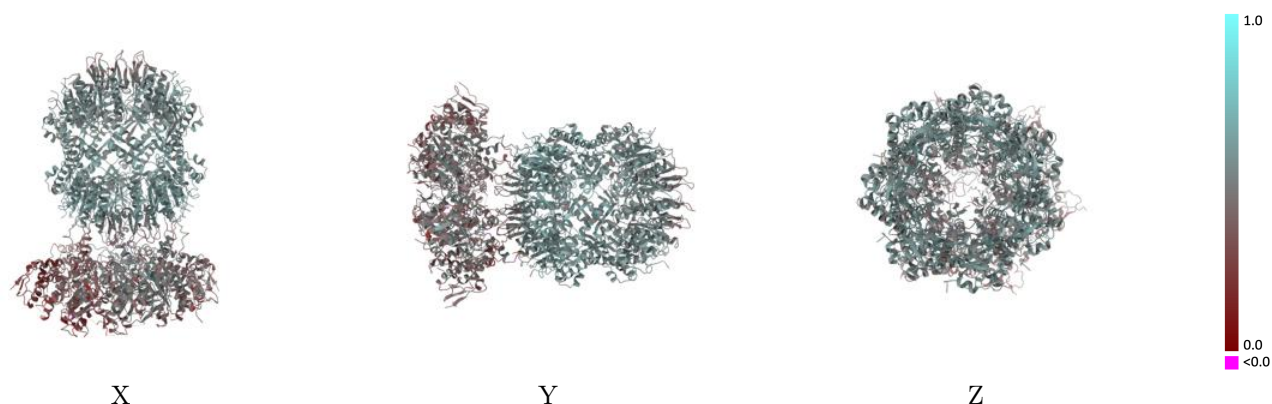
This section contains information regarding the fit between EMDB map EMD-71674 and PDB model 9PIO. Per-residue inclusion information can be found in section [3](#) on page [13](#).

9.1 Map-model overlay [i](#)



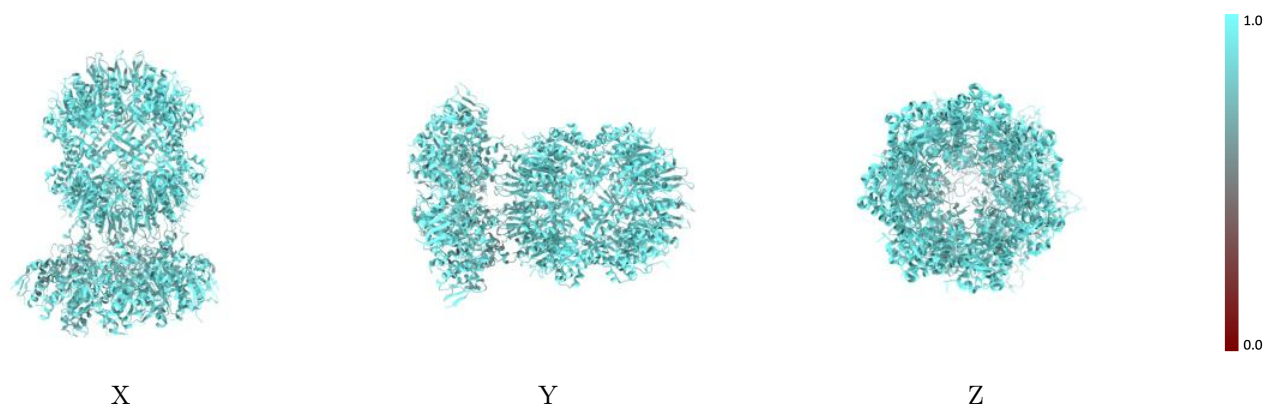
The images above show the 3D surface view of the map at the recommended contour level 0.0577 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



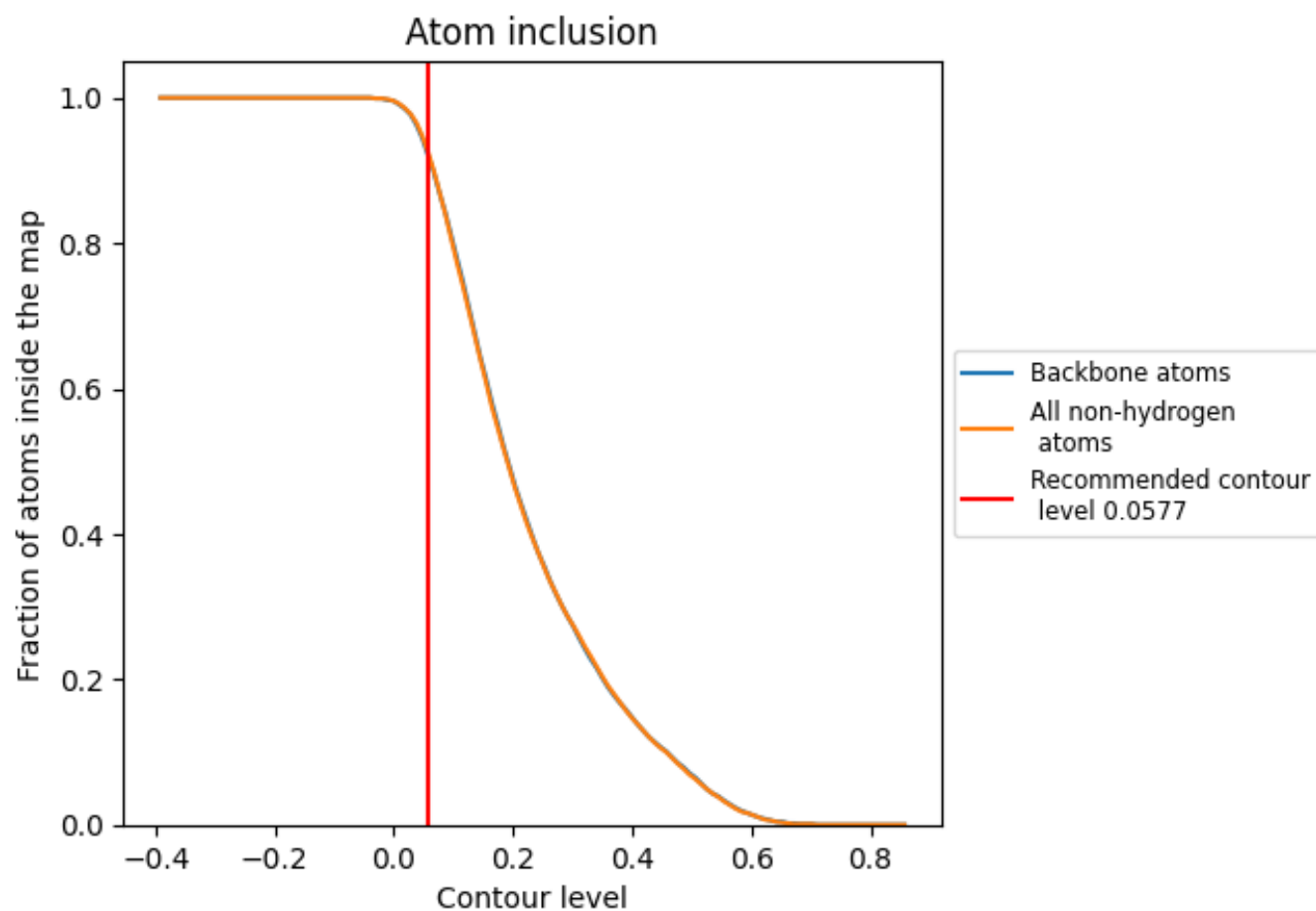
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0577).













































9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 92% 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 (0.0577) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9240	 0.4840
A	 0.8260	 0.2670
B	 0.8630	 0.3630
C	 0.9000	 0.4260
D	 0.9130	 0.4520
E	 0.9070	 0.4500
F	 0.8620	 0.3820
G	 0.8610	 0.4810
H	 0.9670	 0.5750
I	 0.9690	 0.5700
J	 0.9660	 0.5680
K	 0.9670	 0.5680
L	 0.9590	 0.5560
M	 0.9630	 0.5640
N	 0.9700	 0.5710
O	 0.9560	 0.5380
P	 0.9590	 0.5360
Q	 0.9560	 0.5370
R	 0.9570	 0.5360
S	 0.9530	 0.5310
T	 0.9530	 0.5310
U	 0.9560	 0.5350

