Full wwPDB EM Validation Report ⓘ

Oct 28, 2026 – 04:26 PM EDT

PDB ID	:	39QT / pdb_000039qt
EMDB ID	:	EMD-79703
Title	:	SaPIbov1 Rep:dsDNA component 0 frame 0
Authors	:	Shin, H.; Rice, P.A.
Deposited on	:	2026-10-22
Resolution	:	3.35 Å(reported)

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:

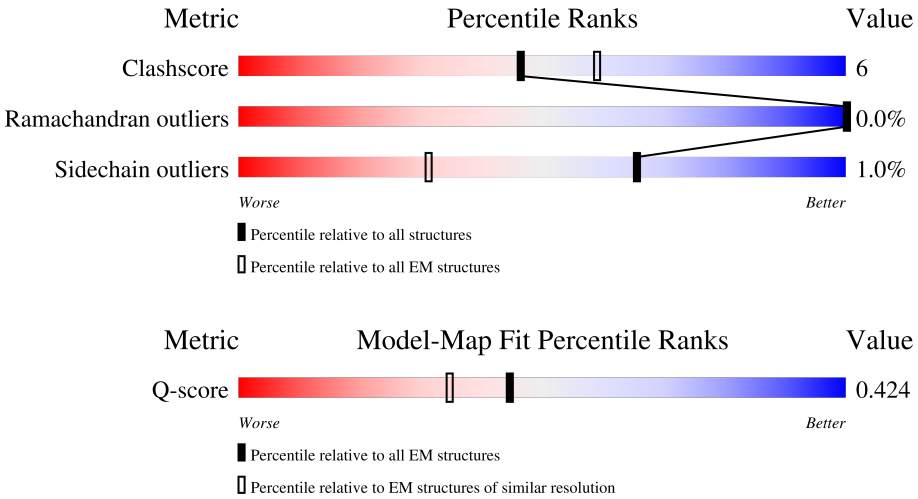
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.2
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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)	:	2.51

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 3.35 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.



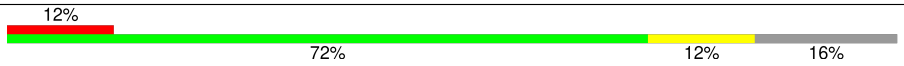
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14390 (2.85 - 3.85)

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	602	12% 68% 16% 16%
1	B	602	• 75% 9% 15%
1	C	602	• 76% 10% • 12%
1	D	602	• 78% 9% 13%

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Mol	Chain	Length	Quality of chain
1	E	602	
1	F	602	
2	G	25	
2	H	25	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 50548 atoms, of which 25177 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 Pathogenicity island protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	F	507	Total	C	H	N	O	S	0	0
			8165	2604	4090	679	781	11		
1	B	509	Total	C	H	N	O	S	0	0
			8182	2607	4094	684	786	11		
1	D	524	Total	C	H	N	O	S	0	0
			8405	2674	4208	703	808	12		
1	A	504	Total	C	H	N	O	S	0	0
			8112	2588	4060	675	778	11		
1	E	524	Total	C	H	N	O	S	0	0
			8415	2677	4215	703	809	11		
1	C	527	Total	C	H	N	O	S	0	0
			8458	2691	4231	711	813	12		

There are 228 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	350	PRO	GLN	conflict	UNP A0A2X2JYA8
F	462	LEU	ILE	conflict	UNP A0A2X2JYA8
F	474	ALA	VAL	conflict	UNP A0A2X2JYA8
F	548	LYS	ARG	conflict	UNP A0A2X2JYA8
F	555	LEU	PHE	conflict	UNP A0A2X2JYA8
F	570	GLY	-	expression tag	UNP A0A2X2JYA8
F	571	SER	-	expression tag	UNP A0A2X2JYA8
F	572	GLY	-	expression tag	UNP A0A2X2JYA8
F	573	SER	-	expression tag	UNP A0A2X2JYA8
F	574	GLY	-	expression tag	UNP A0A2X2JYA8
F	575	TRP	-	expression tag	UNP A0A2X2JYA8
F	576	SER	-	expression tag	UNP A0A2X2JYA8
F	577	HIS	-	expression tag	UNP A0A2X2JYA8
F	578	PRO	-	expression tag	UNP A0A2X2JYA8
F	579	GLN	-	expression tag	UNP A0A2X2JYA8
F	580	PHE	-	expression tag	UNP A0A2X2JYA8
F	581	GLU	-	expression tag	UNP A0A2X2JYA8
F	582	LYS	-	expression tag	UNP A0A2X2JYA8

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Chain	Residue	Modelled	Actual	Comment	Reference
F	583	GLY	-	expression tag	UNP A0A2X2JYA8
F	584	GLY	-	expression tag	UNP A0A2X2JYA8
F	585	GLY	-	expression tag	UNP A0A2X2JYA8
F	586	SER	-	expression tag	UNP A0A2X2JYA8
F	587	GLY	-	expression tag	UNP A0A2X2JYA8
F	588	GLY	-	expression tag	UNP A0A2X2JYA8
F	589	GLY	-	expression tag	UNP A0A2X2JYA8
F	590	SER	-	expression tag	UNP A0A2X2JYA8
F	591	GLY	-	expression tag	UNP A0A2X2JYA8
F	592	GLY	-	expression tag	UNP A0A2X2JYA8
F	593	SER	-	expression tag	UNP A0A2X2JYA8
F	594	ALA	-	expression tag	UNP A0A2X2JYA8
F	595	TRP	-	expression tag	UNP A0A2X2JYA8
F	596	SER	-	expression tag	UNP A0A2X2JYA8
F	597	HIS	-	expression tag	UNP A0A2X2JYA8
F	598	PRO	-	expression tag	UNP A0A2X2JYA8
F	599	GLN	-	expression tag	UNP A0A2X2JYA8
F	600	PHE	-	expression tag	UNP A0A2X2JYA8
F	601	GLU	-	expression tag	UNP A0A2X2JYA8
F	602	LYS	-	expression tag	UNP A0A2X2JYA8
B	350	PRO	GLN	conflict	UNP A0A2X2JYA8
B	462	LEU	ILE	conflict	UNP A0A2X2JYA8
B	474	ALA	VAL	conflict	UNP A0A2X2JYA8
B	548	LYS	ARG	conflict	UNP A0A2X2JYA8
B	555	LEU	PHE	conflict	UNP A0A2X2JYA8
B	570	GLY	-	expression tag	UNP A0A2X2JYA8
B	571	SER	-	expression tag	UNP A0A2X2JYA8
B	572	GLY	-	expression tag	UNP A0A2X2JYA8
B	573	SER	-	expression tag	UNP A0A2X2JYA8
B	574	GLY	-	expression tag	UNP A0A2X2JYA8
B	575	TRP	-	expression tag	UNP A0A2X2JYA8
B	576	SER	-	expression tag	UNP A0A2X2JYA8
B	577	HIS	-	expression tag	UNP A0A2X2JYA8
B	578	PRO	-	expression tag	UNP A0A2X2JYA8
B	579	GLN	-	expression tag	UNP A0A2X2JYA8
B	580	PHE	-	expression tag	UNP A0A2X2JYA8
B	581	GLU	-	expression tag	UNP A0A2X2JYA8
B	582	LYS	-	expression tag	UNP A0A2X2JYA8
B	583	GLY	-	expression tag	UNP A0A2X2JYA8
B	584	GLY	-	expression tag	UNP A0A2X2JYA8
B	585	GLY	-	expression tag	UNP A0A2X2JYA8
B	586	SER	-	expression tag	UNP A0A2X2JYA8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	587	GLY	-	expression tag	UNP A0A2X2JYA8
B	588	GLY	-	expression tag	UNP A0A2X2JYA8
B	589	GLY	-	expression tag	UNP A0A2X2JYA8
B	590	SER	-	expression tag	UNP A0A2X2JYA8
B	591	GLY	-	expression tag	UNP A0A2X2JYA8
B	592	GLY	-	expression tag	UNP A0A2X2JYA8
B	593	SER	-	expression tag	UNP A0A2X2JYA8
B	594	ALA	-	expression tag	UNP A0A2X2JYA8
B	595	TRP	-	expression tag	UNP A0A2X2JYA8
B	596	SER	-	expression tag	UNP A0A2X2JYA8
B	597	HIS	-	expression tag	UNP A0A2X2JYA8
B	598	PRO	-	expression tag	UNP A0A2X2JYA8
B	599	GLN	-	expression tag	UNP A0A2X2JYA8
B	600	PHE	-	expression tag	UNP A0A2X2JYA8
B	601	GLU	-	expression tag	UNP A0A2X2JYA8
B	602	LYS	-	expression tag	UNP A0A2X2JYA8
D	350	PRO	GLN	conflict	UNP A0A2X2JYA8
D	462	LEU	ILE	conflict	UNP A0A2X2JYA8
D	474	ALA	VAL	conflict	UNP A0A2X2JYA8
D	548	LYS	ARG	conflict	UNP A0A2X2JYA8
D	555	LEU	PHE	conflict	UNP A0A2X2JYA8
D	570	GLY	-	expression tag	UNP A0A2X2JYA8
D	571	SER	-	expression tag	UNP A0A2X2JYA8
D	572	GLY	-	expression tag	UNP A0A2X2JYA8
D	573	SER	-	expression tag	UNP A0A2X2JYA8
D	574	GLY	-	expression tag	UNP A0A2X2JYA8
D	575	TRP	-	expression tag	UNP A0A2X2JYA8
D	576	SER	-	expression tag	UNP A0A2X2JYA8
D	577	HIS	-	expression tag	UNP A0A2X2JYA8
D	578	PRO	-	expression tag	UNP A0A2X2JYA8
D	579	GLN	-	expression tag	UNP A0A2X2JYA8
D	580	PHE	-	expression tag	UNP A0A2X2JYA8
D	581	GLU	-	expression tag	UNP A0A2X2JYA8
D	582	LYS	-	expression tag	UNP A0A2X2JYA8
D	583	GLY	-	expression tag	UNP A0A2X2JYA8
D	584	GLY	-	expression tag	UNP A0A2X2JYA8
D	585	GLY	-	expression tag	UNP A0A2X2JYA8
D	586	SER	-	expression tag	UNP A0A2X2JYA8
D	587	GLY	-	expression tag	UNP A0A2X2JYA8
D	588	GLY	-	expression tag	UNP A0A2X2JYA8
D	589	GLY	-	expression tag	UNP A0A2X2JYA8
D	590	SER	-	expression tag	UNP A0A2X2JYA8

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Chain	Residue	Modelled	Actual	Comment	Reference
D	591	GLY	-	expression tag	UNP A0A2X2JYA8
D	592	GLY	-	expression tag	UNP A0A2X2JYA8
D	593	SER	-	expression tag	UNP A0A2X2JYA8
D	594	ALA	-	expression tag	UNP A0A2X2JYA8
D	595	TRP	-	expression tag	UNP A0A2X2JYA8
D	596	SER	-	expression tag	UNP A0A2X2JYA8
D	597	HIS	-	expression tag	UNP A0A2X2JYA8
D	598	PRO	-	expression tag	UNP A0A2X2JYA8
D	599	GLN	-	expression tag	UNP A0A2X2JYA8
D	600	PHE	-	expression tag	UNP A0A2X2JYA8
D	601	GLU	-	expression tag	UNP A0A2X2JYA8
D	602	LYS	-	expression tag	UNP A0A2X2JYA8
A	350	PRO	GLN	conflict	UNP A0A2X2JYA8
A	462	LEU	ILE	conflict	UNP A0A2X2JYA8
A	474	ALA	VAL	conflict	UNP A0A2X2JYA8
A	548	LYS	ARG	conflict	UNP A0A2X2JYA8
A	555	LEU	PHE	conflict	UNP A0A2X2JYA8
A	570	GLY	-	expression tag	UNP A0A2X2JYA8
A	571	SER	-	expression tag	UNP A0A2X2JYA8
A	572	GLY	-	expression tag	UNP A0A2X2JYA8
A	573	SER	-	expression tag	UNP A0A2X2JYA8
A	574	GLY	-	expression tag	UNP A0A2X2JYA8
A	575	TRP	-	expression tag	UNP A0A2X2JYA8
A	576	SER	-	expression tag	UNP A0A2X2JYA8
A	577	HIS	-	expression tag	UNP A0A2X2JYA8
A	578	PRO	-	expression tag	UNP A0A2X2JYA8
A	579	GLN	-	expression tag	UNP A0A2X2JYA8
A	580	PHE	-	expression tag	UNP A0A2X2JYA8
A	581	GLU	-	expression tag	UNP A0A2X2JYA8
A	582	LYS	-	expression tag	UNP A0A2X2JYA8
A	583	GLY	-	expression tag	UNP A0A2X2JYA8
A	584	GLY	-	expression tag	UNP A0A2X2JYA8
A	585	GLY	-	expression tag	UNP A0A2X2JYA8
A	586	SER	-	expression tag	UNP A0A2X2JYA8
A	587	GLY	-	expression tag	UNP A0A2X2JYA8
A	588	GLY	-	expression tag	UNP A0A2X2JYA8
A	589	GLY	-	expression tag	UNP A0A2X2JYA8
A	590	SER	-	expression tag	UNP A0A2X2JYA8
A	591	GLY	-	expression tag	UNP A0A2X2JYA8
A	592	GLY	-	expression tag	UNP A0A2X2JYA8
A	593	SER	-	expression tag	UNP A0A2X2JYA8
A	594	ALA	-	expression tag	UNP A0A2X2JYA8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	595	TRP	-	expression tag	UNP A0A2X2JYA8
A	596	SER	-	expression tag	UNP A0A2X2JYA8
A	597	HIS	-	expression tag	UNP A0A2X2JYA8
A	598	PRO	-	expression tag	UNP A0A2X2JYA8
A	599	GLN	-	expression tag	UNP A0A2X2JYA8
A	600	PHE	-	expression tag	UNP A0A2X2JYA8
A	601	GLU	-	expression tag	UNP A0A2X2JYA8
A	602	LYS	-	expression tag	UNP A0A2X2JYA8
E	350	PRO	GLN	conflict	UNP A0A2X2JYA8
E	462	LEU	ILE	conflict	UNP A0A2X2JYA8
E	474	ALA	VAL	conflict	UNP A0A2X2JYA8
E	548	LYS	ARG	conflict	UNP A0A2X2JYA8
E	555	LEU	PHE	conflict	UNP A0A2X2JYA8
E	570	GLY	-	expression tag	UNP A0A2X2JYA8
E	571	SER	-	expression tag	UNP A0A2X2JYA8
E	572	GLY	-	expression tag	UNP A0A2X2JYA8
E	573	SER	-	expression tag	UNP A0A2X2JYA8
E	574	GLY	-	expression tag	UNP A0A2X2JYA8
E	575	TRP	-	expression tag	UNP A0A2X2JYA8
E	576	SER	-	expression tag	UNP A0A2X2JYA8
E	577	HIS	-	expression tag	UNP A0A2X2JYA8
E	578	PRO	-	expression tag	UNP A0A2X2JYA8
E	579	GLN	-	expression tag	UNP A0A2X2JYA8
E	580	PHE	-	expression tag	UNP A0A2X2JYA8
E	581	GLU	-	expression tag	UNP A0A2X2JYA8
E	582	LYS	-	expression tag	UNP A0A2X2JYA8
E	583	GLY	-	expression tag	UNP A0A2X2JYA8
E	584	GLY	-	expression tag	UNP A0A2X2JYA8
E	585	GLY	-	expression tag	UNP A0A2X2JYA8
E	586	SER	-	expression tag	UNP A0A2X2JYA8
E	587	GLY	-	expression tag	UNP A0A2X2JYA8
E	588	GLY	-	expression tag	UNP A0A2X2JYA8
E	589	GLY	-	expression tag	UNP A0A2X2JYA8
E	590	SER	-	expression tag	UNP A0A2X2JYA8
E	591	GLY	-	expression tag	UNP A0A2X2JYA8
E	592	GLY	-	expression tag	UNP A0A2X2JYA8
E	593	SER	-	expression tag	UNP A0A2X2JYA8
E	594	ALA	-	expression tag	UNP A0A2X2JYA8
E	595	TRP	-	expression tag	UNP A0A2X2JYA8
E	596	SER	-	expression tag	UNP A0A2X2JYA8
E	597	HIS	-	expression tag	UNP A0A2X2JYA8
E	598	PRO	-	expression tag	UNP A0A2X2JYA8

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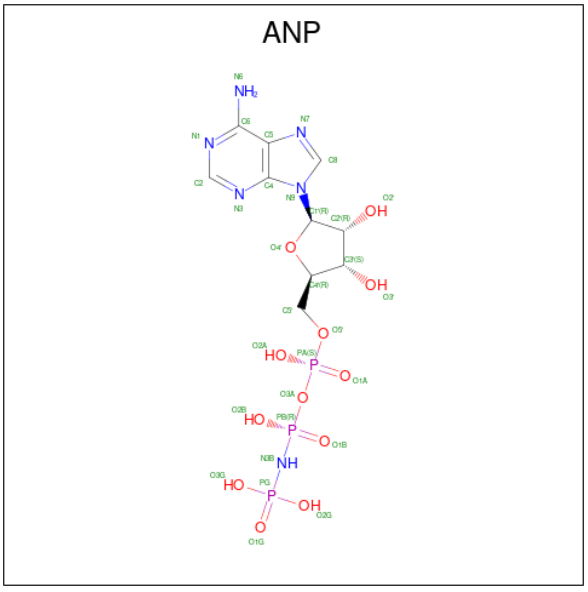
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Chain	Residue	Modelled	Actual	Comment	Reference
E	599	GLN	-	expression tag	UNP A0A2X2JYA8
E	600	PHE	-	expression tag	UNP A0A2X2JYA8
E	601	GLU	-	expression tag	UNP A0A2X2JYA8
E	602	LYS	-	expression tag	UNP A0A2X2JYA8
C	350	PRO	GLN	conflict	UNP A0A2X2JYA8
C	462	LEU	ILE	conflict	UNP A0A2X2JYA8
C	474	ALA	VAL	conflict	UNP A0A2X2JYA8
C	548	LYS	ARG	conflict	UNP A0A2X2JYA8
C	555	LEU	PHE	conflict	UNP A0A2X2JYA8
C	570	GLY	-	expression tag	UNP A0A2X2JYA8
C	571	SER	-	expression tag	UNP A0A2X2JYA8
C	572	GLY	-	expression tag	UNP A0A2X2JYA8
C	573	SER	-	expression tag	UNP A0A2X2JYA8
C	574	GLY	-	expression tag	UNP A0A2X2JYA8
C	575	TRP	-	expression tag	UNP A0A2X2JYA8
C	576	SER	-	expression tag	UNP A0A2X2JYA8
C	577	HIS	-	expression tag	UNP A0A2X2JYA8
C	578	PRO	-	expression tag	UNP A0A2X2JYA8
C	579	GLN	-	expression tag	UNP A0A2X2JYA8
C	580	PHE	-	expression tag	UNP A0A2X2JYA8
C	581	GLU	-	expression tag	UNP A0A2X2JYA8
C	582	LYS	-	expression tag	UNP A0A2X2JYA8
C	583	GLY	-	expression tag	UNP A0A2X2JYA8
C	584	GLY	-	expression tag	UNP A0A2X2JYA8
C	585	GLY	-	expression tag	UNP A0A2X2JYA8
C	586	SER	-	expression tag	UNP A0A2X2JYA8
C	587	GLY	-	expression tag	UNP A0A2X2JYA8
C	588	GLY	-	expression tag	UNP A0A2X2JYA8
C	589	GLY	-	expression tag	UNP A0A2X2JYA8
C	590	SER	-	expression tag	UNP A0A2X2JYA8
C	591	GLY	-	expression tag	UNP A0A2X2JYA8
C	592	GLY	-	expression tag	UNP A0A2X2JYA8
C	593	SER	-	expression tag	UNP A0A2X2JYA8
C	594	ALA	-	expression tag	UNP A0A2X2JYA8
C	595	TRP	-	expression tag	UNP A0A2X2JYA8
C	596	SER	-	expression tag	UNP A0A2X2JYA8
C	597	HIS	-	expression tag	UNP A0A2X2JYA8
C	598	PRO	-	expression tag	UNP A0A2X2JYA8
C	599	GLN	-	expression tag	UNP A0A2X2JYA8
C	600	PHE	-	expression tag	UNP A0A2X2JYA8
C	601	GLU	-	expression tag	UNP A0A2X2JYA8
C	602	LYS	-	expression tag	UNP A0A2X2JYA8

- Molecule 2 is a DNA chain called DNA (25-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
2	G	10	Total	C	H	N	O	P	0	0
			318	98	114	34	62	10		
2	H	10	Total	C	H	N	O	P	0	0
			318	98	114	34	62	10		

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
3	B	1	Total	C	H	N	O	P	0
			44	10	13	6	12	3	
3	D	1	Total	C	H	N	O	P	0
			44	10	13	6	12	3	
3	C	1	Total	C	H	N	O	P	0
			44	10	13	6	12	3	

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

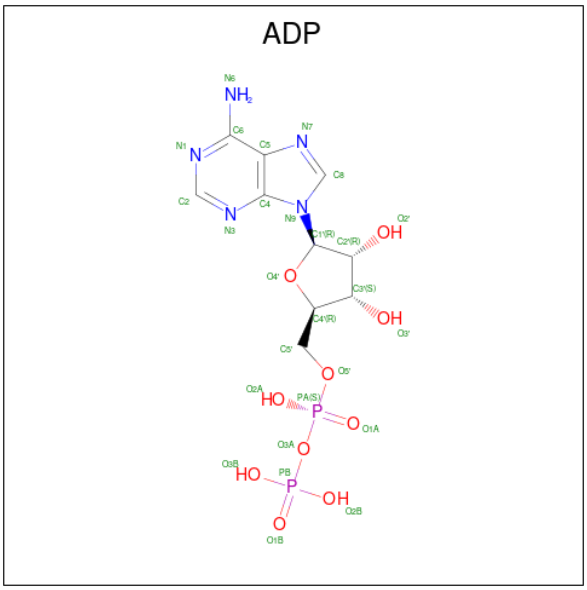
Mol	Chain	Residues	Atoms		AltConf
4	B	1	Total	Mg	0
			1	1	
4	D	1	Total	Mg	0
			1	1	
4	E	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
4	C	1	Total	Mg	0
			1	1	

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



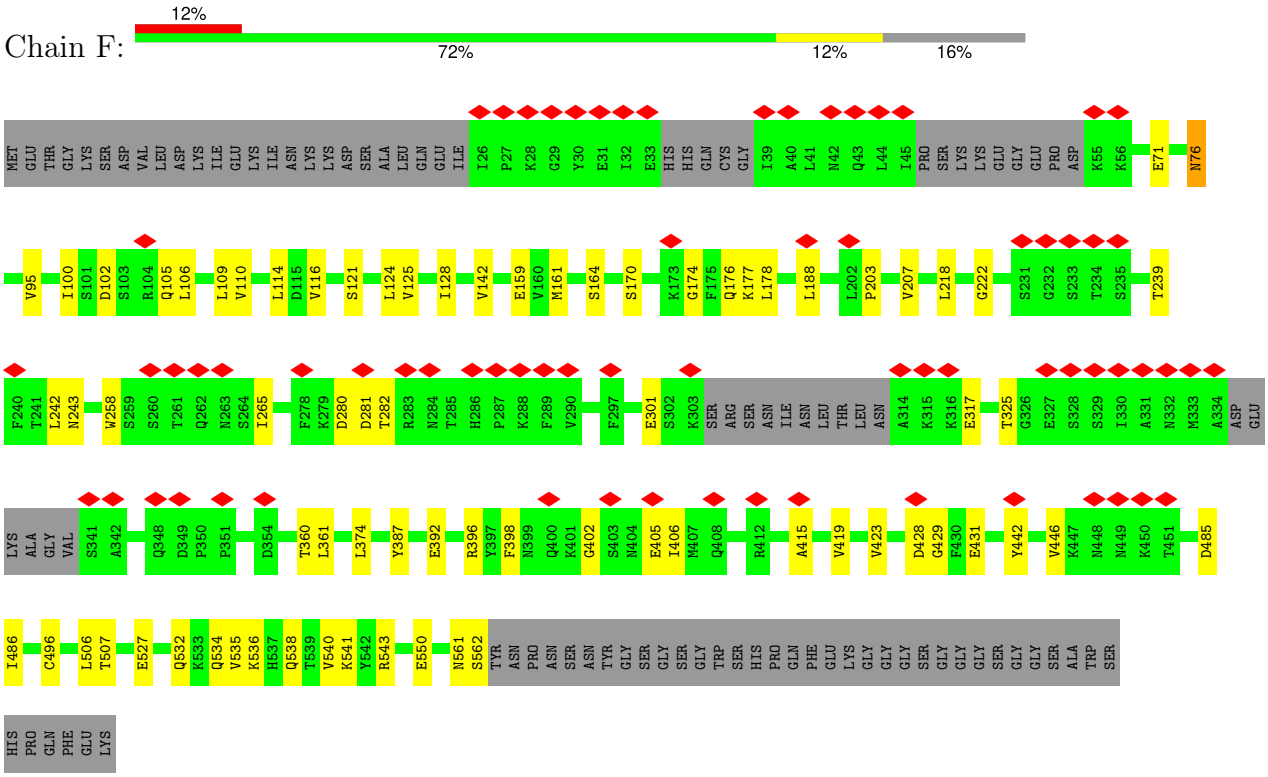
Mol	Chain	Residues	Atoms						AltConf
5	E	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	

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.

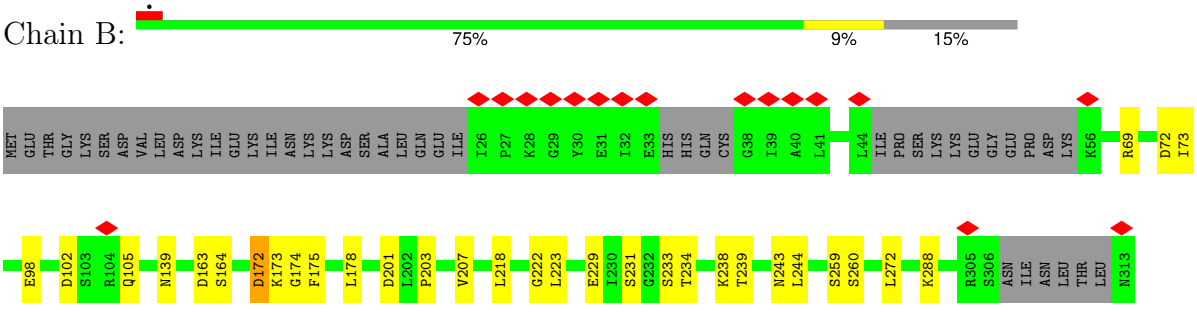
• Molecule 1: Pathogenicity island protein

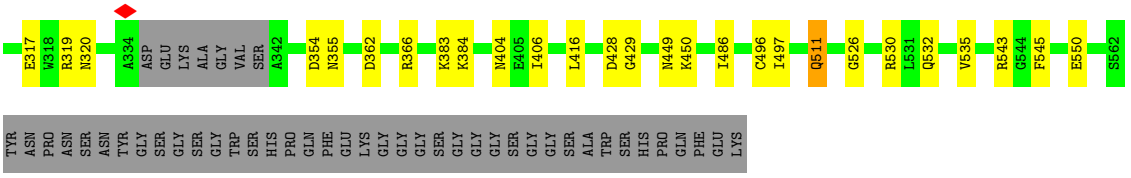
Chain F:



• Molecule 1: Pathogenicity island protein

Chain B:

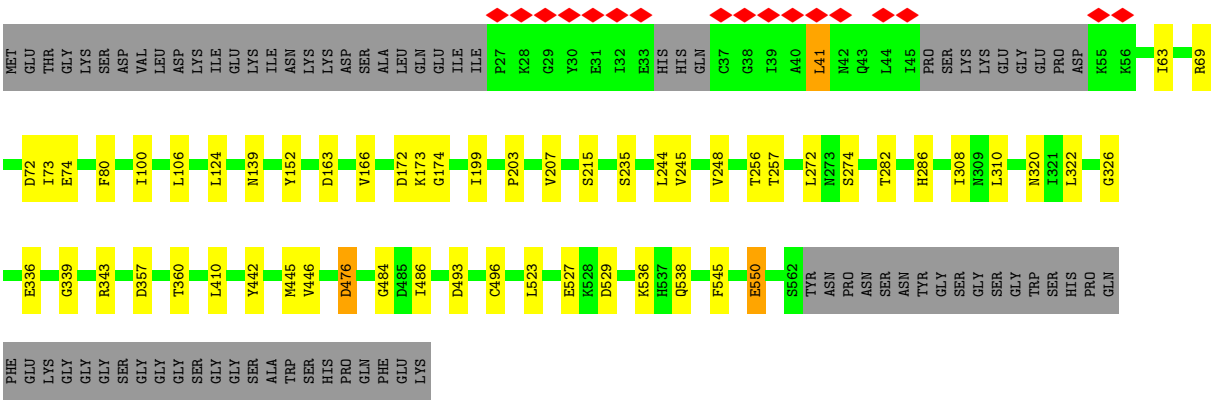




• Molecule 1: Pathogenicity island protein

Chain D:

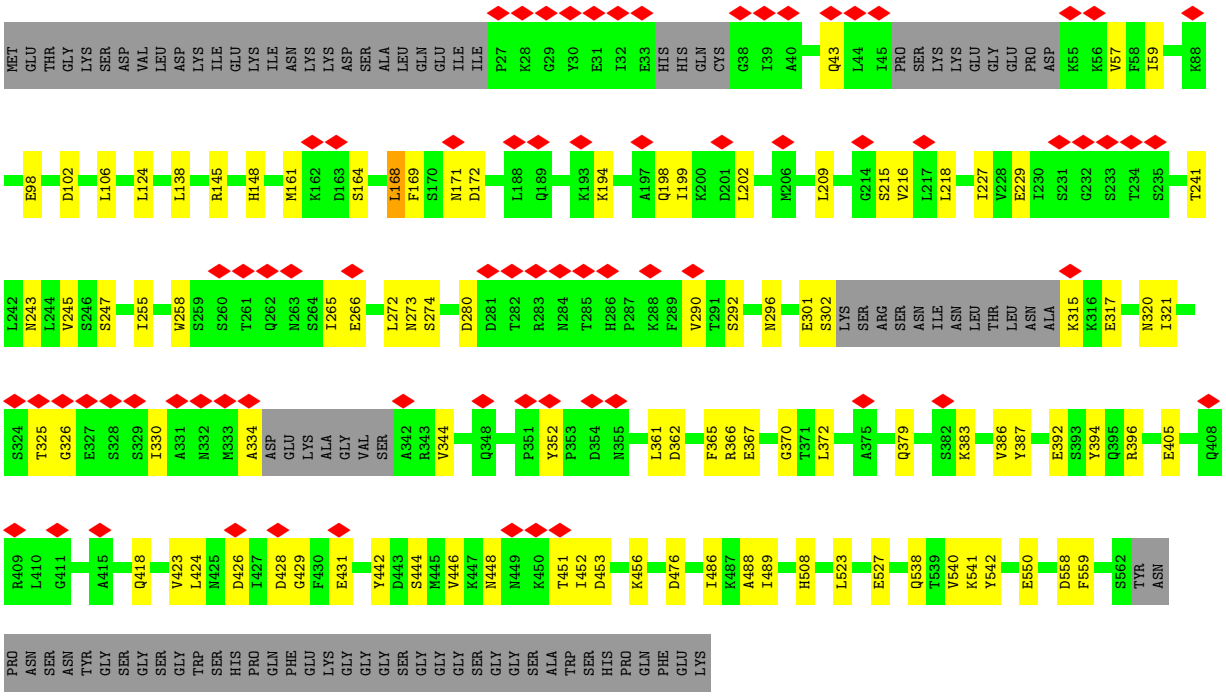




• Molecule 1: Pathogenicity island protein

Chain A:

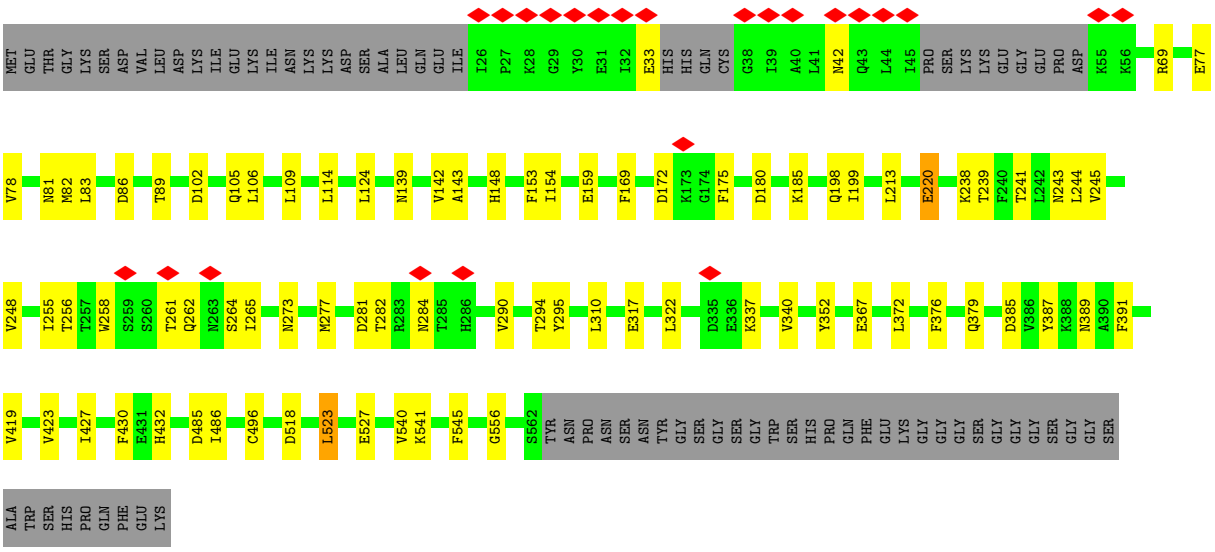




• Molecule 1: Pathogenicity island protein

Chain E:

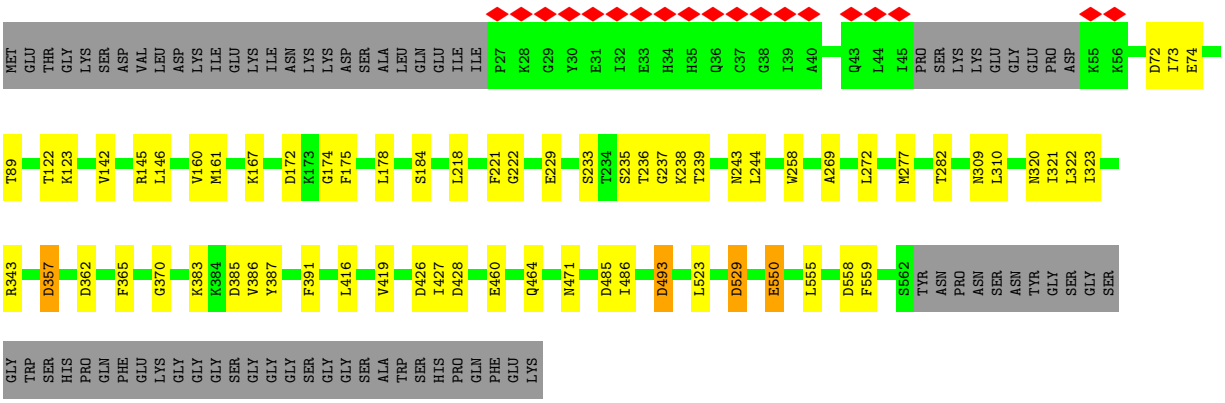




• Molecule 1: Pathogenicity island protein

Chain C:

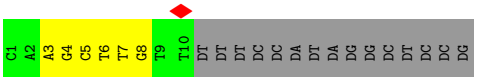




• Molecule 2: DNA (25-MER)

Chain G:

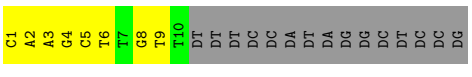




• Molecule 2: DNA (25-MER)

Chain H:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	31581	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	52	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.242	Depositor
Minimum map value	-0.108	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	349.76, 349.76, 349.76	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.093, 1.093, 1.093	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.14	0/4127	0.25	0/5555
1	B	0.22	0/4163	0.28	0/5604
1	C	0.22	0/4307	0.30	0/5802
1	D	0.22	0/4274	0.28	0/5756
1	E	0.18	0/4277	0.26	0/5761
1	F	0.15	0/4150	0.24	0/5587
2	G	0.84	0/227	1.07	0/348
2	H	0.85	0/227	1.15	0/348
All	All	0.22	0/25752	0.31	0/34761

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	4052	4060	4056	64	0
1	B	4088	4094	4088	36	0
1	C	4227	4231	4229	46	0
1	D	4197	4208	4203	36	0
1	E	4200	4215	4211	56	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	4075	4090	4083	55	0
2	G	204	114	115	11	0
2	H	204	114	115	6	0
3	B	31	13	13	4	0
3	C	31	13	13	4	0
3	D	31	13	13	2	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
5	E	27	12	12	2	0
All	All	25371	25177	25151	309	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 6.

All (309) 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:A:215:SER:OG	1:A:274:SER:O	1.87	0.92
1:C:550:GLU:OE1	1:C:550:GLU:N	2.07	0.87
1:D:550:GLU:N	1:D:550:GLU:OE1	2.08	0.86
1:E:317:GLU:N	1:E:317:GLU:OE1	2.10	0.83
1:F:550:GLU:N	1:F:550:GLU:OE1	2.12	0.82
1:B:229:GLU:OE2	1:B:231:SER:OG	1.98	0.82
1:C:237:GLY:N	3:C:701:ANP:O1A	2.12	0.81
1:E:198:GLN:N	1:E:198:GLN:OE1	2.13	0.81
1:F:431:GLU:N	1:F:431:GLU:OE1	2.14	0.81
1:F:527:GLU:OE1	1:F:527:GLU:N	2.14	0.80
1:B:233:SER:O	1:B:238:LYS:NZ	2.15	0.80
1:D:336:GLU:OE1	1:D:336:GLU:N	2.14	0.79
1:B:550:GLU:N	1:B:550:GLU:OE1	2.15	0.79
1:A:145:ARG:NH1	1:A:273:ASN:OD1	2.15	0.79
1:C:272:LEU:O	1:C:320:ASN:ND2	2.16	0.78
1:D:72:ASP:OD1	1:D:73:ILE:N	2.17	0.78
1:A:161:MET:O	1:A:164:SER:OG	2.03	0.76
1:C:493:ASP:OD1	1:C:493:ASP:N	2.17	0.75
1:A:431:GLU:N	1:A:431:GLU:OE1	2.20	0.75
1:F:506:LEU:O	1:F:507:THR:OG1	2.05	0.74
1:A:292:SER:O	1:A:296:ASN:ND2	2.20	0.74
1:E:148:HIS:O	1:E:273:ASN:ND2	2.21	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:GLU:N	1:A:266:GLU:OE1	2.22	0.72
1:A:229:GLU:OE2	1:A:326:GLY:N	2.23	0.72
1:F:301:GLU:N	1:F:301:GLU:OE1	2.24	0.71
1:F:239:THR:O	1:F:243:ASN:ND2	2.23	0.70
1:B:317:GLU:OE2	1:B:319:ARG:NH1	2.23	0.70
1:F:317:GLU:N	1:F:317:GLU:OE1	2.24	0.70
1:F:392:GLU:OE1	1:F:396:ARG:NH1	2.25	0.70
1:A:550:GLU:N	1:A:550:GLU:OE1	2.24	0.69
1:B:172:ASP:OD1	1:B:174:GLY:N	2.24	0.69
1:A:280:ASP:OD1	1:A:325:THR:OG1	2.06	0.69
1:C:161:MET:O	1:C:167:LYS:NZ	2.26	0.68
1:A:379:GLN:NE2	1:A:426:ASP:OD2	2.27	0.67
1:C:172:ASP:OD1	1:C:174:GLY:N	2.28	0.67
1:A:444:SER:O	1:A:448:ASN:ND2	2.29	0.66
1:A:168:LEU:HD12	1:A:169:PHE:N	2.10	0.66
1:A:387:TYR:CE1	1:A:423:VAL:HG12	2.31	0.66
1:F:161:MET:O	1:F:164:SER:OG	2.08	0.65
1:F:387:TYR:CE1	1:F:423:VAL:HG22	2.30	0.65
1:E:33:GLU:OE2	1:E:42:ASN:ND2	2.30	0.65
1:A:199:ILE:HG22	1:A:202:LEU:HD12	1.77	0.65
1:F:174:GLY:O	1:F:177:LYS:NZ	2.30	0.64
1:B:532:GLN:OE1	1:B:543:ARG:NH2	2.31	0.64
1:E:77:GLU:OE1	1:E:78:VAL:N	2.31	0.64
1:E:185:LYS:NZ	1:E:367:GLU:O	2.30	0.63
2:G:7:DT:N3	2:G:8:DG:O6	2.31	0.63
1:D:527:GLU:N	1:D:527:GLU:OE1	2.32	0.63
1:A:362:ASP:OD1	1:A:366:ARG:NH1	2.33	0.62
1:B:234:THR:O	3:B:701:ANP:N3B	2.32	0.62
1:E:391:PHE:HB2	1:E:419:VAL:HG21	1.81	0.62
1:C:239:THR:O	1:C:243:ASN:ND2	2.33	0.62
1:B:239:THR:O	1:B:243:ASN:ND2	2.33	0.61
1:B:511:GLN:N	1:B:511:GLN:OE1	2.34	0.61
1:E:238:LYS:N	5:E:701:ADP:O2A	2.34	0.61
1:B:72:ASP:OD1	1:B:73:ILE:N	2.34	0.61
1:A:301:GLU:N	1:A:301:GLU:OE1	2.34	0.61
1:F:543:ARG:NE	1:E:556:GLY:O	2.29	0.60
1:E:106:LEU:HD21	1:E:124:LEU:HD23	1.84	0.60
1:B:172:ASP:OD1	1:B:173:LYS:N	2.35	0.60
1:A:428:ASP:OD1	1:A:429:GLY:N	2.34	0.59
1:E:385:ASP:O	1:E:389:ASN:ND2	2.34	0.59
1:A:258:TRP:CH2	1:A:290:VAL:HG13	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:233:SER:O	1:C:238:LYS:NZ	2.30	0.59
1:C:236:THR:N	3:C:701:ANP:O1A	2.36	0.59
1:B:404:ASN:OD1	1:B:406:ILE:N	2.34	0.59
1:A:488:ALA:C	1:A:489:ILE:HD12	2.27	0.58
1:E:239:THR:O	1:E:243:ASN:ND2	2.36	0.58
1:D:536:LYS:NZ	1:D:538:GLN:O	2.30	0.58
1:A:405:GLU:OE1	1:A:405:GLU:N	2.36	0.58
1:C:235:SER:H	3:C:701:ANP:HNB1	1.51	0.57
1:E:86:ASP:O	1:E:89:THR:OG1	2.18	0.57
1:F:106:LEU:HD21	1:F:124:LEU:HD23	1.86	0.57
1:F:536:LYS:NZ	1:F:538:GLN:O	2.33	0.57
1:E:159:GLU:OE1	1:E:159:GLU:N	2.37	0.57
1:A:442:TYR:O	1:A:446:VAL:HG23	2.04	0.57
1:F:398:PHE:O	1:F:402:GLY:N	2.35	0.57
1:E:241:THR:HG1	1:E:352:TYR:HH	1.49	0.57
1:F:405:GLU:OE1	1:F:406:ILE:N	2.37	0.57
1:D:322:LEU:HD23	1:D:322:LEU:C	2.29	0.57
1:C:72:ASP:OD1	1:C:73:ILE:N	2.38	0.57
1:F:170:SER:O	1:F:176:GLN:NE2	2.39	0.56
1:A:302:SER:HG	1:A:315:LYS:N	2.04	0.56
1:F:106:LEU:CD2	1:F:116:VAL:HG21	2.35	0.56
1:B:354:ASP:OD1	1:B:355:ASN:N	2.38	0.56
1:E:172:ASP:OD2	1:E:175:PHE:N	2.37	0.56
1:F:71:GLU:O	1:F:142:VAL:HG22	2.07	0.55
1:F:100:ILE:HG23	1:F:128:ILE:HG21	1.87	0.55
1:B:244:LEU:HD23	1:B:244:LEU:C	2.31	0.55
1:A:227:ILE:HB	1:A:344:VAL:HG13	1.89	0.55
1:C:218:LEU:O	1:C:222:GLY:N	2.40	0.55
1:B:102:ASP:OD2	1:B:105:GLN:NE2	2.40	0.55
1:A:558:ASP:OD1	1:A:559:PHE:N	2.39	0.55
1:A:194:LYS:NZ	1:A:367:GLU:OE1	2.41	0.54
1:E:239:THR:OG1	5:E:701:ADP:O3B	2.26	0.54
1:F:218:LEU:O	1:F:222:GLY:N	2.41	0.54
1:A:272:LEU:O	1:A:320:ASN:ND2	2.41	0.54
1:C:529:ASP:OD1	1:C:529:ASP:N	2.39	0.54
2:H:3:DA:H2'	2:H:4:DG:C8	2.43	0.54
1:F:561:ASN:O	1:F:562:SER:OG	2.21	0.53
1:F:280:ASP:OD1	1:F:281:ASP:N	2.41	0.53
3:D:701:ANP:H8	3:D:701:ANP:O5'	2.08	0.53
1:F:258:TRP:NE1	1:F:282:THR:HG22	2.23	0.53
1:D:215:SER:OG	1:D:274:SER:O	2.27	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:430:PHE:O	1:E:432:HIS:ND1	2.40	0.53
1:F:532:GLN:OE1	1:F:532:GLN:N	2.40	0.53
1:F:280:ASP:OD1	1:F:325:THR:OG1	2.26	0.52
2:G:5:DC:H2'	2:G:6:DT:H71	1.90	0.52
1:D:152:TYR:CD1	1:D:166:VAL:HG21	2.43	0.52
1:F:100:ILE:CG2	1:F:128:ILE:HG21	2.40	0.52
1:F:428:ASP:OD1	1:F:429:GLY:N	2.43	0.52
1:C:269:ALA:HB2	1:C:277:MET:HE1	1.92	0.52
1:A:106:LEU:HD21	1:A:124:LEU:HD23	1.92	0.52
1:B:222:GLY:C	1:B:223:LEU:HD12	2.35	0.51
1:C:387:TYR:OH	1:C:426:ASP:OD2	2.27	0.51
2:G:6:DT:H2'	2:G:7:DT:H71	1.92	0.51
1:F:106:LEU:HD21	1:F:116:VAL:HG21	1.93	0.51
1:E:241:THR:OG1	1:E:352:TYR:OH	2.18	0.51
1:A:453:ASP:O	1:A:456:LYS:N	2.43	0.51
1:E:387:TYR:CE1	1:E:423:VAL:HG22	2.45	0.51
1:B:272:LEU:O	1:B:320:ASN:ND2	2.43	0.51
1:E:486:ILE:HD12	1:E:486:ILE:H	1.75	0.51
1:F:496:CYS:SG	1:F:535:VAL:HG21	2.50	0.50
1:B:526:GLY:N	1:B:530:ARG:O	2.37	0.50
1:E:258:TRP:NE1	1:E:282:THR:HG22	2.26	0.50
1:A:321:ILE:N	1:A:321:ILE:HD12	2.27	0.50
1:E:379:GLN:HB2	1:E:427:ILE:HD11	1.92	0.50
1:C:357:ASP:OD1	1:C:357:ASP:N	2.45	0.50
1:D:357:ASP:OD2	1:D:360:THR:OG1	2.27	0.50
1:A:241:THR:HG1	1:A:352:TYR:HH	1.59	0.50
1:D:172:ASP:OD1	1:D:174:GLY:N	2.36	0.50
1:B:175:PHE:O	1:B:178:LEU:N	2.45	0.50
1:F:177:LYS:HG3	1:F:178:LEU:HD22	1.93	0.50
1:A:98:GLU:O	1:A:102:ASP:N	2.45	0.50
1:E:109:LEU:HB2	1:E:114:LEU:HD23	1.95	0.49
2:H:4:DG:H2'	2:H:5:DC:C6	2.47	0.49
1:A:43:GLN:N	1:A:57:VAL:O	2.43	0.49
1:F:188:LEU:C	1:F:188:LEU:HD23	2.36	0.49
1:B:428:ASP:OD1	1:B:429:GLY:N	2.45	0.49
1:A:317:GLU:OE1	1:A:317:GLU:N	2.37	0.49
1:E:213:LEU:HD21	1:E:376:PHE:CD1	2.47	0.49
2:G:4:DG:C4	2:G:5:DC:C5	3.00	0.49
1:D:172:ASP:OD1	1:D:173:LYS:N	2.46	0.49
1:A:265:ILE:HG23	1:A:266:GLU:N	2.27	0.49
1:D:72:ASP:OD1	1:D:74:GLU:N	2.40	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:374:LEU:HD22	1:F:374:LEU:H	1.78	0.49
1:A:383:LYS:O	1:A:386:VAL:HG12	2.13	0.49
1:E:277:MET:O	1:E:322:LEU:HD12	2.13	0.49
1:E:245:VAL:O	1:E:248:VAL:HG12	2.13	0.48
1:B:362:ASP:OD2	3:B:701:ANP:N6	2.45	0.48
1:D:69:ARG:NH2	1:D:139:ASN:OD1	2.45	0.48
1:A:171:ASN:OD1	1:A:172:ASP:N	2.46	0.48
1:C:460:GLU:OE1	1:C:555:LEU:HD13	2.13	0.48
1:A:394:TYR:CG	1:A:418:GLN:NE2	2.81	0.48
1:D:476:ASP:OD1	1:D:476:ASP:N	2.47	0.48
1:E:248:VAL:HG23	1:E:372:LEU:HB3	1.95	0.48
1:C:72:ASP:OD1	1:C:74:GLU:N	2.43	0.48
1:F:203:PRO:O	1:F:207:VAL:HG23	2.13	0.48
1:F:242:LEU:O	1:F:242:LEU:HD23	2.14	0.48
1:E:102:ASP:OD1	1:E:105:GLN:N	2.46	0.48
1:C:175:PHE:O	1:C:178:LEU:N	2.46	0.48
1:C:244:LEU:C	1:C:244:LEU:HD23	2.38	0.48
1:D:272:LEU:O	1:D:320:ASN:ND2	2.44	0.48
1:F:442:TYR:O	1:F:446:VAL:HG23	2.14	0.48
2:H:1:DC:C4	2:H:2:DA:N6	2.81	0.48
1:F:76:ASN:OD1	1:F:76:ASN:N	2.47	0.47
1:A:198:GLN:HG3	1:A:361:LEU:HD13	1.96	0.47
1:E:261:THR:O	1:E:264:SER:OG	2.30	0.47
1:B:69:ARG:NH2	1:B:139:ASN:OD1	2.47	0.47
1:E:69:ARG:NH2	1:E:139:ASN:OD1	2.40	0.47
1:C:184:SER:OG	1:C:370:GLY:O	2.28	0.47
1:C:485:ASP:OD1	1:C:485:ASP:N	2.47	0.47
1:A:489:ILE:HD12	1:A:489:ILE:N	2.30	0.47
1:C:258:TRP:NE1	1:C:282:THR:HG22	2.29	0.47
1:F:387:TYR:CZ	1:F:423:VAL:HG22	2.50	0.47
1:A:392:GLU:OE1	1:A:396:ARG:NH1	2.48	0.47
1:A:486:ILE:HD12	1:A:486:ILE:H	1.80	0.47
1:C:385:ASP:OD1	1:C:386:VAL:N	2.47	0.47
1:B:218:LEU:HD12	1:B:416:LEU:HD11	1.97	0.47
1:D:310:LEU:N	1:D:310:LEU:HD22	2.29	0.47
1:A:320:ASN:N	1:A:320:ASN:OD1	2.47	0.47
1:A:387:TYR:CD1	1:A:423:VAL:HG12	2.50	0.46
1:E:523:LEU:O	1:E:523:LEU:HD12	2.15	0.46
1:F:121:SER:O	1:F:125:VAL:HG23	2.15	0.46
2:G:7:DT:H2"	2:G:8:DG:C8	2.50	0.46
1:F:110:VAL:HG23	1:F:114:LEU:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:486:ILE:H	1:D:486:ILE:HD12	1.81	0.46
1:D:486:ILE:HD12	1:D:486:ILE:N	2.30	0.46
1:C:160:VAL:HG22	1:C:160:VAL:O	2.16	0.46
1:C:391:PHE:HB2	1:C:419:VAL:HG21	1.97	0.46
2:G:6:DT:H2'	2:G:7:DT:C6	2.51	0.46
1:F:486:ILE:HD12	1:F:486:ILE:H	1.81	0.46
1:D:523:LEU:HD12	1:D:523:LEU:O	2.16	0.45
1:C:310:LEU:N	1:C:310:LEU:HD22	2.30	0.45
1:A:451:THR:C	1:A:452:ILE:HD12	2.41	0.45
1:E:154:ILE:N	1:E:154:ILE:HD12	2.31	0.45
1:F:109:LEU:HB2	1:F:114:LEU:HD23	1.96	0.45
1:D:339:GLY:O	1:D:343:ARG:NH1	2.48	0.45
1:A:209:LEU:HD22	1:A:245:VAL:HG12	1.97	0.45
1:A:43:GLN:HB2	1:A:59:ILE:HD11	1.99	0.45
1:C:321:ILE:HG22	1:C:322:LEU:N	2.31	0.45
1:B:201:ASP:OD1	1:B:201:ASP:N	2.48	0.45
1:B:259:SER:O	1:B:260:SER:OG	2.33	0.45
1:D:80:PHE:CD1	1:D:100:ILE:HD11	2.51	0.45
1:A:330:ILE:O	1:A:334:ALA:N	2.49	0.45
1:C:362:ASP:OD2	3:C:701:ANP:N6	2.50	0.45
1:A:365:PHE:CD1	1:A:365:PHE:C	2.95	0.45
1:E:387:TYR:CZ	1:E:423:VAL:HG22	2.52	0.45
1:C:486:ILE:N	1:C:486:ILE:HD12	2.32	0.45
1:D:235:SER:N	3:D:701:ANP:O1B	2.50	0.45
1:D:244:LEU:HD23	1:D:244:LEU:O	2.17	0.45
1:E:486:ILE:HD12	1:E:486:ILE:N	2.31	0.45
1:B:406:ILE:N	1:B:406:ILE:HD12	2.32	0.45
1:D:199:ILE:HD12	1:D:199:ILE:O	2.17	0.45
1:E:180:ASP:N	1:E:180:ASP:OD1	2.50	0.44
1:A:258:TRP:N	1:A:280:ASP:O	2.49	0.44
1:E:518:ASP:HA	1:E:523:LEU:HD11	1.99	0.44
1:A:138:LEU:N	1:A:138:LEU:HD22	2.33	0.44
1:F:387:TYR:CD1	1:F:423:VAL:HG22	2.52	0.44
1:B:497:ILE:N	1:B:545:PHE:O	2.47	0.44
1:A:486:ILE:HD12	1:A:486:ILE:N	2.33	0.44
1:E:142:VAL:HG12	1:E:143:ALA:N	2.33	0.44
1:F:486:ILE:HD12	1:F:486:ILE:N	2.32	0.44
3:B:701:ANP:O2G	1:C:343:ARG:NH1	2.50	0.44
1:D:199:ILE:HD12	1:D:199:ILE:C	2.43	0.44
1:E:337:LYS:O	1:E:340:VAL:HG12	2.18	0.44
1:A:218:LEU:CD2	1:A:321:ILE:HD11	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:SER:O	1:A:370:GLY:N	2.44	0.44
1:B:486:ILE:HD12	1:B:486:ILE:H	1.82	0.44
3:B:701:ANP:O2G	1:C:343:ARG:NH2	2.49	0.44
1:A:540:VAL:HG11	1:A:542:TYR:CZ	2.53	0.44
1:F:419:VAL:O	1:F:423:VAL:HG23	2.18	0.43
1:B:163:ASP:OD1	1:B:164:SER:N	2.51	0.43
1:F:415:ALA:O	1:F:419:VAL:HG23	2.18	0.43
1:E:540:VAL:HG12	1:E:541:LYS:N	2.34	0.43
1:B:486:ILE:HD12	1:B:486:ILE:N	2.34	0.43
1:E:281:ASP:OD2	1:E:284:ASN:ND2	2.51	0.43
1:C:322:LEU:C	1:C:322:LEU:HD23	2.44	0.43
1:E:106:LEU:CD2	1:E:124:LEU:HD23	2.48	0.43
1:E:258:TRP:CD1	1:E:282:THR:HG22	2.53	0.43
2:G:6:DT:C5	2:G:7:DT:H73	2.53	0.43
1:E:153:PHE:C	1:E:154:ILE:HD12	2.44	0.43
1:D:244:LEU:HD23	1:D:244:LEU:C	2.44	0.43
1:B:362:ASP:O	1:B:366:ARG:HG2	2.19	0.43
1:E:255:ILE:HG22	1:E:256:THR:N	2.34	0.43
1:E:379:GLN:CB	1:E:427:ILE:HD11	2.48	0.43
2:G:5:DC:C2'	2:G:6:DT:H71	2.48	0.43
1:E:527:GLU:OE1	1:E:527:GLU:N	2.45	0.42
1:C:558:ASP:OD1	1:C:559:PHE:N	2.53	0.42
1:A:227:ILE:HB	1:A:344:VAL:HG22	2.02	0.42
1:E:290:VAL:O	1:E:294:THR:HG23	2.19	0.42
2:G:3:DA:C4	2:G:4:DG:C8	3.07	0.42
1:F:242:LEU:HD23	1:F:242:LEU:C	2.45	0.42
1:F:540:VAL:HG12	1:F:541:LYS:N	2.34	0.42
1:A:424:LEU:O	1:A:424:LEU:HD23	2.20	0.42
1:A:540:VAL:HG12	1:A:541:LYS:N	2.34	0.42
1:C:323:ILE:N	1:C:323:ILE:HD12	2.34	0.42
1:F:282:THR:HG23	1:F:325:THR:O	2.20	0.42
1:F:360:THR:HG23	1:F:361:LEU:N	2.35	0.42
1:E:485:ASP:N	1:E:485:ASP:OD1	2.52	0.42
1:B:203:PRO:O	1:B:207:VAL:HG23	2.19	0.42
1:D:496:CYS:HA	1:D:545:PHE:O	2.20	0.42
1:F:95:VAL:HG21	1:F:100:ILE:HD11	2.01	0.42
1:B:383:LYS:O	1:B:384:LYS:C	2.63	0.42
1:C:218:LEU:HD11	1:C:416:LEU:HD21	2.02	0.42
1:C:122:THR:HG23	1:C:123:LYS:N	2.35	0.42
1:F:102:ASP:OD1	1:F:105:GLN:N	2.40	0.41
1:D:282:THR:HG22	1:D:326:GLY:HA3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:220:GLU:N	1:E:220:GLU:OE1	2.53	0.41
1:C:309:ASN:C	1:C:310:LEU:HD22	2.45	0.41
2:G:3:DA:C2	2:G:4:DG:C4	3.09	0.41
1:A:362:ASP:HA	1:A:365:PHE:CE2	2.56	0.41
1:A:527:GLU:OE1	1:A:527:GLU:N	2.41	0.41
1:D:442:TYR:O	1:D:446:VAL:HG23	2.20	0.41
1:A:148:HIS:CE1	1:A:216:VAL:HG13	2.56	0.41
1:A:243:ASN:HA	1:A:255:ILE:HD11	2.03	0.41
1:B:496:CYS:HA	1:B:545:PHE:O	2.21	0.41
1:E:310:LEU:HD12	1:E:310:LEU:N	2.36	0.41
2:H:5:DC:H2'	2:H:6:DT:C6	2.56	0.41
1:A:452:ILE:HD12	1:A:452:ILE:N	2.36	0.41
1:E:83:LEU:C	1:E:83:LEU:HD23	2.46	0.41
1:F:265:ILE:HD12	1:F:265:ILE:N	2.36	0.41
1:B:449:ASN:OD1	1:B:450:LYS:N	2.54	0.41
1:D:106:LEU:HD21	1:D:124:LEU:HD23	2.03	0.41
1:D:245:VAL:O	1:D:248:VAL:HG23	2.21	0.41
1:D:256:THR:HG22	1:D:257:THR:N	2.35	0.41
1:D:410:LEU:HD13	1:D:445:MET:HE1	2.02	0.41
1:E:199:ILE:HD13	1:E:244:LEU:HD21	2.03	0.41
1:C:145:ARG:O	1:C:146:LEU:HD23	2.21	0.41
1:C:523:LEU:O	1:C:523:LEU:HD12	2.21	0.41
1:F:159:GLU:OE1	1:F:159:GLU:N	2.37	0.41
1:B:98:GLU:O	1:B:102:ASP:N	2.54	0.41
1:E:262:GLN:O	1:E:265:ILE:N	2.54	0.41
1:C:221:PHE:N	1:C:221:PHE:CD1	2.89	0.41
1:D:41:LEU:HD23	1:D:63:ILE:HG13	2.02	0.40
1:D:484:GLY:O	1:C:471:ASN:ND2	2.53	0.40
1:C:258:TRP:CD1	1:C:282:THR:HA	2.56	0.40
1:C:365:PHE:CD1	1:C:365:PHE:C	3.00	0.40
2:G:7:DT:C4	2:G:8:DG:O6	2.74	0.40
1:E:81:ASN:OD1	1:E:82:MET:N	2.55	0.40
1:C:383:LYS:O	1:C:386:VAL:HG12	2.21	0.40
2:H:8:DG:N2	2:H:9:DT:C2	2.89	0.40
1:F:485:ASP:OD1	1:F:485:ASP:N	2.54	0.40
1:E:496:CYS:HA	1:E:545:PHE:O	2.21	0.40
1:C:427:ILE:HG22	1:C:428:ASP:N	2.36	0.40
1:D:203:PRO:O	1:D:207:VAL:HG23	2.21	0.40
1:A:476:ASP:OD1	1:A:476:ASP:N	2.52	0.40
1:A:508:HIS:O	1:A:508:HIS:CG	2.74	0.40
2:H:5:DC:H2'	2:H:6:DT:H6	1.87	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	494/602 (82%)	473 (96%)	20 (4%)	1 (0%)	43 70
1	B	499/602 (83%)	471 (94%)	28 (6%)	0	100 100
1	C	523/602 (87%)	496 (95%)	27 (5%)	0	100 100
1	D	518/602 (86%)	493 (95%)	25 (5%)	0	100 100
1	E	518/602 (86%)	492 (95%)	26 (5%)	0	100 100
1	F	497/602 (83%)	483 (97%)	14 (3%)	0	100 100
All	All	3049/3612 (84%)	2908 (95%)	140 (5%)	1 (0%)	100 100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	538	GLN

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	454/534 (85%)	451 (99%)	3 (1%)	76 77
1	B	458/534 (86%)	454 (99%)	4 (1%)	70 75
1	C	474/534 (89%)	466 (98%)	8 (2%)	53 67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	470/534 (88%)	462 (98%)	8 (2%)	53 67
1	E	471/534 (88%)	467 (99%)	4 (1%)	73 76
1	F	456/534 (85%)	454 (100%)	2 (0%)	84 82
All	All	2783/3204 (87%)	2754 (99%)	29 (1%)	65 74

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	76	ASN
1	F	534	GLN
1	B	172	ASP
1	B	288	LYS
1	B	511	GLN
1	B	535	VAL
1	D	41	LEU
1	D	163	ASP
1	D	286	HIS
1	D	308	ILE
1	D	476	ASP
1	D	493	ASP
1	D	529	ASP
1	D	550	GLU
1	A	168	LEU
1	A	372	LEU
1	A	523	LEU
1	E	169	PHE
1	E	220	GLU
1	E	295	TYR
1	E	523	LEU
1	C	89	THR
1	C	142	VAL
1	C	229	GLU
1	C	357	ASP
1	C	464	GLN
1	C	493	ASP
1	C	529	ASP
1	C	550	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	263	ASN
1	F	284	ASN
1	F	464	GLN
1	F	469	ASN
1	B	448	ASN
1	D	81	ASN
1	D	355	ASN
1	D	404	ASN
1	A	42	ASN
1	A	296	ASN
1	A	537	HIS
1	E	148	HIS
1	E	273	ASN
1	C	404	ASN
1	C	448	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	$\#\|Z\|>2$
3	ANP	C	701	4	33,33,33	2.17	5 (15%)	45,52,52	1.23	4 (8%)
3	ANP	D	701	4	33,33,33	2.22	5 (15%)	45,52,52	1.36	3 (6%)
5	ADP	E	701	4	28,29,29	1.38	4 (14%)	43,45,45	1.89	11 (25%)
3	ANP	B	701	4	33,33,33	2.16	5 (15%)	45,52,52	1.26	3 (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
3	ANP	C	701	4	-	8/18/38/38	0/3/3/3
3	ANP	D	701	4	-	5/18/38/38	0/3/3/3
5	ADP	E	701	4	-	5/16/32/32	0/3/3/3
3	ANP	B	701	4	-	4/18/38/38	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	701	ANP	PB-O3A	8.61	1.69	1.59
3	C	701	ANP	PB-O3A	8.27	1.69	1.59
3	B	701	ANP	PB-O3A	8.10	1.69	1.59
3	B	701	ANP	PG-N3B	6.05	1.79	1.63
3	D	701	ANP	PG-N3B	5.96	1.78	1.63
3	C	701	ANP	PG-N3B	5.89	1.78	1.63
3	C	701	ANP	PG-O1G	4.57	1.53	1.46
5	E	701	ADP	C5-C4	4.51	1.47	1.39
3	D	701	ANP	PG-O1G	4.48	1.53	1.46
3	B	701	ANP	PG-O1G	4.48	1.53	1.46
5	E	701	ADP	C5-C6	2.67	1.48	1.41
3	D	701	ANP	PB-O1B	2.53	1.50	1.46
3	C	701	ANP	PB-O1B	2.50	1.50	1.46
3	B	701	ANP	PB-O1B	2.48	1.49	1.46
5	E	701	ADP	C8-N7	2.47	1.36	1.31
3	B	701	ANP	PB-O2B	-2.33	1.50	1.56
5	E	701	ADP	C5-N7	-2.28	1.34	1.39
3	C	701	ANP	PB-O2B	-2.28	1.50	1.56
3	D	701	ANP	PB-O2B	-2.27	1.50	1.56

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	701	ADP	C5-C4-N3	-5.58	119.04	126.72
3	D	701	ANP	O1G-PG-N3B	-5.57	103.57	111.77
3	B	701	ANP	O2B-PB-O1B	5.19	121.00	109.87
3	D	701	ANP	O2B-PB-O1B	5.11	120.83	109.87
3	C	701	ANP	O2B-PB-O1B	5.05	120.71	109.87
5	E	701	ADP	N3-C4-N9	4.42	134.69	127.17
3	B	701	ANP	O1G-PG-N3B	-4.10	105.74	111.77
5	E	701	ADP	C2-N3-C4	3.84	121.20	111.83
5	E	701	ADP	N3-C2-N1	-3.81	122.81	128.58
5	E	701	ADP	C4-C5-N7	-3.53	106.55	110.58
3	C	701	ANP	O1G-PG-N3B	-3.52	106.59	111.77
5	E	701	ADP	C4-N9-C8	3.07	108.96	105.74
3	D	701	ANP	O2G-PG-O3G	2.91	115.40	107.59
5	E	701	ADP	C5-N7-C8	2.75	107.78	103.45
3	B	701	ANP	O2G-PG-O3G	2.74	114.96	107.59
3	C	701	ANP	O2G-PG-O3G	2.50	114.30	107.59
5	E	701	ADP	N9-C8-N7	-2.46	110.44	113.94
5	E	701	ADP	C6-C5-N7	2.30	136.52	132.09
5	E	701	ADP	C3'-C2'-C1'	2.18	105.60	101.46
5	E	701	ADP	C2-N1-C6	2.15	122.27	118.73
3	C	701	ANP	O3A-PB-N3B	-2.01	101.03	106.59

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	701	ANP	PG-N3B-PB-O1B
3	B	701	ANP	PA-O3A-PB-O2B
3	B	701	ANP	C5'-O5'-PA-O1A
3	D	701	ANP	PB-N3B-PG-O1G
3	D	701	ANP	PG-N3B-PB-O1B
3	D	701	ANP	C5'-O5'-PA-O1A
3	D	701	ANP	C5'-O5'-PA-O3A
3	C	701	ANP	PG-N3B-PB-O1B
3	C	701	ANP	PA-O3A-PB-O2B
3	C	701	ANP	C5'-O5'-PA-O2A
3	C	701	ANP	C5'-O5'-PA-O3A
5	E	701	ADP	C5'-O5'-PA-O1A
5	E	701	ADP	C5'-O5'-PA-O2A
5	E	701	ADP	C5'-O5'-PA-O3A
5	E	701	ADP	O4'-C4'-C5'-O5'
5	E	701	ADP	C3'-C4'-C5'-O5'
3	C	701	ANP	O4'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	C	701	ANP	C3'-C4'-C5'-O5'
3	D	701	ANP	C5'-O5'-PA-O2A
3	B	701	ANP	PA-O3A-PB-O1B
3	C	701	ANP	PA-O3A-PB-O1B
3	C	701	ANP	PB-N3B-PG-O1G

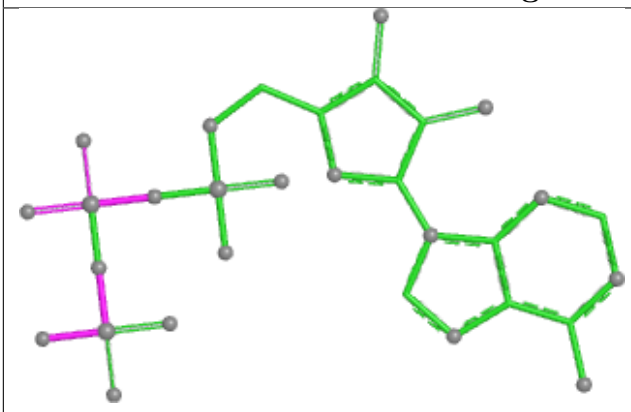
There are no ring outliers.

4 monomers are involved in 12 short contacts:

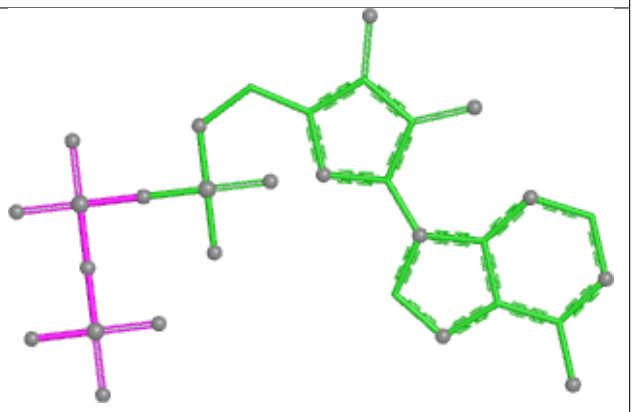
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	701	ANP	4	0
3	D	701	ANP	2	0
5	E	701	ADP	2	0
3	B	701	ANP	4	0

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.

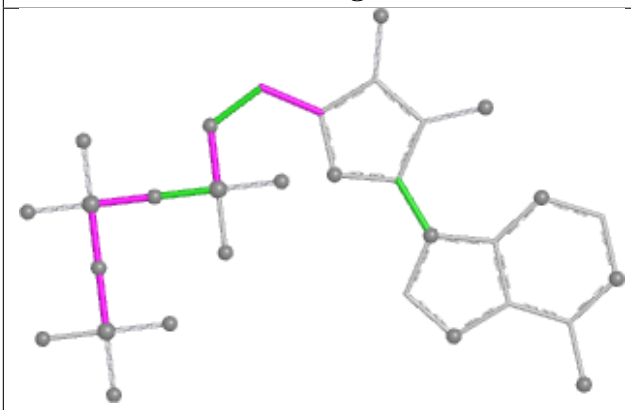
Ligand ANP C 701



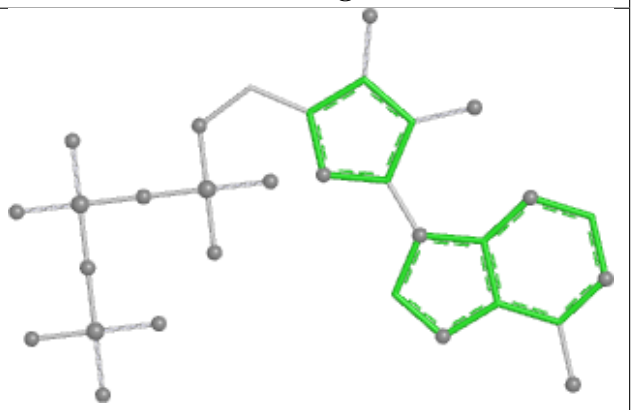
Bond lengths



Bond angles

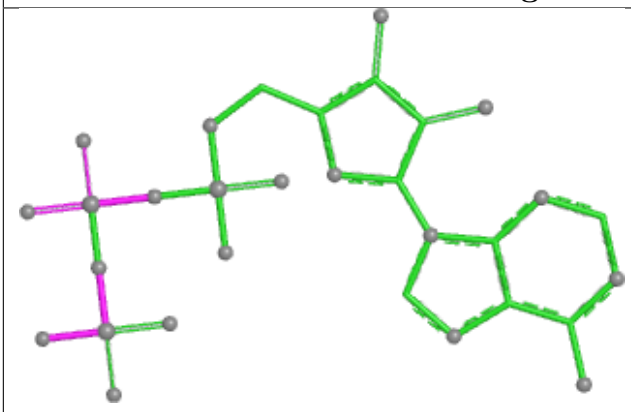


Torsions

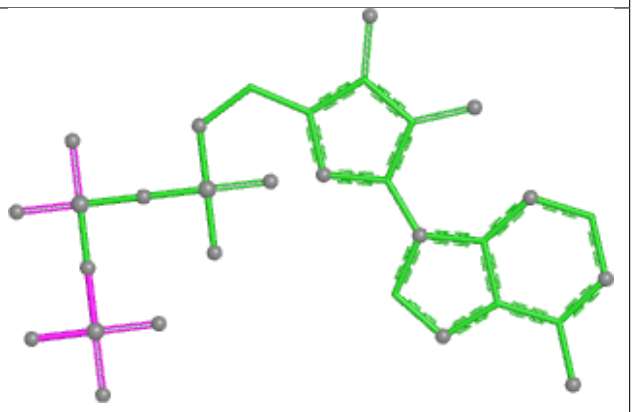


Rings

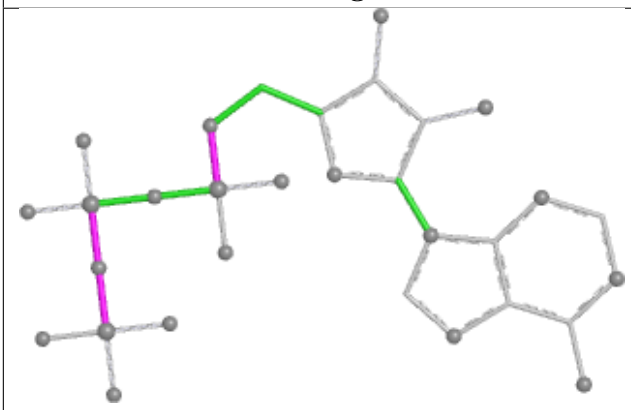
Ligand ANP D 701



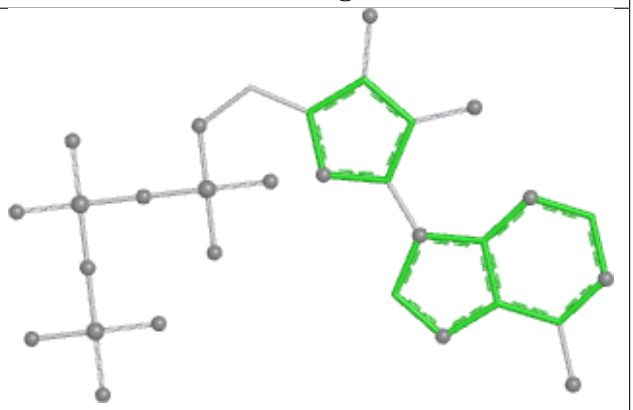
Bond lengths



Bond angles

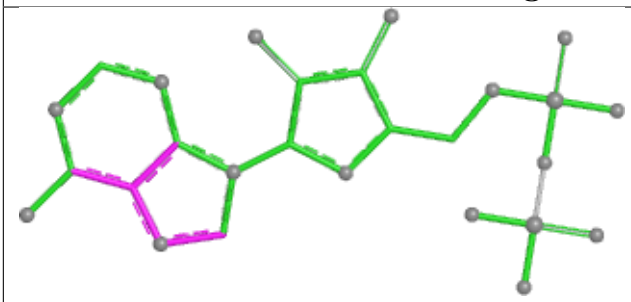


Torsions

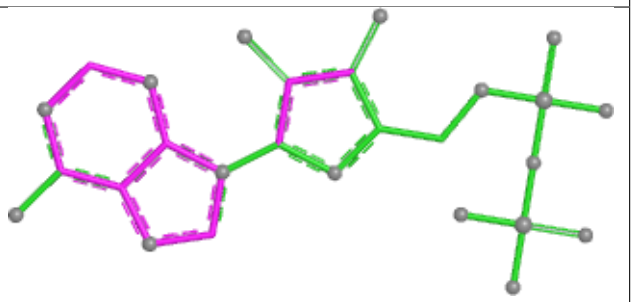


Rings

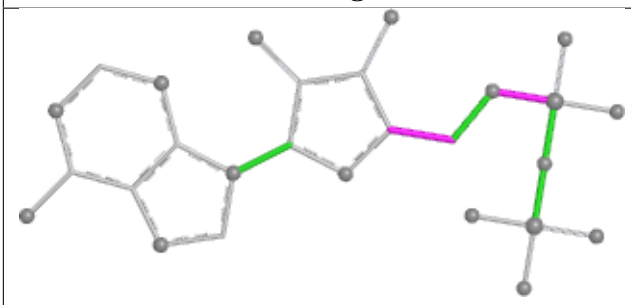
Ligand ADP E 701



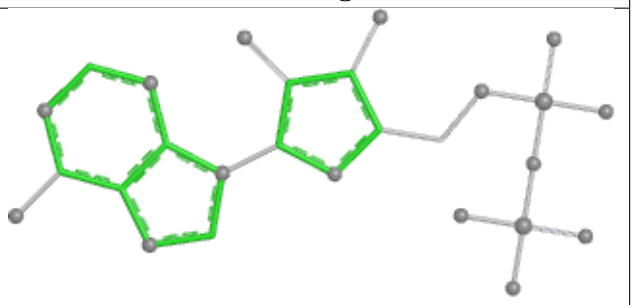
Bond lengths



Bond angles

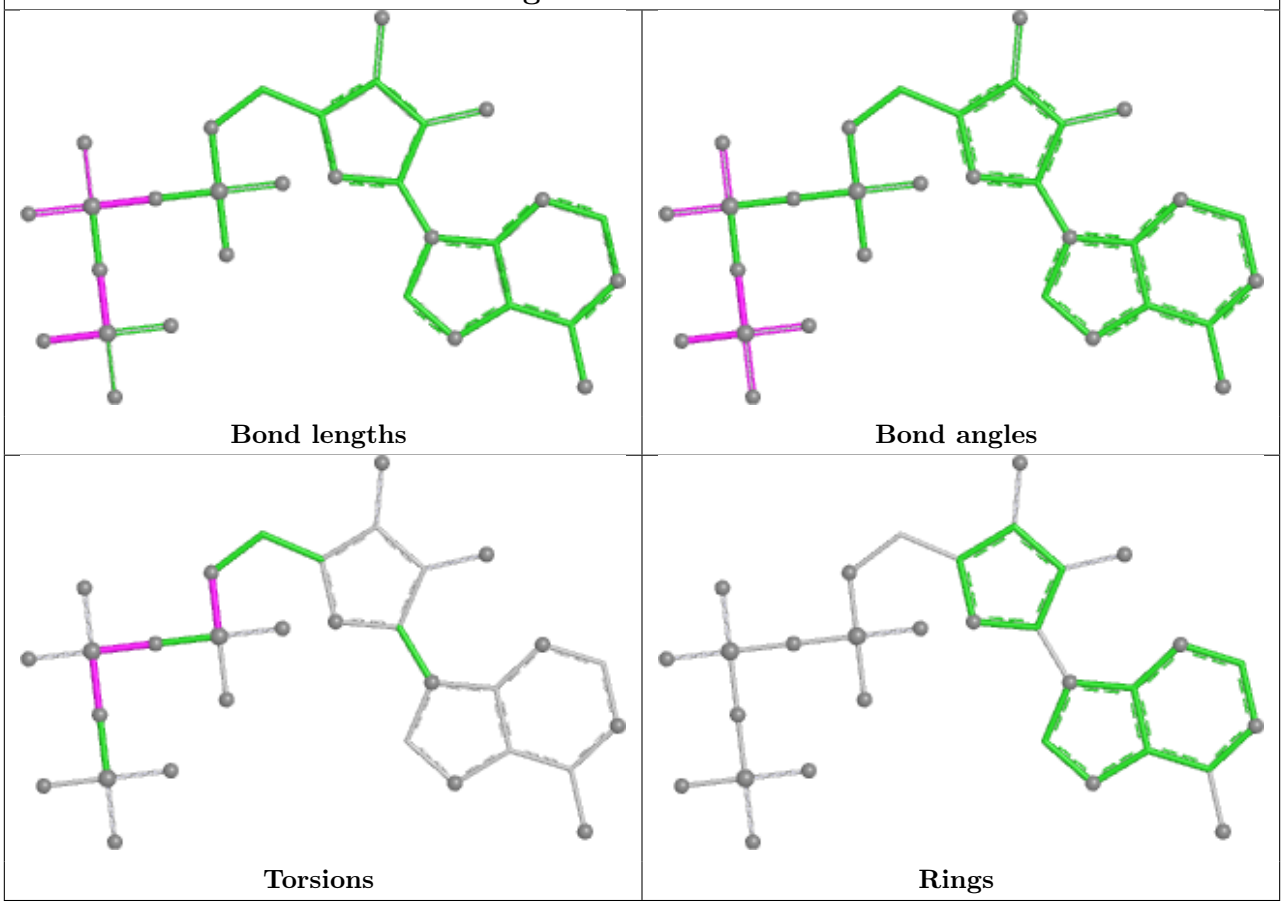


Torsions



Rings

Ligand ANP B 701



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.

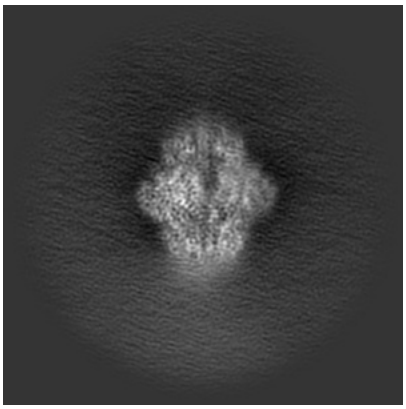
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-79703. These allow visual inspection of the internal detail of the map and identification of artifacts.

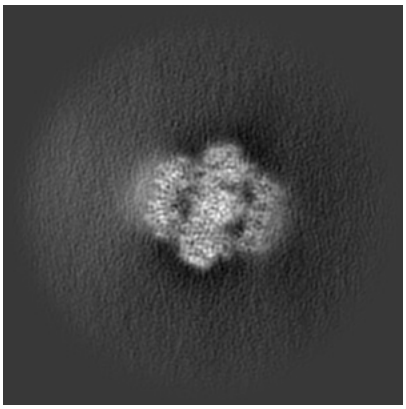
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

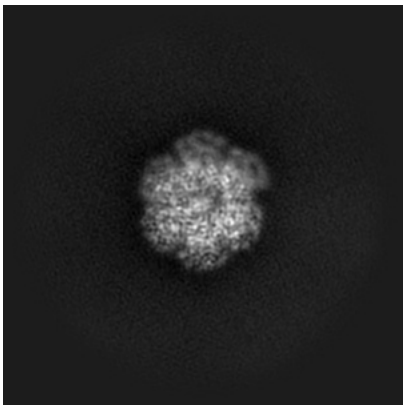
6.1.1 Primary map



X

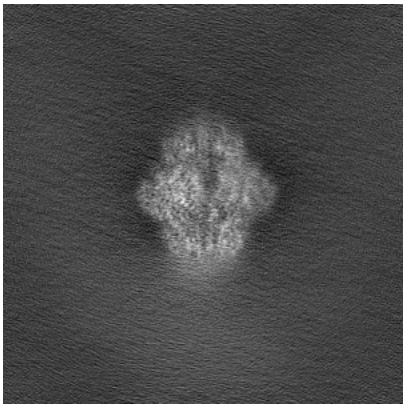


Y

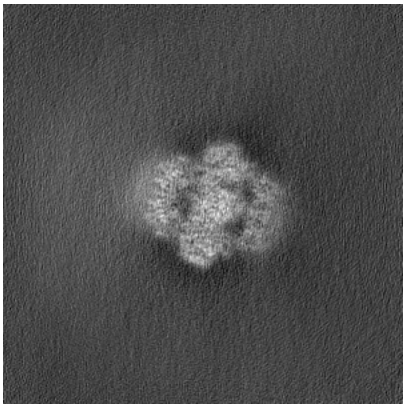


Z

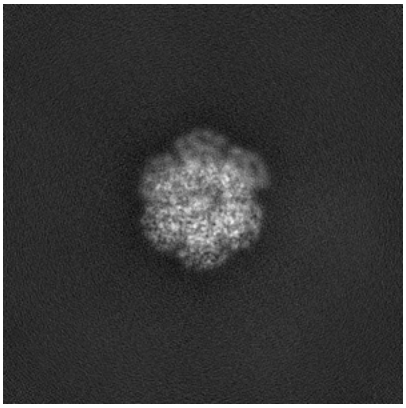
6.1.2 Raw map



X



Y

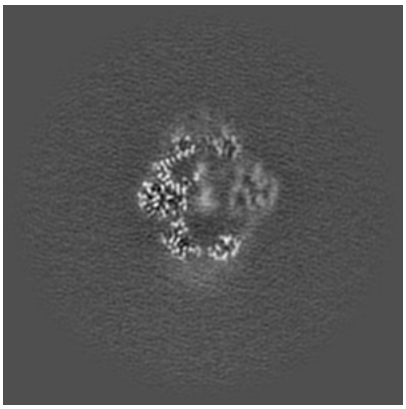


Z

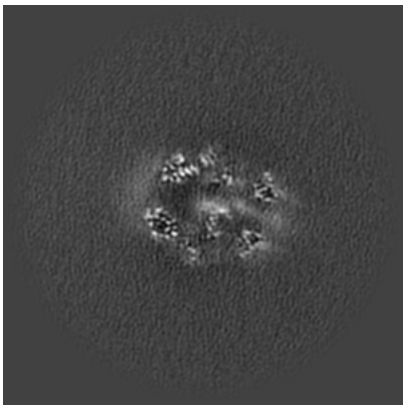
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

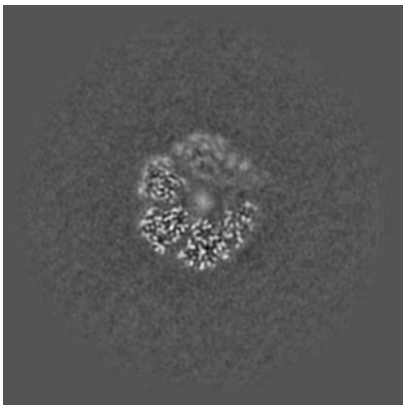
6.2.1 Primary map



X Index: 160

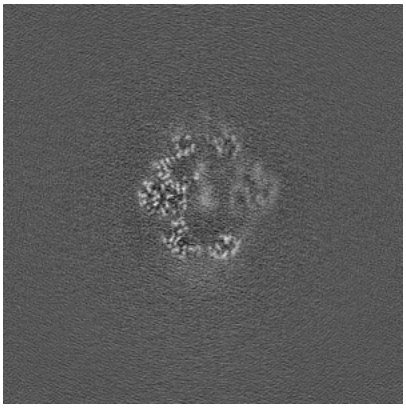


Y Index: 160

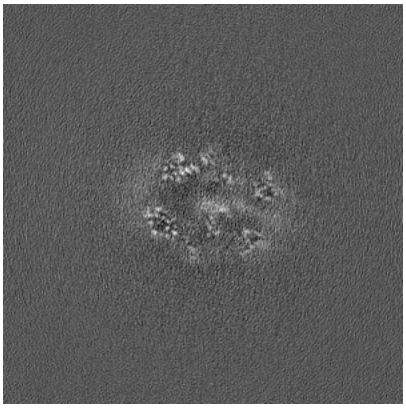


Z Index: 160

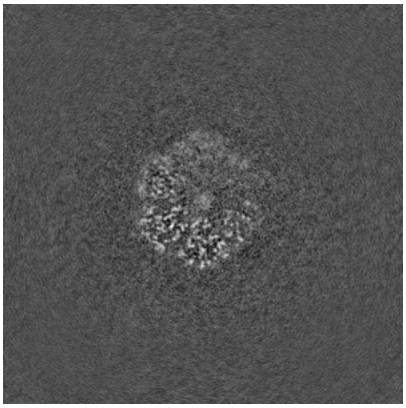
6.2.2 Raw map



X Index: 160



Y Index: 160

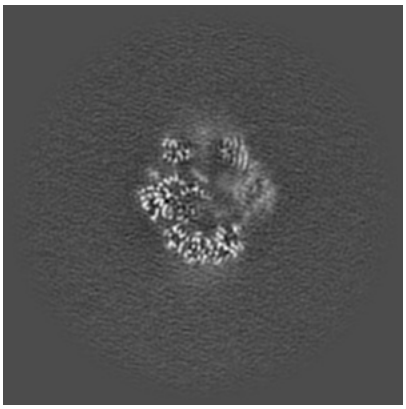


Z Index: 160

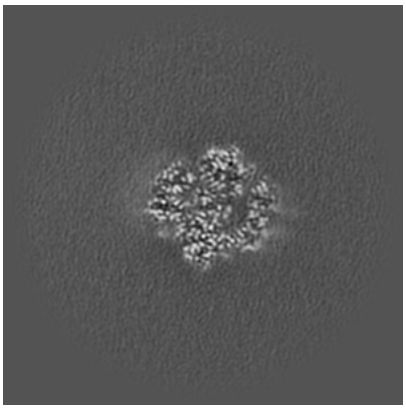
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

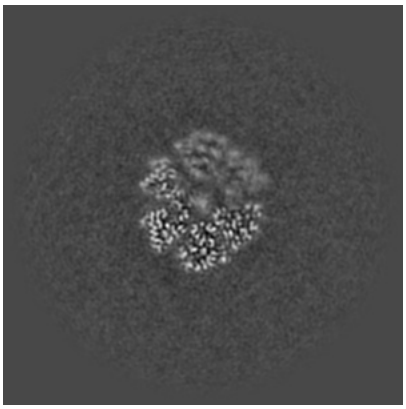
6.3.1 Primary map



X Index: 150

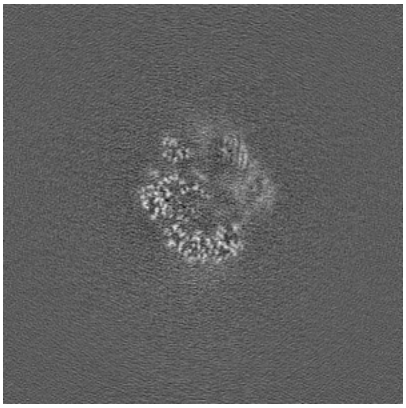


Y Index: 142

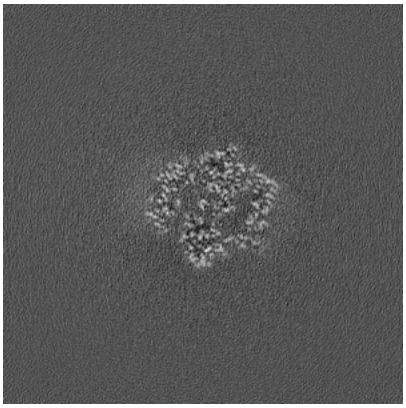


Z Index: 165

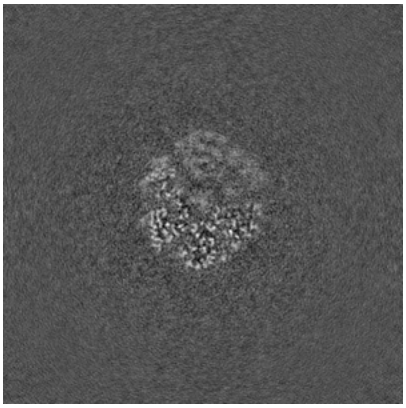
6.3.2 Raw map



X Index: 150



Y Index: 146

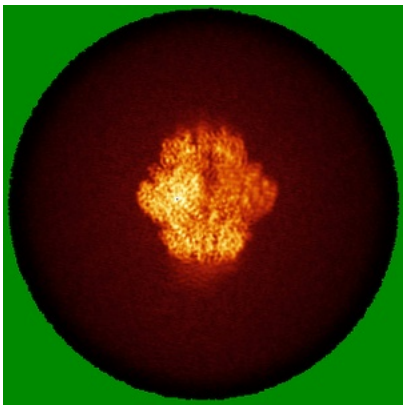


Z Index: 165

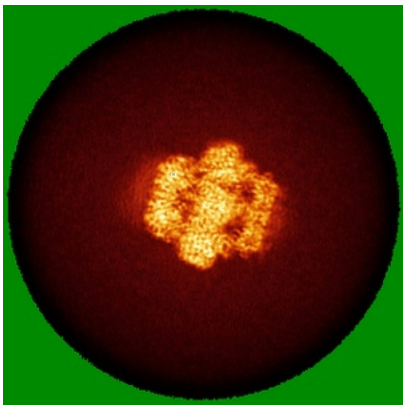
The images above show the largest variance slices of the map in three orthogonal directions.

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

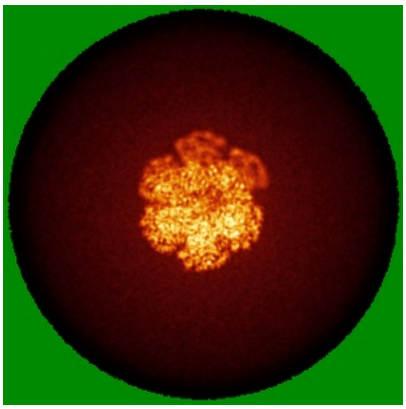
6.4.1 Primary map



X

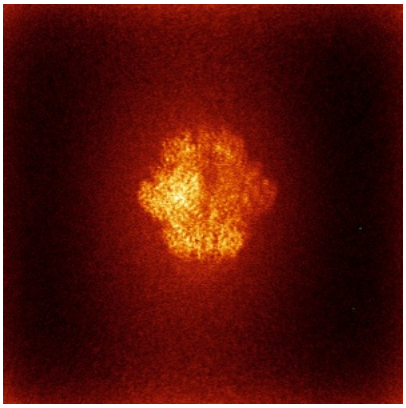


Y

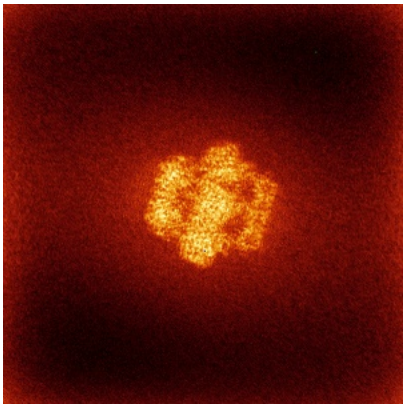


Z

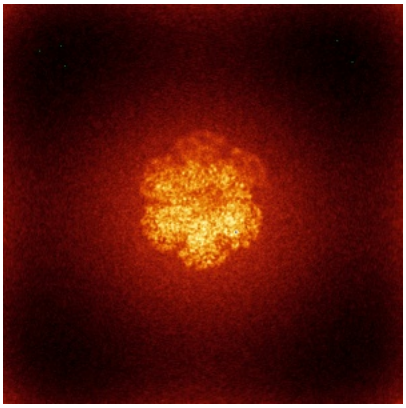
6.4.2 Raw map



X



Y

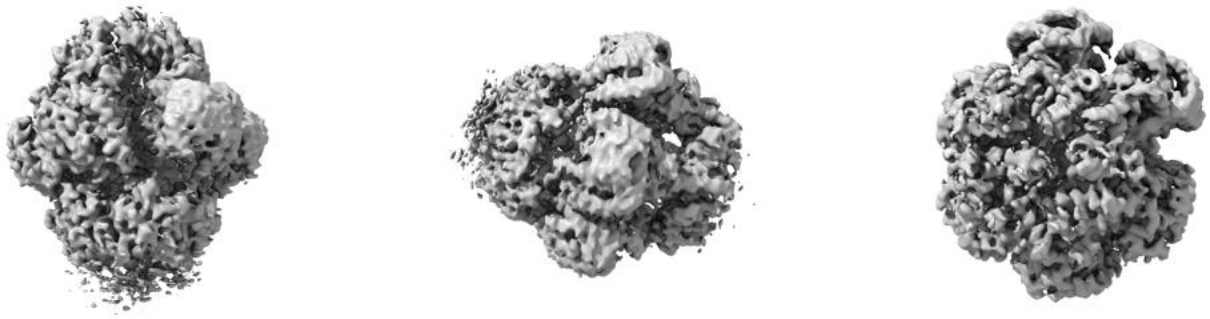


Z

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)

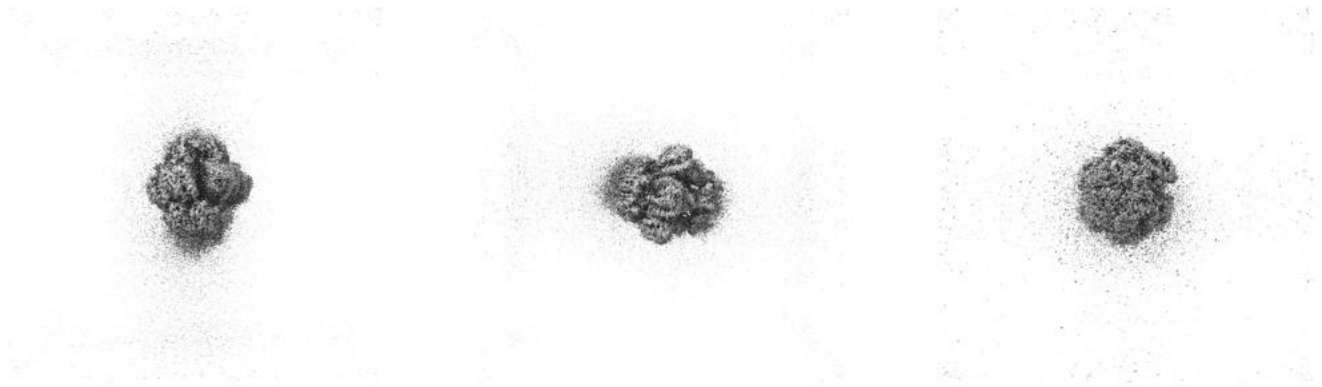
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.04. 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.

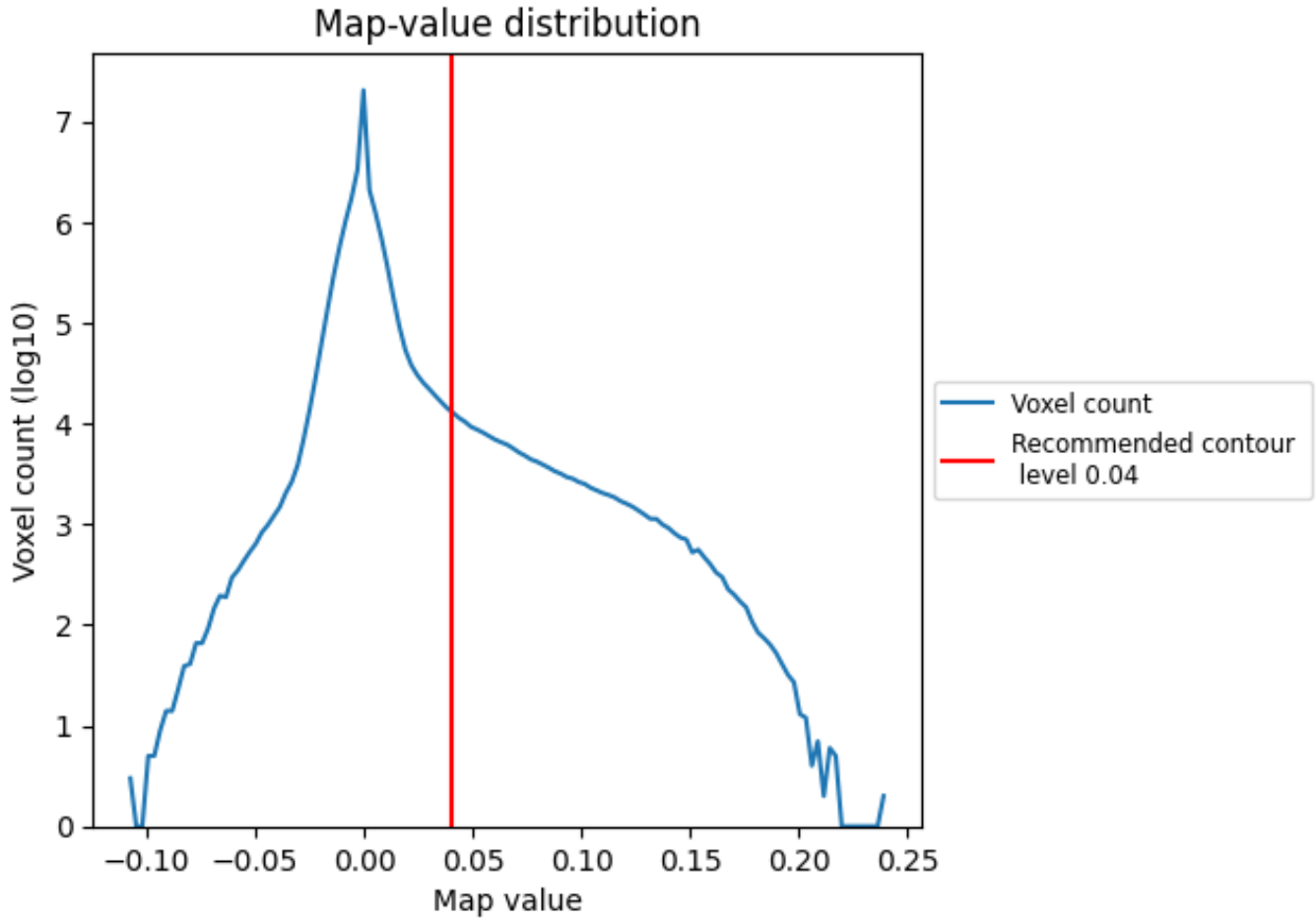
6.6 Mask visualisation (i)

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

7 Map analysis

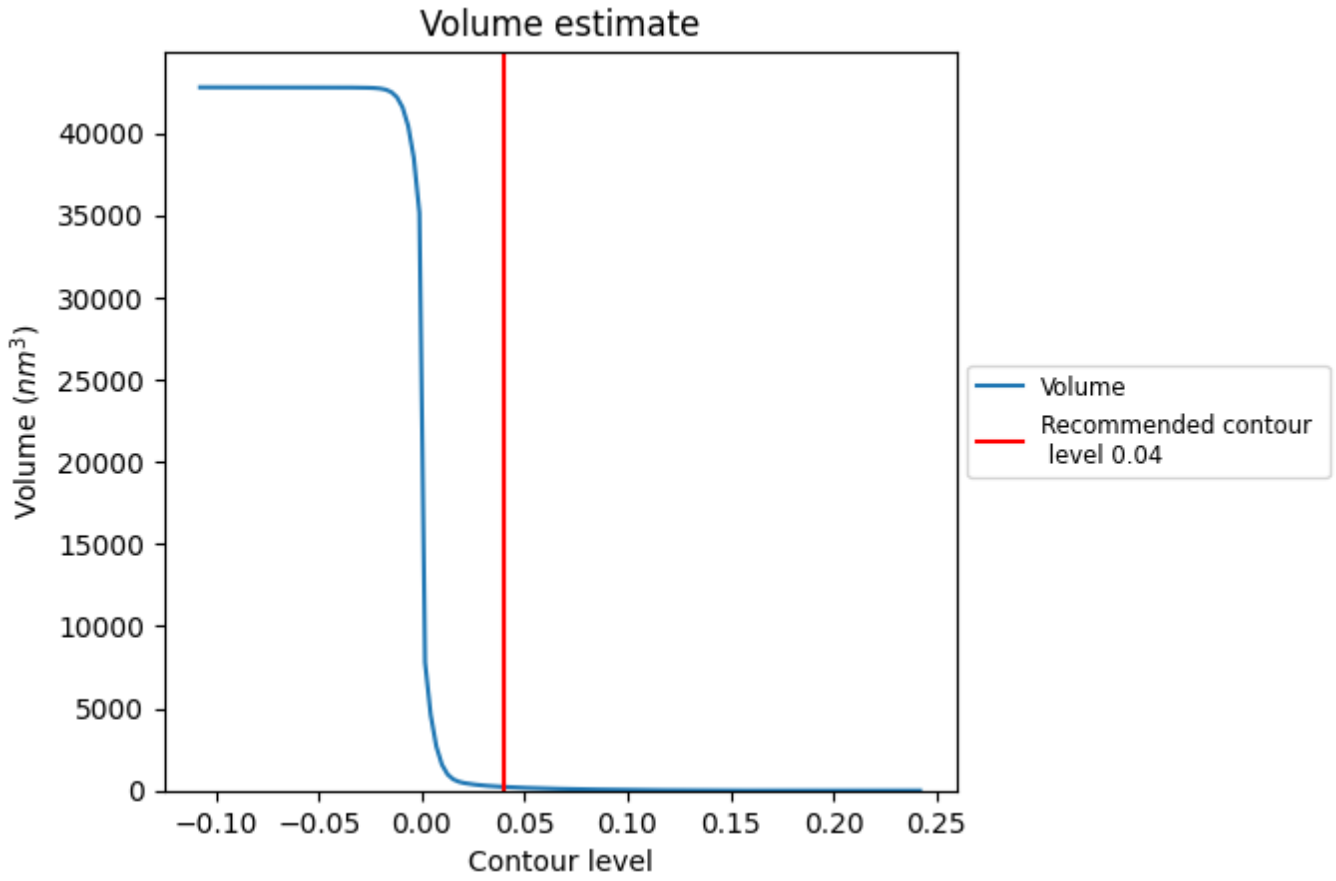
This section contains the results of statistical analysis of the map.

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.

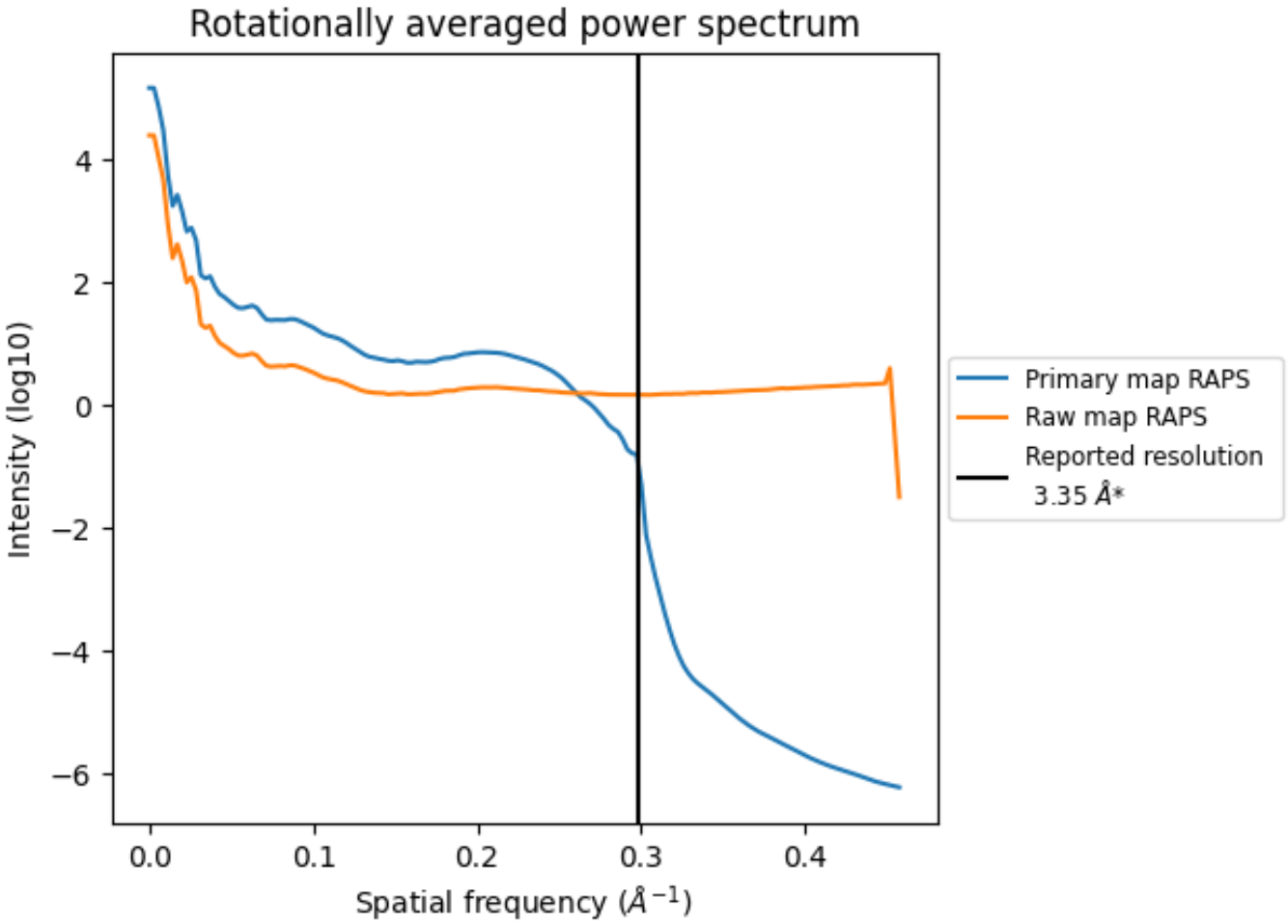
7.2 Volume estimate



The volume at the recommended contour level is 223 nm^3; this corresponds to an approximate mass of 201 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)

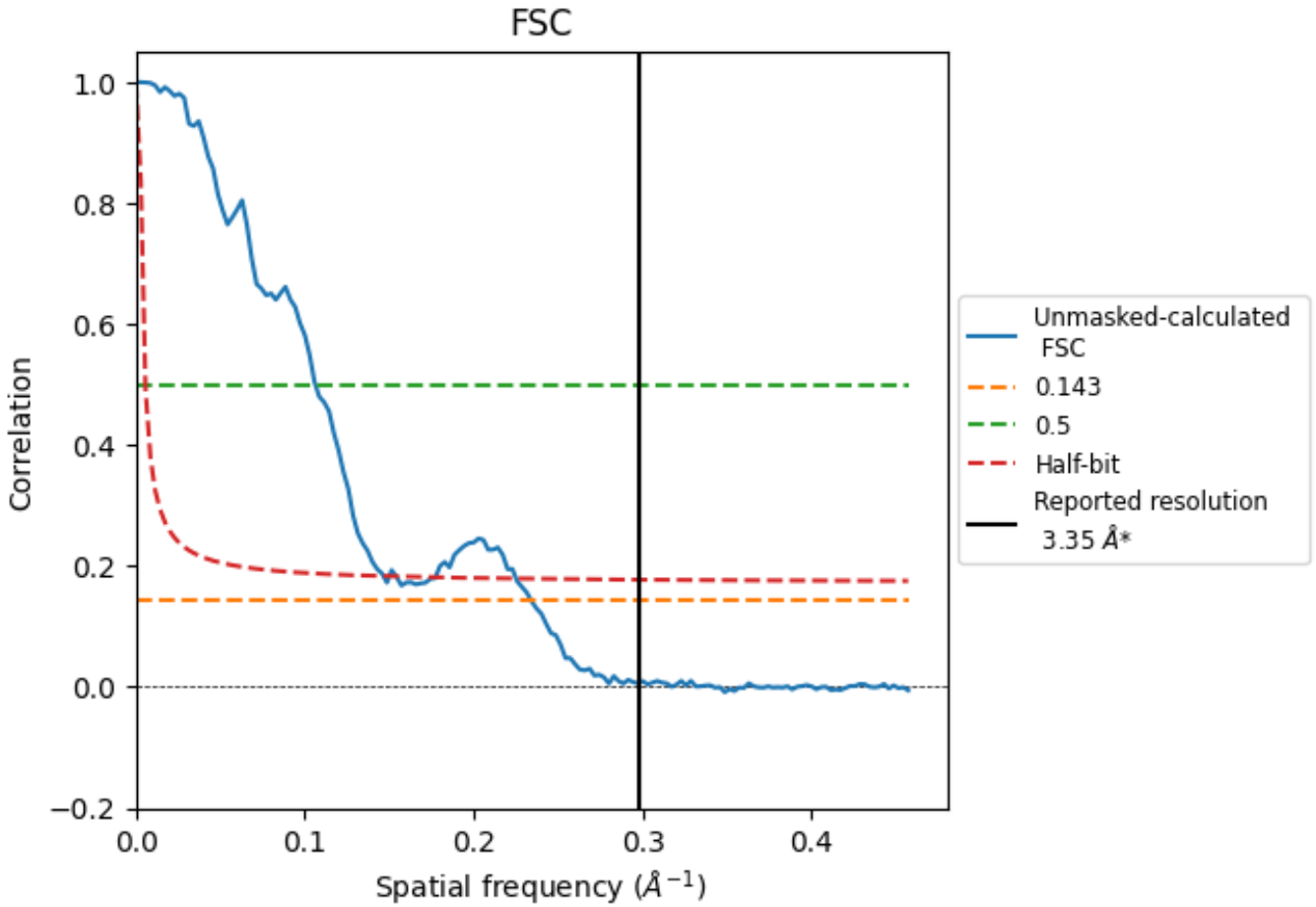


*Reported resolution corresponds to spatial frequency of 0.299 Å^{-1}

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 0.299 Å^{-1}

8.2 Resolution estimates (i)

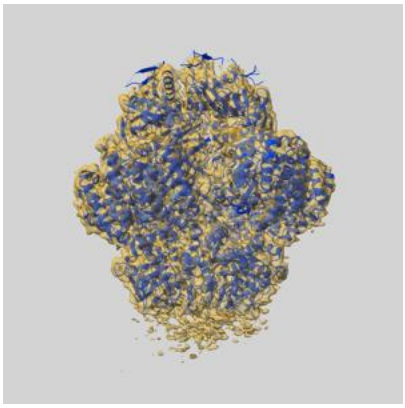
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.35	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.27	9.41	6.82

*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 4.27 differs from the reported value 3.35 by more than 10 %

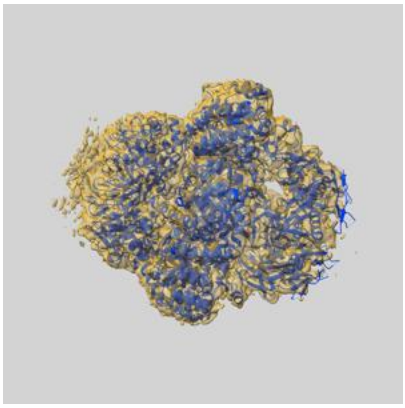
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-79703 and PDB model 39QT. Per-residue inclusion information can be found in section 3 on page 12.

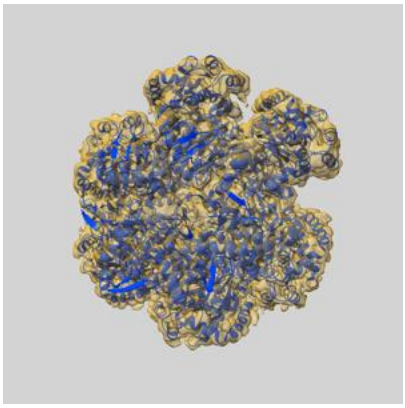
9.1 Map-model overlay



X



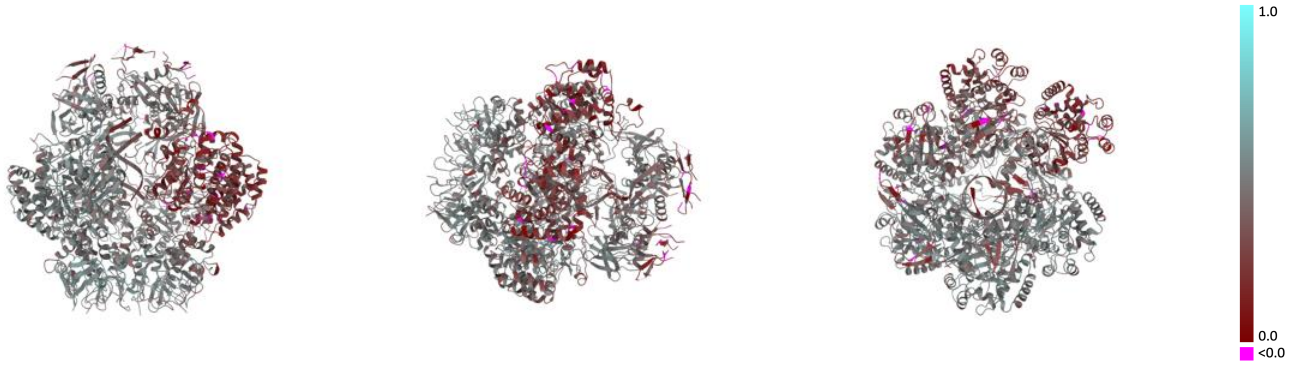
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04 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.

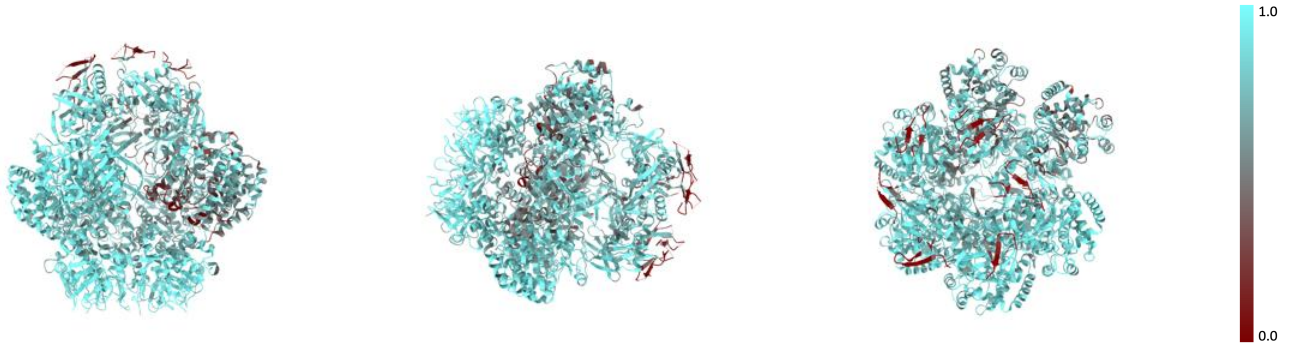
9.2 Q-score mapped to coordinate model (i)



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.

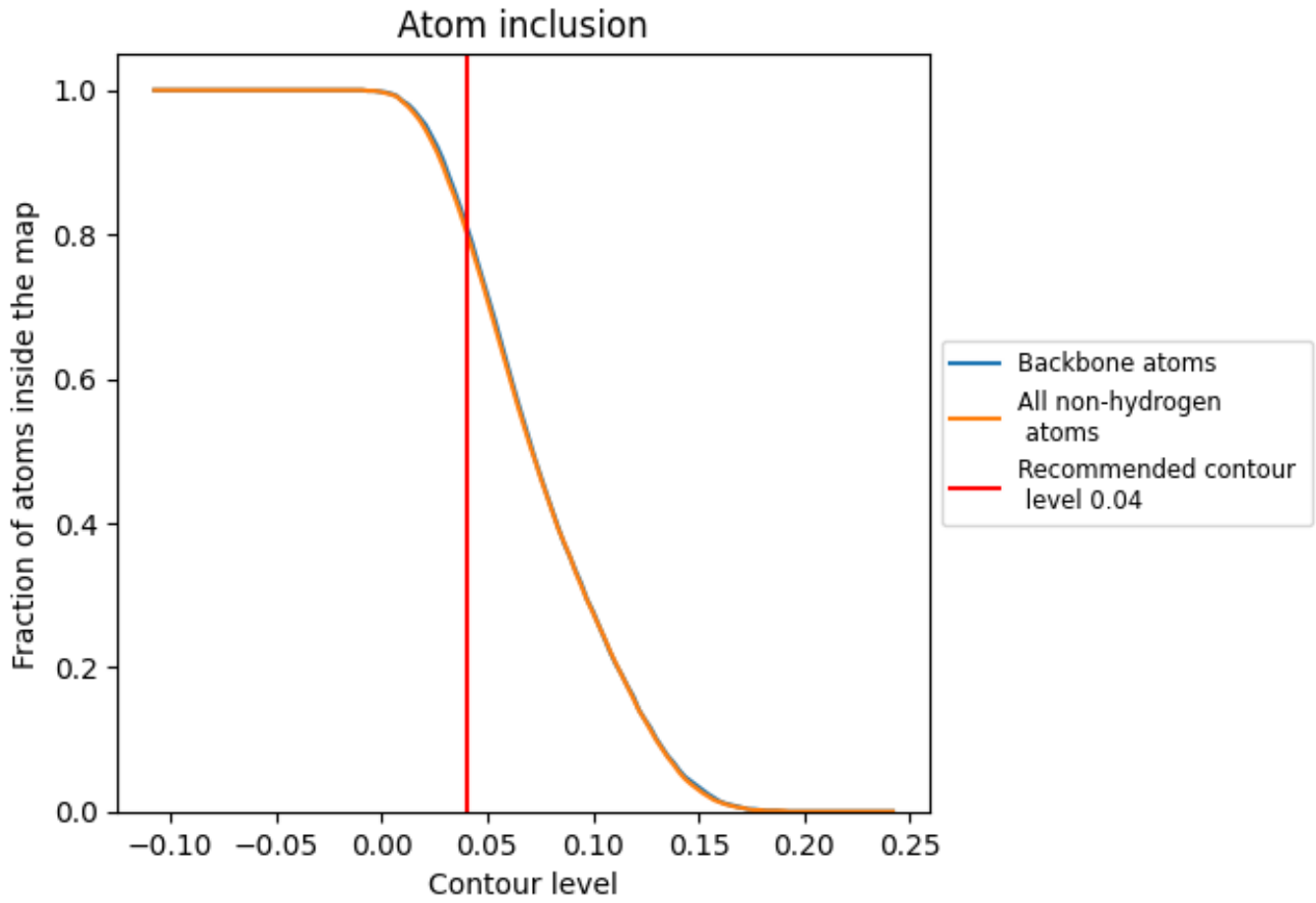
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.04).

9.4 Atom inclusion (i)



At the recommended contour level, 81% of all backbone atoms, 80% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8050	0.4240
A	0.7140	0.3190
B	0.8680	0.4780
C	0.8680	0.4880
D	0.8670	0.4870
E	0.8210	0.4400
F	0.6930	0.3320
G	0.8380	0.2890
H	0.8870	0.3920

