wwPDB EM Validation Summary Report (i)

Mar 25, 2024 – 05:25 PM JST

PDB ID	:	7Y59
EMDB ID	:	EMD-33613
Title	:	The cryo-EM structure of human ERAD retro-translocation complex
Authors	:	Cao, Y.; Rao, B.; Wang, Q.; Yao, D.; Xia, Y.; Li, W.; Li, S.; Shen, Y.
Deposited on	:	2022-06-16
Resolution	:	4.51 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

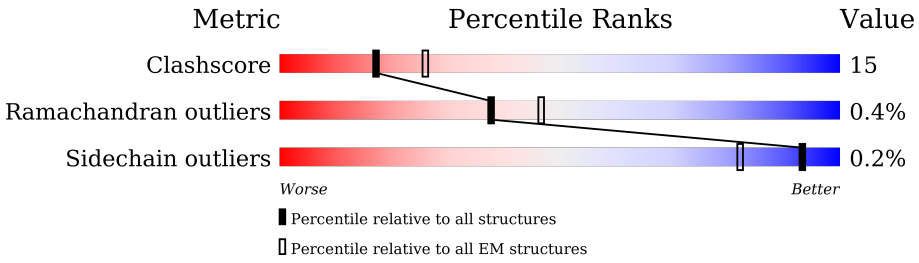
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.51 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	W	267	60% 60% 24% 16%
1	X	267	57% 53% 31% 16%
1	Y	267	69% 81% • 16%
1	Z	267	59% 80% • 16%
2	A	787	10% 63% 31% 5%
2	B	787	11% 60% 35% • 5%
2	C	787	17% 59% 35% • 5%
2	D	787	17% 62% 32% 6%

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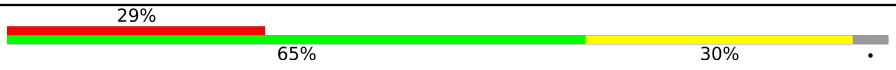
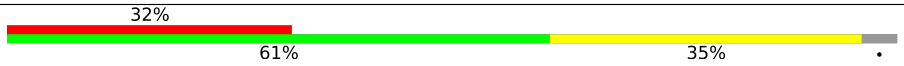
Mol	Chain	Length	Quality of chain
2	E	787	
2	F	787	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 41564 atoms, of which 0 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 Derlin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	W	225	Total	C	N	O	S	0	0
			1870	1267	297	295	11		
1	X	225	Total	C	N	O	S	0	0
			1870	1267	297	295	11		
1	Y	225	Total	C	N	O		0	0
			1144	682	233	229			
1	Z	225	Total	C	N	O		0	0
			1144	682	233	229			

There are 264 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
W	?	-	ARG	deletion	UNP Q9BUN8
W	?	-	GLY	deletion	UNP Q9BUN8
W	?	-	GLY	deletion	UNP Q9BUN8
W	?	-	VAL	deletion	UNP Q9BUN8
W	?	-	SER	deletion	UNP Q9BUN8
W	?	-	GLY	deletion	UNP Q9BUN8
W	?	-	PHE	deletion	UNP Q9BUN8
W	?	-	GLY	deletion	UNP Q9BUN8
W	?	-	VAL	deletion	UNP Q9BUN8
W	?	-	PRO	deletion	UNP Q9BUN8
W	?	-	PRO	deletion	UNP Q9BUN8
W	?	-	ALA	deletion	UNP Q9BUN8
W	?	-	SER	deletion	UNP Q9BUN8
W	?	-	MET	deletion	UNP Q9BUN8
W	?	-	ARG	deletion	UNP Q9BUN8
W	?	-	ARG	deletion	UNP Q9BUN8
W	?	-	ALA	deletion	UNP Q9BUN8
W	?	-	ALA	deletion	UNP Q9BUN8
W	?	-	ASP	deletion	UNP Q9BUN8
W	?	-	GLN	deletion	UNP Q9BUN8
W	?	-	ASN	deletion	UNP Q9BUN8
W	?	-	GLY	deletion	UNP Q9BUN8

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Chain	Residue	Modelled	Actual	Comment	Reference
W	?	-	GLY	deletion	UNP Q9BUN8
W	?	-	GLY	deletion	UNP Q9BUN8
W	?	-	GLY	deletion	UNP Q9BUN8
W	252	ALA	-	expression tag	UNP Q9BUN8
W	253	ALA	-	expression tag	UNP Q9BUN8
W	254	ALA	-	expression tag	UNP Q9BUN8
W	255	LEU	-	expression tag	UNP Q9BUN8
W	256	GLU	-	expression tag	UNP Q9BUN8
W	257	VAL	-	expression tag	UNP Q9BUN8
W	258	LEU	-	expression tag	UNP Q9BUN8
W	259	PHE	-	expression tag	UNP Q9BUN8
W	260	GLN	-	expression tag	UNP Q9BUN8
W	261	GLY	-	expression tag	UNP Q9BUN8
W	262	PRO	-	expression tag	UNP Q9BUN8
W	263	SER	-	expression tag	UNP Q9BUN8
W	264	ALA	-	expression tag	UNP Q9BUN8
W	265	TRP	-	expression tag	UNP Q9BUN8
W	266	SER	-	expression tag	UNP Q9BUN8
W	267	HIS	-	expression tag	UNP Q9BUN8
W	268	PRO	-	expression tag	UNP Q9BUN8
W	269	GLN	-	expression tag	UNP Q9BUN8
W	270	PHE	-	expression tag	UNP Q9BUN8
W	271	GLU	-	expression tag	UNP Q9BUN8
W	272	LYS	-	expression tag	UNP Q9BUN8
W	273	GLY	-	expression tag	UNP Q9BUN8
W	274	GLY	-	expression tag	UNP Q9BUN8
W	275	GLY	-	expression tag	UNP Q9BUN8
W	276	SER	-	expression tag	UNP Q9BUN8
W	277	GLY	-	expression tag	UNP Q9BUN8
W	278	GLY	-	expression tag	UNP Q9BUN8
W	279	GLY	-	expression tag	UNP Q9BUN8
W	280	SER	-	expression tag	UNP Q9BUN8
W	281	GLY	-	expression tag	UNP Q9BUN8
W	282	GLY	-	expression tag	UNP Q9BUN8
W	283	SER	-	expression tag	UNP Q9BUN8
W	284	ALA	-	expression tag	UNP Q9BUN8
W	285	TRP	-	expression tag	UNP Q9BUN8
W	286	SER	-	expression tag	UNP Q9BUN8
W	287	HIS	-	expression tag	UNP Q9BUN8
W	288	PRO	-	expression tag	UNP Q9BUN8
W	289	GLN	-	expression tag	UNP Q9BUN8
W	290	PHE	-	expression tag	UNP Q9BUN8

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Chain	Residue	Modelled	Actual	Comment	Reference
W	291	GLU	-	expression tag	UNP Q9BUN8
W	292	LYS	-	expression tag	UNP Q9BUN8
X	?	-	ARG	deletion	UNP Q9BUN8
X	?	-	GLY	deletion	UNP Q9BUN8
X	?	-	GLY	deletion	UNP Q9BUN8
X	?	-	VAL	deletion	UNP Q9BUN8
X	?	-	SER	deletion	UNP Q9BUN8
X	?	-	GLY	deletion	UNP Q9BUN8
X	?	-	PHE	deletion	UNP Q9BUN8
X	?	-	GLY	deletion	UNP Q9BUN8
X	?	-	VAL	deletion	UNP Q9BUN8
X	?	-	PRO	deletion	UNP Q9BUN8
X	?	-	PRO	deletion	UNP Q9BUN8
X	?	-	ALA	deletion	UNP Q9BUN8
X	?	-	SER	deletion	UNP Q9BUN8
X	?	-	MET	deletion	UNP Q9BUN8
X	?	-	ARG	deletion	UNP Q9BUN8
X	?	-	ARG	deletion	UNP Q9BUN8
X	?	-	ALA	deletion	UNP Q9BUN8
X	?	-	ALA	deletion	UNP Q9BUN8
X	?	-	ASP	deletion	UNP Q9BUN8
X	?	-	GLN	deletion	UNP Q9BUN8
X	?	-	ASN	deletion	UNP Q9BUN8
X	?	-	GLY	deletion	UNP Q9BUN8
X	?	-	GLY	deletion	UNP Q9BUN8
X	?	-	GLY	deletion	UNP Q9BUN8
X	?	-	GLY	deletion	UNP Q9BUN8
X	252	ALA	-	expression tag	UNP Q9BUN8
X	253	ALA	-	expression tag	UNP Q9BUN8
X	254	ALA	-	expression tag	UNP Q9BUN8
X	255	LEU	-	expression tag	UNP Q9BUN8
X	256	GLU	-	expression tag	UNP Q9BUN8
X	257	VAL	-	expression tag	UNP Q9BUN8
X	258	LEU	-	expression tag	UNP Q9BUN8
X	259	PHE	-	expression tag	UNP Q9BUN8
X	260	GLN	-	expression tag	UNP Q9BUN8
X	261	GLY	-	expression tag	UNP Q9BUN8
X	262	PRO	-	expression tag	UNP Q9BUN8
X	263	SER	-	expression tag	UNP Q9BUN8
X	264	ALA	-	expression tag	UNP Q9BUN8
X	265	TRP	-	expression tag	UNP Q9BUN8
X	266	SER	-	expression tag	UNP Q9BUN8

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Chain	Residue	Modelled	Actual	Comment	Reference
X	267	HIS	-	expression tag	UNP Q9BUN8
X	268	PRO	-	expression tag	UNP Q9BUN8
X	269	GLN	-	expression tag	UNP Q9BUN8
X	270	PHE	-	expression tag	UNP Q9BUN8
X	271	GLU	-	expression tag	UNP Q9BUN8
X	272	LYS	-	expression tag	UNP Q9BUN8
X	273	GLY	-	expression tag	UNP Q9BUN8
X	274	GLY	-	expression tag	UNP Q9BUN8
X	275	GLY	-	expression tag	UNP Q9BUN8
X	276	SER	-	expression tag	UNP Q9BUN8
X	277	GLY	-	expression tag	UNP Q9BUN8
X	278	GLY	-	expression tag	UNP Q9BUN8
X	279	GLY	-	expression tag	UNP Q9BUN8
X	280	SER	-	expression tag	UNP Q9BUN8
X	281	GLY	-	expression tag	UNP Q9BUN8
X	282	GLY	-	expression tag	UNP Q9BUN8
X	283	SER	-	expression tag	UNP Q9BUN8
X	284	ALA	-	expression tag	UNP Q9BUN8
X	285	TRP	-	expression tag	UNP Q9BUN8
X	286	SER	-	expression tag	UNP Q9BUN8
X	287	HIS	-	expression tag	UNP Q9BUN8
X	288	PRO	-	expression tag	UNP Q9BUN8
X	289	GLN	-	expression tag	UNP Q9BUN8
X	290	PHE	-	expression tag	UNP Q9BUN8
X	291	GLU	-	expression tag	UNP Q9BUN8
X	292	LYS	-	expression tag	UNP Q9BUN8
Y	?	-	ARG	deletion	UNP Q9BUN8
Y	?	-	GLY	deletion	UNP Q9BUN8
Y	?	-	GLY	deletion	UNP Q9BUN8
Y	?	-	VAL	deletion	UNP Q9BUN8
Y	?	-	SER	deletion	UNP Q9BUN8
Y	?	-	GLY	deletion	UNP Q9BUN8
Y	?	-	PHE	deletion	UNP Q9BUN8
Y	?	-	GLY	deletion	UNP Q9BUN8
Y	?	-	VAL	deletion	UNP Q9BUN8
Y	?	-	PRO	deletion	UNP Q9BUN8
Y	?	-	PRO	deletion	UNP Q9BUN8
Y	?	-	ALA	deletion	UNP Q9BUN8
Y	?	-	SER	deletion	UNP Q9BUN8
Y	?	-	MET	deletion	UNP Q9BUN8
Y	?	-	ARG	deletion	UNP Q9BUN8
Y	?	-	ARG	deletion	UNP Q9BUN8

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Chain	Residue	Modelled	Actual	Comment	Reference
Y	?	-	ALA	deletion	UNP Q9BUN8
Y	?	-	ALA	deletion	UNP Q9BUN8
Y	?	-	ASP	deletion	UNP Q9BUN8
Y	?	-	GLN	deletion	UNP Q9BUN8
Y	?	-	ASN	deletion	UNP Q9BUN8
Y	?	-	GLY	deletion	UNP Q9BUN8
Y	?	-	GLY	deletion	UNP Q9BUN8
Y	?	-	GLY	deletion	UNP Q9BUN8
Y	?	-	GLY	deletion	UNP Q9BUN8
Y	252	ALA	-	expression tag	UNP Q9BUN8
Y	253	ALA	-	expression tag	UNP Q9BUN8
Y	254	ALA	-	expression tag	UNP Q9BUN8
Y	255	LEU	-	expression tag	UNP Q9BUN8
Y	256	GLU	-	expression tag	UNP Q9BUN8
Y	257	VAL	-	expression tag	UNP Q9BUN8
Y	258	LEU	-	expression tag	UNP Q9BUN8
Y	259	PHE	-	expression tag	UNP Q9BUN8
Y	260	GLN	-	expression tag	UNP Q9BUN8
Y	261	GLY	-	expression tag	UNP Q9BUN8
Y	262	PRO	-	expression tag	UNP Q9BUN8
Y	263	SER	-	expression tag	UNP Q9BUN8
Y	264	ALA	-	expression tag	UNP Q9BUN8
Y	265	TRP	-	expression tag	UNP Q9BUN8
Y	266	SER	-	expression tag	UNP Q9BUN8
Y	267	HIS	-	expression tag	UNP Q9BUN8
Y	268	PRO	-	expression tag	UNP Q9BUN8
Y	269	GLN	-	expression tag	UNP Q9BUN8
Y	270	PHE	-	expression tag	UNP Q9BUN8
Y	271	GLU	-	expression tag	UNP Q9BUN8
Y	272	LYS	-	expression tag	UNP Q9BUN8
Y	273	GLY	-	expression tag	UNP Q9BUN8
Y	274	GLY	-	expression tag	UNP Q9BUN8
Y	275	GLY	-	expression tag	UNP Q9BUN8
Y	276	SER	-	expression tag	UNP Q9BUN8
Y	277	GLY	-	expression tag	UNP Q9BUN8
Y	278	GLY	-	expression tag	UNP Q9BUN8
Y	279	GLY	-	expression tag	UNP Q9BUN8
Y	280	SER	-	expression tag	UNP Q9BUN8
Y	281	GLY	-	expression tag	UNP Q9BUN8
Y	282	GLY	-	expression tag	UNP Q9BUN8
Y	283	SER	-	expression tag	UNP Q9BUN8
Y	284	ALA	-	expression tag	UNP Q9BUN8

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Chain	Residue	Modelled	Actual	Comment	Reference
Y	285	TRP	-	expression tag	UNP Q9BUN8
Y	286	SER	-	expression tag	UNP Q9BUN8
Y	287	HIS	-	expression tag	UNP Q9BUN8
Y	288	PRO	-	expression tag	UNP Q9BUN8
Y	289	GLN	-	expression tag	UNP Q9BUN8
Y	290	PHE	-	expression tag	UNP Q9BUN8
Y	291	GLU	-	expression tag	UNP Q9BUN8
Y	292	LYS	-	expression tag	UNP Q9BUN8
Z	?	-	ARG	deletion	UNP Q9BUN8
Z	?	-	GLY	deletion	UNP Q9BUN8
Z	?	-	GLY	deletion	UNP Q9BUN8
Z	?	-	VAL	deletion	UNP Q9BUN8
Z	?	-	SER	deletion	UNP Q9BUN8
Z	?	-	GLY	deletion	UNP Q9BUN8
Z	?	-	PHE	deletion	UNP Q9BUN8
Z	?	-	GLY	deletion	UNP Q9BUN8
Z	?	-	VAL	deletion	UNP Q9BUN8
Z	?	-	PRO	deletion	UNP Q9BUN8
Z	?	-	PRO	deletion	UNP Q9BUN8
Z	?	-	ALA	deletion	UNP Q9BUN8
Z	?	-	SER	deletion	UNP Q9BUN8
Z	?	-	MET	deletion	UNP Q9BUN8
Z	?	-	ARG	deletion	UNP Q9BUN8
Z	?	-	ARG	deletion	UNP Q9BUN8
Z	?	-	ALA	deletion	UNP Q9BUN8
Z	?	-	ALA	deletion	UNP Q9BUN8
Z	?	-	ASP	deletion	UNP Q9BUN8
Z	?	-	GLN	deletion	UNP Q9BUN8
Z	?	-	ASN	deletion	UNP Q9BUN8
Z	?	-	GLY	deletion	UNP Q9BUN8
Z	?	-	GLY	deletion	UNP Q9BUN8
Z	?	-	GLY	deletion	UNP Q9BUN8
Z	?	-	GLY	deletion	UNP Q9BUN8
Z	252	ALA	-	expression tag	UNP Q9BUN8
Z	253	ALA	-	expression tag	UNP Q9BUN8
Z	254	ALA	-	expression tag	UNP Q9BUN8
Z	255	LEU	-	expression tag	UNP Q9BUN8
Z	256	GLU	-	expression tag	UNP Q9BUN8
Z	257	VAL	-	expression tag	UNP Q9BUN8
Z	258	LEU	-	expression tag	UNP Q9BUN8
Z	259	PHE	-	expression tag	UNP Q9BUN8
Z	260	GLN	-	expression tag	UNP Q9BUN8

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Chain	Residue	Modelled	Actual	Comment	Reference
Z	261	GLY	-	expression tag	UNP Q9BUN8
Z	262	PRO	-	expression tag	UNP Q9BUN8
Z	263	SER	-	expression tag	UNP Q9BUN8
Z	264	ALA	-	expression tag	UNP Q9BUN8
Z	265	TRP	-	expression tag	UNP Q9BUN8
Z	266	SER	-	expression tag	UNP Q9BUN8
Z	267	HIS	-	expression tag	UNP Q9BUN8
Z	268	PRO	-	expression tag	UNP Q9BUN8
Z	269	GLN	-	expression tag	UNP Q9BUN8
Z	270	PHE	-	expression tag	UNP Q9BUN8
Z	271	GLU	-	expression tag	UNP Q9BUN8
Z	272	LYS	-	expression tag	UNP Q9BUN8
Z	273	GLY	-	expression tag	UNP Q9BUN8
Z	274	GLY	-	expression tag	UNP Q9BUN8
Z	275	GLY	-	expression tag	UNP Q9BUN8
Z	276	SER	-	expression tag	UNP Q9BUN8
Z	277	GLY	-	expression tag	UNP Q9BUN8
Z	278	GLY	-	expression tag	UNP Q9BUN8
Z	279	GLY	-	expression tag	UNP Q9BUN8
Z	280	SER	-	expression tag	UNP Q9BUN8
Z	281	GLY	-	expression tag	UNP Q9BUN8
Z	282	GLY	-	expression tag	UNP Q9BUN8
Z	283	SER	-	expression tag	UNP Q9BUN8
Z	284	ALA	-	expression tag	UNP Q9BUN8
Z	285	TRP	-	expression tag	UNP Q9BUN8
Z	286	SER	-	expression tag	UNP Q9BUN8
Z	287	HIS	-	expression tag	UNP Q9BUN8
Z	288	PRO	-	expression tag	UNP Q9BUN8
Z	289	GLN	-	expression tag	UNP Q9BUN8
Z	290	PHE	-	expression tag	UNP Q9BUN8
Z	291	GLU	-	expression tag	UNP Q9BUN8
Z	292	LYS	-	expression tag	UNP Q9BUN8

- Molecule 2 is a protein called Transitional endoplasmic reticulum ATPase.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	745	Total	C	N	O	S	0	0
			5846	3667	1035	1113	31		
2	B	745	Total	C	N	O	S	0	0
			5846	3667	1035	1113	31		
2	C	744	Total	C	N	O	S	0	0
			5835	3661	1031	1112	31		

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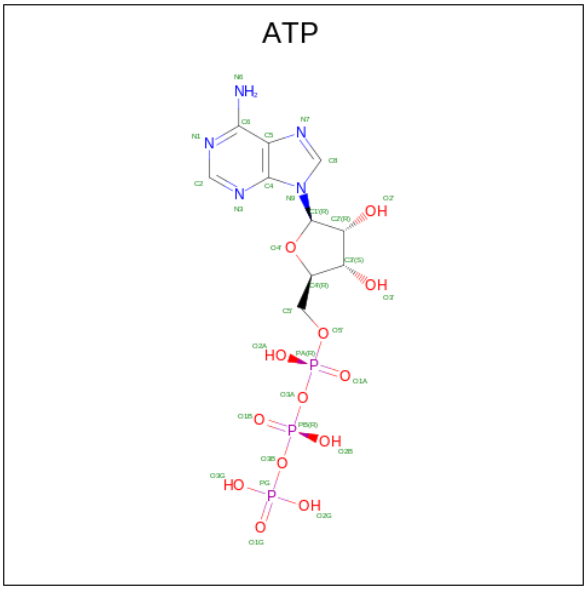
Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	743	Total	C	N	O	S	0	0
			5829	3658	1030	1110	31		
2	E	753	Total	C	N	O	S	0	0
			5911	3712	1046	1122	31		
2	F	755	Total	C	N	O	S	0	0
			5921	3717	1048	1125	31		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	MET	-	initiating methionine	UNP P55072
B	20	MET	-	initiating methionine	UNP P55072
C	20	MET	-	initiating methionine	UNP P55072
D	20	MET	-	initiating methionine	UNP P55072
E	20	MET	-	initiating methionine	UNP P55072
F	20	MET	-	initiating methionine	UNP P55072

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	C	1	Total	C	N	O	P	0
			31	10	5	13	3	

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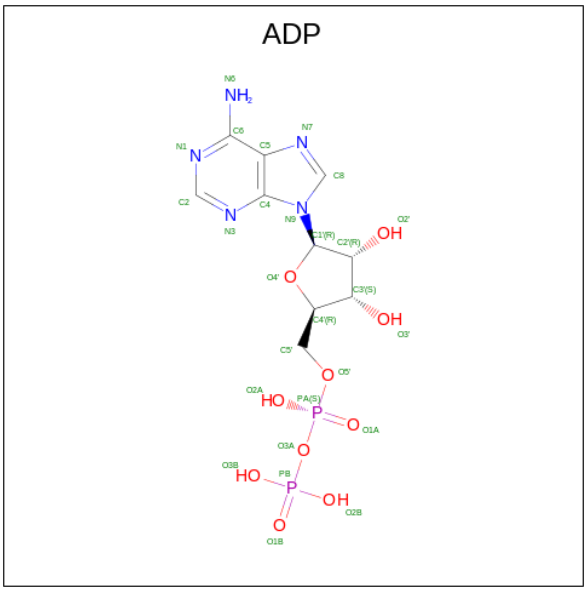
Mol	Chain	Residues	Atoms					AltConf
3	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	E	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	F	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



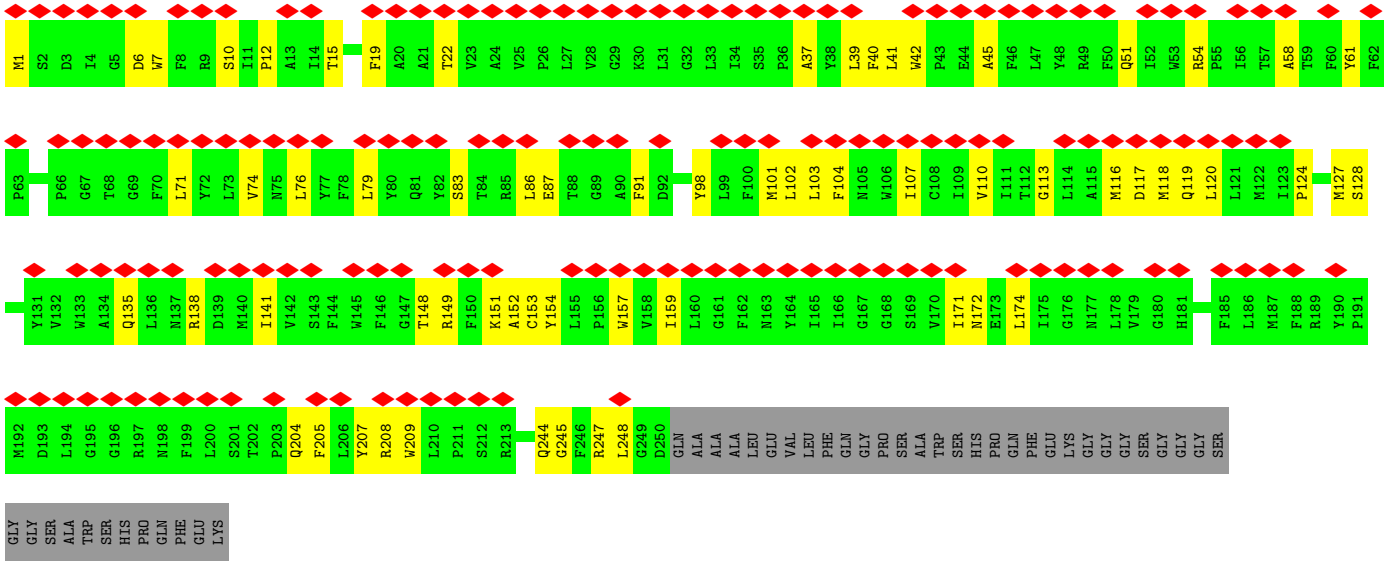
Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	E	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	F	1	Total	C	N	O	P	0
			27	10	5	10	2	

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.

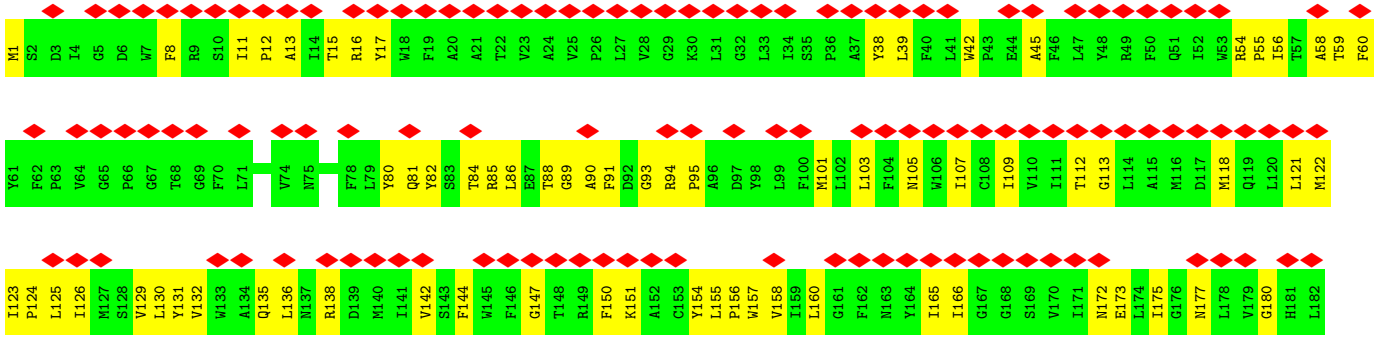
• Molecule 1: Derlin-1

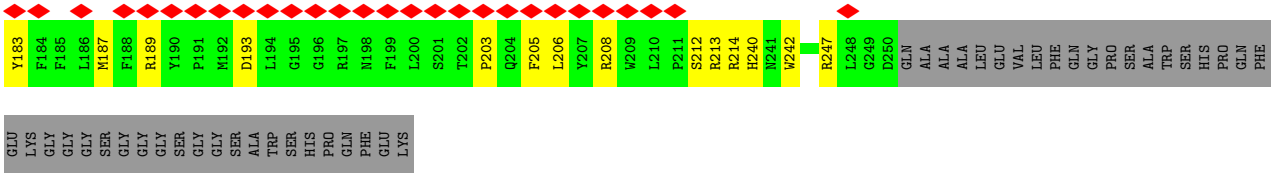
Chain W:



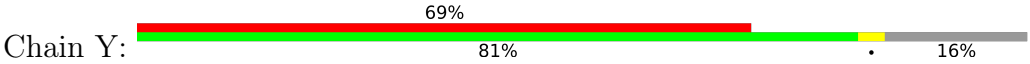
• Molecule 1: Derlin-1

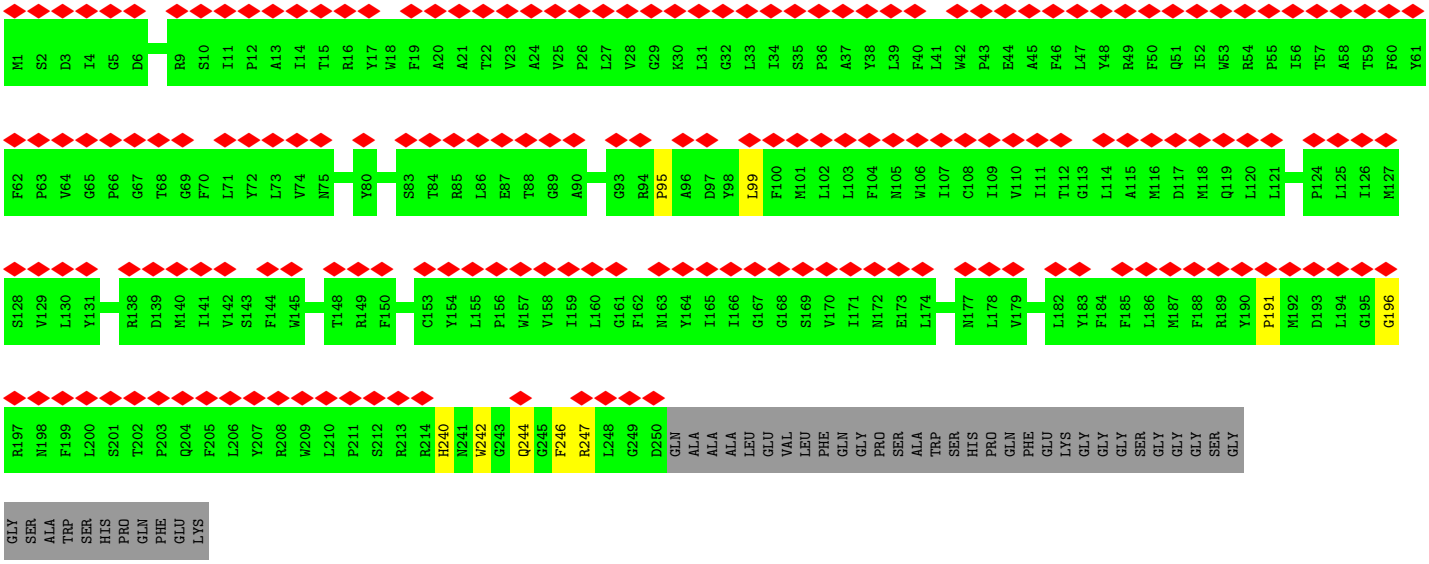
Chain X:



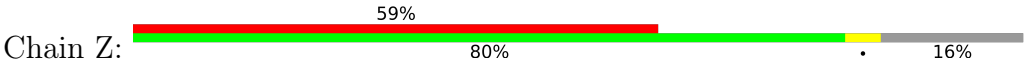


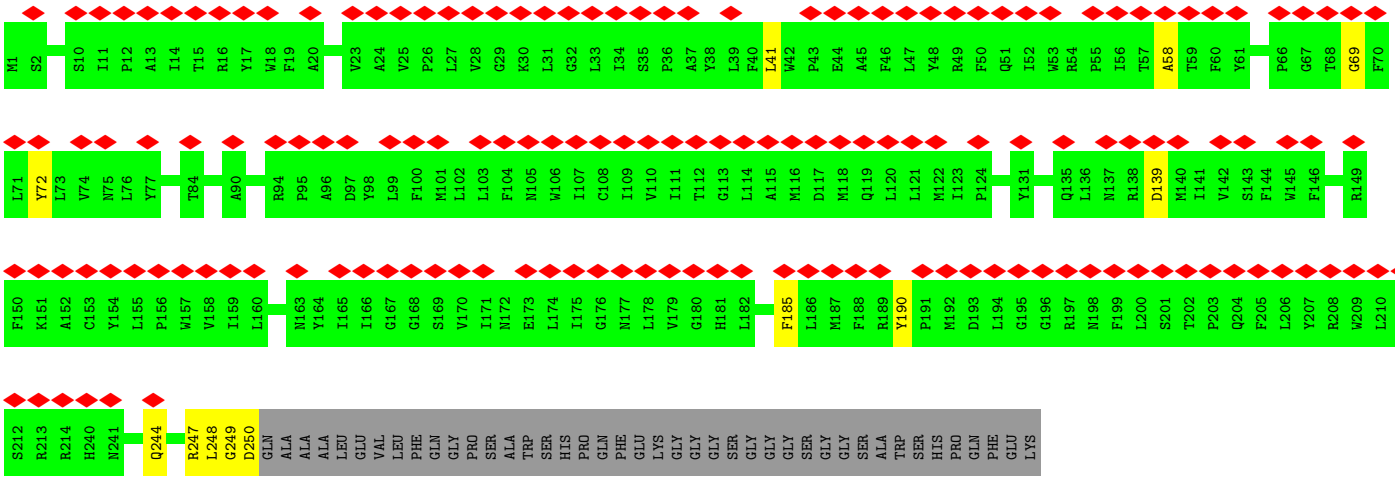
• Molecule 1: Derlin-1



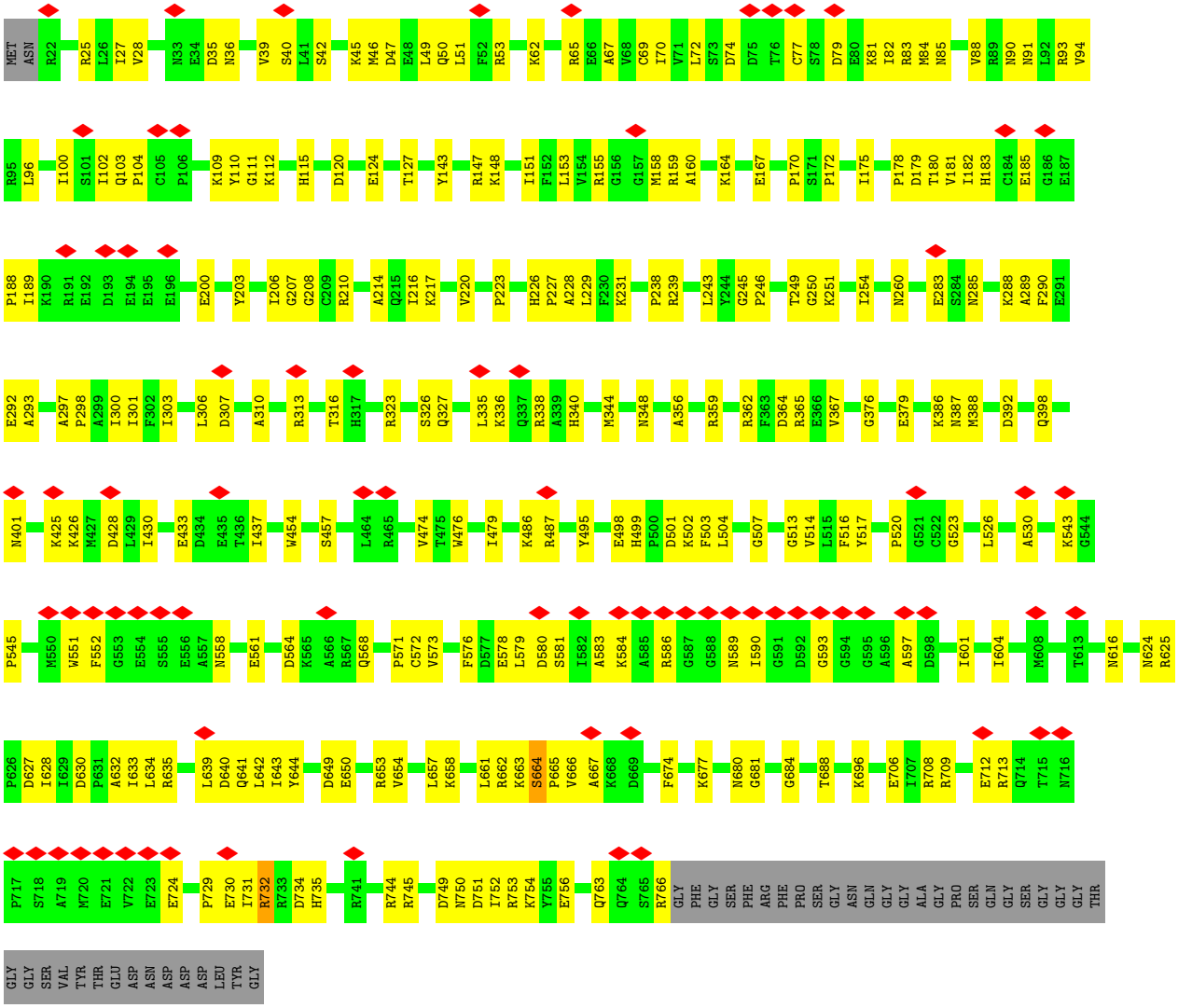


• Molecule 1: Derlin-1



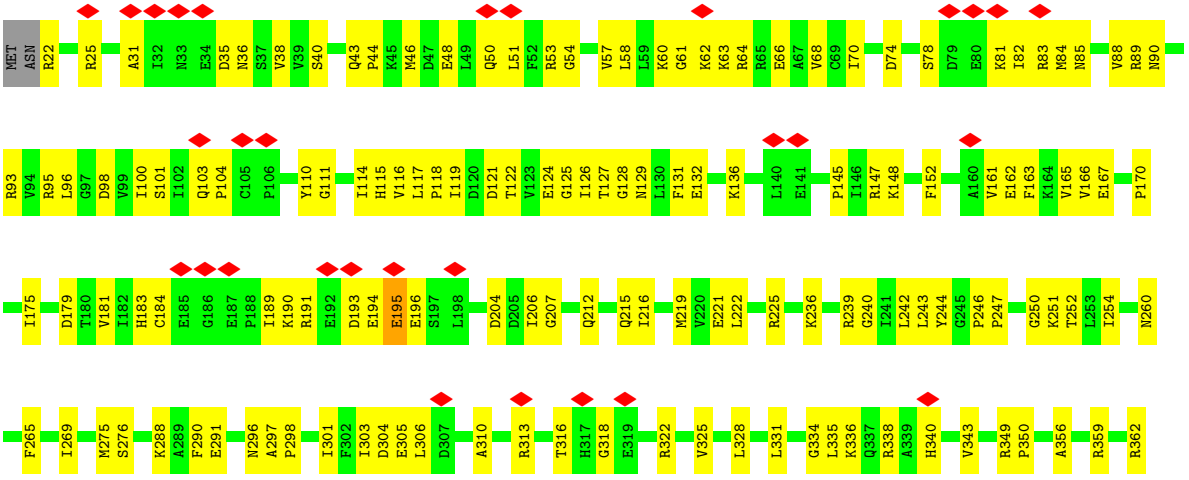


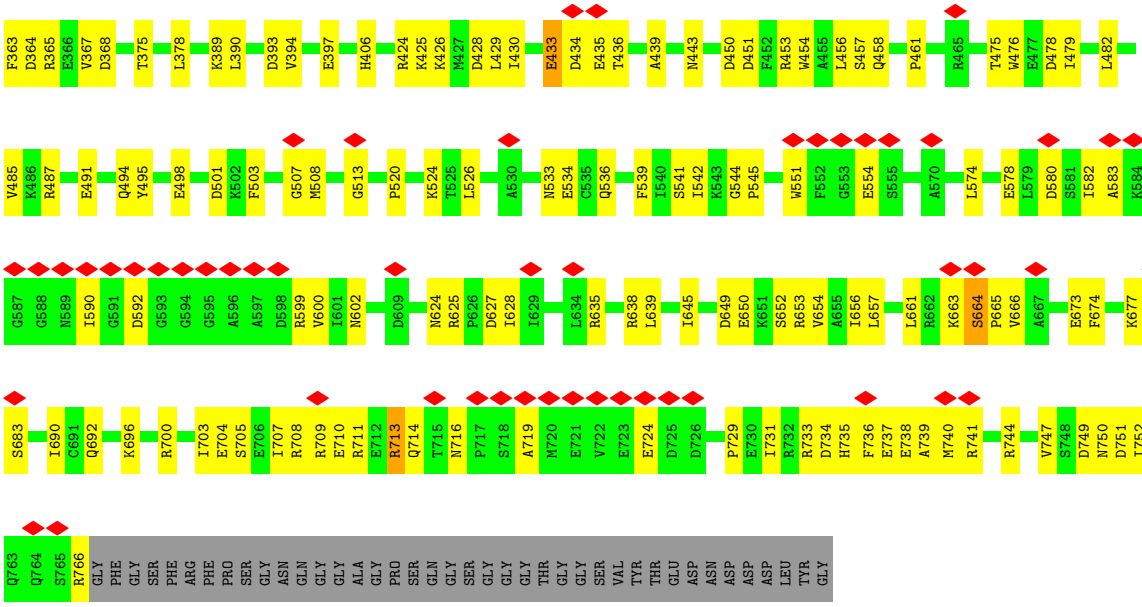
• Molecule 2: Transitional endoplasmic reticulum ATPase



• Molecule 2: Transitional endoplasmic reticulum ATPase

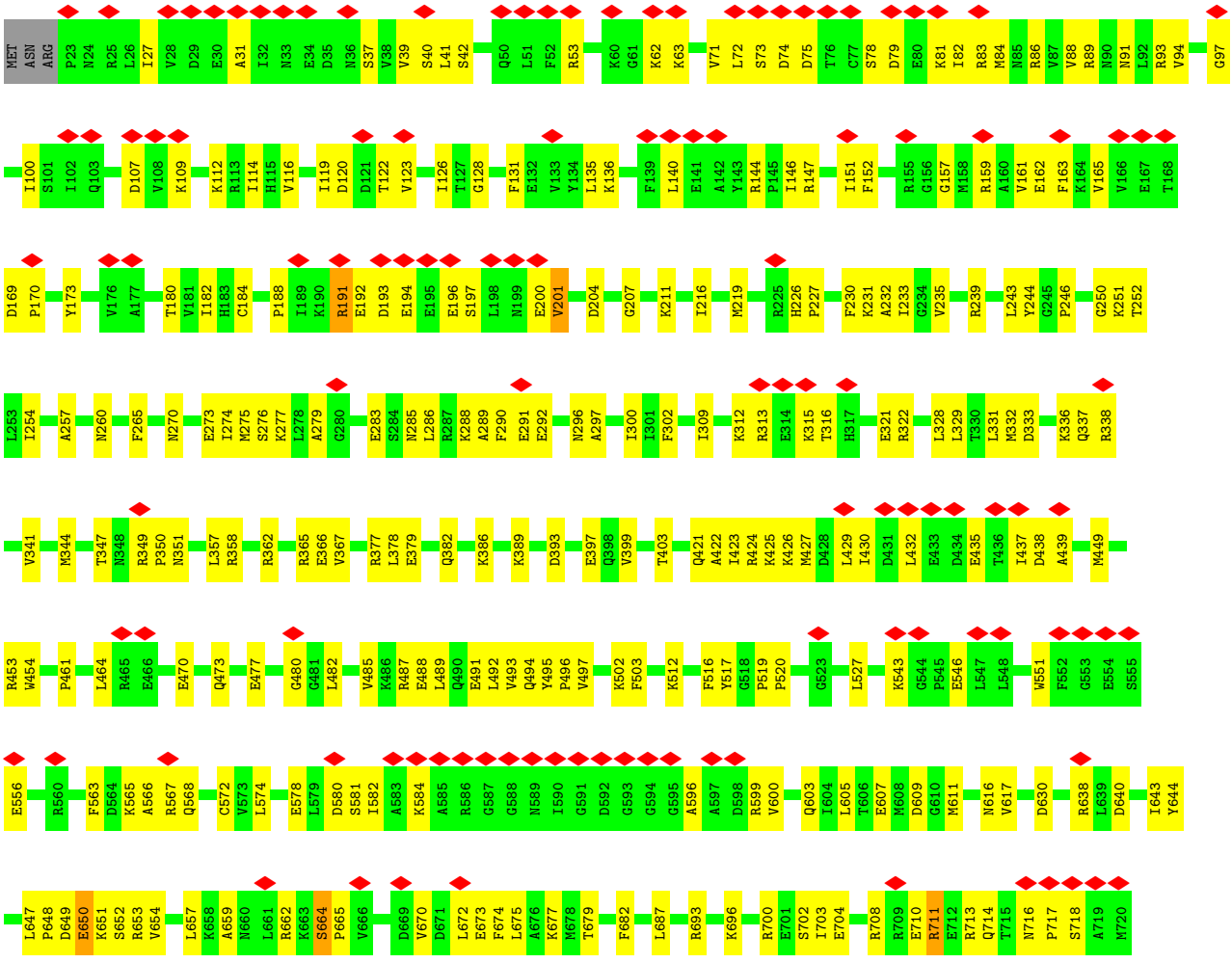
Chain B:

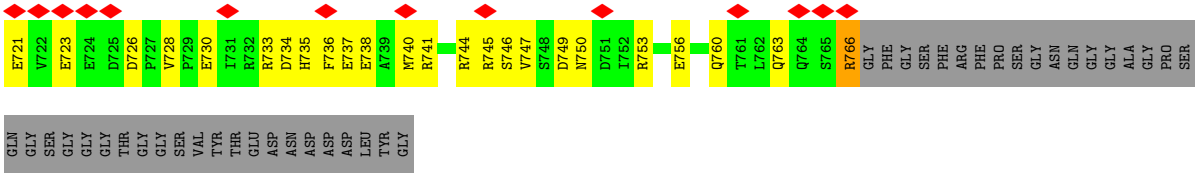




• Molecule 2: Transitional endoplasmic reticulum ATPase

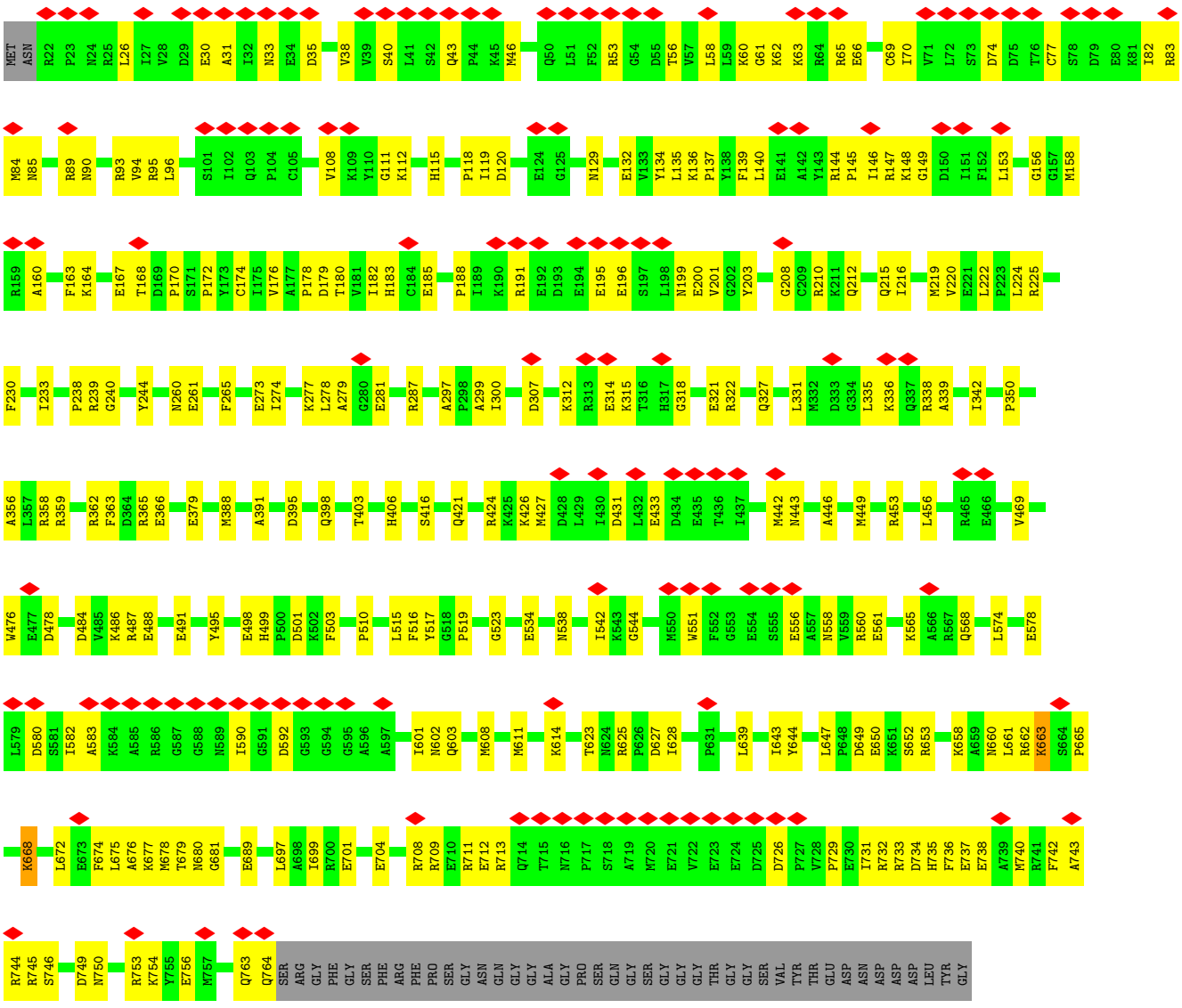
Chain C:





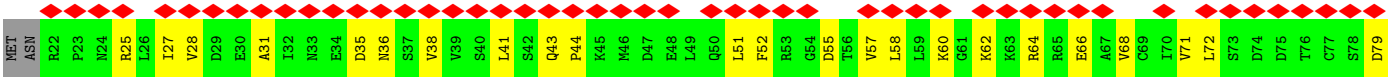
• Molecule 2: Transitional endoplasmic reticulum ATPase

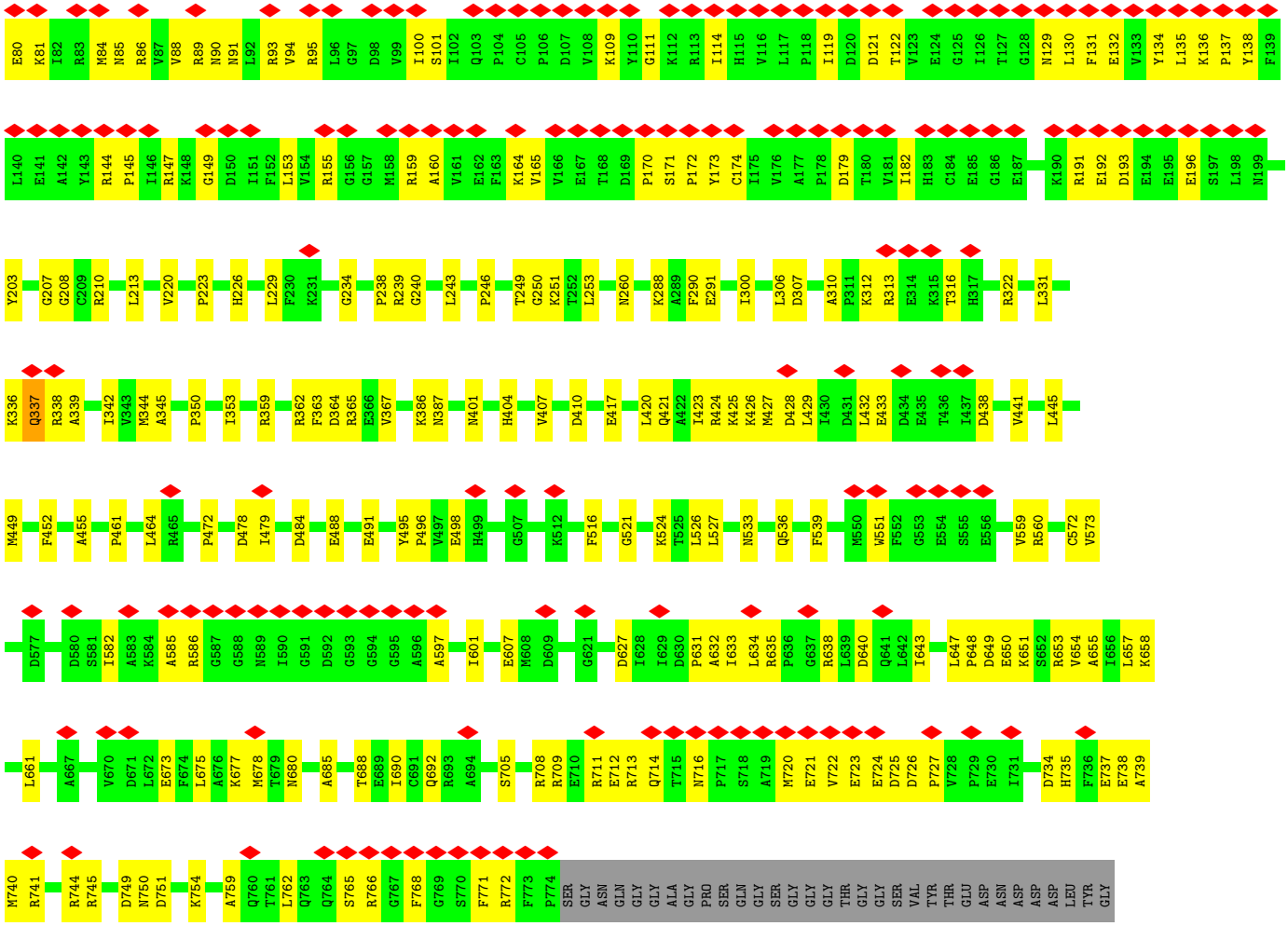
Chain D:



• Molecule 2: Transitional endoplasmic reticulum ATPase

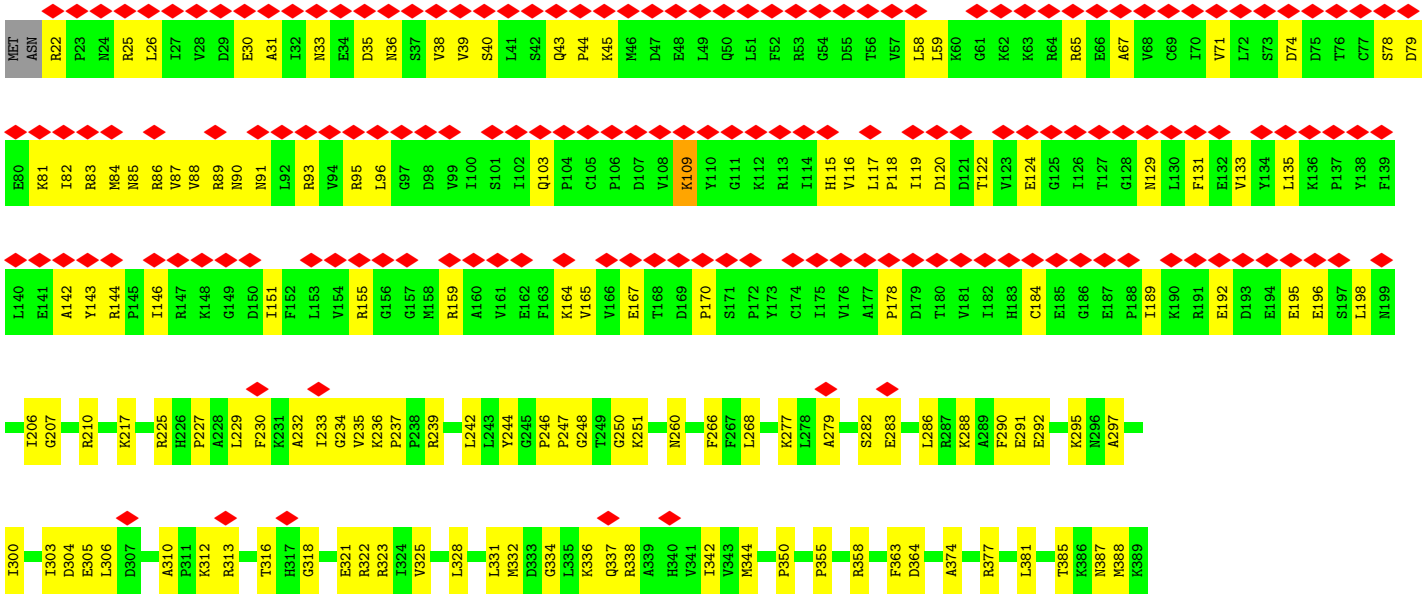
Chain E:

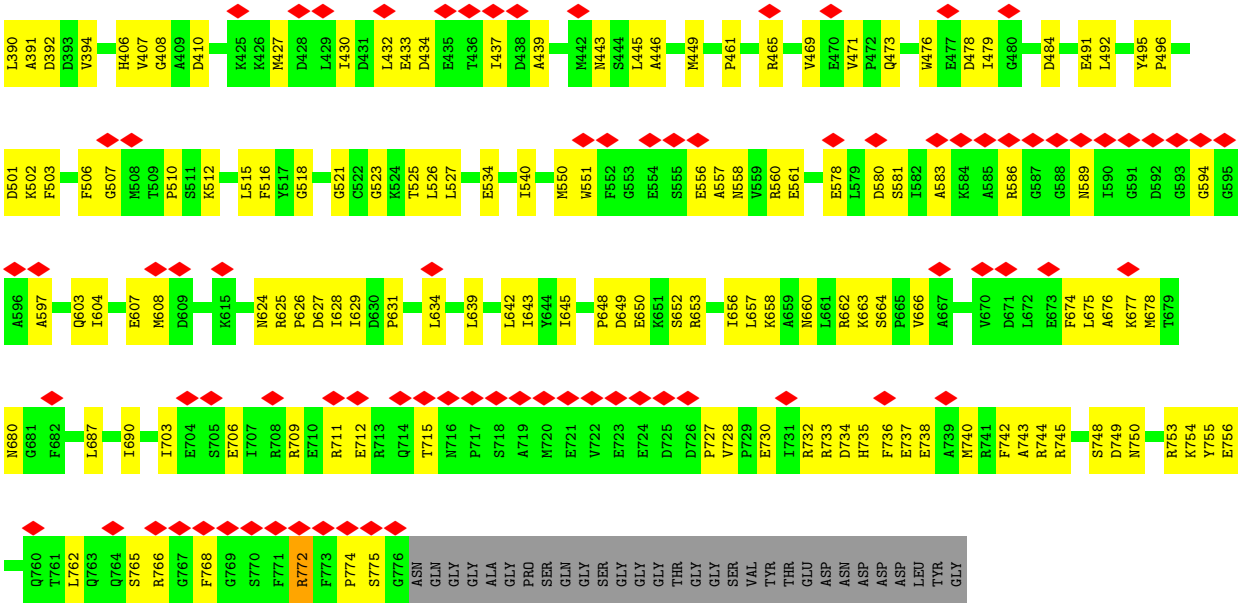




• Molecule 2: Transitional endoplasmic reticulum ATPase

Chain F:




L390 A391 D392 D393 V394 H406 V407 G408 A409 D410 K425 K426 M427 D428 L429 I430 D431 L432 E433 D434 E435 T436 I437 D438 A439 M442 N443 S444 L445 A446 M449 P461 R465 V469 E470 V471 P472 Q473 W476 E477 D478 I479 G480 D484 E491 L492 Y495 P496
D501 K502 F503 F506 G507 M508 T509 P510 S511 K512 L515 F516 Y517 G518 G521 G522 G523 K524 T525 L526 L527 E534 T540 M550 W551 F552 G553 E554 S555 E556 A557 N558 V559 R560 E561 E578 L579 D580 S581 I582 A583 K584 A585 R586 G587 G588 N589 I590 G591 D592 G593 G594 G595
A596 A597 Q603 I604 E607 M608 D609 K615 N624 R625 P626 D627 I628 I629 D630 P631 L634 L639 L642 I643 Y644 I645 P648 D649 E650 K651 S652 R653 I656 L657 K658 A659 N660 L661 R662 K663 S664 P665 V666 A667 V670 D671 L672 E673 F674 L675 A676 K677 M678 T679
N680 G681 F682 L687 I690 I703 E704 S705 E706 I707 R708 R709 E710 R711 E712 R713 Q714 T715 N716 P717 S718 A719 M720 E721 V722 E723 E724 D725 D726 P727 V728 P729 E730 I731 R732 R733 D734 H735 F736 E737 E738 A739 M740 R741 F742 A743 R744 R745 S748 D749 N750 R753 K754 Y755 E756
Q760 T761 L762 Q763 Q764 S765 R766 G767 F768 G769 S770 F771 R772 F773 P774 S775 G776 ASN GLN GLY GLY ALA GLY PRO SER GLN GLY SER GLY GLY GLY THR GLY GLY SER VAL TYR THR GLU ASP ASN ASP ASP ASP LEU TYR GLY

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	62905	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.408	Depositor
Minimum map value	-0.848	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.049	Depositor
Recommended contour level	0.25	Depositor
Map size (Å)	352.0, 352.0, 352.0	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	W	0.26	0/1941	0.52	0/2647
1	X	0.26	0/1941	0.48	0/2647
1	Y	0.24	0/1147	0.47	0/1589
1	Z	0.26	0/1147	0.48	0/1589
2	A	0.27	0/5941	0.51	0/8023
2	B	0.27	0/5941	0.51	0/8023
2	C	0.26	0/5930	0.51	0/8008
2	D	0.26	0/5924	0.52	0/8001
2	E	0.27	0/6010	0.51	0/8115
2	F	0.26	0/6020	0.51	0/8128
All	All	0.27	0/41942	0.51	0/56770

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	W	1870	0	1856	53	0
1	X	1870	0	1856	59	0
1	Y	1144	0	547	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Z	1144	0	547	13	0
2	A	5846	0	5905	188	0
2	B	5846	0	5905	201	0
2	C	5835	0	5893	219	0
2	D	5829	0	5887	207	0
2	E	5911	0	5963	181	0
2	F	5921	0	5971	218	0
3	A	31	0	12	3	0
3	B	31	0	12	5	0
3	C	31	0	12	3	0
3	D	31	0	12	0	0
3	E	31	0	12	3	0
3	F	31	0	12	6	0
4	A	27	0	12	3	0
4	B	27	0	12	1	0
4	C	27	0	12	2	0
4	D	27	0	12	2	0
4	E	27	0	12	5	0
4	F	27	0	12	4	0
All	All	41564	0	40474	1257	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 15.

The worst 5 of 1257 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)
2:B:524:LYS:HE2	2:B:645:ILE:CG1	1.71	1.19
2:B:524:LYS:CE	2:B:645:ILE:HG13	1.70	1.18
2:A:543:LYS:HG3	2:A:545:PRO:HD2	1.48	0.96
2:B:54:GLY:HA2	2:B:70:ILE:HG23	1.60	0.81
1:X:1:MET:HG2	1:Z:139:ASP:HA	1.64	0.80

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	W	223/267 (84%)	202 (91%)	21 (9%)	0	100	100
1	X	223/267 (84%)	202 (91%)	20 (9%)	1 (0%)	34	72
1	Y	223/267 (84%)	195 (87%)	28 (13%)	0	100	100
1	Z	223/267 (84%)	200 (90%)	23 (10%)	0	100	100
2	A	743/787 (94%)	683 (92%)	57 (8%)	3 (0%)	34	72
2	B	743/787 (94%)	686 (92%)	52 (7%)	5 (1%)	22	62
2	C	742/787 (94%)	683 (92%)	54 (7%)	5 (1%)	22	62
2	D	741/787 (94%)	678 (92%)	59 (8%)	4 (0%)	29	68
2	E	751/787 (95%)	691 (92%)	59 (8%)	1 (0%)	51	85
2	F	753/787 (96%)	689 (92%)	61 (8%)	3 (0%)	34	72
All	All	5365/5790 (93%)	4909 (92%)	434 (8%)	22 (0%)	38	72

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	664	SER
2	C	650	GLU
2	D	663	LYS
2	E	337	GLN
2	F	434	ASP

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	W	193/221 (87%)	193 (100%)	0	100	100
1	X	193/221 (87%)	193 (100%)	0	100	100
1	Y	8/221 (4%)	8 (100%)	0	100	100
1	Z	8/221 (4%)	8 (100%)	0	100	100
2	A	636/664 (96%)	635 (100%)	1 (0%)	93	96
2	B	636/664 (96%)	635 (100%)	1 (0%)	93	96
2	C	635/664 (96%)	631 (99%)	4 (1%)	86	92
2	D	634/664 (96%)	632 (100%)	2 (0%)	92	95
2	E	642/664 (97%)	642 (100%)	0	100	100
2	F	643/664 (97%)	641 (100%)	2 (0%)	92	95
All	All	4228/4868 (87%)	4218 (100%)	10 (0%)	93	96

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	713	ARG
2	F	109	LYS
2	F	772	ARG
2	C	386	LYS
2	C	711	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
2	F	558	ASN
2	E	536	GLN
2	C	763	GLN
2	C	714	GLN
2	D	490	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

12 ligands are modelled in this entry.

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	ADP	E	902	-	24,29,29	0.92	1 (4%)	29,45,45	1.42	4 (13%)
3	ATP	B	901	-	26,33,33	0.62	0	31,52,52	0.73	1 (3%)
3	ATP	F	901	-	26,33,33	0.62	0	31,52,52	0.73	2 (6%)
4	ADP	B	902	-	24,29,29	0.93	1 (4%)	29,45,45	1.47	4 (13%)
3	ATP	C	901	-	26,33,33	0.63	0	31,52,52	0.73	2 (6%)
3	ATP	A	901	-	26,33,33	0.62	0	31,52,52	0.74	2 (6%)
4	ADP	D	902	-	24,29,29	0.92	1 (4%)	29,45,45	1.35	4 (13%)
3	ATP	D	901	-	26,33,33	0.62	0	31,52,52	0.76	2 (6%)
3	ATP	E	901	-	26,33,33	0.62	0	31,52,52	0.73	2 (6%)
4	ADP	F	902	-	24,29,29	0.93	1 (4%)	29,45,45	1.36	4 (13%)
4	ADP	C	902	-	24,29,29	0.93	1 (4%)	29,45,45	1.45	4 (13%)
4	ADP	A	902	-	24,29,29	0.93	1 (4%)	29,45,45	1.45	4 (13%)

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	ADP	E	902	-	-	5/12/32/32	0/3/3/3
3	ATP	B	901	-	-	9/18/38/38	0/3/3/3
3	ATP	F	901	-	-	7/18/38/38	0/3/3/3
4	ADP	B	902	-	-	2/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	C	901	-	-	8/18/38/38	0/3/3/3
3	ATP	A	901	-	-	4/18/38/38	0/3/3/3
4	ADP	D	902	-	-	4/12/32/32	0/3/3/3
3	ATP	D	901	-	-	5/18/38/38	0/3/3/3
3	ATP	E	901	-	-	6/18/38/38	0/3/3/3
4	ADP	F	902	-	-	4/12/32/32	0/3/3/3
4	ADP	C	902	-	-	4/12/32/32	0/3/3/3
4	ADP	A	902	-	-	2/12/32/32	0/3/3/3

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	902	ADP	C5-C4	2.41	1.47	1.40
4	C	902	ADP	C5-C4	2.41	1.47	1.40
4	A	902	ADP	C5-C4	2.40	1.47	1.40
4	F	902	ADP	C5-C4	2.36	1.47	1.40
4	E	902	ADP	C5-C4	2.35	1.47	1.40

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	902	ADP	PA-O3A-PB	-3.92	119.36	132.83
4	A	902	ADP	PA-O3A-PB	-3.86	119.57	132.83
4	C	902	ADP	PA-O3A-PB	-3.68	120.21	132.83
4	E	902	ADP	PA-O3A-PB	-3.57	120.57	132.83
4	D	902	ADP	N3-C2-N1	-3.45	123.29	128.68

There are no chirality outliers.

5 of 60 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	901	ATP	O4'-C4'-C5'-O5'
3	A	901	ATP	C3'-C4'-C5'-O5'
3	B	901	ATP	PB-O3A-PA-O5'
3	B	901	ATP	C5'-O5'-PA-O1A
3	B	901	ATP	C5'-O5'-PA-O2A

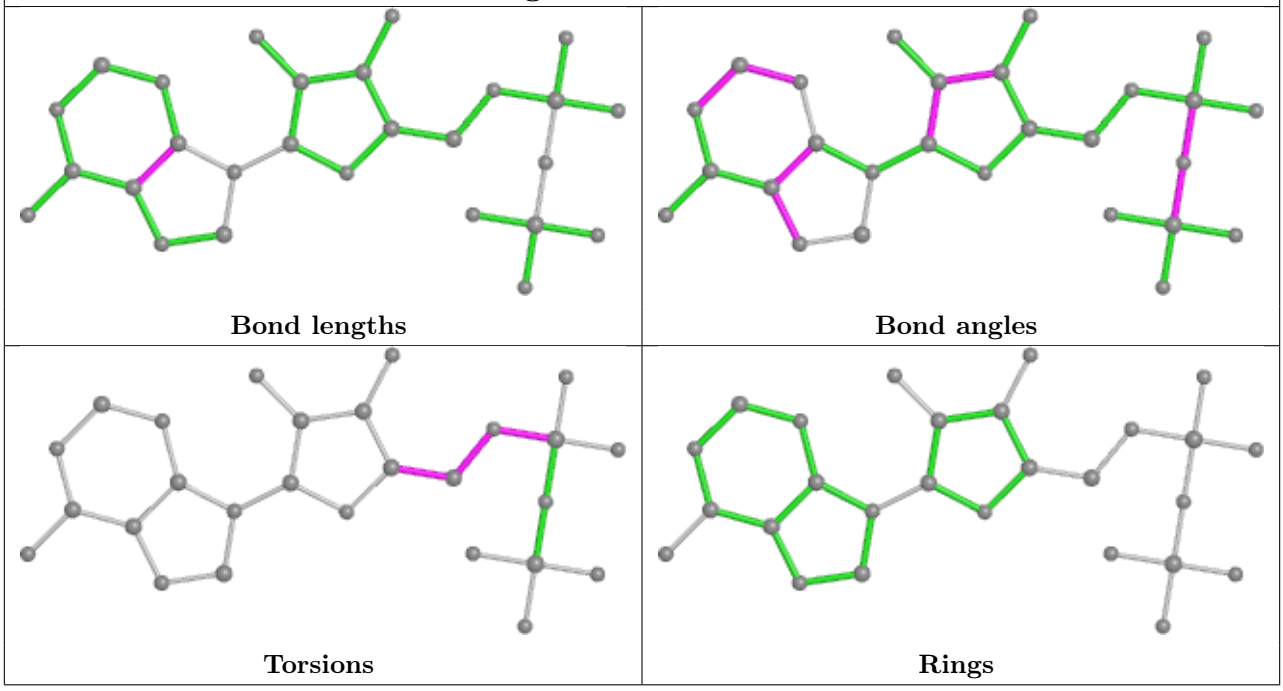
There are no ring outliers.

11 monomers are involved in 37 short contacts:

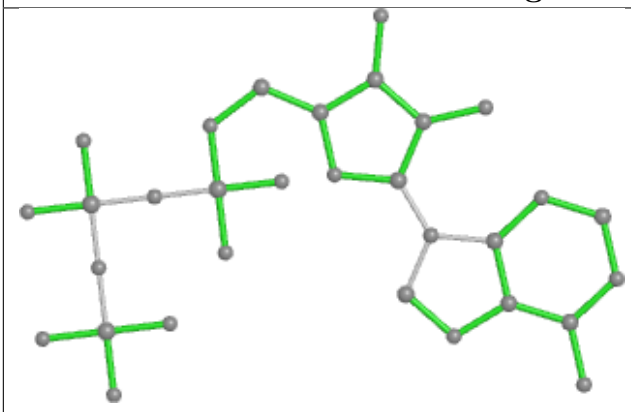
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	902	ADP	5	0
3	B	901	ATP	5	0
3	F	901	ATP	6	0
4	B	902	ADP	1	0
3	C	901	ATP	3	0
3	A	901	ATP	3	0
4	D	902	ADP	2	0
3	E	901	ATP	3	0
4	F	902	ADP	4	0
4	C	902	ADP	2	0
4	A	902	ADP	3	0

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

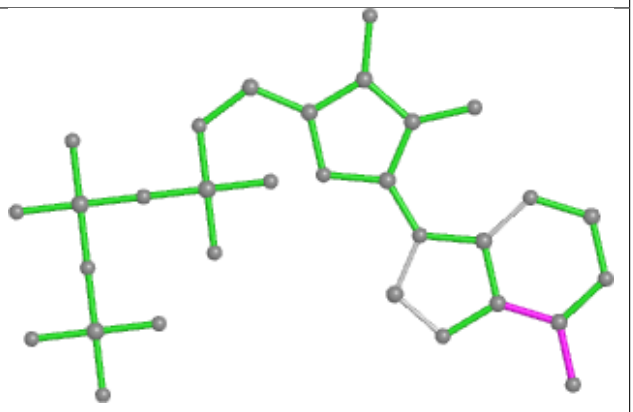
Ligand ADP E 902



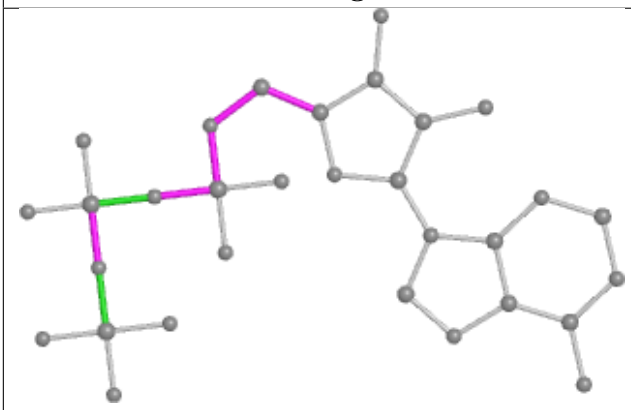
Ligand ATP B 901



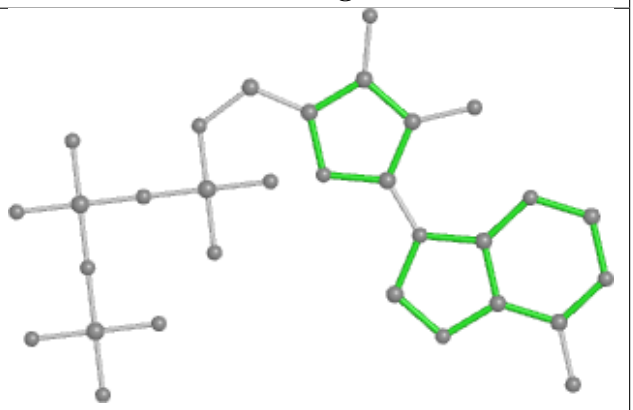
Bond lengths



Bond angles

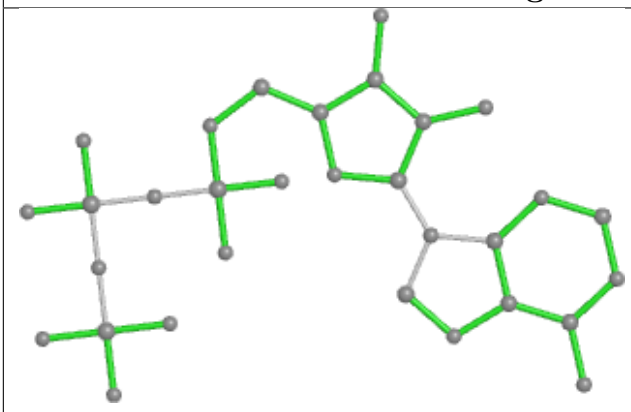


Torsions

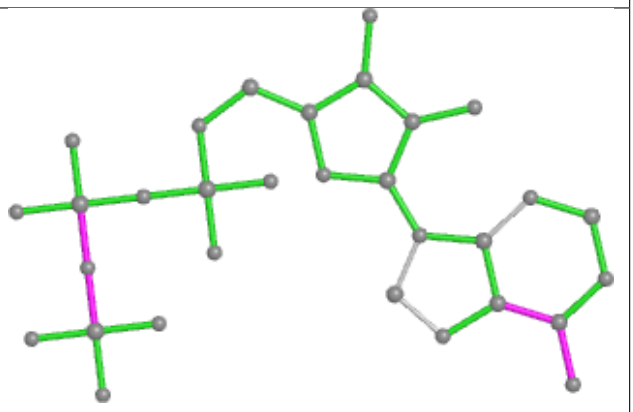


Rings

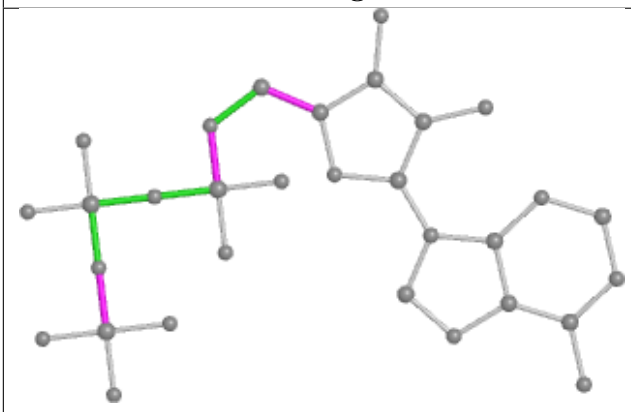
Ligand ATP F 901



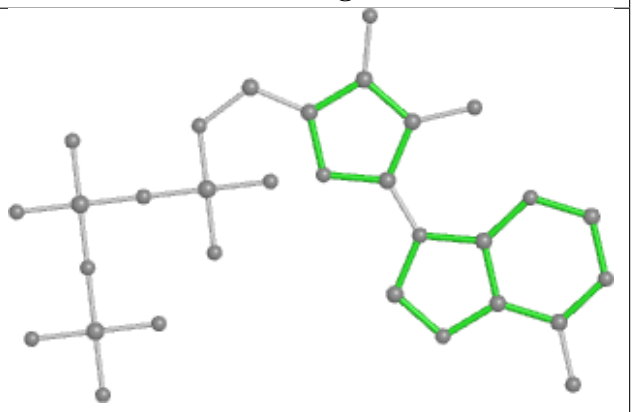
Bond lengths



Bond angles

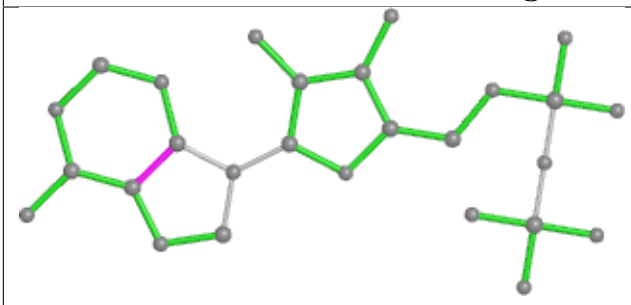


Torsions

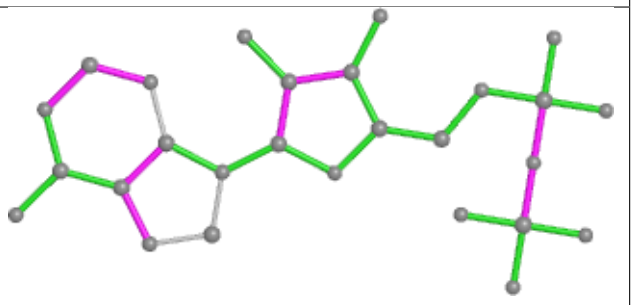


Rings

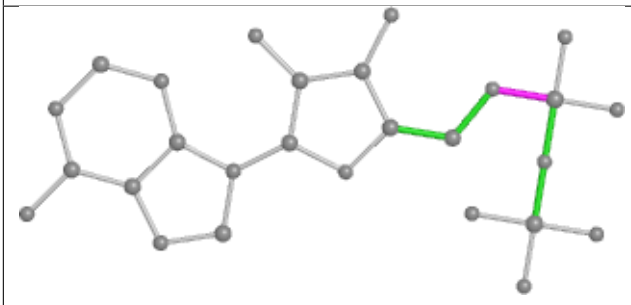
Ligand ADP B 902



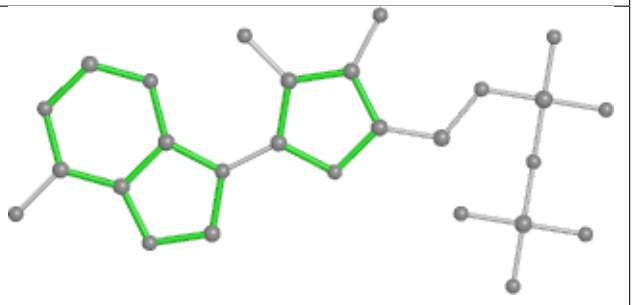
Bond lengths



Bond angles

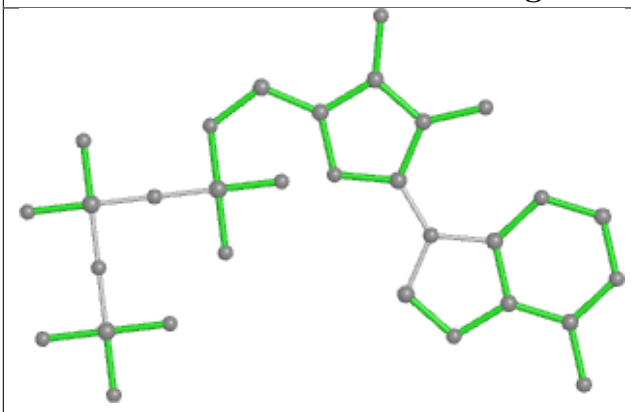


Torsions

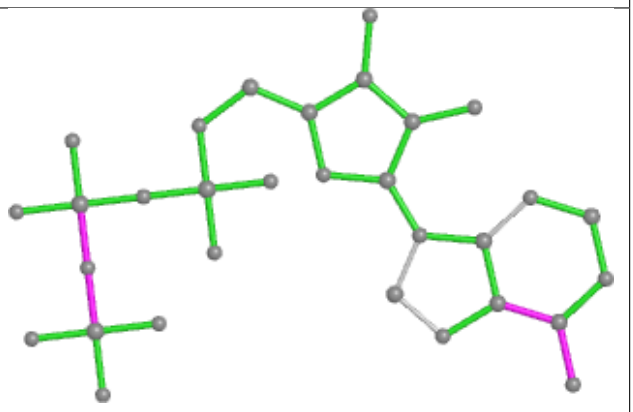


Rings

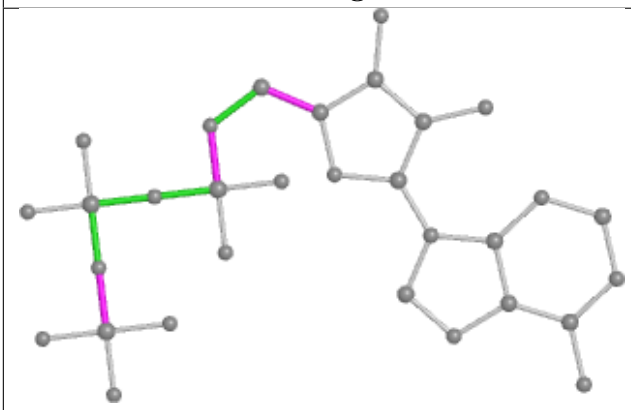
Ligand ATP C 901



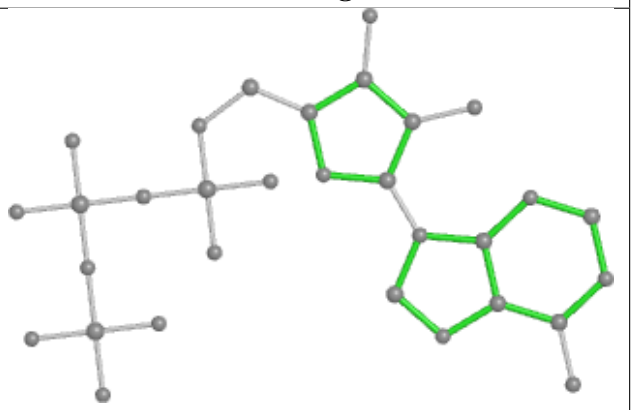
Bond lengths



Bond angles

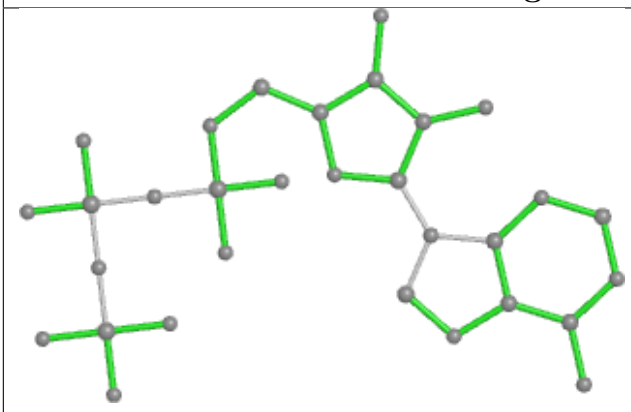


Torsions

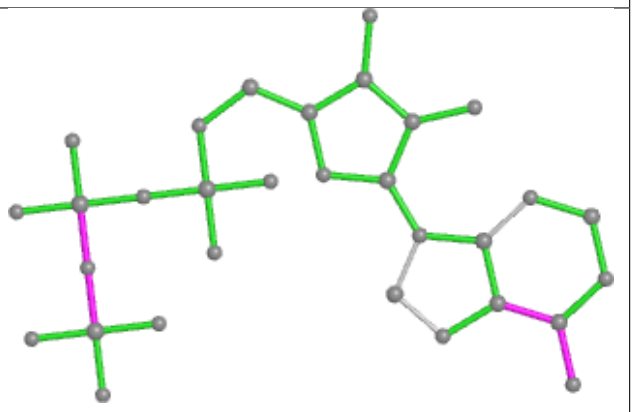


Rings

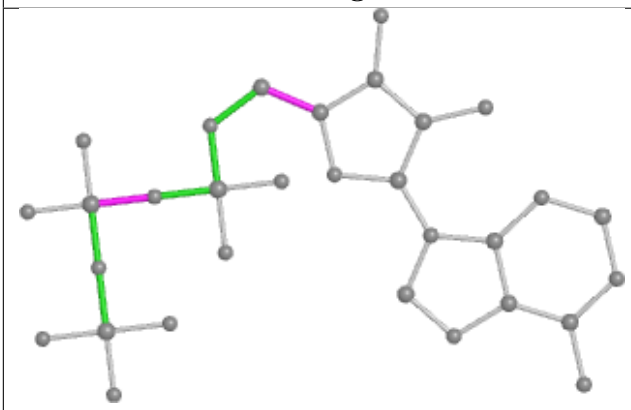
Ligand ATP A 901



Bond lengths



Bond angles



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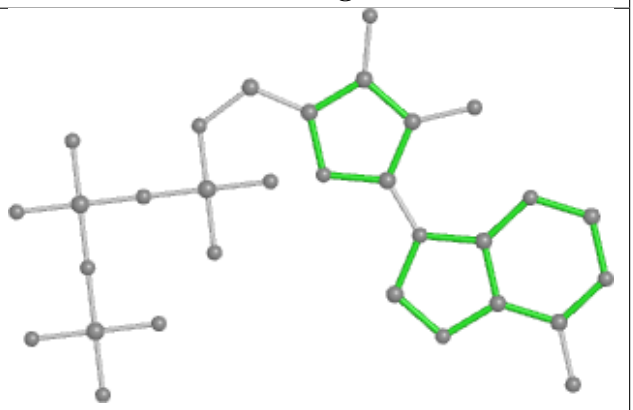
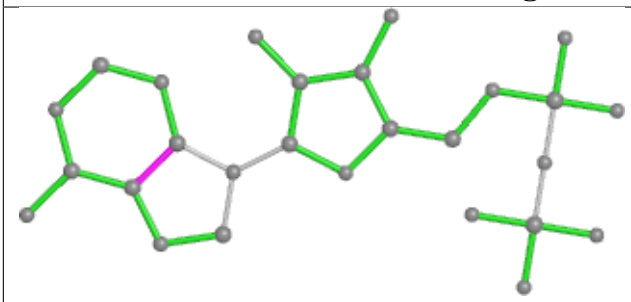
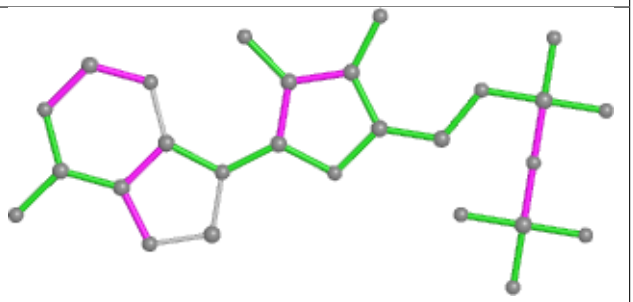


Rings

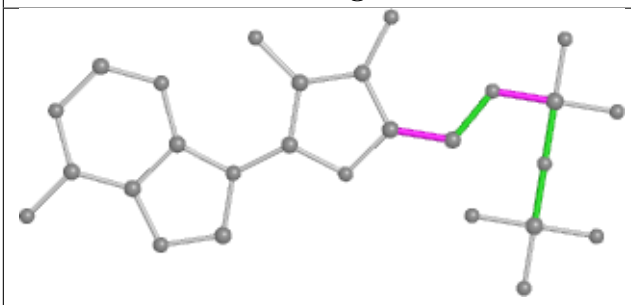
Ligand ADP D 902



Bond lengths



Bond angles



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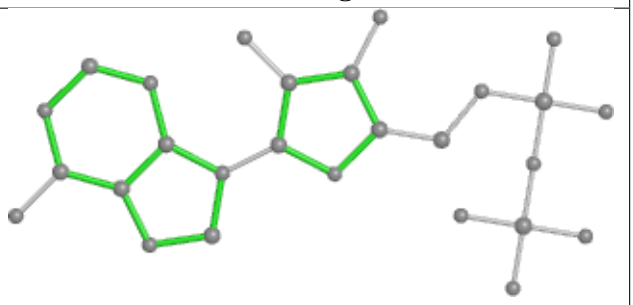
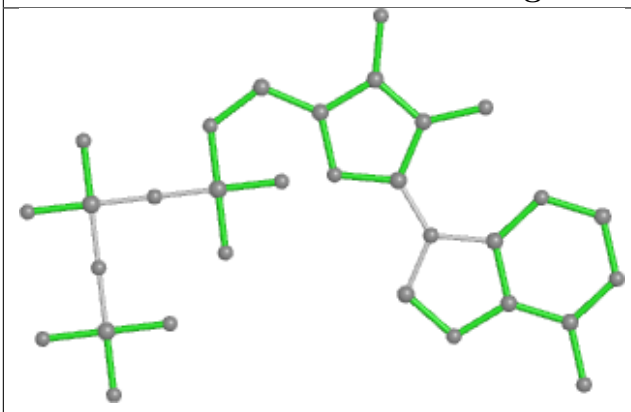
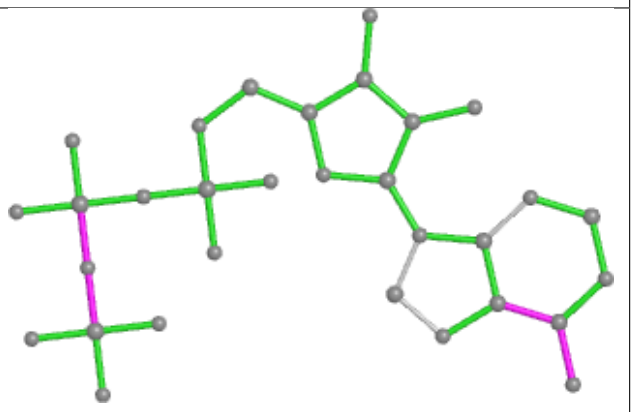


Rings

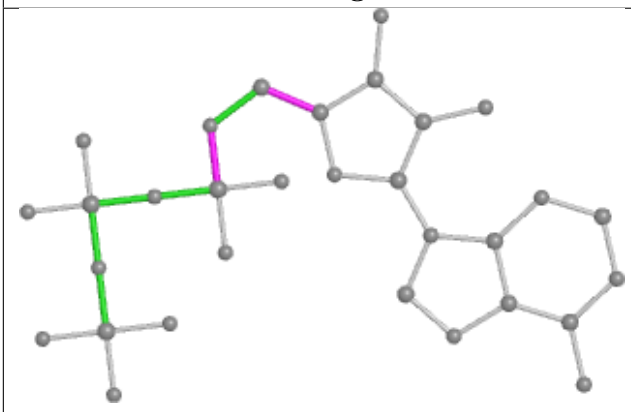
Ligand ATP D 901



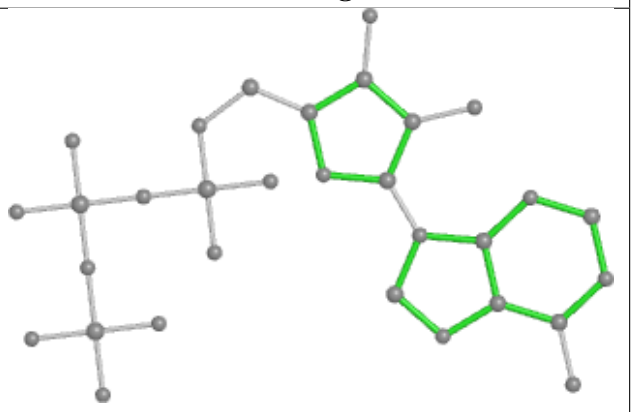
Bond lengths



Bond angles

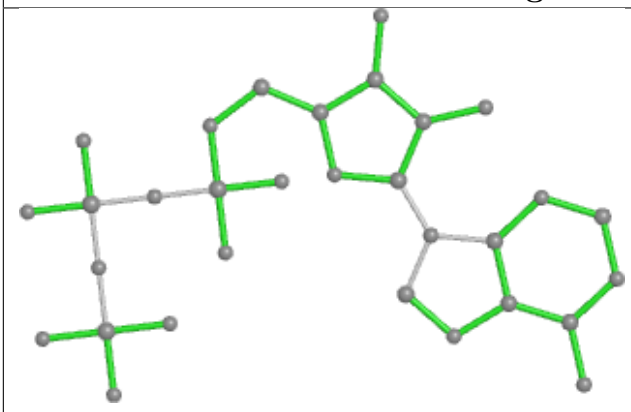


Torsions

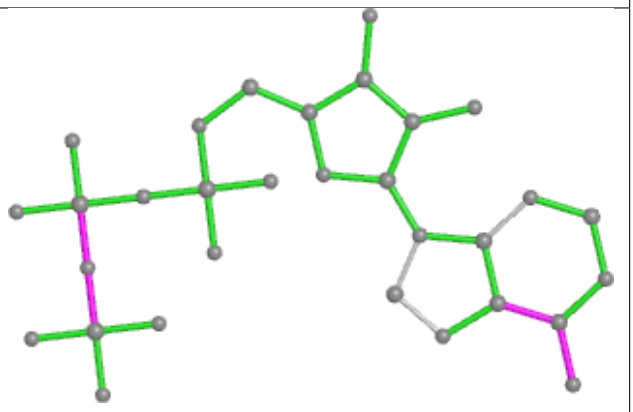


Rings

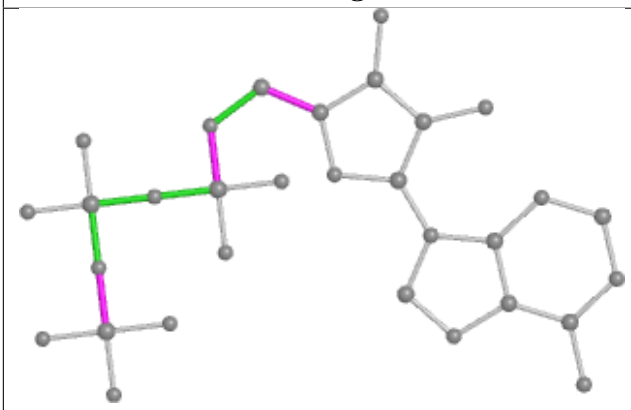
Ligand ATP E 901



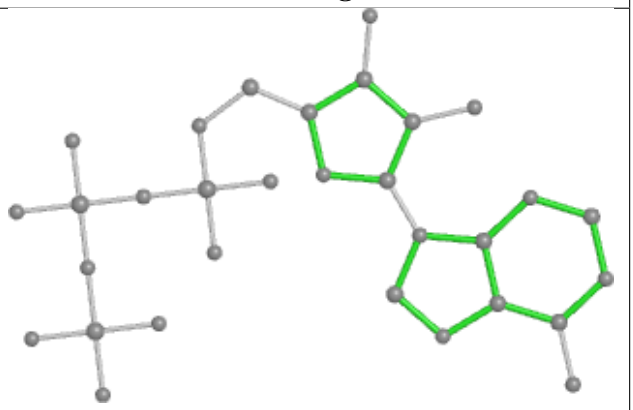
Bond lengths



Bond angles

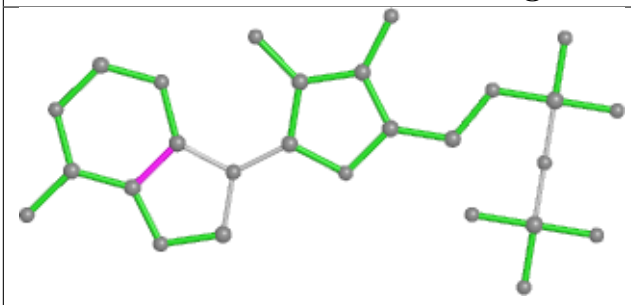


Torsions

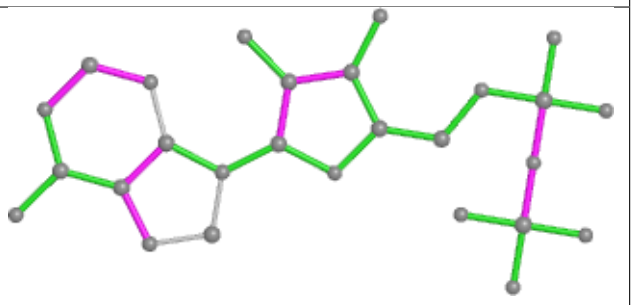


Rings

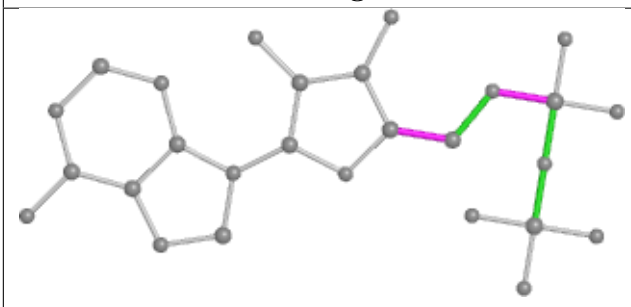
Ligand ADP F 902



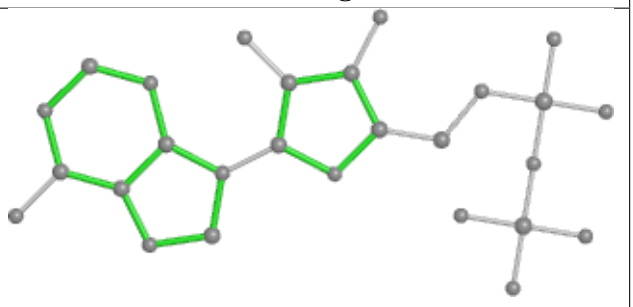
Bond lengths



Bond angles

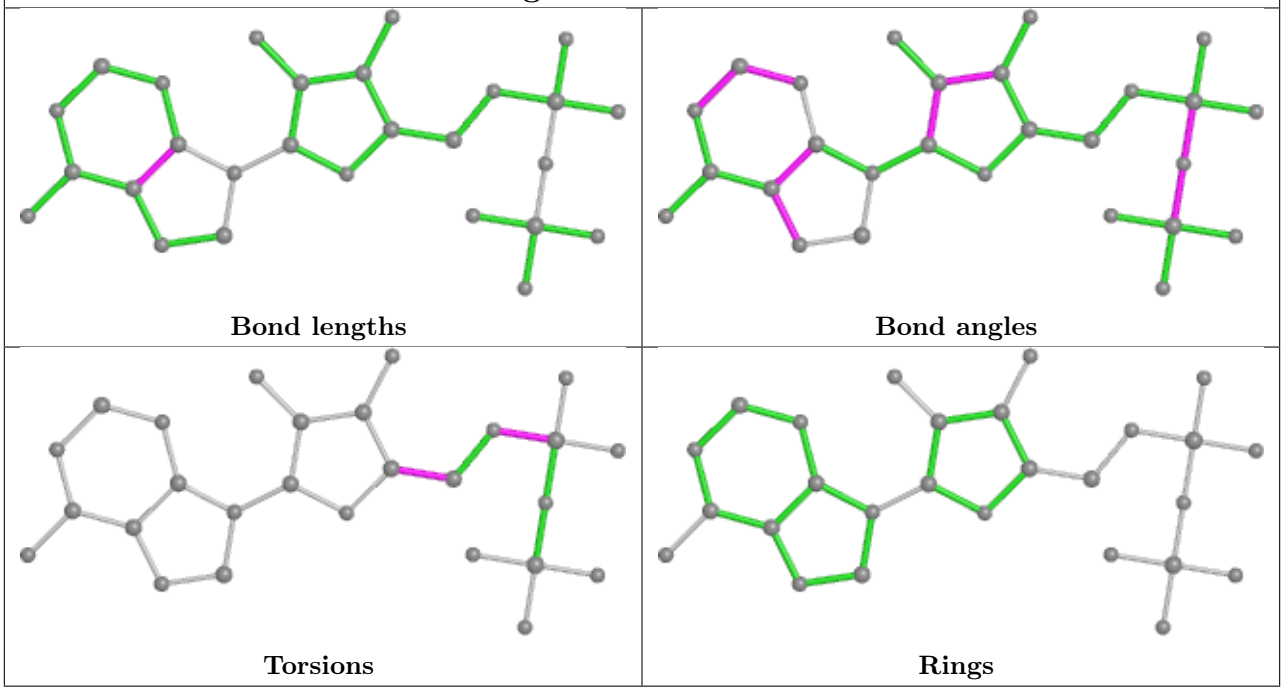


Torsions

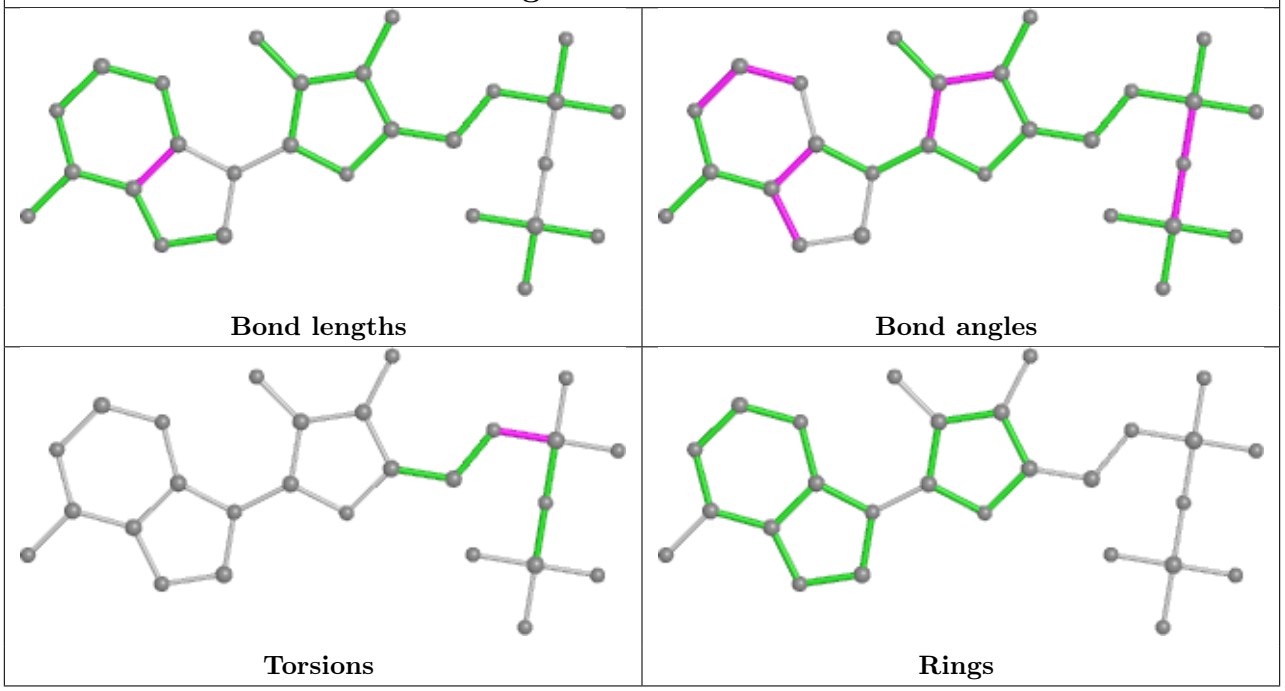


Rings

Ligand ADP C 902



Ligand ADP A 902



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.

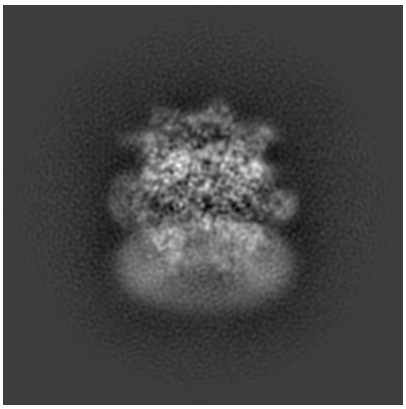
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-33613. These allow visual inspection of the internal detail of the map and identification of artifacts.

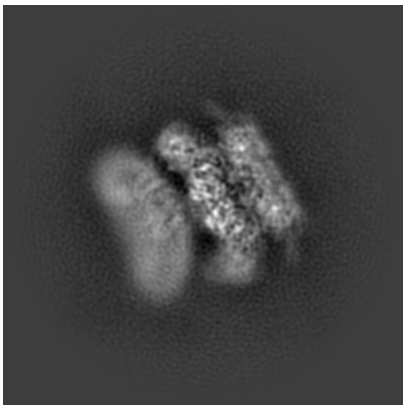
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

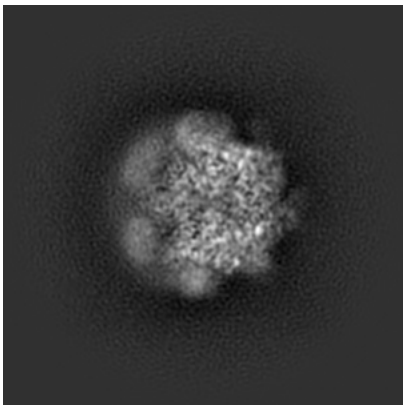
6.1.1 Primary map



X

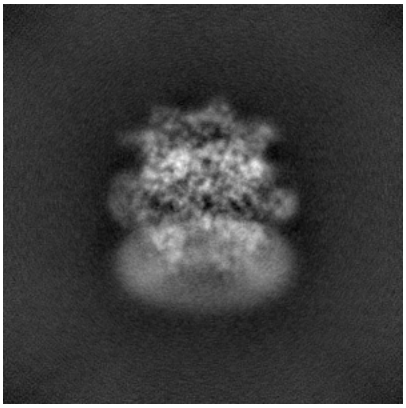


Y

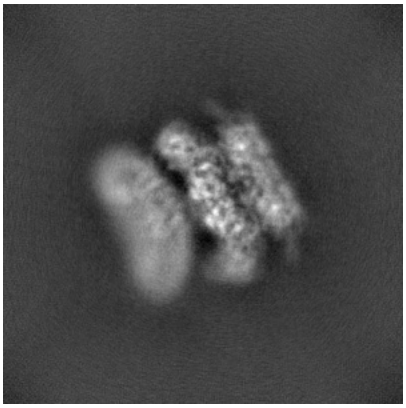


Z

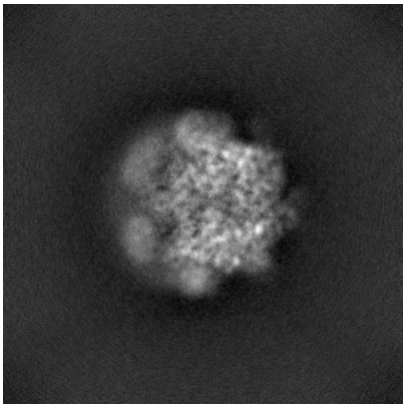
6.1.2 Raw map



X



Y

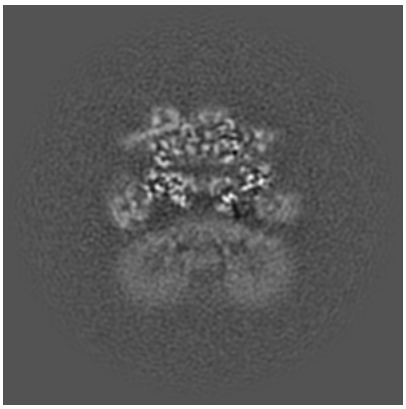


Z

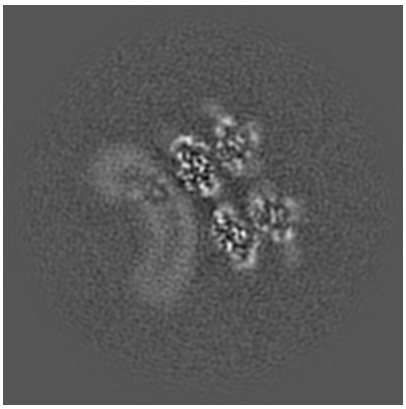
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

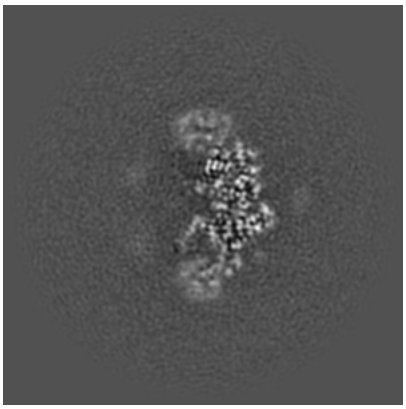
6.2.1 Primary map



X Index: 160

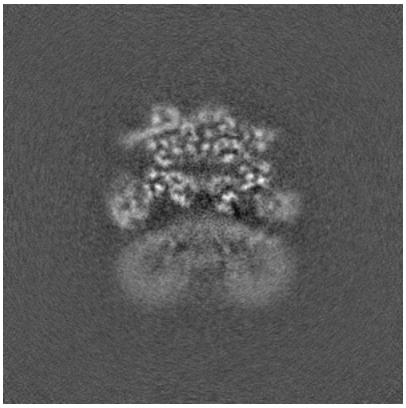


Y Index: 160

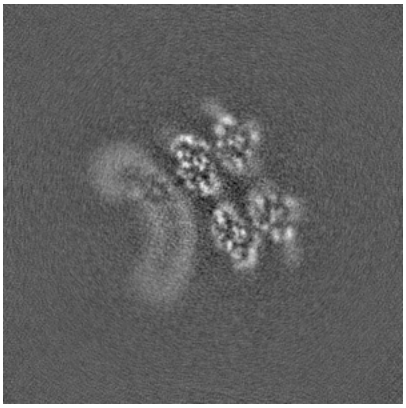


Z Index: 160

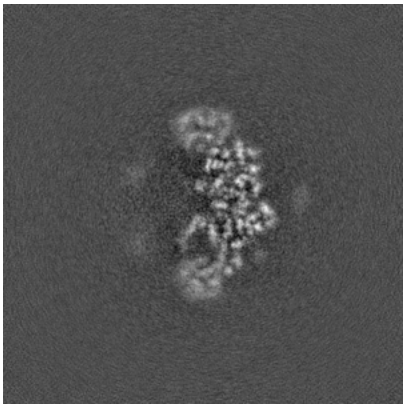
6.2.2 Raw map



X Index: 160



Y Index: 160

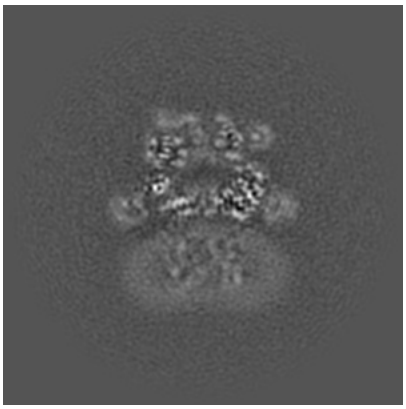


Z Index: 160

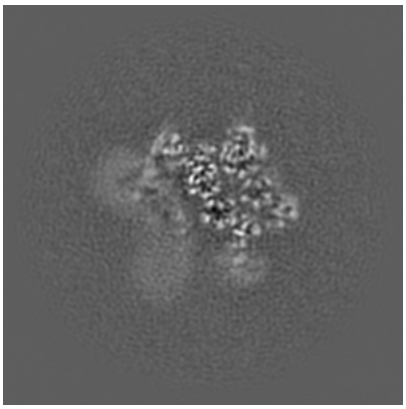
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

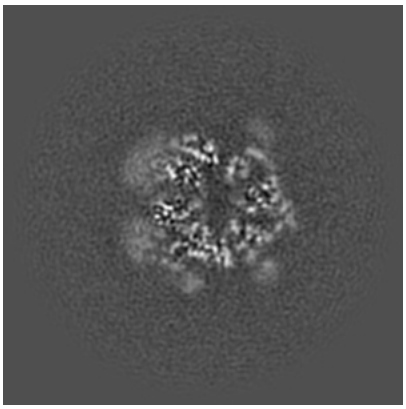
6.3.1 Primary map



X Index: 167

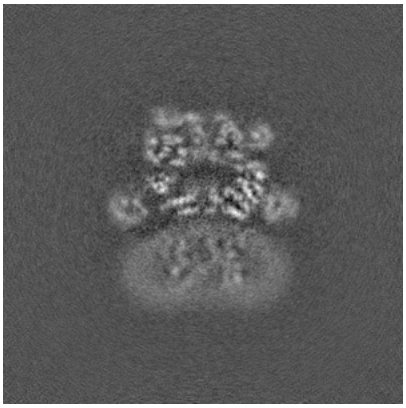


Y Index: 138

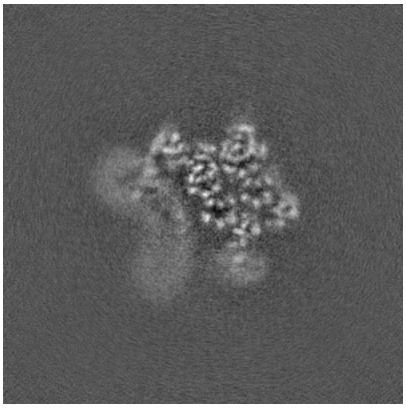


Z Index: 182

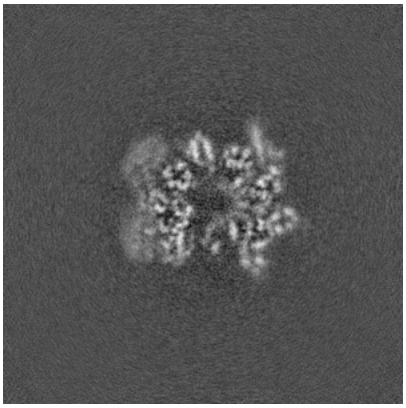
6.3.2 Raw map



X Index: 166



Y Index: 138

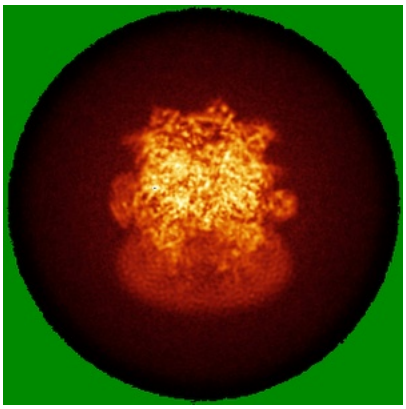


Z Index: 190

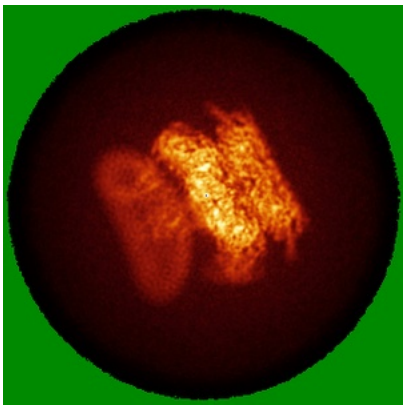
The images above show the largest variance slices of the map in three orthogonal directions.

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

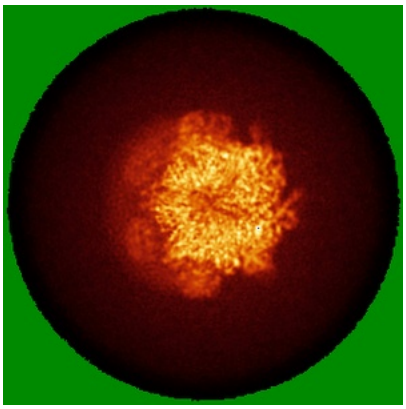
6.4.1 Primary map



X

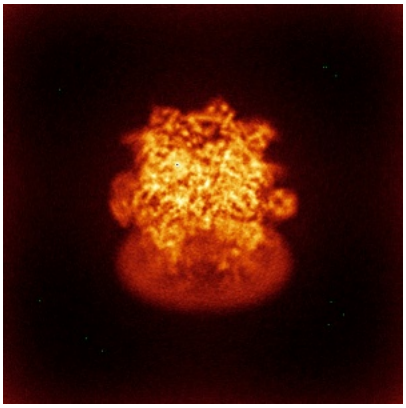


Y

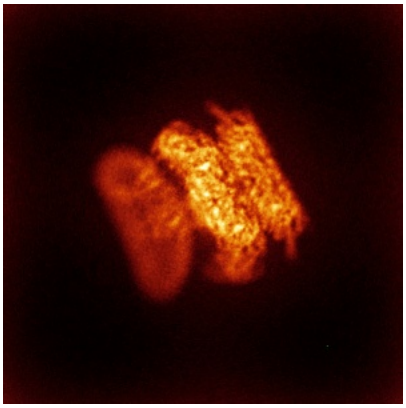


Z

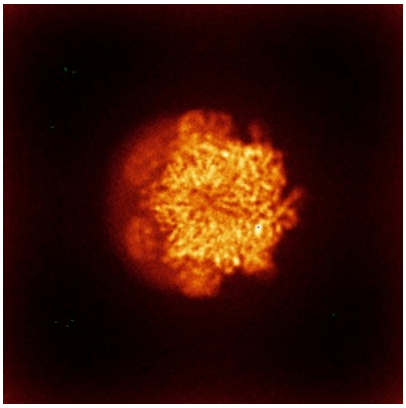
6.4.2 Raw map



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 0.25. 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.

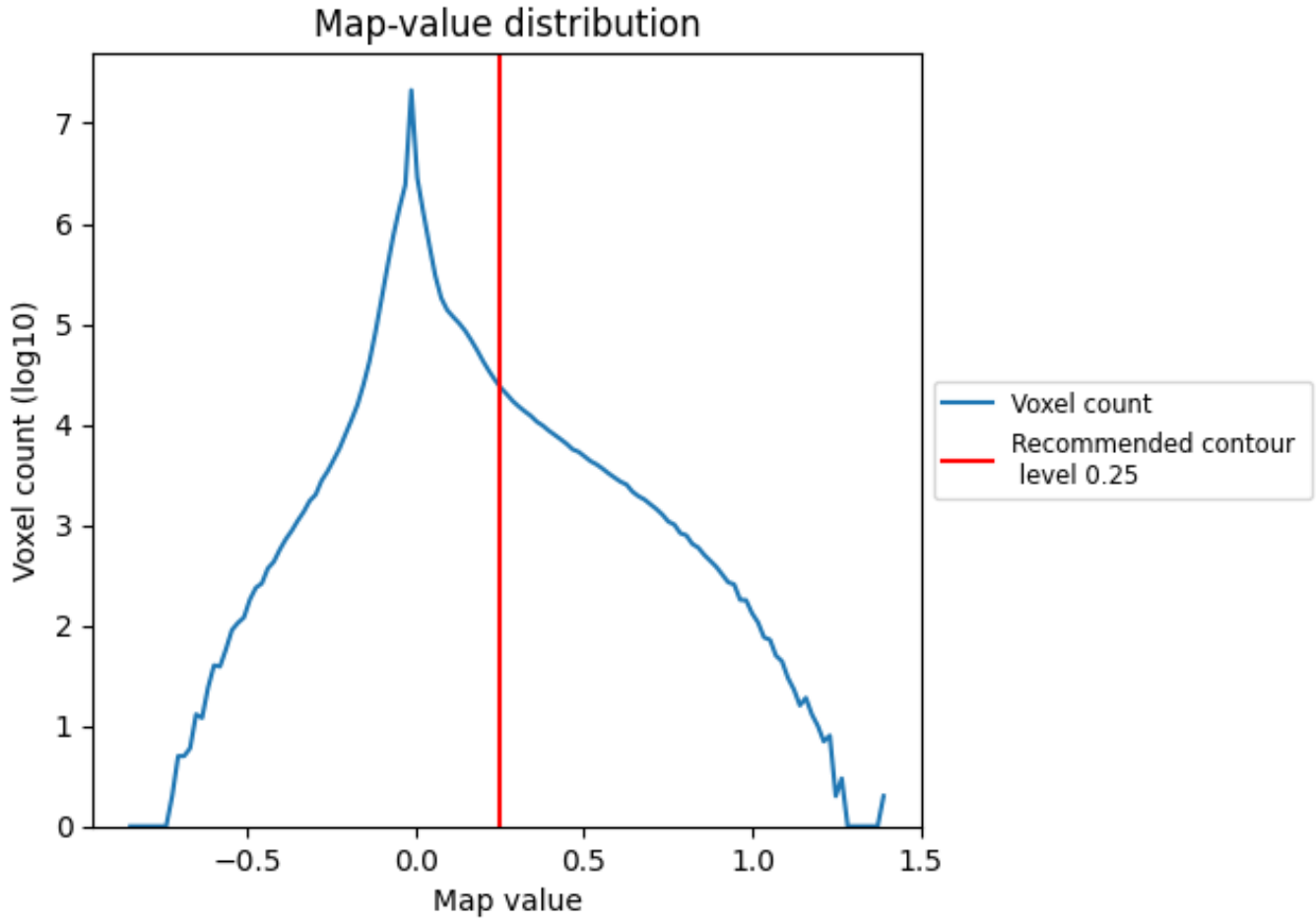
6.6 Mask visualisation (i)

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

7 Map analysis

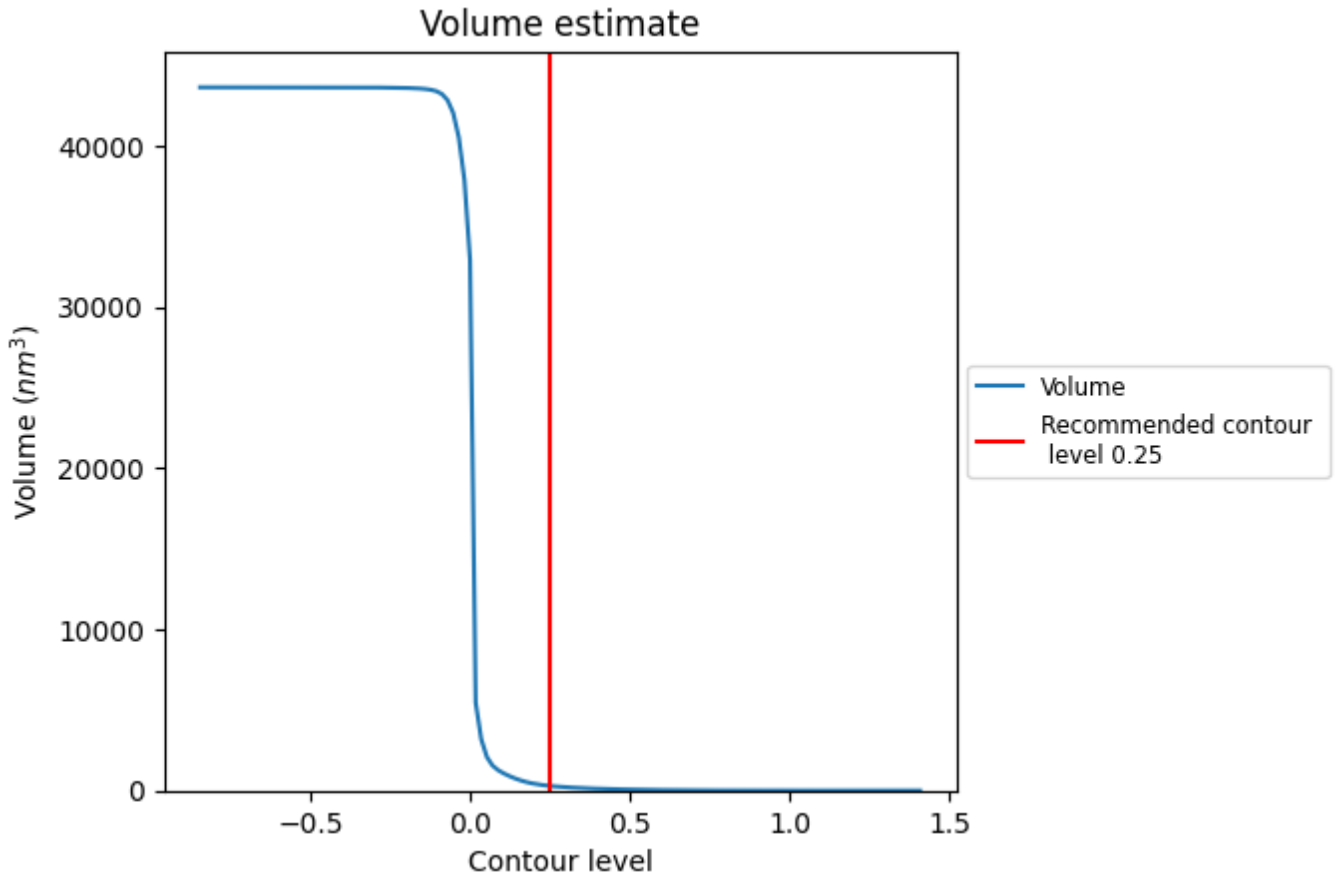
This section contains the results of statistical analysis of the map.

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.

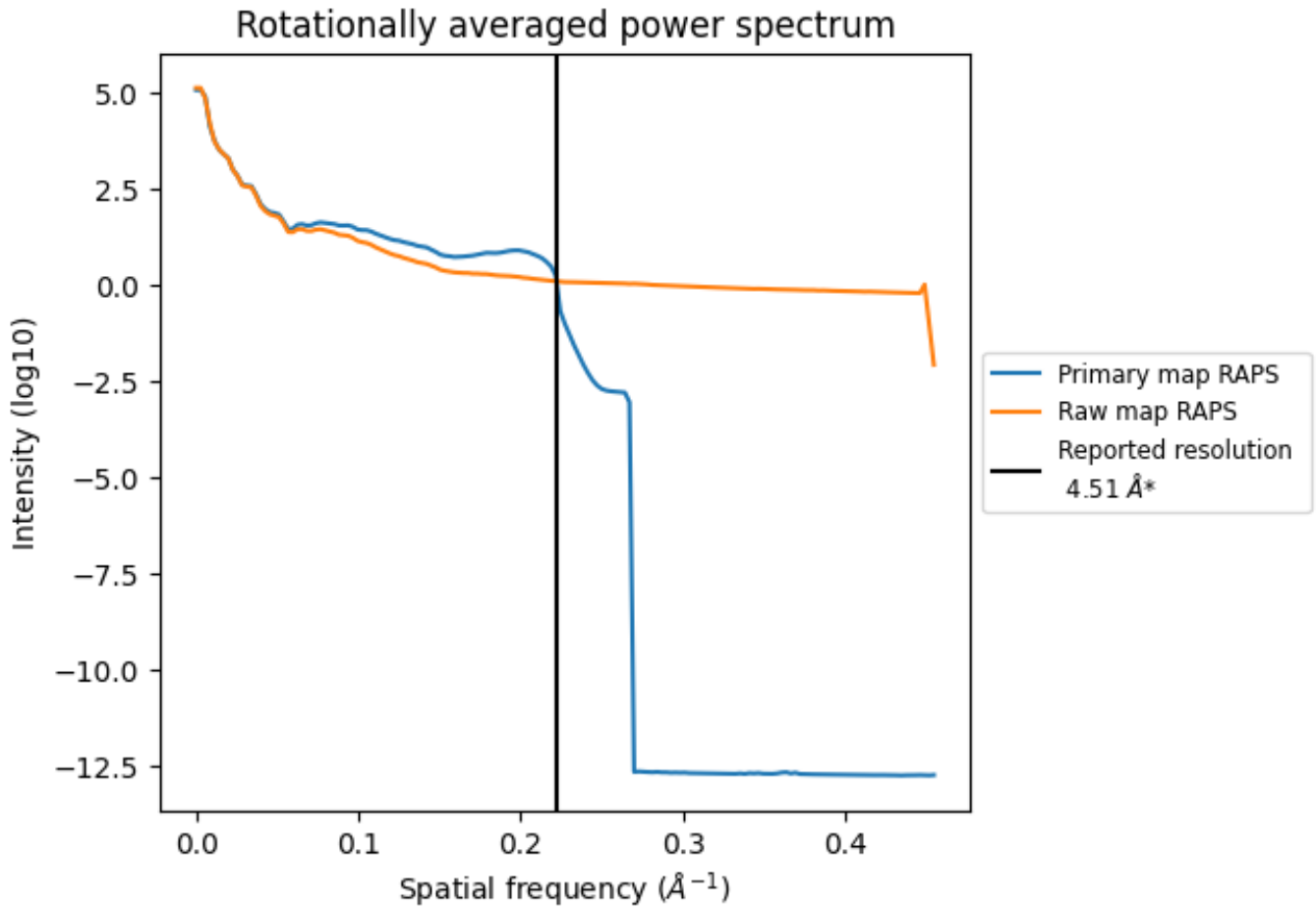
7.2 Volume estimate (i)



The volume at the recommended contour level is 285 nm^3; this corresponds to an approximate mass of 258 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)

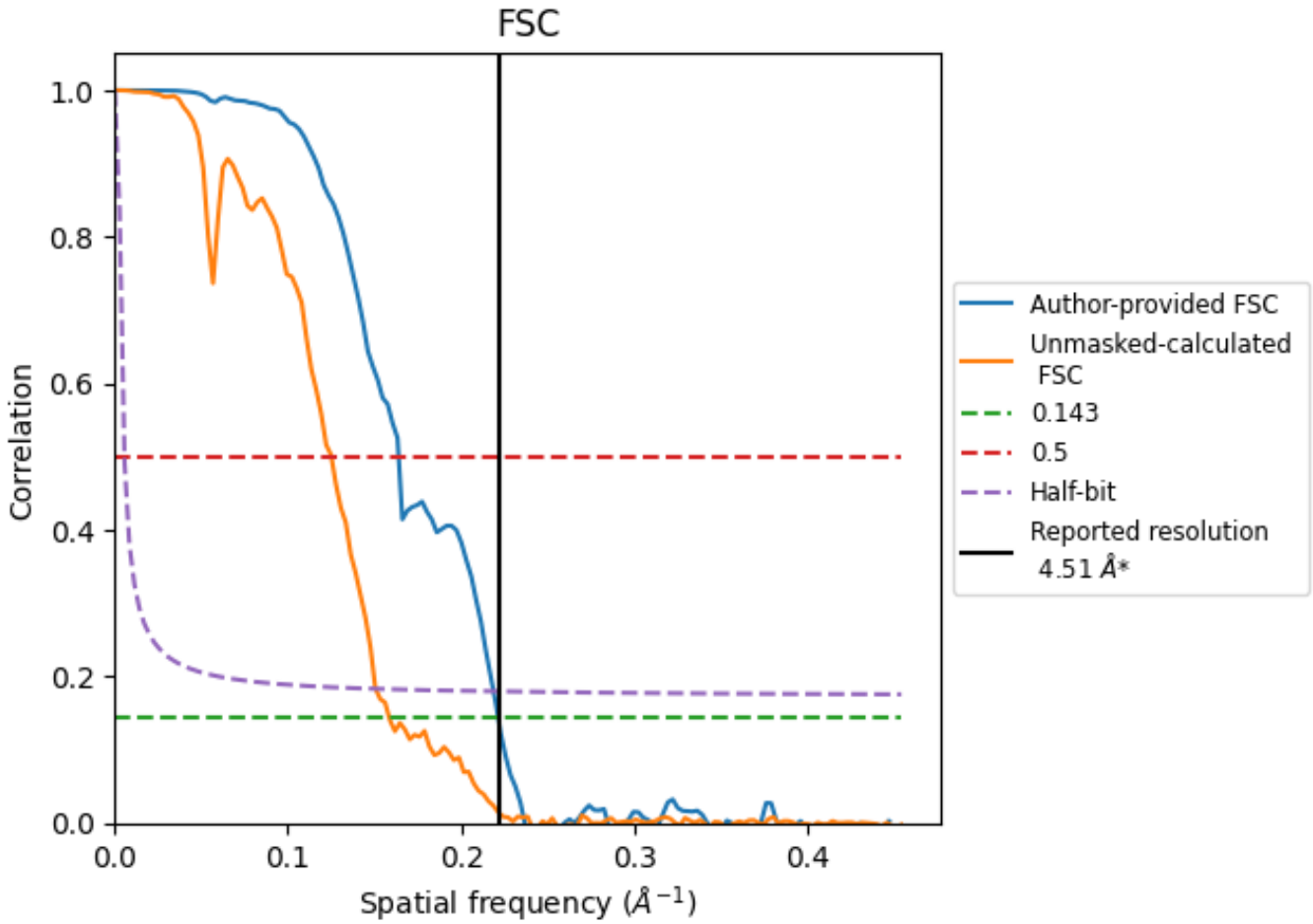


*Reported resolution corresponds to spatial frequency of 0.222 $Å^{-1}$

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 0.222 Å^{-1}

8.2 Resolution estimates (i)

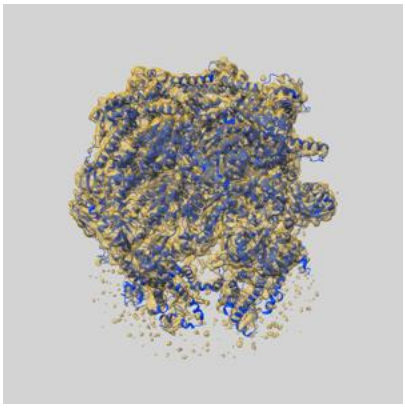
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.51	-	-
Author-provided FSC curve	4.51	6.10	4.57
Unmasked-calculated*	6.30	7.99	6.63

*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 6.30 differs from the reported value 4.51 by more than 10 %

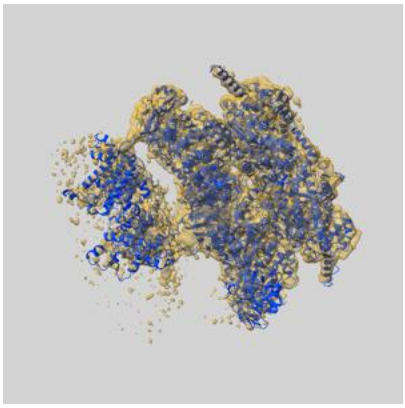
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-33613 and PDB model 7Y59. Per-residue inclusion information can be found in section 3 on page 13.

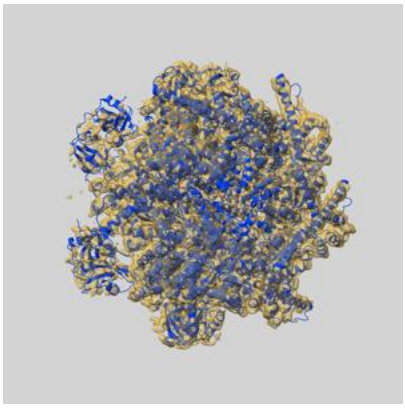
9.1 Map-model overlay



X



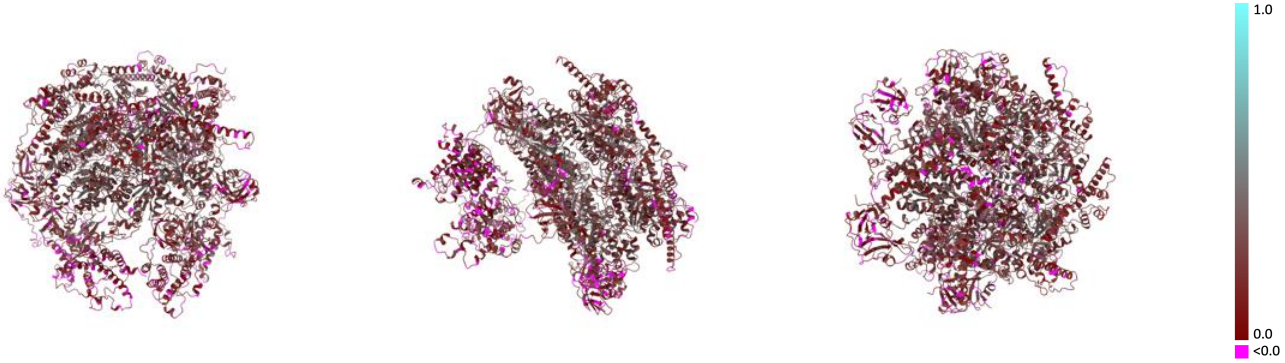
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.25 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.

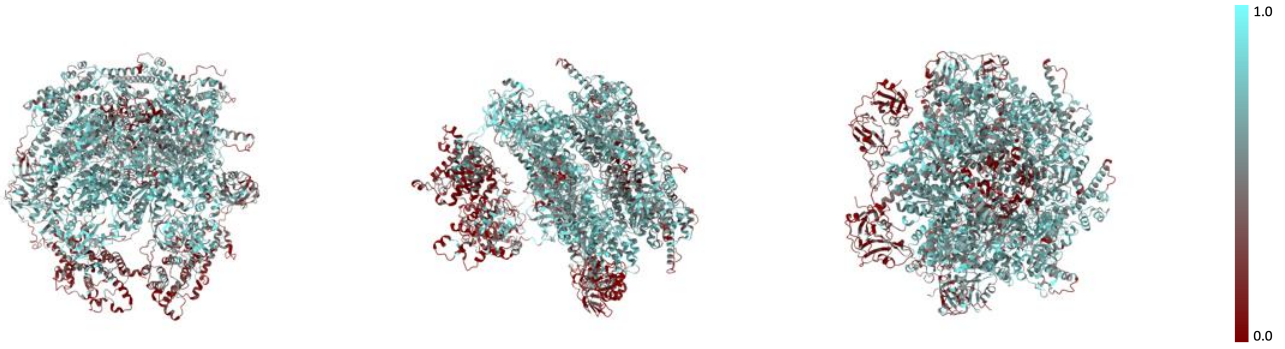
9.2 Q-score mapped to coordinate model (i)



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.

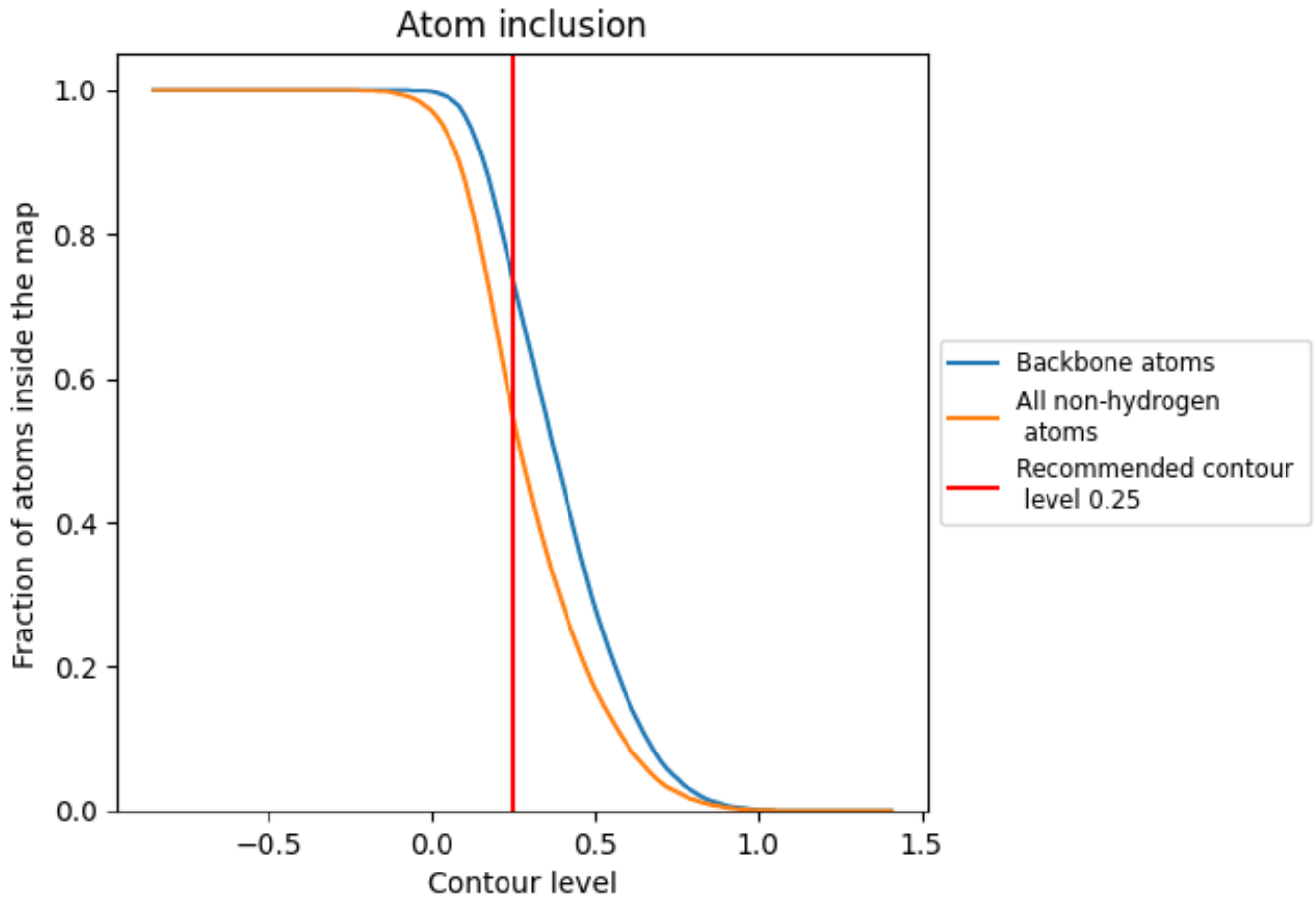
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.25).

9.4 Atom inclusion (i)



At the recommended contour level, 74% of all backbone atoms, 55% 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 (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5480	0.2200
A	0.6620	0.2610
B	0.6510	0.2510
C	0.6090	0.2400
D	0.6040	0.2390
E	0.5260	0.2180
F	0.5100	0.2150
W	0.2800	0.1000
X	0.3020	0.1370
Y	0.2090	0.0980
Z	0.3300	0.1480