



wwPDB EM Validation Summary Report ⓘ

May 4, 2025 – 08:21 PM EDT

PDB ID : 6CRI / pdb_00006cri
EMDB ID : EMD-7563
Title : Structure of the cargo bound AP-1:Arf1:tetherin-Nef stable closed trimer
Authors : Morris, K.L.; Buffalo, C.Z.; Hurley, J.H.
Deposited on : 2018-03-18
Resolution : 6.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

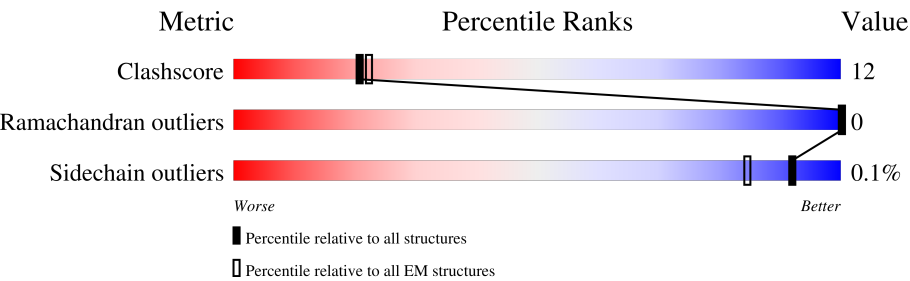
EMDB validation analysis : 0.0.1.dev118
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

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 6.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	N	264	<div><div>32%</div><div>39%</div><div>14%</div><div>47%</div></div>
1	T	264	<div><div>95%</div></div>
1	Y	264	<div><div>12%</div><div>39%</div><div>14%</div><div>47%</div></div>
1	Z	264	<div><div>14%</div><div>38%</div><div>15%</div><div>47%</div></div>
1	c	264	<div><div>95%</div></div>
1	d	264	<div><div>95%</div></div>
2	B	570	<div><div>5%</div><div>71%</div><div>29%</div></div>
2	I	570	<div><div>70%</div><div>30%</div></div>

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Mol	Chain	Length	Quality of chain
2	J	570	
3	C	165	
3	H	165	
3	K	165	
3	L	165	
3	U	165	
3	V	165	
4	G	585	
4	Q	585	
4	R	585	
5	M	422	
5	W	422	
5	X	422	
6	S	142	
6	a	142	
6	b	142	

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 53049 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 Bone marrow stromal antigen 2, Protein Nef chimera.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	T	13	Total	C	N	O	S	0	0
			105	64	16	23	2		
1	N	141	Total	C	N	O	S	0	0
			1165	759	207	196	3		
1	c	13	Total	C	N	O	S	0	0
			105	64	16	23	2		
1	Y	141	Total	C	N	O	S	0	0
			1165	759	207	196	3		
1	d	13	Total	C	N	O	S	0	0
			105	64	16	23	2		
1	Z	141	Total	C	N	O	S	0	0
			1165	759	207	196	3		

There are 228 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	-26	MET	-	expression tag	UNP Q10589
T	-25	SER	-	expression tag	UNP Q10589
T	-24	TYR	-	expression tag	UNP Q10589
T	-23	TYR	-	expression tag	UNP Q10589
T	-22	HIS	-	expression tag	UNP Q10589
T	-21	HIS	-	expression tag	UNP Q10589
T	-20	HIS	-	expression tag	UNP Q10589
T	-19	HIS	-	expression tag	UNP Q10589
T	-18	HIS	-	expression tag	UNP Q10589
T	-17	HIS	-	expression tag	UNP Q10589
T	-16	ASP	-	expression tag	UNP Q10589
T	-15	TYR	-	expression tag	UNP Q10589
T	-14	ASP	-	expression tag	UNP Q10589
T	-13	ILE	-	expression tag	UNP Q10589
T	-12	PRO	-	expression tag	UNP Q10589
T	-11	THR	-	expression tag	UNP Q10589
T	-10	THR	-	expression tag	UNP Q10589
T	-9	GLU	-	expression tag	UNP Q10589

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Chain	Residue	Modelled	Actual	Comment	Reference
T	-8	ASN	-	expression tag	UNP Q10589
T	-7	LEU	-	expression tag	UNP Q10589
T	-6	TYR	-	expression tag	UNP Q10589
T	-5	PHE	-	expression tag	UNP Q10589
T	-4	GLN	-	expression tag	UNP Q10589
T	-3	GLY	-	expression tag	UNP Q10589
T	-2	ALA	-	expression tag	UNP Q10589
T	-1	MET	-	expression tag	UNP Q10589
T	0	GLY	-	expression tag	UNP Q10589
T	1	SER	-	expression tag	UNP Q10589
T	22	GLY	-	linker	UNP Q10589
T	23	SER	-	linker	UNP Q10589
T	24	ASP	-	linker	UNP Q10589
T	25	GLU	-	linker	UNP Q10589
T	26	ALA	-	linker	UNP Q10589
T	27	SER	-	linker	UNP Q10589
T	28	GLU	-	linker	UNP Q10589
T	29	GLY	-	linker	UNP Q10589
T	30	SER	-	linker	UNP Q10589
T	31	GLY	-	linker	UNP Q10589
N	-57	MET	-	expression tag	UNP Q10589
N	-56	SER	-	expression tag	UNP Q10589
N	-55	TYR	-	expression tag	UNP Q10589
N	-54	TYR	-	expression tag	UNP Q10589
N	-53	HIS	-	expression tag	UNP Q10589
N	-52	HIS	-	expression tag	UNP Q10589
N	-51	HIS	-	expression tag	UNP Q10589
N	-50	HIS	-	expression tag	UNP Q10589
N	-49	HIS	-	expression tag	UNP Q10589
N	-48	HIS	-	expression tag	UNP Q10589
N	-47	ASP	-	expression tag	UNP Q10589
N	-46	TYR	-	expression tag	UNP Q10589
N	-45	ASP	-	expression tag	UNP Q10589
N	-44	ILE	-	expression tag	UNP Q10589
N	-43	PRO	-	expression tag	UNP Q10589
N	-42	THR	-	expression tag	UNP Q10589
N	-41	THR	-	expression tag	UNP Q10589
N	-40	GLU	-	expression tag	UNP Q10589
N	-39	ASN	-	expression tag	UNP Q10589
N	-38	LEU	-	expression tag	UNP Q10589
N	-37	TYR	-	expression tag	UNP Q10589
N	-36	PHE	-	expression tag	UNP Q10589

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Chain	Residue	Modelled	Actual	Comment	Reference
N	-35	GLN	-	expression tag	UNP Q10589
N	-34	GLY	-	expression tag	UNP Q10589
N	-33	ALA	-	expression tag	UNP Q10589
N	-32	MET	-	expression tag	UNP Q10589
N	-31	GLY	-	expression tag	UNP Q10589
N	-30	SER	-	expression tag	UNP Q10589
N	-9	GLY	-	linker	UNP Q10589
N	-8	SER	-	linker	UNP Q10589
N	-7	ASP	-	linker	UNP Q10589
N	-6	GLU	-	linker	UNP Q10589
N	-5	ALA	-	linker	UNP Q10589
N	-4	SER	-	linker	UNP Q10589
N	-3	GLU	-	linker	UNP Q10589
N	-2	GLY	-	linker	UNP Q10589
N	-1	SER	-	linker	UNP Q10589
N	0	GLY	-	linker	UNP Q10589
c	-26	MET	-	expression tag	UNP Q10589
c	-25	SER	-	expression tag	UNP Q10589
c	-24	TYR	-	expression tag	UNP Q10589
c	-23	TYR	-	expression tag	UNP Q10589
c	-22	HIS	-	expression tag	UNP Q10589
c	-21	HIS	-	expression tag	UNP Q10589
c	-20	HIS	-	expression tag	UNP Q10589
c	-19	HIS	-	expression tag	UNP Q10589
c	-18	HIS	-	expression tag	UNP Q10589
c	-17	HIS	-	expression tag	UNP Q10589
c	-16	ASP	-	expression tag	UNP Q10589
c	-15	TYR	-	expression tag	UNP Q10589
c	-14	ASP	-	expression tag	UNP Q10589
c	-13	ILE	-	expression tag	UNP Q10589
c	-12	PRO	-	expression tag	UNP Q10589
c	-11	THR	-	expression tag	UNP Q10589
c	-10	THR	-	expression tag	UNP Q10589
c	-9	GLU	-	expression tag	UNP Q10589
c	-8	ASN	-	expression tag	UNP Q10589
c	-7	LEU	-	expression tag	UNP Q10589
c	-6	TYR	-	expression tag	UNP Q10589
c	-5	PHE	-	expression tag	UNP Q10589
c	-4	GLN	-	expression tag	UNP Q10589
c	-3	GLY	-	expression tag	UNP Q10589
c	-2	ALA	-	expression tag	UNP Q10589
c	-1	MET	-	expression tag	UNP Q10589

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Chain	Residue	Modelled	Actual	Comment	Reference
c	0	GLY	-	expression tag	UNP Q10589
c	1	SER	-	expression tag	UNP Q10589
c	22	GLY	-	linker	UNP Q10589
c	23	SER	-	linker	UNP Q10589
c	24	ASP	-	linker	UNP Q10589
c	25	GLU	-	linker	UNP Q10589
c	26	ALA	-	linker	UNP Q10589
c	27	SER	-	linker	UNP Q10589
c	28	GLU	-	linker	UNP Q10589
c	29	GLY	-	linker	UNP Q10589
c	30	SER	-	linker	UNP Q10589
c	31	GLY	-	linker	UNP Q10589
Y	-57	MET	-	expression tag	UNP Q10589
Y	-56	SER	-	expression tag	UNP Q10589
Y	-55	TYR	-	expression tag	UNP Q10589
Y	-54	TYR	-	expression tag	UNP Q10589
Y	-53	HIS	-	expression tag	UNP Q10589
Y	-52	HIS	-	expression tag	UNP Q10589
Y	-51	HIS	-	expression tag	UNP Q10589
Y	-50	HIS	-	expression tag	UNP Q10589
Y	-49	HIS	-	expression tag	UNP Q10589
Y	-48	HIS	-	expression tag	UNP Q10589
Y	-47	ASP	-	expression tag	UNP Q10589
Y	-46	TYR	-	expression tag	UNP Q10589
Y	-45	ASP	-	expression tag	UNP Q10589
Y	-44	ILE	-	expression tag	UNP Q10589
Y	-43	PRO	-	expression tag	UNP Q10589
Y	-42	THR	-	expression tag	UNP Q10589
Y	-41	THR	-	expression tag	UNP Q10589
Y	-40	GLU	-	expression tag	UNP Q10589
Y	-39	ASN	-	expression tag	UNP Q10589
Y	-38	LEU	-	expression tag	UNP Q10589
Y	-37	TYR	-	expression tag	UNP Q10589
Y	-36	PHE	-	expression tag	UNP Q10589
Y	-35	GLN	-	expression tag	UNP Q10589
Y	-34	GLY	-	expression tag	UNP Q10589
Y	-33	ALA	-	expression tag	UNP Q10589
Y	-32	MET	-	expression tag	UNP Q10589
Y	-31	GLY	-	expression tag	UNP Q10589
Y	-30	SER	-	expression tag	UNP Q10589
Y	-9	GLY	-	linker	UNP Q10589
Y	-8	SER	-	linker	UNP Q10589

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Chain	Residue	Modelled	Actual	Comment	Reference
Y	-7	ASP	-	linker	UNP Q10589
Y	-6	GLU	-	linker	UNP Q10589
Y	-5	ALA	-	linker	UNP Q10589
Y	-4	SER	-	linker	UNP Q10589
Y	-3	GLU	-	linker	UNP Q10589
Y	-2	GLY	-	linker	UNP Q10589
Y	-1	SER	-	linker	UNP Q10589
Y	0	GLY	-	linker	UNP Q10589
d	-26	MET	-	expression tag	UNP Q10589
d	-25	SER	-	expression tag	UNP Q10589
d	-24	TYR	-	expression tag	UNP Q10589
d	-23	TYR	-	expression tag	UNP Q10589
d	-22	HIS	-	expression tag	UNP Q10589
d	-21	HIS	-	expression tag	UNP Q10589
d	-20	HIS	-	expression tag	UNP Q10589
d	-19	HIS	-	expression tag	UNP Q10589
d	-18	HIS	-	expression tag	UNP Q10589
d	-17	HIS	-	expression tag	UNP Q10589
d	-16	ASP	-	expression tag	UNP Q10589
d	-15	TYR	-	expression tag	UNP Q10589
d	-14	ASP	-	expression tag	UNP Q10589
d	-13	ILE	-	expression tag	UNP Q10589
d	-12	PRO	-	expression tag	UNP Q10589
d	-11	THR	-	expression tag	UNP Q10589
d	-10	THR	-	expression tag	UNP Q10589
d	-9	GLU	-	expression tag	UNP Q10589
d	-8	ASN	-	expression tag	UNP Q10589
d	-7	LEU	-	expression tag	UNP Q10589
d	-6	TYR	-	expression tag	UNP Q10589
d	-5	PHE	-	expression tag	UNP Q10589
d	-4	GLN	-	expression tag	UNP Q10589
d	-3	GLY	-	expression tag	UNP Q10589
d	-2	ALA	-	expression tag	UNP Q10589
d	-1	MET	-	expression tag	UNP Q10589
d	0	GLY	-	expression tag	UNP Q10589
d	1	SER	-	expression tag	UNP Q10589
d	22	GLY	-	linker	UNP Q10589
d	23	SER	-	linker	UNP Q10589
d	24	ASP	-	linker	UNP Q10589
d	25	GLU	-	linker	UNP Q10589
d	26	ALA	-	linker	UNP Q10589
d	27	SER	-	linker	UNP Q10589

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Chain	Residue	Modelled	Actual	Comment	Reference
d	28	GLU	-	linker	UNP Q10589
d	29	GLY	-	linker	UNP Q10589
d	30	SER	-	linker	UNP Q10589
d	31	GLY	-	linker	UNP Q10589
Z	-57	MET	-	expression tag	UNP Q10589
Z	-56	SER	-	expression tag	UNP Q10589
Z	-55	TYR	-	expression tag	UNP Q10589
Z	-54	TYR	-	expression tag	UNP Q10589
Z	-53	HIS	-	expression tag	UNP Q10589
Z	-52	HIS	-	expression tag	UNP Q10589
Z	-51	HIS	-	expression tag	UNP Q10589
Z	-50	HIS	-	expression tag	UNP Q10589
Z	-49	HIS	-	expression tag	UNP Q10589
Z	-48	HIS	-	expression tag	UNP Q10589
Z	-47	ASP	-	expression tag	UNP Q10589
Z	-46	TYR	-	expression tag	UNP Q10589
Z	-45	ASP	-	expression tag	UNP Q10589
Z	-44	ILE	-	expression tag	UNP Q10589
Z	-43	PRO	-	expression tag	UNP Q10589
Z	-42	THR	-	expression tag	UNP Q10589
Z	-41	THR	-	expression tag	UNP Q10589
Z	-40	GLU	-	expression tag	UNP Q10589
Z	-39	ASN	-	expression tag	UNP Q10589
Z	-38	LEU	-	expression tag	UNP Q10589
Z	-37	TYR	-	expression tag	UNP Q10589
Z	-36	PHE	-	expression tag	UNP Q10589
Z	-35	GLN	-	expression tag	UNP Q10589
Z	-34	GLY	-	expression tag	UNP Q10589
Z	-33	ALA	-	expression tag	UNP Q10589
Z	-32	MET	-	expression tag	UNP Q10589
Z	-31	GLY	-	expression tag	UNP Q10589
Z	-30	SER	-	expression tag	UNP Q10589
Z	-9	GLY	-	linker	UNP Q10589
Z	-8	SER	-	linker	UNP Q10589
Z	-7	ASP	-	linker	UNP Q10589
Z	-6	GLU	-	linker	UNP Q10589
Z	-5	ALA	-	linker	UNP Q10589
Z	-4	SER	-	linker	UNP Q10589
Z	-3	GLU	-	linker	UNP Q10589
Z	-2	GLY	-	linker	UNP Q10589
Z	-1	SER	-	linker	UNP Q10589
Z	0	GLY	-	linker	UNP Q10589

- Molecule 2 is a protein called AP-1 complex subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	570	Total	C	N	O	S	0	0
			4513	2883	741	862	27		
2	I	570	Total	C	N	O	S	0	0
			4513	2883	741	862	27		
2	J	570	Total	C	N	O	S	0	0
			4513	2883	741	862	27		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	359	ARG	LYS	engineered mutation	UNP Q10567
B	476	LYS	GLU	engineered mutation	UNP Q10567
I	359	ARG	LYS	engineered mutation	UNP Q10567
I	476	LYS	GLU	engineered mutation	UNP Q10567
J	359	ARG	LYS	engineered mutation	UNP Q10567
J	476	LYS	GLU	engineered mutation	UNP Q10567

- Molecule 3 is a protein called ADP-ribosylation factor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	165	Total	C	N	O	S	0	0
			1330	842	233	249	6		
3	H	163	Total	C	N	O	S	0	0
			1312	831	229	246	6		
3	K	165	Total	C	N	O	S	0	0
			1330	842	233	249	6		
3	U	163	Total	C	N	O	S	0	0
			1312	831	229	246	6		
3	L	165	Total	C	N	O	S	0	0
			1330	842	233	249	6		
3	V	163	Total	C	N	O	S	0	0
			1312	831	229	246	6		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	71	LEU	GLN	engineered mutation	UNP P84077
H	71	LEU	GLN	engineered mutation	UNP P84077
K	71	LEU	GLN	engineered mutation	UNP P84077
U	71	LEU	GLN	engineered mutation	UNP P84077
L	71	LEU	GLN	engineered mutation	UNP P84077

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Chain	Residue	Modelled	Actual	Comment	Reference
V	71	LEU	GLN	engineered mutation	UNP P84077

- Molecule 4 is a protein called AP-1 complex subunit gamma-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	585	Total	C	N	O	S	0	0
			4633	2914	815	865	39		
4	Q	585	Total	C	N	O	S	0	0
			4633	2914	815	865	39		
4	R	585	Total	C	N	O	S	0	0
			4633	2914	815	865	39		

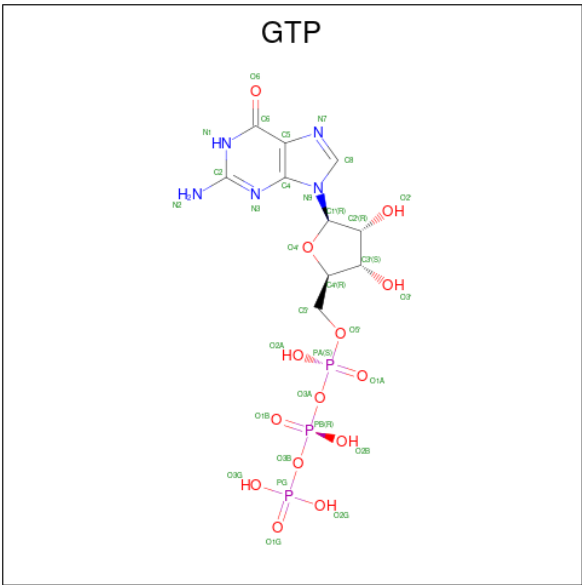
- Molecule 5 is a protein called AP-1 complex subunit mu-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	M	415	Total	C	N	O	S	0	0
			3362	2161	566	621	14		
5	W	415	Total	C	N	O	S	0	0
			3362	2161	566	621	14		
5	X	415	Total	C	N	O	S	0	0
			3362	2161	566	621	14		

- Molecule 6 is a protein called AP-1 complex subunit sigma-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	S	142	Total	C	N	O	S	0	0
			1197	782	197	213	5		
6	a	142	Total	C	N	O	S	0	0
			1197	782	197	213	5		
6	b	142	Total	C	N	O	S	0	0
			1197	782	197	213	5		

- Molecule 7 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

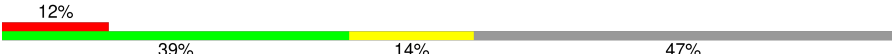


Mol	Chain	Residues	Atoms					AltConf
7	C	1	Total	C	N	O	P	0
			32	10	5	14	3	
7	H	1	Total	C	N	O	P	0
			32	10	5	14	3	
7	K	1	Total	C	N	O	P	0
			32	10	5	14	3	
7	U	1	Total	C	N	O	P	0
			32	10	5	14	3	
7	L	1	Total	C	N	O	P	0
			32	10	5	14	3	
7	V	1	Total	C	N	O	P	0
			32	10	5	14	3	

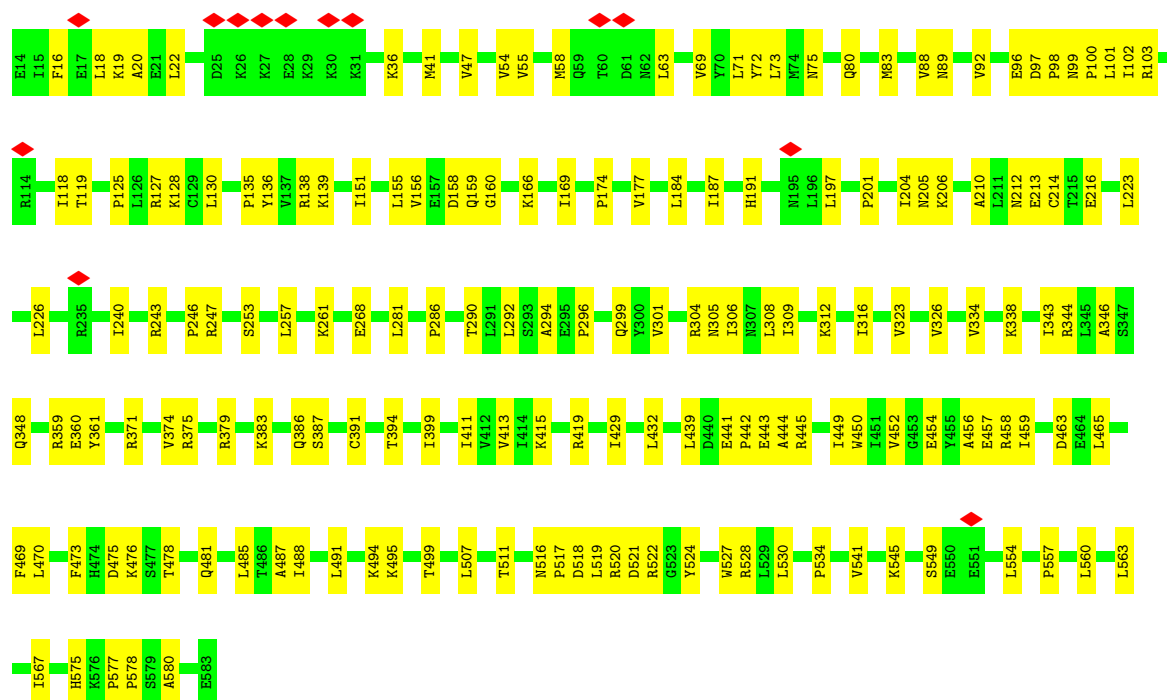
- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
8	C	1	Total	Mg	0
			1	1	
8	H	1	Total	Mg	0
			1	1	
8	K	1	Total	Mg	0
			1	1	
8	U	1	Total	Mg	0
			1	1	
8	L	1	Total	Mg	0
			1	1	
8	V	1	Total	Mg	0
			1	1	

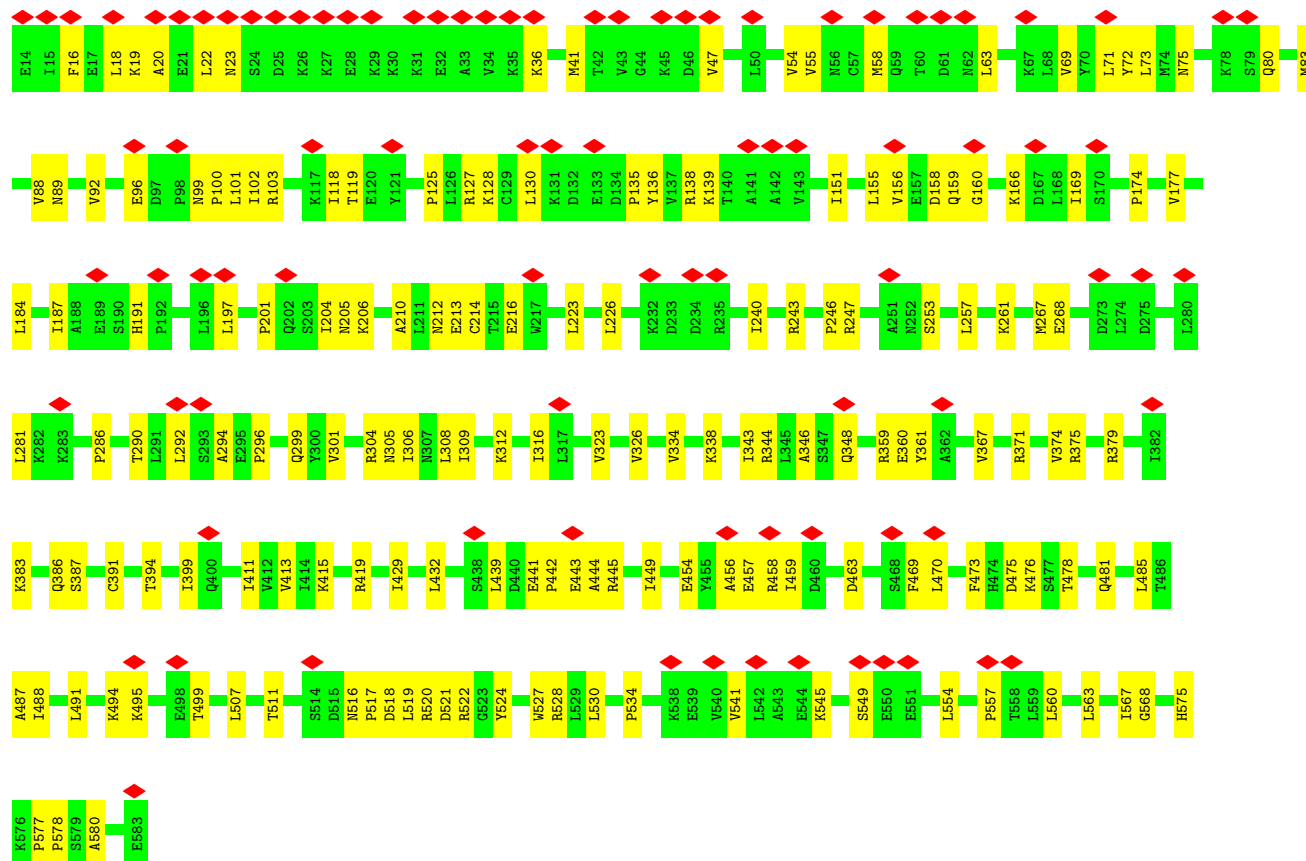
- [illegible]

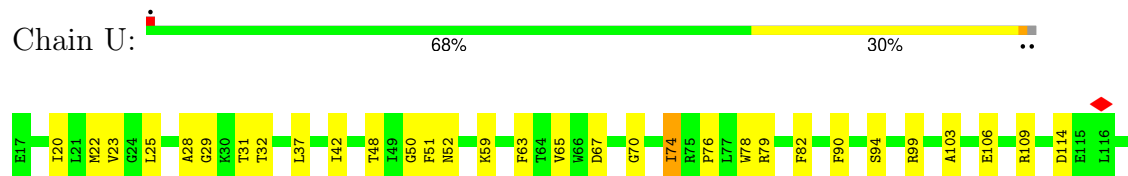
- Chain Y: 
- Met
Tyr
Tyr
Tyr
His
His
His
His
His
Asp
Tyr
Asp
Asp
Ile
Pro
Thr
Thr
Glu
Asn
Leu
Tyr
Phe
Gln
Gly
Ala
Met
Gly
Ser
Ala
Ser
Thr
Ser
Tyr
Tyr
Asp
Cys
Arg
Val
Pro
Met
Glu
Asp
Gly
Asp
Lys
Arg
Cys
Lys
Gly
Ser
Met
Gly
- Gly
Lys
S6
S9
W13
R17
M20
R21
P25
A26
Ala
Asp
Gly
Val
Gly
Ala
Val
Ser
Arg
Asp
Leu
Glu
Lys
His
Gly
Ala
Ile
Thr
Ser
Ser
Asn
Thr
Ala
Ala
Asn
Asn
Ala
Cys
Ala
Trp
Leu
Glu
Ala
Gln
Glu
Glu
E64
E65
V66
G67
F68
P69
V70
- Q73
W74
P75
T80
A83
D86
L87
L91
K92
E93
L100
H101
H102
S103
Q104
R105
R106
Q107
D108
P122
D123
W124
Q125
N126
Y127
T128
P129
G130
P131
G132
V133
R134
L137
T138
F139
G140
W141
K144
V145
Glu
Pro
Asp
Lys
Val
Glu
Glu
Ala
Asn
K158
- P167
Val
Ser
Leu
His
Gly
Met
Asp
Pro
Pro
Glu
Arg
Glu
V130
L131
R184
L189
A190
F191
H192
A195
R196
E197
L198
H199
P200
E201
Y202
F203
K204
Asn
Cys

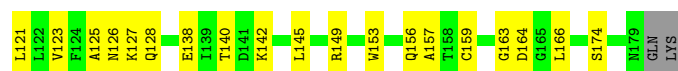
- [illegible]



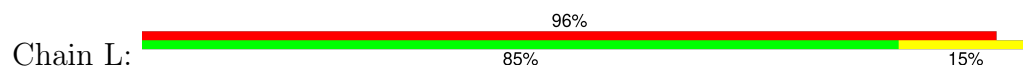
• Molecule 2: AP-1 complex subunit beta-1



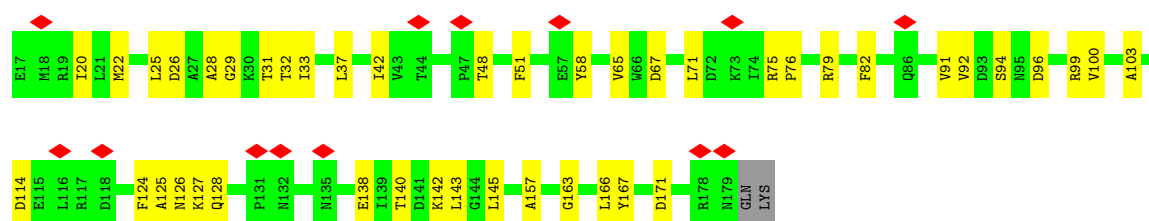




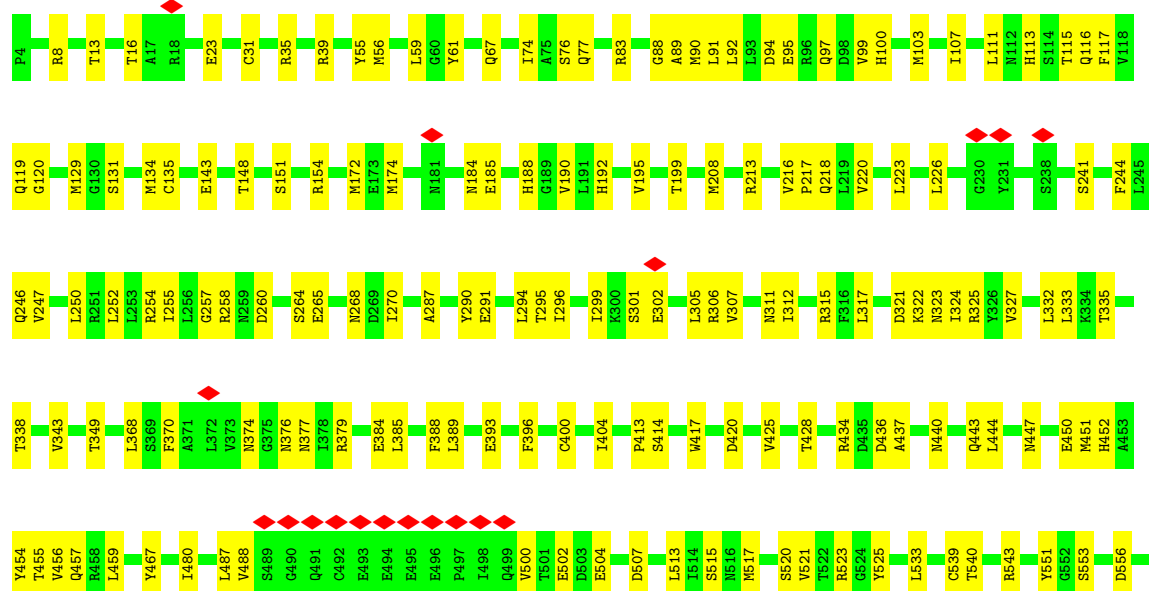
• Molecule 3: ADP-ribosylation factor 1

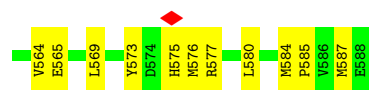


• Molecule 3: ADP-ribosylation factor 1

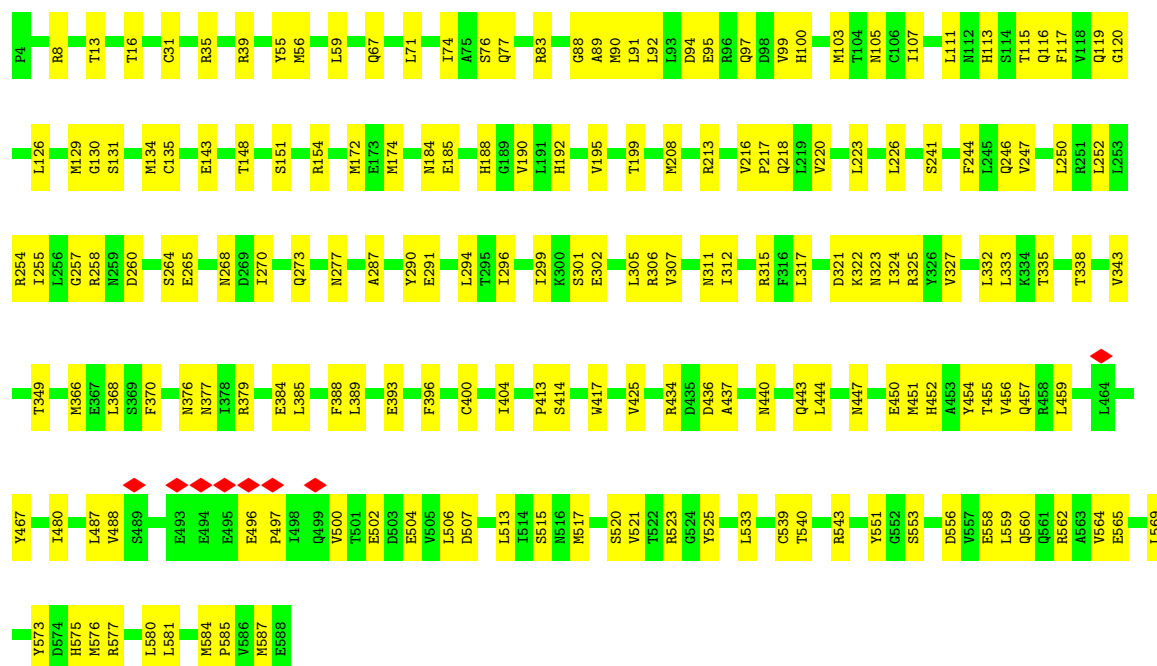


• Molecule 4: AP-1 complex subunit gamma-1

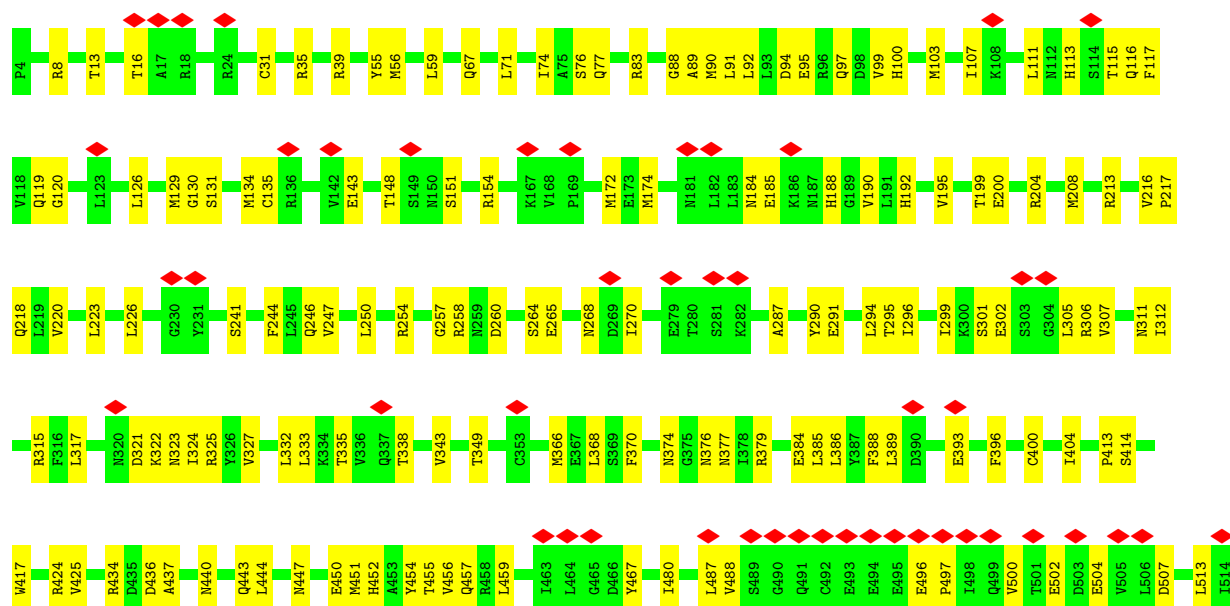




• Molecule 4: AP-1 complex subunit gamma-1

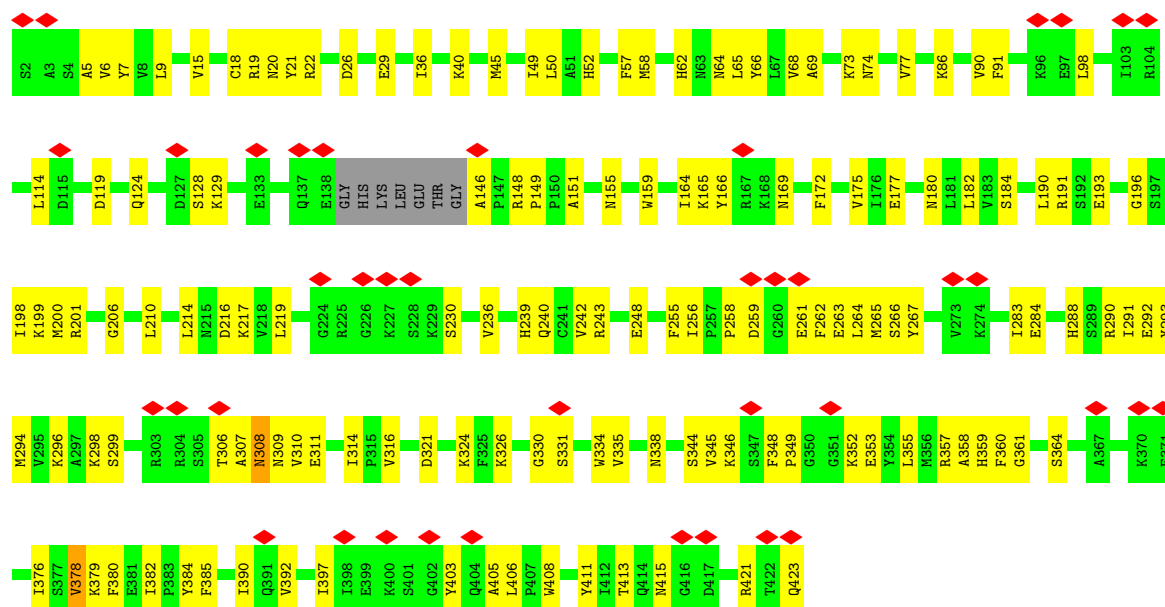


• Molecule 4: AP-1 complex subunit gamma-1

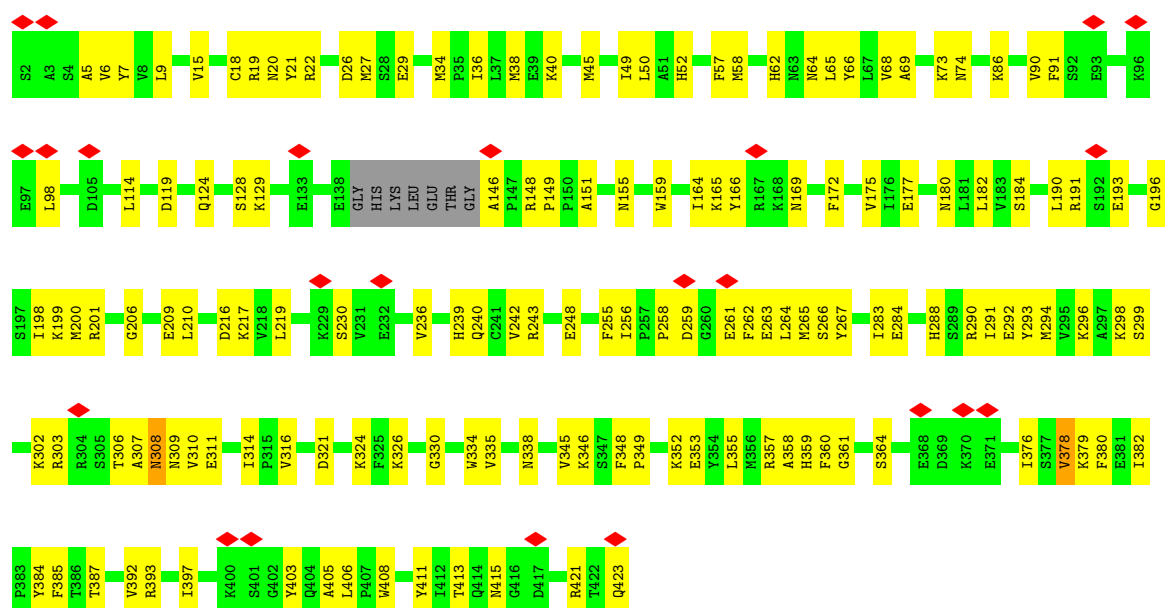




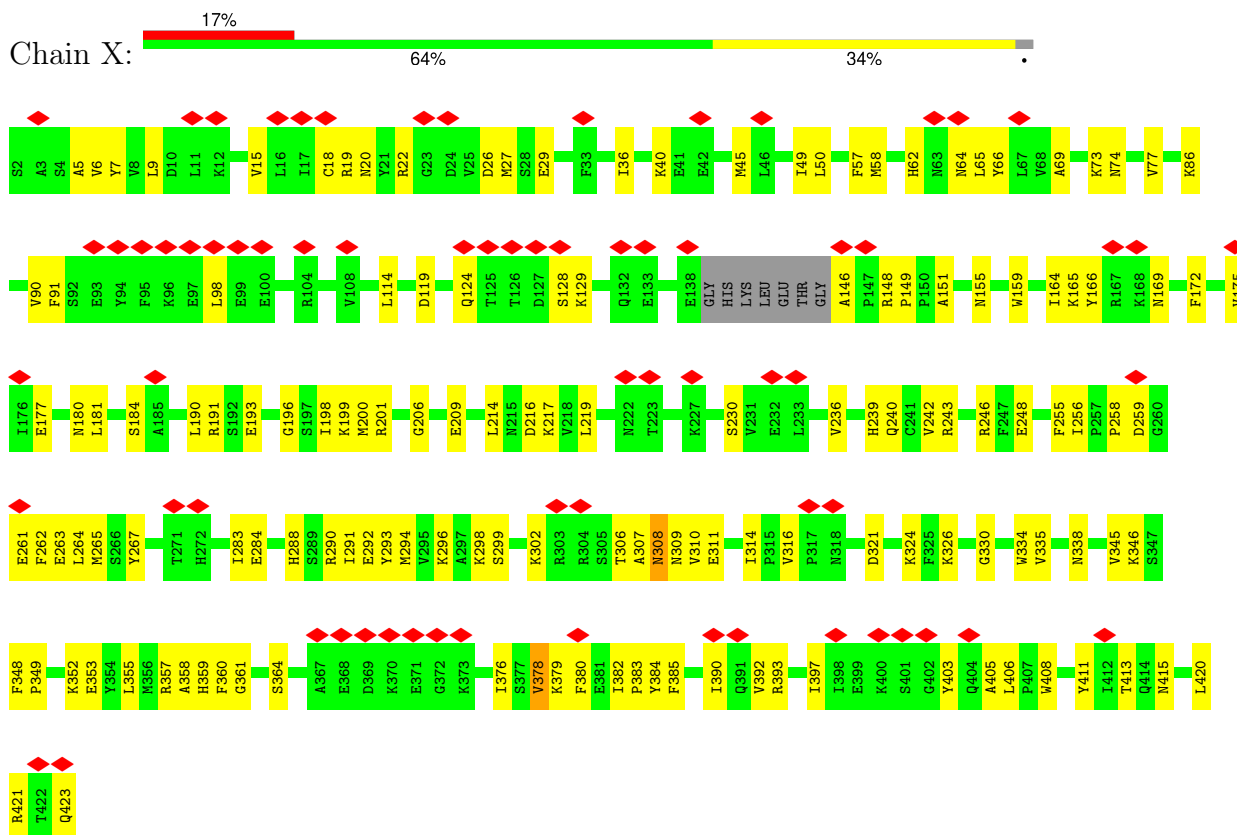
• Molecule 5: AP-1 complex subunit mu-1



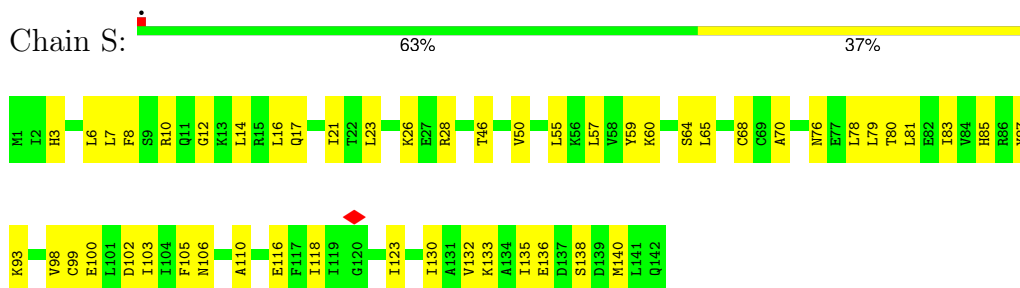
• Molecule 5: AP-1 complex subunit mu-1



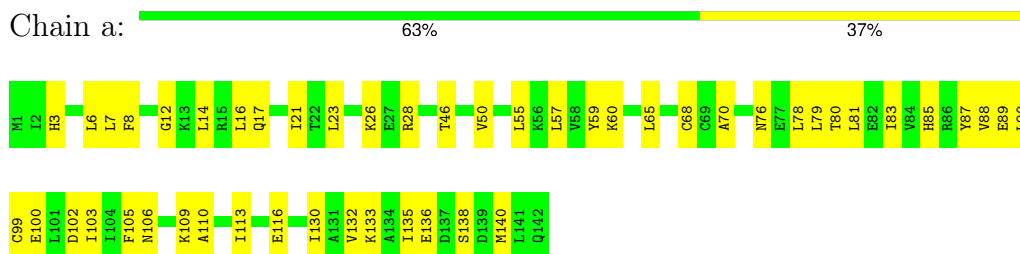
• Molecule 5: AP-1 complex subunit mu-1



• Molecule 6: AP-1 complex subunit sigma-3

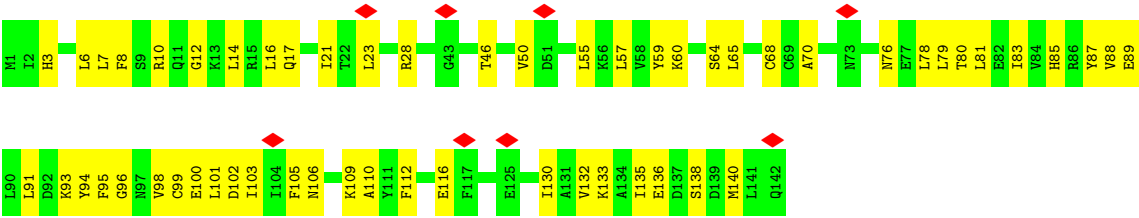


• Molecule 6: AP-1 complex subunit sigma-3



• Molecule 6: AP-1 complex subunit sigma-3





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	11108	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 ($e^-/\text{\AA}^2$)	62.4	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.059	Depositor
Minimum map value	-0.018	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0149	Depositor
Map size (Å)	409.72803, 409.72803, 409.72803	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.067, 1.067, 1.067	Depositor

5 Model quality

5.1 Standard geometry

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

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	N	0.25	0/1205	0.53	0/1636
1	T	0.32	0/107	0.61	0/144
1	Y	0.25	0/1205	0.53	0/1636
1	Z	0.25	0/1205	0.53	0/1636
1	c	0.32	0/107	0.62	0/144
1	d	0.32	0/107	0.61	0/144
2	B	0.34	0/4583	0.60	0/6216
2	I	0.34	0/4583	0.60	0/6216
2	J	0.34	0/4583	0.60	0/6216
3	C	0.27	0/1353	0.53	0/1831
3	H	0.45	0/1335	0.70	0/1808
3	K	0.26	0/1353	0.54	0/1831
3	L	0.24	0/1353	0.52	0/1831
3	U	0.44	0/1335	0.70	2/1808 (0.1%)
3	V	0.36	0/1335	0.64	0/1808
4	G	0.35	0/4697	0.63	1/6338 (0.0%)
4	Q	0.35	0/4697	0.63	1/6338 (0.0%)
4	R	0.35	0/4697	0.63	1/6338 (0.0%)
5	M	0.38	0/3439	0.62	2/4648 (0.0%)
5	W	0.38	0/3439	0.62	2/4648 (0.0%)
5	X	0.38	0/3439	0.62	2/4648 (0.0%)
6	S	0.44	0/1220	0.67	0/1639
6	a	0.44	0/1220	0.67	0/1639
6	b	0.44	0/1220	0.67	0/1639
All	All	0.35	0/53817	0.61	11/72780 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
4	G	0	1
4	Q	0	1
4	R	0	1
All	All	0	3

There are no bond length outliers.

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	Q	543	ARG	N-CA-C	-7.63	104.10	113.41
4	G	543	ARG	N-CA-C	-7.62	104.11	113.41
4	R	543	ARG	N-CA-C	-7.62	104.11	113.41
3	U	74	ILE	CA-C-N	5.62	128.00	120.58
3	U	74	ILE	C-N-CA	5.62	128.00	120.58

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	G	521	VAL	Peptide
4	Q	521	VAL	Peptide
4	R	521	VAL	Peptide

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	N	1165	0	1136	29	0
1	T	105	0	89	3	0
1	Y	1165	0	1136	31	0
1	Z	1165	0	1136	30	0
1	c	105	0	89	4	0
1	d	105	0	89	5	0
2	B	4513	0	4647	119	0
2	I	4513	0	4647	121	0
2	J	4513	0	4647	120	0
3	C	1330	0	1328	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	1312	0	1307	36	0
3	K	1330	0	1328	18	0
3	L	1330	0	1327	17	0
3	U	1312	0	1307	38	0
3	V	1312	0	1307	31	0
4	G	4633	0	4756	108	0
4	Q	4633	0	4756	113	0
4	R	4633	0	4756	112	0
5	M	3362	0	3373	103	0
5	W	3362	0	3373	108	0
5	X	3362	0	3373	104	0
6	S	1197	0	1229	34	0
6	a	1197	0	1229	38	0
6	b	1197	0	1229	40	0
7	C	32	0	12	5	0
7	H	32	0	12	4	0
7	K	32	0	12	4	0
7	L	32	0	12	4	0
7	U	32	0	12	4	0
7	V	32	0	12	3	0
8	C	1	0	0	0	0
8	H	1	0	0	0	0
8	K	1	0	0	0	0
8	L	1	0	0	0	0
8	U	1	0	0	0	0
8	V	1	0	0	0	0
All	All	53049	0	53666	1259	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 12.

The worst 5 of 1259 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)
5:X:324:LYS:HB2	5:X:359:HIS:HB3	1.70	0.73
5:M:324:LYS:HB2	5:M:359:HIS:HB3	1.70	0.73
3:H:25:LEU:HB3	3:H:99:ARG:HH21	1.54	0.73
5:W:324:LYS:HB2	5:W:359:HIS:HB3	1.70	0.72
5:X:302:LYS:HG3	1:Z:69:PRO:HD3	1.73	0.71

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	N	133/264 (50%)	124 (93%)	9 (7%)	0	100	100
1	T	11/264 (4%)	10 (91%)	1 (9%)	0	100	100
1	Y	133/264 (50%)	124 (93%)	9 (7%)	0	100	100
1	Z	133/264 (50%)	124 (93%)	9 (7%)	0	100	100
1	c	11/264 (4%)	10 (91%)	1 (9%)	0	100	100
1	d	11/264 (4%)	10 (91%)	1 (9%)	0	100	100
2	B	568/570 (100%)	537 (94%)	31 (6%)	0	100	100
2	I	568/570 (100%)	537 (94%)	31 (6%)	0	100	100
2	J	568/570 (100%)	537 (94%)	31 (6%)	0	100	100
3	C	163/165 (99%)	153 (94%)	10 (6%)	0	100	100
3	H	161/165 (98%)	151 (94%)	10 (6%)	0	100	100
3	K	163/165 (99%)	154 (94%)	9 (6%)	0	100	100
3	L	163/165 (99%)	153 (94%)	10 (6%)	0	100	100
3	U	161/165 (98%)	149 (92%)	12 (8%)	0	100	100
3	V	161/165 (98%)	153 (95%)	8 (5%)	0	100	100
4	G	583/585 (100%)	556 (95%)	27 (5%)	0	100	100
4	Q	583/585 (100%)	555 (95%)	28 (5%)	0	100	100
4	R	583/585 (100%)	556 (95%)	27 (5%)	0	100	100
5	M	411/422 (97%)	392 (95%)	19 (5%)	0	100	100
5	W	411/422 (97%)	393 (96%)	18 (4%)	0	100	100
5	X	411/422 (97%)	393 (96%)	18 (4%)	0	100	100
6	S	140/142 (99%)	133 (95%)	7 (5%)	0	100	100
6	a	140/142 (99%)	133 (95%)	7 (5%)	0	100	100
6	b	140/142 (99%)	133 (95%)	7 (5%)	0	100	100
All	All	6510/7731 (84%)	6170 (95%)	340 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	N	123/222 (55%)	123 (100%)	0	100	100
1	T	12/222 (5%)	12 (100%)	0	100	100
1	Y	123/222 (55%)	123 (100%)	0	100	100
1	Z	123/222 (55%)	123 (100%)	0	100	100
1	c	12/222 (5%)	12 (100%)	0	100	100
1	d	12/222 (5%)	12 (100%)	0	100	100
2	B	510/510 (100%)	510 (100%)	0	100	100
2	I	510/510 (100%)	510 (100%)	0	100	100
2	J	510/510 (100%)	510 (100%)	0	100	100
3	C	143/143 (100%)	143 (100%)	0	100	100
3	H	141/143 (99%)	141 (100%)	0	100	100
3	K	143/143 (100%)	143 (100%)	0	100	100
3	L	143/143 (100%)	143 (100%)	0	100	100
3	U	141/143 (99%)	141 (100%)	0	100	100
3	V	141/143 (99%)	141 (100%)	0	100	100
4	G	520/520 (100%)	520 (100%)	0	100	100
4	Q	520/520 (100%)	520 (100%)	0	100	100
4	R	520/520 (100%)	520 (100%)	0	100	100
5	M	377/382 (99%)	375 (100%)	2 (0%)	86	89
5	W	377/382 (99%)	375 (100%)	2 (0%)	86	89
5	X	377/382 (99%)	375 (100%)	2 (0%)	86	89
6	S	132/132 (100%)	132 (100%)	0	100	100
6	a	132/132 (100%)	132 (100%)	0	100	100
6	b	132/132 (100%)	132 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	5874/6822 (86%)	5868 (100%)	6 (0%)	92 95

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

Mol	Chain	Res	Type
5	W	392	VAL
5	X	378	VAL
5	X	392	VAL
5	M	392	VAL
5	M	378	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 121 such sidechains are listed below:

Mol	Chain	Res	Type
4	Q	184	ASN
3	V	128	GLN
3	U	152	ASN
3	V	52	ASN
5	X	308	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 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
7	GTP	C	1001	8	29,34,34	1.19	1 (3%)	35,54,54	1.23	3 (8%)
7	GTP	U	1001	8	29,34,34	1.18	1 (3%)	35,54,54	1.20	3 (8%)
7	GTP	H	1001	8	29,34,34	1.18	1 (3%)	35,54,54	1.20	3 (8%)
7	GTP	L	1001	8	29,34,34	1.18	1 (3%)	35,54,54	1.23	3 (8%)
7	GTP	V	1001	8	29,34,34	1.19	1 (3%)	35,54,54	1.20	3 (8%)
7	GTP	K	1001	8	29,34,34	1.18	1 (3%)	35,54,54	1.22	3 (8%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	GTP	C	1001	8	-	6/18/38/38	0/3/3/3
7	GTP	U	1001	8	-	6/18/38/38	0/3/3/3
7	GTP	H	1001	8	-	6/18/38/38	0/3/3/3
7	GTP	L	1001	8	-	6/18/38/38	0/3/3/3
7	GTP	V	1001	8	-	6/18/38/38	0/3/3/3
7	GTP	K	1001	8	-	6/18/38/38	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)
7	V	1001	GTP	C5-C6	-4.17	1.39	1.47
7	U	1001	GTP	C5-C6	-4.15	1.39	1.47
7	C	1001	GTP	C5-C6	-4.14	1.39	1.47
7	H	1001	GTP	C5-C6	-4.14	1.39	1.47
7	L	1001	GTP	C5-C6	-4.13	1.39	1.47

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	L	1001	GTP	C8-N7-C5	3.82	109.05	102.55
7	V	1001	GTP	C8-N7-C5	3.82	109.05	102.55
7	C	1001	GTP	C8-N7-C5	3.81	109.04	102.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	H	1001	GTP	C8-N7-C5	3.81	109.03	102.55
7	U	1001	GTP	C8-N7-C5	3.80	109.02	102.55

There are no chirality outliers.

5 of 36 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	1001	GTP	C5'-O5'-PA-O2A
7	H	1001	GTP	C5'-O5'-PA-O2A
7	K	1001	GTP	C5'-O5'-PA-O2A
7	U	1001	GTP	C5'-O5'-PA-O2A
7	L	1001	GTP	C5'-O5'-PA-O2A

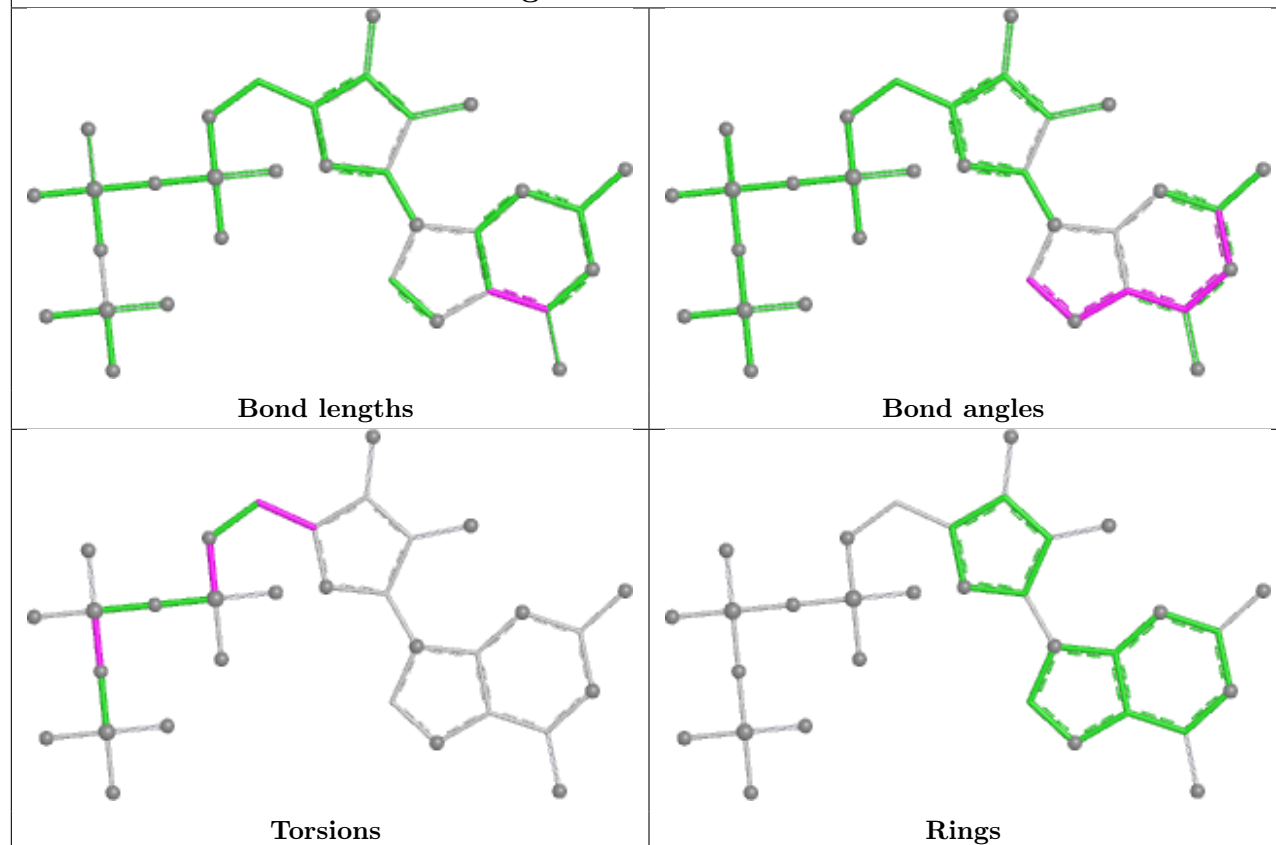
There are no ring outliers.

6 monomers are involved in 24 short contacts:

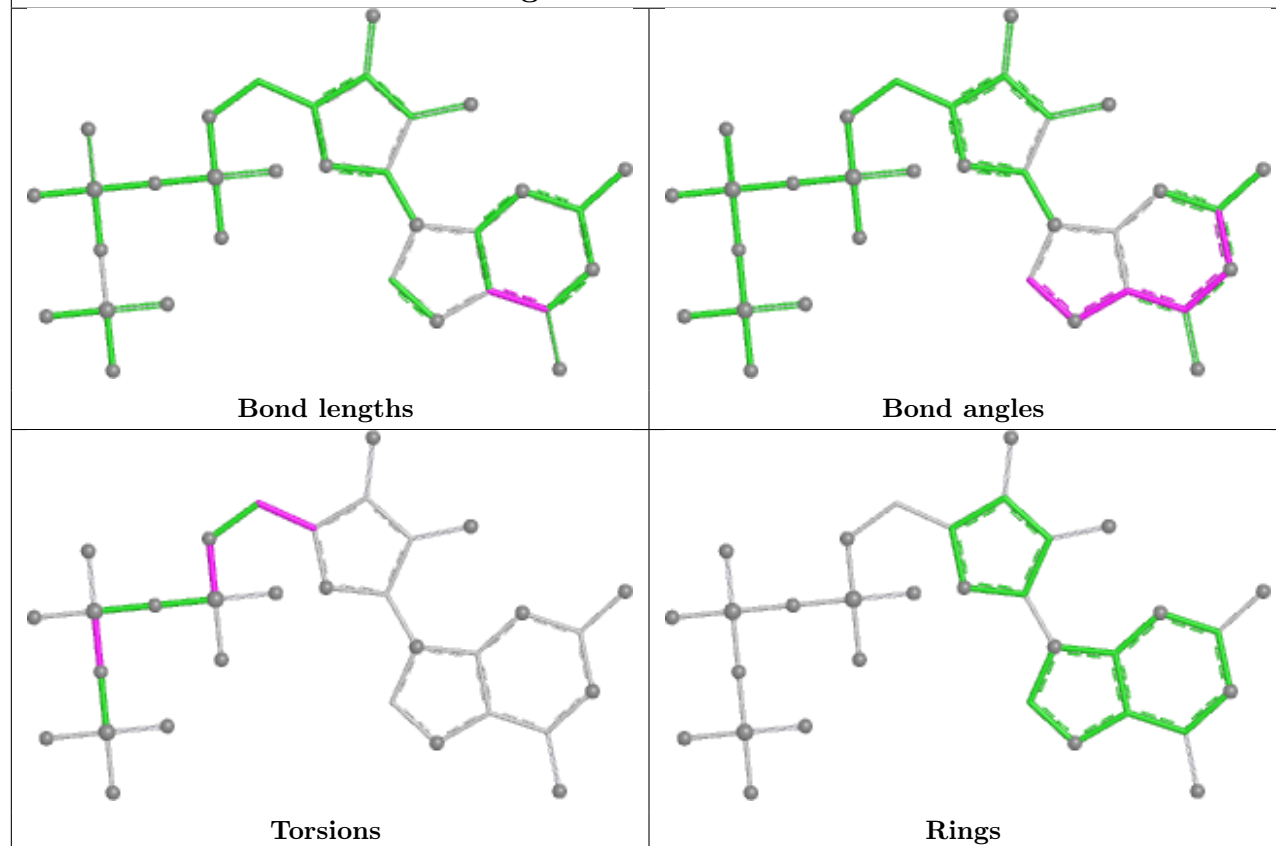
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	1001	GTP	5	0
7	U	1001	GTP	4	0
7	H	1001	GTP	4	0
7	L	1001	GTP	4	0
7	V	1001	GTP	3	0
7	K	1001	GTP	4	0

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

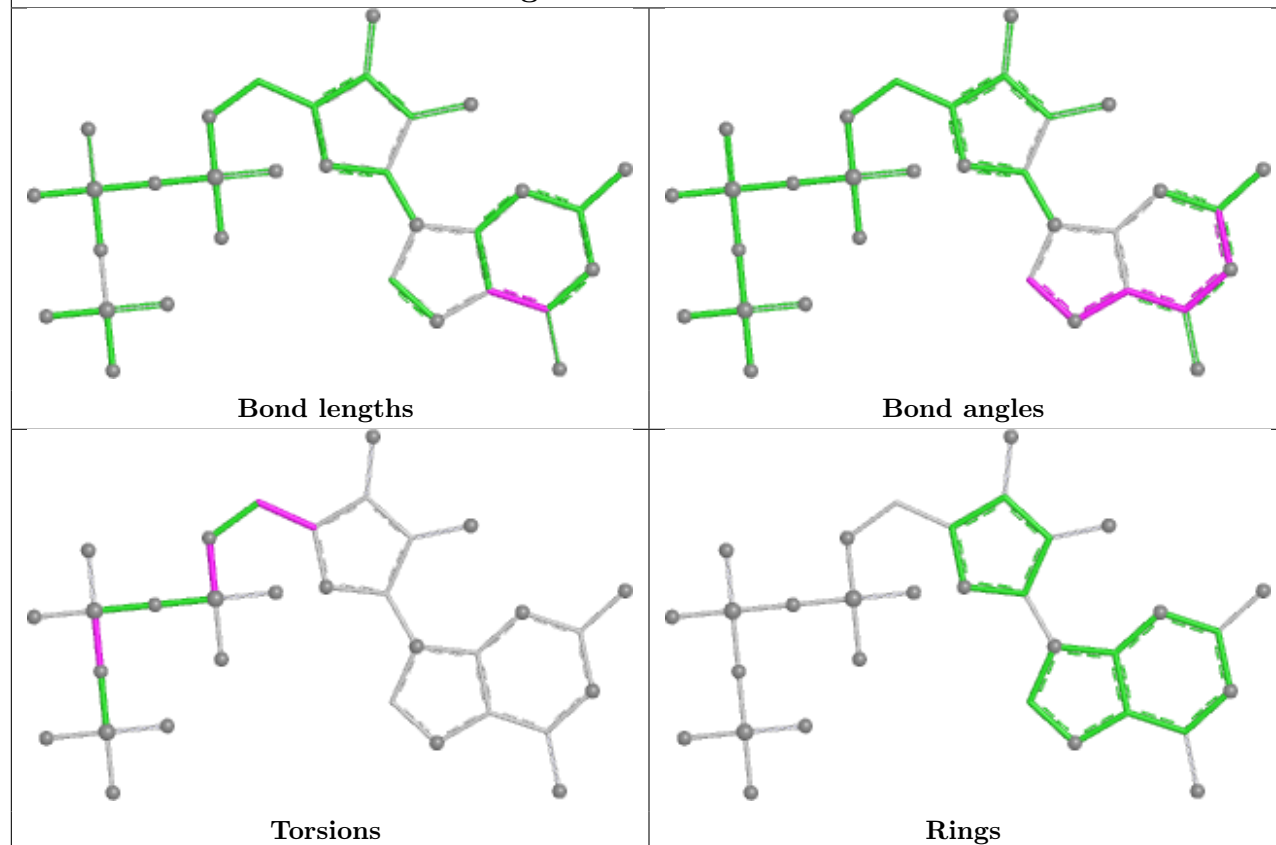
Ligand GTP C 1001



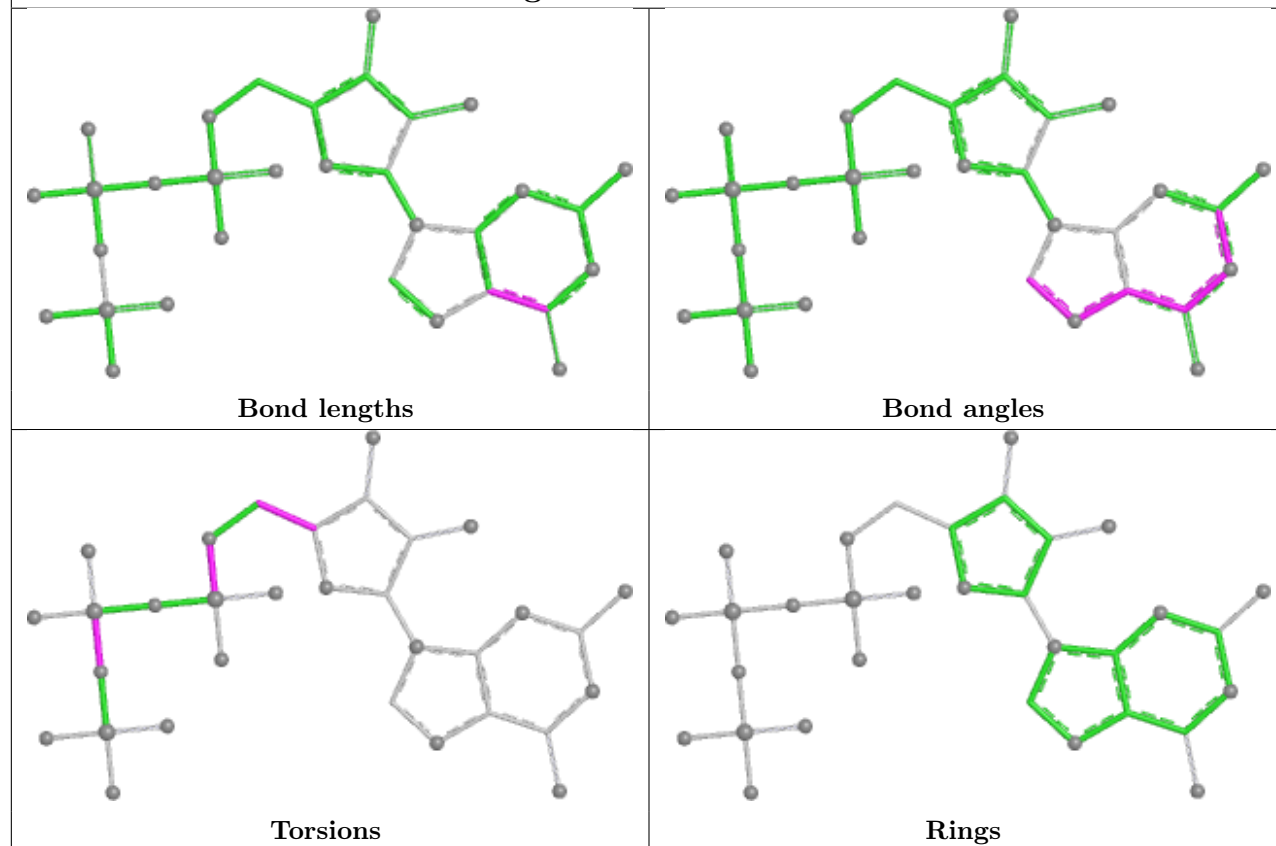
Ligand GTP U 1001



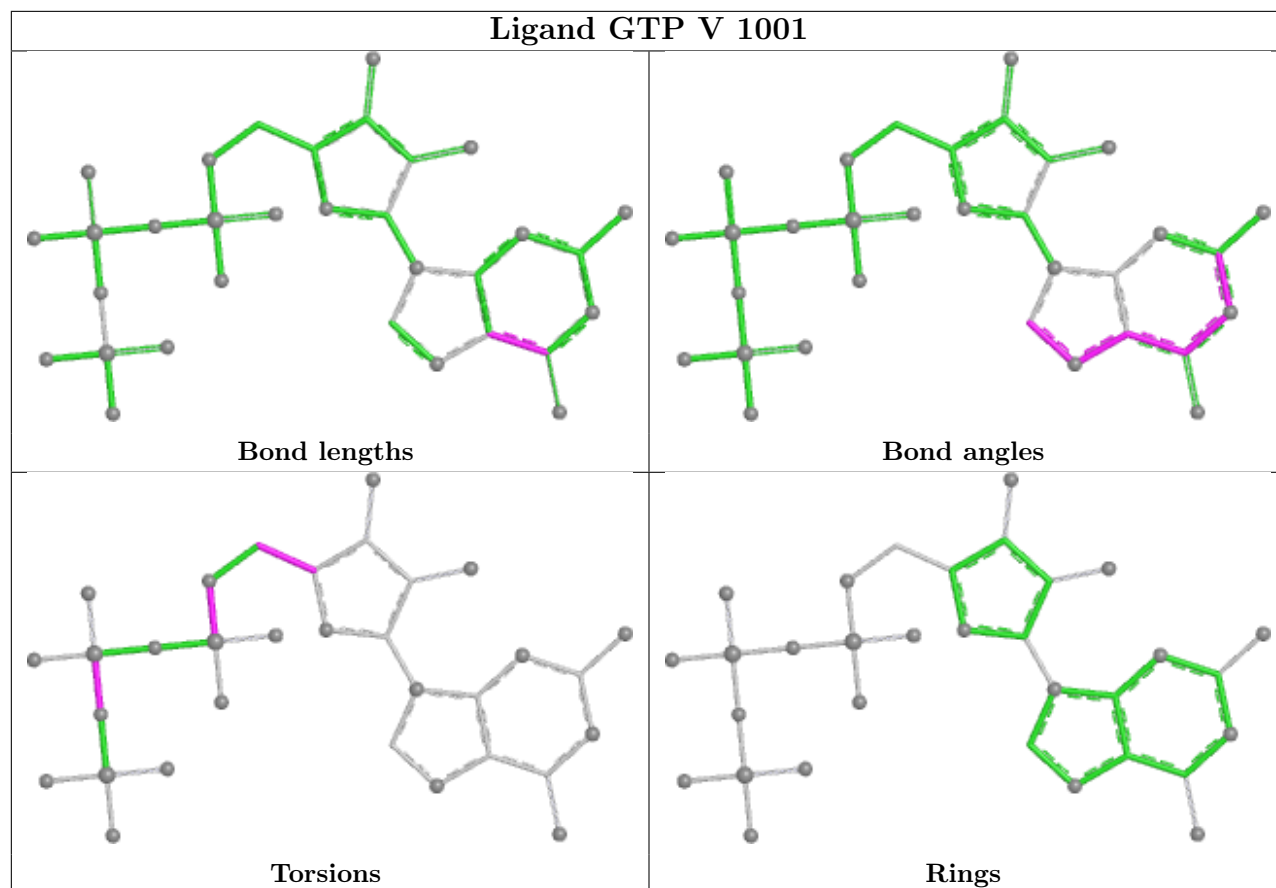
Ligand GTP H 1001



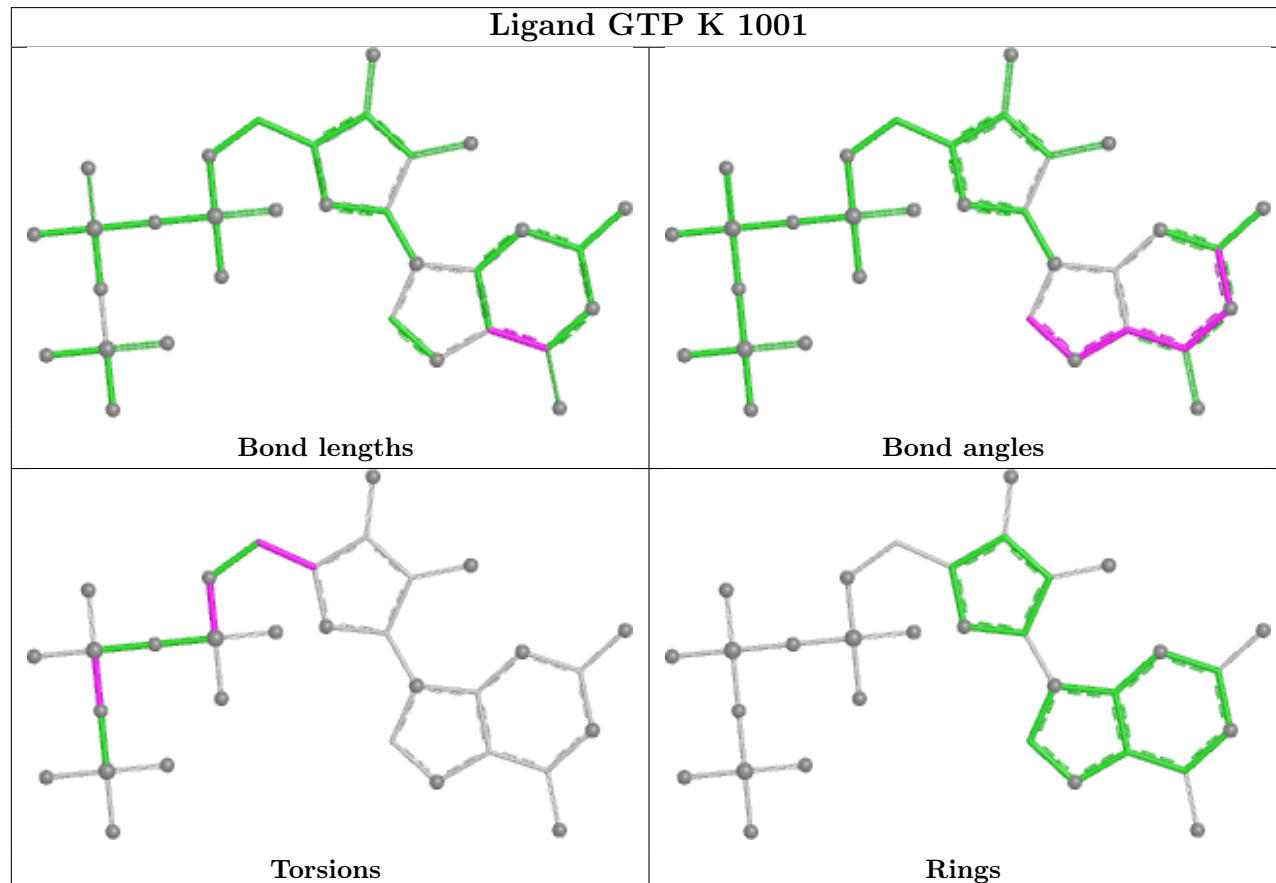
Ligand GTP L 1001



Ligand GTP V 1001



Ligand GTP K 1001



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

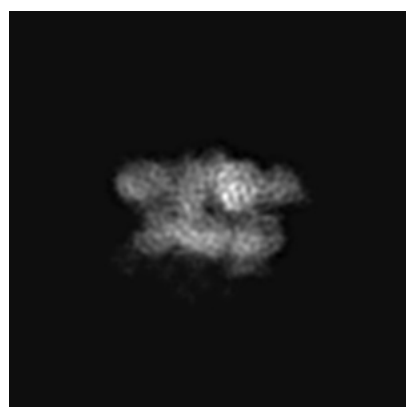
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7563. These allow visual inspection of the internal detail of the map and identification of artifacts.

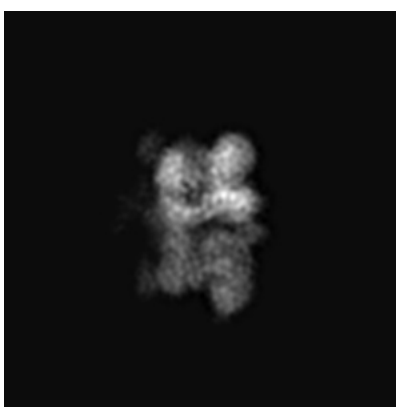
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

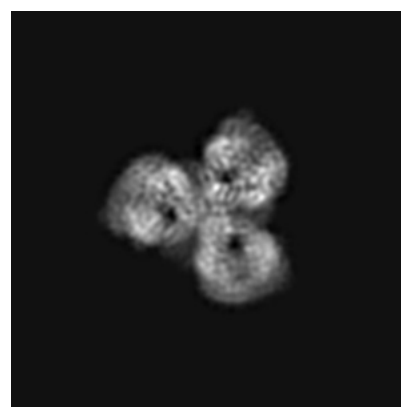
6.1.1 Primary map



X



Y

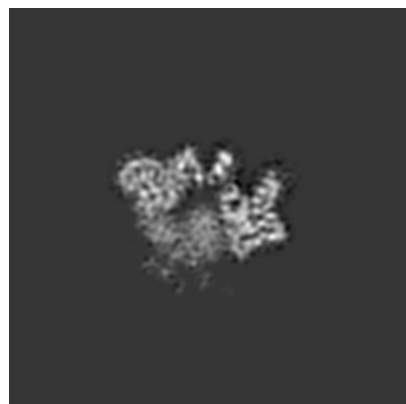


Z

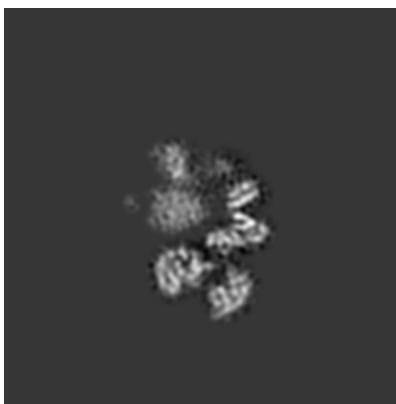
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

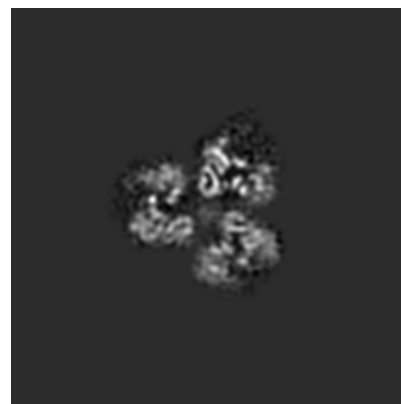
6.2.1 Primary map



X Index: 192



Y Index: 192



Z Index: 192

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: 204



Y Index: 216

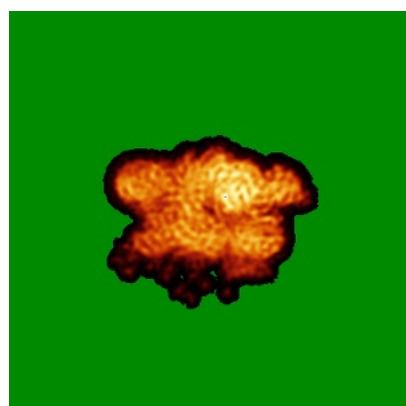


Z Index: 213

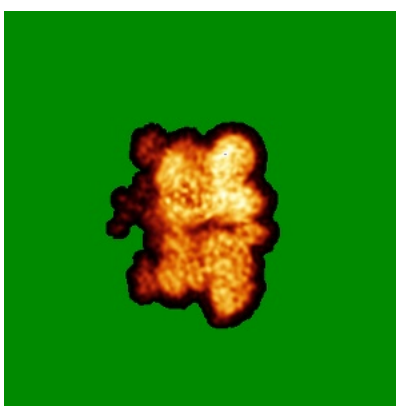
The images above show the largest variance slices of the map in three orthogonal directions.

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

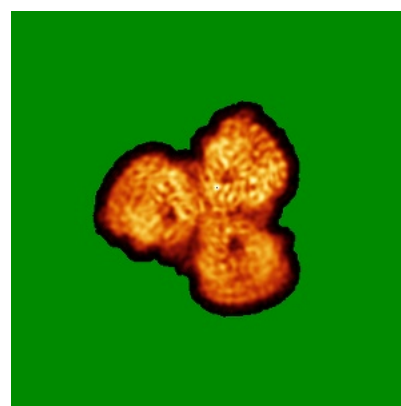
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0149. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

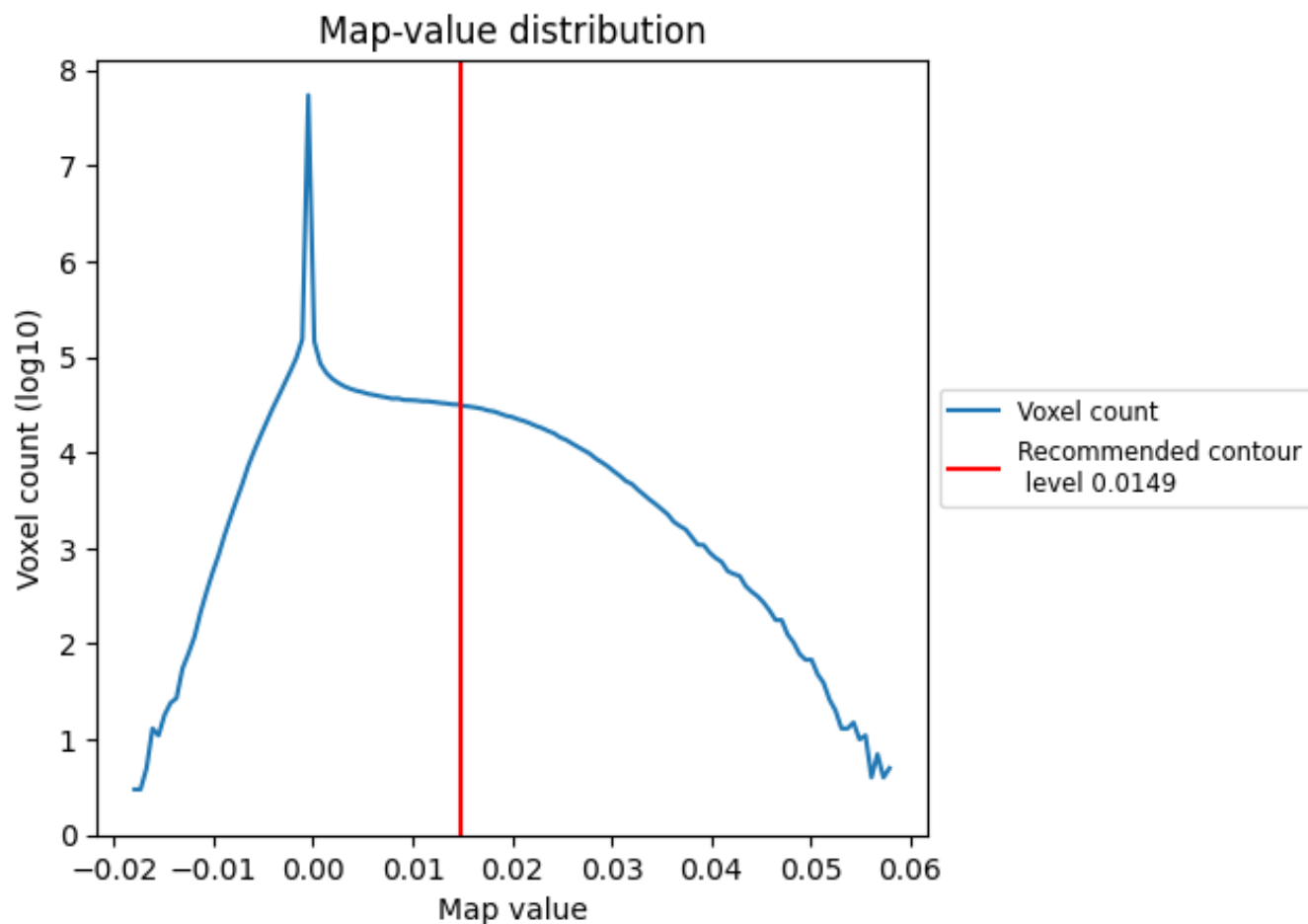
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

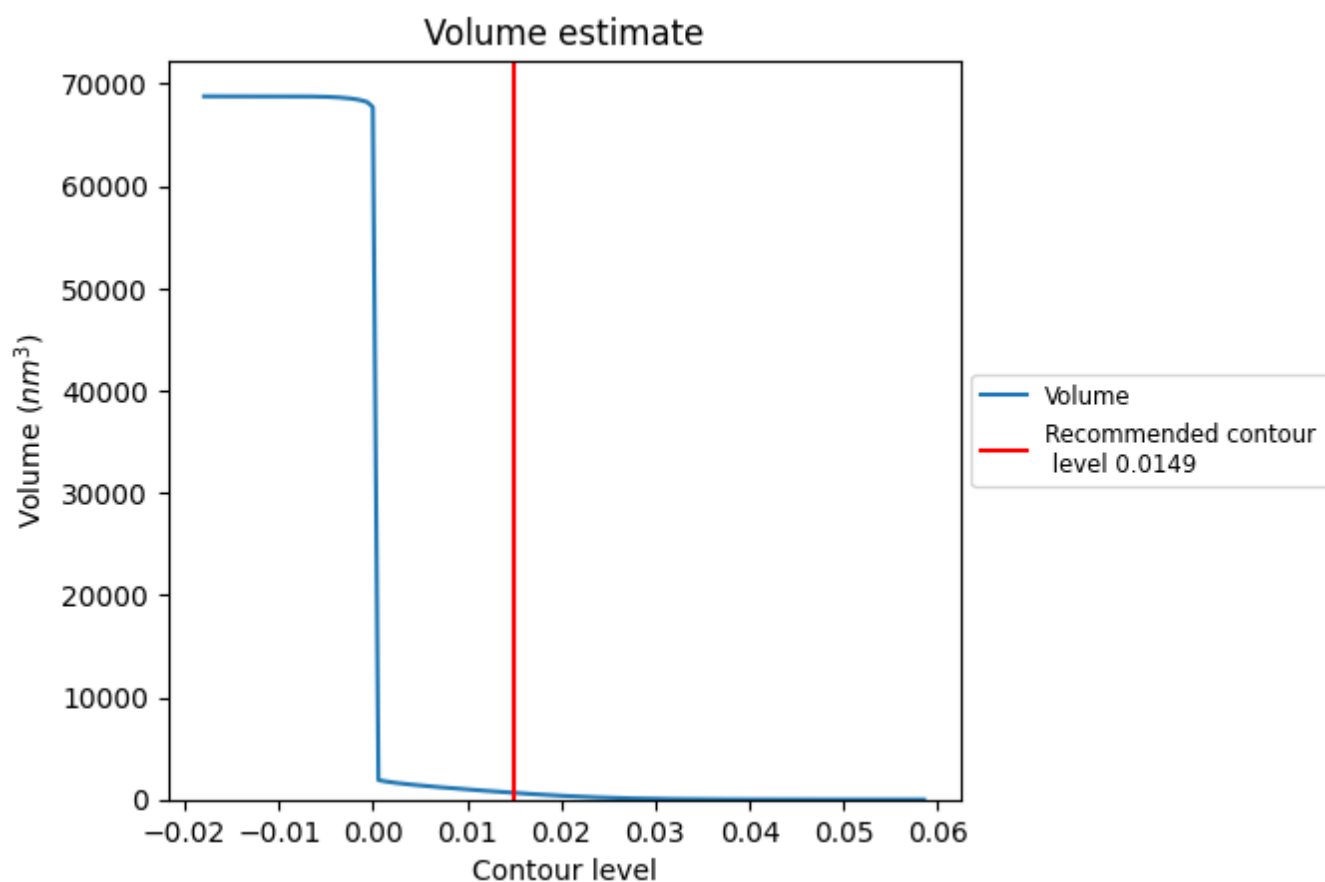
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

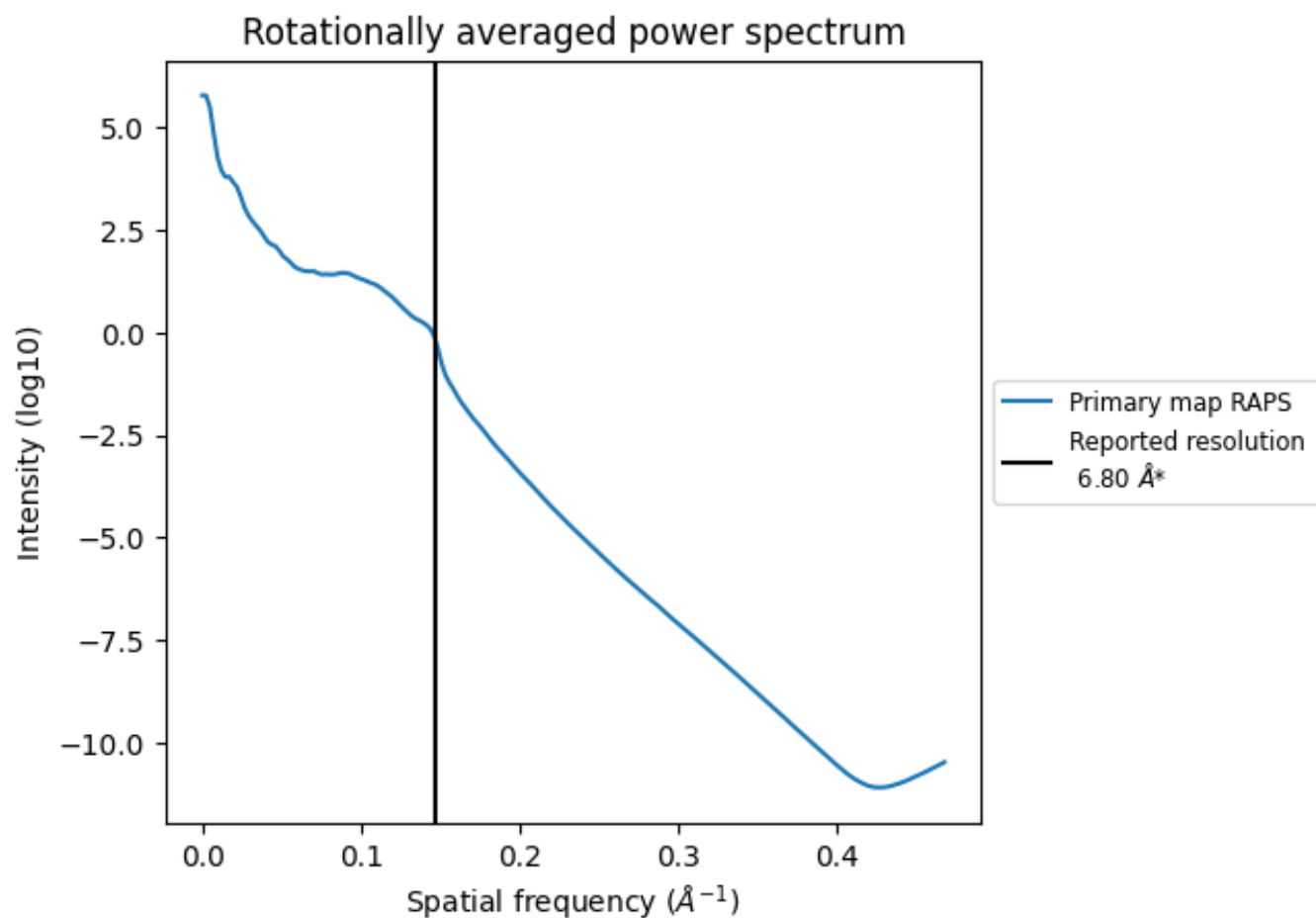
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 663 nm³; this corresponds to an approximate mass of 599 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 ⓘ

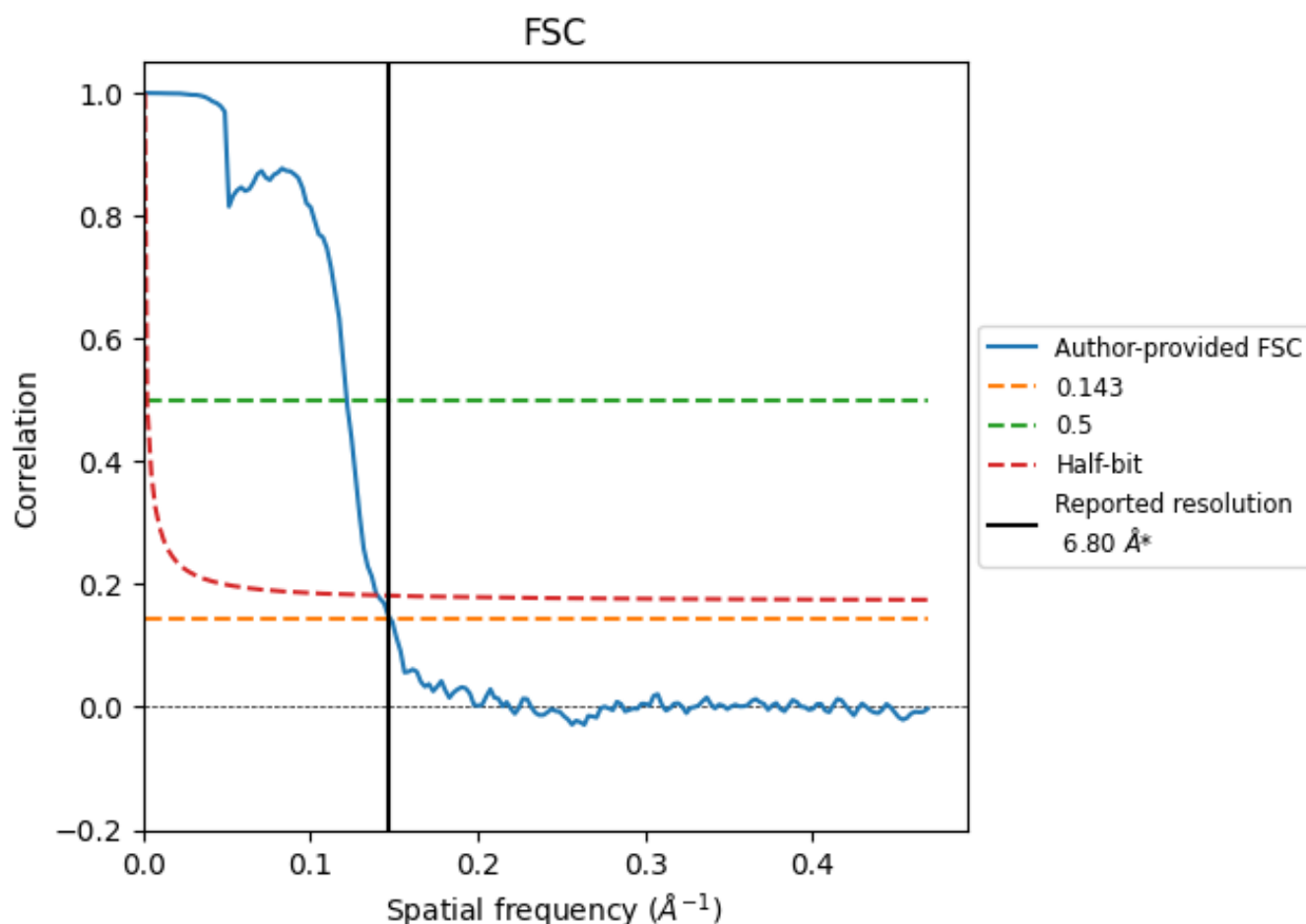


*Reported resolution corresponds to spatial frequency of 0.147 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.147 Å⁻¹

8.2 Resolution estimates [i](#)

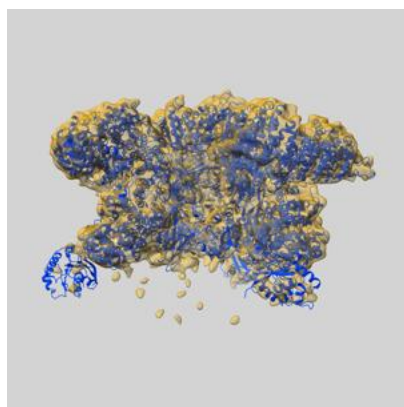
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.80	-	-
Author-provided FSC curve	6.76	8.22	7.14
Unmasked-calculated*	-	-	-

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

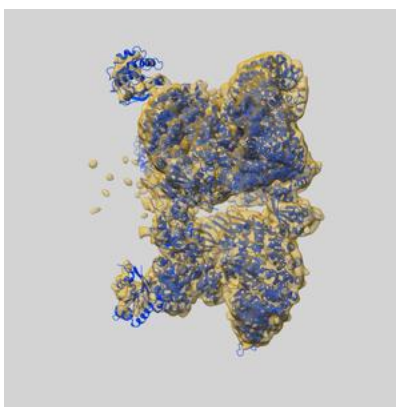
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-7563 and PDB model 6CRI. Per-residue inclusion information can be found in section [3](#) on page [13](#).

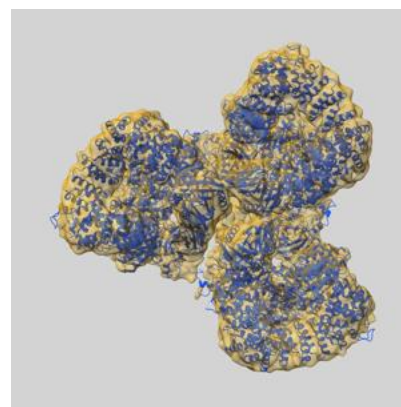
9.1 Map-model overlay [i](#)



X



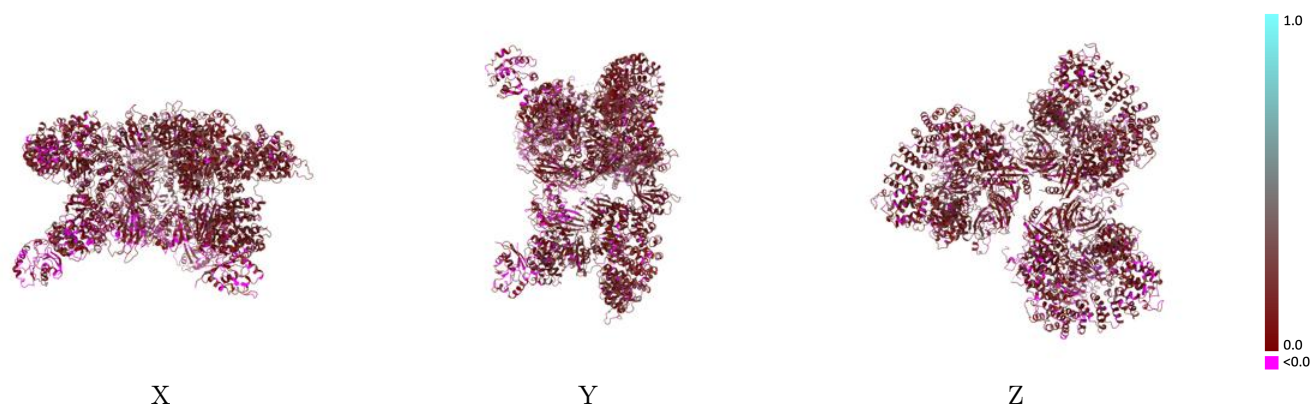
Y



Z

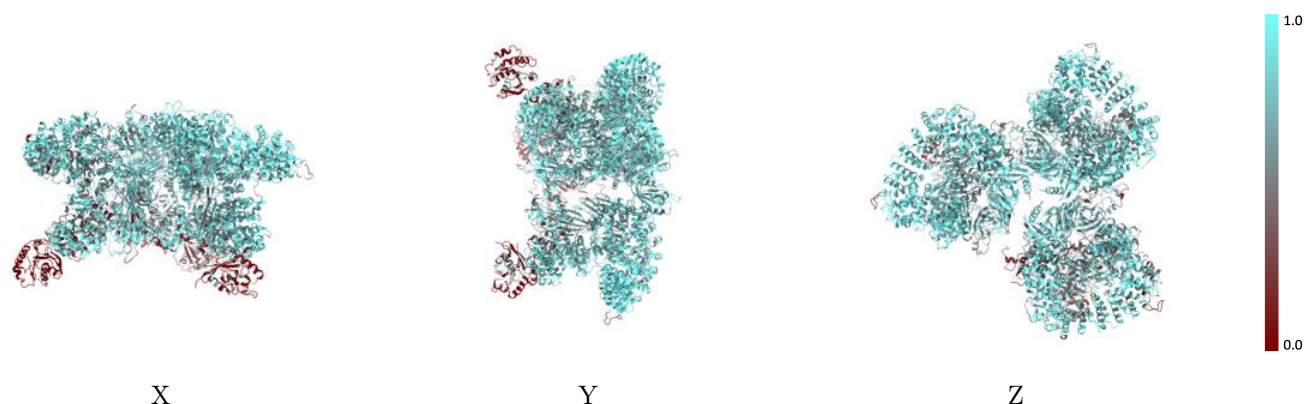
The images above show the 3D surface view of the map at the recommended contour level 0.0149 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



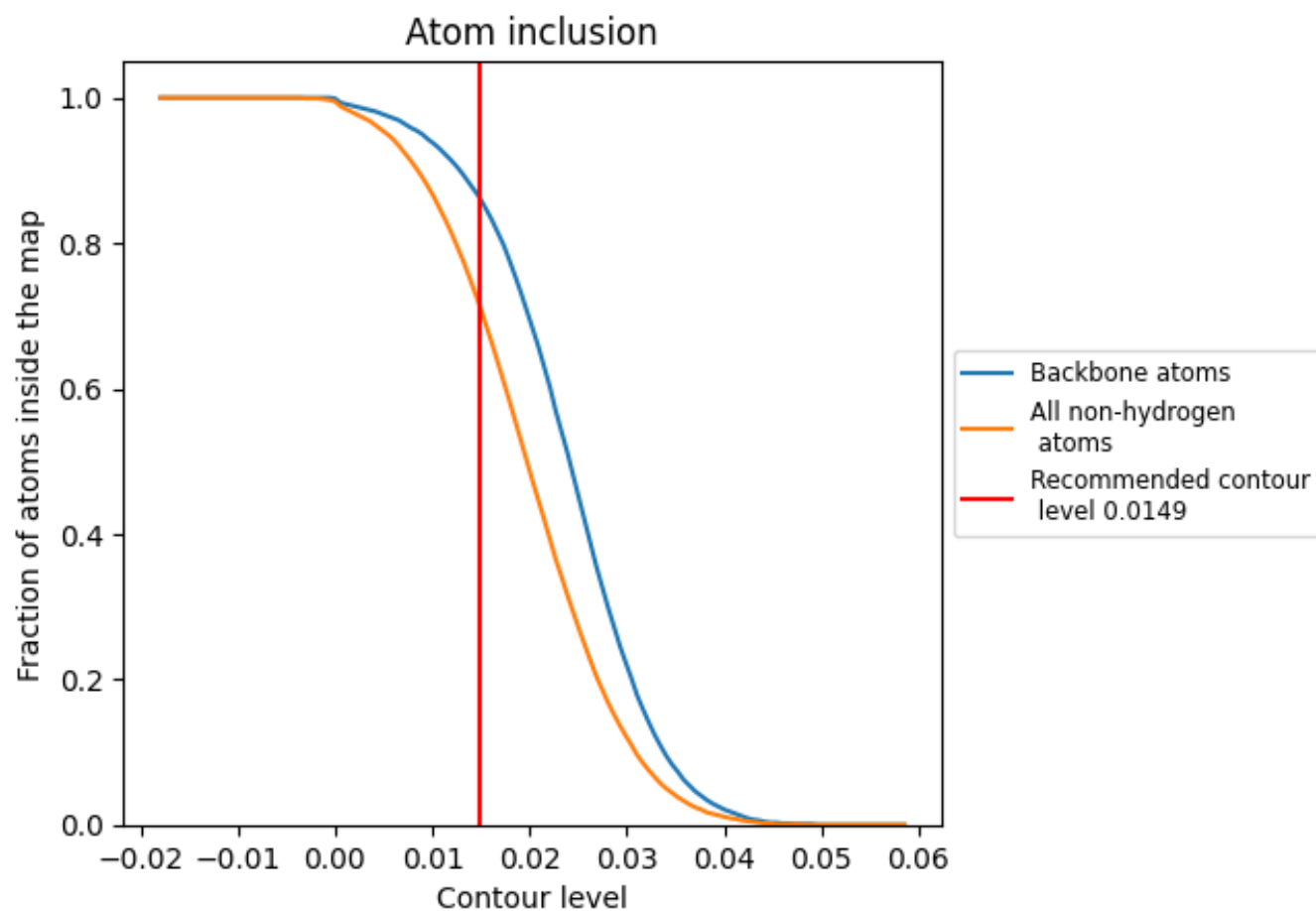
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0149).



















































9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 71% 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 (0.0149) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7130	 0.1340
B	 0.8140	 0.1450
C	 0.2720	 0.0850
G	 0.8370	 0.1550
H	 0.8260	 0.1640
I	 0.7960	 0.1630
J	 0.7140	 0.1280
K	 0.1780	 0.0740
L	 0.0340	 -0.0140
M	 0.7190	 0.1400
N	 0.3270	 0.0520
Q	 0.8330	 0.1570
R	 0.7730	 0.1310
S	 0.7930	 0.1440
T	 0.5640	 -0.0100
U	 0.8200	 0.1690
V	 0.7680	 0.1480
W	 0.7500	 0.1600
X	 0.6600	 0.1320
Y	 0.6820	 0.0840
Z	 0.6280	 0.0830
a	 0.7990	 0.1560
b	 0.7650	 0.1270
c	 0.7520	 0.1480
d	 0.5840	 0.1200

