Full wwPDB EM Validation Report

Dec 21, 2024 – 02:06 PM EST

PDB ID	:	9DC3
EMDB ID	:	EMD-46741
Title	:	AAV8 in complex with the AAVX affinity ligand
Authors	:	Mietzsch, M.; McKenna, R.
Deposited on	:	2024-08-25
Resolution	:	2.31 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (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:

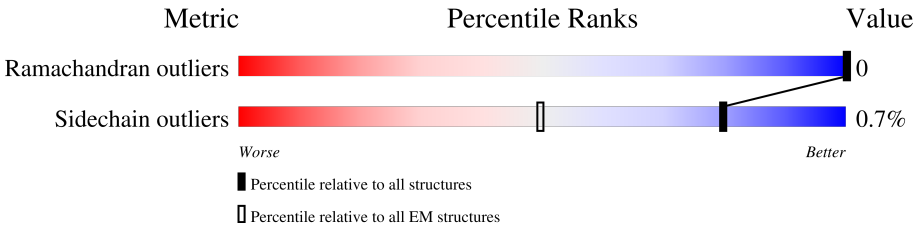
EMDB validation analysis	:	0.0.1.dev113
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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 2.31 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)
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 <=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	1	535	97%
1	2	535	97%
1	3	535	97%
1	4	535	97%
1	5	535	97%
1	6	535	97%
1	7	535	97%
1	8	535	97%
1	A	535	97%

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Mol	Chain	Length	Quality of chain
1	B	535	97%
1	C	535	97%
1	D	535	97%
1	E	535	97%
1	F	535	97%
1	G	535	97%
1	H	535	97%
1	I	535	97%
1	J	535	97%
1	K	535	97%
1	L	535	97%
1	M	535	97%
1	N	535	97%
1	O	535	97%
1	P	535	97%
1	Q	535	97%
1	R	535	97%
1	S	535	97%
1	T	535	97%
1	U	535	97%
1	V	535	97%
1	W	535	97%
1	X	535	97%
1	Y	535	97%
1	Z	535	97%

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Mol	Chain	Length	Quality of chain
1	a	535	97%
1	b	535	97%
1	c	535	97%
1	d	535	97%
1	e	535	97%
1	f	535	97%
1	g	535	97%
1	h	535	97%
1	i	535	97%
1	j	535	97%
1	k	535	97%
1	l	535	97%
1	m	535	97%
1	n	535	97%
1	o	535	97%
1	p	535	97%
1	q	535	97%
1	r	535	97%
1	s	535	97%
1	t	535	97%
1	u	535	97%
1	v	535	97%
1	w	535	97%
1	x	535	97%
1	y	535	97%

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Mol	Chain	Length	Quality of chain
1	z	535	97%
2	12	126	34% 98%
2	22	126	33% 98%
2	32	126	34% 98%
2	42	126	34% 98%
2	52	126	33% 98%
2	62	126	33% 98%
2	72	126	33% 98%
2	82	126	33% 98%
2	A2	126	33% 98%
2	B2	126	33% 98%
2	C2	126	33% 98%
2	D2	126	33% 98%
2	E2	126	34% 98%
2	F2	126	34% 98%
2	G2	126	33% 98%
2	H2	126	33% 98%
2	I2	126	33% 98%
2	J2	126	33% 98%
2	K2	126	33% 98%
2	L2	126	33% 98%
2	M2	126	33% 98%
2	N2	126	33% 98%
2	O2	126	33% 98%
2	P2	126	33% 98%

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Mol	Chain	Length	Quality of chain
2	Q2	126	34% 98%
2	R2	126	33% 98%
2	S2	126	33% 98%
2	T2	126	33% 98%
2	U2	126	33% 98%
2	V2	126	33% 98%
2	W2	126	34% 98%
2	X2	126	33% 98%
2	Y2	126	33% 98%
2	Z2	126	34% 98%
2	a2	126	33% 98%
2	b2	126	33% 98%
2	c2	126	34% 98%
2	d2	126	33% 98%
2	e2	126	33% 98%
2	f2	126	33% 98%
2	g2	126	33% 98%
2	h2	126	33% 98%
2	i2	126	34% 98%
2	j2	126	34% 98%
2	k2	126	34% 98%
2	l2	126	33% 98%
2	m2	126	33% 98%
2	n2	126	34% 98%
2	o2	126	34% 98%

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Mol	Chain	Length	Quality of chain
2	p2	126	34% 98%
2	q2	126	33% 98%
2	r2	126	33% 98%
2	s2	126	33% 98%
2	t2	126	33% 98%
2	u2	126	33% 98%
2	v2	126	32% 98%
2	w2	126	33% 98%
2	x2	126	33% 98%
2	y2	126	33% 98%
2	z2	126	33% 98%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 305280 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 Capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	520	Total	C	N	O	S	0	0
			4141	2612	717	799	13		
1	B	520	Total	C	N	O	S	0	0
			4141	2612	717	799	13		
1	C	520	Total	C	N	O	S	0	0
			4141	2612	717	799	13		
1	D	520	Total	C	N	O	S	0	0
			4141	2612	717	799	13		
1	E	520	Total	C	N	O	S	0	0
			4141	2612	717	799	13		
1	F	520	Total	C	N	O	S	0	0
			4141	2612	717	799	13		
1	G	520	Total	C	N	O	S	0	0
			4141	2612	717	799	13		
1	H	520	Total	C	N	O	S	0	0
			4141	2612	717	799	13		
1	I	520	Total	C	N	O	S	0	0
			4141	2612	717	799	13		
1	J	520	Total	C	N	O	S	0	0
			4141	2612	717	799	13		
1	K	520	Total	C	N	O	S	0	0
			4141	2612	717	799	13		
1	L	520	Total	C	N	O	S	0	0
			4141	2612	717	799	13		
1	M	520	Total	C	N	O	S	0	0
			4141	2612	717	799	13		
1	N	520	Total	C	N	O	S	0	0
			4141	2612	717	799	13		
1	O	520	Total	C	N	O	S	0	0
			4141	2612	717	799	13		
1	P	520	Total	C	N	O	S	0	0
			4141	2612	717	799	13		
1	Q	520	Total	C	N	O	S	0	0
			4141	2612	717	799	13		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	520	Total	C	N	O	S	0	0
			4141	2612	717	799	13		
1	S	520	Total	C	N	O	S	0	0
			4141	2612	717	799	13		
1	T	520	Total	C	N	O	S	0	0
			4141	2612	717	799	13		
1	U	520	Total	C	N	O	S	0	0
			4141	2612	717	799	13		
1	V	520	Total	C	N	O	S	0	0
			4141	2612	717	799	13		
1	W	520	Total	C	N	O	S	0	0
			4141	2612	717	799	13		
1	X	520	Total	C	N	O	S	0	0
			4141	2612	717	799	13		
1	Y	520	Total	C	N	O	S	0	0
			4141	2612	717	799	13		
1	Z	520	Total	C	N	O	S	0	0
			4141	2612	717	799	13		
1	a	520	Total	C	N	O	S	0	0
			4141	2612	717	799	13		
1	b	520	Total	C	N	O	S	0	0
			4141	2612	717	799	13		
1	c	520	Total	C	N	O	S	0	0
			4141	2612	717	799	13		
1	d	520	Total	C	N	O	S	0	0
			4141	2612	717	799	13		
1	e	520	Total	C	N	O	S	0	0
			4141	2612	717	799	13		
1	f	520	Total	C	N	O	S	0	0
			4141	2612	717	799	13		
1	g	520	Total	C	N	O	S	0	0
			4141	2612	717	799	13		
1	h	520	Total	C	N	O	S	0	0
			4141	2612	717	799	13		
1	i	520	Total	C	N	O	S	0	0
			4141	2612	717	799	13		
1	j	520	Total	C	N	O	S	0	0
			4141	2612	717	799	13		
1	k	520	Total	C	N	O	S	0	0
			4141	2612	717	799	13		
1	l	520	Total	C	N	O	S	0	0
			4141	2612	717	799	13		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	m	520	Total	C	N	O	S	0	0
			4141	2612	717	799	13		
1	n	520	Total	C	N	O	S	0	0
			4141	2612	717	799	13		
1	o	520	Total	C	N	O	S	0	0
			4141	2612	717	799	13		
1	p	520	Total	C	N	O	S	0	0
			4141	2612	717	799	13		
1	q	520	Total	C	N	O	S	0	0
			4141	2612	717	799	13		
1	r	520	Total	C	N	O	S	0	0
			4141	2612	717	799	13		
1	s	520	Total	C	N	O	S	0	0
			4141	2612	717	799	13		
1	t	520	Total	C	N	O	S	0	0
			4141	2612	717	799	13		
1	u	520	Total	C	N	O	S	0	0
			4141	2612	717	799	13		
1	v	520	Total	C	N	O	S	0	0
			4141	2612	717	799	13		
1	w	520	Total	C	N	O	S	0	0
			4141	2612	717	799	13		
1	x	520	Total	C	N	O	S	0	0
			4141	2612	717	799	13		
1	y	520	Total	C	N	O	S	0	0
			4141	2612	717	799	13		
1	z	520	Total	C	N	O	S	0	0
			4141	2612	717	799	13		
1	1	520	Total	C	N	O	S	0	0
			4141	2612	717	799	13		
1	2	520	Total	C	N	O	S	0	0
			4141	2612	717	799	13		
1	3	520	Total	C	N	O	S	0	0
			4141	2612	717	799	13		
1	4	520	Total	C	N	O	S	0	0
			4141	2612	717	799	13		
1	5	520	Total	C	N	O	S	0	0
			4141	2612	717	799	13		
1	6	520	Total	C	N	O	S	0	0
			4141	2612	717	799	13		
1	7	520	Total	C	N	O	S	0	0
			4141	2612	717	799	13		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	8	520	Total	C	N	O	S	0	0
			4141	2612	717	799	13		

- Molecule 2 is a protein called AAVX affinity ligand.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A2	125	Total	C	N	O	S	0	0
			947	583	170	188	6		
2	B2	125	Total	C	N	O	S	0	0
			947	583	170	188	6		
2	C2	125	Total	C	N	O	S	0	0
			947	583	170	188	6		
2	D2	125	Total	C	N	O	S	0	0
			947	583	170	188	6		
2	E2	125	Total	C	N	O	S	0	0
			947	583	170	188	6		
2	F2	125	Total	C	N	O	S	0	0
			947	583	170	188	6		
2	G2	125	Total	C	N	O	S	0	0
			947	583	170	188	6		
2	H2	125	Total	C	N	O	S	0	0
			947	583	170	188	6		
2	I2	125	Total	C	N	O	S	0	0
			947	583	170	188	6		
2	J2	125	Total	C	N	O	S	0	0
			947	583	170	188	6		
2	K2	125	Total	C	N	O	S	0	0
			947	583	170	188	6		
2	L2	125	Total	C	N	O	S	0	0
			947	583	170	188	6		
2	M2	125	Total	C	N	O	S	0	0
			947	583	170	188	6		
2	N2	125	Total	C	N	O	S	0	0
			947	583	170	188	6		
2	O2	125	Total	C	N	O	S	0	0
			947	583	170	188	6		
2	P2	125	Total	C	N	O	S	0	0
			947	583	170	188	6		
2	Q2	125	Total	C	N	O	S	0	0
			947	583	170	188	6		
2	R2	125	Total	C	N	O	S	0	0
			947	583	170	188	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	S2	125	Total	C	N	O	S	0	0
			947	583	170	188	6		
2	T2	125	Total	C	N	O	S	0	0
			947	583	170	188	6		
2	U2	125	Total	C	N	O	S	0	0
			947	583	170	188	6		
2	V2	125	Total	C	N	O	S	0	0
			947	583	170	188	6		
2	W2	125	Total	C	N	O	S	0	0
			947	583	170	188	6		
2	X2	125	Total	C	N	O	S	0	0
			947	583	170	188	6		
2	Y2	125	Total	C	N	O	S	0	0
			947	583	170	188	6		
2	Z2	125	Total	C	N	O	S	0	0
			947	583	170	188	6		
2	a2	125	Total	C	N	O	S	0	0
			947	583	170	188	6		
2	b2	125	Total	C	N	O	S	0	0
			947	583	170	188	6		
2	c2	125	Total	C	N	O	S	0	0
			947	583	170	188	6		
2	d2	125	Total	C	N	O	S	0	0
			947	583	170	188	6		
2	e2	125	Total	C	N	O	S	0	0
			947	583	170	188	6		
2	f2	125	Total	C	N	O	S	0	0
			947	583	170	188	6		
2	g2	125	Total	C	N	O	S	0	0
			947	583	170	188	6		
2	h2	125	Total	C	N	O	S	0	0
			947	583	170	188	6		
2	i2	125	Total	C	N	O	S	0	0
			947	583	170	188	6		
2	j2	125	Total	C	N	O	S	0	0
			947	583	170	188	6		
2	k2	125	Total	C	N	O	S	0	0
			947	583	170	188	6		
2	l2	125	Total	C	N	O	S	0	0
			947	583	170	188	6		
2	m2	125	Total	C	N	O	S	0	0
			947	583	170	188	6		

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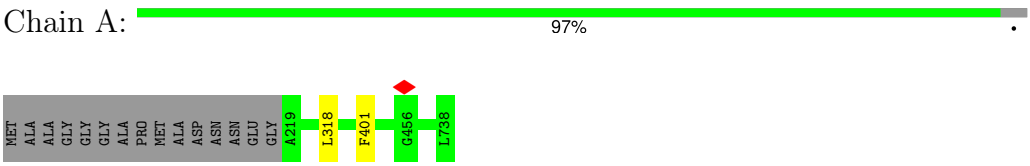
Mol	Chain	Residues	Atoms					AltConf	Trace
2	n2	125	Total	C	N	O	S	0	0
			947	583	170	188	6		
2	o2	125	Total	C	N	O	S	0	0
			947	583	170	188	6		
2	p2	125	Total	C	N	O	S	0	0
			947	583	170	188	6		
2	q2	125	Total	C	N	O	S	0	0
			947	583	170	188	6		
2	r2	125	Total	C	N	O	S	0	0
			947	583	170	188	6		
2	s2	125	Total	C	N	O	S	0	0
			947	583	170	188	6		
2	t2	125	Total	C	N	O	S	0	0
			947	583	170	188	6		
2	u2	125	Total	C	N	O	S	0	0
			947	583	170	188	6		
2	v2	125	Total	C	N	O	S	0	0
			947	583	170	188	6		
2	w2	125	Total	C	N	O	S	0	0
			947	583	170	188	6		
2	x2	125	Total	C	N	O	S	0	0
			947	583	170	188	6		
2	y2	125	Total	C	N	O	S	0	0
			947	583	170	188	6		
2	z2	125	Total	C	N	O	S	0	0
			947	583	170	188	6		
2	12	125	Total	C	N	O	S	0	0
			947	583	170	188	6		
2	22	125	Total	C	N	O	S	0	0
			947	583	170	188	6		
2	32	125	Total	C	N	O	S	0	0
			947	583	170	188	6		
2	42	125	Total	C	N	O	S	0	0
			947	583	170	188	6		
2	52	125	Total	C	N	O	S	0	0
			947	583	170	188	6		
2	62	125	Total	C	N	O	S	0	0
			947	583	170	188	6		
2	72	125	Total	C	N	O	S	0	0
			947	583	170	188	6		
2	82	125	Total	C	N	O	S	0	0
			947	583	170	188	6		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

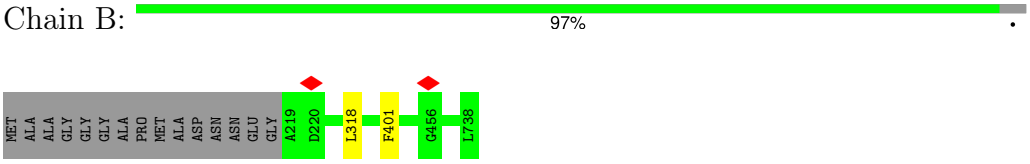
• Molecule 1: Capsid protein

Chain A:



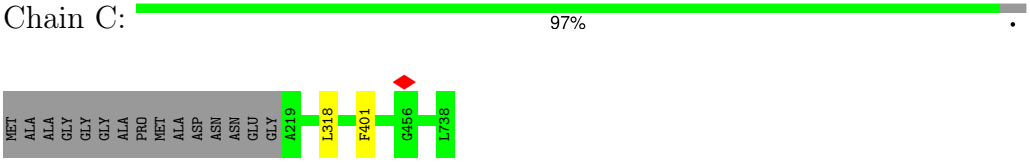
• Molecule 1: Capsid protein

Chain B:



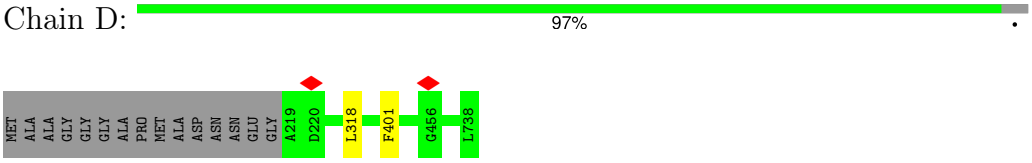
• Molecule 1: Capsid protein

Chain C:



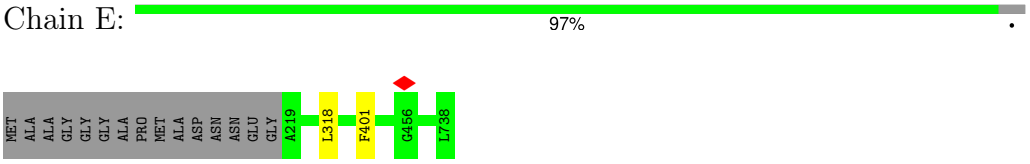
• Molecule 1: Capsid protein

Chain D:



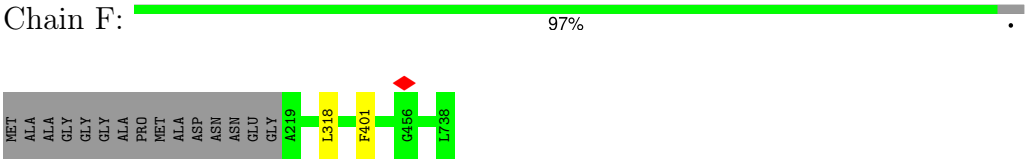
• Molecule 1: Capsid protein

Chain E:



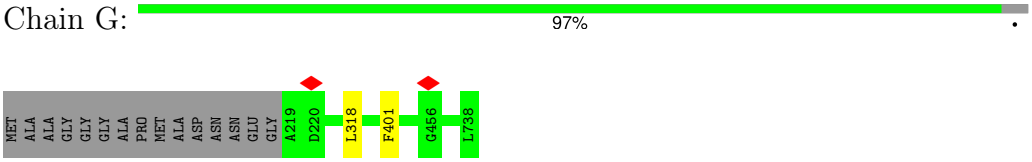
• Molecule 1: Capsid protein

Chain F:



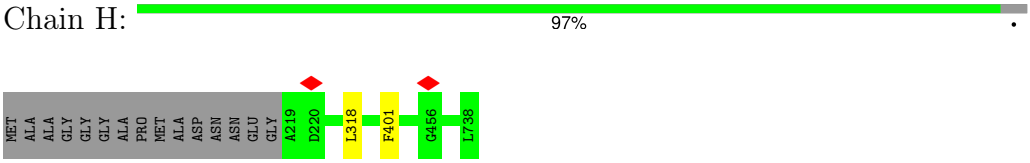
• Molecule 1: Capsid protein

Chain G:



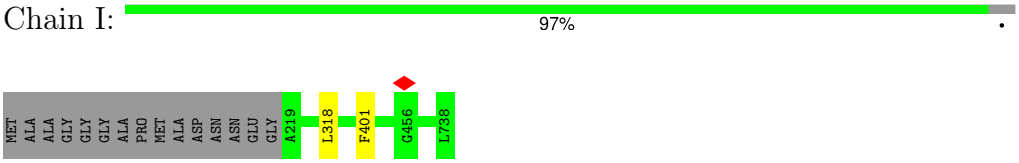
• Molecule 1: Capsid protein

Chain H:



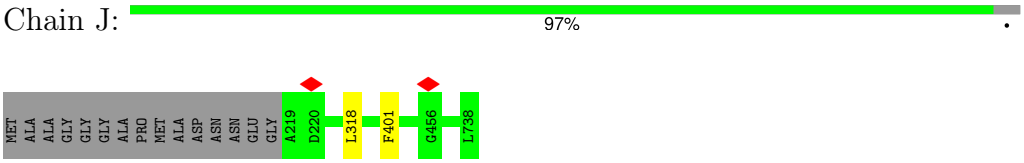
• Molecule 1: Capsid protein

Chain I:



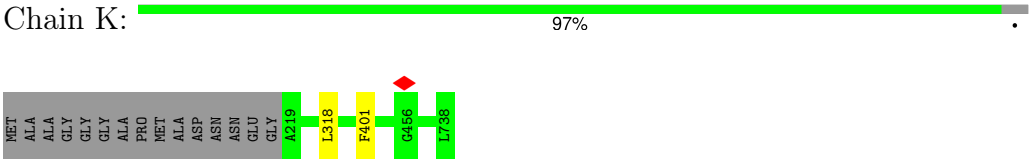
• Molecule 1: Capsid protein

Chain J:



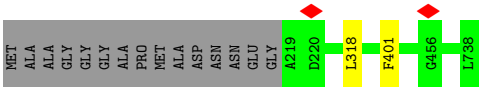
• Molecule 1: Capsid protein

Chain K:



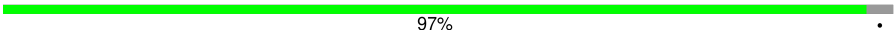
• Molecule 1: Capsid protein

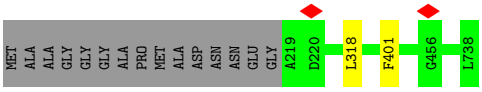
Chain L:



• Molecule 1: Capsid protein

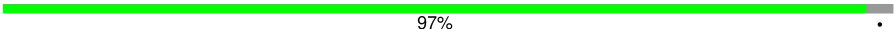
Chain M:

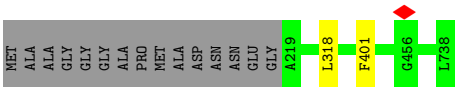




• Molecule 1: Capsid protein

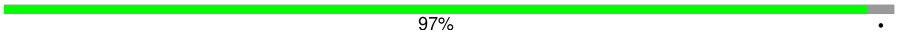
Chain N:

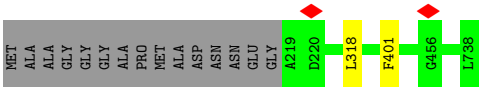




• Molecule 1: Capsid protein

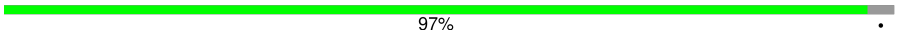
Chain O:

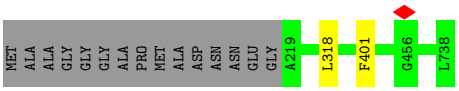




• Molecule 1: Capsid protein

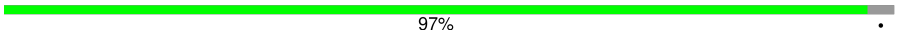
Chain P:

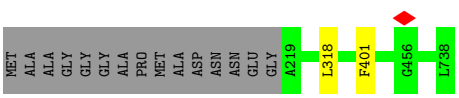




• Molecule 1: Capsid protein

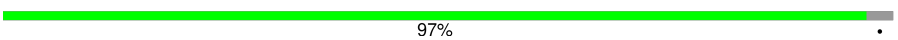
Chain Q:

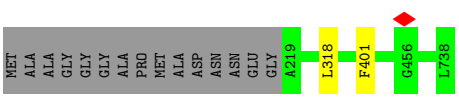




• Molecule 1: Capsid protein

Chain R:



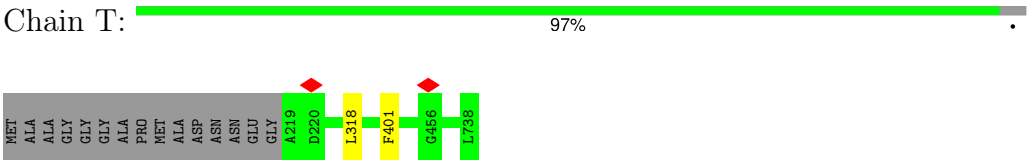


• Molecule 1: Capsid protein

Chain S:

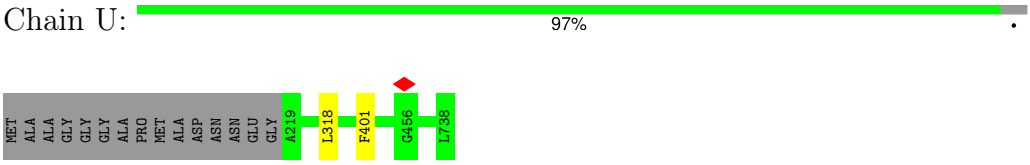
• Molecule 1: Capsid protein

Chain T:



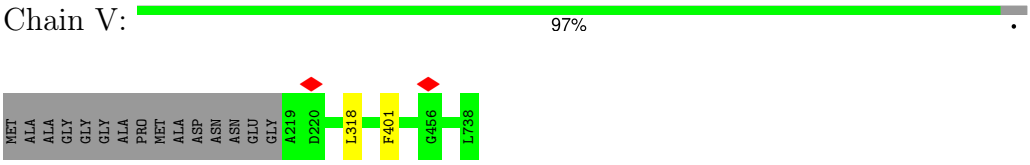
• Molecule 1: Capsid protein

Chain U:



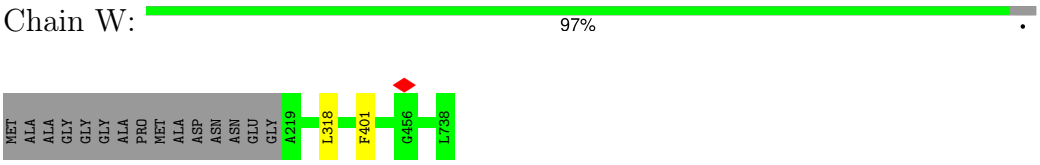
• Molecule 1: Capsid protein

Chain V:



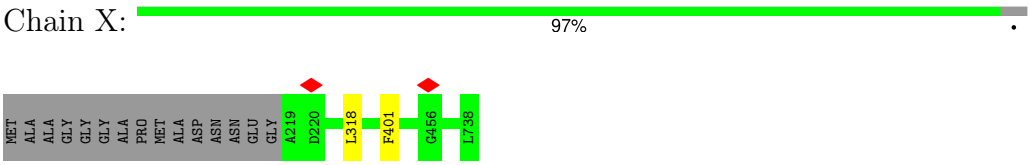
• Molecule 1: Capsid protein

Chain W:



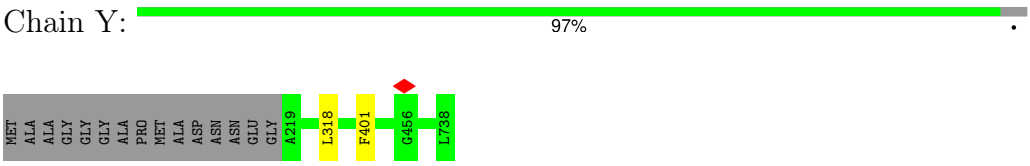
• Molecule 1: Capsid protein

Chain X:



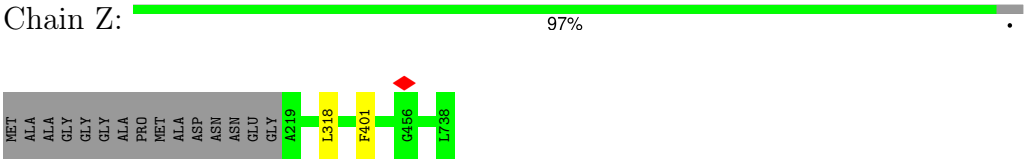
• Molecule 1: Capsid protein

Chain Y:



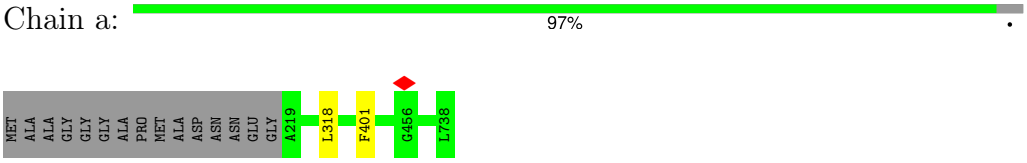
• Molecule 1: Capsid protein

Chain Z:



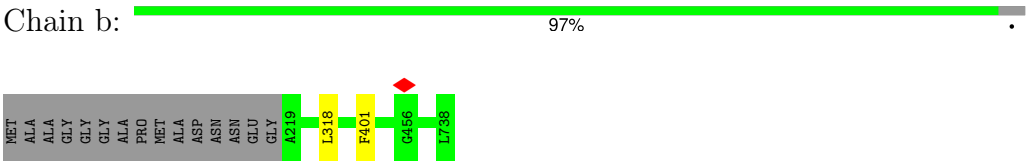
• Molecule 1: Capsid protein

Chain a:



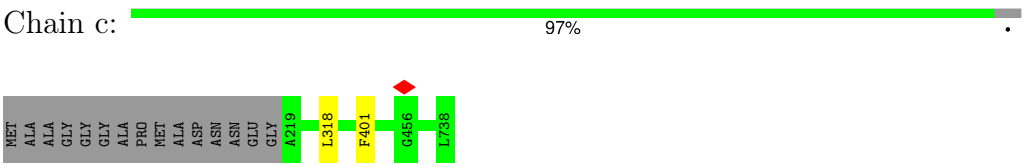
• Molecule 1: Capsid protein

Chain b:



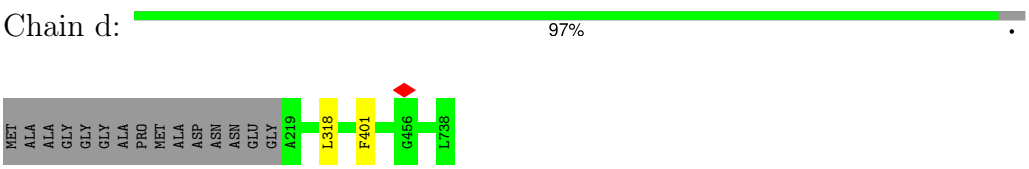
• Molecule 1: Capsid protein

Chain c:



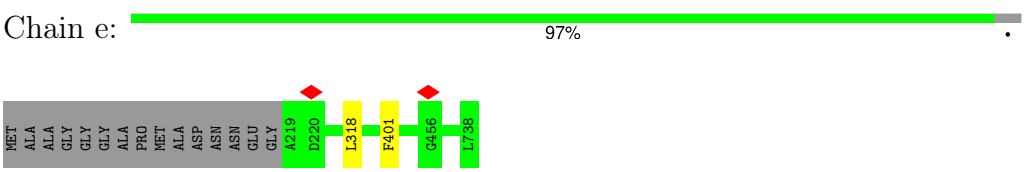
• Molecule 1: Capsid protein

Chain d:



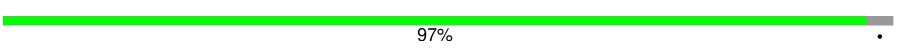
• Molecule 1: Capsid protein

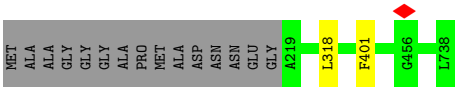
Chain e:



• Molecule 1: Capsid protein

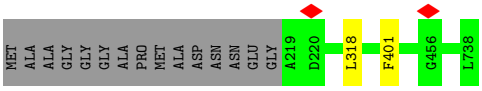
Chain f:





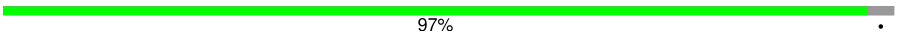
• Molecule 1: Capsid protein

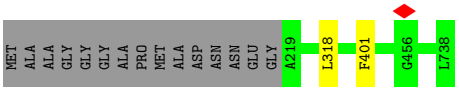
Chain g:



• Molecule 1: Capsid protein

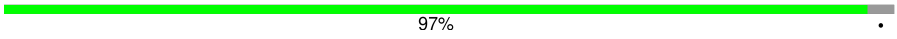
Chain h:

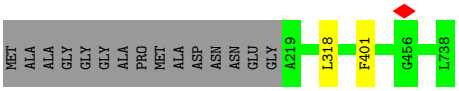




• Molecule 1: Capsid protein

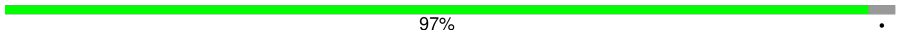
Chain i:

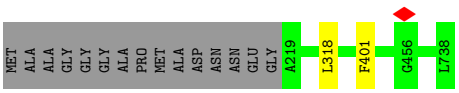




• Molecule 1: Capsid protein

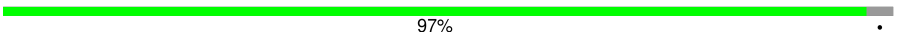
Chain j:

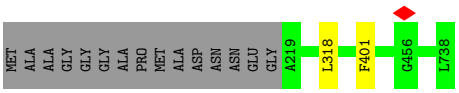




• Molecule 1: Capsid protein

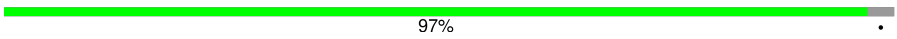
Chain k:

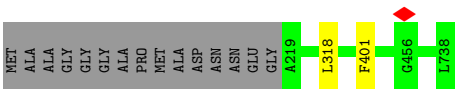




• Molecule 1: Capsid protein

Chain l:



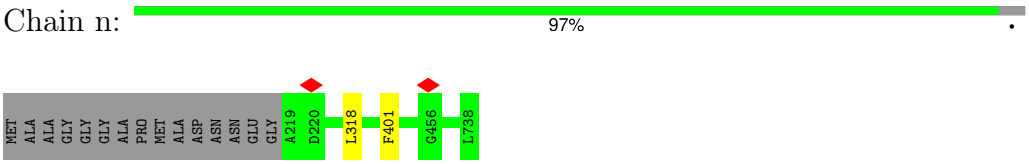


• Molecule 1: Capsid protein

Chain m:

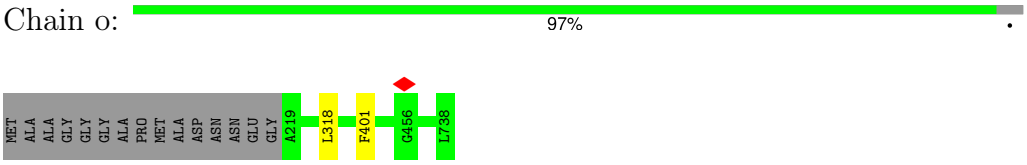
• Molecule 1: Capsid protein

Chain n:



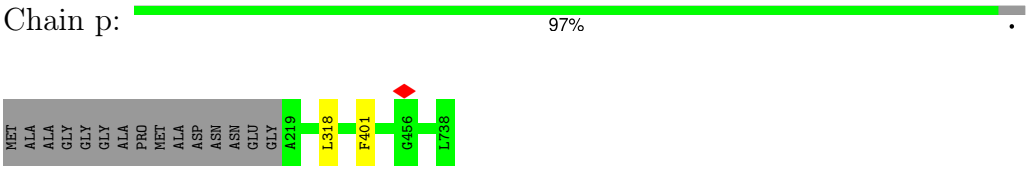
• Molecule 1: Capsid protein

Chain o:



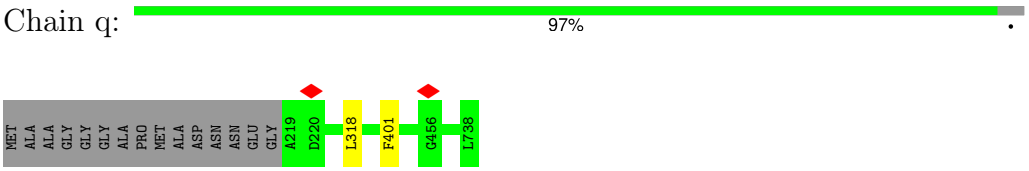
• Molecule 1: Capsid protein

Chain p:



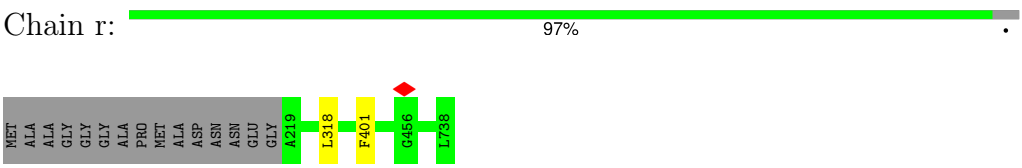
• Molecule 1: Capsid protein

Chain q:



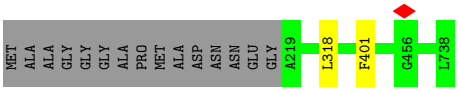
• Molecule 1: Capsid protein

Chain r:



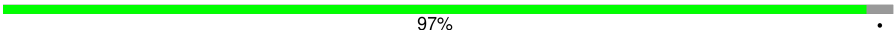
• Molecule 1: Capsid protein

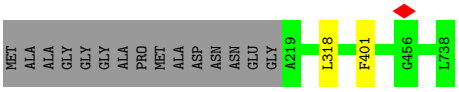
Chain s:



• Molecule 1: Capsid protein

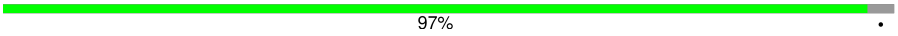
Chain t:

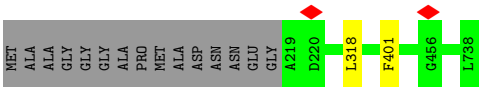




• Molecule 1: Capsid protein

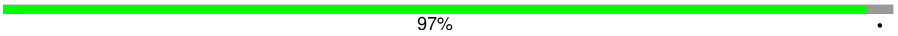
Chain u:

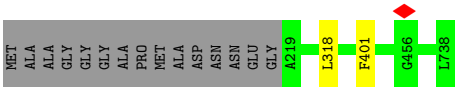




• Molecule 1: Capsid protein

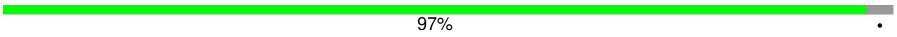
Chain v:

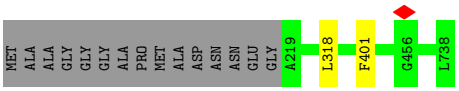




• Molecule 1: Capsid protein

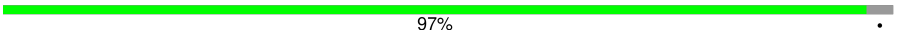
Chain w:

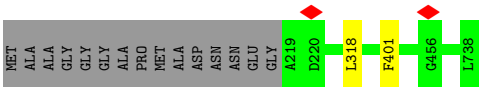




• Molecule 1: Capsid protein

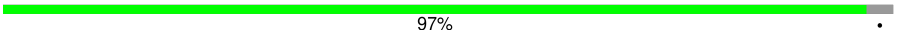
Chain x:

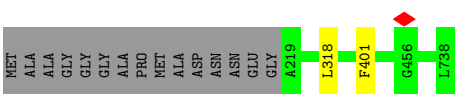




• Molecule 1: Capsid protein

Chain y:



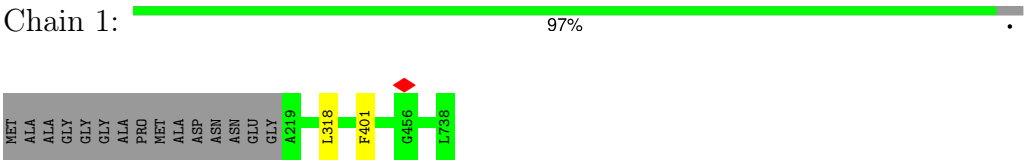


• Molecule 1: Capsid protein

Chain z:

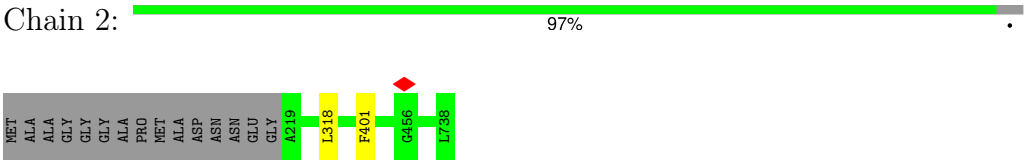
• Molecule 1: Capsid protein

Chain 1:



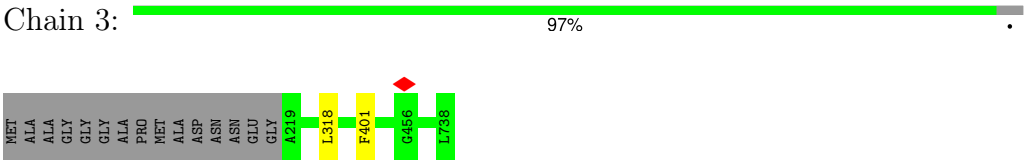
• Molecule 1: Capsid protein

Chain 2:



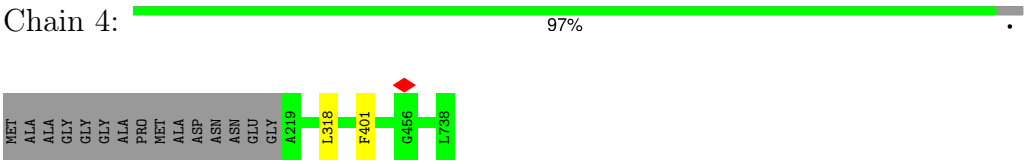
• Molecule 1: Capsid protein

Chain 3:



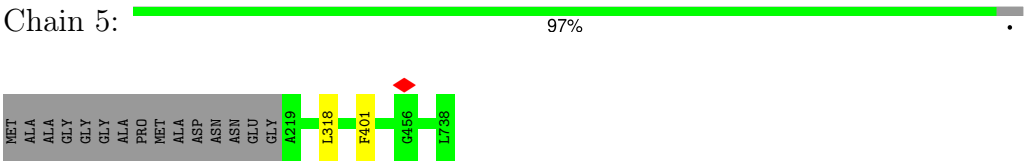
• Molecule 1: Capsid protein

Chain 4:



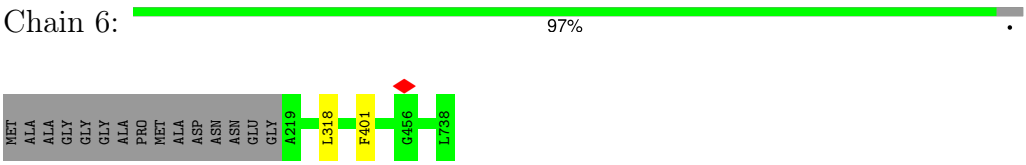
• Molecule 1: Capsid protein

Chain 5:



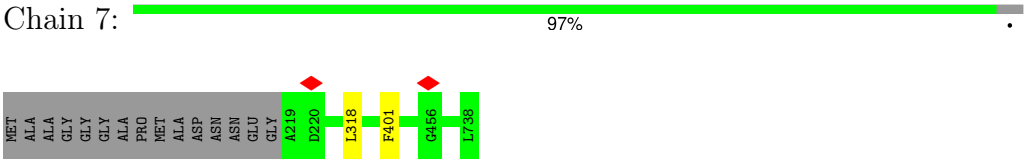
• Molecule 1: Capsid protein

Chain 6:



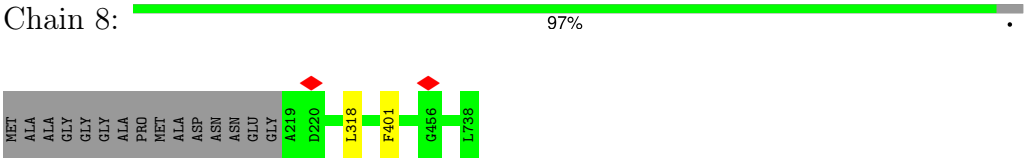
- Molecule 1: Capsid protein

Chain 7:



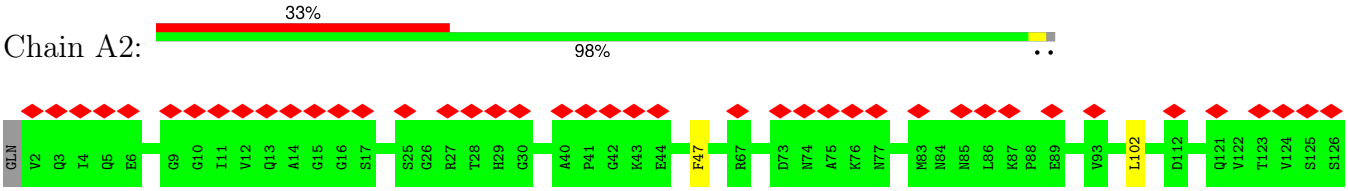
- Molecule 1: Capsid protein

Chain 8:



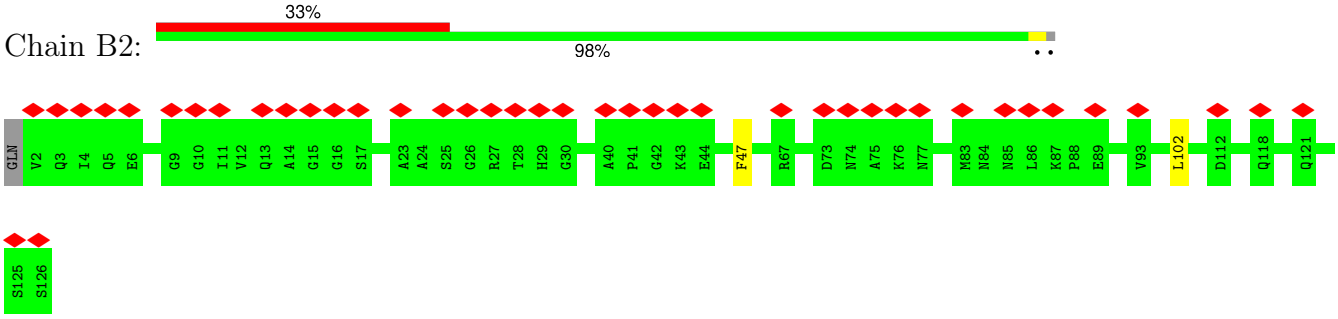
- Molecule 2: AAVX affinity ligand

Chain A2:



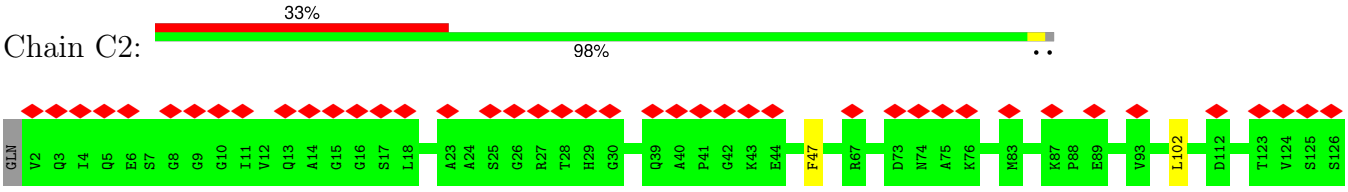
- Molecule 2: AAVX affinity ligand

Chain B2:



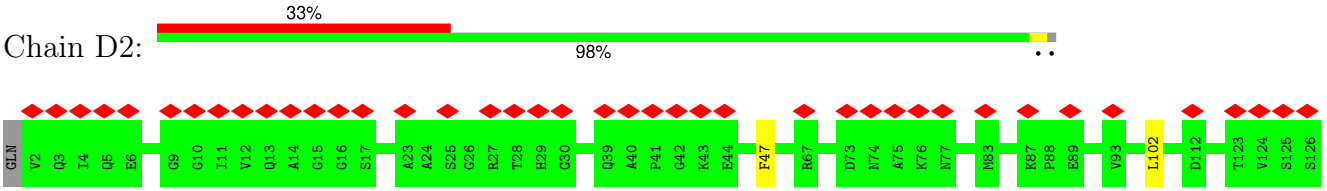
- Molecule 2: AAVX affinity ligand

Chain C2:



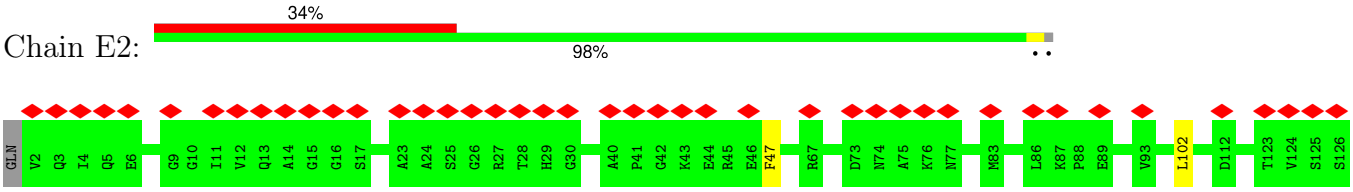
- Molecule 2: AAVX affinity ligand

Chain D2:



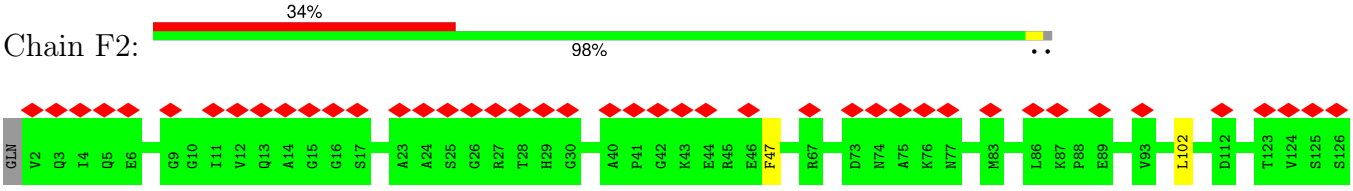
- Molecule 2: AAVX affinity ligand

Chain E2:



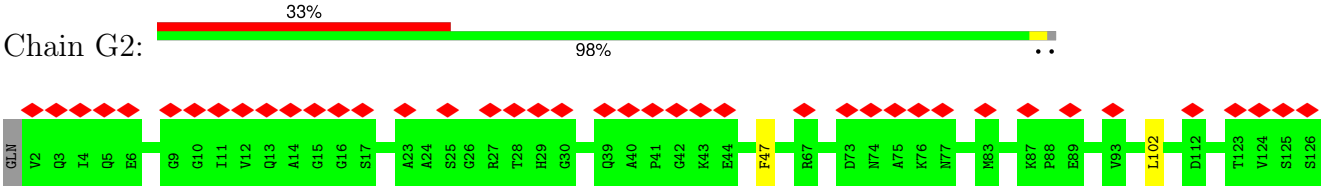
• Molecule 2: AAVX affinity ligand

Chain F2:



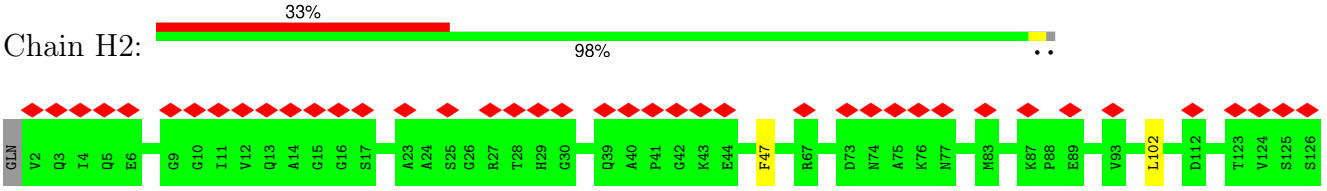
• Molecule 2: AAVX affinity ligand

Chain G2:



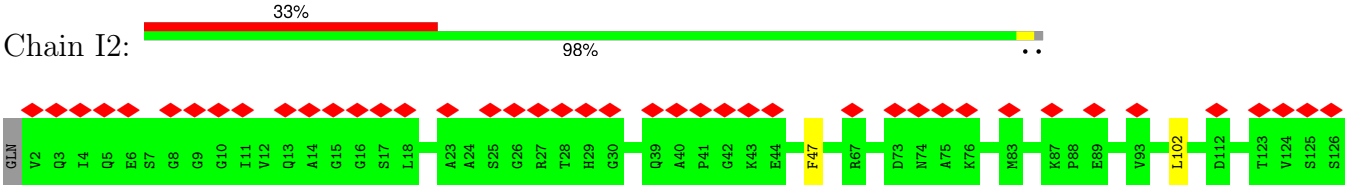
• Molecule 2: AAVX affinity ligand

Chain H2:



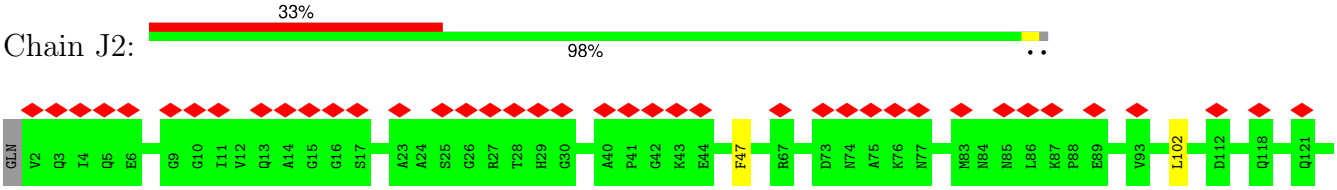
• Molecule 2: AAVX affinity ligand

Chain I2:



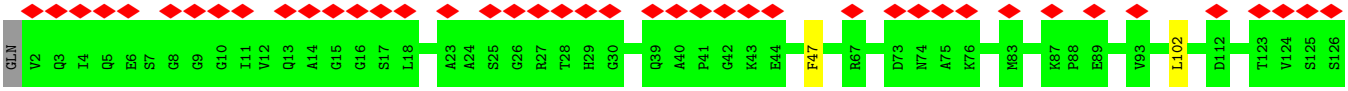
• Molecule 2: AAVX affinity ligand

Chain J2:



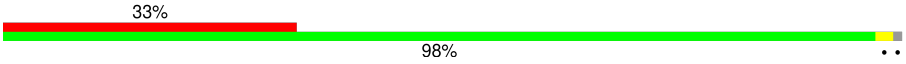
• Molecule 2: AAVX affinity ligand

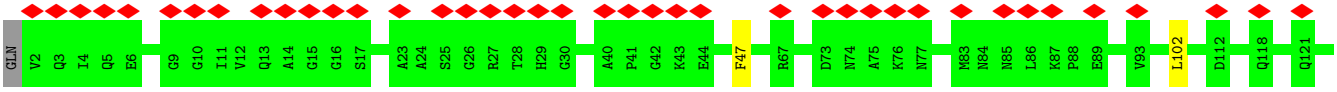
Chain K2:



• Molecule 2: AAVX affinity ligand

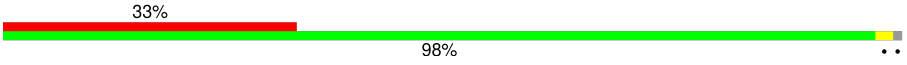
Chain L2:

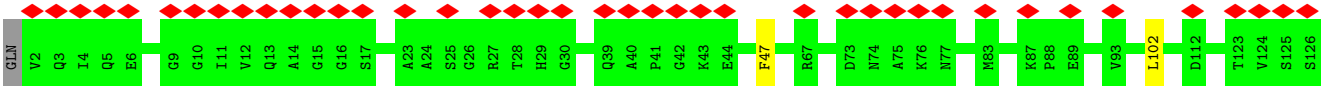




• Molecule 2: AAVX affinity ligand

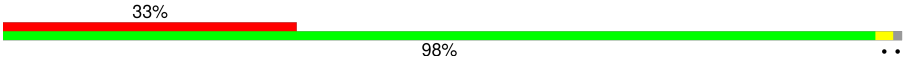
Chain M2:

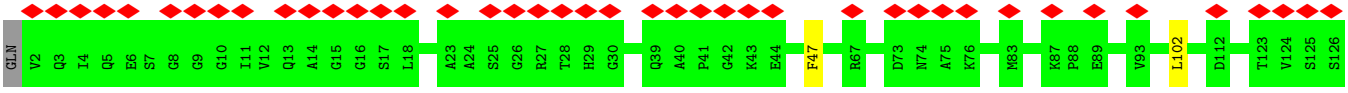




• Molecule 2: AAVX affinity ligand

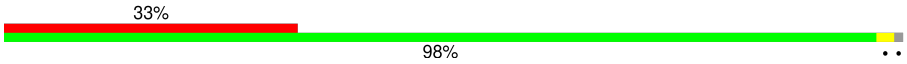
Chain N2:

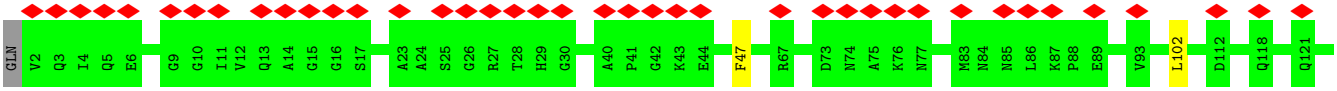




• Molecule 2: AAVX affinity ligand

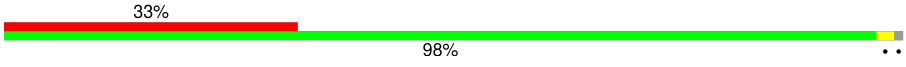
Chain O2:

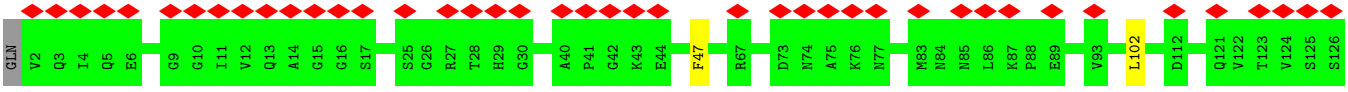




• Molecule 2: AAVX affinity ligand

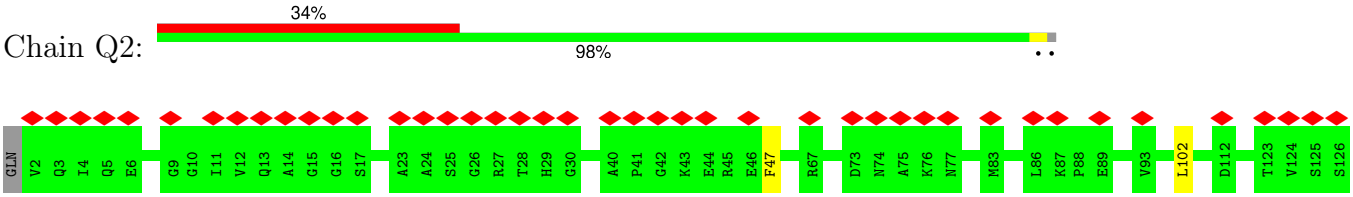
Chain P2:





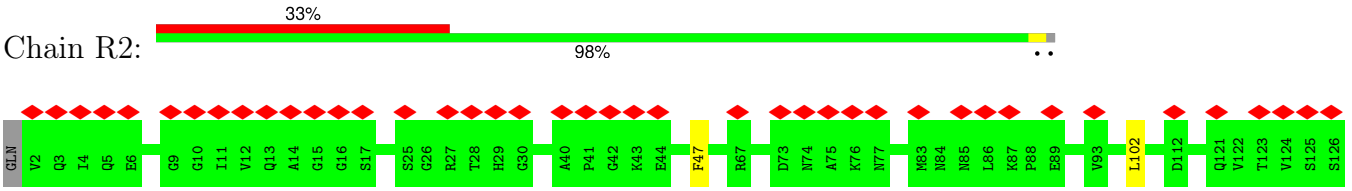
• Molecule 2: AAVX affinity ligand

Chain Q2:



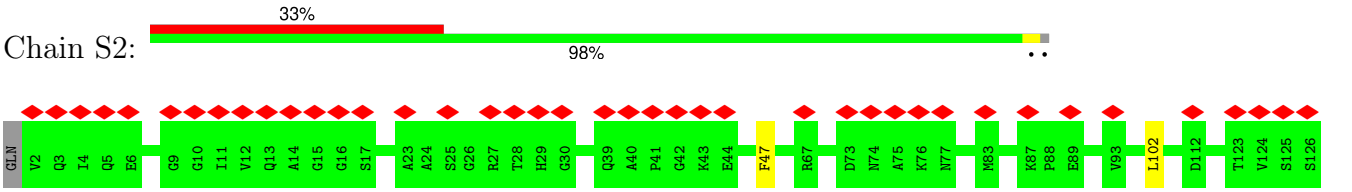
• Molecule 2: AAVX affinity ligand

Chain R2:



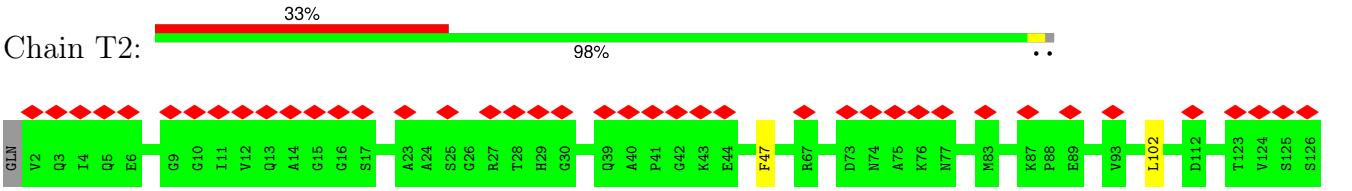
• Molecule 2: AAVX affinity ligand

Chain S2:



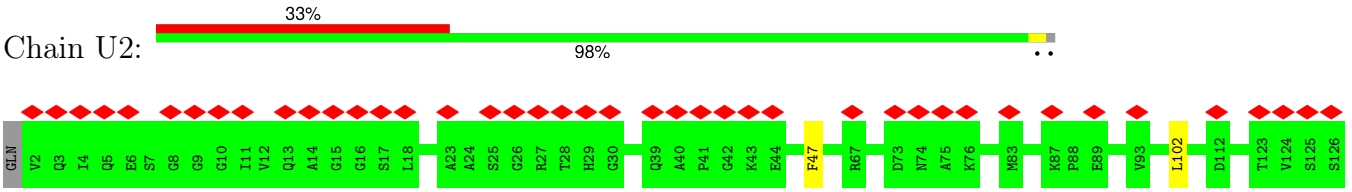
• Molecule 2: AAVX affinity ligand

Chain T2:



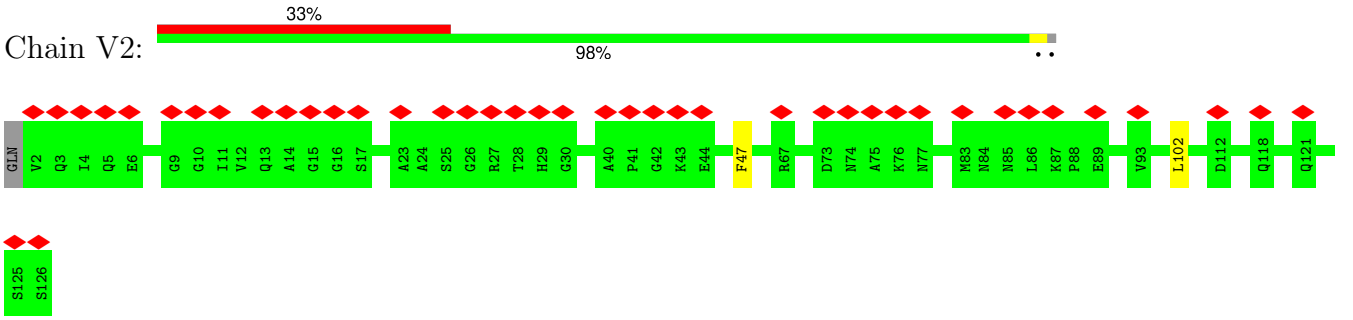
• Molecule 2: AAVX affinity ligand

Chain U2:



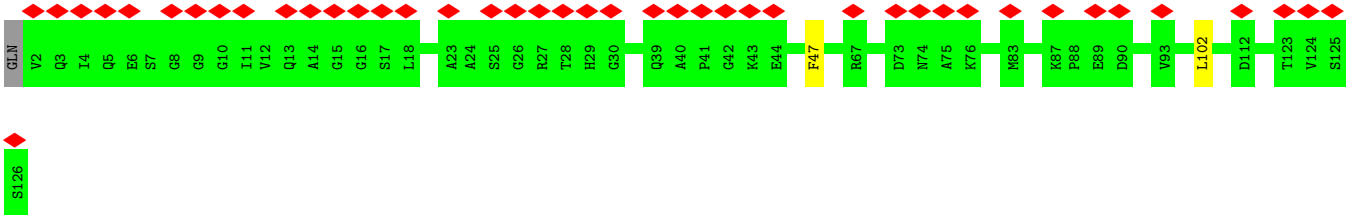
• Molecule 2: AAVX affinity ligand

Chain V2:



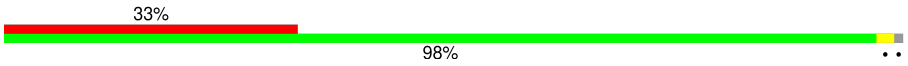
• Molecule 2: AAVX affinity ligand

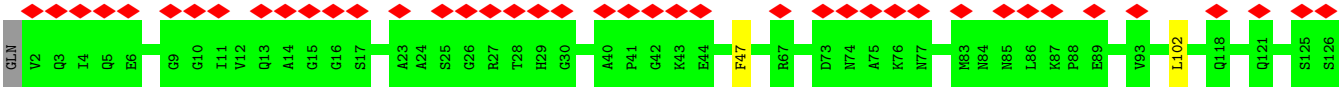
Chain W2:



• Molecule 2: AAVX affinity ligand

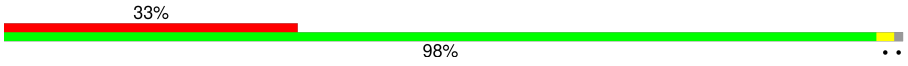
Chain X2:

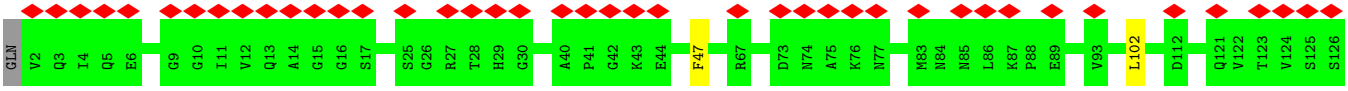




• Molecule 2: AAVX affinity ligand

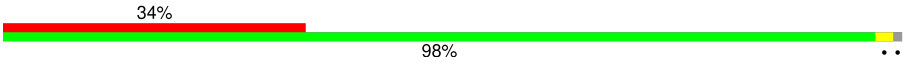
Chain Y2:

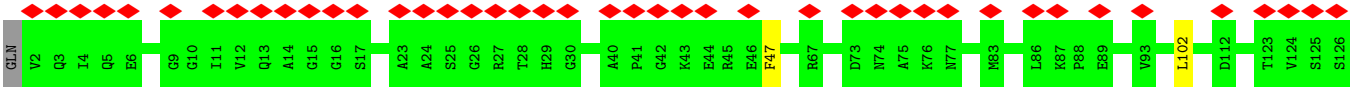




• Molecule 2: AAVX affinity ligand

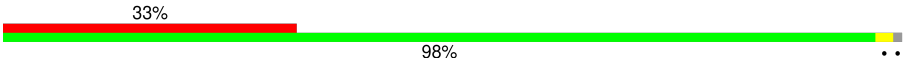
Chain Z2:

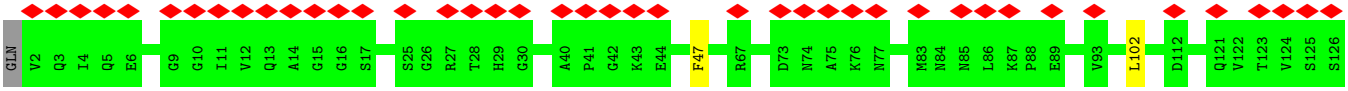




• Molecule 2: AAVX affinity ligand

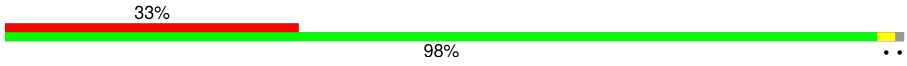
Chain a2:

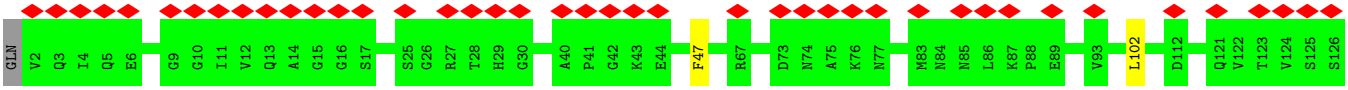




• Molecule 2: AAVX affinity ligand

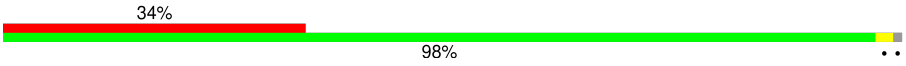
Chain b2:

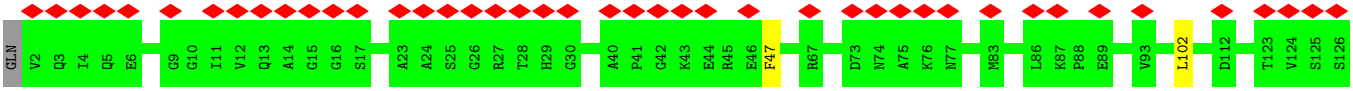




• Molecule 2: AAVX affinity ligand

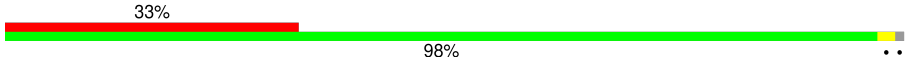
Chain c2:

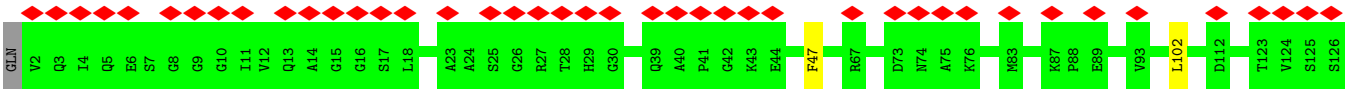




• Molecule 2: AAVX affinity ligand

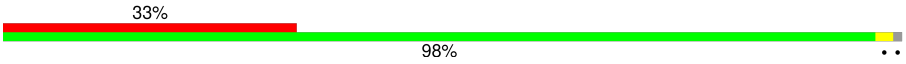
Chain d2:

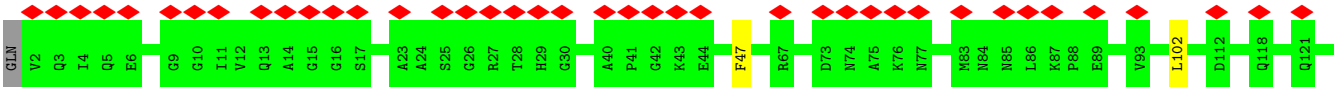




• Molecule 2: AAVX affinity ligand

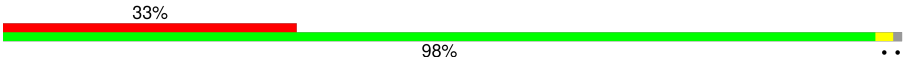
Chain e2:

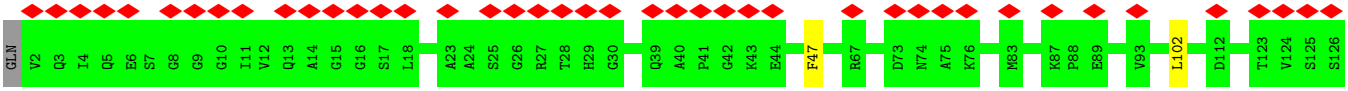




• Molecule 2: AAVX affinity ligand

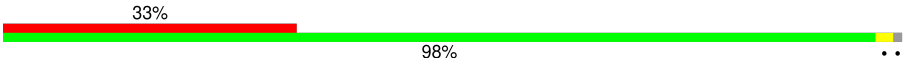
Chain f2:

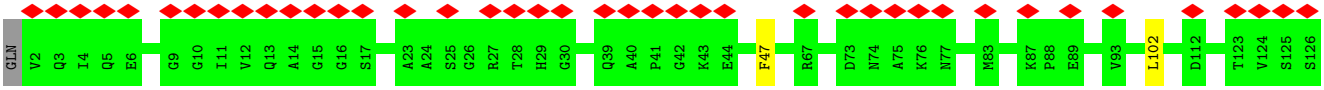




• Molecule 2: AAVX affinity ligand

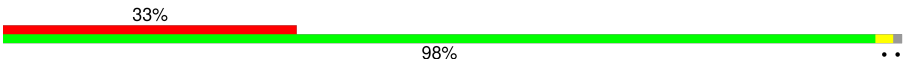
Chain g2:

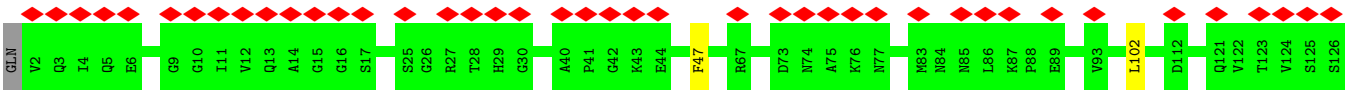




• Molecule 2: AAVX affinity ligand

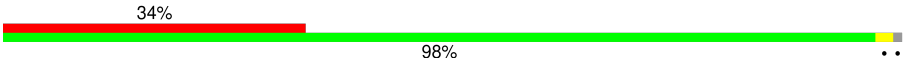
Chain h2:

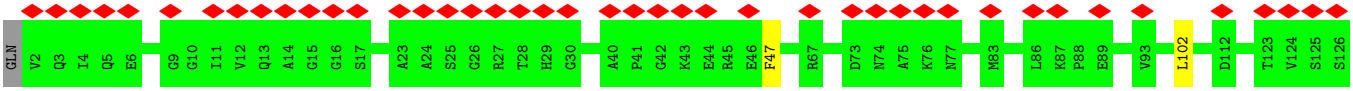




• Molecule 2: AAVX affinity ligand

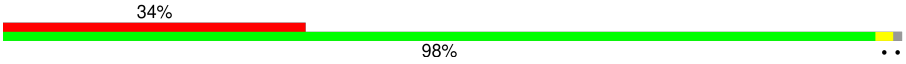
Chain i2:

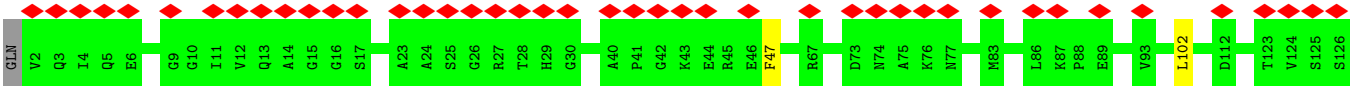




• Molecule 2: AAVX affinity ligand

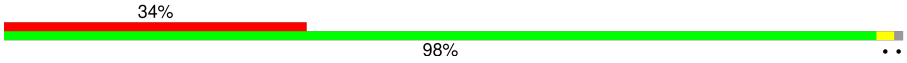
Chain j2:

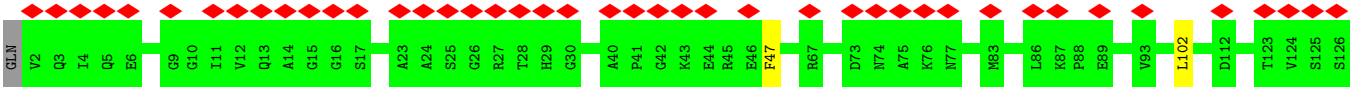




• Molecule 2: AAVX affinity ligand

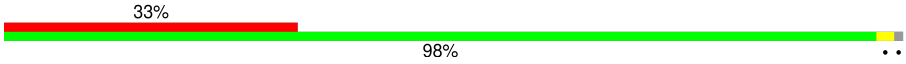
Chain k2:

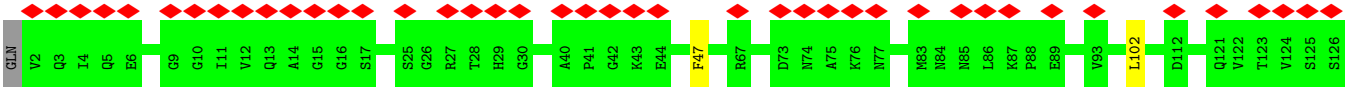




• Molecule 2: AAVX affinity ligand

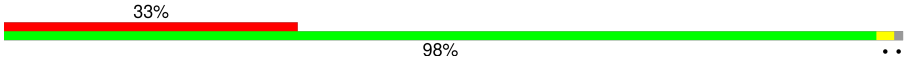
Chain l2:

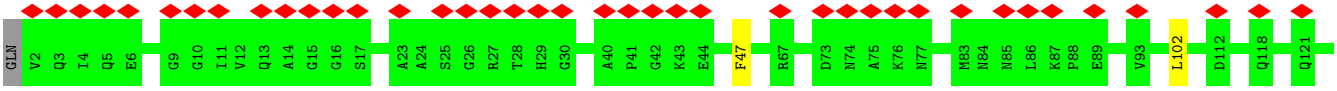




• Molecule 2: AAVX affinity ligand

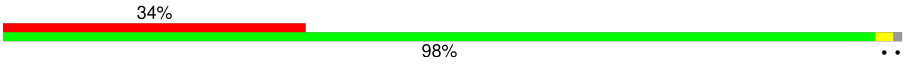
Chain m2:

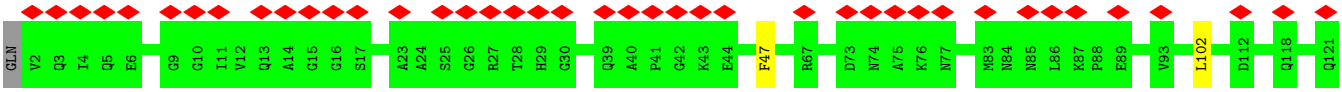




• Molecule 2: AAVX affinity ligand

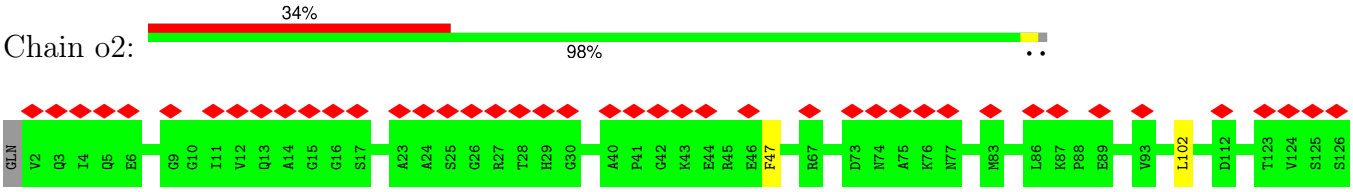
Chain n2:





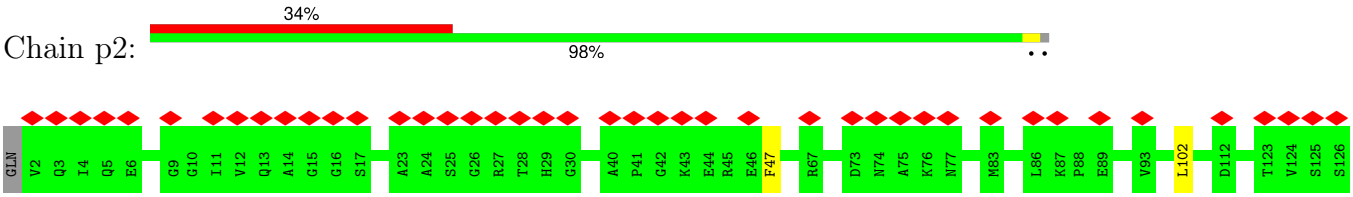
• Molecule 2: AAVX affinity ligand

Chain o2:



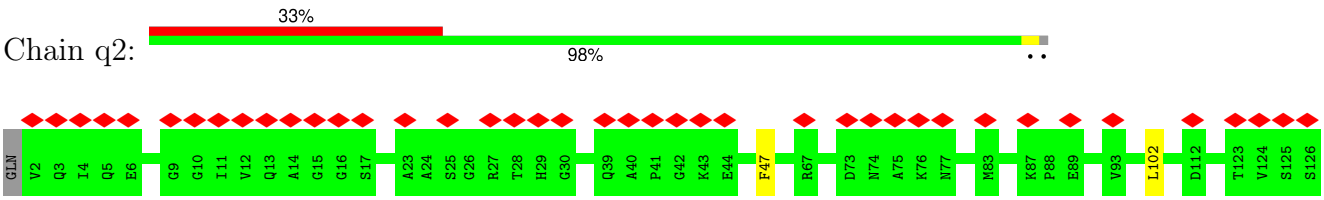
• Molecule 2: AAVX affinity ligand

Chain p2:



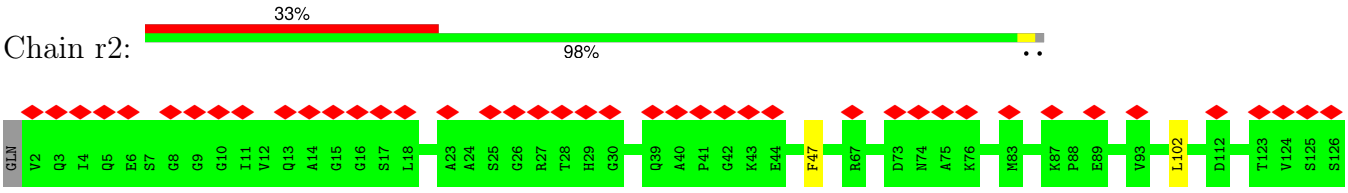
• Molecule 2: AAVX affinity ligand

Chain q2:



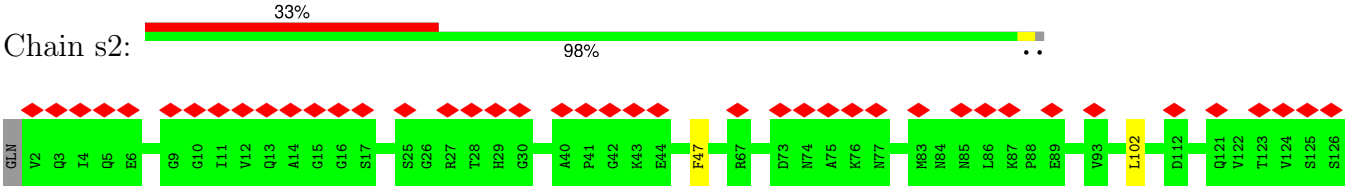
• Molecule 2: AAVX affinity ligand

Chain r2:



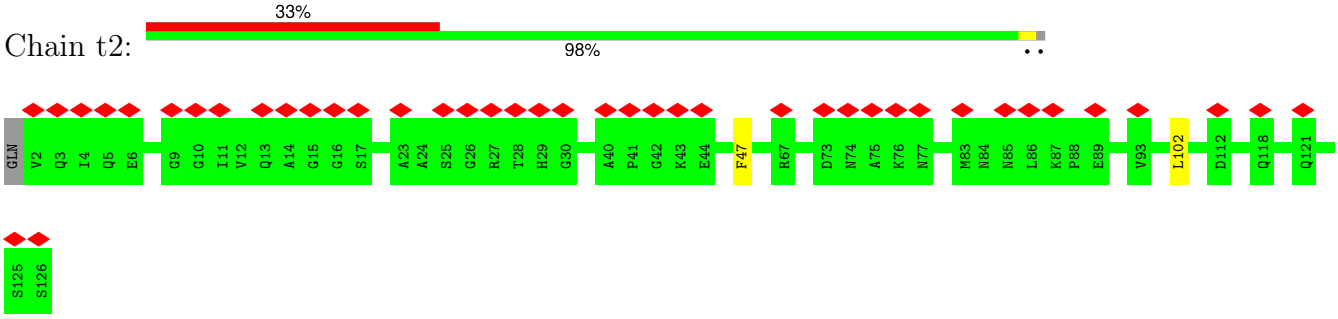
• Molecule 2: AAVX affinity ligand

Chain s2:



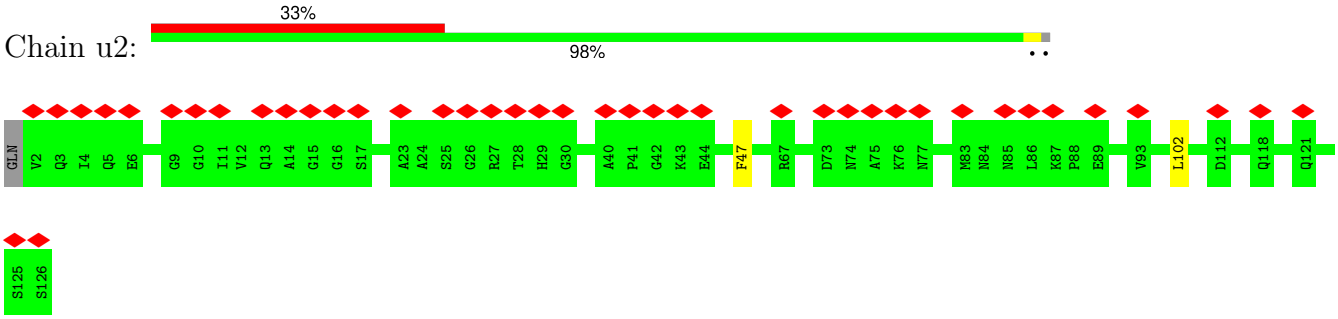
• Molecule 2: AAVX affinity ligand

Chain t2:



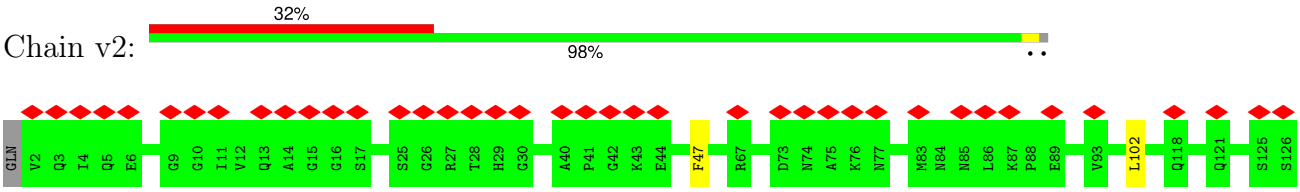
• Molecule 2: AAVX affinity ligand

Chain u2:



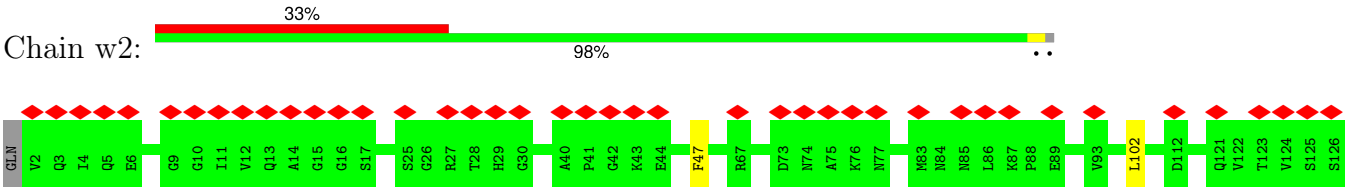
• Molecule 2: AAVX affinity ligand

Chain v2:



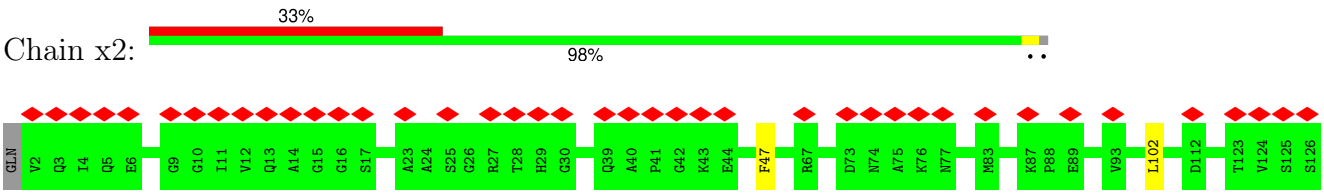
• Molecule 2: AAVX affinity ligand

Chain w2:



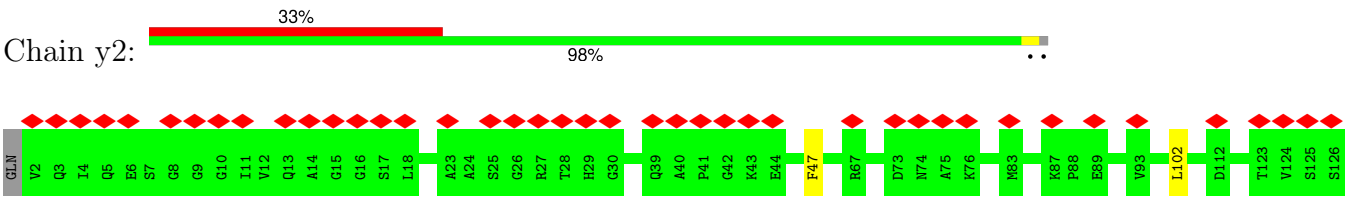
• Molecule 2: AAVX affinity ligand

Chain x2:



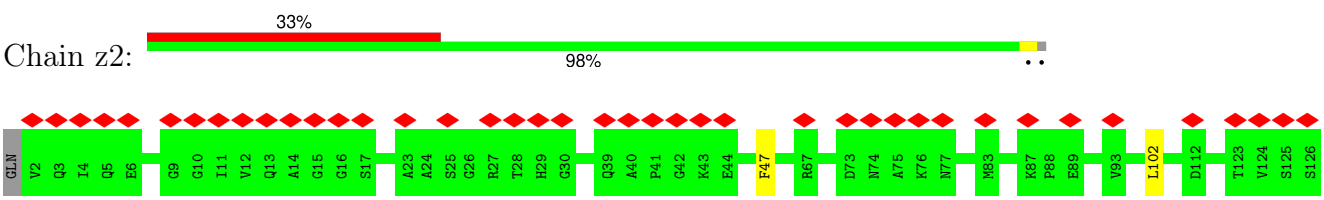
• Molecule 2: AAVX affinity ligand

Chain y2:



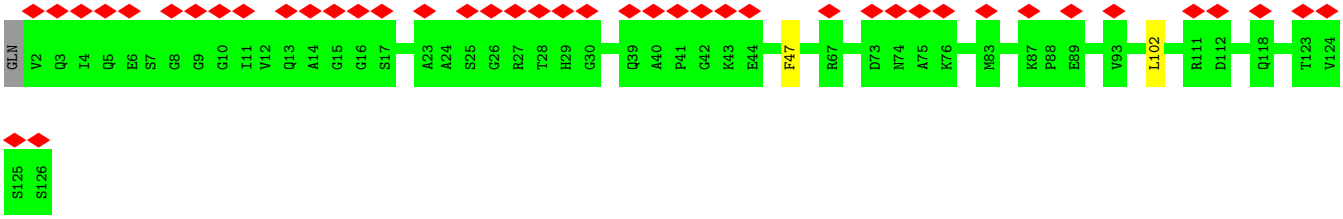
• Molecule 2: AAVX affinity ligand

Chain z2:



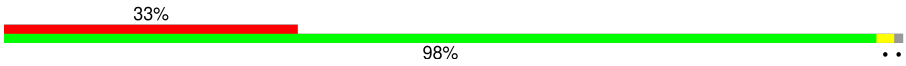
• Molecule 2: AAVX affinity ligand

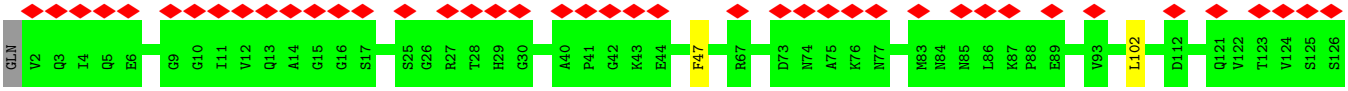
Chain 12:



• Molecule 2: AAVX affinity ligand

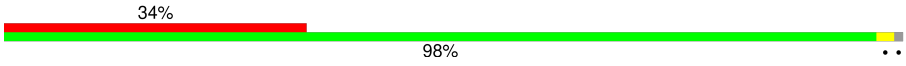
Chain 22:

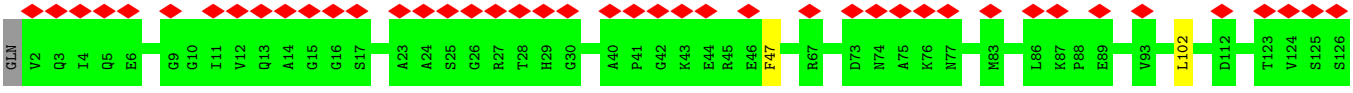




• Molecule 2: AAVX affinity ligand

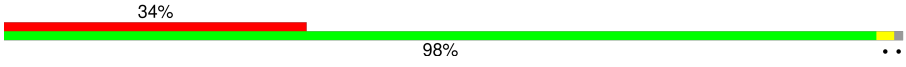
Chain 32:

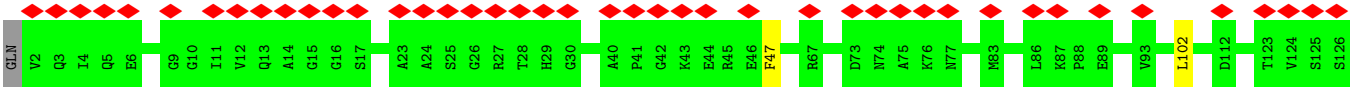




• Molecule 2: AAVX affinity ligand

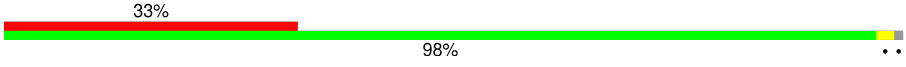
Chain 42:

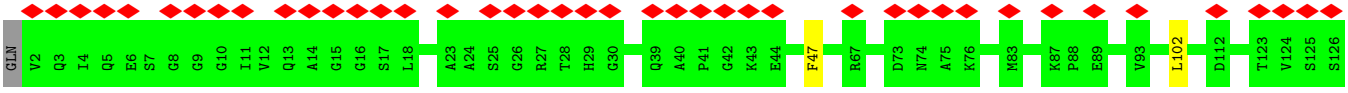




• Molecule 2: AAVX affinity ligand

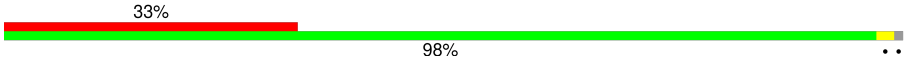
Chain 52:

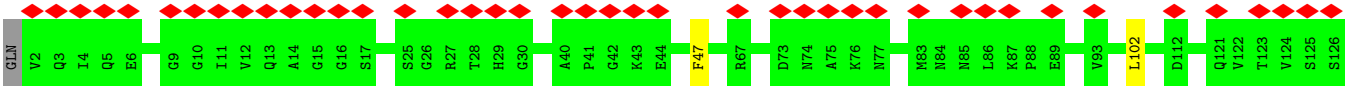




• Molecule 2: AAVX affinity ligand

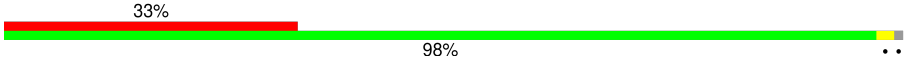
Chain 62:

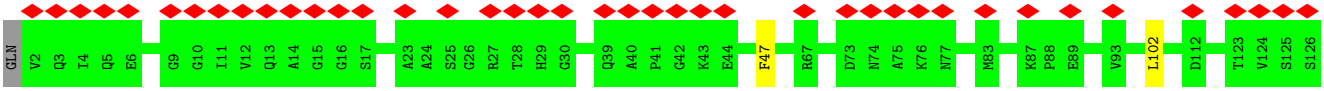




• Molecule 2: AAVX affinity ligand

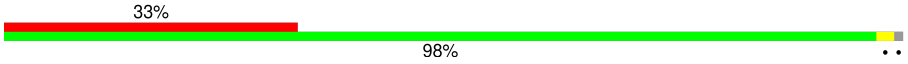
Chain 72:

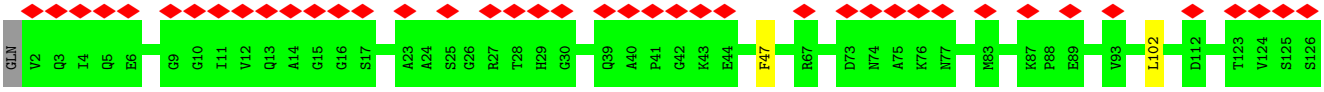




- Molecule 2: AAVX affinity ligand

Chain 82:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	92713	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)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	17.458	Depositor
Minimum map value	-8.409	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	1.4	Depositor
Map size (Å)	420.0, 420.0, 420.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.84, 0.84, 0.84	Depositor

5 Model quality

5.1 Standard geometry

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	1	0.69	0/4264	0.62	0/5818
1	2	0.69	0/4264	0.62	0/5818
1	3	0.69	0/4264	0.62	0/5818
1	4	0.69	0/4264	0.62	0/5818
1	5	0.69	0/4264	0.62	0/5818
1	6	0.69	0/4264	0.62	0/5818
1	7	0.69	0/4264	0.62	0/5818
1	8	0.69	0/4264	0.62	0/5818
1	A	0.69	0/4264	0.62	0/5818
1	B	0.69	0/4264	0.62	0/5818
1	C	0.69	0/4264	0.62	0/5818
1	D	0.69	0/4264	0.62	0/5818
1	E	0.69	0/4264	0.62	0/5818
1	F	0.69	0/4264	0.62	0/5818
1	G	0.69	0/4264	0.62	0/5818
1	H	0.69	0/4264	0.62	0/5818
1	I	0.69	0/4264	0.62	0/5818
1	J	0.69	0/4264	0.62	0/5818
1	K	0.69	0/4264	0.62	0/5818
1	L	0.69	0/4264	0.62	0/5818
1	M	0.69	0/4264	0.62	0/5818
1	N	0.69	0/4264	0.62	0/5818
1	O	0.69	0/4264	0.62	0/5818
1	P	0.69	0/4264	0.62	0/5818
1	Q	0.69	0/4264	0.62	0/5818
1	R	0.69	0/4264	0.62	0/5818
1	S	0.69	0/4264	0.62	0/5818
1	T	0.69	0/4264	0.62	0/5818
1	U	0.69	0/4264	0.62	0/5818
1	V	0.69	0/4264	0.62	0/5818
1	W	0.69	0/4264	0.62	0/5818
1	X	0.69	0/4264	0.62	0/5818
1	Y	0.69	0/4264	0.62	0/5818
1	Z	0.69	0/4264	0.62	0/5818

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	a	0.69	0/4264	0.62	0/5818
1	b	0.69	0/4264	0.62	0/5818
1	c	0.69	0/4264	0.62	0/5818
1	d	0.69	0/4264	0.62	0/5818
1	e	0.69	0/4264	0.62	0/5818
1	f	0.69	0/4264	0.62	0/5818
1	g	0.69	0/4264	0.62	0/5818
1	h	0.69	0/4264	0.62	0/5818
1	i	0.69	0/4264	0.62	0/5818
1	j	0.69	0/4264	0.62	0/5818
1	k	0.69	0/4264	0.62	0/5818
1	l	0.69	0/4264	0.62	0/5818
1	m	0.69	0/4264	0.62	0/5818
1	n	0.69	0/4264	0.62	0/5818
1	o	0.69	0/4264	0.62	0/5818
1	p	0.69	0/4264	0.62	0/5818
1	q	0.69	0/4264	0.62	0/5818
1	r	0.69	0/4264	0.62	0/5818
1	s	0.69	0/4264	0.62	0/5818
1	t	0.69	0/4264	0.62	0/5818
1	u	0.69	0/4264	0.62	0/5818
1	v	0.69	0/4264	0.62	0/5818
1	w	0.69	0/4264	0.62	0/5818
1	x	0.69	0/4264	0.62	0/5818
1	y	0.69	0/4264	0.62	0/5818
1	z	0.69	0/4264	0.62	0/5818
2	12	0.45	0/966	0.53	0/1305
2	22	0.45	0/966	0.53	0/1305
2	32	0.45	0/966	0.53	0/1305
2	42	0.45	0/966	0.53	0/1305
2	52	0.45	0/966	0.53	0/1305
2	62	0.45	0/966	0.53	0/1305
2	72	0.45	0/966	0.53	0/1305
2	82	0.45	0/966	0.53	0/1305
2	A2	0.45	0/966	0.53	0/1305
2	B2	0.45	0/966	0.53	0/1305
2	C2	0.45	0/966	0.53	0/1305
2	D2	0.45	0/966	0.53	0/1305
2	E2	0.45	0/966	0.53	0/1305
2	F2	0.45	0/966	0.53	0/1305
2	G2	0.45	0/966	0.53	0/1305
2	H2	0.45	0/966	0.53	0/1305
2	I2	0.45	0/966	0.53	0/1305

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
2	J2	0.45	0/966	0.53	0/1305
2	K2	0.45	0/966	0.53	0/1305
2	L2	0.45	0/966	0.53	0/1305
2	M2	0.45	0/966	0.53	0/1305
2	N2	0.45	0/966	0.53	0/1305
2	O2	0.45	0/966	0.53	0/1305
2	P2	0.45	0/966	0.53	0/1305
2	Q2	0.45	0/966	0.53	0/1305
2	R2	0.45	0/966	0.53	0/1305
2	S2	0.45	0/966	0.53	0/1305
2	T2	0.45	0/966	0.53	0/1305
2	U2	0.45	0/966	0.53	0/1305
2	V2	0.45	0/966	0.53	0/1305
2	W2	0.45	0/966	0.53	0/1305
2	X2	0.45	0/966	0.53	0/1305
2	Y2	0.45	0/966	0.53	0/1305
2	Z2	0.45	0/966	0.53	0/1305
2	a2	0.45	0/966	0.53	0/1305
2	b2	0.45	0/966	0.53	0/1305
2	c2	0.45	0/966	0.53	0/1305
2	d2	0.45	0/966	0.53	0/1305
2	e2	0.45	0/966	0.53	0/1305
2	f2	0.45	0/966	0.53	0/1305
2	g2	0.45	0/966	0.53	0/1305
2	h2	0.45	0/966	0.53	0/1305
2	i2	0.45	0/966	0.53	0/1305
2	j2	0.45	0/966	0.53	0/1305
2	k2	0.45	0/966	0.53	0/1305
2	l2	0.45	0/966	0.53	0/1305
2	m2	0.45	0/966	0.53	0/1305
2	n2	0.45	0/966	0.53	0/1305
2	o2	0.45	0/966	0.53	0/1305
2	p2	0.45	0/966	0.53	0/1305
2	q2	0.45	0/966	0.53	0/1305
2	r2	0.45	0/966	0.53	0/1305
2	s2	0.45	0/966	0.53	0/1305
2	t2	0.45	0/966	0.53	0/1305
2	u2	0.45	0/966	0.53	0/1305
2	v2	0.45	0/966	0.53	0/1305
2	w2	0.45	0/966	0.53	0/1305
2	x2	0.45	0/966	0.53	0/1305
2	y2	0.45	0/966	0.53	0/1305
2	z2	0.45	0/966	0.53	0/1305

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
All	All	0.65	0/313800	0.61	0/427380

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 (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	1	518/535 (97%)	504 (97%)	14 (3%)	0	100	100
1	2	518/535 (97%)	504 (97%)	14 (3%)	0	100	100
1	3	518/535 (97%)	503 (97%)	15 (3%)	0	100	100
1	4	518/535 (97%)	503 (97%)	15 (3%)	0	100	100
1	5	518/535 (97%)	503 (97%)	15 (3%)	0	100	100
1	6	518/535 (97%)	504 (97%)	14 (3%)	0	100	100
1	7	518/535 (97%)	503 (97%)	15 (3%)	0	100	100
1	8	518/535 (97%)	503 (97%)	15 (3%)	0	100	100
1	A	518/535 (97%)	504 (97%)	14 (3%)	0	100	100
1	B	518/535 (97%)	504 (97%)	14 (3%)	0	100	100
1	C	518/535 (97%)	503 (97%)	15 (3%)	0	100	100
1	D	518/535 (97%)	504 (97%)	14 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	518/535 (97%)	503 (97%)	15 (3%)	0	100	100
1	F	518/535 (97%)	503 (97%)	15 (3%)	0	100	100
1	G	518/535 (97%)	503 (97%)	15 (3%)	0	100	100
1	H	518/535 (97%)	504 (97%)	14 (3%)	0	100	100
1	I	518/535 (97%)	503 (97%)	15 (3%)	0	100	100
1	J	518/535 (97%)	503 (97%)	15 (3%)	0	100	100
1	K	518/535 (97%)	504 (97%)	14 (3%)	0	100	100
1	L	518/535 (97%)	503 (97%)	15 (3%)	0	100	100
1	M	518/535 (97%)	504 (97%)	14 (3%)	0	100	100
1	N	518/535 (97%)	503 (97%)	15 (3%)	0	100	100
1	O	518/535 (97%)	503 (97%)	15 (3%)	0	100	100
1	P	518/535 (97%)	504 (97%)	14 (3%)	0	100	100
1	Q	518/535 (97%)	503 (97%)	15 (3%)	0	100	100
1	R	518/535 (97%)	504 (97%)	14 (3%)	0	100	100
1	S	518/535 (97%)	503 (97%)	15 (3%)	0	100	100
1	T	518/535 (97%)	503 (97%)	15 (3%)	0	100	100
1	U	518/535 (97%)	504 (97%)	14 (3%)	0	100	100
1	V	518/535 (97%)	503 (97%)	15 (3%)	0	100	100
1	W	518/535 (97%)	503 (97%)	15 (3%)	0	100	100
1	X	518/535 (97%)	504 (97%)	14 (3%)	0	100	100
1	Y	518/535 (97%)	504 (97%)	14 (3%)	0	100	100
1	Z	518/535 (97%)	503 (97%)	15 (3%)	0	100	100
1	a	518/535 (97%)	504 (97%)	14 (3%)	0	100	100
1	b	518/535 (97%)	504 (97%)	14 (3%)	0	100	100
1	c	518/535 (97%)	503 (97%)	15 (3%)	0	100	100
1	d	518/535 (97%)	504 (97%)	14 (3%)	0	100	100
1	e	518/535 (97%)	503 (97%)	15 (3%)	0	100	100
1	f	518/535 (97%)	503 (97%)	15 (3%)	0	100	100
1	g	518/535 (97%)	504 (97%)	14 (3%)	0	100	100
1	h	518/535 (97%)	504 (97%)	14 (3%)	0	100	100
1	i	518/535 (97%)	503 (97%)	15 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	j	518/535 (97%)	503 (97%)	15 (3%)	0	100	100
1	k	518/535 (97%)	503 (97%)	15 (3%)	0	100	100
1	l	518/535 (97%)	504 (97%)	14 (3%)	0	100	100
1	m	518/535 (97%)	504 (97%)	14 (3%)	0	100	100
1	n	518/535 (97%)	503 (97%)	15 (3%)	0	100	100
1	o	518/535 (97%)	503 (97%)	15 (3%)	0	100	100
1	p	518/535 (97%)	503 (97%)	15 (3%)	0	100	100
1	q	518/535 (97%)	503 (97%)	15 (3%)	0	100	100
1	r	518/535 (97%)	503 (97%)	15 (3%)	0	100	100
1	s	518/535 (97%)	504 (97%)	14 (3%)	0	100	100
1	t	518/535 (97%)	504 (97%)	14 (3%)	0	100	100
1	u	518/535 (97%)	504 (97%)	14 (3%)	0	100	100
1	v	518/535 (97%)	504 (97%)	14 (3%)	0	100	100
1	w	518/535 (97%)	504 (97%)	14 (3%)	0	100	100
1	x	518/535 (97%)	503 (97%)	15 (3%)	0	100	100
1	y	518/535 (97%)	503 (97%)	15 (3%)	0	100	100
1	z	518/535 (97%)	504 (97%)	14 (3%)	0	100	100
2	12	123/126 (98%)	120 (98%)	3 (2%)	0	100	100
2	22	123/126 (98%)	120 (98%)	3 (2%)	0	100	100
2	32	123/126 (98%)	120 (98%)	3 (2%)	0	100	100
2	42	123/126 (98%)	120 (98%)	3 (2%)	0	100	100
2	52	123/126 (98%)	120 (98%)	3 (2%)	0	100	100
2	62	123/126 (98%)	120 (98%)	3 (2%)	0	100	100
2	72	123/126 (98%)	120 (98%)	3 (2%)	0	100	100
2	82	123/126 (98%)	120 (98%)	3 (2%)	0	100	100
2	A2	123/126 (98%)	120 (98%)	3 (2%)	0	100	100
2	B2	123/126 (98%)	120 (98%)	3 (2%)	0	100	100
2	C2	123/126 (98%)	120 (98%)	3 (2%)	0	100	100
2	D2	123/126 (98%)	120 (98%)	3 (2%)	0	100	100
2	E2	123/126 (98%)	120 (98%)	3 (2%)	0	100	100
2	F2	123/126 (98%)	120 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	G2	123/126 (98%)	120 (98%)	3 (2%)	0	100	100
2	H2	123/126 (98%)	120 (98%)	3 (2%)	0	100	100
2	I2	123/126 (98%)	120 (98%)	3 (2%)	0	100	100
2	J2	123/126 (98%)	120 (98%)	3 (2%)	0	100	100
2	K2	123/126 (98%)	120 (98%)	3 (2%)	0	100	100
2	L2	123/126 (98%)	120 (98%)	3 (2%)	0	100	100
2	M2	123/126 (98%)	120 (98%)	3 (2%)	0	100	100
2	N2	123/126 (98%)	120 (98%)	3 (2%)	0	100	100
2	O2	123/126 (98%)	120 (98%)	3 (2%)	0	100	100
2	P2	123/126 (98%)	120 (98%)	3 (2%)	0	100	100
2	Q2	123/126 (98%)	120 (98%)	3 (2%)	0	100	100
2	R2	123/126 (98%)	120 (98%)	3 (2%)	0	100	100
2	S2	123/126 (98%)	120 (98%)	3 (2%)	0	100	100
2	T2	123/126 (98%)	120 (98%)	3 (2%)	0	100	100
2	U2	123/126 (98%)	120 (98%)	3 (2%)	0	100	100
2	V2	123/126 (98%)	120 (98%)	3 (2%)	0	100	100
2	W2	123/126 (98%)	120 (98%)	3 (2%)	0	100	100
2	X2	123/126 (98%)	120 (98%)	3 (2%)	0	100	100
2	Y2	123/126 (98%)	120 (98%)	3 (2%)	0	100	100
2	Z2	123/126 (98%)	120 (98%)	3 (2%)	0	100	100
2	a2	123/126 (98%)	120 (98%)	3 (2%)	0	100	100
2	b2	123/126 (98%)	120 (98%)	3 (2%)	0	100	100
2	c2	123/126 (98%)	120 (98%)	3 (2%)	0	100	100
2	d2	123/126 (98%)	120 (98%)	3 (2%)	0	100	100
2	e2	123/126 (98%)	120 (98%)	3 (2%)	0	100	100
2	f2	123/126 (98%)	120 (98%)	3 (2%)	0	100	100
2	g2	123/126 (98%)	120 (98%)	3 (2%)	0	100	100
2	h2	123/126 (98%)	120 (98%)	3 (2%)	0	100	100
2	i2	123/126 (98%)	120 (98%)	3 (2%)	0	100	100
2	j2	123/126 (98%)	120 (98%)	3 (2%)	0	100	100
2	k2	123/126 (98%)	120 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	l2	123/126 (98%)	120 (98%)	3 (2%)	0	100	100
2	m2	123/126 (98%)	120 (98%)	3 (2%)	0	100	100
2	n2	123/126 (98%)	120 (98%)	3 (2%)	0	100	100
2	o2	123/126 (98%)	120 (98%)	3 (2%)	0	100	100
2	p2	123/126 (98%)	120 (98%)	3 (2%)	0	100	100
2	q2	123/126 (98%)	120 (98%)	3 (2%)	0	100	100
2	r2	123/126 (98%)	120 (98%)	3 (2%)	0	100	100
2	s2	123/126 (98%)	120 (98%)	3 (2%)	0	100	100
2	t2	123/126 (98%)	120 (98%)	3 (2%)	0	100	100
2	u2	123/126 (98%)	120 (98%)	3 (2%)	0	100	100
2	v2	123/126 (98%)	120 (98%)	3 (2%)	0	100	100
2	w2	123/126 (98%)	120 (98%)	3 (2%)	0	100	100
2	x2	123/126 (98%)	120 (98%)	3 (2%)	0	100	100
2	y2	123/126 (98%)	120 (98%)	3 (2%)	0	100	100
2	z2	123/126 (98%)	120 (98%)	3 (2%)	0	100	100
All	All	38460/39660 (97%)	37407 (97%)	1053 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	453/460 (98%)	451 (100%)	2 (0%)	89	94
1	2	453/460 (98%)	451 (100%)	2 (0%)	89	94
1	3	453/460 (98%)	451 (100%)	2 (0%)	89	94
1	4	453/460 (98%)	451 (100%)	2 (0%)	89	94
1	5	453/460 (98%)	451 (100%)	2 (0%)	89	94
1	6	453/460 (98%)	451 (100%)	2 (0%)	89	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	7	453/460 (98%)	451 (100%)	2 (0%)	89	94
1	8	453/460 (98%)	451 (100%)	2 (0%)	89	94
1	A	453/460 (98%)	451 (100%)	2 (0%)	89	94
1	B	453/460 (98%)	451 (100%)	2 (0%)	89	94
1	C	453/460 (98%)	451 (100%)	2 (0%)	89	94
1	D	453/460 (98%)	451 (100%)	2 (0%)	89	94
1	E	453/460 (98%)	451 (100%)	2 (0%)	89	94
1	F	453/460 (98%)	451 (100%)	2 (0%)	89	94
1	G	453/460 (98%)	451 (100%)	2 (0%)	89	94
1	H	453/460 (98%)	451 (100%)	2 (0%)	89	94
1	I	453/460 (98%)	451 (100%)	2 (0%)	89	94
1	J	453/460 (98%)	451 (100%)	2 (0%)	89	94
1	K	453/460 (98%)	451 (100%)	2 (0%)	89	94
1	L	453/460 (98%)	451 (100%)	2 (0%)	89	94
1	M	453/460 (98%)	451 (100%)	2 (0%)	89	94
1	N	453/460 (98%)	451 (100%)	2 (0%)	89	94
1	O	453/460 (98%)	451 (100%)	2 (0%)	89	94
1	P	453/460 (98%)	451 (100%)	2 (0%)	89	94
1	Q	453/460 (98%)	451 (100%)	2 (0%)	89	94
1	R	453/460 (98%)	451 (100%)	2 (0%)	89	94
1	S	453/460 (98%)	451 (100%)	2 (0%)	89	94
1	T	453/460 (98%)	451 (100%)	2 (0%)	89	94
1	U	453/460 (98%)	451 (100%)	2 (0%)	89	94
1	V	453/460 (98%)	451 (100%)	2 (0%)	89	94
1	W	453/460 (98%)	451 (100%)	2 (0%)	89	94
1	X	453/460 (98%)	451 (100%)	2 (0%)	89	94
1	Y	453/460 (98%)	451 (100%)	2 (0%)	89	94
1	Z	453/460 (98%)	451 (100%)	2 (0%)	89	94
1	a	453/460 (98%)	451 (100%)	2 (0%)	89	94
1	b	453/460 (98%)	451 (100%)	2 (0%)	89	94
1	c	453/460 (98%)	451 (100%)	2 (0%)	89	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	d	453/460 (98%)	451 (100%)	2 (0%)	89	94
1	e	453/460 (98%)	451 (100%)	2 (0%)	89	94
1	f	453/460 (98%)	451 (100%)	2 (0%)	89	94
1	g	453/460 (98%)	451 (100%)	2 (0%)	89	94
1	h	453/460 (98%)	451 (100%)	2 (0%)	89	94
1	i	453/460 (98%)	451 (100%)	2 (0%)	89	94
1	j	453/460 (98%)	451 (100%)	2 (0%)	89	94
1	k	453/460 (98%)	451 (100%)	2 (0%)	89	94
1	l	453/460 (98%)	451 (100%)	2 (0%)	89	94
1	m	453/460 (98%)	451 (100%)	2 (0%)	89	94
1	n	453/460 (98%)	451 (100%)	2 (0%)	89	94
1	o	453/460 (98%)	451 (100%)	2 (0%)	89	94
1	p	453/460 (98%)	451 (100%)	2 (0%)	89	94
1	q	453/460 (98%)	451 (100%)	2 (0%)	89	94
1	r	453/460 (98%)	451 (100%)	2 (0%)	89	94
1	s	453/460 (98%)	451 (100%)	2 (0%)	89	94
1	t	453/460 (98%)	451 (100%)	2 (0%)	89	94
1	u	453/460 (98%)	451 (100%)	2 (0%)	89	94
1	v	453/460 (98%)	451 (100%)	2 (0%)	89	94
1	w	453/460 (98%)	451 (100%)	2 (0%)	89	94
1	x	453/460 (98%)	451 (100%)	2 (0%)	89	94
1	y	453/460 (98%)	451 (100%)	2 (0%)	89	94
1	z	453/460 (98%)	451 (100%)	2 (0%)	89	94
2	12	97/98 (99%)	95 (98%)	2 (2%)	48	65
2	22	97/98 (99%)	95 (98%)	2 (2%)	48	65
2	32	97/98 (99%)	95 (98%)	2 (2%)	48	65
2	42	97/98 (99%)	95 (98%)	2 (2%)	48	65
2	52	97/98 (99%)	95 (98%)	2 (2%)	48	65
2	62	97/98 (99%)	95 (98%)	2 (2%)	48	65
2	72	97/98 (99%)	95 (98%)	2 (2%)	48	65
2	82	97/98 (99%)	95 (98%)	2 (2%)	48	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A2	97/98 (99%)	95 (98%)	2 (2%)	48	65
2	B2	97/98 (99%)	95 (98%)	2 (2%)	48	65
2	C2	97/98 (99%)	95 (98%)	2 (2%)	48	65
2	D2	97/98 (99%)	95 (98%)	2 (2%)	48	65
2	E2	97/98 (99%)	95 (98%)	2 (2%)	48	65
2	F2	97/98 (99%)	95 (98%)	2 (2%)	48	65
2	G2	97/98 (99%)	95 (98%)	2 (2%)	48	65
2	H2	97/98 (99%)	95 (98%)	2 (2%)	48	65
2	I2	97/98 (99%)	95 (98%)	2 (2%)	48	65
2	J2	97/98 (99%)	95 (98%)	2 (2%)	48	65
2	K2	97/98 (99%)	95 (98%)	2 (2%)	48	65
2	L2	97/98 (99%)	95 (98%)	2 (2%)	48	65
2	M2	97/98 (99%)	95 (98%)	2 (2%)	48	65
2	N2	97/98 (99%)	95 (98%)	2 (2%)	48	65
2	O2	97/98 (99%)	95 (98%)	2 (2%)	48	65
2	P2	97/98 (99%)	95 (98%)	2 (2%)	48	65
2	Q2	97/98 (99%)	95 (98%)	2 (2%)	48	65
2	R2	97/98 (99%)	95 (98%)	2 (2%)	48	65
2	S2	97/98 (99%)	95 (98%)	2 (2%)	48	65
2	T2	97/98 (99%)	95 (98%)	2 (2%)	48	65
2	U2	97/98 (99%)	95 (98%)	2 (2%)	48	65
2	V2	97/98 (99%)	95 (98%)	2 (2%)	48	65
2	W2	97/98 (99%)	95 (98%)	2 (2%)	48	65
2	X2	97/98 (99%)	95 (98%)	2 (2%)	48	65
2	Y2	97/98 (99%)	95 (98%)	2 (2%)	48	65
2	Z2	97/98 (99%)	95 (98%)	2 (2%)	48	65
2	a2	97/98 (99%)	95 (98%)	2 (2%)	48	65
2	b2	97/98 (99%)	95 (98%)	2 (2%)	48	65
2	c2	97/98 (99%)	95 (98%)	2 (2%)	48	65
2	d2	97/98 (99%)	95 (98%)	2 (2%)	48	65
2	e2	97/98 (99%)	95 (98%)	2 (2%)	48	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	f2	97/98 (99%)	95 (98%)	2 (2%)	48	65
2	g2	97/98 (99%)	95 (98%)	2 (2%)	48	65
2	h2	97/98 (99%)	95 (98%)	2 (2%)	48	65
2	i2	97/98 (99%)	95 (98%)	2 (2%)	48	65
2	j2	97/98 (99%)	95 (98%)	2 (2%)	48	65
2	k2	97/98 (99%)	95 (98%)	2 (2%)	48	65
2	l2	97/98 (99%)	95 (98%)	2 (2%)	48	65
2	m2	97/98 (99%)	95 (98%)	2 (2%)	48	65
2	n2	97/98 (99%)	95 (98%)	2 (2%)	48	65
2	o2	97/98 (99%)	95 (98%)	2 (2%)	48	65
2	p2	97/98 (99%)	95 (98%)	2 (2%)	48	65
2	q2	97/98 (99%)	95 (98%)	2 (2%)	48	65
2	r2	97/98 (99%)	95 (98%)	2 (2%)	48	65
2	s2	97/98 (99%)	95 (98%)	2 (2%)	48	65
2	t2	97/98 (99%)	95 (98%)	2 (2%)	48	65
2	u2	97/98 (99%)	95 (98%)	2 (2%)	48	65
2	v2	97/98 (99%)	95 (98%)	2 (2%)	48	65
2	w2	97/98 (99%)	95 (98%)	2 (2%)	48	65
2	x2	97/98 (99%)	95 (98%)	2 (2%)	48	65
2	y2	97/98 (99%)	95 (98%)	2 (2%)	48	65
2	z2	97/98 (99%)	95 (98%)	2 (2%)	48	65
All	All	33000/33480 (99%)	32760 (99%)	240 (1%)	80	90

All (240) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	318	LEU
1	A	401	PHE
1	B	318	LEU
1	B	401	PHE
1	C	318	LEU
1	C	401	PHE
1	D	318	LEU
1	D	401	PHE
1	E	318	LEU

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Mol	Chain	Res	Type
1	E	401	PHE
1	F	318	LEU
1	F	401	PHE
1	G	318	LEU
1	G	401	PHE
1	H	318	LEU
1	H	401	PHE
1	I	318	LEU
1	I	401	PHE
1	J	318	LEU
1	J	401	PHE
1	K	318	LEU
1	K	401	PHE
1	L	318	LEU
1	L	401	PHE
1	M	318	LEU
1	M	401	PHE
1	N	318	LEU
1	N	401	PHE
1	O	318	LEU
1	O	401	PHE
1	P	318	LEU
1	P	401	PHE
1	Q	318	LEU
1	Q	401	PHE
1	R	318	LEU
1	R	401	PHE
1	S	318	LEU
1	S	401	PHE
1	T	318	LEU
1	T	401	PHE
1	U	318	LEU
1	U	401	PHE
1	V	318	LEU
1	V	401	PHE
1	W	318	LEU
1	W	401	PHE
1	X	318	LEU
1	X	401	PHE
1	Y	318	LEU
1	Y	401	PHE
1	Z	318	LEU

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Mol	Chain	Res	Type
1	Z	401	PHE
1	a	318	LEU
1	a	401	PHE
1	b	318	LEU
1	b	401	PHE
1	c	318	LEU
1	c	401	PHE
1	d	318	LEU
1	d	401	PHE
1	e	318	LEU
1	e	401	PHE
1	f	318	LEU
1	f	401	PHE
1	g	318	LEU
1	g	401	PHE
1	h	318	LEU
1	h	401	PHE
1	i	318	LEU
1	i	401	PHE
1	j	318	LEU
1	j	401	PHE
1	k	318	LEU
1	k	401	PHE
1	l	318	LEU
1	l	401	PHE
1	m	318	LEU
1	m	401	PHE
1	n	318	LEU
1	n	401	PHE
1	o	318	LEU
1	o	401	PHE
1	p	318	LEU
1	p	401	PHE
1	q	318	LEU
1	q	401	PHE
1	r	318	LEU
1	r	401	PHE
1	s	318	LEU
1	s	401	PHE
1	t	318	LEU
1	t	401	PHE
1	u	318	LEU

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Mol	Chain	Res	Type
1	u	401	PHE
1	v	318	LEU
1	v	401	PHE
1	w	318	LEU
1	w	401	PHE
1	x	318	LEU
1	x	401	PHE
1	y	318	LEU
1	y	401	PHE
1	z	318	LEU
1	z	401	PHE
1	1	318	LEU
1	1	401	PHE
1	2	318	LEU
1	2	401	PHE
1	3	318	LEU
1	3	401	PHE
1	4	318	LEU
1	4	401	PHE
1	5	318	LEU
1	5	401	PHE
1	6	318	LEU
1	6	401	PHE
1	7	318	LEU
1	7	401	PHE
1	8	318	LEU
1	8	401	PHE
2	A2	47	PHE
2	A2	102	LEU
2	B2	47	PHE
2	B2	102	LEU
2	C2	47	PHE
2	C2	102	LEU
2	D2	47	PHE
2	D2	102	LEU
2	E2	47	PHE
2	E2	102	LEU
2	F2	47	PHE
2	F2	102	LEU
2	G2	47	PHE
2	G2	102	LEU
2	H2	47	PHE

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Mol	Chain	Res	Type
2	H2	102	LEU
2	I2	47	PHE
2	I2	102	LEU
2	J2	47	PHE
2	J2	102	LEU
2	K2	47	PHE
2	K2	102	LEU
2	L2	47	PHE
2	L2	102	LEU
2	M2	47	PHE
2	M2	102	LEU
2	N2	47	PHE
2	N2	102	LEU
2	O2	47	PHE
2	O2	102	LEU
2	P2	47	PHE
2	P2	102	LEU
2	Q2	47	PHE
2	Q2	102	LEU
2	R2	47	PHE
2	R2	102	LEU
2	S2	47	PHE
2	S2	102	LEU
2	T2	47	PHE
2	T2	102	LEU
2	U2	47	PHE
2	U2	102	LEU
2	V2	47	PHE
2	V2	102	LEU
2	W2	47	PHE
2	W2	102	LEU
2	X2	47	PHE
2	X2	102	LEU
2	Y2	47	PHE
2	Y2	102	LEU
2	Z2	47	PHE
2	Z2	102	LEU
2	a2	47	PHE
2	a2	102	LEU
2	b2	47	PHE
2	b2	102	LEU
2	c2	47	PHE

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Mol	Chain	Res	Type
2	c2	102	LEU
2	d2	47	PHE
2	d2	102	LEU
2	e2	47	PHE
2	e2	102	LEU
2	f2	47	PHE
2	f2	102	LEU
2	g2	47	PHE
2	g2	102	LEU
2	h2	47	PHE
2	h2	102	LEU
2	i2	47	PHE
2	i2	102	LEU
2	j2	47	PHE
2	j2	102	LEU
2	k2	47	PHE
2	k2	102	LEU
2	l2	47	PHE
2	l2	102	LEU
2	m2	47	PHE
2	m2	102	LEU
2	n2	47	PHE
2	n2	102	LEU
2	o2	47	PHE
2	o2	102	LEU
2	p2	47	PHE
2	p2	102	LEU
2	q2	47	PHE
2	q2	102	LEU
2	r2	47	PHE
2	r2	102	LEU
2	s2	47	PHE
2	s2	102	LEU
2	t2	47	PHE
2	t2	102	LEU
2	u2	47	PHE
2	u2	102	LEU
2	v2	47	PHE
2	v2	102	LEU
2	w2	47	PHE
2	w2	102	LEU
2	x2	47	PHE

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Mol	Chain	Res	Type
2	x2	102	LEU
2	y2	47	PHE
2	y2	102	LEU
2	z2	47	PHE
2	z2	102	LEU
2	12	47	PHE
2	12	102	LEU
2	22	47	PHE
2	22	102	LEU
2	32	47	PHE
2	32	102	LEU
2	42	47	PHE
2	42	102	LEU
2	52	47	PHE
2	52	102	LEU
2	62	47	PHE
2	62	102	LEU
2	72	47	PHE
2	72	102	LEU
2	82	47	PHE
2	82	102	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (653) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	328	GLN
1	A	475	ASN
1	A	548	GLN
1	A	587	GLN
1	A	601	GLN
1	A	610	GLN
1	A	653	ASN
1	A	665	ASN
1	B	328	GLN
1	B	475	ASN
1	B	548	GLN
1	B	587	GLN
1	B	601	GLN
1	B	610	GLN
1	B	653	ASN
1	B	665	ASN
1	C	328	GLN

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Mol	Chain	Res	Type
1	C	475	ASN
1	C	548	GLN
1	C	587	GLN
1	C	601	GLN
1	C	610	GLN
1	C	653	ASN
1	C	665	ASN
1	D	328	GLN
1	D	475	ASN
1	D	548	GLN
1	D	587	GLN
1	D	601	GLN
1	D	610	GLN
1	D	653	ASN
1	D	665	ASN
1	D	675	GLN
1	E	328	GLN
1	E	475	ASN
1	E	548	GLN
1	E	587	GLN
1	E	601	GLN
1	E	610	GLN
1	E	653	ASN
1	E	665	ASN
1	F	328	GLN
1	F	475	ASN
1	F	548	GLN
1	F	587	GLN
1	F	601	GLN
1	F	610	GLN
1	F	653	ASN
1	F	665	ASN
1	F	675	GLN
1	G	328	GLN
1	G	475	ASN
1	G	548	GLN
1	G	587	GLN
1	G	601	GLN
1	G	610	GLN
1	G	653	ASN
1	G	665	ASN
1	H	328	GLN

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Mol	Chain	Res	Type
1	H	475	ASN
1	H	548	GLN
1	H	587	GLN
1	H	601	GLN
1	H	610	GLN
1	H	653	ASN
1	H	665	ASN
1	I	328	GLN
1	I	475	ASN
1	I	548	GLN
1	I	587	GLN
1	I	601	GLN
1	I	610	GLN
1	I	653	ASN
1	I	665	ASN
1	I	675	GLN
1	J	328	GLN
1	J	475	ASN
1	J	548	GLN
1	J	587	GLN
1	J	601	GLN
1	J	610	GLN
1	J	653	ASN
1	J	665	ASN
1	K	328	GLN
1	K	475	ASN
1	K	548	GLN
1	K	587	GLN
1	K	601	GLN
1	K	610	GLN
1	K	653	ASN
1	K	665	ASN
1	L	328	GLN
1	L	475	ASN
1	L	548	GLN
1	L	587	GLN
1	L	601	GLN
1	L	610	GLN
1	L	653	ASN
1	L	665	ASN
1	L	675	GLN
1	M	328	GLN

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Mol	Chain	Res	Type
1	M	475	ASN
1	M	548	GLN
1	M	587	GLN
1	M	601	GLN
1	M	610	GLN
1	M	653	ASN
1	M	665	ASN
1	M	675	GLN
1	N	328	GLN
1	N	475	ASN
1	N	548	GLN
1	N	587	GLN
1	N	601	GLN
1	N	610	GLN
1	N	653	ASN
1	N	665	ASN
1	O	328	GLN
1	O	475	ASN
1	O	548	GLN
1	O	587	GLN
1	O	601	GLN
1	O	610	GLN
1	O	653	ASN
1	O	665	ASN
1	O	675	GLN
1	P	328	GLN
1	P	475	ASN
1	P	548	GLN
1	P	587	GLN
1	P	601	GLN
1	P	610	GLN
1	P	653	ASN
1	P	665	ASN
1	Q	328	GLN
1	Q	475	ASN
1	Q	548	GLN
1	Q	587	GLN
1	Q	601	GLN
1	Q	610	GLN
1	Q	653	ASN
1	Q	665	ASN
1	R	328	GLN

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Mol	Chain	Res	Type
1	R	475	ASN
1	R	548	GLN
1	R	587	GLN
1	R	601	GLN
1	R	610	GLN
1	R	653	ASN
1	R	665	ASN
1	R	675	GLN
1	S	328	GLN
1	S	475	ASN
1	S	548	GLN
1	S	587	GLN
1	S	601	GLN
1	S	610	GLN
1	S	653	ASN
1	S	665	ASN
1	T	328	GLN
1	T	475	ASN
1	T	548	GLN
1	T	587	GLN
1	T	601	GLN
1	T	610	GLN
1	T	653	ASN
1	T	665	ASN
1	U	328	GLN
1	U	475	ASN
1	U	548	GLN
1	U	587	GLN
1	U	601	GLN
1	U	610	GLN
1	U	653	ASN
1	U	665	ASN
1	U	675	GLN
1	V	328	GLN
1	V	475	ASN
1	V	548	GLN
1	V	587	GLN
1	V	601	GLN
1	V	610	GLN
1	V	653	ASN
1	V	665	ASN
1	W	328	GLN

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Mol	Chain	Res	Type
1	W	475	ASN
1	W	548	GLN
1	W	587	GLN
1	W	601	GLN
1	W	610	GLN
1	W	653	ASN
1	W	665	ASN
1	W	675	GLN
1	X	328	GLN
1	X	475	ASN
1	X	548	GLN
1	X	587	GLN
1	X	601	GLN
1	X	610	GLN
1	X	653	ASN
1	X	665	ASN
1	X	675	GLN
1	Y	328	GLN
1	Y	475	ASN
1	Y	548	GLN
1	Y	587	GLN
1	Y	601	GLN
1	Y	610	GLN
1	Y	653	ASN
1	Y	665	ASN
1	Y	675	GLN
1	Z	328	GLN
1	Z	475	ASN
1	Z	548	GLN
1	Z	587	GLN
1	Z	601	GLN
1	Z	610	GLN
1	Z	653	ASN
1	Z	665	ASN
1	a	328	GLN
1	a	475	ASN
1	a	548	GLN
1	a	587	GLN
1	a	601	GLN
1	a	610	GLN
1	a	653	ASN
1	a	665	ASN

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Mol	Chain	Res	Type
1	a	675	GLN
1	b	328	GLN
1	b	475	ASN
1	b	548	GLN
1	b	587	GLN
1	b	601	GLN
1	b	610	GLN
1	b	653	ASN
1	b	665	ASN
1	c	328	GLN
1	c	475	ASN
1	c	548	GLN
1	c	587	GLN
1	c	601	GLN
1	c	610	GLN
1	c	653	ASN
1	c	665	ASN
1	d	328	GLN
1	d	475	ASN
1	d	548	GLN
1	d	587	GLN
1	d	601	GLN
1	d	610	GLN
1	d	653	ASN
1	d	665	ASN
1	e	328	GLN
1	e	475	ASN
1	e	548	GLN
1	e	587	GLN
1	e	601	GLN
1	e	610	GLN
1	e	653	ASN
1	e	665	ASN
1	e	675	GLN
1	f	328	GLN
1	f	475	ASN
1	f	548	GLN
1	f	587	GLN
1	f	601	GLN
1	f	610	GLN
1	f	653	ASN
1	f	665	ASN

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Mol	Chain	Res	Type
1	g	328	GLN
1	g	475	ASN
1	g	548	GLN
1	g	549	ASN
1	g	587	GLN
1	g	601	GLN
1	g	610	GLN
1	g	653	ASN
1	g	665	ASN
1	h	328	GLN
1	h	475	ASN
1	h	548	GLN
1	h	587	GLN
1	h	601	GLN
1	h	610	GLN
1	h	653	ASN
1	h	665	ASN
1	i	328	GLN
1	i	475	ASN
1	i	548	GLN
1	i	587	GLN
1	i	601	GLN
1	i	610	GLN
1	i	653	ASN
1	i	665	ASN
1	i	675	GLN
1	j	328	GLN
1	j	475	ASN
1	j	548	GLN
1	j	587	GLN
1	j	601	GLN
1	j	610	GLN
1	j	653	ASN
1	j	665	ASN
1	k	328	GLN
1	k	475	ASN
1	k	548	GLN
1	k	587	GLN
1	k	601	GLN
1	k	610	GLN
1	k	653	ASN
1	k	665	ASN

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Mol	Chain	Res	Type
1	k	675	GLN
1	l	328	GLN
1	l	475	ASN
1	l	548	GLN
1	l	587	GLN
1	l	601	GLN
1	l	610	GLN
1	l	653	ASN
1	l	665	ASN
1	l	675	GLN
1	m	328	GLN
1	m	475	ASN
1	m	548	GLN
1	m	587	GLN
1	m	601	GLN
1	m	610	GLN
1	m	653	ASN
1	m	665	ASN
1	n	328	GLN
1	n	475	ASN
1	n	548	GLN
1	n	587	GLN
1	n	601	GLN
1	n	610	GLN
1	n	653	ASN
1	n	665	ASN
1	o	328	GLN
1	o	475	ASN
1	o	548	GLN
1	o	587	GLN
1	o	601	GLN
1	o	610	GLN
1	o	653	ASN
1	o	665	ASN
1	p	328	GLN
1	p	475	ASN
1	p	548	GLN
1	p	587	GLN
1	p	601	GLN
1	p	610	GLN
1	p	653	ASN
1	p	665	ASN

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Mol	Chain	Res	Type
1	p	675	GLN
1	q	328	GLN
1	q	475	ASN
1	q	548	GLN
1	q	587	GLN
1	q	601	GLN
1	q	610	GLN
1	q	653	ASN
1	q	665	ASN
1	r	328	GLN
1	r	475	ASN
1	r	548	GLN
1	r	587	GLN
1	r	601	GLN
1	r	610	GLN
1	r	653	ASN
1	r	665	ASN
1	r	675	GLN
1	s	328	GLN
1	s	475	ASN
1	s	548	GLN
1	s	587	GLN
1	s	601	GLN
1	s	610	GLN
1	s	653	ASN
1	s	665	ASN
1	s	675	GLN
1	t	328	GLN
1	t	475	ASN
1	t	548	GLN
1	t	587	GLN
1	t	601	GLN
1	t	610	GLN
1	t	653	ASN
1	t	665	ASN
1	t	675	GLN
1	u	328	GLN
1	u	475	ASN
1	u	548	GLN
1	u	587	GLN
1	u	601	GLN
1	u	610	GLN

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Mol	Chain	Res	Type
1	u	653	ASN
1	u	665	ASN
1	u	675	GLN
1	v	328	GLN
1	v	475	ASN
1	v	548	GLN
1	v	587	GLN
1	v	601	GLN
1	v	610	GLN
1	v	653	ASN
1	v	665	ASN
1	v	675	GLN
1	w	328	GLN
1	w	475	ASN
1	w	548	GLN
1	w	587	GLN
1	w	601	GLN
1	w	610	GLN
1	w	653	ASN
1	w	665	ASN
1	w	675	GLN
1	x	328	GLN
1	x	475	ASN
1	x	548	GLN
1	x	587	GLN
1	x	601	GLN
1	x	610	GLN
1	x	653	ASN
1	x	665	ASN
1	y	328	GLN
1	y	475	ASN
1	y	548	GLN
1	y	587	GLN
1	y	601	GLN
1	y	610	GLN
1	y	653	ASN
1	y	665	ASN
1	y	675	GLN
1	z	328	GLN
1	z	475	ASN
1	z	548	GLN
1	z	587	GLN

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Mol	Chain	Res	Type
1	z	601	GLN
1	z	610	GLN
1	z	653	ASN
1	z	665	ASN
1	z	675	GLN
1	1	328	GLN
1	1	475	ASN
1	1	548	GLN
1	1	587	GLN
1	1	601	GLN
1	1	610	GLN
1	1	653	ASN
1	1	665	ASN
1	2	328	GLN
1	2	475	ASN
1	2	548	GLN
1	2	587	GLN
1	2	601	GLN
1	2	610	GLN
1	2	653	ASN
1	2	665	ASN
1	3	328	GLN
1	3	475	ASN
1	3	548	GLN
1	3	587	GLN
1	3	601	GLN
1	3	610	GLN
1	3	653	ASN
1	3	665	ASN
1	3	675	GLN
1	4	328	GLN
1	4	475	ASN
1	4	548	GLN
1	4	587	GLN
1	4	601	GLN
1	4	610	GLN
1	4	653	ASN
1	4	665	ASN
1	4	675	GLN
1	5	328	GLN
1	5	475	ASN
1	5	548	GLN

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Mol	Chain	Res	Type
1	5	587	GLN
1	5	601	GLN
1	5	610	GLN
1	5	653	ASN
1	5	665	ASN
1	5	675	GLN
1	6	328	GLN
1	6	475	ASN
1	6	548	GLN
1	6	587	GLN
1	6	601	GLN
1	6	610	GLN
1	6	653	ASN
1	6	665	ASN
1	6	675	GLN
1	7	328	GLN
1	7	475	ASN
1	7	548	GLN
1	7	587	GLN
1	7	601	GLN
1	7	610	GLN
1	7	653	ASN
1	7	665	ASN
1	8	328	GLN
1	8	475	ASN
1	8	548	GLN
1	8	587	GLN
1	8	601	GLN
1	8	610	GLN
1	8	653	ASN
1	8	665	ASN
1	8	675	GLN
2	A2	13	GLN
2	A2	29	HIS
2	B2	13	GLN
2	B2	29	HIS
2	B2	51	GLN
2	C2	13	GLN
2	C2	29	HIS
2	D2	13	GLN
2	D2	29	HIS
2	D2	51	GLN

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Mol	Chain	Res	Type
2	E2	13	GLN
2	E2	29	HIS
2	F2	13	GLN
2	F2	29	HIS
2	G2	13	GLN
2	G2	29	HIS
2	H2	13	GLN
2	H2	29	HIS
2	H2	51	GLN
2	I2	13	GLN
2	I2	29	HIS
2	I2	51	GLN
2	J2	13	GLN
2	J2	29	HIS
2	J2	51	GLN
2	K2	13	GLN
2	K2	29	HIS
2	L2	13	GLN
2	L2	29	HIS
2	M2	13	GLN
2	M2	29	HIS
2	M2	51	GLN
2	N2	13	GLN
2	N2	29	HIS
2	O2	13	GLN
2	O2	29	HIS
2	O2	51	GLN
2	P2	13	GLN
2	P2	29	HIS
2	P2	51	GLN
2	Q2	13	GLN
2	Q2	29	HIS
2	R2	13	GLN
2	R2	29	HIS
2	S2	13	GLN
2	S2	29	HIS
2	T2	13	GLN
2	T2	29	HIS
2	T2	51	GLN
2	U2	13	GLN
2	U2	29	HIS
2	U2	51	GLN

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Mol	Chain	Res	Type
2	V2	13	GLN
2	V2	29	HIS
2	W2	13	GLN
2	W2	29	HIS
2	W2	51	GLN
2	X2	13	GLN
2	X2	29	HIS
2	Y2	13	GLN
2	Y2	29	HIS
2	Z2	13	GLN
2	Z2	29	HIS
2	a2	13	GLN
2	a2	29	HIS
2	a2	51	GLN
2	b2	13	GLN
2	b2	29	HIS
2	b2	51	GLN
2	c2	13	GLN
2	c2	29	HIS
2	d2	13	GLN
2	d2	29	HIS
2	e2	13	GLN
2	e2	29	HIS
2	f2	13	GLN
2	f2	29	HIS
2	g2	13	GLN
2	g2	29	HIS
2	h2	13	GLN
2	h2	29	HIS
2	h2	51	GLN
2	i2	13	GLN
2	i2	29	HIS
2	j2	13	GLN
2	j2	29	HIS
2	k2	13	GLN
2	k2	29	HIS
2	l2	13	GLN
2	l2	29	HIS
2	l2	51	GLN
2	m2	13	GLN
2	m2	29	HIS
2	m2	51	GLN

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Mol	Chain	Res	Type
2	n2	13	GLN
2	n2	29	HIS
2	n2	51	GLN
2	o2	13	GLN
2	o2	29	HIS
2	p2	13	GLN
2	p2	29	HIS
2	q2	13	GLN
2	q2	29	HIS
2	r2	13	GLN
2	r2	29	HIS
2	s2	13	GLN
2	s2	29	HIS
2	t2	13	GLN
2	t2	29	HIS
2	u2	13	GLN
2	u2	29	HIS
2	v2	13	GLN
2	v2	29	HIS
2	w2	13	GLN
2	w2	29	HIS
2	x2	13	GLN
2	x2	29	HIS
2	x2	51	GLN
2	y2	13	GLN
2	y2	29	HIS
2	y2	51	GLN
2	z2	13	GLN
2	z2	29	HIS
2	12	13	GLN
2	22	13	GLN
2	22	29	HIS
2	32	13	GLN
2	32	29	HIS
2	32	51	GLN
2	42	13	GLN
2	42	29	HIS
2	42	51	GLN
2	52	13	GLN
2	52	29	HIS
2	52	51	GLN
2	62	13	GLN

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Mol	Chain	Res	Type
2	62	29	HIS
2	72	13	GLN
2	72	29	HIS
2	82	13	GLN
2	82	29	HIS
2	82	51	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

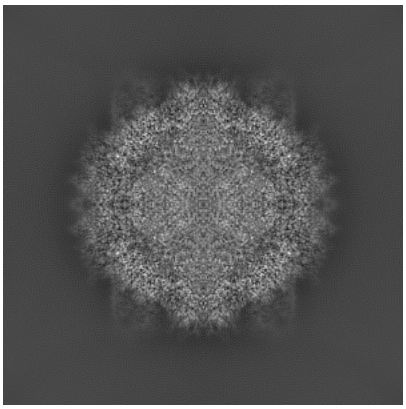
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-46741. These allow visual inspection of the internal detail of the map and identification of artifacts.

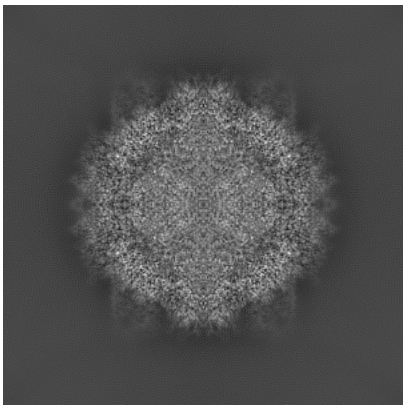
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

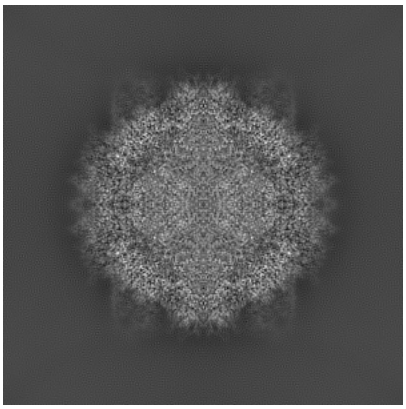
6.1.1 Primary map



X

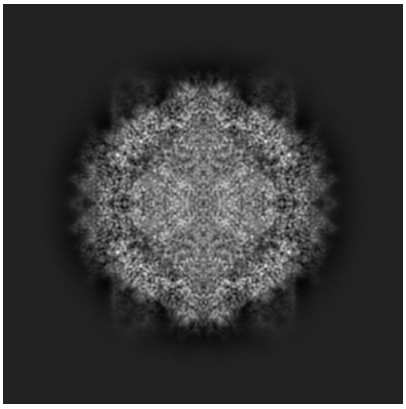


Y

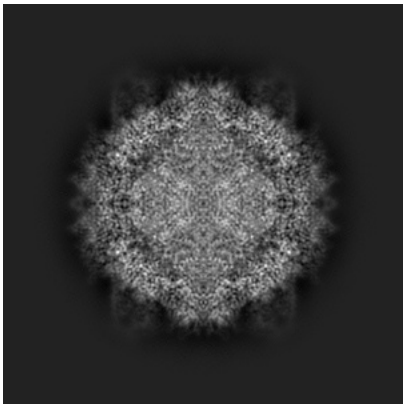


Z

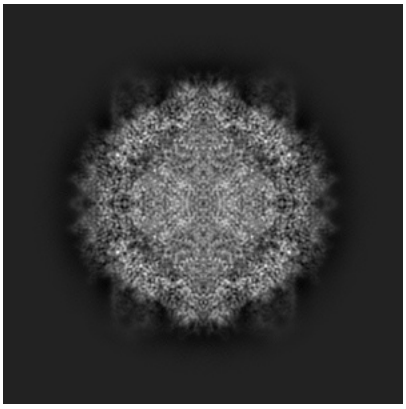
6.1.2 Raw map



X



Y

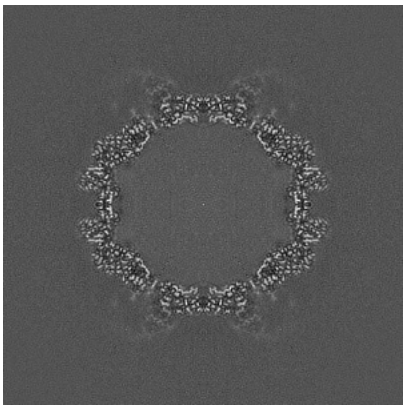


Z

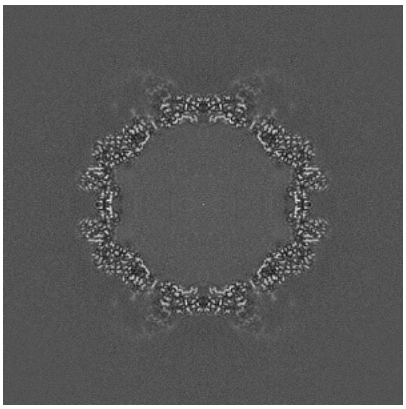
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

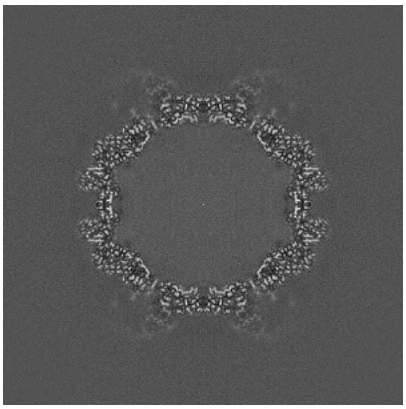
6.2.1 Primary map



X Index: 250

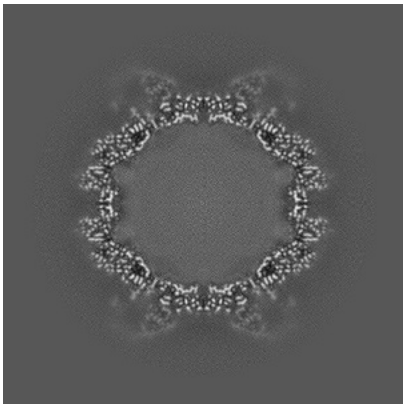


Y Index: 250

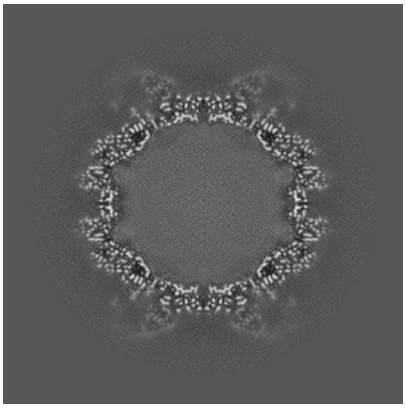


Z Index: 250

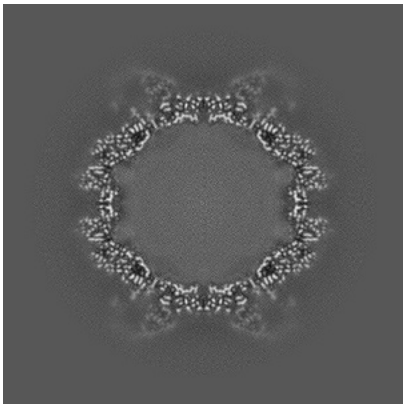
6.2.2 Raw map



X Index: 250



Y Index: 250

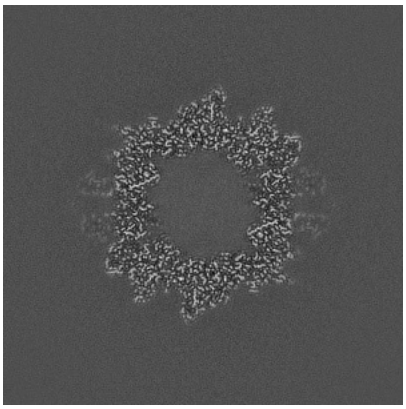


Z Index: 250

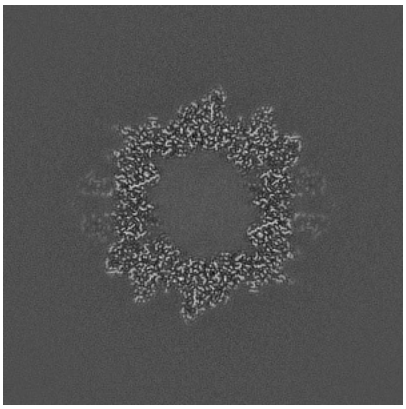
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

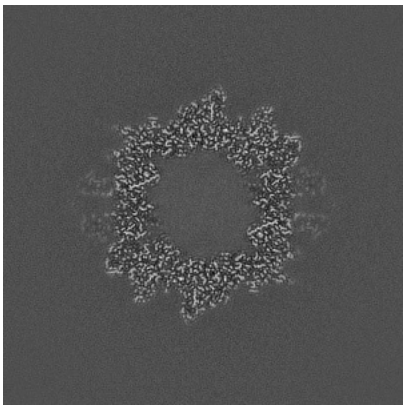
6.3.1 Primary map



X Index: 329

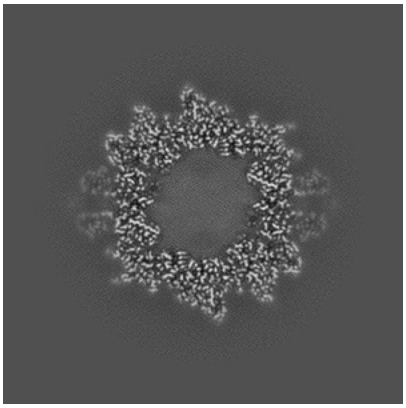


Y Index: 329

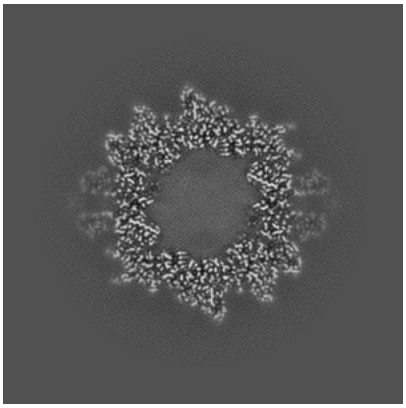


Z Index: 329

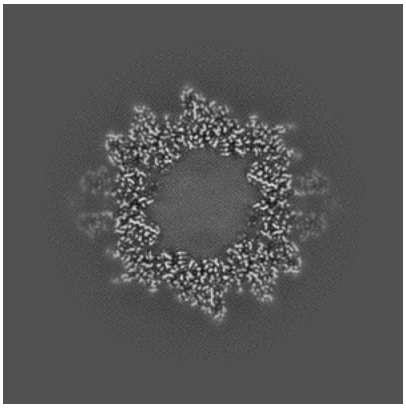
6.3.2 Raw map



X Index: 171



Y Index: 171

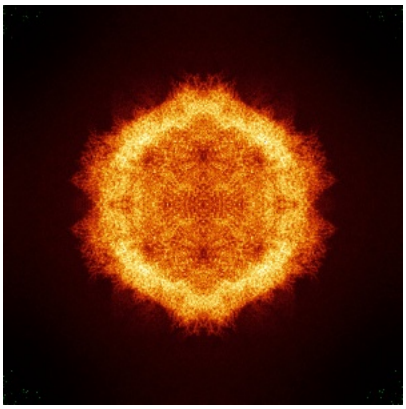


Z Index: 171

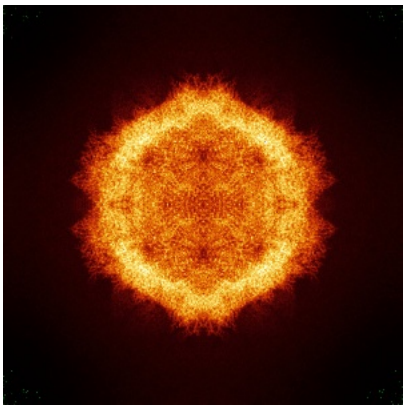
The images above show the largest variance slices of the map in three orthogonal directions.

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

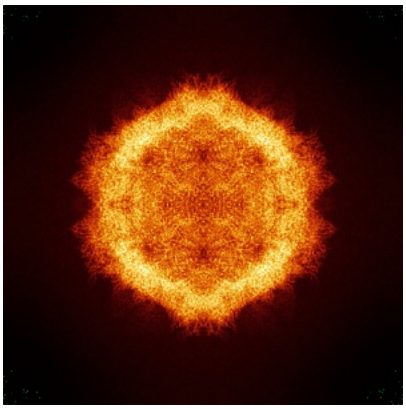
6.4.1 Primary map



X

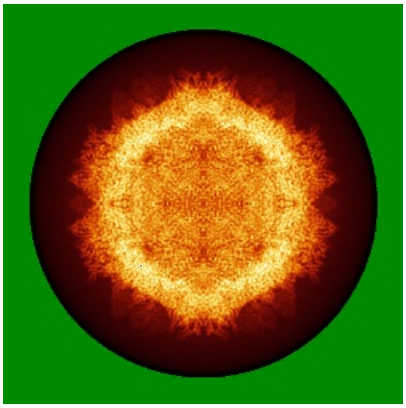


Y

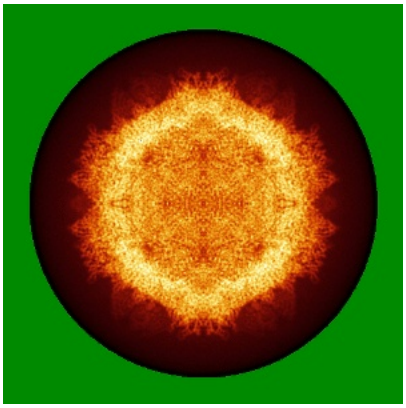


Z

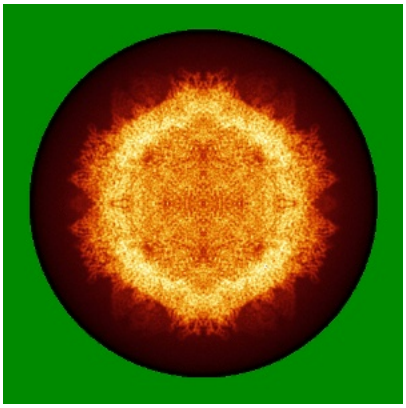
6.4.2 Raw map



X



Y

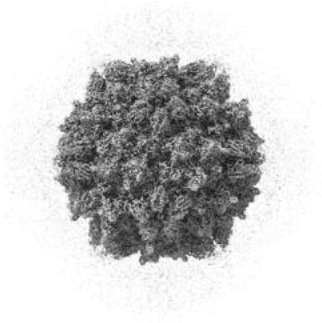


Z

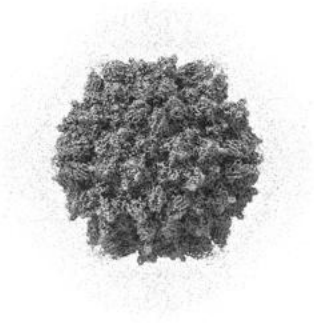
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

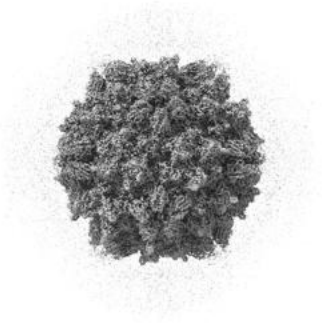
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X

Y

Z

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

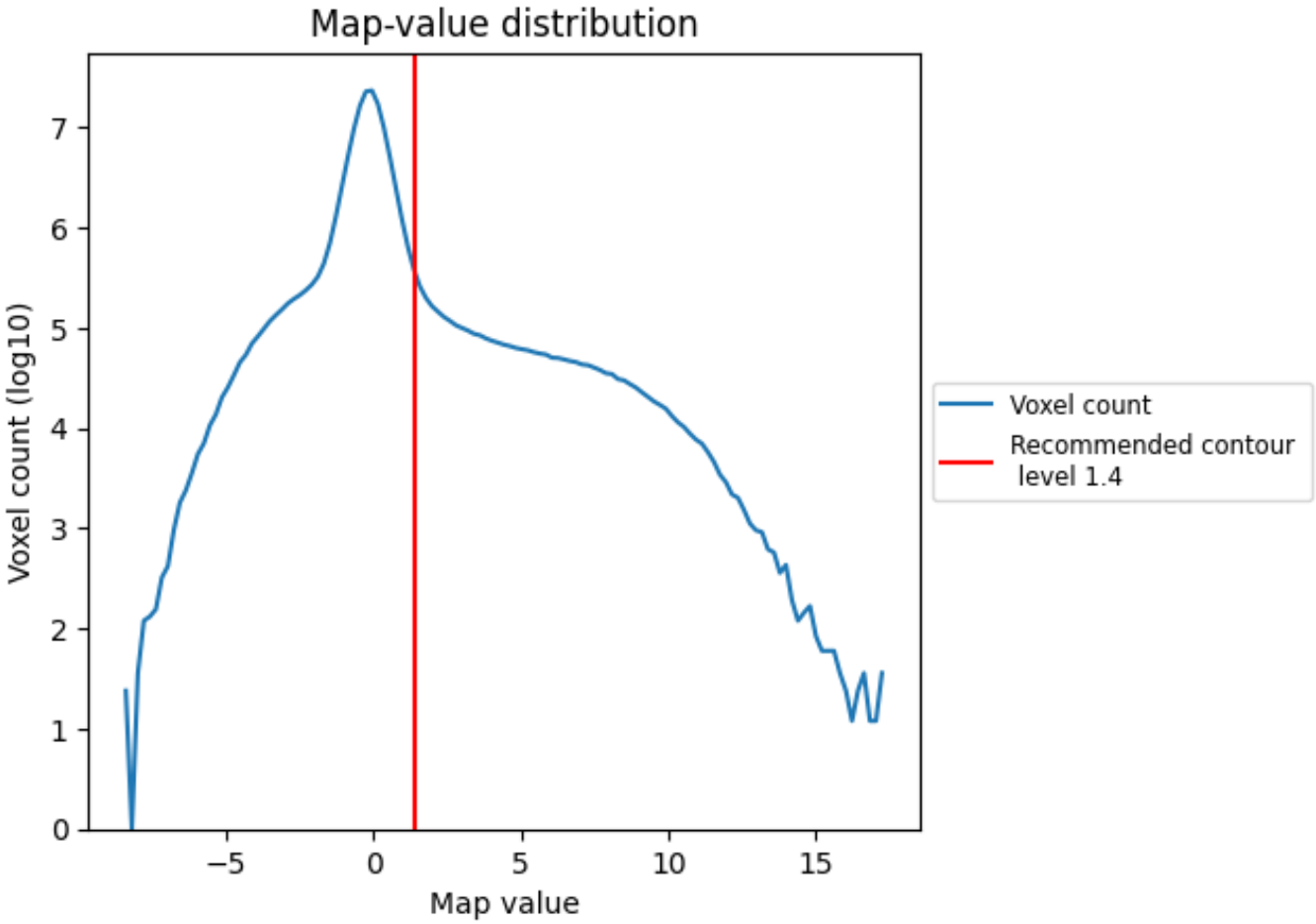
6.6 Mask visualisation (i)

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

7 Map analysis

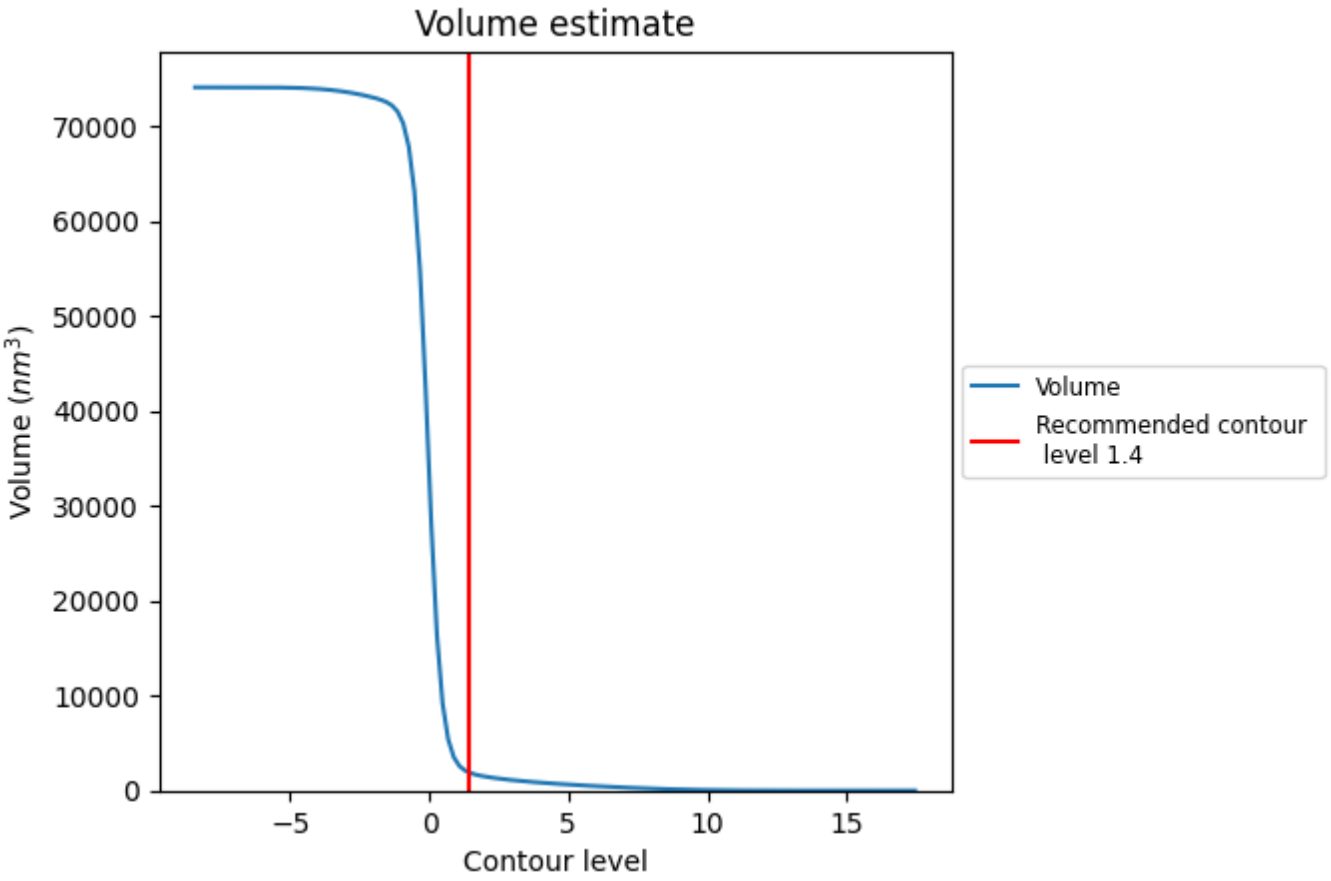
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

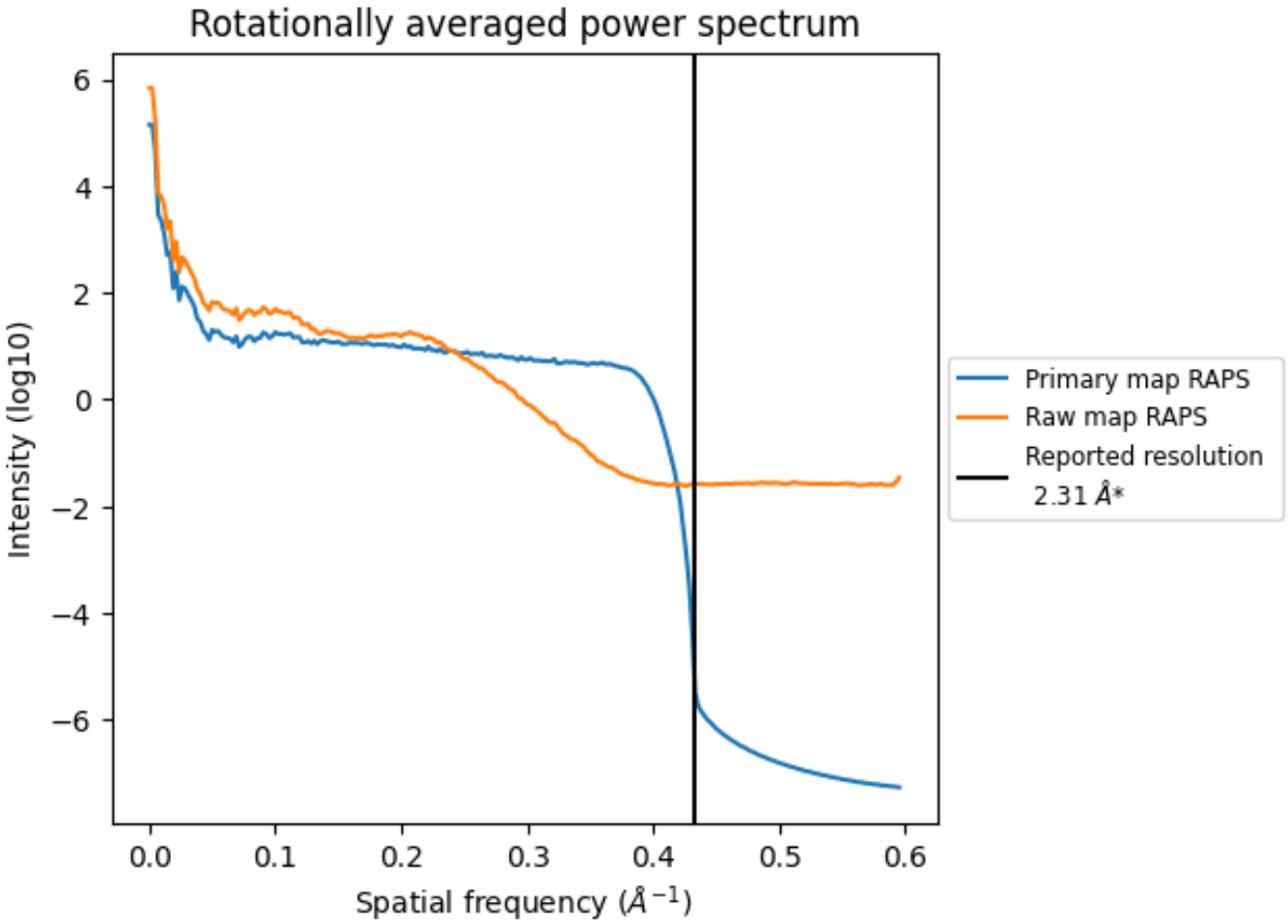
7.2 Volume estimate



The volume at the recommended contour level is 1963 nm^3; this corresponds to an approximate mass of 1773 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)

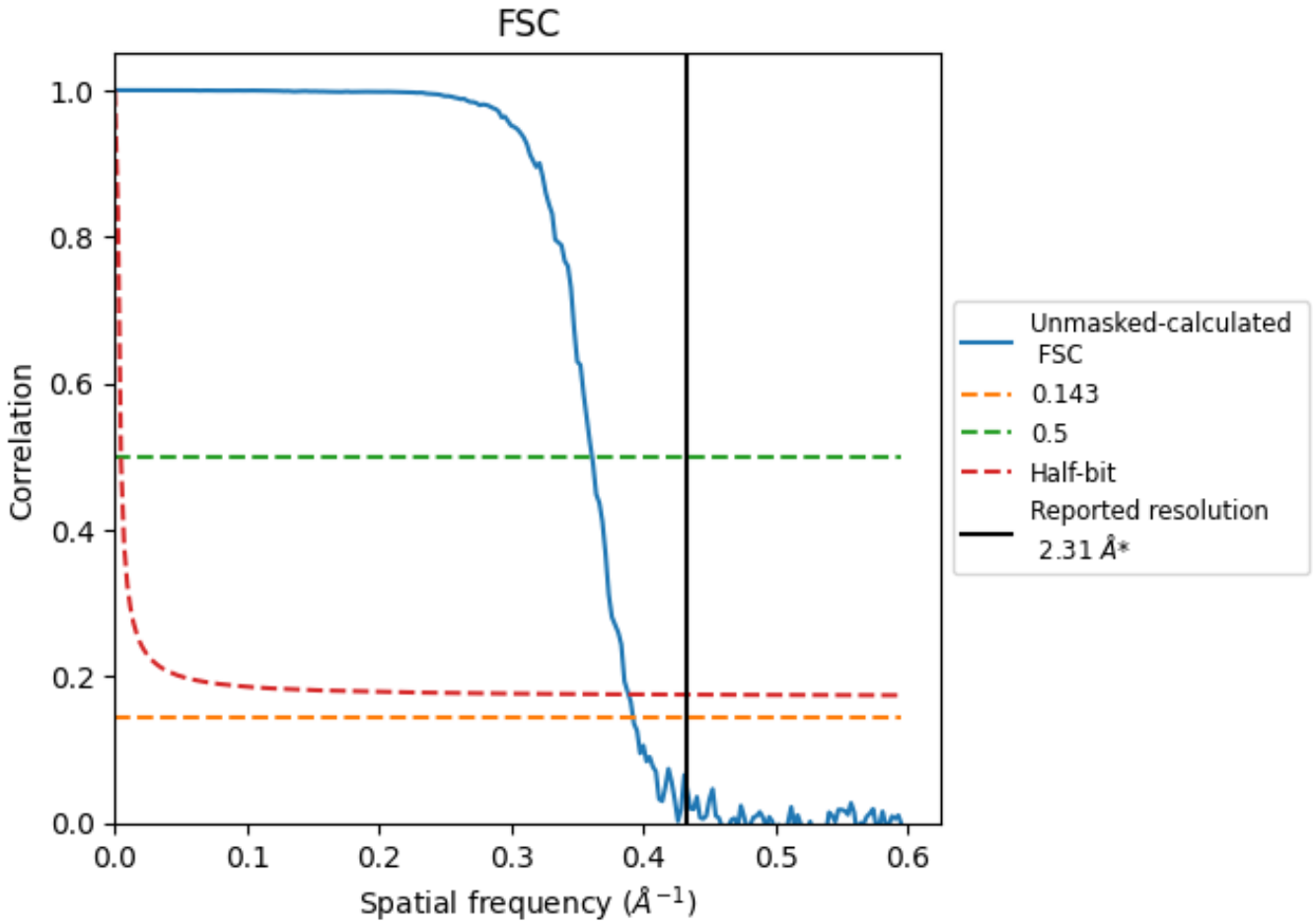


*Reported resolution corresponds to spatial frequency of 0.433 Å^{-1}

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 0.433 Å^{-1}

8.2 Resolution estimates (i)

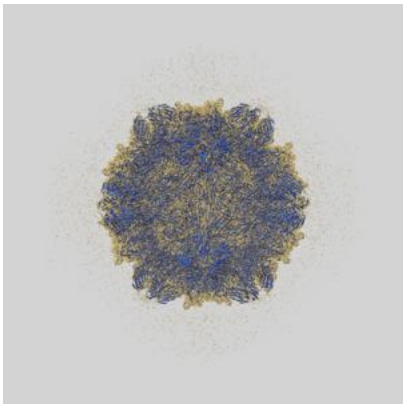
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.31	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.55	2.77	2.57

*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 2.55 differs from the reported value 2.31 by more than 10 %

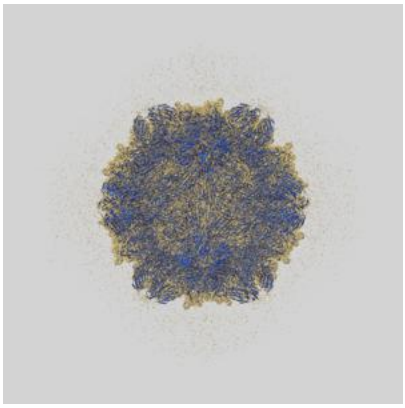
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-46741 and PDB model 9DC3. Per-residue inclusion information can be found in section 3 on page 14.

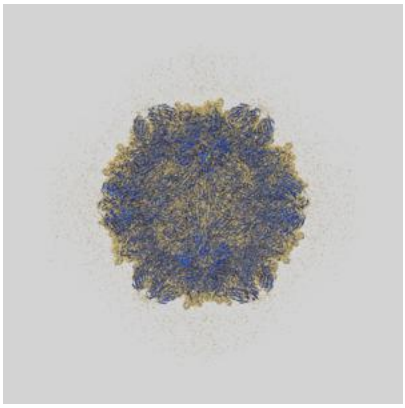
9.1 Map-model overlay



X



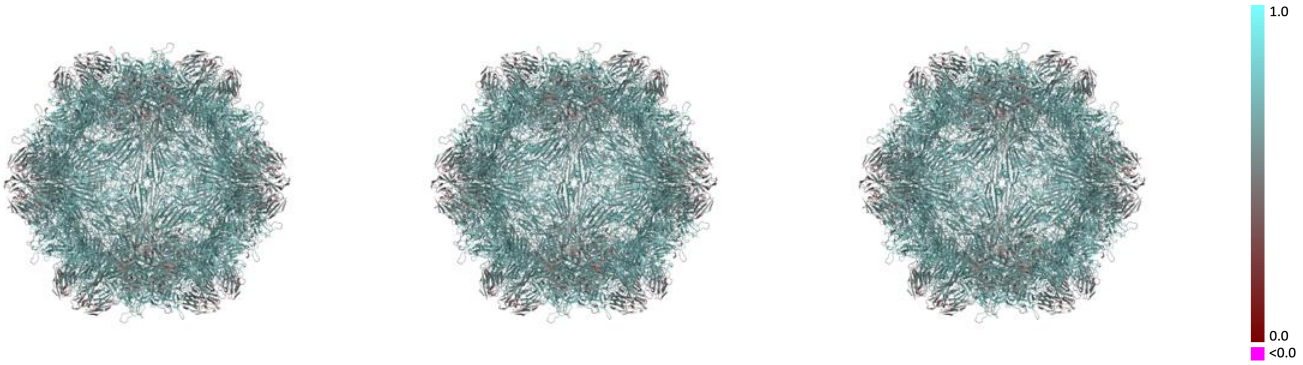
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.4 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.

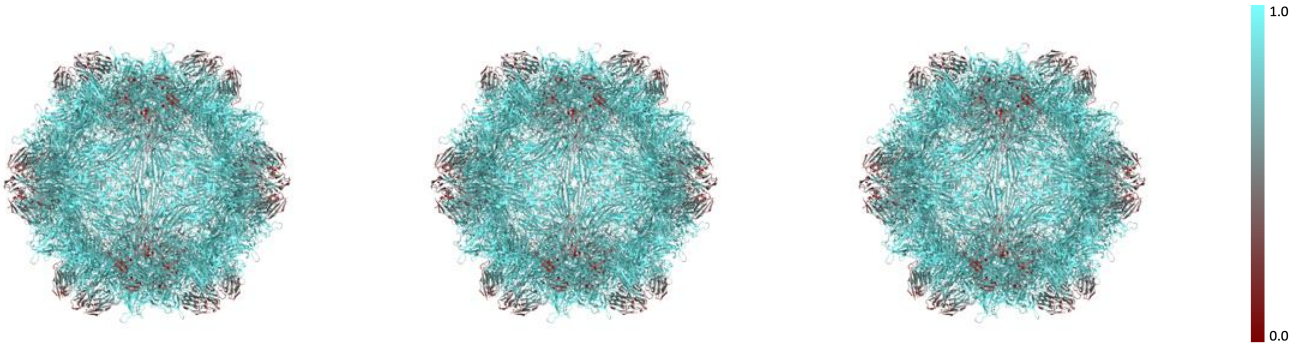
9.2 Q-score mapped to coordinate model (i)



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.

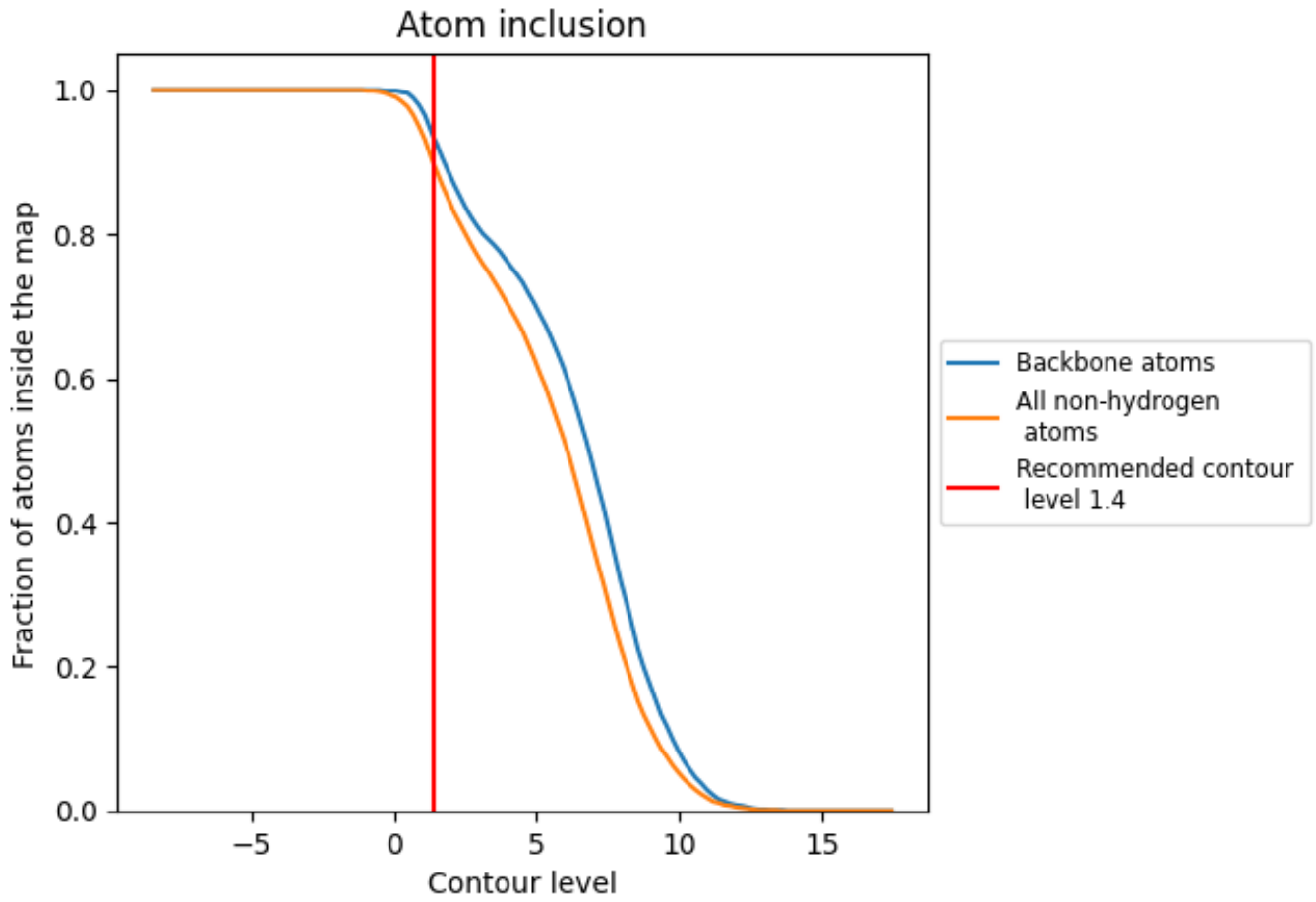
9.3 Atom inclusion mapped to coordinate model (i)



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 (1.4).

9.4 Atom inclusion (i)



At the recommended contour level, 93% of all backbone atoms, 90% 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 (1.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8960	0.6610
1	0.9740	0.6920
12	0.5520	0.5200
2	0.9740	0.6920
22	0.5580	0.5250
3	0.9750	0.6920
32	0.5540	0.5270
4	0.9750	0.6910
42	0.5540	0.5270
5	0.9740	0.6910
52	0.5550	0.5280
6	0.9740	0.6930
62	0.5580	0.5240
7	0.9730	0.6910
72	0.5610	0.5250
8	0.9730	0.6920
82	0.5610	0.5240
A	0.9740	0.6920
A2	0.5580	0.5290
B	0.9730	0.6910
B2	0.5540	0.5270
C	0.9740	0.6920
C2	0.5560	0.5240
D	0.9730	0.6920
D2	0.5600	0.5260
E	0.9750	0.6920
E2	0.5540	0.5260
F	0.9750	0.6910
F2	0.5540	0.5230
G	0.9730	0.6910
G2	0.5610	0.5220
H	0.9730	0.6910
H2	0.5610	0.5260
I	0.9740	0.6910
I2	0.5550	0.5250

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Chain	Atom inclusion	Q-score
J	0.9730	0.6910
J2	0.5540	0.5260
K	0.9740	0.6920
K2	0.5550	0.5270
L	0.9730	0.6910
L2	0.5540	0.5250
M	0.9730	0.6910
M2	0.5600	0.5250
N	0.9740	0.6920
N2	0.5560	0.5260
O	0.9730	0.6910
O2	0.5540	0.5280
P	0.9740	0.6920
P2	0.5580	0.5260
Q	0.9750	0.6920
Q2	0.5540	0.5280
R	0.9740	0.6920
R2	0.5580	0.5260
S	0.9730	0.6920
S2	0.5610	0.5250
T	0.9730	0.6910
T2	0.5600	0.5230
U	0.9740	0.6910
U2	0.5550	0.5270
V	0.9730	0.6910
V2	0.5540	0.5260
W	0.9740	0.6900
W2	0.5560	0.5260
X	0.9730	0.6910
X2	0.5550	0.5250
Y	0.9740	0.6910
Y2	0.5580	0.5280
Z	0.9750	0.6910
Z2	0.5540	0.5250
a	0.9740	0.6920
a2	0.5580	0.5250
b	0.9740	0.6920
b2	0.5580	0.5270
c	0.9750	0.6910
c2	0.5540	0.5270
d	0.9740	0.6910
d2	0.5550	0.5240

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Chain	Atom inclusion	Q-score
e	0.9730	0.6910
e2	0.5540	0.5280
f	0.9740	0.6920
f2	0.5560	0.5240
g	0.9730	0.6910
g2	0.5610	0.5270
h	0.9740	0.6920
h2	0.5580	0.5250
i	0.9750	0.6920
i2	0.5540	0.5280
j	0.9750	0.6920
j2	0.5540	0.5240
k	0.9750	0.6920
k2	0.5540	0.5270
l	0.9740	0.6920
l2	0.5580	0.5270
m	0.9730	0.6910
m2	0.5540	0.5240
n	0.9730	0.6910
n2	0.5520	0.5260
o	0.9750	0.6920
o2	0.5540	0.5260
p	0.9750	0.6900
p2	0.5540	0.5250
q	0.9730	0.6910
q2	0.5600	0.5250
r	0.9740	0.6900
r2	0.5550	0.5250
s	0.9740	0.6910
s2	0.5580	0.5280
t	0.9730	0.6910
t2	0.5540	0.5250
u	0.9730	0.6910
u2	0.5540	0.5240
v	0.9730	0.6910
v2	0.5560	0.5270
w	0.9740	0.6920
w2	0.5580	0.5270
x	0.9730	0.6910
x2	0.5610	0.5250
y	0.9740	0.6900
y2	0.5550	0.5270

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Chain	Atom inclusion	Q-score
z	0.9730	0.6910
z2	0.5610	0.5250