



Full wwPDB EM Validation Report ⓘ

Oct 31, 2022 – 03:38 PM EDT

PDB ID : 8EP9
EMDB ID : EMD-28522
Title : The capsid structure of Human Parvovirus 4
Authors : Mietzsch, M.; McKenna, R.
Deposited on : 2022-10-05
Resolution : 3.12 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

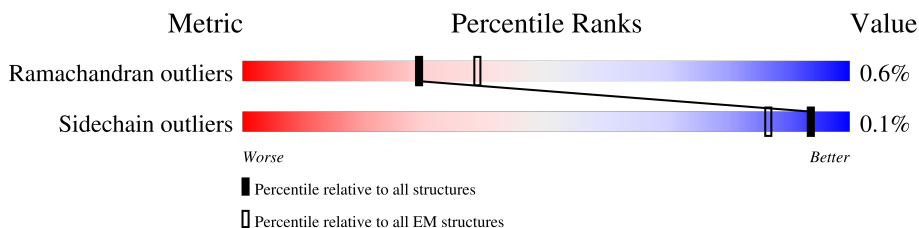
EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.12 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	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	1	552	5% 95% . .
1	2	552	5% 95% . .
1	3	552	5% 95% . .
1	4	552	6% 95% . .
1	5	552	6% 95% . .
1	6	552	6% 95% . .
1	7	552	6% 95% . .
1	8	552	5% 95% . .
1	A	552	5% 95% . .

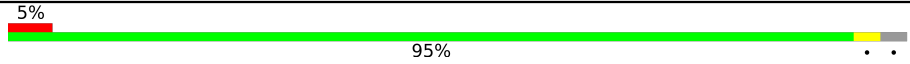
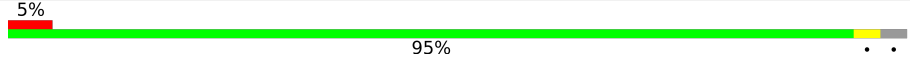
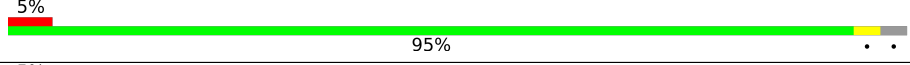
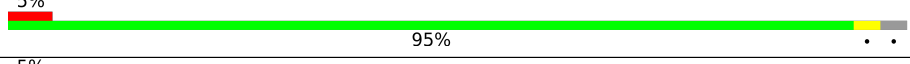
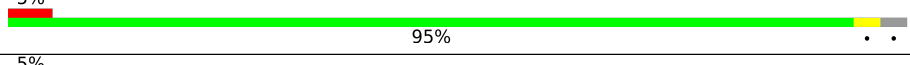
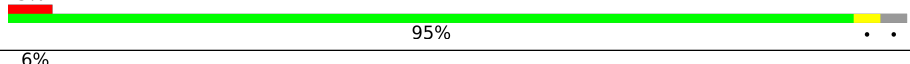
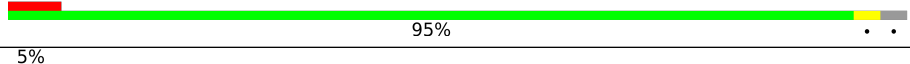
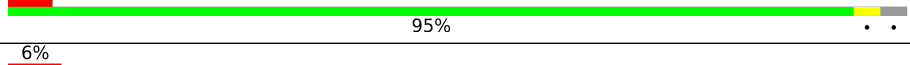
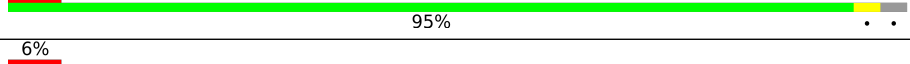
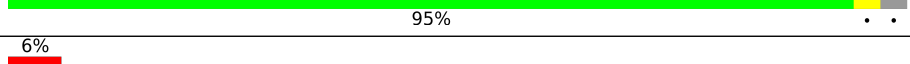
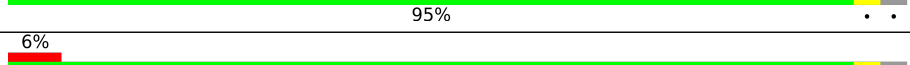

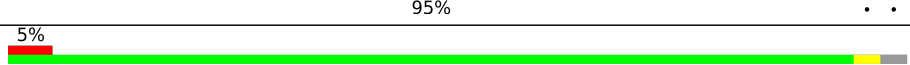
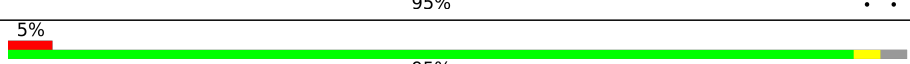
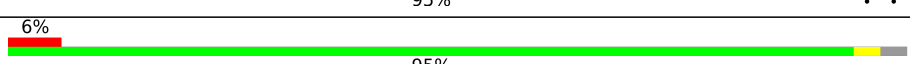
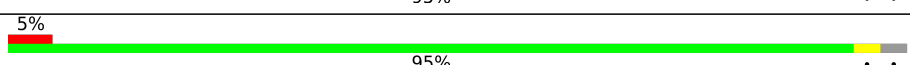
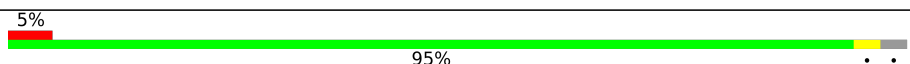
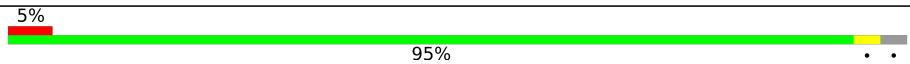
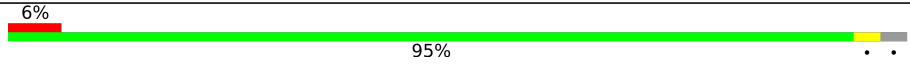
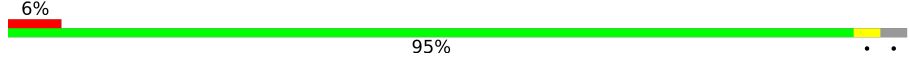
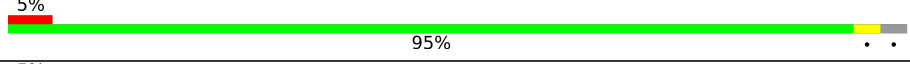
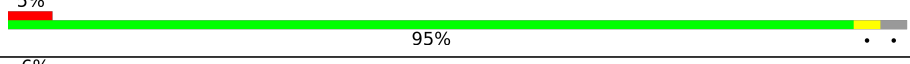
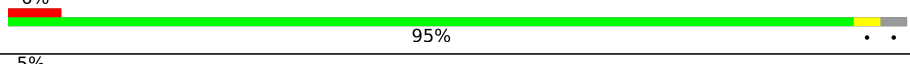
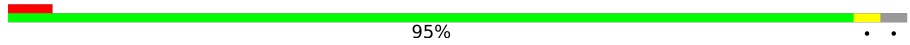

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	B	552	5% 95% ..
1	C	552	6% 95% ..
1	D	552	6% 95% ..
1	E	552	5% 95% ..
1	F	552	5% 95% ..
1	G	552	5% 95% ..
1	H	552	6% 95% ..
1	I	552	6% 95% ..
1	J	552	5% 95% ..
1	K	552	6% 95% ..
1	L	552	5% 95% ..
1	M	552	5% 95% ..
1	N	552	6% 95% ..
1	O	552	5% 95% ..
1	P	552	6% 95% ..
1	Q	552	6% 95% ..
1	R	552	5% 95% ..
1	S	552	5% 95% ..
1	T	552	6% 95% ..
1	U	552	5% 95% ..
1	V	552	6% 95% ..
1	W	552	6% 95% ..
1	X	552	5% 95% ..
1	Y	552	6% 95% ..
1	Z	552	5% 95% ..

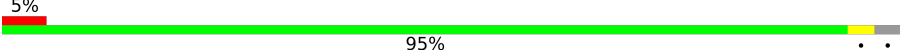
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	a	552	
1	b	552	
1	c	552	
1	d	552	
1	e	552	
1	f	552	
1	g	552	
1	h	552	
1	i	552	
1	j	552	
1	k	552	
1	l	552	
1	m	552	
1	n	552	
1	o	552	
1	p	552	
1	q	552	
1	r	552	
1	s	552	
1	t	552	
1	u	552	
1	v	552	
1	w	552	
1	x	552	
1	y	552	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	z	552	 5% 95% . .

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 256320 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 Human Parvovirus 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	538	4272	2711	746	802	13	0	0
1	B	538	4272	2711	746	802	13	0	0
1	C	538	4272	2711	746	802	13	0	0
1	D	538	4272	2711	746	802	13	0	0
1	E	538	4272	2711	746	802	13	0	0
1	F	538	4272	2711	746	802	13	0	0
1	G	538	4272	2711	746	802	13	0	0
1	H	538	4272	2711	746	802	13	0	0
1	I	538	4272	2711	746	802	13	0	0
1	J	538	4272	2711	746	802	13	0	0
1	K	538	4272	2711	746	802	13	0	0
1	L	538	4272	2711	746	802	13	0	0
1	M	538	4272	2711	746	802	13	0	0
1	N	538	4272	2711	746	802	13	0	0
1	O	538	4272	2711	746	802	13	0	0
1	P	538	4272	2711	746	802	13	0	0
1	Q	538	4272	2711	746	802	13	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	538	Total	C	N	O	S	0	0
			4272	2711	746	802	13		
1	S	538	Total	C	N	O	S	0	0
			4272	2711	746	802	13		
1	T	538	Total	C	N	O	S	0	0
			4272	2711	746	802	13		
1	U	538	Total	C	N	O	S	0	0
			4272	2711	746	802	13		
1	V	538	Total	C	N	O	S	0	0
			4272	2711	746	802	13		
1	W	538	Total	C	N	O	S	0	0
			4272	2711	746	802	13		
1	X	538	Total	C	N	O	S	0	0
			4272	2711	746	802	13		
1	Y	538	Total	C	N	O	S	0	0
			4272	2711	746	802	13		
1	Z	538	Total	C	N	O	S	0	0
			4272	2711	746	802	13		
1	a	538	Total	C	N	O	S	0	0
			4272	2711	746	802	13		
1	b	538	Total	C	N	O	S	0	0
			4272	2711	746	802	13		
1	c	538	Total	C	N	O	S	0	0
			4272	2711	746	802	13		
1	d	538	Total	C	N	O	S	0	0
			4272	2711	746	802	13		
1	e	538	Total	C	N	O	S	0	0
			4272	2711	746	802	13		
1	f	538	Total	C	N	O	S	0	0
			4272	2711	746	802	13		
1	g	538	Total	C	N	O	S	0	0
			4272	2711	746	802	13		
1	h	538	Total	C	N	O	S	0	0
			4272	2711	746	802	13		
1	i	538	Total	C	N	O	S	0	0
			4272	2711	746	802	13		
1	j	538	Total	C	N	O	S	0	0
			4272	2711	746	802	13		
1	k	538	Total	C	N	O	S	0	0
			4272	2711	746	802	13		
1	l	538	Total	C	N	O	S	0	0
			4272	2711	746	802	13		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	m	538	Total	C	N	O	S	0	0
			4272	2711	746	802	13		
1	n	538	Total	C	N	O	S	0	0
			4272	2711	746	802	13		
1	o	538	Total	C	N	O	S	0	0
			4272	2711	746	802	13		
1	p	538	Total	C	N	O	S	0	0
			4272	2711	746	802	13		
1	q	538	Total	C	N	O	S	0	0
			4272	2711	746	802	13		
1	r	538	Total	C	N	O	S	0	0
			4272	2711	746	802	13		
1	s	538	Total	C	N	O	S	0	0
			4272	2711	746	802	13		
1	t	538	Total	C	N	O	S	0	0
			4272	2711	746	802	13		
1	u	538	Total	C	N	O	S	0	0
			4272	2711	746	802	13		
1	v	538	Total	C	N	O	S	0	0
			4272	2711	746	802	13		
1	w	538	Total	C	N	O	S	0	0
			4272	2711	746	802	13		
1	x	538	Total	C	N	O	S	0	0
			4272	2711	746	802	13		
1	y	538	Total	C	N	O	S	0	0
			4272	2711	746	802	13		
1	z	538	Total	C	N	O	S	0	0
			4272	2711	746	802	13		
1	1	538	Total	C	N	O	S	0	0
			4272	2711	746	802	13		
1	2	538	Total	C	N	O	S	0	0
			4272	2711	746	802	13		
1	3	538	Total	C	N	O	S	0	0
			4272	2711	746	802	13		
1	4	538	Total	C	N	O	S	0	0
			4272	2711	746	802	13		
1	5	538	Total	C	N	O	S	0	0
			4272	2711	746	802	13		
1	6	538	Total	C	N	O	S	0	0
			4272	2711	746	802	13		
1	7	538	Total	C	N	O	S	0	0
			4272	2711	746	802	13		

Continued on next page...

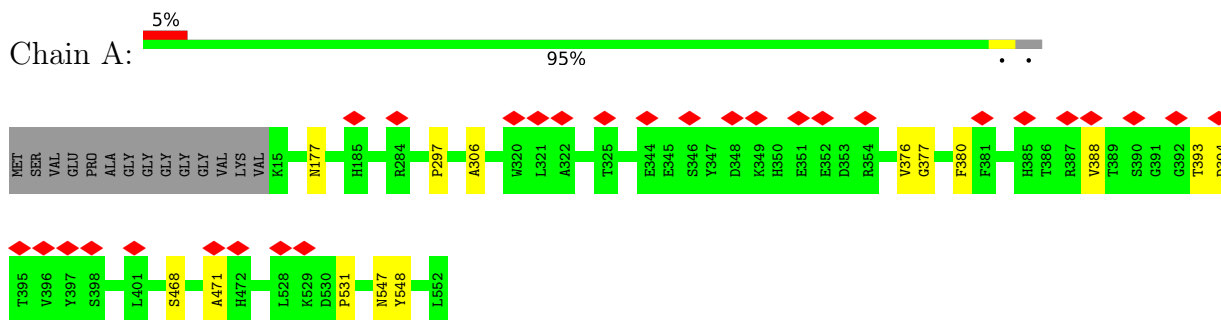
Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	8	538	4272	2711	746	802	13	0	0

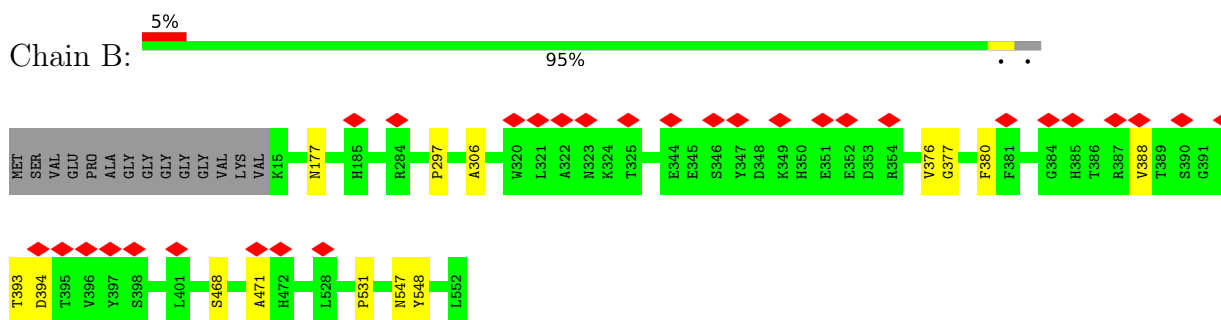
3 Residue-property plots [i](#)

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.

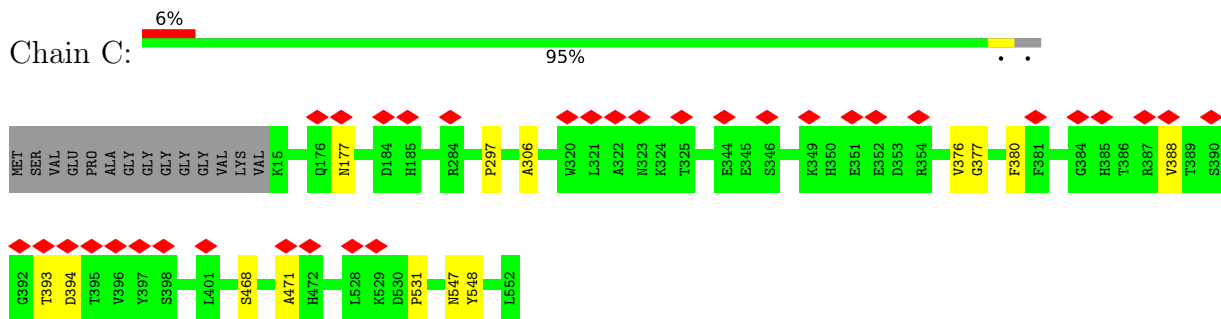
- Molecule 1: Human Parvovirus 4



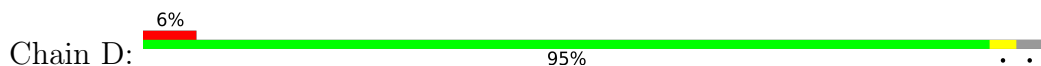
- Molecule 1: Human Parvovirus 4

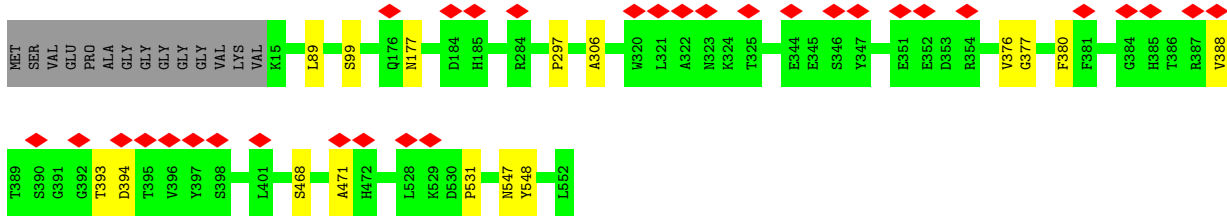


- Molecule 1: Human Parvovirus 4

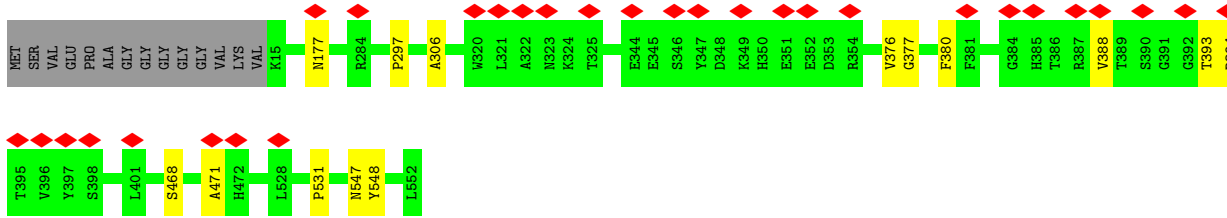
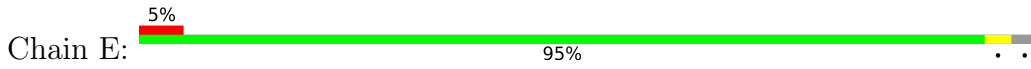


- Molecule 1: Human Parvovirus 4

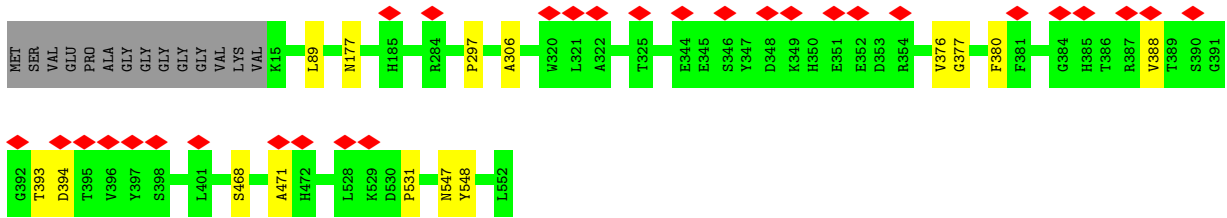




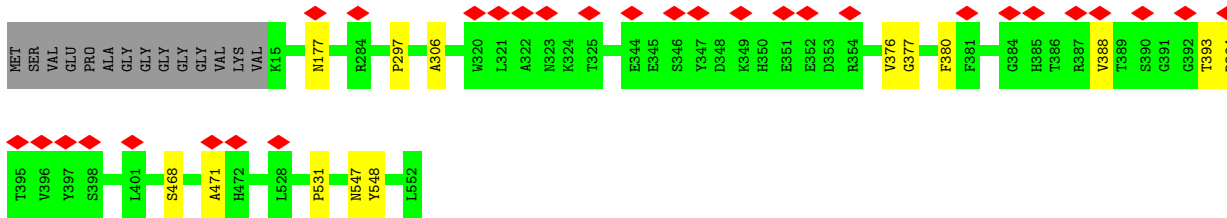
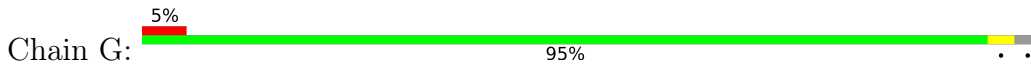
• Molecule 1: Human Parvovirus 4



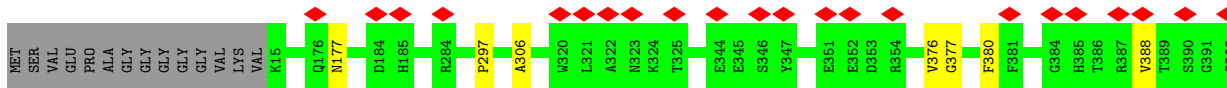
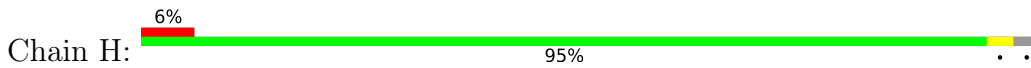
• Molecule 1: Human Parvovirus 4

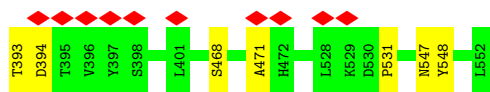


• Molecule 1: Human Parvovirus 4

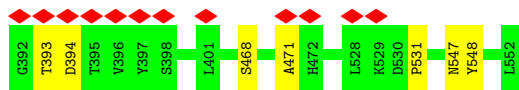
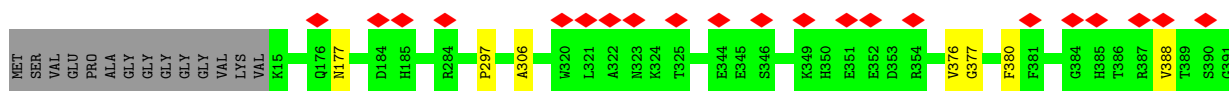
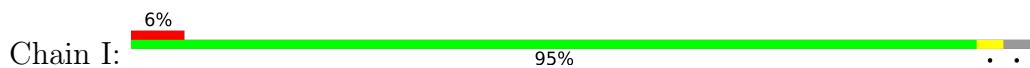


• Molecule 1: Human Parvovirus 4

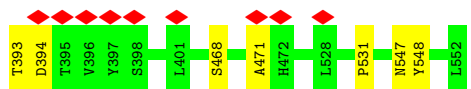
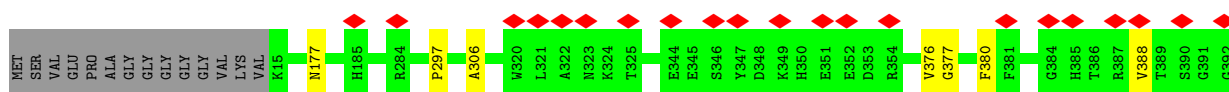
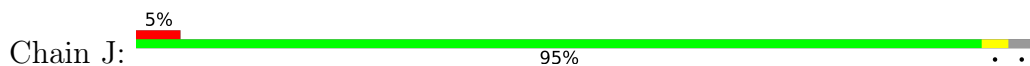




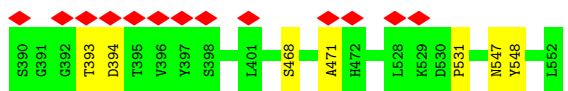
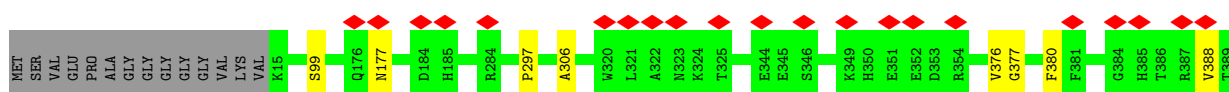
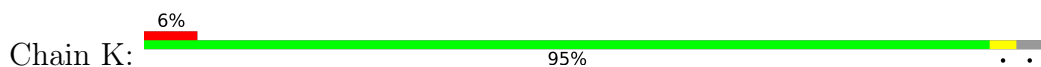
• Molecule 1: Human Parvovirus 4



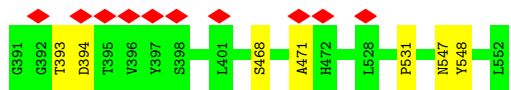
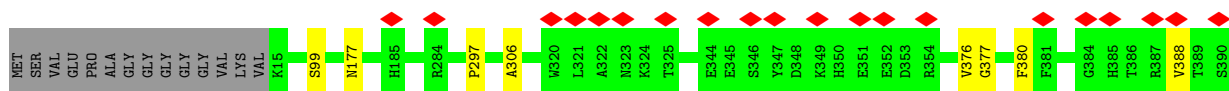
• Molecule 1: Human Parvovirus 4



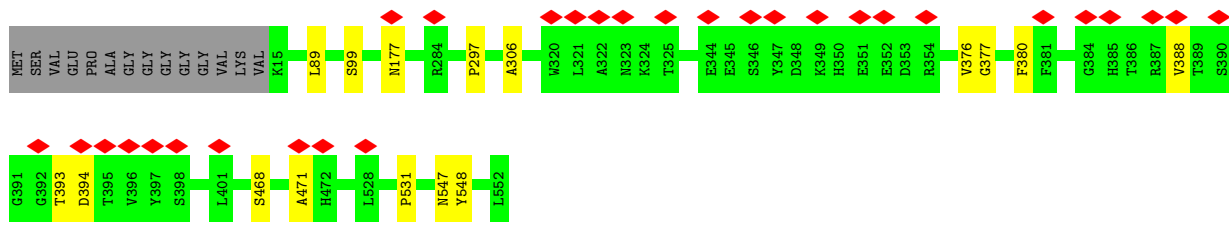
• Molecule 1: Human Parvovirus 4



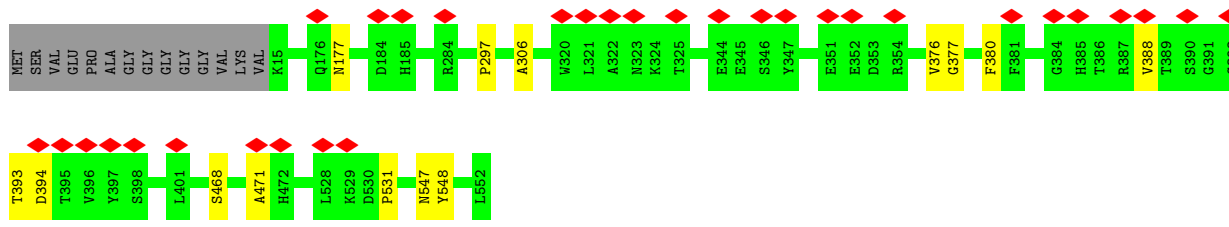
• Molecule 1: Human Parvovirus 4



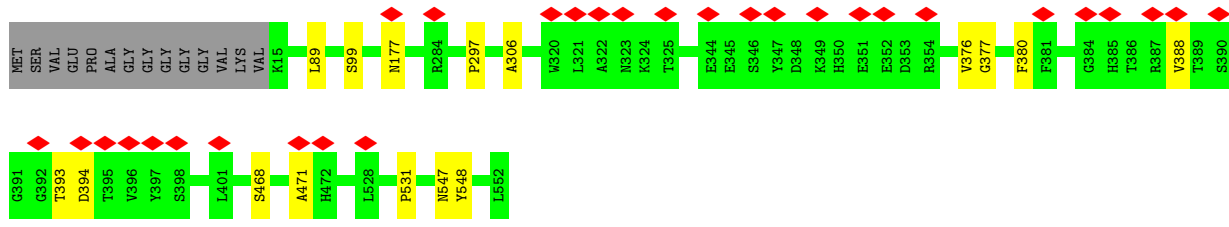
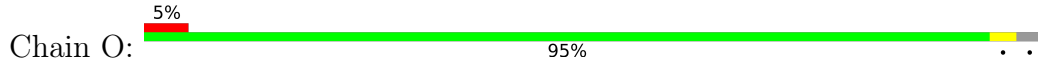
• Molecule 1: Human Parvovirus 4



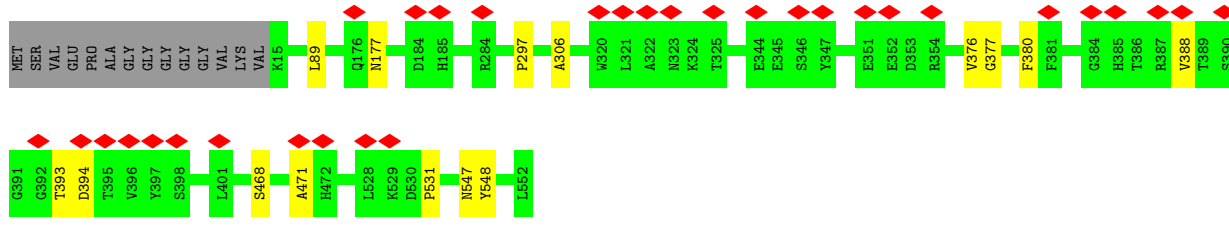
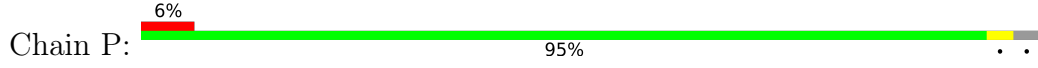
• Molecule 1: Human Parvovirus 4



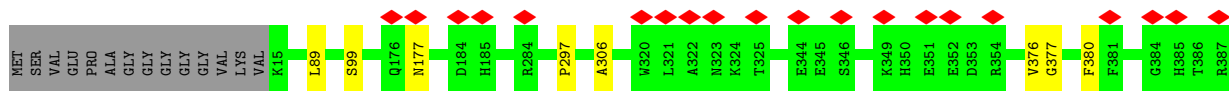
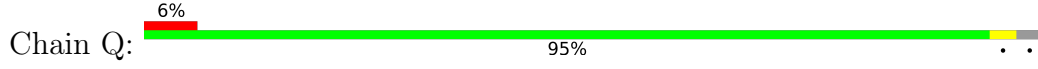
• Molecule 1: Human Parvovirus 4

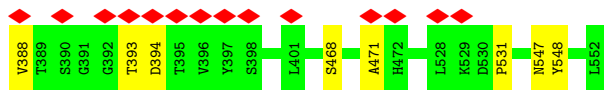


• Molecule 1: Human Parvovirus 4

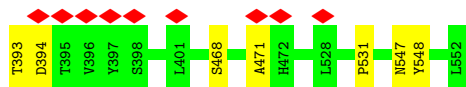
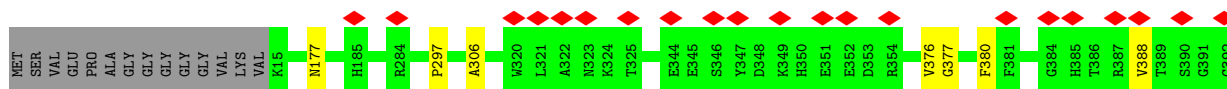


• Molecule 1: Human Parvovirus 4

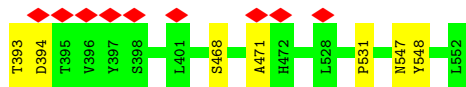
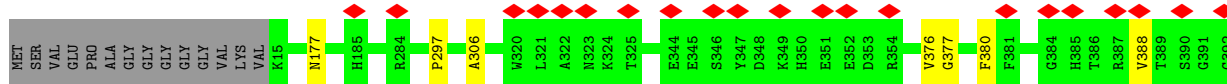




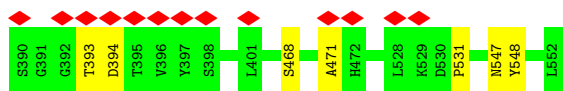
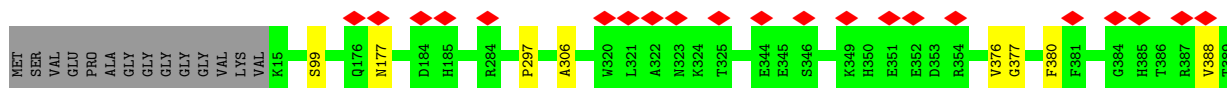
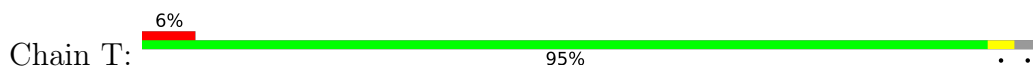
• Molecule 1: Human Parvovirus 4



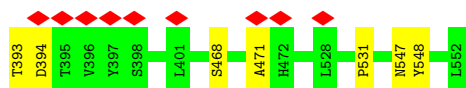
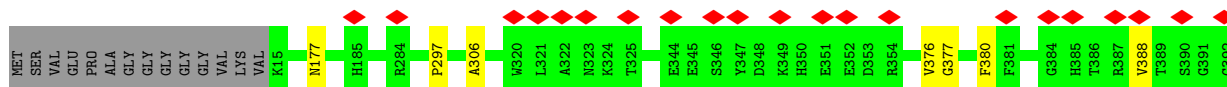
• Molecule 1: Human Parvovirus 4



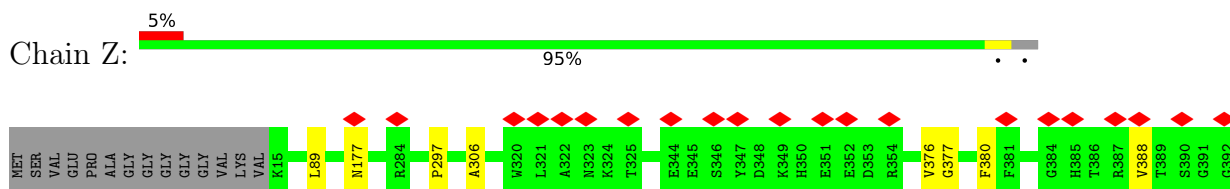
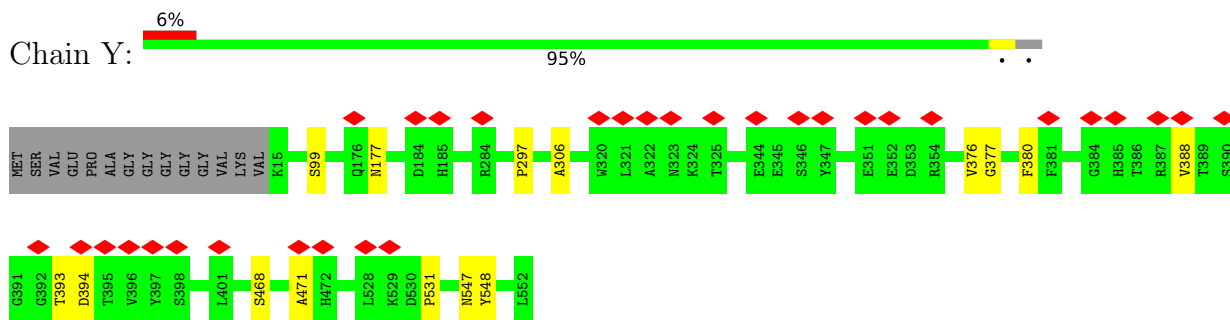
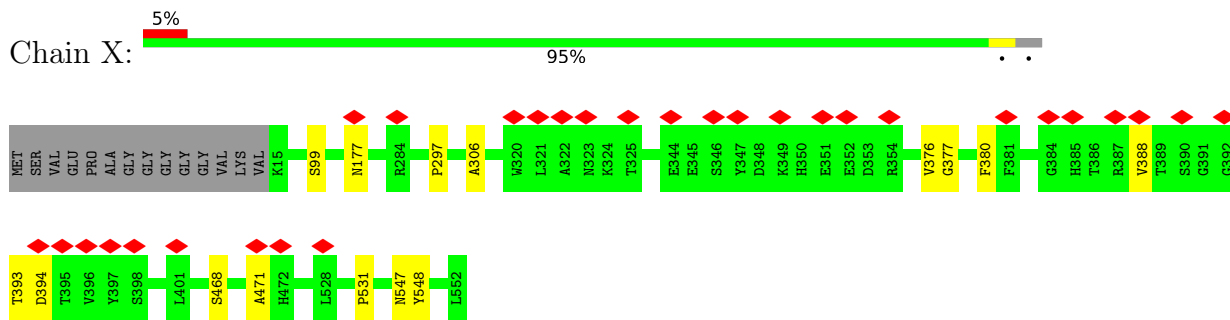
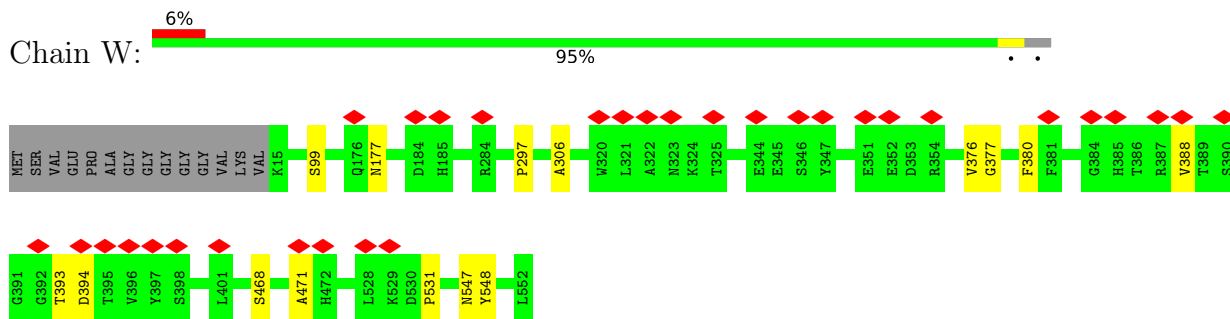
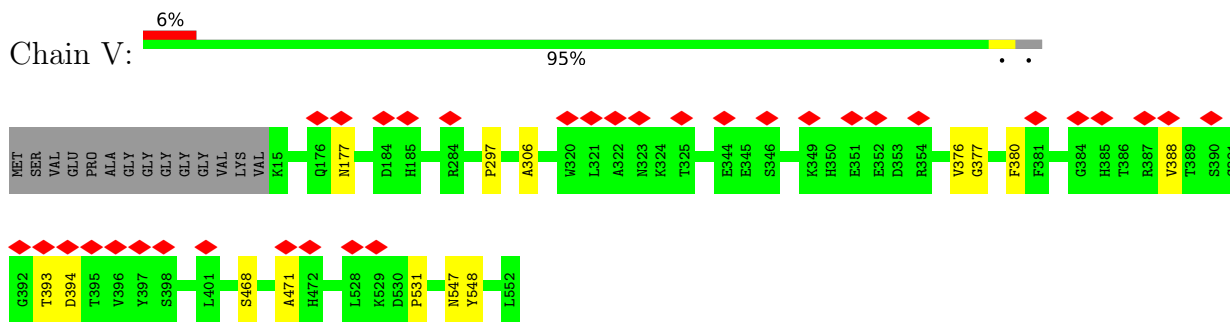
• Molecule 1: Human Parvovirus 4

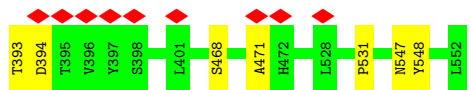


• Molecule 1: Human Parvovirus 4

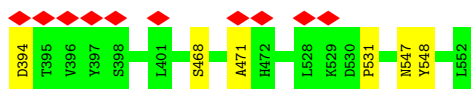
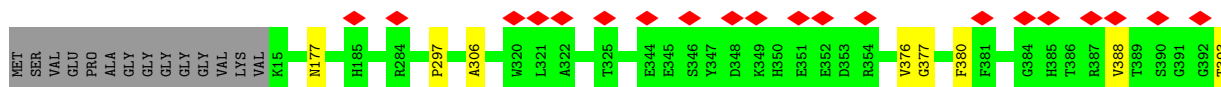
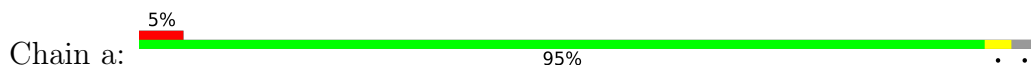


• Molecule 1: Human Parvovirus 4

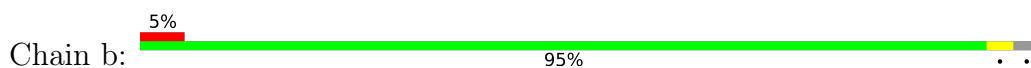




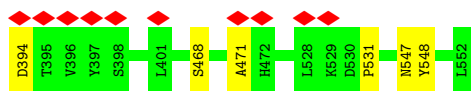
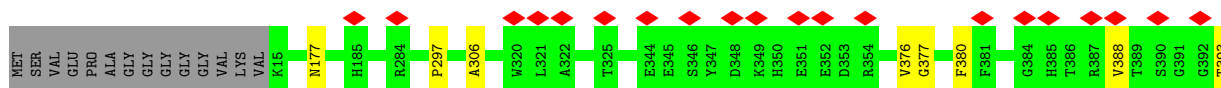
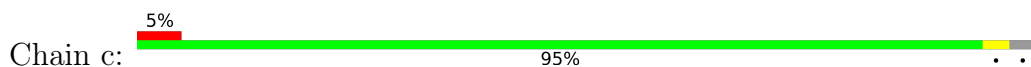
- Molecule 1: Human Parvovirus 4



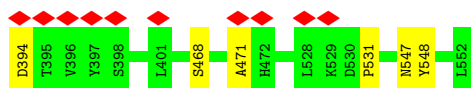
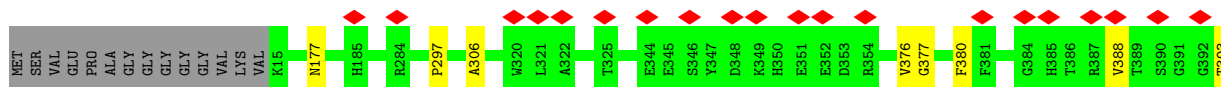
- Molecule 1: Human Parvovirus 4



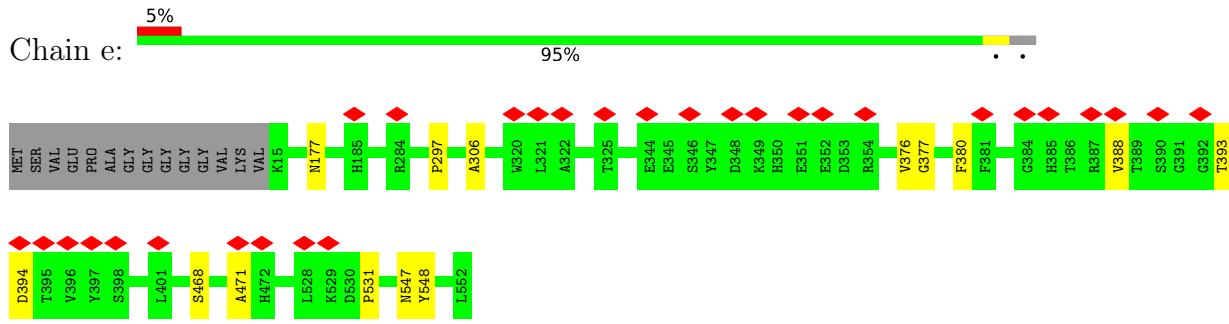
- Molecule 1: Human Parvovirus 4



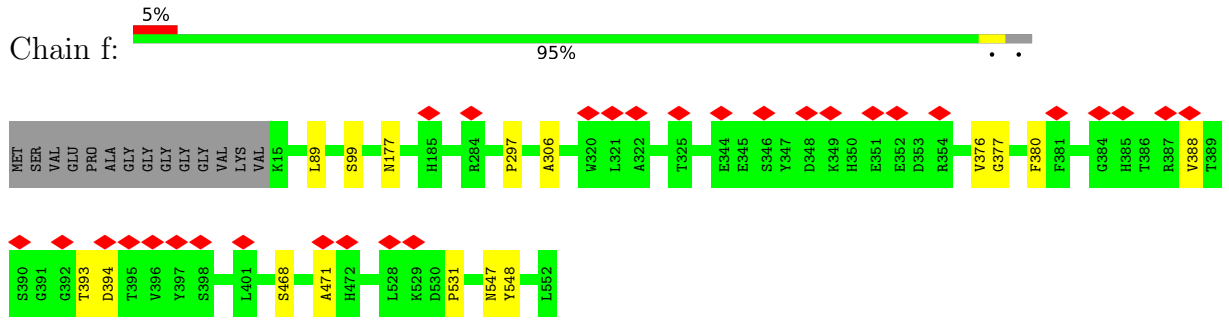
- Molecule 1: Human Parvovirus 4



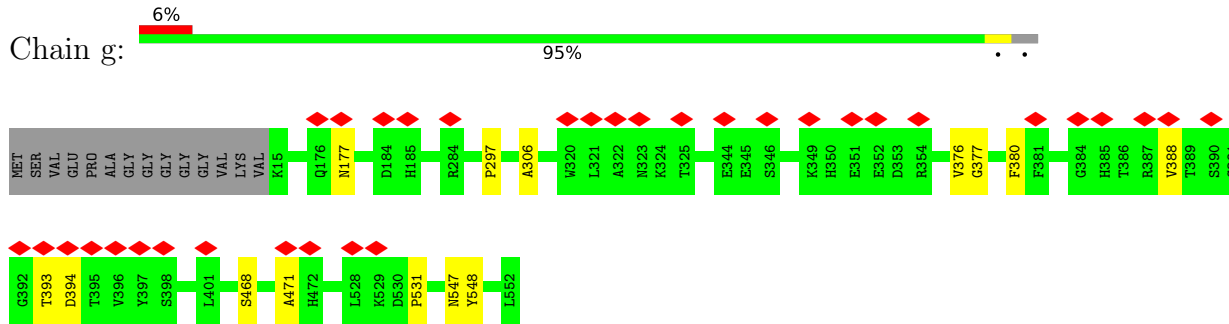
- Molecule 1: Human Parvovirus 4



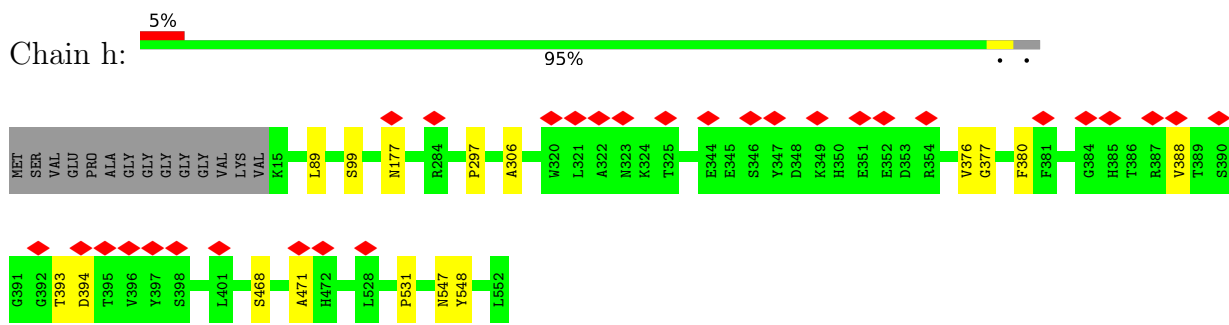
• Molecule 1: Human Parvovirus 4



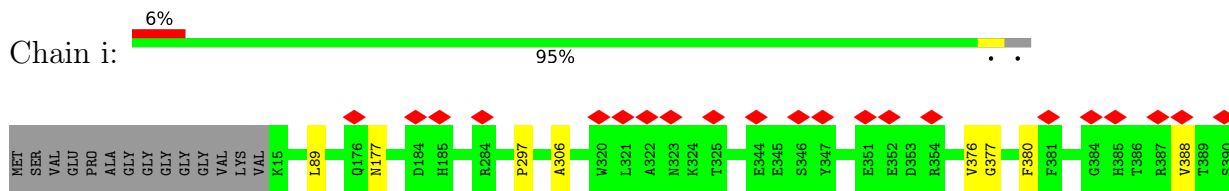
• Molecule 1: Human Parvovirus 4



• Molecule 1: Human Parvovirus 4

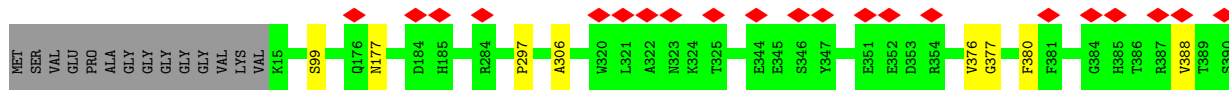
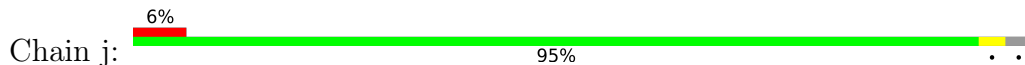


• Molecule 1: Human Parvovirus 4

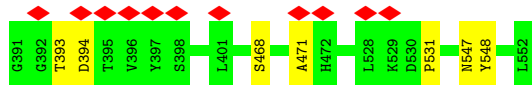
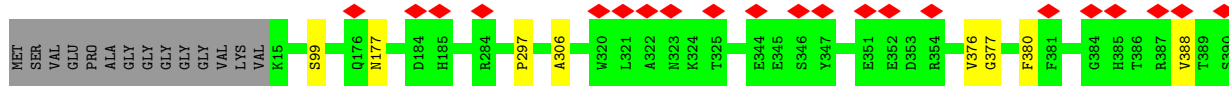




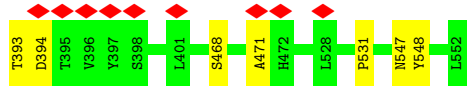
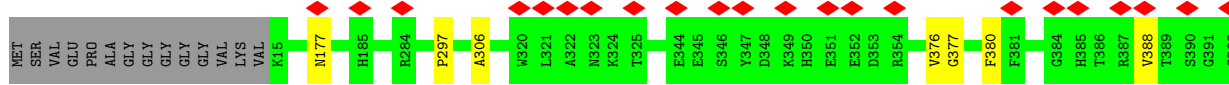
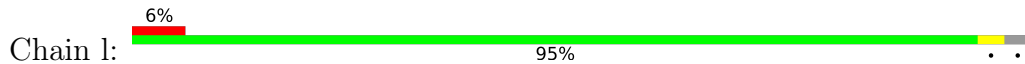
• Molecule 1: Human Parvovirus 4



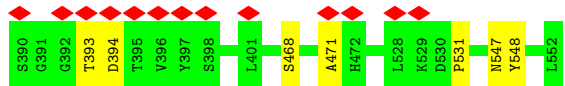
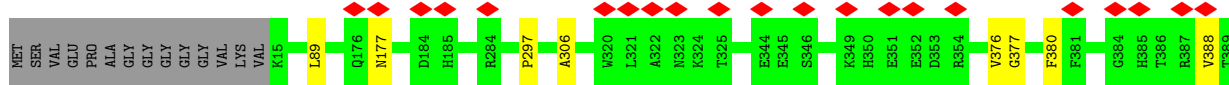
• Molecule 1: Human Parvovirus 4



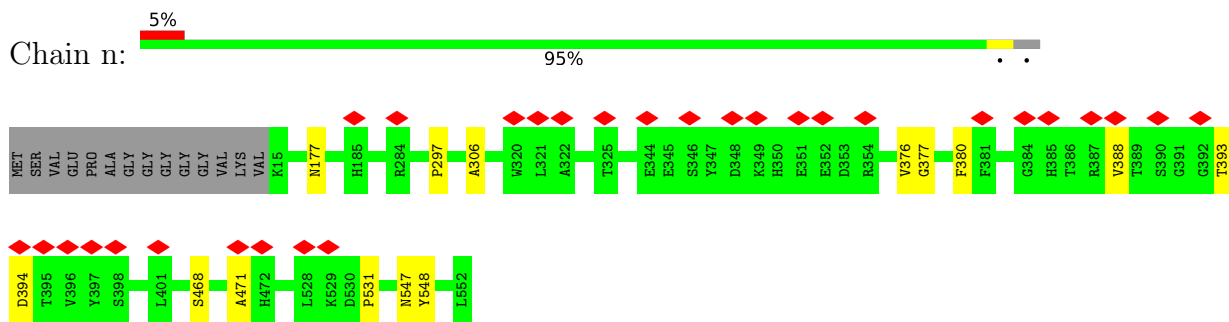
• Molecule 1: Human Parvovirus 4



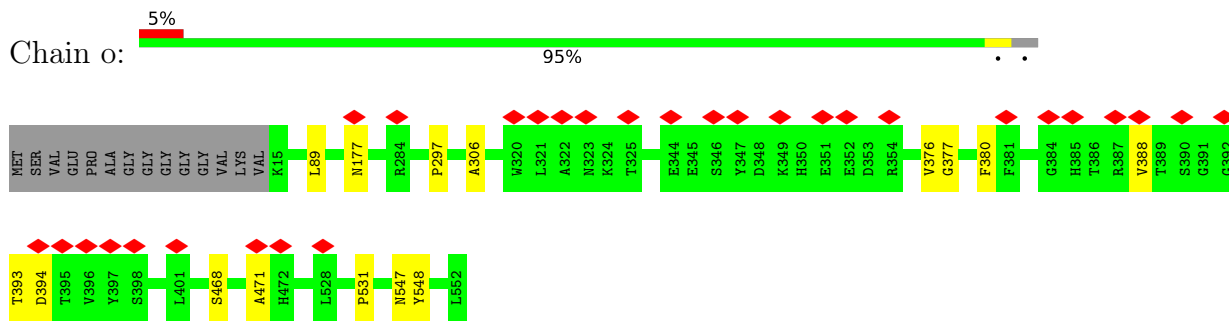
• Molecule 1: Human Parvovirus 4



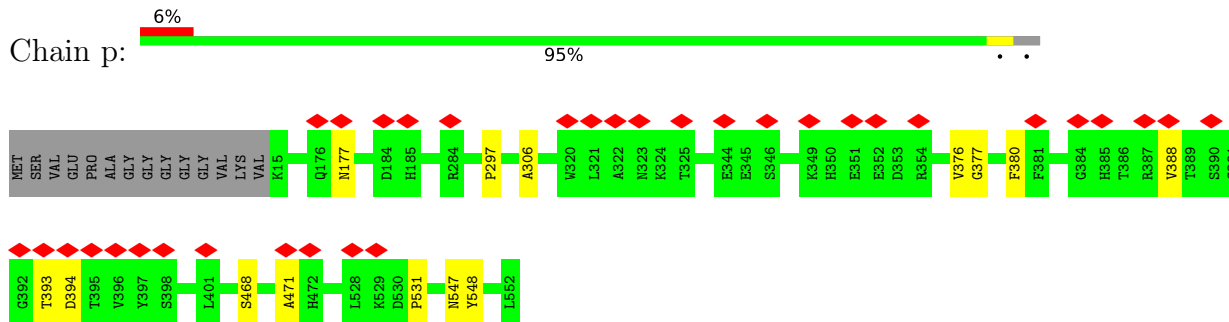
• Molecule 1: Human Parvovirus 4



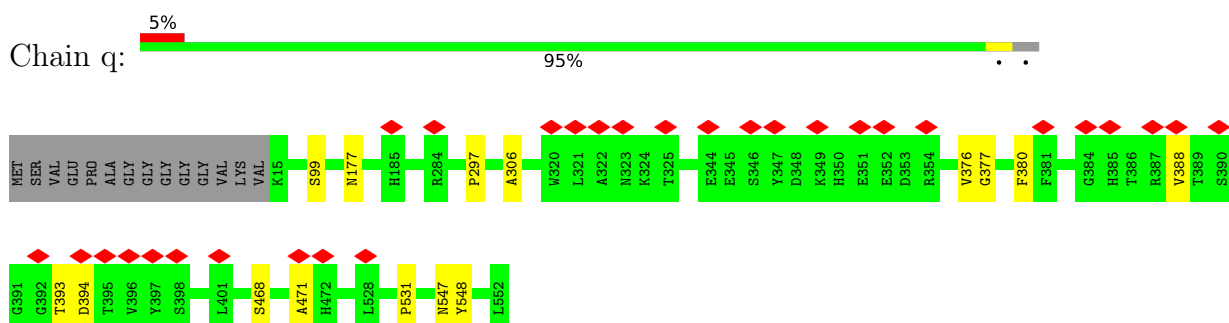
• Molecule 1: Human Parvovirus 4



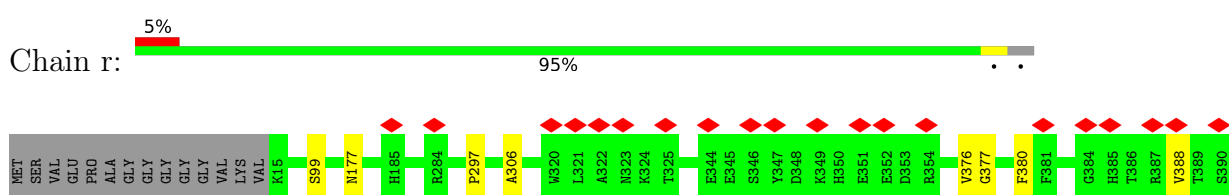
• Molecule 1: Human Parvovirus 4

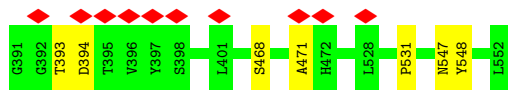


• Molecule 1: Human Parvovirus 4

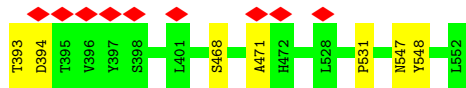
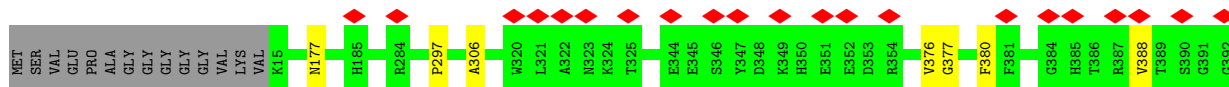


• Molecule 1: Human Parvovirus 4

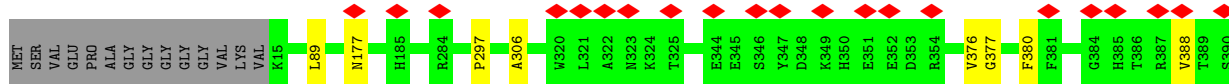
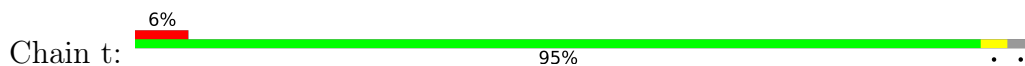




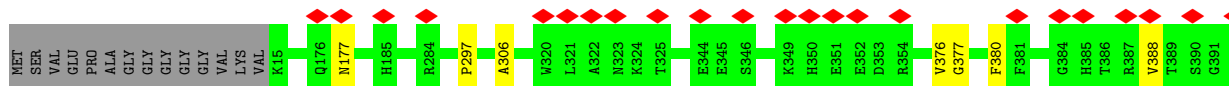
• Molecule 1: Human Parvovirus 4



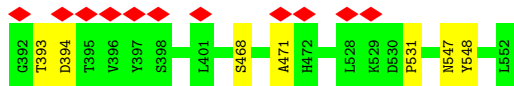
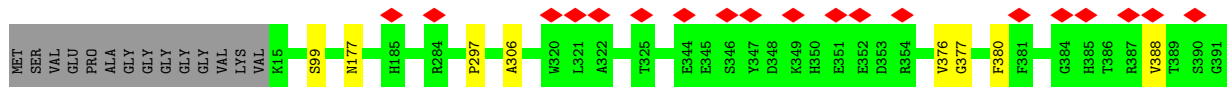
• Molecule 1: Human Parvovirus 4



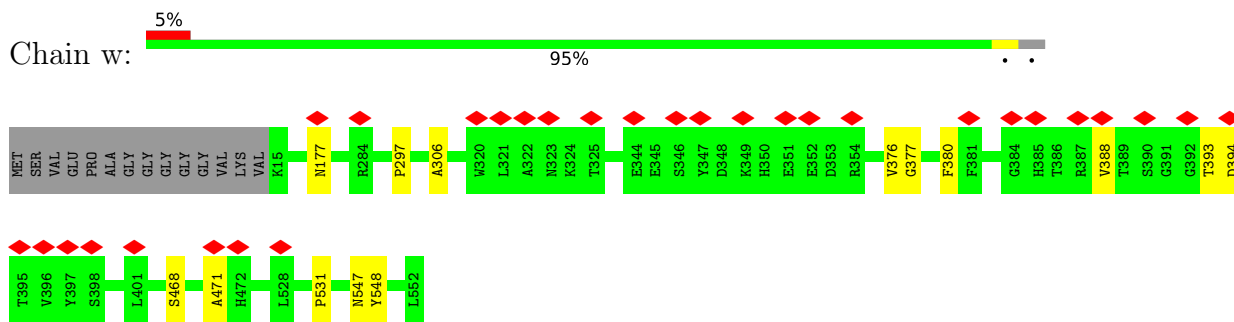
• Molecule 1: Human Parvovirus 4



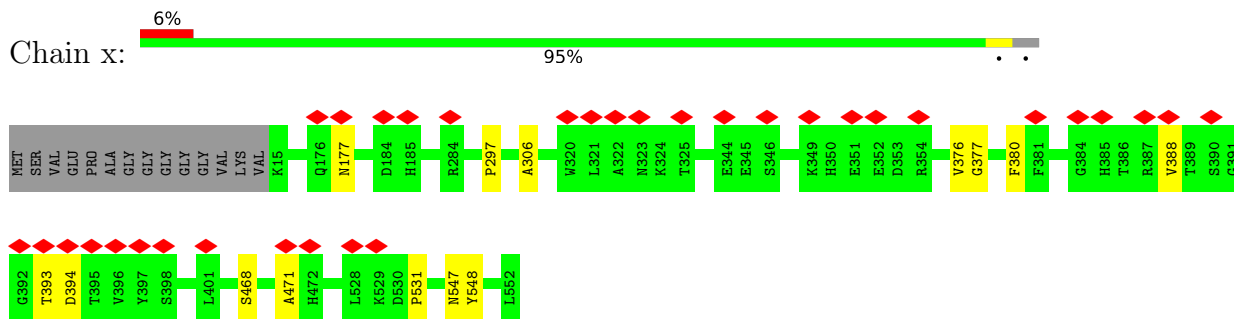
• Molecule 1: Human Parvovirus 4



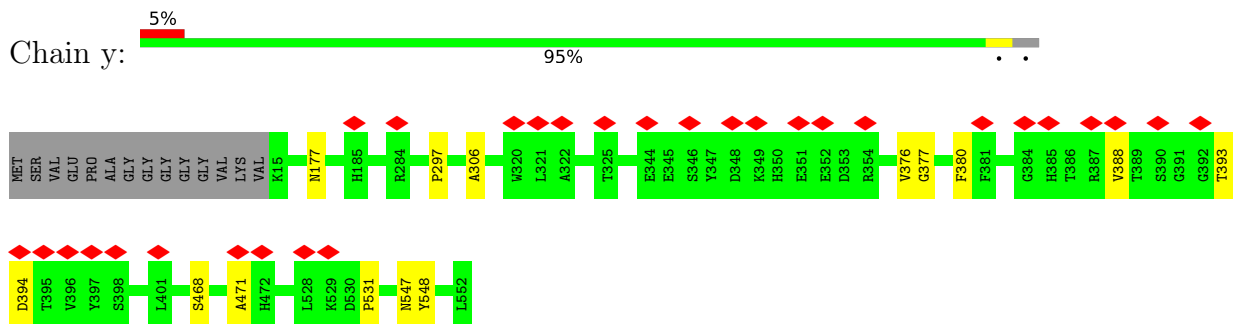
• Molecule 1: Human Parvovirus 4



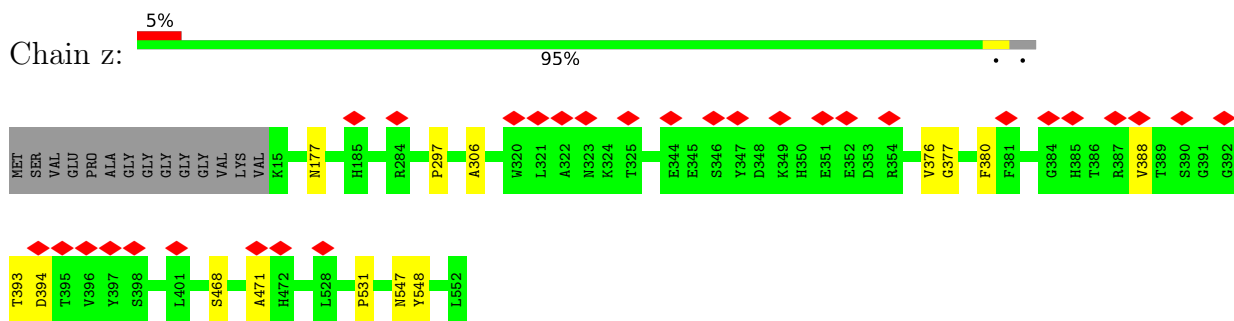
• Molecule 1: Human Parvovirus 4



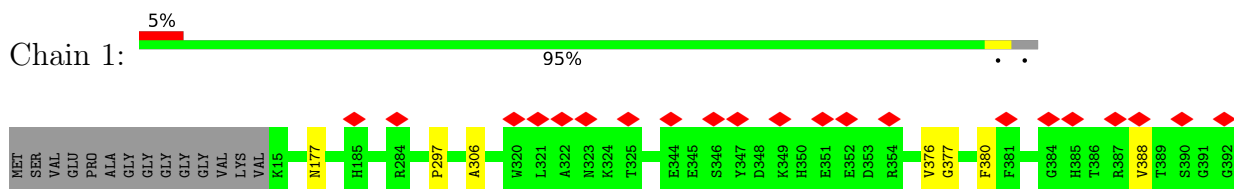
• Molecule 1: Human Parvovirus 4

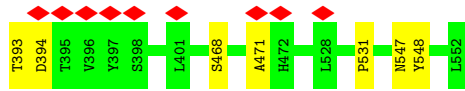


• Molecule 1: Human Parvovirus 4

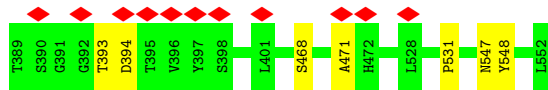
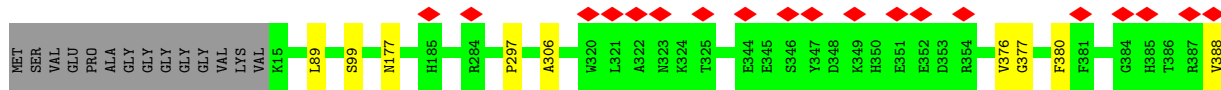


• Molecule 1: Human Parvovirus 4

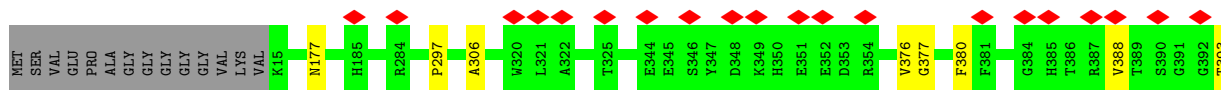
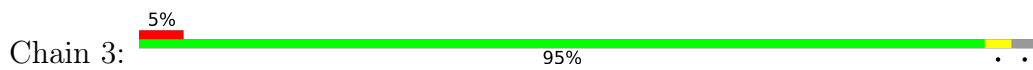




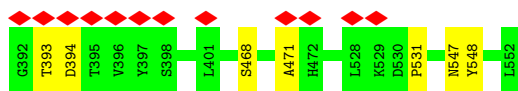
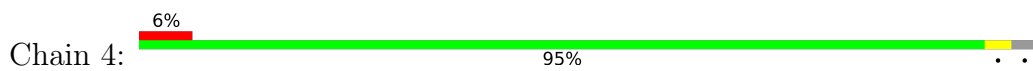
• Molecule 1: Human Parvovirus 4



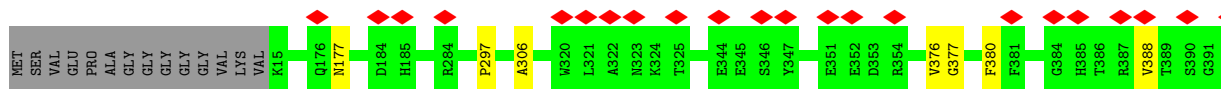
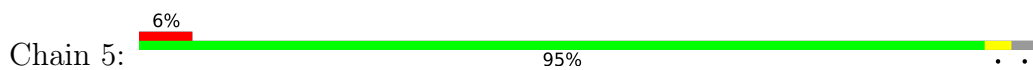
• Molecule 1: Human Parvovirus 4



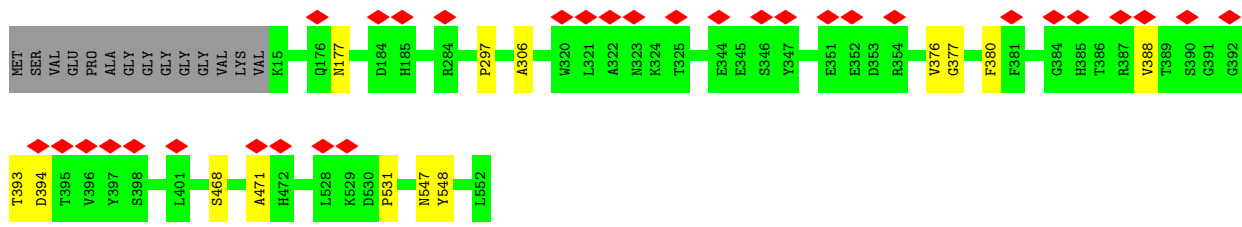
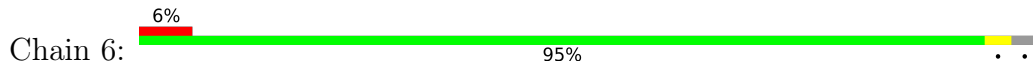
• Molecule 1: Human Parvovirus 4



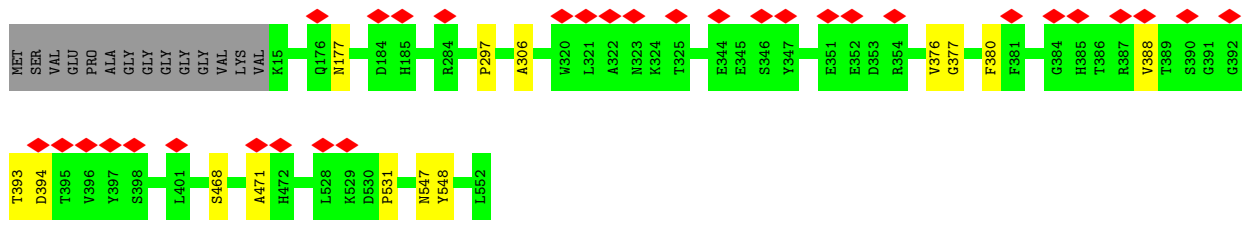
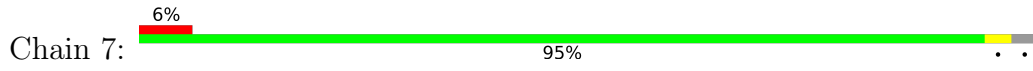
• Molecule 1: Human Parvovirus 4



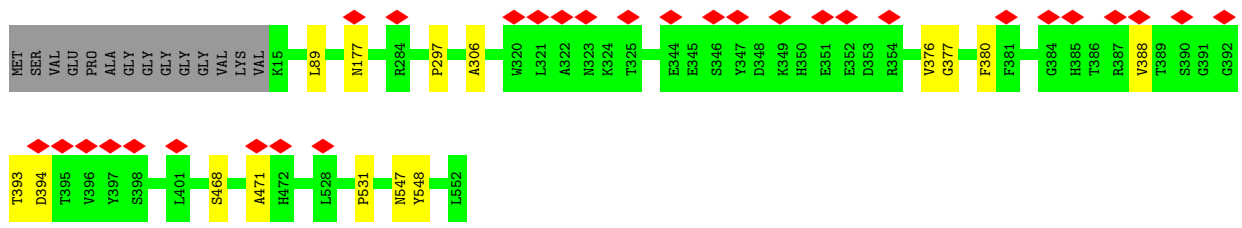
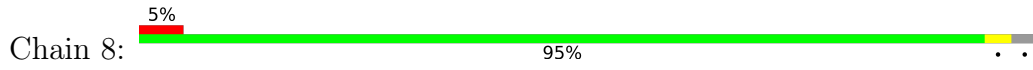
• Molecule 1: Human Parvovirus 4



• Molecule 1: Human Parvovirus 4



• Molecule 1: Human Parvovirus 4



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	5248	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	DIRECT ELECTRON DE-64 (8k x 8k)	Depositor
Maximum map value	18.538	Depositor
Minimum map value	-9.839	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	1.3	Depositor
Map size (\AA)	426.619, 426.619, 426.619	wwPDB
Map dimensions	470, 470, 470	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.9077, 0.9077, 0.9077	Depositor

5 Model quality i

5.1 Standard geometry i

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	0.73	2/4412 (0.0%)	0.76	9/6036 (0.1%)
1	2	0.74	2/4412 (0.0%)	0.76	10/6036 (0.2%)
1	3	0.74	2/4412 (0.0%)	0.76	9/6036 (0.1%)
1	4	0.73	2/4412 (0.0%)	0.76	9/6036 (0.1%)
1	5	0.73	2/4412 (0.0%)	0.76	9/6036 (0.1%)
1	6	0.74	2/4412 (0.0%)	0.76	9/6036 (0.1%)
1	7	0.74	2/4412 (0.0%)	0.76	9/6036 (0.1%)
1	8	0.74	2/4412 (0.0%)	0.76	10/6036 (0.2%)
1	A	0.73	2/4412 (0.0%)	0.76	9/6036 (0.1%)
1	B	0.73	2/4412 (0.0%)	0.76	9/6036 (0.1%)
1	C	0.73	2/4412 (0.0%)	0.76	9/6036 (0.1%)
1	D	0.74	2/4412 (0.0%)	0.76	10/6036 (0.2%)
1	E	0.74	2/4412 (0.0%)	0.76	9/6036 (0.1%)
1	F	0.74	2/4412 (0.0%)	0.76	10/6036 (0.2%)
1	G	0.74	2/4412 (0.0%)	0.76	9/6036 (0.1%)
1	H	0.73	2/4412 (0.0%)	0.76	9/6036 (0.1%)
1	I	0.73	2/4412 (0.0%)	0.76	9/6036 (0.1%)
1	J	0.73	2/4412 (0.0%)	0.76	9/6036 (0.1%)
1	K	0.74	2/4412 (0.0%)	0.76	9/6036 (0.1%)
1	L	0.73	2/4412 (0.0%)	0.76	9/6036 (0.1%)
1	M	0.73	2/4412 (0.0%)	0.76	10/6036 (0.2%)
1	N	0.74	2/4412 (0.0%)	0.76	9/6036 (0.1%)
1	O	0.74	2/4412 (0.0%)	0.76	10/6036 (0.2%)
1	P	0.73	2/4412 (0.0%)	0.76	10/6036 (0.2%)
1	Q	0.73	2/4412 (0.0%)	0.76	10/6036 (0.2%)
1	R	0.73	2/4412 (0.0%)	0.76	9/6036 (0.1%)
1	S	0.74	2/4412 (0.0%)	0.76	9/6036 (0.1%)
1	T	0.74	2/4412 (0.0%)	0.76	9/6036 (0.1%)
1	U	0.73	2/4412 (0.0%)	0.76	9/6036 (0.1%)
1	V	0.74	2/4412 (0.0%)	0.76	9/6036 (0.1%)
1	W	0.74	2/4412 (0.0%)	0.76	9/6036 (0.1%)
1	X	0.74	2/4412 (0.0%)	0.76	9/6036 (0.1%)
1	Y	0.74	2/4412 (0.0%)	0.76	9/6036 (0.1%)
1	Z	0.74	2/4412 (0.0%)	0.76	10/6036 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	a	0.74	2/4412 (0.0%)	0.76	9/6036 (0.1%)
1	b	0.73	2/4412 (0.0%)	0.76	10/6036 (0.2%)
1	c	0.73	2/4412 (0.0%)	0.76	9/6036 (0.1%)
1	d	0.74	2/4412 (0.0%)	0.76	9/6036 (0.1%)
1	e	0.73	2/4412 (0.0%)	0.76	9/6036 (0.1%)
1	f	0.73	2/4412 (0.0%)	0.76	10/6036 (0.2%)
1	g	0.73	2/4412 (0.0%)	0.76	9/6036 (0.1%)
1	h	0.74	2/4412 (0.0%)	0.76	10/6036 (0.2%)
1	i	0.74	2/4412 (0.0%)	0.76	10/6036 (0.2%)
1	j	0.73	2/4412 (0.0%)	0.76	9/6036 (0.1%)
1	k	0.74	2/4412 (0.0%)	0.76	9/6036 (0.1%)
1	l	0.74	2/4412 (0.0%)	0.76	9/6036 (0.1%)
1	m	0.73	2/4412 (0.0%)	0.76	10/6036 (0.2%)
1	n	0.74	2/4412 (0.0%)	0.76	9/6036 (0.1%)
1	o	0.74	2/4412 (0.0%)	0.76	10/6036 (0.2%)
1	p	0.73	2/4412 (0.0%)	0.76	9/6036 (0.1%)
1	q	0.73	2/4412 (0.0%)	0.76	9/6036 (0.1%)
1	r	0.74	2/4412 (0.0%)	0.76	9/6036 (0.1%)
1	s	0.73	2/4412 (0.0%)	0.76	9/6036 (0.1%)
1	t	0.73	2/4412 (0.0%)	0.76	10/6036 (0.2%)
1	u	0.74	2/4412 (0.0%)	0.76	9/6036 (0.1%)
1	v	0.74	2/4412 (0.0%)	0.76	9/6036 (0.1%)
1	w	0.74	2/4412 (0.0%)	0.76	9/6036 (0.1%)
1	x	0.73	2/4412 (0.0%)	0.76	9/6036 (0.1%)
1	y	0.74	2/4412 (0.0%)	0.76	9/6036 (0.1%)
1	z	0.74	2/4412 (0.0%)	0.76	9/6036 (0.1%)
All	All	0.74	120/264720 (0.0%)	0.76	556/362160 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1	1	1
1	2	1	1
1	3	1	1
1	4	1	1
1	5	1	1
1	6	1	1
1	7	1	1
1	8	1	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	1
1	B	1	1
1	C	1	1
1	D	1	1
1	E	1	1
1	F	1	1
1	G	1	1
1	H	1	1
1	I	1	1
1	J	1	1
1	K	1	1
1	L	1	1
1	M	1	1
1	N	1	1
1	O	1	1
1	P	1	1
1	Q	1	1
1	R	1	1
1	S	1	1
1	T	1	1
1	U	1	1
1	V	1	1
1	W	1	1
1	X	1	1
1	Y	1	1
1	Z	1	1
1	a	1	1
1	b	1	1
1	c	1	1
1	d	1	1
1	e	1	1
1	f	1	1
1	g	1	1
1	h	1	1
1	i	1	1
1	j	1	1
1	k	1	1
1	l	1	1
1	m	1	1
1	n	1	1
1	o	1	1
1	p	1	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
1	q	1	1
1	r	1	1
1	s	1	1
1	t	1	1
1	u	1	1
1	v	1	1
1	w	1	1
1	x	1	1
1	y	1	1
1	z	1	1
All	All	60	60

All (120) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	468	SER	C-N	-6.87	1.21	1.34
1	E	468	SER	C-N	-6.84	1.21	1.34
1	Z	468	SER	C-N	-6.84	1.21	1.34
1	h	468	SER	C-N	-6.84	1.21	1.34
1	o	468	SER	C-N	-6.84	1.21	1.34
1	w	468	SER	C-N	-6.84	1.21	1.34
1	8	468	SER	C-N	-6.84	1.21	1.34
1	D	468	SER	C-N	-6.83	1.21	1.34
1	H	468	SER	C-N	-6.83	1.21	1.34
1	Y	468	SER	C-N	-6.83	1.21	1.34
1	i	468	SER	C-N	-6.83	1.21	1.34
1	5	468	SER	C-N	-6.83	1.21	1.34
1	B	468	SER	C-N	-6.83	1.21	1.34
1	J	468	SER	C-N	-6.83	1.21	1.34
1	q	468	SER	C-N	-6.83	1.21	1.34
1	r	468	SER	C-N	-6.83	1.21	1.34
1	s	468	SER	C-N	-6.83	1.21	1.34
1	z	468	SER	C-N	-6.83	1.21	1.34
1	l	468	SER	C-N	-6.83	1.21	1.34
1	C	468	SER	C-N	-6.83	1.21	1.34
1	I	468	SER	C-N	-6.83	1.21	1.34
1	K	468	SER	C-N	-6.83	1.21	1.34
1	u	468	SER	C-N	-6.83	1.21	1.34
1	x	468	SER	C-N	-6.83	1.21	1.34
1	4	468	SER	C-N	-6.83	1.21	1.34
1	e	468	SER	C-N	-6.83	1.21	1.34
1	n	468	SER	C-N	-6.83	1.21	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	468	SER	C-N	-6.82	1.21	1.34
1	F	468	SER	C-N	-6.82	1.21	1.34
1	a	468	SER	C-N	-6.82	1.21	1.34
1	b	468	SER	C-N	-6.82	1.21	1.34
1	c	468	SER	C-N	-6.82	1.21	1.34
1	f	468	SER	C-N	-6.82	1.21	1.34
1	v	468	SER	C-N	-6.82	1.21	1.34
1	y	468	SER	C-N	-6.82	1.21	1.34
1	3	468	SER	C-N	-6.82	1.21	1.34
1	k	468	SER	C-N	-6.82	1.21	1.34
1	N	468	SER	C-N	-6.82	1.21	1.34
1	P	468	SER	C-N	-6.82	1.21	1.34
1	d	468	SER	C-N	-6.82	1.21	1.34
1	6	468	SER	C-N	-6.82	1.21	1.34
1	2	468	SER	C-N	-6.82	1.21	1.34
1	T	468	SER	C-N	-6.81	1.21	1.34
1	V	468	SER	C-N	-6.81	1.21	1.34
1	g	468	SER	C-N	-6.81	1.21	1.34
1	p	468	SER	C-N	-6.81	1.21	1.34
1	G	468	SER	C-N	-6.79	1.21	1.34
1	O	468	SER	C-N	-6.79	1.21	1.34
1	X	468	SER	C-N	-6.79	1.21	1.34
1	t	468	SER	C-N	-6.79	1.21	1.34
1	j	468	SER	C-N	-6.79	1.21	1.34
1	7	468	SER	C-N	-6.79	1.21	1.34
1	Q	468	SER	C-N	-6.79	1.21	1.34
1	m	468	SER	C-N	-6.79	1.21	1.34
1	R	468	SER	C-N	-6.79	1.21	1.34
1	S	468	SER	C-N	-6.79	1.21	1.34
1	U	468	SER	C-N	-6.79	1.21	1.34
1	l	468	SER	C-N	-6.78	1.21	1.34
1	W	468	SER	C-N	-6.78	1.21	1.34
1	L	468	SER	C-N	-6.77	1.21	1.34
1	B	306	ALA	C-N	-6.32	1.22	1.34
1	i	306	ALA	C-N	-6.31	1.22	1.34
1	j	306	ALA	C-N	-6.31	1.22	1.34
1	Z	306	ALA	C-N	-6.30	1.22	1.34
1	t	306	ALA	C-N	-6.30	1.22	1.34
1	8	306	ALA	C-N	-6.30	1.22	1.34
1	l	306	ALA	C-N	-6.30	1.22	1.34
1	L	306	ALA	C-N	-6.29	1.22	1.34
1	N	306	ALA	C-N	-6.29	1.22	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	R	306	ALA	C-N	-6.29	1.22	1.34
1	k	306	ALA	C-N	-6.29	1.22	1.34
1	r	306	ALA	C-N	-6.29	1.22	1.34
1	P	306	ALA	C-N	-6.28	1.22	1.34
1	S	306	ALA	C-N	-6.28	1.22	1.34
1	Y	306	ALA	C-N	-6.28	1.22	1.34
1	s	306	ALA	C-N	-6.28	1.22	1.34
1	1	306	ALA	C-N	-6.28	1.22	1.34
1	2	306	ALA	C-N	-6.28	1.22	1.34
1	I	306	ALA	C-N	-6.27	1.22	1.34
1	Q	306	ALA	C-N	-6.27	1.22	1.34
1	T	306	ALA	C-N	-6.27	1.22	1.34
1	V	306	ALA	C-N	-6.27	1.22	1.34
1	g	306	ALA	C-N	-6.27	1.22	1.34
1	m	306	ALA	C-N	-6.27	1.22	1.34
1	u	306	ALA	C-N	-6.27	1.22	1.34
1	x	306	ALA	C-N	-6.27	1.22	1.34
1	A	306	ALA	C-N	-6.27	1.22	1.34
1	F	306	ALA	C-N	-6.27	1.22	1.34
1	a	306	ALA	C-N	-6.27	1.22	1.34
1	b	306	ALA	C-N	-6.27	1.22	1.34
1	c	306	ALA	C-N	-6.27	1.22	1.34
1	e	306	ALA	C-N	-6.27	1.22	1.34
1	n	306	ALA	C-N	-6.27	1.22	1.34
1	5	306	ALA	C-N	-6.26	1.22	1.34
1	6	306	ALA	C-N	-6.26	1.22	1.34
1	D	306	ALA	C-N	-6.25	1.22	1.34
1	o	306	ALA	C-N	-6.25	1.22	1.34
1	h	306	ALA	C-N	-6.25	1.22	1.34
1	w	306	ALA	C-N	-6.25	1.22	1.34
1	J	306	ALA	C-N	-6.25	1.22	1.34
1	U	306	ALA	C-N	-6.25	1.22	1.34
1	z	306	ALA	C-N	-6.25	1.22	1.34
1	C	306	ALA	C-N	-6.25	1.22	1.34
1	p	306	ALA	C-N	-6.25	1.22	1.34
1	4	306	ALA	C-N	-6.25	1.22	1.34
1	W	306	ALA	C-N	-6.25	1.22	1.34
1	M	306	ALA	C-N	-6.24	1.22	1.34
1	X	306	ALA	C-N	-6.24	1.22	1.34
1	K	306	ALA	C-N	-6.24	1.22	1.34
1	E	306	ALA	C-N	-6.24	1.22	1.34
1	G	306	ALA	C-N	-6.24	1.22	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	306	ALA	C-N	-6.24	1.22	1.34
1	d	306	ALA	C-N	-6.24	1.22	1.34
1	f	306	ALA	C-N	-6.24	1.22	1.34
1	v	306	ALA	C-N	-6.24	1.22	1.34
1	y	306	ALA	C-N	-6.24	1.22	1.34
1	3	306	ALA	C-N	-6.24	1.22	1.34
1	q	306	ALA	C-N	-6.22	1.22	1.34
1	H	306	ALA	C-N	-6.22	1.22	1.34
1	7	306	ALA	C-N	-6.22	1.22	1.34

All (556) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	394	ASP	N-CA-CB	-15.34	82.99	110.60
1	W	394	ASP	N-CA-CB	-15.33	83.00	110.60
1	6	394	ASP	N-CA-CB	-15.33	83.00	110.60
1	Q	394	ASP	N-CA-CB	-15.33	83.01	110.60
1	b	394	ASP	N-CA-CB	-15.33	83.01	110.60
1	c	394	ASP	N-CA-CB	-15.33	83.01	110.60
1	C	394	ASP	N-CA-CB	-15.32	83.02	110.60
1	V	394	ASP	N-CA-CB	-15.32	83.02	110.60
1	7	394	ASP	N-CA-CB	-15.32	83.02	110.60
1	E	394	ASP	N-CA-CB	-15.32	83.03	110.60
1	u	394	ASP	N-CA-CB	-15.32	83.03	110.60
1	D	394	ASP	N-CA-CB	-15.31	83.04	110.60
1	P	394	ASP	N-CA-CB	-15.31	83.04	110.60
1	J	394	ASP	N-CA-CB	-15.31	83.05	110.60
1	L	394	ASP	N-CA-CB	-15.31	83.05	110.60
1	R	394	ASP	N-CA-CB	-15.31	83.05	110.60
1	S	394	ASP	N-CA-CB	-15.31	83.05	110.60
1	U	394	ASP	N-CA-CB	-15.31	83.05	110.60
1	e	394	ASP	N-CA-CB	-15.31	83.05	110.60
1	q	394	ASP	N-CA-CB	-15.31	83.05	110.60
1	r	394	ASP	N-CA-CB	-15.31	83.05	110.60
1	s	394	ASP	N-CA-CB	-15.31	83.05	110.60
1	z	394	ASP	N-CA-CB	-15.31	83.04	110.60
1	l	394	ASP	N-CA-CB	-15.31	83.05	110.60
1	A	394	ASP	N-CA-CB	-15.31	83.05	110.60
1	N	394	ASP	N-CA-CB	-15.31	83.05	110.60
1	T	394	ASP	N-CA-CB	-15.30	83.05	110.60
1	d	394	ASP	N-CA-CB	-15.31	83.05	110.60
1	h	394	ASP	N-CA-CB	-15.31	83.05	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	j	394	ASP	N-CA-CB	-15.31	83.05	110.60
1	3	394	ASP	N-CA-CB	-15.31	83.05	110.60
1	4	394	ASP	N-CA-CB	-15.30	83.06	110.60
1	B	394	ASP	N-CA-CB	-15.30	83.06	110.60
1	I	394	ASP	N-CA-CB	-15.30	83.06	110.60
1	K	394	ASP	N-CA-CB	-15.30	83.06	110.60
1	M	394	ASP	N-CA-CB	-15.30	83.06	110.60
1	O	394	ASP	N-CA-CB	-15.30	83.06	110.60
1	Z	394	ASP	N-CA-CB	-15.30	83.06	110.60
1	g	394	ASP	N-CA-CB	-15.30	83.06	110.60
1	t	394	ASP	N-CA-CB	-15.30	83.06	110.60
1	x	394	ASP	N-CA-CB	-15.30	83.06	110.60
1	2	394	ASP	N-CA-CB	-15.30	83.06	110.60
1	8	394	ASP	N-CA-CB	-15.30	83.06	110.60
1	H	394	ASP	N-CA-CB	-15.29	83.07	110.60
1	X	394	ASP	N-CA-CB	-15.29	83.07	110.60
1	Y	394	ASP	N-CA-CB	-15.29	83.07	110.60
1	i	394	ASP	N-CA-CB	-15.29	83.07	110.60
1	k	394	ASP	N-CA-CB	-15.29	83.07	110.60
1	m	394	ASP	N-CA-CB	-15.29	83.07	110.60
1	p	394	ASP	N-CA-CB	-15.29	83.07	110.60
1	5	394	ASP	N-CA-CB	-15.29	83.07	110.60
1	l	394	ASP	N-CA-CB	-15.29	83.08	110.60
1	w	394	ASP	N-CA-CB	-15.29	83.07	110.60
1	F	394	ASP	N-CA-CB	-15.29	83.08	110.60
1	f	394	ASP	N-CA-CB	-15.29	83.08	110.60
1	n	394	ASP	N-CA-CB	-15.29	83.08	110.60
1	v	394	ASP	N-CA-CB	-15.29	83.08	110.60
1	y	394	ASP	N-CA-CB	-15.29	83.08	110.60
1	o	394	ASP	N-CA-CB	-15.28	83.09	110.60
1	a	394	ASP	N-CA-CB	-15.28	83.10	110.60
1	O	376	VAL	CB-CA-C	-11.72	89.13	111.40
1	j	376	VAL	CB-CA-C	-11.72	89.13	111.40
1	n	376	VAL	CB-CA-C	-11.72	89.14	111.40
1	p	376	VAL	CB-CA-C	-11.72	89.14	111.40
1	y	376	VAL	CB-CA-C	-11.72	89.14	111.40
1	3	376	VAL	CB-CA-C	-11.72	89.14	111.40
1	P	376	VAL	CB-CA-C	-11.71	89.14	111.40
1	U	376	VAL	CB-CA-C	-11.71	89.14	111.40
1	Z	376	VAL	CB-CA-C	-11.71	89.14	111.40
1	q	376	VAL	CB-CA-C	-11.71	89.14	111.40
1	1	376	VAL	CB-CA-C	-11.71	89.14	111.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	376	VAL	CB-CA-C	-11.71	89.14	111.40
1	N	376	VAL	CB-CA-C	-11.71	89.15	111.40
1	J	376	VAL	CB-CA-C	-11.71	89.16	111.40
1	o	376	VAL	CB-CA-C	-11.71	89.16	111.40
1	T	376	VAL	CB-CA-C	-11.71	89.16	111.40
1	t	376	VAL	CB-CA-C	-11.70	89.16	111.40
1	V	376	VAL	CB-CA-C	-11.70	89.17	111.40
1	l	376	VAL	CB-CA-C	-11.70	89.16	111.40
1	x	376	VAL	CB-CA-C	-11.70	89.17	111.40
1	6	376	VAL	CB-CA-C	-11.70	89.17	111.40
1	7	376	VAL	CB-CA-C	-11.70	89.17	111.40
1	S	376	VAL	CB-CA-C	-11.70	89.17	111.40
1	z	376	VAL	CB-CA-C	-11.70	89.17	111.40
1	4	376	VAL	CB-CA-C	-11.70	89.17	111.40
1	A	376	VAL	CB-CA-C	-11.70	89.17	111.40
1	C	376	VAL	CB-CA-C	-11.70	89.17	111.40
1	F	376	VAL	CB-CA-C	-11.70	89.17	111.40
1	I	376	VAL	CB-CA-C	-11.70	89.17	111.40
1	K	376	VAL	CB-CA-C	-11.70	89.17	111.40
1	a	376	VAL	CB-CA-C	-11.70	89.17	111.40
1	b	376	VAL	CB-CA-C	-11.70	89.17	111.40
1	d	376	VAL	CB-CA-C	-11.70	89.17	111.40
1	f	376	VAL	CB-CA-C	-11.70	89.17	111.40
1	g	376	VAL	CB-CA-C	-11.70	89.17	111.40
1	v	376	VAL	CB-CA-C	-11.70	89.17	111.40
1	8	376	VAL	CB-CA-C	-11.70	89.17	111.40
1	H	376	VAL	CB-CA-C	-11.70	89.18	111.40
1	M	376	VAL	CB-CA-C	-11.70	89.18	111.40
1	W	376	VAL	CB-CA-C	-11.70	89.18	111.40
1	X	376	VAL	CB-CA-C	-11.70	89.18	111.40
1	Y	376	VAL	CB-CA-C	-11.70	89.18	111.40
1	h	376	VAL	CB-CA-C	-11.70	89.18	111.40
1	D	376	VAL	CB-CA-C	-11.69	89.18	111.40
1	r	376	VAL	CB-CA-C	-11.69	89.18	111.40
1	m	376	VAL	CB-CA-C	-11.69	89.19	111.40
1	s	376	VAL	CB-CA-C	-11.69	89.19	111.40
1	5	376	VAL	CB-CA-C	-11.69	89.19	111.40
1	Q	376	VAL	CB-CA-C	-11.69	89.19	111.40
1	u	376	VAL	CB-CA-C	-11.69	89.19	111.40
1	w	376	VAL	CB-CA-C	-11.69	89.19	111.40
1	B	376	VAL	CB-CA-C	-11.69	89.19	111.40
1	E	376	VAL	CB-CA-C	-11.69	89.19	111.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	376	VAL	CB-CA-C	-11.69	89.20	111.40
1	L	376	VAL	CB-CA-C	-11.69	89.19	111.40
1	R	376	VAL	CB-CA-C	-11.69	89.19	111.40
1	i	376	VAL	CB-CA-C	-11.69	89.19	111.40
1	k	376	VAL	CB-CA-C	-11.69	89.20	111.40
1	c	376	VAL	CB-CA-C	-11.68	89.21	111.40
1	e	376	VAL	CB-CA-C	-11.68	89.21	111.40
1	m	393	THR	N-CA-C	10.34	138.91	111.00
1	C	393	THR	N-CA-C	10.34	138.91	111.00
1	a	393	THR	N-CA-C	10.33	138.90	111.00
1	l	393	THR	N-CA-C	10.33	138.90	111.00
1	n	393	THR	N-CA-C	10.33	138.90	111.00
1	c	393	THR	N-CA-C	10.33	138.89	111.00
1	i	393	THR	N-CA-C	10.33	138.89	111.00
1	6	393	THR	N-CA-C	10.33	138.89	111.00
1	R	393	THR	N-CA-C	10.33	138.88	111.00
1	s	393	THR	N-CA-C	10.33	138.88	111.00
1	I	393	THR	N-CA-C	10.32	138.87	111.00
1	K	393	THR	N-CA-C	10.32	138.87	111.00
1	V	393	THR	N-CA-C	10.32	138.87	111.00
1	x	393	THR	N-CA-C	10.32	138.87	111.00
1	D	393	THR	N-CA-C	10.32	138.87	111.00
1	M	393	THR	N-CA-C	10.32	138.87	111.00
1	G	393	THR	N-CA-C	10.32	138.87	111.00
1	S	393	THR	N-CA-C	10.32	138.87	111.00
1	o	393	THR	N-CA-C	10.32	138.87	111.00
1	2	393	THR	N-CA-C	10.32	138.86	111.00
1	A	393	THR	N-CA-C	10.32	138.85	111.00
1	b	393	THR	N-CA-C	10.32	138.85	111.00
1	f	393	THR	N-CA-C	10.32	138.85	111.00
1	u	393	THR	N-CA-C	10.32	138.85	111.00
1	p	393	THR	N-CA-C	10.31	138.85	111.00
1	r	393	THR	N-CA-C	10.31	138.85	111.00
1	1	393	THR	N-CA-C	10.31	138.85	111.00
1	L	393	THR	N-CA-C	10.31	138.84	111.00
1	N	393	THR	N-CA-C	10.31	138.84	111.00
1	X	393	THR	N-CA-C	10.31	138.84	111.00
1	Y	393	THR	N-CA-C	10.31	138.84	111.00
1	j	393	THR	N-CA-C	10.31	138.84	111.00
1	5	393	THR	N-CA-C	10.31	138.84	111.00
1	E	393	THR	N-CA-C	10.31	138.84	111.00
1	H	393	THR	N-CA-C	10.31	138.84	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	393	THR	N-CA-C	10.31	138.84	111.00
1	W	393	THR	N-CA-C	10.31	138.84	111.00
1	g	393	THR	N-CA-C	10.31	138.84	111.00
1	3	393	THR	N-CA-C	10.31	138.84	111.00
1	B	393	THR	N-CA-C	10.31	138.83	111.00
1	J	393	THR	N-CA-C	10.31	138.83	111.00
1	U	393	THR	N-CA-C	10.31	138.83	111.00
1	e	393	THR	N-CA-C	10.31	138.83	111.00
1	w	393	THR	N-CA-C	10.31	138.83	111.00
1	z	393	THR	N-CA-C	10.31	138.83	111.00
1	8	393	THR	N-CA-C	10.31	138.83	111.00
1	Q	393	THR	N-CA-C	10.31	138.83	111.00
1	h	393	THR	N-CA-C	10.31	138.82	111.00
1	t	393	THR	N-CA-C	10.31	138.83	111.00
1	y	393	THR	N-CA-C	10.30	138.82	111.00
1	4	393	THR	N-CA-C	10.31	138.83	111.00
1	P	393	THR	N-CA-C	10.30	138.82	111.00
1	T	393	THR	N-CA-C	10.30	138.82	111.00
1	k	393	THR	N-CA-C	10.30	138.82	111.00
1	Z	393	THR	N-CA-C	10.30	138.81	111.00
1	7	393	THR	N-CA-C	10.30	138.81	111.00
1	F	393	THR	N-CA-C	10.30	138.80	111.00
1	d	393	THR	N-CA-C	10.30	138.80	111.00
1	v	393	THR	N-CA-C	10.30	138.80	111.00
1	q	393	THR	N-CA-C	10.29	138.79	111.00
1	B	377	GLY	N-CA-C	-8.26	92.46	113.10
1	n	377	GLY	N-CA-C	-8.26	92.46	113.10
1	C	377	GLY	N-CA-C	-8.25	92.47	113.10
1	p	377	GLY	N-CA-C	-8.25	92.47	113.10
1	a	377	GLY	N-CA-C	-8.25	92.47	113.10
1	i	377	GLY	N-CA-C	-8.25	92.47	113.10
1	y	377	GLY	N-CA-C	-8.25	92.47	113.10
1	L	377	GLY	N-CA-C	-8.25	92.48	113.10
1	U	377	GLY	N-CA-C	-8.25	92.48	113.10
1	r	377	GLY	N-CA-C	-8.25	92.48	113.10
1	u	377	GLY	N-CA-C	-8.25	92.47	113.10
1	v	377	GLY	N-CA-C	-8.25	92.47	113.10
1	T	377	GLY	N-CA-C	-8.25	92.48	113.10
1	Y	377	GLY	N-CA-C	-8.25	92.48	113.10
1	5	377	GLY	N-CA-C	-8.25	92.48	113.10
1	W	377	GLY	N-CA-C	-8.25	92.48	113.10
1	7	377	GLY	N-CA-C	-8.25	92.48	113.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	377	GLY	N-CA-C	-8.24	92.49	113.10
1	2	377	GLY	N-CA-C	-8.24	92.49	113.10
1	G	377	GLY	N-CA-C	-8.24	92.49	113.10
1	M	377	GLY	N-CA-C	-8.24	92.49	113.10
1	l	377	GLY	N-CA-C	-8.24	92.49	113.10
1	m	377	GLY	N-CA-C	-8.24	92.49	113.10
1	4	377	GLY	N-CA-C	-8.24	92.49	113.10
1	A	377	GLY	N-CA-C	-8.24	92.50	113.10
1	F	377	GLY	N-CA-C	-8.24	92.50	113.10
1	K	377	GLY	N-CA-C	-8.24	92.50	113.10
1	J	377	GLY	N-CA-C	-8.24	92.50	113.10
1	V	377	GLY	N-CA-C	-8.24	92.50	113.10
1	b	377	GLY	N-CA-C	-8.24	92.50	113.10
1	c	377	GLY	N-CA-C	-8.24	92.50	113.10
1	d	377	GLY	N-CA-C	-8.24	92.50	113.10
1	e	377	GLY	N-CA-C	-8.24	92.50	113.10
1	f	377	GLY	N-CA-C	-8.24	92.50	113.10
1	g	377	GLY	N-CA-C	-8.24	92.50	113.10
1	s	377	GLY	N-CA-C	-8.24	92.50	113.10
1	w	377	GLY	N-CA-C	-8.24	92.50	113.10
1	8	377	GLY	N-CA-C	-8.24	92.50	113.10
1	O	377	GLY	N-CA-C	-8.24	92.50	113.10
1	I	377	GLY	N-CA-C	-8.24	92.51	113.10
1	x	377	GLY	N-CA-C	-8.24	92.51	113.10
1	S	377	GLY	N-CA-C	-8.23	92.51	113.10
1	q	377	GLY	N-CA-C	-8.23	92.51	113.10
1	z	377	GLY	N-CA-C	-8.23	92.51	113.10
1	l	377	GLY	N-CA-C	-8.23	92.51	113.10
1	D	377	GLY	N-CA-C	-8.23	92.52	113.10
1	H	377	GLY	N-CA-C	-8.23	92.52	113.10
1	P	377	GLY	N-CA-C	-8.23	92.52	113.10
1	k	377	GLY	N-CA-C	-8.23	92.52	113.10
1	j	377	GLY	N-CA-C	-8.23	92.52	113.10
1	6	377	GLY	N-CA-C	-8.23	92.52	113.10
1	Z	377	GLY	N-CA-C	-8.23	92.52	113.10
1	E	377	GLY	N-CA-C	-8.23	92.53	113.10
1	h	377	GLY	N-CA-C	-8.23	92.53	113.10
1	X	377	GLY	N-CA-C	-8.23	92.53	113.10
1	o	377	GLY	N-CA-C	-8.23	92.53	113.10
1	t	377	GLY	N-CA-C	-8.23	92.54	113.10
1	Q	377	GLY	N-CA-C	-8.22	92.54	113.10
1	3	377	GLY	N-CA-C	-8.22	92.54	113.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	377	GLY	N-CA-C	-8.22	92.54	113.10
1	r	376	VAL	N-CA-C	7.92	132.38	111.00
1	W	376	VAL	N-CA-C	7.91	132.36	111.00
1	k	376	VAL	N-CA-C	7.91	132.35	111.00
1	p	376	VAL	N-CA-C	7.91	132.35	111.00
1	D	376	VAL	N-CA-C	7.91	132.35	111.00
1	M	376	VAL	N-CA-C	7.91	132.35	111.00
1	O	376	VAL	N-CA-C	7.91	132.35	111.00
1	X	376	VAL	N-CA-C	7.91	132.35	111.00
1	h	376	VAL	N-CA-C	7.91	132.35	111.00
1	B	376	VAL	N-CA-C	7.90	132.34	111.00
1	C	376	VAL	N-CA-C	7.90	132.34	111.00
1	H	376	VAL	N-CA-C	7.90	132.34	111.00
1	R	376	VAL	N-CA-C	7.90	132.34	111.00
1	g	376	VAL	N-CA-C	7.90	132.34	111.00
1	Z	376	VAL	N-CA-C	7.90	132.34	111.00
1	u	376	VAL	N-CA-C	7.90	132.34	111.00
1	6	376	VAL	N-CA-C	7.90	132.34	111.00
1	7	376	VAL	N-CA-C	7.90	132.34	111.00
1	T	376	VAL	N-CA-C	7.90	132.33	111.00
1	G	376	VAL	N-CA-C	7.90	132.33	111.00
1	P	376	VAL	N-CA-C	7.90	132.33	111.00
1	j	376	VAL	N-CA-C	7.90	132.33	111.00
1	J	376	VAL	N-CA-C	7.90	132.32	111.00
1	b	376	VAL	N-CA-C	7.90	132.32	111.00
1	f	376	VAL	N-CA-C	7.90	132.32	111.00
1	n	376	VAL	N-CA-C	7.90	132.32	111.00
1	y	376	VAL	N-CA-C	7.90	132.32	111.00
1	3	376	VAL	N-CA-C	7.90	132.32	111.00
1	A	376	VAL	N-CA-C	7.90	132.32	111.00
1	I	376	VAL	N-CA-C	7.90	132.32	111.00
1	Q	376	VAL	N-CA-C	7.90	132.32	111.00
1	V	376	VAL	N-CA-C	7.90	132.32	111.00
1	x	376	VAL	N-CA-C	7.90	132.32	111.00
1	E	376	VAL	N-CA-C	7.89	132.31	111.00
1	F	376	VAL	N-CA-C	7.89	132.31	111.00
1	a	376	VAL	N-CA-C	7.89	132.31	111.00
1	d	376	VAL	N-CA-C	7.89	132.32	111.00
1	e	376	VAL	N-CA-C	7.89	132.31	111.00
1	m	376	VAL	N-CA-C	7.89	132.32	111.00
1	w	376	VAL	N-CA-C	7.89	132.31	111.00
1	8	376	VAL	N-CA-C	7.89	132.31	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	376	VAL	N-CA-C	7.89	132.31	111.00
1	N	376	VAL	N-CA-C	7.89	132.31	111.00
1	q	376	VAL	N-CA-C	7.89	132.31	111.00
1	t	376	VAL	N-CA-C	7.89	132.31	111.00
1	i	376	VAL	N-CA-C	7.89	132.31	111.00
1	l	376	VAL	N-CA-C	7.89	132.30	111.00
1	o	376	VAL	N-CA-C	7.89	132.30	111.00
1	4	376	VAL	N-CA-C	7.89	132.30	111.00
1	v	376	VAL	N-CA-C	7.89	132.29	111.00
1	K	376	VAL	N-CA-C	7.88	132.28	111.00
1	S	376	VAL	N-CA-C	7.88	132.29	111.00
1	U	376	VAL	N-CA-C	7.88	132.29	111.00
1	s	376	VAL	N-CA-C	7.88	132.29	111.00
1	z	376	VAL	N-CA-C	7.88	132.29	111.00
1	1	376	VAL	N-CA-C	7.88	132.29	111.00
1	2	376	VAL	N-CA-C	7.88	132.29	111.00
1	c	376	VAL	N-CA-C	7.88	132.28	111.00
1	5	376	VAL	N-CA-C	7.88	132.28	111.00
1	Y	376	VAL	N-CA-C	7.88	132.27	111.00
1	O	547	ASN	N-CA-C	7.47	131.17	111.00
1	W	547	ASN	N-CA-C	7.46	131.15	111.00
1	m	547	ASN	N-CA-C	7.46	131.14	111.00
1	K	547	ASN	N-CA-C	7.46	131.13	111.00
1	L	547	ASN	N-CA-C	7.45	131.12	111.00
1	z	547	ASN	N-CA-C	7.45	131.12	111.00
1	N	547	ASN	N-CA-C	7.45	131.12	111.00
1	Y	547	ASN	N-CA-C	7.45	131.12	111.00
1	6	547	ASN	N-CA-C	7.45	131.12	111.00
1	H	547	ASN	N-CA-C	7.45	131.12	111.00
1	I	547	ASN	N-CA-C	7.45	131.12	111.00
1	g	547	ASN	N-CA-C	7.45	131.12	111.00
1	1	547	ASN	N-CA-C	7.45	131.12	111.00
1	4	547	ASN	N-CA-C	7.45	131.12	111.00
1	U	547	ASN	N-CA-C	7.45	131.11	111.00
1	l	547	ASN	N-CA-C	7.45	131.11	111.00
1	V	547	ASN	N-CA-C	7.45	131.11	111.00
1	a	547	ASN	N-CA-C	7.45	131.10	111.00
1	d	547	ASN	N-CA-C	7.45	131.10	111.00
1	s	547	ASN	N-CA-C	7.45	131.10	111.00
1	8	547	ASN	N-CA-C	7.45	131.10	111.00
1	G	547	ASN	N-CA-C	7.44	131.10	111.00
1	M	547	ASN	N-CA-C	7.44	131.10	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	r	547	ASN	N-CA-C	7.44	131.10	111.00
1	2	547	ASN	N-CA-C	7.44	131.10	111.00
1	A	547	ASN	N-CA-C	7.44	131.09	111.00
1	J	547	ASN	N-CA-C	7.44	131.09	111.00
1	b	547	ASN	N-CA-C	7.44	131.09	111.00
1	c	547	ASN	N-CA-C	7.44	131.09	111.00
1	e	547	ASN	N-CA-C	7.44	131.09	111.00
1	n	547	ASN	N-CA-C	7.44	131.09	111.00
1	t	547	ASN	N-CA-C	7.44	131.09	111.00
1	w	547	ASN	N-CA-C	7.44	131.09	111.00
1	3	547	ASN	N-CA-C	7.44	131.09	111.00
1	Z	547	ASN	N-CA-C	7.44	131.09	111.00
1	y	547	ASN	N-CA-C	7.44	131.09	111.00
1	B	547	ASN	N-CA-C	7.44	131.09	111.00
1	E	547	ASN	N-CA-C	7.44	131.09	111.00
1	R	547	ASN	N-CA-C	7.44	131.09	111.00
1	S	547	ASN	N-CA-C	7.44	131.09	111.00
1	X	547	ASN	N-CA-C	7.44	131.09	111.00
1	h	547	ASN	N-CA-C	7.44	131.09	111.00
1	o	547	ASN	N-CA-C	7.44	131.09	111.00
1	q	547	ASN	N-CA-C	7.44	131.09	111.00
1	F	547	ASN	N-CA-C	7.43	131.07	111.00
1	C	547	ASN	N-CA-C	7.43	131.06	111.00
1	D	547	ASN	N-CA-C	7.43	131.06	111.00
1	P	547	ASN	N-CA-C	7.43	131.06	111.00
1	Q	547	ASN	N-CA-C	7.43	131.06	111.00
1	f	547	ASN	N-CA-C	7.43	131.06	111.00
1	i	547	ASN	N-CA-C	7.43	131.06	111.00
1	j	547	ASN	N-CA-C	7.43	131.06	111.00
1	p	547	ASN	N-CA-C	7.43	131.06	111.00
1	v	547	ASN	N-CA-C	7.43	131.06	111.00
1	x	547	ASN	N-CA-C	7.43	131.06	111.00
1	5	547	ASN	N-CA-C	7.43	131.06	111.00
1	7	547	ASN	N-CA-C	7.43	131.06	111.00
1	T	547	ASN	N-CA-C	7.42	131.05	111.00
1	u	547	ASN	N-CA-C	7.42	131.04	111.00
1	k	547	ASN	N-CA-C	7.42	131.04	111.00
1	S	548	TYR	N-CA-CB	6.67	122.61	110.60
1	4	548	TYR	N-CA-CB	6.67	122.60	110.60
1	I	548	TYR	N-CA-CB	6.67	122.60	110.60
1	K	548	TYR	N-CA-CB	6.67	122.60	110.60
1	b	548	TYR	N-CA-CB	6.67	122.60	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	c	548	TYR	N-CA-CB	6.67	122.60	110.60
1	e	548	TYR	N-CA-CB	6.67	122.60	110.60
1	f	548	TYR	N-CA-CB	6.67	122.60	110.60
1	p	548	TYR	N-CA-CB	6.67	122.60	110.60
1	D	548	TYR	N-CA-CB	6.66	122.59	110.60
1	E	548	TYR	N-CA-CB	6.66	122.59	110.60
1	G	548	TYR	N-CA-CB	6.66	122.59	110.60
1	N	548	TYR	N-CA-CB	6.66	122.59	110.60
1	O	548	TYR	N-CA-CB	6.66	122.59	110.60
1	Q	548	TYR	N-CA-CB	6.66	122.59	110.60
1	Y	548	TYR	N-CA-CB	6.66	122.59	110.60
1	Z	548	TYR	N-CA-CB	6.66	122.59	110.60
1	k	548	TYR	N-CA-CB	6.66	122.59	110.60
1	6	548	TYR	N-CA-CB	6.66	122.59	110.60
1	7	548	TYR	N-CA-CB	6.66	122.59	110.60
1	V	548	TYR	N-CA-CB	6.66	122.59	110.60
1	d	548	TYR	N-CA-CB	6.66	122.59	110.60
1	B	548	TYR	N-CA-CB	6.66	122.59	110.60
1	U	548	TYR	N-CA-CB	6.66	122.59	110.60
1	q	548	TYR	N-CA-CB	6.66	122.58	110.60
1	u	548	TYR	N-CA-CB	6.66	122.59	110.60
1	x	548	TYR	N-CA-CB	6.66	122.58	110.60
1	A	548	TYR	N-CA-CB	6.66	122.58	110.60
1	a	548	TYR	N-CA-CB	6.66	122.58	110.60
1	v	548	TYR	N-CA-CB	6.66	122.58	110.60
1	y	548	TYR	N-CA-CB	6.66	122.58	110.60
1	C	548	TYR	N-CA-CB	6.66	122.58	110.60
1	T	548	TYR	N-CA-CB	6.66	122.58	110.60
1	m	548	TYR	N-CA-CB	6.66	122.58	110.60
1	H	548	TYR	N-CA-CB	6.65	122.58	110.60
1	j	548	TYR	N-CA-CB	6.65	122.58	110.60
1	L	548	TYR	N-CA-CB	6.65	122.58	110.60
1	M	548	TYR	N-CA-CB	6.65	122.58	110.60
1	R	548	TYR	N-CA-CB	6.65	122.57	110.60
1	W	548	TYR	N-CA-CB	6.65	122.58	110.60
1	X	548	TYR	N-CA-CB	6.65	122.58	110.60
1	h	548	TYR	N-CA-CB	6.65	122.58	110.60
1	s	548	TYR	N-CA-CB	6.65	122.58	110.60
1	z	548	TYR	N-CA-CB	6.65	122.58	110.60
1	1	548	TYR	N-CA-CB	6.65	122.58	110.60
1	2	548	TYR	N-CA-CB	6.65	122.57	110.60
1	i	548	TYR	N-CA-CB	6.65	122.57	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	r	548	TYR	N-CA-CB	6.65	122.56	110.60
1	o	548	TYR	N-CA-CB	6.64	122.56	110.60
1	t	548	TYR	N-CA-CB	6.64	122.56	110.60
1	w	548	TYR	N-CA-CB	6.64	122.56	110.60
1	l	548	TYR	N-CA-CB	6.64	122.56	110.60
1	F	548	TYR	N-CA-CB	6.64	122.55	110.60
1	P	548	TYR	N-CA-CB	6.64	122.55	110.60
1	g	548	TYR	N-CA-CB	6.64	122.55	110.60
1	n	548	TYR	N-CA-CB	6.64	122.55	110.60
1	3	548	TYR	N-CA-CB	6.64	122.55	110.60
1	5	548	TYR	N-CA-CB	6.64	122.55	110.60
1	8	548	TYR	N-CA-CB	6.64	122.55	110.60
1	J	548	TYR	N-CA-CB	6.63	122.54	110.60
1	G	388	VAL	N-CA-C	-6.50	93.45	111.00
1	t	388	VAL	N-CA-C	-6.50	93.45	111.00
1	W	388	VAL	N-CA-C	-6.50	93.46	111.00
1	u	388	VAL	N-CA-C	-6.50	93.46	111.00
1	6	388	VAL	N-CA-C	-6.50	93.46	111.00
1	B	388	VAL	N-CA-C	-6.50	93.46	111.00
1	L	388	VAL	N-CA-C	-6.50	93.46	111.00
1	2	388	VAL	N-CA-C	-6.50	93.46	111.00
1	E	388	VAL	N-CA-C	-6.49	93.47	111.00
1	Z	388	VAL	N-CA-C	-6.49	93.47	111.00
1	h	388	VAL	N-CA-C	-6.49	93.47	111.00
1	P	388	VAL	N-CA-C	-6.49	93.47	111.00
1	v	388	VAL	N-CA-C	-6.49	93.47	111.00
1	T	388	VAL	N-CA-C	-6.49	93.48	111.00
1	U	388	VAL	N-CA-C	-6.49	93.48	111.00
1	D	388	VAL	N-CA-C	-6.49	93.48	111.00
1	y	388	VAL	N-CA-C	-6.49	93.48	111.00
1	3	388	VAL	N-CA-C	-6.49	93.48	111.00
1	H	388	VAL	N-CA-C	-6.49	93.49	111.00
1	M	388	VAL	N-CA-C	-6.49	93.49	111.00
1	N	388	VAL	N-CA-C	-6.49	93.49	111.00
1	X	388	VAL	N-CA-C	-6.49	93.49	111.00
1	i	388	VAL	N-CA-C	-6.49	93.49	111.00
1	A	388	VAL	N-CA-C	-6.48	93.49	111.00
1	C	388	VAL	N-CA-C	-6.48	93.49	111.00
1	F	388	VAL	N-CA-C	-6.48	93.49	111.00
1	Q	388	VAL	N-CA-C	-6.48	93.49	111.00
1	V	388	VAL	N-CA-C	-6.48	93.49	111.00
1	c	388	VAL	N-CA-C	-6.48	93.49	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	d	388	VAL	N-CA-C	-6.48	93.49	111.00
1	e	388	VAL	N-CA-C	-6.48	93.49	111.00
1	f	388	VAL	N-CA-C	-6.48	93.49	111.00
1	x	388	VAL	N-CA-C	-6.48	93.49	111.00
1	4	388	VAL	N-CA-C	-6.48	93.49	111.00
1	K	388	VAL	N-CA-C	-6.48	93.50	111.00
1	S	388	VAL	N-CA-C	-6.48	93.50	111.00
1	b	388	VAL	N-CA-C	-6.48	93.50	111.00
1	l	388	VAL	N-CA-C	-6.48	93.50	111.00
1	o	388	VAL	N-CA-C	-6.48	93.50	111.00
1	r	388	VAL	N-CA-C	-6.48	93.50	111.00
1	8	388	VAL	N-CA-C	-6.48	93.50	111.00
1	I	388	VAL	N-CA-C	-6.48	93.51	111.00
1	g	388	VAL	N-CA-C	-6.48	93.51	111.00
1	p	388	VAL	N-CA-C	-6.48	93.51	111.00
1	Y	388	VAL	N-CA-C	-6.48	93.51	111.00
1	m	388	VAL	N-CA-C	-6.48	93.51	111.00
1	l	388	VAL	N-CA-C	-6.48	93.51	111.00
1	k	388	VAL	N-CA-C	-6.48	93.52	111.00
1	J	388	VAL	N-CA-C	-6.47	93.52	111.00
1	R	388	VAL	N-CA-C	-6.47	93.52	111.00
1	q	388	VAL	N-CA-C	-6.47	93.52	111.00
1	s	388	VAL	N-CA-C	-6.47	93.52	111.00
1	w	388	VAL	N-CA-C	-6.47	93.52	111.00
1	z	388	VAL	N-CA-C	-6.47	93.52	111.00
1	n	388	VAL	N-CA-C	-6.47	93.52	111.00
1	j	388	VAL	N-CA-C	-6.47	93.53	111.00
1	5	388	VAL	N-CA-C	-6.47	93.53	111.00
1	7	388	VAL	N-CA-C	-6.47	93.53	111.00
1	O	388	VAL	N-CA-C	-6.47	93.54	111.00
1	a	388	VAL	N-CA-C	-6.46	93.55	111.00
1	Q	471	ALA	CB-CA-C	-6.16	100.86	110.10
1	S	471	ALA	CB-CA-C	-6.15	100.87	110.10
1	G	471	ALA	CB-CA-C	-6.15	100.88	110.10
1	O	471	ALA	CB-CA-C	-6.15	100.88	110.10
1	e	471	ALA	CB-CA-C	-6.14	100.88	110.10
1	f	471	ALA	CB-CA-C	-6.14	100.88	110.10
1	N	471	ALA	CB-CA-C	-6.14	100.89	110.10
1	W	471	ALA	CB-CA-C	-6.14	100.89	110.10
1	6	471	ALA	CB-CA-C	-6.14	100.89	110.10
1	M	471	ALA	CB-CA-C	-6.14	100.89	110.10
1	J	471	ALA	CB-CA-C	-6.14	100.90	110.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	x	471	ALA	CB-CA-C	-6.14	100.89	110.10
1	E	471	ALA	CB-CA-C	-6.13	100.90	110.10
1	T	471	ALA	CB-CA-C	-6.13	100.90	110.10
1	r	471	ALA	CB-CA-C	-6.13	100.90	110.10
1	2	471	ALA	CB-CA-C	-6.13	100.90	110.10
1	8	471	ALA	CB-CA-C	-6.13	100.90	110.10
1	I	471	ALA	CB-CA-C	-6.13	100.90	110.10
1	p	471	ALA	CB-CA-C	-6.13	100.90	110.10
1	u	471	ALA	CB-CA-C	-6.13	100.90	110.10
1	4	471	ALA	CB-CA-C	-6.13	100.90	110.10
1	L	471	ALA	CB-CA-C	-6.13	100.90	110.10
1	K	471	ALA	CB-CA-C	-6.13	100.91	110.10
1	P	471	ALA	CB-CA-C	-6.12	100.91	110.10
1	7	471	ALA	CB-CA-C	-6.12	100.91	110.10
1	B	471	ALA	CB-CA-C	-6.12	100.91	110.10
1	Y	471	ALA	CB-CA-C	-6.12	100.92	110.10
1	a	471	ALA	CB-CA-C	-6.12	100.92	110.10
1	j	471	ALA	CB-CA-C	-6.12	100.92	110.10
1	y	471	ALA	CB-CA-C	-6.12	100.92	110.10
1	3	471	ALA	CB-CA-C	-6.12	100.92	110.10
1	5	471	ALA	CB-CA-C	-6.12	100.92	110.10
1	A	471	ALA	CB-CA-C	-6.12	100.92	110.10
1	c	471	ALA	CB-CA-C	-6.12	100.92	110.10
1	d	471	ALA	CB-CA-C	-6.12	100.92	110.10
1	n	471	ALA	CB-CA-C	-6.12	100.92	110.10
1	g	471	ALA	CB-CA-C	-6.12	100.92	110.10
1	m	471	ALA	CB-CA-C	-6.12	100.92	110.10
1	l	471	ALA	CB-CA-C	-6.12	100.92	110.10
1	R	471	ALA	CB-CA-C	-6.12	100.93	110.10
1	U	471	ALA	CB-CA-C	-6.12	100.93	110.10
1	h	471	ALA	CB-CA-C	-6.12	100.93	110.10
1	C	471	ALA	CB-CA-C	-6.11	100.93	110.10
1	V	471	ALA	CB-CA-C	-6.11	100.93	110.10
1	F	471	ALA	CB-CA-C	-6.11	100.94	110.10
1	v	471	ALA	CB-CA-C	-6.11	100.94	110.10
1	q	471	ALA	CB-CA-C	-6.11	100.94	110.10
1	H	471	ALA	CB-CA-C	-6.11	100.94	110.10
1	i	471	ALA	CB-CA-C	-6.11	100.94	110.10
1	k	471	ALA	CB-CA-C	-6.11	100.94	110.10
1	s	471	ALA	CB-CA-C	-6.11	100.94	110.10
1	t	471	ALA	CB-CA-C	-6.10	100.94	110.10
1	b	471	ALA	CB-CA-C	-6.10	100.95	110.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	471	ALA	CB-CA-C	-6.10	100.95	110.10
1	X	471	ALA	CB-CA-C	-6.10	100.96	110.10
1	o	471	ALA	CB-CA-C	-6.10	100.96	110.10
1	Z	471	ALA	CB-CA-C	-6.09	100.96	110.10
1	w	471	ALA	CB-CA-C	-6.09	100.97	110.10
1	z	471	ALA	CB-CA-C	-6.09	100.97	110.10
1	D	471	ALA	CB-CA-C	-6.09	100.97	110.10
1	i	89	LEU	CB-CG-CD1	-5.04	102.44	111.00
1	F	89	LEU	CB-CG-CD1	-5.01	102.48	111.00
1	o	89	LEU	CB-CG-CD1	-5.01	102.48	111.00
1	D	89	LEU	CB-CG-CD1	-5.01	102.48	111.00
1	M	89	LEU	CB-CG-CD1	-5.01	102.48	111.00
1	h	89	LEU	CB-CG-CD1	-5.01	102.48	111.00
1	t	89	LEU	CB-CG-CD1	-5.01	102.48	111.00
1	2	89	LEU	CB-CG-CD1	-5.01	102.48	111.00
1	8	89	LEU	CB-CG-CD1	-5.01	102.48	111.00
1	O	89	LEU	CB-CG-CD1	-5.01	102.49	111.00
1	Q	89	LEU	CB-CG-CD1	-5.01	102.49	111.00
1	Z	89	LEU	CB-CG-CD1	-5.01	102.49	111.00
1	b	89	LEU	CB-CG-CD1	-5.01	102.49	111.00
1	f	89	LEU	CB-CG-CD1	-5.01	102.49	111.00
1	P	89	LEU	CB-CG-CD1	-5.00	102.49	111.00
1	m	89	LEU	CB-CG-CD1	-5.00	102.50	111.00

All (60) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	393	THR	CA
1	B	393	THR	CA
1	C	393	THR	CA
1	D	393	THR	CA
1	E	393	THR	CA
1	F	393	THR	CA
1	G	393	THR	CA
1	H	393	THR	CA
1	I	393	THR	CA
1	J	393	THR	CA
1	K	393	THR	CA
1	L	393	THR	CA
1	M	393	THR	CA
1	N	393	THR	CA
1	O	393	THR	CA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
1	P	393	THR	CA
1	Q	393	THR	CA
1	R	393	THR	CA
1	S	393	THR	CA
1	T	393	THR	CA
1	U	393	THR	CA
1	V	393	THR	CA
1	W	393	THR	CA
1	X	393	THR	CA
1	Y	393	THR	CA
1	Z	393	THR	CA
1	a	393	THR	CA
1	b	393	THR	CA
1	c	393	THR	CA
1	d	393	THR	CA
1	e	393	THR	CA
1	f	393	THR	CA
1	g	393	THR	CA
1	h	393	THR	CA
1	i	393	THR	CA
1	j	393	THR	CA
1	k	393	THR	CA
1	l	393	THR	CA
1	m	393	THR	CA
1	n	393	THR	CA
1	o	393	THR	CA
1	p	393	THR	CA
1	q	393	THR	CA
1	r	393	THR	CA
1	s	393	THR	CA
1	t	393	THR	CA
1	u	393	THR	CA
1	v	393	THR	CA
1	w	393	THR	CA
1	x	393	THR	CA
1	y	393	THR	CA
1	z	393	THR	CA
1	1	393	THR	CA
1	2	393	THR	CA
1	3	393	THR	CA
1	4	393	THR	CA
1	5	393	THR	CA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
1	6	393	THR	CA
1	7	393	THR	CA
1	8	393	THR	CA

All (60) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	380	PHE	Peptide
1	2	380	PHE	Peptide
1	3	380	PHE	Peptide
1	4	380	PHE	Peptide
1	5	380	PHE	Peptide
1	6	380	PHE	Peptide
1	7	380	PHE	Peptide
1	8	380	PHE	Peptide
1	A	380	PHE	Peptide
1	B	380	PHE	Peptide
1	C	380	PHE	Peptide
1	D	380	PHE	Peptide
1	E	380	PHE	Peptide
1	F	380	PHE	Peptide
1	G	380	PHE	Peptide
1	H	380	PHE	Peptide
1	I	380	PHE	Peptide
1	J	380	PHE	Peptide
1	K	380	PHE	Peptide
1	L	380	PHE	Peptide
1	M	380	PHE	Peptide
1	N	380	PHE	Peptide
1	O	380	PHE	Peptide
1	P	380	PHE	Peptide
1	Q	380	PHE	Peptide
1	R	380	PHE	Peptide
1	S	380	PHE	Peptide
1	T	380	PHE	Peptide
1	U	380	PHE	Peptide
1	V	380	PHE	Peptide
1	W	380	PHE	Peptide
1	X	380	PHE	Peptide
1	Y	380	PHE	Peptide
1	Z	380	PHE	Peptide
1	a	380	PHE	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	b	380	PHE	Peptide
1	c	380	PHE	Peptide
1	d	380	PHE	Peptide
1	e	380	PHE	Peptide
1	f	380	PHE	Peptide
1	g	380	PHE	Peptide
1	h	380	PHE	Peptide
1	i	380	PHE	Peptide
1	j	380	PHE	Peptide
1	k	380	PHE	Peptide
1	l	380	PHE	Peptide
1	m	380	PHE	Peptide
1	n	380	PHE	Peptide
1	o	380	PHE	Peptide
1	p	380	PHE	Peptide
1	q	380	PHE	Peptide
1	r	380	PHE	Peptide
1	s	380	PHE	Peptide
1	t	380	PHE	Peptide
1	u	380	PHE	Peptide
1	v	380	PHE	Peptide
1	w	380	PHE	Peptide
1	x	380	PHE	Peptide
1	y	380	PHE	Peptide
1	z	380	PHE	Peptide

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	536/552 (97%)	514 (96%)	19 (4%)	3 (1%)	25	59
1	2	536/552 (97%)	514 (96%)	19 (4%)	3 (1%)	25	59
1	3	536/552 (97%)	514 (96%)	19 (4%)	3 (1%)	25	59
1	4	536/552 (97%)	514 (96%)	19 (4%)	3 (1%)	25	59
1	5	536/552 (97%)	514 (96%)	19 (4%)	3 (1%)	25	59
1	6	536/552 (97%)	514 (96%)	19 (4%)	3 (1%)	25	59
1	7	536/552 (97%)	514 (96%)	19 (4%)	3 (1%)	25	59
1	8	536/552 (97%)	514 (96%)	19 (4%)	3 (1%)	25	59
1	A	536/552 (97%)	514 (96%)	19 (4%)	3 (1%)	25	59
1	B	536/552 (97%)	514 (96%)	19 (4%)	3 (1%)	25	59
1	C	536/552 (97%)	514 (96%)	19 (4%)	3 (1%)	25	59
1	D	536/552 (97%)	514 (96%)	19 (4%)	3 (1%)	25	59
1	E	536/552 (97%)	514 (96%)	19 (4%)	3 (1%)	25	59
1	F	536/552 (97%)	514 (96%)	19 (4%)	3 (1%)	25	59
1	G	536/552 (97%)	514 (96%)	19 (4%)	3 (1%)	25	59
1	H	536/552 (97%)	514 (96%)	19 (4%)	3 (1%)	25	59
1	I	536/552 (97%)	514 (96%)	19 (4%)	3 (1%)	25	59
1	J	536/552 (97%)	514 (96%)	19 (4%)	3 (1%)	25	59
1	K	536/552 (97%)	514 (96%)	19 (4%)	3 (1%)	25	59
1	L	536/552 (97%)	514 (96%)	19 (4%)	3 (1%)	25	59
1	M	536/552 (97%)	514 (96%)	19 (4%)	3 (1%)	25	59
1	N	536/552 (97%)	514 (96%)	19 (4%)	3 (1%)	25	59
1	O	536/552 (97%)	514 (96%)	19 (4%)	3 (1%)	25	59
1	P	536/552 (97%)	514 (96%)	19 (4%)	3 (1%)	25	59
1	Q	536/552 (97%)	514 (96%)	19 (4%)	3 (1%)	25	59
1	R	536/552 (97%)	514 (96%)	19 (4%)	3 (1%)	25	59
1	S	536/552 (97%)	514 (96%)	19 (4%)	3 (1%)	25	59
1	T	536/552 (97%)	514 (96%)	19 (4%)	3 (1%)	25	59
1	U	536/552 (97%)	514 (96%)	19 (4%)	3 (1%)	25	59
1	V	536/552 (97%)	514 (96%)	19 (4%)	3 (1%)	25	59
1	W	536/552 (97%)	514 (96%)	19 (4%)	3 (1%)	25	59
1	X	536/552 (97%)	514 (96%)	19 (4%)	3 (1%)	25	59

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Y	536/552 (97%)	514 (96%)	19 (4%)	3 (1%)	25	59
1	Z	536/552 (97%)	514 (96%)	19 (4%)	3 (1%)	25	59
1	a	536/552 (97%)	514 (96%)	19 (4%)	3 (1%)	25	59
1	b	536/552 (97%)	514 (96%)	19 (4%)	3 (1%)	25	59
1	c	536/552 (97%)	514 (96%)	19 (4%)	3 (1%)	25	59
1	d	536/552 (97%)	514 (96%)	19 (4%)	3 (1%)	25	59
1	e	536/552 (97%)	514 (96%)	19 (4%)	3 (1%)	25	59
1	f	536/552 (97%)	514 (96%)	19 (4%)	3 (1%)	25	59
1	g	536/552 (97%)	514 (96%)	19 (4%)	3 (1%)	25	59
1	h	536/552 (97%)	514 (96%)	19 (4%)	3 (1%)	25	59
1	i	536/552 (97%)	514 (96%)	19 (4%)	3 (1%)	25	59
1	j	536/552 (97%)	514 (96%)	19 (4%)	3 (1%)	25	59
1	k	536/552 (97%)	514 (96%)	19 (4%)	3 (1%)	25	59
1	l	536/552 (97%)	514 (96%)	19 (4%)	3 (1%)	25	59
1	m	536/552 (97%)	514 (96%)	19 (4%)	3 (1%)	25	59
1	n	536/552 (97%)	514 (96%)	19 (4%)	3 (1%)	25	59
1	o	536/552 (97%)	514 (96%)	19 (4%)	3 (1%)	25	59
1	p	536/552 (97%)	514 (96%)	19 (4%)	3 (1%)	25	59
1	q	536/552 (97%)	514 (96%)	19 (4%)	3 (1%)	25	59
1	r	536/552 (97%)	514 (96%)	19 (4%)	3 (1%)	25	59
1	s	536/552 (97%)	514 (96%)	19 (4%)	3 (1%)	25	59
1	t	536/552 (97%)	514 (96%)	19 (4%)	3 (1%)	25	59
1	u	536/552 (97%)	514 (96%)	19 (4%)	3 (1%)	25	59
1	v	536/552 (97%)	514 (96%)	19 (4%)	3 (1%)	25	59
1	w	536/552 (97%)	514 (96%)	19 (4%)	3 (1%)	25	59
1	x	536/552 (97%)	514 (96%)	19 (4%)	3 (1%)	25	59
1	y	536/552 (97%)	514 (96%)	19 (4%)	3 (1%)	25	59
1	z	536/552 (97%)	514 (96%)	19 (4%)	3 (1%)	25	59
All	All	32160/33120 (97%)	30840 (96%)	1140 (4%)	180 (1%)	29	59

All (180) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	531	PRO
1	K	177	ASN
1	T	177	ASN
1	p	531	PRO
1	A	177	ASN
1	A	531	PRO
1	B	177	ASN
1	C	177	ASN
1	C	531	PRO
1	D	177	ASN
1	D	531	PRO
1	E	177	ASN
1	E	531	PRO
1	F	177	ASN
1	F	531	PRO
1	G	177	ASN
1	G	531	PRO
1	H	177	ASN
1	H	531	PRO
1	I	177	ASN
1	I	531	PRO
1	J	177	ASN
1	J	531	PRO
1	K	531	PRO
1	L	177	ASN
1	L	531	PRO
1	M	177	ASN
1	M	531	PRO
1	N	177	ASN
1	N	531	PRO
1	O	177	ASN
1	O	531	PRO
1	P	177	ASN
1	P	531	PRO
1	Q	177	ASN
1	Q	531	PRO
1	R	177	ASN
1	R	531	PRO
1	S	177	ASN
1	S	531	PRO
1	T	531	PRO
1	U	177	ASN
1	U	531	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	V	177	ASN
1	V	531	PRO
1	W	177	ASN
1	W	531	PRO
1	X	177	ASN
1	X	531	PRO
1	Y	177	ASN
1	Y	531	PRO
1	Z	177	ASN
1	Z	531	PRO
1	a	177	ASN
1	a	531	PRO
1	b	177	ASN
1	b	531	PRO
1	c	177	ASN
1	c	531	PRO
1	d	177	ASN
1	d	531	PRO
1	e	177	ASN
1	e	531	PRO
1	f	177	ASN
1	f	531	PRO
1	g	177	ASN
1	g	531	PRO
1	h	177	ASN
1	h	531	PRO
1	i	177	ASN
1	i	531	PRO
1	j	177	ASN
1	j	531	PRO
1	k	177	ASN
1	k	531	PRO
1	l	177	ASN
1	l	531	PRO
1	m	177	ASN
1	m	531	PRO
1	n	177	ASN
1	n	531	PRO
1	o	177	ASN
1	o	531	PRO
1	p	177	ASN
1	q	177	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	q	531	PRO
1	r	177	ASN
1	r	531	PRO
1	s	177	ASN
1	s	531	PRO
1	t	177	ASN
1	t	531	PRO
1	u	177	ASN
1	u	531	PRO
1	v	177	ASN
1	v	531	PRO
1	w	177	ASN
1	w	531	PRO
1	x	177	ASN
1	x	531	PRO
1	y	177	ASN
1	y	531	PRO
1	z	177	ASN
1	z	531	PRO
1	1	177	ASN
1	1	531	PRO
1	2	177	ASN
1	2	531	PRO
1	3	177	ASN
1	3	531	PRO
1	4	177	ASN
1	4	531	PRO
1	5	177	ASN
1	5	531	PRO
1	6	177	ASN
1	6	531	PRO
1	7	177	ASN
1	7	531	PRO
1	8	177	ASN
1	8	531	PRO
1	A	297	PRO
1	B	297	PRO
1	C	297	PRO
1	D	297	PRO
1	E	297	PRO
1	F	297	PRO
1	G	297	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	297	PRO
1	I	297	PRO
1	J	297	PRO
1	K	297	PRO
1	L	297	PRO
1	M	297	PRO
1	N	297	PRO
1	O	297	PRO
1	P	297	PRO
1	Q	297	PRO
1	R	297	PRO
1	S	297	PRO
1	T	297	PRO
1	U	297	PRO
1	V	297	PRO
1	W	297	PRO
1	X	297	PRO
1	Y	297	PRO
1	Z	297	PRO
1	a	297	PRO
1	b	297	PRO
1	c	297	PRO
1	d	297	PRO
1	e	297	PRO
1	f	297	PRO
1	g	297	PRO
1	h	297	PRO
1	i	297	PRO
1	j	297	PRO
1	k	297	PRO
1	l	297	PRO
1	m	297	PRO
1	n	297	PRO
1	o	297	PRO
1	p	297	PRO
1	q	297	PRO
1	r	297	PRO
1	s	297	PRO
1	t	297	PRO
1	u	297	PRO
1	v	297	PRO
1	w	297	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	x	297	PRO
1	y	297	PRO
1	z	297	PRO
1	1	297	PRO
1	2	297	PRO
1	3	297	PRO
1	4	297	PRO
1	5	297	PRO
1	6	297	PRO
1	7	297	PRO
1	8	297	PRO

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	471/479 (98%)	471 (100%)	0	100	100
1	2	471/479 (98%)	470 (100%)	1 (0%)	93	97
1	3	471/479 (98%)	471 (100%)	0	100	100
1	4	471/479 (98%)	471 (100%)	0	100	100
1	5	471/479 (98%)	471 (100%)	0	100	100
1	6	471/479 (98%)	471 (100%)	0	100	100
1	7	471/479 (98%)	471 (100%)	0	100	100
1	8	471/479 (98%)	471 (100%)	0	100	100
1	A	471/479 (98%)	471 (100%)	0	100	100
1	B	471/479 (98%)	471 (100%)	0	100	100
1	C	471/479 (98%)	471 (100%)	0	100	100
1	D	471/479 (98%)	470 (100%)	1 (0%)	93	97
1	E	471/479 (98%)	471 (100%)	0	100	100
1	F	471/479 (98%)	471 (100%)	0	100	100
1	G	471/479 (98%)	471 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	471/479 (98%)	471 (100%)	0	100	100
1	I	471/479 (98%)	471 (100%)	0	100	100
1	J	471/479 (98%)	471 (100%)	0	100	100
1	K	471/479 (98%)	470 (100%)	1 (0%)	93	97
1	L	471/479 (98%)	470 (100%)	1 (0%)	93	97
1	M	471/479 (98%)	470 (100%)	1 (0%)	93	97
1	N	471/479 (98%)	471 (100%)	0	100	100
1	O	471/479 (98%)	470 (100%)	1 (0%)	93	97
1	P	471/479 (98%)	471 (100%)	0	100	100
1	Q	471/479 (98%)	470 (100%)	1 (0%)	93	97
1	R	471/479 (98%)	471 (100%)	0	100	100
1	S	471/479 (98%)	471 (100%)	0	100	100
1	T	471/479 (98%)	470 (100%)	1 (0%)	93	97
1	U	471/479 (98%)	471 (100%)	0	100	100
1	V	471/479 (98%)	471 (100%)	0	100	100
1	W	471/479 (98%)	470 (100%)	1 (0%)	93	97
1	X	471/479 (98%)	470 (100%)	1 (0%)	93	97
1	Y	471/479 (98%)	470 (100%)	1 (0%)	93	97
1	Z	471/479 (98%)	471 (100%)	0	100	100
1	a	471/479 (98%)	471 (100%)	0	100	100
1	b	471/479 (98%)	470 (100%)	1 (0%)	93	97
1	c	471/479 (98%)	471 (100%)	0	100	100
1	d	471/479 (98%)	471 (100%)	0	100	100
1	e	471/479 (98%)	471 (100%)	0	100	100
1	f	471/479 (98%)	470 (100%)	1 (0%)	93	97
1	g	471/479 (98%)	471 (100%)	0	100	100
1	h	471/479 (98%)	470 (100%)	1 (0%)	93	97
1	i	471/479 (98%)	471 (100%)	0	100	100
1	j	471/479 (98%)	470 (100%)	1 (0%)	93	97
1	k	471/479 (98%)	470 (100%)	1 (0%)	93	97
1	l	471/479 (98%)	471 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	m	471/479 (98%)	471 (100%)	0	100	100
1	n	471/479 (98%)	471 (100%)	0	100	100
1	o	471/479 (98%)	471 (100%)	0	100	100
1	p	471/479 (98%)	471 (100%)	0	100	100
1	q	471/479 (98%)	470 (100%)	1 (0%)	93	97
1	r	471/479 (98%)	470 (100%)	1 (0%)	93	97
1	s	471/479 (98%)	471 (100%)	0	100	100
1	t	471/479 (98%)	471 (100%)	0	100	100
1	u	471/479 (98%)	471 (100%)	0	100	100
1	v	471/479 (98%)	470 (100%)	1 (0%)	93	97
1	w	471/479 (98%)	471 (100%)	0	100	100
1	x	471/479 (98%)	471 (100%)	0	100	100
1	y	471/479 (98%)	471 (100%)	0	100	100
1	z	471/479 (98%)	471 (100%)	0	100	100
All	All	28260/28740 (98%)	28241 (100%)	19 (0%)	93	98

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	99	SER
1	K	99	SER
1	L	99	SER
1	M	99	SER
1	O	99	SER
1	Q	99	SER
1	T	99	SER
1	W	99	SER
1	X	99	SER
1	Y	99	SER
1	b	99	SER
1	f	99	SER
1	h	99	SER
1	j	99	SER
1	k	99	SER
1	q	99	SER
1	r	99	SER
1	v	99	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2	99	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (997) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	GLN
1	A	79	HIS
1	A	153	HIS
1	A	194	HIS
1	A	282	GLN
1	A	323	ASN
1	A	343	HIS
1	A	378	HIS
1	A	385	HIS
1	A	472	HIS
1	A	478	ASN
1	A	486	HIS
1	A	488	HIS
1	A	504	HIS
1	A	526	ASN
1	A	550	HIS
1	B	59	GLN
1	B	79	HIS
1	B	153	HIS
1	B	194	HIS
1	B	282	GLN
1	B	323	ASN
1	B	343	HIS
1	B	378	HIS
1	B	385	HIS
1	B	425	GLN
1	B	472	HIS
1	B	478	ASN
1	B	486	HIS
1	B	488	HIS
1	B	504	HIS
1	B	526	ASN
1	B	550	HIS
1	C	59	GLN
1	C	79	HIS
1	C	153	HIS
1	C	194	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	282	GLN
1	C	323	ASN
1	C	343	HIS
1	C	378	HIS
1	C	385	HIS
1	C	472	HIS
1	C	478	ASN
1	C	486	HIS
1	C	488	HIS
1	C	504	HIS
1	C	526	ASN
1	C	550	HIS
1	D	59	GLN
1	D	79	HIS
1	D	153	HIS
1	D	194	HIS
1	D	282	GLN
1	D	323	ASN
1	D	343	HIS
1	D	378	HIS
1	D	385	HIS
1	D	425	GLN
1	D	472	HIS
1	D	478	ASN
1	D	486	HIS
1	D	488	HIS
1	D	504	HIS
1	D	526	ASN
1	D	550	HIS
1	E	59	GLN
1	E	79	HIS
1	E	153	HIS
1	E	194	HIS
1	E	282	GLN
1	E	323	ASN
1	E	343	HIS
1	E	378	HIS
1	E	385	HIS
1	E	472	HIS
1	E	478	ASN
1	E	486	HIS
1	E	488	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	504	HIS
1	E	526	ASN
1	E	550	HIS
1	F	59	GLN
1	F	79	HIS
1	F	153	HIS
1	F	194	HIS
1	F	282	GLN
1	F	323	ASN
1	F	343	HIS
1	F	378	HIS
1	F	385	HIS
1	F	472	HIS
1	F	478	ASN
1	F	486	HIS
1	F	488	HIS
1	F	504	HIS
1	F	526	ASN
1	F	550	HIS
1	G	59	GLN
1	G	79	HIS
1	G	153	HIS
1	G	194	HIS
1	G	282	GLN
1	G	323	ASN
1	G	343	HIS
1	G	378	HIS
1	G	385	HIS
1	G	425	GLN
1	G	472	HIS
1	G	478	ASN
1	G	486	HIS
1	G	488	HIS
1	G	504	HIS
1	G	526	ASN
1	G	550	HIS
1	H	59	GLN
1	H	79	HIS
1	H	153	HIS
1	H	194	HIS
1	H	282	GLN
1	H	323	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	343	HIS
1	H	378	HIS
1	H	385	HIS
1	H	425	GLN
1	H	472	HIS
1	H	478	ASN
1	H	486	HIS
1	H	488	HIS
1	H	504	HIS
1	H	526	ASN
1	H	550	HIS
1	I	59	GLN
1	I	79	HIS
1	I	153	HIS
1	I	194	HIS
1	I	282	GLN
1	I	323	ASN
1	I	343	HIS
1	I	378	HIS
1	I	385	HIS
1	I	425	GLN
1	I	472	HIS
1	I	478	ASN
1	I	486	HIS
1	I	488	HIS
1	I	504	HIS
1	I	526	ASN
1	I	550	HIS
1	J	59	GLN
1	J	79	HIS
1	J	153	HIS
1	J	194	HIS
1	J	282	GLN
1	J	323	ASN
1	J	343	HIS
1	J	378	HIS
1	J	385	HIS
1	J	425	GLN
1	J	472	HIS
1	J	478	ASN
1	J	486	HIS
1	J	488	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	504	HIS
1	J	526	ASN
1	J	550	HIS
1	K	59	GLN
1	K	79	HIS
1	K	153	HIS
1	K	194	HIS
1	K	282	GLN
1	K	323	ASN
1	K	343	HIS
1	K	378	HIS
1	K	385	HIS
1	K	425	GLN
1	K	472	HIS
1	K	478	ASN
1	K	486	HIS
1	K	488	HIS
1	K	504	HIS
1	K	526	ASN
1	K	550	HIS
1	L	59	GLN
1	L	79	HIS
1	L	153	HIS
1	L	194	HIS
1	L	282	GLN
1	L	323	ASN
1	L	343	HIS
1	L	378	HIS
1	L	385	HIS
1	L	425	GLN
1	L	472	HIS
1	L	478	ASN
1	L	486	HIS
1	L	488	HIS
1	L	504	HIS
1	L	526	ASN
1	L	550	HIS
1	M	59	GLN
1	M	79	HIS
1	M	153	HIS
1	M	194	HIS
1	M	282	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	M	323	ASN
1	M	343	HIS
1	M	378	HIS
1	M	385	HIS
1	M	472	HIS
1	M	478	ASN
1	M	486	HIS
1	M	488	HIS
1	M	504	HIS
1	M	526	ASN
1	M	550	HIS
1	N	59	GLN
1	N	79	HIS
1	N	153	HIS
1	N	194	HIS
1	N	282	GLN
1	N	323	ASN
1	N	343	HIS
1	N	378	HIS
1	N	385	HIS
1	N	425	GLN
1	N	472	HIS
1	N	478	ASN
1	N	486	HIS
1	N	488	HIS
1	N	504	HIS
1	N	526	ASN
1	N	550	HIS
1	O	59	GLN
1	O	79	HIS
1	O	153	HIS
1	O	194	HIS
1	O	282	GLN
1	O	323	ASN
1	O	343	HIS
1	O	378	HIS
1	O	385	HIS
1	O	472	HIS
1	O	478	ASN
1	O	486	HIS
1	O	488	HIS
1	O	504	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	O	526	ASN
1	O	550	HIS
1	P	59	GLN
1	P	79	HIS
1	P	153	HIS
1	P	194	HIS
1	P	282	GLN
1	P	323	ASN
1	P	343	HIS
1	P	378	HIS
1	P	385	HIS
1	P	472	HIS
1	P	478	ASN
1	P	486	HIS
1	P	488	HIS
1	P	504	HIS
1	P	526	ASN
1	P	550	HIS
1	Q	59	GLN
1	Q	79	HIS
1	Q	153	HIS
1	Q	194	HIS
1	Q	282	GLN
1	Q	323	ASN
1	Q	343	HIS
1	Q	378	HIS
1	Q	385	HIS
1	Q	472	HIS
1	Q	478	ASN
1	Q	486	HIS
1	Q	488	HIS
1	Q	504	HIS
1	Q	526	ASN
1	Q	550	HIS
1	R	59	GLN
1	R	79	HIS
1	R	153	HIS
1	R	194	HIS
1	R	282	GLN
1	R	323	ASN
1	R	343	HIS
1	R	378	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	R	385	HIS
1	R	425	GLN
1	R	472	HIS
1	R	478	ASN
1	R	486	HIS
1	R	488	HIS
1	R	504	HIS
1	R	526	ASN
1	R	550	HIS
1	S	59	GLN
1	S	79	HIS
1	S	153	HIS
1	S	194	HIS
1	S	225	ASN
1	S	282	GLN
1	S	323	ASN
1	S	343	HIS
1	S	378	HIS
1	S	385	HIS
1	S	425	GLN
1	S	472	HIS
1	S	478	ASN
1	S	486	HIS
1	S	488	HIS
1	S	504	HIS
1	S	526	ASN
1	S	550	HIS
1	T	59	GLN
1	T	79	HIS
1	T	153	HIS
1	T	194	HIS
1	T	282	GLN
1	T	323	ASN
1	T	343	HIS
1	T	378	HIS
1	T	385	HIS
1	T	472	HIS
1	T	478	ASN
1	T	486	HIS
1	T	488	HIS
1	T	504	HIS
1	T	526	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	T	550	HIS
1	U	59	GLN
1	U	79	HIS
1	U	153	HIS
1	U	194	HIS
1	U	282	GLN
1	U	323	ASN
1	U	343	HIS
1	U	378	HIS
1	U	385	HIS
1	U	425	GLN
1	U	472	HIS
1	U	478	ASN
1	U	486	HIS
1	U	488	HIS
1	U	504	HIS
1	U	526	ASN
1	U	550	HIS
1	V	59	GLN
1	V	79	HIS
1	V	153	HIS
1	V	194	HIS
1	V	282	GLN
1	V	323	ASN
1	V	343	HIS
1	V	378	HIS
1	V	385	HIS
1	V	425	GLN
1	V	472	HIS
1	V	478	ASN
1	V	486	HIS
1	V	488	HIS
1	V	504	HIS
1	V	526	ASN
1	V	550	HIS
1	W	59	GLN
1	W	79	HIS
1	W	153	HIS
1	W	194	HIS
1	W	282	GLN
1	W	323	ASN
1	W	343	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	W	378	HIS
1	W	385	HIS
1	W	472	HIS
1	W	478	ASN
1	W	486	HIS
1	W	488	HIS
1	W	504	HIS
1	W	526	ASN
1	W	550	HIS
1	X	59	GLN
1	X	79	HIS
1	X	153	HIS
1	X	194	HIS
1	X	282	GLN
1	X	323	ASN
1	X	343	HIS
1	X	378	HIS
1	X	385	HIS
1	X	425	GLN
1	X	472	HIS
1	X	478	ASN
1	X	486	HIS
1	X	488	HIS
1	X	504	HIS
1	X	526	ASN
1	X	550	HIS
1	Y	59	GLN
1	Y	79	HIS
1	Y	153	HIS
1	Y	194	HIS
1	Y	282	GLN
1	Y	323	ASN
1	Y	343	HIS
1	Y	378	HIS
1	Y	385	HIS
1	Y	472	HIS
1	Y	478	ASN
1	Y	486	HIS
1	Y	488	HIS
1	Y	504	HIS
1	Y	526	ASN
1	Y	550	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	Z	59	GLN
1	Z	79	HIS
1	Z	153	HIS
1	Z	194	HIS
1	Z	282	GLN
1	Z	323	ASN
1	Z	343	HIS
1	Z	378	HIS
1	Z	385	HIS
1	Z	425	GLN
1	Z	472	HIS
1	Z	478	ASN
1	Z	486	HIS
1	Z	488	HIS
1	Z	504	HIS
1	Z	526	ASN
1	Z	550	HIS
1	a	59	GLN
1	a	79	HIS
1	a	153	HIS
1	a	194	HIS
1	a	282	GLN
1	a	323	ASN
1	a	343	HIS
1	a	378	HIS
1	a	385	HIS
1	a	472	HIS
1	a	478	ASN
1	a	486	HIS
1	a	488	HIS
1	a	504	HIS
1	a	526	ASN
1	a	550	HIS
1	b	59	GLN
1	b	79	HIS
1	b	153	HIS
1	b	194	HIS
1	b	282	GLN
1	b	323	ASN
1	b	343	HIS
1	b	378	HIS
1	b	385	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	b	425	GLN
1	b	472	HIS
1	b	478	ASN
1	b	486	HIS
1	b	488	HIS
1	b	504	HIS
1	b	526	ASN
1	b	550	HIS
1	c	59	GLN
1	c	79	HIS
1	c	153	HIS
1	c	194	HIS
1	c	282	GLN
1	c	323	ASN
1	c	343	HIS
1	c	378	HIS
1	c	385	HIS
1	c	425	GLN
1	c	472	HIS
1	c	478	ASN
1	c	486	HIS
1	c	488	HIS
1	c	504	HIS
1	c	526	ASN
1	c	550	HIS
1	d	59	GLN
1	d	79	HIS
1	d	153	HIS
1	d	194	HIS
1	d	282	GLN
1	d	323	ASN
1	d	343	HIS
1	d	378	HIS
1	d	385	HIS
1	d	472	HIS
1	d	478	ASN
1	d	486	HIS
1	d	488	HIS
1	d	504	HIS
1	d	526	ASN
1	d	550	HIS
1	e	59	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	e	79	HIS
1	e	153	HIS
1	e	194	HIS
1	e	282	GLN
1	e	323	ASN
1	e	343	HIS
1	e	378	HIS
1	e	385	HIS
1	e	425	GLN
1	e	472	HIS
1	e	478	ASN
1	e	486	HIS
1	e	488	HIS
1	e	504	HIS
1	e	526	ASN
1	e	550	HIS
1	f	59	GLN
1	f	79	HIS
1	f	153	HIS
1	f	194	HIS
1	f	282	GLN
1	f	323	ASN
1	f	343	HIS
1	f	378	HIS
1	f	385	HIS
1	f	425	GLN
1	f	472	HIS
1	f	478	ASN
1	f	486	HIS
1	f	488	HIS
1	f	504	HIS
1	f	526	ASN
1	f	550	HIS
1	g	59	GLN
1	g	79	HIS
1	g	153	HIS
1	g	194	HIS
1	g	282	GLN
1	g	323	ASN
1	g	343	HIS
1	g	378	HIS
1	g	385	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	g	472	HIS
1	g	478	ASN
1	g	486	HIS
1	g	488	HIS
1	g	504	HIS
1	g	526	ASN
1	g	550	HIS
1	h	59	GLN
1	h	79	HIS
1	h	153	HIS
1	h	194	HIS
1	h	282	GLN
1	h	323	ASN
1	h	343	HIS
1	h	378	HIS
1	h	385	HIS
1	h	425	GLN
1	h	472	HIS
1	h	478	ASN
1	h	486	HIS
1	h	488	HIS
1	h	504	HIS
1	h	526	ASN
1	h	550	HIS
1	i	59	GLN
1	i	79	HIS
1	i	153	HIS
1	i	194	HIS
1	i	225	ASN
1	i	282	GLN
1	i	323	ASN
1	i	343	HIS
1	i	378	HIS
1	i	385	HIS
1	i	472	HIS
1	i	478	ASN
1	i	486	HIS
1	i	488	HIS
1	i	504	HIS
1	i	526	ASN
1	i	550	HIS
1	j	59	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	j	79	HIS
1	j	153	HIS
1	j	194	HIS
1	j	282	GLN
1	j	323	ASN
1	j	343	HIS
1	j	378	HIS
1	j	385	HIS
1	j	472	HIS
1	j	478	ASN
1	j	486	HIS
1	j	488	HIS
1	j	504	HIS
1	j	526	ASN
1	j	550	HIS
1	k	59	GLN
1	k	79	HIS
1	k	153	HIS
1	k	194	HIS
1	k	282	GLN
1	k	323	ASN
1	k	343	HIS
1	k	378	HIS
1	k	385	HIS
1	k	425	GLN
1	k	472	HIS
1	k	478	ASN
1	k	486	HIS
1	k	488	HIS
1	k	504	HIS
1	k	526	ASN
1	k	550	HIS
1	l	59	GLN
1	l	79	HIS
1	l	153	HIS
1	l	194	HIS
1	l	282	GLN
1	l	323	ASN
1	l	343	HIS
1	l	378	HIS
1	l	385	HIS
1	l	472	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	l	478	ASN
1	l	486	HIS
1	l	488	HIS
1	l	504	HIS
1	l	526	ASN
1	l	550	HIS
1	m	59	GLN
1	m	79	HIS
1	m	153	HIS
1	m	194	HIS
1	m	282	GLN
1	m	323	ASN
1	m	343	HIS
1	m	378	HIS
1	m	385	HIS
1	m	472	HIS
1	m	478	ASN
1	m	486	HIS
1	m	488	HIS
1	m	504	HIS
1	m	526	ASN
1	m	550	HIS
1	n	59	GLN
1	n	79	HIS
1	n	153	HIS
1	n	194	HIS
1	n	282	GLN
1	n	323	ASN
1	n	343	HIS
1	n	378	HIS
1	n	385	HIS
1	n	472	HIS
1	n	478	ASN
1	n	486	HIS
1	n	488	HIS
1	n	504	HIS
1	n	526	ASN
1	n	550	HIS
1	o	59	GLN
1	o	79	HIS
1	o	153	HIS
1	o	194	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	o	282	GLN
1	o	323	ASN
1	o	343	HIS
1	o	378	HIS
1	o	385	HIS
1	o	425	GLN
1	o	472	HIS
1	o	478	ASN
1	o	486	HIS
1	o	488	HIS
1	o	504	HIS
1	o	526	ASN
1	o	550	HIS
1	p	59	GLN
1	p	79	HIS
1	p	153	HIS
1	p	194	HIS
1	p	282	GLN
1	p	323	ASN
1	p	343	HIS
1	p	378	HIS
1	p	385	HIS
1	p	425	GLN
1	p	472	HIS
1	p	478	ASN
1	p	486	HIS
1	p	488	HIS
1	p	504	HIS
1	p	526	ASN
1	p	550	HIS
1	q	59	GLN
1	q	79	HIS
1	q	153	HIS
1	q	194	HIS
1	q	282	GLN
1	q	323	ASN
1	q	343	HIS
1	q	378	HIS
1	q	385	HIS
1	q	425	GLN
1	q	472	HIS
1	q	478	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	q	486	HIS
1	q	488	HIS
1	q	504	HIS
1	q	526	ASN
1	q	550	HIS
1	r	59	GLN
1	r	79	HIS
1	r	153	HIS
1	r	194	HIS
1	r	282	GLN
1	r	323	ASN
1	r	343	HIS
1	r	378	HIS
1	r	385	HIS
1	r	425	GLN
1	r	472	HIS
1	r	478	ASN
1	r	486	HIS
1	r	488	HIS
1	r	504	HIS
1	r	526	ASN
1	r	550	HIS
1	s	59	GLN
1	s	79	HIS
1	s	153	HIS
1	s	194	HIS
1	s	282	GLN
1	s	323	ASN
1	s	343	HIS
1	s	378	HIS
1	s	385	HIS
1	s	425	GLN
1	s	472	HIS
1	s	478	ASN
1	s	486	HIS
1	s	488	HIS
1	s	504	HIS
1	s	526	ASN
1	s	550	HIS
1	t	59	GLN
1	t	79	HIS
1	t	153	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	t	194	HIS
1	t	282	GLN
1	t	323	ASN
1	t	343	HIS
1	t	378	HIS
1	t	385	HIS
1	t	425	GLN
1	t	472	HIS
1	t	478	ASN
1	t	486	HIS
1	t	488	HIS
1	t	504	HIS
1	t	526	ASN
1	t	550	HIS
1	u	59	GLN
1	u	79	HIS
1	u	153	HIS
1	u	194	HIS
1	u	282	GLN
1	u	323	ASN
1	u	343	HIS
1	u	378	HIS
1	u	385	HIS
1	u	425	GLN
1	u	472	HIS
1	u	478	ASN
1	u	486	HIS
1	u	488	HIS
1	u	504	HIS
1	u	526	ASN
1	u	550	HIS
1	v	59	GLN
1	v	79	HIS
1	v	153	HIS
1	v	194	HIS
1	v	282	GLN
1	v	323	ASN
1	v	343	HIS
1	v	378	HIS
1	v	385	HIS
1	v	472	HIS
1	v	478	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	v	486	HIS
1	v	488	HIS
1	v	504	HIS
1	v	526	ASN
1	v	550	HIS
1	w	59	GLN
1	w	79	HIS
1	w	153	HIS
1	w	194	HIS
1	w	282	GLN
1	w	323	ASN
1	w	343	HIS
1	w	378	HIS
1	w	385	HIS
1	w	425	GLN
1	w	472	HIS
1	w	478	ASN
1	w	486	HIS
1	w	488	HIS
1	w	504	HIS
1	w	526	ASN
1	w	550	HIS
1	x	59	GLN
1	x	79	HIS
1	x	153	HIS
1	x	194	HIS
1	x	282	GLN
1	x	323	ASN
1	x	343	HIS
1	x	378	HIS
1	x	385	HIS
1	x	472	HIS
1	x	478	ASN
1	x	486	HIS
1	x	488	HIS
1	x	504	HIS
1	x	526	ASN
1	x	550	HIS
1	y	59	GLN
1	y	79	HIS
1	y	153	HIS
1	y	194	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	y	282	GLN
1	y	323	ASN
1	y	343	HIS
1	y	378	HIS
1	y	385	HIS
1	y	472	HIS
1	y	478	ASN
1	y	486	HIS
1	y	488	HIS
1	y	504	HIS
1	y	526	ASN
1	y	550	HIS
1	z	59	GLN
1	z	79	HIS
1	z	153	HIS
1	z	194	HIS
1	z	282	GLN
1	z	323	ASN
1	z	343	HIS
1	z	378	HIS
1	z	385	HIS
1	z	425	GLN
1	z	472	HIS
1	z	478	ASN
1	z	486	HIS
1	z	488	HIS
1	z	504	HIS
1	z	526	ASN
1	z	550	HIS
1	1	59	GLN
1	1	79	HIS
1	1	153	HIS
1	1	194	HIS
1	1	282	GLN
1	1	323	ASN
1	1	343	HIS
1	1	378	HIS
1	1	385	HIS
1	1	425	GLN
1	1	472	HIS
1	1	478	ASN
1	1	486	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	488	HIS
1	1	504	HIS
1	1	526	ASN
1	1	550	HIS
1	2	59	GLN
1	2	79	HIS
1	2	153	HIS
1	2	194	HIS
1	2	282	GLN
1	2	323	ASN
1	2	343	HIS
1	2	378	HIS
1	2	385	HIS
1	2	425	GLN
1	2	472	HIS
1	2	478	ASN
1	2	486	HIS
1	2	488	HIS
1	2	504	HIS
1	2	526	ASN
1	2	550	HIS
1	3	59	GLN
1	3	79	HIS
1	3	153	HIS
1	3	194	HIS
1	3	282	GLN
1	3	323	ASN
1	3	343	HIS
1	3	378	HIS
1	3	385	HIS
1	3	472	HIS
1	3	478	ASN
1	3	486	HIS
1	3	488	HIS
1	3	504	HIS
1	3	526	ASN
1	3	550	HIS
1	4	59	GLN
1	4	79	HIS
1	4	153	HIS
1	4	194	HIS
1	4	282	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	4	323	ASN
1	4	343	HIS
1	4	378	HIS
1	4	385	HIS
1	4	425	GLN
1	4	472	HIS
1	4	478	ASN
1	4	486	HIS
1	4	488	HIS
1	4	504	HIS
1	4	526	ASN
1	4	550	HIS
1	5	59	GLN
1	5	79	HIS
1	5	153	HIS
1	5	194	HIS
1	5	282	GLN
1	5	323	ASN
1	5	343	HIS
1	5	378	HIS
1	5	385	HIS
1	5	425	GLN
1	5	472	HIS
1	5	478	ASN
1	5	486	HIS
1	5	488	HIS
1	5	504	HIS
1	5	526	ASN
1	5	550	HIS
1	6	59	GLN
1	6	79	HIS
1	6	153	HIS
1	6	194	HIS
1	6	282	GLN
1	6	323	ASN
1	6	343	HIS
1	6	378	HIS
1	6	385	HIS
1	6	472	HIS
1	6	478	ASN
1	6	486	HIS
1	6	488	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	6	504	HIS
1	6	526	ASN
1	6	550	HIS
1	7	59	GLN
1	7	79	HIS
1	7	153	HIS
1	7	194	HIS
1	7	282	GLN
1	7	323	ASN
1	7	343	HIS
1	7	378	HIS
1	7	385	HIS
1	7	472	HIS
1	7	478	ASN
1	7	486	HIS
1	7	488	HIS
1	7	504	HIS
1	7	526	ASN
1	7	550	HIS
1	8	59	GLN
1	8	79	HIS
1	8	153	HIS
1	8	194	HIS
1	8	282	GLN
1	8	323	ASN
1	8	343	HIS
1	8	378	HIS
1	8	385	HIS
1	8	425	GLN
1	8	472	HIS
1	8	478	ASN
1	8	486	HIS
1	8	488	HIS
1	8	504	HIS
1	8	526	ASN
1	8	550	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

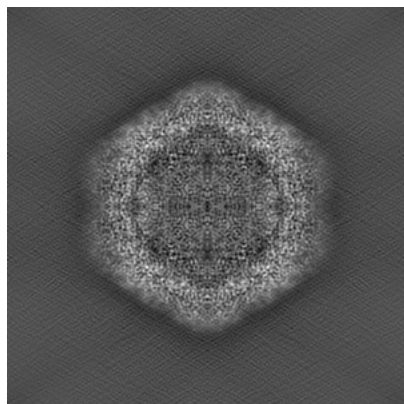
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-28522. These allow visual inspection of the internal detail of the map and identification of artifacts.

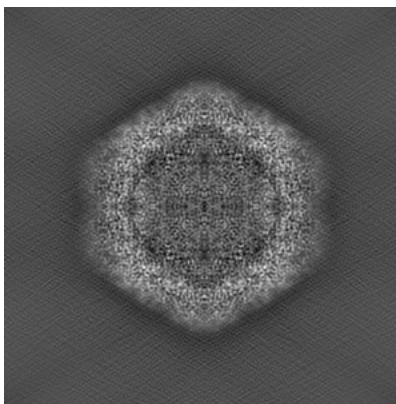
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

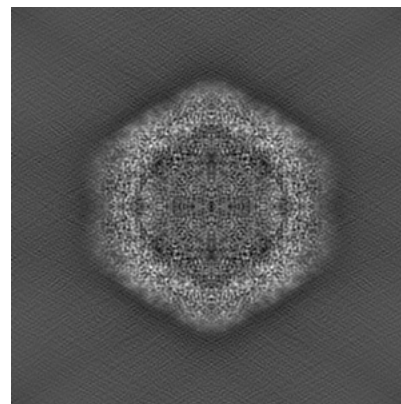
6.1.1 Primary map



X

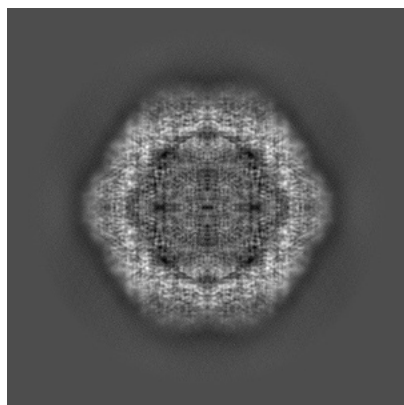


Y

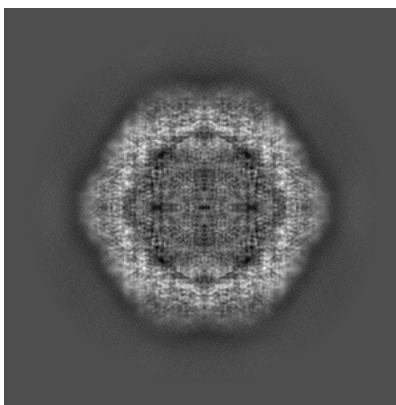


Z

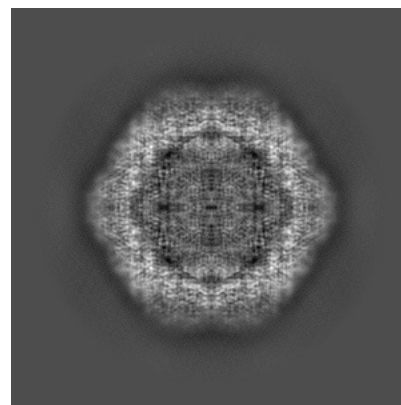
6.1.2 Raw map



X



Y

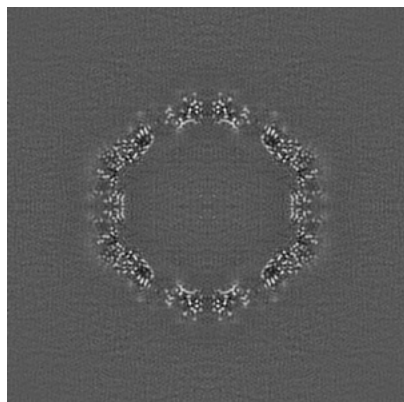


Z

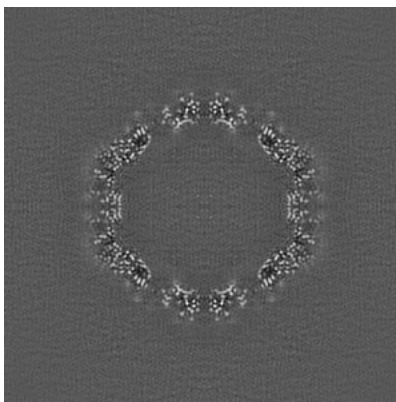
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

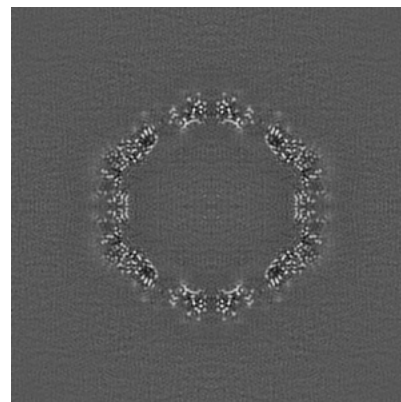
6.2.1 Primary map



X Index: 235

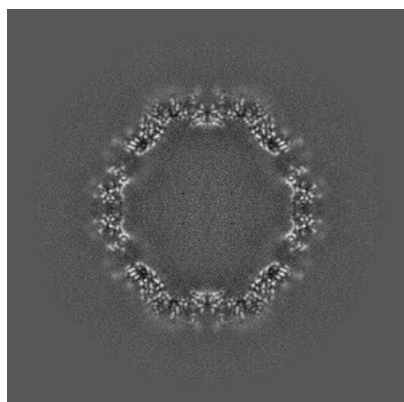


Y Index: 235

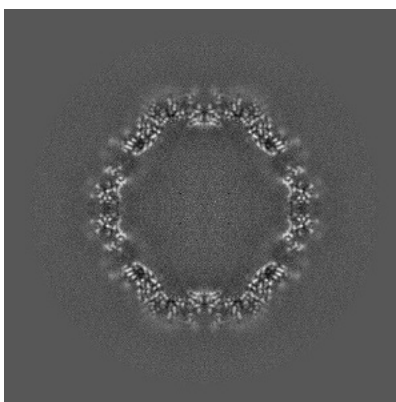


Z Index: 235

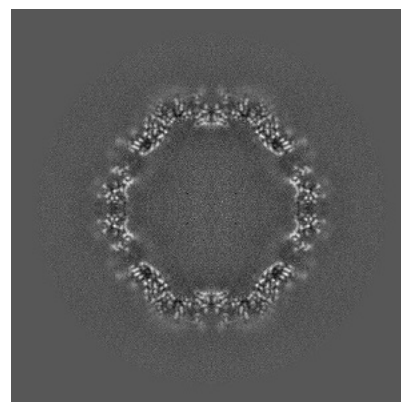
6.2.2 Raw map



X Index: 235



Y Index: 235

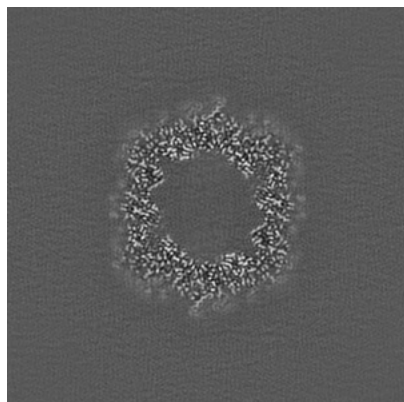


Z Index: 235

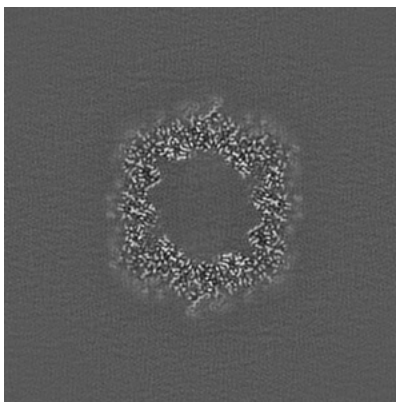
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

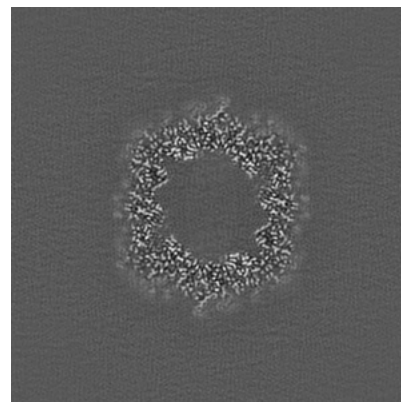
6.3.1 Primary map



X Index: 310

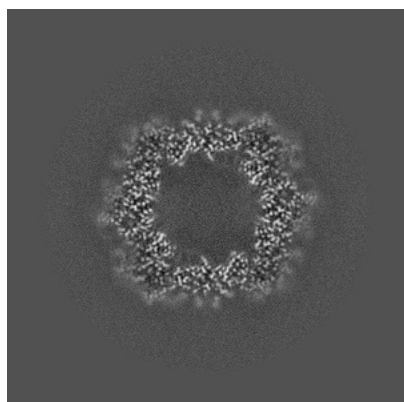


Y Index: 310

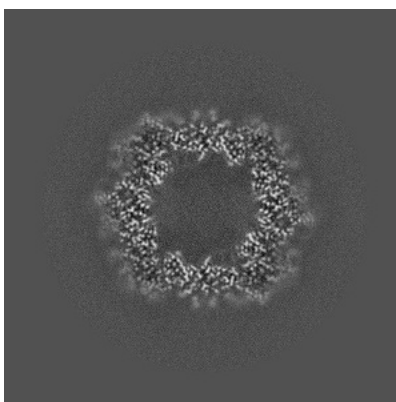


Z Index: 310

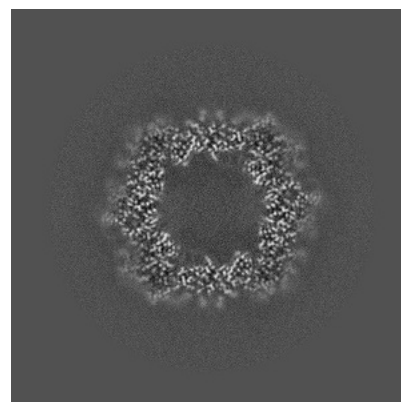
6.3.2 Raw map



X Index: 308



Y Index: 162

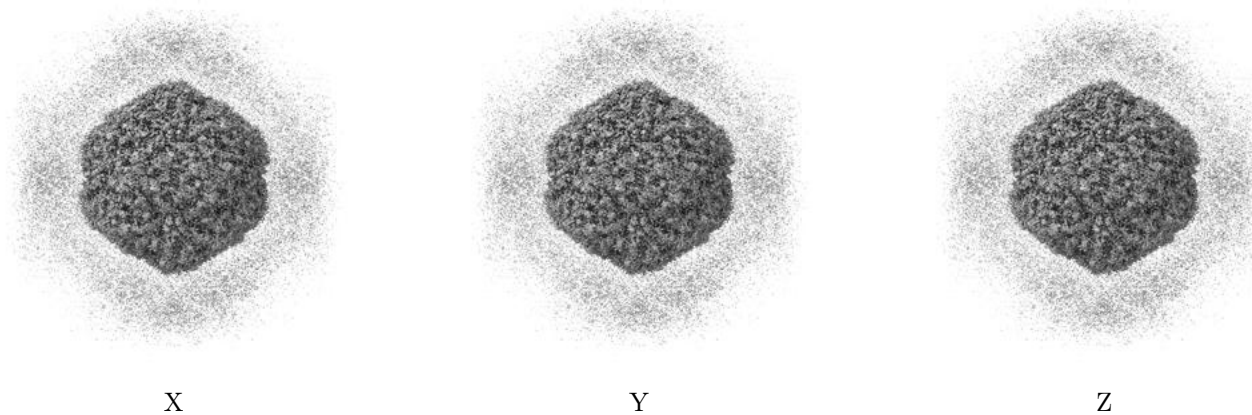


Z Index: 308

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

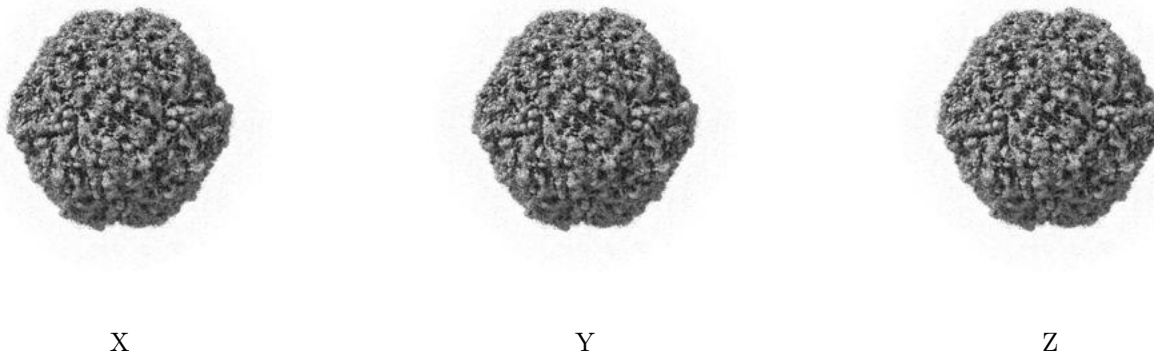
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 1.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



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.

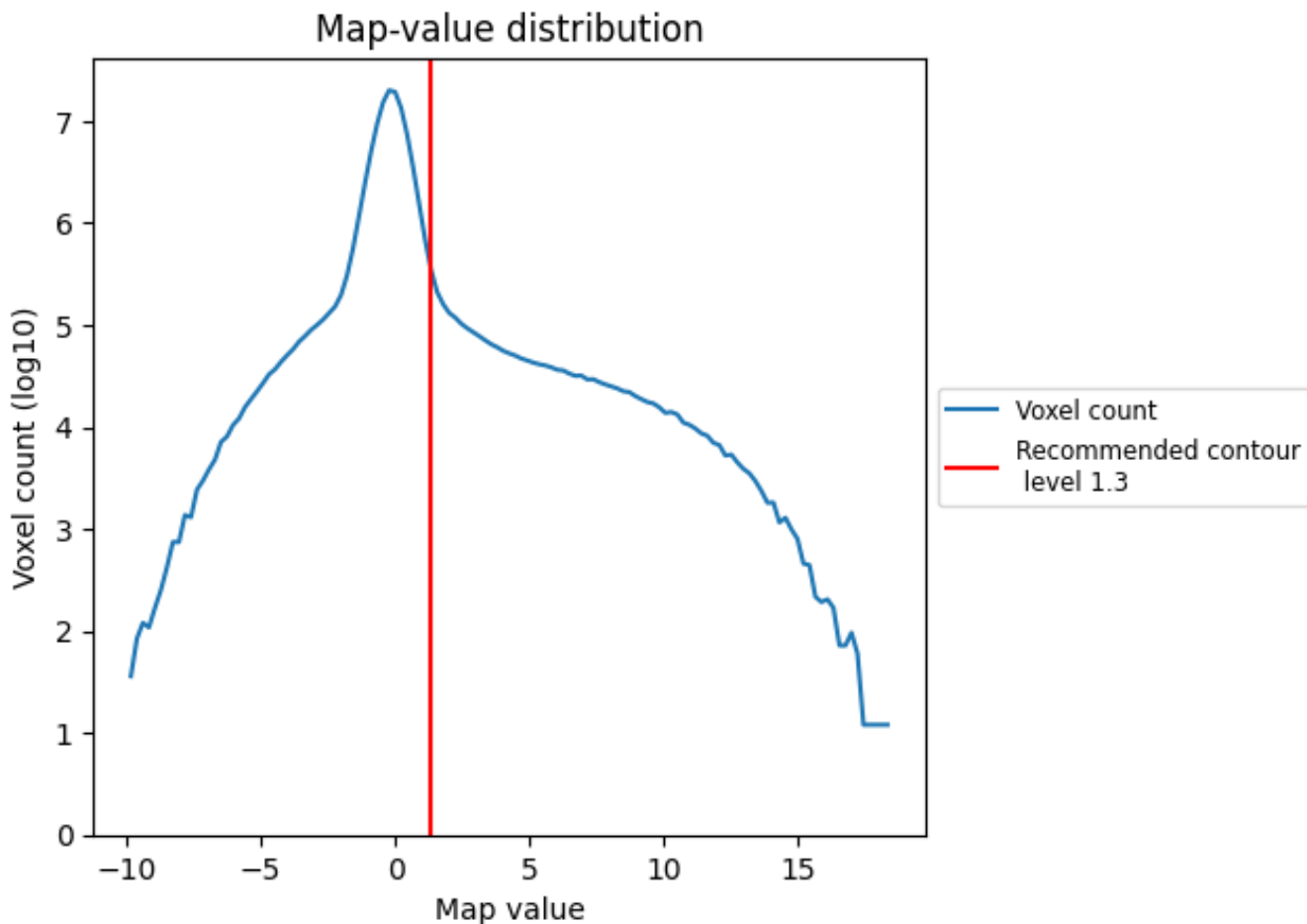
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

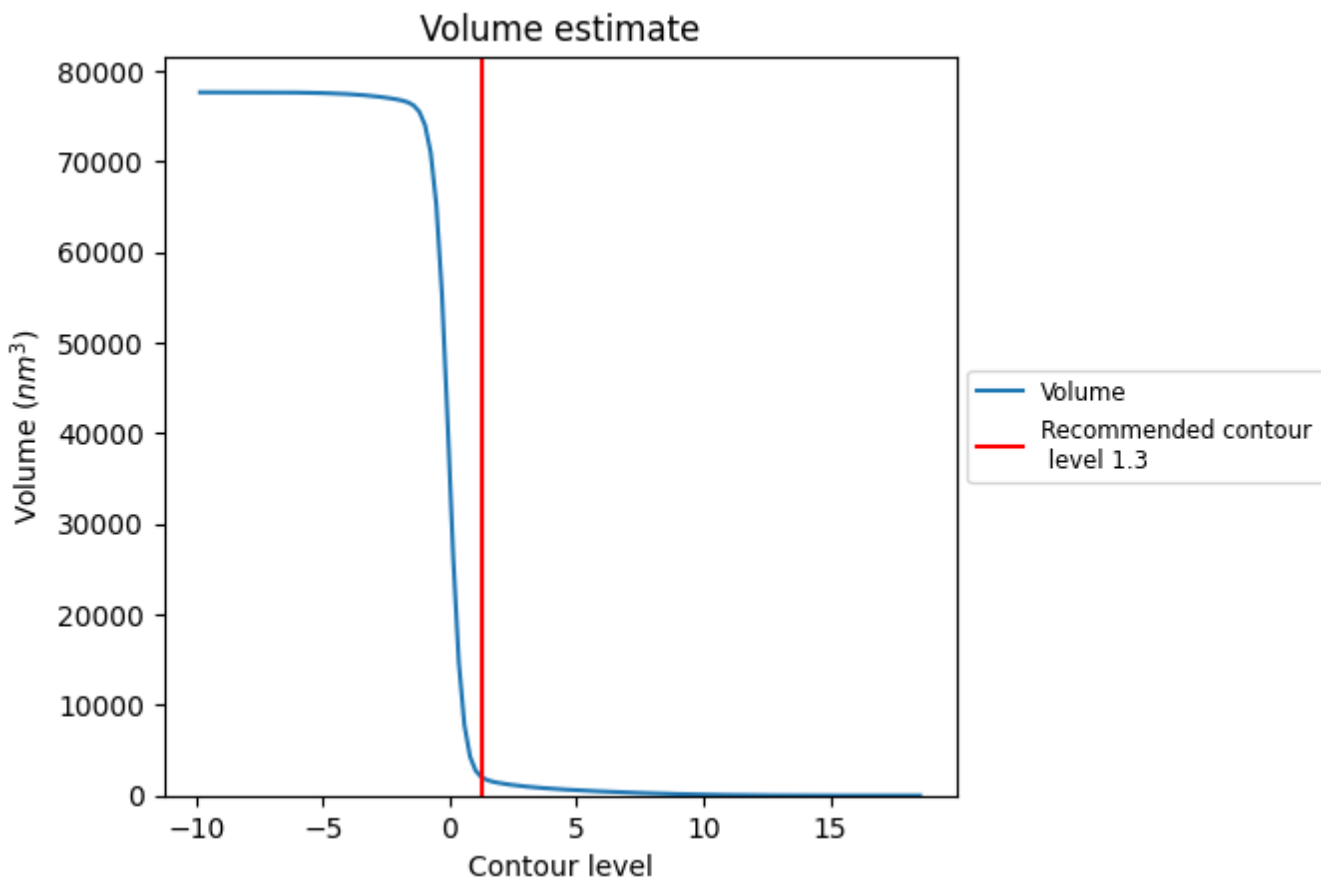
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

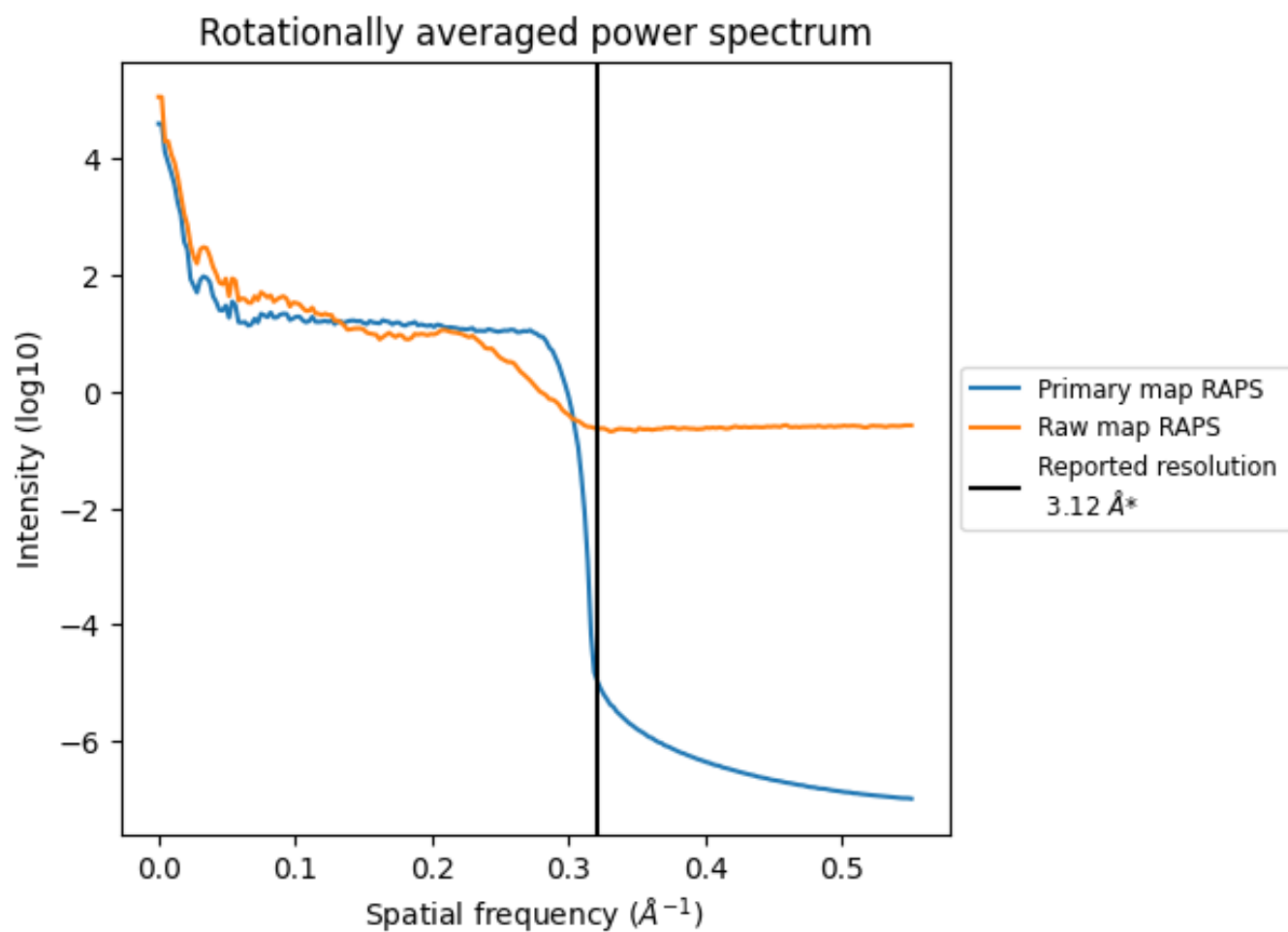
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1971 nm³; this corresponds to an approximate mass of 1780 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

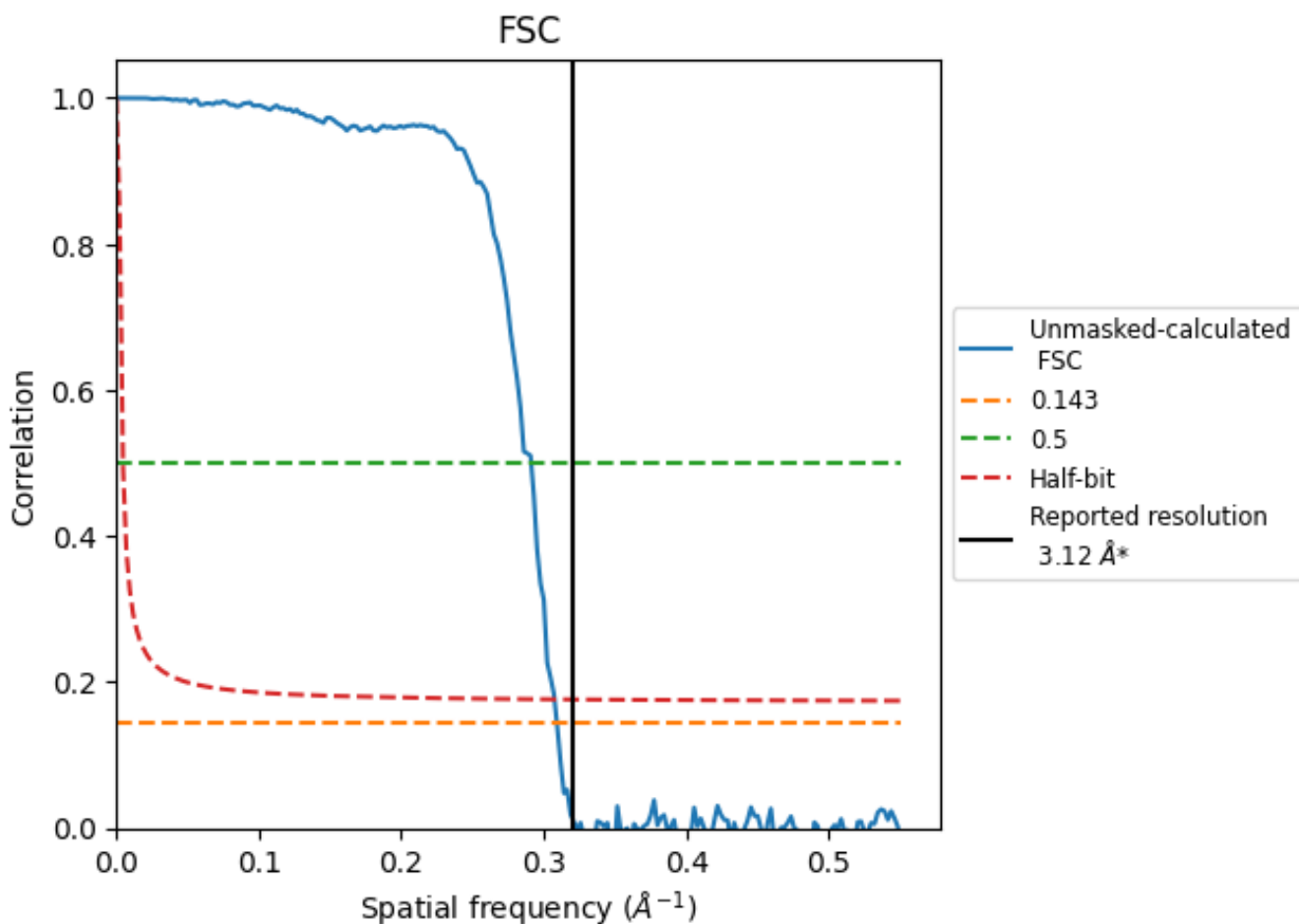


*Reported resolution corresponds to spatial frequency of 0.321 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.321 Å⁻¹

8.2 Resolution estimates [i](#)

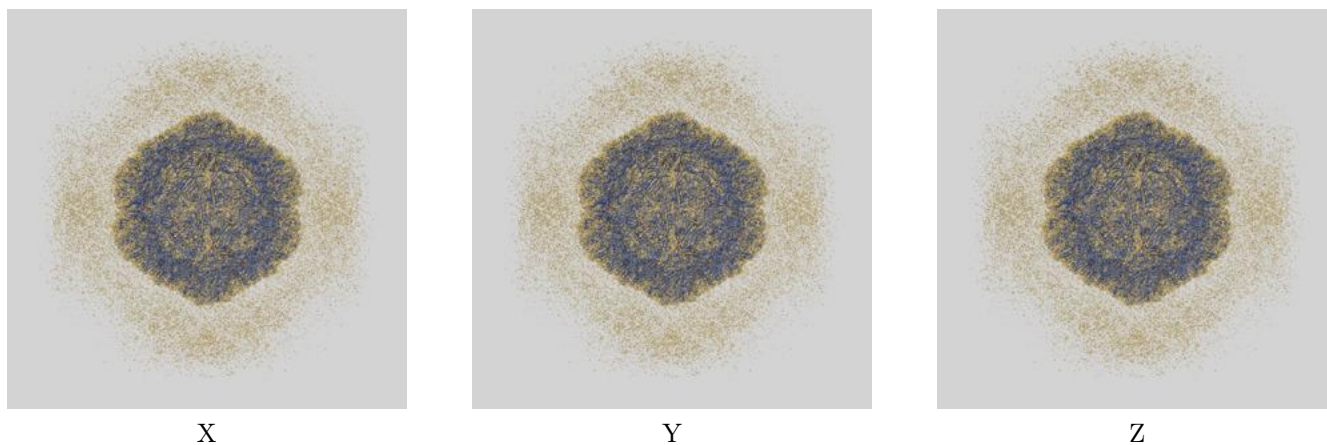
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.12	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.23	3.44	3.25

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

9 Map-model fit [i](#)

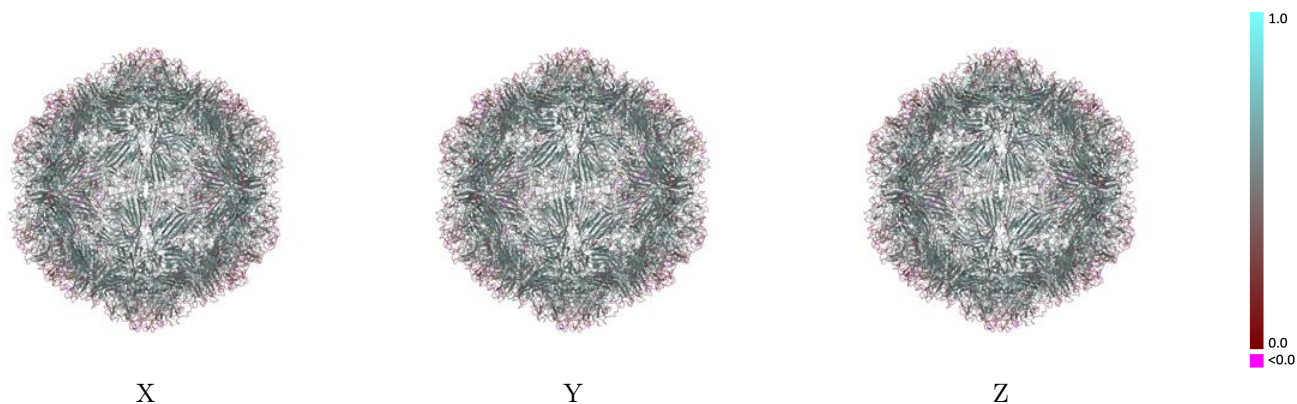
This section contains information regarding the fit between EMDB map EMD-28522 and PDB model 8EP9. Per-residue inclusion information can be found in section 3 on page 10.

9.1 Map-model overlay [i](#)



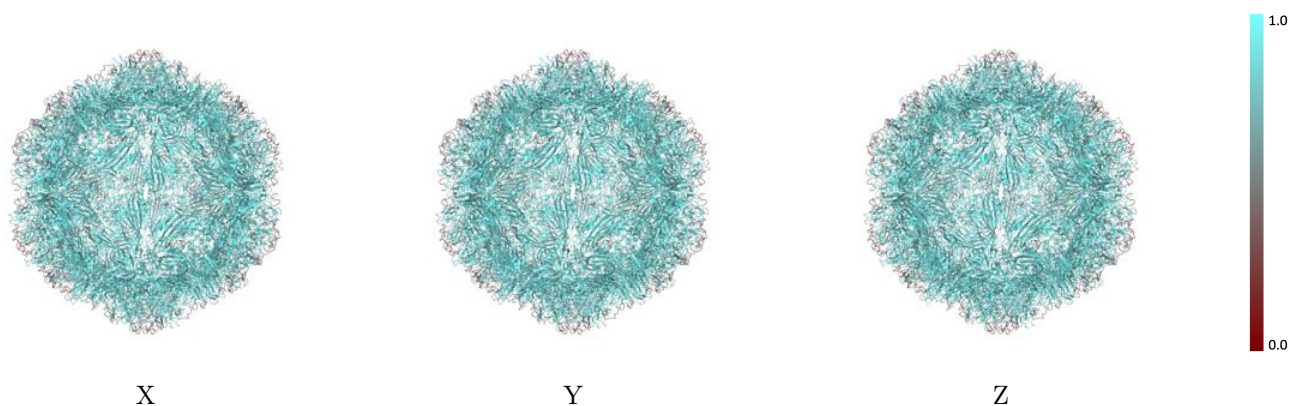
The images above show the 3D surface view of the map at the recommended contour level 1.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



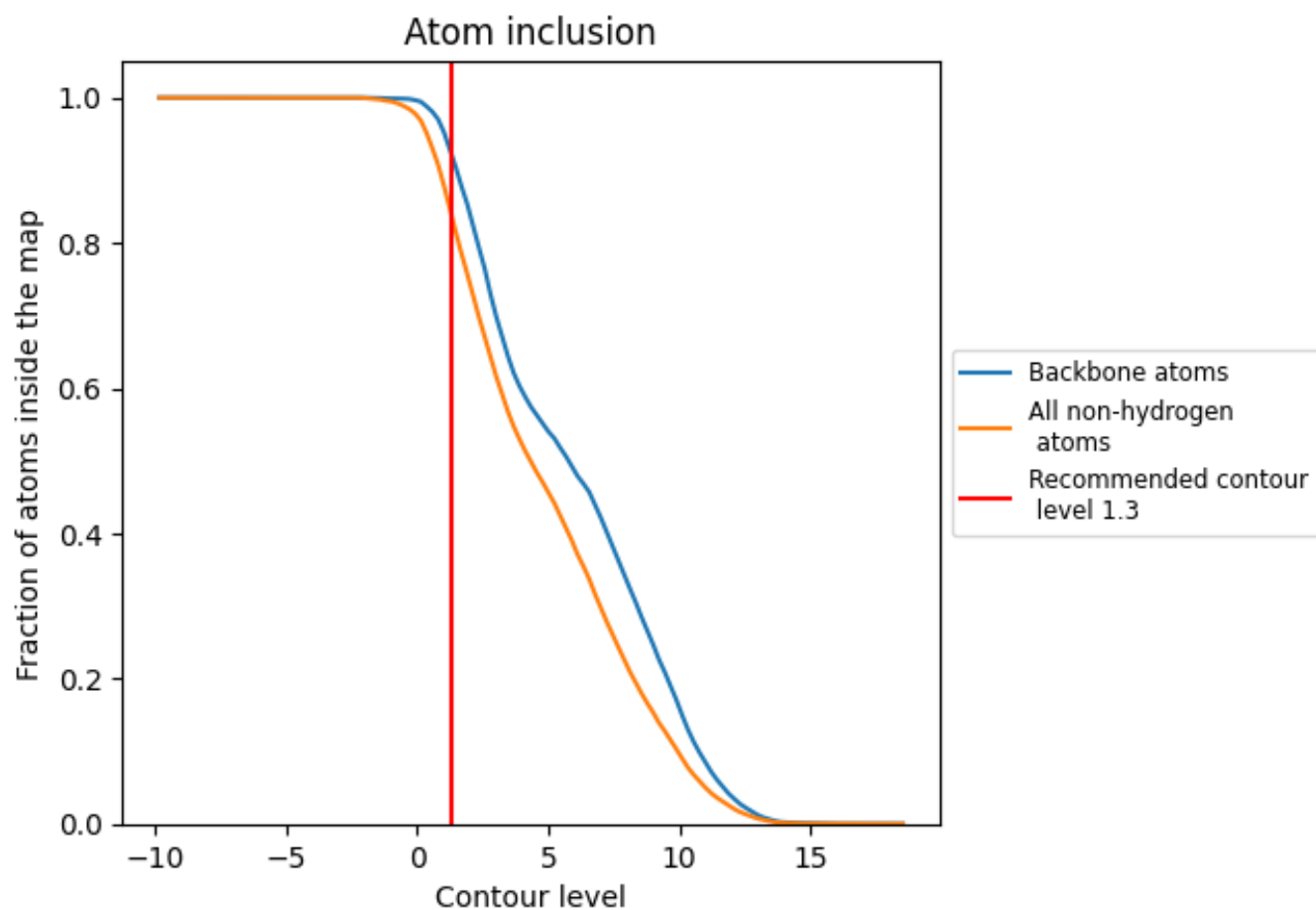
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (1.3).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 84% 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 (1.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8387	 0.4870
1	 0.8418	 0.4870
2	 0.8421	 0.4860
3	 0.8373	 0.4880
4	 0.8349	 0.4860
5	 0.8404	 0.4860
6	 0.8404	 0.4850
7	 0.8404	 0.4860
8	 0.8394	 0.4870
A	 0.8378	 0.4880
B	 0.8418	 0.4870
C	 0.8346	 0.4870
D	 0.8404	 0.4850
E	 0.8394	 0.4880
F	 0.8373	 0.4880
G	 0.8387	 0.4870
H	 0.8404	 0.4860
I	 0.8354	 0.4870
J	 0.8413	 0.4860
K	 0.8354	 0.4850
L	 0.8423	 0.4870
M	 0.8394	 0.4870
N	 0.8404	 0.4860
O	 0.8392	 0.4880
P	 0.8404	 0.4860
Q	 0.8354	 0.4860
R	 0.8421	 0.4870
S	 0.8418	 0.4870
T	 0.8349	 0.4860
U	 0.8421	 0.4870
V	 0.8346	 0.4860
W	 0.8406	 0.4880
X	 0.8394	 0.4860
Y	 0.8404	 0.4860
Z	 0.8392	 0.4870



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
a	 0.8366	 0.4870
b	 0.8373	 0.4880
c	 0.8370	 0.4860
d	 0.8370	 0.4870
e	 0.8375	 0.4870
f	 0.8375	 0.4880
g	 0.8346	 0.4850
h	 0.8394	 0.4870
i	 0.8404	 0.4850
j	 0.8404	 0.4860
k	 0.8404	 0.4850
l	 0.8375	 0.4870
m	 0.8354	 0.4870
n	 0.8373	 0.4860
o	 0.8392	 0.4870
p	 0.8351	 0.4860
q	 0.8418	 0.4860
r	 0.8411	 0.4870
s	 0.8406	 0.4870
t	 0.8397	 0.4860
u	 0.8366	 0.4860
v	 0.8378	 0.4860
w	 0.8390	 0.4870
x	 0.8349	 0.4860
y	 0.8373	 0.4860
z	 0.8421	 0.4870