Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 08:43 PM EST

PDB ID	:	7MTP
EMDB ID	:	EMD-23993
Title	:	Structure of the adeno-associated virus 9 capsid at pH 5.5
Authors	:	Penzes, J.J.; Chipman, P.; Bhattacharya, N.; Zeher, A.; Huang, R.; McKenna, R.; Agbandje-McKenna, M.
Deposited on	:	2021-05-13
Resolution	:	2.79 Å(reported)
Based on initial model	:	3UX1

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:

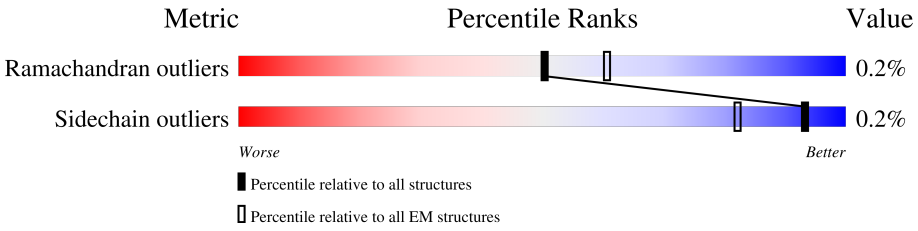
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.79 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 <=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	518	99%
1	2	518	99%
1	3	518	99%
1	4	518	99%
1	5	518	99%
1	6	518	99%
1	7	518	99%
1	8	518	99%
1	A	518	99%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	B	518	99%
1	C	518	99%
1	D	518	99%
1	E	518	99%
1	F	518	99%
1	G	518	99%
1	H	518	99%
1	I	518	99%
1	J	518	99%
1	K	518	99%
1	L	518	99%
1	M	518	99%
1	N	518	99%
1	O	518	99%
1	P	518	99%
1	Q	518	99%
1	R	518	99%
1	S	518	99%
1	T	518	99%
1	U	518	99%
1	V	518	99%
1	W	518	99%
1	X	518	99%
1	Y	518	99%
1	Z	518	99%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	a	518	99%
1	b	518	99%
1	c	518	99%
1	d	518	99%
1	e	518	99%
1	f	518	99%
1	g	518	99%
1	h	518	99%
1	i	518	99%
1	j	518	99%
1	k	518	99%
1	l	518	99%
1	m	518	99%
1	n	518	99%
1	o	518	99%
1	p	518	99%
1	q	518	99%
1	r	518	99%
1	s	518	99%
1	t	518	99%
1	u	518	99%
1	v	518	99%
1	w	518	99%
1	x	518	99%
1	y	518	99%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	z	518	99%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 247860 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Capsid protein VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	518	Total 4131	C 2608	N 718	O 791	S 14	0	0
1	B	518	Total 4131	C 2608	N 718	O 791	S 14	0	0
1	C	518	Total 4131	C 2608	N 718	O 791	S 14	0	0
1	D	518	Total 4131	C 2608	N 718	O 791	S 14	0	0
1	E	518	Total 4131	C 2608	N 718	O 791	S 14	0	0
1	F	518	Total 4131	C 2608	N 718	O 791	S 14	0	0
1	G	518	Total 4131	C 2608	N 718	O 791	S 14	0	0
1	H	518	Total 4131	C 2608	N 718	O 791	S 14	0	0
1	I	518	Total 4131	C 2608	N 718	O 791	S 14	0	0
1	J	518	Total 4131	C 2608	N 718	O 791	S 14	0	0
1	K	518	Total 4131	C 2608	N 718	O 791	S 14	0	0
1	L	518	Total 4131	C 2608	N 718	O 791	S 14	0	0
1	M	518	Total 4131	C 2608	N 718	O 791	S 14	0	0
1	N	518	Total 4131	C 2608	N 718	O 791	S 14	0	0
1	O	518	Total 4131	C 2608	N 718	O 791	S 14	0	0
1	P	518	Total 4131	C 2608	N 718	O 791	S 14	0	0
1	Q	518	Total 4131	C 2608	N 718	O 791	S 14	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	518	Total	C	N	O	S	0	0
			4131	2608	718	791	14		
1	S	518	Total	C	N	O	S	0	0
			4131	2608	718	791	14		
1	T	518	Total	C	N	O	S	0	0
			4131	2608	718	791	14		
1	U	518	Total	C	N	O	S	0	0
			4131	2608	718	791	14		
1	V	518	Total	C	N	O	S	0	0
			4131	2608	718	791	14		
1	W	518	Total	C	N	O	S	0	0
			4131	2608	718	791	14		
1	X	518	Total	C	N	O	S	0	0
			4131	2608	718	791	14		
1	Y	518	Total	C	N	O	S	0	0
			4131	2608	718	791	14		
1	Z	518	Total	C	N	O	S	0	0
			4131	2608	718	791	14		
1	1	518	Total	C	N	O	S	0	0
			4131	2608	718	791	14		
1	2	518	Total	C	N	O	S	0	0
			4131	2608	718	791	14		
1	3	518	Total	C	N	O	S	0	0
			4131	2608	718	791	14		
1	4	518	Total	C	N	O	S	0	0
			4131	2608	718	791	14		
1	5	518	Total	C	N	O	S	0	0
			4131	2608	718	791	14		
1	6	518	Total	C	N	O	S	0	0
			4131	2608	718	791	14		
1	a	518	Total	C	N	O	S	0	0
			4131	2608	718	791	14		
1	b	518	Total	C	N	O	S	0	0
			4131	2608	718	791	14		
1	c	518	Total	C	N	O	S	0	0
			4131	2608	718	791	14		
1	d	518	Total	C	N	O	S	0	0
			4131	2608	718	791	14		
1	e	518	Total	C	N	O	S	0	0
			4131	2608	718	791	14		
1	f	518	Total	C	N	O	S	0	0
			4131	2608	718	791	14		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	g	518	Total	C	N	O	S	0	0
			4131	2608	718	791	14		
1	h	518	Total	C	N	O	S	0	0
			4131	2608	718	791	14		
1	i	518	Total	C	N	O	S	0	0
			4131	2608	718	791	14		
1	j	518	Total	C	N	O	S	0	0
			4131	2608	718	791	14		
1	k	518	Total	C	N	O	S	0	0
			4131	2608	718	791	14		
1	l	518	Total	C	N	O	S	0	0
			4131	2608	718	791	14		
1	m	518	Total	C	N	O	S	0	0
			4131	2608	718	791	14		
1	n	518	Total	C	N	O	S	0	0
			4131	2608	718	791	14		
1	o	518	Total	C	N	O	S	0	0
			4131	2608	718	791	14		
1	p	518	Total	C	N	O	S	0	0
			4131	2608	718	791	14		
1	q	518	Total	C	N	O	S	0	0
			4131	2608	718	791	14		
1	r	518	Total	C	N	O	S	0	0
			4131	2608	718	791	14		
1	s	518	Total	C	N	O	S	0	0
			4131	2608	718	791	14		
1	t	518	Total	C	N	O	S	0	0
			4131	2608	718	791	14		
1	u	518	Total	C	N	O	S	0	0
			4131	2608	718	791	14		
1	v	518	Total	C	N	O	S	0	0
			4131	2608	718	791	14		
1	w	518	Total	C	N	O	S	0	0
			4131	2608	718	791	14		
1	x	518	Total	C	N	O	S	0	0
			4131	2608	718	791	14		
1	y	518	Total	C	N	O	S	0	0
			4131	2608	718	791	14		
1	z	518	Total	C	N	O	S	0	0
			4131	2608	718	791	14		
1	7	518	Total	C	N	O	S	0	0
			4131	2608	718	791	14		

Continued on next page...

Continued from previous page...

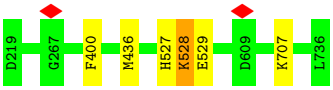
Mol	Chain	Residues	Atoms					AltConf	Trace
1	8	518	Total	C	N	O	S	0	0
			4131	2608	718	791	14		

3 Residue-property plots (i)

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

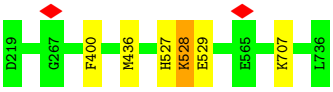
• Molecule 1: Capsid protein VP1

Chain A:



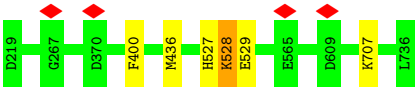
• Molecule 1: Capsid protein VP1

Chain B:



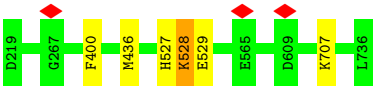
• Molecule 1: Capsid protein VP1

Chain C:



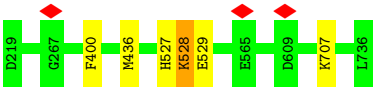
• Molecule 1: Capsid protein VP1

Chain D:



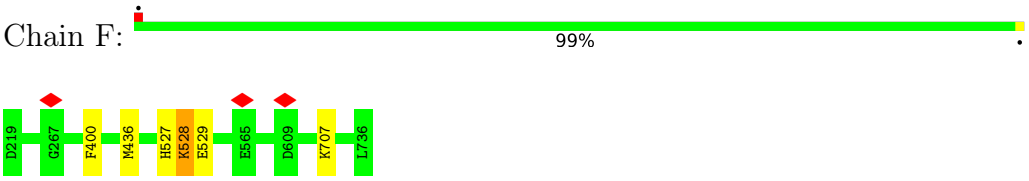
• Molecule 1: Capsid protein VP1

Chain E:



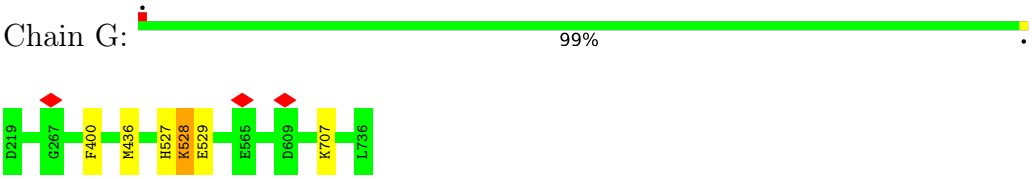
• Molecule 1: Capsid protein VP1

Chain F:



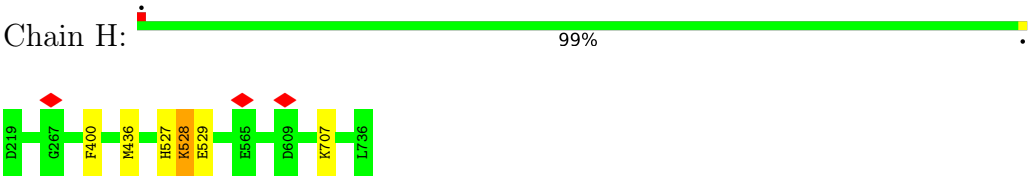
• Molecule 1: Capsid protein VP1

Chain G:



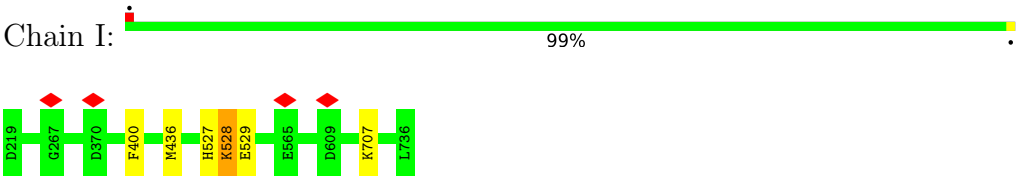
• Molecule 1: Capsid protein VP1

Chain H:



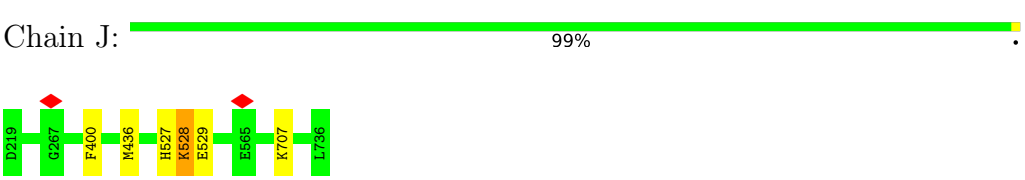
• Molecule 1: Capsid protein VP1

Chain I:



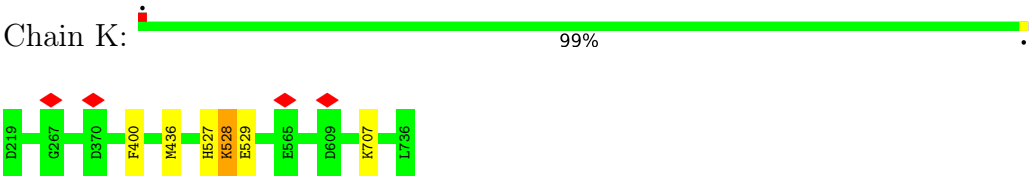
• Molecule 1: Capsid protein VP1

Chain J:



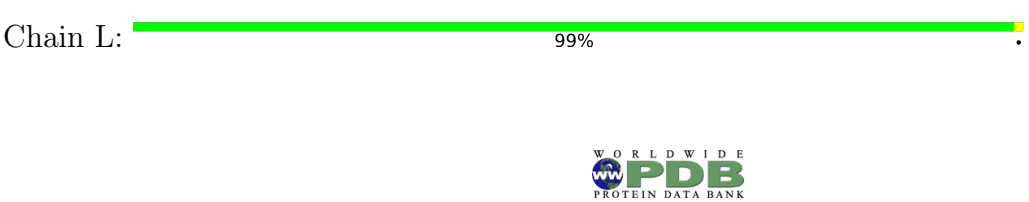
• Molecule 1: Capsid protein VP1

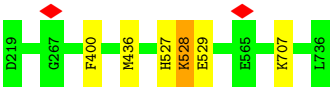
Chain K:



• Molecule 1: Capsid protein VP1

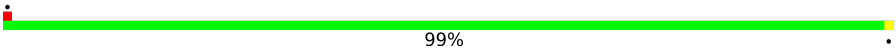
Chain L:

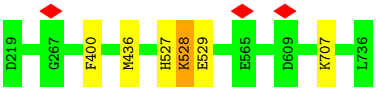




• Molecule 1: Capsid protein VP1

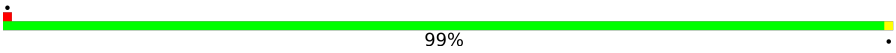
Chain M:

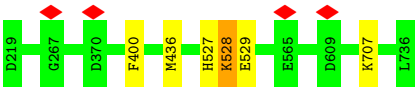




• Molecule 1: Capsid protein VP1

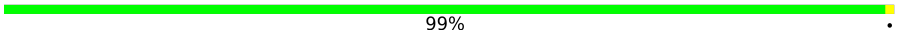
Chain N:

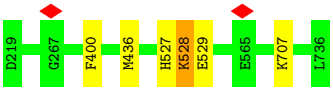




• Molecule 1: Capsid protein VP1

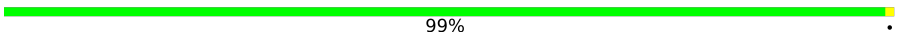
Chain O:

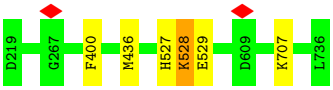




• Molecule 1: Capsid protein VP1

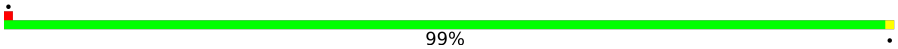
Chain P:

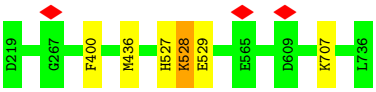




• Molecule 1: Capsid protein VP1

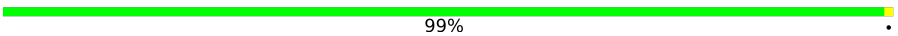
Chain Q:

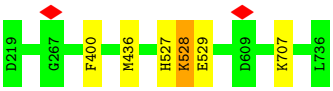




• Molecule 1: Capsid protein VP1

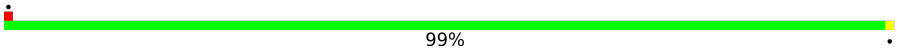
Chain R:

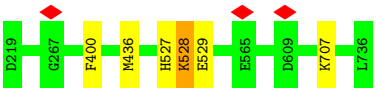




• Molecule 1: Capsid protein VP1

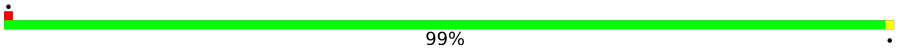
Chain S:

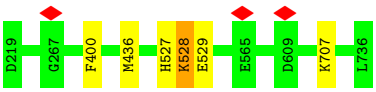




• Molecule 1: Capsid protein VP1

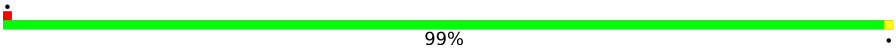
Chain T:

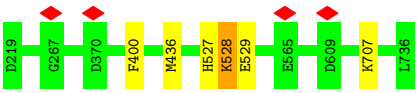




• Molecule 1: Capsid protein VP1

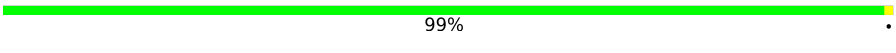
Chain U:

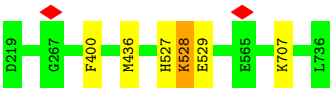




• Molecule 1: Capsid protein VP1

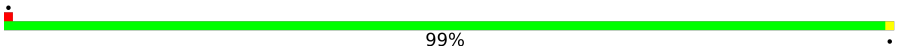
Chain V:

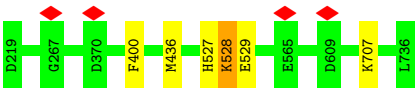




• Molecule 1: Capsid protein VP1

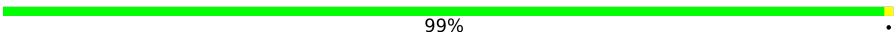
Chain W:

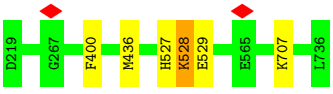




• Molecule 1: Capsid protein VP1

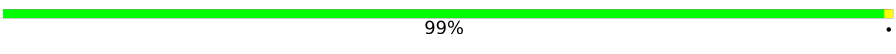
Chain X:

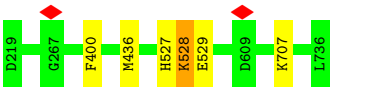




• Molecule 1: Capsid protein VP1

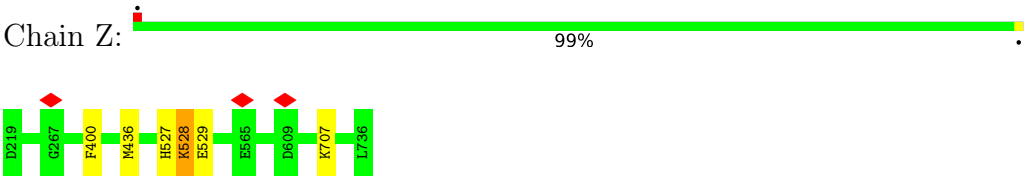
Chain Y:





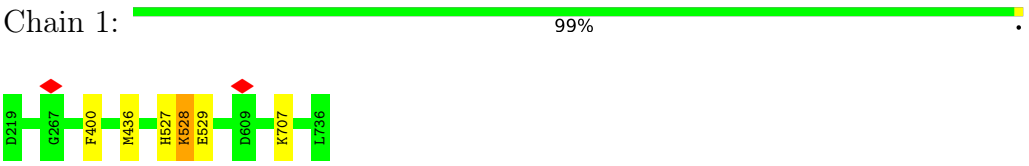
• Molecule 1: Capsid protein VP1

Chain Z:



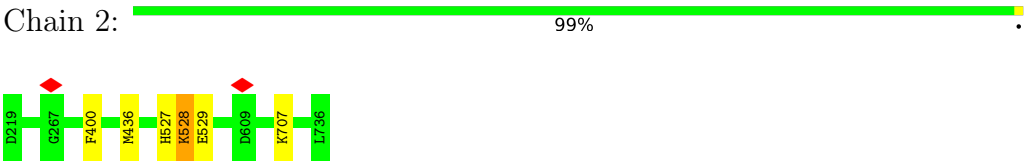
• Molecule 1: Capsid protein VP1

Chain 1:



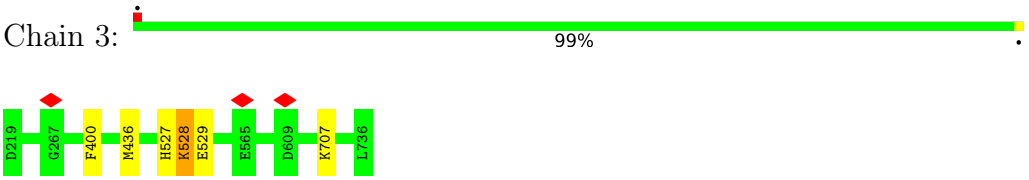
• Molecule 1: Capsid protein VP1

Chain 2:



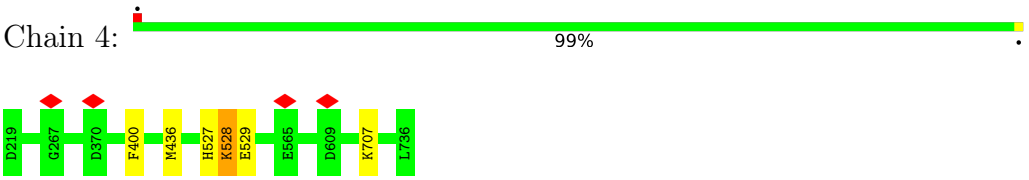
• Molecule 1: Capsid protein VP1

Chain 3:



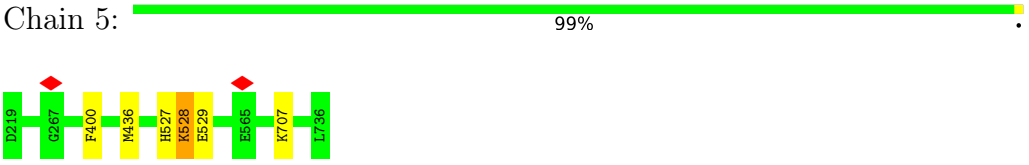
• Molecule 1: Capsid protein VP1

Chain 4:



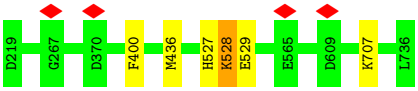
• Molecule 1: Capsid protein VP1

Chain 5:



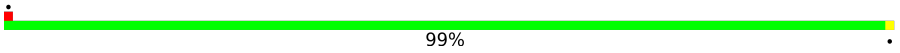
• Molecule 1: Capsid protein VP1

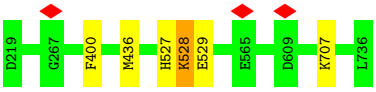
Chain 6:



• Molecule 1: Capsid protein VP1

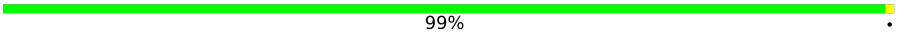
Chain a:

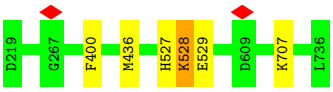




• Molecule 1: Capsid protein VP1

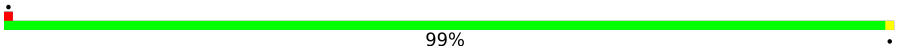
Chain b:

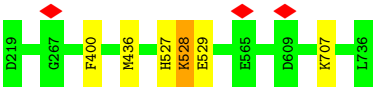




• Molecule 1: Capsid protein VP1

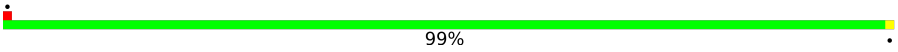
Chain c:

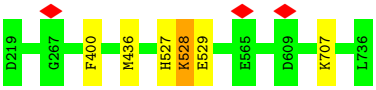




• Molecule 1: Capsid protein VP1

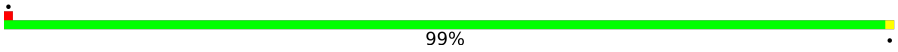
Chain d:

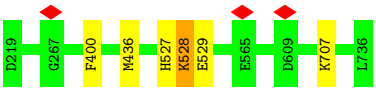




• Molecule 1: Capsid protein VP1

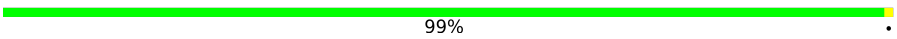
Chain e:

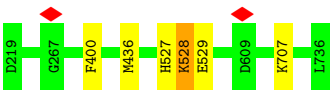




• Molecule 1: Capsid protein VP1

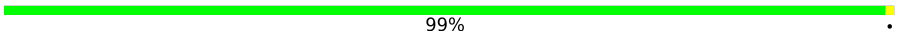
Chain f:

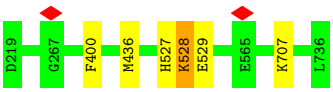




• Molecule 1: Capsid protein VP1

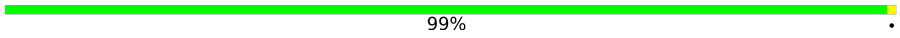
Chain g:

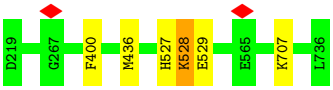




• Molecule 1: Capsid protein VP1

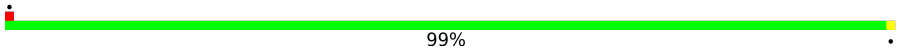
Chain h:

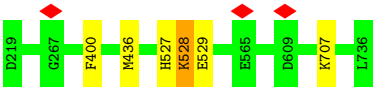




• Molecule 1: Capsid protein VP1

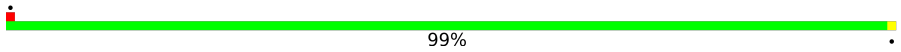
Chain i:

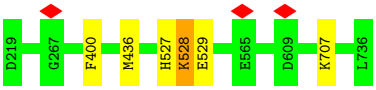




• Molecule 1: Capsid protein VP1

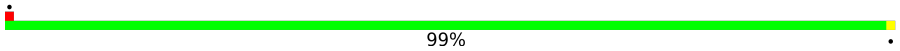
Chain j:

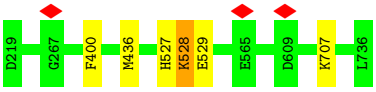




• Molecule 1: Capsid protein VP1

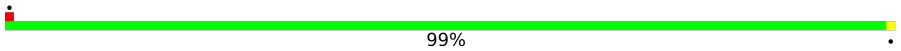
Chain k:

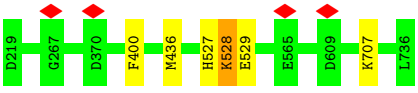




• Molecule 1: Capsid protein VP1

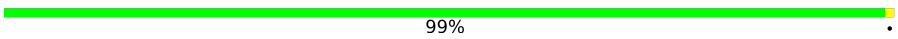
Chain l:

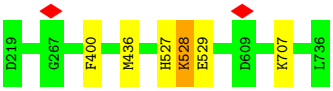




• Molecule 1: Capsid protein VP1

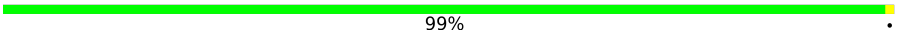
Chain m:

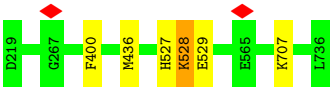




• Molecule 1: Capsid protein VP1

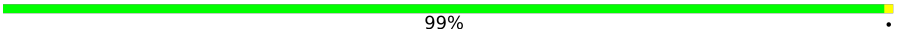
Chain n:

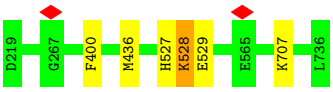




• Molecule 1: Capsid protein VP1

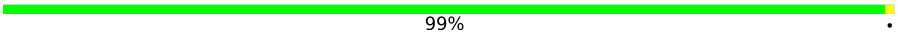
Chain o:

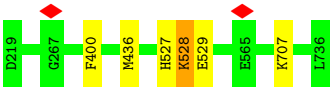




• Molecule 1: Capsid protein VP1

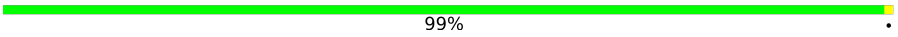
Chain p:

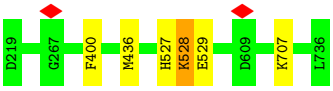




• Molecule 1: Capsid protein VP1

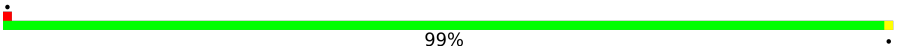
Chain q:

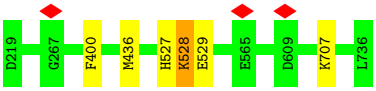




• Molecule 1: Capsid protein VP1

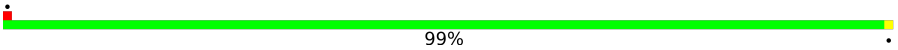
Chain r:

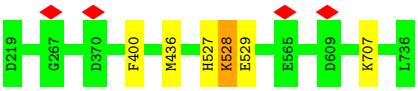




• Molecule 1: Capsid protein VP1

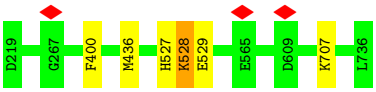
Chain s:





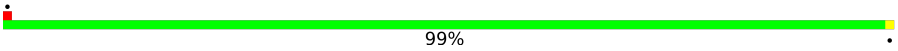
• Molecule 1: Capsid protein VP1

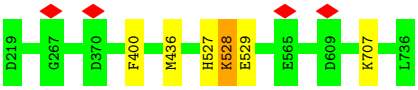
Chain t:



• Molecule 1: Capsid protein VP1

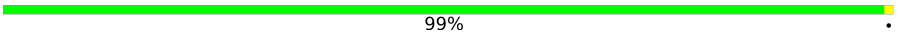
Chain u:

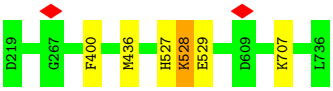




• Molecule 1: Capsid protein VP1

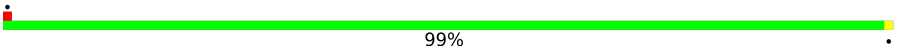
Chain v:

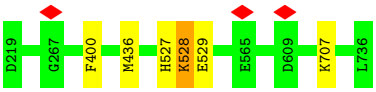




• Molecule 1: Capsid protein VP1

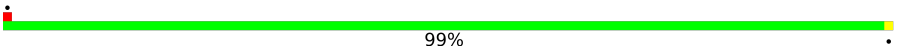
Chain w:

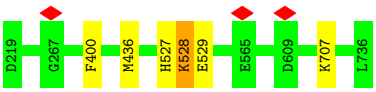




• Molecule 1: Capsid protein VP1

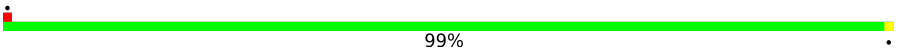
Chain x:

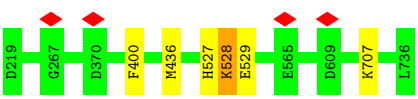




• Molecule 1: Capsid protein VP1

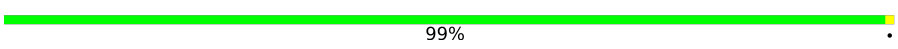
Chain y:

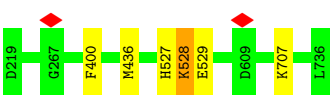




• Molecule 1: Capsid protein VP1

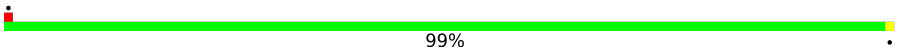
Chain z:

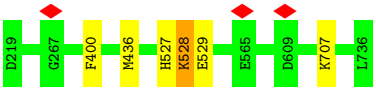




• Molecule 1: Capsid protein VP1

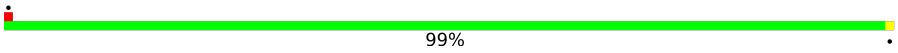
Chain 7:

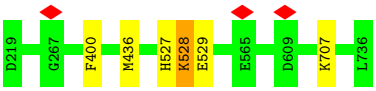




• Molecule 1: Capsid protein VP1

Chain 8:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	99899	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	27.988	Depositor
Minimum map value	-13.725	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	2.0	Depositor
Map size (Å)	479.367, 479.367, 479.367	wwPDB
Map dimensions	441, 441, 441	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.087, 1.087, 1.087	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	1	0.57	1/4256 (0.0%)	0.64	7/5800 (0.1%)
1	2	0.57	1/4256 (0.0%)	0.64	7/5800 (0.1%)
1	3	0.57	1/4256 (0.0%)	0.64	7/5800 (0.1%)
1	4	0.57	1/4256 (0.0%)	0.64	7/5800 (0.1%)
1	5	0.57	1/4256 (0.0%)	0.64	7/5800 (0.1%)
1	6	0.57	1/4256 (0.0%)	0.64	7/5800 (0.1%)
1	7	0.57	1/4256 (0.0%)	0.64	7/5800 (0.1%)
1	8	0.57	1/4256 (0.0%)	0.64	7/5800 (0.1%)
1	A	0.57	1/4256 (0.0%)	0.64	7/5800 (0.1%)
1	B	0.57	1/4256 (0.0%)	0.64	7/5800 (0.1%)
1	C	0.57	1/4256 (0.0%)	0.64	7/5800 (0.1%)
1	D	0.57	1/4256 (0.0%)	0.64	7/5800 (0.1%)
1	E	0.57	1/4256 (0.0%)	0.64	7/5800 (0.1%)
1	F	0.57	1/4256 (0.0%)	0.64	7/5800 (0.1%)
1	G	0.57	1/4256 (0.0%)	0.64	7/5800 (0.1%)
1	H	0.57	1/4256 (0.0%)	0.64	7/5800 (0.1%)
1	I	0.57	1/4256 (0.0%)	0.64	7/5800 (0.1%)
1	J	0.57	1/4256 (0.0%)	0.64	7/5800 (0.1%)
1	K	0.57	1/4256 (0.0%)	0.64	7/5800 (0.1%)
1	L	0.57	1/4256 (0.0%)	0.64	7/5800 (0.1%)
1	M	0.57	1/4256 (0.0%)	0.64	7/5800 (0.1%)
1	N	0.57	1/4256 (0.0%)	0.64	7/5800 (0.1%)
1	O	0.57	1/4256 (0.0%)	0.64	7/5800 (0.1%)
1	P	0.57	1/4256 (0.0%)	0.64	7/5800 (0.1%)
1	Q	0.57	1/4256 (0.0%)	0.64	7/5800 (0.1%)
1	R	0.57	1/4256 (0.0%)	0.64	7/5800 (0.1%)
1	S	0.57	1/4256 (0.0%)	0.64	7/5800 (0.1%)
1	T	0.57	1/4256 (0.0%)	0.64	7/5800 (0.1%)
1	U	0.57	1/4256 (0.0%)	0.64	7/5800 (0.1%)
1	V	0.57	1/4256 (0.0%)	0.64	7/5800 (0.1%)
1	W	0.57	1/4256 (0.0%)	0.64	7/5800 (0.1%)
1	X	0.57	1/4256 (0.0%)	0.64	7/5800 (0.1%)
1	Y	0.57	1/4256 (0.0%)	0.64	7/5800 (0.1%)
1	Z	0.57	1/4256 (0.0%)	0.64	7/5800 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	a	0.57	1/4256 (0.0%)	0.64	7/5800 (0.1%)
1	b	0.57	1/4256 (0.0%)	0.64	7/5800 (0.1%)
1	c	0.57	1/4256 (0.0%)	0.64	7/5800 (0.1%)
1	d	0.57	1/4256 (0.0%)	0.64	7/5800 (0.1%)
1	e	0.57	1/4256 (0.0%)	0.64	7/5800 (0.1%)
1	f	0.57	1/4256 (0.0%)	0.64	7/5800 (0.1%)
1	g	0.57	1/4256 (0.0%)	0.64	7/5800 (0.1%)
1	h	0.57	1/4256 (0.0%)	0.64	7/5800 (0.1%)
1	i	0.57	1/4256 (0.0%)	0.64	7/5800 (0.1%)
1	j	0.57	1/4256 (0.0%)	0.64	7/5800 (0.1%)
1	k	0.57	1/4256 (0.0%)	0.64	7/5800 (0.1%)
1	l	0.57	1/4256 (0.0%)	0.64	7/5800 (0.1%)
1	m	0.57	1/4256 (0.0%)	0.64	7/5800 (0.1%)
1	n	0.57	1/4256 (0.0%)	0.64	7/5800 (0.1%)
1	o	0.57	1/4256 (0.0%)	0.64	7/5800 (0.1%)
1	p	0.57	1/4256 (0.0%)	0.64	7/5800 (0.1%)
1	q	0.57	1/4256 (0.0%)	0.64	7/5800 (0.1%)
1	r	0.57	1/4256 (0.0%)	0.64	7/5800 (0.1%)
1	s	0.57	1/4256 (0.0%)	0.64	7/5800 (0.1%)
1	t	0.57	1/4256 (0.0%)	0.64	7/5800 (0.1%)
1	u	0.57	1/4256 (0.0%)	0.64	7/5800 (0.1%)
1	v	0.57	1/4256 (0.0%)	0.64	7/5800 (0.1%)
1	w	0.57	1/4256 (0.0%)	0.64	7/5800 (0.1%)
1	x	0.57	1/4256 (0.0%)	0.64	7/5800 (0.1%)
1	y	0.57	1/4256 (0.0%)	0.64	7/5800 (0.1%)
1	z	0.57	1/4256 (0.0%)	0.64	7/5800 (0.1%)
All	All	0.57	60/255360 (0.0%)	0.64	420/348000 (0.1%)

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	0	1
1	2	0	1
1	3	0	1
1	4	0	1
1	5	0	1
1	6	0	1
1	7	0	1
1	8	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
1	G	0	1
1	H	0	1
1	I	0	1
1	J	0	1
1	K	0	1
1	L	0	1
1	M	0	1
1	N	0	1
1	O	0	1
1	P	0	1
1	Q	0	1
1	R	0	1
1	S	0	1
1	T	0	1
1	U	0	1
1	V	0	1
1	W	0	1
1	X	0	1
1	Y	0	1
1	Z	0	1
1	a	0	1
1	b	0	1
1	c	0	1
1	d	0	1
1	e	0	1
1	f	0	1
1	g	0	1
1	h	0	1
1	i	0	1
1	j	0	1
1	k	0	1
1	l	0	1
1	m	0	1
1	n	0	1
1	o	0	1
1	p	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
1	q	0	1
1	r	0	1
1	s	0	1
1	t	0	1
1	u	0	1
1	v	0	1
1	w	0	1
1	x	0	1
1	y	0	1
1	z	0	1
All	All	0	60

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	h	400	PHE	C-N	-10.13	1.15	1.34
1	n	400	PHE	C-N	-10.13	1.15	1.34
1	C	400	PHE	C-N	-10.13	1.15	1.34
1	I	400	PHE	C-N	-10.13	1.15	1.34
1	O	400	PHE	C-N	-10.13	1.15	1.34
1	W	400	PHE	C-N	-10.13	1.15	1.34
1	l	400	PHE	C-N	-10.13	1.15	1.34
1	s	400	PHE	C-N	-10.13	1.15	1.34
1	F	400	PHE	C-N	-10.12	1.15	1.34
1	Z	400	PHE	C-N	-10.12	1.15	1.34
1	d	400	PHE	C-N	-10.12	1.15	1.34
1	j	400	PHE	C-N	-10.12	1.15	1.34
1	G	400	PHE	C-N	-10.12	1.15	1.34
1	M	400	PHE	C-N	-10.12	1.15	1.34
1	S	400	PHE	C-N	-10.12	1.15	1.34
1	T	400	PHE	C-N	-10.12	1.15	1.34
1	7	400	PHE	C-N	-10.12	1.15	1.34
1	8	400	PHE	C-N	-10.12	1.15	1.34
1	K	400	PHE	C-N	-10.11	1.15	1.34
1	U	400	PHE	C-N	-10.11	1.15	1.34
1	4	400	PHE	C-N	-10.11	1.15	1.34
1	g	400	PHE	C-N	-10.11	1.15	1.34
1	y	400	PHE	C-N	-10.11	1.15	1.34
1	D	400	PHE	C-N	-10.11	1.15	1.34
1	H	400	PHE	C-N	-10.11	1.15	1.34
1	a	400	PHE	C-N	-10.11	1.15	1.34
1	k	400	PHE	C-N	-10.11	1.15	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	r	400	PHE	C-N	-10.11	1.15	1.34
1	t	400	PHE	C-N	-10.11	1.15	1.34
1	A	400	PHE	C-N	-10.09	1.15	1.34
1	P	400	PHE	C-N	-10.09	1.15	1.34
1	R	400	PHE	C-N	-10.09	1.15	1.34
1	Y	400	PHE	C-N	-10.09	1.15	1.34
1	1	400	PHE	C-N	-10.09	1.15	1.34
1	2	400	PHE	C-N	-10.09	1.15	1.34
1	b	400	PHE	C-N	-10.09	1.15	1.34
1	f	400	PHE	C-N	-10.09	1.15	1.34
1	m	400	PHE	C-N	-10.09	1.15	1.34
1	q	400	PHE	C-N	-10.09	1.15	1.34
1	v	400	PHE	C-N	-10.09	1.15	1.34
1	z	400	PHE	C-N	-10.09	1.15	1.34
1	B	400	PHE	C-N	-10.09	1.15	1.34
1	E	400	PHE	C-N	-10.09	1.15	1.34
1	L	400	PHE	C-N	-10.09	1.15	1.34
1	V	400	PHE	C-N	-10.09	1.15	1.34
1	e	400	PHE	C-N	-10.09	1.15	1.34
1	x	400	PHE	C-N	-10.09	1.15	1.34
1	3	400	PHE	C-N	-10.09	1.15	1.34
1	i	400	PHE	C-N	-10.09	1.15	1.34
1	J	400	PHE	C-N	-10.08	1.15	1.34
1	X	400	PHE	C-N	-10.08	1.15	1.34
1	5	400	PHE	C-N	-10.08	1.15	1.34
1	o	400	PHE	C-N	-10.08	1.15	1.34
1	p	400	PHE	C-N	-10.08	1.15	1.34
1	6	400	PHE	C-N	-10.08	1.15	1.34
1	u	400	PHE	C-N	-10.08	1.15	1.34
1	N	400	PHE	C-N	-10.06	1.15	1.34
1	Q	400	PHE	C-N	-10.05	1.15	1.34
1	c	400	PHE	C-N	-10.05	1.15	1.34
1	w	400	PHE	C-N	-10.05	1.15	1.34

All (420) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	527	HIS	N-CA-C	-13.77	73.82	111.00
1	b	527	HIS	N-CA-C	-13.77	73.82	111.00
1	v	527	HIS	N-CA-C	-13.77	73.82	111.00
1	I	527	HIS	N-CA-C	-13.77	73.83	111.00
1	R	527	HIS	N-CA-C	-13.77	73.82	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	527	HIS	N-CA-C	-13.77	73.83	111.00
1	Y	527	HIS	N-CA-C	-13.77	73.82	111.00
1	1	527	HIS	N-CA-C	-13.77	73.82	111.00
1	5	527	HIS	N-CA-C	-13.77	73.83	111.00
1	m	527	HIS	N-CA-C	-13.77	73.82	111.00
1	o	527	HIS	N-CA-C	-13.77	73.83	111.00
1	p	527	HIS	N-CA-C	-13.77	73.83	111.00
1	q	527	HIS	N-CA-C	-13.77	73.82	111.00
1	z	527	HIS	N-CA-C	-13.77	73.82	111.00
1	V	527	HIS	N-CA-C	-13.77	73.83	111.00
1	h	527	HIS	N-CA-C	-13.77	73.83	111.00
1	n	527	HIS	N-CA-C	-13.77	73.83	111.00
1	M	527	HIS	N-CA-C	-13.77	73.83	111.00
1	N	527	HIS	N-CA-C	-13.77	73.83	111.00
1	k	527	HIS	N-CA-C	-13.77	73.83	111.00
1	r	527	HIS	N-CA-C	-13.77	73.83	111.00
1	B	527	HIS	N-CA-C	-13.76	73.84	111.00
1	L	527	HIS	N-CA-C	-13.76	73.84	111.00
1	W	527	HIS	N-CA-C	-13.76	73.84	111.00
1	3	527	HIS	N-CA-C	-13.76	73.84	111.00
1	f	527	HIS	N-CA-C	-13.76	73.84	111.00
1	l	527	HIS	N-CA-C	-13.76	73.84	111.00
1	s	527	HIS	N-CA-C	-13.76	73.84	111.00
1	C	527	HIS	N-CA-C	-13.76	73.85	111.00
1	G	527	HIS	N-CA-C	-13.76	73.85	111.00
1	J	527	HIS	N-CA-C	-13.76	73.86	111.00
1	K	527	HIS	N-CA-C	-13.76	73.86	111.00
1	O	527	HIS	N-CA-C	-13.76	73.86	111.00
1	P	527	HIS	N-CA-C	-13.76	73.86	111.00
1	S	527	HIS	N-CA-C	-13.76	73.86	111.00
1	T	527	HIS	N-CA-C	-13.76	73.86	111.00
1	U	527	HIS	N-CA-C	-13.76	73.86	111.00
1	2	527	HIS	N-CA-C	-13.76	73.86	111.00
1	4	527	HIS	N-CA-C	-13.76	73.86	111.00
1	6	527	HIS	N-CA-C	-13.76	73.86	111.00
1	g	527	HIS	N-CA-C	-13.76	73.86	111.00
1	u	527	HIS	N-CA-C	-13.76	73.86	111.00
1	y	527	HIS	N-CA-C	-13.76	73.86	111.00
1	7	527	HIS	N-CA-C	-13.76	73.86	111.00
1	8	527	HIS	N-CA-C	-13.76	73.86	111.00
1	D	527	HIS	N-CA-C	-13.75	73.86	111.00
1	a	527	HIS	N-CA-C	-13.75	73.86	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	t	527	HIS	N-CA-C	-13.75	73.86	111.00
1	A	527	HIS	N-CA-C	-13.75	73.87	111.00
1	E	527	HIS	N-CA-C	-13.75	73.87	111.00
1	F	527	HIS	N-CA-C	-13.75	73.87	111.00
1	Q	527	HIS	N-CA-C	-13.75	73.87	111.00
1	Z	527	HIS	N-CA-C	-13.75	73.87	111.00
1	c	527	HIS	N-CA-C	-13.75	73.87	111.00
1	d	527	HIS	N-CA-C	-13.75	73.87	111.00
1	e	527	HIS	N-CA-C	-13.75	73.87	111.00
1	i	527	HIS	N-CA-C	-13.75	73.87	111.00
1	j	527	HIS	N-CA-C	-13.75	73.87	111.00
1	w	527	HIS	N-CA-C	-13.75	73.87	111.00
1	x	527	HIS	N-CA-C	-13.75	73.87	111.00
1	D	528	LYS	N-CA-C	-12.82	76.38	111.00
1	M	528	LYS	N-CA-C	-12.82	76.38	111.00
1	A	528	LYS	N-CA-C	-12.82	76.39	111.00
1	H	528	LYS	N-CA-C	-12.82	76.39	111.00
1	Z	528	LYS	N-CA-C	-12.82	76.38	111.00
1	2	528	LYS	N-CA-C	-12.82	76.39	111.00
1	5	528	LYS	N-CA-C	-12.82	76.39	111.00
1	k	528	LYS	N-CA-C	-12.82	76.39	111.00
1	o	528	LYS	N-CA-C	-12.82	76.39	111.00
1	r	528	LYS	N-CA-C	-12.82	76.39	111.00
1	C	528	LYS	N-CA-C	-12.82	76.39	111.00
1	E	528	LYS	N-CA-C	-12.82	76.39	111.00
1	F	528	LYS	N-CA-C	-12.82	76.39	111.00
1	G	528	LYS	N-CA-C	-12.82	76.39	111.00
1	I	528	LYS	N-CA-C	-12.82	76.39	111.00
1	a	528	LYS	N-CA-C	-12.82	76.39	111.00
1	d	528	LYS	N-CA-C	-12.82	76.39	111.00
1	j	528	LYS	N-CA-C	-12.82	76.39	111.00
1	t	528	LYS	N-CA-C	-12.82	76.39	111.00
1	W	528	LYS	N-CA-C	-12.81	76.40	111.00
1	l	528	LYS	N-CA-C	-12.81	76.40	111.00
1	s	528	LYS	N-CA-C	-12.81	76.40	111.00
1	g	528	LYS	N-CA-C	-12.81	76.41	111.00
1	S	528	LYS	N-CA-C	-12.81	76.41	111.00
1	T	528	LYS	N-CA-C	-12.81	76.41	111.00
1	7	528	LYS	N-CA-C	-12.81	76.41	111.00
1	8	528	LYS	N-CA-C	-12.81	76.41	111.00
1	P	528	LYS	N-CA-C	-12.81	76.42	111.00
1	Q	528	LYS	N-CA-C	-12.81	76.41	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	R	528	LYS	N-CA-C	-12.81	76.42	111.00
1	c	528	LYS	N-CA-C	-12.81	76.41	111.00
1	e	528	LYS	N-CA-C	-12.81	76.41	111.00
1	f	528	LYS	N-CA-C	-12.81	76.42	111.00
1	i	528	LYS	N-CA-C	-12.81	76.41	111.00
1	w	528	LYS	N-CA-C	-12.81	76.41	111.00
1	x	528	LYS	N-CA-C	-12.81	76.41	111.00
1	B	528	LYS	N-CA-C	-12.81	76.42	111.00
1	J	528	LYS	N-CA-C	-12.81	76.42	111.00
1	L	528	LYS	N-CA-C	-12.81	76.42	111.00
1	O	528	LYS	N-CA-C	-12.81	76.42	111.00
1	V	528	LYS	N-CA-C	-12.81	76.42	111.00
1	X	528	LYS	N-CA-C	-12.81	76.42	111.00
1	Y	528	LYS	N-CA-C	-12.81	76.42	111.00
1	1	528	LYS	N-CA-C	-12.81	76.42	111.00
1	b	528	LYS	N-CA-C	-12.81	76.42	111.00
1	h	528	LYS	N-CA-C	-12.81	76.42	111.00
1	m	528	LYS	N-CA-C	-12.81	76.42	111.00
1	p	528	LYS	N-CA-C	-12.81	76.42	111.00
1	q	528	LYS	N-CA-C	-12.81	76.42	111.00
1	v	528	LYS	N-CA-C	-12.81	76.42	111.00
1	z	528	LYS	N-CA-C	-12.81	76.42	111.00
1	K	528	LYS	N-CA-C	-12.81	76.42	111.00
1	U	528	LYS	N-CA-C	-12.81	76.42	111.00
1	4	528	LYS	N-CA-C	-12.81	76.42	111.00
1	6	528	LYS	N-CA-C	-12.81	76.42	111.00
1	N	528	LYS	N-CA-C	-12.80	76.43	111.00
1	3	528	LYS	N-CA-C	-12.80	76.43	111.00
1	u	528	LYS	N-CA-C	-12.81	76.42	111.00
1	y	528	LYS	N-CA-C	-12.81	76.42	111.00
1	n	528	LYS	N-CA-C	-12.80	76.43	111.00
1	D	529	GLU	N-CA-CB	-9.15	94.13	110.60
1	K	529	GLU	N-CA-CB	-9.15	94.13	110.60
1	U	529	GLU	N-CA-CB	-9.15	94.13	110.60
1	4	529	GLU	N-CA-CB	-9.15	94.13	110.60
1	y	529	GLU	N-CA-CB	-9.15	94.13	110.60
1	6	529	GLU	N-CA-CB	-9.14	94.14	110.60
1	u	529	GLU	N-CA-CB	-9.14	94.14	110.60
1	Q	529	GLU	N-CA-CB	-9.14	94.14	110.60
1	c	529	GLU	N-CA-CB	-9.14	94.14	110.60
1	w	529	GLU	N-CA-CB	-9.14	94.14	110.60
1	m	529	GLU	N-CA-CB	-9.13	94.16	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	q	529	GLU	N-CA-CB	-9.13	94.16	110.60
1	e	529	GLU	N-CA-CB	-9.13	94.16	110.60
1	i	529	GLU	N-CA-CB	-9.13	94.16	110.60
1	x	529	GLU	N-CA-CB	-9.13	94.16	110.60
1	M	529	GLU	N-CA-CB	-9.13	94.17	110.60
1	k	529	GLU	N-CA-CB	-9.13	94.17	110.60
1	r	529	GLU	N-CA-CB	-9.13	94.17	110.60
1	S	529	GLU	N-CA-CB	-9.13	94.17	110.60
1	T	529	GLU	N-CA-CB	-9.13	94.17	110.60
1	Y	529	GLU	N-CA-CB	-9.13	94.17	110.60
1	7	529	GLU	N-CA-CB	-9.13	94.17	110.60
1	8	529	GLU	N-CA-CB	-9.13	94.17	110.60
1	N	529	GLU	N-CA-CB	-9.12	94.18	110.60
1	X	529	GLU	N-CA-CB	-9.12	94.18	110.60
1	5	529	GLU	N-CA-CB	-9.12	94.17	110.60
1	o	529	GLU	N-CA-CB	-9.12	94.17	110.60
1	p	529	GLU	N-CA-CB	-9.12	94.18	110.60
1	E	529	GLU	N-CA-CB	-9.12	94.18	110.60
1	F	529	GLU	N-CA-CB	-9.12	94.18	110.60
1	I	529	GLU	N-CA-CB	-9.12	94.18	110.60
1	W	529	GLU	N-CA-CB	-9.12	94.18	110.60
1	Z	529	GLU	N-CA-CB	-9.12	94.18	110.60
1	d	529	GLU	N-CA-CB	-9.12	94.18	110.60
1	g	529	GLU	N-CA-CB	-9.12	94.18	110.60
1	j	529	GLU	N-CA-CB	-9.12	94.18	110.60
1	l	529	GLU	N-CA-CB	-9.12	94.18	110.60
1	s	529	GLU	N-CA-CB	-9.12	94.18	110.60
1	C	529	GLU	N-CA-CB	-9.12	94.19	110.60
1	V	529	GLU	N-CA-CB	-9.12	94.19	110.60
1	h	529	GLU	N-CA-CB	-9.12	94.19	110.60
1	n	529	GLU	N-CA-CB	-9.12	94.19	110.60
1	P	529	GLU	N-CA-CB	-9.12	94.19	110.60
1	2	529	GLU	N-CA-CB	-9.12	94.19	110.60
1	B	529	GLU	N-CA-CB	-9.11	94.20	110.60
1	3	529	GLU	N-CA-CB	-9.11	94.20	110.60
1	J	529	GLU	N-CA-CB	-9.11	94.20	110.60
1	L	529	GLU	N-CA-CB	-9.11	94.20	110.60
1	A	529	GLU	N-CA-CB	-9.11	94.20	110.60
1	G	529	GLU	N-CA-CB	-9.11	94.20	110.60
1	O	529	GLU	N-CA-CB	-9.11	94.20	110.60
1	b	529	GLU	N-CA-CB	-9.11	94.20	110.60
1	v	529	GLU	N-CA-CB	-9.11	94.20	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	529	GLU	N-CA-CB	-9.10	94.21	110.60
1	a	529	GLU	N-CA-CB	-9.10	94.21	110.60
1	t	529	GLU	N-CA-CB	-9.10	94.21	110.60
1	R	529	GLU	N-CA-CB	-9.10	94.22	110.60
1	1	529	GLU	N-CA-CB	-9.10	94.22	110.60
1	f	529	GLU	N-CA-CB	-9.10	94.22	110.60
1	z	529	GLU	N-CA-CB	-9.10	94.22	110.60
1	W	527	HIS	CB-CA-C	7.58	125.56	110.40
1	l	527	HIS	CB-CA-C	7.58	125.56	110.40
1	s	527	HIS	CB-CA-C	7.58	125.56	110.40
1	g	527	HIS	CB-CA-C	7.58	125.56	110.40
1	J	527	HIS	CB-CA-C	7.58	125.56	110.40
1	X	527	HIS	CB-CA-C	7.58	125.56	110.40
1	Z	527	HIS	CB-CA-C	7.58	125.56	110.40
1	p	527	HIS	CB-CA-C	7.58	125.56	110.40
1	8	527	HIS	CB-CA-C	7.58	125.55	110.40
1	E	527	HIS	CB-CA-C	7.57	125.55	110.40
1	F	527	HIS	CB-CA-C	7.57	125.55	110.40
1	Q	527	HIS	CB-CA-C	7.57	125.55	110.40
1	c	527	HIS	CB-CA-C	7.57	125.55	110.40
1	d	527	HIS	CB-CA-C	7.57	125.55	110.40
1	e	527	HIS	CB-CA-C	7.57	125.55	110.40
1	i	527	HIS	CB-CA-C	7.57	125.55	110.40
1	j	527	HIS	CB-CA-C	7.57	125.55	110.40
1	w	527	HIS	CB-CA-C	7.57	125.55	110.40
1	x	527	HIS	CB-CA-C	7.57	125.55	110.40
1	G	527	HIS	CB-CA-C	7.57	125.55	110.40
1	6	527	HIS	CB-CA-C	7.57	125.54	110.40
1	u	527	HIS	CB-CA-C	7.57	125.54	110.40
1	B	527	HIS	CB-CA-C	7.57	125.54	110.40
1	S	527	HIS	CB-CA-C	7.57	125.53	110.40
1	T	527	HIS	CB-CA-C	7.57	125.53	110.40
1	7	527	HIS	CB-CA-C	7.57	125.53	110.40
1	P	527	HIS	CB-CA-C	7.57	125.53	110.40
1	3	527	HIS	CB-CA-C	7.57	125.53	110.40
1	f	527	HIS	CB-CA-C	7.57	125.53	110.40
1	Y	527	HIS	CB-CA-C	7.56	125.53	110.40
1	q	527	HIS	CB-CA-C	7.56	125.53	110.40
1	C	527	HIS	CB-CA-C	7.56	125.53	110.40
1	5	527	HIS	CB-CA-C	7.56	125.52	110.40
1	o	527	HIS	CB-CA-C	7.56	125.52	110.40
1	O	527	HIS	CB-CA-C	7.56	125.52	110.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	R	527	HIS	CB-CA-C	7.55	125.51	110.40
1	1	527	HIS	CB-CA-C	7.55	125.51	110.40
1	b	527	HIS	CB-CA-C	7.55	125.51	110.40
1	m	527	HIS	CB-CA-C	7.55	125.51	110.40
1	v	527	HIS	CB-CA-C	7.55	125.51	110.40
1	z	527	HIS	CB-CA-C	7.55	125.51	110.40
1	I	527	HIS	CB-CA-C	7.55	125.50	110.40
1	A	527	HIS	CB-CA-C	7.55	125.50	110.40
1	D	527	HIS	CB-CA-C	7.55	125.50	110.40
1	L	527	HIS	CB-CA-C	7.55	125.50	110.40
1	2	527	HIS	CB-CA-C	7.55	125.50	110.40
1	a	527	HIS	CB-CA-C	7.55	125.50	110.40
1	t	527	HIS	CB-CA-C	7.55	125.50	110.40
1	M	527	HIS	CB-CA-C	7.55	125.50	110.40
1	V	527	HIS	CB-CA-C	7.55	125.50	110.40
1	h	527	HIS	CB-CA-C	7.55	125.50	110.40
1	k	527	HIS	CB-CA-C	7.55	125.50	110.40
1	n	527	HIS	CB-CA-C	7.55	125.50	110.40
1	r	527	HIS	CB-CA-C	7.55	125.50	110.40
1	K	527	HIS	CB-CA-C	7.54	125.49	110.40
1	N	527	HIS	CB-CA-C	7.54	125.49	110.40
1	U	527	HIS	CB-CA-C	7.54	125.49	110.40
1	4	527	HIS	CB-CA-C	7.54	125.49	110.40
1	y	527	HIS	CB-CA-C	7.54	125.49	110.40
1	H	527	HIS	CB-CA-C	7.54	125.48	110.40
1	2	528	LYS	CB-CA-C	-7.17	96.06	110.40
1	n	528	LYS	CB-CA-C	-7.17	96.06	110.40
1	G	528	LYS	CB-CA-C	-7.17	96.06	110.40
1	V	528	LYS	CB-CA-C	-7.17	96.06	110.40
1	h	528	LYS	CB-CA-C	-7.17	96.06	110.40
1	A	528	LYS	CB-CA-C	-7.15	96.09	110.40
1	L	528	LYS	CB-CA-C	-7.15	96.09	110.40
1	P	528	LYS	CB-CA-C	-7.15	96.10	110.40
1	R	528	LYS	CB-CA-C	-7.15	96.10	110.40
1	Y	528	LYS	CB-CA-C	-7.15	96.10	110.40
1	1	528	LYS	CB-CA-C	-7.15	96.10	110.40
1	b	528	LYS	CB-CA-C	-7.15	96.10	110.40
1	f	528	LYS	CB-CA-C	-7.15	96.10	110.40
1	g	528	LYS	CB-CA-C	-7.15	96.09	110.40
1	m	528	LYS	CB-CA-C	-7.15	96.10	110.40
1	q	528	LYS	CB-CA-C	-7.15	96.10	110.40
1	v	528	LYS	CB-CA-C	-7.15	96.10	110.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	z	528	LYS	CB-CA-C	-7.15	96.10	110.40
1	E	528	LYS	CB-CA-C	-7.15	96.10	110.40
1	F	528	LYS	CB-CA-C	-7.15	96.10	110.40
1	S	528	LYS	CB-CA-C	-7.15	96.10	110.40
1	T	528	LYS	CB-CA-C	-7.15	96.10	110.40
1	W	528	LYS	CB-CA-C	-7.15	96.10	110.40
1	Z	528	LYS	CB-CA-C	-7.15	96.10	110.40
1	a	528	LYS	CB-CA-C	-7.15	96.10	110.40
1	d	528	LYS	CB-CA-C	-7.15	96.10	110.40
1	j	528	LYS	CB-CA-C	-7.15	96.10	110.40
1	l	528	LYS	CB-CA-C	-7.15	96.10	110.40
1	s	528	LYS	CB-CA-C	-7.15	96.10	110.40
1	t	528	LYS	CB-CA-C	-7.15	96.10	110.40
1	7	528	LYS	CB-CA-C	-7.15	96.10	110.40
1	8	528	LYS	CB-CA-C	-7.15	96.10	110.40
1	N	528	LYS	CB-CA-C	-7.15	96.10	110.40
1	Q	528	LYS	CB-CA-C	-7.14	96.11	110.40
1	c	528	LYS	CB-CA-C	-7.14	96.11	110.40
1	e	528	LYS	CB-CA-C	-7.14	96.11	110.40
1	i	528	LYS	CB-CA-C	-7.14	96.11	110.40
1	w	528	LYS	CB-CA-C	-7.14	96.11	110.40
1	x	528	LYS	CB-CA-C	-7.14	96.11	110.40
1	B	528	LYS	CB-CA-C	-7.14	96.12	110.40
1	J	528	LYS	CB-CA-C	-7.14	96.12	110.40
1	O	528	LYS	CB-CA-C	-7.14	96.12	110.40
1	X	528	LYS	CB-CA-C	-7.14	96.12	110.40
1	5	528	LYS	CB-CA-C	-7.14	96.12	110.40
1	o	528	LYS	CB-CA-C	-7.14	96.12	110.40
1	p	528	LYS	CB-CA-C	-7.14	96.12	110.40
1	D	528	LYS	CB-CA-C	-7.14	96.12	110.40
1	H	528	LYS	CB-CA-C	-7.14	96.12	110.40
1	K	528	LYS	CB-CA-C	-7.14	96.12	110.40
1	M	528	LYS	CB-CA-C	-7.14	96.12	110.40
1	U	528	LYS	CB-CA-C	-7.14	96.12	110.40
1	4	528	LYS	CB-CA-C	-7.14	96.12	110.40
1	k	528	LYS	CB-CA-C	-7.14	96.12	110.40
1	r	528	LYS	CB-CA-C	-7.14	96.12	110.40
1	y	528	LYS	CB-CA-C	-7.14	96.12	110.40
1	3	528	LYS	CB-CA-C	-7.14	96.13	110.40
1	C	528	LYS	CB-CA-C	-7.13	96.13	110.40
1	I	528	LYS	CB-CA-C	-7.13	96.13	110.40
1	6	528	LYS	CB-CA-C	-7.13	96.13	110.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	u	528	LYS	CB-CA-C	-7.13	96.13	110.40
1	m	529	GLU	N-CA-C	6.99	129.88	111.00
1	q	529	GLU	N-CA-C	6.99	129.88	111.00
1	Y	529	GLU	N-CA-C	6.99	129.87	111.00
1	Q	529	GLU	N-CA-C	6.98	129.86	111.00
1	c	529	GLU	N-CA-C	6.98	129.86	111.00
1	w	529	GLU	N-CA-C	6.98	129.86	111.00
1	i	529	GLU	N-CA-C	6.98	129.85	111.00
1	S	529	GLU	N-CA-C	6.98	129.84	111.00
1	T	529	GLU	N-CA-C	6.98	129.84	111.00
1	7	529	GLU	N-CA-C	6.98	129.84	111.00
1	8	529	GLU	N-CA-C	6.98	129.84	111.00
1	V	529	GLU	N-CA-C	6.97	129.83	111.00
1	g	529	GLU	N-CA-C	6.97	129.83	111.00
1	h	529	GLU	N-CA-C	6.97	129.83	111.00
1	n	529	GLU	N-CA-C	6.97	129.83	111.00
1	K	529	GLU	N-CA-C	6.97	129.82	111.00
1	U	529	GLU	N-CA-C	6.97	129.82	111.00
1	4	529	GLU	N-CA-C	6.97	129.82	111.00
1	y	529	GLU	N-CA-C	6.97	129.82	111.00
1	C	529	GLU	N-CA-C	6.97	129.82	111.00
1	D	529	GLU	N-CA-C	6.97	129.81	111.00
1	E	529	GLU	N-CA-C	6.97	129.81	111.00
1	F	529	GLU	N-CA-C	6.97	129.81	111.00
1	R	529	GLU	N-CA-C	6.97	129.81	111.00
1	Z	529	GLU	N-CA-C	6.97	129.81	111.00
1	1	529	GLU	N-CA-C	6.97	129.81	111.00
1	b	529	GLU	N-CA-C	6.97	129.81	111.00
1	d	529	GLU	N-CA-C	6.97	129.81	111.00
1	f	529	GLU	N-CA-C	6.97	129.81	111.00
1	j	529	GLU	N-CA-C	6.97	129.81	111.00
1	v	529	GLU	N-CA-C	6.97	129.81	111.00
1	z	529	GLU	N-CA-C	6.97	129.81	111.00
1	I	529	GLU	N-CA-C	6.97	129.81	111.00
1	W	529	GLU	N-CA-C	6.97	129.81	111.00
1	l	529	GLU	N-CA-C	6.96	129.80	111.00
1	s	529	GLU	N-CA-C	6.96	129.80	111.00
1	O	529	GLU	N-CA-C	6.96	129.80	111.00
1	X	529	GLU	N-CA-C	6.96	129.80	111.00
1	p	529	GLU	N-CA-C	6.96	129.80	111.00
1	6	529	GLU	N-CA-C	6.96	129.79	111.00
1	u	529	GLU	N-CA-C	6.96	129.79	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	529	GLU	N-CA-C	6.96	129.79	111.00
1	N	529	GLU	N-CA-C	6.95	129.78	111.00
1	G	529	GLU	N-CA-C	6.95	129.77	111.00
1	J	529	GLU	N-CA-C	6.95	129.77	111.00
1	L	529	GLU	N-CA-C	6.95	129.77	111.00
1	5	529	GLU	N-CA-C	6.95	129.77	111.00
1	o	529	GLU	N-CA-C	6.95	129.77	111.00
1	H	529	GLU	N-CA-C	6.95	129.77	111.00
1	P	529	GLU	N-CA-C	6.95	129.76	111.00
1	2	529	GLU	N-CA-C	6.95	129.76	111.00
1	a	529	GLU	N-CA-C	6.95	129.77	111.00
1	t	529	GLU	N-CA-C	6.95	129.77	111.00
1	3	529	GLU	N-CA-C	6.95	129.76	111.00
1	e	529	GLU	N-CA-C	6.95	129.76	111.00
1	x	529	GLU	N-CA-C	6.95	129.76	111.00
1	B	529	GLU	N-CA-C	6.95	129.75	111.00
1	M	529	GLU	N-CA-C	6.94	129.75	111.00
1	k	529	GLU	N-CA-C	6.94	129.75	111.00
1	r	529	GLU	N-CA-C	6.94	129.75	111.00
1	V	528	LYS	N-CA-CB	-6.30	99.27	110.60
1	h	528	LYS	N-CA-CB	-6.30	99.27	110.60
1	Y	528	LYS	N-CA-CB	-6.29	99.27	110.60
1	1	528	LYS	N-CA-CB	-6.29	99.27	110.60
1	b	528	LYS	N-CA-CB	-6.29	99.27	110.60
1	m	528	LYS	N-CA-CB	-6.29	99.27	110.60
1	q	528	LYS	N-CA-CB	-6.29	99.27	110.60
1	v	528	LYS	N-CA-CB	-6.29	99.27	110.60
1	z	528	LYS	N-CA-CB	-6.29	99.27	110.60
1	B	528	LYS	N-CA-CB	-6.29	99.28	110.60
1	J	528	LYS	N-CA-CB	-6.29	99.28	110.60
1	L	528	LYS	N-CA-CB	-6.29	99.28	110.60
1	O	528	LYS	N-CA-CB	-6.29	99.28	110.60
1	X	528	LYS	N-CA-CB	-6.29	99.28	110.60
1	p	528	LYS	N-CA-CB	-6.29	99.28	110.60
1	6	528	LYS	N-CA-CB	-6.29	99.28	110.60
1	u	528	LYS	N-CA-CB	-6.29	99.28	110.60
1	D	528	LYS	N-CA-CB	-6.29	99.28	110.60
1	M	528	LYS	N-CA-CB	-6.29	99.28	110.60
1	3	528	LYS	N-CA-CB	-6.29	99.28	110.60
1	N	528	LYS	N-CA-CB	-6.28	99.29	110.60
1	G	528	LYS	N-CA-CB	-6.28	99.29	110.60
1	K	528	LYS	N-CA-CB	-6.28	99.29	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	U	528	LYS	N-CA-CB	-6.28	99.29	110.60
1	4	528	LYS	N-CA-CB	-6.28	99.29	110.60
1	y	528	LYS	N-CA-CB	-6.28	99.29	110.60
1	2	528	LYS	N-CA-CB	-6.28	99.31	110.60
1	a	528	LYS	N-CA-CB	-6.28	99.31	110.60
1	g	528	LYS	N-CA-CB	-6.28	99.30	110.60
1	t	528	LYS	N-CA-CB	-6.28	99.31	110.60
1	A	528	LYS	N-CA-CB	-6.27	99.31	110.60
1	P	528	LYS	N-CA-CB	-6.27	99.31	110.60
1	Q	528	LYS	N-CA-CB	-6.27	99.31	110.60
1	R	528	LYS	N-CA-CB	-6.27	99.31	110.60
1	S	528	LYS	N-CA-CB	-6.27	99.31	110.60
1	T	528	LYS	N-CA-CB	-6.27	99.31	110.60
1	W	528	LYS	N-CA-CB	-6.27	99.31	110.60
1	c	528	LYS	N-CA-CB	-6.27	99.31	110.60
1	e	528	LYS	N-CA-CB	-6.27	99.31	110.60
1	f	528	LYS	N-CA-CB	-6.27	99.31	110.60
1	i	528	LYS	N-CA-CB	-6.27	99.31	110.60
1	l	528	LYS	N-CA-CB	-6.27	99.31	110.60
1	s	528	LYS	N-CA-CB	-6.27	99.31	110.60
1	w	528	LYS	N-CA-CB	-6.27	99.31	110.60
1	x	528	LYS	N-CA-CB	-6.27	99.31	110.60
1	7	528	LYS	N-CA-CB	-6.27	99.31	110.60
1	8	528	LYS	N-CA-CB	-6.27	99.31	110.60
1	Z	528	LYS	N-CA-CB	-6.27	99.31	110.60
1	n	528	LYS	N-CA-CB	-6.27	99.31	110.60
1	C	528	LYS	N-CA-CB	-6.27	99.31	110.60
1	H	528	LYS	N-CA-CB	-6.27	99.32	110.60
1	I	528	LYS	N-CA-CB	-6.27	99.31	110.60
1	k	528	LYS	N-CA-CB	-6.27	99.32	110.60
1	r	528	LYS	N-CA-CB	-6.27	99.32	110.60
1	5	528	LYS	N-CA-CB	-6.27	99.32	110.60
1	o	528	LYS	N-CA-CB	-6.27	99.32	110.60
1	E	528	LYS	N-CA-CB	-6.26	99.34	110.60
1	F	528	LYS	N-CA-CB	-6.26	99.34	110.60
1	d	528	LYS	N-CA-CB	-6.26	99.34	110.60
1	j	528	LYS	N-CA-CB	-6.26	99.34	110.60

There are no chirality outliers.

All (60) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	528	LYS	Mainchain
1	2	528	LYS	Mainchain
1	3	528	LYS	Mainchain
1	4	528	LYS	Mainchain
1	5	528	LYS	Mainchain
1	6	528	LYS	Mainchain
1	7	528	LYS	Mainchain
1	8	528	LYS	Mainchain
1	A	528	LYS	Mainchain
1	B	528	LYS	Mainchain
1	C	528	LYS	Mainchain
1	D	528	LYS	Mainchain
1	E	528	LYS	Mainchain
1	F	528	LYS	Mainchain
1	G	528	LYS	Mainchain
1	H	528	LYS	Mainchain
1	I	528	LYS	Mainchain
1	J	528	LYS	Mainchain
1	K	528	LYS	Mainchain
1	L	528	LYS	Mainchain
1	M	528	LYS	Mainchain
1	N	528	LYS	Mainchain
1	O	528	LYS	Mainchain
1	P	528	LYS	Mainchain
1	Q	528	LYS	Mainchain
1	R	528	LYS	Mainchain
1	S	528	LYS	Mainchain
1	T	528	LYS	Mainchain
1	U	528	LYS	Mainchain
1	V	528	LYS	Mainchain
1	W	528	LYS	Mainchain
1	X	528	LYS	Mainchain
1	Y	528	LYS	Mainchain
1	Z	528	LYS	Mainchain
1	a	528	LYS	Mainchain
1	b	528	LYS	Mainchain
1	c	528	LYS	Mainchain
1	d	528	LYS	Mainchain
1	e	528	LYS	Mainchain
1	f	528	LYS	Mainchain
1	g	528	LYS	Mainchain
1	h	528	LYS	Mainchain
1	i	528	LYS	Mainchain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	j	528	LYS	Mainchain
1	k	528	LYS	Mainchain
1	l	528	LYS	Mainchain
1	m	528	LYS	Mainchain
1	n	528	LYS	Mainchain
1	o	528	LYS	Mainchain
1	p	528	LYS	Mainchain
1	q	528	LYS	Mainchain
1	r	528	LYS	Mainchain
1	s	528	LYS	Mainchain
1	t	528	LYS	Mainchain
1	u	528	LYS	Mainchain
1	v	528	LYS	Mainchain
1	w	528	LYS	Mainchain
1	x	528	LYS	Mainchain
1	y	528	LYS	Mainchain
1	z	528	LYS	Mainchain

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	516/518 (100%)	500 (97%)	15 (3%)	1 (0%)	47 78
1	2	516/518 (100%)	500 (97%)	15 (3%)	1 (0%)	47 78
1	3	516/518 (100%)	500 (97%)	15 (3%)	1 (0%)	47 78
1	4	516/518 (100%)	500 (97%)	15 (3%)	1 (0%)	47 78
1	5	516/518 (100%)	500 (97%)	15 (3%)	1 (0%)	47 78

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	6	516/518 (100%)	500 (97%)	15 (3%)	1 (0%)	47	78
1	7	516/518 (100%)	500 (97%)	15 (3%)	1 (0%)	47	78
1	8	516/518 (100%)	500 (97%)	15 (3%)	1 (0%)	47	78
1	A	516/518 (100%)	500 (97%)	15 (3%)	1 (0%)	47	78
1	B	516/518 (100%)	500 (97%)	15 (3%)	1 (0%)	47	78
1	C	516/518 (100%)	500 (97%)	15 (3%)	1 (0%)	47	78
1	D	516/518 (100%)	500 (97%)	15 (3%)	1 (0%)	47	78
1	E	516/518 (100%)	500 (97%)	15 (3%)	1 (0%)	47	78
1	F	516/518 (100%)	500 (97%)	15 (3%)	1 (0%)	47	78
1	G	516/518 (100%)	500 (97%)	15 (3%)	1 (0%)	47	78
1	H	516/518 (100%)	500 (97%)	15 (3%)	1 (0%)	47	78
1	I	516/518 (100%)	500 (97%)	15 (3%)	1 (0%)	47	78
1	J	516/518 (100%)	500 (97%)	15 (3%)	1 (0%)	47	78
1	K	516/518 (100%)	500 (97%)	15 (3%)	1 (0%)	47	78
1	L	516/518 (100%)	500 (97%)	15 (3%)	1 (0%)	47	78
1	M	516/518 (100%)	500 (97%)	15 (3%)	1 (0%)	47	78
1	N	516/518 (100%)	500 (97%)	15 (3%)	1 (0%)	47	78
1	O	516/518 (100%)	500 (97%)	15 (3%)	1 (0%)	47	78
1	P	516/518 (100%)	500 (97%)	15 (3%)	1 (0%)	47	78
1	Q	516/518 (100%)	500 (97%)	15 (3%)	1 (0%)	47	78
1	R	516/518 (100%)	500 (97%)	15 (3%)	1 (0%)	47	78
1	S	516/518 (100%)	500 (97%)	15 (3%)	1 (0%)	47	78
1	T	516/518 (100%)	500 (97%)	15 (3%)	1 (0%)	47	78
1	U	516/518 (100%)	500 (97%)	15 (3%)	1 (0%)	47	78
1	V	516/518 (100%)	500 (97%)	15 (3%)	1 (0%)	47	78
1	W	516/518 (100%)	500 (97%)	15 (3%)	1 (0%)	47	78
1	X	516/518 (100%)	500 (97%)	15 (3%)	1 (0%)	47	78
1	Y	516/518 (100%)	500 (97%)	15 (3%)	1 (0%)	47	78
1	Z	516/518 (100%)	500 (97%)	15 (3%)	1 (0%)	47	78
1	a	516/518 (100%)	500 (97%)	15 (3%)	1 (0%)	47	78
1	b	516/518 (100%)	500 (97%)	15 (3%)	1 (0%)	47	78

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	c	516/518 (100%)	500 (97%)	15 (3%)	1 (0%)	47	78
1	d	516/518 (100%)	500 (97%)	15 (3%)	1 (0%)	47	78
1	e	516/518 (100%)	500 (97%)	15 (3%)	1 (0%)	47	78
1	f	516/518 (100%)	500 (97%)	15 (3%)	1 (0%)	47	78
1	g	516/518 (100%)	500 (97%)	15 (3%)	1 (0%)	47	78
1	h	516/518 (100%)	500 (97%)	15 (3%)	1 (0%)	47	78
1	i	516/518 (100%)	500 (97%)	15 (3%)	1 (0%)	47	78
1	j	516/518 (100%)	500 (97%)	15 (3%)	1 (0%)	47	78
1	k	516/518 (100%)	500 (97%)	15 (3%)	1 (0%)	47	78
1	l	516/518 (100%)	500 (97%)	15 (3%)	1 (0%)	47	78
1	m	516/518 (100%)	500 (97%)	15 (3%)	1 (0%)	47	78
1	n	516/518 (100%)	500 (97%)	15 (3%)	1 (0%)	47	78
1	o	516/518 (100%)	500 (97%)	15 (3%)	1 (0%)	47	78
1	p	516/518 (100%)	500 (97%)	15 (3%)	1 (0%)	47	78
1	q	516/518 (100%)	500 (97%)	15 (3%)	1 (0%)	47	78
1	r	516/518 (100%)	500 (97%)	15 (3%)	1 (0%)	47	78
1	s	516/518 (100%)	500 (97%)	15 (3%)	1 (0%)	47	78
1	t	516/518 (100%)	500 (97%)	15 (3%)	1 (0%)	47	78
1	u	516/518 (100%)	500 (97%)	15 (3%)	1 (0%)	47	78
1	v	516/518 (100%)	500 (97%)	15 (3%)	1 (0%)	47	78
1	w	516/518 (100%)	500 (97%)	15 (3%)	1 (0%)	47	78
1	x	516/518 (100%)	500 (97%)	15 (3%)	1 (0%)	47	78
1	y	516/518 (100%)	500 (97%)	15 (3%)	1 (0%)	47	78
1	z	516/518 (100%)	500 (97%)	15 (3%)	1 (0%)	47	78
All	All	30960/31080 (100%)	30000 (97%)	900 (3%)	60 (0%)	50	78

All (60) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	707	LYS
1	B	707	LYS
1	C	707	LYS
1	D	707	LYS
1	E	707	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	707	LYS
1	G	707	LYS
1	H	707	LYS
1	I	707	LYS
1	J	707	LYS
1	K	707	LYS
1	L	707	LYS
1	M	707	LYS
1	N	707	LYS
1	O	707	LYS
1	P	707	LYS
1	Q	707	LYS
1	R	707	LYS
1	S	707	LYS
1	T	707	LYS
1	U	707	LYS
1	V	707	LYS
1	W	707	LYS
1	X	707	LYS
1	Y	707	LYS
1	Z	707	LYS
1	1	707	LYS
1	2	707	LYS
1	3	707	LYS
1	4	707	LYS
1	5	707	LYS
1	6	707	LYS
1	a	707	LYS
1	b	707	LYS
1	c	707	LYS
1	d	707	LYS
1	e	707	LYS
1	f	707	LYS
1	g	707	LYS
1	h	707	LYS
1	i	707	LYS
1	j	707	LYS
1	k	707	LYS
1	l	707	LYS
1	m	707	LYS
1	n	707	LYS
1	o	707	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	p	707	LYS
1	q	707	LYS
1	r	707	LYS
1	s	707	LYS
1	t	707	LYS
1	u	707	LYS
1	v	707	LYS
1	w	707	LYS
1	x	707	LYS
1	y	707	LYS
1	z	707	LYS
1	7	707	LYS
1	8	707	LYS

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	453/453 (100%)	452 (100%)	1 (0%)	93	98
1	2	453/453 (100%)	452 (100%)	1 (0%)	93	98
1	3	453/453 (100%)	452 (100%)	1 (0%)	93	98
1	4	453/453 (100%)	452 (100%)	1 (0%)	93	98
1	5	453/453 (100%)	452 (100%)	1 (0%)	93	98
1	6	453/453 (100%)	452 (100%)	1 (0%)	93	98
1	7	453/453 (100%)	452 (100%)	1 (0%)	93	98
1	8	453/453 (100%)	452 (100%)	1 (0%)	93	98
1	A	453/453 (100%)	452 (100%)	1 (0%)	93	98
1	B	453/453 (100%)	452 (100%)	1 (0%)	93	98
1	C	453/453 (100%)	452 (100%)	1 (0%)	93	98
1	D	453/453 (100%)	452 (100%)	1 (0%)	93	98
1	E	453/453 (100%)	452 (100%)	1 (0%)	93	98
1	F	453/453 (100%)	452 (100%)	1 (0%)	93	98

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	453/453 (100%)	452 (100%)	1 (0%)	93	98
1	H	453/453 (100%)	452 (100%)	1 (0%)	93	98
1	I	453/453 (100%)	452 (100%)	1 (0%)	93	98
1	J	453/453 (100%)	452 (100%)	1 (0%)	93	98
1	K	453/453 (100%)	452 (100%)	1 (0%)	93	98
1	L	453/453 (100%)	452 (100%)	1 (0%)	93	98
1	M	453/453 (100%)	452 (100%)	1 (0%)	93	98
1	N	453/453 (100%)	452 (100%)	1 (0%)	93	98
1	O	453/453 (100%)	452 (100%)	1 (0%)	93	98
1	P	453/453 (100%)	452 (100%)	1 (0%)	93	98
1	Q	453/453 (100%)	452 (100%)	1 (0%)	93	98
1	R	453/453 (100%)	452 (100%)	1 (0%)	93	98
1	S	453/453 (100%)	452 (100%)	1 (0%)	93	98
1	T	453/453 (100%)	452 (100%)	1 (0%)	93	98
1	U	453/453 (100%)	452 (100%)	1 (0%)	93	98
1	V	453/453 (100%)	452 (100%)	1 (0%)	93	98
1	W	453/453 (100%)	452 (100%)	1 (0%)	93	98
1	X	453/453 (100%)	452 (100%)	1 (0%)	93	98
1	Y	453/453 (100%)	452 (100%)	1 (0%)	93	98
1	Z	453/453 (100%)	452 (100%)	1 (0%)	93	98
1	a	453/453 (100%)	452 (100%)	1 (0%)	93	98
1	b	453/453 (100%)	452 (100%)	1 (0%)	93	98
1	c	453/453 (100%)	452 (100%)	1 (0%)	93	98
1	d	453/453 (100%)	452 (100%)	1 (0%)	93	98
1	e	453/453 (100%)	452 (100%)	1 (0%)	93	98
1	f	453/453 (100%)	452 (100%)	1 (0%)	93	98
1	g	453/453 (100%)	452 (100%)	1 (0%)	93	98
1	h	453/453 (100%)	452 (100%)	1 (0%)	93	98
1	i	453/453 (100%)	452 (100%)	1 (0%)	93	98
1	j	453/453 (100%)	452 (100%)	1 (0%)	93	98
1	k	453/453 (100%)	452 (100%)	1 (0%)	93	98

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	l	453/453 (100%)	452 (100%)	1 (0%)	93	98
1	m	453/453 (100%)	452 (100%)	1 (0%)	93	98
1	n	453/453 (100%)	452 (100%)	1 (0%)	93	98
1	o	453/453 (100%)	452 (100%)	1 (0%)	93	98
1	p	453/453 (100%)	452 (100%)	1 (0%)	93	98
1	q	453/453 (100%)	452 (100%)	1 (0%)	93	98
1	r	453/453 (100%)	452 (100%)	1 (0%)	93	98
1	s	453/453 (100%)	452 (100%)	1 (0%)	93	98
1	t	453/453 (100%)	452 (100%)	1 (0%)	93	98
1	u	453/453 (100%)	452 (100%)	1 (0%)	93	98
1	v	453/453 (100%)	452 (100%)	1 (0%)	93	98
1	w	453/453 (100%)	452 (100%)	1 (0%)	93	98
1	x	453/453 (100%)	452 (100%)	1 (0%)	93	98
1	y	453/453 (100%)	452 (100%)	1 (0%)	93	98
1	z	453/453 (100%)	452 (100%)	1 (0%)	93	98
All	All	27180/27180 (100%)	27120 (100%)	60 (0%)	93	98

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	436	MET
1	B	436	MET
1	C	436	MET
1	D	436	MET
1	E	436	MET
1	F	436	MET
1	G	436	MET
1	H	436	MET
1	I	436	MET
1	J	436	MET
1	K	436	MET
1	L	436	MET
1	M	436	MET
1	N	436	MET
1	O	436	MET
1	P	436	MET
1	Q	436	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	R	436	MET
1	S	436	MET
1	T	436	MET
1	U	436	MET
1	V	436	MET
1	W	436	MET
1	X	436	MET
1	Y	436	MET
1	Z	436	MET
1	1	436	MET
1	2	436	MET
1	3	436	MET
1	4	436	MET
1	5	436	MET
1	6	436	MET
1	a	436	MET
1	b	436	MET
1	c	436	MET
1	d	436	MET
1	e	436	MET
1	f	436	MET
1	g	436	MET
1	h	436	MET
1	i	436	MET
1	j	436	MET
1	k	436	MET
1	l	436	MET
1	m	436	MET
1	n	436	MET
1	o	436	MET
1	p	436	MET
1	q	436	MET
1	r	436	MET
1	s	436	MET
1	t	436	MET
1	u	436	MET
1	v	436	MET
1	w	436	MET
1	x	436	MET
1	y	436	MET
1	z	436	MET
1	7	436	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	8	436	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (867) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	229	HIS
1	A	253	ASN
1	A	290	HIS
1	A	337	ASN
1	A	423	HIS
1	A	428	HIS
1	A	497	ASN
1	A	579	GLN
1	A	585	GLN
1	A	624	HIS
1	A	646	GLN
1	A	651	ASN
1	A	673	GLN
1	A	700	GLN
1	B	229	HIS
1	B	253	ASN
1	B	290	HIS
1	B	337	ASN
1	B	343	GLN
1	B	423	HIS
1	B	428	HIS
1	B	497	ASN
1	B	579	GLN
1	B	585	GLN
1	B	624	HIS
1	B	646	GLN
1	B	651	ASN
1	B	673	GLN
1	B	700	GLN
1	C	229	HIS
1	C	253	ASN
1	C	290	HIS
1	C	337	ASN
1	C	343	GLN
1	C	423	HIS
1	C	428	HIS
1	C	497	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	579	GLN
1	C	585	GLN
1	C	624	HIS
1	C	646	GLN
1	C	651	ASN
1	C	673	GLN
1	C	700	GLN
1	D	229	HIS
1	D	253	ASN
1	D	290	HIS
1	D	337	ASN
1	D	343	GLN
1	D	423	HIS
1	D	428	HIS
1	D	497	ASN
1	D	579	GLN
1	D	585	GLN
1	D	624	HIS
1	D	646	GLN
1	D	651	ASN
1	D	673	GLN
1	D	700	GLN
1	E	229	HIS
1	E	253	ASN
1	E	290	HIS
1	E	337	ASN
1	E	423	HIS
1	E	428	HIS
1	E	497	ASN
1	E	579	GLN
1	E	585	GLN
1	E	624	HIS
1	E	646	GLN
1	E	673	GLN
1	E	700	GLN
1	F	229	HIS
1	F	253	ASN
1	F	290	HIS
1	F	337	ASN
1	F	343	GLN
1	F	423	HIS
1	F	428	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	497	ASN
1	F	579	GLN
1	F	585	GLN
1	F	624	HIS
1	F	646	GLN
1	F	651	ASN
1	F	673	GLN
1	F	700	GLN
1	G	229	HIS
1	G	253	ASN
1	G	290	HIS
1	G	337	ASN
1	G	343	GLN
1	G	423	HIS
1	G	428	HIS
1	G	497	ASN
1	G	579	GLN
1	G	585	GLN
1	G	624	HIS
1	G	646	GLN
1	G	673	GLN
1	G	700	GLN
1	H	229	HIS
1	H	253	ASN
1	H	290	HIS
1	H	337	ASN
1	H	343	GLN
1	H	423	HIS
1	H	428	HIS
1	H	497	ASN
1	H	579	GLN
1	H	585	GLN
1	H	624	HIS
1	H	646	GLN
1	H	673	GLN
1	H	700	GLN
1	I	229	HIS
1	I	253	ASN
1	I	290	HIS
1	I	337	ASN
1	I	343	GLN
1	I	423	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	428	HIS
1	I	497	ASN
1	I	579	GLN
1	I	585	GLN
1	I	624	HIS
1	I	646	GLN
1	I	651	ASN
1	I	673	GLN
1	I	700	GLN
1	J	229	HIS
1	J	253	ASN
1	J	290	HIS
1	J	337	ASN
1	J	343	GLN
1	J	423	HIS
1	J	428	HIS
1	J	497	ASN
1	J	579	GLN
1	J	585	GLN
1	J	624	HIS
1	J	646	GLN
1	J	651	ASN
1	J	673	GLN
1	J	700	GLN
1	K	229	HIS
1	K	253	ASN
1	K	290	HIS
1	K	337	ASN
1	K	343	GLN
1	K	423	HIS
1	K	428	HIS
1	K	497	ASN
1	K	579	GLN
1	K	585	GLN
1	K	624	HIS
1	K	646	GLN
1	K	651	ASN
1	K	673	GLN
1	K	700	GLN
1	L	229	HIS
1	L	253	ASN
1	L	290	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L	337	ASN
1	L	343	GLN
1	L	423	HIS
1	L	428	HIS
1	L	497	ASN
1	L	579	GLN
1	L	585	GLN
1	L	624	HIS
1	L	646	GLN
1	L	651	ASN
1	L	673	GLN
1	L	700	GLN
1	M	229	HIS
1	M	253	ASN
1	M	290	HIS
1	M	337	ASN
1	M	423	HIS
1	M	428	HIS
1	M	497	ASN
1	M	579	GLN
1	M	585	GLN
1	M	624	HIS
1	M	646	GLN
1	M	651	ASN
1	M	673	GLN
1	M	700	GLN
1	N	229	HIS
1	N	253	ASN
1	N	290	HIS
1	N	337	ASN
1	N	423	HIS
1	N	428	HIS
1	N	497	ASN
1	N	579	GLN
1	N	585	GLN
1	N	624	HIS
1	N	646	GLN
1	N	673	GLN
1	N	700	GLN
1	O	229	HIS
1	O	253	ASN
1	O	290	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	O	337	ASN
1	O	423	HIS
1	O	428	HIS
1	O	497	ASN
1	O	579	GLN
1	O	585	GLN
1	O	624	HIS
1	O	646	GLN
1	O	651	ASN
1	O	673	GLN
1	O	700	GLN
1	P	229	HIS
1	P	253	ASN
1	P	290	HIS
1	P	337	ASN
1	P	423	HIS
1	P	428	HIS
1	P	497	ASN
1	P	579	GLN
1	P	585	GLN
1	P	624	HIS
1	P	646	GLN
1	P	651	ASN
1	P	673	GLN
1	P	700	GLN
1	Q	229	HIS
1	Q	253	ASN
1	Q	290	HIS
1	Q	337	ASN
1	Q	343	GLN
1	Q	423	HIS
1	Q	428	HIS
1	Q	497	ASN
1	Q	579	GLN
1	Q	585	GLN
1	Q	624	HIS
1	Q	646	GLN
1	Q	651	ASN
1	Q	673	GLN
1	Q	700	GLN
1	R	229	HIS
1	R	253	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	R	290	HIS
1	R	337	ASN
1	R	423	HIS
1	R	428	HIS
1	R	497	ASN
1	R	579	GLN
1	R	585	GLN
1	R	624	HIS
1	R	646	GLN
1	R	673	GLN
1	R	700	GLN
1	S	229	HIS
1	S	253	ASN
1	S	290	HIS
1	S	337	ASN
1	S	423	HIS
1	S	428	HIS
1	S	497	ASN
1	S	579	GLN
1	S	585	GLN
1	S	624	HIS
1	S	646	GLN
1	S	651	ASN
1	S	673	GLN
1	S	700	GLN
1	T	229	HIS
1	T	253	ASN
1	T	290	HIS
1	T	337	ASN
1	T	423	HIS
1	T	428	HIS
1	T	497	ASN
1	T	579	GLN
1	T	585	GLN
1	T	624	HIS
1	T	646	GLN
1	T	651	ASN
1	T	673	GLN
1	T	700	GLN
1	U	229	HIS
1	U	253	ASN
1	U	290	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	U	337	ASN
1	U	343	GLN
1	U	423	HIS
1	U	428	HIS
1	U	497	ASN
1	U	579	GLN
1	U	585	GLN
1	U	624	HIS
1	U	646	GLN
1	U	651	ASN
1	U	673	GLN
1	U	700	GLN
1	V	229	HIS
1	V	253	ASN
1	V	290	HIS
1	V	337	ASN
1	V	423	HIS
1	V	428	HIS
1	V	497	ASN
1	V	579	GLN
1	V	585	GLN
1	V	624	HIS
1	V	646	GLN
1	V	651	ASN
1	V	673	GLN
1	V	700	GLN
1	W	229	HIS
1	W	253	ASN
1	W	290	HIS
1	W	337	ASN
1	W	423	HIS
1	W	428	HIS
1	W	497	ASN
1	W	579	GLN
1	W	585	GLN
1	W	624	HIS
1	W	646	GLN
1	W	651	ASN
1	W	673	GLN
1	W	700	GLN
1	X	229	HIS
1	X	253	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	X	290	HIS
1	X	337	ASN
1	X	343	GLN
1	X	423	HIS
1	X	428	HIS
1	X	497	ASN
1	X	579	GLN
1	X	585	GLN
1	X	624	HIS
1	X	646	GLN
1	X	651	ASN
1	X	673	GLN
1	X	700	GLN
1	Y	229	HIS
1	Y	253	ASN
1	Y	290	HIS
1	Y	337	ASN
1	Y	423	HIS
1	Y	428	HIS
1	Y	497	ASN
1	Y	579	GLN
1	Y	585	GLN
1	Y	624	HIS
1	Y	646	GLN
1	Y	651	ASN
1	Y	673	GLN
1	Y	700	GLN
1	Z	229	HIS
1	Z	253	ASN
1	Z	290	HIS
1	Z	337	ASN
1	Z	343	GLN
1	Z	423	HIS
1	Z	428	HIS
1	Z	497	ASN
1	Z	579	GLN
1	Z	585	GLN
1	Z	624	HIS
1	Z	646	GLN
1	Z	651	ASN
1	Z	673	GLN
1	Z	700	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	229	HIS
1	1	253	ASN
1	1	290	HIS
1	1	337	ASN
1	1	343	GLN
1	1	423	HIS
1	1	428	HIS
1	1	497	ASN
1	1	579	GLN
1	1	585	GLN
1	1	624	HIS
1	1	646	GLN
1	1	651	ASN
1	1	673	GLN
1	1	700	GLN
1	2	229	HIS
1	2	290	HIS
1	2	337	ASN
1	2	343	GLN
1	2	376	GLN
1	2	423	HIS
1	2	428	HIS
1	2	497	ASN
1	2	579	GLN
1	2	585	GLN
1	2	624	HIS
1	2	646	GLN
1	2	651	ASN
1	2	673	GLN
1	2	700	GLN
1	3	229	HIS
1	3	253	ASN
1	3	290	HIS
1	3	337	ASN
1	3	343	GLN
1	3	423	HIS
1	3	428	HIS
1	3	497	ASN
1	3	579	GLN
1	3	585	GLN
1	3	624	HIS
1	3	646	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	3	651	ASN
1	3	673	GLN
1	3	700	GLN
1	4	229	HIS
1	4	253	ASN
1	4	290	HIS
1	4	337	ASN
1	4	343	GLN
1	4	423	HIS
1	4	428	HIS
1	4	497	ASN
1	4	579	GLN
1	4	585	GLN
1	4	624	HIS
1	4	646	GLN
1	4	651	ASN
1	4	673	GLN
1	4	700	GLN
1	5	229	HIS
1	5	253	ASN
1	5	290	HIS
1	5	337	ASN
1	5	423	HIS
1	5	428	HIS
1	5	497	ASN
1	5	579	GLN
1	5	585	GLN
1	5	624	HIS
1	5	646	GLN
1	5	651	ASN
1	5	673	GLN
1	5	700	GLN
1	6	229	HIS
1	6	253	ASN
1	6	290	HIS
1	6	337	ASN
1	6	423	HIS
1	6	428	HIS
1	6	497	ASN
1	6	579	GLN
1	6	585	GLN
1	6	624	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	6	646	GLN
1	6	673	GLN
1	6	700	GLN
1	a	229	HIS
1	a	253	ASN
1	a	290	HIS
1	a	337	ASN
1	a	343	GLN
1	a	423	HIS
1	a	428	HIS
1	a	497	ASN
1	a	579	GLN
1	a	585	GLN
1	a	624	HIS
1	a	646	GLN
1	a	651	ASN
1	a	673	GLN
1	a	700	GLN
1	b	229	HIS
1	b	253	ASN
1	b	290	HIS
1	b	337	ASN
1	b	423	HIS
1	b	428	HIS
1	b	497	ASN
1	b	579	GLN
1	b	585	GLN
1	b	624	HIS
1	b	646	GLN
1	b	651	ASN
1	b	673	GLN
1	b	700	GLN
1	c	229	HIS
1	c	253	ASN
1	c	290	HIS
1	c	337	ASN
1	c	343	GLN
1	c	423	HIS
1	c	428	HIS
1	c	497	ASN
1	c	579	GLN
1	c	585	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	c	624	HIS
1	c	646	GLN
1	c	651	ASN
1	c	673	GLN
1	c	700	GLN
1	d	229	HIS
1	d	253	ASN
1	d	290	HIS
1	d	337	ASN
1	d	343	GLN
1	d	423	HIS
1	d	428	HIS
1	d	497	ASN
1	d	579	GLN
1	d	585	GLN
1	d	624	HIS
1	d	646	GLN
1	d	651	ASN
1	d	673	GLN
1	d	700	GLN
1	e	229	HIS
1	e	253	ASN
1	e	290	HIS
1	e	337	ASN
1	e	423	HIS
1	e	428	HIS
1	e	497	ASN
1	e	579	GLN
1	e	585	GLN
1	e	624	HIS
1	e	646	GLN
1	e	673	GLN
1	e	700	GLN
1	f	229	HIS
1	f	253	ASN
1	f	290	HIS
1	f	337	ASN
1	f	423	HIS
1	f	428	HIS
1	f	497	ASN
1	f	579	GLN
1	f	585	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	f	624	HIS
1	f	646	GLN
1	f	673	GLN
1	f	700	GLN
1	g	229	HIS
1	g	253	ASN
1	g	290	HIS
1	g	337	ASN
1	g	343	GLN
1	g	423	HIS
1	g	428	HIS
1	g	497	ASN
1	g	579	GLN
1	g	585	GLN
1	g	624	HIS
1	g	646	GLN
1	g	651	ASN
1	g	673	GLN
1	g	700	GLN
1	h	229	HIS
1	h	253	ASN
1	h	290	HIS
1	h	337	ASN
1	h	423	HIS
1	h	428	HIS
1	h	497	ASN
1	h	579	GLN
1	h	585	GLN
1	h	624	HIS
1	h	646	GLN
1	h	651	ASN
1	h	673	GLN
1	h	700	GLN
1	i	229	HIS
1	i	253	ASN
1	i	290	HIS
1	i	337	ASN
1	i	343	GLN
1	i	423	HIS
1	i	428	HIS
1	i	497	ASN
1	i	579	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	i	585	GLN
1	i	624	HIS
1	i	646	GLN
1	i	651	ASN
1	i	673	GLN
1	i	700	GLN
1	j	229	HIS
1	j	253	ASN
1	j	290	HIS
1	j	337	ASN
1	j	343	GLN
1	j	423	HIS
1	j	428	HIS
1	j	497	ASN
1	j	579	GLN
1	j	585	GLN
1	j	624	HIS
1	j	646	GLN
1	j	651	ASN
1	j	673	GLN
1	j	700	GLN
1	k	229	HIS
1	k	253	ASN
1	k	290	HIS
1	k	337	ASN
1	k	343	GLN
1	k	423	HIS
1	k	428	HIS
1	k	497	ASN
1	k	579	GLN
1	k	585	GLN
1	k	624	HIS
1	k	646	GLN
1	k	673	GLN
1	k	700	GLN
1	l	229	HIS
1	l	253	ASN
1	l	290	HIS
1	l	337	ASN
1	l	423	HIS
1	l	428	HIS
1	l	497	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	l	579	GLN
1	l	585	GLN
1	l	624	HIS
1	l	646	GLN
1	l	651	ASN
1	l	673	GLN
1	l	700	GLN
1	m	229	HIS
1	m	253	ASN
1	m	290	HIS
1	m	337	ASN
1	m	423	HIS
1	m	428	HIS
1	m	497	ASN
1	m	579	GLN
1	m	585	GLN
1	m	624	HIS
1	m	646	GLN
1	m	651	ASN
1	m	673	GLN
1	m	700	GLN
1	n	229	HIS
1	n	253	ASN
1	n	290	HIS
1	n	337	ASN
1	n	343	GLN
1	n	423	HIS
1	n	428	HIS
1	n	497	ASN
1	n	579	GLN
1	n	585	GLN
1	n	624	HIS
1	n	646	GLN
1	n	651	ASN
1	n	673	GLN
1	n	700	GLN
1	o	229	HIS
1	o	253	ASN
1	o	290	HIS
1	o	337	ASN
1	o	343	GLN
1	o	423	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	o	428	HIS
1	o	497	ASN
1	o	579	GLN
1	o	585	GLN
1	o	624	HIS
1	o	646	GLN
1	o	651	ASN
1	o	673	GLN
1	o	700	GLN
1	p	229	HIS
1	p	253	ASN
1	p	290	HIS
1	p	337	ASN
1	p	343	GLN
1	p	423	HIS
1	p	428	HIS
1	p	497	ASN
1	p	579	GLN
1	p	585	GLN
1	p	624	HIS
1	p	646	GLN
1	p	651	ASN
1	p	673	GLN
1	p	700	GLN
1	q	229	HIS
1	q	253	ASN
1	q	290	HIS
1	q	337	ASN
1	q	343	GLN
1	q	423	HIS
1	q	428	HIS
1	q	497	ASN
1	q	579	GLN
1	q	585	GLN
1	q	624	HIS
1	q	646	GLN
1	q	673	GLN
1	q	700	GLN
1	r	229	HIS
1	r	253	ASN
1	r	290	HIS
1	r	337	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	r	343	GLN
1	r	423	HIS
1	r	428	HIS
1	r	497	ASN
1	r	579	GLN
1	r	585	GLN
1	r	624	HIS
1	r	646	GLN
1	r	673	GLN
1	r	700	GLN
1	s	229	HIS
1	s	253	ASN
1	s	290	HIS
1	s	337	ASN
1	s	343	GLN
1	s	423	HIS
1	s	428	HIS
1	s	497	ASN
1	s	579	GLN
1	s	585	GLN
1	s	624	HIS
1	s	646	GLN
1	s	673	GLN
1	s	700	GLN
1	t	229	HIS
1	t	253	ASN
1	t	290	HIS
1	t	337	ASN
1	t	423	HIS
1	t	428	HIS
1	t	497	ASN
1	t	579	GLN
1	t	585	GLN
1	t	624	HIS
1	t	646	GLN
1	t	651	ASN
1	t	673	GLN
1	t	700	GLN
1	u	229	HIS
1	u	253	ASN
1	u	290	HIS
1	u	337	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	u	343	GLN
1	u	423	HIS
1	u	428	HIS
1	u	497	ASN
1	u	579	GLN
1	u	585	GLN
1	u	624	HIS
1	u	646	GLN
1	u	673	GLN
1	u	700	GLN
1	v	229	HIS
1	v	253	ASN
1	v	290	HIS
1	v	337	ASN
1	v	343	GLN
1	v	376	GLN
1	v	423	HIS
1	v	428	HIS
1	v	497	ASN
1	v	579	GLN
1	v	585	GLN
1	v	624	HIS
1	v	646	GLN
1	v	651	ASN
1	v	673	GLN
1	v	700	GLN
1	w	229	HIS
1	w	253	ASN
1	w	290	HIS
1	w	337	ASN
1	w	343	GLN
1	w	423	HIS
1	w	428	HIS
1	w	497	ASN
1	w	579	GLN
1	w	585	GLN
1	w	624	HIS
1	w	646	GLN
1	w	651	ASN
1	w	673	GLN
1	w	700	GLN
1	x	229	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	x	253	ASN
1	x	290	HIS
1	x	337	ASN
1	x	343	GLN
1	x	423	HIS
1	x	428	HIS
1	x	497	ASN
1	x	579	GLN
1	x	585	GLN
1	x	624	HIS
1	x	646	GLN
1	x	651	ASN
1	x	673	GLN
1	x	700	GLN
1	y	229	HIS
1	y	253	ASN
1	y	290	HIS
1	y	337	ASN
1	y	343	GLN
1	y	423	HIS
1	y	428	HIS
1	y	497	ASN
1	y	579	GLN
1	y	585	GLN
1	y	624	HIS
1	y	646	GLN
1	y	651	ASN
1	y	673	GLN
1	y	700	GLN
1	z	229	HIS
1	z	253	ASN
1	z	290	HIS
1	z	337	ASN
1	z	343	GLN
1	z	423	HIS
1	z	428	HIS
1	z	497	ASN
1	z	579	GLN
1	z	585	GLN
1	z	624	HIS
1	z	646	GLN
1	z	651	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	z	673	GLN
1	z	700	GLN
1	7	229	HIS
1	7	253	ASN
1	7	290	HIS
1	7	337	ASN
1	7	343	GLN
1	7	423	HIS
1	7	428	HIS
1	7	497	ASN
1	7	579	GLN
1	7	585	GLN
1	7	624	HIS
1	7	646	GLN
1	7	651	ASN
1	7	673	GLN
1	7	700	GLN
1	8	229	HIS
1	8	253	ASN
1	8	290	HIS
1	8	337	ASN
1	8	343	GLN
1	8	423	HIS
1	8	428	HIS
1	8	497	ASN
1	8	579	GLN
1	8	585	GLN
1	8	624	HIS
1	8	646	GLN
1	8	651	ASN
1	8	673	GLN
1	8	700	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1
1	B	1
1	C	1
1	D	1
1	E	1
1	F	1
1	G	1
1	H	1
1	I	1
1	J	1
1	K	1
1	L	1
1	M	1
1	N	1
1	O	1
1	P	1
1	Q	1
1	R	1
1	S	1
1	T	1
1	U	1
1	V	1
1	W	1
1	X	1
1	Y	1

Continued on next page...

Continued from previous page...

Mol	Chain	Number of breaks
1	Z	1
1	1	1
1	2	1
1	3	1
1	4	1
1	5	1
1	6	1
1	a	1
1	b	1
1	c	1
1	d	1
1	e	1
1	f	1
1	g	1
1	h	1
1	i	1
1	j	1
1	k	1
1	l	1
1	m	1
1	n	1
1	o	1
1	p	1
1	q	1
1	r	1
1	s	1
1	t	1
1	u	1
1	v	1
1	w	1
1	x	1
1	y	1
1	z	1
1	7	1
1	8	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	400:PHE	C	401:PRO	N	1.15
1	B	400:PHE	C	401:PRO	N	1.15
1	C	400:PHE	C	401:PRO	N	1.15
1	D	400:PHE	C	401:PRO	N	1.15

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	400:PHE	C	401:PRO	N	1.15
1	F	400:PHE	C	401:PRO	N	1.15
1	G	400:PHE	C	401:PRO	N	1.15
1	H	400:PHE	C	401:PRO	N	1.15
1	I	400:PHE	C	401:PRO	N	1.15
1	J	400:PHE	C	401:PRO	N	1.15
1	K	400:PHE	C	401:PRO	N	1.15
1	L	400:PHE	C	401:PRO	N	1.15
1	M	400:PHE	C	401:PRO	N	1.15
1	N	400:PHE	C	401:PRO	N	1.15
1	O	400:PHE	C	401:PRO	N	1.15
1	P	400:PHE	C	401:PRO	N	1.15
1	Q	400:PHE	C	401:PRO	N	1.15
1	R	400:PHE	C	401:PRO	N	1.15
1	S	400:PHE	C	401:PRO	N	1.15
1	T	400:PHE	C	401:PRO	N	1.15
1	U	400:PHE	C	401:PRO	N	1.15
1	V	400:PHE	C	401:PRO	N	1.15
1	W	400:PHE	C	401:PRO	N	1.15
1	X	400:PHE	C	401:PRO	N	1.15
1	Y	400:PHE	C	401:PRO	N	1.15
1	Z	400:PHE	C	401:PRO	N	1.15
1	1	400:PHE	C	401:PRO	N	1.15
1	2	400:PHE	C	401:PRO	N	1.15
1	3	400:PHE	C	401:PRO	N	1.15
1	4	400:PHE	C	401:PRO	N	1.15
1	5	400:PHE	C	401:PRO	N	1.15
1	6	400:PHE	C	401:PRO	N	1.15
1	a	400:PHE	C	401:PRO	N	1.15
1	b	400:PHE	C	401:PRO	N	1.15
1	c	400:PHE	C	401:PRO	N	1.15
1	d	400:PHE	C	401:PRO	N	1.15
1	e	400:PHE	C	401:PRO	N	1.15
1	f	400:PHE	C	401:PRO	N	1.15
1	g	400:PHE	C	401:PRO	N	1.15
1	h	400:PHE	C	401:PRO	N	1.15
1	i	400:PHE	C	401:PRO	N	1.15
1	j	400:PHE	C	401:PRO	N	1.15
1	k	400:PHE	C	401:PRO	N	1.15
1	l	400:PHE	C	401:PRO	N	1.15
1	m	400:PHE	C	401:PRO	N	1.15
1	n	400:PHE	C	401:PRO	N	1.15

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	o	400:PHE	C	401:PRO	N	1.15
1	p	400:PHE	C	401:PRO	N	1.15
1	q	400:PHE	C	401:PRO	N	1.15
1	r	400:PHE	C	401:PRO	N	1.15
1	s	400:PHE	C	401:PRO	N	1.15
1	t	400:PHE	C	401:PRO	N	1.15
1	u	400:PHE	C	401:PRO	N	1.15
1	v	400:PHE	C	401:PRO	N	1.15
1	w	400:PHE	C	401:PRO	N	1.15
1	x	400:PHE	C	401:PRO	N	1.15
1	y	400:PHE	C	401:PRO	N	1.15
1	z	400:PHE	C	401:PRO	N	1.15
1	7	400:PHE	C	401:PRO	N	1.15
1	8	400:PHE	C	401:PRO	N	1.15

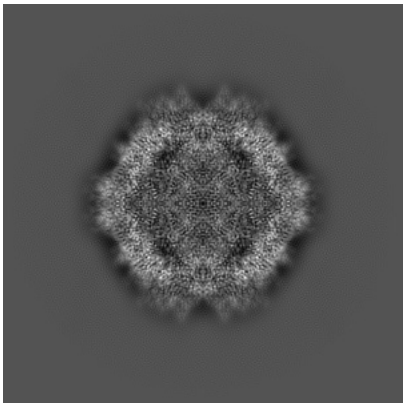
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-23993. These allow visual inspection of the internal detail of the map and identification of artifacts.

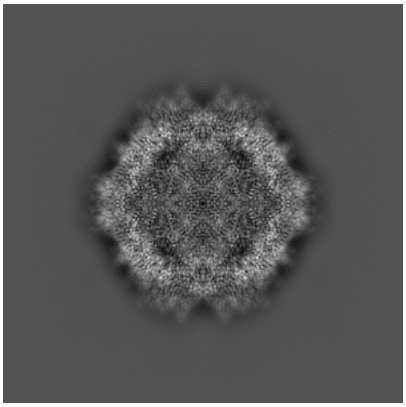
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

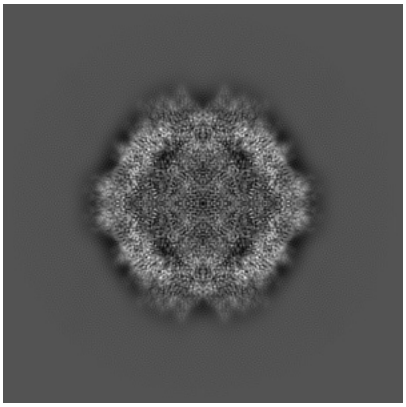
6.1.1 Primary map



X



Y

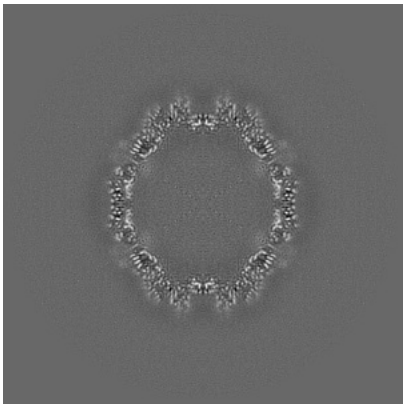


Z

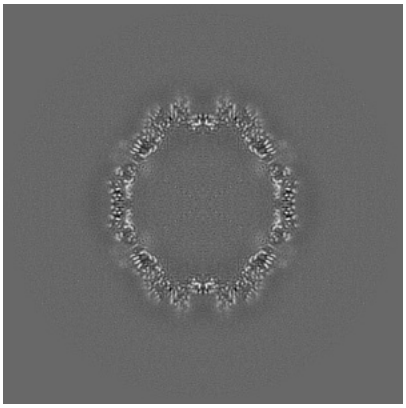
The images above show the map projected in three orthogonal directions.

6.2 Central slices

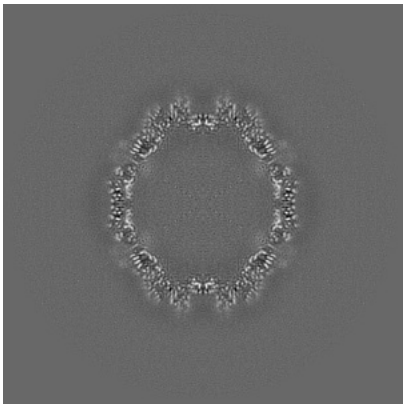
6.2.1 Primary map



X Index: 220



Y Index: 220

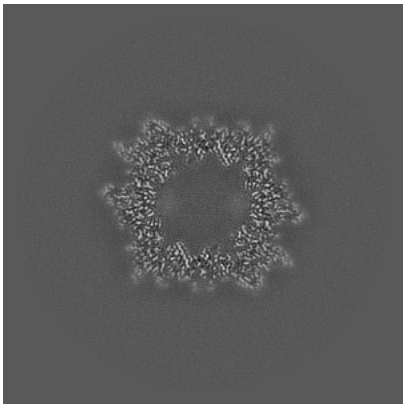


Z Index: 220

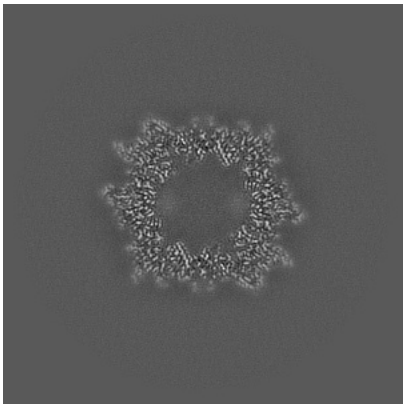
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

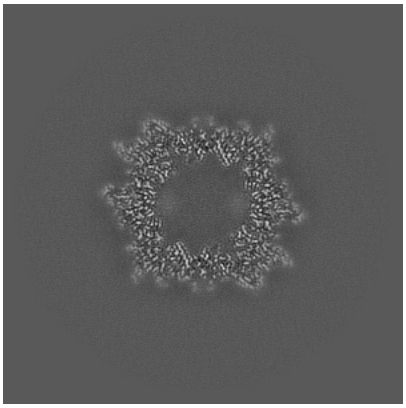
6.3.1 Primary map



X Index: 280



Y Index: 280

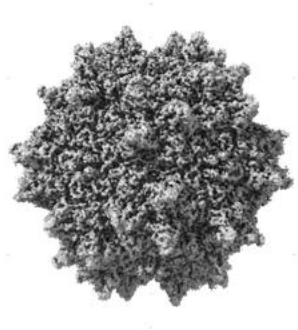


Z Index: 280

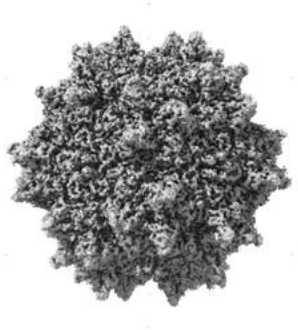
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

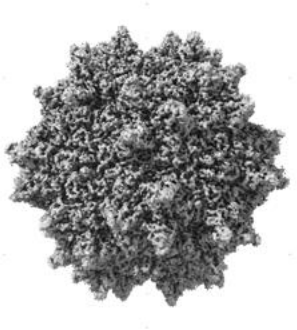
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

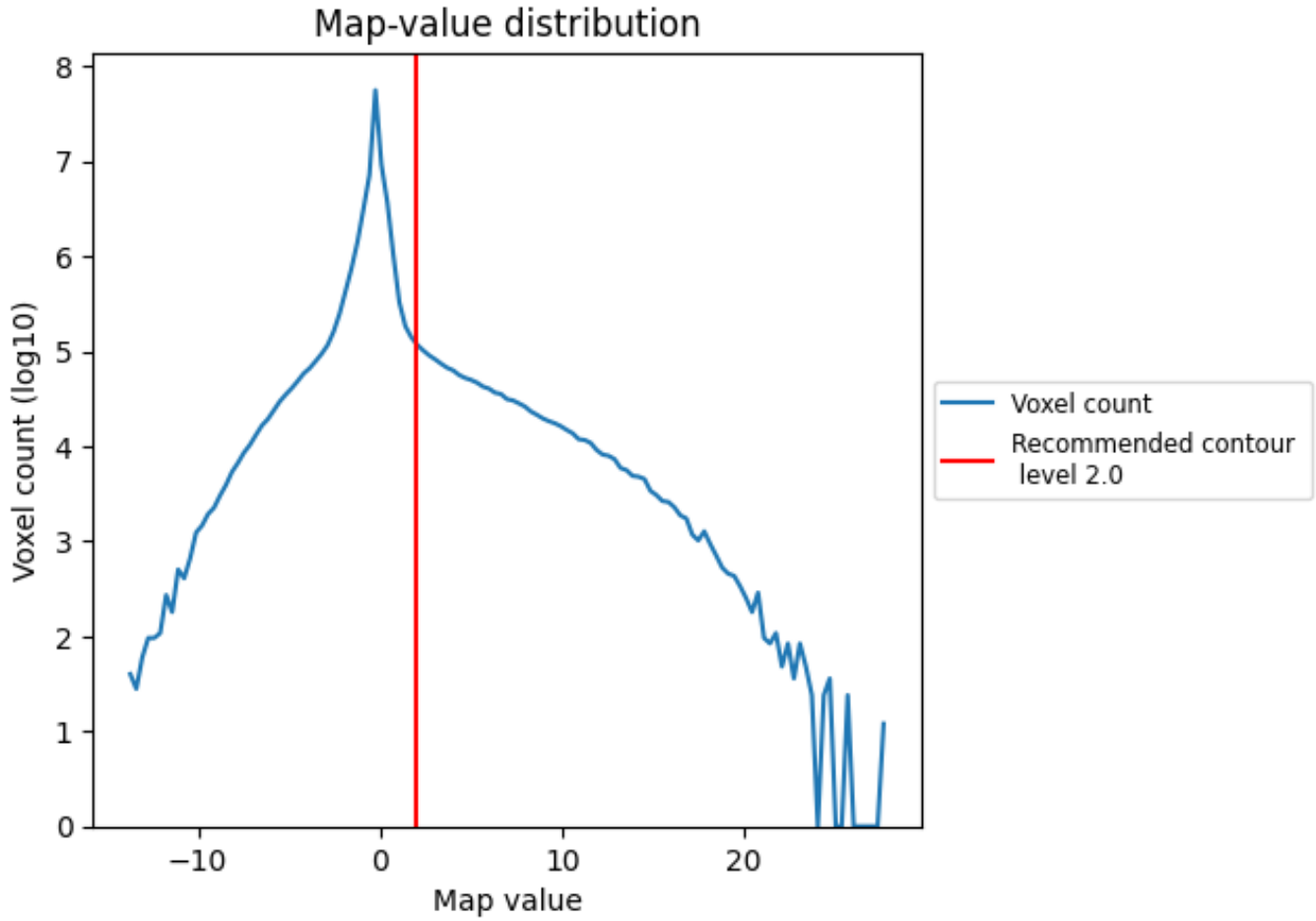
6.5 Mask visualisation (i)

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

7 Map analysis

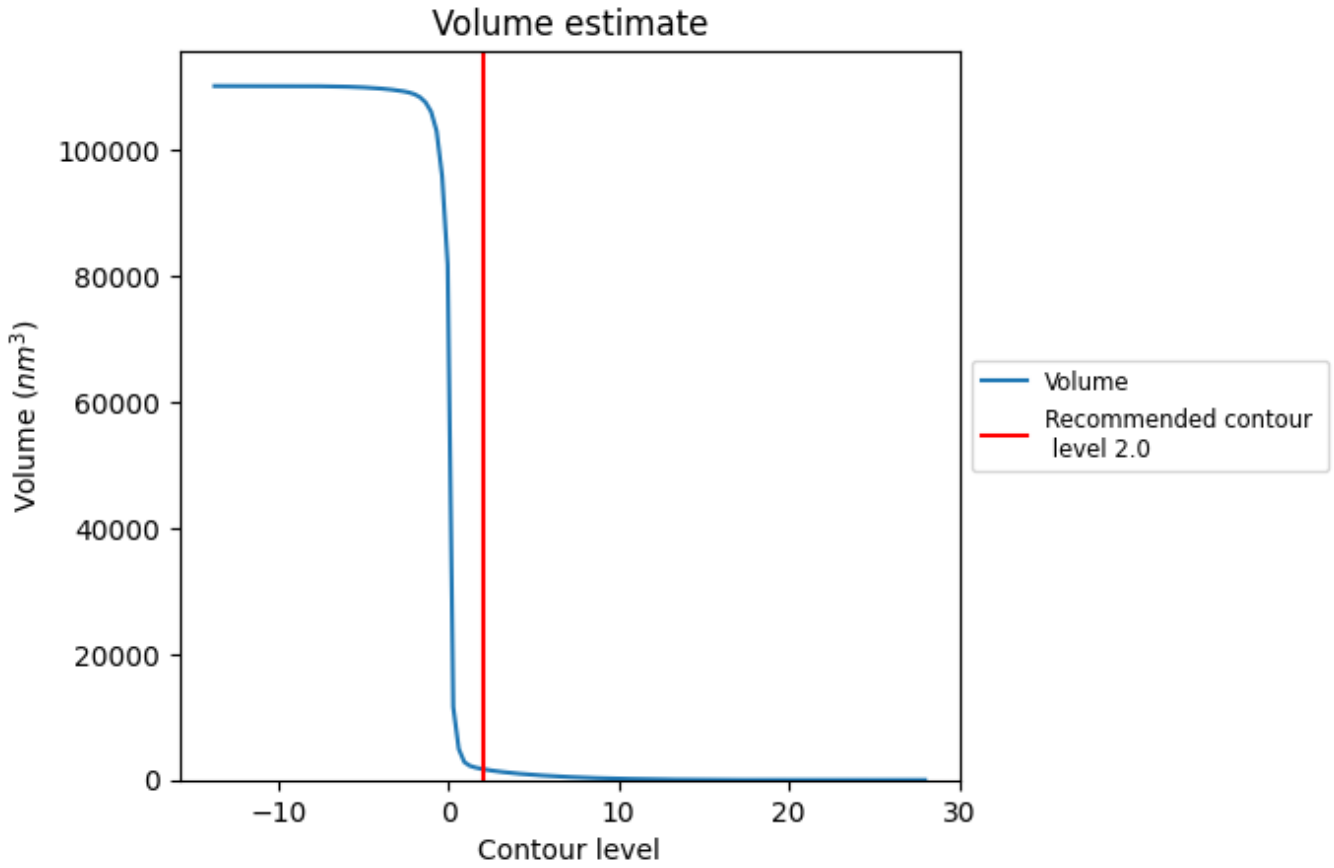
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

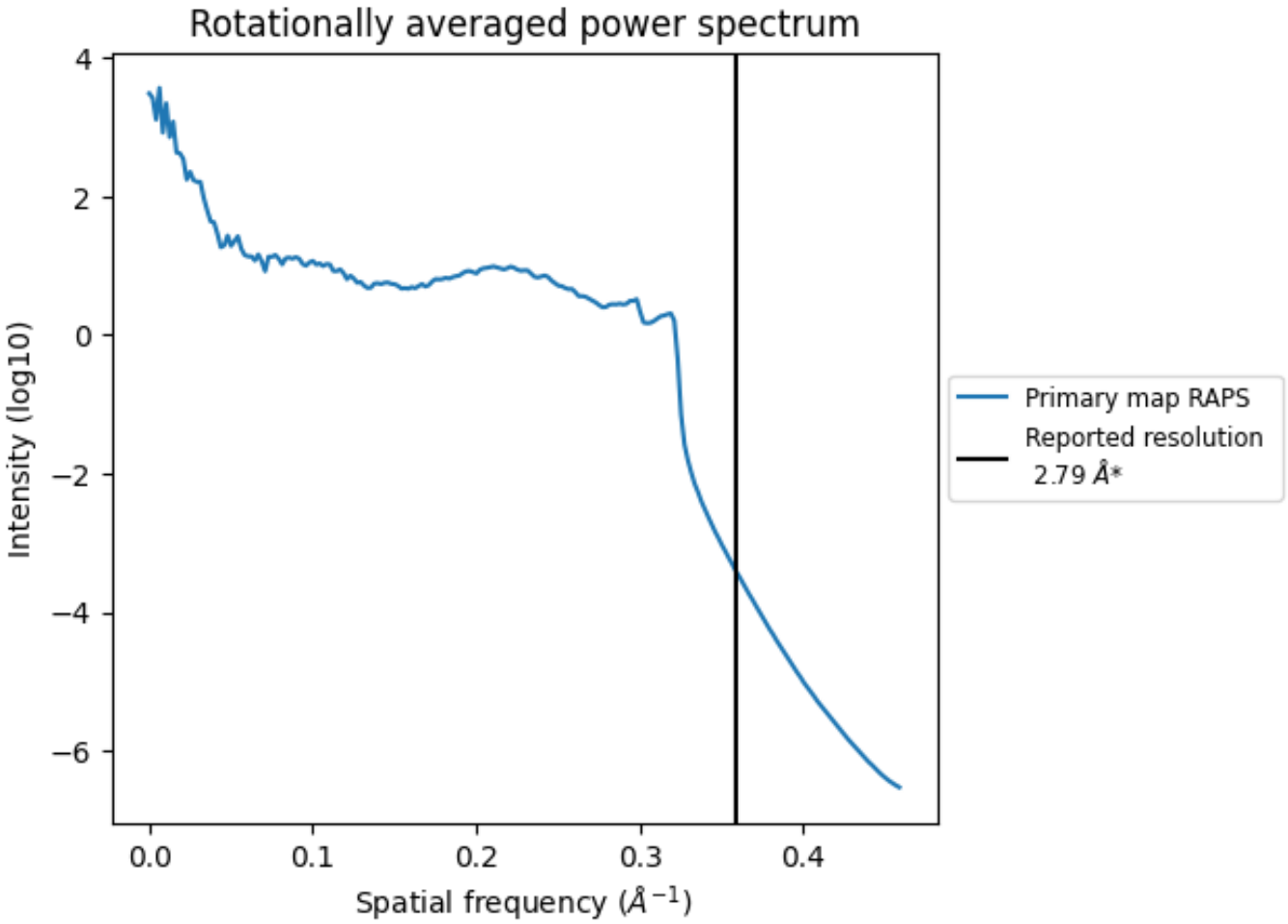
7.2 Volume estimate



The volume at the recommended contour level is 1737 nm^3; this corresponds to an approximate mass of 1569 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 0.358 Å^{-1}

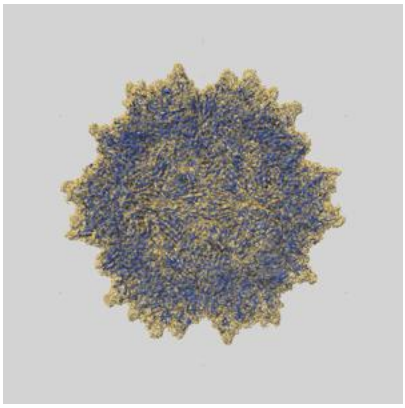
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

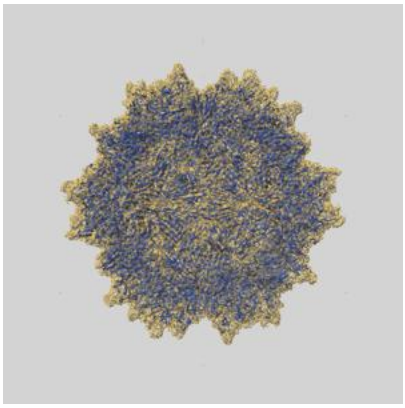
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-23993 and PDB model 7MTP. Per-residue inclusion information can be found in section 3 on page 10.

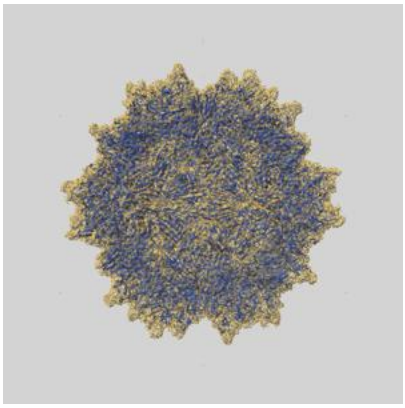
9.1 Map-model overlay



X



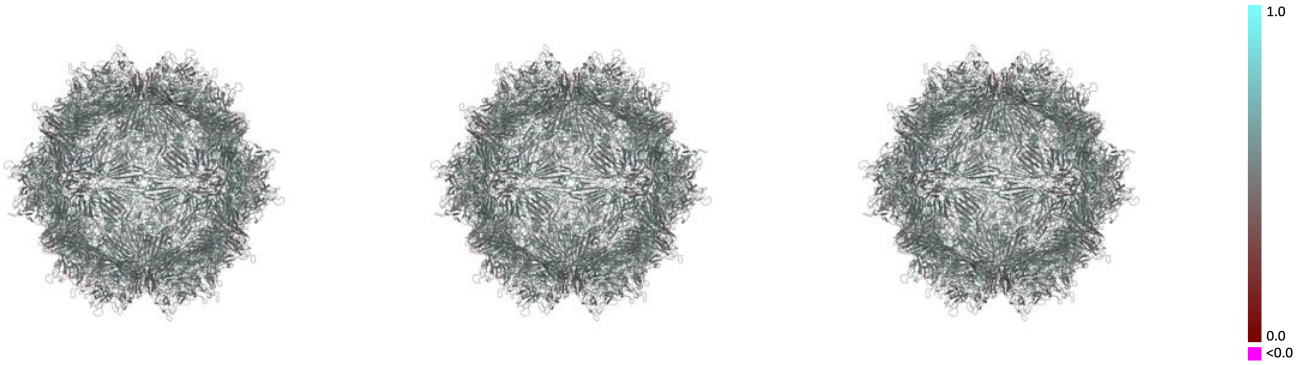
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

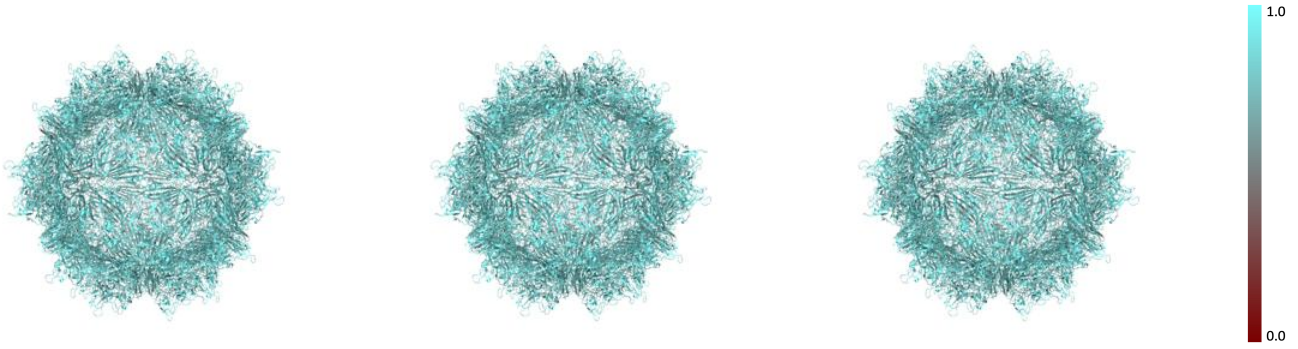
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

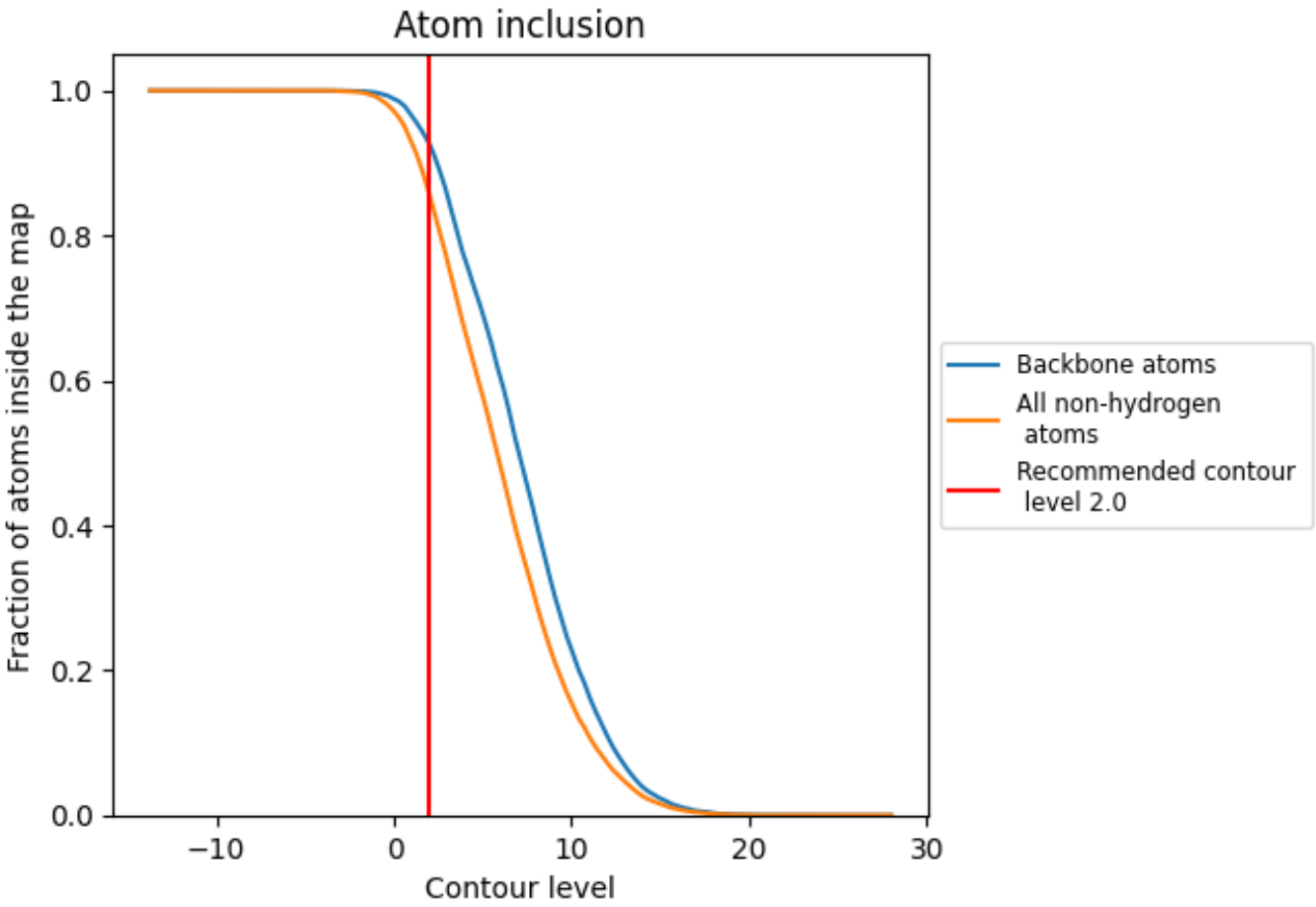
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (2.0).

9.4 Atom inclusion (i)



At the recommended contour level, 93% of all backbone atoms, 86% 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 (2.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8564	0.5180
1	0.8558	0.5180
2	0.8558	0.5190
3	0.8563	0.5190
4	0.8551	0.5180
5	0.8585	0.5180
6	0.8548	0.5190
7	0.8558	0.5190
8	0.8558	0.5170
A	0.8560	0.5170
B	0.8580	0.5170
C	0.8553	0.5180
D	0.8556	0.5180
E	0.8565	0.5180
F	0.8565	0.5190
G	0.8558	0.5170
H	0.8558	0.5150
I	0.8551	0.5170
J	0.8590	0.5170
K	0.8551	0.5180
L	0.8583	0.5170
M	0.8558	0.5180
N	0.8570	0.5180
O	0.8590	0.5170
P	0.8560	0.5180
Q	0.8565	0.5180
R	0.8558	0.5180
S	0.8558	0.5180
T	0.8558	0.5170
U	0.8551	0.5180
V	0.8590	0.5200
W	0.8551	0.5160
X	0.8585	0.5180
Y	0.8558	0.5170
Z	0.8565	0.5180

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
a	0.8556	0.5180
b	0.8558	0.5170
c	0.8565	0.5170
d	0.8565	0.5180
e	0.8563	0.5190
f	0.8558	0.5180
g	0.8580	0.5170
h	0.8590	0.5190
i	0.8565	0.5190
j	0.8565	0.5180
k	0.8558	0.5160
l	0.8551	0.5160
m	0.8558	0.5170
n	0.8590	0.5180
o	0.8585	0.5180
p	0.8585	0.5190
q	0.8558	0.5170
r	0.8558	0.5160
s	0.8551	0.5170
t	0.8556	0.5180
u	0.8548	0.5180
v	0.8558	0.5190
w	0.8565	0.5170
x	0.8563	0.5180
y	0.8551	0.5180
z	0.8558	0.5190