Full wwPDB EM Validation Report ⓘ

Mar 2, 2024 – 02:18 PM EST

PDB ID	:	5VLZ
EMDB ID	:	EMD-8709
Title	:	Backbone model for phage Qbeta capsid
Authors	:	Cui, Z.; Zhang, J.
Deposited on	:	2017-04-26
Resolution	:	4.40 Å(reported)

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

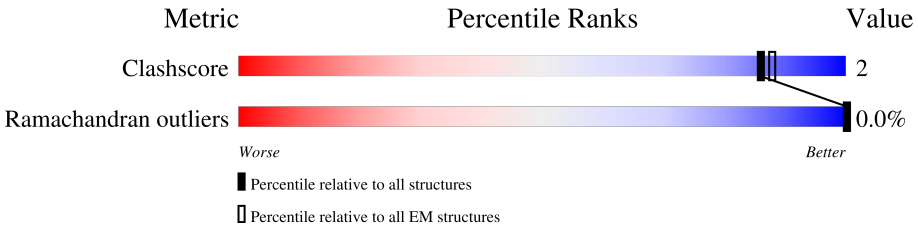
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.40 Å.

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



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

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	AA	133	98%
1	AB	133	6% 96%
1	AC	133	98%
1	AD	133	98%
1	AE	133	98%
1	AF	133	96%
1	AG	133	98%
1	AH	133	98%
1	AI	133	98%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	AJ	133	96%
1	AK	133	5% 96%
1	AL	133	6% 98%
1	AM	133	96%
1	AN	133	96%
1	BA	133	98%
1	BB	133	98%
1	BC	133	99%
1	BD	133	5% 98%
1	BE	133	96%
1	BF	133	96%
1	BG	133	98%
1	BH	133	96%
1	BI	133	96%
1	BJ	133	96%
1	BK	133	96%
1	BL	133	96%
1	BM	133	98%
1	BN	133	5% 96%
1	CA	133	96%
1	CB	133	96%
1	CC	133	5% 99%
1	CD	133	98%
1	CE	133	98%
1	CF	133	96%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	CG	133	99%
1	CH	133	96%
1	CI	133	96%
1	CJ	133	99%
1	CK	133	6% 97%
1	CL	133	12% 96%
1	CM	133	10% 96%
1	CN	133	96%
1	DA	133	5% 96%
1	DB	133	53% 96%
1	DC	133	5% 98%
1	DD	133	99%
1	DE	133	98%
1	DF	133	99%
1	DG	133	96%
1	DH	133	96%
1	DI	133	96%
1	DJ	133	95%
1	DK	133	98%
1	DL	133	5% 96%
1	DN	133	95%
1	EA	133	5% 96%
1	EB	133	8% 96%
1	EC	133	95% 5%
1	ED	133	15% 96%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	EE	133	97%
1	EF	133	7% 98%
1	EG	133	96%
1	EH	133	98%
1	EI	133	96%
1	EK	133	6% 98%
1	EL	133	98%
1	EM	133	96%
1	EN	133	6% 96%
1	FA	133	98%
1	FB	133	98%
1	FC	133	5% 98%
1	FD	133	96%
1	FE	133	96%
1	FF	133	96%
1	FH	133	98%
1	FI	133	99%
1	FJ	133	96%
1	FK	133	99%
1	FL	133	96%
1	FM	133	98%
1	FN	133	96%
1	GA	133	99%
1	GB	133	5% 96%
1	GC	133	96%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	GD	133	57% 96%
1	GE	133	96%
1	GF	133	98%
1	GG	133	96%
1	GH	133	96%
1	GI	133	96%
1	GJ	133	98%
1	GK	133	98%
1	GL	133	96%
1	GM	133	98%
1	GN	133	98%
1	HA	133	96%
1	HB	133	5% 96%
1	HC	133	99%
1	HD	133	98%
1	HE	133	5% 98%
1	HF	133	98%
1	HG	133	7% 96%
1	HH	133	96%
1	HI	133	98%
1	HJ	133	98%
1	HK	133	98%
1	HL	133	96%
1	HM	133	98%
1	HN	133	98%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	IA	133	98%
1	IB	133	98%
1	IC	133	96%
1	ID	133	98%
1	IE	133	96%
1	IF	133	96%
1	IG	133	99%
1	IH	133	98%
1	II	133	98%
1	IJ	133	96%
1	IK	133	96%
1	IL	133	96%
1	IM	133	96%
1	IN	133	96%
1	JA	133	96%
1	JB	133	98%
1	JC	133	98%
1	JD	133	98%
1	JE	133	98%
1	JF	133	98%
1	JG	133	98%
1	JH	133	96%
1	JI	133	96%
1	JJ	133	98%
1	JK	133	6% 96%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	JL	133	99%
1	JM	133	8% 96%
1	JN	133	96%
1	KA	133	99%
1	KB	133	5% 98%
1	KC	133	96%
1	KD	133	96%
1	KE	133	96%
1	KF	133	96%
1	KG	133	98%
1	KH	133	96%
1	KI	133	5% 96%
1	KJ	133	96%
1	KK	133	98%
1	KL	133	96%
1	KM	133	98%
1	KN	133	98%
1	LA	133	98%
1	LB	133	99%
1	LC	133	98%
1	LD	133	96%
1	LE	133	98%
1	LF	133	98%
1	LG	133	98%
1	LH	133	96%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	LI	133	98%
1	LJ	133	96%
1	LK	133	96%
1	LL	133	98%
1	LM	133	5% 98%
1	LN	133	98%
1	MA	133	99%
1	MB	133	5% 98%
1	MC	133	96%
1	MD	133	98%
1	ME	133	5% 98%
1	MF	133	96%
1	MG	133	98%
1	MH	133	99%
1	MI	133	96%
1	MJ	133	96%
1	MK	133	98%
1	ML	133	98%
1	MM	133	98%
1	MN	133	98%
1	NA	133	98%
2	EJ	420	19% 99%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 96897 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Capsid protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	AH	132	Total 529	C 264	N 132	O 133	0	0
1	GN	132	Total 529	C 264	N 132	O 133	0	0
1	HA	132	Total 529	C 264	N 132	O 133	0	0
1	HB	132	Total 529	C 264	N 132	O 133	0	0
1	HC	132	Total 529	C 264	N 132	O 133	0	0
1	HD	132	Total 529	C 264	N 132	O 133	0	0
1	HE	132	Total 529	C 264	N 132	O 133	0	0
1	HF	132	Total 529	C 264	N 132	O 133	0	0
1	HG	132	Total 529	C 264	N 132	O 133	0	0
1	HH	132	Total 529	C 264	N 132	O 133	0	0
1	HI	132	Total 529	C 264	N 132	O 133	0	0
1	AI	132	Total 529	C 264	N 132	O 133	0	0
1	HJ	132	Total 529	C 264	N 132	O 133	0	0
1	HK	132	Total 529	C 264	N 132	O 133	0	0
1	HL	132	Total 529	C 264	N 132	O 133	0	0
1	HM	132	Total 529	C 264	N 132	O 133	0	0
1	HN	132	Total 529	C 264	N 132	O 133	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
1	IA	132	Total 529	C 264	N 132	O 133	0	0
1	IB	132	Total 529	C 264	N 132	O 133	0	0
1	IC	132	Total 529	C 264	N 132	O 133	0	0
1	ID	132	Total 529	C 264	N 132	O 133	0	0
1	IE	132	Total 529	C 264	N 132	O 133	0	0
1	AJ	132	Total 529	C 264	N 132	O 133	0	0
1	IF	132	Total 529	C 264	N 132	O 133	0	0
1	IG	132	Total 529	C 264	N 132	O 133	0	0
1	IH	132	Total 529	C 264	N 132	O 133	0	0
1	II	132	Total 529	C 264	N 132	O 133	0	0
1	IJ	132	Total 529	C 264	N 132	O 133	0	0
1	IK	132	Total 529	C 264	N 132	O 133	0	0
1	IL	132	Total 529	C 264	N 132	O 133	0	0
1	IM	132	Total 529	C 264	N 132	O 133	0	0
1	IN	132	Total 529	C 264	N 132	O 133	0	0
1	JA	132	Total 529	C 264	N 132	O 133	0	0
1	AK	132	Total 529	C 264	N 132	O 133	0	0
1	JB	132	Total 529	C 264	N 132	O 133	0	0
1	JC	132	Total 529	C 264	N 132	O 133	0	0
1	JD	132	Total 529	C 264	N 132	O 133	0	0
1	JE	132	Total 529	C 264	N 132	O 133	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
1	JF	132	Total 529	C 264	N 132	O 133	0	0
1	JG	132	Total 529	C 264	N 132	O 133	0	0
1	JH	132	Total 529	C 264	N 132	O 133	0	0
1	JI	132	Total 529	C 264	N 132	O 133	0	0
1	JJ	132	Total 529	C 264	N 132	O 133	0	0
1	JK	132	Total 529	C 264	N 132	O 133	0	0
1	AL	132	Total 529	C 264	N 132	O 133	0	0
1	JL	132	Total 529	C 264	N 132	O 133	0	0
1	JM	132	Total 529	C 264	N 132	O 133	0	0
1	JN	132	Total 529	C 264	N 132	O 133	0	0
1	KA	132	Total 529	C 264	N 132	O 133	0	0
1	KB	132	Total 529	C 264	N 132	O 133	0	0
1	KC	132	Total 529	C 264	N 132	O 133	0	0
1	KD	132	Total 529	C 264	N 132	O 133	0	0
1	KE	132	Total 529	C 264	N 132	O 133	0	0
1	KF	132	Total 529	C 264	N 132	O 133	0	0
1	KG	132	Total 529	C 264	N 132	O 133	0	0
1	AM	132	Total 529	C 264	N 132	O 133	0	0
1	KH	132	Total 529	C 264	N 132	O 133	0	0
1	KI	132	Total 529	C 264	N 132	O 133	0	0
1	KJ	132	Total 529	C 264	N 132	O 133	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
1	KK	132	Total 529	C 264	N 132	O 133	0	0
1	KL	132	Total 529	C 264	N 132	O 133	0	0
1	KM	132	Total 529	C 264	N 132	O 133	0	0
1	KN	132	Total 529	C 264	N 132	O 133	0	0
1	LA	132	Total 529	C 264	N 132	O 133	0	0
1	LB	132	Total 529	C 264	N 132	O 133	0	0
1	LC	132	Total 529	C 264	N 132	O 133	0	0
1	AN	132	Total 529	C 264	N 132	O 133	0	0
1	LD	132	Total 529	C 264	N 132	O 133	0	0
1	LE	132	Total 529	C 264	N 132	O 133	0	0
1	LF	132	Total 529	C 264	N 132	O 133	0	0
1	LG	132	Total 529	C 264	N 132	O 133	0	0
1	LH	132	Total 529	C 264	N 132	O 133	0	0
1	LI	132	Total 529	C 264	N 132	O 133	0	0
1	LJ	132	Total 529	C 264	N 132	O 133	0	0
1	LK	132	Total 529	C 264	N 132	O 133	0	0
1	LL	132	Total 529	C 264	N 132	O 133	0	0
1	LM	132	Total 529	C 264	N 132	O 133	0	0
1	BA	132	Total 529	C 264	N 132	O 133	0	0
1	LN	132	Total 529	C 264	N 132	O 133	0	0
1	MA	132	Total 529	C 264	N 132	O 133	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
1	MB	132	Total 529	C 264	N 132	O 133	0	0
1	MC	132	Total 529	C 264	N 132	O 133	0	0
1	MD	132	Total 529	C 264	N 132	O 133	0	0
1	ME	132	Total 529	C 264	N 132	O 133	0	0
1	MF	132	Total 529	C 264	N 132	O 133	0	0
1	MG	132	Total 529	C 264	N 132	O 133	0	0
1	MH	132	Total 529	C 264	N 132	O 133	0	0
1	MI	132	Total 529	C 264	N 132	O 133	0	0
1	BB	132	Total 529	C 264	N 132	O 133	0	0
1	MJ	132	Total 529	C 264	N 132	O 133	0	0
1	MK	132	Total 529	C 264	N 132	O 133	0	0
1	ML	132	Total 529	C 264	N 132	O 133	0	0
1	MM	132	Total 529	C 264	N 132	O 133	0	0
1	MN	132	Total 529	C 264	N 132	O 133	0	0
1	NA	132	Total 529	C 264	N 132	O 133	0	0
1	BC	132	Total 529	C 264	N 132	O 133	0	0
1	BD	132	Total 529	C 264	N 132	O 133	0	0
1	BE	132	Total 529	C 264	N 132	O 133	0	0
1	BF	132	Total 529	C 264	N 132	O 133	0	0
1	BG	132	Total 529	C 264	N 132	O 133	0	0
1	BH	132	Total 529	C 264	N 132	O 133	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
1	BI	132	Total 529	C 264	N 132	O 133	0	0
1	BJ	132	Total 529	C 264	N 132	O 133	0	0
1	BK	132	Total 529	C 264	N 132	O 133	0	0
1	BL	132	Total 529	C 264	N 132	O 133	0	0
1	BM	132	Total 529	C 264	N 132	O 133	0	0
1	AA	132	Total 529	C 264	N 132	O 133	0	0
1	BN	132	Total 529	C 264	N 132	O 133	0	0
1	CA	132	Total 529	C 264	N 132	O 133	0	0
1	CB	132	Total 529	C 264	N 132	O 133	0	0
1	CC	132	Total 529	C 264	N 132	O 133	0	0
1	CD	132	Total 529	C 264	N 132	O 133	0	0
1	CE	132	Total 529	C 264	N 132	O 133	0	0
1	CF	132	Total 529	C 264	N 132	O 133	0	0
1	CG	132	Total 529	C 264	N 132	O 133	0	0
1	CH	132	Total 529	C 264	N 132	O 133	0	0
1	CI	132	Total 529	C 264	N 132	O 133	0	0
1	AB	132	Total 529	C 264	N 132	O 133	0	0
1	CJ	132	Total 529	C 264	N 132	O 133	0	0
1	CK	132	Total 529	C 264	N 132	O 133	0	0
1	CL	132	Total 529	C 264	N 132	O 133	0	0
1	CM	132	Total 529	C 264	N 132	O 133	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
1	CN	132	Total 529	C 264	N 132	O 133	0	0
1	DA	132	Total 529	C 264	N 132	O 133	0	0
1	DB	132	Total 529	C 264	N 132	O 133	0	0
1	DC	132	Total 529	C 264	N 132	O 133	0	0
1	DD	132	Total 529	C 264	N 132	O 133	0	0
1	DE	132	Total 529	C 264	N 132	O 133	0	0
1	AC	132	Total 529	C 264	N 132	O 133	0	0
1	DF	132	Total 529	C 264	N 132	O 133	0	0
1	DG	132	Total 529	C 264	N 132	O 133	0	0
1	DH	132	Total 529	C 264	N 132	O 133	0	0
1	DI	132	Total 529	C 264	N 132	O 133	0	0
1	DJ	132	Total 529	C 264	N 132	O 133	0	0
1	DK	132	Total 529	C 264	N 132	O 133	0	0
1	DL	132	Total 529	C 264	N 132	O 133	0	0
1	DN	132	Total 529	C 264	N 132	O 133	0	0
1	EA	132	Total 529	C 264	N 132	O 133	0	0
1	AD	132	Total 529	C 264	N 132	O 133	0	0
1	EB	132	Total 529	C 264	N 132	O 133	0	0
1	EC	132	Total 529	C 264	N 132	O 133	0	0
1	ED	132	Total 529	C 264	N 132	O 133	0	0
1	EE	132	Total 529	C 264	N 132	O 133	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
1	EF	132	Total 529	C 264	N 132	O 133	0	0
1	EG	132	Total 529	C 264	N 132	O 133	0	0
1	EH	132	Total 529	C 264	N 132	O 133	0	0
1	EI	132	Total 529	C 264	N 132	O 133	0	0
1	EK	132	Total 529	C 264	N 132	O 133	0	0
1	AE	132	Total 529	C 264	N 132	O 133	0	0
1	EL	132	Total 529	C 264	N 132	O 133	0	0
1	EM	132	Total 529	C 264	N 132	O 133	0	0
1	EN	132	Total 529	C 264	N 132	O 133	0	0
1	FA	132	Total 529	C 264	N 132	O 133	0	0
1	FB	132	Total 529	C 264	N 132	O 133	0	0
1	FC	132	Total 529	C 264	N 132	O 133	0	0
1	FD	132	Total 529	C 264	N 132	O 133	0	0
1	FE	132	Total 529	C 264	N 132	O 133	0	0
1	FF	132	Total 529	C 264	N 132	O 133	0	0
1	AF	132	Total 529	C 264	N 132	O 133	0	0
1	FH	132	Total 529	C 264	N 132	O 133	0	0
1	FI	132	Total 529	C 264	N 132	O 133	0	0
1	FJ	132	Total 529	C 264	N 132	O 133	0	0
1	FK	132	Total 529	C 264	N 132	O 133	0	0
1	FL	132	Total 529	C 264	N 132	O 133	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
1	FM	132	Total 529	C 264	N 132	O 133	0	0
1	FN	132	Total 529	C 264	N 132	O 133	0	0
1	GA	132	Total 529	C 264	N 132	O 133	0	0
1	GB	132	Total 529	C 264	N 132	O 133	0	0
1	GC	132	Total 529	C 264	N 132	O 133	0	0
1	AG	132	Total 529	C 264	N 132	O 133	0	0
1	GD	132	Total 529	C 264	N 132	O 133	0	0
1	GE	132	Total 529	C 264	N 132	O 133	0	0
1	GF	132	Total 529	C 264	N 132	O 133	0	0
1	GG	132	Total 529	C 264	N 132	O 133	0	0
1	GH	132	Total 529	C 264	N 132	O 133	0	0
1	GI	132	Total 529	C 264	N 132	O 133	0	0
1	GJ	132	Total 529	C 264	N 132	O 133	0	0
1	GK	132	Total 529	C 264	N 132	O 133	0	0
1	GL	132	Total 529	C 264	N 132	O 133	0	0
1	GM	132	Total 529	C 264	N 132	O 133	0	0

- Molecule 2 is a protein called Maturation protein A2.

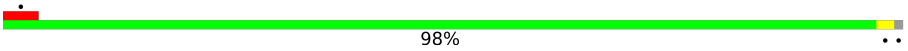
Mol	Chain	Residues	Atoms				AltConf	Trace
2	EJ	419	Total 1677	C 838	N 419	O 420	0	0

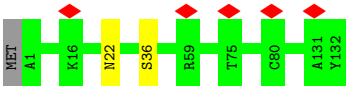
3 Residue-property plots (i)

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

• Molecule 1: Capsid protein

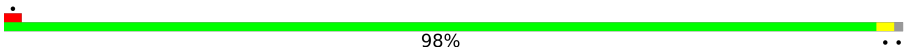
Chain AH:

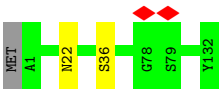




• Molecule 1: Capsid protein

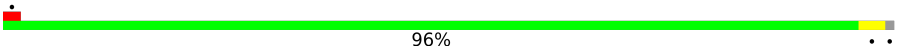
Chain GN:

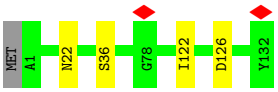




• Molecule 1: Capsid protein

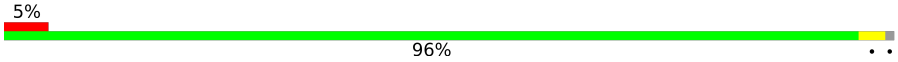
Chain HA:

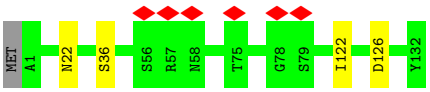




• Molecule 1: Capsid protein

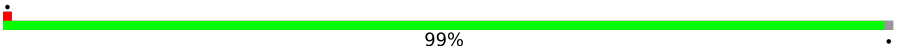
Chain HB:

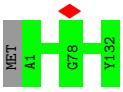




• Molecule 1: Capsid protein

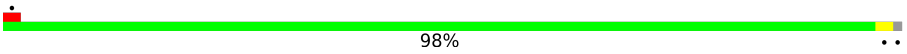
Chain HC:

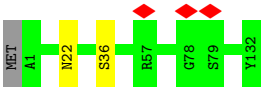




• Molecule 1: Capsid protein

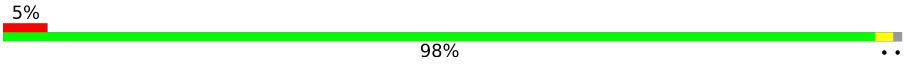
Chain HD:

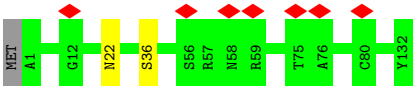




• Molecule 1: Capsid protein

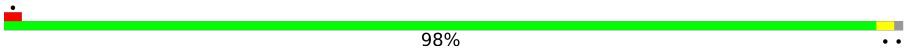
Chain HE:

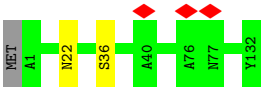




• Molecule 1: Capsid protein

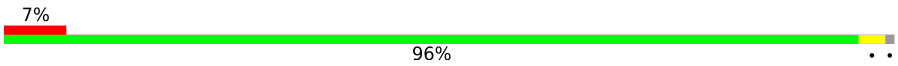
Chain HF:

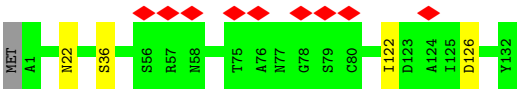




• Molecule 1: Capsid protein

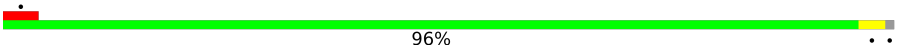
Chain HG:

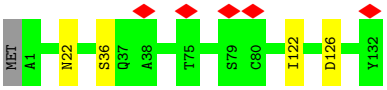




• Molecule 1: Capsid protein

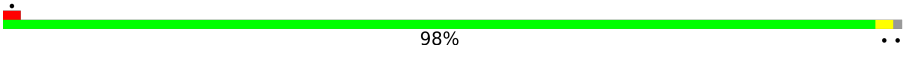
Chain HH:

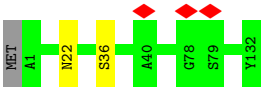




• Molecule 1: Capsid protein

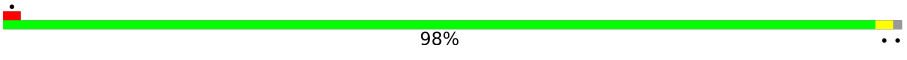
Chain HI:

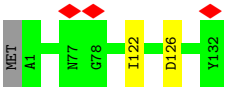




• Molecule 1: Capsid protein

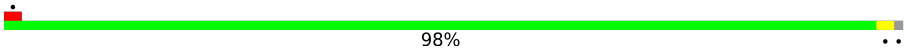
Chain AI:

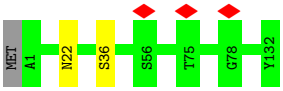




• Molecule 1: Capsid protein

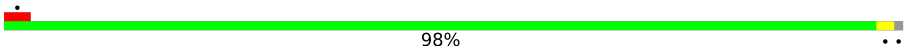
Chain HJ:

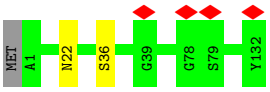




• Molecule 1: Capsid protein

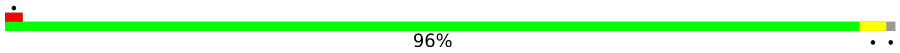
Chain HK:

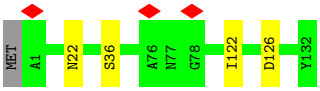




• Molecule 1: Capsid protein

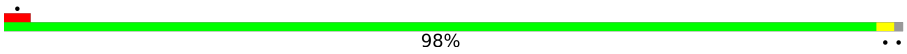
Chain HL:

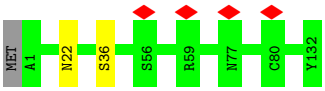




• Molecule 1: Capsid protein

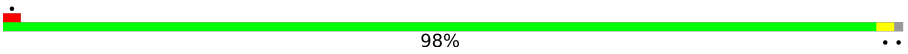
Chain HM:

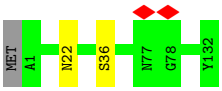




• Molecule 1: Capsid protein

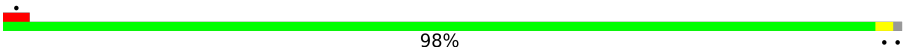
Chain HN:

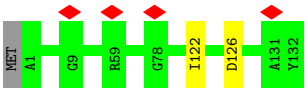




• Molecule 1: Capsid protein

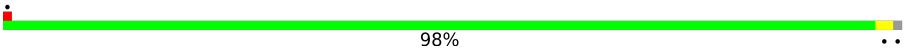
Chain IA:

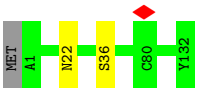




• Molecule 1: Capsid protein

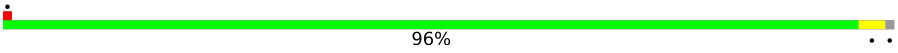
Chain IB:

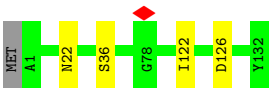




• Molecule 1: Capsid protein

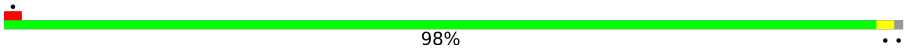
Chain IC:

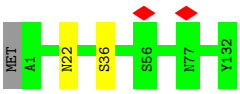




• Molecule 1: Capsid protein

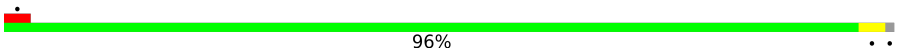
Chain ID:

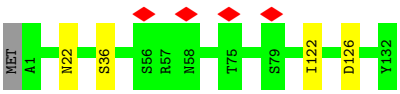




• Molecule 1: Capsid protein

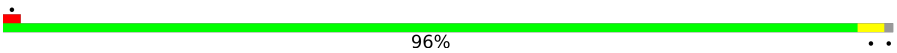
Chain IE:

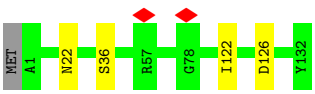




• Molecule 1: Capsid protein

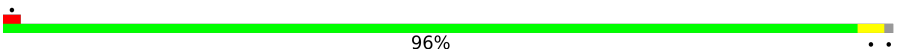
Chain AJ:

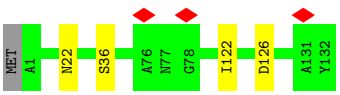




• Molecule 1: Capsid protein

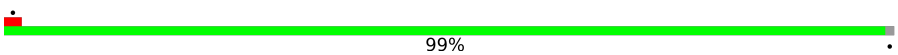
Chain IF:

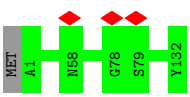




• Molecule 1: Capsid protein

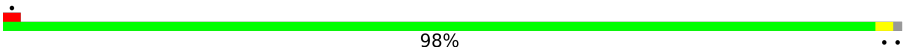
Chain IG:

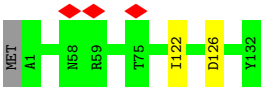




• Molecule 1: Capsid protein

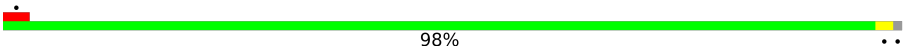
Chain IH:

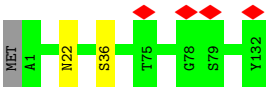




• Molecule 1: Capsid protein

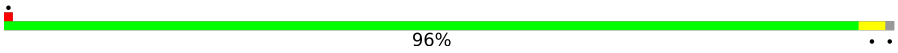
Chain II:

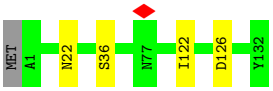




• Molecule 1: Capsid protein

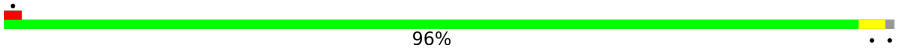
Chain IJ:





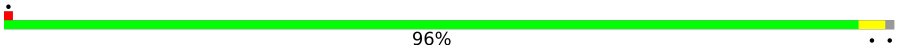
• Molecule 1: Capsid protein

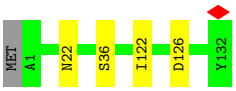
Chain IK:



• Molecule 1: Capsid protein

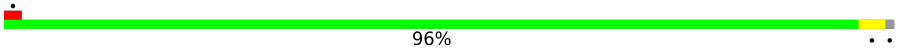
Chain IL:

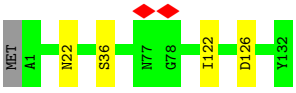




• Molecule 1: Capsid protein

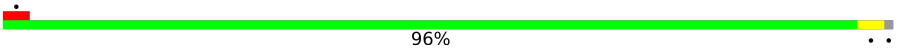
Chain IM:

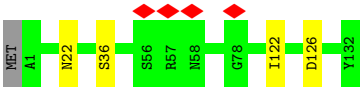




• Molecule 1: Capsid protein

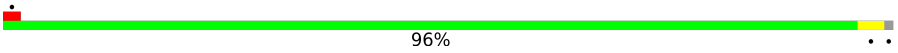
Chain IN:

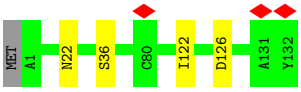




• Molecule 1: Capsid protein

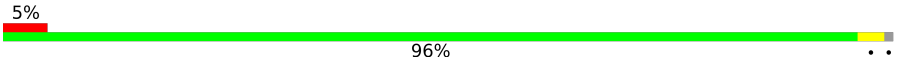
Chain JA:

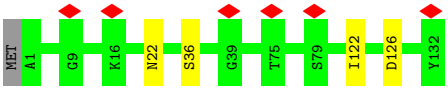




• Molecule 1: Capsid protein

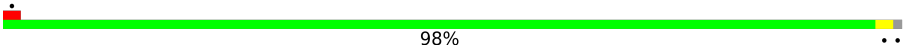
Chain AK:

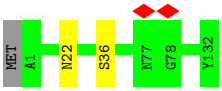




• Molecule 1: Capsid protein

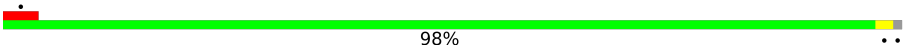
Chain JB:

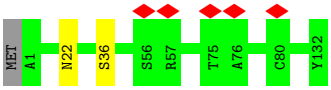




• Molecule 1: Capsid protein

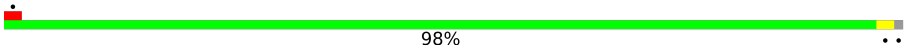
Chain JC:

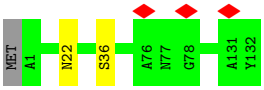




• Molecule 1: Capsid protein

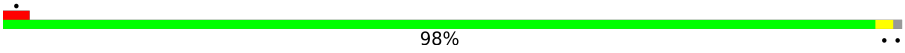
Chain JD:

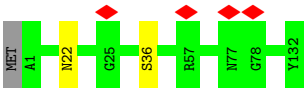




• Molecule 1: Capsid protein

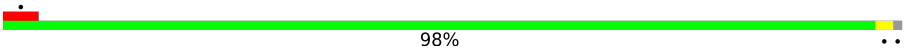
Chain JE:

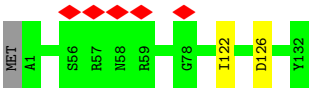




• Molecule 1: Capsid protein

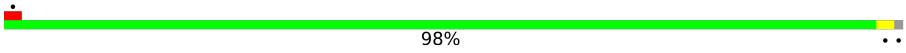
Chain JF:

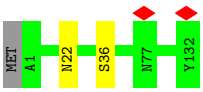




• Molecule 1: Capsid protein

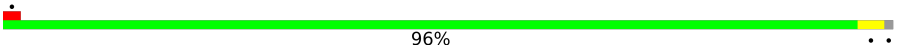
Chain JG:

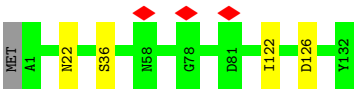




• Molecule 1: Capsid protein

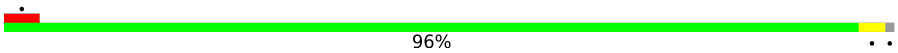
Chain JH:

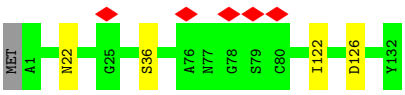




• Molecule 1: Capsid protein

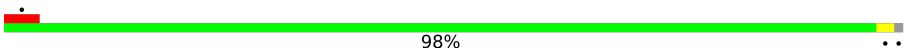
Chain JI:

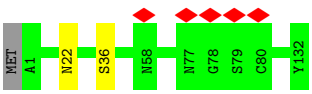




• Molecule 1: Capsid protein

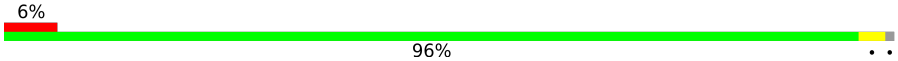
Chain JJ:

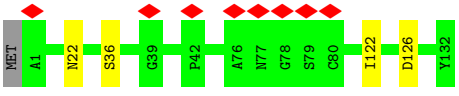




• Molecule 1: Capsid protein

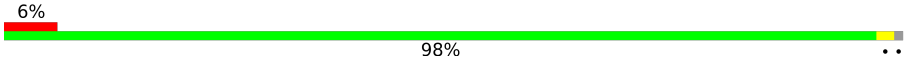
Chain JK:

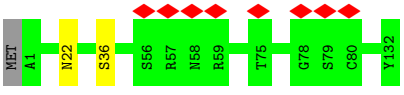




• Molecule 1: Capsid protein

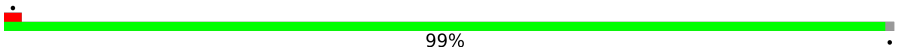
Chain AL:

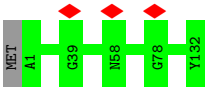




• Molecule 1: Capsid protein

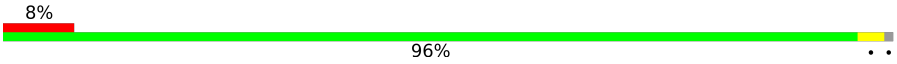
Chain JL:

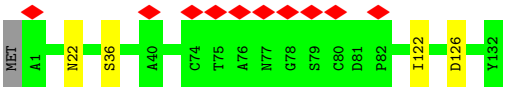




• Molecule 1: Capsid protein

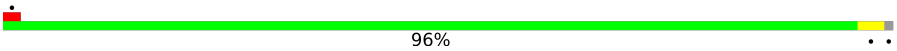
Chain JM:

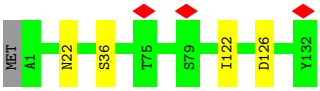




• Molecule 1: Capsid protein

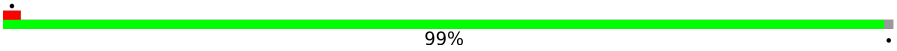
Chain JN:

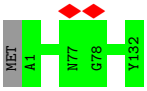




• Molecule 1: Capsid protein

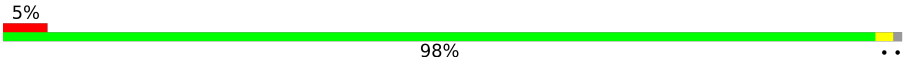
Chain KA:

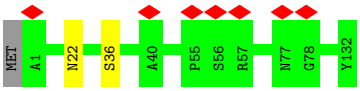




• Molecule 1: Capsid protein

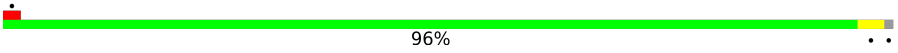
Chain KB:

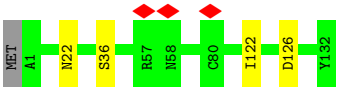




• Molecule 1: Capsid protein

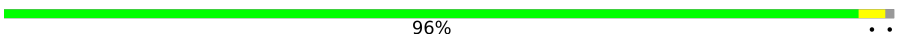
Chain KC:

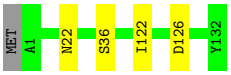




• Molecule 1: Capsid protein

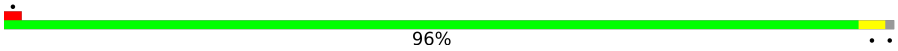
Chain KD:

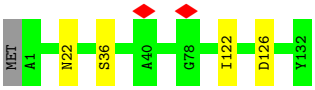




• Molecule 1: Capsid protein

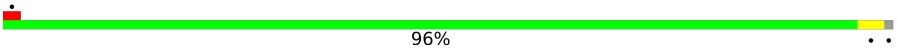
Chain KE:

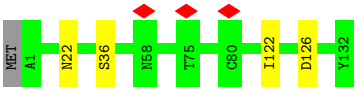




• Molecule 1: Capsid protein

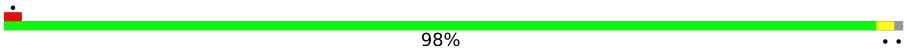
Chain KF:

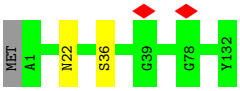




• Molecule 1: Capsid protein

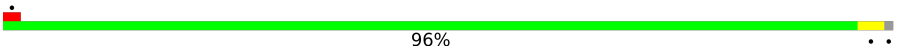
Chain KG:

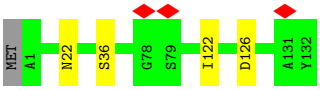




• Molecule 1: Capsid protein

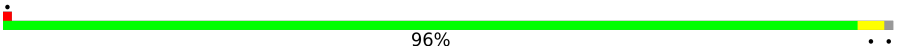
Chain AM:

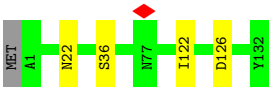




• Molecule 1: Capsid protein

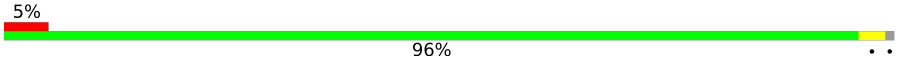
Chain KH:

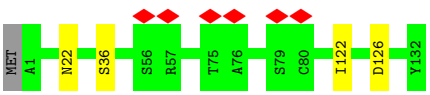




• Molecule 1: Capsid protein

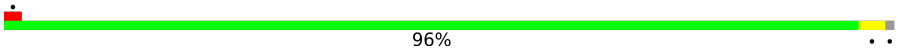
Chain KI:

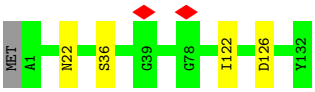




• Molecule 1: Capsid protein

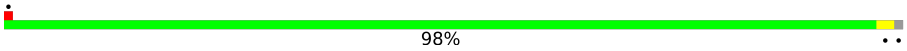
Chain KJ:

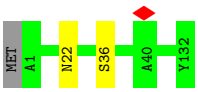




• Molecule 1: Capsid protein

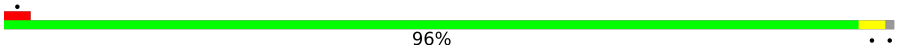
Chain KK:

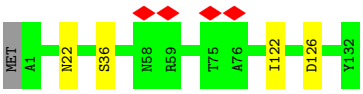




• Molecule 1: Capsid protein

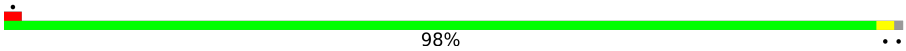
Chain KL:

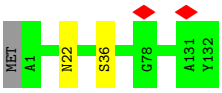




• Molecule 1: Capsid protein

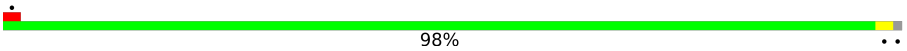
Chain KM:

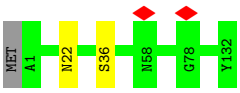




• Molecule 1: Capsid protein

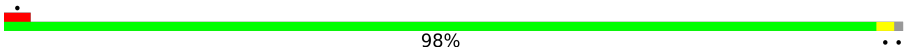
Chain KN:

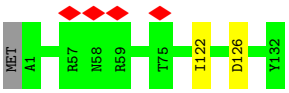




• Molecule 1: Capsid protein

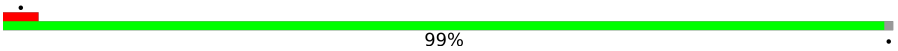
Chain LA:

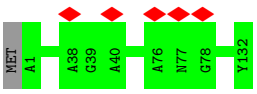




• Molecule 1: Capsid protein

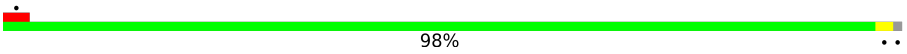
Chain LB:

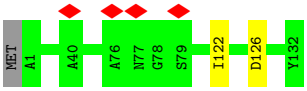




• Molecule 1: Capsid protein

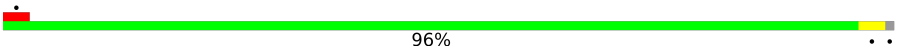
Chain LC:

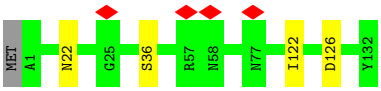




• Molecule 1: Capsid protein

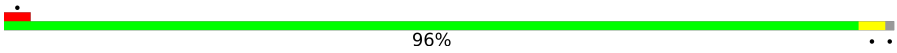
Chain AN:

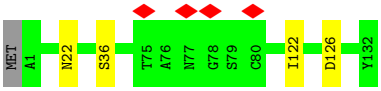




• Molecule 1: Capsid protein

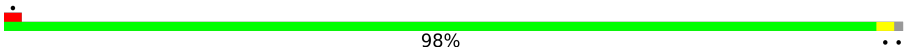
Chain LD:

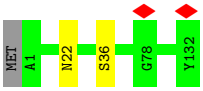




• Molecule 1: Capsid protein

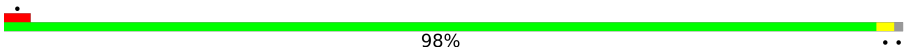
Chain LE:

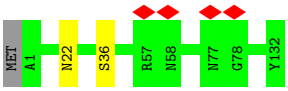




• Molecule 1: Capsid protein

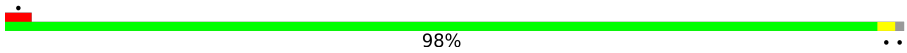
Chain LF:





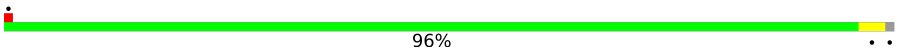
• Molecule 1: Capsid protein

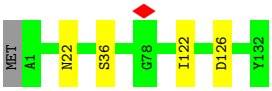
Chain LG:



• Molecule 1: Capsid protein

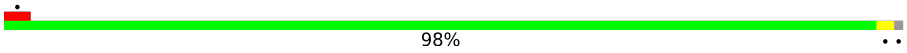
Chain LH:

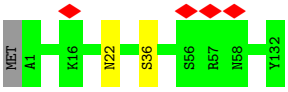




• Molecule 1: Capsid protein

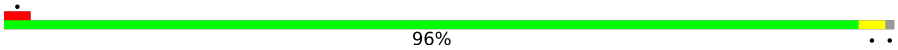
Chain LI:

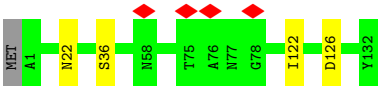




• Molecule 1: Capsid protein

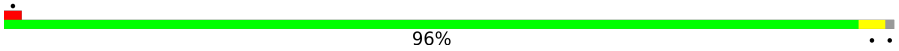
Chain LJ:

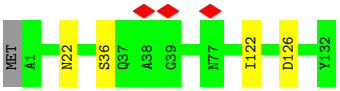




• Molecule 1: Capsid protein

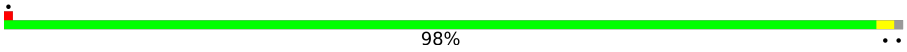
Chain LK:

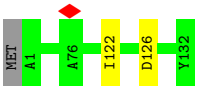




• Molecule 1: Capsid protein

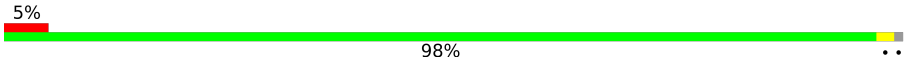
Chain LL:

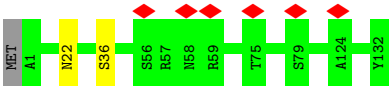




• Molecule 1: Capsid protein

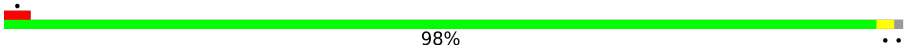
Chain LM:

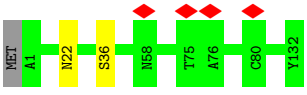




• Molecule 1: Capsid protein

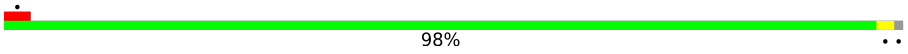
Chain BA:

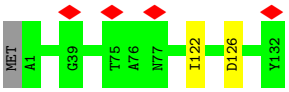




• Molecule 1: Capsid protein

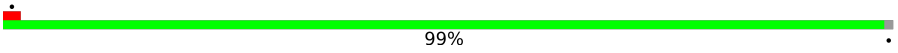
Chain LN:

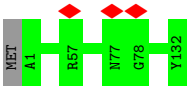




• Molecule 1: Capsid protein

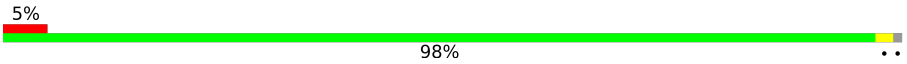
Chain MA:

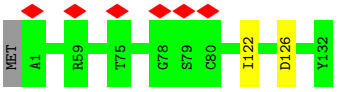




• Molecule 1: Capsid protein

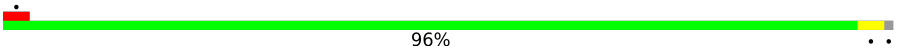
Chain MB:

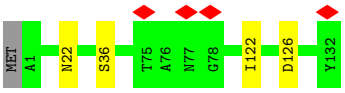




• Molecule 1: Capsid protein

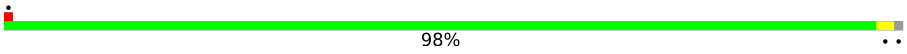
Chain MC:

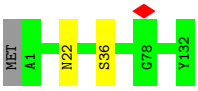




• Molecule 1: Capsid protein

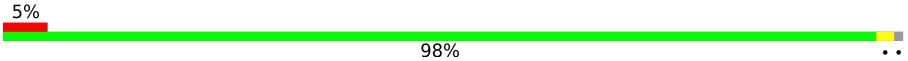
Chain MD:

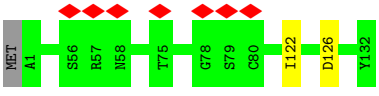




• Molecule 1: Capsid protein

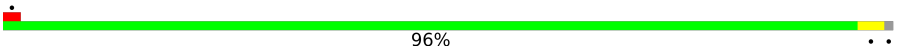
Chain ME:

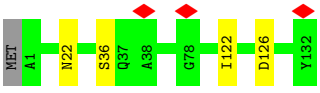




• Molecule 1: Capsid protein

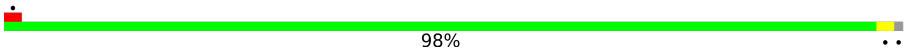
Chain MF:

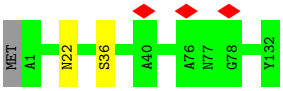




• Molecule 1: Capsid protein

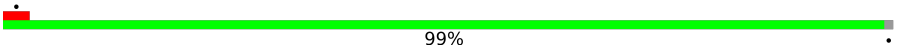
Chain MG:

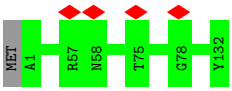




• Molecule 1: Capsid protein

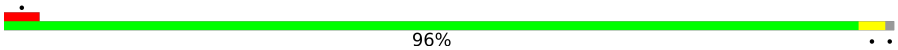
Chain MH:

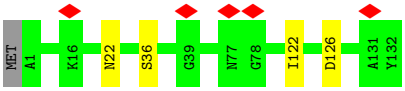




• Molecule 1: Capsid protein

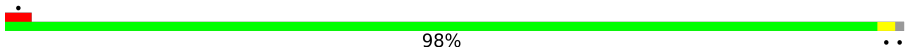
Chain MI:

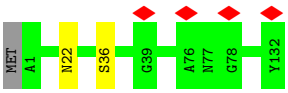




• Molecule 1: Capsid protein

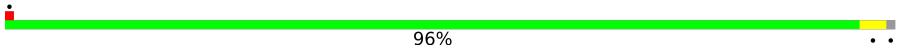
Chain BB:

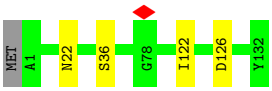




• Molecule 1: Capsid protein

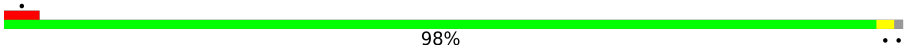
Chain MJ:

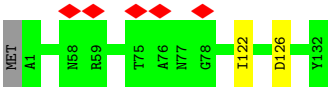




• Molecule 1: Capsid protein

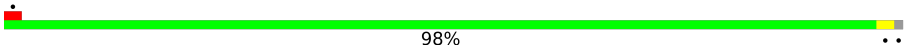
Chain MK:

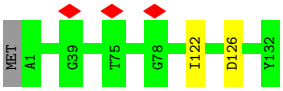




• Molecule 1: Capsid protein

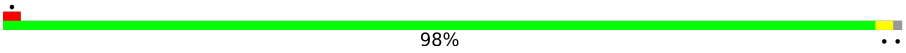
Chain ML:

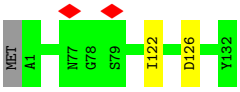




• Molecule 1: Capsid protein

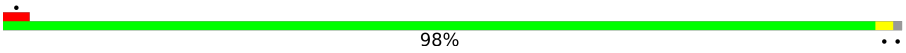
Chain MM:

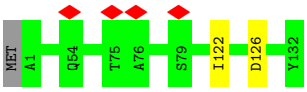




• Molecule 1: Capsid protein

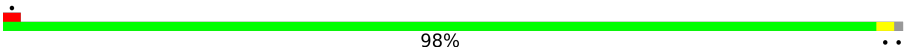
Chain MN:

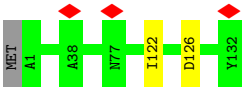




• Molecule 1: Capsid protein

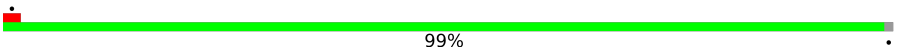
Chain NA:

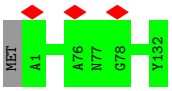




• Molecule 1: Capsid protein

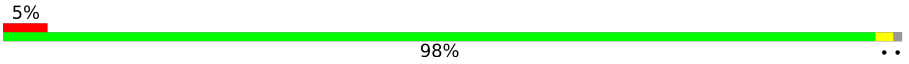
Chain BC:

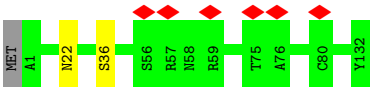




• Molecule 1: Capsid protein

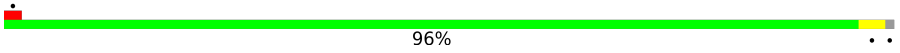
Chain BD:

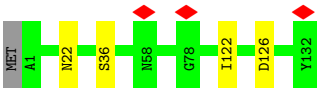




• Molecule 1: Capsid protein

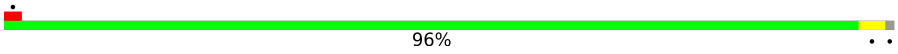
Chain BE:

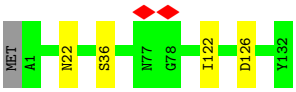




• Molecule 1: Capsid protein

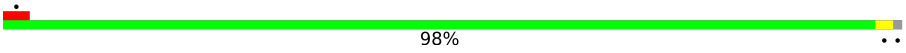
Chain BF:

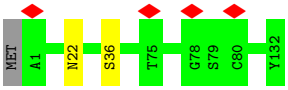




• Molecule 1: Capsid protein

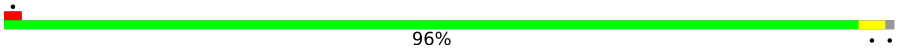
Chain BG:

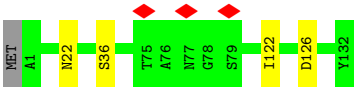




• Molecule 1: Capsid protein

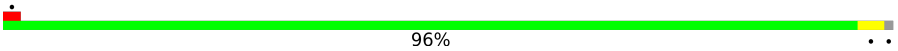
Chain BH:

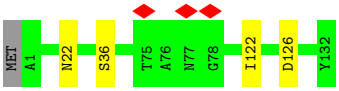




• Molecule 1: Capsid protein

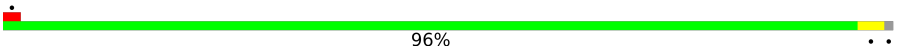
Chain BI:

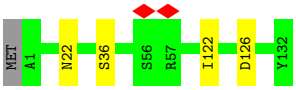




• Molecule 1: Capsid protein

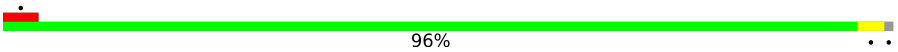
Chain BJ:

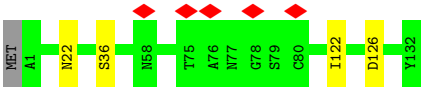




• Molecule 1: Capsid protein

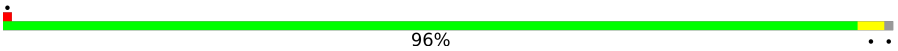
Chain BK:

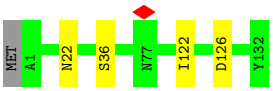




• Molecule 1: Capsid protein

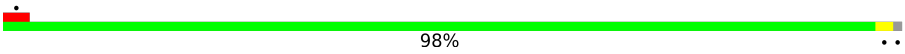
Chain BL:

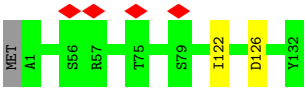




• Molecule 1: Capsid protein

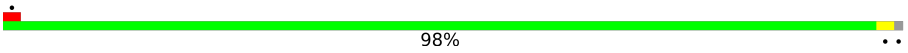
Chain BM:

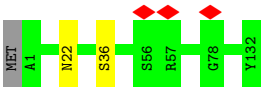




• Molecule 1: Capsid protein

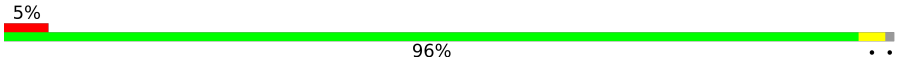
Chain AA:

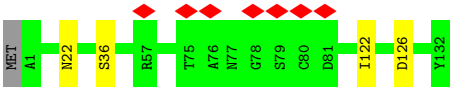




• Molecule 1: Capsid protein

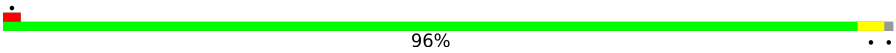
Chain BN:

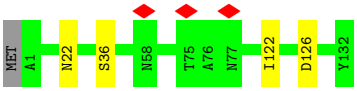




• Molecule 1: Capsid protein

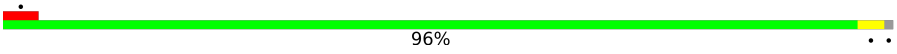
Chain CA:

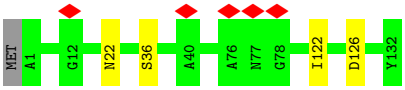




• Molecule 1: Capsid protein

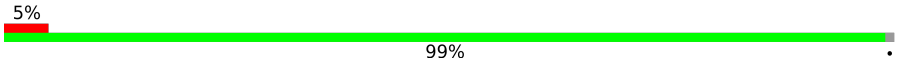
Chain CB:

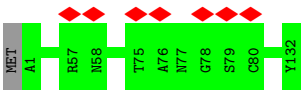




• Molecule 1: Capsid protein

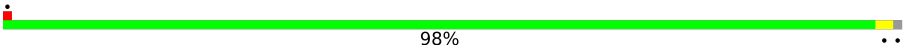
Chain CC:

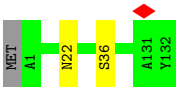




• Molecule 1: Capsid protein

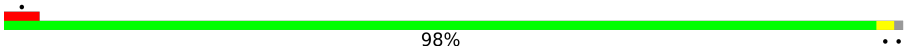
Chain CD:

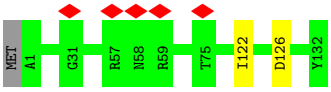




• Molecule 1: Capsid protein

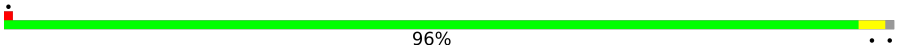
Chain CE:

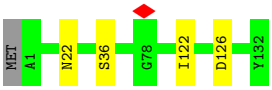




• Molecule 1: Capsid protein

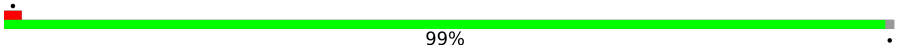
Chain CF:

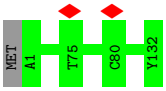




• Molecule 1: Capsid protein

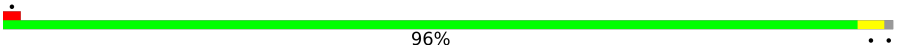
Chain CG:

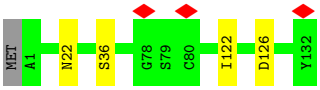




• Molecule 1: Capsid protein

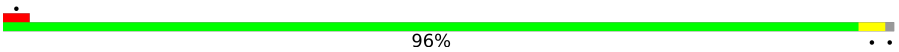
Chain CH:

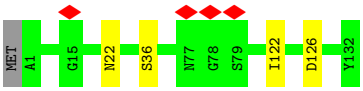




• Molecule 1: Capsid protein

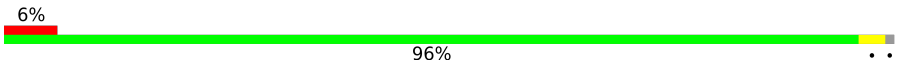
Chain CI:

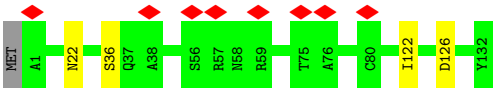




• Molecule 1: Capsid protein

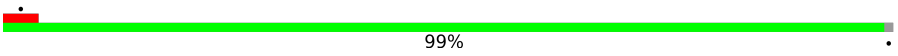
Chain AB:

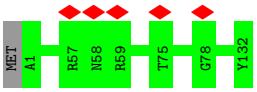




• Molecule 1: Capsid protein

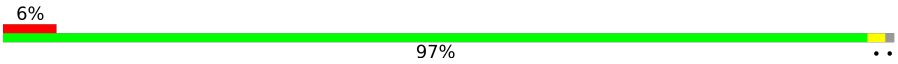
Chain CJ:

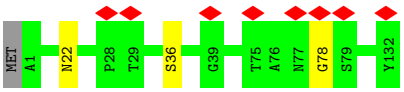




• Molecule 1: Capsid protein

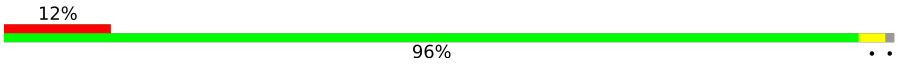
Chain CK:

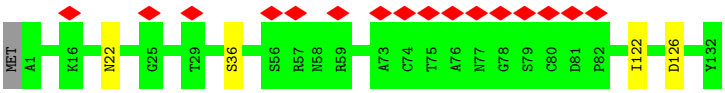




• Molecule 1: Capsid protein

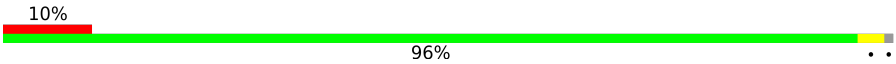
Chain CL:

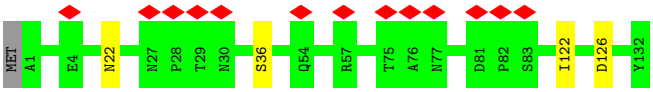




• Molecule 1: Capsid protein

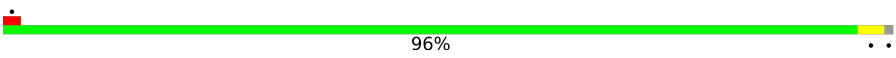
Chain CM:

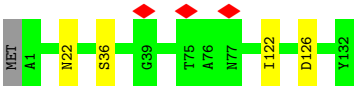




• Molecule 1: Capsid protein

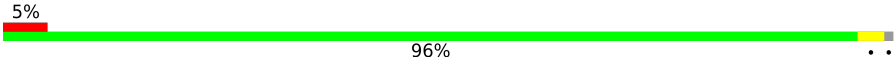
Chain CN:

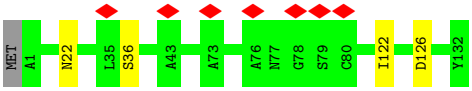




• Molecule 1: Capsid protein

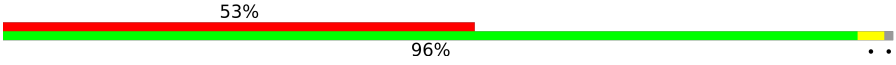
Chain DA:

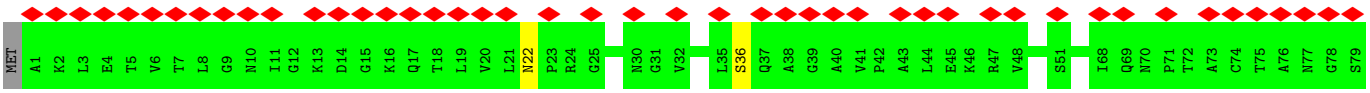


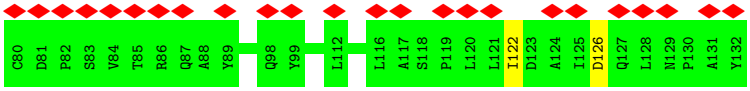


• Molecule 1: Capsid protein

Chain DB:

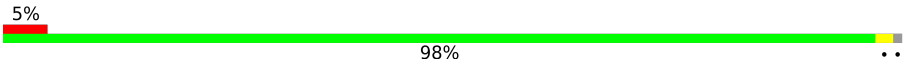


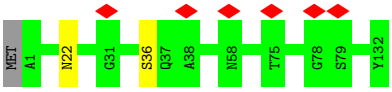




• Molecule 1: Capsid protein

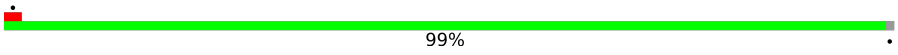
Chain DC:

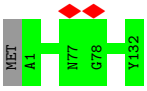




• Molecule 1: Capsid protein

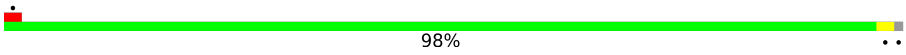
Chain DD:

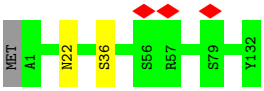




• Molecule 1: Capsid protein

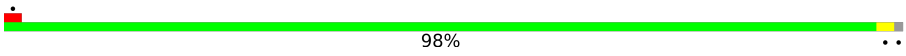
Chain DE:

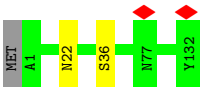




• Molecule 1: Capsid protein

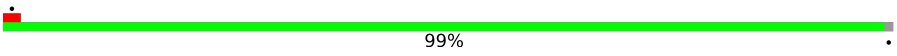
Chain AC:

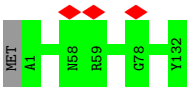




• Molecule 1: Capsid protein

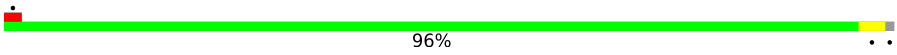
Chain DF:

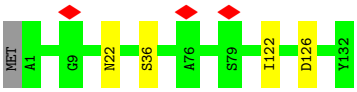




• Molecule 1: Capsid protein

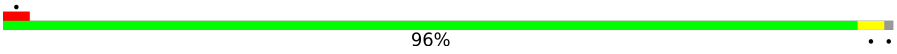
Chain DG:

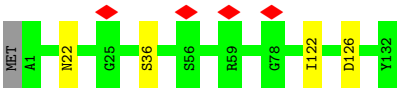




• Molecule 1: Capsid protein

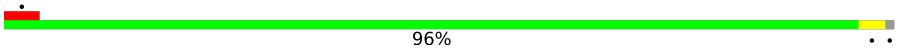
Chain DH:

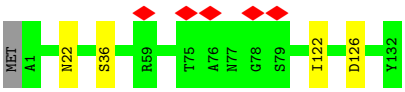




• Molecule 1: Capsid protein

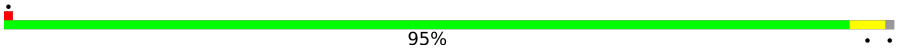
Chain DI:

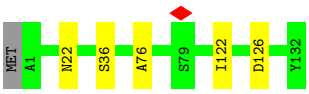




• Molecule 1: Capsid protein

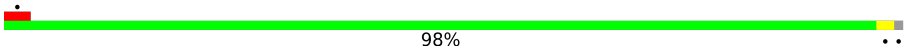
Chain DJ:

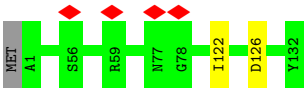




• Molecule 1: Capsid protein

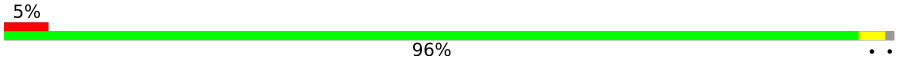
Chain DK:

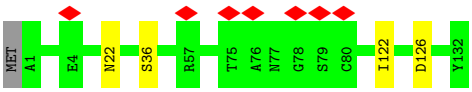




• Molecule 1: Capsid protein

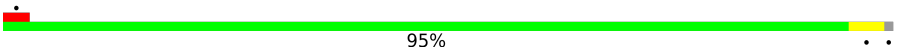
Chain DL:

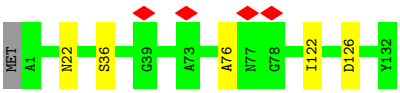




• Molecule 1: Capsid protein

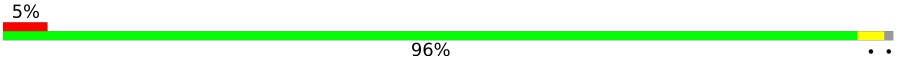
Chain DN:

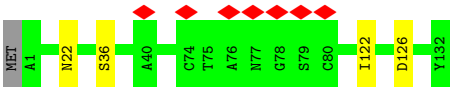




• Molecule 1: Capsid protein

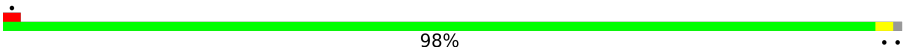
Chain EA:

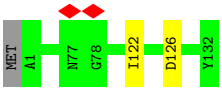




• Molecule 1: Capsid protein

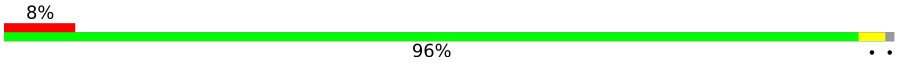
Chain AD:

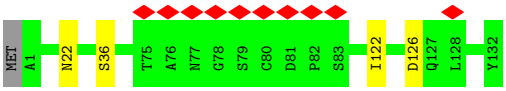




• Molecule 1: Capsid protein

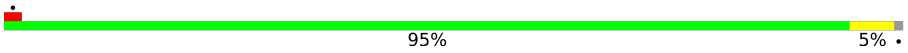
Chain EB:

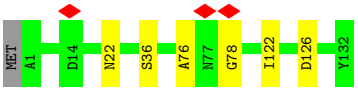




• Molecule 1: Capsid protein

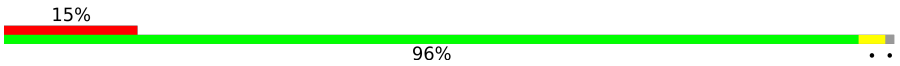
Chain EC:

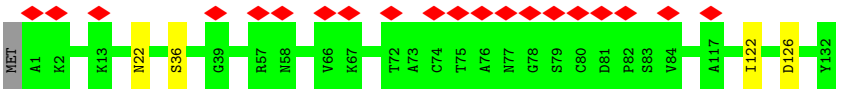




• Molecule 1: Capsid protein

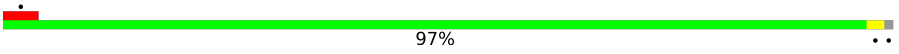
Chain ED:

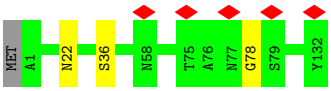




• Molecule 1: Capsid protein

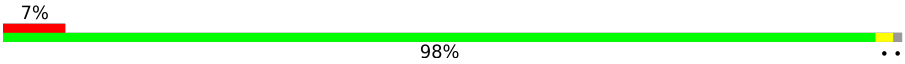
Chain EE:

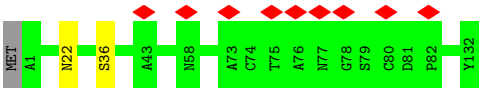




• Molecule 1: Capsid protein

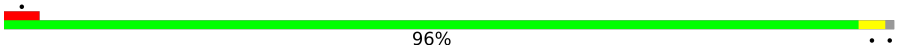
Chain EF:

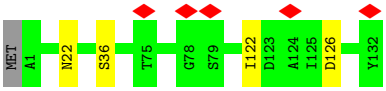




• Molecule 1: Capsid protein

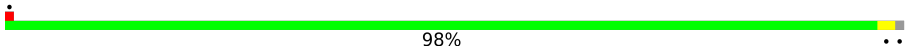
Chain EG:

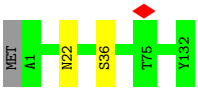




• Molecule 1: Capsid protein

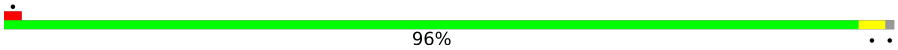
Chain EH:

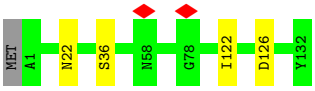




• Molecule 1: Capsid protein

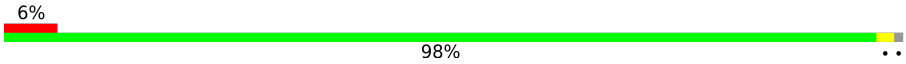
Chain EI:

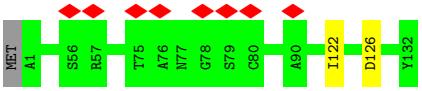




• Molecule 1: Capsid protein

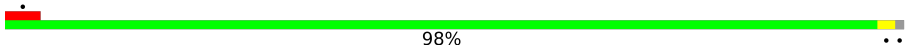
Chain EK:

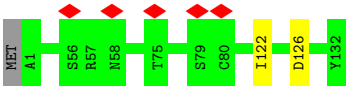




• Molecule 1: Capsid protein

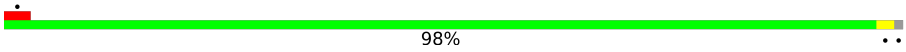
Chain AE:

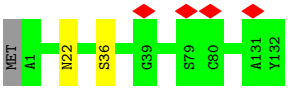




• Molecule 1: Capsid protein

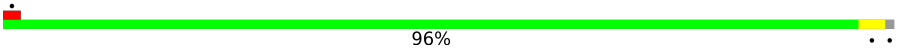
Chain EL:

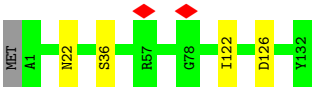




• Molecule 1: Capsid protein

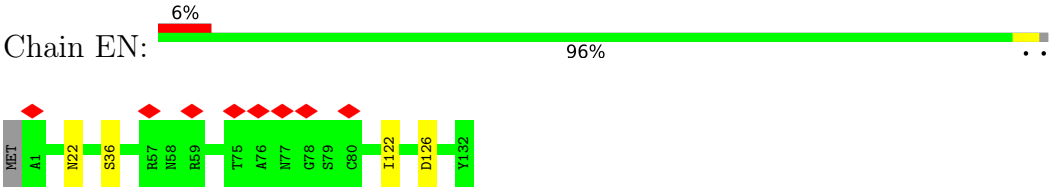
Chain EM:





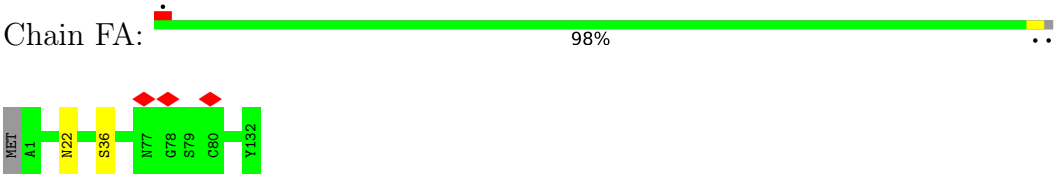
• Molecule 1: Capsid protein

Chain EN:



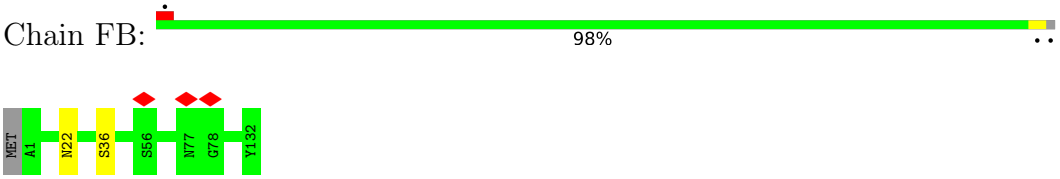
• Molecule 1: Capsid protein

Chain FA:



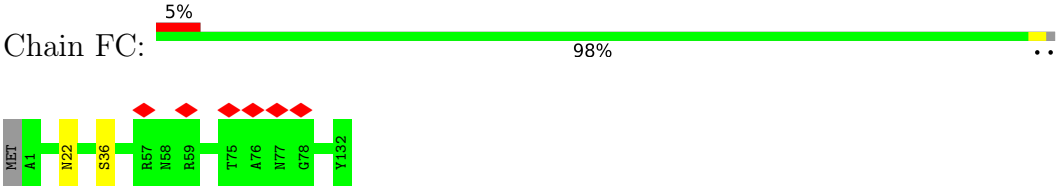
• Molecule 1: Capsid protein

Chain FB:



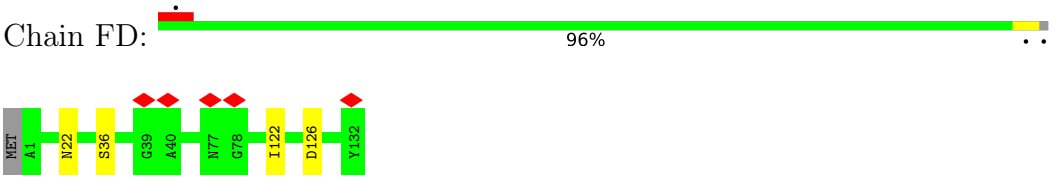
• Molecule 1: Capsid protein

Chain FC:



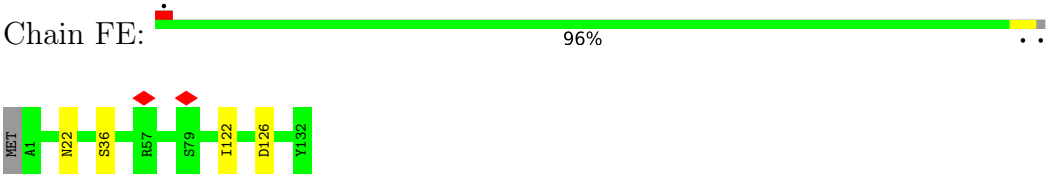
• Molecule 1: Capsid protein

Chain FD:



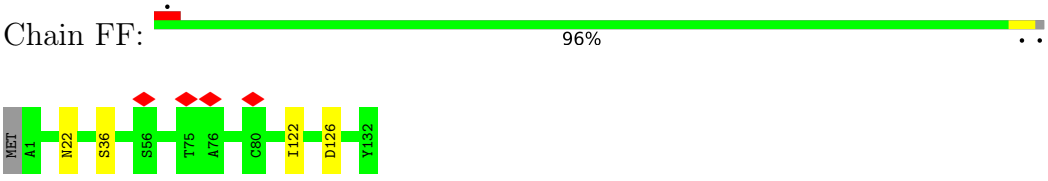
• Molecule 1: Capsid protein

Chain FE:



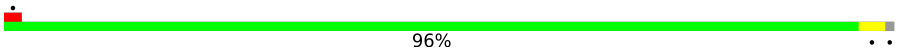
• Molecule 1: Capsid protein

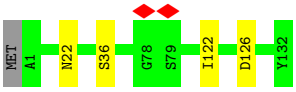
Chain FF:



• Molecule 1: Capsid protein

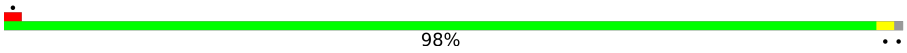
Chain AF:

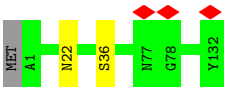




• Molecule 1: Capsid protein

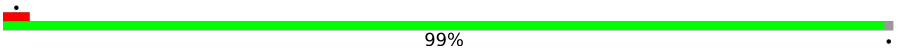
Chain FH:

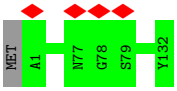




• Molecule 1: Capsid protein

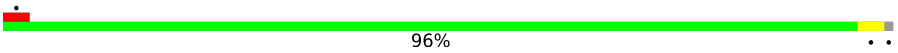
Chain FI:

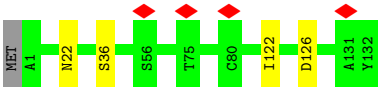




• Molecule 1: Capsid protein

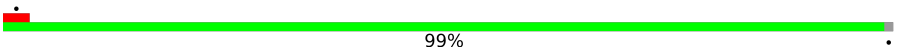
Chain FJ:

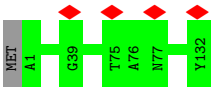




• Molecule 1: Capsid protein

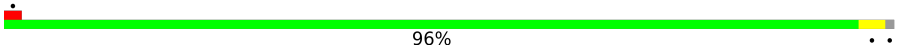
Chain FK:

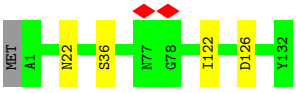




• Molecule 1: Capsid protein

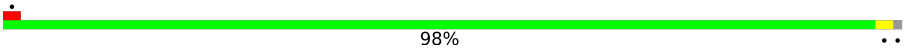
Chain FL:

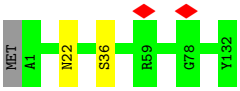




• Molecule 1: Capsid protein

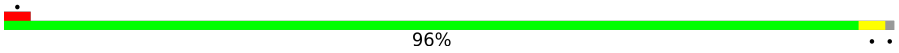
Chain FM:

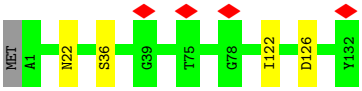




• Molecule 1: Capsid protein

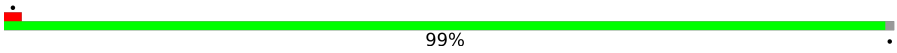
Chain FN:

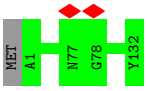




• Molecule 1: Capsid protein

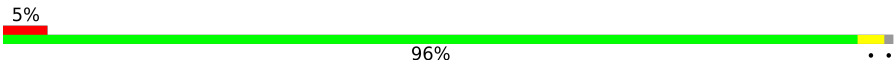
Chain GA:

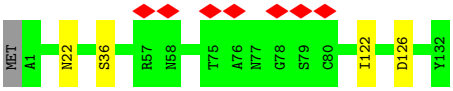




• Molecule 1: Capsid protein

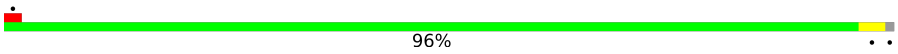
Chain GB:

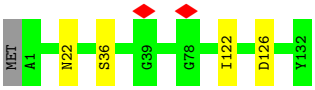




• Molecule 1: Capsid protein

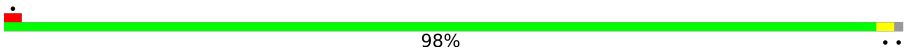
Chain GC:

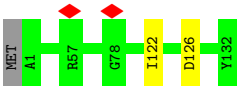




• Molecule 1: Capsid protein

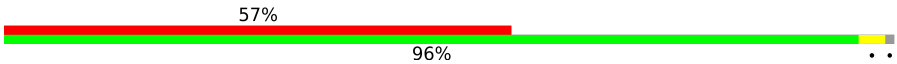
Chain AG:

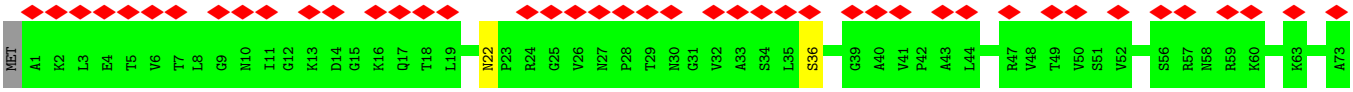


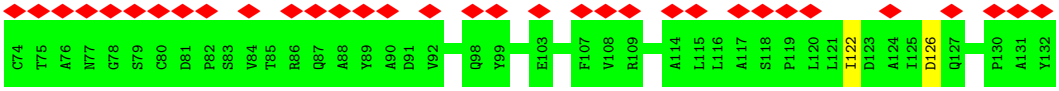


• Molecule 1: Capsid protein

Chain GD:

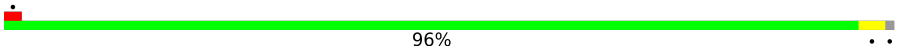


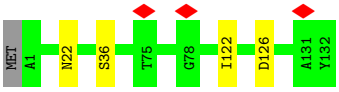




• Molecule 1: Capsid protein

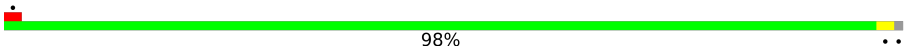
Chain GE:

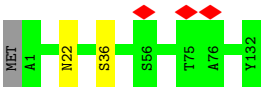




• Molecule 1: Capsid protein

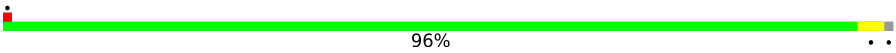
Chain GF:

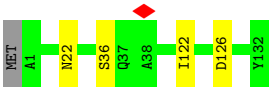




• Molecule 1: Capsid protein

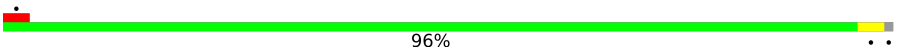
Chain GG:

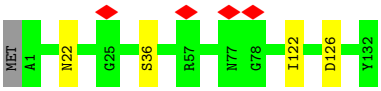




• Molecule 1: Capsid protein

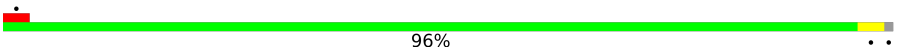
Chain GH:

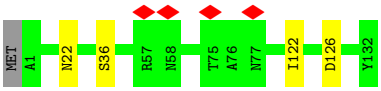




• Molecule 1: Capsid protein

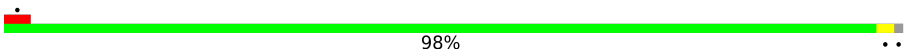
Chain GI:

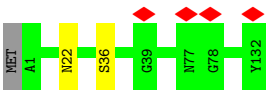




• Molecule 1: Capsid protein

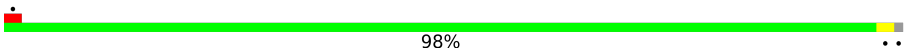
Chain GJ:





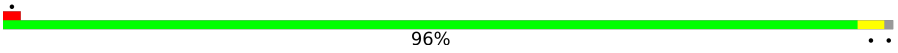
• Molecule 1: Capsid protein

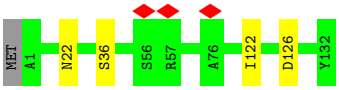
Chain GK:



• Molecule 1: Capsid protein

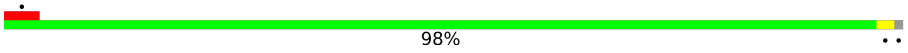
Chain GL:

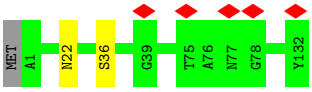




• Molecule 1: Capsid protein

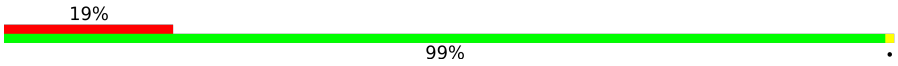
Chain GM:

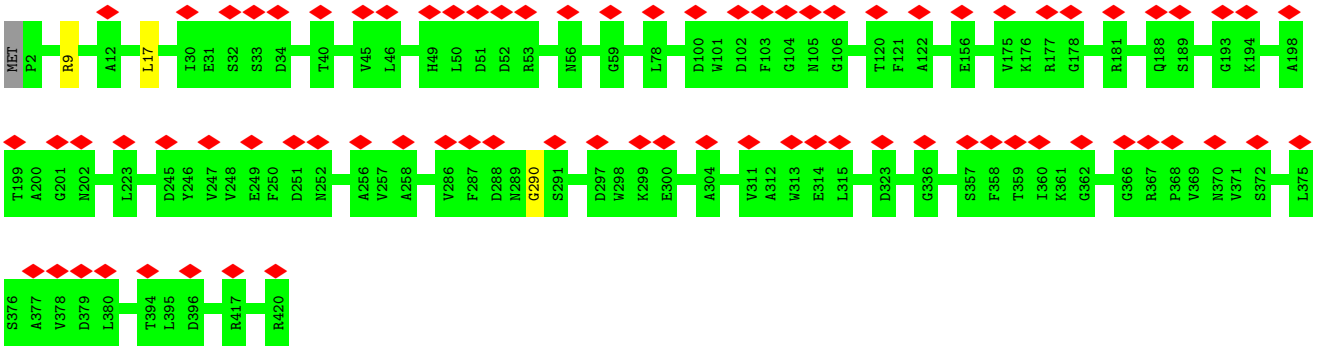




• Molecule 2: Maturation protein A2

Chain EJ:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	46471	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL 3200FSC	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	1	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	30000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.075	Depositor
Minimum map value	-0.044	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	389.12, 389.12, 389.12	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.216, 1.216, 1.216	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	AA	0.38	0/528	0.55	0/657
1	AB	0.38	0/528	0.55	0/657
1	AC	0.38	0/528	0.55	0/657
1	AD	0.38	0/528	0.55	0/657
1	AE	0.38	0/528	0.55	0/657
1	AF	0.38	0/528	0.55	0/657
1	AG	0.38	0/528	0.55	0/657
1	AH	0.38	0/528	0.55	0/657
1	AI	0.38	0/528	0.55	0/657
1	AJ	0.38	0/528	0.55	0/657
1	AK	0.38	0/528	0.55	0/657
1	AL	0.38	0/528	0.55	0/657
1	AM	0.38	0/528	0.55	0/657
1	AN	0.38	0/528	0.55	0/657
1	BA	0.38	0/528	0.54	0/657
1	BB	0.38	0/528	0.55	0/657
1	BC	0.38	0/528	0.55	0/657
1	BD	0.38	0/528	0.55	0/657
1	BE	0.38	0/528	0.55	0/657
1	BF	0.38	0/528	0.55	0/657
1	BG	0.38	0/528	0.55	0/657
1	BH	0.38	0/528	0.55	0/657
1	BI	0.38	0/528	0.54	0/657
1	BJ	0.38	0/528	0.55	0/657
1	BK	0.38	0/528	0.55	0/657
1	BL	0.38	0/528	0.55	0/657
1	BM	0.38	0/528	0.55	0/657
1	BN	0.38	0/528	0.55	0/657
1	CA	0.38	0/528	0.55	0/657
1	CB	0.38	0/528	0.55	0/657
1	CC	0.38	0/528	0.55	0/657
1	CD	0.38	0/528	0.55	0/657
1	CE	0.38	0/528	0.55	0/657
1	CF	0.38	0/528	0.55	0/657

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	CG	0.38	0/528	0.55	0/657
1	CH	0.38	0/528	0.54	0/657
1	CI	0.38	0/528	0.55	0/657
1	CJ	0.38	0/528	0.55	0/657
1	CK	0.38	0/528	0.55	0/657
1	CL	0.38	0/528	0.55	0/657
1	CM	0.38	0/528	0.55	0/657
1	CN	0.38	0/528	0.55	0/657
1	DA	0.38	0/528	0.55	0/657
1	DB	0.38	0/528	0.55	0/657
1	DC	0.38	0/528	0.55	0/657
1	DD	0.38	0/528	0.55	0/657
1	DE	0.38	0/528	0.55	0/657
1	DF	0.38	0/528	0.55	0/657
1	DG	0.38	0/528	0.55	0/657
1	DH	0.38	0/528	0.54	0/657
1	DI	0.37	0/528	0.55	0/657
1	DJ	0.38	0/528	0.55	0/657
1	DK	0.38	0/528	0.55	0/657
1	DL	0.38	0/528	0.55	0/657
1	DN	0.38	0/528	0.55	0/657
1	EA	0.38	0/528	0.55	0/657
1	EB	0.38	0/528	0.55	0/657
1	EC	0.38	0/528	0.55	0/657
1	ED	0.38	0/528	0.55	0/657
1	EE	0.38	0/528	0.55	0/657
1	EF	0.38	0/528	0.55	0/657
1	EG	0.38	0/528	0.55	0/657
1	EH	0.38	0/528	0.55	0/657
1	EI	0.38	0/528	0.55	0/657
1	EK	0.38	0/528	0.55	0/657
1	EL	0.38	0/528	0.55	0/657
1	EM	0.38	0/528	0.55	0/657
1	EN	0.38	0/528	0.55	0/657
1	FA	0.38	0/528	0.55	0/657
1	FB	0.38	0/528	0.55	0/657
1	FC	0.38	0/528	0.55	0/657
1	FD	0.38	0/528	0.55	0/657
1	FE	0.38	0/528	0.55	0/657
1	FF	0.38	0/528	0.55	0/657
1	FH	0.38	0/528	0.55	0/657
1	FI	0.38	0/528	0.55	0/657
1	FJ	0.38	0/528	0.55	0/657

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	FK	0.38	0/528	0.55	0/657
1	FL	0.38	0/528	0.55	0/657
1	FM	0.38	0/528	0.55	0/657
1	FN	0.38	0/528	0.55	0/657
1	GA	0.38	0/528	0.55	0/657
1	GB	0.38	0/528	0.55	0/657
1	GC	0.38	0/528	0.55	0/657
1	GD	0.38	0/528	0.55	0/657
1	GE	0.38	0/528	0.55	0/657
1	GF	0.38	0/528	0.55	0/657
1	GG	0.38	0/528	0.55	0/657
1	GH	0.38	0/528	0.55	0/657
1	GI	0.38	0/528	0.55	0/657
1	GJ	0.38	0/528	0.55	0/657
1	GK	0.38	0/528	0.55	0/657
1	GL	0.38	0/528	0.55	0/657
1	GM	0.38	0/528	0.55	0/657
1	GN	0.38	0/528	0.55	0/657
1	HA	0.38	0/528	0.54	0/657
1	HB	0.38	0/528	0.55	0/657
1	HC	0.38	0/528	0.55	0/657
1	HD	0.38	0/528	0.55	0/657
1	HE	0.38	0/528	0.55	0/657
1	HF	0.38	0/528	0.55	0/657
1	HG	0.38	0/528	0.55	0/657
1	HH	0.38	0/528	0.55	0/657
1	HI	0.38	0/528	0.55	0/657
1	HJ	0.38	0/528	0.55	0/657
1	HK	0.38	0/528	0.54	0/657
1	HL	0.38	0/528	0.55	0/657
1	HM	0.38	0/528	0.55	0/657
1	HN	0.38	0/528	0.55	0/657
1	IA	0.38	0/528	0.55	0/657
1	IB	0.38	0/528	0.54	0/657
1	IC	0.38	0/528	0.55	0/657
1	ID	0.38	0/528	0.55	0/657
1	IE	0.38	0/528	0.55	0/657
1	IF	0.38	0/528	0.55	0/657
1	IG	0.37	0/528	0.55	0/657
1	IH	0.38	0/528	0.55	0/657
1	II	0.38	0/528	0.55	0/657
1	IJ	0.38	0/528	0.55	0/657
1	IK	0.38	0/528	0.54	0/657

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	IL	0.38	0/528	0.55	0/657
1	IM	0.38	0/528	0.55	0/657
1	IN	0.38	0/528	0.55	0/657
1	JA	0.38	0/528	0.55	0/657
1	JB	0.38	0/528	0.54	0/657
1	JC	0.38	0/528	0.55	0/657
1	JD	0.38	0/528	0.55	0/657
1	JE	0.38	0/528	0.55	0/657
1	JF	0.38	0/528	0.54	0/657
1	JG	0.38	0/528	0.55	0/657
1	JH	0.38	0/528	0.55	0/657
1	JI	0.38	0/528	0.55	0/657
1	JJ	0.38	0/528	0.55	0/657
1	JK	0.38	0/528	0.55	0/657
1	JL	0.38	0/528	0.55	0/657
1	JM	0.38	0/528	0.55	0/657
1	JN	0.38	0/528	0.55	0/657
1	KA	0.38	0/528	0.55	0/657
1	KB	0.38	0/528	0.55	0/657
1	KC	0.38	0/528	0.55	0/657
1	KD	0.38	0/528	0.55	0/657
1	KE	0.38	0/528	0.55	0/657
1	KF	0.38	0/528	0.55	0/657
1	KG	0.38	0/528	0.55	0/657
1	KH	0.38	0/528	0.55	0/657
1	KI	0.38	0/528	0.55	0/657
1	KJ	0.38	0/528	0.55	0/657
1	KK	0.38	0/528	0.55	0/657
1	KL	0.38	0/528	0.55	0/657
1	KM	0.38	0/528	0.55	0/657
1	KN	0.38	0/528	0.54	0/657
1	LA	0.38	0/528	0.55	0/657
1	LB	0.38	0/528	0.55	0/657
1	LC	0.38	0/528	0.55	0/657
1	LD	0.38	0/528	0.55	0/657
1	LE	0.38	0/528	0.55	0/657
1	LF	0.38	0/528	0.55	0/657
1	LG	0.38	0/528	0.55	0/657
1	LH	0.38	0/528	0.55	0/657
1	LI	0.38	0/528	0.54	0/657
1	LJ	0.38	0/528	0.55	0/657
1	LK	0.38	0/528	0.55	0/657
1	LL	0.38	0/528	0.55	0/657

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	LM	0.38	0/528	0.55	0/657
1	LN	0.38	0/528	0.55	0/657
1	MA	0.38	0/528	0.55	0/657
1	MB	0.38	0/528	0.54	0/657
1	MC	0.38	0/528	0.55	0/657
1	MD	0.38	0/528	0.55	0/657
1	ME	0.38	0/528	0.55	0/657
1	MF	0.38	0/528	0.55	0/657
1	MG	0.38	0/528	0.55	0/657
1	MH	0.38	0/528	0.55	0/657
1	MI	0.38	0/528	0.55	0/657
1	MJ	0.38	0/528	0.55	0/657
1	MK	0.38	0/528	0.55	0/657
1	ML	0.38	0/528	0.55	0/657
1	MM	0.38	0/528	0.55	0/657
1	MN	0.38	0/528	0.55	0/657
1	NA	0.38	0/528	0.55	0/657
2	EJ	0.27	0/1676	0.58	0/2092
All	All	0.38	0/96716	0.55	0/120352

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	529	0	140	1	0
1	AB	529	0	140	2	0
1	AC	529	0	140	1	0
1	AD	529	0	140	1	0
1	AE	529	0	140	1	0
1	AF	529	0	140	2	0
1	AG	529	0	140	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AH	529	0	140	1	0
1	AI	529	0	140	1	0
1	AJ	529	0	140	2	0
1	AK	529	0	140	2	0
1	AL	529	0	140	1	0
1	AM	529	0	140	2	0
1	AN	529	0	140	2	0
1	BA	529	0	140	1	0
1	BB	529	0	140	1	0
1	BC	529	0	140	0	0
1	BD	529	0	140	1	0
1	BE	529	0	140	2	0
1	BF	529	0	140	2	0
1	BG	529	0	140	1	0
1	BH	529	0	140	2	0
1	BI	529	0	140	2	0
1	BJ	529	0	140	2	0
1	BK	529	0	140	2	0
1	BL	529	0	140	2	0
1	BM	529	0	140	1	0
1	BN	529	0	140	2	0
1	CA	529	0	140	2	0
1	CB	529	0	140	2	0
1	CC	529	0	140	0	0
1	CD	529	0	140	1	0
1	CE	529	0	140	1	0
1	CF	529	0	140	2	0
1	CG	529	0	140	0	0
1	CH	529	0	140	2	0
1	CI	529	0	140	2	0
1	CJ	529	0	140	0	0
1	CK	529	0	140	2	0
1	CL	529	0	140	2	0
1	CM	529	0	140	2	0
1	CN	529	0	140	2	0
1	DA	529	0	140	2	0
1	DB	529	0	140	2	0
1	DC	529	0	140	1	0
1	DD	529	0	140	0	0
1	DE	529	0	140	1	0
1	DF	529	0	140	0	0
1	DG	529	0	140	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	DH	529	0	140	2	0
1	DI	529	0	140	2	0
1	DJ	529	0	140	3	0
1	DK	529	0	140	1	0
1	DL	529	0	140	2	0
1	DN	529	0	140	3	0
1	EA	529	0	140	2	0
1	EB	529	0	140	2	0
1	EC	529	0	140	4	0
1	ED	529	0	140	2	0
1	EE	529	0	140	2	0
1	EF	529	0	140	1	0
1	EG	529	0	140	2	0
1	EH	529	0	140	1	0
1	EI	529	0	140	2	0
1	EK	529	0	140	1	0
1	EL	529	0	140	1	0
1	EM	529	0	140	2	0
1	EN	529	0	140	2	0
1	FA	529	0	140	1	0
1	FB	529	0	140	1	0
1	FC	529	0	140	1	0
1	FD	529	0	140	2	0
1	FE	529	0	140	2	0
1	FF	529	0	140	2	0
1	FH	529	0	140	1	0
1	FI	529	0	140	0	0
1	FJ	529	0	140	2	0
1	FK	529	0	140	0	0
1	FL	529	0	140	2	0
1	FM	529	0	140	1	0
1	FN	529	0	140	2	0
1	GA	529	0	140	0	0
1	GB	529	0	140	2	0
1	GC	529	0	140	2	0
1	GD	529	0	140	2	0
1	GE	529	0	140	2	0
1	GF	529	0	140	1	0
1	GG	529	0	140	2	0
1	GH	529	0	140	2	0
1	GI	529	0	140	2	0
1	GJ	529	0	140	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	GK	529	0	140	1	0
1	GL	529	0	140	2	0
1	GM	529	0	140	1	0
1	GN	529	0	140	1	0
1	HA	529	0	140	2	0
1	HB	529	0	140	2	0
1	HC	529	0	140	0	0
1	HD	529	0	140	1	0
1	HE	529	0	140	1	0
1	HF	529	0	140	1	0
1	HG	529	0	140	2	0
1	HH	529	0	140	2	0
1	HI	529	0	140	1	0
1	HJ	529	0	140	1	0
1	HK	529	0	140	1	0
1	HL	529	0	140	2	0
1	HM	529	0	140	1	0
1	HN	529	0	140	1	0
1	IA	529	0	140	1	0
1	IB	529	0	140	1	0
1	IC	529	0	140	2	0
1	ID	529	0	140	1	0
1	IE	529	0	140	2	0
1	IF	529	0	140	2	0
1	IG	529	0	140	0	0
1	IH	529	0	140	1	0
1	II	529	0	140	1	0
1	IJ	529	0	140	2	0
1	IK	529	0	140	2	0
1	IL	529	0	140	2	0
1	IM	529	0	140	2	0
1	IN	529	0	140	2	0
1	JA	529	0	140	2	0
1	JB	529	0	140	1	0
1	JC	529	0	140	1	0
1	JD	529	0	140	1	0
1	JE	529	0	140	1	0
1	JF	529	0	140	1	0
1	JG	529	0	140	1	0
1	JH	529	0	140	2	0
1	JI	529	0	140	2	0
1	JJ	529	0	140	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	JK	529	0	140	2	0
1	JL	529	0	140	0	0
1	JM	529	0	140	2	0
1	JN	529	0	140	2	0
1	KA	529	0	140	0	0
1	KB	529	0	140	1	0
1	KC	529	0	140	2	0
1	KD	529	0	140	2	0
1	KE	529	0	140	2	0
1	KF	529	0	140	2	0
1	KG	529	0	140	1	0
1	KH	529	0	140	2	0
1	KI	529	0	140	2	0
1	KJ	529	0	140	2	0
1	KK	529	0	140	1	0
1	KL	529	0	140	2	0
1	KM	529	0	140	1	0
1	KN	529	0	140	1	0
1	LA	529	0	140	1	0
1	LB	529	0	140	0	0
1	LC	529	0	140	1	0
1	LD	529	0	140	2	0
1	LE	529	0	140	1	0
1	LF	529	0	140	1	0
1	LG	529	0	140	1	0
1	LH	529	0	140	2	0
1	LI	529	0	140	1	0
1	LJ	529	0	140	2	0
1	LK	529	0	140	2	0
1	LL	529	0	140	1	0
1	LM	529	0	140	1	0
1	LN	529	0	140	1	0
1	MA	529	0	140	0	0
1	MB	529	0	140	1	0
1	MC	529	0	140	2	0
1	MD	529	0	140	1	0
1	ME	529	0	140	1	0
1	MF	529	0	140	2	0
1	MG	529	0	140	1	0
1	MH	529	0	140	0	0
1	MI	529	0	140	2	0
1	MJ	529	0	140	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	MK	529	0	140	1	0
1	ML	529	0	140	1	0
1	MM	529	0	140	1	0
1	MN	529	0	140	1	0
1	NA	529	0	140	1	0
2	EJ	1677	0	456	1	0
All	All	96897	0	25656	255	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (255) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DN:76:ALA:O	1:EC:78:GLY:O	2.27	0.52
1:EC:76:ALA:O	1:EE:78:GLY:O	2.30	0.48
1:JD:22:ASN:N	1:JD:36:SER:O	2.44	0.47
1:KL:22:ASN:N	1:KL:36:SER:O	2.44	0.47
1:CL:22:ASN:N	1:CL:36:SER:O	2.44	0.47
1:HD:22:ASN:N	1:HD:36:SER:O	2.44	0.47
1:IN:22:ASN:N	1:IN:36:SER:O	2.44	0.47
1:LM:22:ASN:N	1:LM:36:SER:O	2.44	0.47
1:GJ:22:ASN:N	1:GJ:36:SER:O	2.44	0.47
1:HH:22:ASN:N	1:HH:36:SER:O	2.44	0.46
1:KK:22:ASN:N	1:KK:36:SER:O	2.44	0.46
1:DB:22:ASN:N	1:DB:36:SER:O	2.44	0.46
1:BD:22:ASN:N	1:BD:36:SER:O	2.44	0.46
1:IK:22:ASN:N	1:IK:36:SER:O	2.44	0.46
1:GD:22:ASN:N	1:GD:36:SER:O	2.44	0.46
1:BI:22:ASN:N	1:BI:36:SER:O	2.44	0.46
1:BB:22:ASN:N	1:BB:36:SER:O	2.44	0.46
1:FF:22:ASN:N	1:FF:36:SER:O	2.44	0.46
1:KI:22:ASN:N	1:KI:36:SER:O	2.44	0.46
1:KM:22:ASN:N	1:KM:36:SER:O	2.44	0.46
1:LE:22:ASN:N	1:LE:36:SER:O	2.44	0.46
1:GC:22:ASN:N	1:GC:36:SER:O	2.44	0.46
1:IM:22:ASN:N	1:IM:36:SER:O	2.44	0.45
1:KJ:22:ASN:N	1:KJ:36:SER:O	2.44	0.45
1:IE:22:ASN:N	1:IE:36:SER:O	2.44	0.45
1:LF:22:ASN:N	1:LF:36:SER:O	2.44	0.45
1:LK:22:ASN:N	1:LK:36:SER:O	2.44	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DA:22:ASN:N	1:DA:36:SER:O	2.44	0.45
1:EM:22:ASN:N	1:EM:36:SER:O	2.44	0.45
1:KB:22:ASN:N	1:KB:36:SER:O	2.44	0.45
1:EE:22:ASN:N	1:EE:36:SER:O	2.44	0.45
1:GB:22:ASN:N	1:GB:36:SER:O	2.44	0.45
1:JN:22:ASN:N	1:JN:36:SER:O	2.44	0.45
1:KC:22:ASN:N	1:KC:36:SER:O	2.44	0.45
1:EC:22:ASN:N	1:EC:36:SER:O	2.44	0.45
1:FH:22:ASN:N	1:FH:36:SER:O	2.44	0.45
1:ID:22:ASN:N	1:ID:36:SER:O	2.44	0.45
1:MC:22:ASN:N	1:MC:36:SER:O	2.44	0.45
1:IL:22:ASN:N	1:IL:36:SER:O	2.44	0.45
1:KE:22:ASN:N	1:KE:36:SER:O	2.44	0.45
1:ED:22:ASN:N	1:ED:36:SER:O	2.44	0.45
1:EI:22:ASN:N	1:EI:36:SER:O	2.44	0.45
1:FL:22:ASN:N	1:FL:36:SER:O	2.44	0.45
1:FN:22:ASN:N	1:FN:36:SER:O	2.44	0.45
1:HN:22:ASN:N	1:HN:36:SER:O	2.44	0.45
1:JM:22:ASN:N	1:JM:36:SER:O	2.44	0.45
1:LD:22:ASN:N	1:LD:36:SER:O	2.44	0.45
1:EF:22:ASN:N	1:EF:36:SER:O	2.44	0.45
1:IC:22:ASN:N	1:IC:36:SER:O	2.44	0.45
1:ED:122:ILE:O	1:ED:126:ASP:N	2.48	0.45
1:FE:122:ILE:O	1:FE:126:ASP:N	2.48	0.45
1:HH:122:ILE:O	1:HH:126:ASP:N	2.48	0.45
1:AM:122:ILE:O	1:AM:126:ASP:N	2.48	0.45
1:CE:122:ILE:O	1:CE:126:ASP:N	2.48	0.45
1:EK:122:ILE:O	1:EK:126:ASP:N	2.48	0.45
1:EN:22:ASN:N	1:EN:36:SER:O	2.44	0.45
1:JA:22:ASN:N	1:JA:36:SER:O	2.44	0.45
1:DK:122:ILE:O	1:DK:126:ASP:N	2.48	0.45
1:JB:22:ASN:N	1:JB:36:SER:O	2.44	0.44
1:LN:122:ILE:O	1:LN:126:ASP:N	2.48	0.44
1:HL:122:ILE:O	1:HL:126:ASP:N	2.48	0.44
1:IN:122:ILE:O	1:IN:126:ASP:N	2.48	0.44
1:AK:122:ILE:O	1:AK:126:ASP:N	2.48	0.44
1:KD:22:ASN:N	1:KD:36:SER:O	2.44	0.44
1:MG:22:ASN:N	1:MG:36:SER:O	2.44	0.44
1:BN:122:ILE:O	1:BN:126:ASP:N	2.48	0.44
1:DI:122:ILE:O	1:DI:126:ASP:N	2.48	0.44
1:GM:22:ASN:N	1:GM:36:SER:O	2.44	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:HG:22:ASN:N	1:HG:36:SER:O	2.44	0.44
1:DJ:22:ASN:N	1:DJ:36:SER:O	2.44	0.44
1:EH:22:ASN:N	1:EH:36:SER:O	2.44	0.44
1:JH:122:ILE:O	1:JH:126:ASP:N	2.48	0.44
1:JK:22:ASN:N	1:JK:36:SER:O	2.44	0.44
1:IJ:22:ASN:N	1:IJ:36:SER:O	2.44	0.44
1:AK:22:ASN:N	1:AK:36:SER:O	2.44	0.44
1:MF:122:ILE:O	1:MF:126:ASP:N	2.48	0.44
1:CI:22:ASN:N	1:CI:36:SER:O	2.44	0.44
1:FF:122:ILE:O	1:FF:126:ASP:N	2.48	0.44
1:GG:22:ASN:N	1:GG:36:SER:O	2.44	0.44
1:BA:22:ASN:N	1:BA:36:SER:O	2.44	0.44
1:BH:22:ASN:N	1:BH:36:SER:O	2.44	0.44
1:CA:22:ASN:N	1:CA:36:SER:O	2.44	0.44
1:CD:22:ASN:N	1:CD:36:SER:O	2.44	0.44
1:DH:22:ASN:N	1:DH:36:SER:O	2.44	0.44
1:DL:122:ILE:O	1:DL:126:ASP:N	2.48	0.44
1:GK:22:ASN:N	1:GK:36:SER:O	2.44	0.44
1:GN:22:ASN:N	1:GN:36:SER:O	2.44	0.44
1:DE:22:ASN:N	1:DE:36:SER:O	2.44	0.44
1:FB:22:ASN:N	1:FB:36:SER:O	2.44	0.44
1:FE:22:ASN:N	1:FE:36:SER:O	2.44	0.44
1:AF:22:ASN:N	1:AF:36:SER:O	2.44	0.44
1:HB:122:ILE:O	1:HB:126:ASP:N	2.48	0.44
1:LI:22:ASN:N	1:LI:36:SER:O	2.44	0.44
1:DI:22:ASN:N	1:DI:36:SER:O	2.44	0.44
1:GD:122:ILE:O	1:GD:126:ASP:N	2.48	0.44
1:IF:122:ILE:O	1:IF:126:ASP:N	2.48	0.43
1:MI:22:ASN:N	1:MI:36:SER:O	2.44	0.43
1:MJ:22:ASN:N	1:MJ:36:SER:O	2.44	0.43
1:BL:22:ASN:N	1:BL:36:SER:O	2.44	0.43
1:EG:22:ASN:N	1:EG:36:SER:O	2.44	0.43
1:HF:22:ASN:N	1:HF:36:SER:O	2.44	0.43
1:IB:22:ASN:N	1:IB:36:SER:O	2.44	0.43
1:AJ:122:ILE:O	1:AJ:126:ASP:N	2.48	0.43
1:AM:22:ASN:N	1:AM:36:SER:O	2.44	0.43
1:KH:122:ILE:O	1:KH:126:ASP:N	2.48	0.43
1:CF:122:ILE:O	1:CF:126:ASP:N	2.48	0.43
1:EL:22:ASN:N	1:EL:36:SER:O	2.44	0.43
1:EN:122:ILE:O	1:EN:126:ASP:N	2.48	0.43
1:GI:22:ASN:N	1:GI:36:SER:O	2.44	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:122:ILE:O	1:CA:126:ASP:N	2.48	0.43
1:AB:22:ASN:N	1:AB:36:SER:O	2.44	0.43
1:DN:22:ASN:N	1:DN:36:SER:O	2.44	0.43
1:GE:122:ILE:O	1:GE:126:ASP:N	2.48	0.43
1:IH:122:ILE:O	1:IH:126:ASP:N	2.48	0.43
1:AN:122:ILE:O	1:AN:126:ASP:N	2.48	0.43
1:BF:22:ASN:N	1:BF:36:SER:O	2.44	0.43
1:BK:122:ILE:O	1:BK:126:ASP:N	2.48	0.43
1:BN:22:ASN:N	1:BN:36:SER:O	2.44	0.43
1:JC:22:ASN:N	1:JC:36:SER:O	2.44	0.43
1:CF:22:ASN:N	1:CF:36:SER:O	2.44	0.43
1:DJ:122:ILE:O	1:DJ:126:ASP:N	2.48	0.43
1:DN:122:ILE:O	1:DN:126:ASP:N	2.48	0.43
1:EB:122:ILE:O	1:EB:126:ASP:N	2.48	0.43
1:FD:122:ILE:O	1:FD:126:ASP:N	2.48	0.43
1:GC:122:ILE:O	1:GC:126:ASP:N	2.48	0.43
1:JF:122:ILE:O	1:JF:126:ASP:N	2.48	0.43
1:LA:122:ILE:O	1:LA:126:ASP:N	2.48	0.43
1:LC:122:ILE:O	1:LC:126:ASP:N	2.48	0.43
1:CN:122:ILE:O	1:CN:126:ASP:N	2.48	0.43
1:IK:122:ILE:O	1:IK:126:ASP:N	2.48	0.43
1:KF:122:ILE:O	1:KF:126:ASP:N	2.48	0.43
1:KJ:122:ILE:O	1:KJ:126:ASP:N	2.48	0.43
1:NA:122:ILE:O	1:NA:126:ASP:N	2.48	0.43
1:DB:122:ILE:O	1:DB:126:ASP:N	2.48	0.43
1:FD:22:ASN:N	1:FD:36:SER:O	2.44	0.43
1:AG:122:ILE:O	1:AG:126:ASP:N	2.48	0.43
1:LG:22:ASN:N	1:LG:36:SER:O	2.44	0.43
1:FA:22:ASN:N	1:FA:36:SER:O	2.44	0.43
1:GI:122:ILE:O	1:GI:126:ASP:N	2.48	0.43
1:JG:22:ASN:N	1:JG:36:SER:O	2.44	0.43
1:JJ:22:ASN:N	1:JJ:36:SER:O	2.44	0.43
1:KD:122:ILE:O	1:KD:126:ASP:N	2.48	0.43
1:KF:22:ASN:N	1:KF:36:SER:O	2.44	0.43
1:LL:122:ILE:O	1:LL:126:ASP:N	2.48	0.43
1:GL:122:ILE:O	1:GL:126:ASP:N	2.48	0.43
1:HI:22:ASN:N	1:HI:36:SER:O	2.44	0.42
1:JE:22:ASN:N	1:JE:36:SER:O	2.44	0.42
1:JN:122:ILE:O	1:JN:126:ASP:N	2.48	0.42
1:DC:22:ASN:N	1:DC:36:SER:O	2.44	0.42
1:EG:122:ILE:O	1:EG:126:ASP:N	2.48	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FC:22:ASN:N	1:FC:36:SER:O	2.44	0.42
1:AF:122:ILE:O	1:AF:126:ASP:N	2.48	0.42
1:AI:122:ILE:O	1:AI:126:ASP:N	2.48	0.42
1:BE:22:ASN:N	1:BE:36:SER:O	2.44	0.42
1:IC:122:ILE:O	1:IC:126:ASP:N	2.48	0.42
1:LD:122:ILE:O	1:LD:126:ASP:N	2.48	0.42
1:ME:122:ILE:O	1:ME:126:ASP:N	2.48	0.42
1:CH:22:ASN:N	1:CH:36:SER:O	2.44	0.42
1:CM:122:ILE:O	1:CM:126:ASP:N	2.48	0.42
1:CN:22:ASN:N	1:CN:36:SER:O	2.44	0.42
1:AD:122:ILE:O	1:AD:126:ASP:N	2.48	0.42
1:GB:122:ILE:O	1:GB:126:ASP:N	2.48	0.42
1:IE:122:ILE:O	1:IE:126:ASP:N	2.48	0.42
1:IL:122:ILE:O	1:IL:126:ASP:N	2.48	0.42
1:JH:22:ASN:N	1:JH:36:SER:O	2.44	0.42
1:AL:22:ASN:N	1:AL:36:SER:O	2.44	0.42
1:LJ:122:ILE:O	1:LJ:126:ASP:N	2.48	0.42
1:CM:22:ASN:N	1:CM:36:SER:O	2.44	0.42
1:KC:122:ILE:O	1:KC:126:ASP:N	2.48	0.42
1:DH:122:ILE:O	1:DH:126:ASP:N	2.48	0.42
2:EJ:9:ARG:N	2:EJ:17:LEU:O	2.39	0.42
1:FL:122:ILE:O	1:FL:126:ASP:N	2.48	0.42
1:JA:122:ILE:O	1:JA:126:ASP:N	2.48	0.42
1:LK:122:ILE:O	1:LK:126:ASP:N	2.48	0.42
1:MC:122:ILE:O	1:MC:126:ASP:N	2.48	0.42
1:BI:122:ILE:O	1:BI:126:ASP:N	2.48	0.42
1:EA:22:ASN:N	1:EA:36:SER:O	2.44	0.42
1:AE:122:ILE:O	1:AE:126:ASP:N	2.48	0.42
1:HK:22:ASN:N	1:HK:36:SER:O	2.44	0.42
1:JK:122:ILE:O	1:JK:126:ASP:N	2.48	0.42
1:EC:122:ILE:O	1:EC:126:ASP:N	2.48	0.42
1:FN:122:ILE:O	1:FN:126:ASP:N	2.48	0.42
1:LH:122:ILE:O	1:LH:126:ASP:N	2.48	0.42
1:GG:122:ILE:O	1:GG:126:ASP:N	2.48	0.42
1:AH:22:ASN:N	1:AH:36:SER:O	2.44	0.42
1:IA:122:ILE:O	1:IA:126:ASP:N	2.48	0.42
1:KE:122:ILE:O	1:KE:126:ASP:N	2.48	0.42
1:BE:122:ILE:O	1:BE:126:ASP:N	2.48	0.42
1:BF:122:ILE:O	1:BF:126:ASP:N	2.48	0.42
1:GF:22:ASN:N	1:GF:36:SER:O	2.44	0.42
1:HA:122:ILE:O	1:HA:126:ASP:N	2.48	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:MB:122:ILE:O	1:MB:126:ASP:N	2.48	0.42
1:BK:22:ASN:N	1:BK:36:SER:O	2.44	0.42
1:FJ:22:ASN:N	1:FJ:36:SER:O	2.44	0.42
1:ML:122:ILE:O	1:ML:126:ASP:N	2.48	0.41
1:HA:22:ASN:N	1:HA:36:SER:O	2.44	0.41
1:HG:122:ILE:O	1:HG:126:ASP:N	2.48	0.41
1:MF:22:ASN:N	1:MF:36:SER:O	2.44	0.41
1:CI:122:ILE:O	1:CI:126:ASP:N	2.48	0.41
1:BL:122:ILE:O	1:BL:126:ASP:N	2.48	0.41
1:AC:22:ASN:N	1:AC:36:SER:O	2.44	0.41
1:EI:122:ILE:O	1:EI:126:ASP:N	2.48	0.41
1:GH:22:ASN:N	1:GH:36:SER:O	2.44	0.41
1:HB:22:ASN:N	1:HB:36:SER:O	2.44	0.41
1:JI:22:ASN:N	1:JI:36:SER:O	2.44	0.41
1:JI:122:ILE:O	1:JI:126:ASP:N	2.48	0.41
1:MD:22:ASN:N	1:MD:36:SER:O	2.44	0.41
1:BH:122:ILE:O	1:BH:126:ASP:N	2.48	0.41
1:HE:22:ASN:N	1:HE:36:SER:O	2.44	0.41
1:HJ:22:ASN:N	1:HJ:36:SER:O	2.44	0.41
1:HM:22:ASN:N	1:HM:36:SER:O	2.44	0.41
1:KN:22:ASN:N	1:KN:36:SER:O	2.44	0.41
1:BJ:22:ASN:N	1:BJ:36:SER:O	2.44	0.41
1:CK:22:ASN:N	1:CK:36:SER:O	2.44	0.41
1:EM:122:ILE:O	1:EM:126:ASP:N	2.48	0.41
1:GL:22:ASN:N	1:GL:36:SER:O	2.44	0.41
1:KG:22:ASN:N	1:KG:36:SER:O	2.44	0.41
1:AN:22:ASN:N	1:AN:36:SER:O	2.44	0.41
1:BM:122:ILE:O	1:BM:126:ASP:N	2.48	0.41
1:EB:22:ASN:N	1:EB:36:SER:O	2.44	0.41
1:GH:122:ILE:O	1:GH:126:ASP:N	2.48	0.41
1:IF:22:ASN:N	1:IF:36:SER:O	2.44	0.41
1:IM:122:ILE:O	1:IM:126:ASP:N	2.48	0.41
1:AA:22:ASN:N	1:AA:36:SER:O	2.44	0.41
1:EA:122:ILE:O	1:EA:126:ASP:N	2.48	0.41
1:HL:22:ASN:N	1:HL:36:SER:O	2.44	0.41
1:AJ:22:ASN:N	1:AJ:36:SER:O	2.44	0.41
1:KH:22:ASN:N	1:KH:36:SER:O	2.44	0.41
1:MI:122:ILE:O	1:MI:126:ASP:N	2.48	0.41
1:BJ:122:ILE:O	1:BJ:126:ASP:N	2.48	0.41
1:CH:122:ILE:O	1:CH:126:ASP:N	2.48	0.41
1:DA:122:ILE:O	1:DA:126:ASP:N	2.48	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DG:22:ASN:N	1:DG:36:SER:O	2.44	0.41
1:FJ:122:ILE:O	1:FJ:126:ASP:N	2.48	0.41
1:KI:122:ILE:O	1:KI:126:ASP:N	2.48	0.41
1:LJ:22:ASN:N	1:LJ:36:SER:O	2.44	0.41
1:MJ:122:ILE:O	1:MJ:126:ASP:N	2.48	0.41
1:MM:122:ILE:O	1:MM:126:ASP:N	2.48	0.41
1:BG:22:ASN:N	1:BG:36:SER:O	2.44	0.41
1:CK:78:GLY:O	1:DJ:76:ALA:O	2.39	0.41
1:JM:122:ILE:O	1:JM:126:ASP:N	2.48	0.40
1:MK:122:ILE:O	1:MK:126:ASP:N	2.48	0.40
1:CL:122:ILE:O	1:CL:126:ASP:N	2.48	0.40
1:DG:122:ILE:O	1:DG:126:ASP:N	2.48	0.40
1:DL:22:ASN:N	1:DL:36:SER:O	2.44	0.40
1:AB:122:ILE:O	1:AB:126:ASP:N	2.48	0.40
1:LH:22:ASN:N	1:LH:36:SER:O	2.44	0.40
1:CB:22:ASN:N	1:CB:36:SER:O	2.44	0.40
1:GE:22:ASN:N	1:GE:36:SER:O	2.44	0.40
1:II:22:ASN:N	1:II:36:SER:O	2.44	0.40
1:IJ:122:ILE:O	1:IJ:126:ASP:N	2.48	0.40
1:KL:122:ILE:O	1:KL:126:ASP:N	2.48	0.40
1:MN:122:ILE:O	1:MN:126:ASP:N	2.48	0.40
1:CB:122:ILE:O	1:CB:126:ASP:N	2.48	0.40
1:FM:22:ASN:N	1:FM:36:SER:O	2.44	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AA	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	AB	130/133 (98%)	122 (94%)	8 (6%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AC	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	AD	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	AE	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	AF	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	AG	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	AH	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	AI	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	AJ	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	AK	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	AL	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	AM	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	AN	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	BA	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	BB	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	BC	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	BD	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	BE	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	BF	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	BG	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	BH	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	BI	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	BJ	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	BK	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	BL	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	BM	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	BN	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	CA	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	CB	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	CC	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	CD	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	CE	130/133 (98%)	122 (94%)	8 (6%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	CF	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	CG	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	CH	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	CI	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	CJ	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	CK	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	CL	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	CM	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	CN	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	DA	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	DB	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	DC	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	DD	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	DE	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	DF	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	DG	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	DH	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	DI	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	DJ	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	DK	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	DL	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	DN	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	EA	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	EB	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	EC	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	ED	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	EE	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	EF	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	EG	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	EH	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	EI	130/133 (98%)	122 (94%)	8 (6%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	EK	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	EL	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	EM	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	EN	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	FA	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	FB	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	FC	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	FD	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	FE	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	FF	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	FH	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	FI	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	FJ	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	FK	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	FL	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	FM	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	FN	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	GA	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	GB	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	GC	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	GD	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	GE	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	GF	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	GG	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	GH	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	GI	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	GJ	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	GK	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	GL	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	GM	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	GN	130/133 (98%)	122 (94%)	8 (6%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	HA	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	HB	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	HC	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	HD	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	HE	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	HF	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	HG	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	HH	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	HI	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	HJ	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	HK	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	HL	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	HM	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	HN	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	IA	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	IB	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	IC	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	ID	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	IE	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	IF	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	IG	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	IH	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	II	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	IJ	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	IK	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	IL	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	IM	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	IN	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	JA	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	JB	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	JC	130/133 (98%)	122 (94%)	8 (6%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	JD	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	JE	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	JF	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	JG	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	JH	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	JI	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	JJ	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	JK	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	JL	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	JM	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	JN	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	KA	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	KB	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	KC	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	KD	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	KE	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	KF	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	KG	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	KH	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	KI	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	KJ	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	KK	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	KL	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	KM	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	KN	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	LA	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	LB	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	LC	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	LD	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	LE	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	LF	130/133 (98%)	122 (94%)	8 (6%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	LG	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	LH	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	LI	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	LJ	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	LK	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	LL	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	LM	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	LN	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	MA	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	MB	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	MC	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	MD	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	ME	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	MF	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	MG	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	MH	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	MI	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	MJ	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	MK	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	ML	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	MM	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	MN	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
1	NA	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
2	EJ	417/420 (99%)	399 (96%)	17 (4%)	1 (0%)	47	81
All	All	23817/24360 (98%)	22359 (94%)	1457 (6%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	EJ	290	GLY

5.3.2 Protein sidechains

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

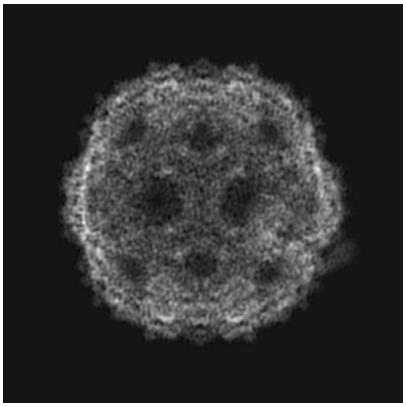
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-8709. These allow visual inspection of the internal detail of the map and identification of artifacts.

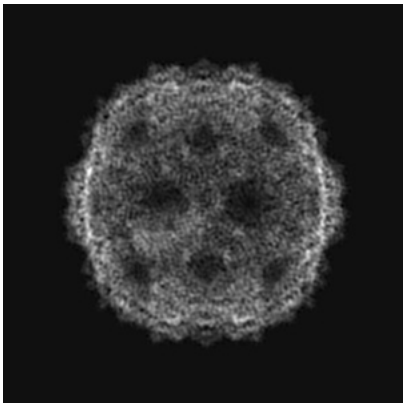
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

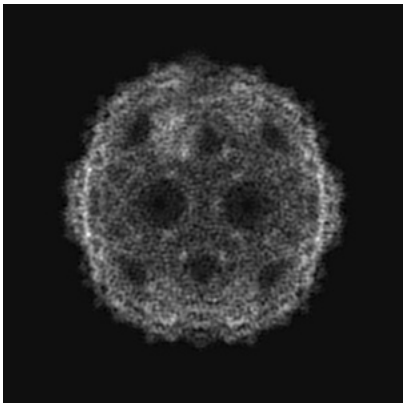
6.1.1 Primary map



X



Y

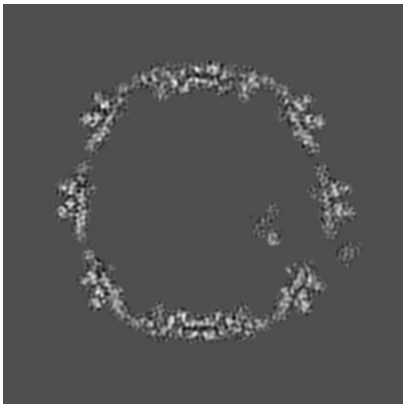


Z

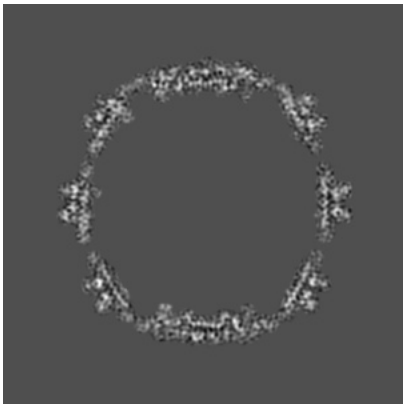
The images above show the map projected in three orthogonal directions.

6.2 Central slices

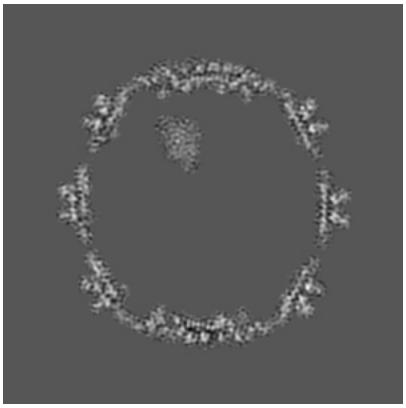
6.2.1 Primary map



X Index: 160



Y Index: 160

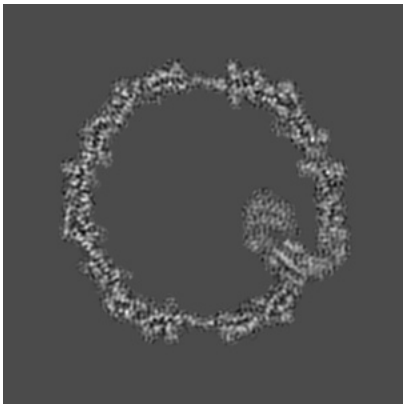


Z Index: 160

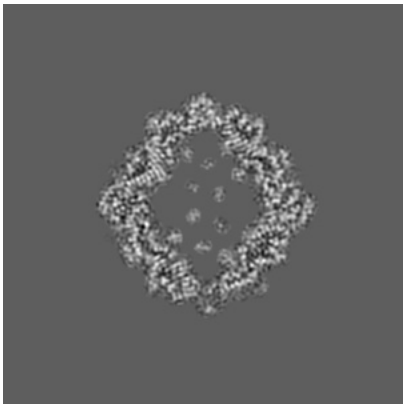
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

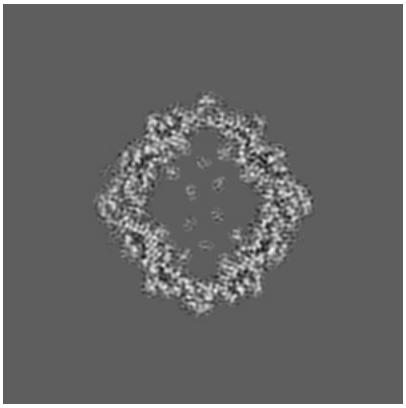
6.3.1 Primary map



X Index: 136



Y Index: 76

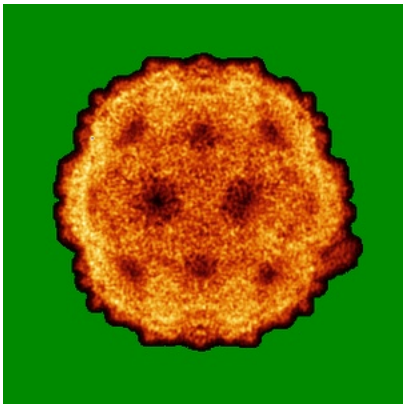


Z Index: 243

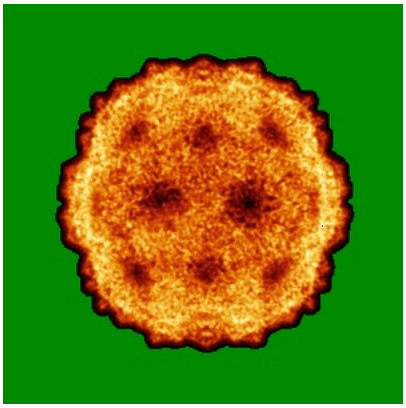
The images above show the largest variance slices of the map in three orthogonal directions.

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

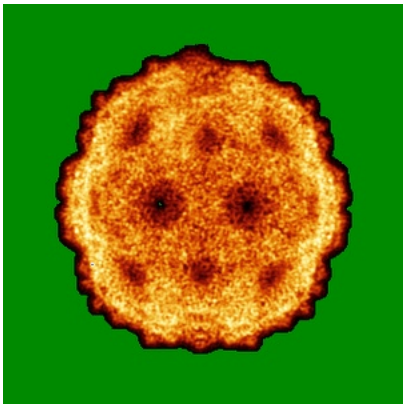
6.4.1 Primary map



X



Y

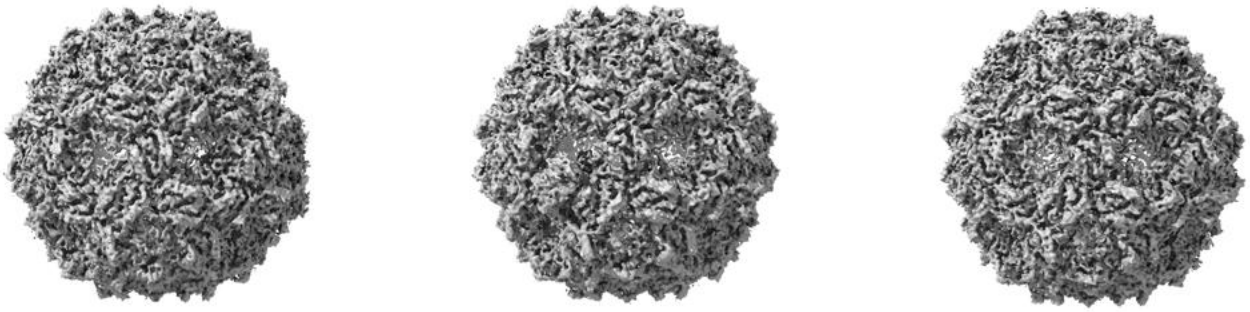


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

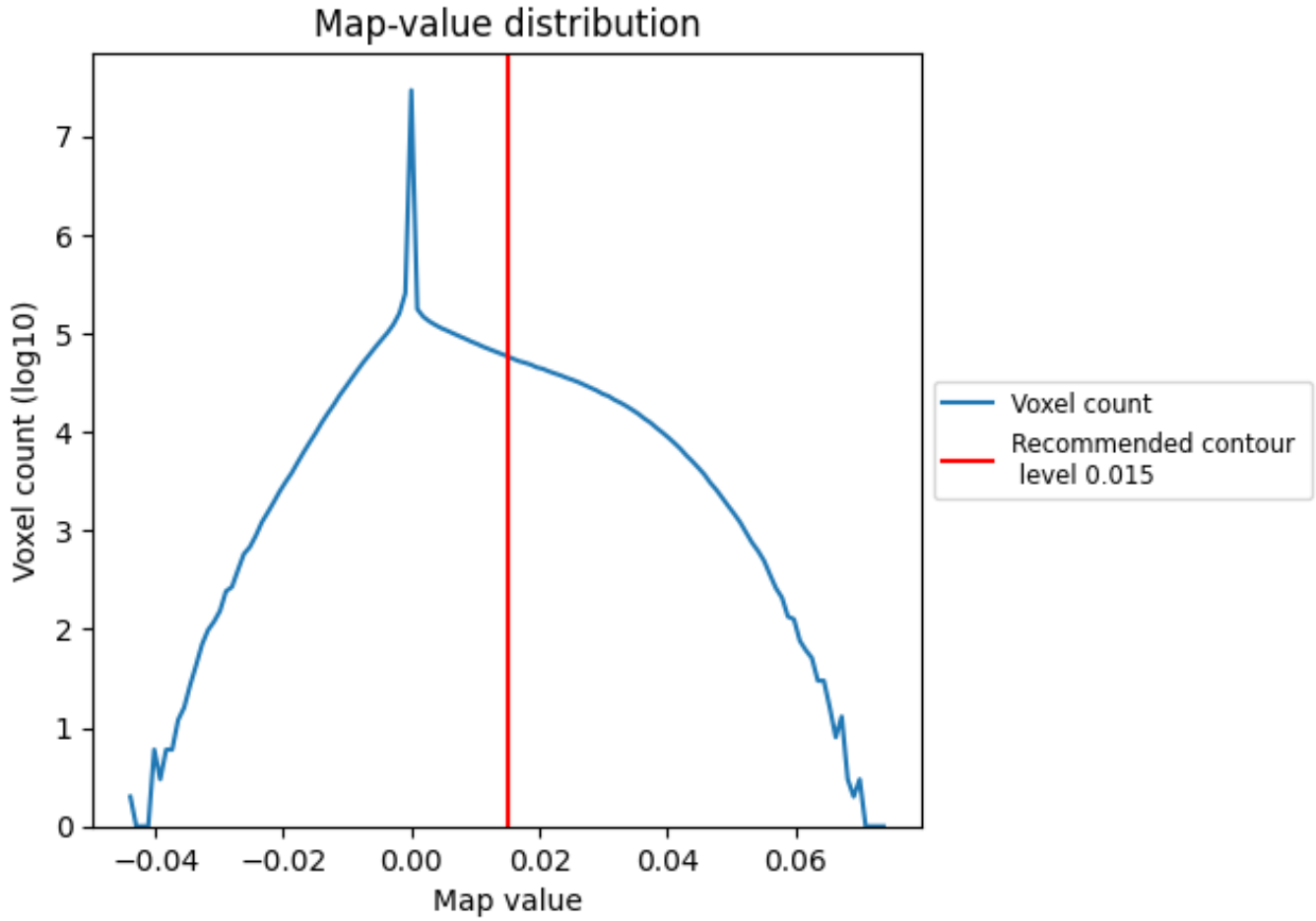
6.6 Mask visualisation (i)

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

7 Map analysis

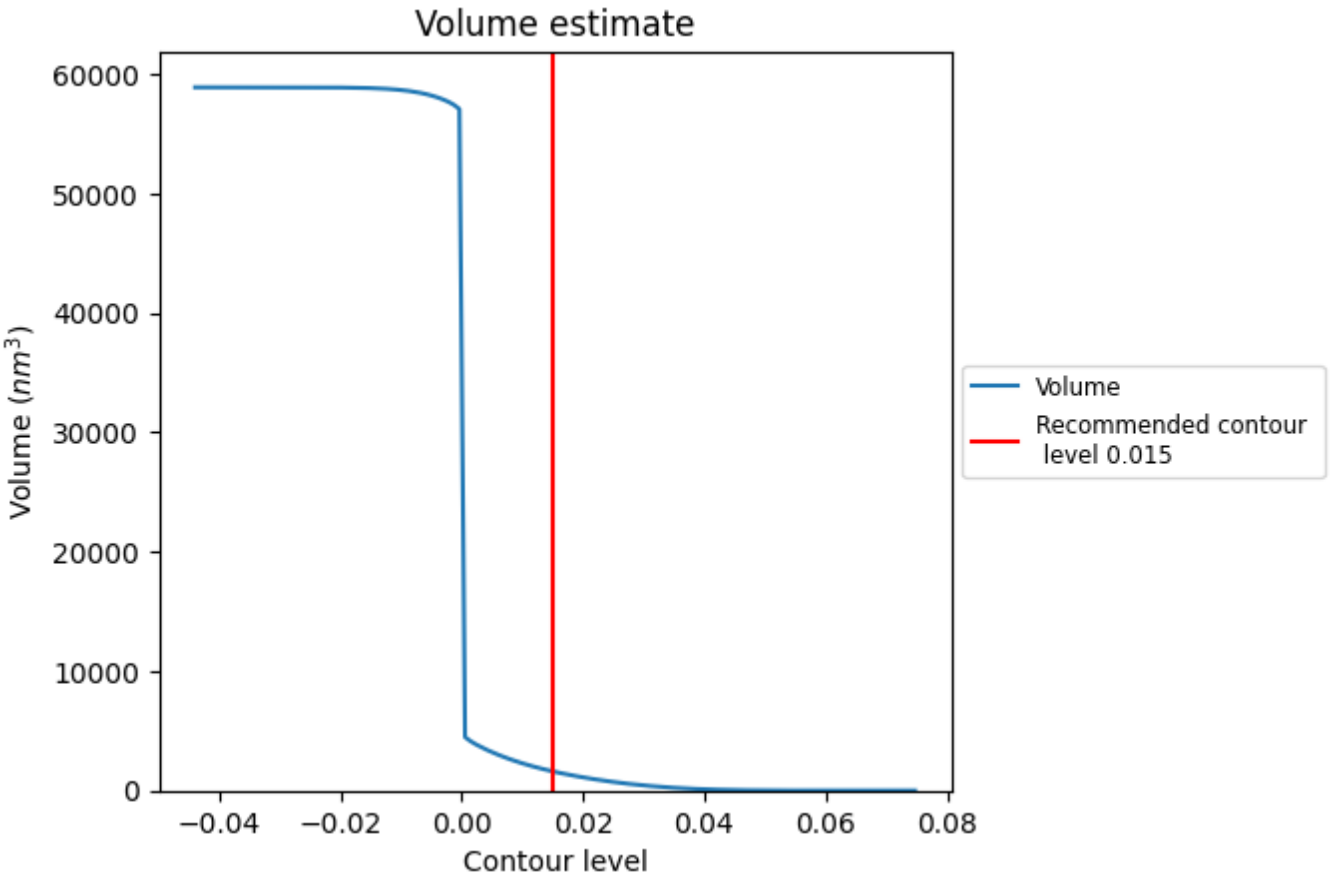
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

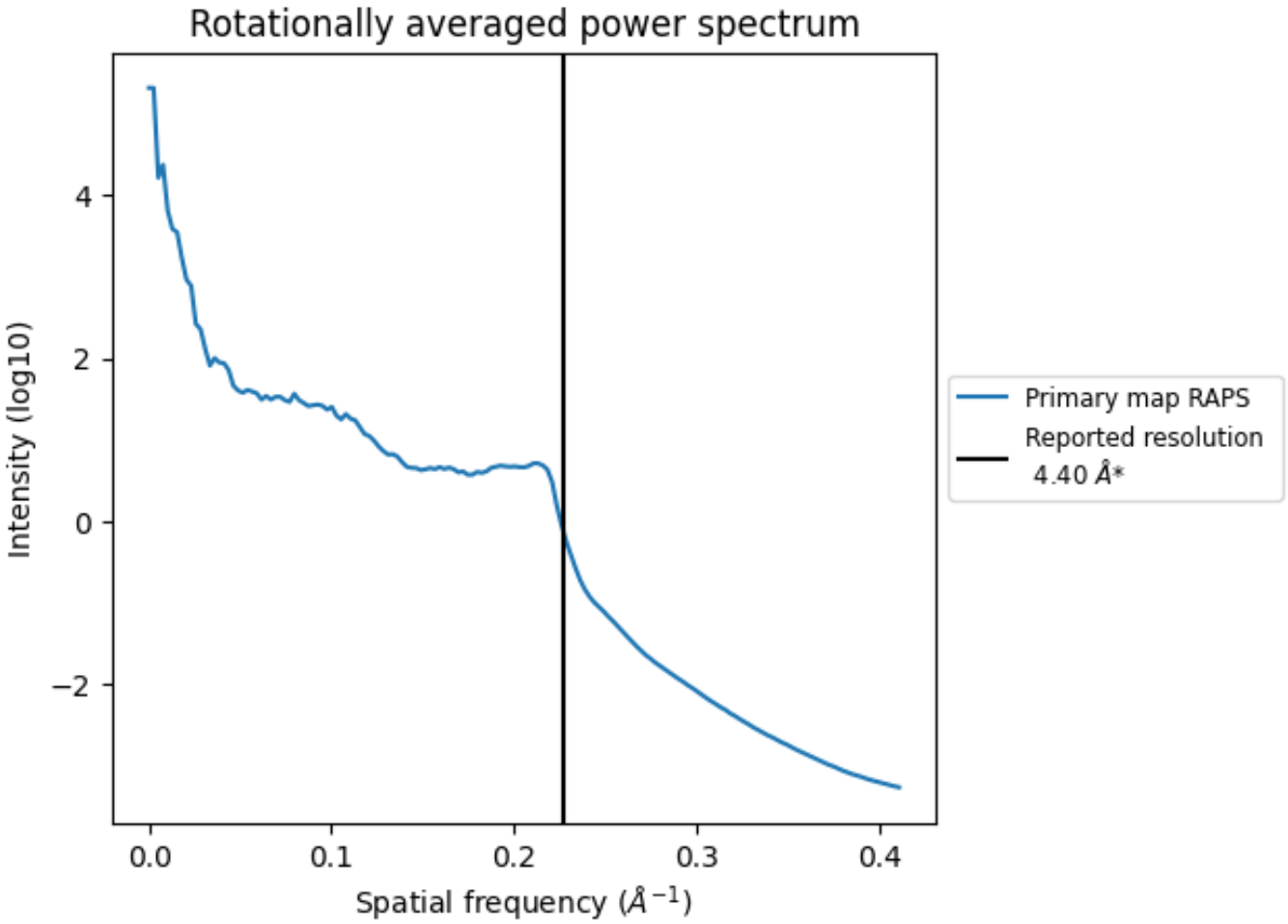
7.2 Volume estimate (i)



The volume at the recommended contour level is 1612 nm^3; this corresponds to an approximate mass of 1456 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 0.227 $Å^{-1}$

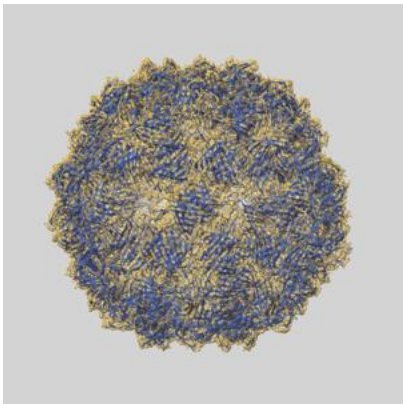
8 Fourier-Shell correlation (i)

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

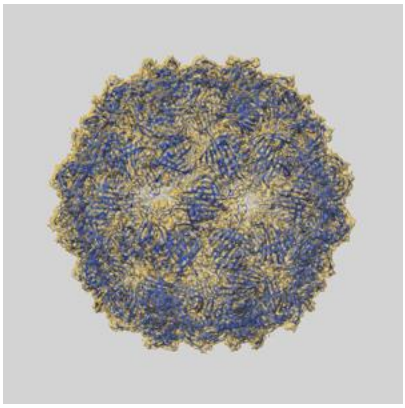
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-8709 and PDB model 5VLZ. Per-residue inclusion information can be found in section 3 on page 19.

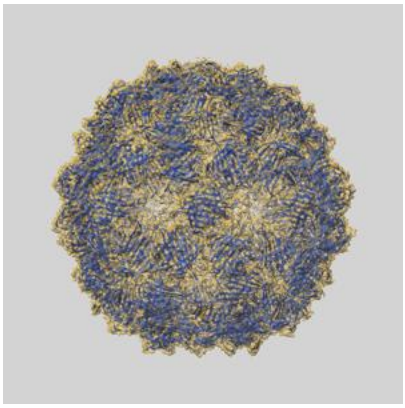
9.1 Map-model overlay



X



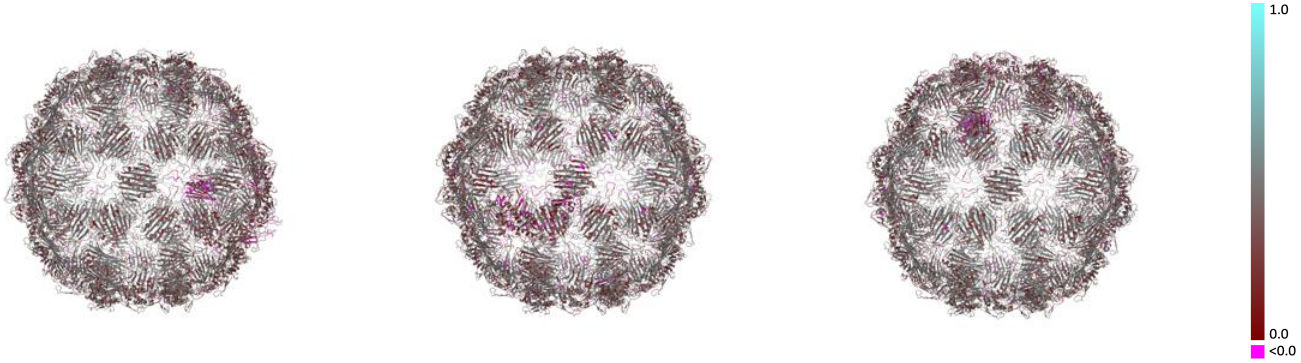
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.015 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.

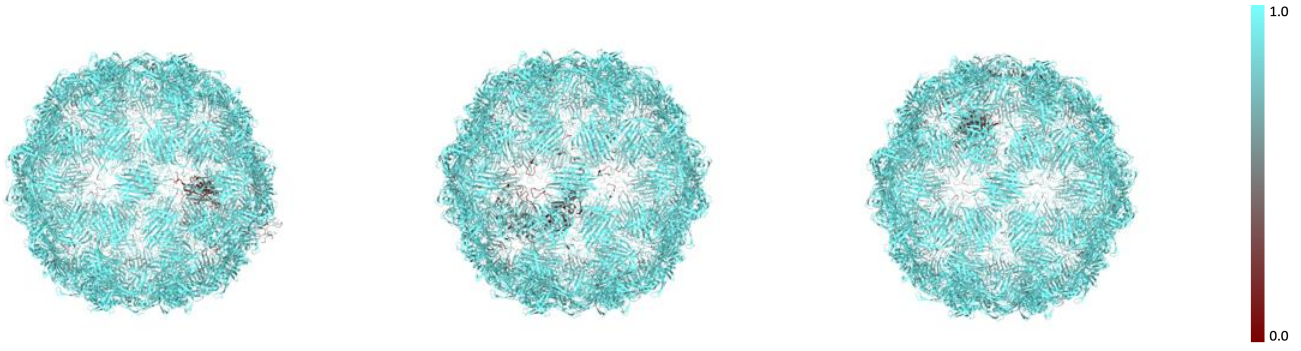
9.2 Q-score mapped to coordinate model



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.

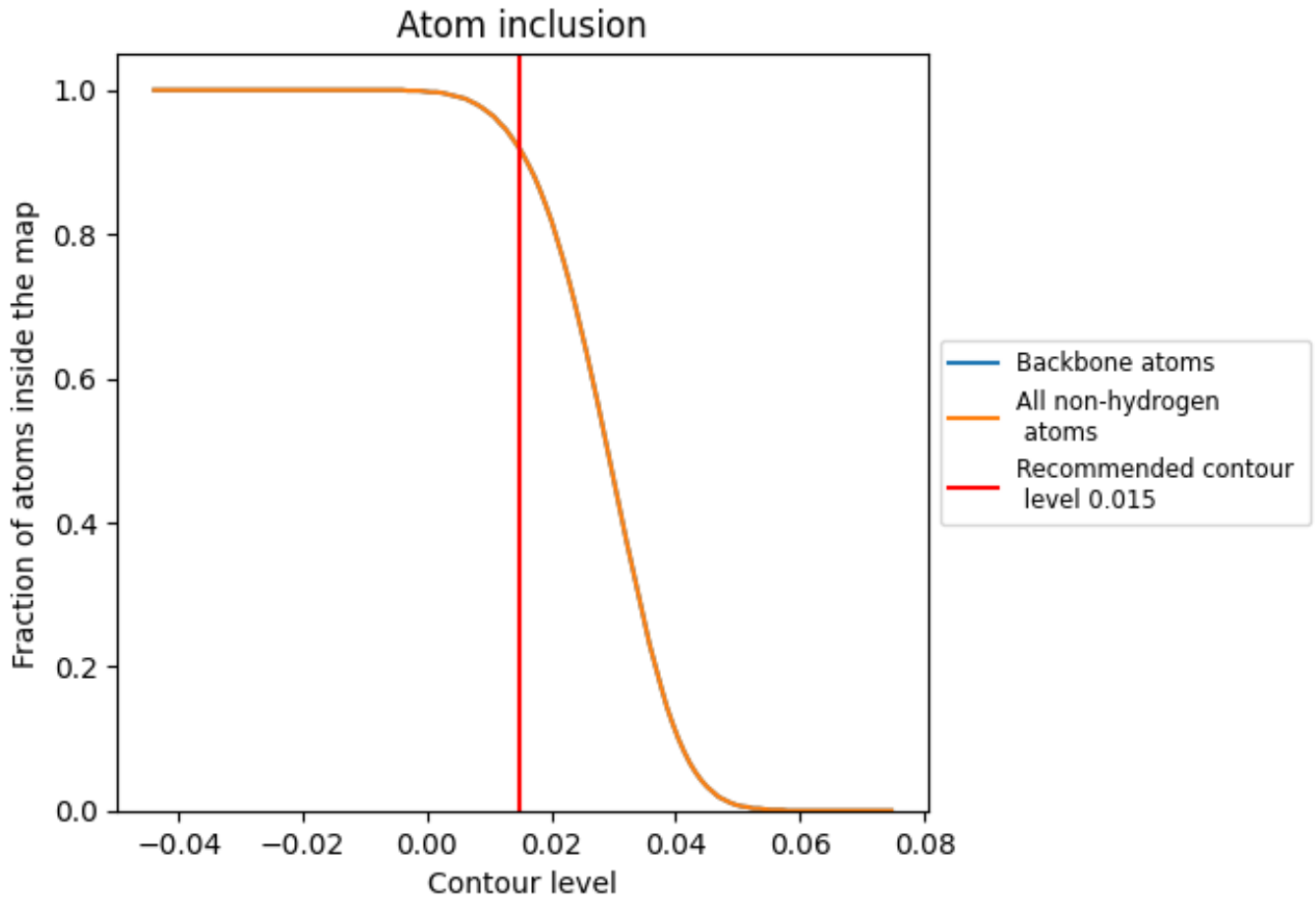
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.015).

9.4 Atom inclusion (i)



At the recommended contour level, 92% of all backbone atoms, 92% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9170	0.3730
AA	0.9400	0.3730
AB	0.9130	0.3790
AC	0.9360	0.3870
AD	0.9400	0.3780
AE	0.9170	0.3720
AF	0.9580	0.4050
AG	0.9410	0.3910
AH	0.9220	0.3720
AI	0.9360	0.3830
AJ	0.9340	0.3720
AK	0.9240	0.3790
AL	0.9090	0.3950
AM	0.9320	0.3920
AN	0.9400	0.4000
BA	0.9340	0.3970
BB	0.9490	0.3930
BC	0.9490	0.3930
BD	0.9170	0.3920
BE	0.9280	0.3880
BF	0.9410	0.3850
BG	0.9210	0.3640
BH	0.9400	0.3910
BI	0.9340	0.3920
BJ	0.9470	0.3870
BK	0.9210	0.3690
BL	0.9410	0.3940
BM	0.9260	0.3830
BN	0.9000	0.3610
CA	0.9470	0.3920
CB	0.9190	0.3830
CC	0.9190	0.3680
CD	0.9450	0.3830
CE	0.9130	0.3720
CF	0.9620	0.4000

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
CG	0.9400	0.3930
CH	0.9450	0.3730
CI	0.9260	0.3990
CJ	0.9110	0.3780
CK	0.8900	0.3430
CL	0.8090	0.2900
CM	0.8130	0.2820
CN	0.9360	0.3760
DA	0.8980	0.3260
DB	0.3630	0.0750
DC	0.9210	0.3600
DD	0.9430	0.3840
DE	0.9300	0.3760
DF	0.9260	0.3850
DG	0.9340	0.3580
DH	0.9360	0.3930
DI	0.9130	0.3660
DJ	0.9300	0.3600
DK	0.9210	0.3780
DL	0.8560	0.3300
DN	0.9070	0.3570
EA	0.8960	0.3400
EB	0.8490	0.3180
EC	0.9220	0.3680
ED	0.7900	0.2730
EE	0.9220	0.3750
EF	0.8660	0.3350
EG	0.9090	0.3810
EH	0.9470	0.3740
EI	0.9320	0.3760
EJ	0.7110	0.2090
EK	0.8920	0.3540
EL	0.9240	0.3660
EM	0.9530	0.3860
EN	0.9040	0.3640
FA	0.9380	0.3950
FB	0.9380	0.3970
FC	0.9130	0.3880
FD	0.9410	0.3930
FE	0.9400	0.3870
FF	0.9260	0.4090
FH	0.9410	0.3890

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
FI	0.9340	0.3860
FJ	0.9340	0.3800
FK	0.9360	0.3920
FL	0.9470	0.4070
FM	0.9380	0.3970
FN	0.9430	0.4050
GA	0.9470	0.3750
GB	0.9090	0.3890
GC	0.9320	0.3850
GD	0.3310	0.0910
GE	0.9380	0.3990
GF	0.9240	0.3900
GG	0.9490	0.3940
GH	0.9240	0.3920
GI	0.9190	0.3890
GJ	0.9380	0.3980
GK	0.9400	0.3840
GL	0.9400	0.3950
GM	0.9410	0.3830
GN	0.9400	0.4060
HA	0.9320	0.3840
HB	0.9220	0.3910
HC	0.9470	0.3920
HD	0.9300	0.3800
HE	0.9130	0.3790
HF	0.9430	0.3830
HG	0.9070	0.3640
HH	0.9340	0.3670
HI	0.9450	0.3870
HJ	0.9210	0.3590
HK	0.9360	0.3820
HL	0.9430	0.3930
HM	0.9050	0.3780
HN	0.9360	0.3820
IA	0.9400	0.3730
IB	0.9260	0.3930
IC	0.9430	0.3960
ID	0.9410	0.4050
IE	0.9280	0.3880
IF	0.9300	0.3920
IG	0.9410	0.3910
IH	0.9320	0.4000

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
II	0.9380	0.3820
IJ	0.9410	0.3890
IK	0.9260	0.3960
IL	0.9410	0.3920
IM	0.9450	0.4040
IN	0.9040	0.3670
JA	0.9360	0.3870
JB	0.9400	0.3990
JC	0.9190	0.3760
JD	0.9210	0.3520
JE	0.9260	0.3770
JF	0.9190	0.3700
JG	0.9410	0.3780
JH	0.9380	0.3740
JI	0.9300	0.3990
JJ	0.9170	0.3330
JK	0.8730	0.3400
JL	0.9190	0.3460
JM	0.8620	0.3110
JN	0.9170	0.3690
KA	0.9400	0.3850
KB	0.9130	0.3800
KC	0.9210	0.3840
KD	0.9510	0.3880
KE	0.9400	0.3950
KF	0.9280	0.3890
KG	0.9400	0.3910
KH	0.9700	0.4120
KI	0.9150	0.3780
KJ	0.9340	0.3790
KK	0.9360	0.3870
KL	0.9380	0.4060
KM	0.9550	0.4020
KN	0.9410	0.4020
LA	0.9240	0.3820
LB	0.9210	0.3710
LC	0.9490	0.4090
LD	0.9280	0.3900
LE	0.9430	0.3780
LF	0.9380	0.3730
LG	0.9150	0.3810
LH	0.9470	0.3940

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
LI	0.9260	0.3860
LJ	0.9380	0.3820
LK	0.9260	0.3810
LL	0.9510	0.3840
LM	0.9050	0.3790
LN	0.9340	0.3870
MA	0.9360	0.3840
MB	0.9190	0.3730
MC	0.9380	0.3840
MD	0.9240	0.3850
ME	0.9110	0.3730
MF	0.9340	0.3610
MG	0.9340	0.3850
MH	0.9380	0.3950
MI	0.9260	0.3890
MJ	0.9430	0.3780
MK	0.9240	0.3800
ML	0.9430	0.3750
MM	0.9450	0.3970
MN	0.9280	0.3760
NA	0.9340	0.3820