



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 03:52 PM UTC

PDB ID : 6H82 / pdb_00006h82
EMDB ID : EMD-0172
Title : Cryo-EM structure of the archaeal extremophilic internal membrane containing Haloarcula hispanica icosahedral virus 2 (HHIV-2) at 3.78 Angstroms resolution.
Authors : Abrescia, N.G.; Santos-Perez, I.; Charro, D.
Deposited on : 2018-08-01
Resolution : 3.78 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:

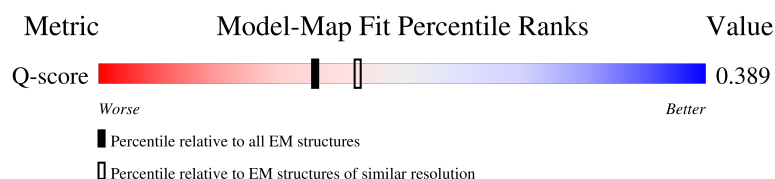
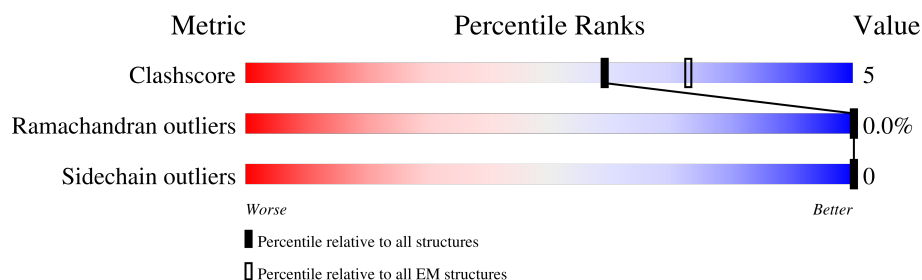
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 3.78 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10074 (3.28 - 4.27)

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

Mol	Chain	Length	Quality of chain
1	A	229	45% 93% 7%
1	B	229	45% 94% 6%
1	C	229	45% 90% 10%
1	G	229	34% 94% 6%

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Mol	Chain	Length	Quality of chain
1	H	229	33% 93% 7%
1	O	229	34% 93% 7%
1	P	229	36% 90% 10%
1	Q	229	39% 91% 9%
1	U	229	34% 93% 7%
1	V	229	41% 91% 9%
1	X	229	31% 92% 8%
1	Z	229	34% 91% 9%
2	D	172	36% 87% 13%
2	J	172	35% 85% 15%
2	T	172	38% 82% 18%
2	W	172	33% 84% 16%
3	E	175	38% 83% 17%
3	F	175	39% 85% 15%
3	K	175	35% 85% 15%
3	M	175	36% 84% 16%
3	N	175	37% 86% 14%
3	R	175	36% 84% 16%
3	S	175	34% 85% 15%
3	a	175	36% 85% 15%
4	I	161	31% 84% 16%
4	L	161	31% 84% 16%
4	Y	161	32% 86% 14%
5	b	135	34% 93% 6% ..
6	g	217	100% 99% .

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Mol	Chain	Length	Quality of chain
7	c	105	100%
			100%
7	d	105	100%
			99% .
8	m	25	100%
			100%

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 86022 atoms, of which 41714 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 VP4.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	229	Total	C	H	N	O	S	0	0
			3492	1125	1687	301	377	2		
1	C	229	Total	C	H	N	O	S	0	0
			3492	1125	1687	301	377	2		
1	B	229	Total	C	H	N	O	S	0	0
			3492	1125	1687	301	377	2		
1	Q	229	Total	C	H	N	O	S	0	0
			3492	1125	1687	301	377	2		
1	P	229	Total	C	H	N	O	S	0	0
			3492	1125	1687	301	377	2		
1	O	229	Total	C	H	N	O	S	0	0
			3492	1125	1687	301	377	2		
1	U	229	Total	C	H	N	O	S	0	0
			3492	1125	1687	301	377	2		
1	Z	229	Total	C	H	N	O	S	0	0
			3492	1125	1687	301	377	2		
1	V	229	Total	C	H	N	O	S	0	0
			3492	1125	1687	301	377	2		
1	H	229	Total	C	H	N	O	S	0	0
			3492	1125	1687	301	377	2		
1	G	229	Total	C	H	N	O	S	0	0
			3492	1125	1687	301	377	2		
1	X	229	Total	C	H	N	O	S	0	0
			3492	1125	1687	301	377	2		

- Molecule 2 is a protein called VP7.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	D	172	Total	C	H	N	O	S	0	0
			2541	797	1247	220	272	5		
2	T	172	Total	C	H	N	O	S	0	0
			2541	797	1247	220	272	5		
2	J	172	Total	C	H	N	O	S	0	0
			2541	797	1247	220	272	5		

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Mol	Chain	Residues	Atoms						AltConf	Trace
2	W	172	Total	C	H	N	O	S	0	0
			2541	797	1247	220	272	5		

- Molecule 3 is a protein called VP7.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	E	175	Total	C	H	N	O	S	0	0
			2598	813	1277	227	276	5		
3	F	175	Total	C	H	N	O	S	0	0
			2598	813	1277	227	276	5		
3	R	175	Total	C	H	N	O	S	0	0
			2598	813	1277	227	276	5		
3	S	175	Total	C	H	N	O	S	0	0
			2598	813	1277	227	276	5		
3	K	175	Total	C	H	N	O	S	0	0
			2598	813	1277	227	276	5		
3	M	175	Total	C	H	N	O	S	0	0
			2598	813	1277	227	276	5		
3	N	175	Total	C	H	N	O	S	0	0
			2598	813	1277	227	276	5		
3	a	175	Total	C	H	N	O	S	0	0
			2598	813	1277	227	276	5		

- Molecule 4 is a protein called VP7.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	L	161	Total	C	H	N	O	S	0	0
			2387	749	1172	208	253	5		
4	I	161	Total	C	H	N	O	S	0	0
			2387	749	1172	208	253	5		
4	Y	161	Total	C	H	N	O	S	0	0
			2387	749	1172	208	253	5		

- Molecule 5 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	b	135	Total	C	H	N	O	S	0	0
			1950	622	951	165	210	2		

- Molecule 6 is a protein called VP16 (vertex complex).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	g	217	Total	C	H	N	O	0	0
			1952	651	867	217	217		

- Molecule 7 is a protein called GPS III.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	c	105	Total	C	H	N	O	0	0
			943	315	418	105	105		
7	d	105	Total	C	H	N	O	0	0
			943	315	418	105	105		

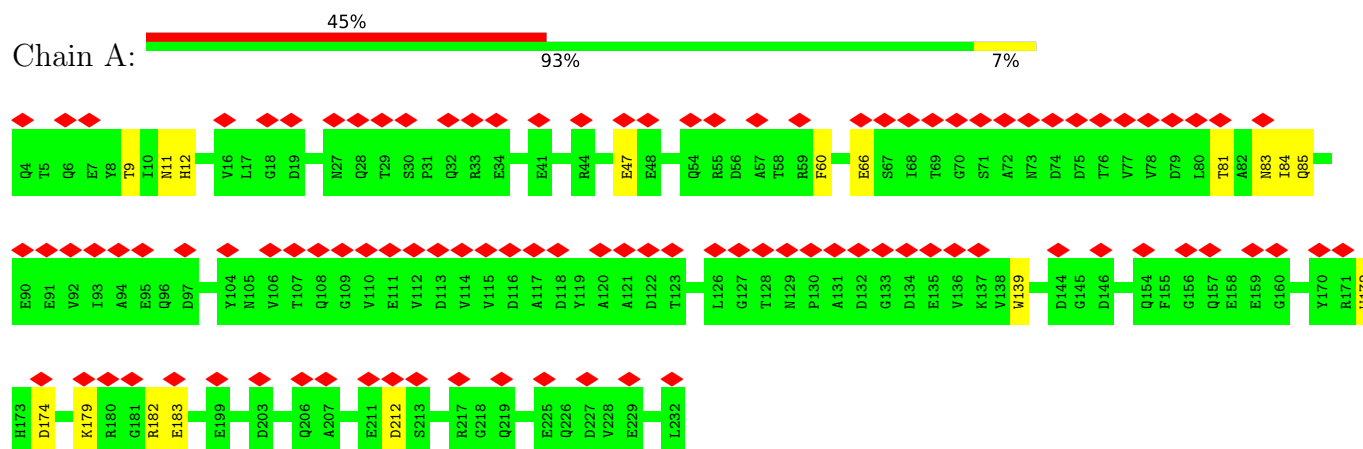
- Molecule 8 is a protein called polypeptide stretch (vertex complex).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	m	25	Total	C	H	N	O	0	0
			221	74	96	25	26		

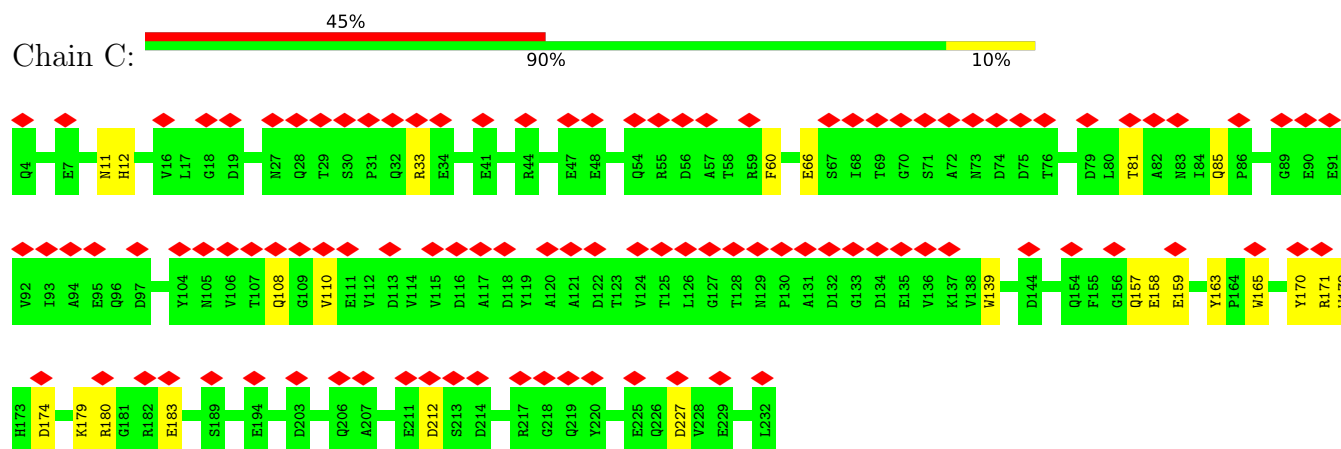
3 Residue-property plots

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.

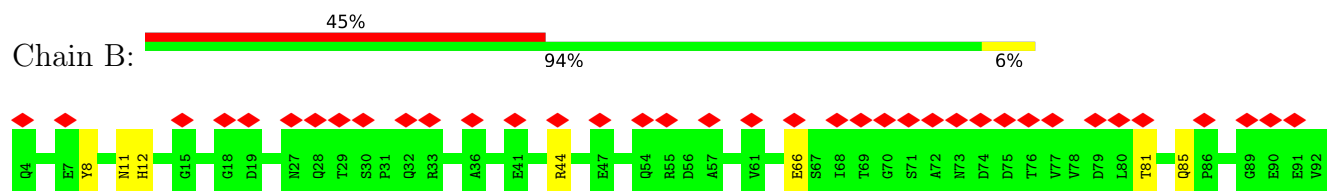
• Molecule 1: VP4

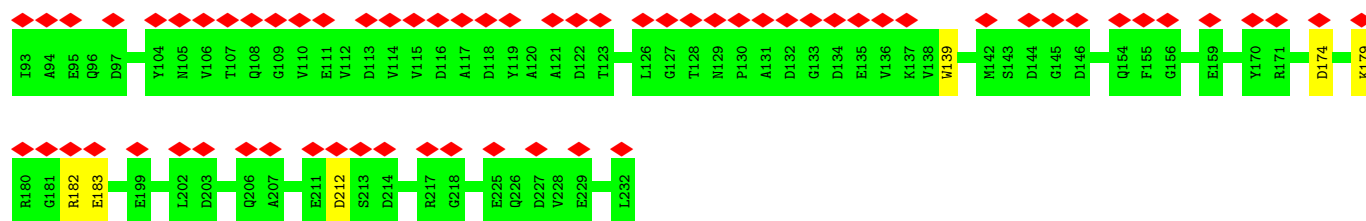


• Molecule 1: VP4

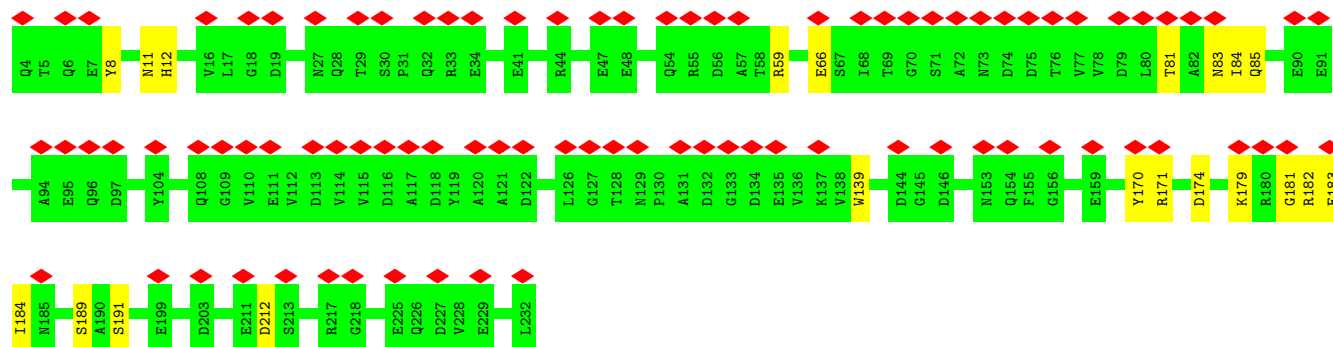
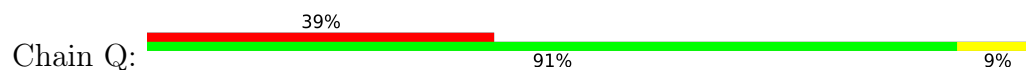


• Molecule 1: VP4

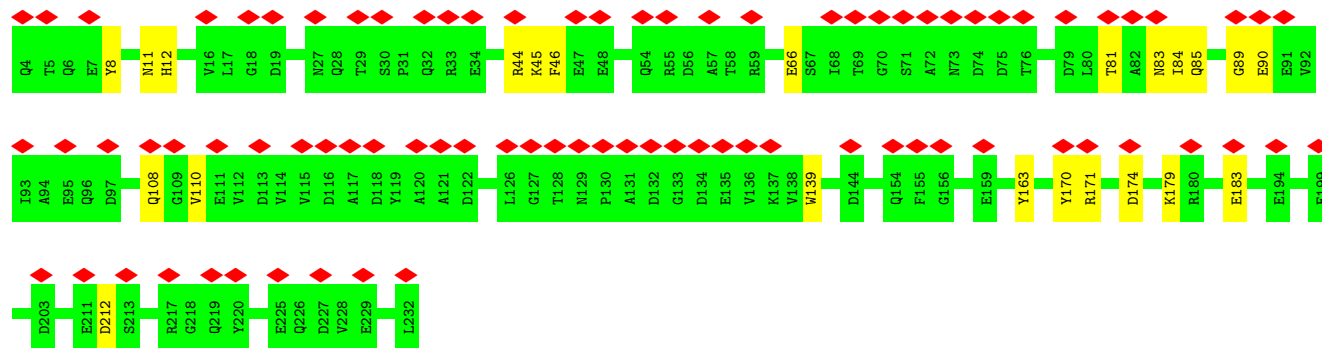
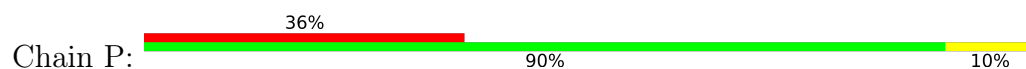




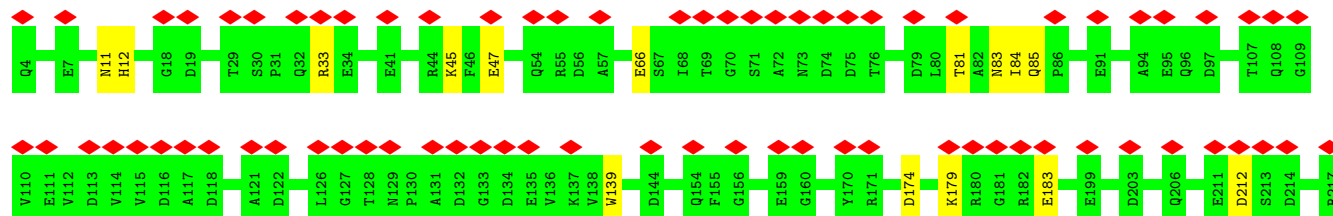
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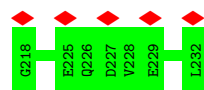


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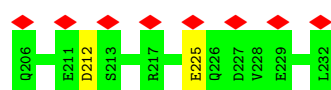
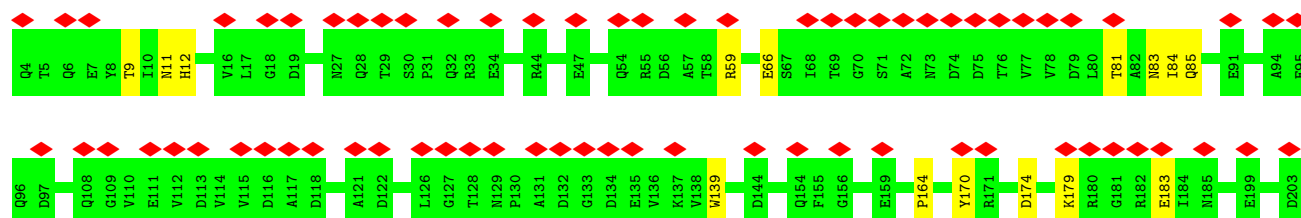


• Molecule 1: VP4

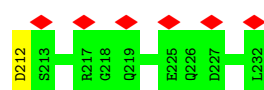
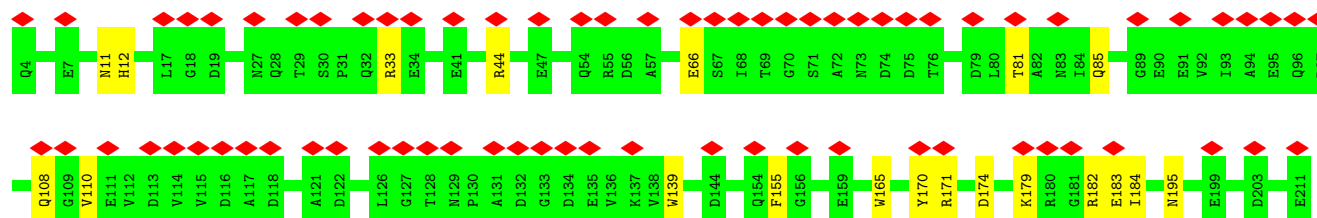




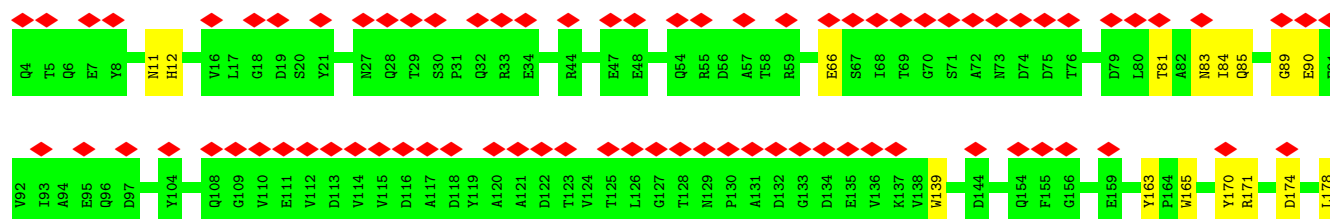
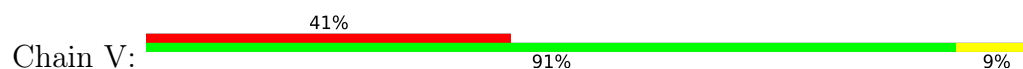
• Molecule 1: VP4



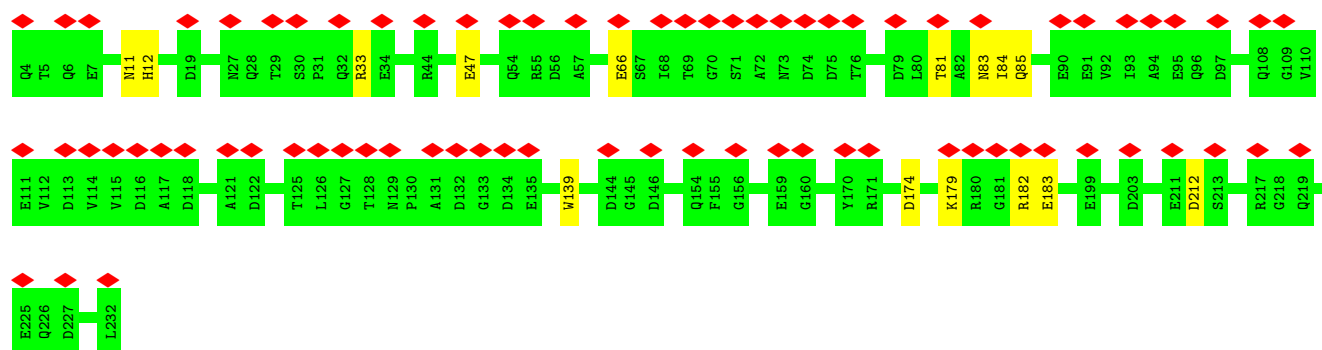
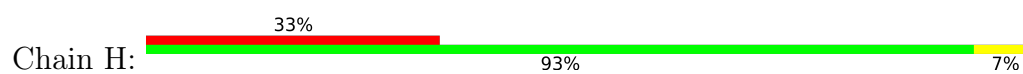
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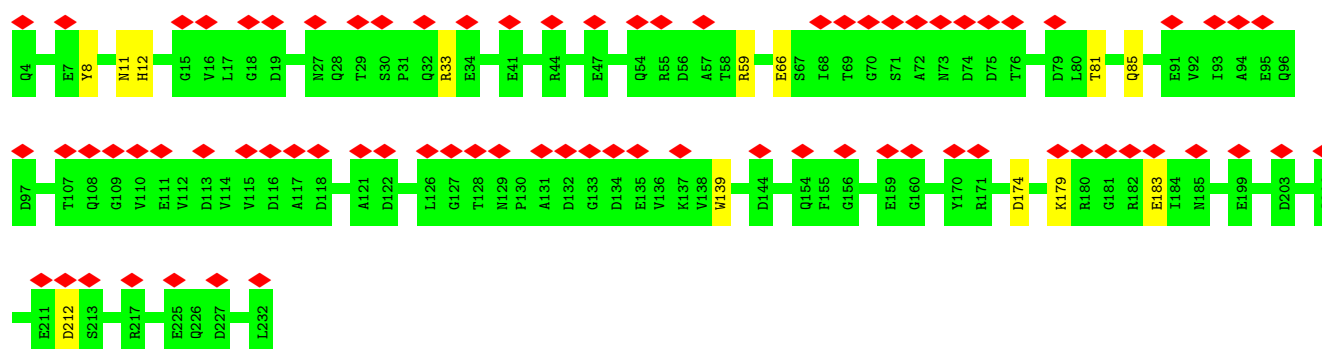
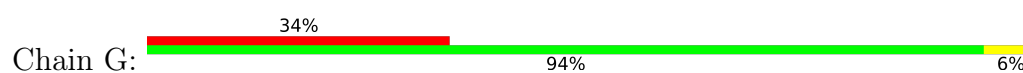
• Molecule 1: VP4



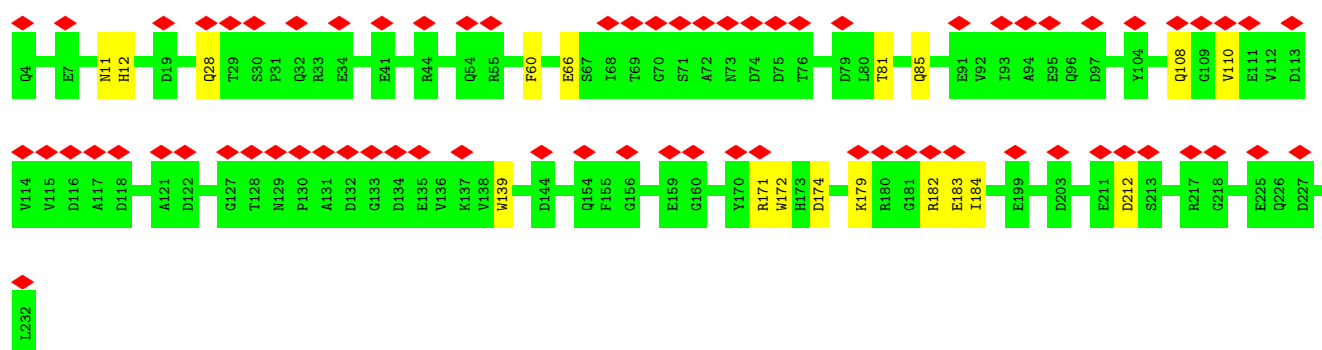
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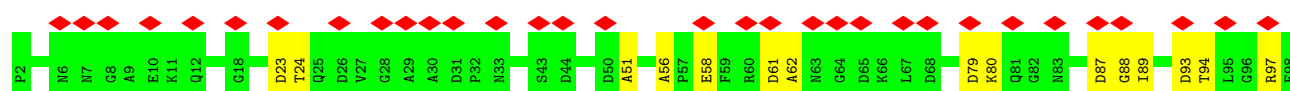
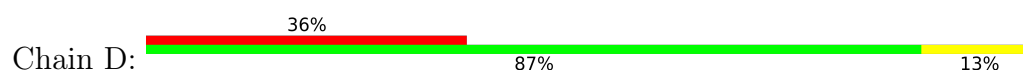
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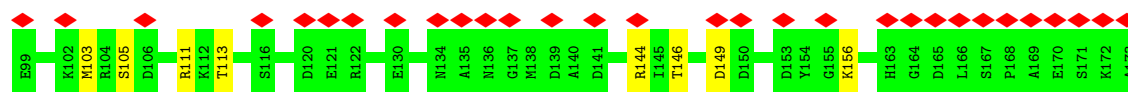


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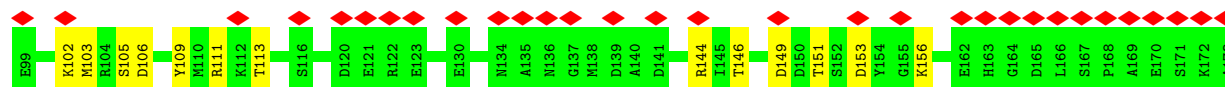
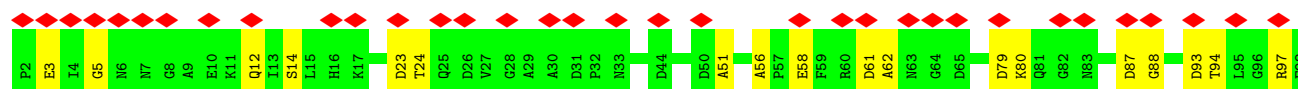
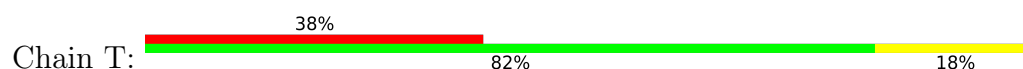


• Molecule 2: VP7

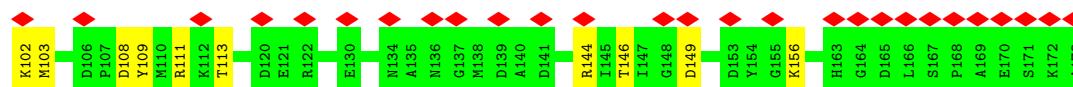
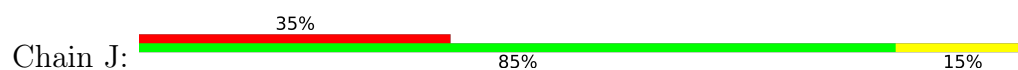




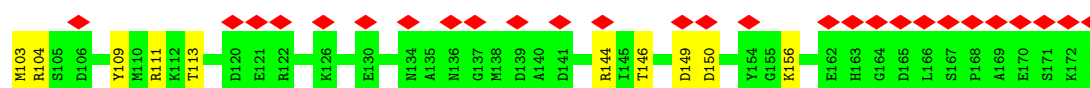
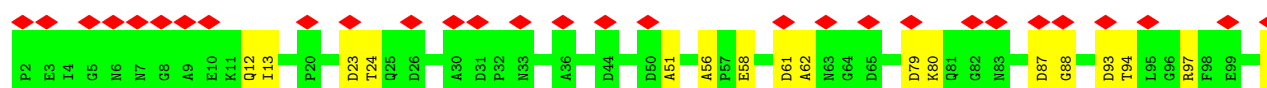
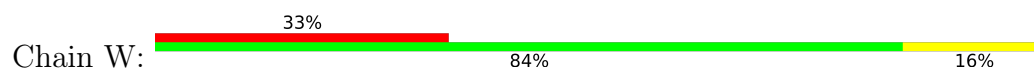
• Molecule 2: VP7



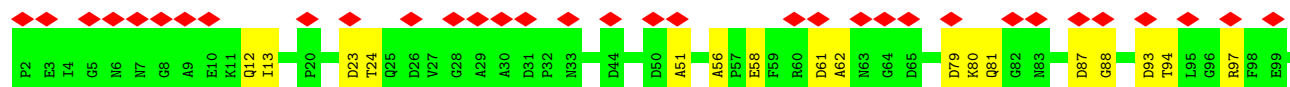
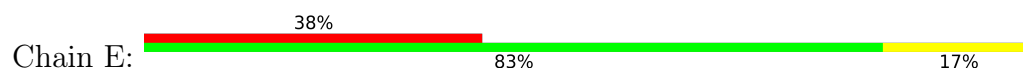
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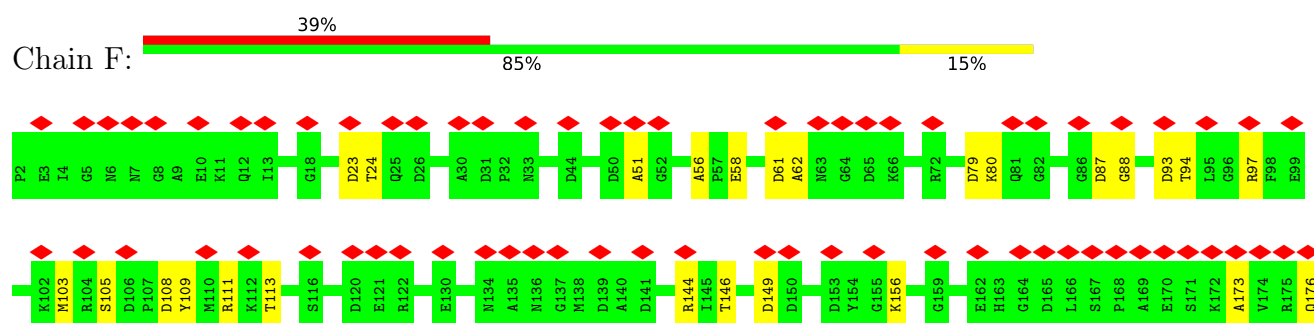
• Molecule 2: VP7



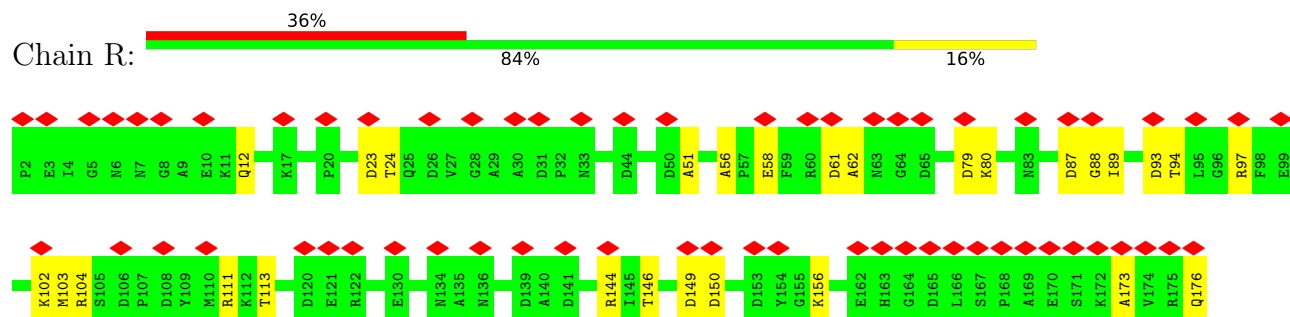
• Molecule 3: VP7



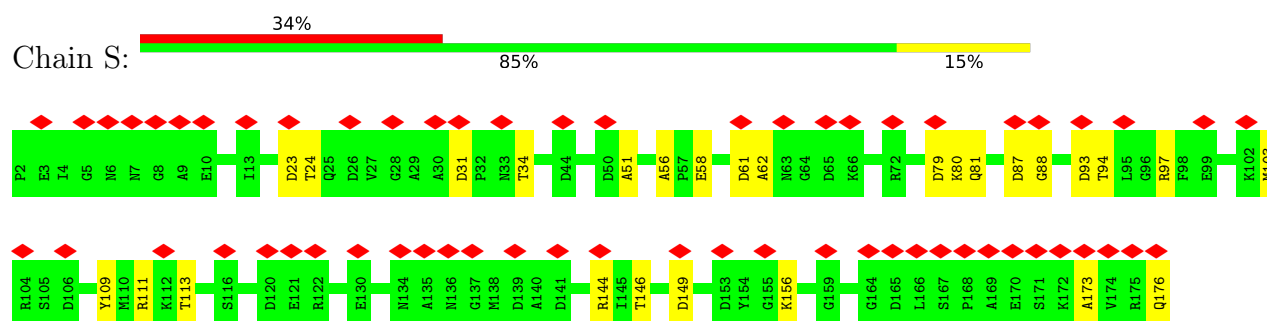
• Molecule 3: VP7



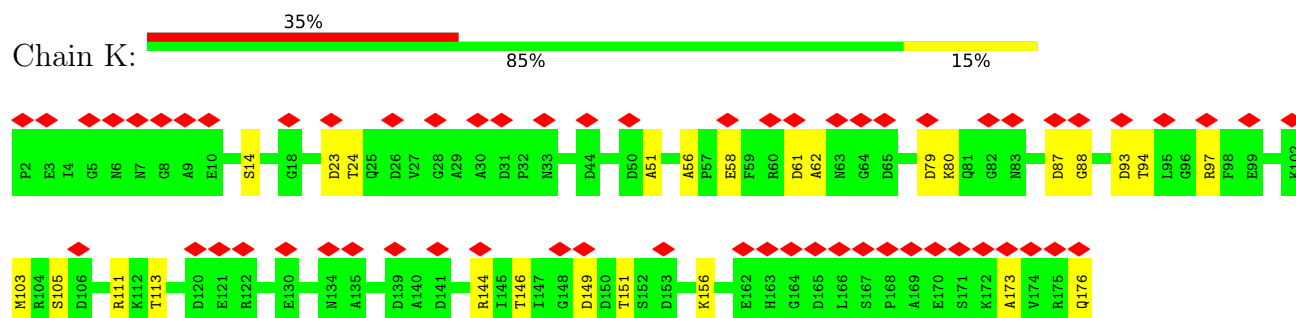
- Molecule 3: VP7



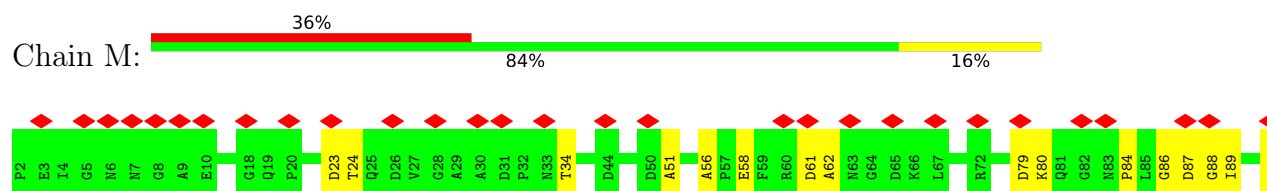
- Molecule 3: VP7

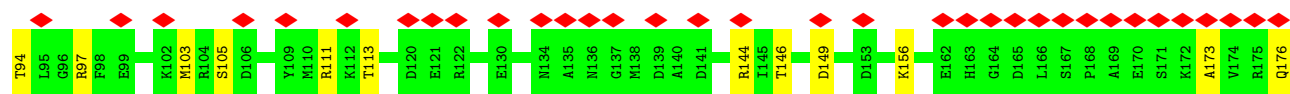


- Molecule 3: VP7

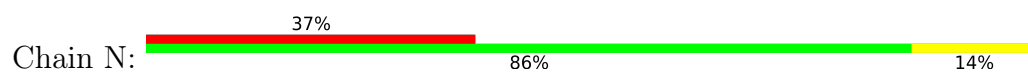


- Molecule 3: VP7

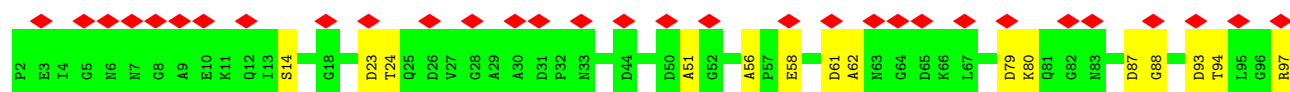
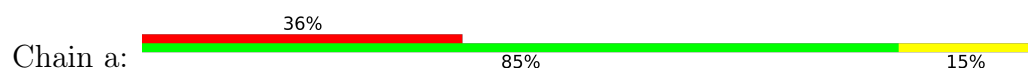




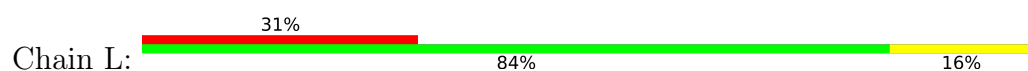
- Molecule 3: VP7



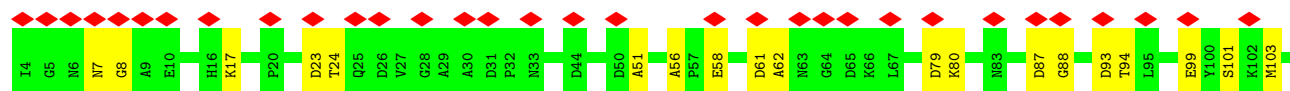
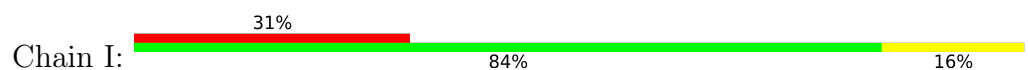
- Molecule 3: VP7



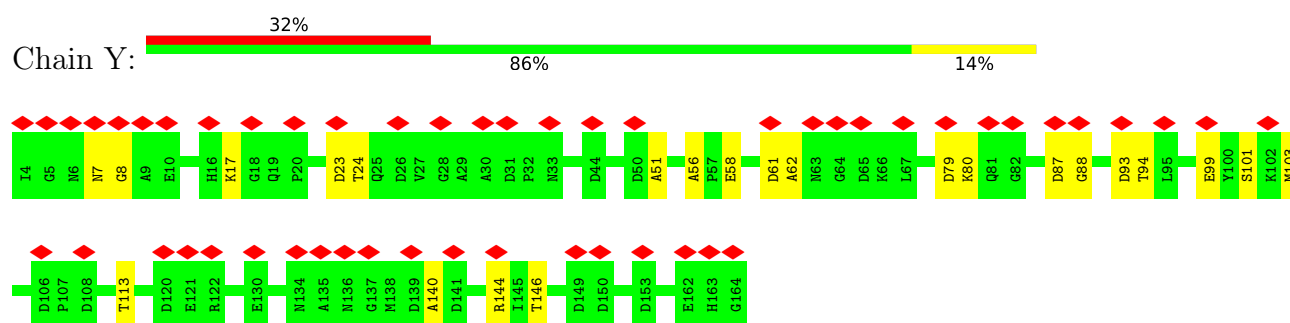
- Molecule 4: VP7



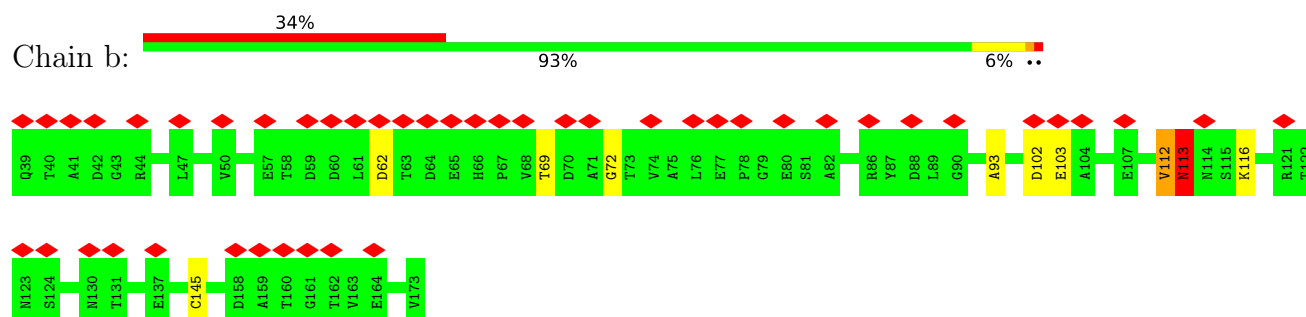
- Molecule 4: VP7



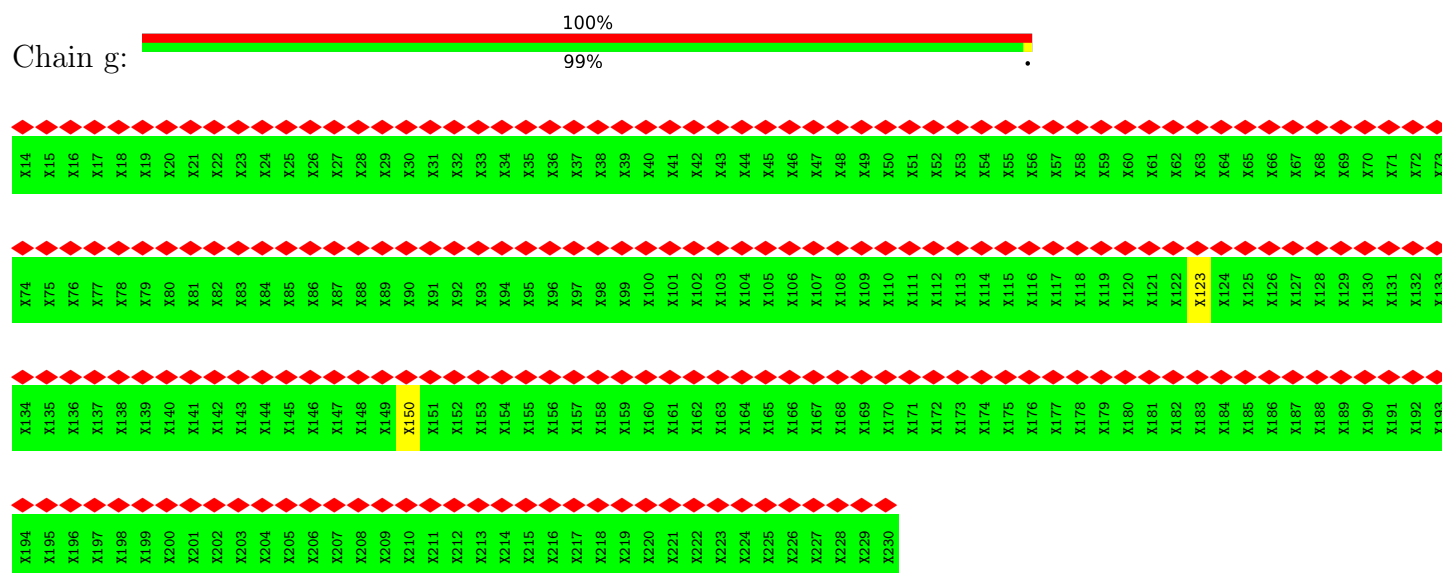
- Molecule 4: VP7



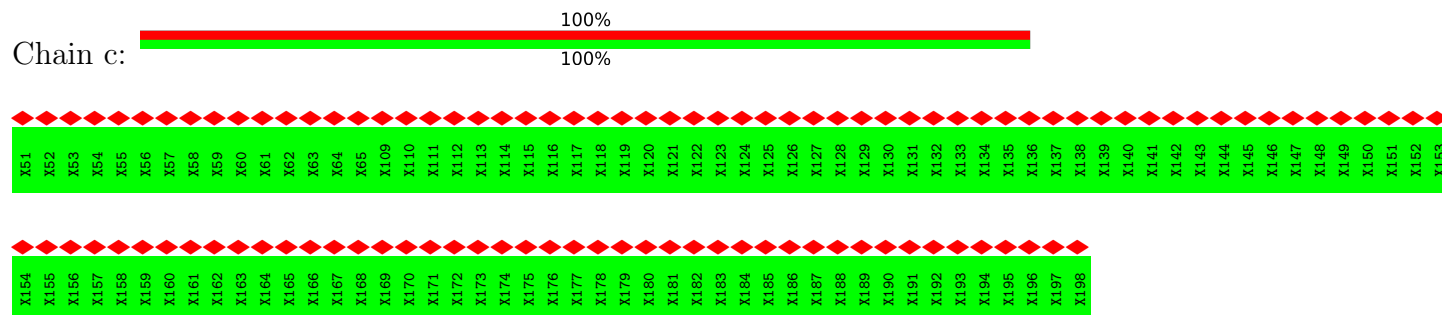
• Molecule 5: Uncharacterized protein



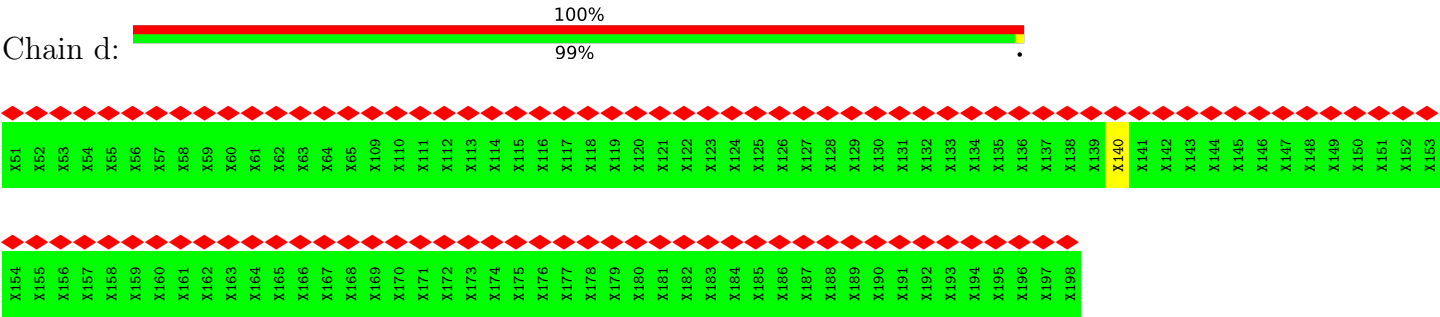
• Molecule 6: VP16 (vertex complex)



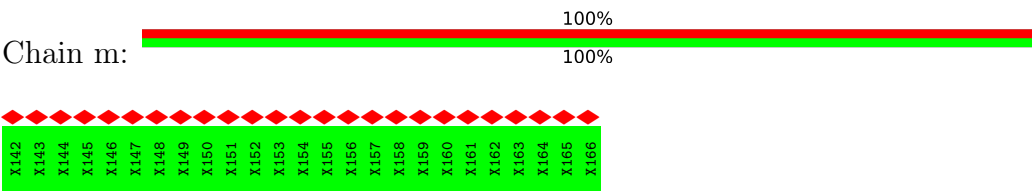
• Molecule 7: GPS III



● Molecule 7: GPS III



● Molecule 8: polypeptide stretch (vertex complex)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	11446	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	35	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.167	Depositor
Minimum map value	-0.056	Depositor
Average map value	0.010	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.067	Depositor
Map size (Å)	1018.4, 1018.4, 1018.4	wwPDB
Map dimensions	760, 760, 760	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.34, 1.34, 1.34	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	A	0.40	0/1845	0.53	0/2528
1	B	0.40	0/1845	0.53	0/2528
1	C	0.40	0/1845	0.53	0/2528
1	G	0.40	0/1845	0.53	0/2528
1	H	0.40	0/1845	0.53	0/2528
1	O	0.40	0/1845	0.53	0/2528
1	P	0.40	0/1845	0.53	0/2528
1	Q	0.40	0/1845	0.53	0/2528
1	U	0.40	0/1845	0.53	0/2528
1	V	0.40	0/1845	0.53	0/2528
1	X	0.40	0/1845	0.53	0/2528
1	Z	0.40	0/1845	0.53	0/2528
2	D	0.36	0/1317	0.46	0/1787
2	J	0.36	0/1317	0.46	0/1787
2	T	0.36	0/1317	0.46	0/1787
2	W	0.36	0/1317	0.46	0/1787
3	E	0.37	0/1344	0.47	0/1823
3	F	0.37	0/1344	0.47	0/1823
3	K	0.37	0/1344	0.47	0/1823
3	M	0.37	0/1344	0.47	0/1823
3	N	0.37	0/1344	0.47	0/1823
3	R	0.37	0/1344	0.47	0/1823
3	S	0.37	0/1344	0.47	0/1823
3	a	0.37	0/1344	0.47	0/1823
4	I	0.33	0/1236	0.43	0/1677
4	L	0.33	0/1236	0.43	0/1677
4	Y	0.33	0/1236	0.43	0/1677
5	b	0.37	0/1019	0.57	1/1398 (0.1%)
All	All	0.38	0/42887	0.50	1/58497 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
5	b	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	b	113	ASN	O-C-N	-5.19	115.68	122.59

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	b	112	VAL	Peptide
5	b	113	ASN	Mainchain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1805	1687	1687	11	0
1	B	1805	1687	1687	11	0
1	C	1805	1687	1687	28	0
1	G	1805	1687	1687	10	0
1	H	1805	1687	1687	11	0
1	O	1805	1687	1687	14	0
1	P	1805	1687	1687	23	0
1	Q	1805	1687	1687	21	0
1	U	1805	1687	1687	12	0
1	V	1805	1687	1687	26	0
1	X	1805	1687	1687	14	0
1	Z	1805	1687	1687	24	0
2	D	1294	1247	1247	14	0
2	J	1294	1247	1247	20	0
2	T	1294	1247	1247	26	0
2	W	1294	1247	1247	25	0
3	E	1321	1277	1277	28	0
3	F	1321	1277	1277	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	K	1321	1277	1277	20	0
3	M	1321	1277	1277	18	0
3	N	1321	1277	1277	13	0
3	R	1321	1277	1277	21	0
3	S	1321	1277	1277	23	0
3	a	1321	1277	1277	16	0
4	I	1215	1172	1172	13	0
4	L	1215	1172	1172	14	0
4	Y	1215	1172	1172	12	0
5	b	999	951	951	6	0
6	g	1085	867	277	1	0
7	c	525	418	126	0	0
7	d	525	418	126	1	0
8	m	125	96	34	0	0
All	All	44308	41714	40478	386	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 5.

All (386) 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)
3:E:81:GLN:HG2	1:O:45:LYS:HD2	1.34	1.04
1:P:44:ARG:HE	1:Z:44:ARG:HD2	1.19	1.02
1:C:171:ARG:NH2	3:E:149:ASP:OD1	2.04	0.90
1:P:44:ARG:NE	1:Z:44:ARG:HD2	1.87	0.89
1:C:179:LYS:HG2	3:F:109:TYR:CE1	2.09	0.87
3:E:80:LYS:NZ	1:O:47:GLU:OE2	2.07	0.86
3:E:81:GLN:HG2	1:O:45:LYS:CD	2.07	0.84
1:C:163:TYR:OH	3:E:12:GLN:O	1.96	0.83
1:P:171:ARG:NH2	3:R:150:ASP:O	2.12	0.83
1:V:163:TYR:OH	2:W:12:GLN:O	1.97	0.82
1:C:171:ARG:NH2	3:E:150:ASP:O	2.14	0.81
3:S:34:THR:OG1	1:Z:33:ARG:NH2	2.15	0.78
2:J:109:TYR:CE1	1:V:179:LYS:HG2	2.19	0.78
1:V:171:ARG:NH2	2:W:149:ASP:OD1	2.18	0.77
1:V:171:ARG:NH2	2:W:150:ASP:O	2.18	0.76
5:b:69:THR:OG1	5:b:72:GLY:O	2.04	0.76
1:C:33:ARG:NH2	3:M:34:THR:OG1	2.19	0.75
1:P:174:ASP:OD2	3:R:104:ARG:NH2	2.20	0.74
2:T:12:GLN:NE2	7:d:140:UNK:O	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:31:ASP:OD1	1:Z:33:ARG:NH2	2.22	0.71
4:Y:58:GLU:OE1	4:Y:144:ARG:NH2	2.23	0.71
4:I:58:GLU:OE1	4:I:144:ARG:NH2	2.23	0.71
1:A:47:GLU:OE2	2:T:80:LYS:NZ	2.23	0.71
4:L:58:GLU:OE1	4:L:144:ARG:NH2	2.23	0.70
2:D:89:ILE:HG21	1:B:8:TYR:OH	1.92	0.70
2:J:58:GLU:OE1	2:J:144:ARG:NH2	2.25	0.70
2:D:58:GLU:OE1	2:D:144:ARG:NH2	2.25	0.69
2:T:58:GLU:OE1	2:T:144:ARG:NH2	2.25	0.69
2:W:58:GLU:OE1	2:W:144:ARG:NH2	2.25	0.69
1:Q:179:LYS:O	1:Q:183:GLU:N	2.27	0.68
1:P:171:ARG:NH2	3:R:149:ASP:OD1	2.25	0.68
1:H:179:LYS:O	1:H:183:GLU:N	2.27	0.68
1:O:179:LYS:O	1:O:183:GLU:N	2.27	0.68
1:C:179:LYS:O	1:C:183:GLU:N	2.27	0.68
2:T:51:ALA:O	2:T:113:THR:OG1	2.12	0.68
1:Z:179:LYS:O	1:Z:183:GLU:N	2.27	0.68
1:A:179:LYS:O	1:A:183:GLU:N	2.27	0.68
1:G:179:LYS:O	1:G:183:GLU:N	2.27	0.68
2:D:51:ALA:O	2:D:113:THR:OG1	2.12	0.68
3:R:58:GLU:OE1	3:R:144:ARG:NH2	2.27	0.68
3:a:58:GLU:OE1	3:a:144:ARG:NH2	2.26	0.68
3:K:58:GLU:OE1	3:K:144:ARG:NH2	2.26	0.68
1:X:179:LYS:O	1:X:183:GLU:N	2.27	0.68
1:B:179:LYS:O	1:B:183:GLU:N	2.27	0.68
3:F:58:GLU:OE1	3:F:144:ARG:NH2	2.27	0.68
3:S:58:GLU:OE1	3:S:144:ARG:NH2	2.27	0.68
1:V:179:LYS:O	1:V:183:GLU:N	2.27	0.68
4:Y:51:ALA:O	4:Y:113:THR:OG1	2.12	0.68
3:E:58:GLU:OE1	3:E:144:ARG:NH2	2.27	0.68
3:N:58:GLU:OE1	3:N:144:ARG:NH2	2.27	0.67
2:J:51:ALA:O	2:J:113:THR:OG1	2.12	0.67
3:M:58:GLU:OE1	3:M:144:ARG:NH2	2.27	0.67
2:W:51:ALA:O	2:W:113:THR:OG1	2.12	0.67
1:Q:171:ARG:HH12	2:T:14:SER:HB3	1.59	0.67
1:U:179:LYS:O	1:U:183:GLU:N	2.27	0.67
1:P:179:LYS:O	1:P:183:GLU:N	2.27	0.67
3:F:51:ALA:O	3:F:113:THR:OG1	2.13	0.66
1:C:159:GLU:O	3:M:86:GLY:N	2.28	0.66
4:L:51:ALA:O	4:L:113:THR:OG1	2.12	0.66
3:E:81:GLN:CG	1:O:45:LYS:HD2	2.18	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:97:ARG:NH1	1:V:227:ASP:OD1	2.26	0.66
1:O:139:TRP:NE1	1:O:212:ASP:OD2	2.29	0.66
1:A:139:TRP:NE1	1:A:212:ASP:OD2	2.29	0.66
1:C:139:TRP:NE1	1:C:212:ASP:OD2	2.29	0.66
1:V:139:TRP:NE1	1:V:212:ASP:OD2	2.29	0.66
1:H:139:TRP:NE1	1:H:212:ASP:OD2	2.29	0.66
1:X:139:TRP:NE1	1:X:212:ASP:OD2	2.29	0.66
1:Q:139:TRP:NE1	1:Q:212:ASP:OD2	2.29	0.65
1:B:139:TRP:NE1	1:B:212:ASP:OD2	2.29	0.65
1:G:139:TRP:NE1	1:G:212:ASP:OD2	2.29	0.65
3:a:51:ALA:O	3:a:113:THR:OG1	2.13	0.65
2:D:149:ASP:N	2:D:156:LYS:O	2.30	0.65
1:P:163:TYR:OH	3:R:12:GLN:O	2.14	0.65
1:Z:139:TRP:NE1	1:Z:212:ASP:OD2	2.29	0.65
1:P:139:TRP:NE1	1:P:212:ASP:OD2	2.29	0.65
3:R:51:ALA:O	3:R:113:THR:OG1	2.13	0.65
4:I:51:ALA:O	4:I:113:THR:OG1	2.12	0.65
2:J:149:ASP:N	2:J:156:LYS:O	2.30	0.65
1:V:174:ASP:OD2	2:W:104:ARG:NH2	2.25	0.65
2:W:149:ASP:N	2:W:156:LYS:O	2.30	0.64
3:K:80:LYS:NZ	1:H:47:GLU:OE2	2.30	0.64
1:U:139:TRP:NE1	1:U:212:ASP:OD2	2.29	0.64
3:S:51:ALA:O	3:S:113:THR:OG1	2.13	0.64
3:M:51:ALA:O	3:M:113:THR:OG1	2.13	0.64
3:K:51:ALA:O	3:K:113:THR:OG1	2.13	0.63
1:Q:85:GLN:NE2	1:Q:174:ASP:OD1	2.32	0.63
1:X:182:ARG:NE	3:a:105:SER:O	2.32	0.63
1:C:85:GLN:NE2	1:C:174:ASP:OD1	2.32	0.63
1:O:85:GLN:NE2	1:O:174:ASP:OD1	2.32	0.63
1:V:85:GLN:NE2	1:V:174:ASP:OD1	2.32	0.63
1:H:85:GLN:NE2	1:H:174:ASP:OD1	2.32	0.63
1:C:179:LYS:HG2	3:F:109:TYR:HE1	1.62	0.62
1:B:85:GLN:NE2	1:B:174:ASP:OD1	2.32	0.62
2:T:149:ASP:N	2:T:156:LYS:O	2.30	0.62
1:Z:85:GLN:NE2	1:Z:174:ASP:OD1	2.32	0.62
1:X:85:GLN:NE2	1:X:174:ASP:OD1	2.32	0.62
1:U:85:GLN:NE2	1:U:174:ASP:OD1	2.32	0.62
3:N:51:ALA:O	3:N:113:THR:OG1	2.13	0.62
1:A:85:GLN:NE2	1:A:174:ASP:OD1	2.32	0.62
3:S:81:GLN:NE2	1:Z:165:TRP:CZ2	2.67	0.62
3:E:51:ALA:O	3:E:113:THR:OG1	2.13	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:85:GLN:NE2	1:P:174:ASP:OD1	2.32	0.61
1:G:85:GLN:NE2	1:G:174:ASP:OD1	2.32	0.61
1:B:11:ASN:OD1	1:B:12:HIS:ND1	2.34	0.61
1:G:11:ASN:OD1	1:G:12:HIS:ND1	2.34	0.61
1:X:11:ASN:OD1	1:X:12:HIS:ND1	2.34	0.61
1:A:11:ASN:OD1	1:A:12:HIS:ND1	2.34	0.60
1:C:11:ASN:OD1	1:C:12:HIS:ND1	2.34	0.60
1:O:11:ASN:OD1	1:O:12:HIS:ND1	2.34	0.60
1:Q:11:ASN:OD1	1:Q:12:HIS:ND1	2.34	0.60
1:P:11:ASN:OD1	1:P:12:HIS:ND1	2.34	0.60
1:H:11:ASN:OD1	1:H:12:HIS:ND1	2.34	0.60
1:P:45:LYS:HA	1:Z:195:ASN:ND2	2.16	0.60
1:U:11:ASN:OD1	1:U:12:HIS:ND1	2.34	0.60
1:V:11:ASN:OD1	1:V:12:HIS:ND1	2.34	0.60
1:Z:11:ASN:OD1	1:Z:12:HIS:ND1	2.34	0.59
2:D:56:ALA:HB1	2:D:103:MET:HE3	1.85	0.59
3:a:56:ALA:HB1	3:a:103:MET:HE3	1.85	0.59
3:E:56:ALA:HB1	3:E:103:MET:HE3	1.85	0.58
2:J:56:ALA:HB1	2:J:103:MET:HE3	1.85	0.58
3:F:56:ALA:HB1	3:F:103:MET:HE3	1.85	0.58
3:S:56:ALA:HB1	3:S:103:MET:HE3	1.85	0.58
3:E:149:ASP:N	3:E:156:LYS:O	2.35	0.58
1:P:179:LYS:HG2	3:S:109:TYR:CE1	2.39	0.58
3:R:56:ALA:HB1	3:R:103:MET:HE3	1.85	0.58
1:U:66:GLU:OE2	1:U:81:THR:OG1	2.17	0.58
3:K:56:ALA:HB1	3:K:103:MET:HE3	1.85	0.57
3:N:56:ALA:HB1	3:N:103:MET:HE3	1.85	0.57
1:X:184:ILE:HG23	3:a:151:THR:HB	1.85	0.57
3:F:149:ASP:N	3:F:156:LYS:O	2.35	0.57
4:I:17:LYS:NZ	4:I:140:ALA:O	2.35	0.57
3:S:149:ASP:N	3:S:156:LYS:O	2.35	0.57
2:T:56:ALA:HB1	2:T:103:MET:HE3	1.85	0.57
3:K:149:ASP:N	3:K:156:LYS:O	2.35	0.57
4:I:56:ALA:HB1	4:I:103:MET:HE3	1.87	0.57
1:P:66:GLU:OE2	1:P:81:THR:OG1	2.17	0.57
2:D:79:ASP:OD2	5:b:116:LYS:NZ	2.35	0.57
1:Q:59:ARG:HH11	3:R:97:ARG:HB3	1.70	0.57
3:M:56:ALA:HB1	3:M:103:MET:HE3	1.85	0.57
1:Q:66:GLU:OE2	1:Q:81:THR:OG1	2.17	0.56
2:W:56:ALA:HB1	2:W:103:MET:HE3	1.85	0.56
1:Q:182:ARG:HH21	2:T:106:ASP:HA	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:66:GLU:OE2	1:C:81:THR:OG1	2.17	0.56
3:R:149:ASP:N	3:R:156:LYS:O	2.35	0.56
1:C:180:ARG:HG2	3:F:108:ASP:O	2.05	0.56
1:O:66:GLU:OE2	1:O:81:THR:OG1	2.17	0.56
4:Y:17:LYS:NZ	4:Y:140:ALA:O	2.35	0.56
3:M:149:ASP:N	3:M:156:LYS:O	2.35	0.56
1:C:165:TRP:CD1	3:E:13:ILE:HG22	2.41	0.55
3:N:97:ARG:O	3:N:111:ARG:NH2	2.40	0.55
3:M:97:ARG:O	3:M:111:ARG:NH2	2.40	0.55
3:a:97:ARG:O	3:a:111:ARG:NH2	2.40	0.55
3:F:97:ARG:O	3:F:111:ARG:NH2	2.40	0.55
1:Q:182:ARG:NE	2:T:105:SER:O	2.40	0.55
3:R:97:ARG:O	3:R:111:ARG:NH2	2.40	0.55
3:S:97:ARG:O	3:S:111:ARG:NH2	2.40	0.55
1:Z:66:GLU:OE2	1:Z:81:THR:OG1	2.17	0.55
4:Y:56:ALA:HB1	4:Y:103:MET:HE3	1.87	0.55
3:K:97:ARG:O	3:K:111:ARG:NH2	2.40	0.55
4:L:56:ALA:HB1	4:L:103:MET:HE3	1.87	0.55
3:a:149:ASP:N	3:a:156:LYS:O	2.35	0.55
1:C:158:GLU:OE1	3:M:84:PRO:HG3	2.07	0.55
1:B:66:GLU:OE2	1:B:81:THR:OG1	2.17	0.54
4:L:17:LYS:NZ	4:L:140:ALA:O	2.35	0.54
3:E:97:ARG:O	3:E:111:ARG:NH2	2.40	0.54
3:N:149:ASP:N	3:N:156:LYS:O	2.35	0.54
1:H:66:GLU:OE2	1:H:81:THR:OG1	2.17	0.54
1:Z:184:ILE:HG23	3:K:151:THR:HB	1.90	0.54
3:S:93:ASP:OD1	3:S:94:THR:N	2.41	0.53
1:C:165:TRP:NE1	3:E:13:ILE:HG21	2.23	0.53
1:H:182:ARG:NE	3:M:105:SER:O	2.42	0.53
1:Q:182:ARG:NH2	2:T:106:ASP:HA	2.24	0.53
3:R:93:ASP:OD1	3:R:94:THR:N	2.41	0.53
1:C:165:TRP:CD1	3:E:13:ILE:CG2	2.92	0.53
1:Z:11:ASN:OD1	1:Z:12:HIS:N	2.42	0.53
1:Q:182:ARG:NH1	2:T:105:SER:OG	2.42	0.53
3:S:61:ASP:OD1	3:S:62:ALA:N	2.42	0.53
3:K:93:ASP:OD1	3:K:94:THR:N	2.41	0.53
1:V:170:TYR:CE2	2:W:144:ARG:NH2	2.77	0.53
2:W:61:ASP:OD1	2:W:62:ALA:N	2.42	0.53
4:Y:61:ASP:OD1	4:Y:62:ALA:N	2.42	0.53
2:J:23:ASP:OD1	2:J:24:THR:N	2.43	0.52
4:I:61:ASP:OD1	4:I:62:ALA:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:23:ASP:OD1	2:D:24:THR:N	2.43	0.52
3:F:93:ASP:OD1	3:F:94:THR:N	2.41	0.52
2:T:23:ASP:OD1	2:T:24:THR:N	2.43	0.52
1:V:66:GLU:OE2	1:V:81:THR:OG1	2.17	0.52
1:G:8:TYR:OH	4:L:89:ILE:HG21	2.09	0.52
1:G:66:GLU:OE2	1:G:81:THR:OG1	2.17	0.52
3:N:93:ASP:OD1	3:N:94:THR:N	2.41	0.52
3:E:93:ASP:OD1	3:E:94:THR:N	2.41	0.52
1:Q:189:SER:O	2:T:5:GLY:N	2.40	0.52
3:a:93:ASP:OD1	3:a:94:THR:N	2.41	0.52
1:O:11:ASN:OD1	1:O:12:HIS:N	2.42	0.52
4:L:79:ASP:OD1	4:L:80:LYS:N	2.43	0.52
1:Q:171:ARG:NH1	2:T:14:SER:HB3	2.24	0.52
4:I:23:ASP:OD1	4:I:24:THR:N	2.43	0.52
3:a:61:ASP:OD1	3:a:62:ALA:N	2.42	0.52
3:E:61:ASP:OD1	3:E:62:ALA:N	2.42	0.52
1:H:11:ASN:OD1	1:H:12:HIS:N	2.42	0.52
4:Y:23:ASP:OD1	4:Y:24:THR:N	2.43	0.52
3:K:23:ASP:OD1	3:K:24:THR:N	2.43	0.52
2:W:23:ASP:OD1	2:W:24:THR:N	2.43	0.52
2:D:61:ASP:OD1	2:D:62:ALA:N	2.42	0.51
4:L:23:ASP:OD1	4:L:24:THR:N	2.43	0.51
3:a:23:ASP:OD1	3:a:24:THR:N	2.43	0.51
2:T:61:ASP:OD1	2:T:62:ALA:N	2.42	0.51
2:T:79:ASP:OD1	2:T:80:LYS:N	2.43	0.51
2:J:79:ASP:OD1	2:J:80:LYS:N	2.43	0.51
3:K:61:ASP:OD1	3:K:62:ALA:N	2.42	0.51
1:G:11:ASN:OD1	1:G:12:HIS:N	2.42	0.51
4:L:61:ASP:OD1	4:L:62:ALA:N	2.42	0.51
4:Y:79:ASP:OD1	4:Y:80:LYS:N	2.43	0.51
1:A:66:GLU:OE2	1:A:81:THR:OG1	2.17	0.51
1:B:44:ARG:NH1	5:b:62:ASP:OD2	2.43	0.51
3:N:79:ASP:OD1	3:N:80:LYS:N	2.43	0.51
1:A:11:ASN:OD1	1:A:12:HIS:N	2.42	0.51
3:F:61:ASP:OD1	3:F:62:ALA:N	2.42	0.51
3:R:61:ASP:OD1	3:R:62:ALA:N	2.42	0.51
1:P:170:TYR:CE2	3:R:144:ARG:NH2	2.78	0.51
1:U:11:ASN:OD1	1:U:12:HIS:N	2.42	0.51
1:O:33:ARG:CZ	1:H:33:ARG:CZ	2.89	0.51
3:S:173:ALA:O	3:S:176:GLN:NE2	2.44	0.51
3:M:23:ASP:OD1	3:M:24:THR:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:66:GLU:OE2	1:X:81:THR:OG1	2.17	0.51
3:R:173:ALA:O	3:R:176:GLN:NE2	2.44	0.51
3:M:61:ASP:OD1	3:M:62:ALA:N	2.42	0.51
3:E:23:ASP:OD1	3:E:24:THR:N	2.43	0.51
3:M:93:ASP:OD1	3:M:94:THR:N	2.41	0.50
3:N:23:ASP:OD1	3:N:24:THR:N	2.43	0.50
3:F:173:ALA:O	3:F:176:GLN:NE2	2.44	0.50
2:W:79:ASP:OD1	2:W:80:LYS:N	2.43	0.50
3:N:61:ASP:OD1	3:N:62:ALA:N	2.42	0.50
3:E:173:ALA:O	3:E:176:GLN:NE2	2.44	0.50
3:R:23:ASP:OD1	3:R:24:THR:N	2.43	0.50
3:K:79:ASP:OD1	3:K:80:LYS:N	2.43	0.50
3:M:79:ASP:OD1	3:M:80:LYS:N	2.43	0.50
2:D:79:ASP:OD1	2:D:80:LYS:N	2.43	0.50
3:N:173:ALA:O	3:N:176:GLN:NE2	2.44	0.50
3:M:173:ALA:O	3:M:176:GLN:NE2	2.44	0.50
3:S:23:ASP:OD1	3:S:24:THR:N	2.43	0.50
1:U:170:TYR:OH	2:J:144:ARG:NH1	2.45	0.50
2:J:61:ASP:OD1	2:J:62:ALA:N	2.42	0.50
3:a:173:ALA:O	3:a:176:GLN:NE2	2.44	0.50
5:b:112:VAL:HG12	5:b:113:ASN:H	1.76	0.49
3:S:79:ASP:OD1	3:S:80:LYS:N	2.43	0.49
3:K:173:ALA:O	3:K:176:GLN:NE2	2.44	0.49
1:C:11:ASN:OD1	1:C:12:HIS:N	2.42	0.49
4:I:79:ASP:OD1	4:I:80:LYS:N	2.43	0.49
1:X:171:ARG:HH12	3:a:14:SER:HB3	1.78	0.49
2:D:87:ASP:OD1	2:D:88:GLY:N	2.45	0.49
2:W:87:ASP:OD1	2:W:88:GLY:N	2.45	0.49
1:C:227:ASP:OD1	3:F:97:ARG:NH1	2.31	0.49
1:B:11:ASN:OD1	1:B:12:HIS:N	2.42	0.49
2:T:87:ASP:OD1	2:T:88:GLY:N	2.45	0.49
3:S:34:THR:OG1	1:Z:33:ARG:NE	2.45	0.49
3:E:79:ASP:OD1	3:E:80:LYS:N	2.43	0.49
3:R:79:ASP:OD1	3:R:80:LYS:N	2.43	0.49
1:V:174:ASP:CG	2:W:104:ARG:HH21	2.18	0.49
1:X:11:ASN:OD1	1:X:12:HIS:N	2.42	0.49
1:Q:184:ILE:HG23	2:T:151:THR:HB	1.94	0.49
3:F:23:ASP:OD1	3:F:24:THR:N	2.43	0.49
1:P:11:ASN:OD1	1:P:12:HIS:N	2.42	0.49
2:J:87:ASP:OD1	2:J:88:GLY:N	2.45	0.49
3:F:79:ASP:OD1	3:F:80:LYS:N	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:11:ASN:OD1	1:V:12:HIS:N	2.42	0.49
2:T:56:ALA:HB3	2:T:146:THR:OG1	2.13	0.48
1:B:182:ARG:NH1	3:F:105:SER:OG	2.46	0.48
3:S:31:ASP:CG	1:Z:33:ARG:HH22	2.21	0.48
2:J:93:ASP:OD1	2:J:94:THR:N	2.44	0.48
4:Y:87:ASP:OD1	4:Y:88:GLY:N	2.46	0.48
2:W:93:ASP:OD1	2:W:94:THR:N	2.44	0.48
4:L:87:ASP:OD1	4:L:88:GLY:N	2.46	0.48
3:E:81:GLN:HA	1:O:45:LYS:HD2	1.96	0.48
1:P:179:LYS:HG2	3:S:109:TYR:HE1	1.76	0.48
3:S:34:THR:CB	1:Z:33:ARG:HH21	2.25	0.48
2:J:109:TYR:OH	1:V:179:LYS:HE2	2.14	0.48
2:D:56:ALA:HB3	2:D:146:THR:OG1	2.13	0.48
2:W:56:ALA:HB3	2:W:146:THR:OG1	2.13	0.48
1:Q:11:ASN:OD1	1:Q:12:HIS:N	2.42	0.48
3:a:79:ASP:OD1	3:a:80:LYS:N	2.43	0.48
2:J:56:ALA:HB3	2:J:146:THR:OG1	2.13	0.47
4:I:87:ASP:OD1	4:I:88:GLY:N	2.46	0.47
3:F:56:ALA:HB3	3:F:146:THR:OG1	2.15	0.47
3:S:34:THR:OG1	1:Z:33:ARG:CZ	2.62	0.47
3:M:56:ALA:HB3	3:M:146:THR:OG1	2.15	0.47
4:Y:99:GLU:OE2	4:Y:101:SER:OG	2.31	0.47
3:E:56:ALA:HB3	3:E:146:THR:OG1	2.15	0.47
1:U:225:GLU:OE1	3:K:97:ARG:HD3	2.15	0.47
1:V:89:GLY:O	2:W:102:LYS:HE3	2.15	0.47
4:L:99:GLU:OE2	4:L:101:SER:OG	2.31	0.47
3:a:56:ALA:HB3	3:a:146:THR:OG1	2.15	0.47
2:D:93:ASP:OD1	2:D:94:THR:N	2.44	0.47
3:R:56:ALA:HB3	3:R:146:THR:OG1	2.15	0.47
1:U:59:ARG:HH11	3:K:97:ARG:HB3	1.80	0.47
6:g:123:UNK:O	6:g:150:UNK:N	2.48	0.47
3:E:87:ASP:OD1	3:E:88:GLY:N	2.49	0.46
4:I:99:GLU:OE2	4:I:101:SER:OG	2.31	0.46
3:S:56:ALA:HB3	3:S:146:THR:OG1	2.15	0.46
3:N:56:ALA:HB3	3:N:146:THR:OG1	2.15	0.46
3:S:34:THR:CB	1:Z:33:ARG:NH2	2.78	0.46
4:Y:56:ALA:HB3	4:Y:146:THR:OG1	2.15	0.46
1:A:9:THR:HG21	3:E:97:ARG:NH2	2.31	0.46
3:R:87:ASP:OD1	3:R:88:GLY:N	2.49	0.46
1:V:171:ARG:HH22	2:W:149:ASP:HA	1.80	0.46
3:F:87:ASP:OD1	3:F:88:GLY:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:93:ASP:OD1	4:I:94:THR:N	2.45	0.46
1:U:9:THR:HG21	3:K:97:ARG:NH2	2.31	0.46
1:Z:171:ARG:HH12	3:K:14:SER:HB3	1.80	0.46
3:M:87:ASP:OD1	3:M:88:GLY:N	2.49	0.46
3:a:87:ASP:OD1	3:a:88:GLY:N	2.49	0.46
3:K:56:ALA:HB3	3:K:146:THR:OG1	2.15	0.46
4:I:56:ALA:HB3	4:I:146:THR:OG1	2.15	0.46
3:N:87:ASP:OD1	3:N:88:GLY:N	2.49	0.46
3:S:87:ASP:OD1	3:S:88:GLY:N	2.49	0.45
1:G:33:ARG:NH1	1:X:28:GLN:OE1	2.50	0.45
1:C:174:ASP:OD2	3:E:104:ARG:NH2	2.46	0.45
2:T:93:ASP:OD1	2:T:94:THR:N	2.44	0.45
3:K:87:ASP:OD1	3:K:88:GLY:N	2.49	0.45
1:G:33:ARG:NH1	1:X:28:GLN:CD	2.75	0.45
4:L:56:ALA:HB3	4:L:146:THR:OG1	2.15	0.45
4:Y:93:ASP:OD1	4:Y:94:THR:N	2.45	0.45
1:C:179:LYS:CG	3:F:109:TYR:CE1	2.93	0.45
1:B:182:ARG:NE	3:F:105:SER:O	2.49	0.45
1:P:46:PHE:CE1	1:Z:155:PHE:CE1	3.04	0.45
1:V:89:GLY:C	2:W:102:LYS:HZ1	2.25	0.45
5:b:102:ASP:OD1	5:b:103:GLU:N	2.50	0.45
3:E:81:GLN:HG2	1:O:45:LYS:CE	2.47	0.45
2:J:108:ASP:O	1:V:180:ARG:CD	2.65	0.45
2:J:109:TYR:HE1	1:V:179:LYS:HG2	1.75	0.45
1:A:182:ARG:NH1	2:D:105:SER:OG	2.50	0.44
1:C:157:GLN:HE21	3:M:89:ILE:HD13	1.81	0.44
1:V:165:TRP:CD1	2:W:13:ILE:CG2	3.00	0.44
1:Q:170:TYR:OH	2:T:144:ARG:NH1	2.50	0.44
1:C:179:LYS:CG	3:F:109:TYR:HE1	2.28	0.44
1:P:8:TYR:OH	1:Z:155:PHE:CD2	2.65	0.44
1:C:227:ASP:CG	3:F:97:ARG:HH12	2.21	0.44
4:L:93:ASP:OD1	4:L:94:THR:N	2.45	0.44
1:G:59:ARG:HH11	4:L:97:ARG:HB3	1.82	0.44
1:C:170:TYR:HE2	3:E:104:ARG:HH22	1.65	0.44
1:P:179:LYS:HE2	3:S:109:TYR:OH	2.17	0.44
5:b:93:ALA:N	5:b:145:CYS:O	2.47	0.43
1:B:182:ARG:CZ	3:F:105:SER:OG	2.66	0.43
1:Q:189:SER:OG	2:T:5:GLY:HA3	2.18	0.43
1:Z:170:TYR:OH	3:K:144:ARG:NH1	2.52	0.43
1:X:182:ARG:HH21	3:a:106:ASP:HA	1.83	0.42
1:Q:181:GLY:HA2	2:T:153:ASP:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:8:TYR:OH	3:R:89:ILE:HG21	2.20	0.42
1:U:164:PRO:HG2	2:J:11:LYS:HE2	2.02	0.42
2:J:97:ARG:O	2:J:111:ARG:NH2	2.53	0.42
1:V:90:GLU:CA	2:W:102:LYS:HZ1	2.33	0.42
1:V:90:GLU:HA	2:W:102:LYS:HZ1	1.84	0.42
2:T:97:ARG:O	2:T:111:ARG:NH2	2.53	0.42
1:Z:182:ARG:NE	3:K:105:SER:O	2.53	0.42
4:I:120:ASP:OD1	4:I:121:GLU:N	2.49	0.42
2:D:97:ARG:O	2:D:111:ARG:NH2	2.53	0.41
1:C:179:LYS:HE2	3:F:109:TYR:OH	2.20	0.41
3:N:120:ASP:OD1	3:N:121:GLU:N	2.49	0.41
4:Y:7:ASN:OD1	4:Y:8:GLY:N	2.53	0.41
1:A:60:PHE:O	1:A:172:TRP:NE1	2.52	0.41
4:I:7:ASN:OD1	4:I:8:GLY:N	2.53	0.41
1:C:60:PHE:O	1:C:172:TRP:NE1	2.52	0.41
1:P:108:GLN:O	1:P:110:VAL:N	2.54	0.41
2:W:97:ARG:O	2:W:111:ARG:NH2	2.53	0.41
4:L:7:ASN:OD1	4:L:8:GLY:N	2.53	0.41
3:E:120:ASP:OD1	3:E:121:GLU:N	2.49	0.41
1:V:165:TRP:CD1	2:W:13:ILE:HG21	2.55	0.41
1:C:108:GLN:O	1:C:110:VAL:N	2.54	0.41
1:P:89:GLY:O	3:R:102:LYS:HE3	2.20	0.41
1:Z:108:GLN:O	1:Z:110:VAL:N	2.54	0.41
1:X:60:PHE:O	1:X:172:TRP:NE1	2.52	0.41
1:P:90:GLU:HA	3:R:102:LYS:HZ1	1.85	0.41
1:A:83:ASN:OD1	1:A:84:ILE:N	2.55	0.40
1:Q:83:ASN:OD1	1:Q:84:ILE:N	2.55	0.40
1:Q:191:SER:O	2:T:3:GLU:N	2.55	0.40
1:O:83:ASN:OD1	1:O:84:ILE:N	2.54	0.40
1:U:83:ASN:OD1	1:U:84:ILE:N	2.55	0.40
2:J:109:TYR:CE1	1:V:178:LEU:O	2.74	0.40
1:V:83:ASN:OD1	1:V:84:ILE:N	2.55	0.40
2:T:102:LYS:HB2	2:T:109:TYR:CE2	2.56	0.40
2:J:102:LYS:HB2	2:J:109:TYR:CE2	2.56	0.40
2:W:102:LYS:HB2	2:W:109:TYR:CE2	2.56	0.40
1:H:182:ARG:NH1	3:M:105:SER:OG	2.55	0.40
1:P:83:ASN:OD1	1:P:84:ILE:N	2.55	0.40
1:H:83:ASN:OD1	1:H:84:ILE:N	2.55	0.40
1:X:108:GLN:O	1:X:110:VAL:N	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	227/229 (99%)	197 (87%)	30 (13%)	0	100	100
1	B	227/229 (99%)	197 (87%)	30 (13%)	0	100	100
1	C	227/229 (99%)	196 (86%)	31 (14%)	0	100	100
1	G	227/229 (99%)	196 (86%)	31 (14%)	0	100	100
1	H	227/229 (99%)	196 (86%)	31 (14%)	0	100	100
1	O	227/229 (99%)	196 (86%)	31 (14%)	0	100	100
1	P	227/229 (99%)	197 (87%)	30 (13%)	0	100	100
1	Q	227/229 (99%)	196 (86%)	31 (14%)	0	100	100
1	U	227/229 (99%)	196 (86%)	31 (14%)	0	100	100
1	V	227/229 (99%)	196 (86%)	31 (14%)	0	100	100
1	X	227/229 (99%)	196 (86%)	31 (14%)	0	100	100
1	Z	227/229 (99%)	196 (86%)	31 (14%)	0	100	100
2	D	170/172 (99%)	156 (92%)	14 (8%)	0	100	100
2	J	170/172 (99%)	155 (91%)	15 (9%)	0	100	100
2	T	170/172 (99%)	156 (92%)	14 (8%)	0	100	100
2	W	170/172 (99%)	156 (92%)	14 (8%)	0	100	100
3	E	173/175 (99%)	160 (92%)	13 (8%)	0	100	100
3	F	173/175 (99%)	160 (92%)	13 (8%)	0	100	100
3	K	173/175 (99%)	160 (92%)	13 (8%)	0	100	100
3	M	173/175 (99%)	160 (92%)	13 (8%)	0	100	100
3	N	173/175 (99%)	160 (92%)	13 (8%)	0	100	100
3	R	173/175 (99%)	160 (92%)	13 (8%)	0	100	100
3	S	173/175 (99%)	160 (92%)	13 (8%)	0	100	100
3	a	173/175 (99%)	160 (92%)	13 (8%)	0	100	100
4	I	159/161 (99%)	148 (93%)	11 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	L	159/161 (99%)	148 (93%)	11 (7%)	0	100	100
4	Y	159/161 (99%)	148 (93%)	11 (7%)	0	100	100
5	b	133/135 (98%)	119 (90%)	13 (10%)	1 (1%)	16	47
All	All	5398/5454 (99%)	4821 (89%)	576 (11%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	b	113	ASN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	198/198 (100%)	198 (100%)	0	100	100
1	B	198/198 (100%)	198 (100%)	0	100	100
1	C	198/198 (100%)	198 (100%)	0	100	100
1	G	198/198 (100%)	198 (100%)	0	100	100
1	H	198/198 (100%)	198 (100%)	0	100	100
1	O	198/198 (100%)	198 (100%)	0	100	100
1	P	198/198 (100%)	198 (100%)	0	100	100
1	Q	198/198 (100%)	198 (100%)	0	100	100
1	U	198/198 (100%)	198 (100%)	0	100	100
1	V	198/198 (100%)	198 (100%)	0	100	100
1	X	198/198 (100%)	198 (100%)	0	100	100
1	Z	198/198 (100%)	198 (100%)	0	100	100
2	D	143/143 (100%)	143 (100%)	0	100	100
2	J	143/143 (100%)	143 (100%)	0	100	100
2	T	143/143 (100%)	143 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	W	143/143 (100%)	143 (100%)	0	100	100
3	E	146/146 (100%)	146 (100%)	0	100	100
3	F	146/146 (100%)	146 (100%)	0	100	100
3	K	146/146 (100%)	146 (100%)	0	100	100
3	M	146/146 (100%)	146 (100%)	0	100	100
3	N	146/146 (100%)	146 (100%)	0	100	100
3	R	146/146 (100%)	146 (100%)	0	100	100
3	S	146/146 (100%)	146 (100%)	0	100	100
3	a	146/146 (100%)	146 (100%)	0	100	100
4	I	134/134 (100%)	134 (100%)	0	100	100
4	L	134/134 (100%)	134 (100%)	0	100	100
4	Y	134/134 (100%)	134 (100%)	0	100	100
5	b	107/107 (100%)	107 (100%)	0	100	100
All	All	4625/4625 (100%)	4625 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	C	32	GLN
1	C	157	GLN
1	B	32	GLN
1	B	187	HIS
1	Q	32	GLN
1	P	32	GLN
1	O	32	GLN
1	O	187	HIS
1	U	32	GLN
1	Z	32	GLN
1	Z	195	ASN
3	K	83	ASN
1	V	32	GLN
1	H	32	GLN
1	G	32	GLN
1	G	187	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	X	32	GLN
5	b	91	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
7	c	1
7	d	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	c	65:UNK	C	109:UNK	N	25.20
1	d	65:UNK	C	109:UNK	N	25.20

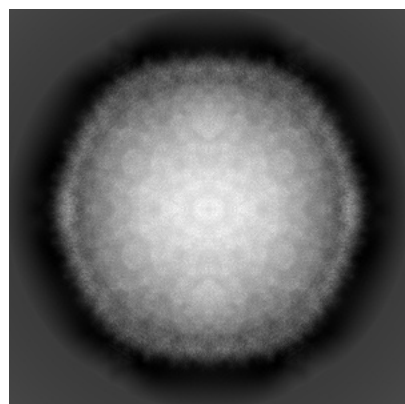
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0172. These allow visual inspection of the internal detail of the map and identification of artifacts.

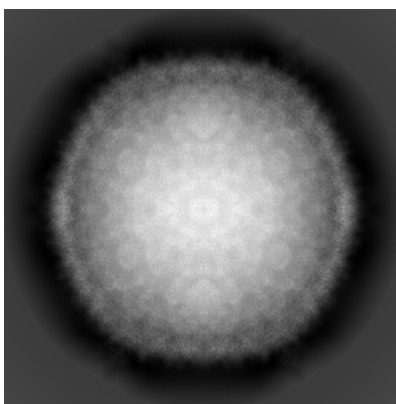
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

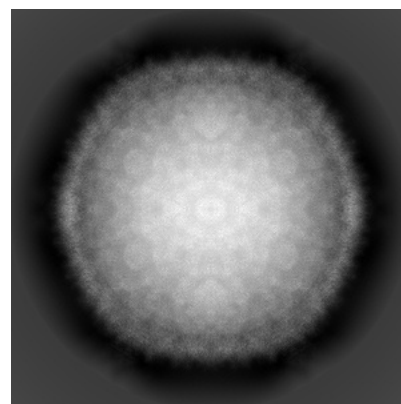
6.1.1 Primary map



X

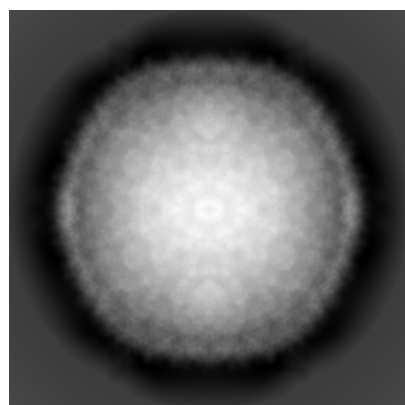


Y

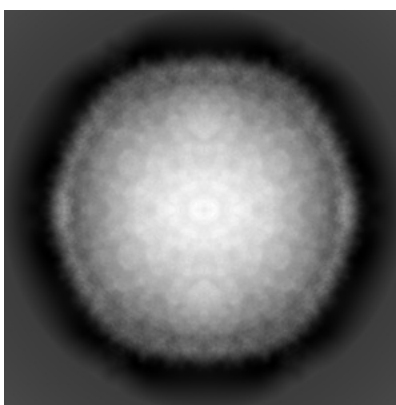


Z

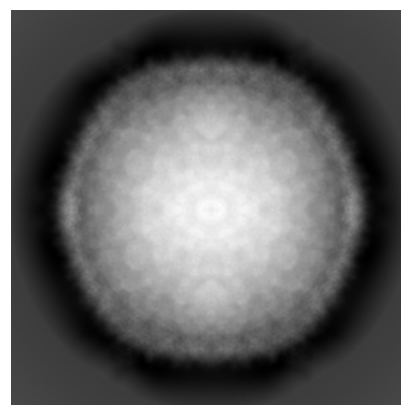
6.1.2 Raw map



X



Y

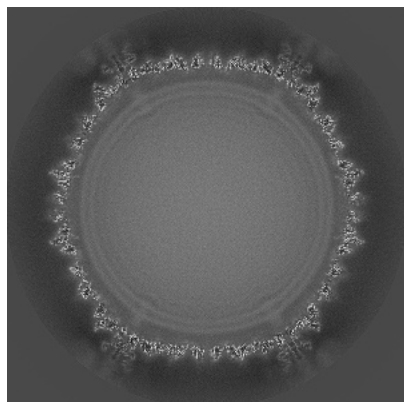


Z

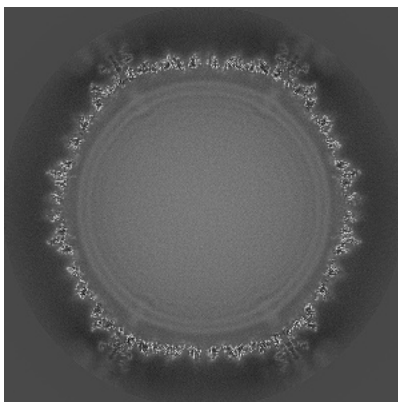
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

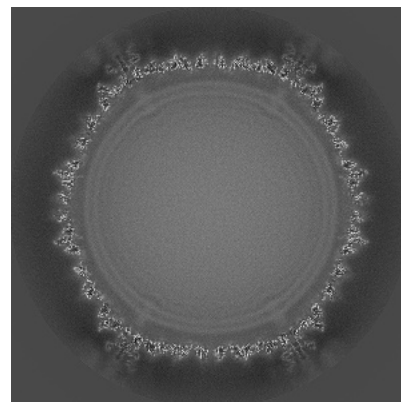
6.2.1 Primary map



X Index: 380

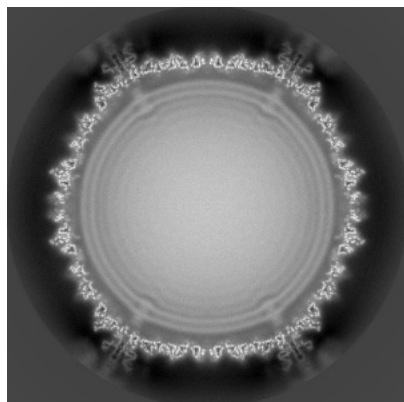


Y Index: 380

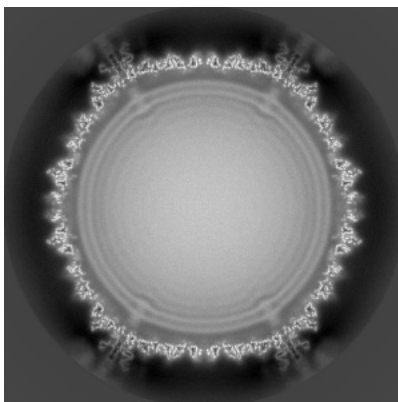


Z Index: 380

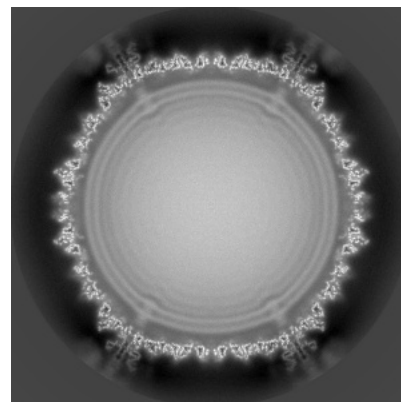
6.2.2 Raw map



X Index: 380



Y Index: 380

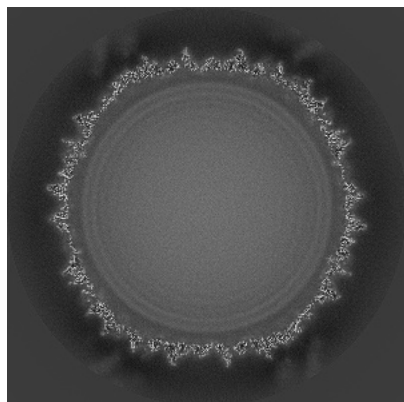


Z Index: 380

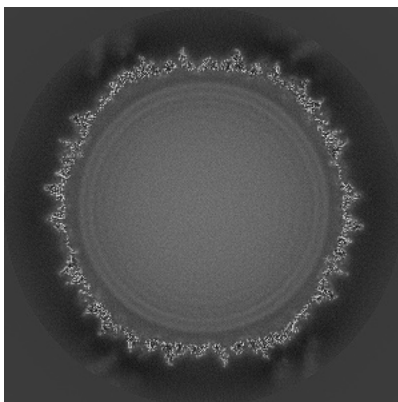
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

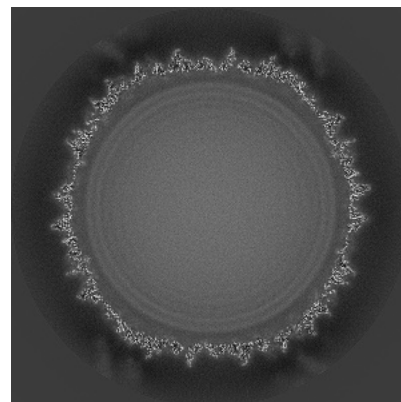
6.3.1 Primary map



X Index: 338

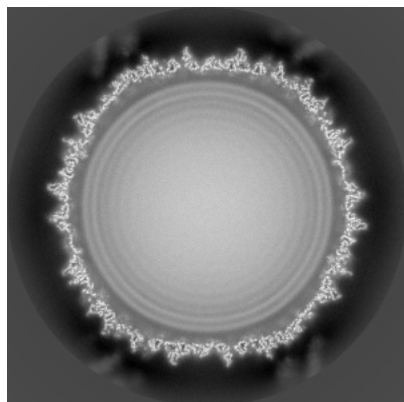


Y Index: 338

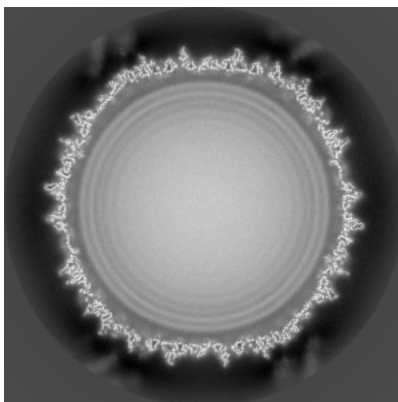


Z Index: 420

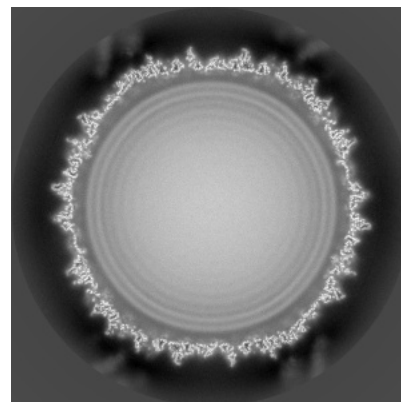
6.3.2 Raw map



X Index: 339



Y Index: 339

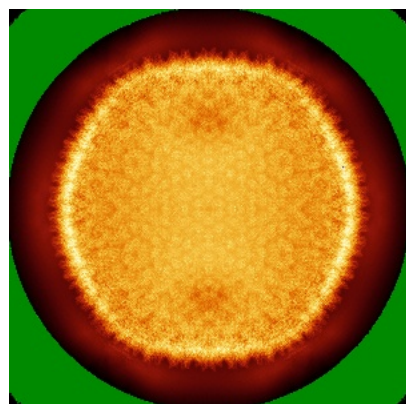


Z Index: 339

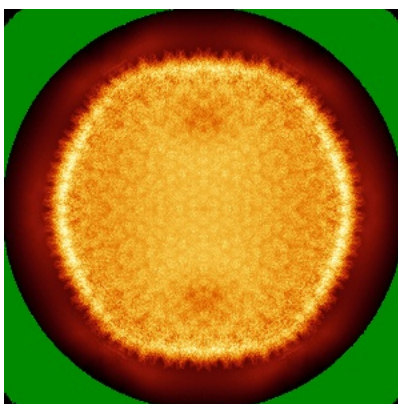
The images above show the largest variance slices of the map in three orthogonal directions.

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

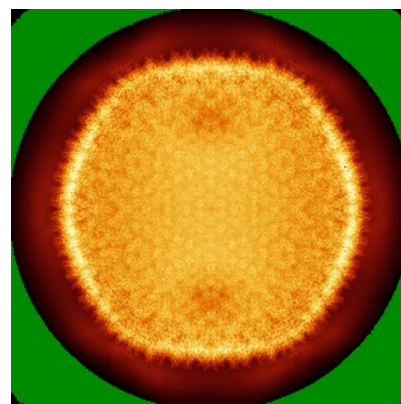
6.4.1 Primary map



X

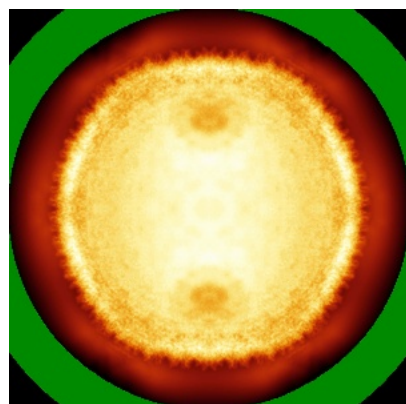


Y

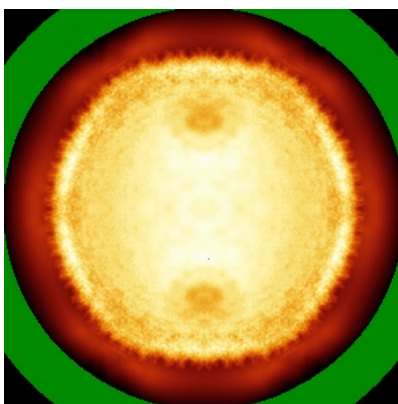


Z

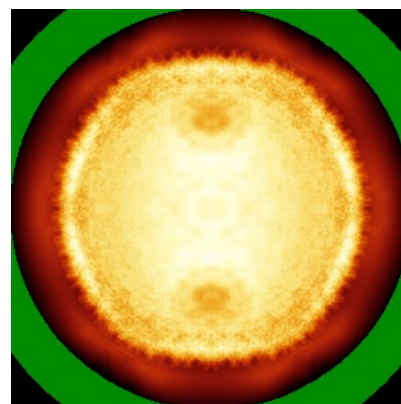
6.4.2 Raw map



X



Y

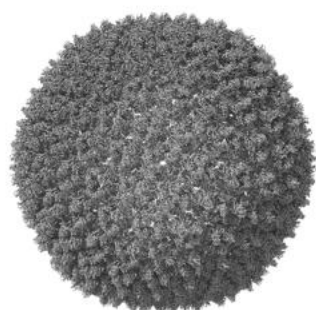


Z

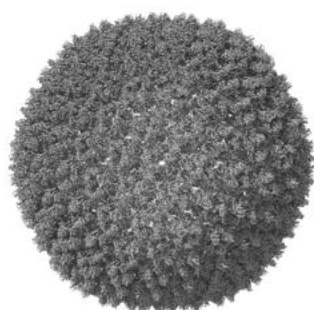
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

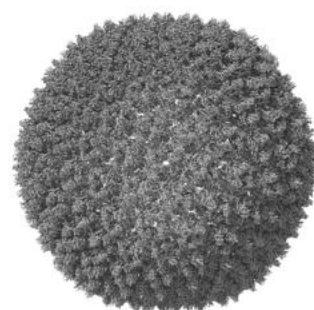
6.5.1 Primary map



X



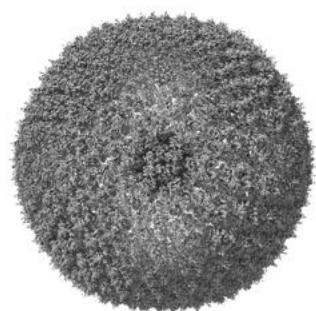
Y



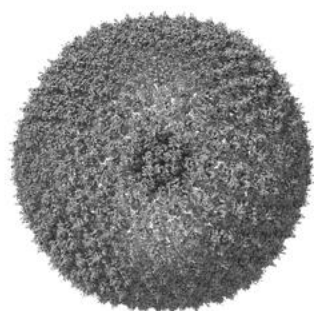
Z

The images above show the 3D surface view of the map at the recommended contour level 0.067. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

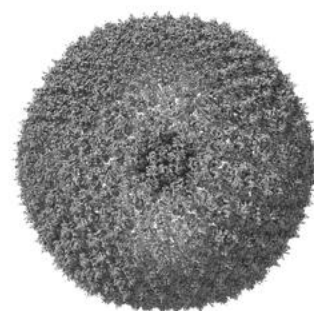
6.5.2 Raw map



X



Y



Z

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

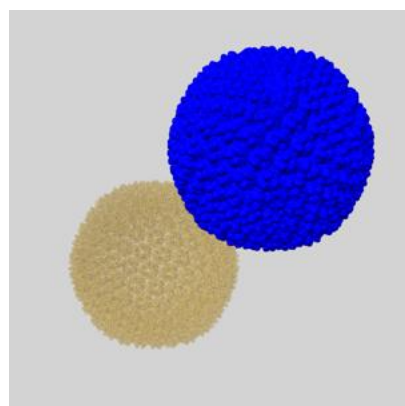
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

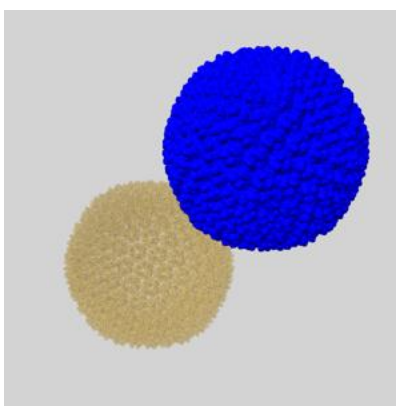
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

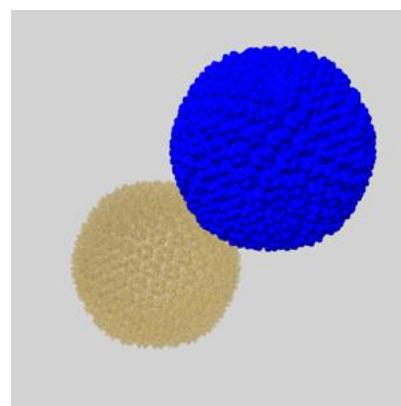
6.6.1 emd_0172_msk_1.map [i](#)



X



Y

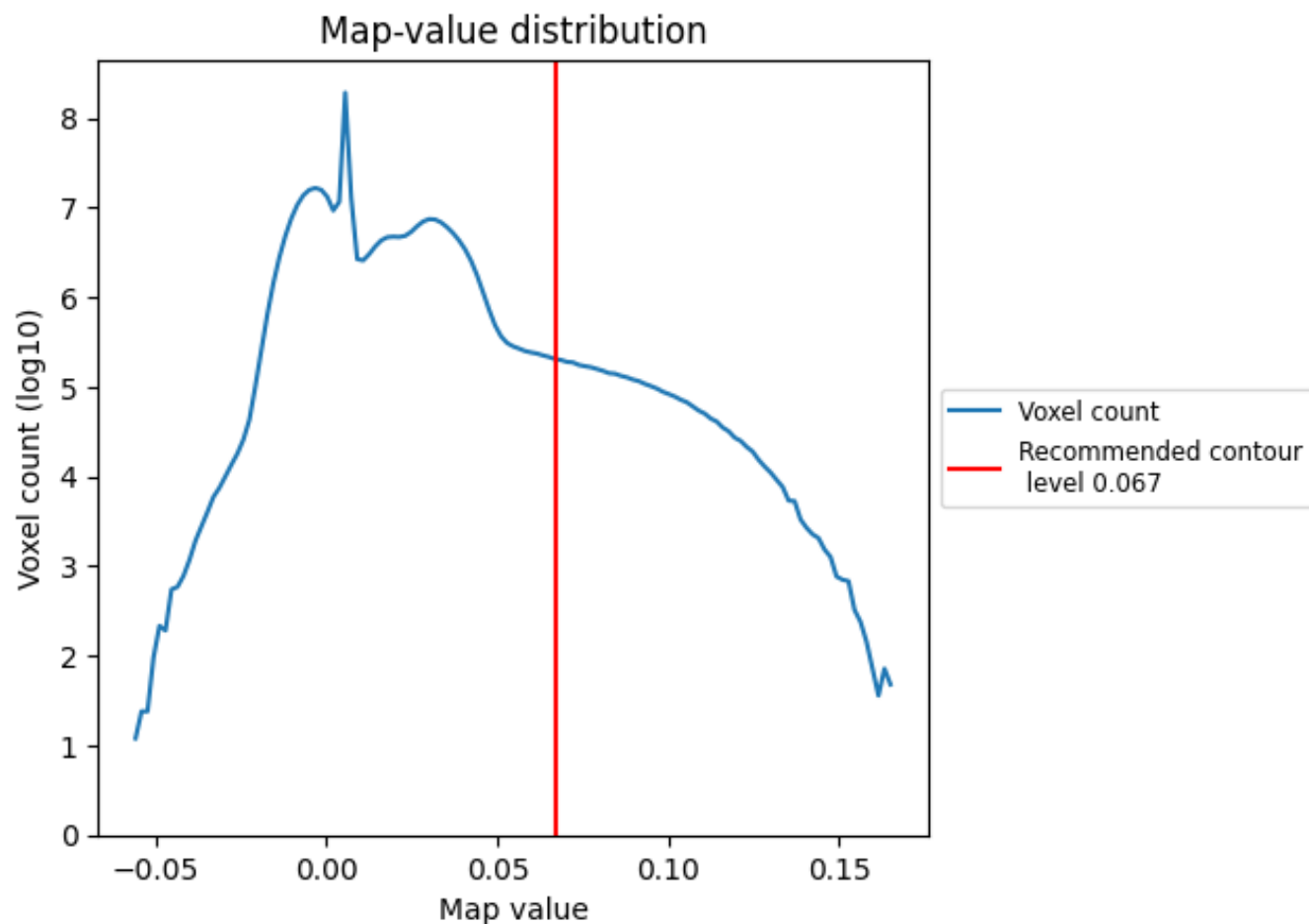


Z

7 Map analysis [i](#)

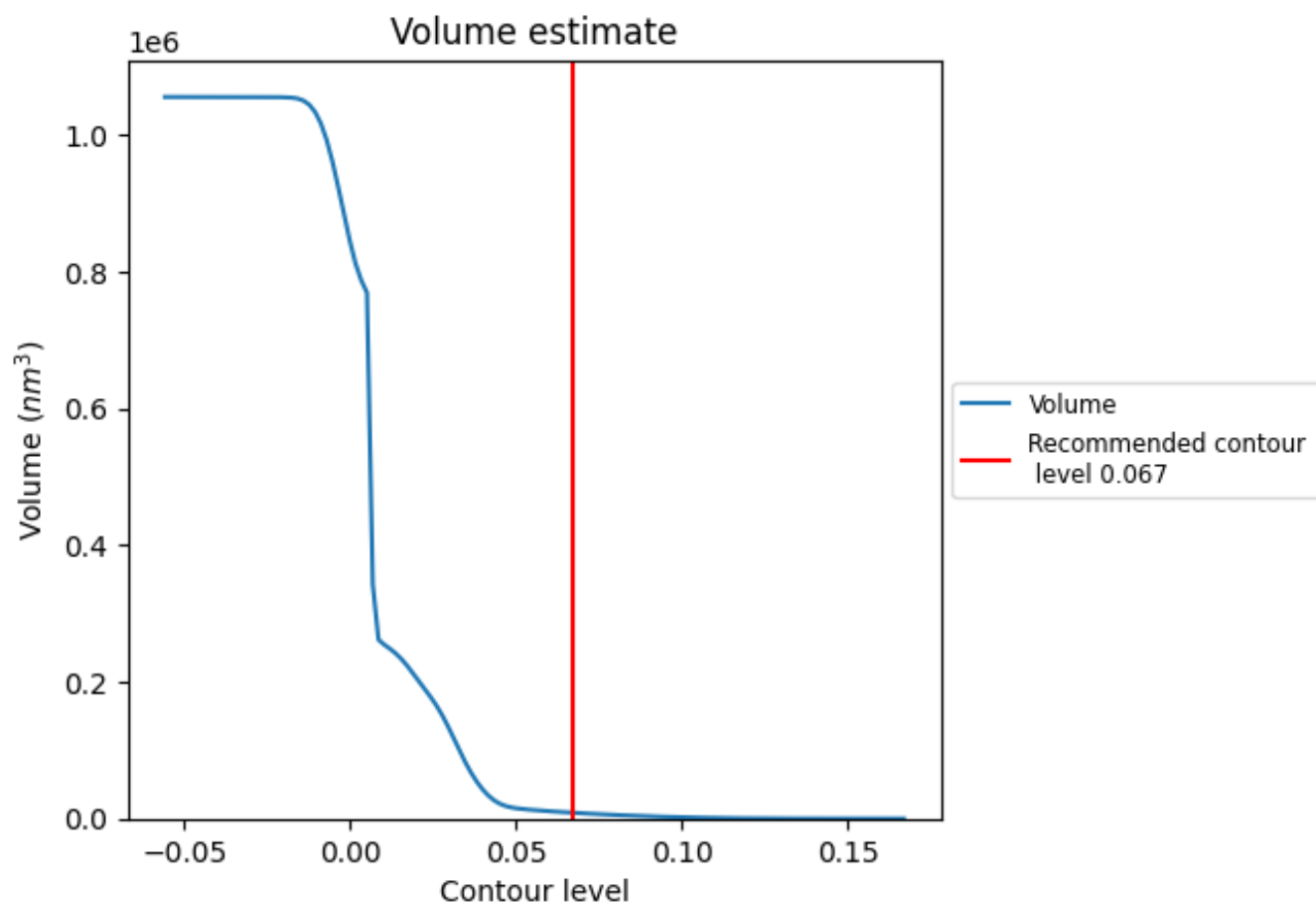
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

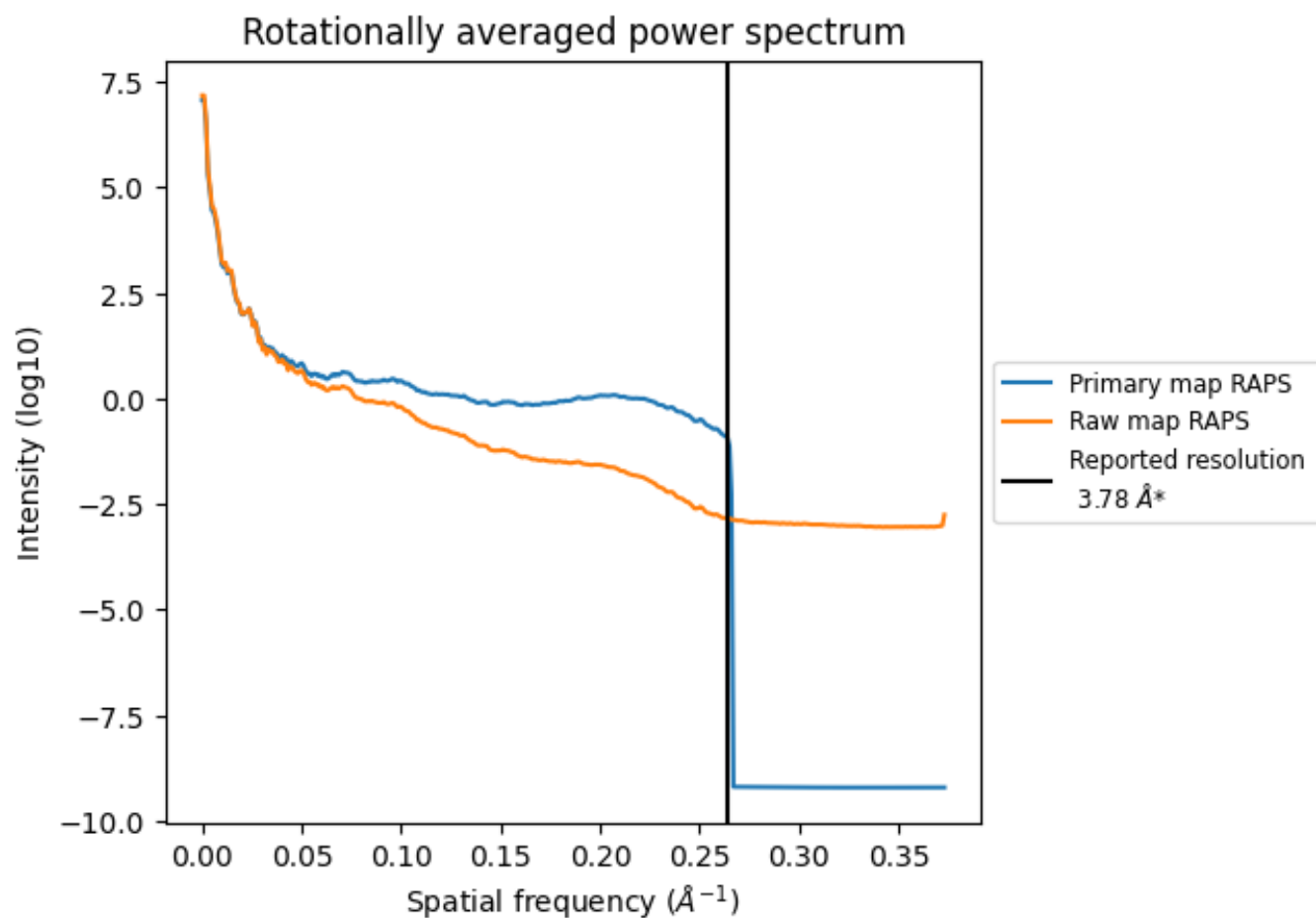
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 8614 nm³; this corresponds to an approximate mass of 7782 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

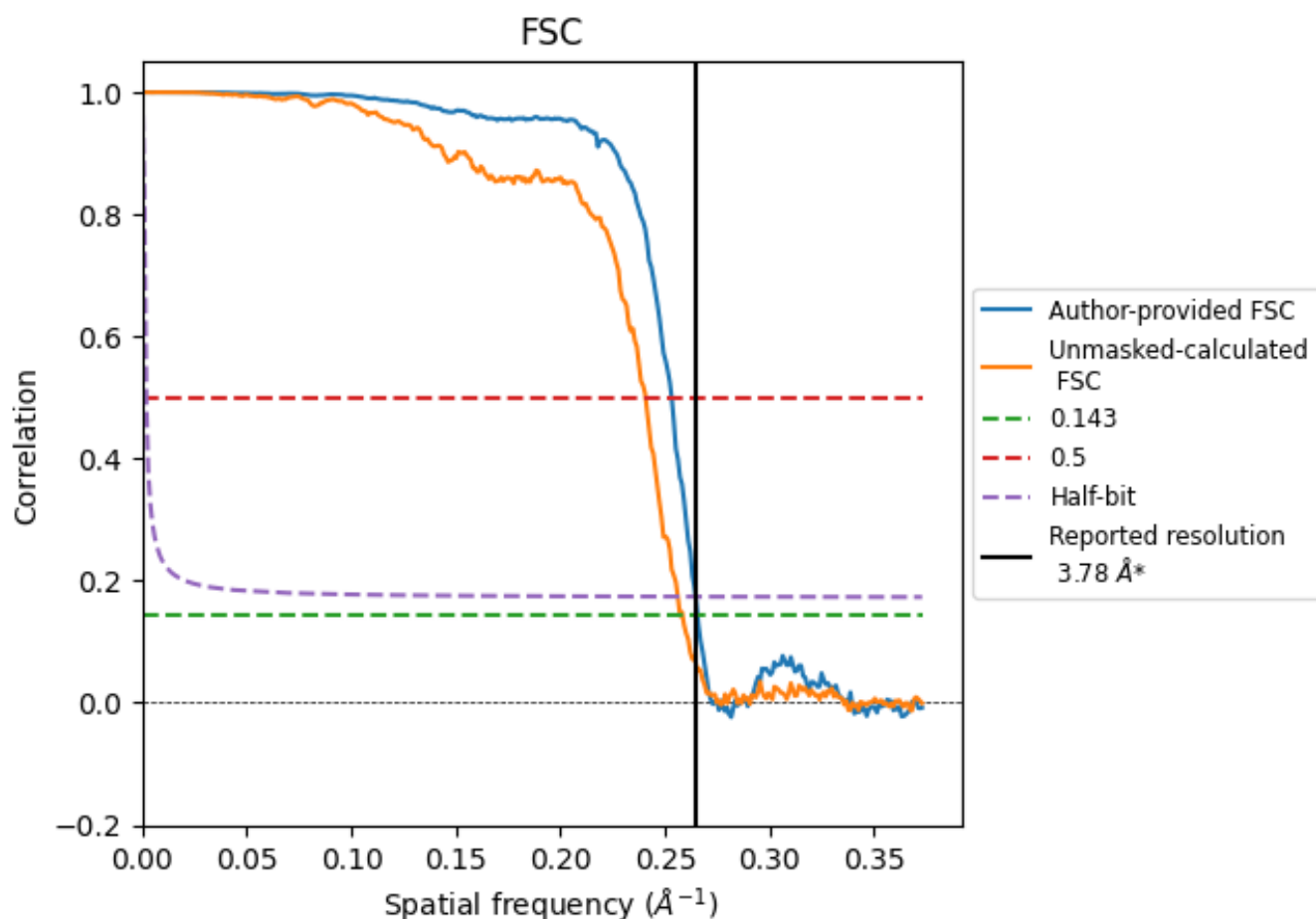


*Reported resolution corresponds to spatial frequency of 0.265 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.265 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.78	-	-
Author-provided FSC curve	3.76	3.95	3.78
Unmasked-calculated*	3.89	4.15	3.90

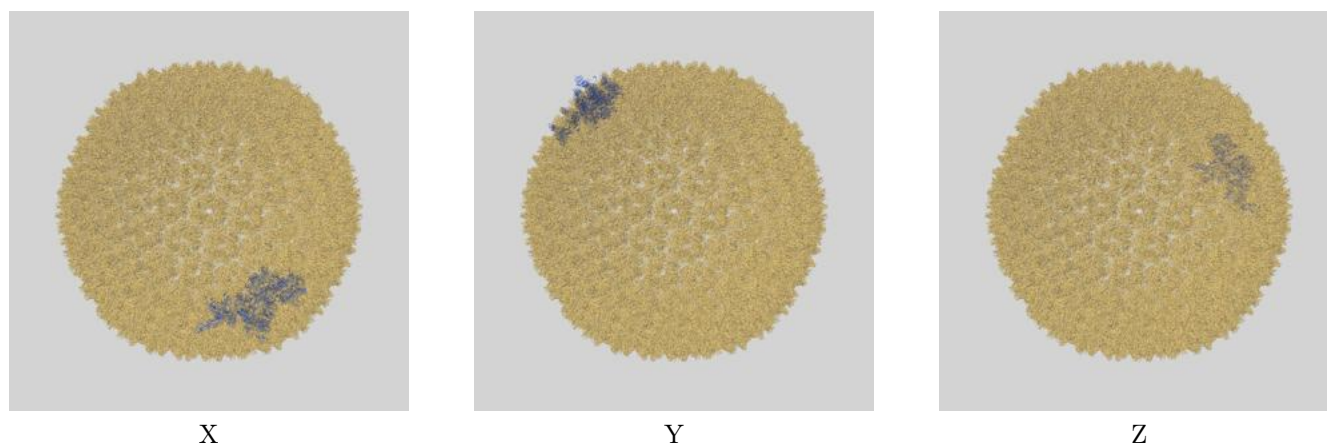
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

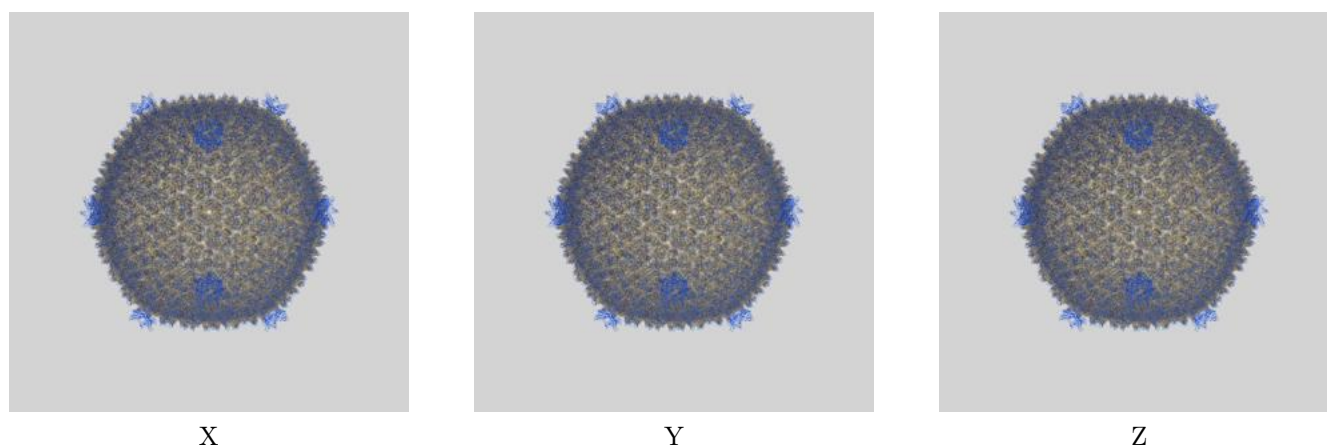
This section contains information regarding the fit between EMDB map EMD-0172 and PDB model 6H82. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)



9.1.2 Map-model assembly overlay [i](#)



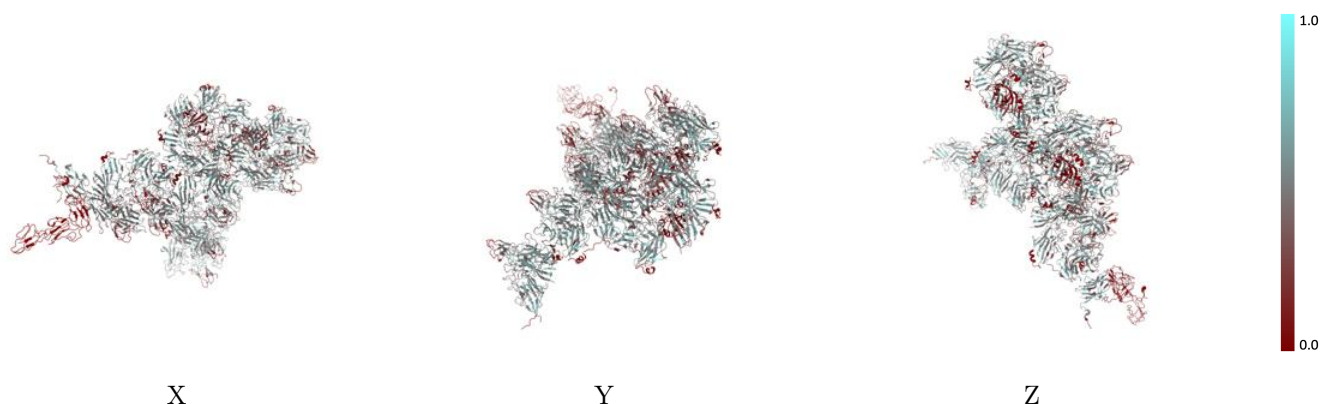
The images above show the 3D surface view of the map at the recommended contour level 0.067 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



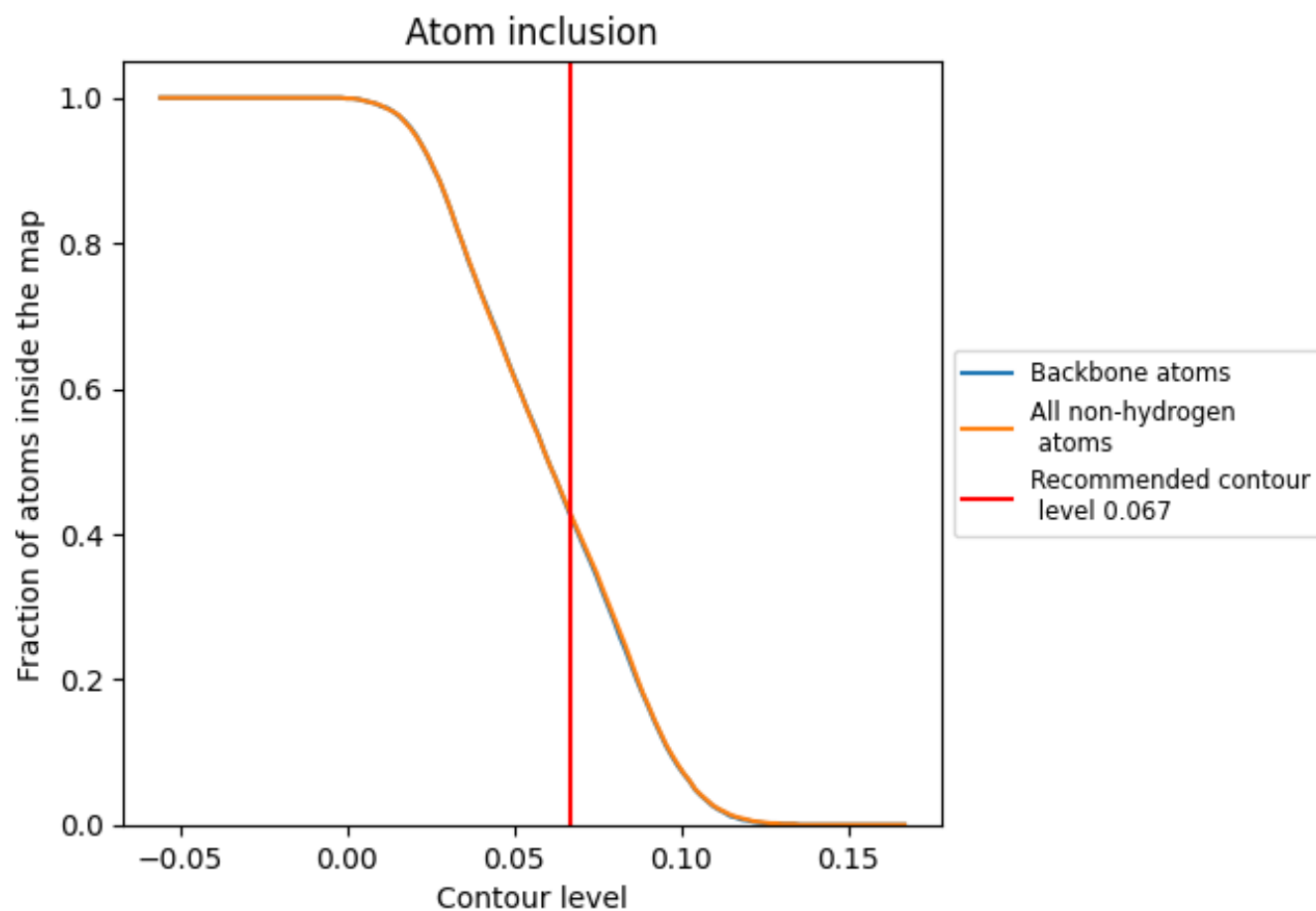
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.067).

9.4 Atom inclusion [i](#)



At the recommended contour level, 42% of all backbone atoms, 43% 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 (0.067) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4260	 0.3890
A	 0.4150	 0.3850
B	 0.4160	 0.3770
C	 0.4130	 0.3730
D	 0.4490	 0.4030
E	 0.4370	 0.3840
F	 0.4290	 0.3990
G	 0.4650	 0.3890
H	 0.4680	 0.3890
I	 0.4810	 0.4140
J	 0.4590	 0.3970
K	 0.4540	 0.3950
L	 0.4810	 0.4180
M	 0.4550	 0.4040
N	 0.4620	 0.3890
O	 0.4590	 0.3900
P	 0.4460	 0.3760
Q	 0.4580	 0.3840
R	 0.4530	 0.3900
S	 0.4580	 0.3970
T	 0.4480	 0.4050
U	 0.4700	 0.3900
V	 0.4490	 0.3730
W	 0.4740	 0.4010
X	 0.4750	 0.3840
Y	 0.4880	 0.4110
Z	 0.4770	 0.3870
a	 0.4640	 0.3890
b	 0.4380	 0.4050
c	 0.0190	 0.4090
d	 0.0000	 0.3500
g	 0.0020	 0.3240
m	 0.0240	 0.4540

