



wwPDB EM Validation Summary Report ⓘ

Oct 8, 2024 – 10:23 AM EDT

PDB ID : 4V7Q
EMDB ID : EMD-5199
Title : Atomic model of an infectious rotavirus particle
Authors : Settembre, E.C.; Chen, J.Z.; Dormitzer, P.R.; Grigorieff, N.; Harrison, S.C.
Deposited on : 2010-05-13
Resolution : 3.80 Å(reported)

This is a wwPDB EM Validation Summary 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.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

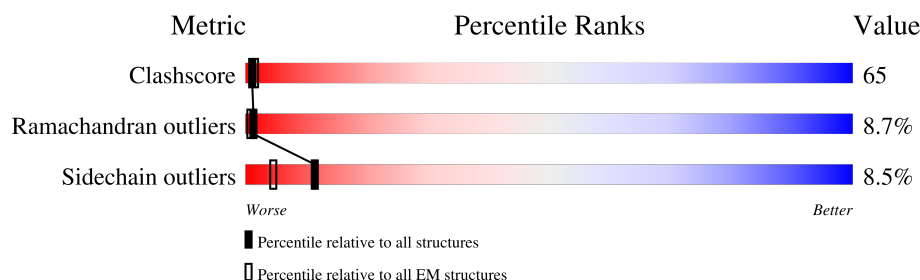
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	AA	800	<div> <div>12%</div> <div>18%</div> <div>57%</div> <div>20%</div> <div>• •</div> </div>
1	AB	800	<div> <div>12%</div> <div>20%</div> <div>57%</div> <div>22%</div> <div>•</div> </div>
2	AC	397	<div> <div>8%</div> <div>56%</div> <div>37%</div> <div>7%</div> <div>•</div> </div>
2	AD	397	<div> <div>10%</div> <div>57%</div> <div>36%</div> <div>7%</div> <div>•</div> </div>
2	AE	397	<div> <div>8%</div> <div>56%</div> <div>37%</div> <div>7%</div> <div>•</div> </div>
2	AF	397	<div> <div>11%</div> <div>59%</div> <div>34%</div> <div>6%</div> <div>•</div> </div>
2	AG	397	<div> <div>14%</div> <div>57%</div> <div>36%</div> <div>7%</div> <div>•</div> </div>
2	AH	397	<div> <div>8%</div> <div>54%</div> <div>39%</div> <div>7%</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
2	AI	397	
2	AJ	397	
2	AK	397	
2	AL	397	
2	AM	397	
2	AN	397	
2	AO	397	
3	BA	276	
3	BF	276	
3	BG	276	
3	BH	276	
3	BI	276	
3	BJ	276	
3	BK	276	
3	BL	276	
3	BM	276	
3	BN	276	
3	BO	276	
3	BP	276	
3	BQ	276	
4	BX	776	
4	BY	776	
4	BZ	776	
5	A	2	
5	B	2	

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Mol	Chain	Length	Quality of chain
5	C	2	<div> <div>100%</div> <div>50%50%</div> </div>
5	D	2	<div> <div>100%</div> <div>50%50%</div> </div>
5	E	2	<div> <div>100%</div> <div>50%50%</div> </div>
5	F	2	<div> <div>50%</div> <div>50%100%</div> </div>
5	G	2	<div> <div>100%</div> <div>100%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NAG	G	1	X	-	-	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 97287 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 Core scaffold protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AA	781	Total	C	N	O	S	0	0
			6379	4052	1101	1190	36		
1	AB	800	Total	C	N	O	S	0	0
			6545	4159	1127	1223	36		

- Molecule 2 is a protein called Intermediate capsid protein VP6.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AC	397	Total	C	N	O	S	0	0
			3163	2004	551	593	15		
2	AD	397	Total	C	N	O	S	0	0
			3163	2004	551	593	15		
2	AE	397	Total	C	N	O	S	0	0
			3163	2004	551	593	15		
2	AF	397	Total	C	N	O	S	0	0
			3163	2004	551	593	15		
2	AG	397	Total	C	N	O	S	0	0
			3163	2004	551	593	15		
2	AH	397	Total	C	N	O	S	0	0
			3163	2004	551	593	15		
2	AI	397	Total	C	N	O	S	0	0
			3163	2004	551	593	15		
2	AJ	397	Total	C	N	O	S	0	0
			3163	2004	551	593	15		
2	AK	397	Total	C	N	O	S	0	0
			3163	2004	551	593	15		
2	AL	397	Total	C	N	O	S	0	0
			3163	2004	551	593	15		
2	AM	397	Total	C	N	O	S	0	0
			3163	2004	551	593	15		
2	AN	397	Total	C	N	O	S	0	0
			3163	2004	551	593	15		
2	AO	397	Total	C	N	O	S	0	0
			3163	2004	551	593	15		

- Molecule 3 is a protein called Outer layer protein VP7.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	BA	255	Total	C	N	O	S	0	0
			2011	1277	314	404	16		
3	BF	263	Total	C	N	O	S	0	0
			2072	1311	329	416	16		
3	BG	273	Total	C	N	O	S	0	0
			2160	1372	341	431	16		
3	BH	255	Total	C	N	O	S	0	0
			2011	1277	314	404	16		
3	BI	273	Total	C	N	O	S	0	0
			2160	1372	341	431	16		
3	BJ	274	Total	C	N	O	S	0	0
			2171	1378	345	432	16		
3	BK	269	Total	C	N	O	S	0	0
			2117	1341	336	424	16		
3	BL	272	Total	C	N	O	S	0	0
			2148	1363	340	429	16		
3	BM	255	Total	C	N	O	S	0	0
			2011	1277	314	404	16		
3	BN	275	Total	C	N	O	S	0	0
			2179	1384	346	433	16		
3	BO	274	Total	C	N	O	S	0	0
			2171	1378	345	432	16		
3	BP	273	Total	C	N	O	S	0	0
			2157	1368	342	431	16		
3	BQ	255	Total	C	N	O	S	0	0
			2011	1277	314	404	16		

- Molecule 4 is a protein called Outer capsid protein VP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	BX	735	Total	C	N	O	S	0	0
			5783	3643	967	1152	21		
4	BY	738	Total	C	N	O	S	0	0
			5809	3660	972	1156	21		
4	BZ	517	Total	C	N	O	S	0	0
			4058	2551	689	802	16		

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BX	37	LEU	PRO	conflict	UNP C3RX20
BX	180	GLU	LYS	conflict	UNP C3RX20

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Chain	Residue	Modelled	Actual	Comment	Reference
BX	187	LYS	ARG	conflict	UNP C3RX20
BX	267	TYR	CYS	conflict	UNP C3RX20
BX	379	ILE	THR	conflict	UNP C3RX20
BY	37	LEU	PRO	conflict	UNP C3RX20
BY	180	GLU	LYS	conflict	UNP C3RX20
BY	187	LYS	ARG	conflict	UNP C3RX20
BY	267	TYR	CYS	conflict	UNP C3RX20
BY	379	ILE	THR	conflict	UNP C3RX20
BZ	37	LEU	PRO	conflict	UNP C3RX20
BZ	180	GLU	LYS	conflict	UNP C3RX20
BZ	187	LYS	ARG	conflict	UNP C3RX20
BZ	267	TYR	CYS	conflict	UNP C3RX20
BZ	379	ILE	THR	conflict	UNP C3RX20

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
5	A	2	Total	C	N	O	0	0
			28	16	2	10		
5	B	2	Total	C	N	O	0	0
			28	16	2	10		
5	C	2	Total	C	N	O	0	0
			28	16	2	10		
5	D	2	Total	C	N	O	0	0
			28	16	2	10		
5	E	2	Total	C	N	O	0	0
			28	16	2	10		
5	F	2	Total	C	N	O	0	0
			28	16	2	10		
5	G	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

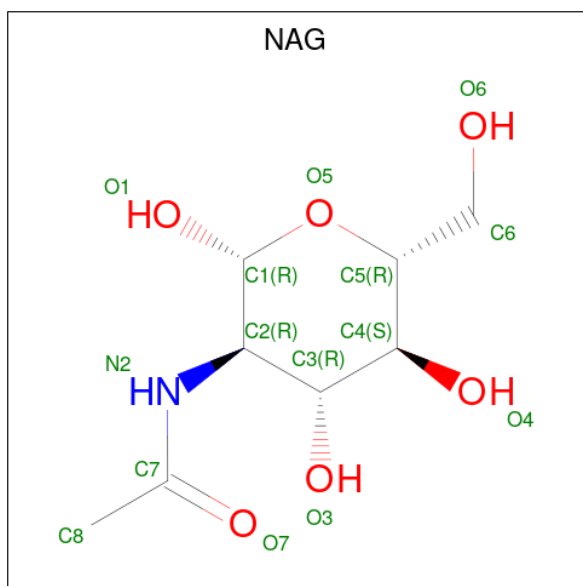
Mol	Chain	Residues	Atoms		AltConf
6	AC	1	Total	Zn	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
6	AF	1	Total	Zn	0
			1	1	
6	AK	1	Total	Zn	0
			1	1	
6	AN	1	Total	Zn	0
			1	1	
6	AO	1	Total	Zn	0
			1	1	

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

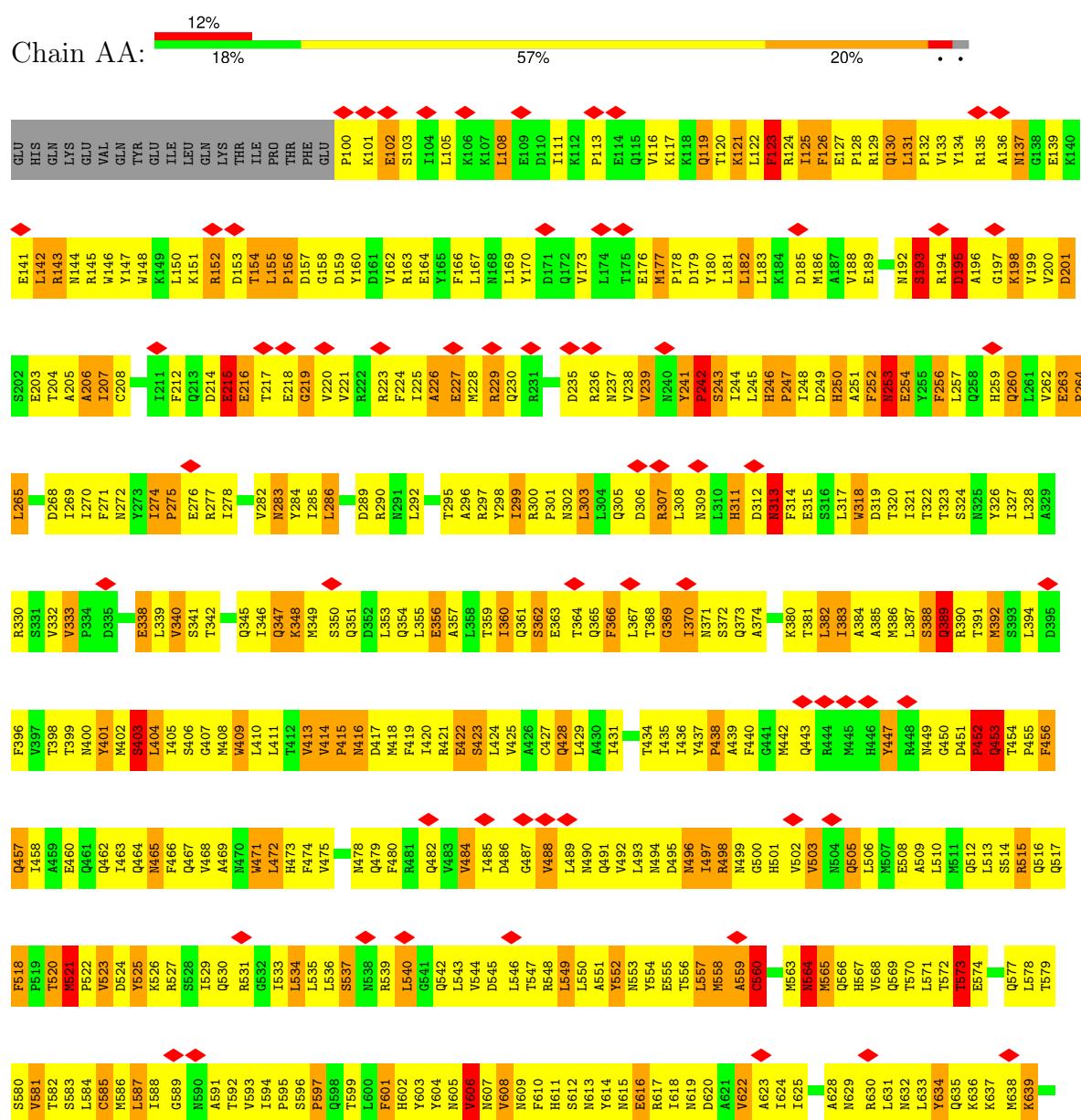


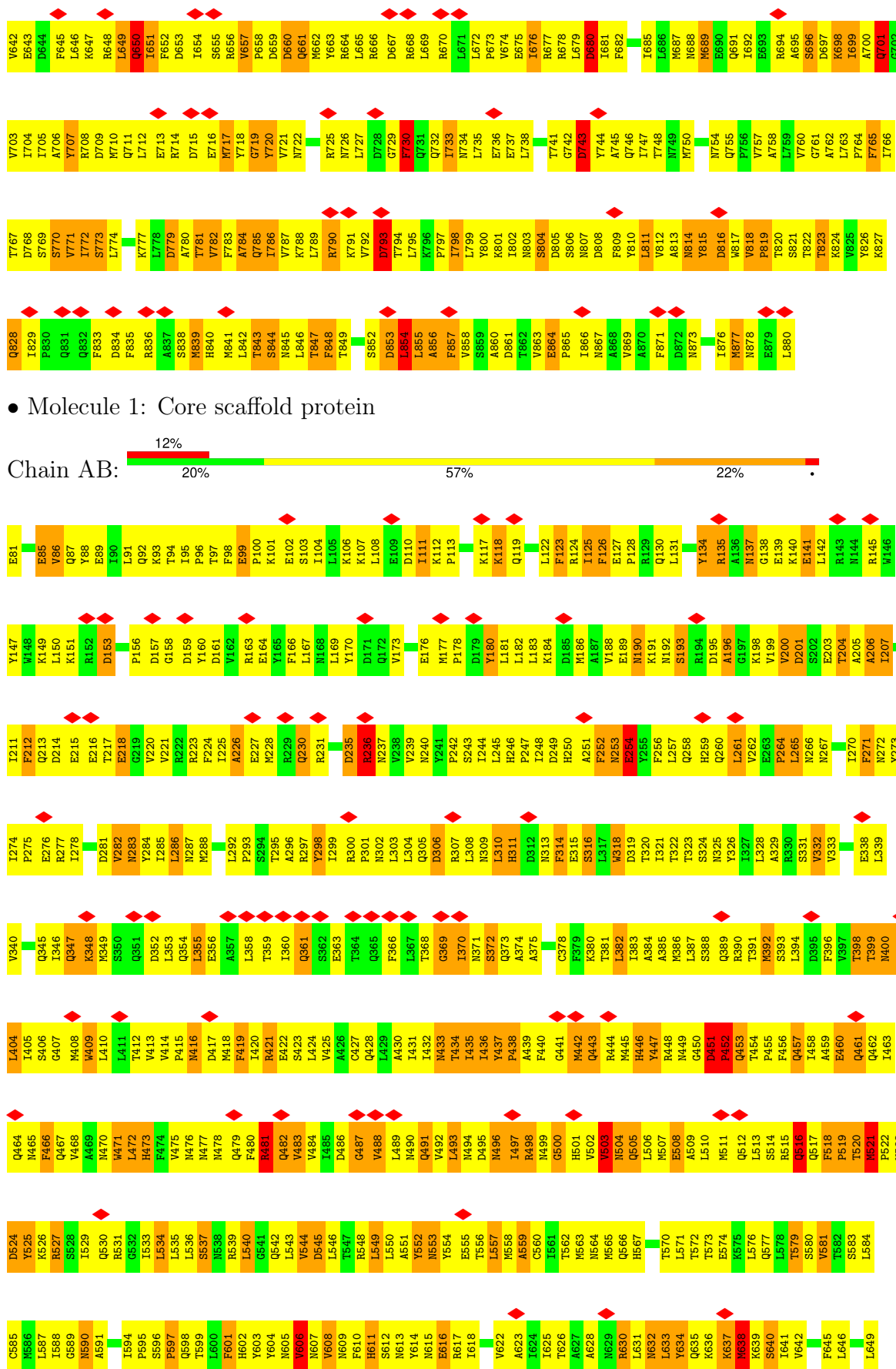
Mol	Chain	Residues	Atoms				AltConf
7	BM	1	Total	C	N	O	0
			14	8	1	5	

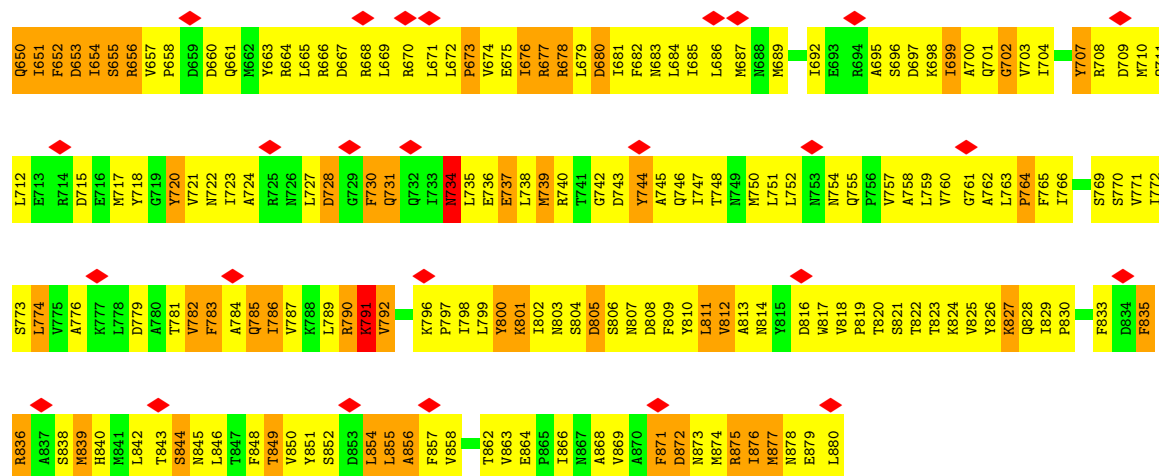
3 Residue-property plots

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.

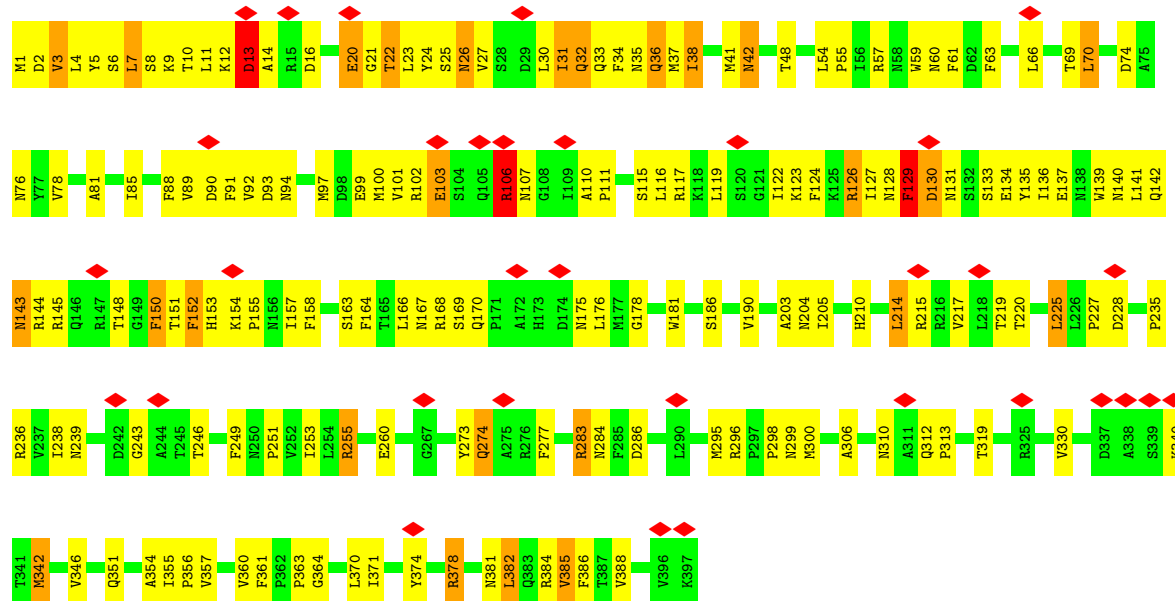
• Molecule 1: Core scaffold protein



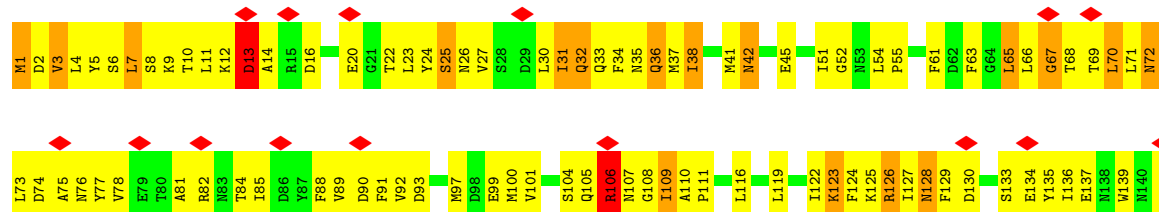


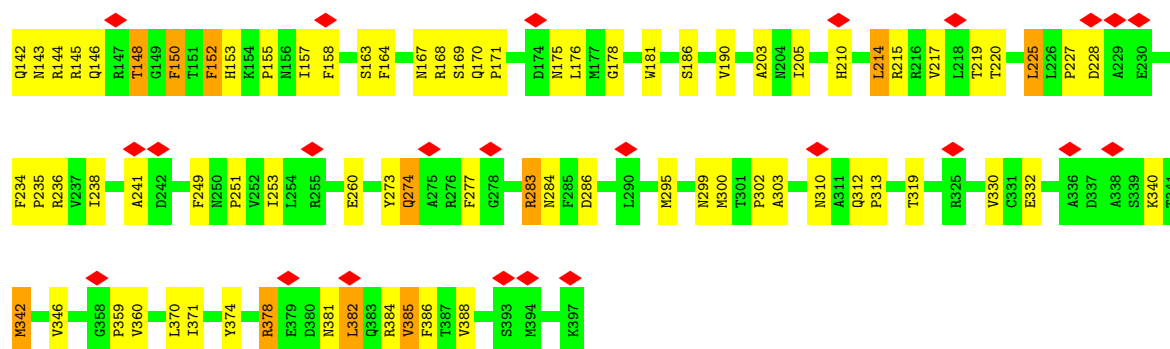


• Molecule 2: Intermediate capsid protein VP6

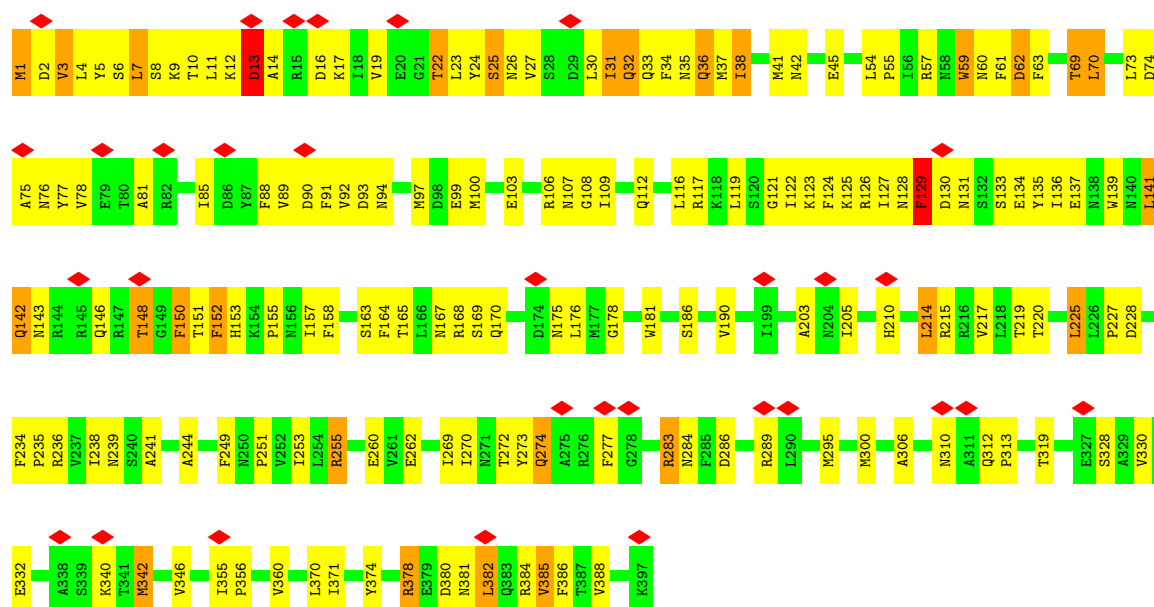


• Molecule 2: Intermediate capsid protein VP6

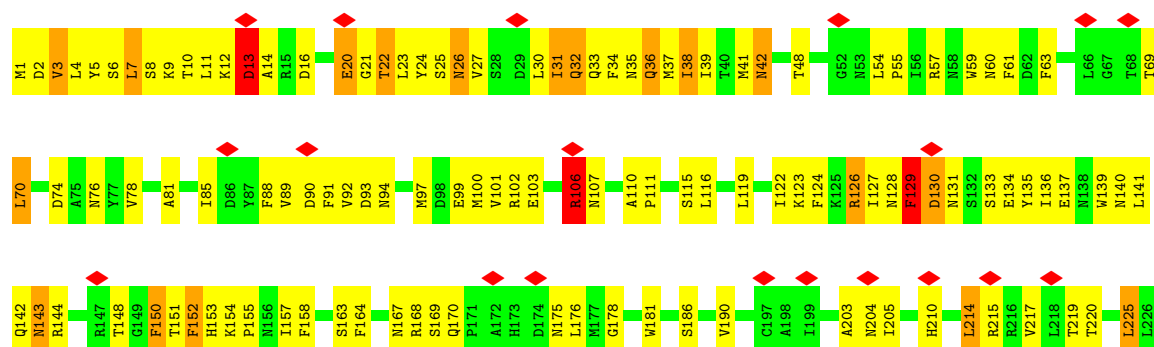


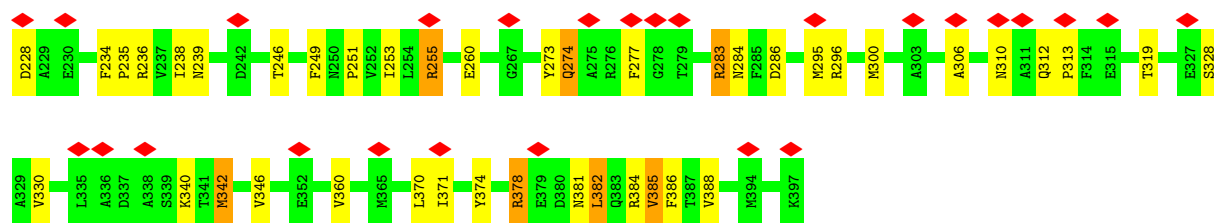


• Molecule 2: Intermediate capsid protein VP6

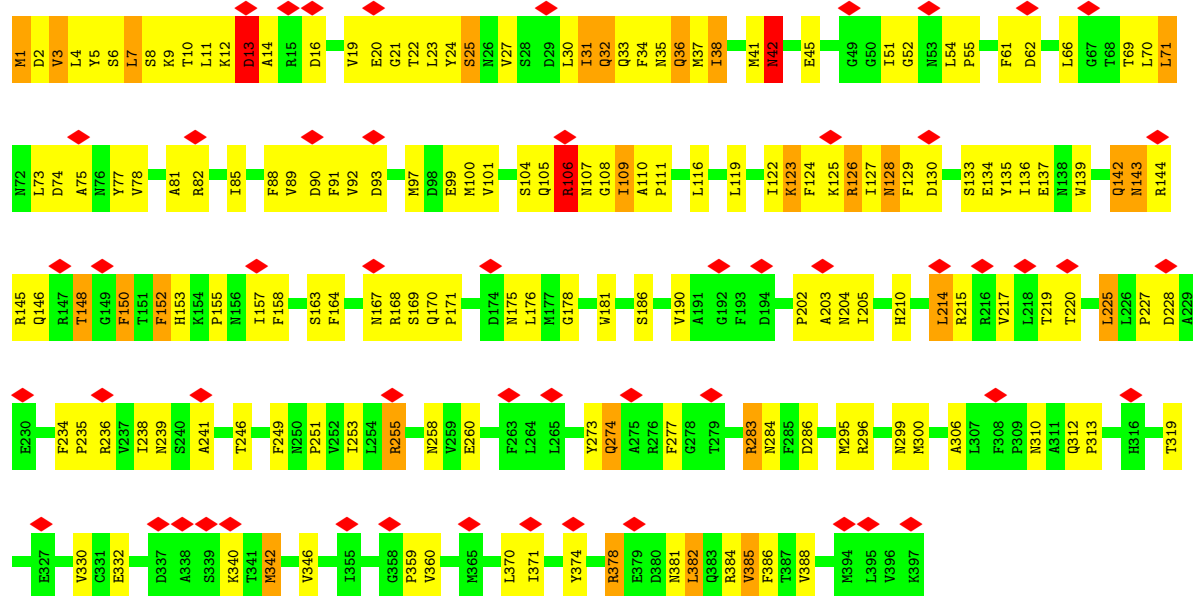


• Molecule 2: Intermediate capsid protein VP6

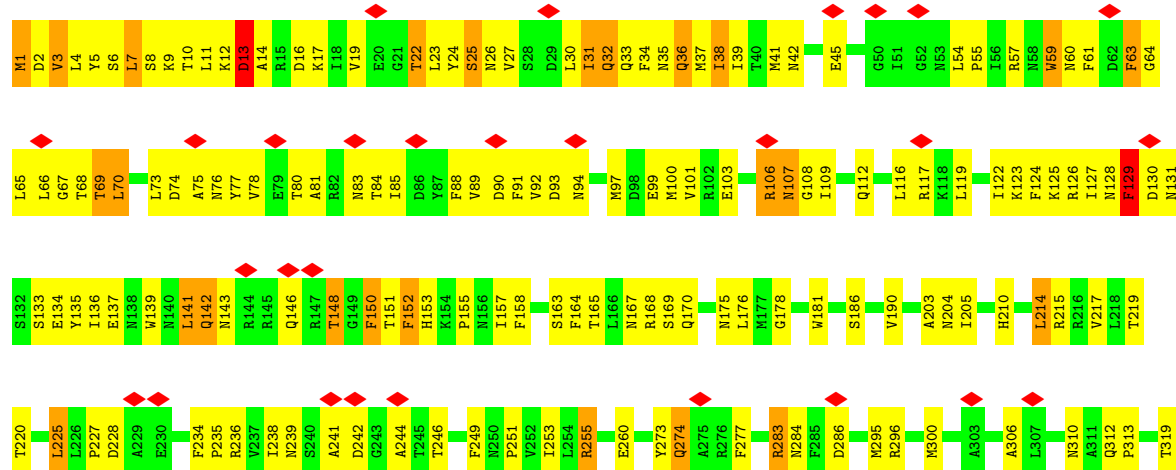




• Molecule 2: Intermediate capsid protein VP6

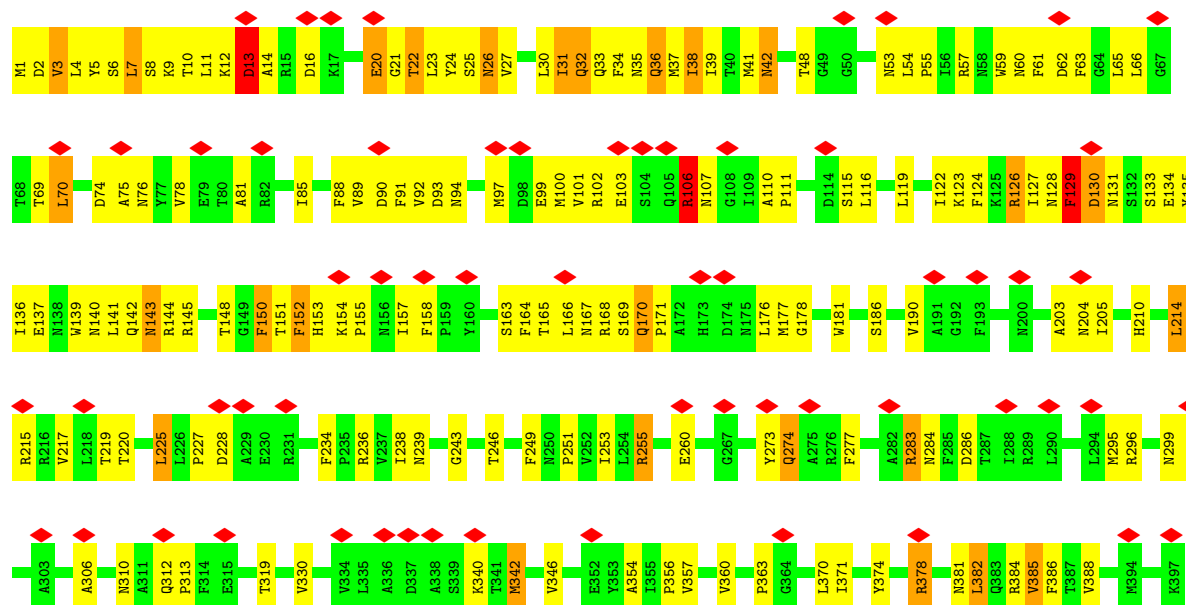


• Molecule 2: Intermediate capsid protein VP6

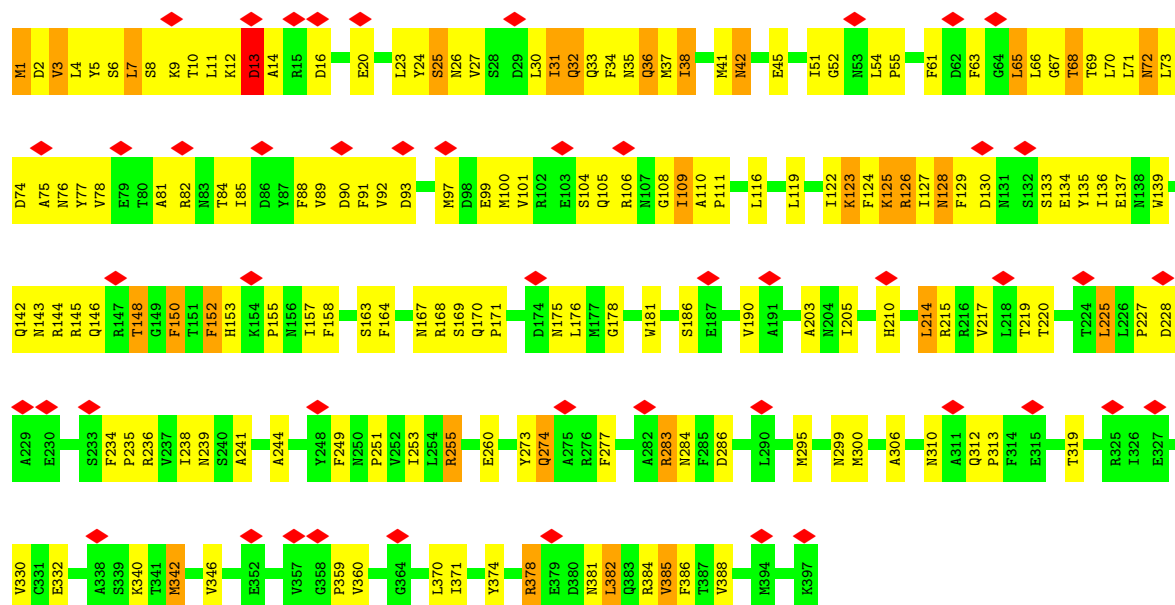




• Molecule 2: Intermediate capsid protein VP6

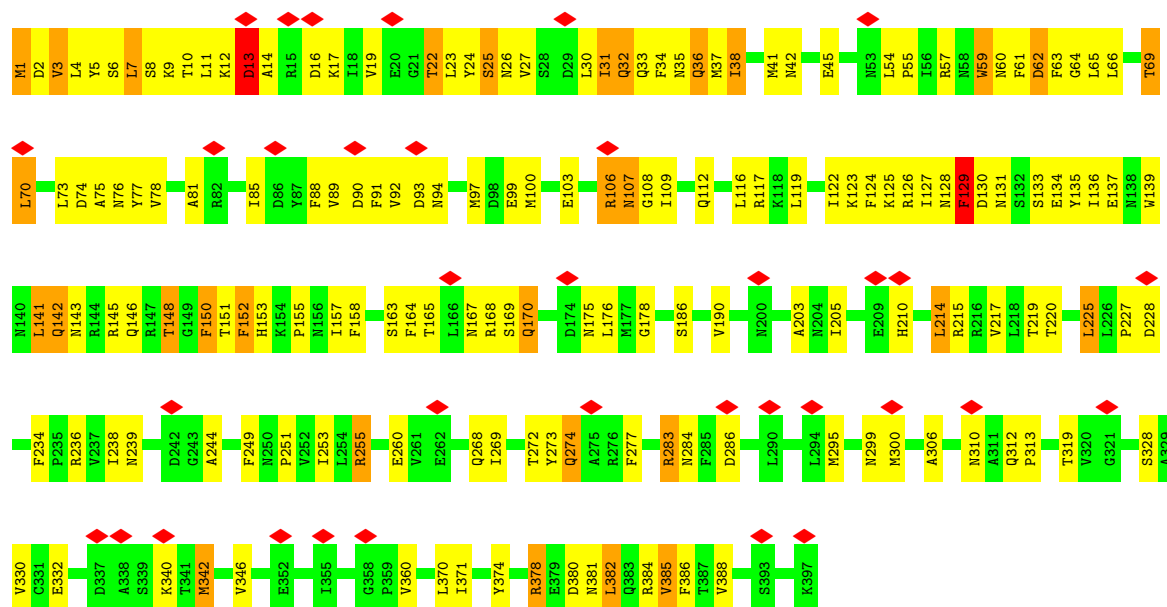


• Molecule 2: Intermediate capsid protein VP6



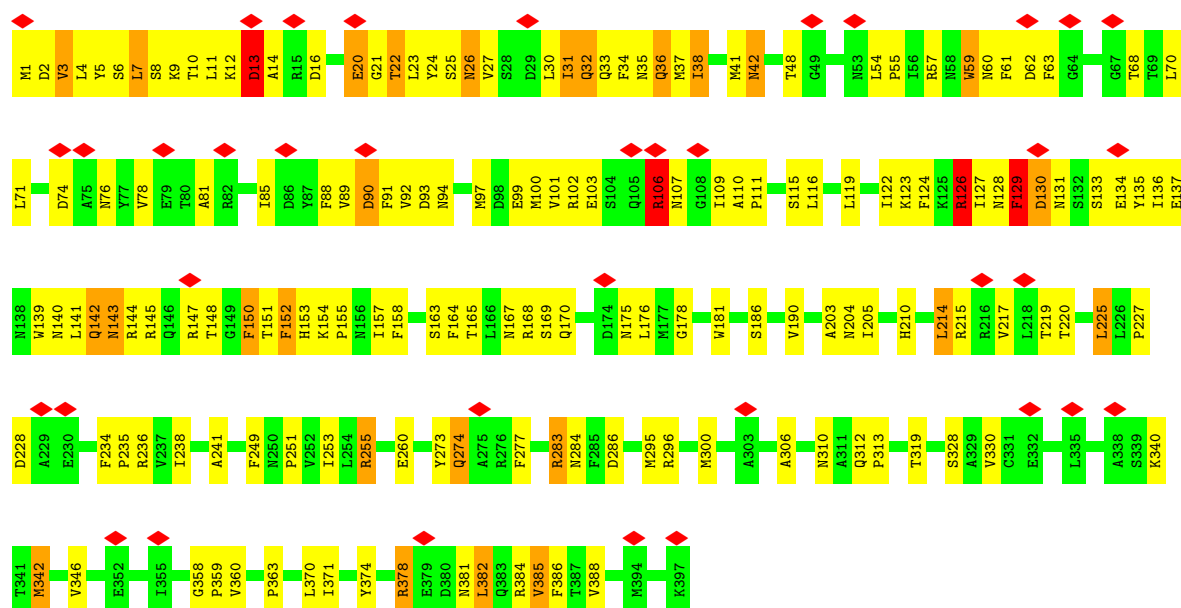
• Molecule 2: Intermediate capsid protein VP6

Chain AK: 



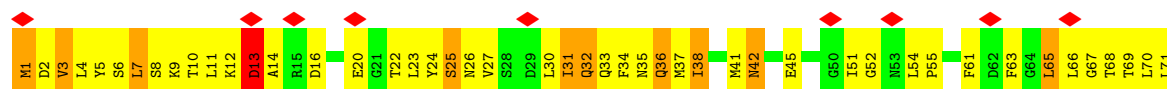
• Molecule 2: Intermediate capsid protein VP6

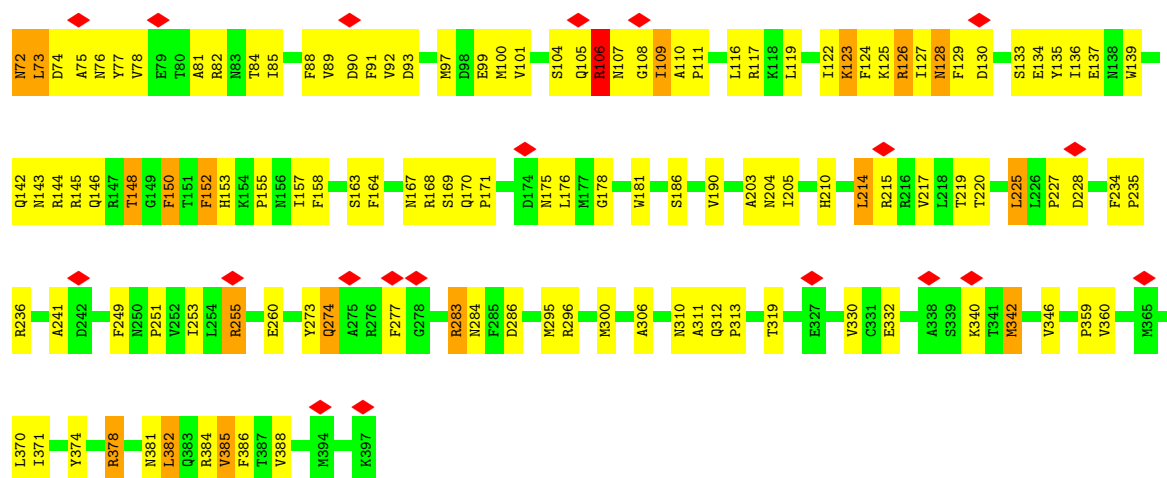
Chain AL: 



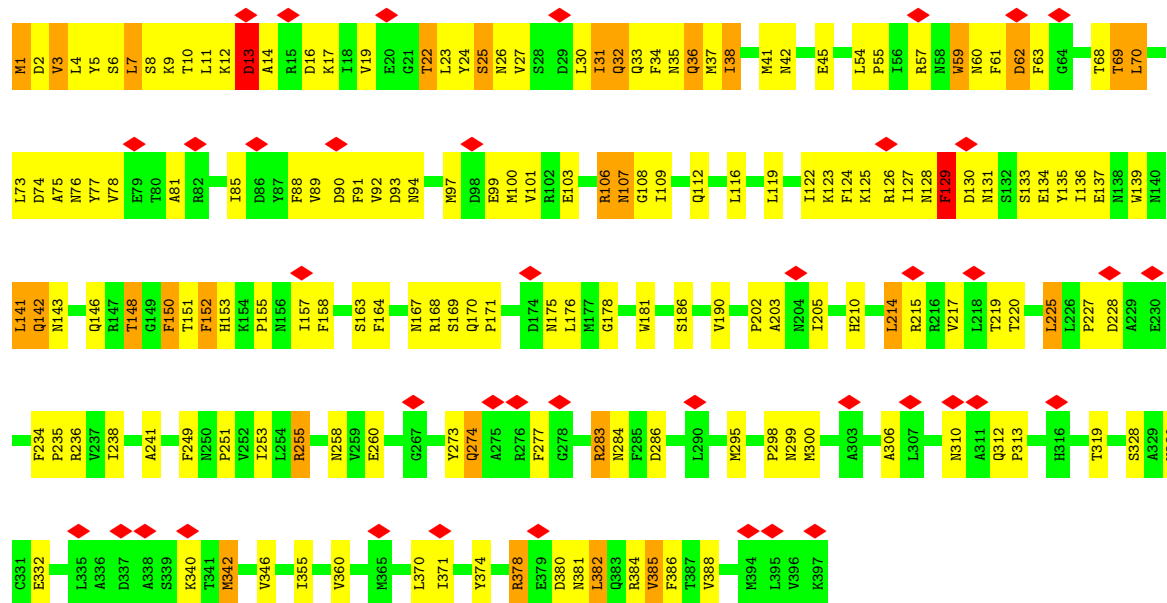
• Molecule 2: Intermediate capsid protein VP6

Chain AM: 

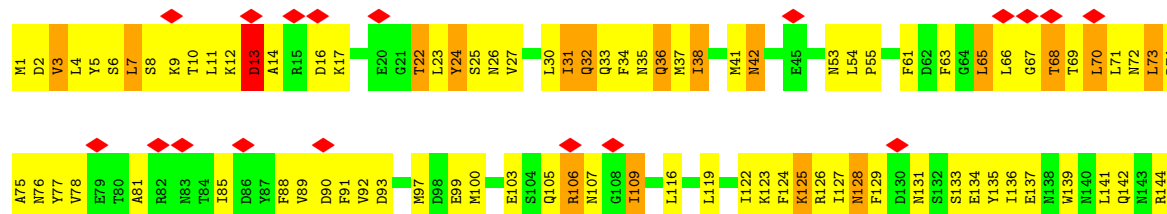




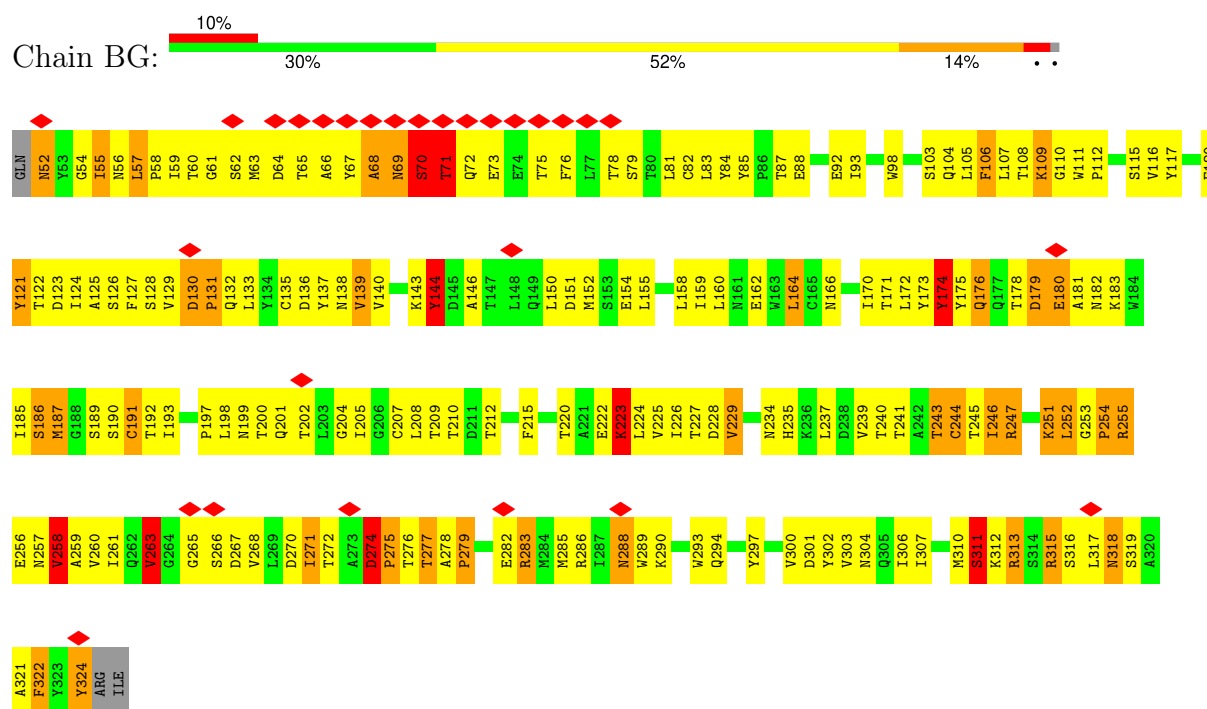
• Molecule 2: Intermediate capsid protein VP6



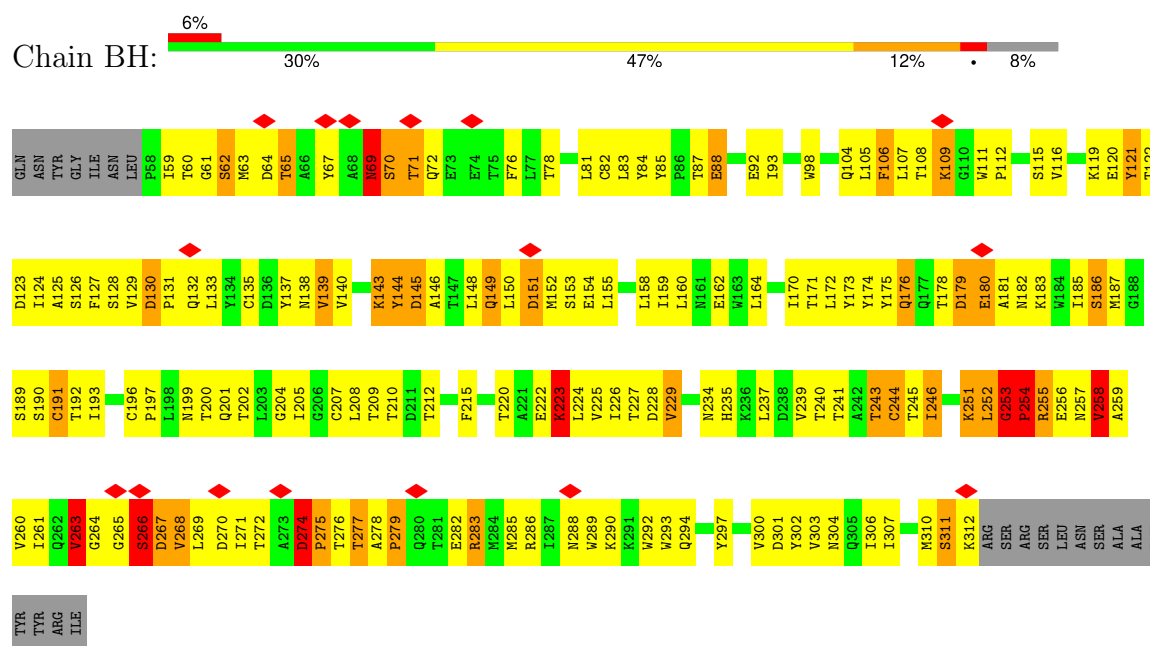
• Molecule 2: Intermediate capsid protein VP6



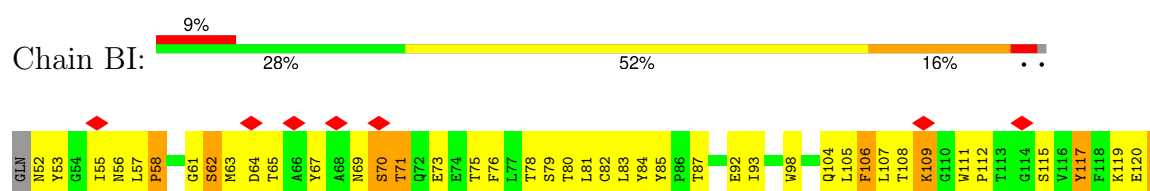
- Molecule 3: Outer layer protein VP7



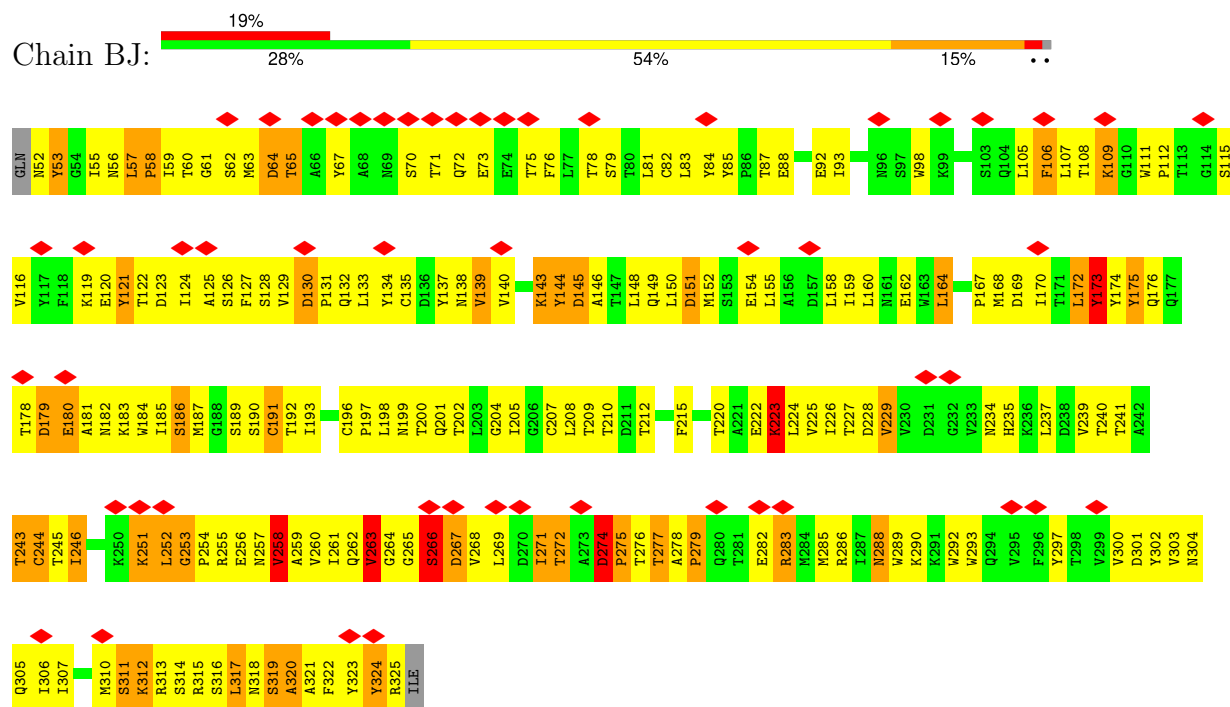
- Molecule 3: Outer layer protein VP7



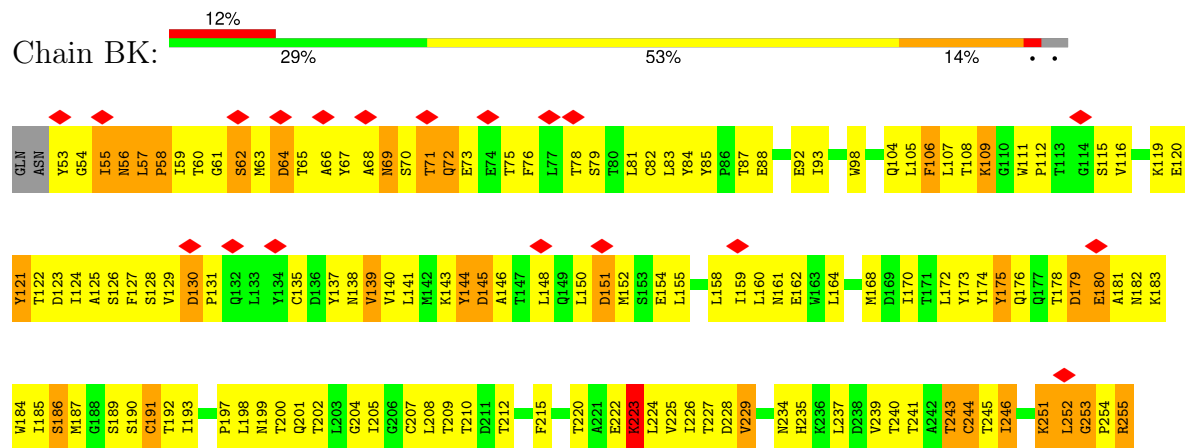
- Molecule 3: Outer layer protein VP7

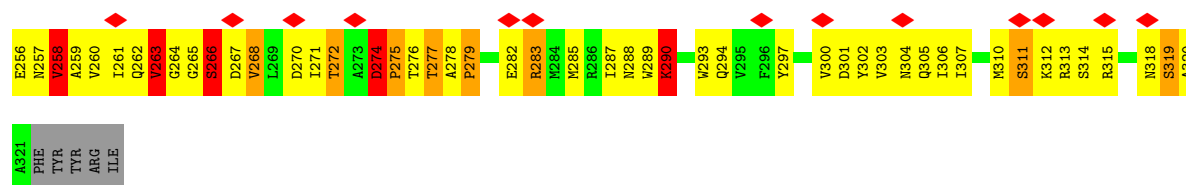


- Molecule 3: Outer layer protein VP7

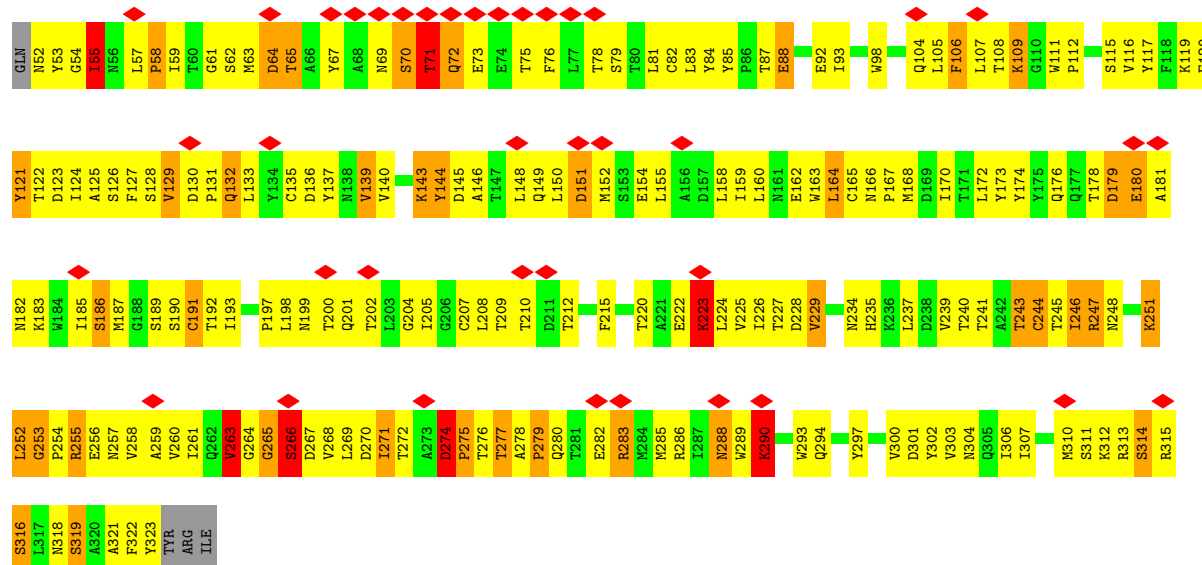


- Molecule 3: Outer layer protein VP7

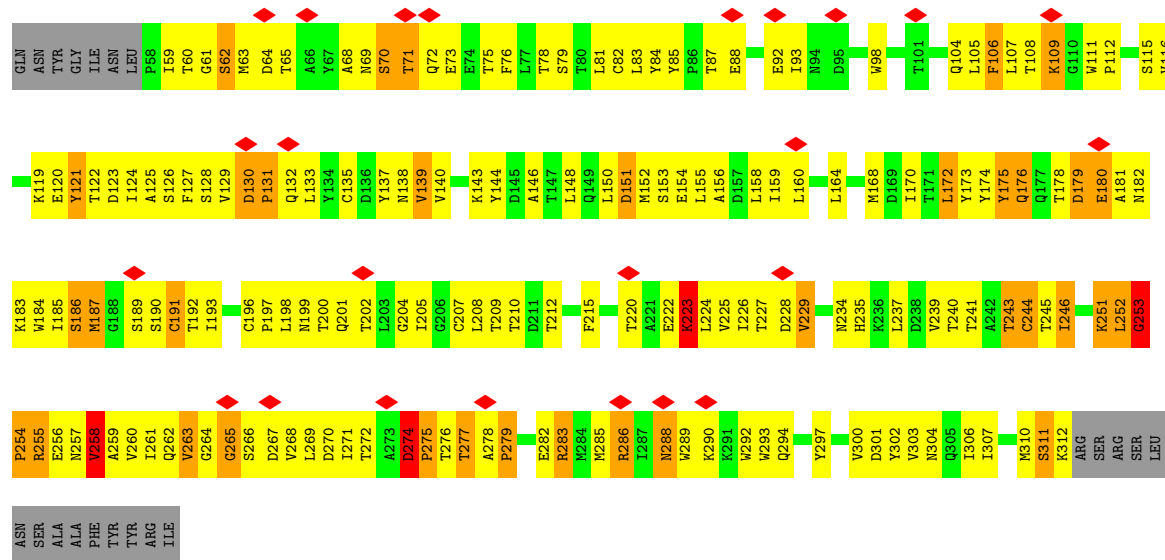




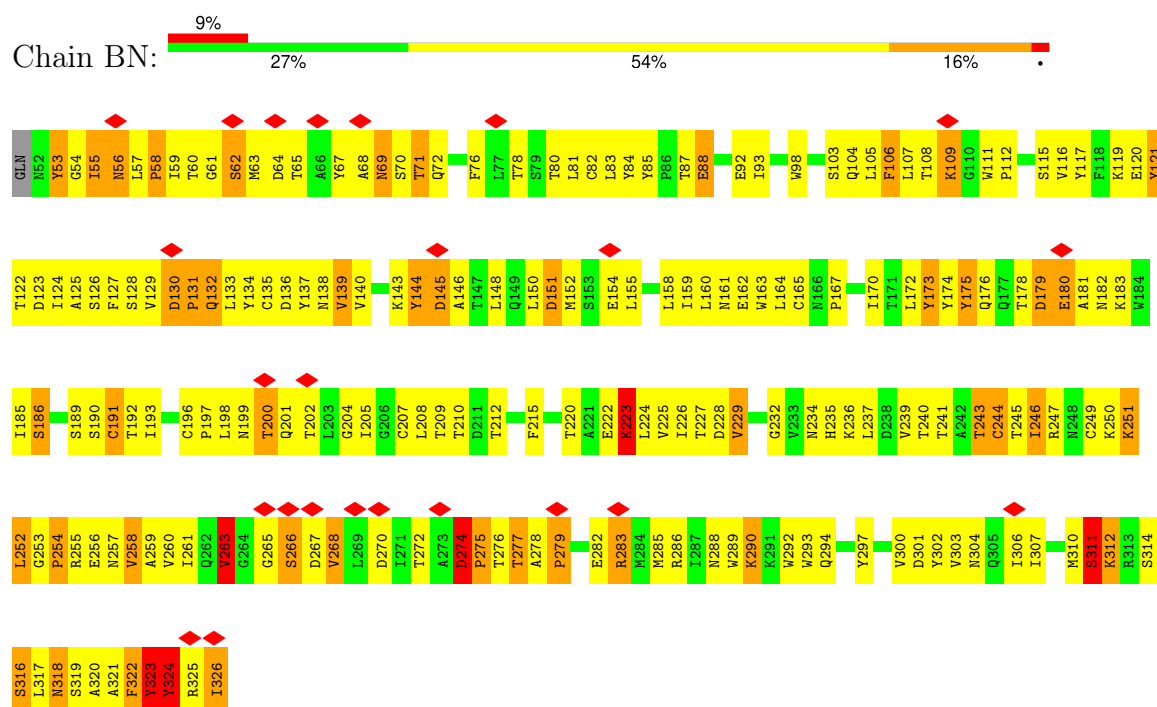
• Molecule 3: Outer layer protein VP7



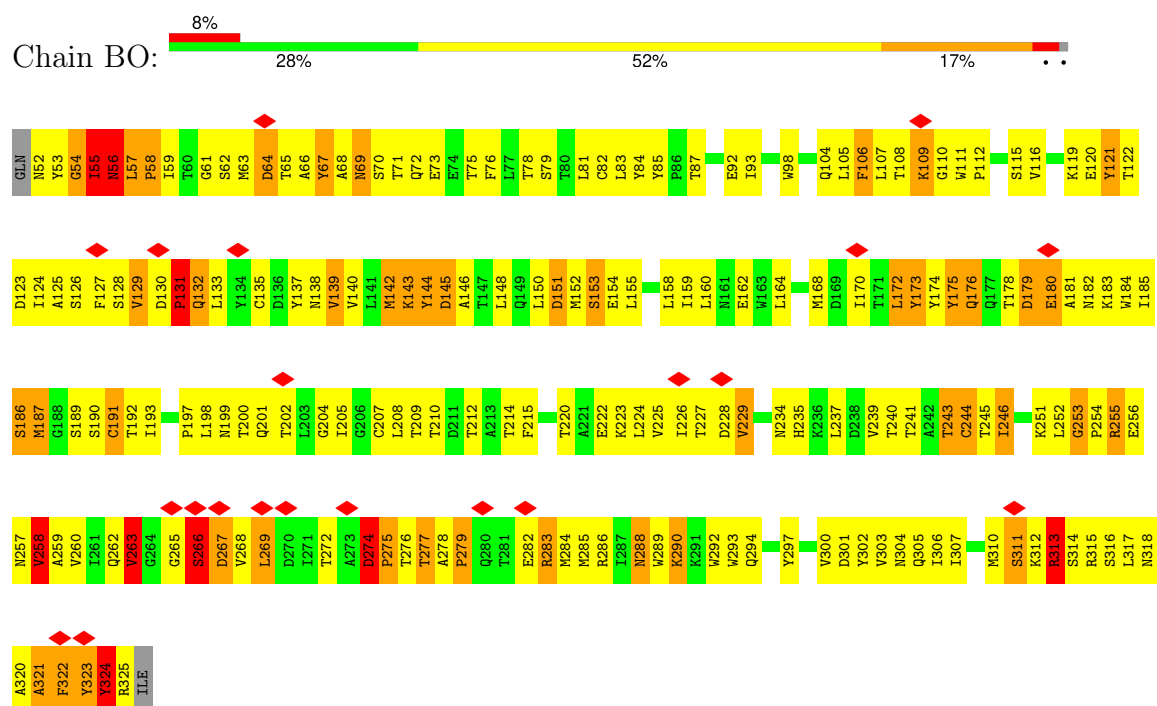
• Molecule 3: Outer layer protein VP7



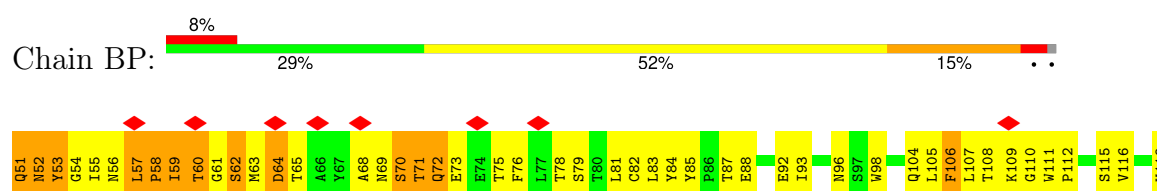
• Molecule 3: Outer layer protein VP7

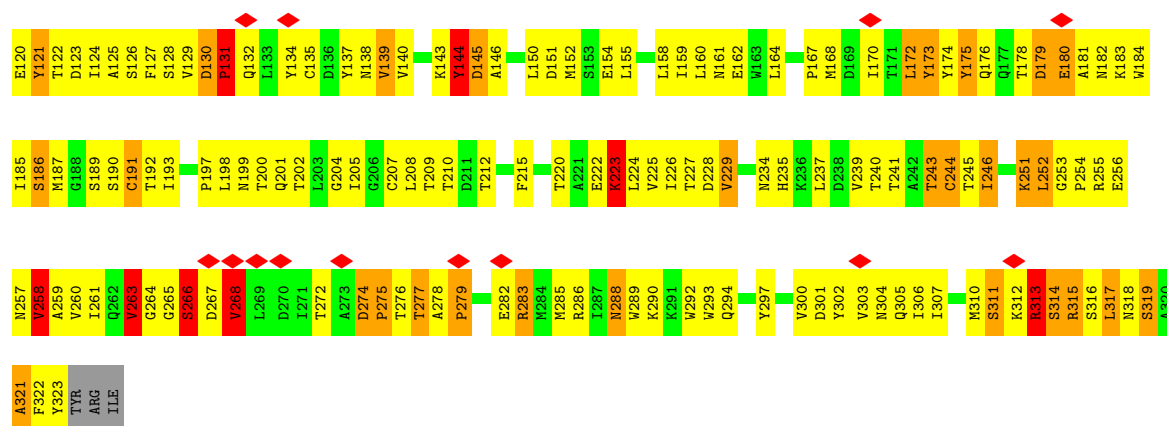


• Molecule 3: Outer layer protein VP7



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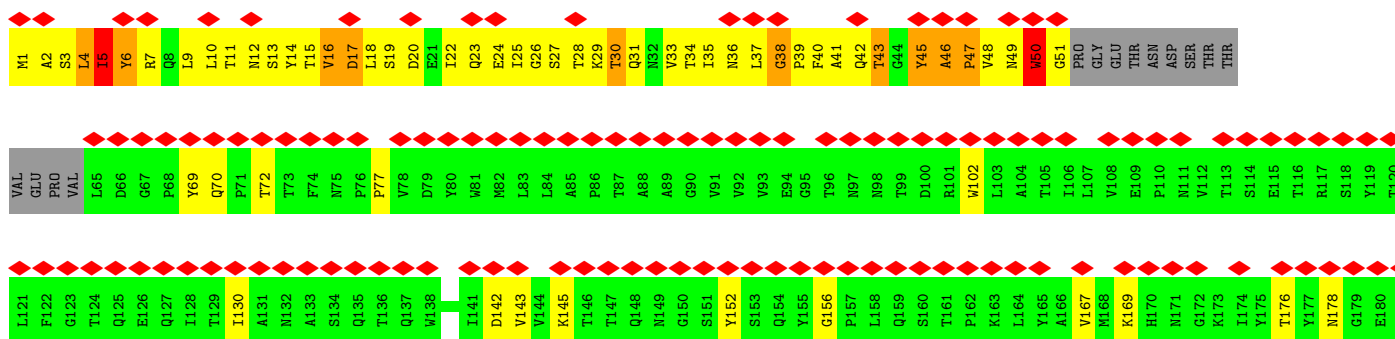
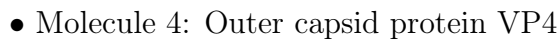


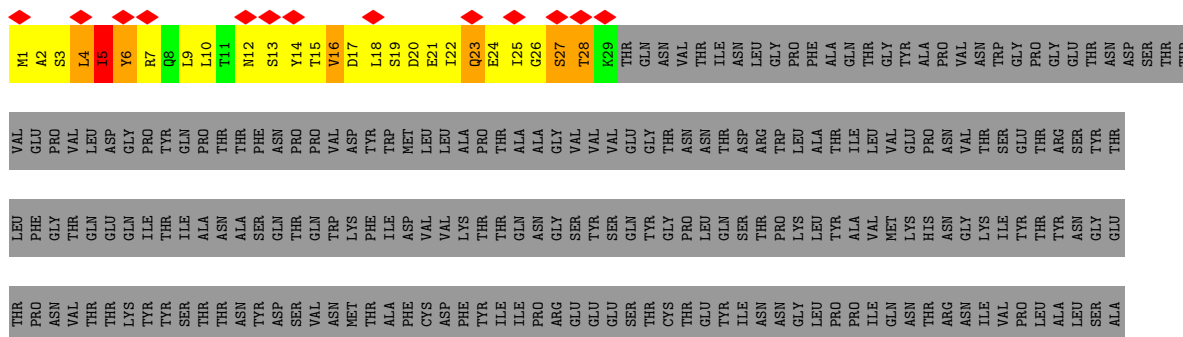
• Molecule 3: Outer layer protein VP7

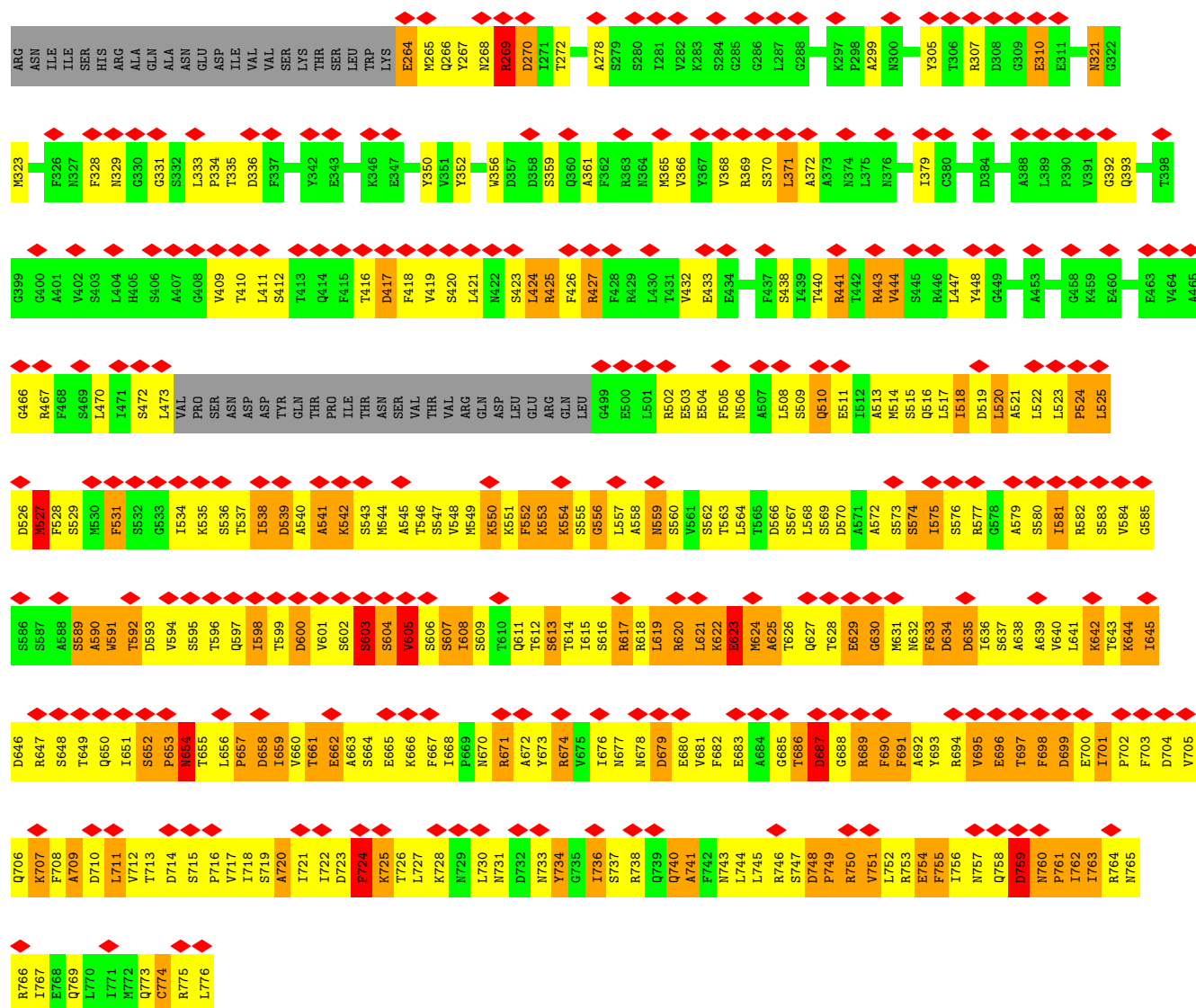


• Molecule 4: Outer capsid protein VP4









- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	4187	Depositor
Resolution determination method	Not provided	
CTF correction method	individual particle	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	56772	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	0.486	Depositor
Minimum map value	-0.323	Depositor
Average map value	-0.013	Depositor
Map value standard deviation	0.041	Depositor
Recommended contour level	0.12	Depositor
Map size (\AA)	615.0, 615.0, 615.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.23, 1.23, 1.23	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, ZN

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	0.60	3/6495 (0.0%)	0.89	12/8810 (0.1%)
1	AB	0.57	1/6665 (0.0%)	0.86	10/9041 (0.1%)
2	AC	0.51	0/3233	0.76	5/4397 (0.1%)
2	AD	0.51	0/3233	0.76	5/4397 (0.1%)
2	AE	0.51	0/3233	0.76	5/4397 (0.1%)
2	AF	0.51	0/3233	0.76	5/4397 (0.1%)
2	AG	0.52	0/3233	0.79	8/4397 (0.2%)
2	AH	0.52	0/3233	0.78	8/4397 (0.2%)
2	AI	0.51	0/3233	0.76	5/4397 (0.1%)
2	AJ	0.52	0/3233	0.77	5/4397 (0.1%)
2	AK	0.52	1/3233 (0.0%)	0.76	5/4397 (0.1%)
2	AL	0.52	0/3233	0.76	5/4397 (0.1%)
2	AM	0.52	0/3233	0.76	5/4397 (0.1%)
2	AN	0.51	0/3233	0.76	5/4397 (0.1%)
2	AO	0.52	0/3233	0.76	5/4397 (0.1%)
3	BA	0.94	9/2053 (0.4%)	1.33	30/2806 (1.1%)
3	BF	0.72	6/2114 (0.3%)	1.28	30/2887 (1.0%)
3	BG	0.79	7/2206 (0.3%)	1.23	25/3014 (0.8%)
3	BH	0.76	8/2053 (0.4%)	1.21	25/2806 (0.9%)
3	BI	0.82	11/2206 (0.5%)	1.41	37/3014 (1.2%)
3	BJ	0.80	9/2217 (0.4%)	1.27	30/3028 (1.0%)
3	BK	0.80	8/2160 (0.4%)	1.32	33/2951 (1.1%)
3	BL	0.70	4/2193 (0.2%)	1.22	24/2996 (0.8%)
3	BM	0.75	6/2053 (0.3%)	1.17	17/2806 (0.6%)
3	BN	0.79	8/2225 (0.4%)	1.18	24/3039 (0.8%)
3	BO	0.73	5/2217 (0.2%)	1.35	32/3028 (1.1%)
3	BP	0.80	8/2202 (0.4%)	1.31	37/3008 (1.2%)
3	BQ	0.73	6/2053 (0.3%)	1.24	23/2806 (0.8%)
4	BX	0.71	4/5897 (0.1%)	0.88	4/8017 (0.0%)
4	BY	0.74	2/5925 (0.0%)	0.91	10/8056 (0.1%)
4	BZ	0.61	1/4128 (0.0%)	0.82	1/5586 (0.0%)
All	All	0.64	107/99091 (0.1%)	0.97	475/134860 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AB	0	1

The worst 5 of 107 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	BY	485	THR	CB-OG1	-23.88	0.95	1.43
3	BA	116	VAL	CB-CG2	-21.24	1.08	1.52
4	BX	257	SER	CB-OG	17.14	1.64	1.42
3	BA	116	VAL	CB-CG1	13.05	1.80	1.52
4	BY	485	THR	CB-CG2	11.03	1.88	1.52

The worst 5 of 475 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	BO	57	LEU	C-N-CD	-24.11	67.55	120.60
3	BA	116	VAL	CA-CB-CG2	21.33	142.90	110.90
4	BX	46	ALA	C-N-CD	-20.07	76.44	120.60
4	BY	485	THR	CA-CB-CG2	-17.76	87.54	112.40
3	BK	57	LEU	C-N-CD	-17.58	81.93	120.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AB	452	PRO	Mainchain

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	6379	0	6408	1177	0
1	AB	6545	0	6569	1213	0
2	AC	3163	0	3112	246	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	AD	3163	0	3111	207	0
2	AE	3163	0	3110	229	0
2	AF	3163	0	3112	167	0
2	AG	3163	0	3111	249	0
2	AH	3163	0	3111	270	0
2	AI	3163	0	3111	265	0
2	AJ	3163	0	3112	226	0
2	AK	3163	0	3112	227	0
2	AL	3163	0	3112	244	0
2	AM	3163	0	3111	206	0
2	AN	3163	0	3111	208	0
2	AO	3163	0	3112	143	0
3	BA	2011	0	1955	287	0
3	BF	2072	0	2019	461	0
3	BG	2160	0	2095	511	0
3	BH	2011	0	1954	418	0
3	BI	2160	0	2095	441	0
3	BJ	2171	0	2109	538	0
3	BK	2117	0	2064	471	0
3	BL	2148	0	2087	510	0
3	BM	2011	0	1956	442	0
3	BN	2179	0	2120	519	0
3	BO	2171	0	2108	537	0
3	BP	2157	0	2095	526	0
3	BQ	2011	0	1953	401	0
4	BX	5783	0	5650	1001	0
4	BY	5809	0	5668	1166	0
4	BZ	4058	0	4001	777	0
5	A	28	0	25	2	0
5	B	28	0	25	4	0
5	C	28	0	25	4	0
5	D	28	0	25	2	0
5	E	28	0	25	3	0
5	F	28	0	25	3	0
5	G	28	0	25	0	0
6	AC	1	0	0	0	0
6	AF	1	0	0	0	0
6	AK	1	0	0	0	0
6	AN	1	0	0	0	0
6	AO	1	0	0	0	0
7	BM	14	0	13	4	0
All	All	97287	0	95542	12547	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 65.

The worst 5 of 12547 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:BA:116:VAL:CG1	3:BA:116:VAL:CB	1.80	1.58
4:BX:32:ASN:HB3	4:BY:484:ILE:CG2	1.33	1.58
3:BI:69:ASN:HD21	5:D:1:NAG:C1	1.11	1.55
2:AE:203:ALA:CB	4:BY:775:ARG:HH12	1.15	1.55
3:BN:174:TYR:CD2	3:BN:198:LEU:HD11	1.43	1.53

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	779/800 (97%)	431 (55%)	210 (27%)	138 (18%)	0	2
1	AB	798/800 (100%)	463 (58%)	209 (26%)	126 (16%)	0	2
2	AC	395/397 (100%)	327 (83%)	48 (12%)	20 (5%)	1	17
2	AD	395/397 (100%)	331 (84%)	42 (11%)	22 (6%)	1	16
2	AE	395/397 (100%)	332 (84%)	44 (11%)	19 (5%)	2	18
2	AF	395/397 (100%)	327 (83%)	48 (12%)	20 (5%)	1	17
2	AG	395/397 (100%)	334 (85%)	42 (11%)	19 (5%)	2	18
2	AH	395/397 (100%)	331 (84%)	45 (11%)	19 (5%)	2	18
2	AI	395/397 (100%)	327 (83%)	48 (12%)	20 (5%)	1	17
2	AJ	395/397 (100%)	334 (85%)	40 (10%)	21 (5%)	1	17
2	AK	395/397 (100%)	334 (85%)	42 (11%)	19 (5%)	2	18
2	AL	395/397 (100%)	327 (83%)	48 (12%)	20 (5%)	1	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AM	395/397 (100%)	333 (84%)	40 (10%)	22 (6%)	1	16
2	AN	395/397 (100%)	332 (84%)	44 (11%)	19 (5%)	2	18
2	AO	395/397 (100%)	321 (81%)	51 (13%)	23 (6%)	1	16
3	BA	253/276 (92%)	209 (83%)	28 (11%)	16 (6%)	1	15
3	BF	261/276 (95%)	216 (83%)	28 (11%)	17 (6%)	1	14
3	BG	271/276 (98%)	214 (79%)	39 (14%)	18 (7%)	1	14
3	BH	253/276 (92%)	210 (83%)	27 (11%)	16 (6%)	1	15
3	BI	271/276 (98%)	214 (79%)	34 (12%)	23 (8%)	0	9
3	BJ	272/276 (99%)	221 (81%)	32 (12%)	19 (7%)	1	12
3	BK	267/276 (97%)	213 (80%)	34 (13%)	20 (8%)	1	12
3	BL	270/276 (98%)	218 (81%)	34 (13%)	18 (7%)	1	13
3	BM	253/276 (92%)	214 (85%)	24 (10%)	15 (6%)	1	15
3	BN	273/276 (99%)	222 (81%)	30 (11%)	21 (8%)	1	11
3	BO	272/276 (99%)	219 (80%)	31 (11%)	22 (8%)	1	10
3	BP	271/276 (98%)	220 (81%)	33 (12%)	18 (7%)	1	14
3	BQ	253/276 (92%)	211 (83%)	28 (11%)	14 (6%)	1	16
4	BX	729/776 (94%)	514 (70%)	105 (14%)	110 (15%)	0	3
4	BY	732/776 (94%)	521 (71%)	119 (16%)	92 (13%)	0	4
4	BZ	511/776 (66%)	326 (64%)	95 (19%)	90 (18%)	0	2
All	All	12124/12677 (96%)	9346 (77%)	1722 (14%)	1056 (9%)	1	9

5 of 1056 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AA	102	GLU
1	AA	123	PHE
1	AA	131	LEU
1	AA	154	THR
1	AA	155	LEU

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	AA	717/736 (97%)	636 (89%)	81 (11%)	4	21
1	AB	736/736 (100%)	644 (88%)	92 (12%)	3	19
2	AC	350/350 (100%)	329 (94%)	21 (6%)	16	41
2	AD	350/350 (100%)	329 (94%)	21 (6%)	16	41
2	AE	350/350 (100%)	329 (94%)	21 (6%)	16	41
2	AF	350/350 (100%)	329 (94%)	21 (6%)	16	41
2	AG	350/350 (100%)	328 (94%)	22 (6%)	15	40
2	AH	350/350 (100%)	330 (94%)	20 (6%)	17	43
2	AI	350/350 (100%)	329 (94%)	21 (6%)	16	41
2	AJ	350/350 (100%)	329 (94%)	21 (6%)	16	41
2	AK	350/350 (100%)	329 (94%)	21 (6%)	16	41
2	AL	350/350 (100%)	328 (94%)	22 (6%)	15	40
2	AM	350/350 (100%)	328 (94%)	22 (6%)	15	40
2	AN	350/350 (100%)	329 (94%)	21 (6%)	16	41
2	AO	350/350 (100%)	331 (95%)	19 (5%)	18	43
3	BA	229/247 (93%)	206 (90%)	23 (10%)	6	24
3	BF	236/247 (96%)	212 (90%)	24 (10%)	6	24
3	BG	244/247 (99%)	214 (88%)	30 (12%)	4	19
3	BH	229/247 (93%)	204 (89%)	25 (11%)	5	22
3	BI	244/247 (99%)	215 (88%)	29 (12%)	4	20
3	BJ	245/247 (99%)	218 (89%)	27 (11%)	5	22
3	BK	240/247 (97%)	214 (89%)	26 (11%)	5	22
3	BL	243/247 (98%)	215 (88%)	28 (12%)	4	21
3	BM	229/247 (93%)	205 (90%)	24 (10%)	5	23
3	BN	246/247 (100%)	221 (90%)	25 (10%)	6	24
3	BO	245/247 (99%)	213 (87%)	32 (13%)	3	18
3	BP	244/247 (99%)	219 (90%)	25 (10%)	6	24
3	BQ	229/247 (93%)	206 (90%)	23 (10%)	6	24
4	BX	652/688 (95%)	608 (93%)	44 (7%)	13	38
4	BY	654/688 (95%)	605 (92%)	49 (8%)	11	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	BZ	456/688 (66%)	416 (91%)	40 (9%)	8	30
All	All	10868/11297 (96%)	9948 (92%)	920 (8%)	11	31

5 of 920 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	BA	262	GLN
4	BZ	323	MET
3	BI	290	LYS
4	BY	748	ASP
4	BX	500	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 343 such sidechains are listed below:

Mol	Chain	Res	Type
3	BH	176	GLN
3	BP	56	ASN
3	BI	235	HIS
3	BL	248	ASN
3	BQ	305	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](#)

14 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	A	1	5	14,14,15	0.61	0	17,19,21	1.44	2 (11%)
5	NAG	A	2	5	14,14,15	1.09	1 (7%)	17,19,21	1.73	5 (29%)
5	NAG	B	1	5	14,14,15	0.63	0	17,19,21	1.45	2 (11%)
5	NAG	B	2	5	14,14,15	1.08	1 (7%)	17,19,21	1.73	5 (29%)
5	NAG	C	1	5	14,14,15	0.60	0	17,19,21	1.44	2 (11%)
5	NAG	C	2	5	14,14,15	1.08	1 (7%)	17,19,21	1.73	5 (29%)
5	NAG	D	1	5	14,14,15	0.60	0	17,19,21	1.44	2 (11%)
5	NAG	D	2	5	14,14,15	1.08	1 (7%)	17,19,21	1.74	5 (29%)
5	NAG	E	1	5	14,14,15	0.62	0	17,19,21	1.44	2 (11%)
5	NAG	E	2	5	14,14,15	1.07	1 (7%)	17,19,21	1.74	5 (29%)
5	NAG	F	1	5	14,14,15	0.62	0	17,19,21	1.44	2 (11%)
5	NAG	F	2	5	14,14,15	1.08	1 (7%)	17,19,21	1.74	5 (29%)
5	NAG	G	1	3,5	14,14,15	0.60	0	17,19,21	1.43	2 (11%)
5	NAG	G	2	5	14,14,15	1.08	1 (7%)	17,19,21	1.74	5 (29%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	1	5	-	0/6/23/26	0/1/1/1
5	NAG	A	2	5	-	1/6/23/26	0/1/1/1
5	NAG	B	1	5	-	0/6/23/26	0/1/1/1
5	NAG	B	2	5	-	1/6/23/26	0/1/1/1
5	NAG	C	1	5	-	0/6/23/26	0/1/1/1
5	NAG	C	2	5	-	1/6/23/26	0/1/1/1
5	NAG	D	1	5	-	0/6/23/26	0/1/1/1
5	NAG	D	2	5	-	1/6/23/26	0/1/1/1
5	NAG	E	1	5	-	0/6/23/26	0/1/1/1
5	NAG	E	2	5	-	1/6/23/26	0/1/1/1
5	NAG	F	1	5	-	0/6/23/26	0/1/1/1
5	NAG	F	2	5	-	1/6/23/26	0/1/1/1
5	NAG	G	1	3,5	1/1/5/7	0/6/23/26	0/1/1/1
5	NAG	G	2	5	-	1/6/23/26	0/1/1/1

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	2	NAG	C1-C2	3.06	1.56	1.52
5	F	2	NAG	C1-C2	3.05	1.56	1.52
5	B	2	NAG	C1-C2	3.04	1.56	1.52
5	D	2	NAG	C1-C2	3.02	1.56	1.52
5	G	2	NAG	C1-C2	3.00	1.56	1.52

The worst 5 of 49 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	2	NAG	C2-N2-C7	3.87	128.09	122.90
5	B	2	NAG	C2-N2-C7	3.87	128.09	122.90
5	D	2	NAG	C2-N2-C7	3.83	128.04	122.90
5	E	2	NAG	C2-N2-C7	3.83	128.04	122.90
5	C	2	NAG	C2-N2-C7	3.82	128.02	122.90

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	G	1	NAG	C1

5 of 7 torsion outliers are listed below:

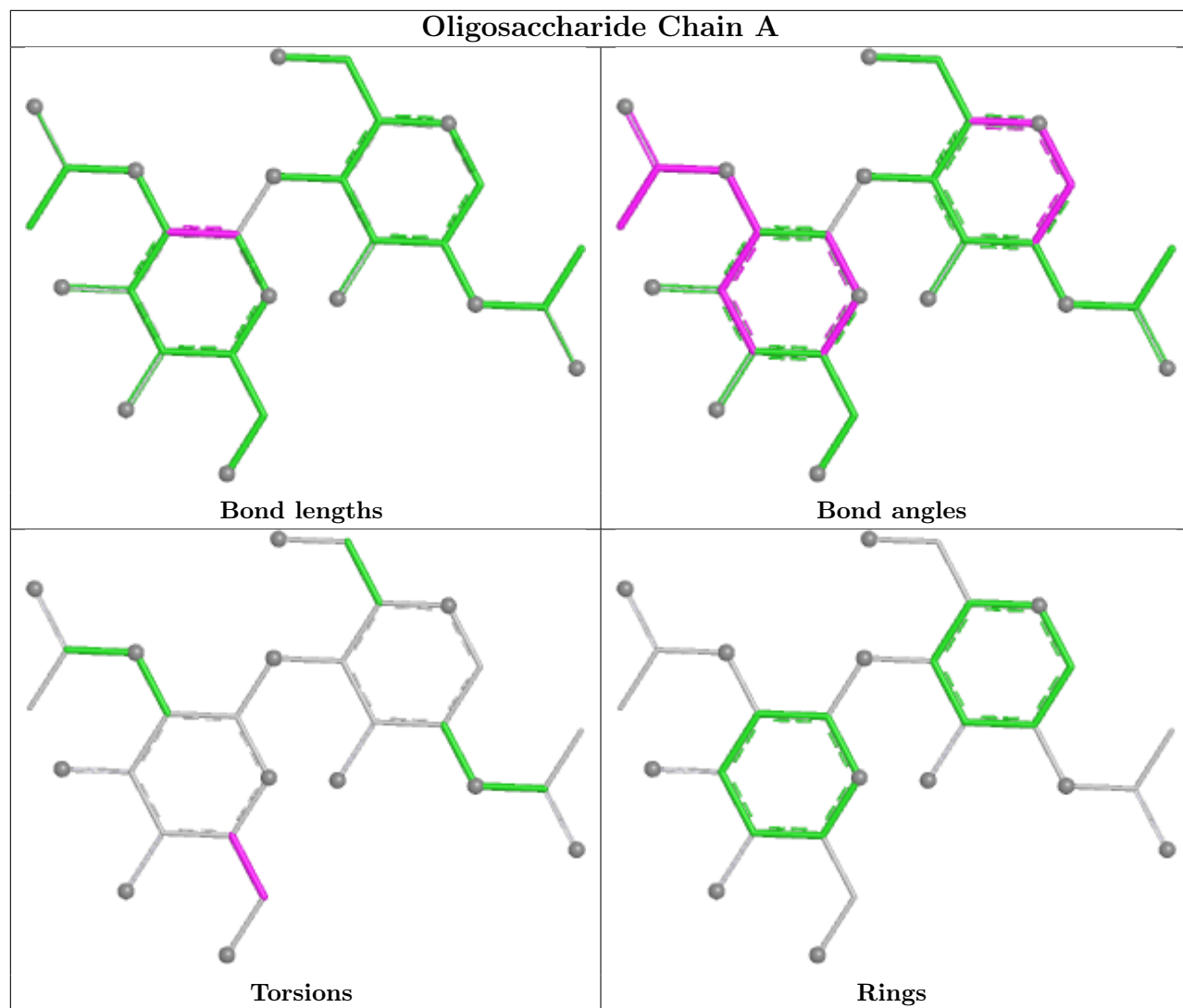
Mol	Chain	Res	Type	Atoms
5	A	2	NAG	O5-C5-C6-O6
5	B	2	NAG	O5-C5-C6-O6
5	D	2	NAG	O5-C5-C6-O6
5	E	2	NAG	O5-C5-C6-O6
5	F	2	NAG	O5-C5-C6-O6

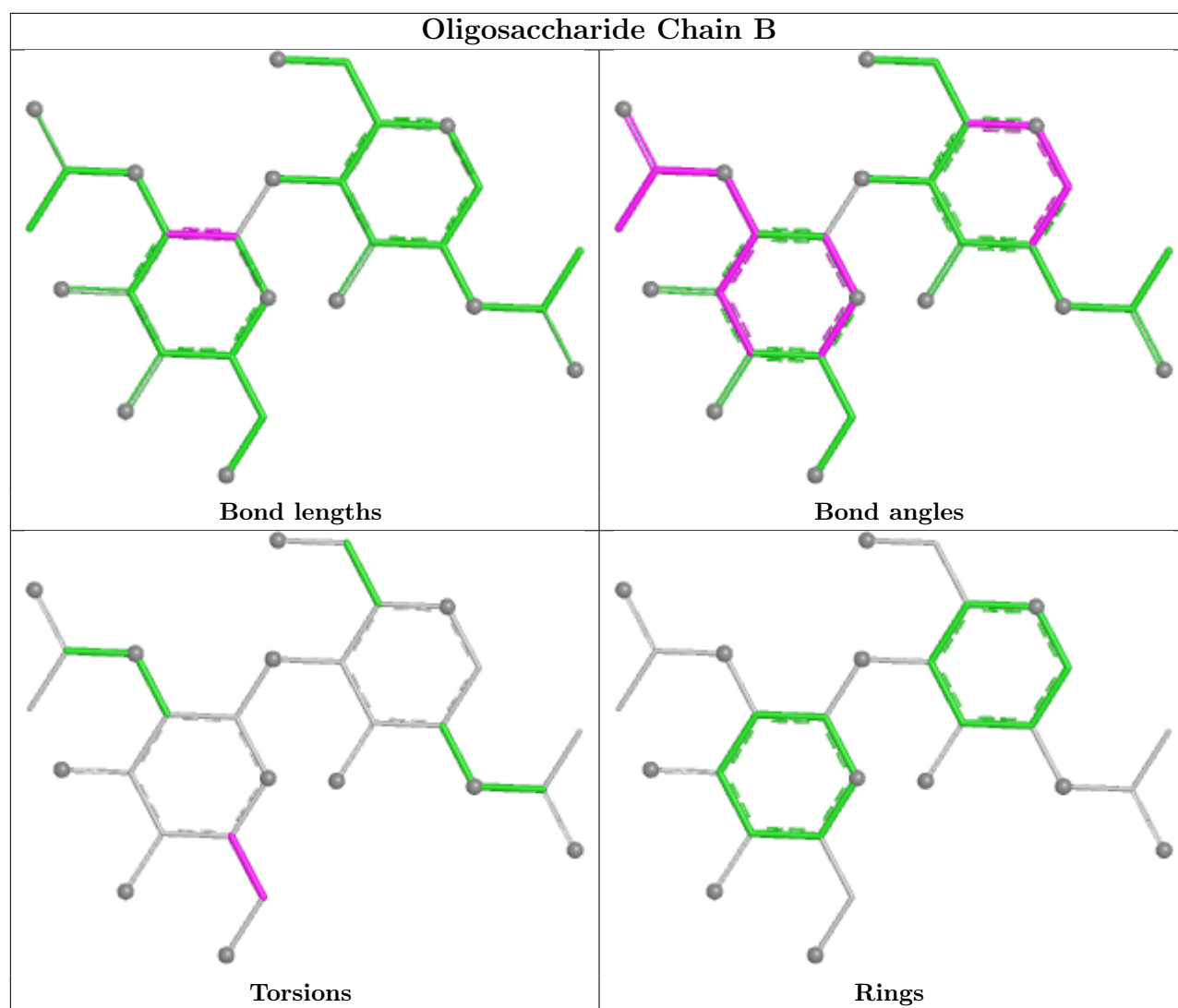
There are no ring outliers.

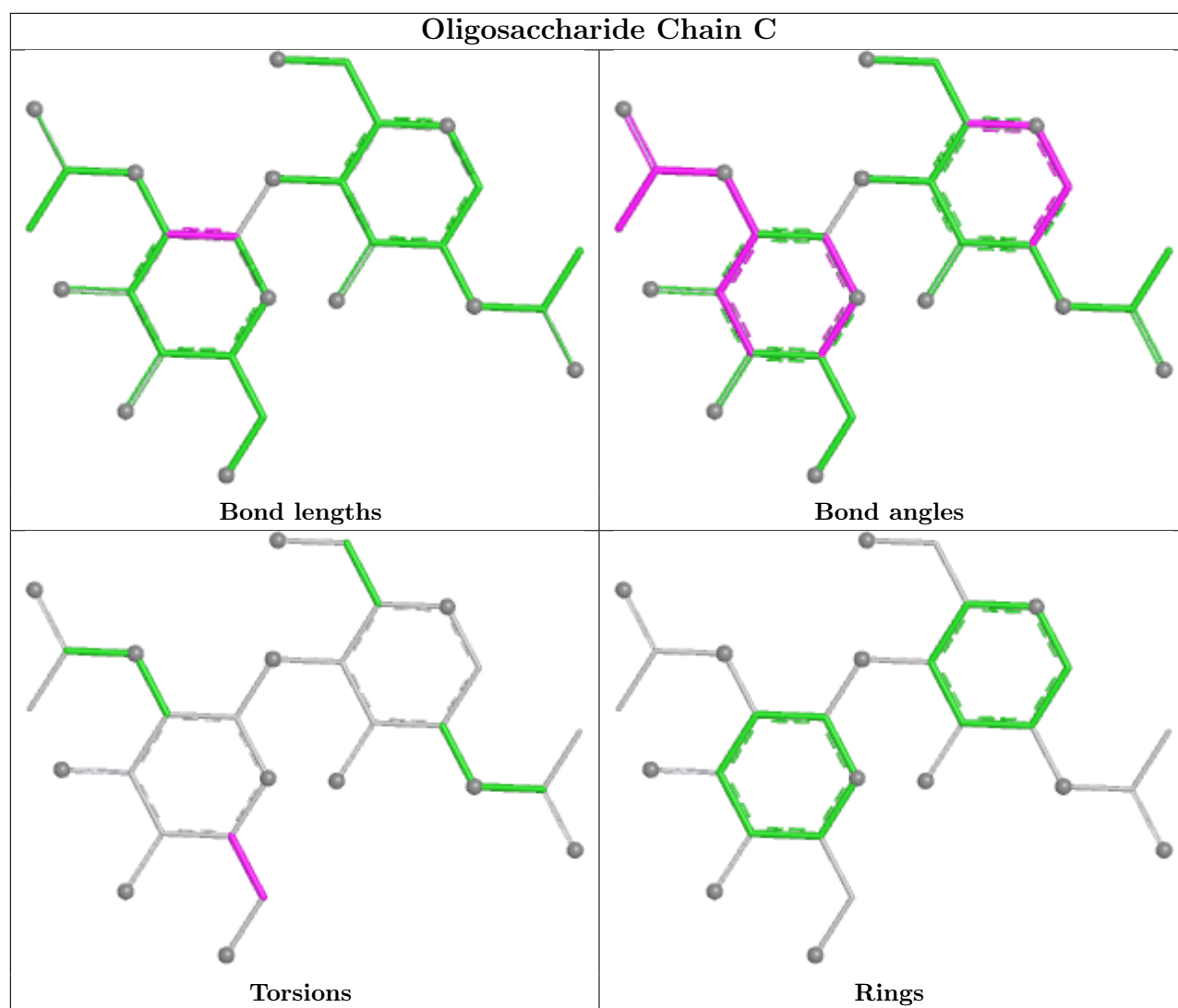
6 monomers are involved in 18 short contacts:

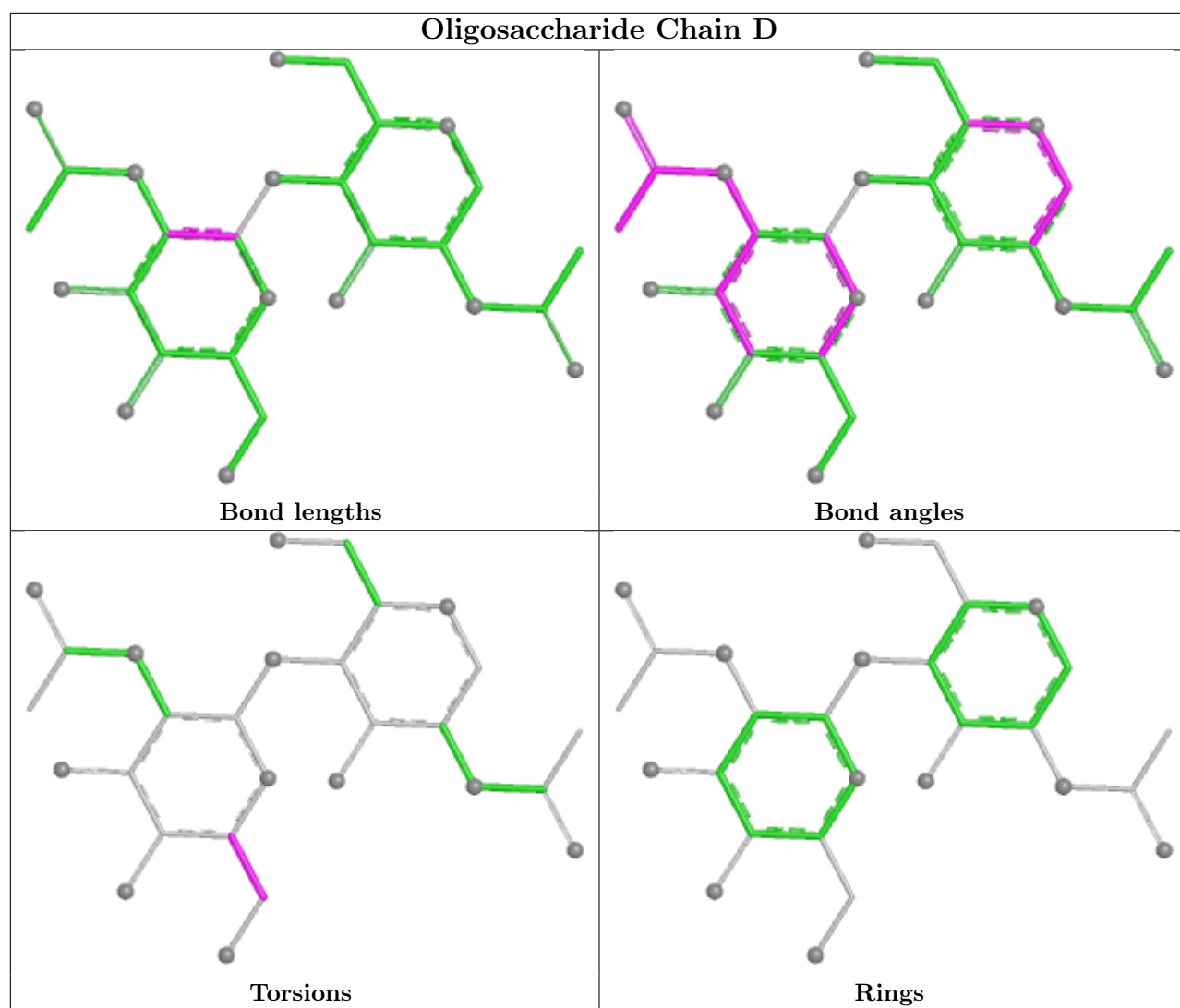
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1	NAG	4	0
5	F	1	NAG	3	0
5	E	1	NAG	3	0
5	D	1	NAG	2	0
5	A	1	NAG	2	0
5	B	1	NAG	4	0

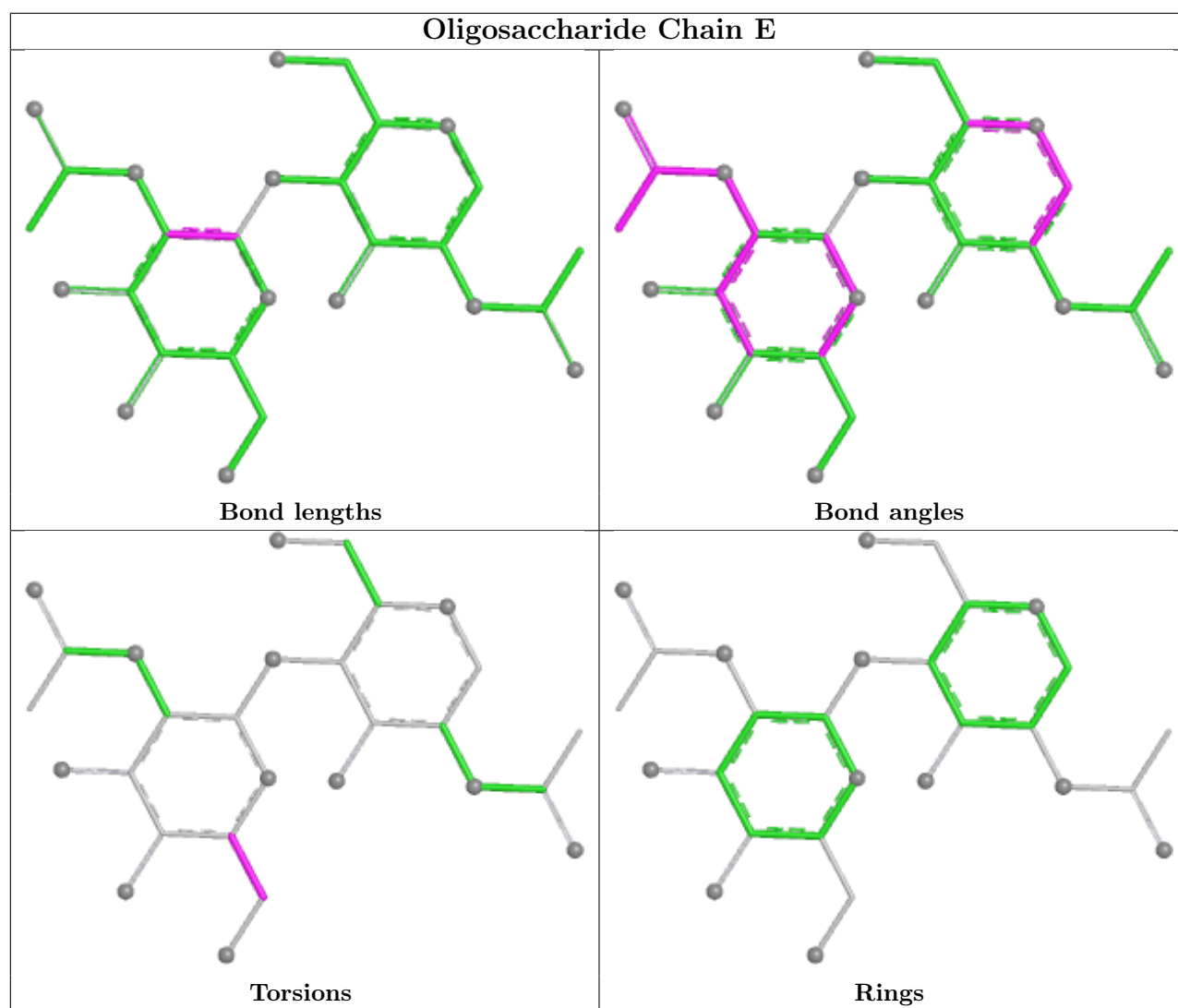
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

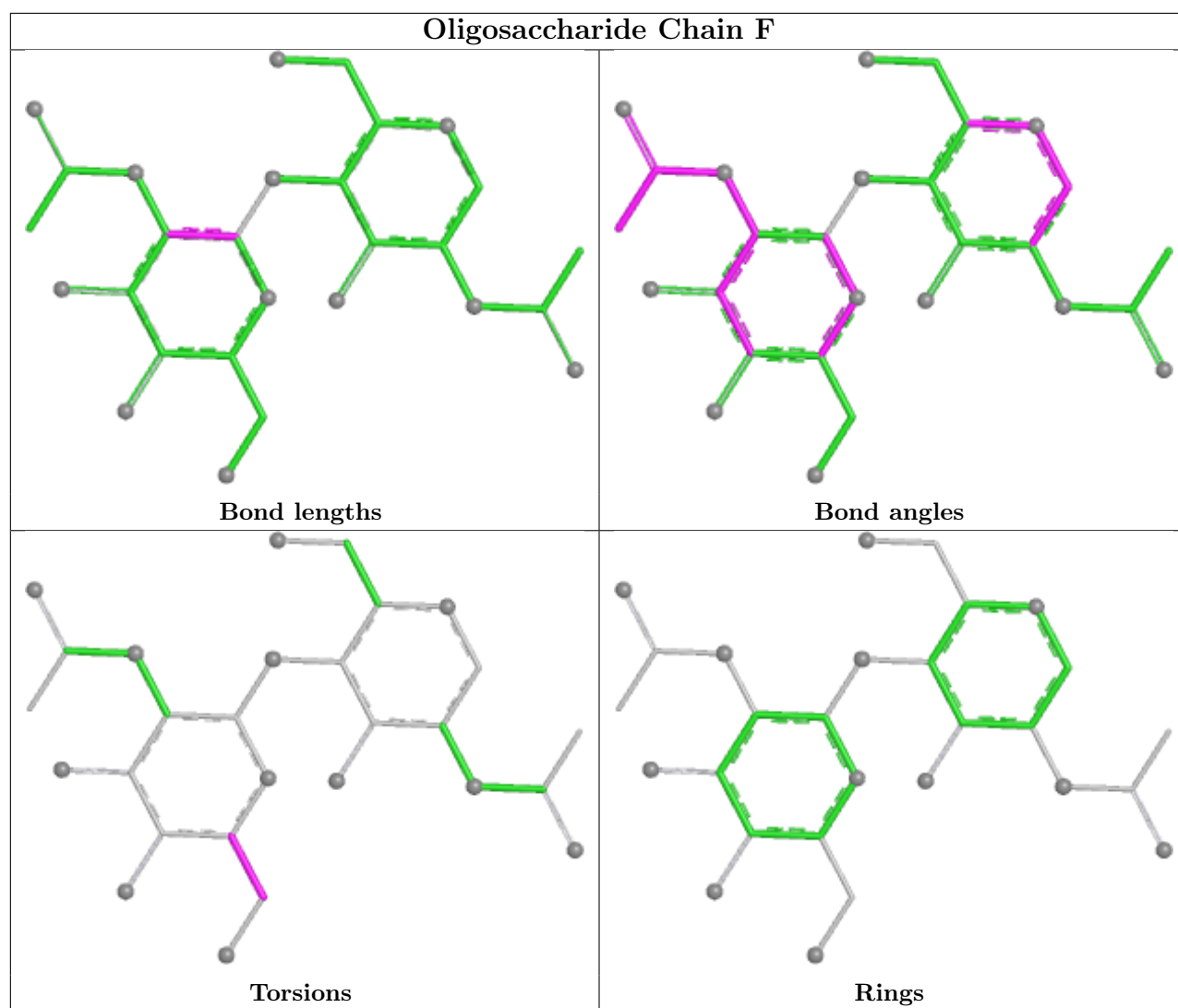


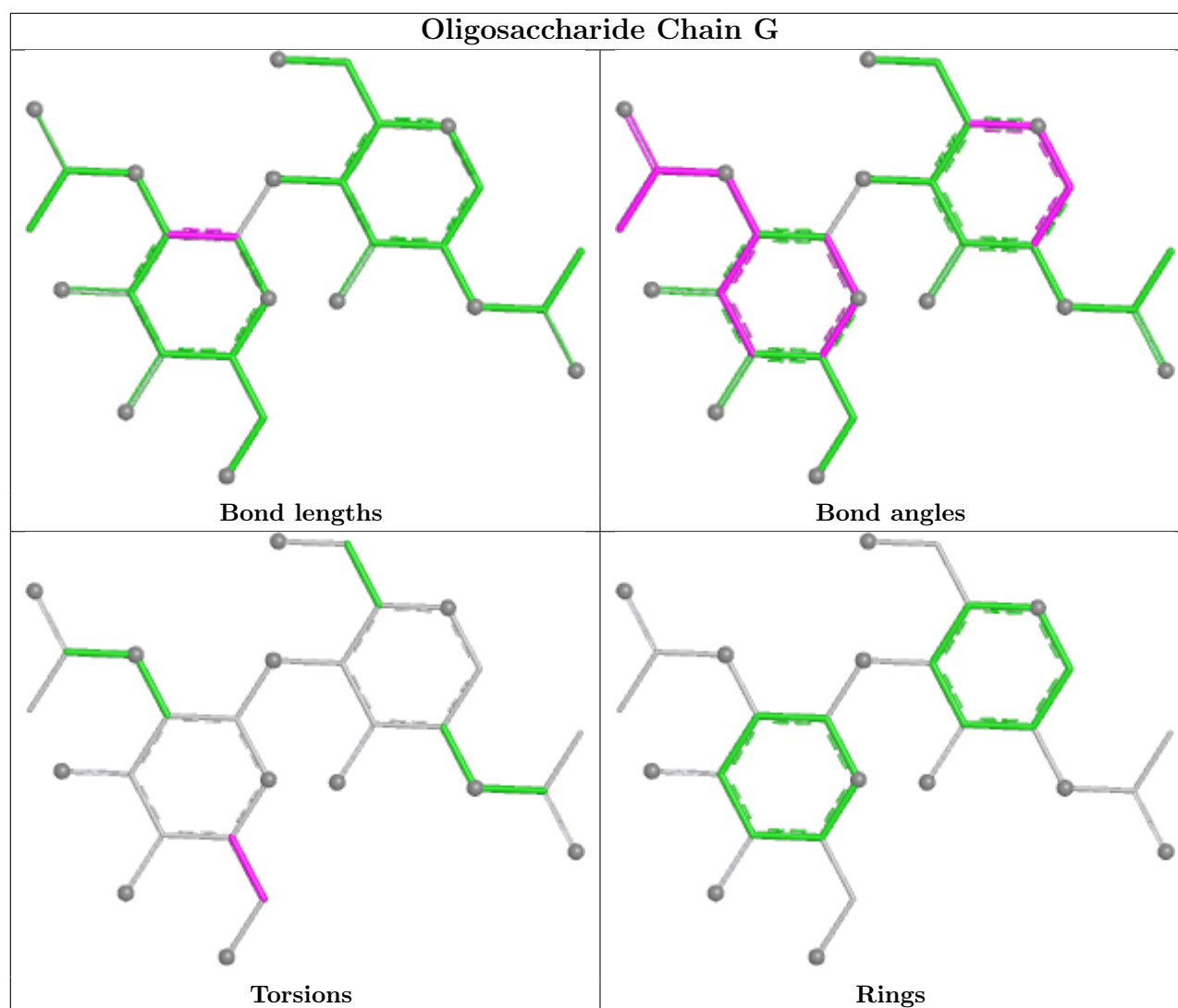












5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 5 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	NAG	BM	401	-	14,14,15	0.62	0	17,19,21	1.43	2 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	BM	401	-	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	BM	401	NAG	C1-O5-C5	3.65	117.08	112.19
7	BM	401	NAG	O5-C1-C2	-3.19	106.35	111.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	BM	401	NAG	4	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

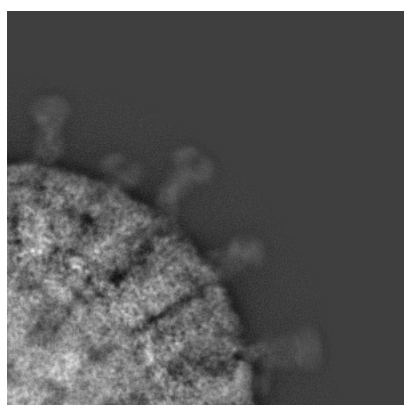
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-5199. These allow visual inspection of the internal detail of the map and identification of artifacts.

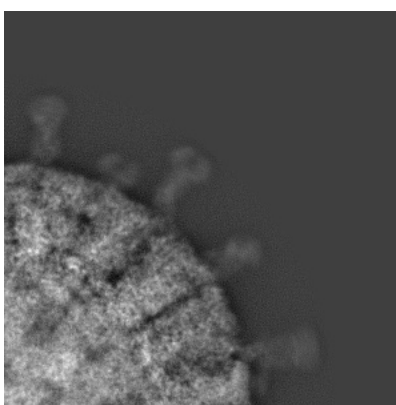
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

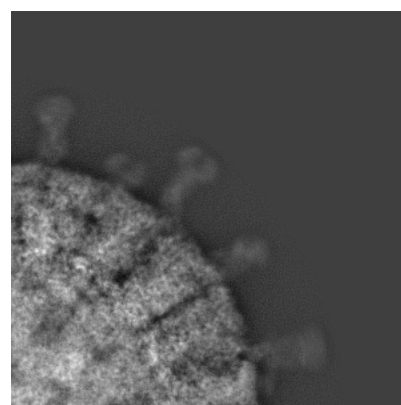
6.1.1 Primary map



X



Y

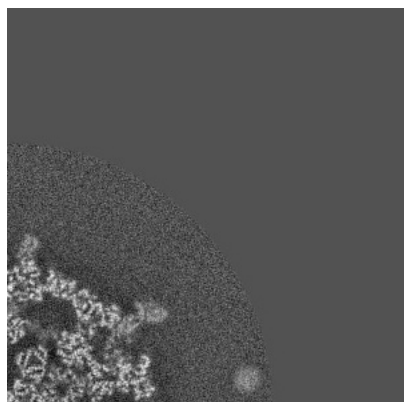


Z

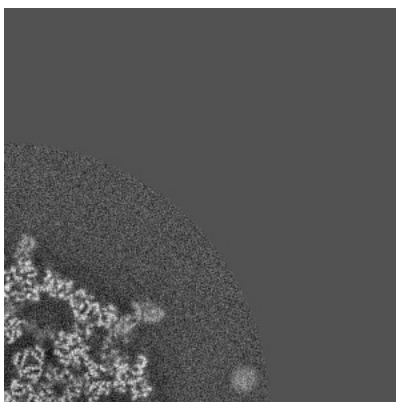
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

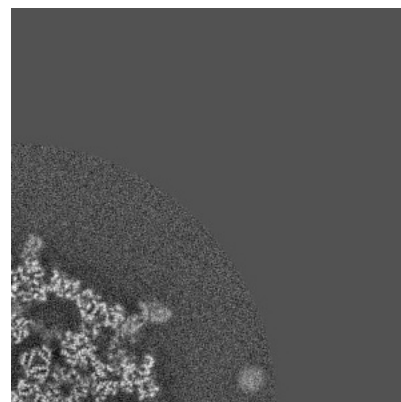
6.2.1 Primary map



X Index: 250



Y Index: 250

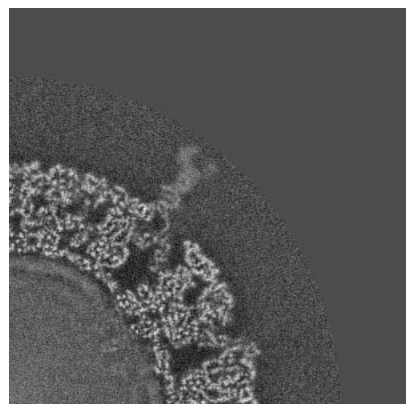


Z Index: 250

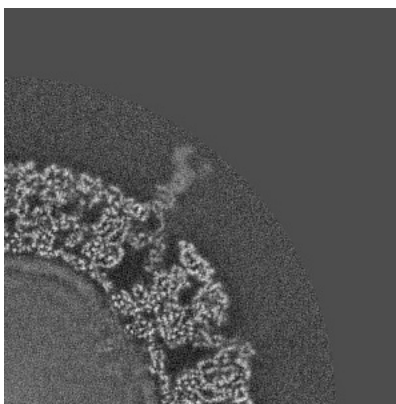
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

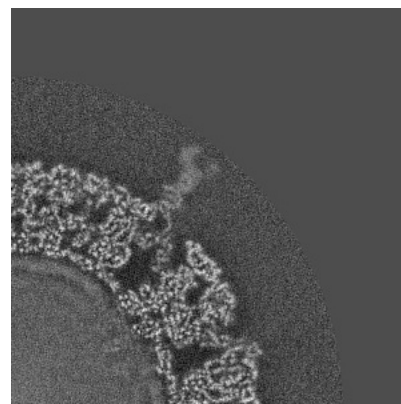
6.3.1 Primary map



X Index: 22



Y Index: 22

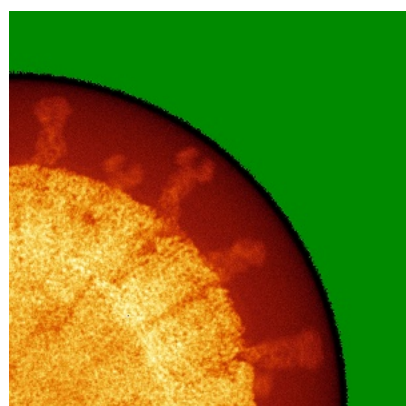


Z Index: 22

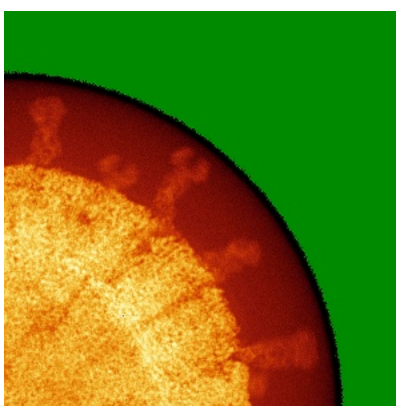
The images above show the largest variance slices of the map in three orthogonal directions.

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

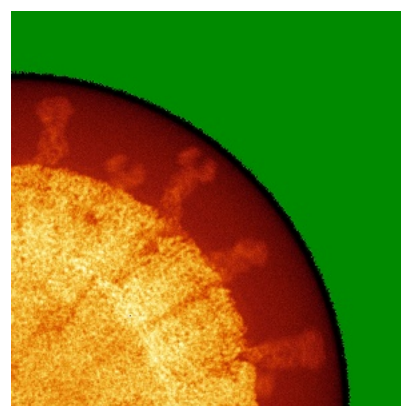
6.4.1 Primary map



X



Y

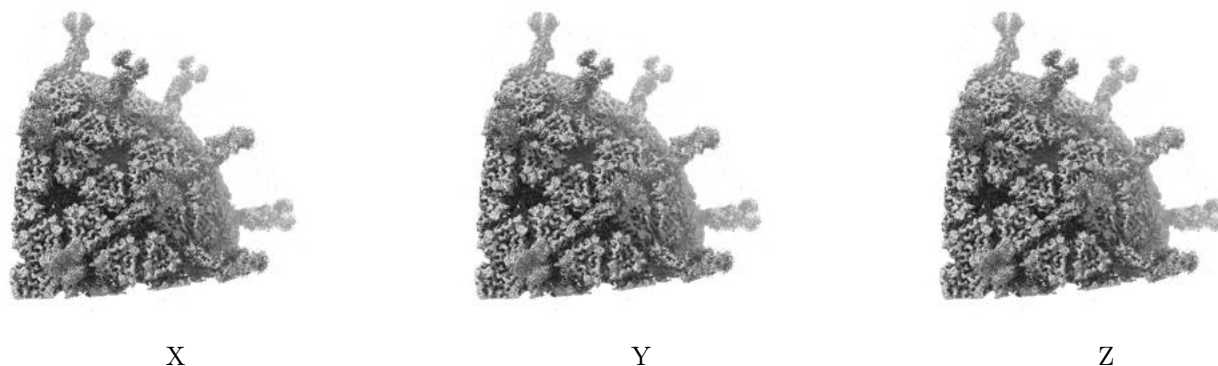


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.12. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

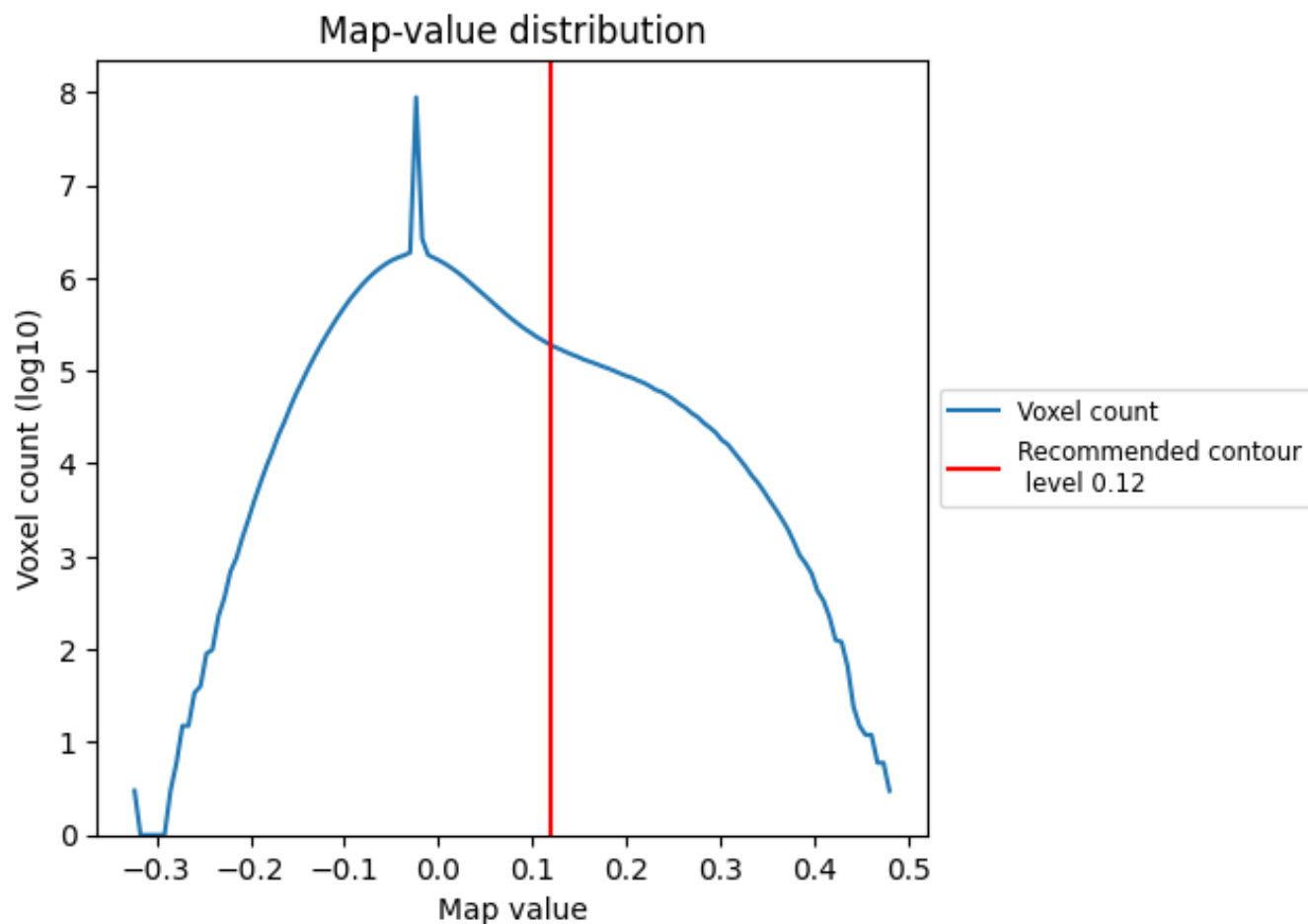
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

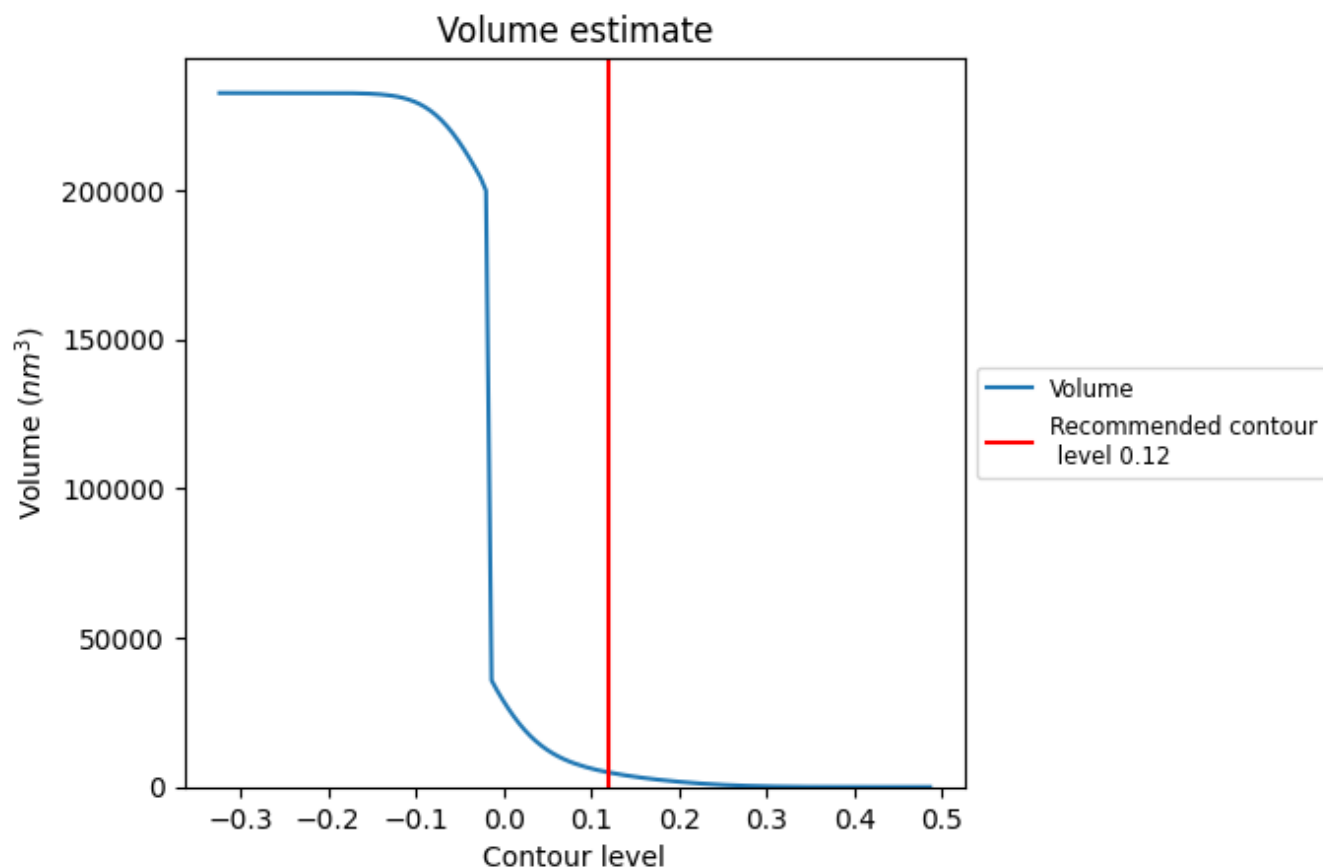
This section contains the results of statistical analysis of the map.

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.

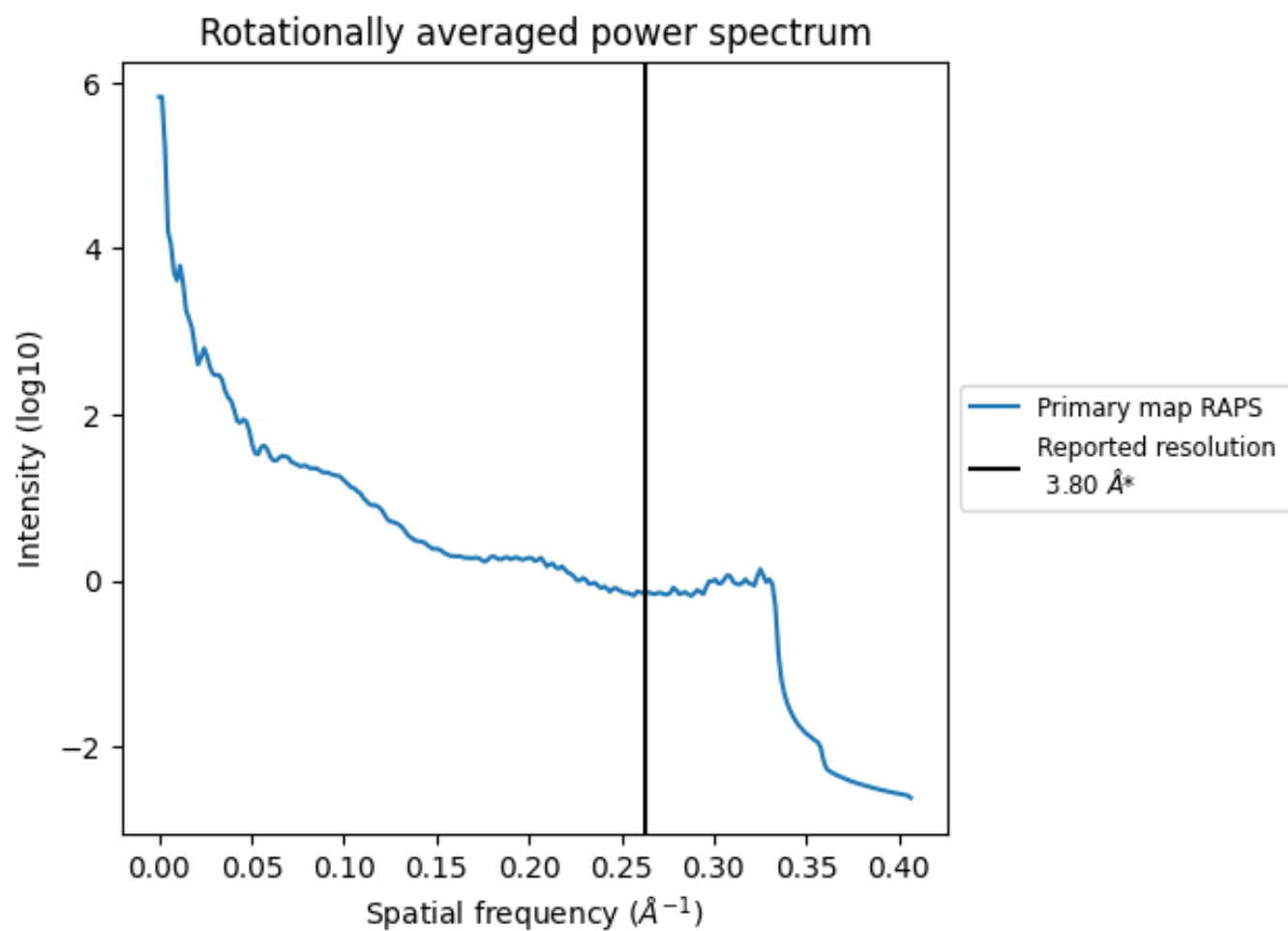
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 4878 nm^3 ; this corresponds to an approximate mass of 4406 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 0.263 Å⁻¹

8 Fourier-Shell correlation

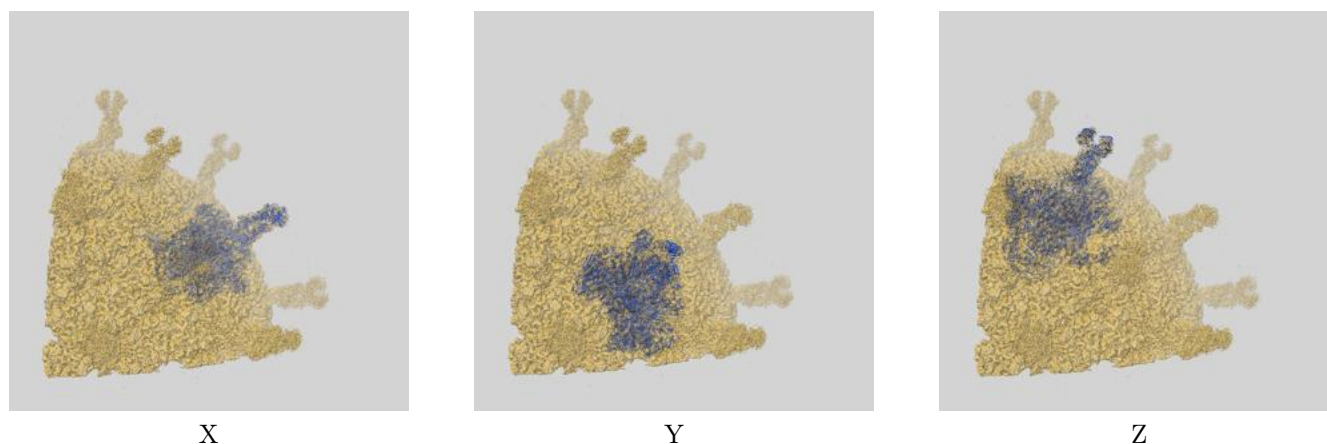
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

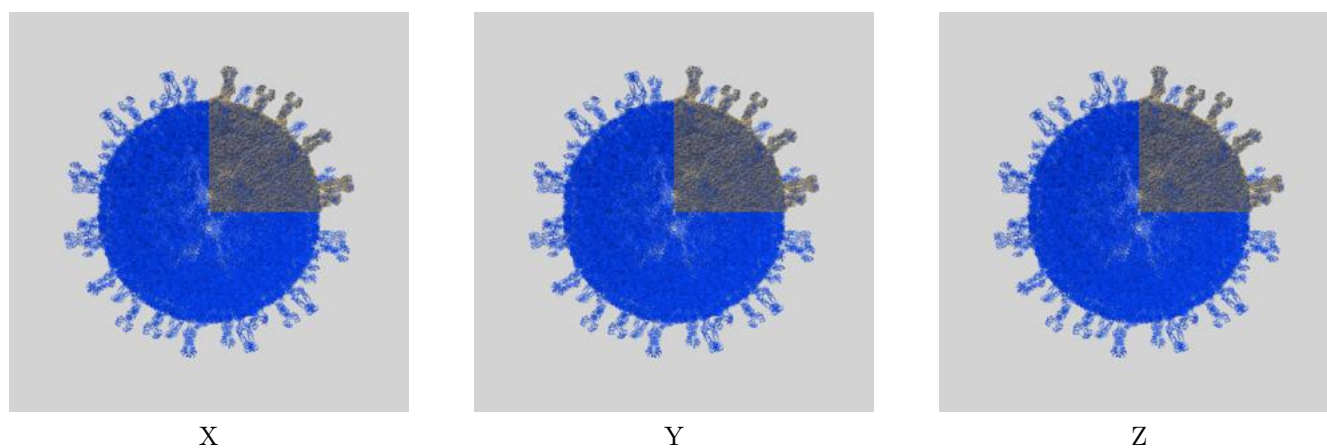
This section contains information regarding the fit between EMDB map EMD-5199 and PDB model 4V7Q. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

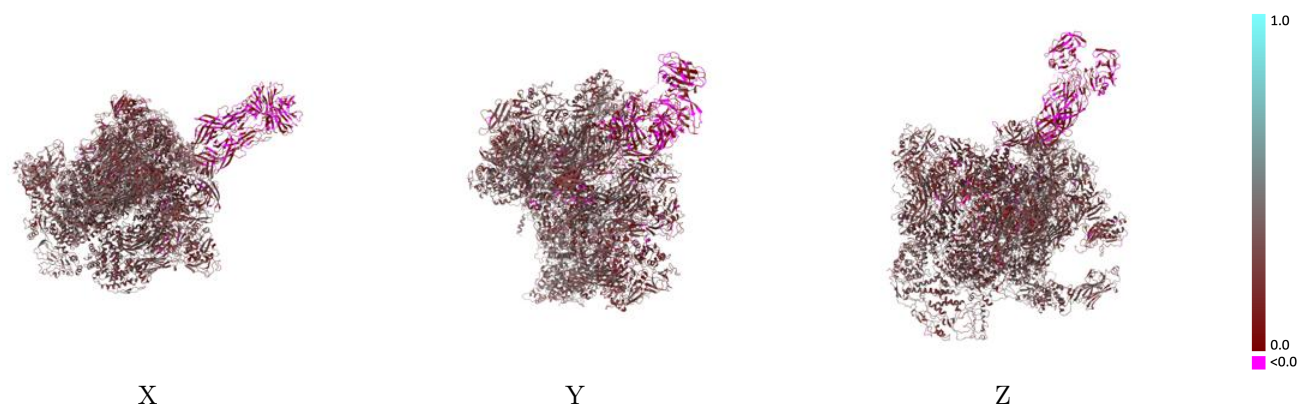


9.1.2 Map-model assembly overlay [i](#)



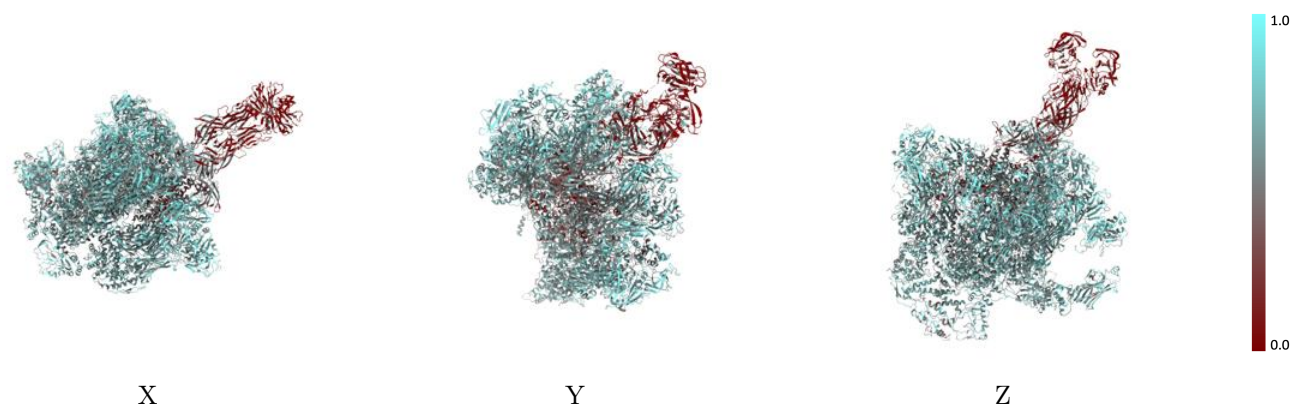
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



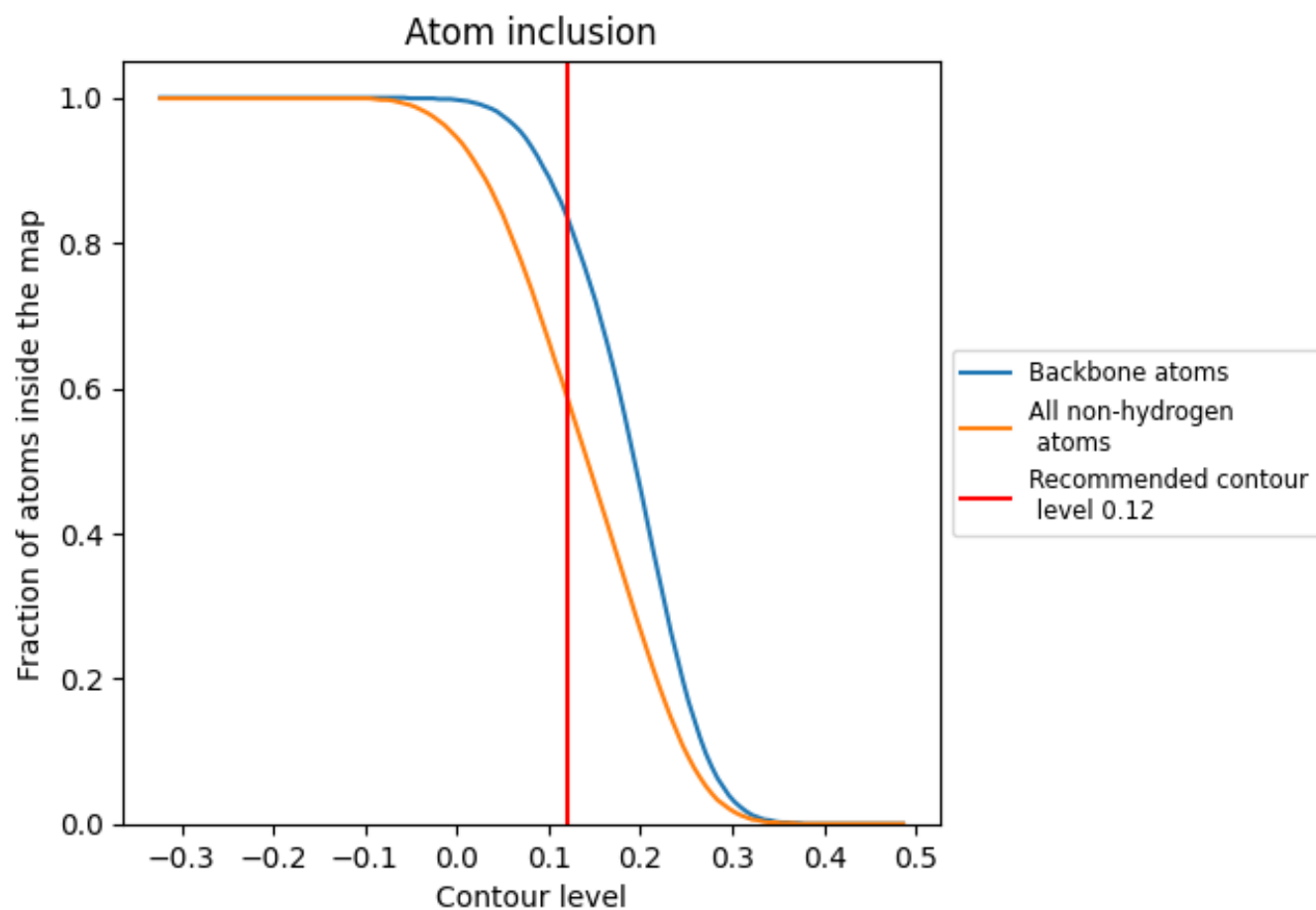
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.12).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 59% 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 (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5880	 0.2770
A	 0.1070	 0.1760
AA	 0.6230	 0.3070
AB	 0.6380	 0.3210
AC	 0.6460	 0.3230
AD	 0.6390	 0.3160
AE	 0.6460	 0.3200
AF	 0.6240	 0.3100
AG	 0.6080	 0.2980
AH	 0.6380	 0.3340
AI	 0.6050	 0.2960
AJ	 0.6370	 0.2950
AK	 0.6320	 0.3190
AL	 0.6270	 0.3180
AM	 0.6450	 0.3240
AN	 0.6390	 0.3320
AO	 0.6360	 0.3150
B	 0.2860	 0.2760
BA	 0.6730	 0.2510
BF	 0.6910	 0.2710
BG	 0.6670	 0.2710
BH	 0.6850	 0.2660
BI	 0.6710	 0.2740
BJ	 0.6020	 0.2080
BK	 0.6590	 0.2520
BL	 0.6150	 0.2240
BM	 0.6620	 0.2090
BN	 0.6760	 0.2600
BO	 0.6800	 0.2760
BP	 0.6800	 0.2820
BQ	 0.6930	 0.2760
BX	 0.2720	 0.1600
BY	 0.2760	 0.1590
BZ	 0.4000	 0.2490
C	 0.1790	 0.1830



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Chain	Atom inclusion	Q-score
D	 0.1070	 0.0980
E	 0.1790	 0.0830
F	 0.2140	 0.1900
G	 0.1430	 0.1670