



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:37 PM BST

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 Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

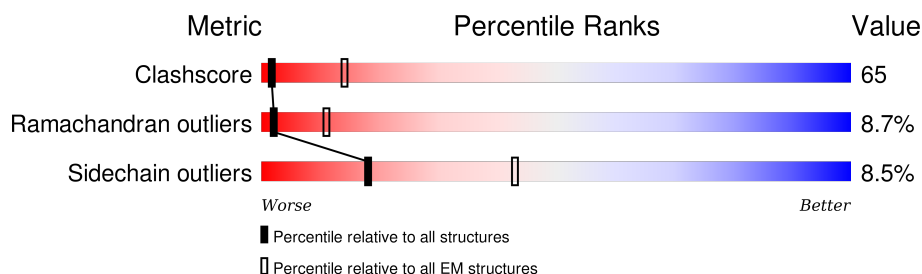
1 Overall quality at a glance

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.














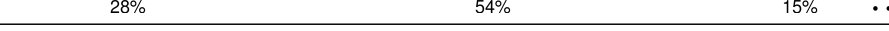


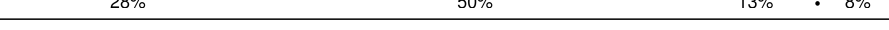




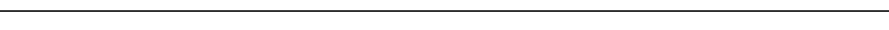

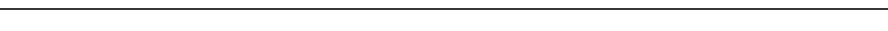
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	AA	800	18% 57% 20% . .
1	AB	800	20% 57% 22% .
2	AC	397	56% 37% 7% .
2	AD	397	57% 36% 7% .
2	AE	397	56% 37% 7% .
2	AF	397	59% 34% 6% .
2	AG	397	57% 36% 7% .
2	AH	397	54% 39% 7% .
2	AI	397	55% 37% 7% .

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Mol	Chain	Length	Quality of chain
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	

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
6	NAG	BQ	401	X	-	-	-

2 Entry composition

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

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

- Molecule 6 is a polymer of unknown type called N-ACETYL-D-GLUCOSAMINE.

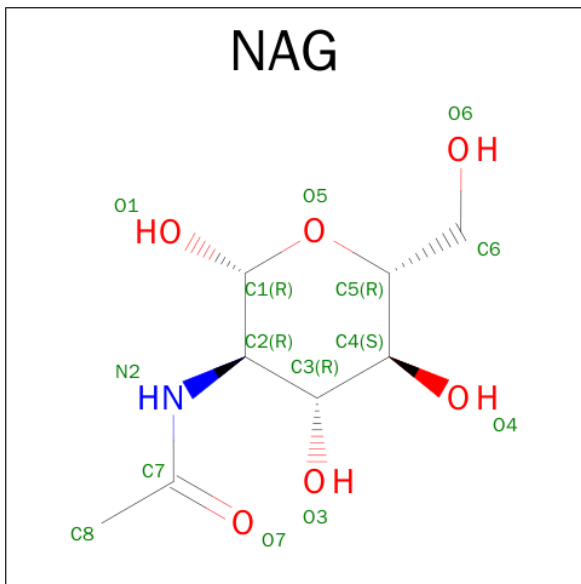
Mol	Chain	Residues	Atoms				AltConf
6	BA	2	Total	C	N	O	0
			28	16	2	10	
6	BF	2	Total	C	N	O	0
			28	16	2	10	
6	BH	2	Total	C	N	O	0
			28	16	2	10	
6	BI	2	Total	C	N	O	0
			28	16	2	10	
6	BN	2	Total	C	N	O	0
			28	16	2	10	

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Mol	Chain	Residues	Atoms				AltConf
6	BO	2	Total	C	N	O	0
			28	16	2	10	
6	BQ	2	Total	C	N	O	0
			28	16	2	10	

- Molecule 7 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

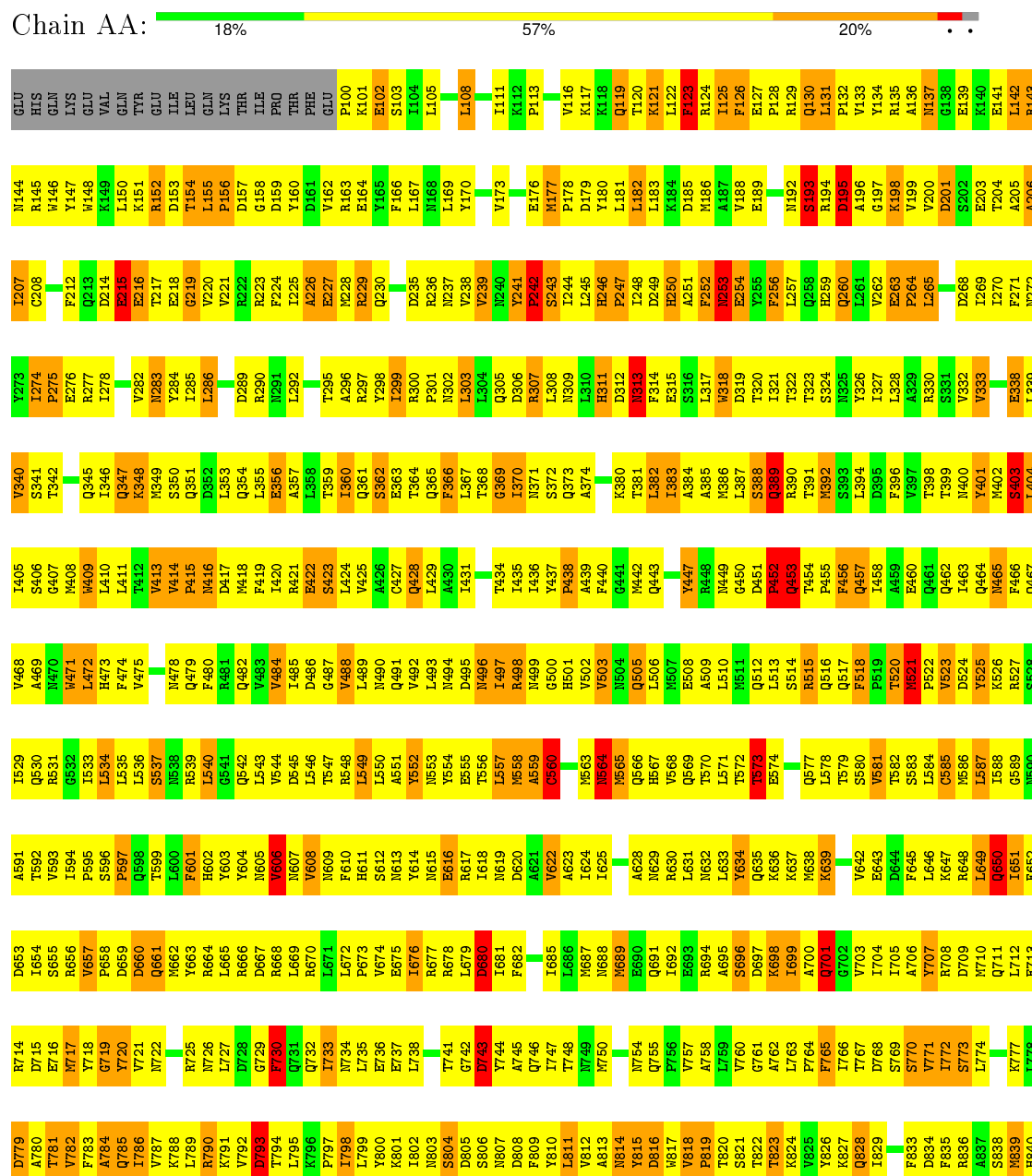


Mol	Chain	Residues	Atoms				AltConf
7	BM	1	Total	C	N	O	0
			14	8	1	5	

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

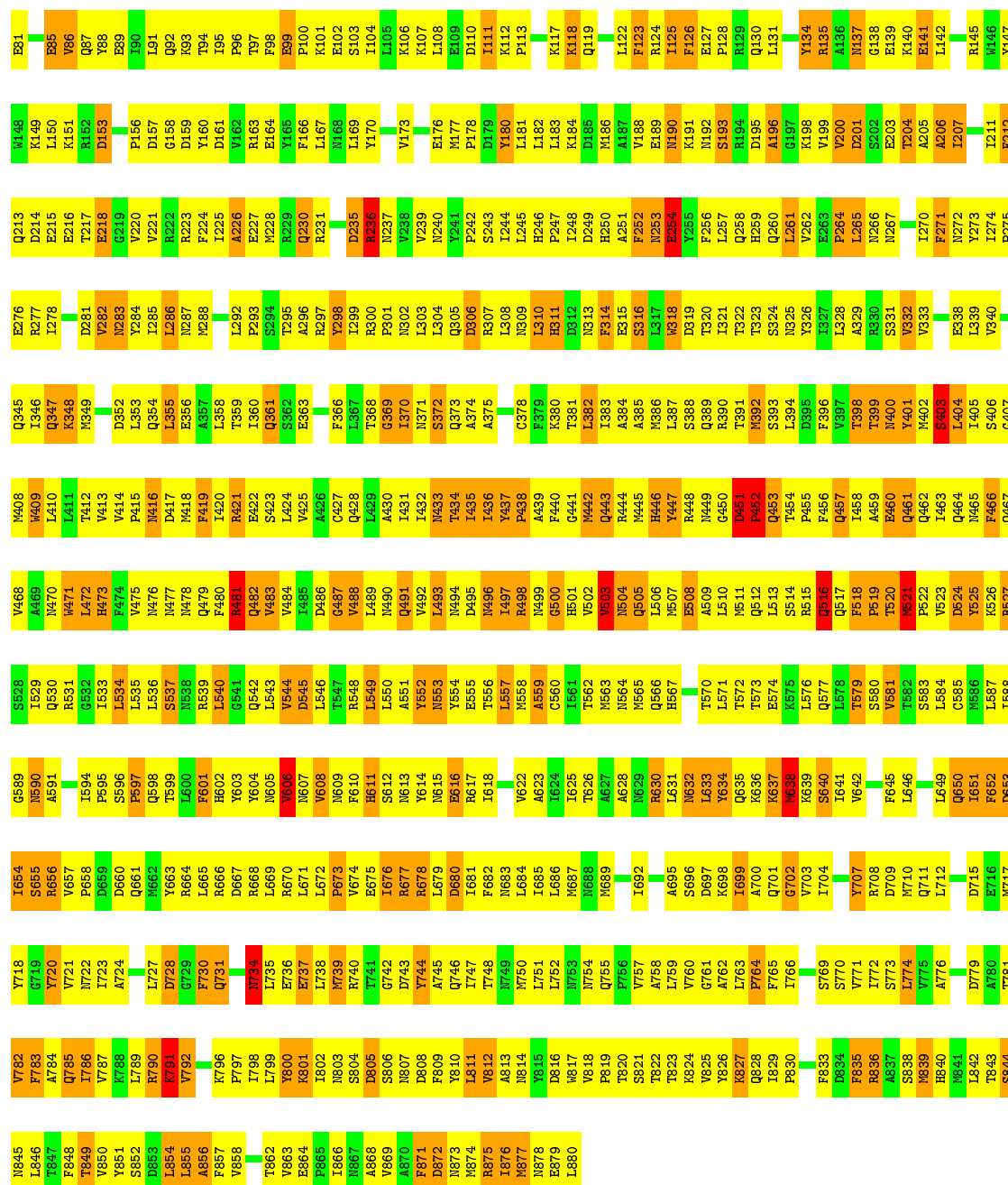
- Molecule 1: Core scaffold protein





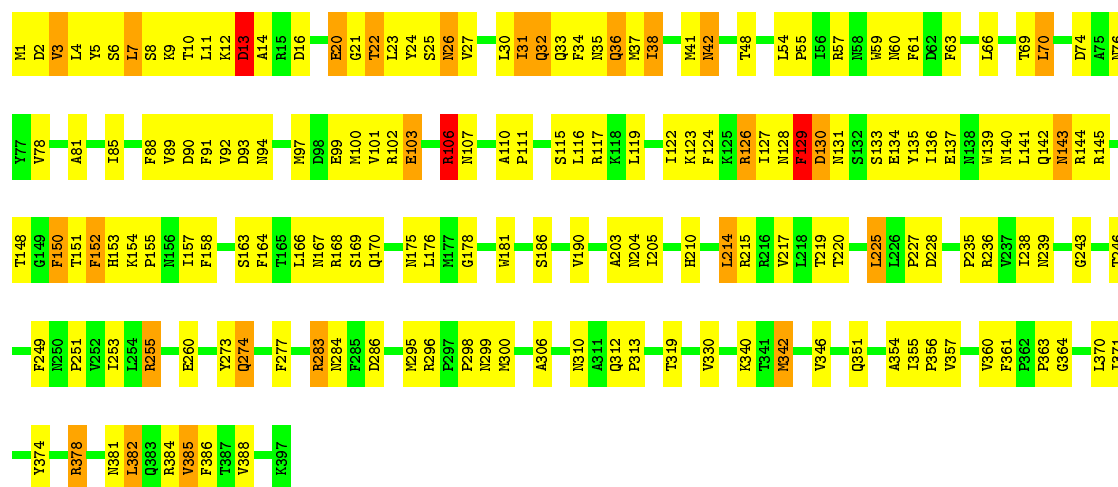
• Molecule 1: Core scaffold protein

Chain AB: 20% 57% 22%



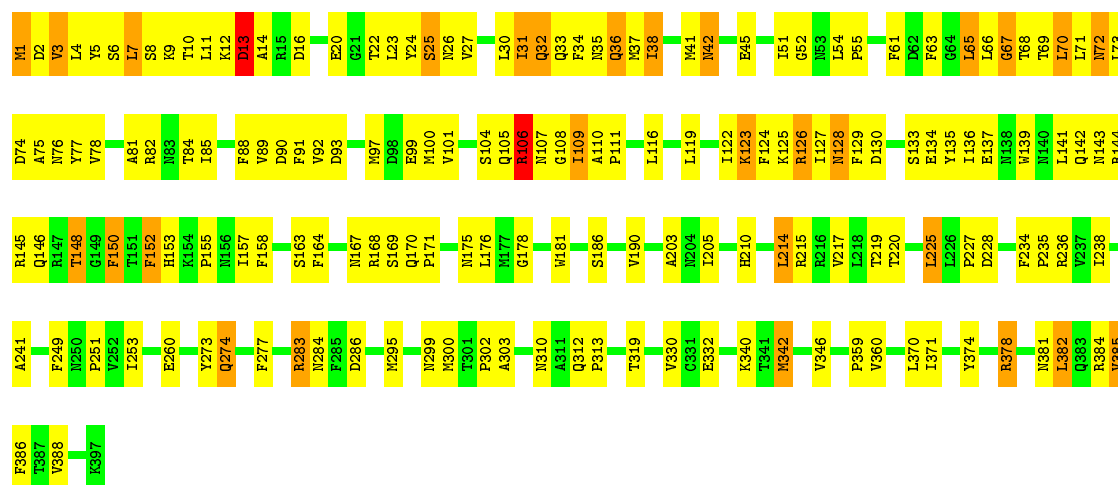
• Molecule 2: Intermediate capsid protein VP6

Chain AC: 56% 37% 7%



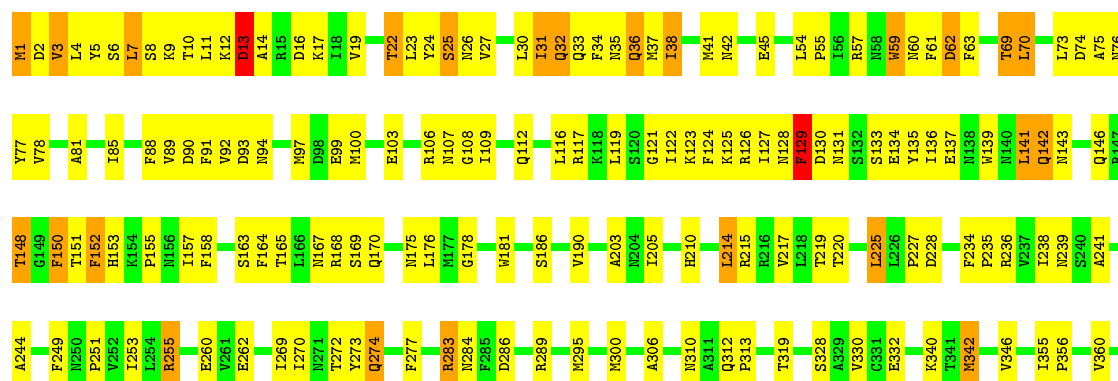
• Molecule 2: Intermediate capsid protein VP6

Chain AD: 57% 36% 7%



• Molecule 2: Intermediate capsid protein VP6

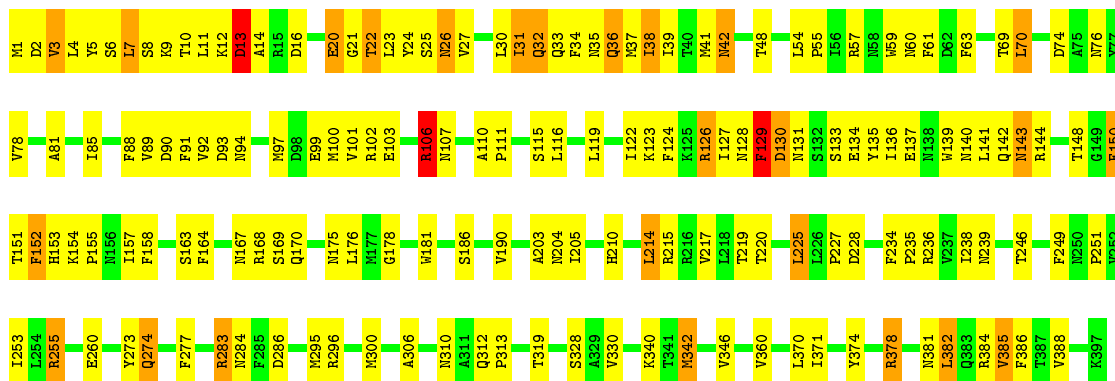
Chain AE: 56% 37% 7%

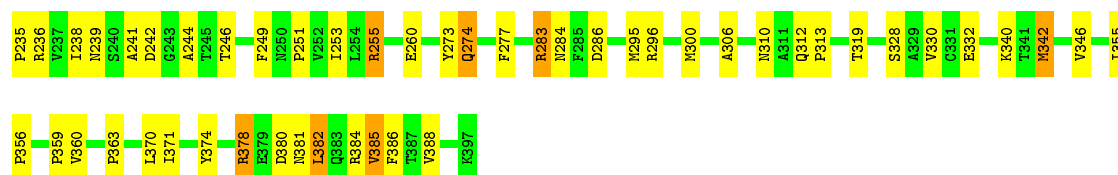




• Molecule 2: Intermediate capsid protein VP6

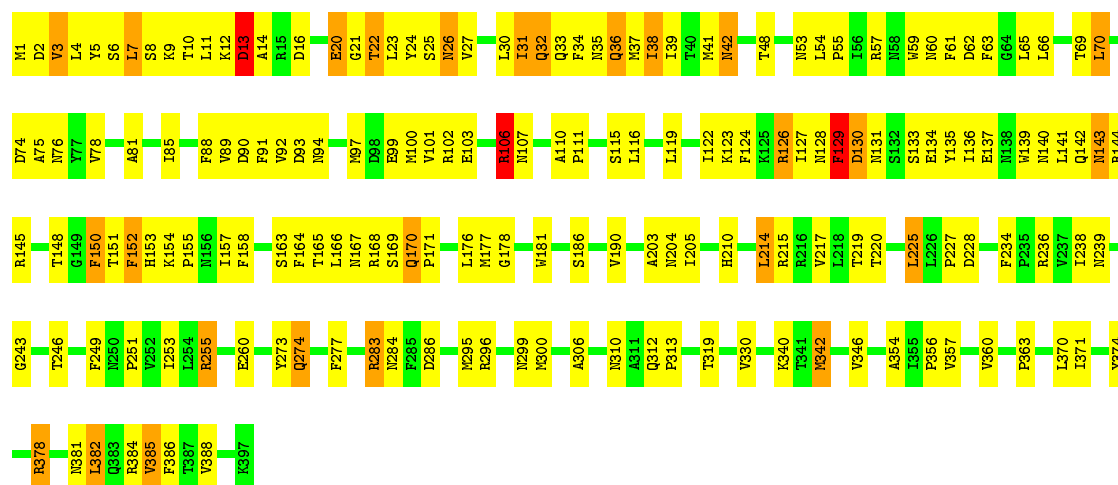
Chain AF: 59% 34% 6% •





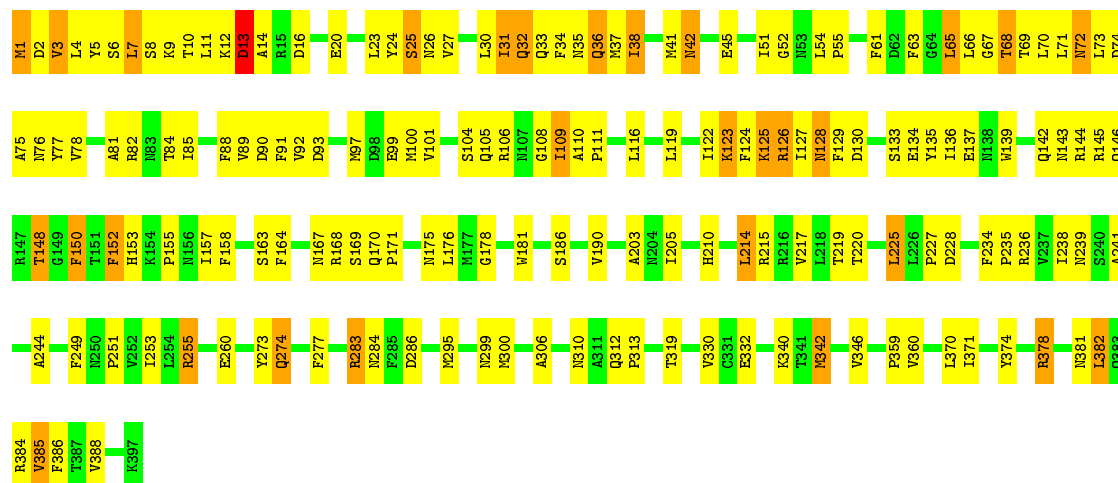
• Molecule 2: Intermediate capsid protein VP6

Chain AI: 55% 37% 7%



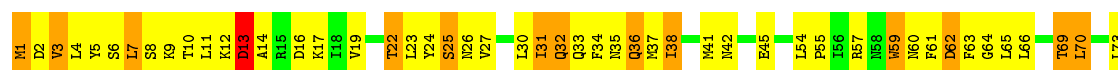
• Molecule 2: Intermediate capsid protein VP6

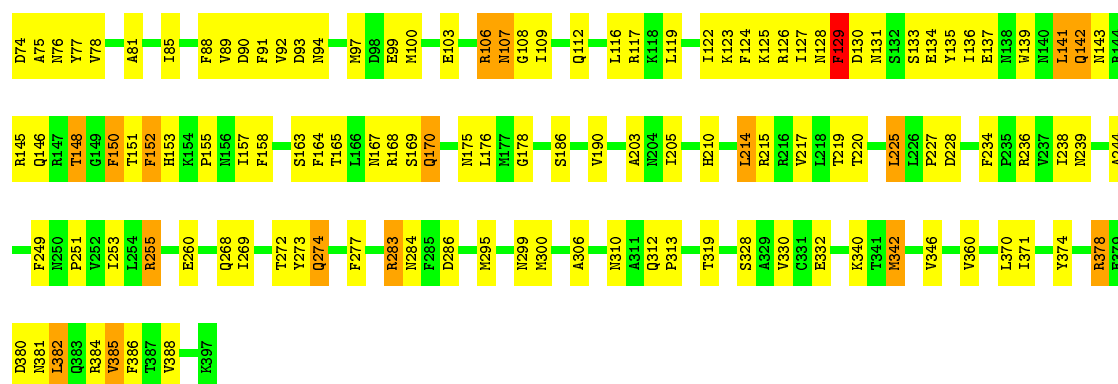
Chain AJ: 57% 35% 7%



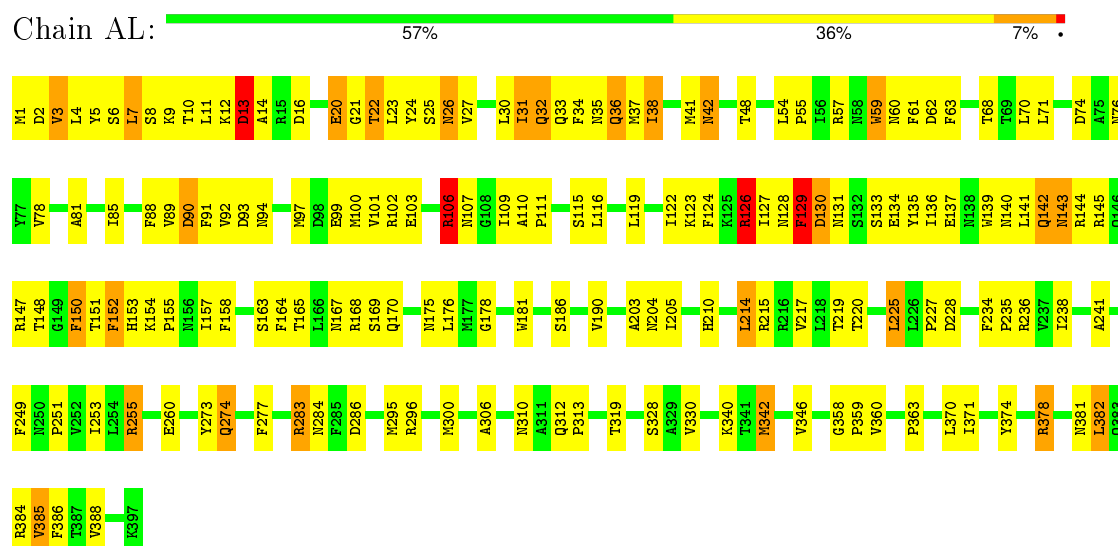
• Molecule 2: Intermediate capsid protein VP6

Chain AK: 57% 35% 8%

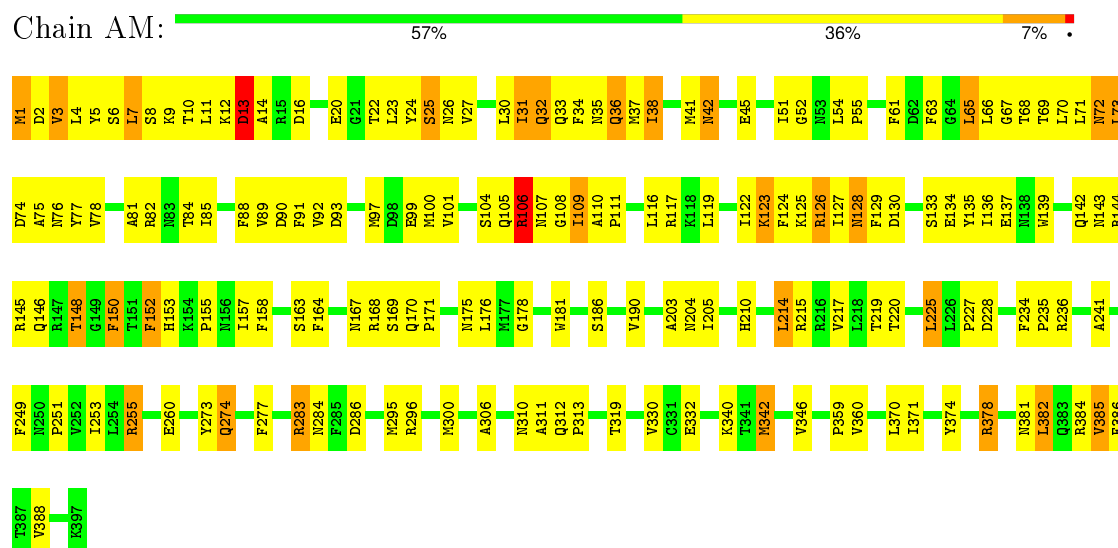




• Molecule 2: Intermediate capsid protein VP6

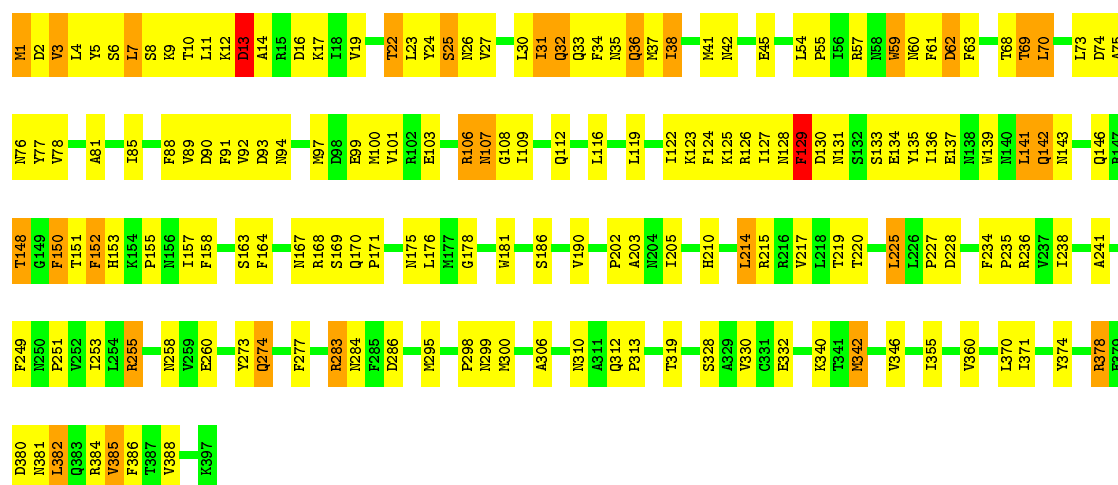


• Molecule 2: Intermediate capsid protein VP6



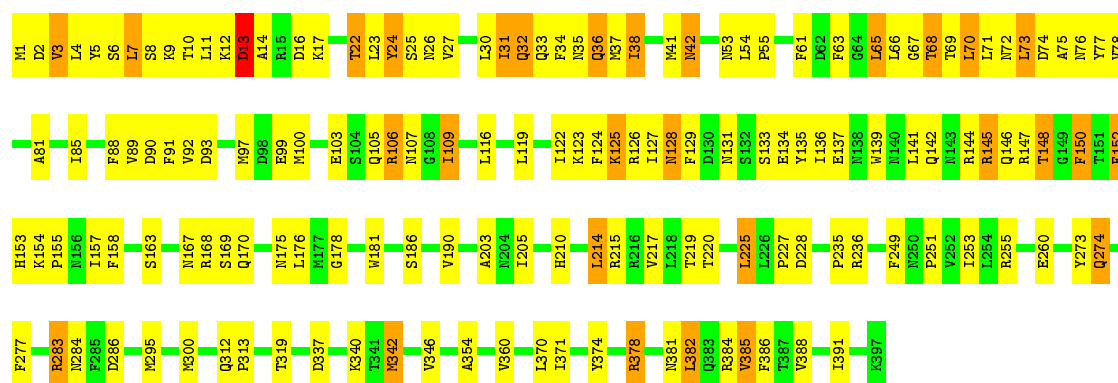
• Molecule 2: Intermediate capsid protein VP6

Chain AN: 



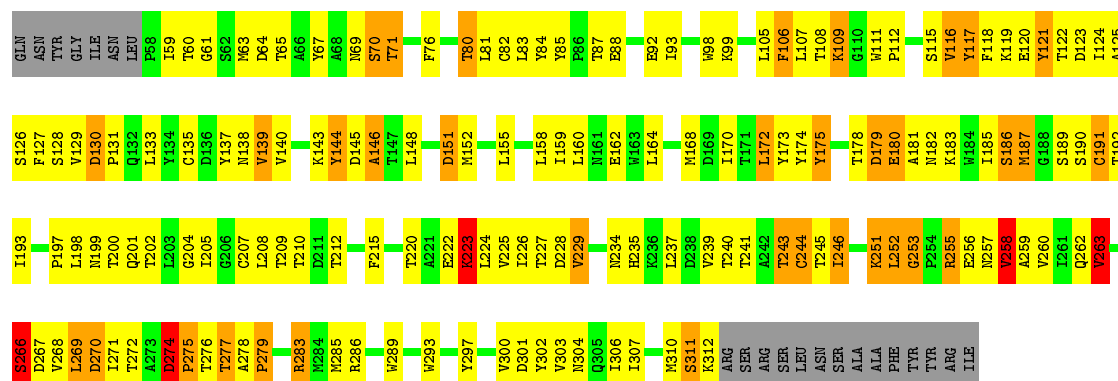
• Molecule 2: Intermediate capsid protein VP6

Chain AO: 

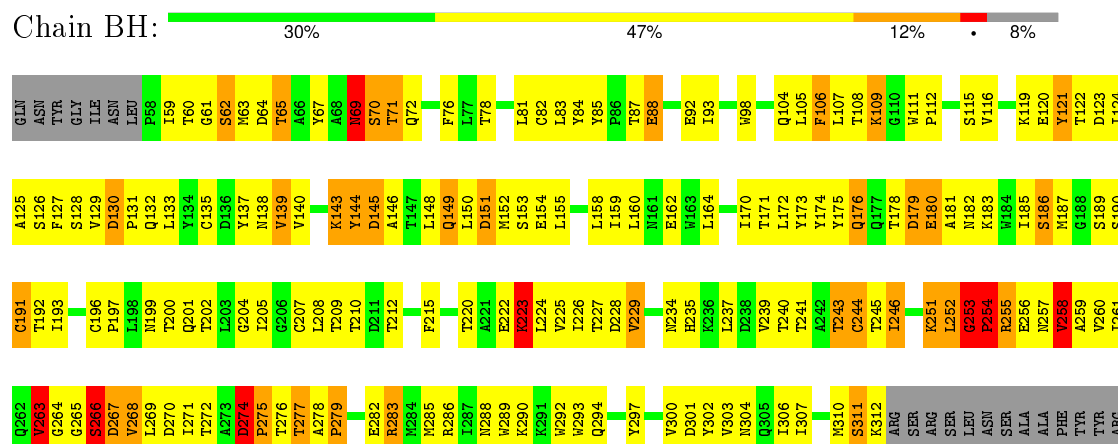


• Molecule 3: Outer layer protein VP7

Chain BA: 


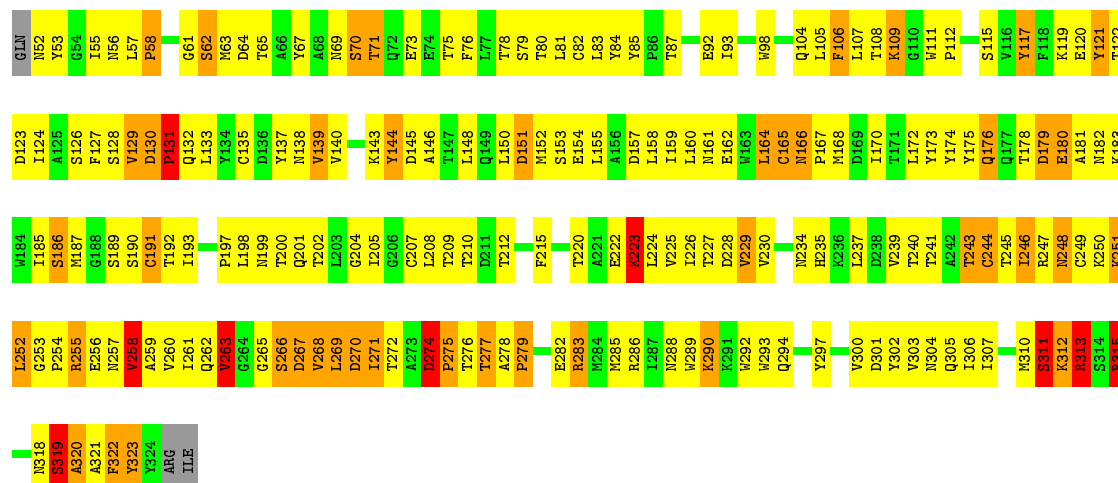


• Molecule 3: Outer layer protein VP7

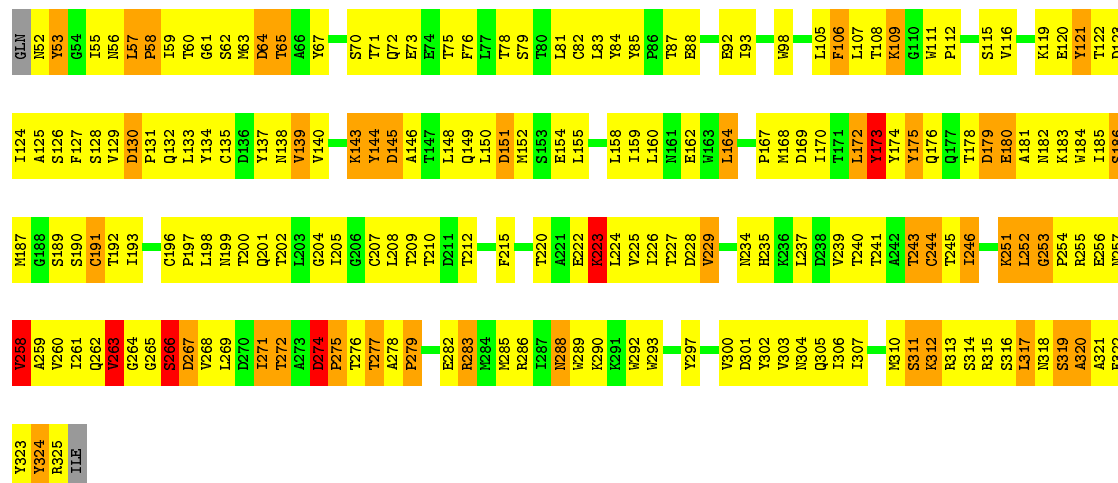


ILE

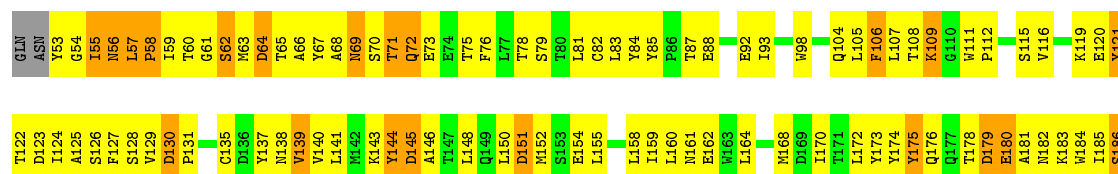
- Molecule 3: Outer layer protein VP7

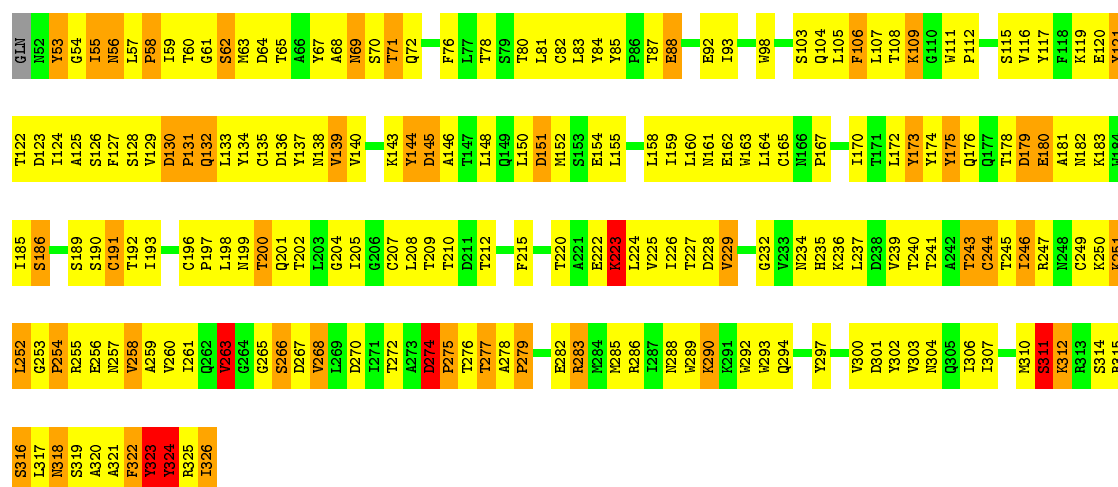
Chain BI:  28% 52% 16% ..

- Molecule 3: Outer layer protein VP7

Chain BJ:  28% 54% 15% ..

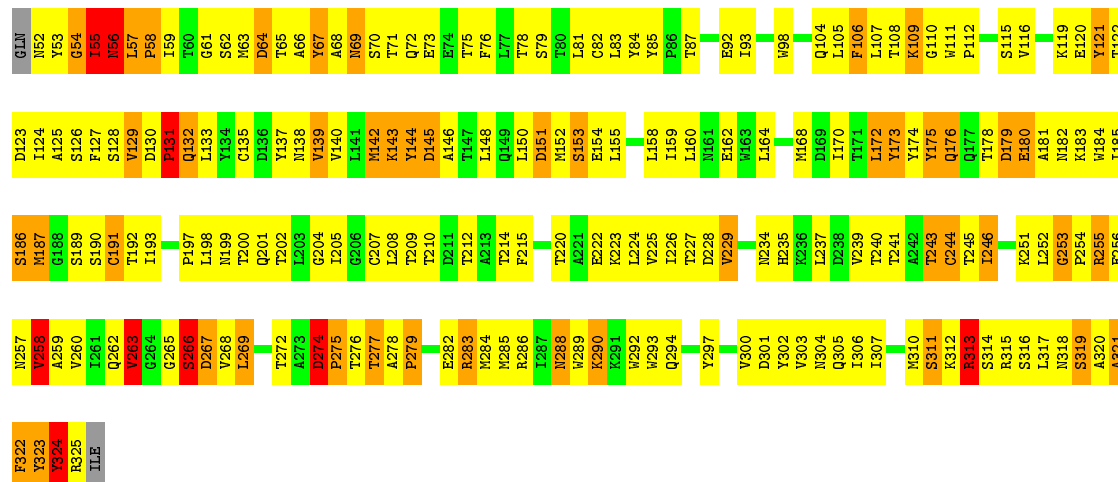
- Molecule 3: Outer layer protein VP7

Chain BK:  29% 53% 14% ..



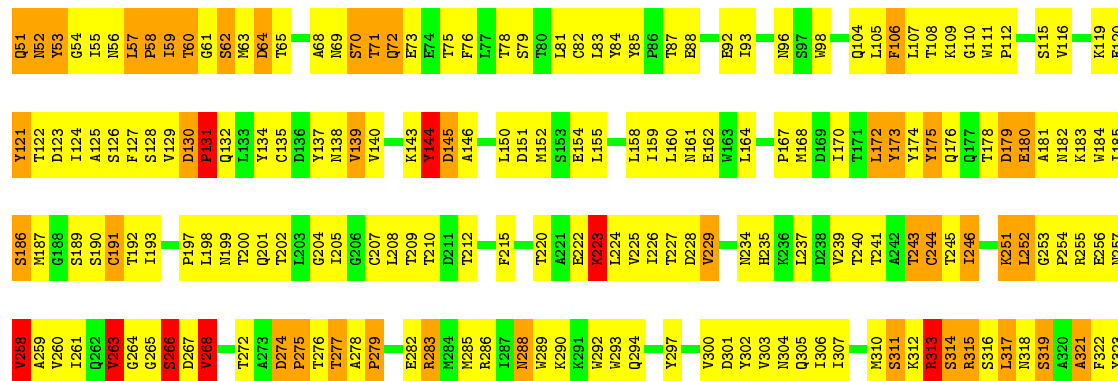
• Molecule 3: Outer layer protein VP7

Chain BO: 28% 52% 17%



• Molecule 3: Outer layer protein VP7

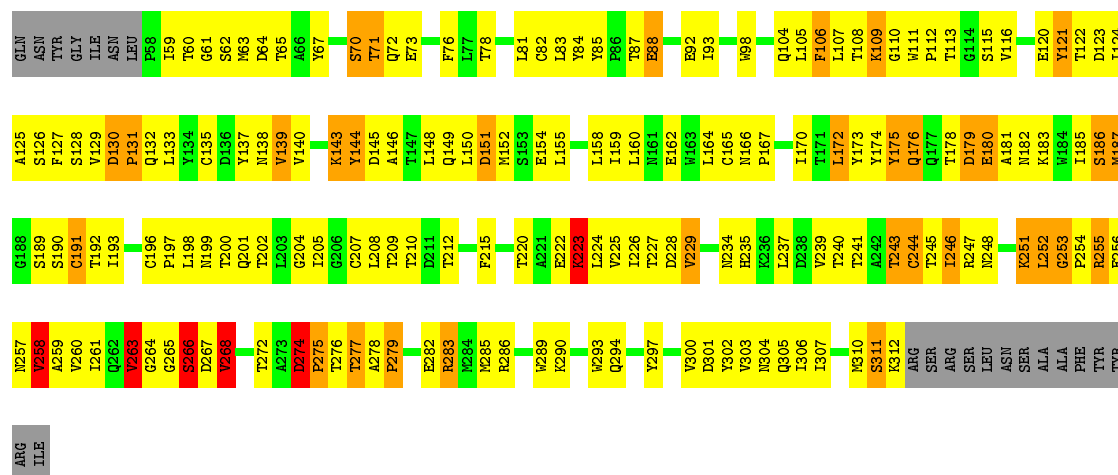
Chain BP: 29% 52% 15%



TYR
ARG
ILE

• Molecule 3: Outer layer protein VP7

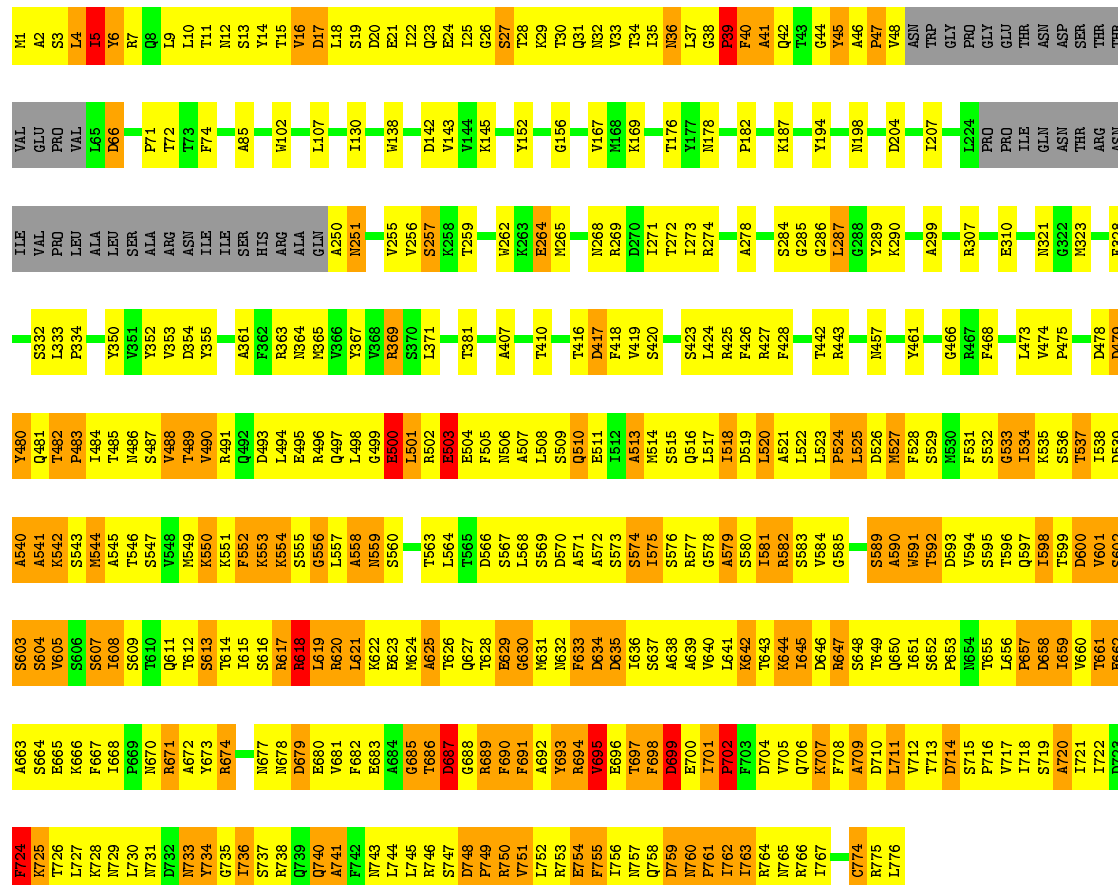
Chain BQ: 29% 49% 12% 8%



ARG
ILE

• Molecule 4: Outer capsid protein VP4

Chain BX: 42% 36% 15% 5%



I718	I598	S536	VAL	
S719	T599	T337	PRO	
A720	D600	I538	SER	
I721	V601	D539	ASN	
I722	B602	A540	ASP	
D723	S603	A541	ASP	
F724	S604	X542	TYR	
K725	V605	S543	GLN	
I726	B606	S544	THR	
I727	S607	A545	PRO	
K728	I608	T546	ILE	
	S609	S547	THR	
N729	P609	V548	ASN	
L730	T610	V549	SER	
N731	Q611	K550	VAL	
D732	T612	K551	THR	
N733	S613	K552	VAL	
Y734	T614	F553	ARG	
I736	I615	X553	GLN	
G735	S616	X554	ASP	
I736	S617	S555	LEU	
S737	R618	G556	LEU	
R738	R619	L557	GLU	
Q739	B620	A558	ARG	
Q740	R621	N559	GLN	
A741	L621	S560	LEU	
F742	K622	S561	G499	
N743	B623	S562	R502	
L744	M624	T563	D417	
L745	A625	T564	F418	
R746	T626	L564	E504	
S747	Q627	T565	E504	
D748	T628	D566	F505	
R749	B629	S567	A420	
R750	F630	L568	L421	
V751	M631	S569	A422	
L752	N632	D570	S423	
R753	F633	A571	S509	
R754	D634	A572	Q510	
F755	D635	S573	E511	
I756	I636	S574	I512	
N757	S637	T575	A513	
F758	A638	S576	M514	
D759	A639	R577	S515	
N760	V640	A578	Q516	
P761	L641	A579	L517	
I762	K642	S580	I518	
I763	T643	T581	D519	
R764	K644	R582	L520	
N765	I645	S583	A521	
R766	D646	V584	L522	
I767	R647	Q585	L523	
E768	S648		P624	
Q769	T649	S589	L525	
	Q650	A590	D526	
Q773	I651	A591	R527	
C774	S652	T592	Q466	
R775	P653	D593	R467	
L776	X654	V594	X630	
	T655	S595	F631	
	L656	T596	I471	
	P657	Q597	S472	
			L473	

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
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	59000	Depositor
Image detector	Kodak SO163	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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 >2	RMSZ	# Z >2
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
6	BQ	1	0
All	All	1	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

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	BQ	401	NAG	C1

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AB	452	PRO	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	AA	6379	0	6408	1177	0
1	AB	6545	0	6569	1213	0
2	AC	3163	0	3112	246	0
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	AC	1	0	0	0	0
5	AF	1	0	0	0	0
5	AK	1	0	0	0	0
5	AN	1	0	0	0	0
5	AO	1	0	0	0	0
6	BA	28	0	25	2	0
6	BF	28	0	25	4	0
6	BH	28	0	25	4	0
6	BI	28	0	25	2	0
6	BN	28	0	25	3	0
6	BO	28	0	25	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	BQ	28	0	25	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:CB	3:BA:116:VAL:CG1	1.80	1.58
4:BX:32:ASN:HB3	4:BY:484:ILE:CG2	1.33	1.58
3:BI:69:ASN:HD21	6:BI:401: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	3
1	AB	798/800 (100%)	463 (58%)	209 (26%)	126 (16%)	0	5
2	AC	395/397 (100%)	327 (83%)	48 (12%)	20 (5%)	2	31
2	AD	395/397 (100%)	331 (84%)	42 (11%)	22 (6%)	2	29
2	AE	395/397 (100%)	332 (84%)	44 (11%)	19 (5%)	3	32
2	AF	395/397 (100%)	327 (83%)	48 (12%)	20 (5%)	2	31
2	AG	395/397 (100%)	334 (85%)	42 (11%)	19 (5%)	3	32
2	AH	395/397 (100%)	331 (84%)	45 (11%)	19 (5%)	3	32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AI	395/397 (100%)	327 (83%)	48 (12%)	20 (5%)	2	31
2	AJ	395/397 (100%)	334 (85%)	40 (10%)	21 (5%)	2	30
2	AK	395/397 (100%)	334 (85%)	42 (11%)	19 (5%)	3	32
2	AL	395/397 (100%)	327 (83%)	48 (12%)	20 (5%)	2	31
2	AM	395/397 (100%)	333 (84%)	40 (10%)	22 (6%)	2	29
2	AN	395/397 (100%)	332 (84%)	44 (11%)	19 (5%)	3	32
2	AO	395/397 (100%)	321 (81%)	51 (13%)	23 (6%)	2	28
3	BA	253/276 (92%)	209 (83%)	28 (11%)	16 (6%)	2	26
3	BF	261/276 (95%)	216 (83%)	28 (11%)	17 (6%)	1	25
3	BG	271/276 (98%)	214 (79%)	39 (14%)	18 (7%)	1	25
3	BH	253/276 (92%)	210 (83%)	27 (11%)	16 (6%)	2	26
3	BI	271/276 (98%)	214 (79%)	34 (12%)	23 (8%)	1	17
3	BJ	272/276 (99%)	221 (81%)	32 (12%)	19 (7%)	1	23
3	BK	267/276 (97%)	213 (80%)	34 (13%)	20 (8%)	1	20
3	BL	270/276 (98%)	218 (81%)	34 (13%)	18 (7%)	1	25
3	BM	253/276 (92%)	214 (85%)	24 (10%)	15 (6%)	2	27
3	BN	273/276 (99%)	222 (81%)	30 (11%)	21 (8%)	1	20
3	BO	272/276 (99%)	219 (80%)	31 (11%)	22 (8%)	1	18
3	BP	271/276 (98%)	220 (81%)	33 (12%)	18 (7%)	1	25
3	BQ	253/276 (92%)	211 (83%)	28 (11%)	14 (6%)	2	29
4	BX	729/776 (94%)	514 (70%)	105 (14%)	110 (15%)	0	5
4	BY	732/776 (94%)	521 (71%)	119 (16%)	92 (13%)	0	8
4	BZ	511/776 (66%)	326 (64%)	95 (19%)	90 (18%)	0	3
All	All	12124/12677 (96%)	9346 (77%)	1722 (14%)	1056 (9%)	2	16

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%)	7	38
1	AB	736/736 (100%)	644 (88%)	92 (12%)	6	33
2	AC	350/350 (100%)	329 (94%)	21 (6%)	24	65
2	AD	350/350 (100%)	329 (94%)	21 (6%)	24	65
2	AE	350/350 (100%)	329 (94%)	21 (6%)	24	65
2	AF	350/350 (100%)	329 (94%)	21 (6%)	24	65
2	AG	350/350 (100%)	328 (94%)	22 (6%)	22	63
2	AH	350/350 (100%)	330 (94%)	20 (6%)	25	67
2	AI	350/350 (100%)	329 (94%)	21 (6%)	24	65
2	AJ	350/350 (100%)	329 (94%)	21 (6%)	24	65
2	AK	350/350 (100%)	329 (94%)	21 (6%)	24	65
2	AL	350/350 (100%)	328 (94%)	22 (6%)	22	63
2	AM	350/350 (100%)	328 (94%)	22 (6%)	22	63
2	AN	350/350 (100%)	329 (94%)	21 (6%)	24	65
2	AO	350/350 (100%)	331 (95%)	19 (5%)	27	68
3	BA	229/247 (93%)	206 (90%)	23 (10%)	9	43
3	BF	236/247 (96%)	212 (90%)	24 (10%)	9	43
3	BG	244/247 (99%)	214 (88%)	30 (12%)	6	34
3	BH	229/247 (93%)	204 (89%)	25 (11%)	8	40
3	BI	244/247 (99%)	215 (88%)	29 (12%)	6	35
3	BJ	245/247 (99%)	218 (89%)	27 (11%)	8	39
3	BK	240/247 (97%)	214 (89%)	26 (11%)	8	41
3	BL	243/247 (98%)	215 (88%)	28 (12%)	7	37
3	BM	229/247 (93%)	205 (90%)	24 (10%)	8	41
3	BN	246/247 (100%)	221 (90%)	25 (10%)	9	43
3	BO	245/247 (99%)	213 (87%)	32 (13%)	5	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	BP	244/247 (99%)	219 (90%)	25 (10%)	9	43
3	BQ	229/247 (93%)	206 (90%)	23 (10%)	9	43
4	BX	652/688 (95%)	608 (93%)	44 (7%)	20	62
4	BY	654/688 (95%)	605 (92%)	49 (8%)	17	57
4	BZ	456/688 (66%)	416 (91%)	40 (9%)	12	50
All	All	10868/11297 (96%)	9948 (92%)	920 (8%)	18	52

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

Mol	Chain	Res	Type
2	AN	170	GLN
3	BG	263	VAL
4	BY	496	ARG
2	AO	103	GLU
3	BA	277	THR

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

Mol	Chain	Res	Type
2	AK	53	ASN
2	AN	167	ASN
4	BY	198	ASN
2	AK	167	ASN
2	AM	94	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

14 carbohydrates 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
6	NAG	BA	401	6	14,14,15	0.58	0	15,19,21	1.19	1 (6%)
6	NAG	BA	402	6	14,14,15	1.01	1 (7%)	15,19,21	1.72	5 (33%)
6	NAG	BF	401	6	14,14,15	0.60	0	15,19,21	1.19	1 (6%)
6	NAG	BF	402	6	14,14,15	1.01	1 (7%)	15,19,21	1.72	5 (33%)
6	NAG	BH	401	6	14,14,15	0.57	0	15,19,21	1.19	1 (6%)
6	NAG	BH	402	6	14,14,15	1.00	1 (7%)	15,19,21	1.72	5 (33%)
6	NAG	BI	401	6	14,14,15	0.57	0	15,19,21	1.19	1 (6%)
6	NAG	BI	402	6	14,14,15	1.01	1 (7%)	15,19,21	1.73	5 (33%)
6	NAG	BN	401	6	14,14,15	0.59	0	15,19,21	1.20	1 (6%)
6	NAG	BN	402	6	14,14,15	1.00	1 (7%)	15,19,21	1.73	5 (33%)
6	NAG	BO	401	6	14,14,15	0.59	0	15,19,21	1.19	1 (6%)
6	NAG	BO	402	6	14,14,15	1.01	1 (7%)	15,19,21	1.73	5 (33%)
6	NAG	BQ	401	3,6	14,14,15	0.57	0	15,19,21	1.19	1 (6%)
6	NAG	BQ	402	6	14,14,15	1.01	1 (7%)	15,19,21	1.73	5 (33%)

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
6	NAG	BA	401	6	-	0/6/23/26	0/1/1/1
6	NAG	BA	402	6	-	0/6/23/26	0/1/1/1
6	NAG	BF	401	6	-	0/6/23/26	0/1/1/1
6	NAG	BF	402	6	-	0/6/23/26	0/1/1/1
6	NAG	BH	401	6	-	0/6/23/26	0/1/1/1
6	NAG	BH	402	6	-	0/6/23/26	0/1/1/1
6	NAG	BI	401	6	-	0/6/23/26	0/1/1/1
6	NAG	BI	402	6	-	0/6/23/26	0/1/1/1
6	NAG	BN	401	6	-	0/6/23/26	0/1/1/1
6	NAG	BN	402	6	-	0/6/23/26	0/1/1/1
6	NAG	BO	401	6	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	BO	402	6	-	0/6/23/26	0/1/1/1
6	NAG	BQ	401	3,6	1/1/5/7	0/6/23/26	0/1/1/1
6	NAG	BQ	402	6	-	0/6/23/26	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)
6	BN	402	NAG	C1-C2	2.74	1.56	1.52
6	BH	402	NAG	C1-C2	2.75	1.56	1.52
6	BQ	402	NAG	C1-C2	2.80	1.56	1.52
6	BI	402	NAG	C1-C2	2.82	1.56	1.52
6	BF	402	NAG	C1-C2	2.83	1.56	1.52

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	BN	402	NAG	O7-C7-C8	-2.61	117.26	122.07
6	BQ	402	NAG	O7-C7-C8	-2.60	117.29	122.07
6	BO	402	NAG	O7-C7-C8	-2.60	117.29	122.07
6	BA	402	NAG	O7-C7-C8	-2.58	117.32	122.07
6	BF	402	NAG	O7-C7-C8	-2.58	117.32	122.07

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	BQ	401	NAG	C1

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	BA	401	NAG	2	0
6	BF	401	NAG	4	0
6	BH	401	NAG	4	0
6	BI	401	NAG	2	0
6	BN	401	NAG	3	0
6	BO	401	NAG	3	0

5.6 Ligand geometry

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	0.59	0	15,19,21	1.19	1 (6%)

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 (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
7	BM	401	NAG	C1-O5-C5	3.36	117.08	112.14

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

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.