



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 12:26 AM UTC

PDB ID : 6Y67 / pdb_00006y67
Title : Structure of apo Finch Polyomavirus VP1
Authors : Stroh, L.J.; Rustmeier, N.H.; Stehle, T.
Deposited on : 2020-02-26
Resolution : 2.62 Å(reported)

This is a wwPDB X-ray Structure 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/XrayValidationReportHelp>

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:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

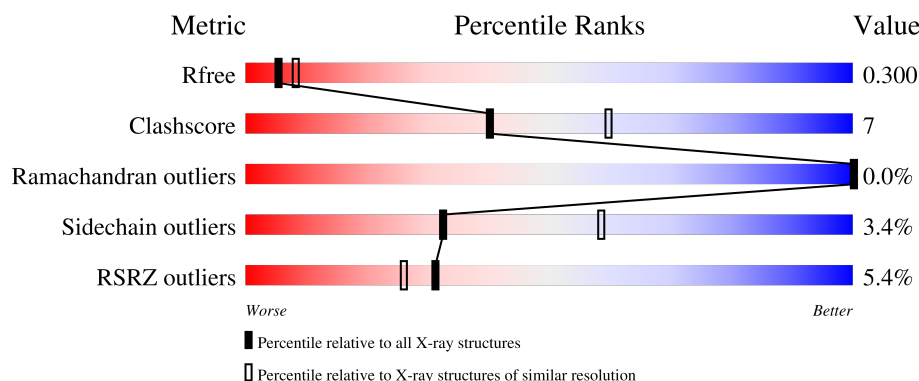
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.62 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4951 (2.64-2.60)
Clashscore	190562	5303 (2.64-2.60)
Ramachandran outliers	187476	5217 (2.64-2.60)
Sidechain outliers	187428	5217 (2.64-2.60)
RSRZ outliers	180081	4950 (2.64-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AAA	293	3% 82% 8% 10%
1	BBB	293	5% 78% 14% 8%
1	CCC	293	2% 78% 13% 9%
1	DDD	293	0% 77% 14% 9%
1	EEE	293	2% 81% 11% 8%

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Mol	Chain	Length	Quality of chain
1	FFF	293	
1	GGG	293	
1	HHH	293	
1	III	293	
1	JJJ	293	
1	KKK	293	
1	LLL	293	
1	MMM	293	
1	NNN	293	
1	OOO	293	
1	PPP	293	
1	QQQ	293	
1	RRR	293	
1	SSS	293	
1	TTT	293	
1	UUU	293	
1	VVV	293	
1	WWW	293	
1	XXX	293	
1	YYY	293	
1	ZZZ	293	
1	aaa	293	
1	bbb	293	
1	ccc	293	
1	ddd	293	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 59801 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Capsid protein VP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	263	Total	C	N	O	S	0	0	0
			1971	1250	330	383	8			
1	BBB	270	Total	C	N	O	S	0	0	0
			2000	1265	335	392	8			
1	CCC	268	Total	C	N	O	S	0	0	0
			2009	1272	336	393	8			
1	DDD	267	Total	C	N	O	S	0	0	0
			1998	1263	334	393	8			
1	EEE	270	Total	C	N	O	S	0	0	0
			2014	1278	336	392	8			
1	FFF	270	Total	C	N	O	S	0	0	0
			2003	1263	336	396	8			
1	GGG	268	Total	C	N	O	S	0	0	0
			2005	1265	336	396	8			
1	HHH	265	Total	C	N	O	S	0	0	0
			1976	1253	332	383	8			
1	III	269	Total	C	N	O	S	0	1	0
			2009	1272	338	391	8			
1	JJJ	262	Total	C	N	O	S	0	0	0
			1959	1238	331	382	8			
1	KKK	268	Total	C	N	O	S	0	0	0
			2018	1279	336	395	8			
1	LLL	268	Total	C	N	O	S	0	0	0
			2002	1264	336	394	8			
1	MMM	258	Total	C	N	O	S	0	0	0
			1924	1214	322	380	8			
1	NNN	266	Total	C	N	O	S	0	1	0
			1934	1217	328	381	8			
1	OOO	270	Total	C	N	O	S	0	0	0
			1984	1253	335	388	8			
1	PPP	264	Total	C	N	O	S	0	0	0
			1972	1252	334	378	8			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	QQQ	269	Total	C	N	O	S	0	1	0
			2017	1275	335	399	8			
1	RRR	263	Total	C	N	O	S	0	0	0
			1959	1239	330	382	8			
1	SSS	268	Total	C	N	O	S	0	1	0
			2015	1270	338	399	8			
1	TTT	270	Total	C	N	O	S	0	0	0
			1997	1261	336	392	8			
1	UUU	261	Total	C	N	O	S	0	0	0
			1944	1228	328	380	8			
1	VVV	261	Total	C	N	O	S	0	0	0
			1873	1179	323	363	8			
1	WWW	268	Total	C	N	O	S	0	0	0
			1922	1209	330	375	8			
1	XXX	267	Total	C	N	O	S	0	1	0
			1975	1246	331	390	8			
1	YYY	262	Total	C	N	O	S	0	0	0
			1909	1202	327	372	8			
1	ZZZ	259	Total	C	N	O	S	0	0	0
			1911	1211	318	374	8			
1	aaa	266	Total	C	N	O	S	0	0	0
			1971	1247	328	388	8			
1	bbb	253	Total	C	N	O	S	0	0	0
			1906	1209	320	369	8			
1	ccc	255	Total	C	N	O	S	0	0	0
			1900	1200	320	372	8			
1	ddd	260	Total	C	N	O	S	0	0	0
			1902	1194	325	375	8			

There are 750 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-1	MET	-	initiating methionine	UNP R4UMH0
AAA	0	GLY	-	expression tag	UNP R4UMH0
AAA	1	SER	-	expression tag	UNP R4UMH0
AAA	2	SER	-	expression tag	UNP R4UMH0
AAA	3	HIS	-	expression tag	UNP R4UMH0
AAA	4	HIS	-	expression tag	UNP R4UMH0
AAA	5	HIS	-	expression tag	UNP R4UMH0
AAA	6	HIS	-	expression tag	UNP R4UMH0
AAA	7	HIS	-	expression tag	UNP R4UMH0
AAA	8	HIS	-	expression tag	UNP R4UMH0
AAA	9	SER	-	expression tag	UNP R4UMH0

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Chain	Residue	Modelled	Actual	Comment	Reference
AAA	10	SER	-	expression tag	UNP R4UMH0
AAA	11	GLY	-	expression tag	UNP R4UMH0
AAA	12	GLU	-	expression tag	UNP R4UMH0
AAA	13	ASN	-	expression tag	UNP R4UMH0
AAA	14	LEU	-	expression tag	UNP R4UMH0
AAA	15	TYR	-	expression tag	UNP R4UMH0
AAA	16	PHE	-	expression tag	UNP R4UMH0
AAA	17	GLN	-	expression tag	UNP R4UMH0
AAA	18	GLY	-	expression tag	UNP R4UMH0
AAA	19	SER	-	expression tag	UNP R4UMH0
AAA	20	HIS	-	expression tag	UNP R4UMH0
AAA	21	MET	-	expression tag	UNP R4UMH0
AAA	78	SER	CYS	conflict	UNP R4UMH0
AAA	92	SER	CYS	conflict	UNP R4UMH0
BBB	-1	MET	-	initiating methionine	UNP R4UMH0
BBB	0	GLY	-	expression tag	UNP R4UMH0
BBB	1	SER	-	expression tag	UNP R4UMH0
BBB	2	SER	-	expression tag	UNP R4UMH0
BBB	3	HIS	-	expression tag	UNP R4UMH0
BBB	4	HIS	-	expression tag	UNP R4UMH0
BBB	5	HIS	-	expression tag	UNP R4UMH0
BBB	6	HIS	-	expression tag	UNP R4UMH0
BBB	7	HIS	-	expression tag	UNP R4UMH0
BBB	8	HIS	-	expression tag	UNP R4UMH0
BBB	9	SER	-	expression tag	UNP R4UMH0
BBB	10	SER	-	expression tag	UNP R4UMH0
BBB	11	GLY	-	expression tag	UNP R4UMH0
BBB	12	GLU	-	expression tag	UNP R4UMH0
BBB	13	ASN	-	expression tag	UNP R4UMH0
BBB	14	LEU	-	expression tag	UNP R4UMH0
BBB	15	TYR	-	expression tag	UNP R4UMH0
BBB	16	PHE	-	expression tag	UNP R4UMH0
BBB	17	GLN	-	expression tag	UNP R4UMH0
BBB	18	GLY	-	expression tag	UNP R4UMH0
BBB	19	SER	-	expression tag	UNP R4UMH0
BBB	20	HIS	-	expression tag	UNP R4UMH0
BBB	21	MET	-	expression tag	UNP R4UMH0
BBB	78	SER	CYS	conflict	UNP R4UMH0
BBB	92	SER	CYS	conflict	UNP R4UMH0
CCC	-1	MET	-	initiating methionine	UNP R4UMH0
CCC	0	GLY	-	expression tag	UNP R4UMH0
CCC	1	SER	-	expression tag	UNP R4UMH0

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Chain	Residue	Modelled	Actual	Comment	Reference
CCC	2	SER	-	expression tag	UNP R4UMH0
CCC	3	HIS	-	expression tag	UNP R4UMH0
CCC	4	HIS	-	expression tag	UNP R4UMH0
CCC	5	HIS	-	expression tag	UNP R4UMH0
CCC	6	HIS	-	expression tag	UNP R4UMH0
CCC	7	HIS	-	expression tag	UNP R4UMH0
CCC	8	HIS	-	expression tag	UNP R4UMH0
CCC	9	SER	-	expression tag	UNP R4UMH0
CCC	10	SER	-	expression tag	UNP R4UMH0
CCC	11	GLY	-	expression tag	UNP R4UMH0
CCC	12	GLU	-	expression tag	UNP R4UMH0
CCC	13	ASN	-	expression tag	UNP R4UMH0
CCC	14	LEU	-	expression tag	UNP R4UMH0
CCC	15	TYR	-	expression tag	UNP R4UMH0
CCC	16	PHE	-	expression tag	UNP R4UMH0
CCC	17	GLN	-	expression tag	UNP R4UMH0
CCC	18	GLY	-	expression tag	UNP R4UMH0
CCC	19	SER	-	expression tag	UNP R4UMH0
CCC	20	HIS	-	expression tag	UNP R4UMH0
CCC	21	MET	-	expression tag	UNP R4UMH0
CCC	78	SER	CYS	conflict	UNP R4UMH0
CCC	92	SER	CYS	conflict	UNP R4UMH0
DDD	-1	MET	-	initiating methionine	UNP R4UMH0
DDD	0	GLY	-	expression tag	UNP R4UMH0
DDD	1	SER	-	expression tag	UNP R4UMH0
DDD	2	SER	-	expression tag	UNP R4UMH0
DDD	3	HIS	-	expression tag	UNP R4UMH0
DDD	4	HIS	-	expression tag	UNP R4UMH0
DDD	5	HIS	-	expression tag	UNP R4UMH0
DDD	6	HIS	-	expression tag	UNP R4UMH0
DDD	7	HIS	-	expression tag	UNP R4UMH0
DDD	8	HIS	-	expression tag	UNP R4UMH0
DDD	9	SER	-	expression tag	UNP R4UMH0
DDD	10	SER	-	expression tag	UNP R4UMH0
DDD	11	GLY	-	expression tag	UNP R4UMH0
DDD	12	GLU	-	expression tag	UNP R4UMH0
DDD	13	ASN	-	expression tag	UNP R4UMH0
DDD	14	LEU	-	expression tag	UNP R4UMH0
DDD	15	TYR	-	expression tag	UNP R4UMH0
DDD	16	PHE	-	expression tag	UNP R4UMH0
DDD	17	GLN	-	expression tag	UNP R4UMH0
DDD	18	GLY	-	expression tag	UNP R4UMH0

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Chain	Residue	Modelled	Actual	Comment	Reference
DDD	19	SER	-	expression tag	UNP R4UMH0
DDD	20	HIS	-	expression tag	UNP R4UMH0
DDD	21	MET	-	expression tag	UNP R4UMH0
DDD	78	SER	CYS	conflict	UNP R4UMH0
DDD	92	SER	CYS	conflict	UNP R4UMH0
EEE	-1	MET	-	initiating methionine	UNP R4UMH0
EEE	0	GLY	-	expression tag	UNP R4UMH0
EEE	1	SER	-	expression tag	UNP R4UMH0
EEE	2	SER	-	expression tag	UNP R4UMH0
EEE	3	HIS	-	expression tag	UNP R4UMH0
EEE	4	HIS	-	expression tag	UNP R4UMH0
EEE	5	HIS	-	expression tag	UNP R4UMH0
EEE	6	HIS	-	expression tag	UNP R4UMH0
EEE	7	HIS	-	expression tag	UNP R4UMH0
EEE	8	HIS	-	expression tag	UNP R4UMH0
EEE	9	SER	-	expression tag	UNP R4UMH0
EEE	10	SER	-	expression tag	UNP R4UMH0
EEE	11	GLY	-	expression tag	UNP R4UMH0
EEE	12	GLU	-	expression tag	UNP R4UMH0
EEE	13	ASN	-	expression tag	UNP R4UMH0
EEE	14	LEU	-	expression tag	UNP R4UMH0
EEE	15	TYR	-	expression tag	UNP R4UMH0
EEE	16	PHE	-	expression tag	UNP R4UMH0
EEE	17	GLN	-	expression tag	UNP R4UMH0
EEE	18	GLY	-	expression tag	UNP R4UMH0
EEE	19	SER	-	expression tag	UNP R4UMH0
EEE	20	HIS	-	expression tag	UNP R4UMH0
EEE	21	MET	-	expression tag	UNP R4UMH0
EEE	78	SER	CYS	conflict	UNP R4UMH0
EEE	92	SER	CYS	conflict	UNP R4UMH0
FFF	-1	MET	-	initiating methionine	UNP R4UMH0
FFF	0	GLY	-	expression tag	UNP R4UMH0
FFF	1	SER	-	expression tag	UNP R4UMH0
FFF	2	SER	-	expression tag	UNP R4UMH0
FFF	3	HIS	-	expression tag	UNP R4UMH0
FFF	4	HIS	-	expression tag	UNP R4UMH0
FFF	5	HIS	-	expression tag	UNP R4UMH0
FFF	6	HIS	-	expression tag	UNP R4UMH0
FFF	7	HIS	-	expression tag	UNP R4UMH0
FFF	8	HIS	-	expression tag	UNP R4UMH0
FFF	9	SER	-	expression tag	UNP R4UMH0
FFF	10	SER	-	expression tag	UNP R4UMH0

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Chain	Residue	Modelled	Actual	Comment	Reference
FFF	11	GLY	-	expression tag	UNP R4UMH0
FFF	12	GLU	-	expression tag	UNP R4UMH0
FFF	13	ASN	-	expression tag	UNP R4UMH0
FFF	14	LEU	-	expression tag	UNP R4UMH0
FFF	15	TYR	-	expression tag	UNP R4UMH0
FFF	16	PHE	-	expression tag	UNP R4UMH0
FFF	17	GLN	-	expression tag	UNP R4UMH0
FFF	18	GLY	-	expression tag	UNP R4UMH0
FFF	19	SER	-	expression tag	UNP R4UMH0
FFF	20	HIS	-	expression tag	UNP R4UMH0
FFF	21	MET	-	expression tag	UNP R4UMH0
FFF	78	SER	CYS	conflict	UNP R4UMH0
FFF	92	SER	CYS	conflict	UNP R4UMH0
GGG	-1	MET	-	initiating methionine	UNP R4UMH0
GGG	0	GLY	-	expression tag	UNP R4UMH0
GGG	1	SER	-	expression tag	UNP R4UMH0
GGG	2	SER	-	expression tag	UNP R4UMH0
GGG	3	HIS	-	expression tag	UNP R4UMH0
GGG	4	HIS	-	expression tag	UNP R4UMH0
GGG	5	HIS	-	expression tag	UNP R4UMH0
GGG	6	HIS	-	expression tag	UNP R4UMH0
GGG	7	HIS	-	expression tag	UNP R4UMH0
GGG	8	HIS	-	expression tag	UNP R4UMH0
GGG	9	SER	-	expression tag	UNP R4UMH0
GGG	10	SER	-	expression tag	UNP R4UMH0
GGG	11	GLY	-	expression tag	UNP R4UMH0
GGG	12	GLU	-	expression tag	UNP R4UMH0
GGG	13	ASN	-	expression tag	UNP R4UMH0
GGG	14	LEU	-	expression tag	UNP R4UMH0
GGG	15	TYR	-	expression tag	UNP R4UMH0
GGG	16	PHE	-	expression tag	UNP R4UMH0
GGG	17	GLN	-	expression tag	UNP R4UMH0
GGG	18	GLY	-	expression tag	UNP R4UMH0
GGG	19	SER	-	expression tag	UNP R4UMH0
GGG	20	HIS	-	expression tag	UNP R4UMH0
GGG	21	MET	-	expression tag	UNP R4UMH0
GGG	78	SER	CYS	conflict	UNP R4UMH0
GGG	92	SER	CYS	conflict	UNP R4UMH0
HHH	-1	MET	-	initiating methionine	UNP R4UMH0
HHH	0	GLY	-	expression tag	UNP R4UMH0
HHH	1	SER	-	expression tag	UNP R4UMH0
HHH	2	SER	-	expression tag	UNP R4UMH0

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Chain	Residue	Modelled	Actual	Comment	Reference
HHH	3	HIS	-	expression tag	UNP R4UMH0
HHH	4	HIS	-	expression tag	UNP R4UMH0
HHH	5	HIS	-	expression tag	UNP R4UMH0
HHH	6	HIS	-	expression tag	UNP R4UMH0
HHH	7	HIS	-	expression tag	UNP R4UMH0
HHH	8	HIS	-	expression tag	UNP R4UMH0
HHH	9	SER	-	expression tag	UNP R4UMH0
HHH	10	SER	-	expression tag	UNP R4UMH0
HHH	11	GLY	-	expression tag	UNP R4UMH0
HHH	12	GLU	-	expression tag	UNP R4UMH0
HHH	13	ASN	-	expression tag	UNP R4UMH0
HHH	14	LEU	-	expression tag	UNP R4UMH0
HHH	15	TYR	-	expression tag	UNP R4UMH0
HHH	16	PHE	-	expression tag	UNP R4UMH0
HHH	17	GLN	-	expression tag	UNP R4UMH0
HHH	18	GLY	-	expression tag	UNP R4UMH0
HHH	19	SER	-	expression tag	UNP R4UMH0
HHH	20	HIS	-	expression tag	UNP R4UMH0
HHH	21	MET	-	expression tag	UNP R4UMH0
HHH	78	SER	CYS	conflict	UNP R4UMH0
HHH	92	SER	CYS	conflict	UNP R4UMH0
III	-1	MET	-	initiating methionine	UNP R4UMH0
III	0	GLY	-	expression tag	UNP R4UMH0
III	1	SER	-	expression tag	UNP R4UMH0
III	2	SER	-	expression tag	UNP R4UMH0
III	3	HIS	-	expression tag	UNP R4UMH0
III	4	HIS	-	expression tag	UNP R4UMH0
III	5	HIS	-	expression tag	UNP R4UMH0
III	6	HIS	-	expression tag	UNP R4UMH0
III	7	HIS	-	expression tag	UNP R4UMH0
III	8	HIS	-	expression tag	UNP R4UMH0
III	9	SER	-	expression tag	UNP R4UMH0
III	10	SER	-	expression tag	UNP R4UMH0
III	11	GLY	-	expression tag	UNP R4UMH0
III	12	GLU	-	expression tag	UNP R4UMH0
III	13	ASN	-	expression tag	UNP R4UMH0
III	14	LEU	-	expression tag	UNP R4UMH0
III	15	TYR	-	expression tag	UNP R4UMH0
III	16	PHE	-	expression tag	UNP R4UMH0
III	17	GLN	-	expression tag	UNP R4UMH0
III	18	GLY	-	expression tag	UNP R4UMH0
III	19	SER	-	expression tag	UNP R4UMH0

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Chain	Residue	Modelled	Actual	Comment	Reference
III	20	HIS	-	expression tag	UNP R4UMH0
III	21	MET	-	expression tag	UNP R4UMH0
III	78	SER	CYS	conflict	UNP R4UMH0
III	92	SER	CYS	conflict	UNP R4UMH0
JJJ	-1	MET	-	initiating methionine	UNP R4UMH0
JJJ	0	GLY	-	expression tag	UNP R4UMH0
JJJ	1	SER	-	expression tag	UNP R4UMH0
JJJ	2	SER	-	expression tag	UNP R4UMH0
JJJ	3	HIS	-	expression tag	UNP R4UMH0
JJJ	4	HIS	-	expression tag	UNP R4UMH0
JJJ	5	HIS	-	expression tag	UNP R4UMH0
JJJ	6	HIS	-	expression tag	UNP R4UMH0
JJJ	7	HIS	-	expression tag	UNP R4UMH0
JJJ	8	HIS	-	expression tag	UNP R4UMH0
JJJ	9	SER	-	expression tag	UNP R4UMH0
JJJ	10	SER	-	expression tag	UNP R4UMH0
JJJ	11	GLY	-	expression tag	UNP R4UMH0
JJJ	12	GLU	-	expression tag	UNP R4UMH0
JJJ	13	ASN	-	expression tag	UNP R4UMH0
JJJ	14	LEU	-	expression tag	UNP R4UMH0
JJJ	15	TYR	-	expression tag	UNP R4UMH0
JJJ	16	PHE	-	expression tag	UNP R4UMH0
JJJ	17	GLN	-	expression tag	UNP R4UMH0
JJJ	18	GLY	-	expression tag	UNP R4UMH0
JJJ	19	SER	-	expression tag	UNP R4UMH0
JJJ	20	HIS	-	expression tag	UNP R4UMH0
JJJ	21	MET	-	expression tag	UNP R4UMH0
JJJ	78	SER	CYS	conflict	UNP R4UMH0
JJJ	92	SER	CYS	conflict	UNP R4UMH0
KKK	-1	MET	-	initiating methionine	UNP R4UMH0
KKK	0	GLY	-	expression tag	UNP R4UMH0
KKK	1	SER	-	expression tag	UNP R4UMH0
KKK	2	SER	-	expression tag	UNP R4UMH0
KKK	3	HIS	-	expression tag	UNP R4UMH0
KKK	4	HIS	-	expression tag	UNP R4UMH0
KKK	5	HIS	-	expression tag	UNP R4UMH0
KKK	6	HIS	-	expression tag	UNP R4UMH0
KKK	7	HIS	-	expression tag	UNP R4UMH0
KKK	8	HIS	-	expression tag	UNP R4UMH0
KKK	9	SER	-	expression tag	UNP R4UMH0
KKK	10	SER	-	expression tag	UNP R4UMH0
KKK	11	GLY	-	expression tag	UNP R4UMH0

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Chain	Residue	Modelled	Actual	Comment	Reference
KKK	12	GLU	-	expression tag	UNP R4UMH0
KKK	13	ASN	-	expression tag	UNP R4UMH0
KKK	14	LEU	-	expression tag	UNP R4UMH0
KKK	15	TYR	-	expression tag	UNP R4UMH0
KKK	16	PHE	-	expression tag	UNP R4UMH0
KKK	17	GLN	-	expression tag	UNP R4UMH0
KKK	18	GLY	-	expression tag	UNP R4UMH0
KKK	19	SER	-	expression tag	UNP R4UMH0
KKK	20	HIS	-	expression tag	UNP R4UMH0
KKK	21	MET	-	expression tag	UNP R4UMH0
KKK	78	SER	CYS	conflict	UNP R4UMH0
KKK	92	SER	CYS	conflict	UNP R4UMH0
LLL	-1	MET	-	initiating methionine	UNP R4UMH0
LLL	0	GLY	-	expression tag	UNP R4UMH0
LLL	1	SER	-	expression tag	UNP R4UMH0
LLL	2	SER	-	expression tag	UNP R4UMH0
LLL	3	HIS	-	expression tag	UNP R4UMH0
LLL	4	HIS	-	expression tag	UNP R4UMH0
LLL	5	HIS	-	expression tag	UNP R4UMH0
LLL	6	HIS	-	expression tag	UNP R4UMH0
LLL	7	HIS	-	expression tag	UNP R4UMH0
LLL	8	HIS	-	expression tag	UNP R4UMH0
LLL	9	SER	-	expression tag	UNP R4UMH0
LLL	10	SER	-	expression tag	UNP R4UMH0
LLL	11	GLY	-	expression tag	UNP R4UMH0
LLL	12	GLU	-	expression tag	UNP R4UMH0
LLL	13	ASN	-	expression tag	UNP R4UMH0
LLL	14	LEU	-	expression tag	UNP R4UMH0
LLL	15	TYR	-	expression tag	UNP R4UMH0
LLL	16	PHE	-	expression tag	UNP R4UMH0
LLL	17	GLN	-	expression tag	UNP R4UMH0
LLL	18	GLY	-	expression tag	UNP R4UMH0
LLL	19	SER	-	expression tag	UNP R4UMH0
LLL	20	HIS	-	expression tag	UNP R4UMH0
LLL	21	MET	-	expression tag	UNP R4UMH0
LLL	78	SER	CYS	conflict	UNP R4UMH0
LLL	92	SER	CYS	conflict	UNP R4UMH0
MMM	-1	MET	-	initiating methionine	UNP R4UMH0
MMM	0	GLY	-	expression tag	UNP R4UMH0
MMM	1	SER	-	expression tag	UNP R4UMH0
MMM	2	SER	-	expression tag	UNP R4UMH0
MMM	3	HIS	-	expression tag	UNP R4UMH0

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Chain	Residue	Modelled	Actual	Comment	Reference
MMM	4	HIS	-	expression tag	UNP R4UMH0
MMM	5	HIS	-	expression tag	UNP R4UMH0
MMM	6	HIS	-	expression tag	UNP R4UMH0
MMM	7	HIS	-	expression tag	UNP R4UMH0
MMM	8	HIS	-	expression tag	UNP R4UMH0
MMM	9	SER	-	expression tag	UNP R4UMH0
MMM	10	SER	-	expression tag	UNP R4UMH0
MMM	11	GLY	-	expression tag	UNP R4UMH0
MMM	12	GLU	-	expression tag	UNP R4UMH0
MMM	13	ASN	-	expression tag	UNP R4UMH0
MMM	14	LEU	-	expression tag	UNP R4UMH0
MMM	15	TYR	-	expression tag	UNP R4UMH0
MMM	16	PHE	-	expression tag	UNP R4UMH0
MMM	17	GLN	-	expression tag	UNP R4UMH0
MMM	18	GLY	-	expression tag	UNP R4UMH0
MMM	19	SER	-	expression tag	UNP R4UMH0
MMM	20	HIS	-	expression tag	UNP R4UMH0
MMM	21	MET	-	expression tag	UNP R4UMH0
MMM	78	SER	CYS	conflict	UNP R4UMH0
MMM	92	SER	CYS	conflict	UNP R4UMH0
NNN	-1	MET	-	initiating methionine	UNP R4UMH0
NNN	0	GLY	-	expression tag	UNP R4UMH0
NNN	1	SER	-	expression tag	UNP R4UMH0
NNN	2	SER	-	expression tag	UNP R4UMH0
NNN	3	HIS	-	expression tag	UNP R4UMH0
NNN	4	HIS	-	expression tag	UNP R4UMH0
NNN	5	HIS	-	expression tag	UNP R4UMH0
NNN	6	HIS	-	expression tag	UNP R4UMH0
NNN	7	HIS	-	expression tag	UNP R4UMH0
NNN	8	HIS	-	expression tag	UNP R4UMH0
NNN	9	SER	-	expression tag	UNP R4UMH0
NNN	10	SER	-	expression tag	UNP R4UMH0
NNN	11	GLY	-	expression tag	UNP R4UMH0
NNN	12	GLU	-	expression tag	UNP R4UMH0
NNN	13	ASN	-	expression tag	UNP R4UMH0
NNN	14	LEU	-	expression tag	UNP R4UMH0
NNN	15	TYR	-	expression tag	UNP R4UMH0
NNN	16	PHE	-	expression tag	UNP R4UMH0
NNN	17	GLN	-	expression tag	UNP R4UMH0
NNN	18	GLY	-	expression tag	UNP R4UMH0
NNN	19	SER	-	expression tag	UNP R4UMH0
NNN	20	HIS	-	expression tag	UNP R4UMH0

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Chain	Residue	Modelled	Actual	Comment	Reference
NNN	21	MET	-	expression tag	UNP R4UMH0
NNN	78	SER	CYS	conflict	UNP R4UMH0
NNN	92	SER	CYS	conflict	UNP R4UMH0
OOO	-1	MET	-	initiating methionine	UNP R4UMH0
OOO	0	GLY	-	expression tag	UNP R4UMH0
OOO	1	SER	-	expression tag	UNP R4UMH0
OOO	2	SER	-	expression tag	UNP R4UMH0
OOO	3	HIS	-	expression tag	UNP R4UMH0
OOO	4	HIS	-	expression tag	UNP R4UMH0
OOO	5	HIS	-	expression tag	UNP R4UMH0
OOO	6	HIS	-	expression tag	UNP R4UMH0
OOO	7	HIS	-	expression tag	UNP R4UMH0
OOO	8	HIS	-	expression tag	UNP R4UMH0
OOO	9	SER	-	expression tag	UNP R4UMH0
OOO	10	SER	-	expression tag	UNP R4UMH0
OOO	11	GLY	-	expression tag	UNP R4UMH0
OOO	12	GLU	-	expression tag	UNP R4UMH0
OOO	13	ASN	-	expression tag	UNP R4UMH0
OOO	14	LEU	-	expression tag	UNP R4UMH0
OOO	15	TYR	-	expression tag	UNP R4UMH0
OOO	16	PHE	-	expression tag	UNP R4UMH0
OOO	17	GLN	-	expression tag	UNP R4UMH0
OOO	18	GLY	-	expression tag	UNP R4UMH0
OOO	19	SER	-	expression tag	UNP R4UMH0
OOO	20	HIS	-	expression tag	UNP R4UMH0
OOO	21	MET	-	expression tag	UNP R4UMH0
OOO	78	SER	CYS	conflict	UNP R4UMH0
OOO	92	SER	CYS	conflict	UNP R4UMH0
PPP	-1	MET	-	initiating methionine	UNP R4UMH0
PPP	0	GLY	-	expression tag	UNP R4UMH0
PPP	1	SER	-	expression tag	UNP R4UMH0
PPP	2	SER	-	expression tag	UNP R4UMH0
PPP	3	HIS	-	expression tag	UNP R4UMH0
PPP	4	HIS	-	expression tag	UNP R4UMH0
PPP	5	HIS	-	expression tag	UNP R4UMH0
PPP	6	HIS	-	expression tag	UNP R4UMH0
PPP	7	HIS	-	expression tag	UNP R4UMH0
PPP	8	HIS	-	expression tag	UNP R4UMH0
PPP	9	SER	-	expression tag	UNP R4UMH0
PPP	10	SER	-	expression tag	UNP R4UMH0
PPP	11	GLY	-	expression tag	UNP R4UMH0
PPP	12	GLU	-	expression tag	UNP R4UMH0

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Chain	Residue	Modelled	Actual	Comment	Reference
PPP	13	ASN	-	expression tag	UNP R4UMH0
PPP	14	LEU	-	expression tag	UNP R4UMH0
PPP	15	TYR	-	expression tag	UNP R4UMH0
PPP	16	PHE	-	expression tag	UNP R4UMH0
PPP	17	GLN	-	expression tag	UNP R4UMH0
PPP	18	GLY	-	expression tag	UNP R4UMH0
PPP	19	SER	-	expression tag	UNP R4UMH0
PPP	20	HIS	-	expression tag	UNP R4UMH0
PPP	21	MET	-	expression tag	UNP R4UMH0
PPP	78	SER	CYS	conflict	UNP R4UMH0
PPP	92	SER	CYS	conflict	UNP R4UMH0
QQQ	-1	MET	-	initiating methionine	UNP R4UMH0
QQQ	0	GLY	-	expression tag	UNP R4UMH0
QQQ	1	SER	-	expression tag	UNP R4UMH0
QQQ	2	SER	-	expression tag	UNP R4UMH0
QQQ	3	HIS	-	expression tag	UNP R4UMH0
QQQ	4	HIS	-	expression tag	UNP R4UMH0
QQQ	5	HIS	-	expression tag	UNP R4UMH0
QQQ	6	HIS	-	expression tag	UNP R4UMH0
QQQ	7	HIS	-	expression tag	UNP R4UMH0
QQQ	8	HIS	-	expression tag	UNP R4UMH0
QQQ	9	SER	-	expression tag	UNP R4UMH0
QQQ	10	SER	-	expression tag	UNP R4UMH0
QQQ	11	GLY	-	expression tag	UNP R4UMH0
QQQ	12	GLU	-	expression tag	UNP R4UMH0
QQQ	13	ASN	-	expression tag	UNP R4UMH0
QQQ	14	LEU	-	expression tag	UNP R4UMH0
QQQ	15	TYR	-	expression tag	UNP R4UMH0
QQQ	16	PHE	-	expression tag	UNP R4UMH0
QQQ	17	GLN	-	expression tag	UNP R4UMH0
QQQ	18	GLY	-	expression tag	UNP R4UMH0
QQQ	19	SER	-	expression tag	UNP R4UMH0
QQQ	20	HIS	-	expression tag	UNP R4UMH0
QQQ	21	MET	-	expression tag	UNP R4UMH0
QQQ	78	SER	CYS	conflict	UNP R4UMH0
QQQ	92	SER	CYS	conflict	UNP R4UMH0
RRR	-1	MET	-	initiating methionine	UNP R4UMH0
RRR	0	GLY	-	expression tag	UNP R4UMH0
RRR	1	SER	-	expression tag	UNP R4UMH0
RRR	2	SER	-	expression tag	UNP R4UMH0
RRR	3	HIS	-	expression tag	UNP R4UMH0
RRR	4	HIS	-	expression tag	UNP R4UMH0

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Chain	Residue	Modelled	Actual	Comment	Reference
RRR	5	HIS	-	expression tag	UNP R4UMH0
RRR	6	HIS	-	expression tag	UNP R4UMH0
RRR	7	HIS	-	expression tag	UNP R4UMH0
RRR	8	HIS	-	expression tag	UNP R4UMH0
RRR	9	SER	-	expression tag	UNP R4UMH0
RRR	10	SER	-	expression tag	UNP R4UMH0
RRR	11	GLY	-	expression tag	UNP R4UMH0
RRR	12	GLU	-	expression tag	UNP R4UMH0
RRR	13	ASN	-	expression tag	UNP R4UMH0
RRR	14	LEU	-	expression tag	UNP R4UMH0
RRR	15	TYR	-	expression tag	UNP R4UMH0
RRR	16	PHE	-	expression tag	UNP R4UMH0
RRR	17	GLN	-	expression tag	UNP R4UMH0
RRR	18	GLY	-	expression tag	UNP R4UMH0
RRR	19	SER	-	expression tag	UNP R4UMH0
RRR	20	HIS	-	expression tag	UNP R4UMH0
RRR	21	MET	-	expression tag	UNP R4UMH0
RRR	78	SER	CYS	conflict	UNP R4UMH0
RRR	92	SER	CYS	conflict	UNP R4UMH0
SSS	-1	MET	-	initiating methionine	UNP R4UMH0
SSS	0	GLY	-	expression tag	UNP R4UMH0
SSS	1	SER	-	expression tag	UNP R4UMH0
SSS	2	SER	-	expression tag	UNP R4UMH0
SSS	3	HIS	-	expression tag	UNP R4UMH0
SSS	4	HIS	-	expression tag	UNP R4UMH0
SSS	5	HIS	-	expression tag	UNP R4UMH0
SSS	6	HIS	-	expression tag	UNP R4UMH0
SSS	7	HIS	-	expression tag	UNP R4UMH0
SSS	8	HIS	-	expression tag	UNP R4UMH0
SSS	9	SER	-	expression tag	UNP R4UMH0
SSS	10	SER	-	expression tag	UNP R4UMH0
SSS	11	GLY	-	expression tag	UNP R4UMH0
SSS	12	GLU	-	expression tag	UNP R4UMH0
SSS	13	ASN	-	expression tag	UNP R4UMH0
SSS	14	LEU	-	expression tag	UNP R4UMH0
SSS	15	TYR	-	expression tag	UNP R4UMH0
SSS	16	PHE	-	expression tag	UNP R4UMH0
SSS	17	GLN	-	expression tag	UNP R4UMH0
SSS	18	GLY	-	expression tag	UNP R4UMH0
SSS	19	SER	-	expression tag	UNP R4UMH0
SSS	20	HIS	-	expression tag	UNP R4UMH0
SSS	21	MET	-	expression tag	UNP R4UMH0

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Chain	Residue	Modelled	Actual	Comment	Reference
SSS	78	SER	CYS	conflict	UNP R4UMH0
SSS	92	SER	CYS	conflict	UNP R4UMH0
TTT	-1	MET	-	initiating methionine	UNP R4UMH0
TTT	0	GLY	-	expression tag	UNP R4UMH0
TTT	1	SER	-	expression tag	UNP R4UMH0
TTT	2	SER	-	expression tag	UNP R4UMH0
TTT	3	HIS	-	expression tag	UNP R4UMH0
TTT	4	HIS	-	expression tag	UNP R4UMH0
TTT	5	HIS	-	expression tag	UNP R4UMH0
TTT	6	HIS	-	expression tag	UNP R4UMH0
TTT	7	HIS	-	expression tag	UNP R4UMH0
TTT	8	HIS	-	expression tag	UNP R4UMH0
TTT	9	SER	-	expression tag	UNP R4UMH0
TTT	10	SER	-	expression tag	UNP R4UMH0
TTT	11	GLY	-	expression tag	UNP R4UMH0
TTT	12	GLU	-	expression tag	UNP R4UMH0
TTT	13	ASN	-	expression tag	UNP R4UMH0
TTT	14	LEU	-	expression tag	UNP R4UMH0
TTT	15	TYR	-	expression tag	UNP R4UMH0
TTT	16	PHE	-	expression tag	UNP R4UMH0
TTT	17	GLN	-	expression tag	UNP R4UMH0
TTT	18	GLY	-	expression tag	UNP R4UMH0
TTT	19	SER	-	expression tag	UNP R4UMH0
TTT	20	HIS	-	expression tag	UNP R4UMH0
TTT	21	MET	-	expression tag	UNP R4UMH0
TTT	78	SER	CYS	conflict	UNP R4UMH0
TTT	92	SER	CYS	conflict	UNP R4UMH0
UUU	-1	MET	-	initiating methionine	UNP R4UMH0
UUU	0	GLY	-	expression tag	UNP R4UMH0
UUU	1	SER	-	expression tag	UNP R4UMH0
UUU	2	SER	-	expression tag	UNP R4UMH0
UUU	3	HIS	-	expression tag	UNP R4UMH0
UUU	4	HIS	-	expression tag	UNP R4UMH0
UUU	5	HIS	-	expression tag	UNP R4UMH0
UUU	6	HIS	-	expression tag	UNP R4UMH0
UUU	7	HIS	-	expression tag	UNP R4UMH0
UUU	8	HIS	-	expression tag	UNP R4UMH0
UUU	9	SER	-	expression tag	UNP R4UMH0
UUU	10	SER	-	expression tag	UNP R4UMH0
UUU	11	GLY	-	expression tag	UNP R4UMH0
UUU	12	GLU	-	expression tag	UNP R4UMH0
UUU	13	ASN	-	expression tag	UNP R4UMH0

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Chain	Residue	Modelled	Actual	Comment	Reference
UUU	14	LEU	-	expression tag	UNP R4UMH0
UUU	15	TYR	-	expression tag	UNP R4UMH0
UUU	16	PHE	-	expression tag	UNP R4UMH0
UUU	17	GLN	-	expression tag	UNP R4UMH0
UUU	18	GLY	-	expression tag	UNP R4UMH0
UUU	19	SER	-	expression tag	UNP R4UMH0
UUU	20	HIS	-	expression tag	UNP R4UMH0
UUU	21	MET	-	expression tag	UNP R4UMH0
UUU	78	SER	CYS	conflict	UNP R4UMH0
UUU	92	SER	CYS	conflict	UNP R4UMH0
VVV	-1	MET	-	initiating methionine	UNP R4UMH0
VVV	0	GLY	-	expression tag	UNP R4UMH0
VVV	1	SER	-	expression tag	UNP R4UMH0
VVV	2	SER	-	expression tag	UNP R4UMH0
VVV	3	HIS	-	expression tag	UNP R4UMH0
VVV	4	HIS	-	expression tag	UNP R4UMH0
VVV	5	HIS	-	expression tag	UNP R4UMH0
VVV	6	HIS	-	expression tag	UNP R4UMH0
VVV	7	HIS	-	expression tag	UNP R4UMH0
VVV	8	HIS	-	expression tag	UNP R4UMH0
VVV	9	SER	-	expression tag	UNP R4UMH0
VVV	10	SER	-	expression tag	UNP R4UMH0
VVV	11	GLY	-	expression tag	UNP R4UMH0
VVV	12	GLU	-	expression tag	UNP R4UMH0
VVV	13	ASN	-	expression tag	UNP R4UMH0
VVV	14	LEU	-	expression tag	UNP R4UMH0
VVV	15	TYR	-	expression tag	UNP R4UMH0
VVV	16	PHE	-	expression tag	UNP R4UMH0
VVV	17	GLN	-	expression tag	UNP R4UMH0
VVV	18	GLY	-	expression tag	UNP R4UMH0
VVV	19	SER	-	expression tag	UNP R4UMH0
VVV	20	HIS	-	expression tag	UNP R4UMH0
VVV	21	MET	-	expression tag	UNP R4UMH0
VVV	78	SER	CYS	conflict	UNP R4UMH0
VVV	92	SER	CYS	conflict	UNP R4UMH0
WWW	-1	MET	-	initiating methionine	UNP R4UMH0
WWW	0	GLY	-	expression tag	UNP R4UMH0
WWW	1	SER	-	expression tag	UNP R4UMH0
WWW	2	SER	-	expression tag	UNP R4UMH0
WWW	3	HIS	-	expression tag	UNP R4UMH0
WWW	4	HIS	-	expression tag	UNP R4UMH0
WWW	5	HIS	-	expression tag	UNP R4UMH0

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Chain	Residue	Modelled	Actual	Comment	Reference
WWW	6	HIS	-	expression tag	UNP R4UMH0
WWW	7	HIS	-	expression tag	UNP R4UMH0
WWW	8	HIS	-	expression tag	UNP R4UMH0
WWW	9	SER	-	expression tag	UNP R4UMH0
WWW	10	SER	-	expression tag	UNP R4UMH0
WWW	11	GLY	-	expression tag	UNP R4UMH0
WWW	12	GLU	-	expression tag	UNP R4UMH0
WWW	13	ASN	-	expression tag	UNP R4UMH0
WWW	14	LEU	-	expression tag	UNP R4UMH0
WWW	15	TYR	-	expression tag	UNP R4UMH0
WWW	16	PHE	-	expression tag	UNP R4UMH0
WWW	17	GLN	-	expression tag	UNP R4UMH0
WWW	18	GLY	-	expression tag	UNP R4UMH0
WWW	19	SER	-	expression tag	UNP R4UMH0
WWW	20	HIS	-	expression tag	UNP R4UMH0
WWW	21	MET	-	expression tag	UNP R4UMH0
WWW	78	SER	CYS	conflict	UNP R4UMH0
WWW	92	SER	CYS	conflict	UNP R4UMH0
XXX	-1	MET	-	initiating methionine	UNP R4UMH0
XXX	0	GLY	-	expression tag	UNP R4UMH0
XXX	1	SER	-	expression tag	UNP R4UMH0
XXX	2	SER	-	expression tag	UNP R4UMH0
XXX	3	HIS	-	expression tag	UNP R4UMH0
XXX	4	HIS	-	expression tag	UNP R4UMH0
XXX	5	HIS	-	expression tag	UNP R4UMH0
XXX	6	HIS	-	expression tag	UNP R4UMH0
XXX	7	HIS	-	expression tag	UNP R4UMH0
XXX	8	HIS	-	expression tag	UNP R4UMH0
XXX	9	SER	-	expression tag	UNP R4UMH0
XXX	10	SER	-	expression tag	UNP R4UMH0
XXX	11	GLY	-	expression tag	UNP R4UMH0
XXX	12	GLU	-	expression tag	UNP R4UMH0
XXX	13	ASN	-	expression tag	UNP R4UMH0
XXX	14	LEU	-	expression tag	UNP R4UMH0
XXX	15	TYR	-	expression tag	UNP R4UMH0
XXX	16	PHE	-	expression tag	UNP R4UMH0
XXX	17	GLN	-	expression tag	UNP R4UMH0
XXX	18	GLY	-	expression tag	UNP R4UMH0
XXX	19	SER	-	expression tag	UNP R4UMH0
XXX	20	HIS	-	expression tag	UNP R4UMH0
XXX	21	MET	-	expression tag	UNP R4UMH0
XXX	78	SER	CYS	conflict	UNP R4UMH0

Continued on next page...

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Chain	Residue	Modelled	Actual	Comment	Reference
XXX	92	SER	CYS	conflict	UNP R4UMH0
YYY	-1	MET	-	initiating methionine	UNP R4UMH0
YYY	0	GLY	-	expression tag	UNP R4UMH0
YYY	1	SER	-	expression tag	UNP R4UMH0
YYY	2	SER	-	expression tag	UNP R4UMH0
YYY	3	HIS	-	expression tag	UNP R4UMH0
YYY	4	HIS	-	expression tag	UNP R4UMH0
YYY	5	HIS	-	expression tag	UNP R4UMH0
YYY	6	HIS	-	expression tag	UNP R4UMH0
YYY	7	HIS	-	expression tag	UNP R4UMH0
YYY	8	HIS	-	expression tag	UNP R4UMH0
YYY	9	SER	-	expression tag	UNP R4UMH0
YYY	10	SER	-	expression tag	UNP R4UMH0
YYY	11	GLY	-	expression tag	UNP R4UMH0
YYY	12	GLU	-	expression tag	UNP R4UMH0
YYY	13	ASN	-	expression tag	UNP R4UMH0
YYY	14	LEU	-	expression tag	UNP R4UMH0
YYY	15	TYR	-	expression tag	UNP R4UMH0
YYY	16	PHE	-	expression tag	UNP R4UMH0
YYY	17	GLN	-	expression tag	UNP R4UMH0
YYY	18	GLY	-	expression tag	UNP R4UMH0
YYY	19	SER	-	expression tag	UNP R4UMH0
YYY	20	HIS	-	expression tag	UNP R4UMH0
YYY	21	MET	-	expression tag	UNP R4UMH0
YYY	78	SER	CYS	conflict	UNP R4UMH0
YYY	92	SER	CYS	conflict	UNP R4UMH0
ZZZ	-1	MET	-	initiating methionine	UNP R4UMH0
ZZZ	0	GLY	-	expression tag	UNP R4UMH0
ZZZ	1	SER	-	expression tag	UNP R4UMH0
ZZZ	2	SER	-	expression tag	UNP R4UMH0
ZZZ	3	HIS	-	expression tag	UNP R4UMH0
ZZZ	4	HIS	-	expression tag	UNP R4UMH0
ZZZ	5	HIS	-	expression tag	UNP R4UMH0
ZZZ	6	HIS	-	expression tag	UNP R4UMH0
ZZZ	7	HIS	-	expression tag	UNP R4UMH0
ZZZ	8	HIS	-	expression tag	UNP R4UMH0
ZZZ	9	SER	-	expression tag	UNP R4UMH0
ZZZ	10	SER	-	expression tag	UNP R4UMH0
ZZZ	11	GLY	-	expression tag	UNP R4UMH0
ZZZ	12	GLU	-	expression tag	UNP R4UMH0
ZZZ	13	ASN	-	expression tag	UNP R4UMH0
ZZZ	14	LEU	-	expression tag	UNP R4UMH0

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Chain	Residue	Modelled	Actual	Comment	Reference
ZZZ	15	TYR	-	expression tag	UNP R4UMH0
ZZZ	16	PHE	-	expression tag	UNP R4UMH0
ZZZ	17	GLN	-	expression tag	UNP R4UMH0
ZZZ	18	GLY	-	expression tag	UNP R4UMH0
ZZZ	19	SER	-	expression tag	UNP R4UMH0
ZZZ	20	HIS	-	expression tag	UNP R4UMH0
ZZZ	21	MET	-	expression tag	UNP R4UMH0
ZZZ	78	SER	CYS	conflict	UNP R4UMH0
ZZZ	92	SER	CYS	conflict	UNP R4UMH0
aaa	-1	MET	-	initiating methionine	UNP R4UMH0
aaa	0	GLY	-	expression tag	UNP R4UMH0
aaa	1	SER	-	expression tag	UNP R4UMH0
aaa	2	SER	-	expression tag	UNP R4UMH0
aaa	3	HIS	-	expression tag	UNP R4UMH0
aaa	4	HIS	-	expression tag	UNP R4UMH0
aaa	5	HIS	-	expression tag	UNP R4UMH0
aaa	6	HIS	-	expression tag	UNP R4UMH0
aaa	7	HIS	-	expression tag	UNP R4UMH0
aaa	8	HIS	-	expression tag	UNP R4UMH0
aaa	9	SER	-	expression tag	UNP R4UMH0
aaa	10	SER	-	expression tag	UNP R4UMH0
aaa	11	GLY	-	expression tag	UNP R4UMH0
aaa	12	GLU	-	expression tag	UNP R4UMH0
aaa	13	ASN	-	expression tag	UNP R4UMH0
aaa	14	LEU	-	expression tag	UNP R4UMH0
aaa	15	TYR	-	expression tag	UNP R4UMH0
aaa	16	PHE	-	expression tag	UNP R4UMH0
aaa	17	GLN	-	expression tag	UNP R4UMH0
aaa	18	GLY	-	expression tag	UNP R4UMH0
aaa	19	SER	-	expression tag	UNP R4UMH0
aaa	20	HIS	-	expression tag	UNP R4UMH0
aaa	21	MET	-	expression tag	UNP R4UMH0
aaa	78	SER	CYS	conflict	UNP R4UMH0
aaa	92	SER	CYS	conflict	UNP R4UMH0
bbb	-1	MET	-	initiating methionine	UNP R4UMH0
bbb	0	GLY	-	expression tag	UNP R4UMH0
bbb	1	SER	-	expression tag	UNP R4UMH0
bbb	2	SER	-	expression tag	UNP R4UMH0
bbb	3	HIS	-	expression tag	UNP R4UMH0
bbb	4	HIS	-	expression tag	UNP R4UMH0
bbb	5	HIS	-	expression tag	UNP R4UMH0
bbb	6	HIS	-	expression tag	UNP R4UMH0

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Chain	Residue	Modelled	Actual	Comment	Reference
bbb	7	HIS	-	expression tag	UNP R4UMH0
bbb	8	HIS	-	expression tag	UNP R4UMH0
bbb	9	SER	-	expression tag	UNP R4UMH0
bbb	10	SER	-	expression tag	UNP R4UMH0
bbb	11	GLY	-	expression tag	UNP R4UMH0
bbb	12	GLU	-	expression tag	UNP R4UMH0
bbb	13	ASN	-	expression tag	UNP R4UMH0
bbb	14	LEU	-	expression tag	UNP R4UMH0
bbb	15	TYR	-	expression tag	UNP R4UMH0
bbb	16	PHE	-	expression tag	UNP R4UMH0
bbb	17	GLN	-	expression tag	UNP R4UMH0
bbb	18	GLY	-	expression tag	UNP R4UMH0
bbb	19	SER	-	expression tag	UNP R4UMH0
bbb	20	HIS	-	expression tag	UNP R4UMH0
bbb	21	MET	-	expression tag	UNP R4UMH0
bbb	78	SER	CYS	conflict	UNP R4UMH0
bbb	92	SER	CYS	conflict	UNP R4UMH0
ccc	-1	MET	-	initiating methionine	UNP R4UMH0
ccc	0	GLY	-	expression tag	UNP R4UMH0
ccc	1	SER	-	expression tag	UNP R4UMH0
ccc	2	SER	-	expression tag	UNP R4UMH0
ccc	3	HIS	-	expression tag	UNP R4UMH0
ccc	4	HIS	-	expression tag	UNP R4UMH0
ccc	5	HIS	-	expression tag	UNP R4UMH0
ccc	6	HIS	-	expression tag	UNP R4UMH0
ccc	7	HIS	-	expression tag	UNP R4UMH0
ccc	8	HIS	-	expression tag	UNP R4UMH0
ccc	9	SER	-	expression tag	UNP R4UMH0
ccc	10	SER	-	expression tag	UNP R4UMH0
ccc	11	GLY	-	expression tag	UNP R4UMH0
ccc	12	GLU	-	expression tag	UNP R4UMH0
ccc	13	ASN	-	expression tag	UNP R4UMH0
ccc	14	LEU	-	expression tag	UNP R4UMH0
ccc	15	TYR	-	expression tag	UNP R4UMH0
ccc	16	PHE	-	expression tag	UNP R4UMH0
ccc	17	GLN	-	expression tag	UNP R4UMH0
ccc	18	GLY	-	expression tag	UNP R4UMH0
ccc	19	SER	-	expression tag	UNP R4UMH0
ccc	20	HIS	-	expression tag	UNP R4UMH0
ccc	21	MET	-	expression tag	UNP R4UMH0
ccc	78	SER	CYS	conflict	UNP R4UMH0
ccc	92	SER	CYS	conflict	UNP R4UMH0

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Chain	Residue	Modelled	Actual	Comment	Reference
ddd	-1	MET	-	initiating methionine	UNP R4UMH0
ddd	0	GLY	-	expression tag	UNP R4UMH0
ddd	1	SER	-	expression tag	UNP R4UMH0
ddd	2	SER	-	expression tag	UNP R4UMH0
ddd	3	HIS	-	expression tag	UNP R4UMH0
ddd	4	HIS	-	expression tag	UNP R4UMH0
ddd	5	HIS	-	expression tag	UNP R4UMH0
ddd	6	HIS	-	expression tag	UNP R4UMH0
ddd	7	HIS	-	expression tag	UNP R4UMH0
ddd	8	HIS	-	expression tag	UNP R4UMH0
ddd	9	SER	-	expression tag	UNP R4UMH0
ddd	10	SER	-	expression tag	UNP R4UMH0
ddd	11	GLY	-	expression tag	UNP R4UMH0
ddd	12	GLU	-	expression tag	UNP R4UMH0
ddd	13	ASN	-	expression tag	UNP R4UMH0
ddd	14	LEU	-	expression tag	UNP R4UMH0
ddd	15	TYR	-	expression tag	UNP R4UMH0
ddd	16	PHE	-	expression tag	UNP R4UMH0
ddd	17	GLN	-	expression tag	UNP R4UMH0
ddd	18	GLY	-	expression tag	UNP R4UMH0
ddd	19	SER	-	expression tag	UNP R4UMH0
ddd	20	HIS	-	expression tag	UNP R4UMH0
ddd	21	MET	-	expression tag	UNP R4UMH0
ddd	78	SER	CYS	conflict	UNP R4UMH0
ddd	92	SER	CYS	conflict	UNP R4UMH0

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	AAA	3	Total Cl 3 3	0	0
2	BBB	5	Total Cl 5 5	0	0
2	CCC	3	Total Cl 3 3	0	0
2	DDD	1	Total Cl 1 1	0	0
2	EEE	1	Total Cl 1 1	0	0
2	FFF	3	Total Cl 3 3	0	0
2	GGG	3	Total Cl 3 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	HHH	3	Total 3	Cl 3	0	0
2	III	3	Total 3	Cl 3	0	0
2	JJJ	3	Total 3	Cl 3	0	0
2	KKK	3	Total 3	Cl 3	0	0
2	LLL	5	Total 5	Cl 5	0	0
2	MMM	2	Total 2	Cl 2	0	0
2	NNN	1	Total 1	Cl 1	0	0
2	OOO	4	Total 4	Cl 4	0	0
2	PPP	3	Total 3	Cl 3	0	0
2	QQQ	2	Total 2	Cl 2	0	0
2	RRR	3	Total 3	Cl 3	0	0
2	SSS	1	Total 1	Cl 1	0	0
2	TTT	1	Total 1	Cl 1	0	0
2	UUU	2	Total 2	Cl 2	0	0
2	VVV	1	Total 1	Cl 1	0	0
2	WWW	1	Total 1	Cl 1	0	0
2	XXX	3	Total 3	Cl 3	0	0
2	YYY	2	Total 2	Cl 2	0	0
2	ZZZ	1	Total 1	Cl 1	0	0
2	aaa	2	Total 2	Cl 2	0	0
2	bbb	3	Total 3	Cl 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	ccc	1	Total 1	Cl 1	0	0
2	ddd	2	Total 2	Cl 2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	AAA	32	Total 32	O 32	0	0
3	BBB	36	Total 36	O 36	0	0
3	CCC	37	Total 37	O 37	0	0
3	DDD	33	Total 33	O 33	0	0
3	EEE	30	Total 30	O 30	0	0
3	FFF	22	Total 22	O 22	0	0
3	GGG	34	Total 34	O 34	0	0
3	HHH	44	Total 44	O 44	0	0
3	III	44	Total 44	O 44	0	0
3	JJJ	30	Total 30	O 30	0	0
3	KKK	35	Total 35	O 35	0	0
3	LLL	20	Total 20	O 20	0	0
3	MMM	20	Total 20	O 20	0	0
3	NNN	17	Total 17	O 17	0	0
3	OOO	19	Total 19	O 19	0	0
3	PPP	33	Total 33	O 33	0	0
3	QQQ	34	Total 34	O 34	0	0

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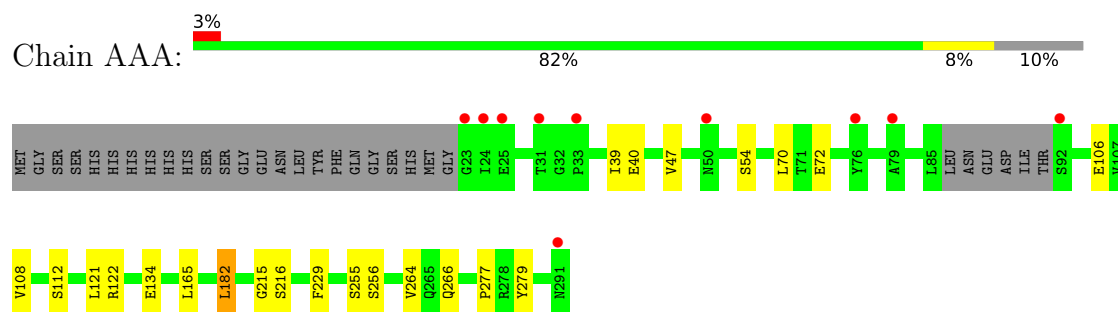
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	RRR	23	Total 23	O 23	0	0
3	SSS	9	Total 9	O 9	0	0
3	TTT	25	Total 25	O 25	0	0
3	UUU	19	Total 19	O 19	0	0
3	VVV	9	Total 9	O 9	0	0
3	WWW	13	Total 13	O 13	0	0
3	XXX	18	Total 18	O 18	0	0
3	YYY	24	Total 24	O 24	0	0
3	ZZZ	15	Total 15	O 15	0	0
3	aaa	27	Total 27	O 27	0	0
3	bbb	21	Total 21	O 21	0	0
3	ccc	9	Total 9	O 9	0	0
3	ddd	19	Total 19	O 19	0	0

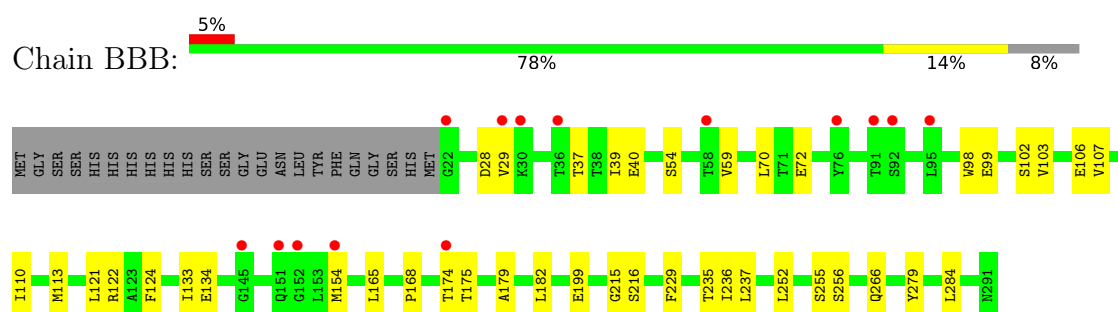
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

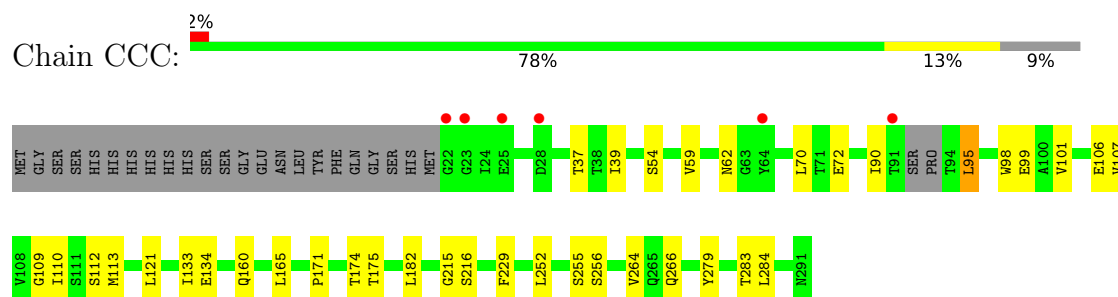
- Molecule 1: Capsid protein VP1



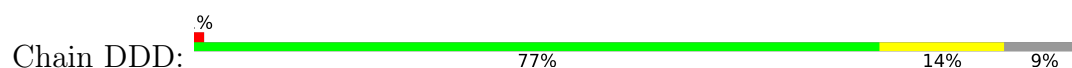
- Molecule 1: Capsid protein VP1

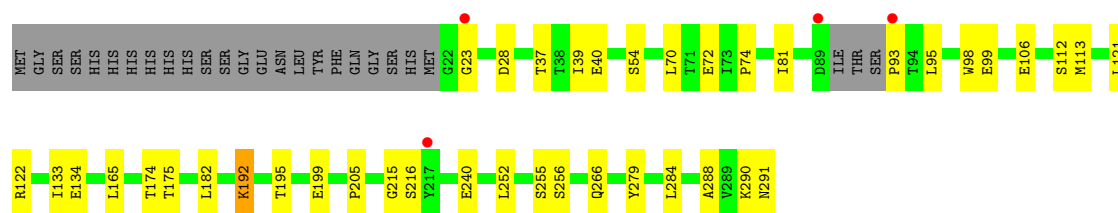


- Molecule 1: Capsid protein VP1

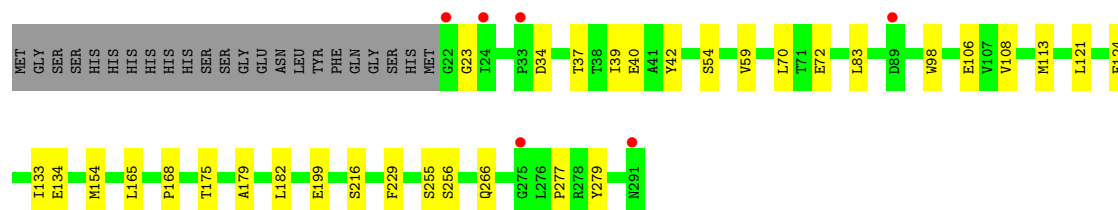
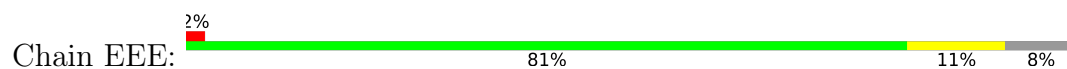


- Molecule 1: Capsid protein VP1

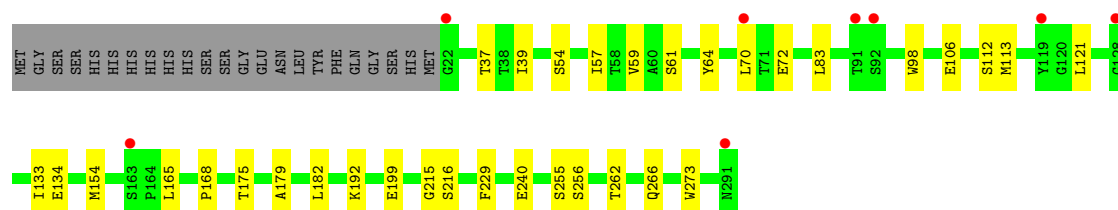
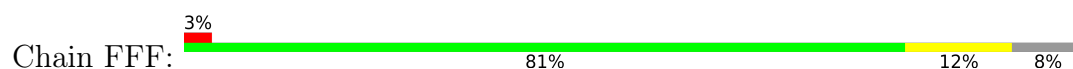




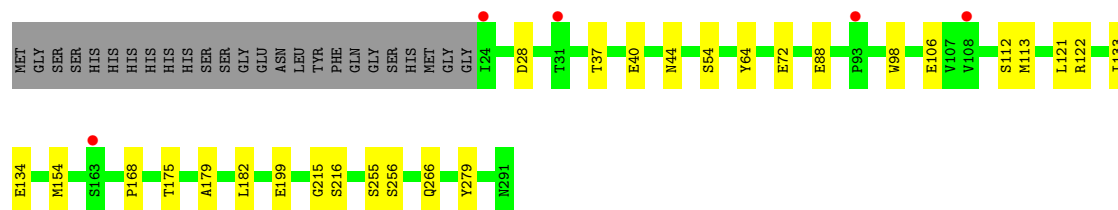
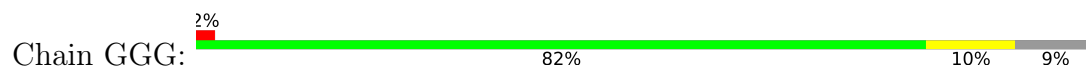
• Molecule 1: Capsid protein VP1



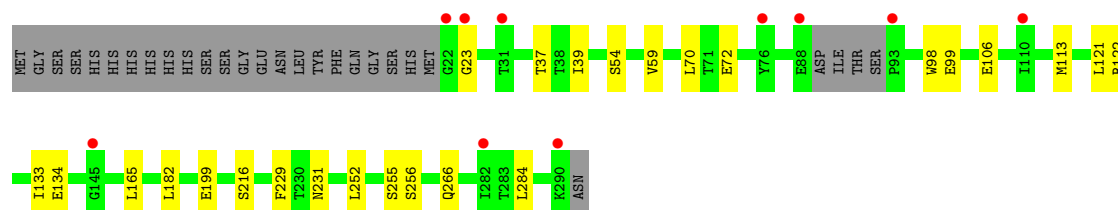
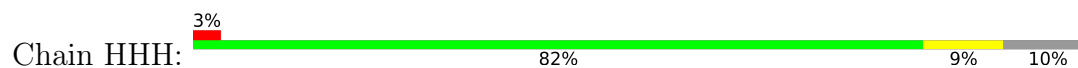
• Molecule 1: Capsid protein VP1



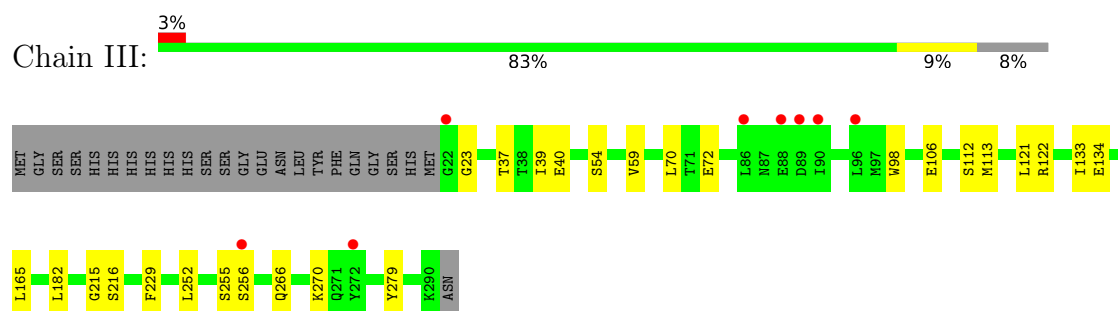
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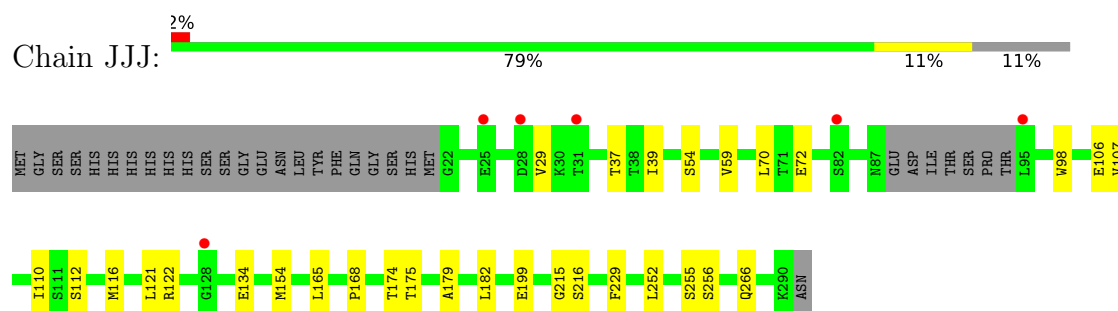
• Molecule 1: Capsid protein VP1



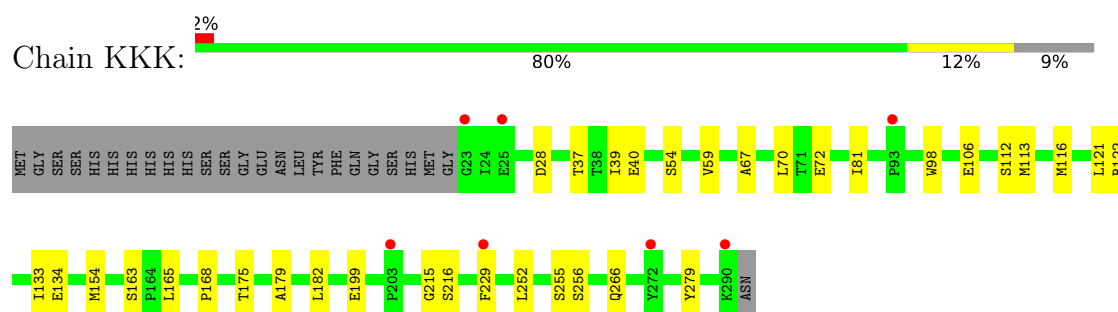
● Molecule 1: Capsid protein VP1



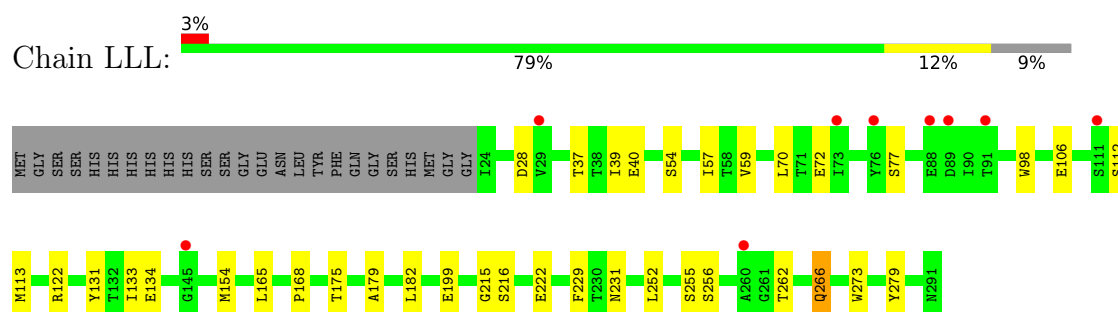
● Molecule 1: Capsid protein VP1



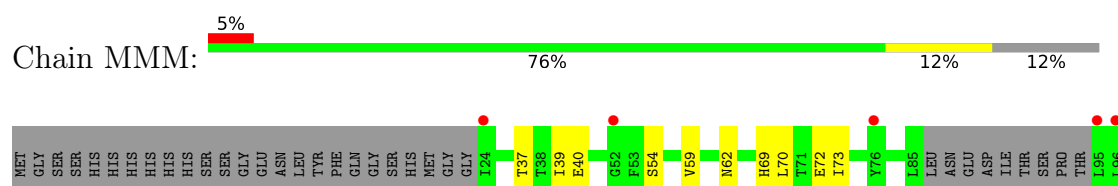
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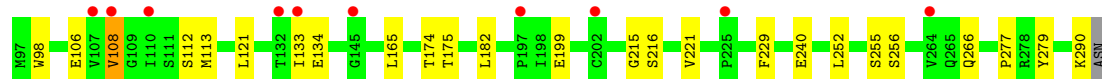


● Molecule 1: Capsid protein VP1

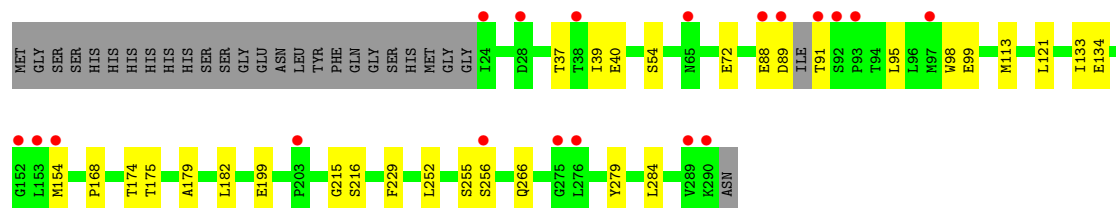
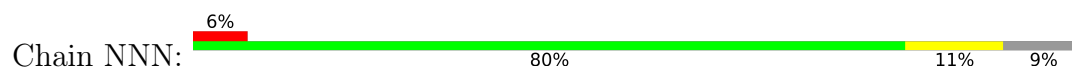


● Molecule 1: Capsid protein VP1

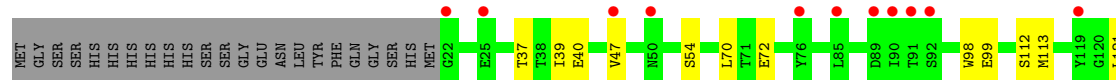
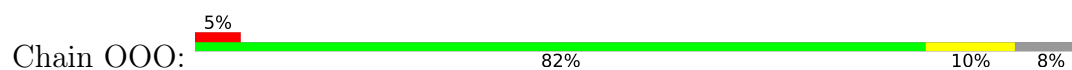




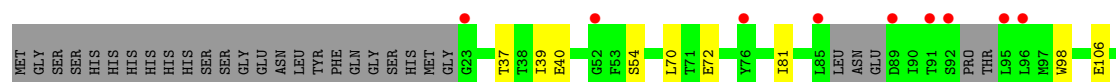
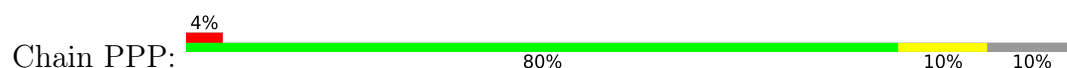
- Molecule 1: Capsid protein VP1



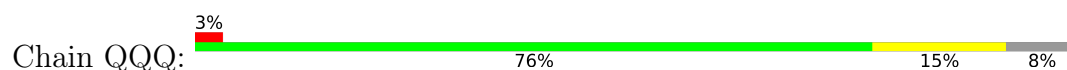
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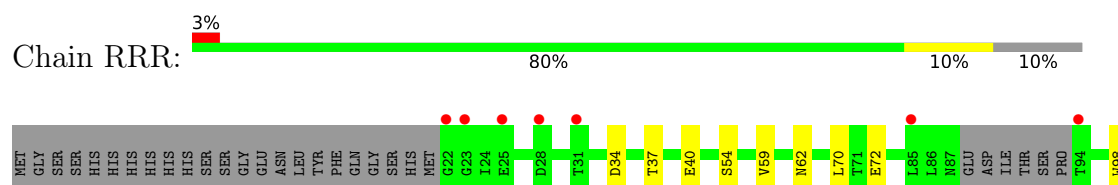
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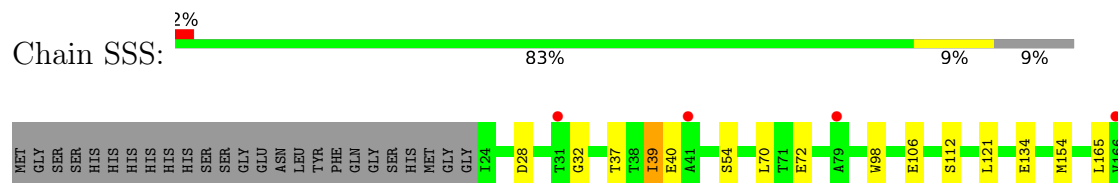
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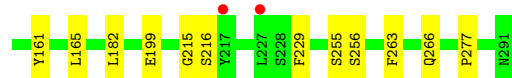
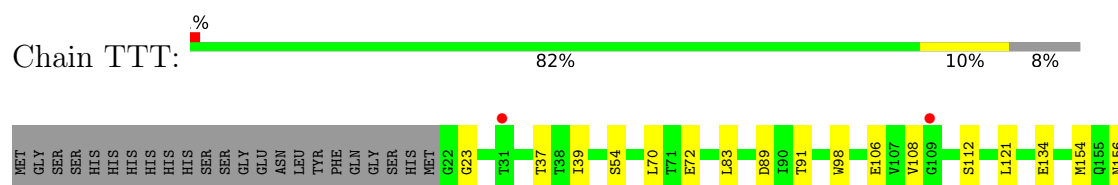
- Molecule 1: Capsid protein VP1



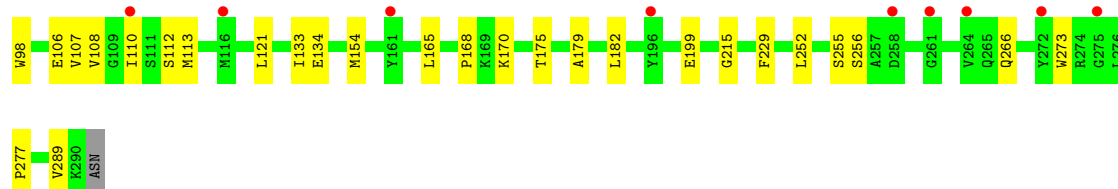
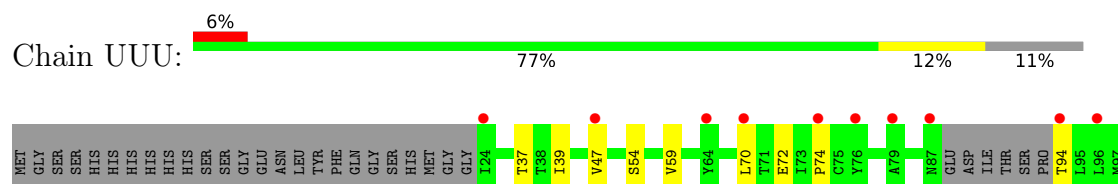
- Molecule 1: Capsid protein VP1



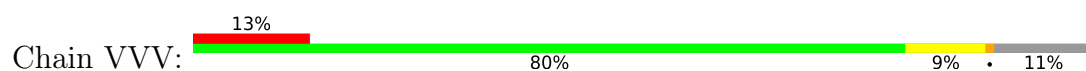
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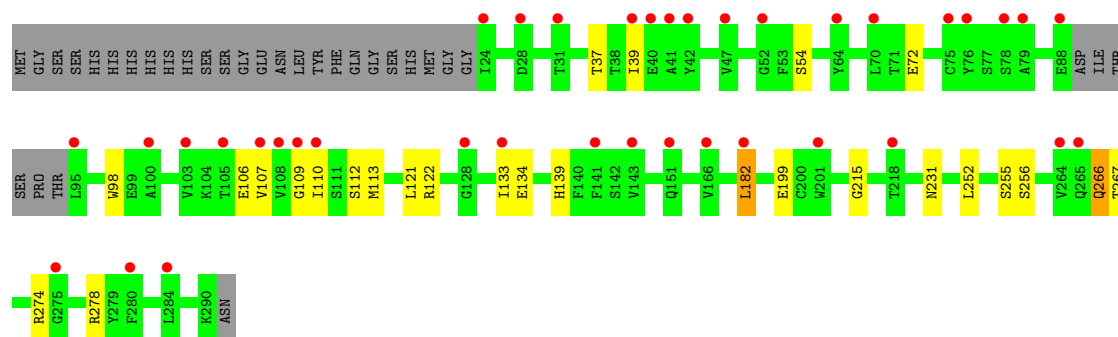


- Molecule 1: Capsid protein VP1

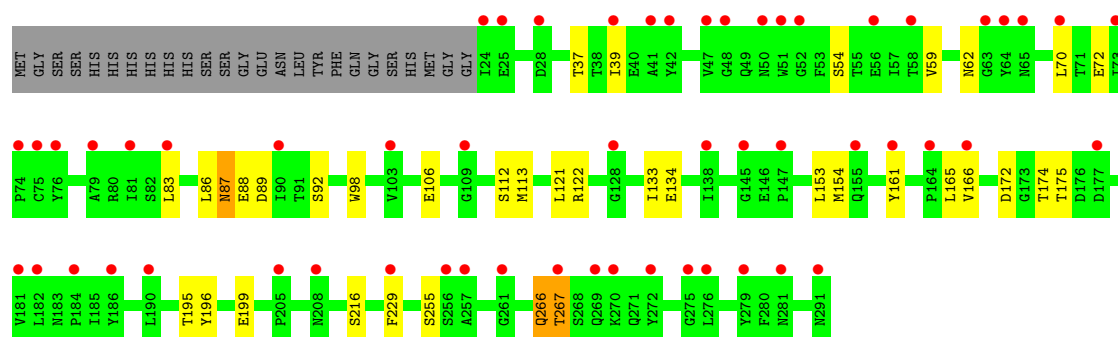
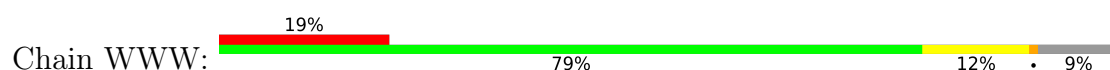


- Molecule 1: Capsid protein VP1

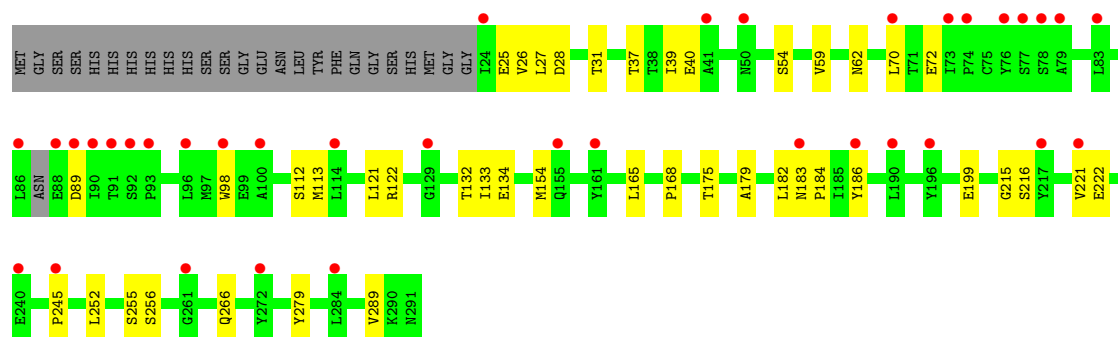
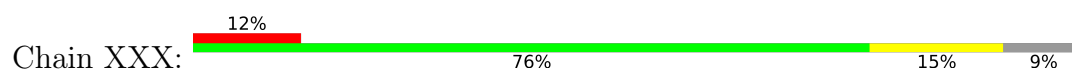




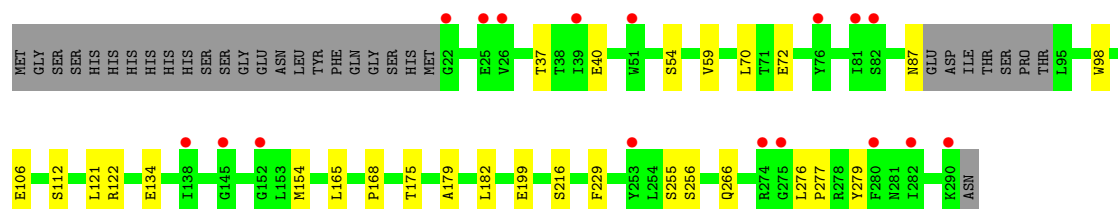
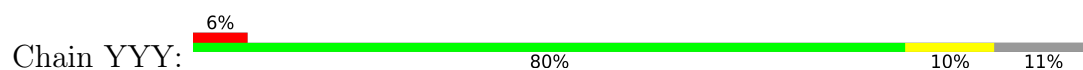
• Molecule 1: Capsid protein VP1



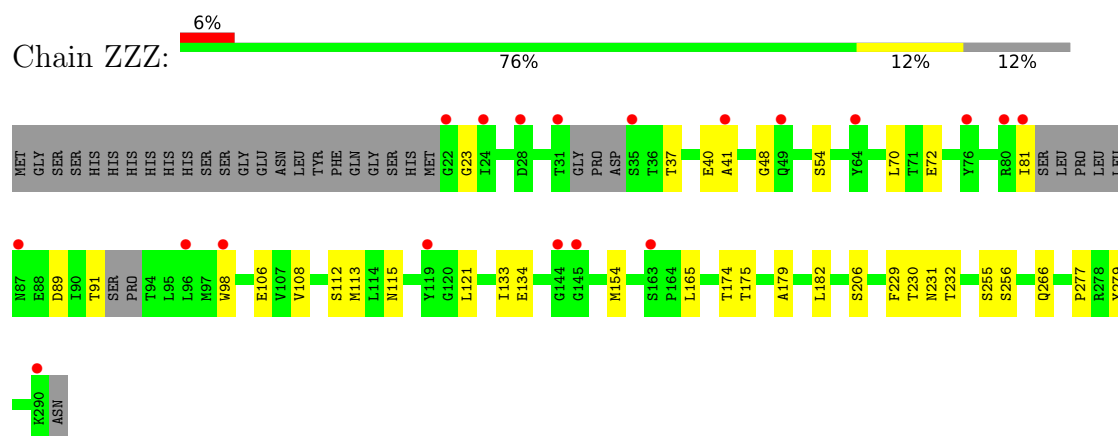
• Molecule 1: Capsid protein VP1



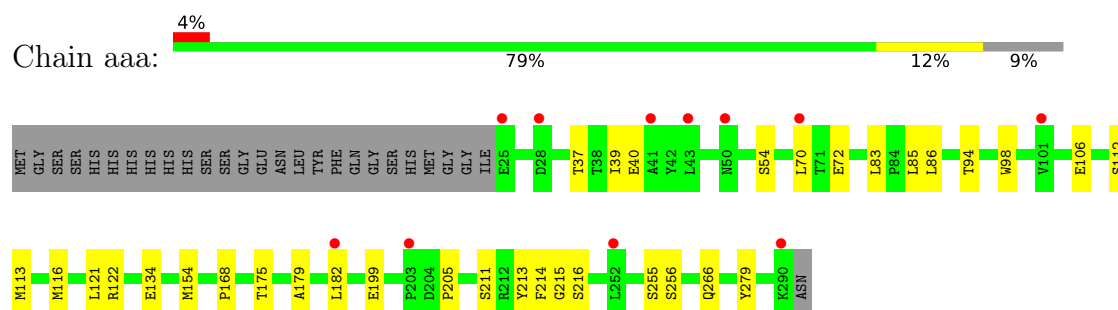
• Molecule 1: Capsid protein VP1



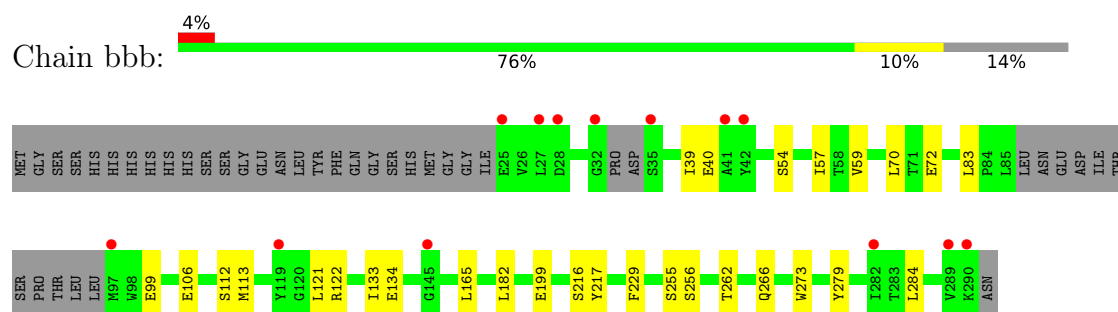
- Molecule 1: Capsid protein VP1



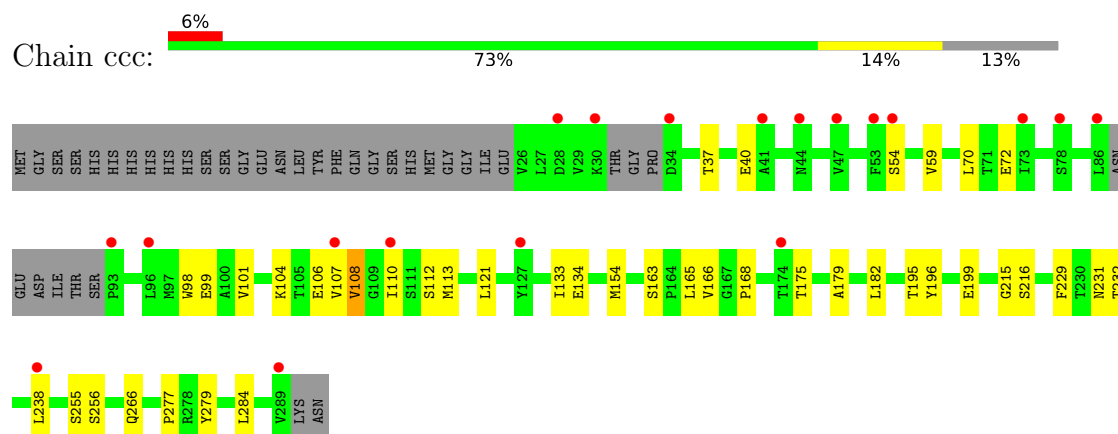
- Molecule 1: Capsid protein VP1



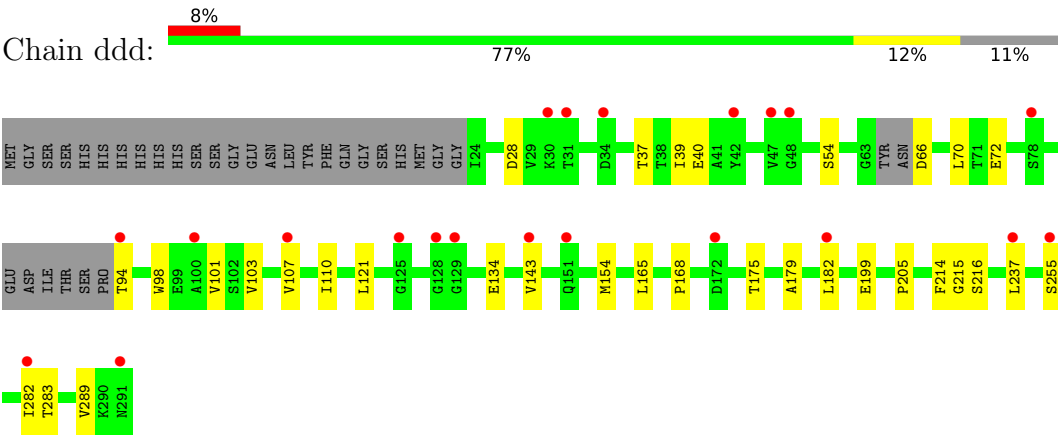
- Molecule 1: Capsid protein VP1



- Molecule 1: Capsid protein VP1



● Molecule 1: Capsid protein VP1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	145.05Å 91.61Å 352.33Å 90.00° 92.10° 90.00°	Depositor
Resolution (Å)	48.07 – 2.62 48.07 – 2.62	Depositor EDS
% Data completeness (in resolution range)	98.5 (48.07-2.62) 98.5 (48.07-2.62)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.11 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.270 , 0.300 0.269 , 0.300	Depositor DCC
R_{free} test set	2748 reflections (1.00%)	wwPDB-VP
Wilson B-factor (Å ²)	49.4	Xtriage
Anisotropy	0.592	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 37.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	59801	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.06% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	AAA	1.03	0/2023	1.24	1/2766 (0.0%)
1	BBB	1.02	0/2053	1.25	1/2811 (0.0%)
1	CCC	1.04	0/2059	1.27	2/2813 (0.1%)
1	DDD	1.04	1/2049 (0.0%)	1.28	6/2800 (0.2%)
1	EEE	1.04	1/2067 (0.0%)	1.27	2/2830 (0.1%)
1	FFF	1.03	0/2056	1.26	0/2817
1	GGG	1.03	0/2058	1.25	2/2819 (0.1%)
1	HHH	1.01	0/2028	1.24	2/2773 (0.1%)
1	III	1.03	0/2062	1.24	2/2822 (0.1%)
1	JJJ	1.01	0/2010	1.24	0/2746
1	KKK	1.01	0/2071	1.23	1/2834 (0.0%)
1	LLL	1.01	0/2055	1.23	1/2813 (0.0%)
1	MMM	1.00	0/1975	1.24	1/2703 (0.0%)
1	NNN	1.04	0/1986	1.26	1/2721 (0.0%)
1	OOO	1.01	0/2037	1.25	0/2790
1	PPP	1.01	0/2021	1.26	1/2760 (0.0%)
1	QQQ	1.05	1/2073 (0.0%)	1.27	2/2837 (0.1%)
1	RRR	1.01	0/2010	1.24	0/2746
1	SSS	1.06	0/2068	1.27	2/2830 (0.1%)
1	TTT	1.03	0/2049	1.27	3/2805 (0.1%)
1	UUU	1.01	0/1994	1.23	0/2725
1	VVV	1.04	0/1919	1.27	1/2629 (0.0%)
1	WWW	1.04	0/1970	1.29	3/2703 (0.1%)
1	XXX	1.04	0/2027	1.25	2/2777 (0.1%)
1	YYY	1.03	0/1959	1.25	1/2680 (0.0%)
1	ZZZ	1.04	0/1957	1.26	2/2675 (0.1%)
1	aaa	1.07	2/2024 (0.1%)	1.27	1/2773 (0.0%)
1	bbb	1.00	0/1955	1.23	0/2668
1	ccc	1.01	0/1948	1.23	0/2659
1	ddd	1.03	0/1949	1.26	1/2666 (0.0%)
All	All	1.03	5/60512 (0.0%)	1.25	41/82791 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	aaa	85	LEU	C-O	-7.19	1.15	1.23
1	EEE	34	ASP	C-O	-6.71	1.14	1.23
1	DDD	290	LYS	C-O	6.67	1.32	1.23
1	aaa	94	THR	C-O	-6.37	1.15	1.24
1	QQQ	88	GLU	C-O	5.29	1.30	1.23

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	SSS	28	ASP	CA-CB-CG	-8.86	103.74	112.60
1	XXX	28	ASP	CA-CB-CG	-8.84	103.77	112.60
1	GGG	28	ASP	CA-CB-CG	-8.30	104.30	112.60
1	DDD	28	ASP	CA-CB-CG	-7.84	104.76	112.60
1	YYY	87	ASN	CA-C-O	-7.70	107.71	120.80

There are no chirality outliers.

There are no planarity outliers.

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	AAA	1971	0	1838	18	0
1	BBB	2000	0	1834	39	0
1	CCC	2009	0	1898	28	0
1	DDD	1998	0	1859	24	0
1	EEE	2014	0	1883	29	0
1	FFF	2003	0	1841	34	0
1	GGG	2005	0	1854	19	0
1	HHH	1976	0	1852	16	0
1	III	2009	0	1878	18	0
1	JJJ	1959	0	1827	33	0
1	KKK	2018	0	1906	35	0
1	LLL	2002	0	1855	39	0
1	MMM	1924	0	1770	28	0
1	NNN	1934	0	1712	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	OOO	1984	0	1813	26	0
1	PPP	1972	0	1853	23	0
1	QQQ	2017	0	1885	47	0
1	RRR	1959	0	1821	20	0
1	SSS	2015	0	1871	15	0
1	TTT	1997	0	1845	18	0
1	UUU	1944	0	1809	37	0
1	VVV	1873	0	1689	30	0
1	WWW	1922	0	1731	33	0
1	XXX	1975	0	1797	43	0
1	YYY	1909	0	1731	17	0
1	ZZZ	1911	0	1759	38	0
1	aaa	1971	0	1812	40	0
1	bbb	1906	0	1787	31	0
1	ccc	1900	0	1769	38	0
1	ddd	1902	0	1729	31	0
2	AAA	3	0	0	0	0
2	BBB	5	0	0	0	0
2	CCC	3	0	0	0	0
2	DDD	1	0	0	0	0
2	EEE	1	0	0	0	0
2	FFF	3	0	0	0	0
2	GGG	3	0	0	0	0
2	HHH	3	0	0	0	0
2	III	3	0	0	0	0
2	JJJ	3	0	0	0	0
2	KKK	3	0	0	0	0
2	LLL	5	0	0	0	0
2	MMM	2	0	0	0	0
2	NNN	1	0	0	0	0
2	OOO	4	0	0	0	0
2	PPP	3	0	0	0	0
2	QQQ	2	0	0	0	0
2	RRR	3	0	0	0	0
2	SSS	1	0	0	0	0
2	TTT	1	0	0	0	0
2	UUU	2	0	0	0	0
2	VVV	1	0	0	0	0
2	WWW	1	0	0	0	0
2	XXX	3	0	0	0	0
2	YYY	2	0	0	0	0
2	ZZZ	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	aaa	2	0	0	0	0
2	bbb	3	0	0	0	0
2	ccc	1	0	0	0	0
2	ddd	2	0	0	0	0
3	AAA	32	0	0	0	0
3	BBB	36	0	0	1	0
3	CCC	37	0	0	2	0
3	DDD	33	0	0	2	0
3	EEE	30	0	0	0	0
3	FFF	22	0	0	1	0
3	GGG	34	0	0	1	0
3	HHH	44	0	0	0	0
3	III	44	0	0	1	0
3	JJJ	30	0	0	0	0
3	KKK	35	0	0	1	0
3	LLL	20	0	0	3	0
3	MMM	20	0	0	1	0
3	NNN	17	0	0	0	0
3	OOO	19	0	0	0	0
3	PPP	33	0	0	0	0
3	QQQ	34	0	0	0	0
3	RRR	23	0	0	2	0
3	SSS	9	0	0	0	0
3	TTT	25	0	0	1	0
3	UUU	19	0	0	0	0
3	VVV	9	0	0	2	0
3	WWW	13	0	0	0	0
3	XXX	18	0	0	3	0
3	YYY	24	0	0	0	0
3	ZZZ	15	0	0	2	0
3	aaa	27	0	0	0	0
3	bbb	21	0	0	0	0
3	ccc	9	0	0	0	0
3	ddd	19	0	0	1	0
All	All	59801	0	54508	744	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 7.

The worst 5 of 744 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:aaa:113:MET:HE3	1:bbb:217:TYR:CE2	1.73	1.21
1:ddd:103:VAL:CG2	1:ddd:237:LEU:HD11	1.75	1.15
1:KKK:116:MET:HE2	1:LLL:273:TRP:CH2	1.86	1.10
1:VVV:107:VAL:HG23	1:VVV:110:ILE:HD11	1.33	1.09
1:ddd:103:VAL:HG23	1:ddd:237:LEU:HD11	1.34	1.09

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 X-ray entries followed by that with respect to entries of similar resolution.

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	AAA	259/293 (88%)	248 (96%)	11 (4%)	0	100	100
1	BBB	268/293 (92%)	258 (96%)	10 (4%)	0	100	100
1	CCC	264/293 (90%)	254 (96%)	10 (4%)	0	100	100
1	DDD	263/293 (90%)	253 (96%)	10 (4%)	0	100	100
1	EEE	268/293 (92%)	260 (97%)	8 (3%)	0	100	100
1	FFF	268/293 (92%)	260 (97%)	8 (3%)	0	100	100
1	GGG	266/293 (91%)	257 (97%)	9 (3%)	0	100	100
1	HHH	261/293 (89%)	252 (97%)	9 (3%)	0	100	100
1	III	268/293 (92%)	258 (96%)	10 (4%)	0	100	100
1	JJJ	258/293 (88%)	248 (96%)	10 (4%)	0	100	100
1	KKK	266/293 (91%)	257 (97%)	9 (3%)	0	100	100
1	LLL	266/293 (91%)	256 (96%)	10 (4%)	0	100	100
1	MMM	254/293 (87%)	245 (96%)	9 (4%)	0	100	100
1	NNN	263/293 (90%)	253 (96%)	10 (4%)	0	100	100
1	OOO	268/293 (92%)	258 (96%)	10 (4%)	0	100	100
1	PPP	258/293 (88%)	248 (96%)	10 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	QQQ	268/293 (92%)	254 (95%)	14 (5%)	0	100	100
1	RRR	259/293 (88%)	248 (96%)	11 (4%)	0	100	100
1	SSS	267/293 (91%)	257 (96%)	10 (4%)	0	100	100
1	TTT	268/293 (92%)	258 (96%)	10 (4%)	0	100	100
1	UUU	257/293 (88%)	246 (96%)	11 (4%)	0	100	100
1	VVV	257/293 (88%)	246 (96%)	11 (4%)	0	100	100
1	WWW	266/293 (91%)	255 (96%)	10 (4%)	1 (0%)	30	49
1	XXX	264/293 (90%)	255 (97%)	9 (3%)	0	100	100
1	YYY	258/293 (88%)	247 (96%)	11 (4%)	0	100	100
1	ZZZ	251/293 (86%)	241 (96%)	10 (4%)	0	100	100
1	aaa	264/293 (90%)	254 (96%)	10 (4%)	0	100	100
1	bbb	247/293 (84%)	238 (96%)	9 (4%)	0	100	100
1	ccc	249/293 (85%)	239 (96%)	10 (4%)	0	100	100
1	ddd	254/293 (87%)	245 (96%)	9 (4%)	0	100	100
All	All	7847/8790 (89%)	7548 (96%)	298 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	WWW	87	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 X-ray entries followed by that with respect to entries of similar resolution.

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	AAA	205/250 (82%)	198 (97%)	7 (3%)	32	58
1	BBB	203/250 (81%)	196 (97%)	7 (3%)	32	58
1	CCC	212/250 (85%)	204 (96%)	8 (4%)	29	54
1	DDD	208/250 (83%)	199 (96%)	9 (4%)	26	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	EEE	209/250 (84%)	202 (97%)	7 (3%)	33	59
1	FFF	207/250 (83%)	200 (97%)	7 (3%)	32	58
1	GGG	210/250 (84%)	203 (97%)	7 (3%)	33	59
1	HHH	206/250 (82%)	199 (97%)	7 (3%)	32	58
1	III	209/250 (84%)	202 (97%)	7 (3%)	33	59
1	JJJ	204/250 (82%)	197 (97%)	7 (3%)	32	58
1	KKK	215/250 (86%)	207 (96%)	8 (4%)	30	55
1	LLL	209/250 (84%)	203 (97%)	6 (3%)	37	63
1	MMM	200/250 (80%)	192 (96%)	8 (4%)	28	53
1	NNN	188/250 (75%)	182 (97%)	6 (3%)	34	60
1	OOO	200/250 (80%)	194 (97%)	6 (3%)	36	62
1	PPP	203/250 (81%)	197 (97%)	6 (3%)	36	62
1	QQQ	213/250 (85%)	207 (97%)	6 (3%)	38	64
1	RRR	202/250 (81%)	195 (96%)	7 (4%)	32	57
1	SSS	212/250 (85%)	204 (96%)	8 (4%)	29	54
1	TTT	205/250 (82%)	198 (97%)	7 (3%)	32	58
1	UUU	202/250 (81%)	196 (97%)	6 (3%)	36	62
1	VVV	182/250 (73%)	176 (97%)	6 (3%)	33	59
1	WWW	188/250 (75%)	183 (97%)	5 (3%)	39	65
1	XXX	201/250 (80%)	195 (97%)	6 (3%)	36	62
1	YYY	190/250 (76%)	183 (96%)	7 (4%)	30	55
1	ZZZ	194/250 (78%)	188 (97%)	6 (3%)	35	61
1	aaa	203/250 (81%)	196 (97%)	7 (3%)	32	58
1	bbb	199/250 (80%)	192 (96%)	7 (4%)	32	57
1	ccc	198/250 (79%)	189 (96%)	9 (4%)	24	48
1	ddd	193/250 (77%)	187 (97%)	6 (3%)	35	61
All	All	6070/7500 (81%)	5864 (97%)	206 (3%)	32	58

5 of 206 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	QQQ	216	SER
1	UUU	182	LEU

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Mol	Chain	Res	Type
1	ccc	266	GLN
1	RRR	106	GLU
1	SSS	216	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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](#)

Of 71 ligands modelled in this entry, 71 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AAA	263/293 (89%)	0.42	10 (3%) 44 39	32, 49, 70, 117	0
1	BBB	270/293 (92%)	0.46	14 (5%) 33 27	37, 52, 80, 124	0
1	CCC	268/293 (91%)	0.30	6 (2%) 62 57	35, 47, 67, 89	0
1	DDD	267/293 (91%)	0.23	4 (1%) 72 68	30, 44, 58, 84	0
1	EEE	270/293 (92%)	0.28	6 (2%) 62 57	32, 46, 68, 97	0
1	FFF	270/293 (92%)	0.40	8 (2%) 52 47	32, 51, 67, 91	0
1	GGG	268/293 (91%)	0.34	5 (1%) 66 62	34, 49, 63, 79	0
1	HHH	265/293 (90%)	0.42	10 (3%) 44 39	35, 50, 70, 114	0
1	III	269/293 (91%)	0.30	8 (2%) 52 47	24, 47, 71, 111	1 (0%)
1	JJJ	262/293 (89%)	0.41	6 (2%) 61 56	35, 51, 71, 93	0
1	KKK	268/293 (91%)	0.42	7 (2%) 57 52	38, 51, 67, 107	0
1	LLL	268/293 (91%)	0.45	9 (3%) 48 43	34, 52, 74, 130	0
1	MMM	258/293 (88%)	0.73	15 (5%) 29 24	45, 60, 76, 94	0
1	NNN	266/293 (90%)	0.75	19 (7%) 22 18	33, 62, 82, 112	1 (0%)
1	OOO	270/293 (92%)	0.65	16 (5%) 28 23	37, 59, 77, 117	0
1	PPP	264/293 (90%)	0.56	13 (4%) 35 29	39, 54, 74, 95	0
1	QQQ	269/293 (91%)	0.54	9 (3%) 49 44	34, 52, 67, 86	1 (0%)
1	RRR	263/293 (89%)	0.55	9 (3%) 48 43	40, 55, 72, 93	0
1	SSS	268/293 (91%)	0.49	5 (1%) 66 62	27, 55, 71, 81	1 (0%)
1	TTT	270/293 (92%)	0.42	4 (1%) 72 68	40, 54, 68, 95	0
1	UUU	261/293 (89%)	0.82	19 (7%) 21 17	42, 60, 79, 100	0
1	VVV	261/293 (89%)	1.15	38 (14%) 6 4	46, 74, 92, 107	0
1	WWW	268/293 (91%)	1.37	56 (20%) 2 2	43, 73, 94, 114	0
1	XXX	267/293 (91%)	1.01	36 (13%) 7 5	32, 63, 81, 98	1 (0%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	YYY	262/293 (89%)	0.86	17 (6%) 25 20	43, 63, 83, 93	0
1	ZZZ	259/293 (88%)	0.92	19 (7%) 21 17	42, 64, 86, 110	0
1	aaa	266/293 (90%)	0.68	11 (4%) 41 36	40, 61, 86, 122	0
1	bbb	253/293 (86%)	0.47	13 (5%) 33 28	36, 55, 82, 103	0
1	ccc	255/293 (87%)	0.73	19 (7%) 20 16	43, 63, 85, 134	0
1	ddd	260/293 (88%)	0.88	22 (8%) 16 13	44, 65, 85, 106	0
All	All	7948/8790 (90%)	0.60	433 (5%) 31 26	24, 55, 81, 134	5 (0%)

The worst 5 of 433 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	WWW	261	GLY	7.2
1	WWW	275	GLY	7.0
1	WWW	76	TYR	5.7
1	YYY	76	TYR	5.4
1	OOO	275	GLY	5.3

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	CL	OOO	303	1/1	0.83	0.18	81,81,81,81	0
2	CL	BBB	304	1/1	0.85	0.19	90,90,90,90	0
2	CL	SSS	301	1/1	0.86	0.09	84,84,84,84	0
2	CL	bbb	301	1/1	0.87	0.16	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CL	LLL	301	1/1	0.88	0.13	80,80,80,80	0
2	CL	HHH	301	1/1	0.88	0.13	79,79,79,79	0
2	CL	GGG	303	1/1	0.89	0.16	79,79,79,79	0
2	CL	CCC	303	1/1	0.89	0.12	79,79,79,79	0
2	CL	QQQ	302	1/1	0.90	0.12	70,70,70,70	0
2	CL	MMM	301	1/1	0.90	0.15	71,71,71,71	0
2	CL	EEE	301	1/1	0.90	0.10	58,58,58,58	0
2	CL	bbb	302	1/1	0.90	0.12	68,68,68,68	0
2	CL	FFF	303	1/1	0.91	0.07	68,68,68,68	0
2	CL	LLL	303	1/1	0.91	0.09	84,84,84,84	0
2	CL	bbb	303	1/1	0.91	0.15	73,73,73,73	0
2	CL	III	302	1/1	0.92	0.12	68,68,68,68	0
2	CL	AAA	301	1/1	0.93	0.12	61,61,61,61	0
2	CL	KKK	302	1/1	0.93	0.11	66,66,66,66	0
2	CL	NNN	301	1/1	0.93	0.10	74,74,74,74	0
2	CL	OOO	302	1/1	0.93	0.08	70,70,70,70	0
2	CL	BBB	302	1/1	0.93	0.07	73,73,73,73	0
2	CL	FFF	302	1/1	0.94	0.10	71,71,71,71	0
2	CL	OOO	304	1/1	0.94	0.14	63,63,63,63	0
2	CL	QQQ	301	1/1	0.94	0.11	68,68,68,68	0
2	CL	LLL	302	1/1	0.94	0.09	75,75,75,75	0
2	CL	AAA	302	1/1	0.94	0.07	69,69,69,69	0
2	CL	VVV	301	1/1	0.94	0.09	62,62,62,62	0
2	CL	WWW	301	1/1	0.94	0.16	61,61,61,61	0
2	CL	YYY	301	1/1	0.94	0.07	66,66,66,66	0
2	CL	YYY	302	1/1	0.94	0.07	53,53,53,53	0
2	CL	JJJ	302	1/1	0.94	0.10	71,71,71,71	0
2	CL	KKK	301	1/1	0.94	0.15	58,58,58,58	0
2	CL	AAA	303	1/1	0.94	0.23	59,59,59,59	0
2	CL	ddd	301	1/1	0.94	0.11	74,74,74,74	0
2	CL	BBB	301	1/1	0.95	0.06	65,65,65,65	0
2	CL	HHH	303	1/1	0.95	0.09	63,63,63,63	0
2	CL	XXX	303	1/1	0.95	0.12	69,69,69,69	0
2	CL	CCC	301	1/1	0.95	0.08	55,55,55,55	0
2	CL	JJJ	301	1/1	0.95	0.14	56,56,56,56	0
2	CL	GGG	302	1/1	0.95	0.09	65,65,65,65	0
2	CL	RRR	303	1/1	0.95	0.12	66,66,66,66	0
2	CL	FFF	301	1/1	0.95	0.13	62,62,62,62	0
2	CL	UUU	301	1/1	0.95	0.12	63,63,63,63	0
2	CL	ddd	302	1/1	0.95	0.07	61,61,61,61	0
2	CL	PPP	302	1/1	0.96	0.12	65,65,65,65	0
2	CL	III	303	1/1	0.96	0.06	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CL	XXX	301	1/1	0.96	0.10	66,66,66,66	0
2	CL	OOO	301	1/1	0.96	0.08	66,66,66,66	0
2	CL	RRR	301	1/1	0.96	0.08	58,58,58,58	0
2	CL	RRR	302	1/1	0.96	0.08	68,68,68,68	0
2	CL	ZZZ	301	1/1	0.96	0.07	62,62,62,62	0
2	CL	aaa	301	1/1	0.96	0.16	60,60,60,60	0
2	CL	aaa	302	1/1	0.96	0.08	66,66,66,66	0
2	CL	III	301	1/1	0.96	0.06	59,59,59,59	0
2	CL	LLL	305	1/1	0.96	0.10	67,67,67,67	0
2	CL	TTT	301	1/1	0.96	0.13	65,65,65,65	0
2	CL	ccc	301	1/1	0.96	0.05	56,56,56,56	0
2	CL	BBB	305	1/1	0.96	0.08	69,69,69,69	0
2	CL	UUU	302	1/1	0.96	0.15	62,62,62,62	0
2	CL	MMM	302	1/1	0.97	0.13	65,65,65,65	0
2	CL	PPP	303	1/1	0.97	0.11	61,61,61,61	0
2	CL	LLL	304	1/1	0.98	0.13	62,62,62,62	0
2	CL	PPP	301	1/1	0.98	0.06	60,60,60,60	0
2	CL	JJJ	303	1/1	0.98	0.06	48,48,48,48	0
2	CL	BBB	303	1/1	0.98	0.10	51,51,51,51	0
2	CL	DDD	301	1/1	0.98	0.12	69,69,69,69	0
2	CL	KKK	303	1/1	0.98	0.10	61,61,61,61	0
2	CL	CCC	302	1/1	0.98	0.13	48,48,48,48	0
2	CL	XXX	302	1/1	0.98	0.13	59,59,59,59	0
2	CL	HHH	302	1/1	0.98	0.06	62,62,62,62	0
2	CL	GGG	301	1/1	0.98	0.11	60,60,60,60	0

6.5 Other polymers [i](#)

There are no such residues in this entry.