Full wwPDB X-ray Structure Validation Report ⓘ

Jan 13, 2024 – 02:54 pm GMT

PDB ID	:	6Y67
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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/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:

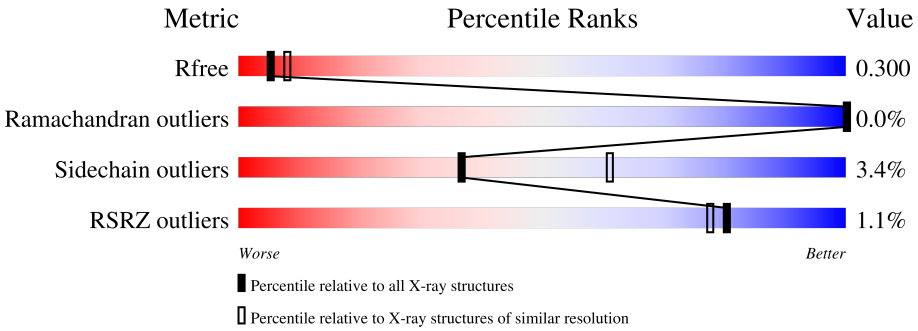
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
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}	130704	3797 (2.64-2.60)
Ramachandran outliers	138981	4093 (2.64-2.60)
Sidechain outliers	138945	4093 (2.64-2.60)
RSRZ outliers	127900	3731 (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 <=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	87% · 10%
1	BBB	293	% 89% · 8%
1	CCC	293	89% · 9%
1	DDD	293	88% · 9%
1	EEE	293	90% · 8%
1	FFF	293	90% · 8%

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Mol	Chain	Length	Quality of chain
1	GGG	293	89% 9%
1	HHH	293	88% 10%
1	III	293	89% 8%
1	JJJ	293	87% 11%
1	KKK	293	89% 9%
1	LLL	293	89% 9%
1	MMM	293	3% 85% 12%
1	NNN	293	89% 9%
1	OOO	293	90% 8%
1	PPP	293	88% 10%
1	QQQ	293	89% 8%
1	RRR	293	87% 10%
1	SSS	293	89% 9%
1	TTT	293	90% 8%
1	UUU	293	87% 11%
1	VVV	293	87% 11%
1	WWW	293	5% 89% 9%
1	XXX	293	89% 9%
1	YYY	293	87% 11%
1	ZZZ	293	86% 12%
1	aaa	293	88% 9%
1	bbb	293	84% 14%
1	ccc	293	84% 13%
1	ddd	293	87% 11%

2 Entry composition (i)

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

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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 (three-letter code: 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 Cl 3 3	0	0
2	III	3	Total Cl 3 3	0	0
2	JJJ	3	Total Cl 3 3	0	0
2	KKK	3	Total Cl 3 3	0	0
2	LLL	5	Total Cl 5 5	0	0
2	MMM	2	Total Cl 2 2	0	0
2	NNN	1	Total Cl 1 1	0	0
2	OOO	4	Total Cl 4 4	0	0
2	PPP	3	Total Cl 3 3	0	0
2	QQQ	2	Total Cl 2 2	0	0
2	RRR	3	Total Cl 3 3	0	0
2	SSS	1	Total Cl 1 1	0	0
2	TTT	1	Total Cl 1 1	0	0
2	UUU	2	Total Cl 2 2	0	0
2	VVV	1	Total Cl 1 1	0	0
2	WWW	1	Total Cl 1 1	0	0
2	XXX	3	Total Cl 3 3	0	0
2	YYY	2	Total Cl 2 2	0	0
2	ZZZ	1	Total Cl 1 1	0	0
2	aaa	2	Total Cl 2 2	0	0
2	bbb	3	Total Cl 3 3	0	0

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

- Molecule 3 is water.

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

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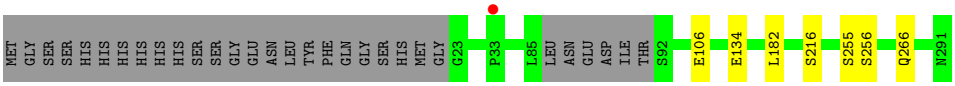
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	RRR	23	Total O 23 23	0	0
3	SSS	9	Total O 9 9	0	0
3	TTT	25	Total O 25 25	0	0
3	UUU	19	Total O 19 19	0	0
3	VVV	9	Total O 9 9	0	0
3	WWW	13	Total O 13 13	0	0
3	XXX	18	Total O 18 18	0	0
3	YYY	24	Total O 24 24	0	0
3	ZZZ	15	Total O 15 15	0	0
3	aaa	27	Total O 27 27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

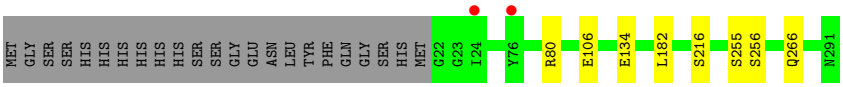
• Molecule 1: Capsid protein VP1

Chain AAA:



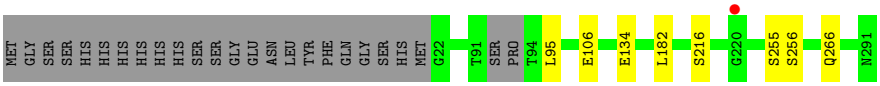
• Molecule 1: Capsid protein VP1

Chain BBB:



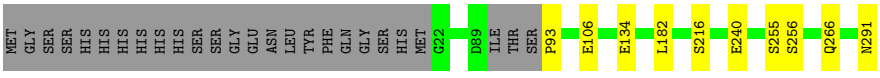
• Molecule 1: Capsid protein VP1

Chain CCC:



• Molecule 1: Capsid protein VP1

Chain DDD:

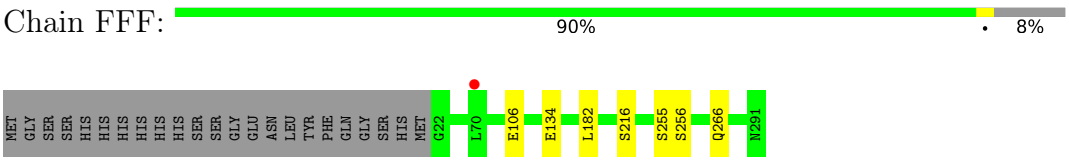


• Molecule 1: Capsid protein VP1

Chain EEE:

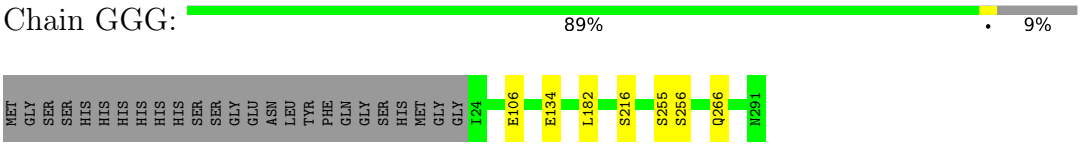
• Molecule 1: Capsid protein VP1

Chain FFF:



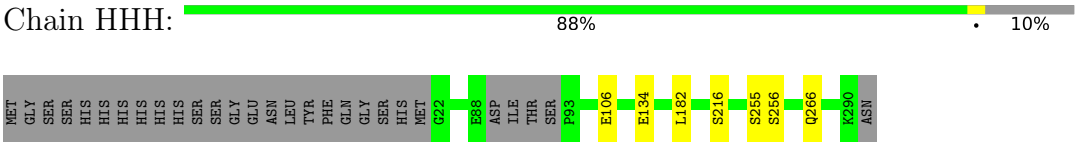
• Molecule 1: Capsid protein VP1

Chain GGG:



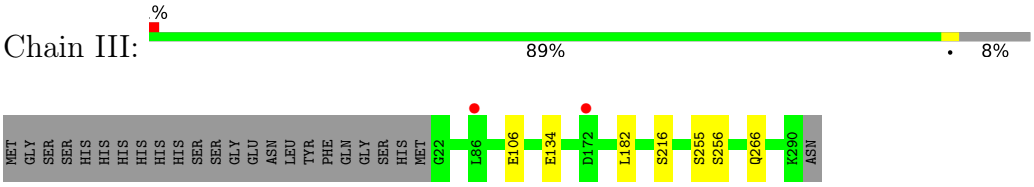
• Molecule 1: Capsid protein VP1

Chain HHH:



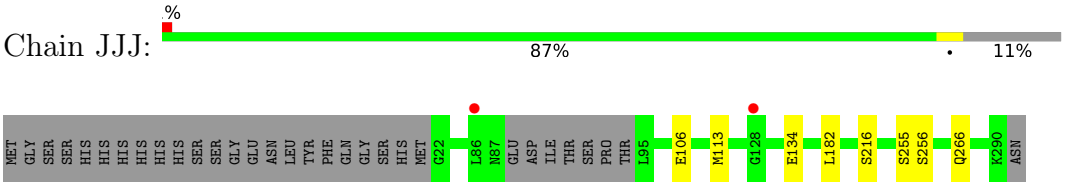
• Molecule 1: Capsid protein VP1

Chain III:



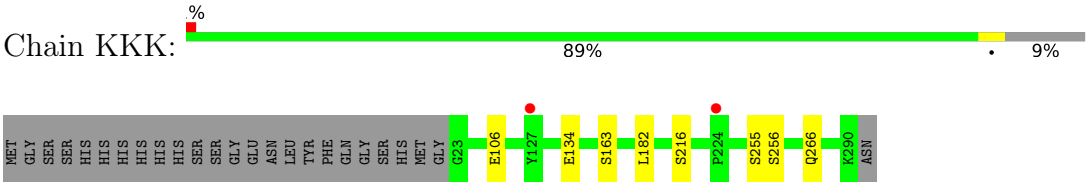
• Molecule 1: Capsid protein VP1

Chain JJJ:



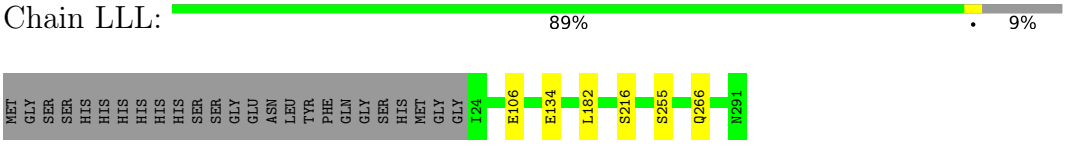
• Molecule 1: Capsid protein VP1

Chain KKK:



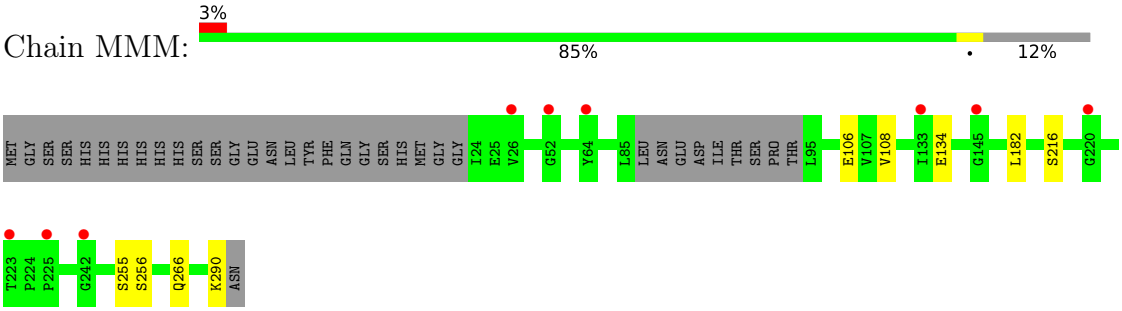
• Molecule 1: Capsid protein VP1

Chain LLL:



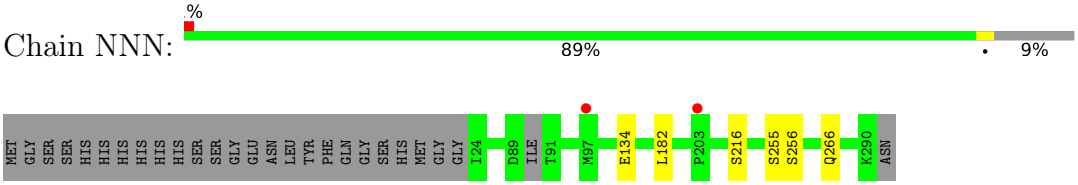
• Molecule 1: Capsid protein VP1

Chain MMM:



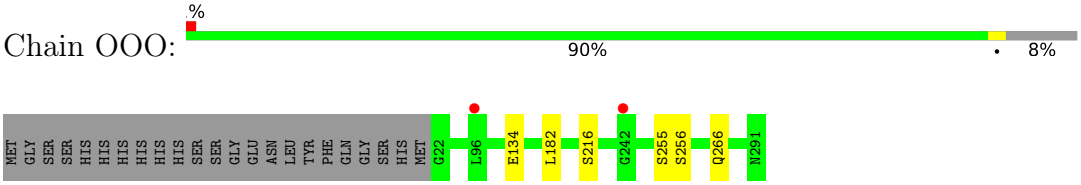
• Molecule 1: Capsid protein VP1

Chain NNN:



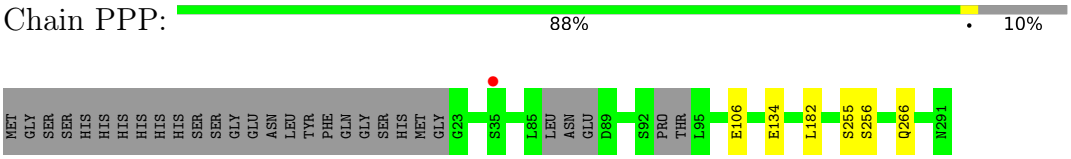
• Molecule 1: Capsid protein VP1

Chain OOO:



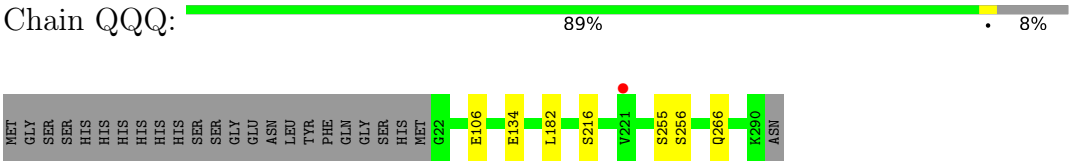
• Molecule 1: Capsid protein VP1

Chain PPP:



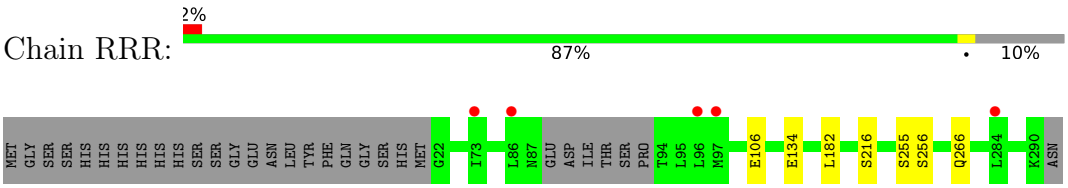
• Molecule 1: Capsid protein VP1

Chain QQQ:



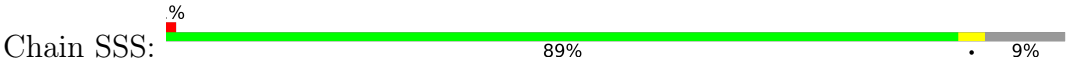
• Molecule 1: Capsid protein VP1

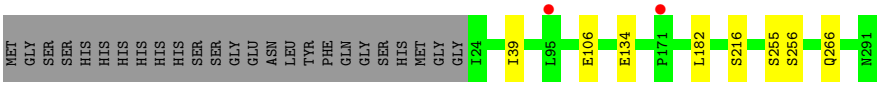
Chain RRR:



• Molecule 1: Capsid protein VP1

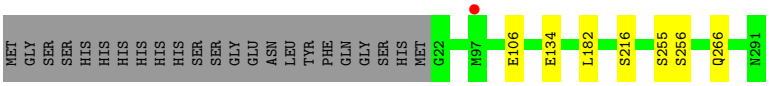
Chain SSS:





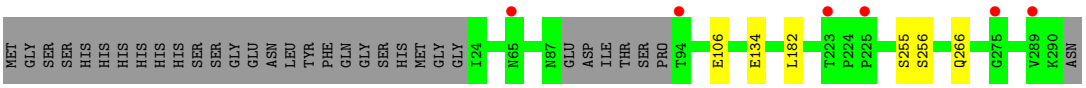
• Molecule 1: Capsid protein VP1

Chain TTT:



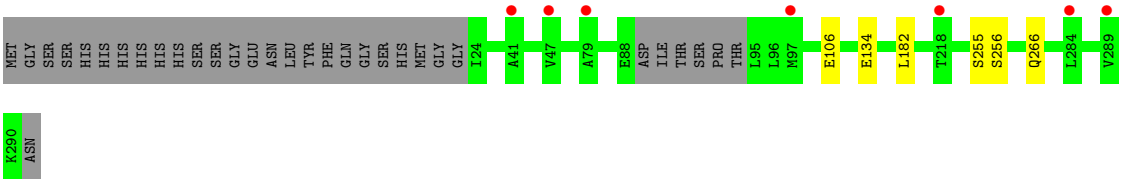
• Molecule 1: Capsid protein VP1

Chain UUU:



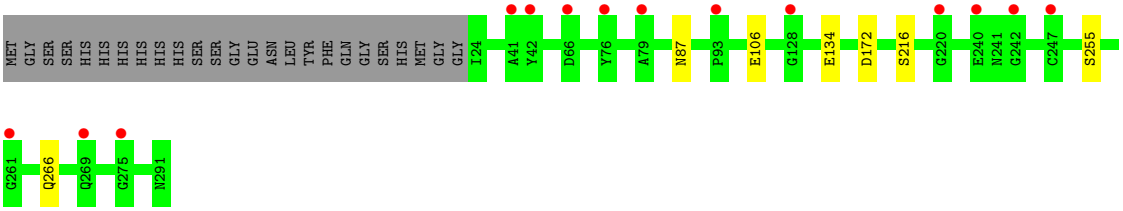
• Molecule 1: Capsid protein VP1

Chain VVV:



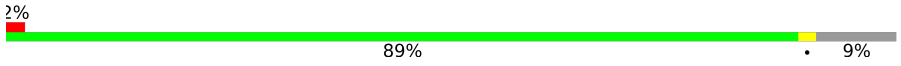
• Molecule 1: Capsid protein VP1

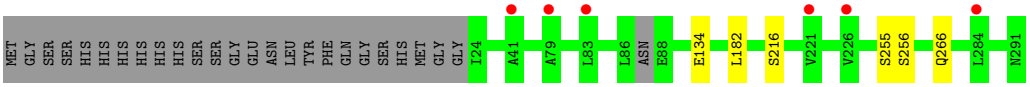
Chain WWW:



• Molecule 1: Capsid protein VP1

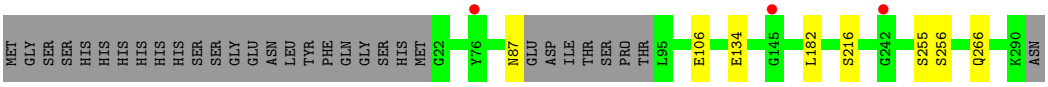
Chain XXX:





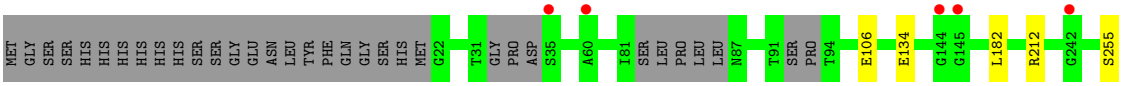
• Molecule 1: Capsid protein VP1

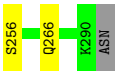
Chain YYY:



• Molecule 1: Capsid protein VP1

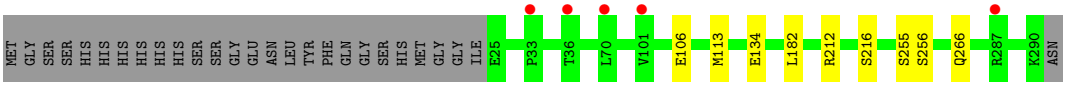
Chain ZZZ:





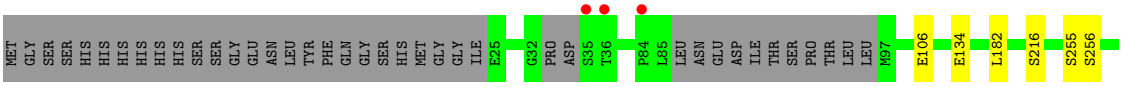
• Molecule 1: Capsid protein VP1

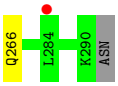
Chain aaa:



• Molecule 1: Capsid protein VP1

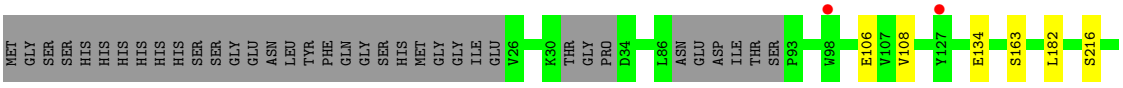
Chain bbb:

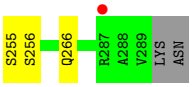




• Molecule 1: Capsid protein VP1

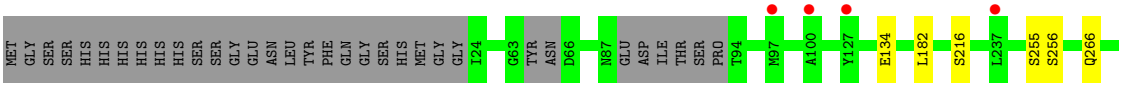
Chain ccc:





• Molecule 1: Capsid protein VP1

Chain ddd:



N291

4 Data and refinement statistics (i)

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) 98.6 (48.07-2.62)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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 , 39.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-l	Xtriage
F_o,F_c correlation	0.91	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.68	0/2023	0.79	0/2766
1	BBB	0.66	0/2053	0.79	1/2811 (0.0%)
1	CCC	0.69	0/2059	0.80	0/2813
1	DDD	0.68	0/2049	0.80	1/2800 (0.0%)
1	EEE	0.69	0/2067	0.79	0/2830
1	FFF	0.68	0/2056	0.78	0/2817
1	GGG	0.68	0/2058	0.78	0/2819
1	HHH	0.66	0/2028	0.76	0/2773
1	III	0.67	0/2062	0.76	0/2822
1	JJJ	0.67	0/2010	0.78	1/2746 (0.0%)
1	KKK	0.66	0/2071	0.77	0/2834
1	LLL	0.66	0/2055	0.76	0/2813
1	MMM	0.65	0/1975	0.78	1/2703 (0.0%)
1	NNN	0.67	0/1986	0.78	0/2721
1	OOO	0.65	0/2037	0.77	0/2790
1	PPP	0.67	0/2021	0.79	0/2760
1	QQQ	0.69	0/2073	0.82	1/2837 (0.0%)
1	RRR	0.66	0/2010	0.77	0/2746
1	SSS	0.70	0/2068	0.79	0/2830
1	TTT	0.68	0/2049	0.79	0/2805
1	UUU	0.67	0/1994	0.78	0/2725
1	VVV	0.69	0/1919	0.79	0/2629
1	WWW	0.67	0/1970	0.81	1/2703 (0.0%)
1	XXX	0.68	0/2027	0.79	0/2777
1	YYY	0.67	0/1959	0.77	1/2680 (0.0%)
1	ZZZ	0.70	0/1957	0.80	1/2675 (0.0%)
1	aaa	0.70	0/2024	0.80	2/2773 (0.1%)
1	bbb	0.65	0/1955	0.76	0/2668
1	ccc	0.66	0/1948	0.76	0/2659
1	ddd	0.68	0/1949	0.78	0/2666
All	All	0.67	0/60512	0.78	10/82791 (0.0%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	QQQ	134	GLU	CB-CA-C	-7.26	95.87	110.40
1	WWW	172	ASP	CB-CA-C	-7.05	96.30	110.40
1	JJJ	113	MET	CG-SD-CE	6.17	110.07	100.20
1	ZZZ	212	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	DDD	93	PRO	N-CA-CB	5.93	110.42	103.30
1	YYY	87	ASN	CA-C-O	-5.90	107.71	120.10
1	BBB	80	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	MMM	290	LYS	CA-C-O	5.44	131.52	120.10
1	aaa	212	ARG	NE-CZ-NH1	5.27	122.93	120.30
1	aaa	113	MET	CG-SD-CE	5.01	108.22	100.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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 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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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%)	34	55
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 (i)

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%)	37	61
1	BBB	203/250 (81%)	196 (97%)	7 (3%)	37	61
1	CCC	212/250 (85%)	204 (96%)	8 (4%)	33	57
1	DDD	208/250 (83%)	199 (96%)	9 (4%)	29	53
1	EEE	209/250 (84%)	202 (97%)	7 (3%)	38	62
1	FFF	207/250 (83%)	200 (97%)	7 (3%)	37	61
1	GGG	210/250 (84%)	203 (97%)	7 (3%)	38	62
1	HHH	206/250 (82%)	199 (97%)	7 (3%)	37	61
1	III	209/250 (84%)	202 (97%)	7 (3%)	38	62
1	JJJ	204/250 (82%)	197 (97%)	7 (3%)	37	61
1	KKK	215/250 (86%)	207 (96%)	8 (4%)	34	58
1	LLL	209/250 (84%)	203 (97%)	6 (3%)	42	67
1	MMM	200/250 (80%)	192 (96%)	8 (4%)	31	55
1	NNN	188/250 (75%)	182 (97%)	6 (3%)	39	63
1	OOO	200/250 (80%)	194 (97%)	6 (3%)	41	66
1	PPP	203/250 (81%)	197 (97%)	6 (3%)	41	66
1	QQQ	213/250 (85%)	207 (97%)	6 (3%)	43	68
1	RRR	202/250 (81%)	195 (96%)	7 (4%)	36	60
1	SSS	212/250 (85%)	204 (96%)	8 (4%)	33	57
1	TTT	205/250 (82%)	198 (97%)	7 (3%)	37	61
1	UUU	202/250 (81%)	196 (97%)	6 (3%)	41	66
1	VVV	182/250 (73%)	176 (97%)	6 (3%)	38	62
1	WWW	188/250 (75%)	183 (97%)	5 (3%)	44	69
1	XXX	201/250 (80%)	195 (97%)	6 (3%)	41	66
1	YYY	190/250 (76%)	183 (96%)	7 (4%)	34	58
1	ZZZ	194/250 (78%)	188 (97%)	6 (3%)	40	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	aaa	203/250 (81%)	196 (97%)	7 (3%)	37 61
1	bbb	199/250 (80%)	192 (96%)	7 (4%)	36 60
1	ccc	198/250 (79%)	189 (96%)	9 (4%)	27 50
1	ddd	193/250 (77%)	187 (97%)	6 (3%)	40 65
All	All	6070/7500 (81%)	5864 (97%)	206 (3%)	37 61

All (206) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	106	GLU
1	AAA	134	GLU
1	AAA	182	LEU
1	AAA	216	SER
1	AAA	255	SER
1	AAA	256	SER
1	AAA	266	GLN
1	BBB	106	GLU
1	BBB	134	GLU
1	BBB	182	LEU
1	BBB	216	SER
1	BBB	255	SER
1	BBB	256	SER
1	BBB	266	GLN
1	CCC	95	LEU
1	CCC	106	GLU
1	CCC	134	GLU
1	CCC	182	LEU
1	CCC	216	SER
1	CCC	255	SER
1	CCC	256	SER
1	CCC	266	GLN
1	DDD	106	GLU
1	DDD	134	GLU
1	DDD	182	LEU
1	DDD	216	SER
1	DDD	240	GLU
1	DDD	255	SER
1	DDD	256	SER
1	DDD	266	GLN
1	DDD	291	ASN
1	EEE	106	GLU

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Mol	Chain	Res	Type
1	EEE	134	GLU
1	EEE	182	LEU
1	EEE	216	SER
1	EEE	255	SER
1	EEE	256	SER
1	EEE	266	GLN
1	FFF	106	GLU
1	FFF	134	GLU
1	FFF	182	LEU
1	FFF	216	SER
1	FFF	255	SER
1	FFF	256	SER
1	FFF	266	GLN
1	GGG	106	GLU
1	GGG	134	GLU
1	GGG	182	LEU
1	GGG	216	SER
1	GGG	255	SER
1	GGG	256	SER
1	GGG	266	GLN
1	HHH	106	GLU
1	HHH	134	GLU
1	HHH	182	LEU
1	HHH	216	SER
1	HHH	255	SER
1	HHH	256	SER
1	HHH	266	GLN
1	III	106	GLU
1	III	134	GLU
1	III	182	LEU
1	III	216	SER
1	III	255	SER
1	III	256	SER
1	III	266	GLN
1	JJJ	106	GLU
1	JJJ	134	GLU
1	JJJ	182	LEU
1	JJJ	216	SER
1	JJJ	255	SER
1	JJJ	256	SER
1	JJJ	266	GLN
1	KKK	106	GLU

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Mol	Chain	Res	Type
1	KKK	134	GLU
1	KKK	163	SER
1	KKK	182	LEU
1	KKK	216	SER
1	KKK	255	SER
1	KKK	256	SER
1	KKK	266	GLN
1	LLL	106	GLU
1	LLL	134	GLU
1	LLL	182	LEU
1	LLL	216	SER
1	LLL	255	SER
1	LLL	266	GLN
1	MMM	106	GLU
1	MMM	108	VAL
1	MMM	134	GLU
1	MMM	182	LEU
1	MMM	216	SER
1	MMM	255	SER
1	MMM	256	SER
1	MMM	266	GLN
1	NNN	134	GLU
1	NNN	182	LEU
1	NNN	216	SER
1	NNN	255	SER
1	NNN	256	SER
1	NNN	266	GLN
1	OOO	134	GLU
1	OOO	182	LEU
1	OOO	216	SER
1	OOO	255	SER
1	OOO	256	SER
1	OOO	266	GLN
1	PPP	106	GLU
1	PPP	134	GLU
1	PPP	182	LEU
1	PPP	255	SER
1	PPP	256	SER
1	PPP	266	GLN
1	QQQ	106	GLU
1	QQQ	182	LEU
1	QQQ	216	SER

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Mol	Chain	Res	Type
1	QQQ	255	SER
1	QQQ	256	SER
1	QQQ	266	GLN
1	RRR	106	GLU
1	RRR	134	GLU
1	RRR	182	LEU
1	RRR	216	SER
1	RRR	255	SER
1	RRR	256	SER
1	RRR	266	GLN
1	SSS	39	ILE
1	SSS	106	GLU
1	SSS	134	GLU
1	SSS	182	LEU
1	SSS	216	SER
1	SSS	255	SER
1	SSS	256	SER
1	SSS	266	GLN
1	TTT	106	GLU
1	TTT	134	GLU
1	TTT	182	LEU
1	TTT	216	SER
1	TTT	255	SER
1	TTT	256	SER
1	TTT	266	GLN
1	UUU	106	GLU
1	UUU	134	GLU
1	UUU	182	LEU
1	UUU	255	SER
1	UUU	256	SER
1	UUU	266	GLN
1	VVV	106	GLU
1	VVV	134	GLU
1	VVV	182	LEU
1	VVV	255	SER
1	VVV	256	SER
1	VVV	266	GLN
1	WWW	106	GLU
1	WWW	134	GLU
1	WWW	216	SER
1	WWW	255	SER
1	WWW	266	GLN

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Mol	Chain	Res	Type
1	XXX	134	GLU
1	XXX	182	LEU
1	XXX	216	SER
1	XXX	255	SER
1	XXX	256	SER
1	XXX	266	GLN
1	YYY	106	GLU
1	YYY	134	GLU
1	YYY	182	LEU
1	YYY	216	SER
1	YYY	255	SER
1	YYY	256	SER
1	YYY	266	GLN
1	ZZZ	106	GLU
1	ZZZ	134	GLU
1	ZZZ	182	LEU
1	ZZZ	255	SER
1	ZZZ	256	SER
1	ZZZ	266	GLN
1	aaa	106	GLU
1	aaa	134	GLU
1	aaa	182	LEU
1	aaa	216	SER
1	aaa	255	SER
1	aaa	256	SER
1	aaa	266	GLN
1	bbb	106	GLU
1	bbb	134	GLU
1	bbb	182	LEU
1	bbb	216	SER
1	bbb	255	SER
1	bbb	256	SER
1	bbb	266	GLN
1	ccc	106	GLU
1	ccc	108	VAL
1	ccc	134	GLU
1	ccc	163	SER
1	ccc	182	LEU
1	ccc	216	SER
1	ccc	255	SER
1	ccc	256	SER
1	ccc	266	GLN

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Mol	Chain	Res	Type
1	ddd	134	GLU
1	ddd	182	LEU
1	ddd	216	SER
1	ddd	255	SER
1	ddd	256	SER
1	ddd	266	GLN

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

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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

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

6.1 Protein, DNA and RNA chains

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, 95^{th} 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%)	-0.15	1 (0%)	92	91	32, 49, 70, 117	0
1	BBB	270/293 (92%)	-0.10	2 (0%)	87	85	37, 52, 80, 124	0
1	CCC	268/293 (91%)	-0.21	1 (0%)	92	91	35, 47, 67, 89	0
1	DDD	267/293 (91%)	-0.23	0	100	100	30, 44, 58, 84	0
1	EEE	270/293 (92%)	-0.13	0	100	100	32, 46, 68, 97	0
1	FFF	270/293 (92%)	-0.08	1 (0%)	92	91	32, 51, 67, 91	0
1	GGG	268/293 (91%)	-0.15	0	100	100	34, 49, 63, 79	0
1	HHH	265/293 (90%)	-0.13	0	100	100	35, 50, 70, 114	0
1	III	269/293 (91%)	-0.12	2 (0%)	87	85	33, 47, 71, 111	0
1	JJJ	262/293 (89%)	-0.12	2 (0%)	86	84	35, 51, 71, 93	0
1	KKK	268/293 (91%)	-0.08	2 (0%)	87	85	38, 51, 67, 107	0
1	LLL	268/293 (91%)	-0.10	0	100	100	34, 52, 74, 130	0
1	MMM	258/293 (88%)	0.09	9 (3%)	44	37	45, 60, 76, 94	0
1	NNN	266/293 (90%)	-0.03	2 (0%)	86	84	45, 62, 82, 112	0
1	OOO	270/293 (92%)	0.02	2 (0%)	87	85	37, 59, 77, 117	0
1	PPP	264/293 (90%)	0.01	1 (0%)	92	91	39, 54, 74, 95	0
1	QQQ	269/293 (91%)	-0.01	1 (0%)	92	91	38, 52, 67, 86	0
1	RRR	263/293 (89%)	-0.01	5 (1%)	66	62	40, 55, 72, 93	0
1	SSS	268/293 (91%)	-0.05	2 (0%)	87	85	36, 55, 71, 81	0
1	TTT	270/293 (92%)	-0.14	1 (0%)	92	91	40, 54, 68, 95	0
1	UUU	261/293 (89%)	0.19	6 (2%)	60	55	42, 60, 79, 100	0
1	VVV	261/293 (89%)	0.27	7 (2%)	54	49	46, 74, 92, 107	0
1	WWW	268/293 (91%)	0.39	14 (5%)	27	21	43, 73, 94, 114	0
1	XXX	267/293 (91%)	0.23	6 (2%)	62	57	43, 63, 81, 98	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å^2)	Q<0.9
1	YYY	262/293 (89%)	0.08	3 (1%)	80 78	43, 63, 83, 93	0
1	ZZZ	259/293 (88%)	0.19	5 (1%)	66 62	42, 64, 86, 110	0
1	aaa	266/293 (90%)	0.11	5 (1%)	66 62	40, 61, 86, 122	0
1	bbb	253/293 (86%)	-0.01	4 (1%)	72 68	36, 55, 82, 103	0
1	ccc	255/293 (87%)	0.05	3 (1%)	79 76	43, 63, 85, 134	0
1	ddd	260/293 (88%)	0.18	4 (1%)	73 70	44, 65, 85, 106	0
All	All	7948/8790 (90%)	-0.00	91 (1%)	80 78	30, 55, 81, 134	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	WWW	128	GLY	4.0
1	WWW	79	ALA	3.9
1	WWW	275	GLY	3.8
1	RRR	86	LEU	3.6
1	MMM	242	GLY	3.5
1	UUU	275	GLY	3.4
1	RRR	96	LEU	3.4
1	YYY	145	GLY	3.3
1	AAA	33	PRO	3.2
1	WWW	76	TYR	3.2
1	VVV	284	LEU	3.1
1	JJJ	86	LEU	3.1
1	ZZZ	35	SER	3.1
1	MMM	145	GLY	3.1
1	VVV	41	ALA	3.0
1	ZZZ	60	ALA	3.0
1	ZZZ	242	GLY	3.0
1	VVV	79	ALA	3.0
1	OOO	96	LEU	2.9
1	RRR	284	LEU	2.9
1	MMM	52	GLY	2.8
1	XXX	83	LEU	2.8
1	MMM	225	PRO	2.8
1	UUU	65	ASN	2.8
1	WWW	269	GLN	2.7
1	aaa	33	PRO	2.7
1	ccc	127	TYR	2.7
1	WWW	93	PRO	2.7
1	ddd	97	MET	2.6

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Mol	Chain	Res	Type	RSRZ
1	VVV	97	MET	2.6
1	ZZZ	144	GLY	2.6
1	YYY	76	TYR	2.6
1	BBB	24	ILE	2.6
1	QQQ	221	VAL	2.6
1	NNN	97	MET	2.6
1	aaa	101	VAL	2.6
1	III	86	LEU	2.5
1	WWW	220	GLY	2.5
1	aaa	287	ARG	2.5
1	UUU	94	THR	2.5
1	ZZZ	145	GLY	2.5
1	bbb	35	SER	2.5
1	VVV	218	THR	2.5
1	WWW	242	GLY	2.4
1	bbb	284	LEU	2.4
1	BBB	76	TYR	2.4
1	XXX	41	ALA	2.4
1	UUU	289	VAL	2.4
1	TTT	97	MET	2.4
1	OOO	242	GLY	2.4
1	XXX	284	LEU	2.3
1	NNN	203	PRO	2.3
1	ccc	287	ARG	2.3
1	WWW	261	GLY	2.3
1	MMM	223	THR	2.3
1	YYY	242	GLY	2.3
1	ddd	127	TYR	2.3
1	bbb	84	PRO	2.2
1	aaa	36	THR	2.2
1	UUU	225	PRO	2.2
1	MMM	64	TYR	2.2
1	XXX	79	ALA	2.2
1	VVV	47	VAL	2.2
1	CCC	220	GLY	2.2
1	XXX	221	VAL	2.2
1	FFF	70	LEU	2.2
1	WWW	240	GLU	2.2
1	ccc	98	TRP	2.2
1	WWW	42	TYR	2.1
1	III	172	ASP	2.1
1	aaa	70	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	WWW	41	ALA	2.1
1	bbb	36	THR	2.1
1	SSS	95	LEU	2.1
1	KKK	224	PRO	2.1
1	PPP	35	SER	2.1
1	MMM	220	GLY	2.1
1	MMM	26	VAL	2.0
1	XXX	226	VAL	2.0
1	RRR	97	MET	2.0
1	UUU	223	THR	2.0
1	MMM	133	ILE	2.0
1	RRR	73	ILE	2.0
1	SSS	171	PRO	2.0
1	ddd	100	ALA	2.0
1	WWW	66	ASP	2.0
1	VVV	289	VAL	2.0
1	KKK	127	TYR	2.0
1	JJJ	128	GLY	2.0
1	WWW	247	CYS	2.0
1	ddd	237	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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, 95^{th} 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	BBB	304	1/1	0.71	0.26	90,90,90,90	0
2	CL	bbb	302	1/1	0.71	0.17	68,68,68,68	0
2	CL	OOO	303	1/1	0.74	0.10	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CL	DDD	301	1/1	0.74	0.09	69,69,69,69	0
2	CL	SSS	301	1/1	0.76	0.38	84,84,84,84	0
2	CL	NNN	301	1/1	0.78	0.10	74,74,74,74	0
2	CL	JJJ	302	1/1	0.80	0.10	71,71,71,71	0
2	CL	bbb	301	1/1	0.84	0.10	80,80,80,80	0
2	CL	BBB	302	1/1	0.85	0.14	73,73,73,73	0
2	CL	LLL	303	1/1	0.86	0.09	84,84,84,84	0
2	CL	ddd	301	1/1	0.86	0.08	74,74,74,74	0
2	CL	MMM	301	1/1	0.87	0.14	71,71,71,71	0
2	CL	QQQ	302	1/1	0.87	0.09	70,70,70,70	0
2	CL	HHH	301	1/1	0.87	0.07	79,79,79,79	0
2	CL	OOO	302	1/1	0.88	0.07	70,70,70,70	0
2	CL	KKK	301	1/1	0.89	0.12	58,58,58,58	0
2	CL	LLL	301	1/1	0.90	0.10	80,80,80,80	0
2	CL	LLL	302	1/1	0.90	0.09	75,75,75,75	0
2	CL	AAA	301	1/1	0.90	0.13	61,61,61,61	0
2	CL	III	303	1/1	0.90	0.10	73,73,73,73	0
2	CL	FFF	303	1/1	0.90	0.08	68,68,68,68	0
2	CL	GGG	303	1/1	0.90	0.17	79,79,79,79	0
2	CL	TTT	301	1/1	0.91	0.21	65,65,65,65	0
2	CL	UUU	301	1/1	0.91	0.29	63,63,63,63	0
2	CL	CCC	301	1/1	0.91	0.09	55,55,55,55	0
2	CL	FFF	302	1/1	0.91	0.32	71,71,71,71	0
2	CL	KKK	302	1/1	0.91	0.15	66,66,66,66	0
2	CL	aaa	301	1/1	0.92	0.12	60,60,60,60	0
2	CL	BBB	305	1/1	0.92	0.07	69,69,69,69	0
2	CL	GGG	302	1/1	0.92	0.15	65,65,65,65	0
2	CL	III	302	1/1	0.92	0.18	68,68,68,68	0
2	CL	AAA	302	1/1	0.93	0.14	69,69,69,69	0
2	CL	UUU	302	1/1	0.93	0.19	62,62,62,62	0
2	CL	XXX	301	1/1	0.93	0.21	66,66,66,66	0
2	CL	XXX	303	1/1	0.93	0.11	69,69,69,69	0
2	CL	ZZZ	301	1/1	0.93	0.15	62,62,62,62	0
2	CL	PPP	302	1/1	0.93	0.12	65,65,65,65	0
2	CL	aaa	302	1/1	0.93	0.09	66,66,66,66	0
2	CL	FFF	301	1/1	0.93	0.25	62,62,62,62	0
2	CL	OOO	301	1/1	0.93	0.13	66,66,66,66	0
2	CL	CCC	303	1/1	0.93	0.11	79,79,79,79	0
2	CL	ddd	302	1/1	0.93	0.07	61,61,61,61	0
2	CL	RRR	303	1/1	0.94	0.13	66,66,66,66	0
2	CL	QQQ	301	1/1	0.94	0.08	68,68,68,68	0
2	CL	AAA	303	1/1	0.94	0.34	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CL	XXX	302	1/1	0.94	0.20	59,59,59,59	0
2	CL	EEE	301	1/1	0.95	0.13	58,58,58,58	0
2	CL	YYY	301	1/1	0.95	0.12	66,66,66,66	0
2	CL	HHH	302	1/1	0.95	0.11	62,62,62,62	0
2	CL	LLL	305	1/1	0.95	0.06	67,67,67,67	0
2	CL	KKK	303	1/1	0.95	0.18	61,61,61,61	0
2	CL	MMM	302	1/1	0.95	0.22	65,65,65,65	0
2	CL	WWW	301	1/1	0.95	0.29	61,61,61,61	0
2	CL	bbb	303	1/1	0.95	0.25	73,73,73,73	0
2	CL	III	301	1/1	0.95	0.06	59,59,59,59	0
2	CL	RRR	302	1/1	0.95	0.09	68,68,68,68	0
2	CL	PPP	301	1/1	0.96	0.13	60,60,60,60	0
2	CL	YYY	302	1/1	0.96	0.07	53,53,53,53	0
2	CL	PPP	303	1/1	0.96	0.28	61,61,61,61	0
2	CL	RRR	301	1/1	0.96	0.18	58,58,58,58	0
2	CL	VVV	301	1/1	0.96	0.17	62,62,62,62	0
2	CL	BBB	301	1/1	0.97	0.12	65,65,65,65	0
2	CL	LLL	304	1/1	0.97	0.18	62,62,62,62	0
2	CL	ccc	301	1/1	0.97	0.09	56,56,56,56	0
2	CL	GGG	301	1/1	0.97	0.22	60,60,60,60	0
2	CL	HHH	303	1/1	0.97	0.13	63,63,63,63	0
2	CL	JJJ	303	1/1	0.98	0.17	48,48,48,48	0
2	CL	BBB	303	1/1	0.98	0.16	51,51,51,51	0
2	CL	CCC	302	1/1	0.98	0.24	48,48,48,48	0
2	CL	OOO	304	1/1	0.98	0.24	63,63,63,63	0
2	CL	JJJ	301	1/1	0.99	0.11	56,56,56,56	0

6.5 Other polymers (i)

There are no such residues in this entry.