



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 19, 2016 – 10:39 PM GMT

PDB ID : 4WIZ  
Title : Crystal structure of Grouper nervous necrosis virus-like particle at 3.6Å  
Authors : Chen, N.C.; Chen, C.J.; Yoshimura, M.; Guan, H.H.; Chen, T.Y.  
Deposited on : 2014-09-28  
Resolution : 3.60 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : unknown  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026982  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20026982

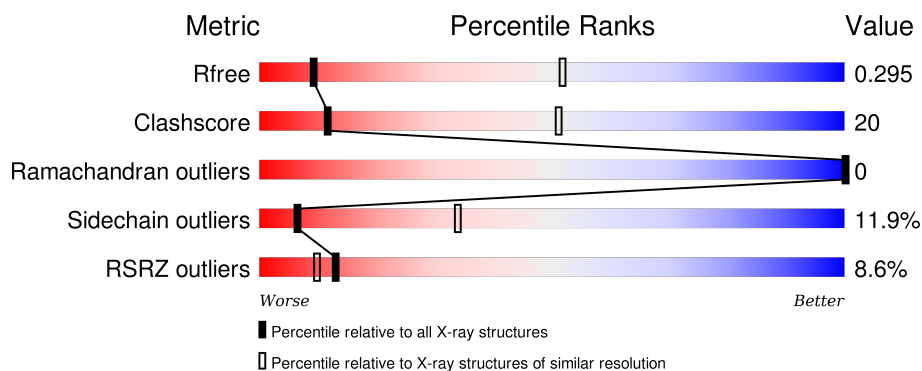
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.60 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))
$R_{free}$	91344	1408 (3.80-3.40)
Clashscore	102246	1010 (3.74-3.46)
Ramachandran outliers	100387	1007 (3.76-3.44)
Sidechain outliers	100360	1007 (3.76-3.44)
RSRZ outliers	91569	1003 (3.78-3.42)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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	AA	338	<div> <div>18%</div> <div>49% 33% 15%</div> </div>
1	AB	338	<div> <div>8%</div> <div>48% 33% 15%</div> </div>
1	AC	338	<div> <div>5%</div> <div>47% 33% 15%</div> </div>
1	AD	338	<div> <div>2%</div> <div>48% 31% 5% 15%</div> </div>
1	AE	338	<div> <div>2%</div> <div>51% 29% 15%</div> </div>

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Mol	Chain	Length	Quality of chain
1	AF	338	
1	AG	338	
1	AH	338	
1	AI	338	
1	AJ	338	
1	AK	338	
1	AL	338	
1	AM	338	
1	AN	338	
1	AO	338	
1	AP	338	
1	AQ	338	
1	AR	338	
1	AS	338	
1	AT	338	
1	AU	338	
1	AV	338	
1	AW	338	
1	AX	338	
1	AY	338	
1	AZ	338	
1	Aa	338	
1	Ab	338	
1	Ac	338	
1	Ad	338	

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Mol	Chain	Length	Quality of chain
1	BA	338	
1	BB	338	
1	BC	338	
1	BD	338	
1	BE	338	
1	BF	338	
1	BG	338	
1	BH	338	
1	BI	338	
1	BJ	338	
1	BK	338	
1	BL	338	
1	BM	338	
1	BN	338	
1	BO	338	
1	BP	338	
1	BQ	338	
1	BR	338	
1	BS	338	
1	BT	338	
1	BU	338	
1	BV	338	
1	BW	338	
1	BX	338	
1	BY	338	

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Mol	Chain	Length	Quality of chain
1	BZ	338	
1	Ba	338	
1	Bb	338	
1	Bc	338	
1	Bd	338	
1	CA	338	
1	CB	338	
1	CC	338	
1	CD	338	
1	CE	338	
1	CF	338	
1	CG	338	
1	CH	338	
1	CI	338	
1	CJ	338	
1	CK	338	
1	CL	338	
1	CM	338	
1	CN	338	
1	CO	338	
1	CP	338	
1	CQ	338	
1	CR	338	
1	CS	338	
1	CT	338	

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Mol	Chain	Length	Quality of chain
1	CU	338	
1	CV	338	
1	CW	338	
1	CX	338	
1	CY	338	
1	CZ	338	
1	Ca	338	
1	Cb	338	
1	Cc	338	
1	Cd	338	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 203250 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 Coat protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	BA	286	Total	C	N	O	S	0	0	0
			2214	1401	381	425	7			
1	AA	287	Total	C	N	O	S	0	0	0
			2218	1403	382	426	7			
1	CA	304	Total	C	N	O	S	0	0	0
			2340	1477	406	450	7			
1	BB	286	Total	C	N	O	S	0	0	0
			2214	1401	381	425	7			
1	AB	287	Total	C	N	O	S	0	0	0
			2218	1403	382	426	7			
1	CB	304	Total	C	N	O	S	0	0	0
			2340	1477	406	450	7			
1	BC	286	Total	C	N	O	S	0	0	0
			2214	1401	381	425	7			
1	AC	287	Total	C	N	O	S	0	0	0
			2218	1403	382	426	7			
1	CC	304	Total	C	N	O	S	0	0	0
			2340	1477	406	450	7			
1	BD	286	Total	C	N	O	S	0	0	0
			2214	1401	381	425	7			
1	AD	287	Total	C	N	O	S	0	0	0
			2218	1403	382	426	7			
1	CD	304	Total	C	N	O	S	0	0	0
			2340	1477	406	450	7			
1	BE	286	Total	C	N	O	S	0	0	0
			2214	1401	381	425	7			
1	AE	287	Total	C	N	O	S	0	0	0
			2218	1403	382	426	7			
1	CE	304	Total	C	N	O	S	0	0	0
			2340	1477	406	450	7			
1	BF	286	Total	C	N	O	S	0	0	0
			2214	1401	381	425	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AF	287	Total	C	N	O	S	0	0	0
			2218	1403	382	426	7			
1	CF	304	Total	C	N	O	S	0	0	0
			2340	1477	406	450	7			
1	BG	286	Total	C	N	O	S	0	0	0
			2214	1401	381	425	7			
1	AG	287	Total	C	N	O	S	0	0	0
			2218	1403	382	426	7			
1	CG	304	Total	C	N	O	S	0	0	0
			2340	1477	406	450	7			
1	BH	286	Total	C	N	O	S	0	0	0
			2214	1401	381	425	7			
1	AH	287	Total	C	N	O	S	0	0	0
			2218	1403	382	426	7			
1	CH	304	Total	C	N	O	S	0	0	0
			2340	1477	406	450	7			
1	BI	286	Total	C	N	O	S	0	0	0
			2214	1401	381	425	7			
1	AI	287	Total	C	N	O	S	0	0	0
			2218	1403	382	426	7			
1	CI	304	Total	C	N	O	S	0	0	0
			2340	1477	406	450	7			
1	BJ	286	Total	C	N	O	S	0	0	0
			2214	1401	381	425	7			
1	AJ	287	Total	C	N	O	S	0	0	0
			2218	1403	382	426	7			
1	CJ	304	Total	C	N	O	S	0	0	0
			2340	1477	406	450	7			
1	BK	286	Total	C	N	O	S	0	0	0
			2214	1401	381	425	7			
1	AK	287	Total	C	N	O	S	0	0	0
			2218	1403	382	426	7			
1	CK	304	Total	C	N	O	S	0	0	0
			2340	1477	406	450	7			
1	BL	286	Total	C	N	O	S	0	0	0
			2214	1401	381	425	7			
1	AL	287	Total	C	N	O	S	0	0	0
			2218	1403	382	426	7			
1	CL	304	Total	C	N	O	S	0	0	0
			2340	1477	406	450	7			
1	BM	286	Total	C	N	O	S	0	0	0
			2214	1401	381	425	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AM	287	Total	C	N	O	S	0	0	0
			2218	1403	382	426	7			
1	CM	304	Total	C	N	O	S	0	0	0
			2340	1477	406	450	7			
1	BN	286	Total	C	N	O	S	0	0	0
			2214	1401	381	425	7			
1	AN	287	Total	C	N	O	S	0	0	0
			2218	1403	382	426	7			
1	CN	304	Total	C	N	O	S	0	0	0
			2340	1477	406	450	7			
1	BO	286	Total	C	N	O	S	0	0	0
			2214	1401	381	425	7			
1	AO	287	Total	C	N	O	S	0	0	0
			2218	1403	382	426	7			
1	CO	304	Total	C	N	O	S	0	0	0
			2340	1477	406	450	7			
1	BP	286	Total	C	N	O	S	0	0	0
			2214	1401	381	425	7			
1	AP	287	Total	C	N	O	S	0	0	0
			2218	1403	382	426	7			
1	CP	304	Total	C	N	O	S	0	0	0
			2340	1477	406	450	7			
1	BQ	286	Total	C	N	O	S	0	0	0
			2214	1401	381	425	7			
1	AQ	287	Total	C	N	O	S	0	0	0
			2218	1403	382	426	7			
1	CQ	304	Total	C	N	O	S	0	0	0
			2340	1477	406	450	7			
1	BR	286	Total	C	N	O	S	0	0	0
			2214	1401	381	425	7			
1	AR	287	Total	C	N	O	S	0	0	0
			2218	1403	382	426	7			
1	CR	304	Total	C	N	O	S	0	0	0
			2340	1477	406	450	7			
1	BS	286	Total	C	N	O	S	0	0	0
			2214	1401	381	425	7			
1	AS	287	Total	C	N	O	S	0	0	0
			2218	1403	382	426	7			
1	CS	304	Total	C	N	O	S	0	0	0
			2340	1477	406	450	7			
1	BT	286	Total	C	N	O	S	0	0	0
			2214	1401	381	425	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AT	287	Total	C	N	O	S	0	0	0
			2218	1403	382	426	7			
1	CT	304	Total	C	N	O	S	0	0	0
			2340	1477	406	450	7			
1	BU	286	Total	C	N	O	S	0	0	0
			2214	1401	381	425	7			
1	AU	287	Total	C	N	O	S	0	0	0
			2218	1403	382	426	7			
1	CU	304	Total	C	N	O	S	0	0	0
			2340	1477	406	450	7			
1	BV	286	Total	C	N	O	S	0	0	0
			2214	1401	381	425	7			
1	AV	287	Total	C	N	O	S	0	0	0
			2218	1403	382	426	7			
1	CV	304	Total	C	N	O	S	0	0	0
			2340	1477	406	450	7			
1	BW	286	Total	C	N	O	S	0	0	0
			2214	1401	381	425	7			
1	AW	287	Total	C	N	O	S	0	0	0
			2218	1403	382	426	7			
1	CW	304	Total	C	N	O	S	0	0	0
			2340	1477	406	450	7			
1	BX	286	Total	C	N	O	S	0	0	0
			2214	1401	381	425	7			
1	AX	287	Total	C	N	O	S	0	0	0
			2218	1403	382	426	7			
1	CX	304	Total	C	N	O	S	0	0	0
			2340	1477	406	450	7			
1	BY	286	Total	C	N	O	S	0	0	0
			2214	1401	381	425	7			
1	AY	287	Total	C	N	O	S	0	0	0
			2218	1403	382	426	7			
1	CY	304	Total	C	N	O	S	0	0	0
			2340	1477	406	450	7			
1	BZ	286	Total	C	N	O	S	0	0	0
			2214	1401	381	425	7			
1	AZ	287	Total	C	N	O	S	0	0	0
			2218	1403	382	426	7			
1	CZ	304	Total	C	N	O	S	0	0	0
			2340	1477	406	450	7			
1	Ba	286	Total	C	N	O	S	0	0	0
			2214	1401	381	425	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Aa	287	Total	C	N	O	S	0	0	0
			2218	1403	382	426	7			
1	Ca	304	Total	C	N	O	S	0	0	0
			2340	1477	406	450	7			
1	Bb	286	Total	C	N	O	S	0	0	0
			2214	1401	381	425	7			
1	Ab	287	Total	C	N	O	S	0	0	0
			2218	1403	382	426	7			
1	Cb	304	Total	C	N	O	S	0	0	0
			2340	1477	406	450	7			
1	Bc	286	Total	C	N	O	S	0	0	0
			2214	1401	381	425	7			
1	Ac	287	Total	C	N	O	S	0	0	0
			2218	1403	382	426	7			
1	Cc	304	Total	C	N	O	S	0	0	0
			2340	1477	406	450	7			
1	Bd	286	Total	C	N	O	S	0	0	0
			2214	1401	381	425	7			
1	Ad	287	Total	C	N	O	S	0	0	0
			2218	1403	382	426	7			
1	Cd	304	Total	C	N	O	S	0	0	0
			2340	1477	406	450	7			

There are 90 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BA	214	ASN	THR	engineered mutation	UNP Q8JNX5
AA	214	ASN	THR	engineered mutation	UNP Q8JNX5
CA	214	ASN	THR	engineered mutation	UNP Q8JNX5
BB	214	ASN	THR	engineered mutation	UNP Q8JNX5
AB	214	ASN	THR	engineered mutation	UNP Q8JNX5
CB	214	ASN	THR	engineered mutation	UNP Q8JNX5
BC	214	ASN	THR	engineered mutation	UNP Q8JNX5
AC	214	ASN	THR	engineered mutation	UNP Q8JNX5
CC	214	ASN	THR	engineered mutation	UNP Q8JNX5
BD	214	ASN	THR	engineered mutation	UNP Q8JNX5
AD	214	ASN	THR	engineered mutation	UNP Q8JNX5
CD	214	ASN	THR	engineered mutation	UNP Q8JNX5
BE	214	ASN	THR	engineered mutation	UNP Q8JNX5
AE	214	ASN	THR	engineered mutation	UNP Q8JNX5
CE	214	ASN	THR	engineered mutation	UNP Q8JNX5
BF	214	ASN	THR	engineered mutation	UNP Q8JNX5
AF	214	ASN	THR	engineered mutation	UNP Q8JNX5

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Chain	Residue	Modelled	Actual	Comment	Reference
CF	214	ASN	THR	engineered mutation	UNP Q8JNX5
BG	214	ASN	THR	engineered mutation	UNP Q8JNX5
AG	214	ASN	THR	engineered mutation	UNP Q8JNX5
CG	214	ASN	THR	engineered mutation	UNP Q8JNX5
BH	214	ASN	THR	engineered mutation	UNP Q8JNX5
AH	214	ASN	THR	engineered mutation	UNP Q8JNX5
CH	214	ASN	THR	engineered mutation	UNP Q8JNX5
BI	214	ASN	THR	engineered mutation	UNP Q8JNX5
AI	214	ASN	THR	engineered mutation	UNP Q8JNX5
CI	214	ASN	THR	engineered mutation	UNP Q8JNX5
BJ	214	ASN	THR	engineered mutation	UNP Q8JNX5
AJ	214	ASN	THR	engineered mutation	UNP Q8JNX5
CJ	214	ASN	THR	engineered mutation	UNP Q8JNX5
BK	214	ASN	THR	engineered mutation	UNP Q8JNX5
AK	214	ASN	THR	engineered mutation	UNP Q8JNX5
CK	214	ASN	THR	engineered mutation	UNP Q8JNX5
BL	214	ASN	THR	engineered mutation	UNP Q8JNX5
AL	214	ASN	THR	engineered mutation	UNP Q8JNX5
CL	214	ASN	THR	engineered mutation	UNP Q8JNX5
BM	214	ASN	THR	engineered mutation	UNP Q8JNX5
AM	214	ASN	THR	engineered mutation	UNP Q8JNX5
CM	214	ASN	THR	engineered mutation	UNP Q8JNX5
BN	214	ASN	THR	engineered mutation	UNP Q8JNX5
AN	214	ASN	THR	engineered mutation	UNP Q8JNX5
CN	214	ASN	THR	engineered mutation	UNP Q8JNX5
BO	214	ASN	THR	engineered mutation	UNP Q8JNX5
AO	214	ASN	THR	engineered mutation	UNP Q8JNX5
CO	214	ASN	THR	engineered mutation	UNP Q8JNX5
BP	214	ASN	THR	engineered mutation	UNP Q8JNX5
AP	214	ASN	THR	engineered mutation	UNP Q8JNX5
CP	214	ASN	THR	engineered mutation	UNP Q8JNX5
BQ	214	ASN	THR	engineered mutation	UNP Q8JNX5
AQ	214	ASN	THR	engineered mutation	UNP Q8JNX5
CQ	214	ASN	THR	engineered mutation	UNP Q8JNX5
BR	214	ASN	THR	engineered mutation	UNP Q8JNX5
AR	214	ASN	THR	engineered mutation	UNP Q8JNX5
CR	214	ASN	THR	engineered mutation	UNP Q8JNX5
BS	214	ASN	THR	engineered mutation	UNP Q8JNX5
AS	214	ASN	THR	engineered mutation	UNP Q8JNX5
CS	214	ASN	THR	engineered mutation	UNP Q8JNX5
BT	214	ASN	THR	engineered mutation	UNP Q8JNX5
AT	214	ASN	THR	engineered mutation	UNP Q8JNX5

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Chain	Residue	Modelled	Actual	Comment	Reference
CT	214	ASN	THR	engineered mutation	UNP Q8JNX5
BU	214	ASN	THR	engineered mutation	UNP Q8JNX5
AU	214	ASN	THR	engineered mutation	UNP Q8JNX5
CU	214	ASN	THR	engineered mutation	UNP Q8JNX5
BV	214	ASN	THR	engineered mutation	UNP Q8JNX5
AV	214	ASN	THR	engineered mutation	UNP Q8JNX5
CV	214	ASN	THR	engineered mutation	UNP Q8JNX5
BW	214	ASN	THR	engineered mutation	UNP Q8JNX5
AW	214	ASN	THR	engineered mutation	UNP Q8JNX5
CW	214	ASN	THR	engineered mutation	UNP Q8JNX5
BX	214	ASN	THR	engineered mutation	UNP Q8JNX5
AX	214	ASN	THR	engineered mutation	UNP Q8JNX5
CX	214	ASN	THR	engineered mutation	UNP Q8JNX5
BY	214	ASN	THR	engineered mutation	UNP Q8JNX5
AY	214	ASN	THR	engineered mutation	UNP Q8JNX5
CY	214	ASN	THR	engineered mutation	UNP Q8JNX5
BZ	214	ASN	THR	engineered mutation	UNP Q8JNX5
AZ	214	ASN	THR	engineered mutation	UNP Q8JNX5
CZ	214	ASN	THR	engineered mutation	UNP Q8JNX5
Ba	214	ASN	THR	engineered mutation	UNP Q8JNX5
Aa	214	ASN	THR	engineered mutation	UNP Q8JNX5
Ca	214	ASN	THR	engineered mutation	UNP Q8JNX5
Bb	214	ASN	THR	engineered mutation	UNP Q8JNX5
Ab	214	ASN	THR	engineered mutation	UNP Q8JNX5
Cb	214	ASN	THR	engineered mutation	UNP Q8JNX5
Bc	214	ASN	THR	engineered mutation	UNP Q8JNX5
Ac	214	ASN	THR	engineered mutation	UNP Q8JNX5
Cc	214	ASN	THR	engineered mutation	UNP Q8JNX5
Bd	214	ASN	THR	engineered mutation	UNP Q8JNX5
Ad	214	ASN	THR	engineered mutation	UNP Q8JNX5
Cd	214	ASN	THR	engineered mutation	UNP Q8JNX5

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	AP	1	Total Ca 1 1	0	0
2	BA	2	Total Ca 2 2	0	0
2	AK	1	Total Ca 1 1	0	0
2	AB	1	Total Ca 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	BL	2	Total 2	Ca 2	0	0
2	Ac	1	Total 1	Ca 1	0	0
2	BE	2	Total 2	Ca 2	0	0
2	AW	1	Total 1	Ca 1	0	0
2	Bd	2	Total 2	Ca 2	0	0
2	AN	1	Total 1	Ca 1	0	0
2	BP	2	Total 2	Ca 2	0	0
2	AX	1	Total 1	Ca 1	0	0
2	BI	2	Total 2	Ca 2	0	0
2	AS	1	Total 1	Ca 1	0	0
2	BB	2	Total 2	Ca 2	0	0
2	AJ	1	Total 1	Ca 1	0	0
2	BT	2	Total 2	Ca 2	0	0
2	Ba	2	Total 2	Ca 2	0	0
2	AE	1	Total 1	Ca 1	0	0
2	BM	2	Total 2	Ca 2	0	0
2	Ab	1	Total 1	Ca 1	0	0
2	BF	2	Total 2	Ca 2	0	0
2	AV	1	Total 1	Ca 1	0	0
2	BX	2	Total 2	Ca 2	0	0
2	AA	1	Total 1	Ca 1	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	BQ	2	Total 2	Ca 2	0	0
2	BJ	2	Total 2	Ca 2	0	0
2	AR	1	Total 1	Ca 1	0	0
2	BC	2	Total 2	Ca 2	0	0
2	AM	1	Total 1	Ca 1	0	0
2	BU	2	Total 2	Ca 2	0	0
2	Bb	2	Total 2	Ca 2	0	0
2	AD	1	Total 1	Ca 1	0	0
2	BN	2	Total 2	Ca 2	0	0
2	BG	2	Total 2	Ca 2	0	0
2	AI	1	Total 1	Ca 1	0	0
2	BY	2	Total 2	Ca 2	0	0
2	BR	2	Total 2	Ca 2	0	0
2	AZ	1	Total 1	Ca 1	0	0
2	Aa	1	Total 1	Ca 1	0	0
2	BK	2	Total 2	Ca 2	0	0
2	AU	1	Total 1	Ca 1	0	0
2	AL	1	Total 1	Ca 1	0	0
2	BV	2	Total 2	Ca 2	0	0
2	Bc	2	Total 2	Ca 2	0	0
2	AG	1	Total 1	Ca 1	0	0

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*Continued from previous page...*

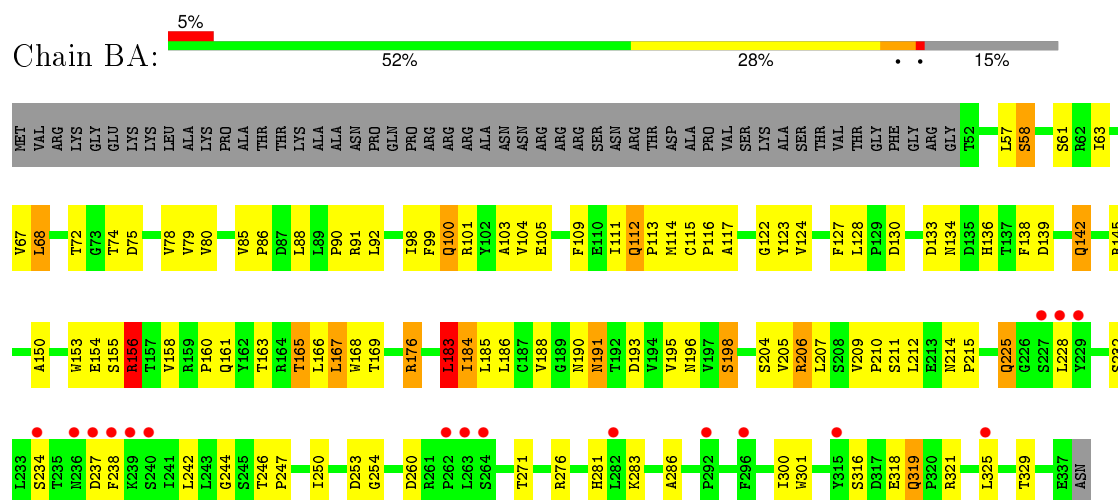
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	BO	2	Total 2	Ca 2	0	0
2	AQ	1	Total 1	Ca 1	0	0
2	Ad	1	Total 1	Ca 1	0	0
2	AH	1	Total 1	Ca 1	0	0
2	BZ	2	Total 2	Ca 2	0	0
2	AC	1	Total 1	Ca 1	0	0
2	BS	2	Total 2	Ca 2	0	0
2	BD	2	Total 2	Ca 2	0	0
2	AT	1	Total 1	Ca 1	0	0
2	AO	1	Total 1	Ca 1	0	0
2	BW	2	Total 2	Ca 2	0	0
2	AY	1	Total 1	Ca 1	0	0
2	AF	1	Total 1	Ca 1	0	0
2	BH	2	Total 2	Ca 2	0	0



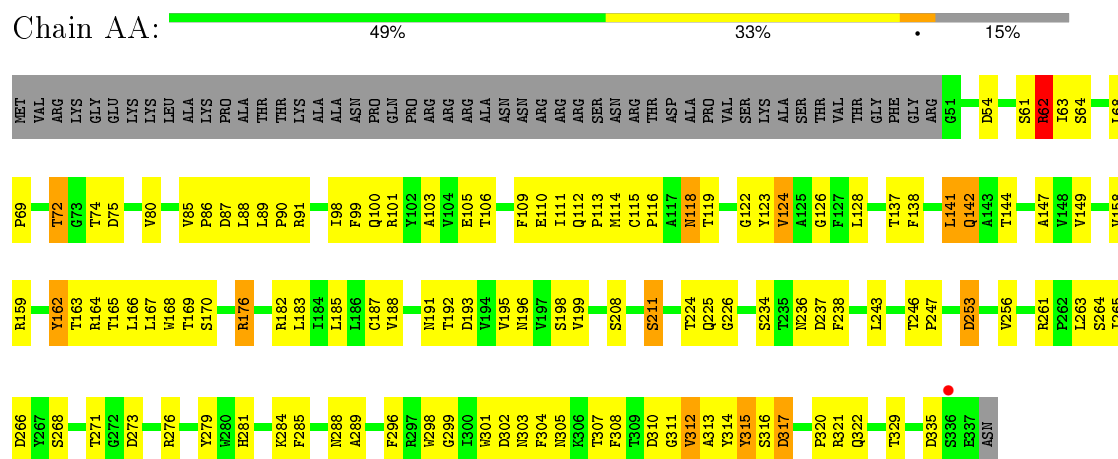
### 3 Residue-property plots

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

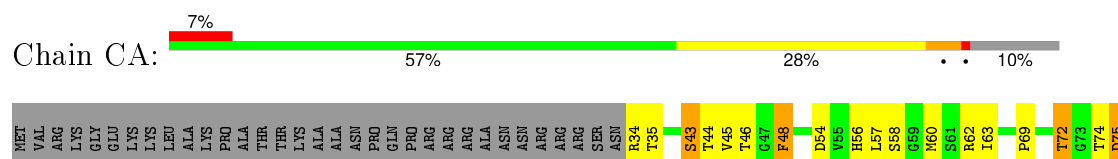
#### • Molecule 1: Coat protein

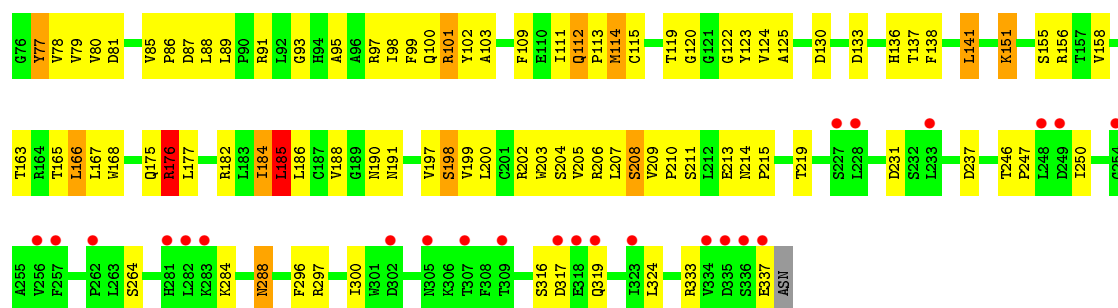


#### • Molecule 1: Coat protein

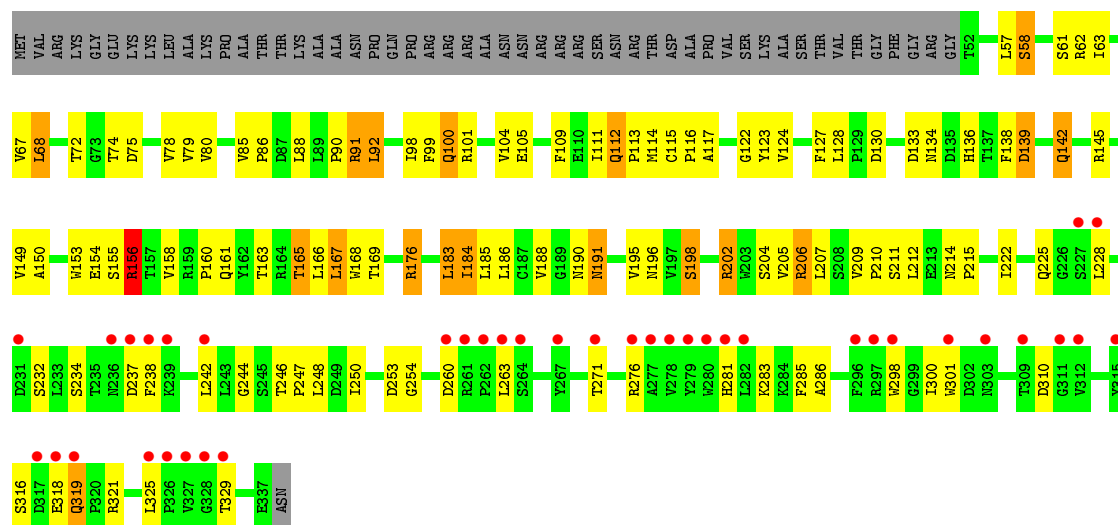


#### • Molecule 1: Coat protein

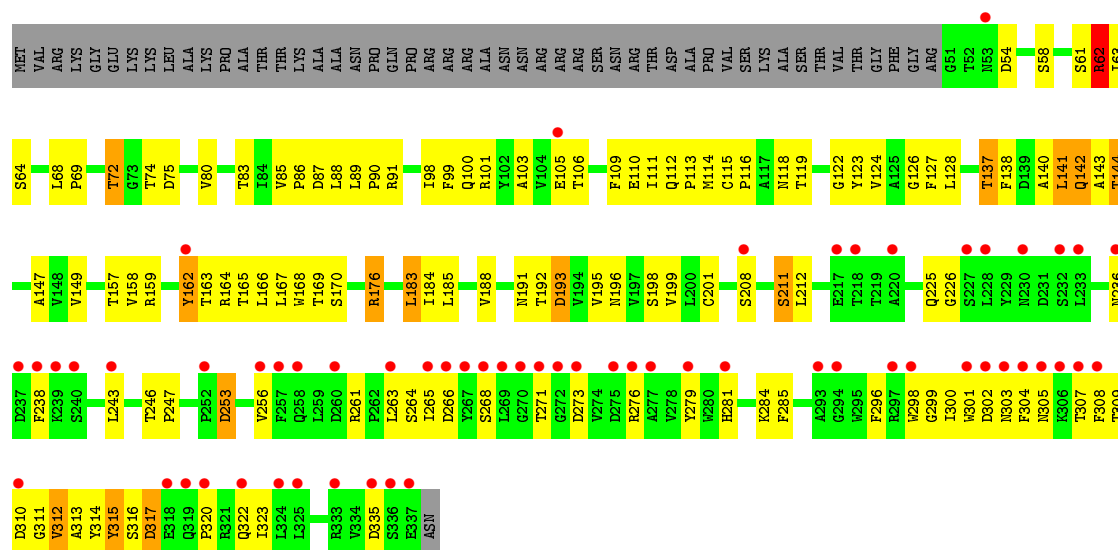




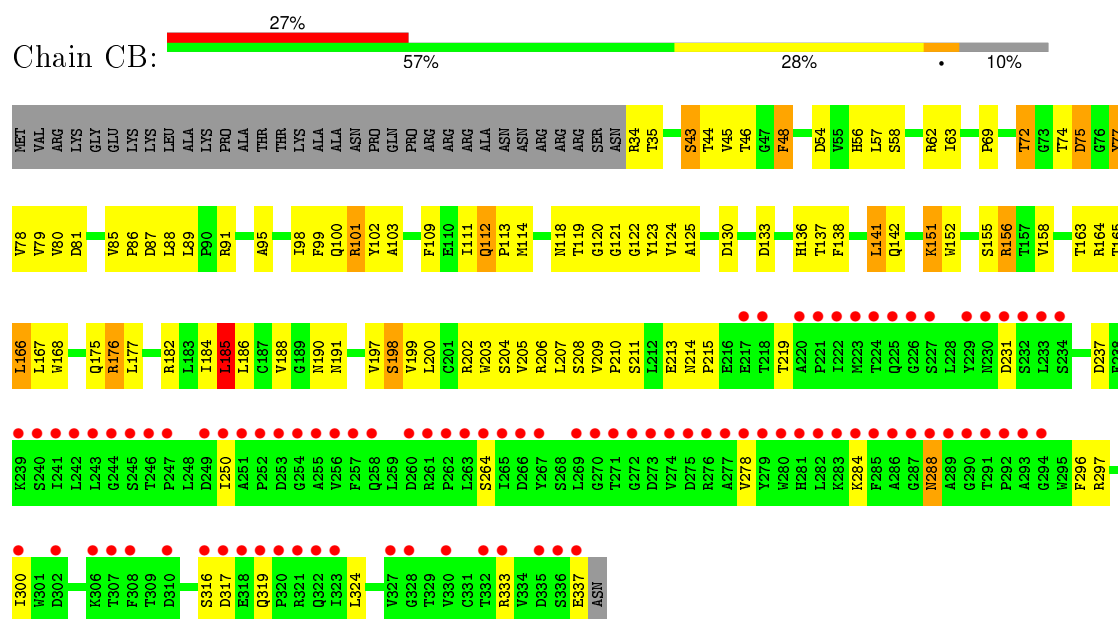
• Molecule 1: Coat protein



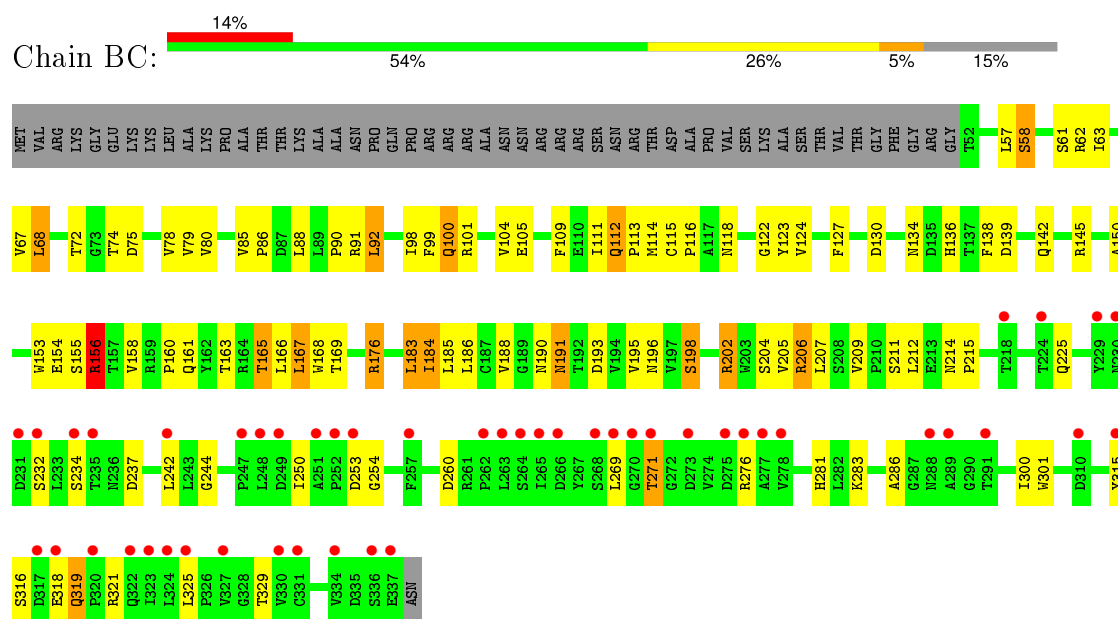
• Molecule 1: Coat protein



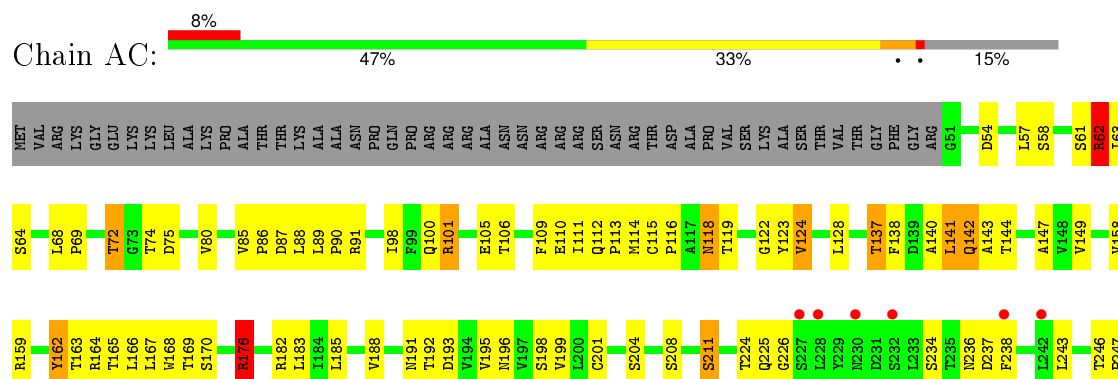
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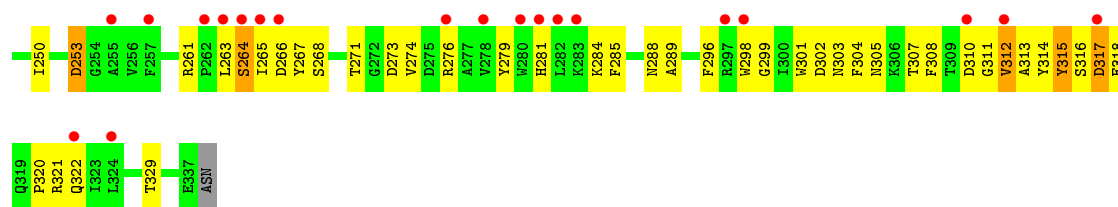


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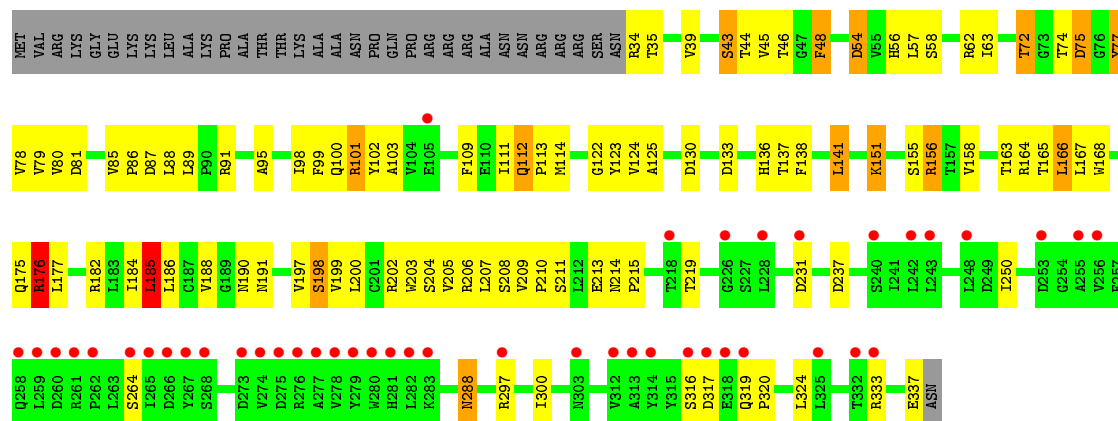


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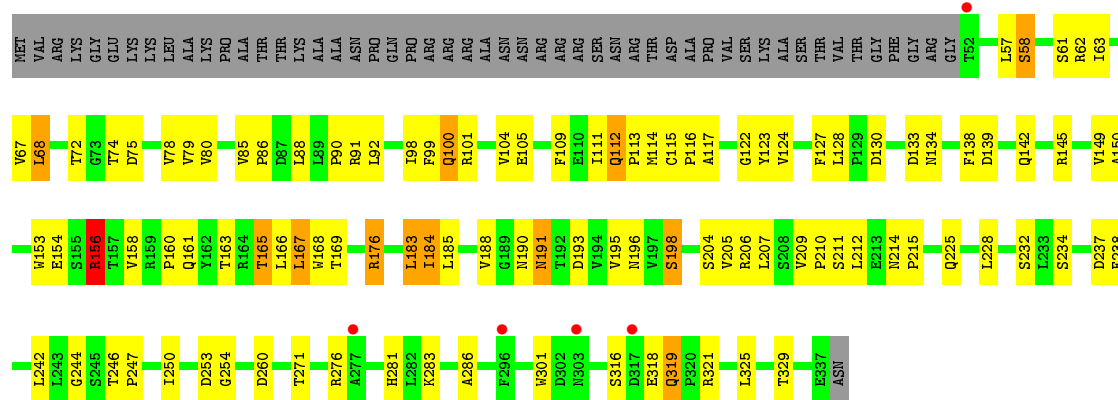




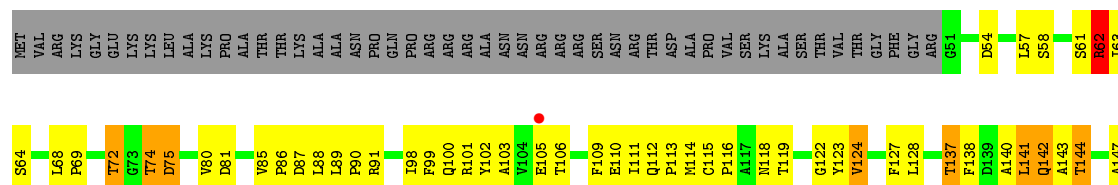
● Molecule 1: Coat protein

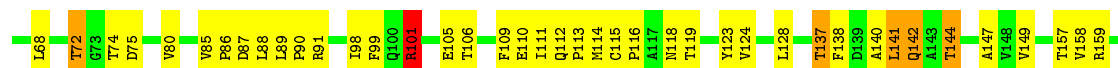


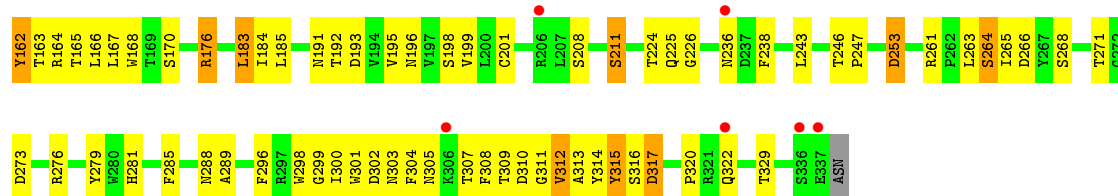
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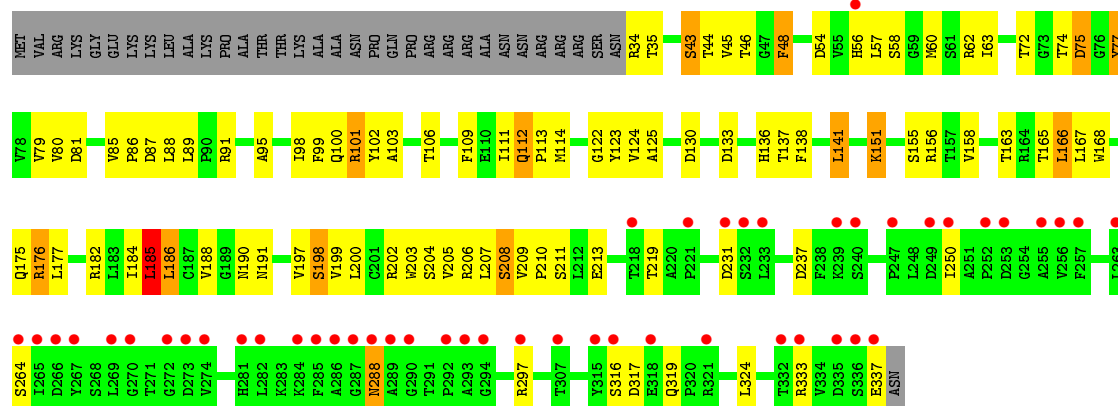
● Molecule 1: Coat protein



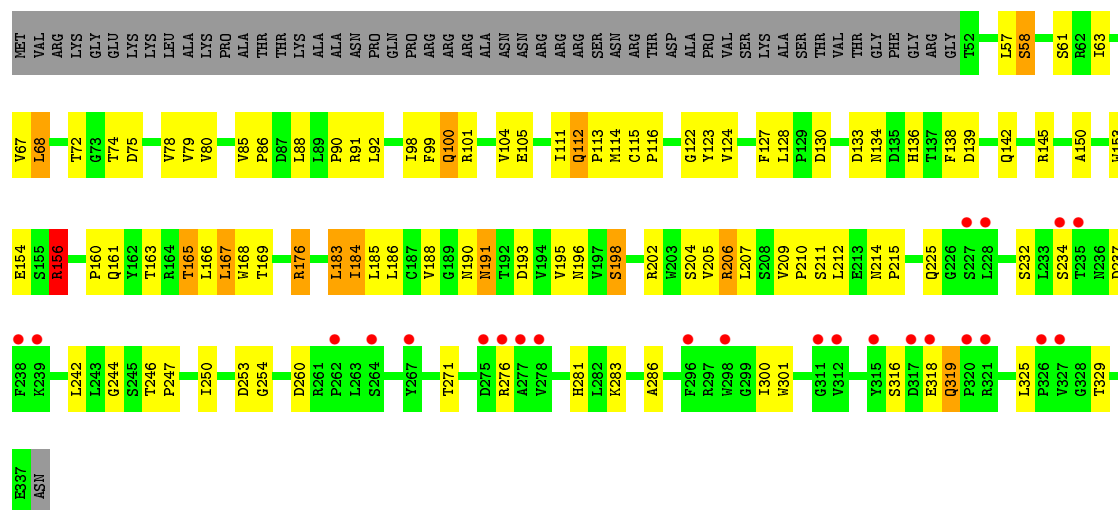




• Molecule 1: Coat protein



• Molecule 1: Coat protein



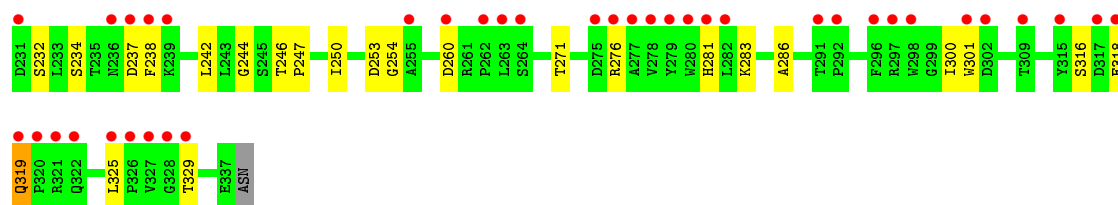
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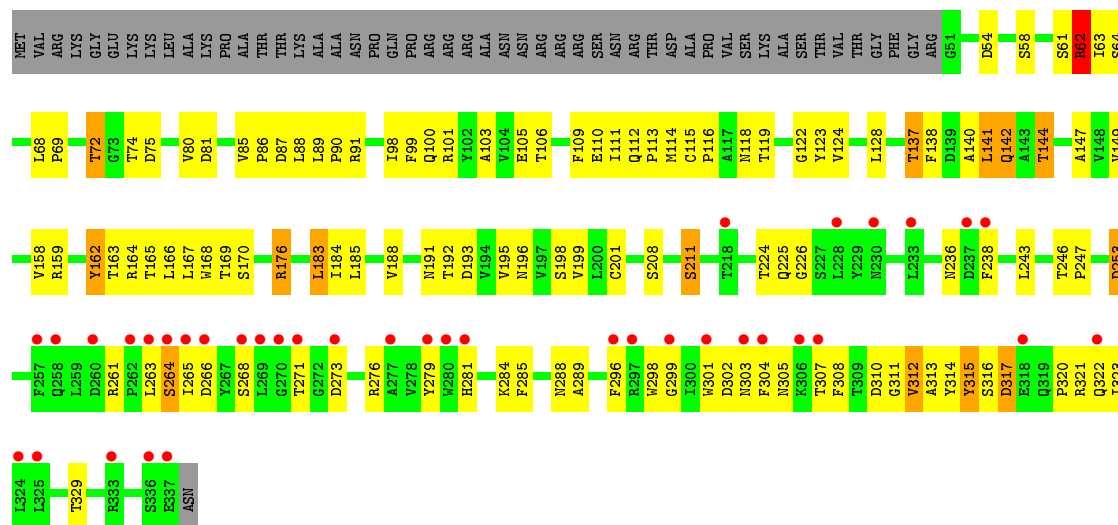




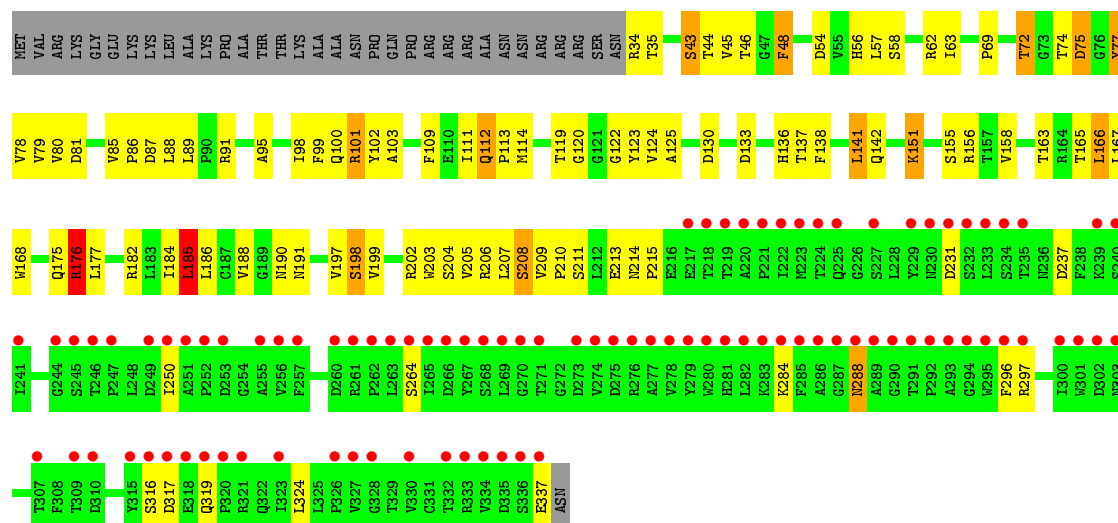




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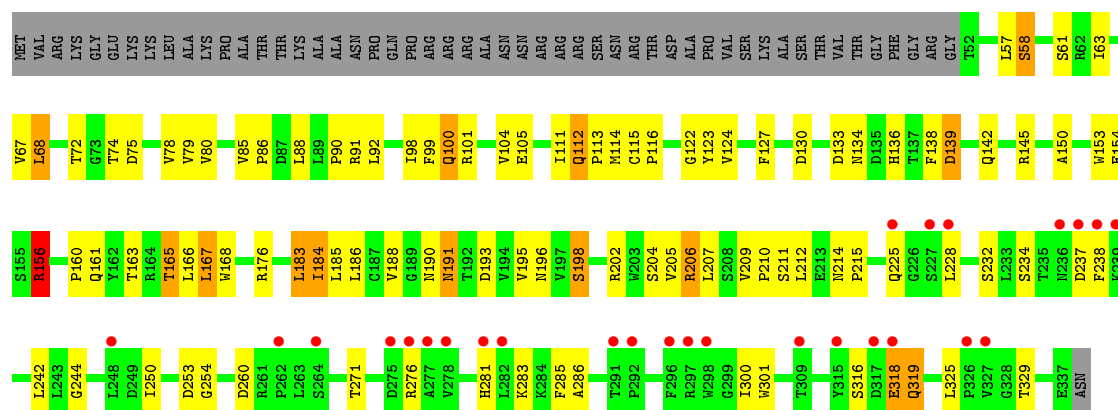


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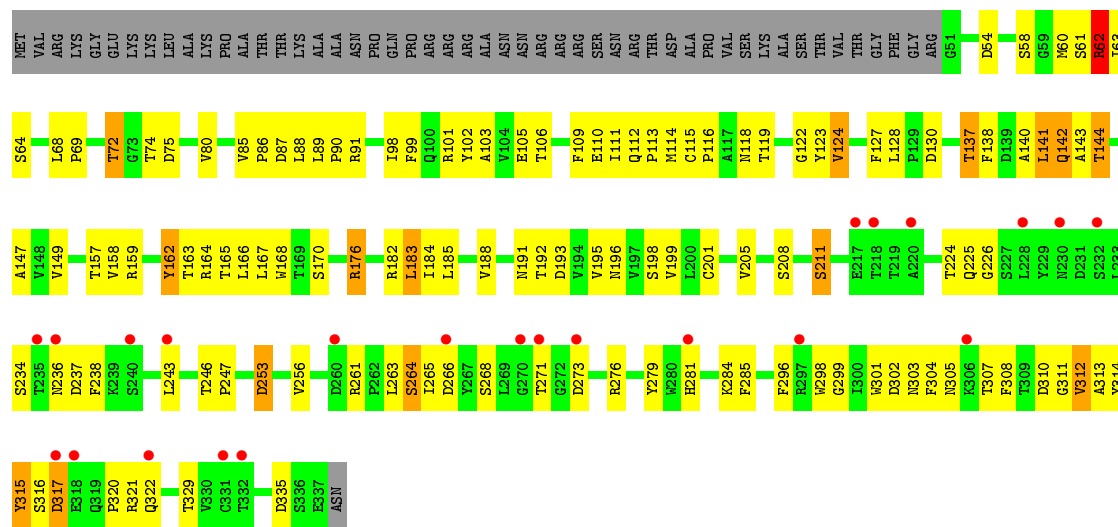


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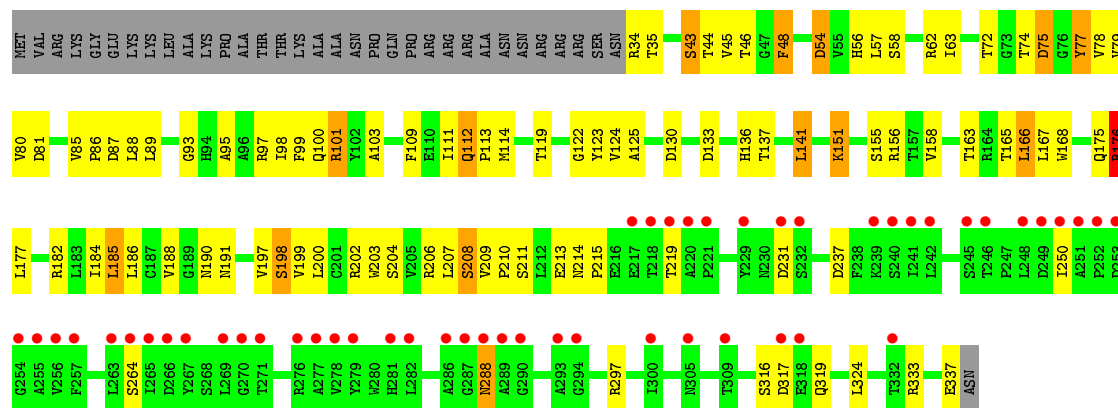




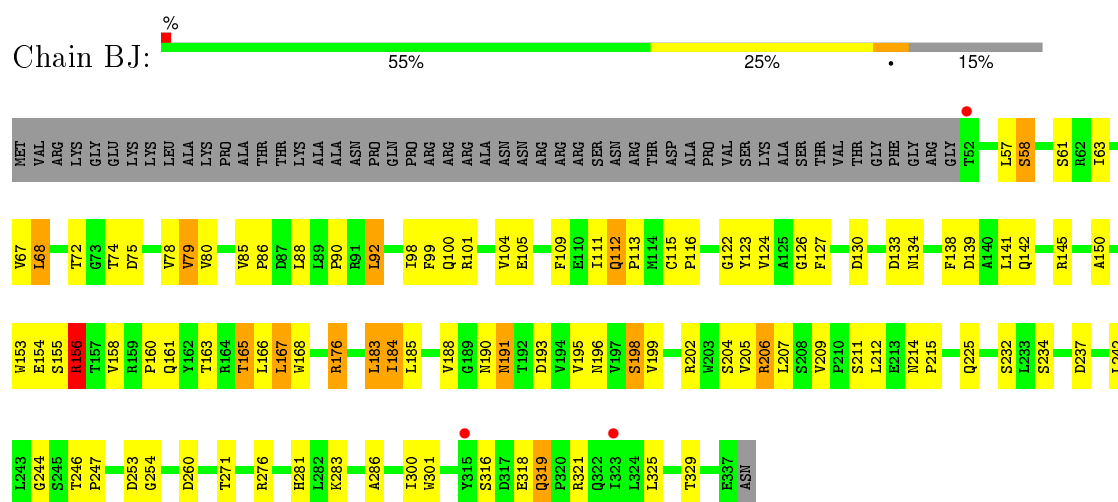
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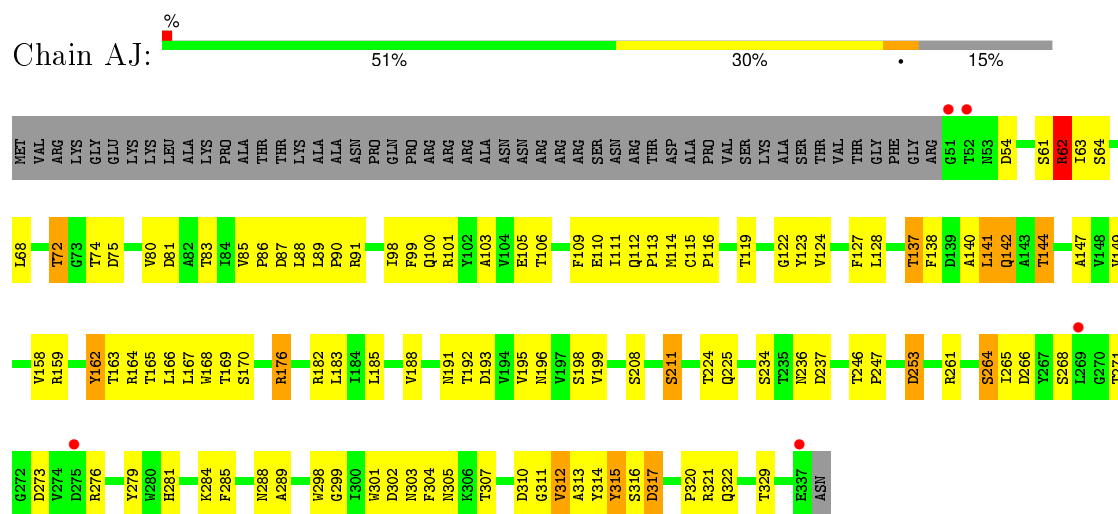
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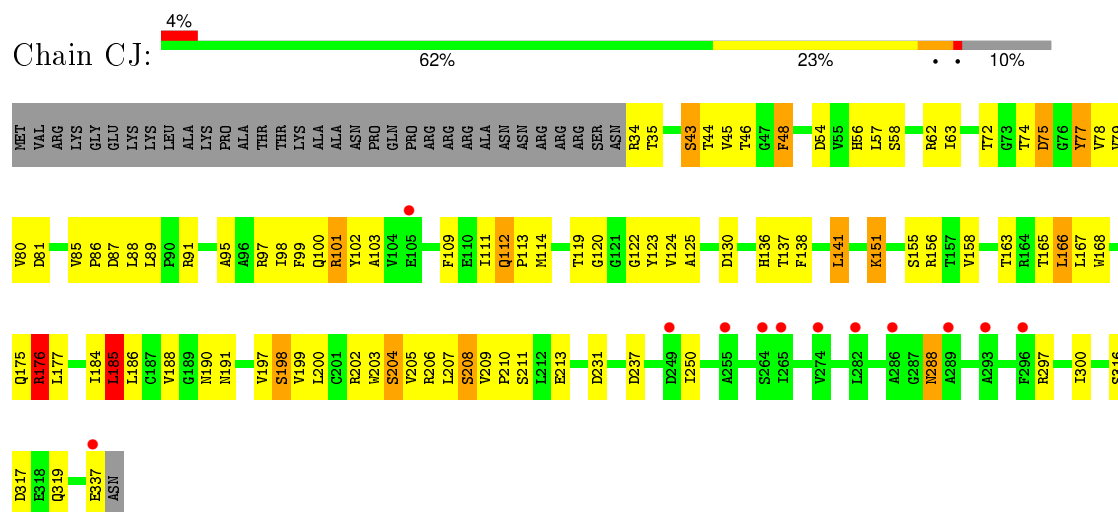
• Molecule 1: Coat protein



- Molecule 1: Coat protein

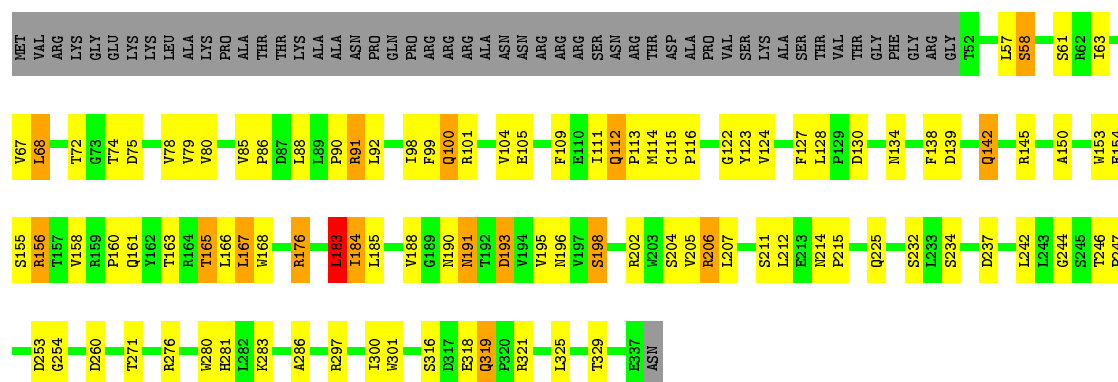


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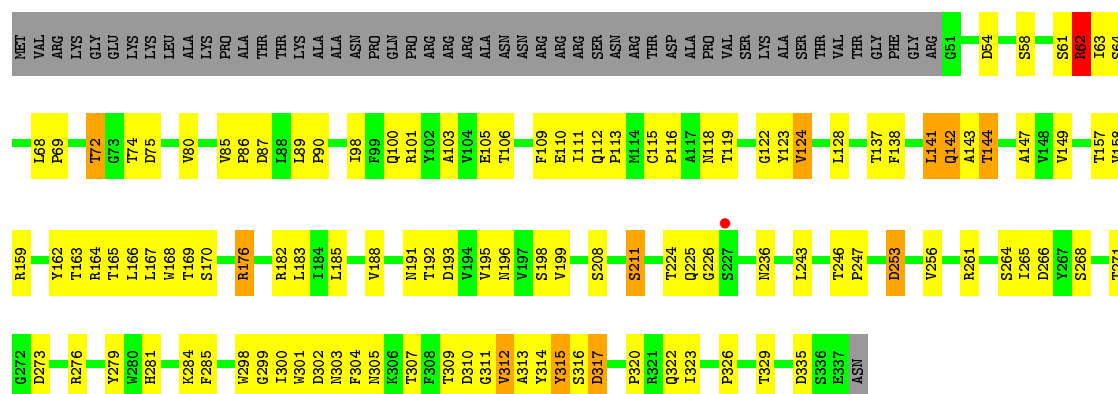


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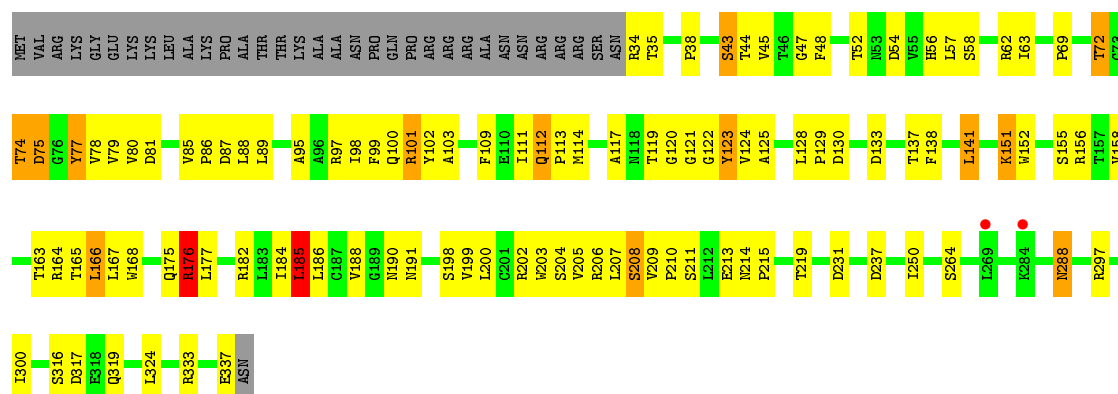




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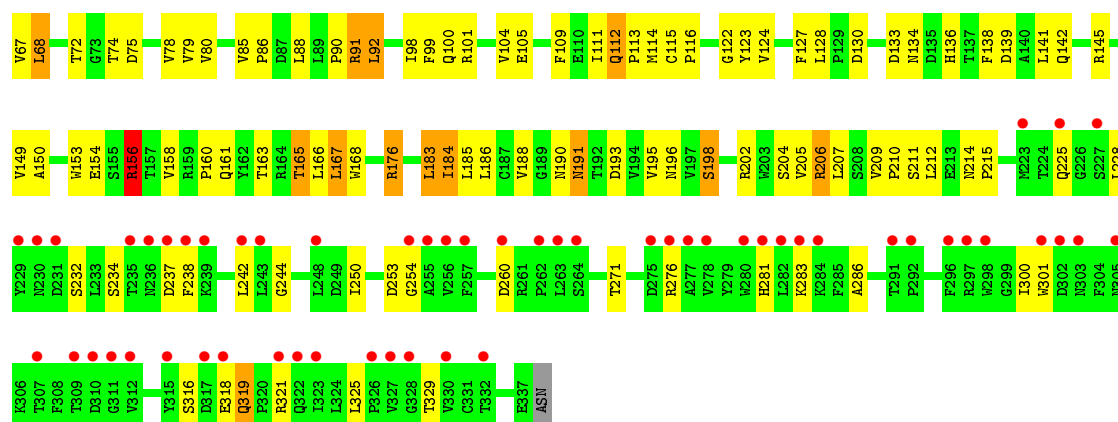


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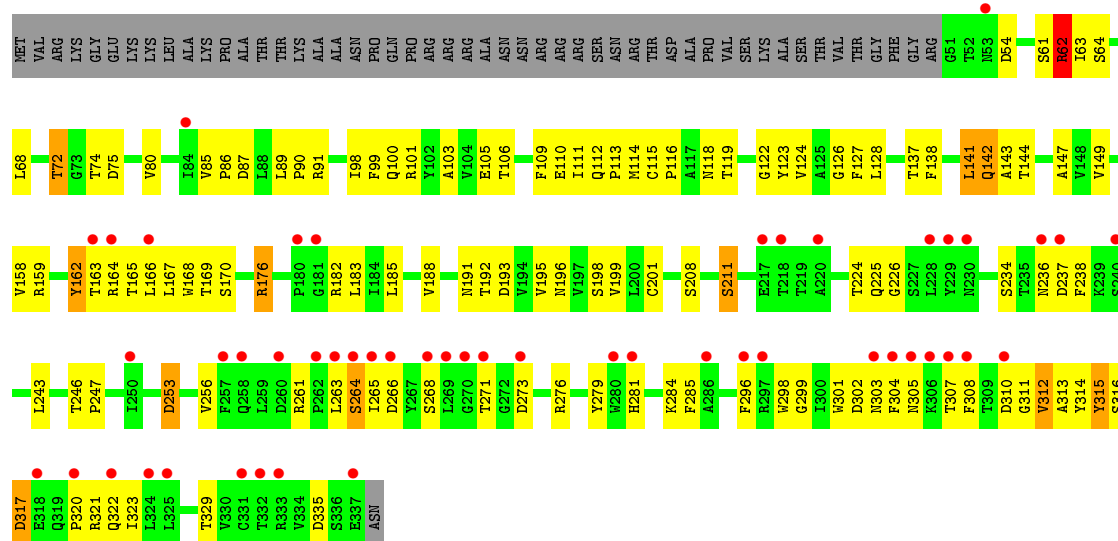


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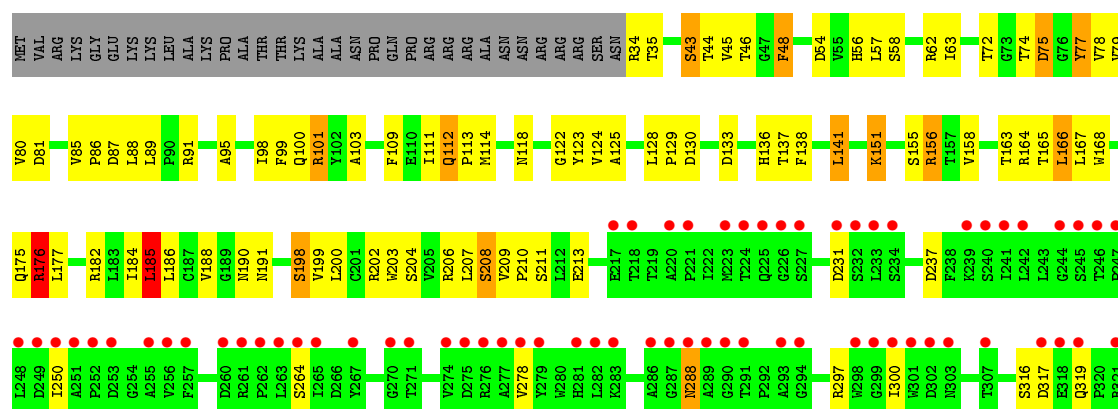


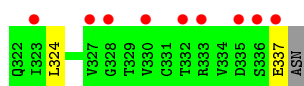


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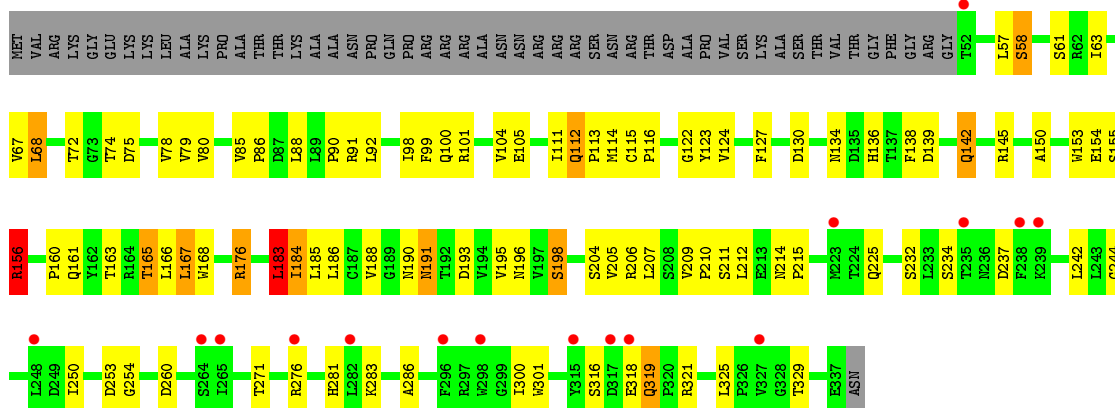


• Molecule 1: Coat protein





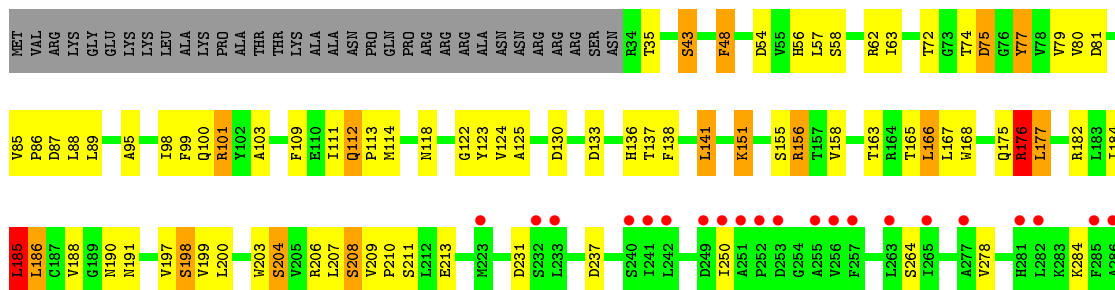
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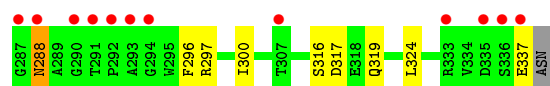


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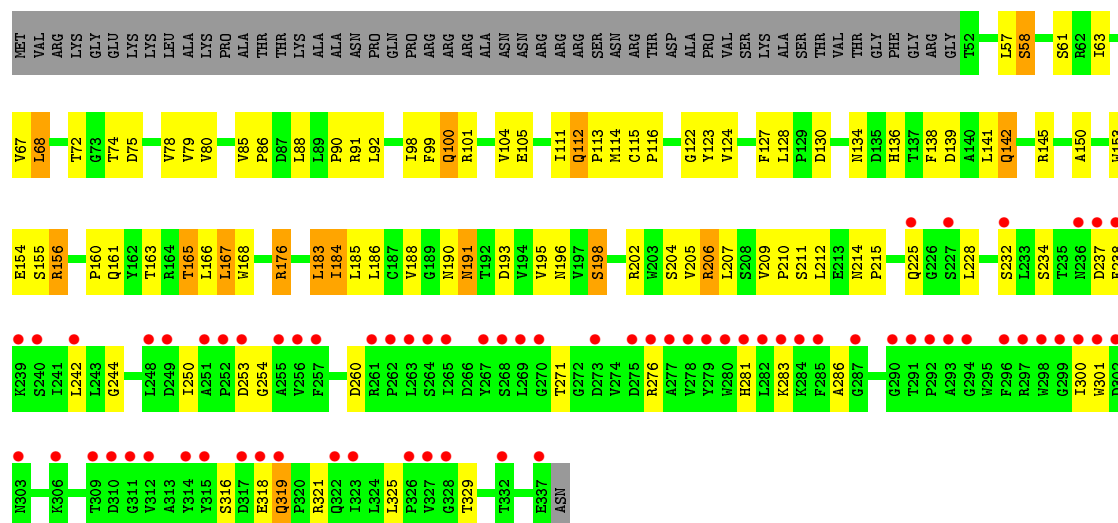


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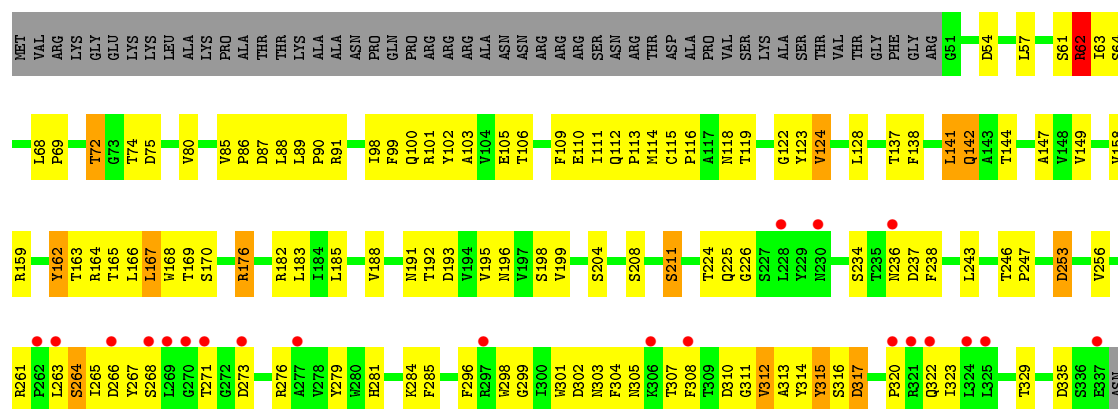




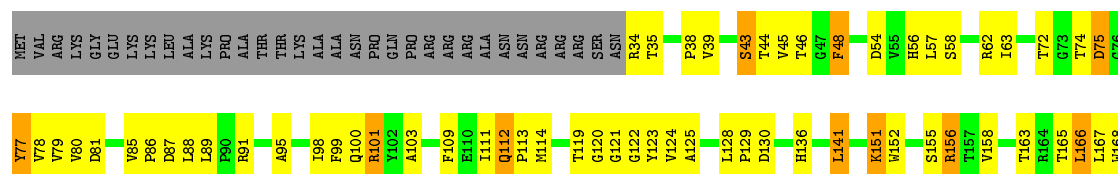
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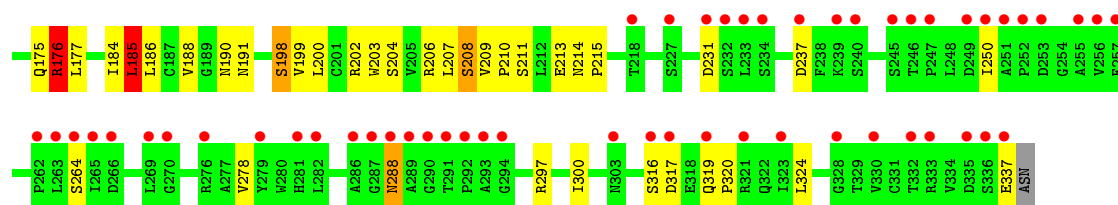
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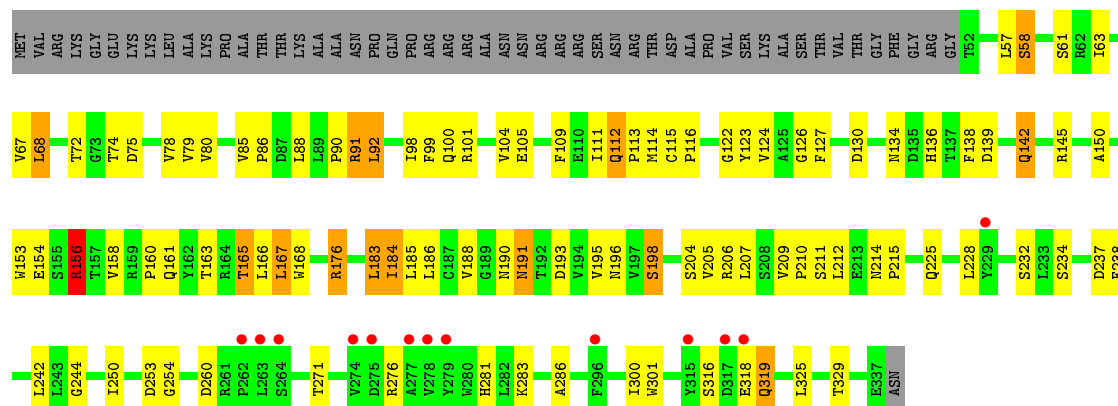
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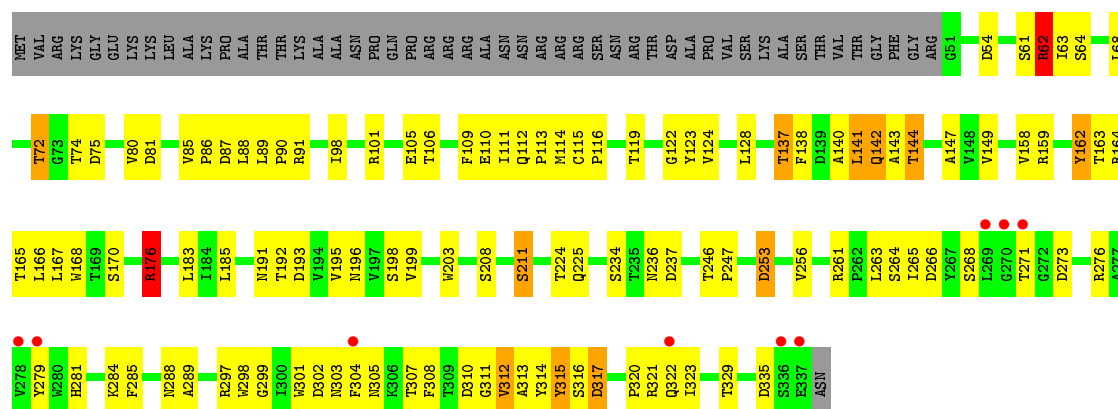




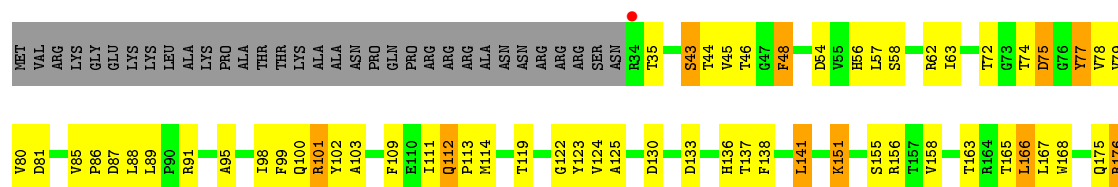
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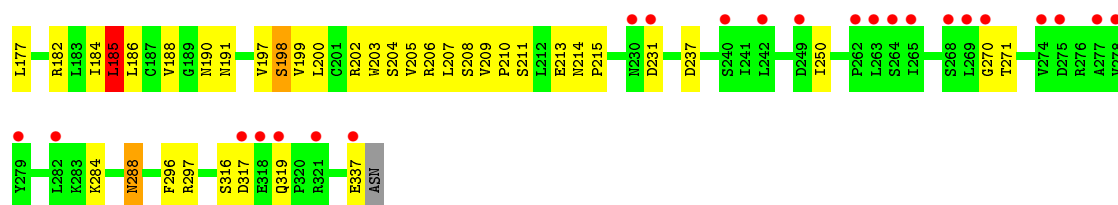


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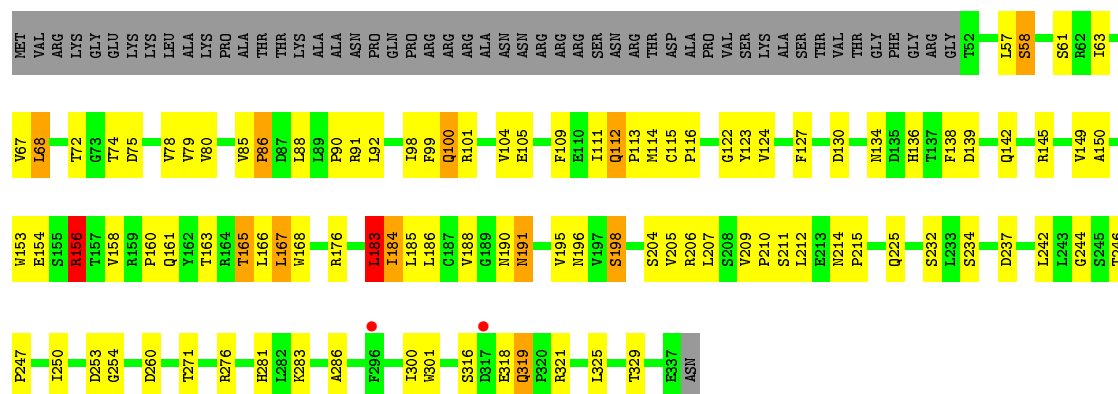


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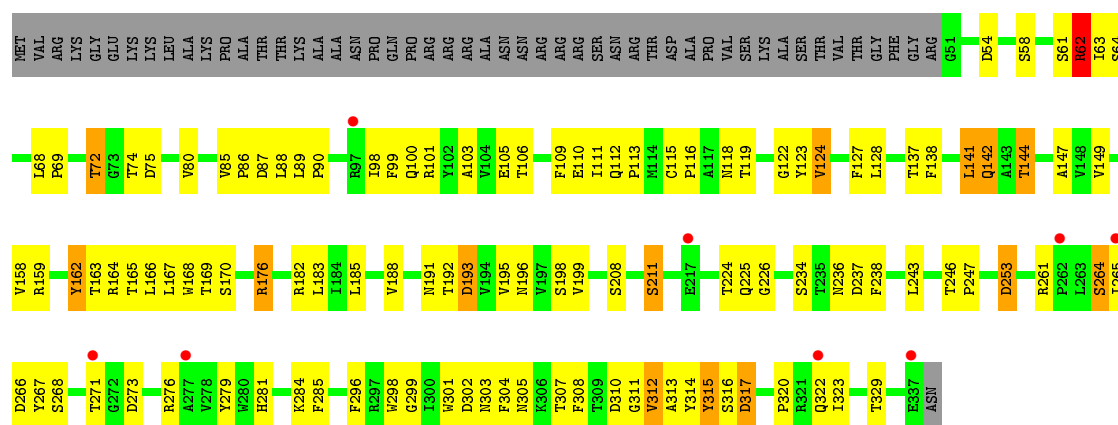




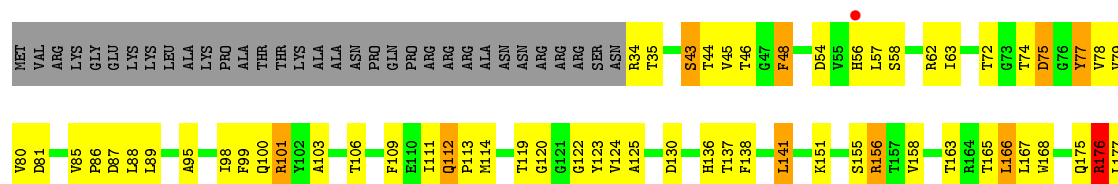
• Molecule 1: Coat protein

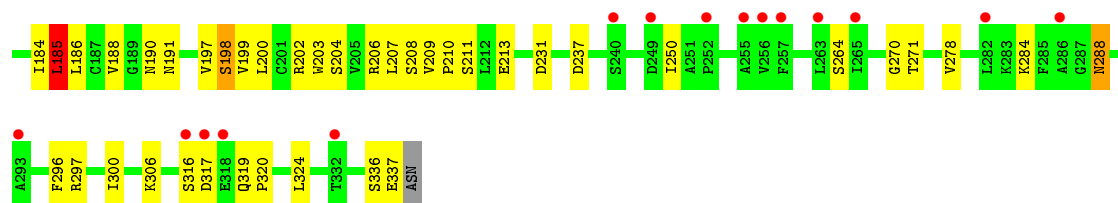


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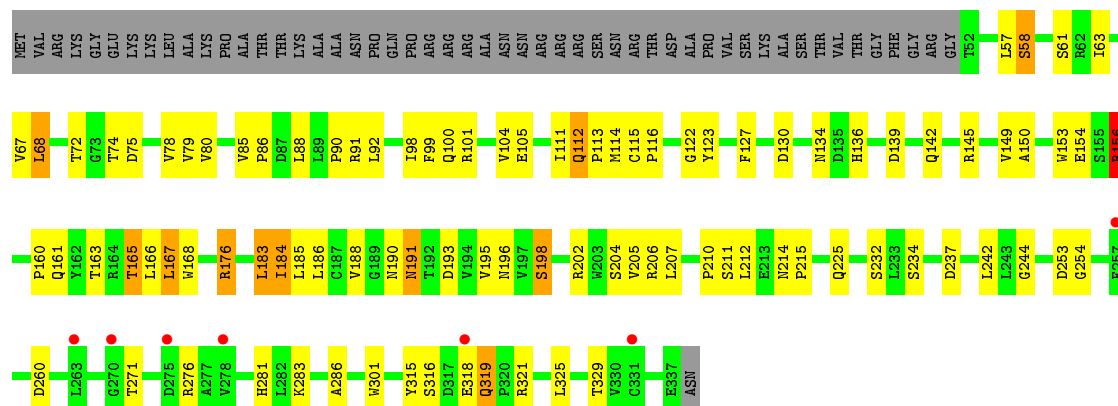


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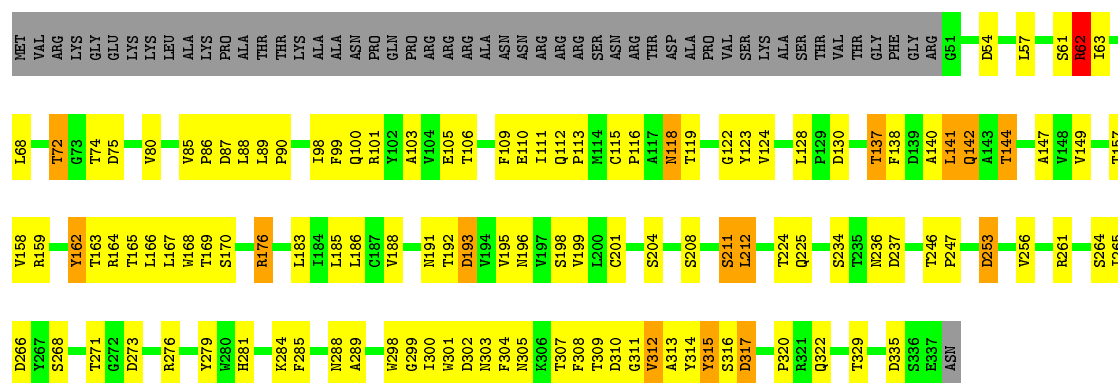




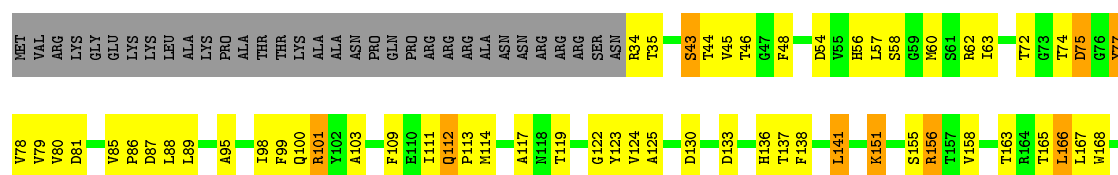
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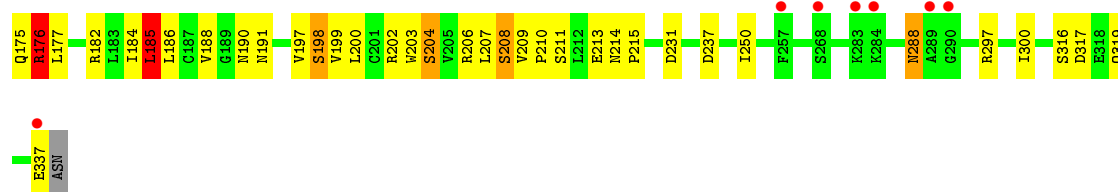


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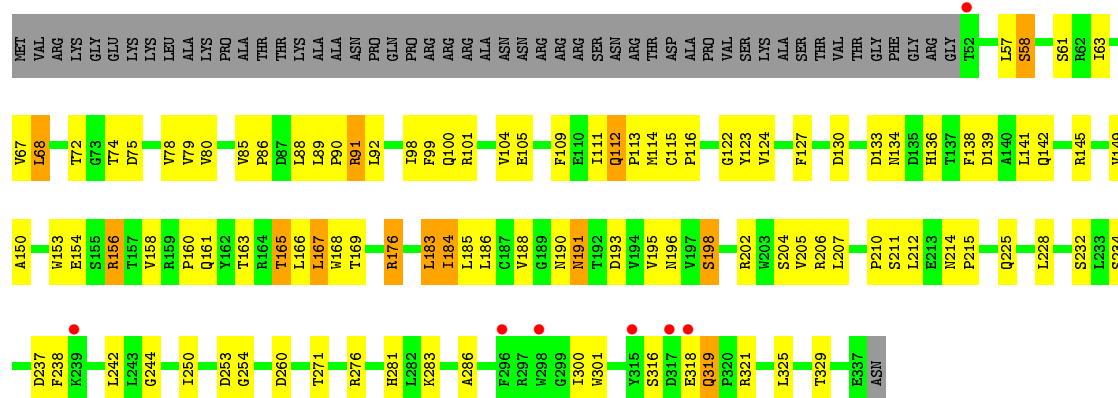


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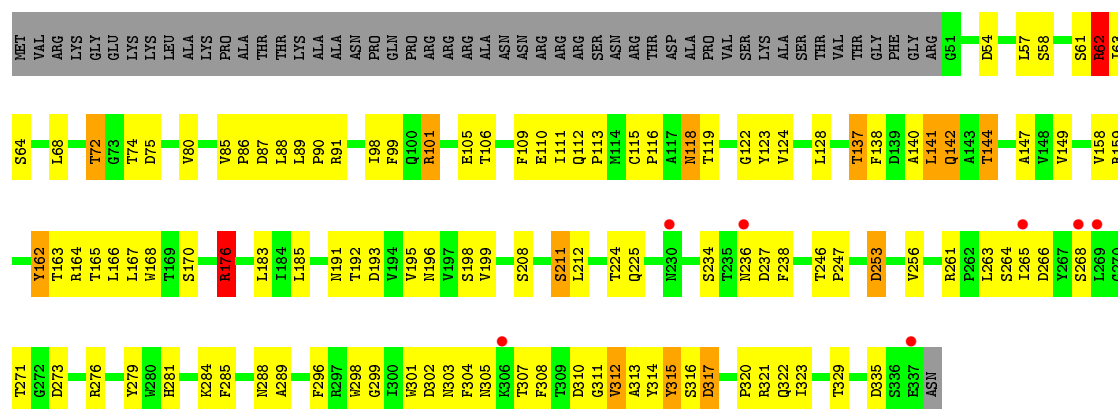




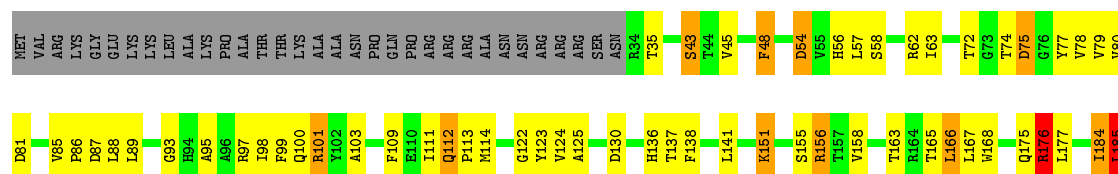
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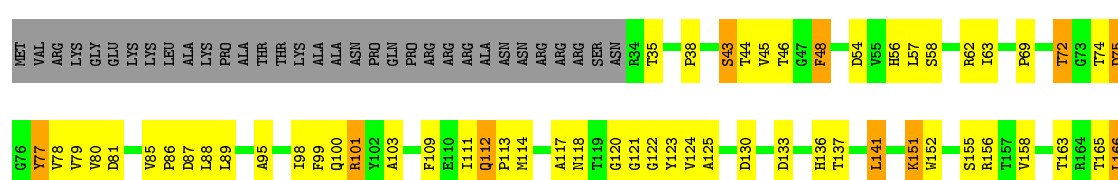


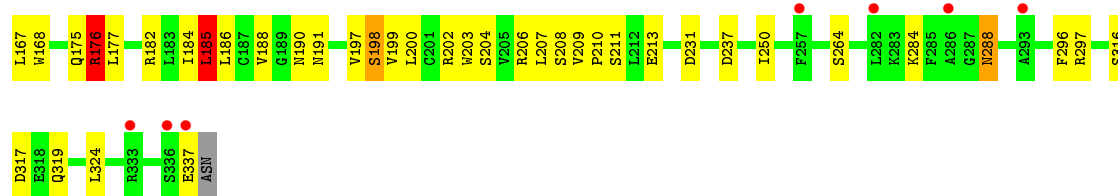
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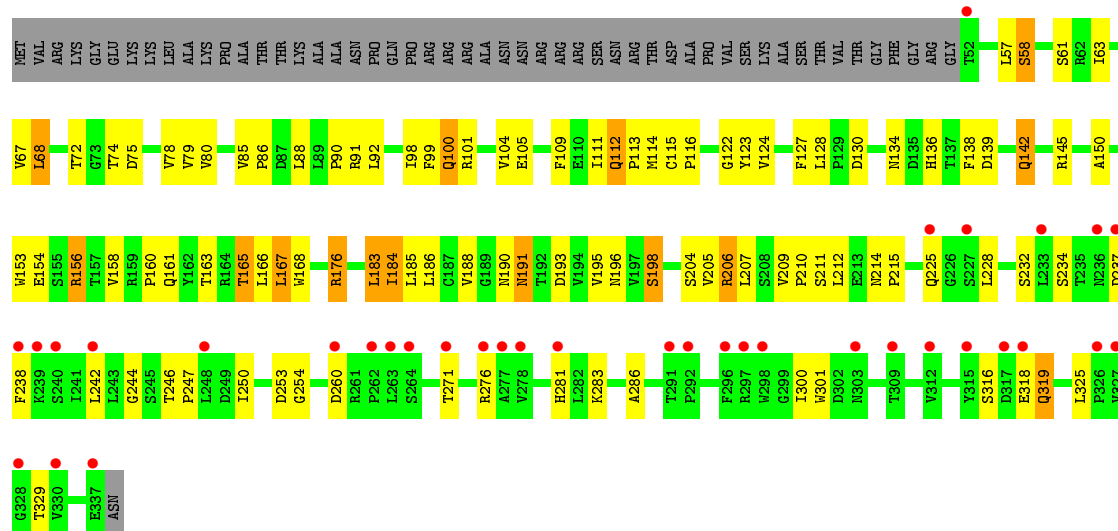
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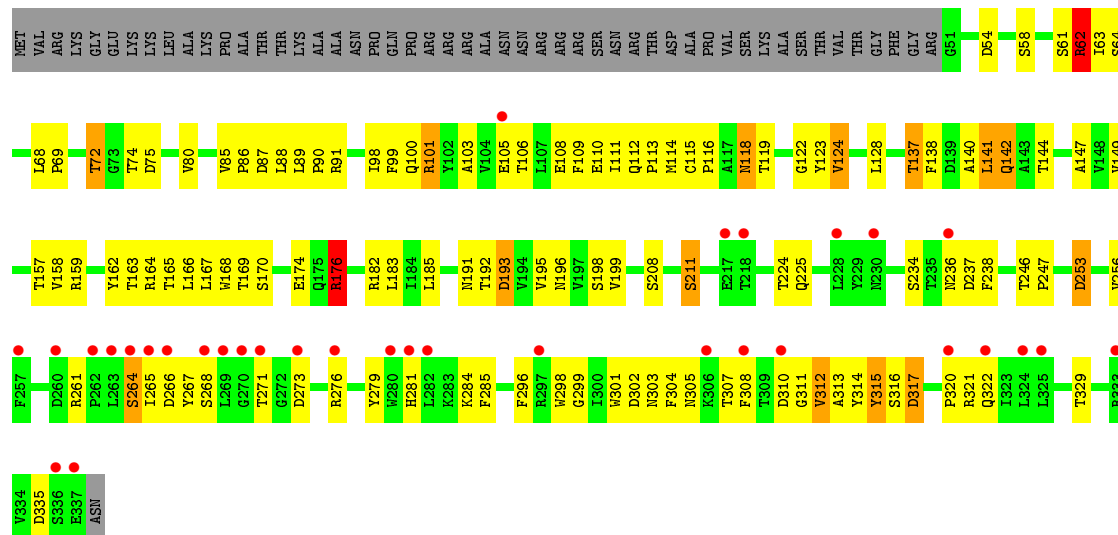




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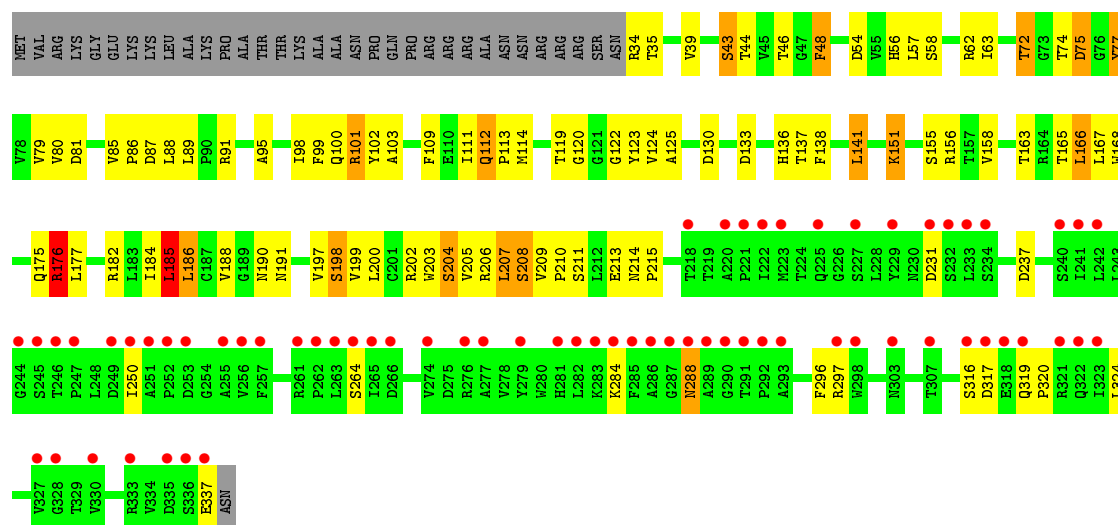


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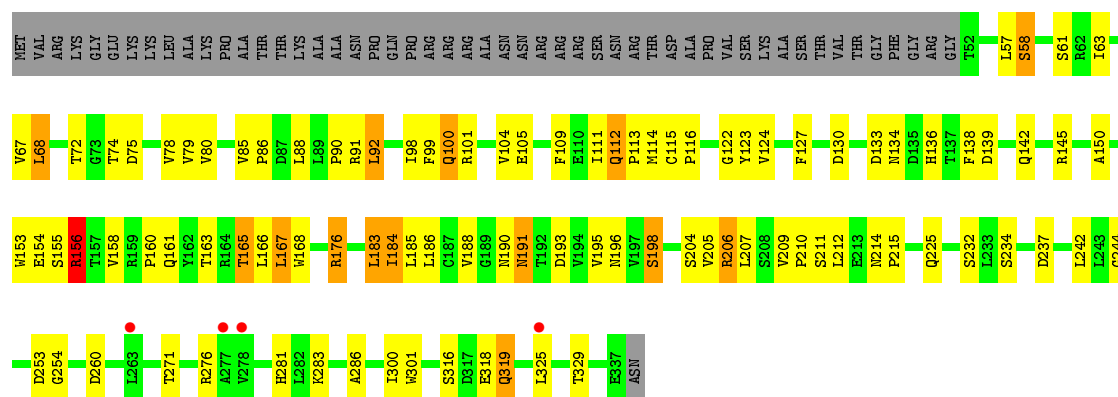


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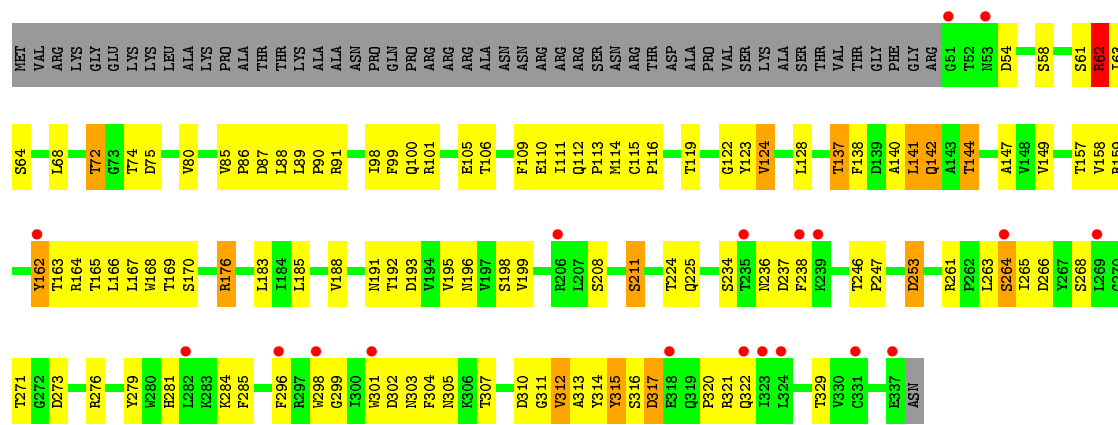




- Molecule 1: Coat protein



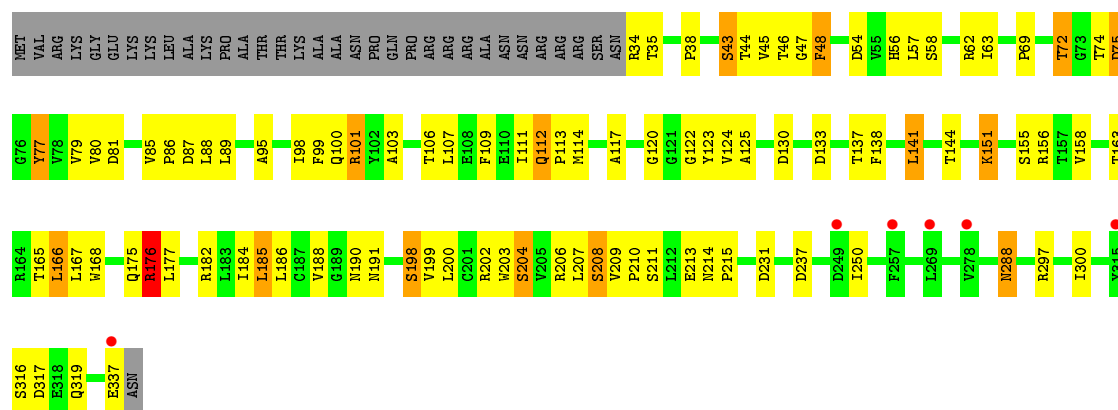
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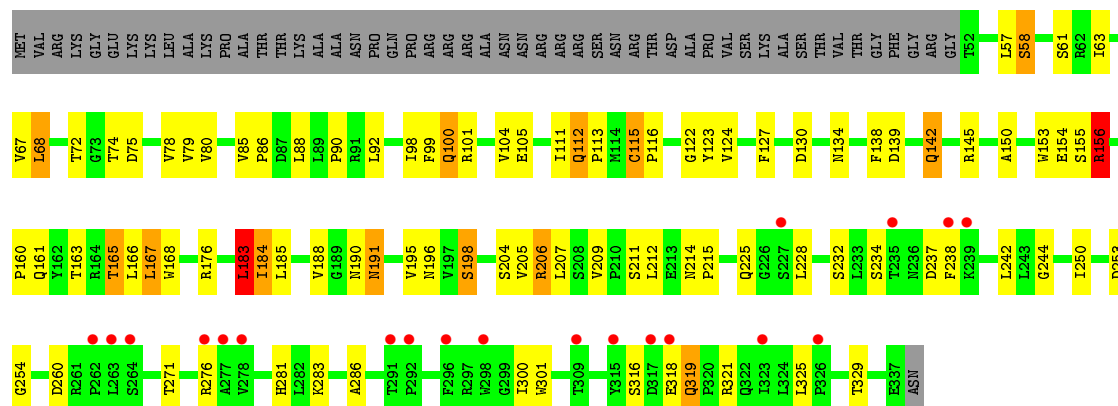
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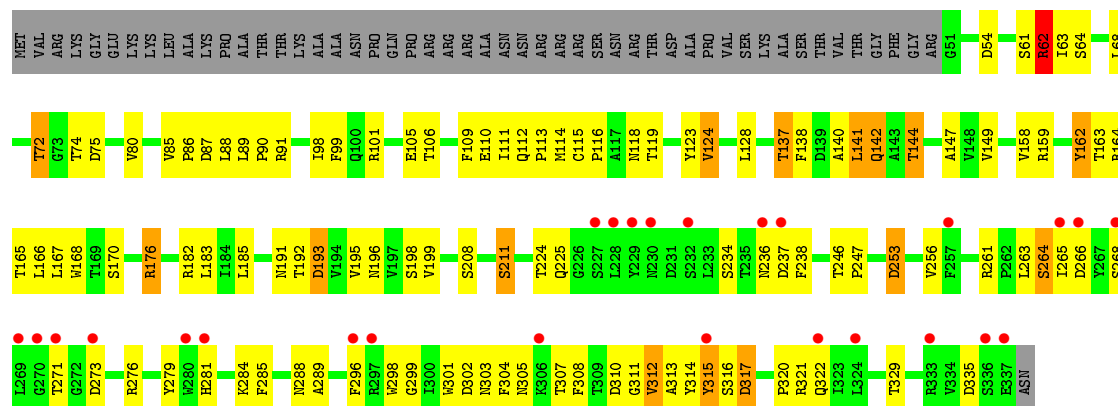




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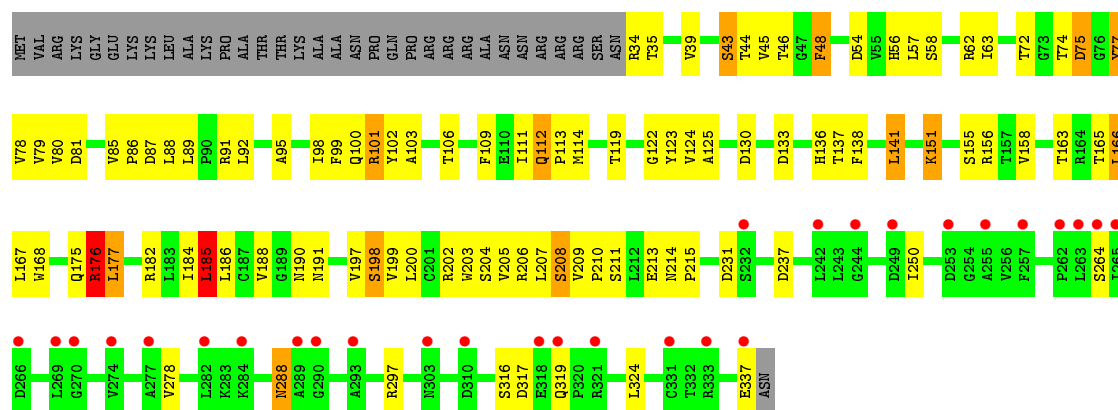
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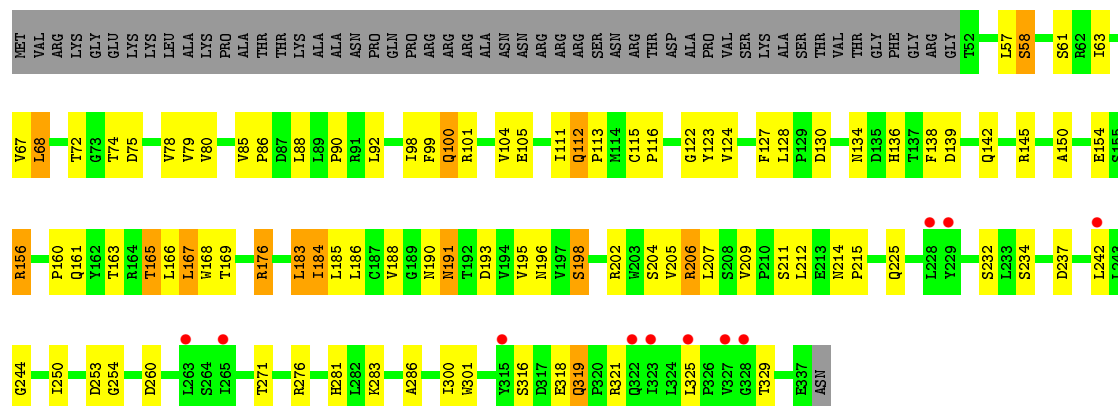
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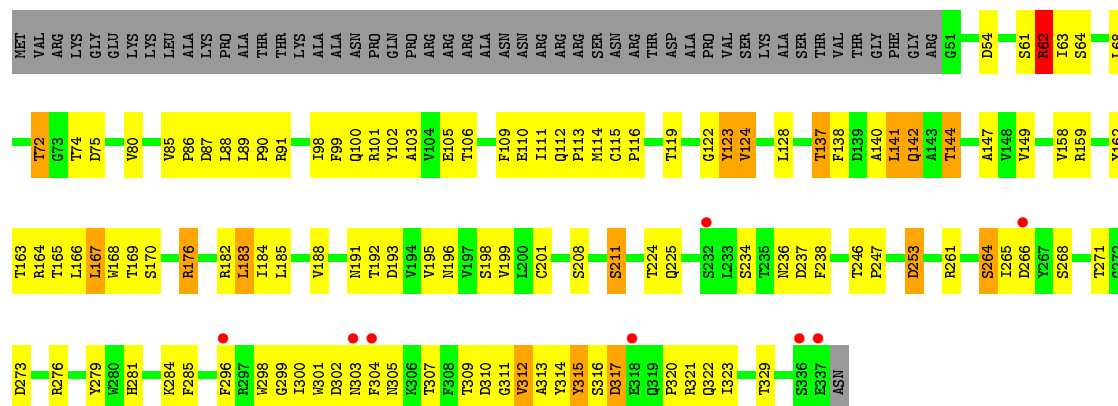




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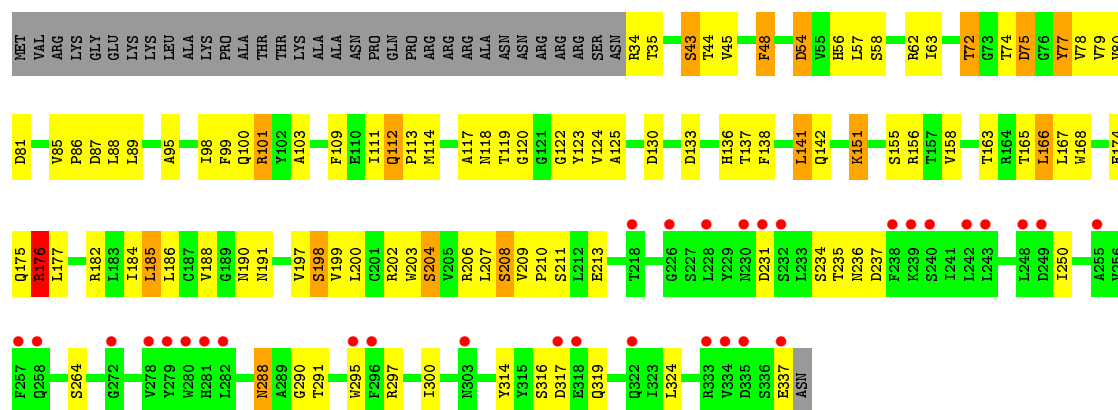


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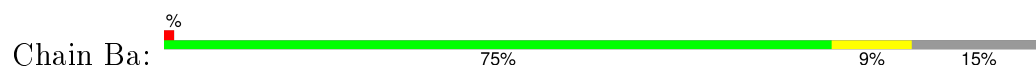


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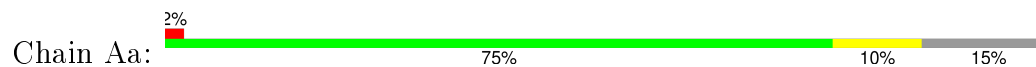




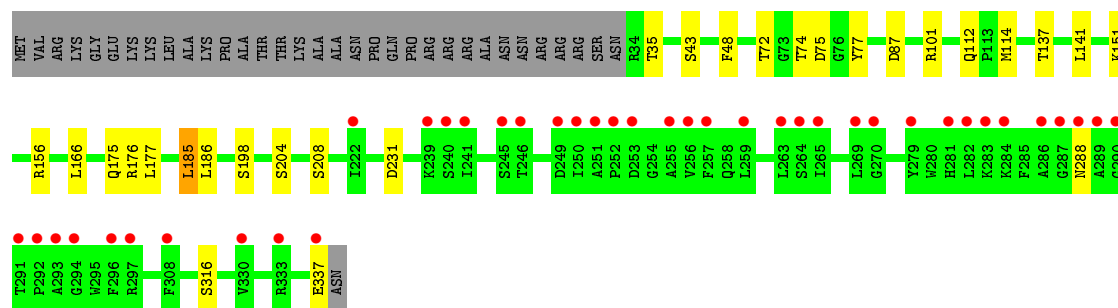
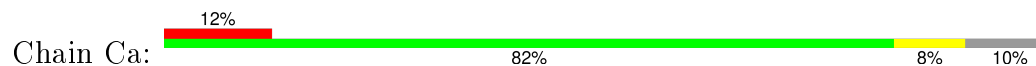
• Molecule 1: Coat protein



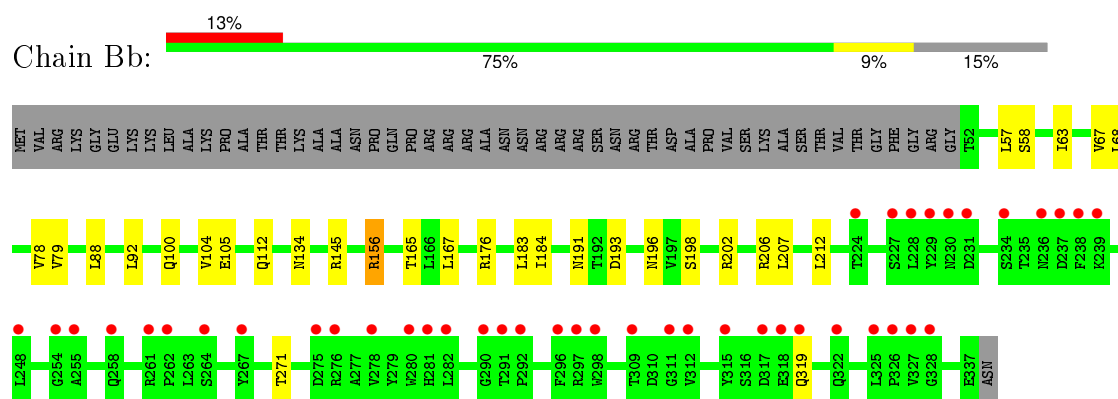
• Molecule 1: Coat protein



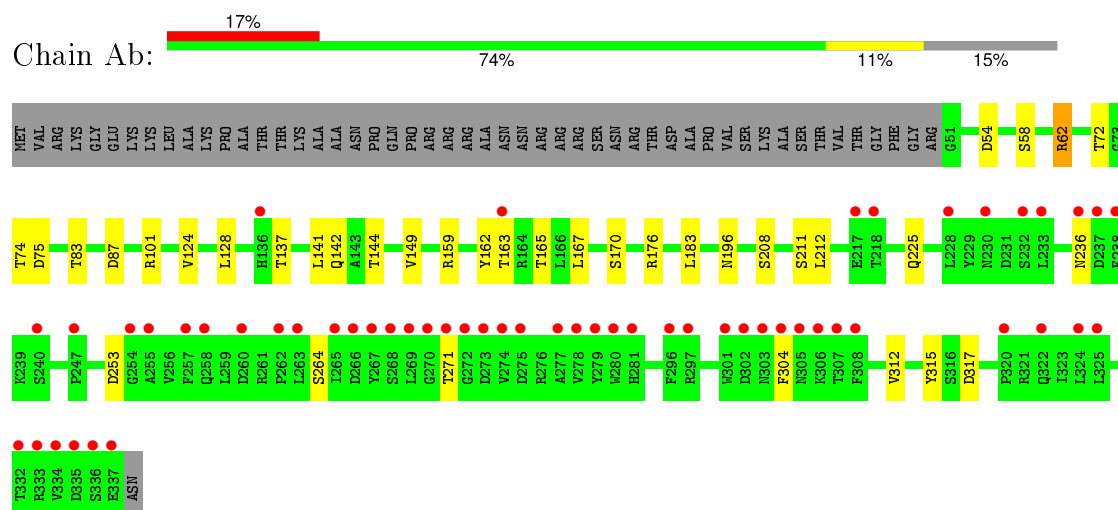
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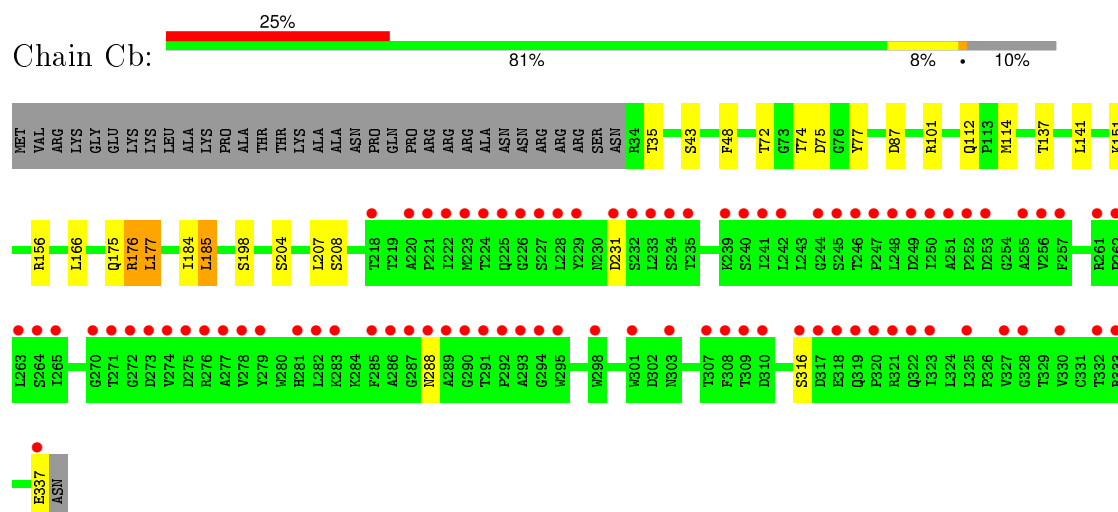
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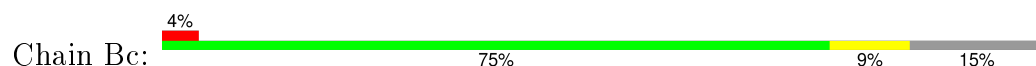
- Molecule 1: Coat protein

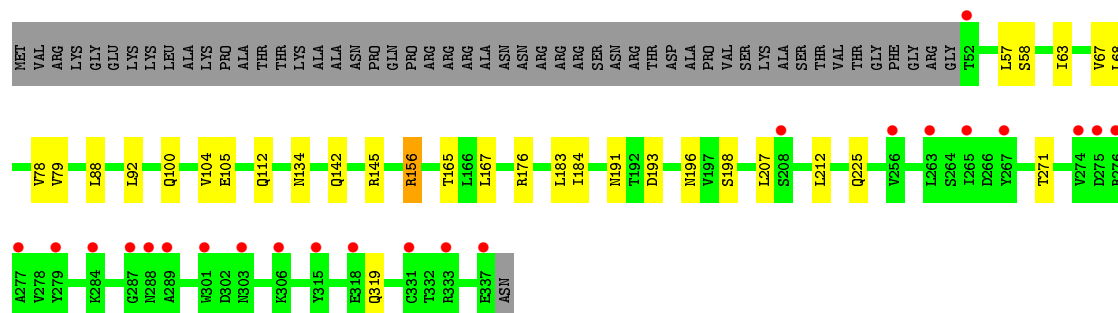


- Molecule 1: Coat protein



- Molecule 1: Coat protein







## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	477.36 Å   422.74 Å   337.89 Å 90.00°   134.03°   90.00°	Depositor
Resolution (Å)	263.91 – 3.60 263.91 – 3.60	Depositor EDS
% Data completeness (in resolution range)	99.2 (263.91-3.60) 99.3 (263.91-3.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.85 (at 3.58 Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, $R_{free}$	0.255 , 0.297 0.255 , 0.295	Depositor DCC
$R_{free}$ test set	27556 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	75.1	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 72.0	EDS
Estimated twinning fraction	0.000 for h+2*l,k,-h-l 0.000 for h,-k,-h-l 0.000 for -h-2*l,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	4 of 549703 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.85	EDS
Total number of atoms	203250	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.66% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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:  
CA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	AA	0.71	0/2274	0.89	4/3112 (0.1%)
1	AB	0.80	0/2274	0.92	3/3112 (0.1%)
1	AC	0.79	0/2274	0.90	4/3112 (0.1%)
1	AD	0.73	0/2274	0.90	2/3112 (0.1%)
1	AE	0.75	0/2274	0.92	3/3112 (0.1%)
1	AF	0.77	1/2274 (0.0%)	0.92	3/3112 (0.1%)
1	AG	0.72	0/2274	0.89	3/3112 (0.1%)
1	AH	0.77	0/2274	0.90	2/3112 (0.1%)
1	AI	0.73	0/2274	0.89	3/3112 (0.1%)
1	AJ	0.78	0/2274	0.92	3/3112 (0.1%)
1	AK	0.92	0/2274	0.99	3/3112 (0.1%)
1	AL	0.85	0/2274	0.95	3/3112 (0.1%)
1	AM	0.72	0/2274	0.88	2/3112 (0.1%)
1	AN	0.72	0/2274	0.89	2/3112 (0.1%)
1	AO	0.76	0/2274	0.91	2/3112 (0.1%)
1	AP	0.77	0/2274	0.91	2/3112 (0.1%)
1	AQ	0.74	0/2274	0.91	4/3112 (0.1%)
1	AR	0.78	0/2274	0.91	3/3112 (0.1%)
1	AS	0.80	0/2274	0.91	2/3112 (0.1%)
1	AT	0.71	0/2274	0.89	3/3112 (0.1%)
1	AU	0.81	2/2274 (0.1%)	0.92	5/3112 (0.2%)
1	AV	0.72	0/2274	0.89	2/3112 (0.1%)
1	AW	0.80	0/2274	0.93	4/3112 (0.1%)
1	AX	0.77	0/2274	0.91	4/3112 (0.1%)
1	AY	0.78	0/2274	0.91	3/3112 (0.1%)
1	AZ	0.75	1/2274 (0.0%)	0.89	4/3112 (0.1%)
1	Aa	0.71	0/2274	0.88	2/3112 (0.1%)
1	Ab	0.78	0/2274	0.92	3/3112 (0.1%)
1	Ac	0.76	0/2274	0.92	5/3112 (0.2%)
1	Ad	0.82	0/2274	0.94	3/3112 (0.1%)
1	BA	0.76	0/2270	0.94	5/3107 (0.2%)
1	BB	0.87	0/2270	0.99	7/3107 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	BC	0.77	0/2270	0.92	5/3107 (0.2%)
1	BD	0.78	0/2270	0.92	3/3107 (0.1%)
1	BE	0.79	0/2270	0.95	6/3107 (0.2%)
1	BF	0.80	0/2270	0.95	6/3107 (0.2%)
1	BG	0.80	0/2270	0.94	4/3107 (0.1%)
1	BH	0.81	0/2270	0.95	5/3107 (0.2%)
1	BI	0.79	1/2270 (0.0%)	0.93	4/3107 (0.1%)
1	BJ	0.86	0/2270	0.97	7/3107 (0.2%)
1	BK	0.92	1/2270 (0.0%)	0.98	5/3107 (0.2%)
1	BL	0.93	0/2270	0.98	8/3107 (0.3%)
1	BM	0.83	0/2270	0.95	5/3107 (0.2%)
1	BN	0.80	0/2270	0.95	5/3107 (0.2%)
1	BO	0.82	0/2270	0.96	6/3107 (0.2%)
1	BP	0.80	0/2270	0.94	5/3107 (0.2%)
1	BQ	0.80	0/2270	0.93	4/3107 (0.1%)
1	BR	0.83	0/2270	0.93	4/3107 (0.1%)
1	BS	0.85	0/2270	0.97	4/3107 (0.1%)
1	BT	0.77	0/2270	0.94	5/3107 (0.2%)
1	BU	0.84	0/2270	0.96	4/3107 (0.1%)
1	BV	0.78	0/2270	0.92	5/3107 (0.2%)
1	BW	0.87	0/2270	0.95	4/3107 (0.1%)
1	BX	0.79	1/2270 (0.0%)	0.93	4/3107 (0.1%)
1	BY	0.79	0/2270	0.92	4/3107 (0.1%)
1	BZ	0.77	0/2270	0.93	4/3107 (0.1%)
1	Ba	0.79	0/2270	0.93	4/3107 (0.1%)
1	Bb	0.85	0/2270	0.98	6/3107 (0.2%)
1	Bc	0.80	0/2270	0.93	4/3107 (0.1%)
1	Bd	0.82	0/2270	0.94	3/3107 (0.1%)
1	CA	0.72	0/2398	0.87	5/3280 (0.2%)
1	CB	0.78	0/2398	0.86	2/3280 (0.1%)
1	CC	0.84	0/2398	0.90	4/3280 (0.1%)
1	CD	0.75	0/2398	0.87	5/3280 (0.2%)
1	CE	0.79	0/2398	0.88	2/3280 (0.1%)
1	CF	0.80	1/2398 (0.0%)	0.88	3/3280 (0.1%)
1	CG	0.73	0/2398	0.86	4/3280 (0.1%)
1	CH	0.75	0/2398	0.87	3/3280 (0.1%)
1	CI	0.73	0/2398	0.86	3/3280 (0.1%)
1	CJ	0.80	0/2398	0.88	5/3280 (0.2%)
1	CK	0.94	0/2398	0.98	4/3280 (0.1%)
1	CL	0.87	1/2398 (0.0%)	0.92	4/3280 (0.1%)
1	CM	0.76	0/2398	0.88	3/3280 (0.1%)
1	CN	0.74	0/2398	0.86	4/3280 (0.1%)
1	CO	0.78	0/2398	0.89	4/3280 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	CP	0.75	0/2398	0.86	2/3280 (0.1%)
1	CQ	0.77	0/2398	0.87	4/3280 (0.1%)
1	CR	0.76	0/2398	0.87	4/3280 (0.1%)
1	CS	0.82	0/2398	0.91	4/3280 (0.1%)
1	CT	0.74	0/2398	0.88	4/3280 (0.1%)
1	CU	0.81	0/2398	0.90	4/3280 (0.1%)
1	CV	0.73	0/2398	0.86	3/3280 (0.1%)
1	CW	0.81	0/2398	0.91	4/3280 (0.1%)
1	CX	0.77	0/2398	0.87	3/3280 (0.1%)
1	CY	0.78	0/2398	0.88	4/3280 (0.1%)
1	CZ	0.74	1/2398 (0.0%)	0.87	3/3280 (0.1%)
1	Ca	0.74	0/2398	0.86	2/3280 (0.1%)
1	Cb	0.79	0/2398	0.88	5/3280 (0.2%)
1	Cc	0.78	0/2398	0.88	5/3280 (0.2%)
1	Cd	0.86	1/2398 (0.0%)	0.94	4/3280 (0.1%)
All	All	0.79	11/208260 (0.0%)	0.91	346/284970 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	CU	0	1
1	Cb	0	1
All	All	0	2

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	BI	318	GLU	CD-OE2	7.13	1.33	1.25
1	Cd	174	GLU	CD-OE1	6.83	1.33	1.25
1	CF	174	GLU	CD-OE1	6.23	1.32	1.25
1	AF	174	GLU	CD-OE2	5.70	1.31	1.25
1	AU	108	GLU	CD-OE1	5.60	1.31	1.25

The worst 5 of 346 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CO	176	ARG	NE-CZ-NH2	8.79	124.70	120.30
1	AE	62	ARG	NE-CZ-NH1	8.55	124.58	120.30
1	CT	176	ARG	NE-CZ-NH2	8.44	124.52	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CU	176	ARG	NE-CZ-NH2	8.25	124.42	120.30
1	CW	176	ARG	NE-CZ-NH2	8.08	124.34	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	CU	207	LEU	Peptide
1	Cb	207	LEU	Peptide

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	2218	0	2155	158	0
1	AB	2218	0	2155	156	0
1	AC	2218	0	2155	146	19
1	AD	2218	0	2155	161	0
1	AE	2218	0	2155	128	0
1	AF	2218	0	2155	132	0
1	AG	2218	0	2155	144	0
1	AH	2218	0	2155	136	0
1	AI	2218	0	2155	142	0
1	AJ	2218	0	2155	136	1
1	AK	2218	0	2155	127	0
1	AL	2218	0	2155	117	0
1	AM	2218	0	2155	139	0
1	AN	2218	0	2155	138	0
1	AO	2218	0	2155	137	0
1	AP	2218	0	2155	130	1
1	AQ	2218	0	2155	127	0
1	AR	2218	0	2155	122	0
1	AS	2218	0	2155	136	0
1	AT	2218	0	2155	136	0
1	AU	2218	0	2155	135	0
1	AV	2218	0	2155	133	0
1	AW	2218	0	2155	136	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AX	2218	0	2155	125	0
1	AY	2218	0	2155	131	0
1	AZ	2218	0	2155	135	0
1	Aa	2218	0	2155	0	0
1	Ab	2218	0	2155	0	0
1	Ac	2218	0	2155	0	0
1	Ad	2218	0	2155	0	0
1	BA	2214	0	2153	114	0
1	BB	2214	0	2153	125	0
1	BC	2214	0	2153	116	13
1	BD	2214	0	2153	118	0
1	BE	2214	0	2153	83	0
1	BF	2214	0	2153	92	0
1	BG	2214	0	2153	92	0
1	BH	2214	0	2153	106	0
1	BI	2214	0	2153	93	8
1	BJ	2214	0	2153	84	1
1	BK	2214	0	2153	94	0
1	BL	2214	0	2153	88	7
1	BM	2214	0	2153	101	0
1	BN	2214	0	2153	84	0
1	BO	2214	0	2153	97	0
1	BP	2214	0	2153	92	0
1	BQ	2214	0	2153	94	0
1	BR	2214	0	2153	85	1
1	BS	2214	0	2153	95	0
1	BT	2214	0	2153	92	0
1	BU	2214	0	2153	88	0
1	BV	2214	0	2153	93	0
1	BW	2214	0	2153	89	6
1	BX	2214	0	2153	79	1
1	BY	2214	0	2153	97	0
1	BZ	2214	0	2153	79	0
1	Ba	2214	0	2153	0	11
1	Bb	2214	0	2153	0	0
1	Bc	2214	0	2153	0	1
1	Bd	2214	0	2153	0	0
1	CA	2340	0	2280	135	1
1	CB	2340	0	2280	154	0
1	CC	2340	0	2280	136	0
1	CD	2340	0	2280	162	0
1	CE	2340	0	2280	110	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	CF	2340	0	2280	121	0
1	CG	2340	0	2280	110	0
1	CH	2340	0	2280	119	0
1	CI	2340	0	2280	116	0
1	CJ	2340	0	2280	114	0
1	CK	2340	0	2280	123	6
1	CL	2340	0	2280	125	1
1	CM	2340	0	2280	120	0
1	CN	2340	0	2280	99	0
1	CO	2340	0	2280	120	0
1	CP	2340	0	2280	111	2
1	CQ	2340	0	2280	118	11
1	CR	2340	0	2280	116	1
1	CS	2340	0	2280	102	0
1	CT	2340	0	2280	116	2
1	CU	2340	0	2280	112	0
1	CV	2340	0	2280	112	0
1	CW	2340	0	2280	120	0
1	CX	2340	0	2280	109	0
1	CY	2340	0	2280	117	0
1	CZ	2340	0	2280	113	32
1	Ca	2340	0	2280	0	0
1	Cb	2340	0	2280	0	0
1	Cc	2340	0	2280	0	0
1	Cd	2340	0	2280	0	7
2	AA	1	0	0	0	0
2	AB	1	0	0	0	0
2	AC	1	0	0	0	0
2	AD	1	0	0	0	0
2	AE	1	0	0	0	0
2	AF	1	0	0	0	0
2	AG	1	0	0	0	0
2	AH	1	0	0	0	0
2	AI	1	0	0	0	0
2	AJ	1	0	0	0	0
2	AK	1	0	0	0	0
2	AL	1	0	0	0	0
2	AM	1	0	0	0	0
2	AN	1	0	0	0	0
2	AO	1	0	0	0	0
2	AP	1	0	0	0	0
2	AQ	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	AR	1	0	0	0	0
2	AS	1	0	0	0	0
2	AT	1	0	0	0	0
2	AU	1	0	0	0	0
2	AV	1	0	0	0	0
2	AW	1	0	0	0	0
2	AX	1	0	0	0	0
2	AY	1	0	0	0	0
2	AZ	1	0	0	0	0
2	Aa	1	0	0	0	0
2	Ab	1	0	0	0	0
2	Ac	1	0	0	0	0
2	Ad	1	0	0	0	0
2	BA	2	0	0	0	0
2	BB	2	0	0	0	0
2	BC	2	0	0	0	0
2	BD	2	0	0	0	0
2	BE	2	0	0	0	0
2	BF	2	0	0	0	0
2	BG	2	0	0	0	0
2	BH	2	0	0	0	0
2	BI	2	0	0	0	0
2	BJ	2	0	0	0	0
2	BK	2	0	0	0	0
2	BL	2	0	0	0	0
2	BM	2	0	0	0	0
2	BN	2	0	0	0	0
2	BO	2	0	0	0	0
2	BP	2	0	0	0	0
2	BQ	2	0	0	0	0
2	BR	2	0	0	0	0
2	BS	2	0	0	0	0
2	BT	2	0	0	0	0
2	BU	2	0	0	0	0
2	BV	2	0	0	0	0
2	BW	2	0	0	0	0
2	BX	2	0	0	0	0
2	BY	2	0	0	0	0
2	BZ	2	0	0	0	0
2	Ba	2	0	0	0	0
2	Bb	2	0	0	0	0
2	Bc	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Bd	2	0	0	0	0
All	All	203250	0	197640	8152	71

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 20.

The worst 5 of 8152 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:AD:298:TRP:NE1	1:AD:312:VAL:HG12	1.23	1.53
1:AA:298:TRP:NE1	1:AA:312:VAL:HG12	1.24	1.53
1:AK:298:TRP:NE1	1:AK:312:VAL:HG12	1.21	1.50
1:AI:298:TRP:NE1	1:AI:312:VAL:HG12	1.24	1.50
1:AB:298:TRP:NE1	1:AB:312:VAL:HG12	1.23	1.49

The worst 5 of 71 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BL:297:ARG:CZ	1:Cd:271:THR:OG1[4_546]	0.58	1.62
1:AC:318:GLU:CD	1:CZ:235:THR:CA[4_545]	0.93	1.27
1:BI:318:GLU:OE1	1:BI:318:GLU:OE2[2_656]	1.02	1.18
1:CQ:271:THR:O	1:Ba:290:GLY:O[4_555]	1.05	1.15
1:AC:318:GLU:CG	1:CZ:235:THR:CA[4_545]	1.06	1.14

## 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	AA	285/338 (84%)	277 (97%)	8 (3%)	0	100	100
1	AB	285/338 (84%)	278 (98%)	7 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AC	285/338 (84%)	277 (97%)	8 (3%)	0	100	100
1	AD	285/338 (84%)	276 (97%)	9 (3%)	0	100	100
1	AE	285/338 (84%)	277 (97%)	8 (3%)	0	100	100
1	AF	285/338 (84%)	278 (98%)	7 (2%)	0	100	100
1	AG	285/338 (84%)	276 (97%)	9 (3%)	0	100	100
1	AH	285/338 (84%)	277 (97%)	8 (3%)	0	100	100
1	AI	285/338 (84%)	278 (98%)	7 (2%)	0	100	100
1	AJ	285/338 (84%)	277 (97%)	8 (3%)	0	100	100
1	AK	285/338 (84%)	277 (97%)	8 (3%)	0	100	100
1	AL	285/338 (84%)	275 (96%)	10 (4%)	0	100	100
1	AM	285/338 (84%)	279 (98%)	6 (2%)	0	100	100
1	AN	285/338 (84%)	276 (97%)	9 (3%)	0	100	100
1	AO	285/338 (84%)	277 (97%)	8 (3%)	0	100	100
1	AP	285/338 (84%)	277 (97%)	8 (3%)	0	100	100
1	AQ	285/338 (84%)	276 (97%)	9 (3%)	0	100	100
1	AR	285/338 (84%)	278 (98%)	7 (2%)	0	100	100
1	AS	285/338 (84%)	276 (97%)	9 (3%)	0	100	100
1	AT	285/338 (84%)	278 (98%)	7 (2%)	0	100	100
1	AU	285/338 (84%)	276 (97%)	9 (3%)	0	100	100
1	AV	285/338 (84%)	276 (97%)	9 (3%)	0	100	100
1	AW	285/338 (84%)	275 (96%)	10 (4%)	0	100	100
1	AX	285/338 (84%)	278 (98%)	7 (2%)	0	100	100
1	AY	285/338 (84%)	276 (97%)	9 (3%)	0	100	100
1	AZ	285/338 (84%)	279 (98%)	6 (2%)	0	100	100
1	Aa	285/338 (84%)	278 (98%)	7 (2%)	0	100	100
1	Ab	285/338 (84%)	277 (97%)	8 (3%)	0	100	100
1	Ac	285/338 (84%)	276 (97%)	9 (3%)	0	100	100
1	Ad	285/338 (84%)	276 (97%)	9 (3%)	0	100	100
1	BA	284/338 (84%)	281 (99%)	3 (1%)	0	100	100
1	BB	284/338 (84%)	280 (99%)	4 (1%)	0	100	100
1	BC	284/338 (84%)	281 (99%)	3 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	BD	284/338 (84%)	282 (99%)	2 (1%)	0	100	100
1	BE	284/338 (84%)	282 (99%)	2 (1%)	0	100	100
1	BF	284/338 (84%)	280 (99%)	4 (1%)	0	100	100
1	BG	284/338 (84%)	281 (99%)	3 (1%)	0	100	100
1	BH	284/338 (84%)	282 (99%)	2 (1%)	0	100	100
1	BI	284/338 (84%)	281 (99%)	3 (1%)	0	100	100
1	BJ	284/338 (84%)	280 (99%)	4 (1%)	0	100	100
1	BK	284/338 (84%)	280 (99%)	4 (1%)	0	100	100
1	BL	284/338 (84%)	281 (99%)	3 (1%)	0	100	100
1	BM	284/338 (84%)	280 (99%)	4 (1%)	0	100	100
1	BN	284/338 (84%)	282 (99%)	2 (1%)	0	100	100
1	BO	284/338 (84%)	281 (99%)	3 (1%)	0	100	100
1	BP	284/338 (84%)	279 (98%)	5 (2%)	0	100	100
1	BQ	284/338 (84%)	281 (99%)	3 (1%)	0	100	100
1	BR	284/338 (84%)	278 (98%)	6 (2%)	0	100	100
1	BS	284/338 (84%)	282 (99%)	2 (1%)	0	100	100
1	BT	284/338 (84%)	281 (99%)	3 (1%)	0	100	100
1	BU	284/338 (84%)	282 (99%)	2 (1%)	0	100	100
1	BV	284/338 (84%)	283 (100%)	1 (0%)	0	100	100
1	BW	284/338 (84%)	281 (99%)	3 (1%)	0	100	100
1	BX	284/338 (84%)	282 (99%)	2 (1%)	0	100	100
1	BY	284/338 (84%)	282 (99%)	2 (1%)	0	100	100
1	BZ	284/338 (84%)	280 (99%)	4 (1%)	0	100	100
1	Ba	284/338 (84%)	279 (98%)	5 (2%)	0	100	100
1	Bb	284/338 (84%)	282 (99%)	2 (1%)	0	100	100
1	Bc	284/338 (84%)	281 (99%)	3 (1%)	0	100	100
1	Bd	284/338 (84%)	281 (99%)	3 (1%)	0	100	100
1	CA	302/338 (89%)	288 (95%)	14 (5%)	0	100	100
1	CB	302/338 (89%)	287 (95%)	15 (5%)	0	100	100
1	CC	302/338 (89%)	288 (95%)	14 (5%)	0	100	100
1	CD	302/338 (89%)	288 (95%)	14 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	CE	302/338 (89%)	288 (95%)	14 (5%)	0	100	100
1	CF	302/338 (89%)	287 (95%)	15 (5%)	0	100	100
1	CG	302/338 (89%)	288 (95%)	14 (5%)	0	100	100
1	CH	302/338 (89%)	288 (95%)	14 (5%)	0	100	100
1	CI	302/338 (89%)	287 (95%)	15 (5%)	0	100	100
1	CJ	302/338 (89%)	289 (96%)	13 (4%)	0	100	100
1	CK	302/338 (89%)	286 (95%)	16 (5%)	0	100	100
1	CL	302/338 (89%)	287 (95%)	15 (5%)	0	100	100
1	CM	302/338 (89%)	287 (95%)	15 (5%)	0	100	100
1	CN	302/338 (89%)	287 (95%)	15 (5%)	0	100	100
1	CO	302/338 (89%)	288 (95%)	14 (5%)	0	100	100
1	CP	302/338 (89%)	287 (95%)	15 (5%)	0	100	100
1	CQ	302/338 (89%)	287 (95%)	15 (5%)	0	100	100
1	CR	302/338 (89%)	287 (95%)	15 (5%)	0	100	100
1	CS	302/338 (89%)	290 (96%)	12 (4%)	0	100	100
1	CT	302/338 (89%)	285 (94%)	17 (6%)	0	100	100
1	CU	302/338 (89%)	285 (94%)	17 (6%)	0	100	100
1	CV	302/338 (89%)	286 (95%)	16 (5%)	0	100	100
1	CW	302/338 (89%)	286 (95%)	16 (5%)	0	100	100
1	CX	302/338 (89%)	289 (96%)	13 (4%)	0	100	100
1	CY	302/338 (89%)	287 (95%)	15 (5%)	0	100	100
1	CZ	302/338 (89%)	286 (95%)	16 (5%)	0	100	100
1	Ca	302/338 (89%)	287 (95%)	15 (5%)	0	100	100
1	Cb	302/338 (89%)	287 (95%)	15 (5%)	0	100	100
1	Cc	302/338 (89%)	290 (96%)	12 (4%)	0	100	100
1	Cd	302/338 (89%)	289 (96%)	13 (4%)	0	100	100
All	All	26130/30420 (86%)	25356 (97%)	774 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	AA	242/283 (86%)	209 (86%)	33 (14%)	5	29
1	AB	242/283 (86%)	206 (85%)	36 (15%)	4	25
1	AC	242/283 (86%)	207 (86%)	35 (14%)	4	26
1	AD	242/283 (86%)	208 (86%)	34 (14%)	4	28
1	AE	242/283 (86%)	206 (85%)	36 (15%)	4	25
1	AF	242/283 (86%)	208 (86%)	34 (14%)	4	28
1	AG	242/283 (86%)	208 (86%)	34 (14%)	4	28
1	AH	242/283 (86%)	209 (86%)	33 (14%)	5	29
1	AI	242/283 (86%)	206 (85%)	36 (15%)	4	25
1	AJ	242/283 (86%)	209 (86%)	33 (14%)	5	29
1	AK	242/283 (86%)	209 (86%)	33 (14%)	5	29
1	AL	242/283 (86%)	207 (86%)	35 (14%)	4	26
1	AM	242/283 (86%)	211 (87%)	31 (13%)	5	31
1	AN	242/283 (86%)	209 (86%)	33 (14%)	5	29
1	AO	242/283 (86%)	209 (86%)	33 (14%)	5	29
1	AP	242/283 (86%)	210 (87%)	32 (13%)	5	30
1	AQ	242/283 (86%)	208 (86%)	34 (14%)	4	28
1	AR	242/283 (86%)	205 (85%)	37 (15%)	3	24
1	AS	242/283 (86%)	207 (86%)	35 (14%)	4	26
1	AT	242/283 (86%)	208 (86%)	34 (14%)	4	28
1	AU	242/283 (86%)	207 (86%)	35 (14%)	4	26
1	AV	242/283 (86%)	207 (86%)	35 (14%)	4	26
1	AW	242/283 (86%)	208 (86%)	34 (14%)	4	28
1	AX	242/283 (86%)	208 (86%)	34 (14%)	4	28
1	AY	242/283 (86%)	210 (87%)	32 (13%)	5	30
1	AZ	242/283 (86%)	210 (87%)	32 (13%)	5	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Aa	242/283 (86%)	208 (86%)	34 (14%)	4	28
1	Ab	242/283 (86%)	206 (85%)	36 (15%)	4	25
1	Ac	242/283 (86%)	208 (86%)	34 (14%)	4	28
1	Ad	242/283 (86%)	209 (86%)	33 (14%)	5	29
1	BA	242/283 (86%)	213 (88%)	29 (12%)	6	33
1	BB	242/283 (86%)	212 (88%)	30 (12%)	6	32
1	BC	242/283 (86%)	214 (88%)	28 (12%)	7	36
1	BD	242/283 (86%)	215 (89%)	27 (11%)	7	38
1	BE	242/283 (86%)	215 (89%)	27 (11%)	7	38
1	BF	242/283 (86%)	214 (88%)	28 (12%)	7	36
1	BG	242/283 (86%)	214 (88%)	28 (12%)	7	36
1	BH	242/283 (86%)	216 (89%)	26 (11%)	8	40
1	BI	242/283 (86%)	213 (88%)	29 (12%)	6	33
1	BJ	242/283 (86%)	215 (89%)	27 (11%)	7	38
1	BK	242/283 (86%)	215 (89%)	27 (11%)	7	38
1	BL	242/283 (86%)	214 (88%)	28 (12%)	7	36
1	BM	242/283 (86%)	214 (88%)	28 (12%)	7	36
1	BN	242/283 (86%)	214 (88%)	28 (12%)	7	36
1	BO	242/283 (86%)	214 (88%)	28 (12%)	7	36
1	BP	242/283 (86%)	214 (88%)	28 (12%)	7	36
1	BQ	242/283 (86%)	215 (89%)	27 (11%)	7	38
1	BR	242/283 (86%)	215 (89%)	27 (11%)	7	38
1	BS	242/283 (86%)	215 (89%)	27 (11%)	7	38
1	BT	242/283 (86%)	214 (88%)	28 (12%)	7	36
1	BU	242/283 (86%)	214 (88%)	28 (12%)	7	36
1	BV	242/283 (86%)	215 (89%)	27 (11%)	7	38
1	BW	242/283 (86%)	216 (89%)	26 (11%)	8	40
1	BX	242/283 (86%)	215 (89%)	27 (11%)	7	38
1	BY	242/283 (86%)	215 (89%)	27 (11%)	7	38
1	BZ	242/283 (86%)	214 (88%)	28 (12%)	7	36
1	Ba	242/283 (86%)	215 (89%)	27 (11%)	7	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Bb	242/283 (86%)	214 (88%)	28 (12%)	7	36
1	Bc	242/283 (86%)	213 (88%)	29 (12%)	6	33
1	Bd	242/283 (86%)	213 (88%)	29 (12%)	6	33
1	CA	255/283 (90%)	229 (90%)	26 (10%)	9	42
1	CB	255/283 (90%)	230 (90%)	25 (10%)	10	44
1	CC	255/283 (90%)	229 (90%)	26 (10%)	9	42
1	CD	255/283 (90%)	229 (90%)	26 (10%)	9	42
1	CE	255/283 (90%)	227 (89%)	28 (11%)	8	39
1	CF	255/283 (90%)	230 (90%)	25 (10%)	10	44
1	CG	255/283 (90%)	226 (89%)	29 (11%)	7	36
1	CH	255/283 (90%)	229 (90%)	26 (10%)	9	42
1	CI	255/283 (90%)	228 (89%)	27 (11%)	8	40
1	CJ	255/283 (90%)	229 (90%)	26 (10%)	9	42
1	CK	255/283 (90%)	228 (89%)	27 (11%)	8	40
1	CL	255/283 (90%)	231 (91%)	24 (9%)	11	47
1	CM	255/283 (90%)	229 (90%)	26 (10%)	9	42
1	CN	255/283 (90%)	228 (89%)	27 (11%)	8	40
1	CO	255/283 (90%)	230 (90%)	25 (10%)	10	44
1	CP	255/283 (90%)	230 (90%)	25 (10%)	10	44
1	CQ	255/283 (90%)	229 (90%)	26 (10%)	9	42
1	CR	255/283 (90%)	230 (90%)	25 (10%)	10	44
1	CS	255/283 (90%)	228 (89%)	27 (11%)	8	40
1	CT	255/283 (90%)	230 (90%)	25 (10%)	10	44
1	CU	255/283 (90%)	228 (89%)	27 (11%)	8	40
1	CV	255/283 (90%)	227 (89%)	28 (11%)	8	39
1	CW	255/283 (90%)	228 (89%)	27 (11%)	8	40
1	CX	255/283 (90%)	228 (89%)	27 (11%)	8	40
1	CY	255/283 (90%)	228 (89%)	27 (11%)	8	40
1	CZ	255/283 (90%)	228 (89%)	27 (11%)	8	40
1	Ca	255/283 (90%)	228 (89%)	27 (11%)	8	40
1	Cb	255/283 (90%)	229 (90%)	26 (10%)	9	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Cc	255/283 (90%)	228 (89%)	27 (11%)	8	40
1	Cd	255/283 (90%)	231 (91%)	24 (9%)	11	47
All	All	22170/25470 (87%)	19531 (88%)	2639 (12%)	6	34

5 of 2639 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AN	176	ARG
1	CQ	114	MET
1	Cb	43	SER
1	CN	204	SER
1	BP	191	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 487 such sidechains are listed below:

Mol	Chain	Res	Type
1	AN	118	ASN
1	AQ	225	GLN
1	Ab	236	ASN
1	AN	258	GLN
1	BP	142	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 90 ligands modelled in this entry, 90 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	AA	287/338 (84%)	-0.02	1 (0%) 94 90	44, 93, 184, 235	0
1	AB	287/338 (84%)	1.14	61 (21%) 1 1	31, 79, 239, 363	0
1	AC	287/338 (84%)	0.35	26 (9%) 11 8	32, 75, 244, 339	0
1	AD	287/338 (84%)	0.37	16 (5%) 28 19	40, 82, 155, 215	0
1	AE	287/338 (84%)	0.23	6 (2%) 67 52	44, 88, 179, 251	0
1	AF	287/338 (84%)	0.37	20 (6%) 19 13	37, 80, 176, 225	0
1	AG	287/338 (84%)	0.65	36 (12%) 5 5	42, 89, 208, 293	0
1	AH	287/338 (84%)	0.65	38 (13%) 4 4	39, 86, 244, 334	0
1	AI	287/338 (84%)	0.38	23 (8%) 15 10	38, 93, 255, 333	0
1	AJ	287/338 (84%)	0.04	5 (1%) 73 59	36, 75, 146, 223	0
1	AK	287/338 (84%)	0.01	2 (0%) 89 81	31, 63, 120, 191	0
1	AL	287/338 (84%)	0.05	1 (0%) 94 90	32, 69, 138, 194	0
1	AM	287/338 (84%)	1.06	51 (17%) 2 2	41, 91, 249, 306	0
1	AN	287/338 (84%)	-0.16	4 (1%) 78 65	41, 85, 200, 285	0
1	AO	287/338 (84%)	0.50	21 (7%) 18 12	36, 83, 203, 294	0
1	AP	287/338 (84%)	0.10	9 (3%) 52 38	41, 81, 187, 253	0
1	AQ	287/338 (84%)	0.07	8 (2%) 56 42	46, 83, 172, 212	0
1	AR	287/338 (84%)	-0.08	0 100 100	40, 77, 141, 197	0
1	AS	287/338 (84%)	-0.07	7 (2%) 62 47	28, 78, 171, 271	0
1	AT	287/338 (84%)	0.17	3 (1%) 84 73	46, 89, 169, 226	0
1	AU	287/338 (84%)	0.71	33 (11%) 6 6	32, 86, 200, 301	0
1	AV	287/338 (84%)	0.38	19 (6%) 22 14	45, 90, 183, 234	0
1	AW	287/338 (84%)	0.07	2 (0%) 89 81	37, 72, 129, 194	0
1	AX	287/338 (84%)	0.47	26 (9%) 11 8	37, 79, 185, 294	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	AY	287/338 (84%)	0.12	7 (2%) 62 47	37, 77, 153, 206	0
1	AZ	287/338 (84%)	0.16	8 (2%) 56 42	39, 84, 178, 279	0
1	Aa	287/338 (84%)	0.02	7 (2%) 62 47	41, 90, 182, 222	0
1	Ab	287/338 (84%)	1.24	56 (19%) 1 1	38, 81, 245, 357	0
1	Ac	287/338 (84%)	0.30	16 (5%) 28 19	45, 82, 169, 236	0
1	Ad	287/338 (84%)	0.31	11 (3%) 44 32	43, 77, 141, 218	0
1	BA	286/338 (84%)	0.28	17 (5%) 26 17	37, 88, 199, 239	0
1	BB	286/338 (84%)	0.80	39 (13%) 4 4	25, 71, 229, 336	0
1	BC	286/338 (84%)	0.86	48 (16%) 2 2	30, 79, 265, 341	0
1	BD	286/338 (84%)	0.04	5 (1%) 73 59	34, 79, 172, 283	0
1	BE	286/338 (84%)	0.36	17 (5%) 26 17	41, 81, 199, 285	0
1	BF	286/338 (84%)	0.32	24 (8%) 14 10	32, 75, 188, 271	0
1	BG	286/338 (84%)	0.84	37 (12%) 5 4	39, 81, 215, 307	0
1	BH	286/338 (84%)	0.84	45 (15%) 3 2	36, 78, 245, 329	0
1	BI	286/338 (84%)	0.38	27 (9%) 11 8	35, 82, 280, 360	0
1	BJ	286/338 (84%)	0.05	3 (1%) 84 73	24, 67, 162, 275	0
1	BK	286/338 (84%)	0.19	4 (1%) 78 65	27, 62, 144, 203	0
1	BL	286/338 (84%)	-0.00	0 100 100	29, 66, 129, 190	0
1	BM	286/338 (84%)	1.13	57 (19%) 1 1	32, 79, 256, 365	0
1	BN	286/338 (84%)	0.15	16 (5%) 28 19	37, 80, 201, 324	0
1	BO	286/338 (84%)	1.22	69 (24%) 1 1	29, 76, 223, 315	0
1	BP	286/338 (84%)	0.18	13 (4%) 37 26	37, 81, 198, 270	0
1	BQ	286/338 (84%)	-0.00	2 (0%) 89 81	35, 78, 180, 295	0
1	BR	286/338 (84%)	0.29	7 (2%) 62 47	37, 80, 149, 225	0
1	BS	286/338 (84%)	0.08	7 (2%) 62 47	27, 67, 180, 308	0
1	BT	286/338 (84%)	0.17	5 (1%) 73 59	38, 84, 176, 270	0
1	BU	286/338 (84%)	0.64	36 (12%) 5 5	32, 75, 209, 323	0
1	BV	286/338 (84%)	0.01	4 (1%) 78 65	38, 86, 183, 243	0
1	BW	286/338 (84%)	-0.06	1 (0%) 94 90	33, 66, 123, 203	0
1	BX	286/338 (84%)	0.39	20 (6%) 19 13	35, 80, 198, 263	0
1	BY	286/338 (84%)	0.53	20 (6%) 19 13	35, 78, 150, 213	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	BZ	286/338 (84%)	0.22	11 (3%) 44 32	38, 83, 195, 246	0
1	Ba	286/338 (84%)	0.06	5 (1%) 73 59	34, 81, 197, 330	0
1	Bb	286/338 (84%)	0.76	43 (15%) 3 3	30, 69, 249, 342	0
1	Bc	286/338 (84%)	0.27	13 (4%) 37 26	33, 79, 214, 279	0
1	Bd	286/338 (84%)	0.51	23 (8%) 15 10	37, 79, 168, 230	0
1	CA	304/338 (89%)	0.30	24 (7%) 15 10	40, 78, 206, 252	0
1	CB	304/338 (89%)	1.66	91 (29%) 1 1	29, 75, 282, 357	0
1	CC	304/338 (89%)	0.59	45 (14%) 3 3	28, 72, 269, 370	0
1	CD	304/338 (89%)	0.10	13 (4%) 39 27	38, 76, 190, 273	0
1	CE	304/338 (89%)	0.71	49 (16%) 3 2	34, 76, 239, 323	0
1	CF	304/338 (89%)	0.79	51 (16%) 2 2	34, 72, 234, 326	0
1	CG	304/338 (89%)	1.95	90 (29%) 1 1	39, 83, 269, 342	0
1	CH	304/338 (89%)	1.96	94 (30%) 1 1	37, 79, 323, 403	0
1	CI	304/338 (89%)	0.73	51 (16%) 2 2	34, 81, 284, 396	0
1	CJ	304/338 (89%)	0.12	12 (3%) 43 31	26, 70, 200, 287	0
1	CK	304/338 (89%)	0.13	2 (0%) 89 81	28, 64, 113, 174	0
1	CL	304/338 (89%)	0.03	2 (0%) 89 81	26, 66, 129, 190	0
1	CM	304/338 (89%)	1.37	76 (25%) 1 1	33, 75, 306, 389	0
1	CN	304/338 (89%)	0.43	33 (10%) 7 6	39, 77, 229, 320	0
1	CO	304/338 (89%)	0.91	53 (17%) 2 2	30, 74, 258, 396	0
1	CP	304/338 (89%)	0.33	24 (7%) 15 10	33, 81, 201, 288	0
1	CQ	304/338 (89%)	0.22	16 (5%) 30 21	39, 80, 187, 294	0
1	CR	304/338 (89%)	0.12	7 (2%) 64 48	34, 79, 153, 209	0
1	CS	304/338 (89%)	0.34	24 (7%) 15 10	28, 66, 226, 306	0
1	CT	304/338 (89%)	0.10	7 (2%) 64 48	37, 76, 186, 299	0
1	CU	304/338 (89%)	1.15	68 (22%) 1 1	31, 70, 249, 303	0
1	CV	304/338 (89%)	0.24	13 (4%) 39 27	41, 80, 196, 237	0
1	CW	304/338 (89%)	0.00	6 (1%) 68 54	30, 75, 137, 176	0
1	CX	304/338 (89%)	0.07	16 (5%) 30 21	39, 78, 244, 302	0
1	CY	304/338 (89%)	0.53	29 (9%) 10 8	33, 73, 176, 256	0
1	CZ	304/338 (89%)	0.38	32 (10%) 8 6	43, 82, 187, 293	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	Ca	304/338 (89%)	0.68	40 (13%) 4 4	35, 78, 209, 267	0
1	Cb	304/338 (89%)	1.89	84 (27%) 1 1	30, 73, 298, 419	0
1	Cc	304/338 (89%)	0.64	47 (15%) 3 2	38, 80, 263, 325	0
1	Cd	304/338 (89%)	0.21	13 (4%) 39 27	35, 75, 137, 221	0
All	All	26310/30420 (86%)	0.45	2253 (8%) 13 10	24, 78, 223, 419	0

The worst 5 of 2253 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Cb	232	SER	28.1
1	CG	265	ILE	22.5
1	CH	337	GLU	21.4
1	Cb	227	SER	20.3
1	BG	317	ASP	20.0

## 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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	CA	AE	401	1/1	0.96	0.18	-0.53	38,38,38,38	0
2	CA	BS	401	1/1	0.99	0.20	-0.58	23,23,23,23	0
2	CA	AF	401	1/1	0.99	0.18	-0.62	50,50,50,50	0
2	CA	AZ	401	1/1	0.99	0.18	-0.65	36,36,36,36	0
2	CA	Ba	401	1/1	0.98	0.19	-0.67	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CA	Aa	401	1/1	0.98	0.15	-0.69	45,45,45,45	0
2	CA	AK	401	1/1	0.98	0.19	-0.74	36,36,36,36	0
2	CA	AN	401	1/1	0.99	0.17	-0.85	42,42,42,42	0
2	CA	BA	401	1/1	0.99	0.16	-0.88	35,35,35,35	0
2	CA	AC	401	1/1	0.98	0.18	-0.89	28,28,28,28	0
2	CA	AW	401	1/1	0.99	0.17	-0.90	39,39,39,39	0
2	CA	AI	401	1/1	0.98	0.17	-1.00	43,43,43,43	0
2	CA	AO	401	1/1	0.99	0.16	-1.03	47,47,47,47	0
2	CA	BT	401	1/1	0.98	0.16	-1.04	19,19,19,19	0
2	CA	AR	401	1/1	0.99	0.14	-1.07	40,40,40,40	0
2	CA	AV	401	1/1	0.99	0.15	-1.10	39,39,39,39	0
2	CA	BE	401	1/1	0.99	0.15	-1.14	35,35,35,35	0
2	CA	Bc	401	1/1	0.98	0.14	-1.16	29,29,29,29	0
2	CA	BP	402	1/1	0.98	0.13	-1.19	35,35,35,35	0
2	CA	BE	402	1/1	0.99	0.18	-1.19	33,33,33,33	0
2	CA	Ac	401	1/1	0.99	0.15	-1.20	48,48,48,48	0
2	CA	AA	401	1/1	0.99	0.14	-1.22	57,57,57,57	0
2	CA	Bc	402	1/1	1.00	0.16	-1.23	43,43,43,43	0
2	CA	BJ	401	1/1	0.97	0.16	-1.28	27,27,27,27	0
2	CA	BP	401	1/1	0.98	0.17	-1.32	33,33,33,33	0
2	CA	BI	401	1/1	0.94	0.15	-1.33	43,43,43,43	0
2	CA	AH	401	1/1	0.98	0.13	-1.35	34,34,34,34	0
2	CA	AS	401	1/1	0.99	0.16	-1.35	27,27,27,27	0
2	CA	BO	401	1/1	0.98	0.18	-1.37	34,34,34,34	0
2	CA	BN	401	1/1	0.98	0.17	-1.38	39,39,39,39	0
2	CA	AB	401	1/1	0.99	0.14	-1.40	40,40,40,40	0
2	CA	BC	402	1/1	0.98	0.14	-1.42	38,38,38,38	0
2	CA	BU	402	1/1	0.98	0.15	-1.45	29,29,29,29	0
2	CA	AD	401	1/1	0.99	0.14	-1.45	36,36,36,36	0
2	CA	AY	401	1/1	0.99	0.14	-1.46	30,30,30,30	0
2	CA	BC	401	1/1	0.98	0.16	-1.47	22,22,22,22	0
2	CA	Ad	401	1/1	0.99	0.15	-1.49	42,42,42,42	0
2	CA	BA	402	1/1	0.98	0.13	-1.52	41,41,41,41	0
2	CA	AG	401	1/1	0.99	0.11	-1.52	44,44,44,44	0
2	CA	Bb	401	1/1	0.97	0.17	-1.55	24,24,24,24	0
2	CA	BH	401	1/1	0.99	0.12	-1.58	34,34,34,34	0
2	CA	BK	401	1/1	0.98	0.16	-1.59	22,22,22,22	0
2	CA	BX	402	1/1	0.99	0.12	-1.60	31,31,31,31	0
2	CA	BF	401	1/1	0.98	0.16	-1.60	27,27,27,27	0
2	CA	BI	402	1/1	0.98	0.14	-1.64	54,54,54,54	0
2	CA	Bd	402	1/1	0.98	0.12	-1.65	48,48,48,48	0
2	CA	BS	402	1/1	0.99	0.16	-1.68	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CA	AM	401	1/1	0.99	0.12	-1.70	45,45,45,45	0
2	CA	BL	402	1/1	0.98	0.14	-1.74	34,34,34,34	0
2	CA	BW	401	1/1	0.99	0.14	-1.75	25,25,25,25	0
2	CA	BF	402	1/1	0.99	0.14	-1.79	36,36,36,36	0
2	CA	BL	401	1/1	0.98	0.15	-1.81	24,24,24,24	0
2	CA	AX	401	1/1	0.99	0.13	-1.81	38,38,38,38	0
2	CA	BO	402	1/1	0.91	0.14	-1.85	52,52,52,52	0
2	CA	BQ	402	1/1	0.96	0.12	-1.86	43,43,43,43	0
2	CA	AJ	401	1/1	0.99	0.14	-1.86	38,38,38,38	0
2	CA	BH	402	1/1	0.98	0.11	-1.86	41,41,41,41	0
2	CA	BZ	401	1/1	0.97	0.14	-1.88	36,36,36,36	0
2	CA	AP	401	1/1	0.98	0.12	-1.88	42,42,42,42	0
2	CA	AL	401	1/1	0.99	0.15	-1.93	41,41,41,41	0
2	CA	BB	402	1/1	0.96	0.12	-1.95	35,35,35,35	0
2	CA	BY	402	1/1	0.95	0.12	-1.95	33,33,33,33	0
2	CA	BV	402	1/1	0.95	0.12	-1.99	57,57,57,57	0
2	CA	BX	401	1/1	0.97	0.14	-2.01	35,35,35,35	0
2	CA	BG	402	1/1	0.98	0.13	-2.04	54,54,54,54	0
2	CA	BV	401	1/1	0.96	0.12	-2.04	36,36,36,36	0
2	CA	AQ	401	1/1	0.99	0.11	-2.05	57,57,57,57	0
2	CA	BD	401	1/1	0.95	0.14	-2.07	36,36,36,36	0
2	CA	Ab	401	1/1	0.98	0.10	-2.09	38,38,38,38	0
2	CA	AT	401	1/1	0.98	0.12	-2.10	36,36,36,36	0
2	CA	Ba	402	1/1	0.95	0.10	-2.13	42,42,42,42	0
2	CA	BJ	402	1/1	0.99	0.12	-2.15	29,29,29,29	0
2	CA	BD	402	1/1	0.99	0.14	-2.16	44,44,44,44	0
2	CA	BU	401	1/1	0.98	0.13	-2.16	32,32,32,32	0
2	CA	BW	402	1/1	0.99	0.16	-2.17	42,42,42,42	0
2	CA	BR	401	1/1	0.98	0.13	-2.18	26,26,26,26	0
2	CA	BZ	402	1/1	0.98	0.10	-2.24	57,57,57,57	0
2	CA	BM	402	1/1	0.99	0.12	-2.26	33,33,33,33	0
2	CA	BY	401	1/1	0.99	0.12	-2.27	31,31,31,31	0
2	CA	BR	402	1/1	0.99	0.10	-2.30	53,53,53,53	0
2	CA	BN	402	1/1	0.95	0.11	-2.30	50,50,50,50	0
2	CA	BQ	401	1/1	0.96	0.14	-2.35	32,32,32,32	0
2	CA	Bd	401	1/1	0.99	0.13	-2.37	37,37,37,37	0
2	CA	AU	401	1/1	0.97	0.12	-2.41	30,30,30,30	0
2	CA	Bb	402	1/1	0.99	0.16	-2.41	33,33,33,33	0
2	CA	BK	402	1/1	0.99	0.12	-2.52	31,31,31,31	0
2	CA	BB	401	1/1	0.97	0.12	-2.53	26,26,26,26	0
2	CA	BM	401	1/1	0.96	0.08	-2.77	39,39,39,39	0
2	CA	BG	401	1/1	0.98	0.11	-3.20	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CA	BT	402	1/1	0.99	0.13	-3.25	42,42,42,42	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.