wwPDB X-ray Structure Validation Summary Report (i)

Jun 24, 2024 – 07:12 PM EDT

PDB ID	:	6YFD
Title	:	Virus-like particle of Beihai levi-like virus 14
Authors	:	Rumnieks, J.; Kalnins, G.; Sisovs, M.; Lieknina, I.; Tars, K.
Deposited on	:	2020-03-26
Resolution	:	3.30 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

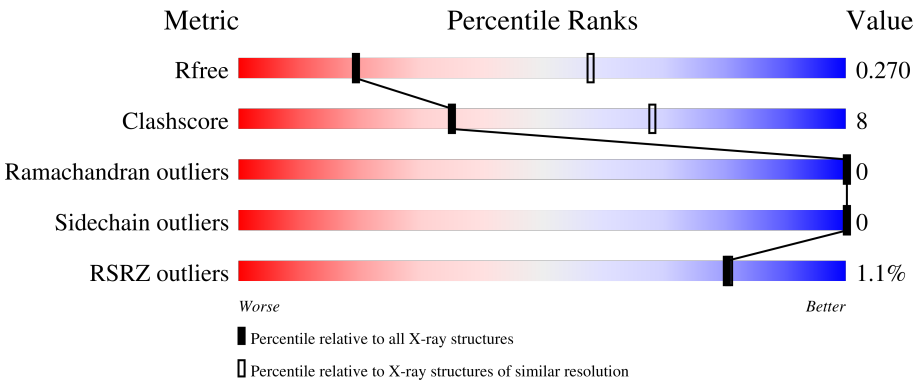
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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	AA	208	72% 23% 5%
1	AB	208	71% 20% 9%
1	AC	208	73% 16% 11%
1	AD	208	% 72% 24% 5%
1	AE	208	% 68% 23% 9%

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Mol	Chain	Length	Quality of chain
1	AF	208	2% 71% 19% 11%
1	AG	208	74% 21% 5%
1	AH	208	72% 19% 9%
1	AI	208	81% 8% 11%
1	AJ	208	73% 23% 5%
1	AK	208	70% 21% 9%
1	AL	208	71% 19% 11%
1	AM	208	75% 20% 5%
1	AN	208	73% 18% 9%
1	AO	208	79% 10% 11%
1	AP	208	74% 21% 5%
1	AQ	208	72% 19% 9%
1	AR	208	72% 18% 11%
1	AS	208	73% 22% 5%
1	AT	208	70% 21% 9%
1	AU	208	71% 18% 11%
1	AV	208	% 75% 21% 5%
1	AW	208	72% 19% 9%
1	AX	208	80% 9% 11%
1	AY	208	% 75% 21% 5%
1	AZ	208	% 71% 20% 9%
1	BA	208	% 73% 17% 11%
1	BB	208	% 73% 22% 5%
1	BC	208	% 71% 20% 9%
1	BD	208	72% 17% 11%

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Mol	Chain	Length	Quality of chain
1	BE	208	2% 73% 22% 5%
1	BF	208	3% 70% 21% 9%
1	BG	208	3% 72% 17% 11%
1	BH	208	2% 74% 22% 5%
1	BI	208	% 71% 20% 9%
1	BJ	208	4% 73% 17% 11%
1	BK	208	% 74% 22% 5%
1	BL	208	3% 72% 19% 9%
1	BM	208	73% 16% 11%
1	BN	208	73% 23% 5%
1	BO	208	% 74% 17% 9%
1	BP	208	73% 17% 11%
1	BQ	208	72% 23% 5%
1	BR	208	70% 21% 9%
1	BS	208	72% 18% 11%
1	BT	208	74% 22% 5%
1	BU	208	% 70% 21% 9%
1	BV	208	3% 80% 9% 11%
1	BW	208	73% 23% 5%
1	BX	208	70% 21% 9%
1	BY	208	73% 16% 11%
1	BZ	208	75% 20% 5%
1	CA	208	71% 20% 9%
1	CB	208	80% 10% 11%
1	CC	208	6% 73% 22% 5%

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Mol	Chain	Length	Quality of chain
1	CD	208	70% 21% 9%
1	CE	208	2% 73% 17% 11%
1	CF	208	74% 22% 5%
1	CG	208	72% 19% 9%
1	CH	208	% 78% 11% 11%
1	CI	208	73% 23% 5%
1	CJ	208	% 70% 21% 9%
1	CK	208	72% 17% 11%
1	CL	208	% 74% 21% 5%
1	CM	208	% 72% 19% 9%
1	CN	208	% 73% 17% 11%
1	CO	208	74% 22% 5%
1	CP	208	% 68% 23% 9%
1	CQ	208	71% 19% 11%
1	CR	208	% 75% 21% 5%
1	CS	208	2% 72% 19% 9%
1	CT	208	2% 74% 15% 11%
1	CU	208	71% 25% 5%
1	CV	208	69% 22% 9%
1	CW	208	72% 17% 11%
1	CX	208	2% 75% 21% 5%
1	CY	208	% 71% 20% 9%
1	CZ	208	4% 73% 17% 11%
1	DA	208	2% 73% 23% 5%
1	DB	208	2% 71% 20% 9%

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Mol	Chain	Length	Quality of chain
1	DC	208	3% 73% 16% 11%
1	DD	208	74% 22% 5%
1	DE	208	2% 72% 19% 9%
1	DF	208	4% 73% 16% 11%
1	DG	208	% 74% 22% 5%
1	DH	208	72% 19% 9%
1	DI	208	74% 16% 11%
1	DJ	208	74% 22% 5%
1	DK	208	70% 21% 9%
1	DL	208	% 71% 19% 11%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 126960 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
			Total	C	N	O	S			
1	AA	198	1463	910	261	286	6	0	0	0
			Total	C	N	O	S			
1	AB	189	1396	869	249	273	5	0	0	0
			Total	C	N	O	S			
1	AC	186	1373	854	245	269	5	0	0	0
			Total	C	N	O	S			
1	AD	198	1463	910	261	286	6	0	0	0
			Total	C	N	O	S			
1	AE	189	1396	869	249	273	5	0	0	0
			Total	C	N	O	S			
1	AF	186	1373	854	245	269	5	0	0	0
			Total	C	N	O	S			
1	AG	198	1463	910	261	286	6	0	0	0
			Total	C	N	O	S			
1	AH	189	1396	869	249	273	5	0	0	0
			Total	C	N	O	S			
1	AI	186	1373	854	245	269	5	0	0	0
			Total	C	N	O	S			
1	AJ	198	1463	910	261	286	6	0	0	0
			Total	C	N	O	S			
1	AK	189	1396	869	249	273	5	0	0	0
			Total	C	N	O	S			
1	AL	186	1373	854	245	269	5	0	0	0
			Total	C	N	O	S			
1	AM	198	1463	910	261	286	6	0	0	0
			Total	C	N	O	S			
1	AN	189	1396	869	249	273	5	0	0	0
			Total	C	N	O	S			
1	AO	186	1373	854	245	269	5	0	0	0
			Total	C	N	O	S			
1	AP	198	1463	910	261	286	6	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	AQ	189	1396	869	249	273	5	0	0	0
			Total	C	N	O	S			
1	AR	186	1373	854	245	269	5	0	0	0
			Total	C	N	O	S			
1	AS	198	1463	910	261	286	6	0	0	0
			Total	C	N	O	S			
1	AT	189	1396	869	249	273	5	0	0	0
			Total	C	N	O	S			
1	AU	186	1373	854	245	269	5	0	0	0
			Total	C	N	O	S			
1	AV	198	1463	910	261	286	6	0	0	0
			Total	C	N	O	S			
1	AW	189	1396	869	249	273	5	0	0	0
			Total	C	N	O	S			
1	AX	186	1373	854	245	269	5	0	0	0
			Total	C	N	O	S			
1	AY	198	1463	910	261	286	6	0	0	0
			Total	C	N	O	S			
1	AZ	189	1396	869	249	273	5	0	0	0
			Total	C	N	O	S			
1	BA	186	1373	854	245	269	5	0	0	0
			Total	C	N	O	S			
1	BB	198	1463	910	261	286	6	0	0	0
			Total	C	N	O	S			
1	BC	189	1396	869	249	273	5	0	0	0
			Total	C	N	O	S			
1	BD	186	1373	854	245	269	5	0	0	0
			Total	C	N	O	S			
1	BE	198	1463	910	261	286	6	0	0	0
			Total	C	N	O	S			
1	BF	189	1396	869	249	273	5	0	0	0
			Total	C	N	O	S			
1	BG	186	1373	854	245	269	5	0	0	0
			Total	C	N	O	S			
1	BH	198	1463	910	261	286	6	0	0	0
			Total	C	N	O	S			
1	BI	189	1396	869	249	273	5	0	0	0
			Total	C	N	O	S			
1	BJ	186	1373	854	245	269	5	0	0	0
			Total	C	N	O	S			
1	BK	198	1463	910	261	286	6	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	BL	189	1396	869	249	273	5	0	0	0
			Total	C	N	O	S			
1	BM	186	1373	854	245	269	5	0	0	0
			Total	C	N	O	S			
1	BN	198	1463	910	261	286	6	0	0	0
			Total	C	N	O	S			
1	BO	189	1396	869	249	273	5	0	0	0
			Total	C	N	O	S			
1	BP	186	1373	854	245	269	5	0	0	0
			Total	C	N	O	S			
1	BQ	198	1463	910	261	286	6	0	0	0
			Total	C	N	O	S			
1	BR	189	1396	869	249	273	5	0	0	0
			Total	C	N	O	S			
1	BS	186	1373	854	245	269	5	0	0	0
			Total	C	N	O	S			
1	BT	198	1463	910	261	286	6	0	0	0
			Total	C	N	O	S			
1	BU	189	1396	869	249	273	5	0	0	0
			Total	C	N	O	S			
1	BV	186	1373	854	245	269	5	0	0	0
			Total	C	N	O	S			
1	BW	198	1463	910	261	286	6	0	0	0
			Total	C	N	O	S			
1	BX	189	1396	869	249	273	5	0	0	0
			Total	C	N	O	S			
1	BY	186	1373	854	245	269	5	0	0	0
			Total	C	N	O	S			
1	BZ	198	1463	910	261	286	6	0	0	0
			Total	C	N	O	S			
1	CA	189	1396	869	249	273	5	0	0	0
			Total	C	N	O	S			
1	CB	186	1373	854	245	269	5	0	0	0
			Total	C	N	O	S			
1	CC	198	1463	910	261	286	6	0	0	0
			Total	C	N	O	S			
1	CD	189	1396	869	249	273	5	0	0	0
			Total	C	N	O	S			
1	CE	186	1373	854	245	269	5	0	0	0
			Total	C	N	O	S			
1	CF	198	1463	910	261	286	6	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	CG	189	1396	869	249	273	5	0	0	0
			Total	C	N	O	S			
1	CH	186	1373	854	245	269	5	0	0	0
			Total	C	N	O	S			
1	CI	198	1463	910	261	286	6	0	0	0
			Total	C	N	O	S			
1	CJ	189	1396	869	249	273	5	0	0	0
			Total	C	N	O	S			
1	CK	186	1373	854	245	269	5	0	0	0
			Total	C	N	O	S			
1	CL	198	1463	910	261	286	6	0	0	0
			Total	C	N	O	S			
1	CM	189	1396	869	249	273	5	0	0	0
			Total	C	N	O	S			
1	CN	186	1373	854	245	269	5	0	0	0
			Total	C	N	O	S			
1	CO	198	1463	910	261	286	6	0	0	0
			Total	C	N	O	S			
1	CP	189	1396	869	249	273	5	0	0	0
			Total	C	N	O	S			
1	CQ	186	1373	854	245	269	5	0	0	0
			Total	C	N	O	S			
1	CR	198	1463	910	261	286	6	0	0	0
			Total	C	N	O	S			
1	CS	189	1396	869	249	273	5	0	0	0
			Total	C	N	O	S			
1	CT	186	1373	854	245	269	5	0	0	0
			Total	C	N	O	S			
1	CU	198	1463	910	261	286	6	0	0	0
			Total	C	N	O	S			
1	CV	189	1396	869	249	273	5	0	0	0
			Total	C	N	O	S			
1	CW	186	1373	854	245	269	5	0	0	0
			Total	C	N	O	S			
1	CX	198	1463	910	261	286	6	0	0	0
			Total	C	N	O	S			
1	CY	189	1396	869	249	273	5	0	0	0
			Total	C	N	O	S			
1	CZ	186	1373	854	245	269	5	0	0	0
			Total	C	N	O	S			
1	DA	198	1463	910	261	286	6	0	0	0

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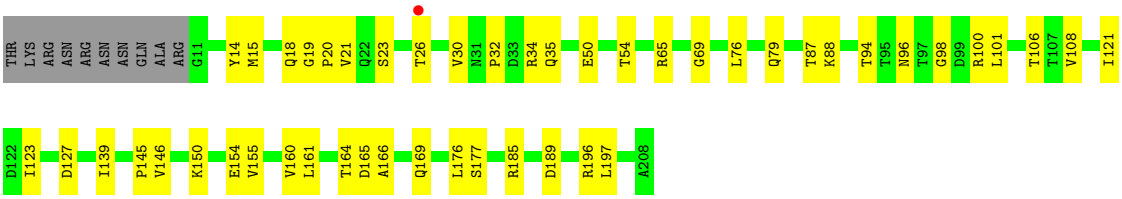
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	DB	189	1396	869	249	273	5	0	0	0
			Total	C	N	O	S			
1	DC	186	1373	854	245	269	5	0	0	0
			Total	C	N	O	S			
1	DD	198	1463	910	261	286	6	0	0	0
			Total	C	N	O	S			
1	DE	189	1396	869	249	273	5	0	0	0
			Total	C	N	O	S			
1	DF	186	1373	854	245	269	5	0	0	0
			Total	C	N	O	S			
1	DG	198	1463	910	261	286	6	0	0	0
			Total	C	N	O	S			
1	DH	189	1396	869	249	273	5	0	0	0
			Total	C	N	O	S			
1	DI	186	1373	854	245	269	5	0	0	0
			Total	C	N	O	S			
1	DJ	198	1463	910	261	286	6	0	0	0
			Total	C	N	O	S			
1	DK	189	1396	869	249	273	5	0	0	0
			Total	C	N	O	S			
1	DL	186	1373	854	245	269	5	0	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.

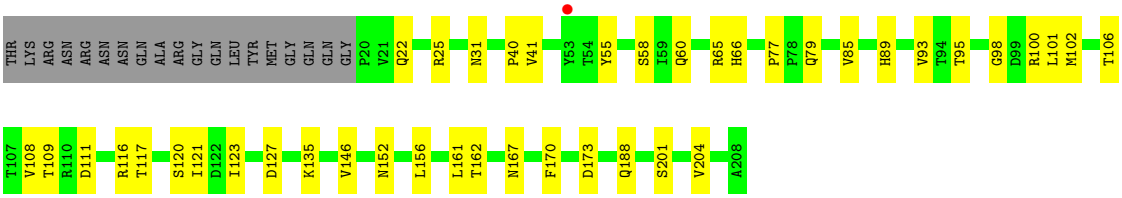
• Molecule 1: coat protein

Chain AA:



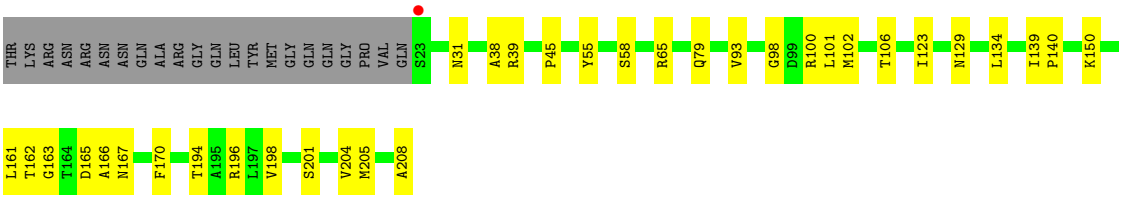
• Molecule 1: coat protein

Chain AB:



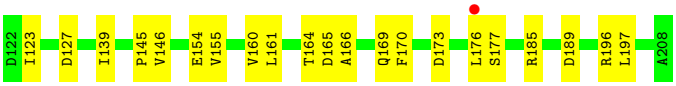
• Molecule 1: coat protein

Chain AC:



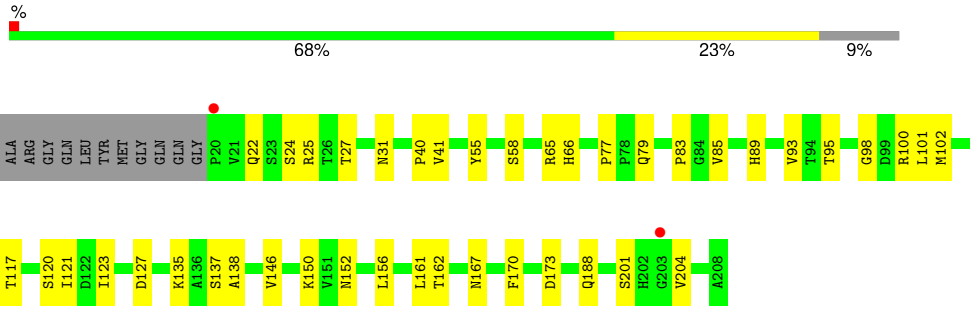
• Molecule 1: coat protein

Chain AD:



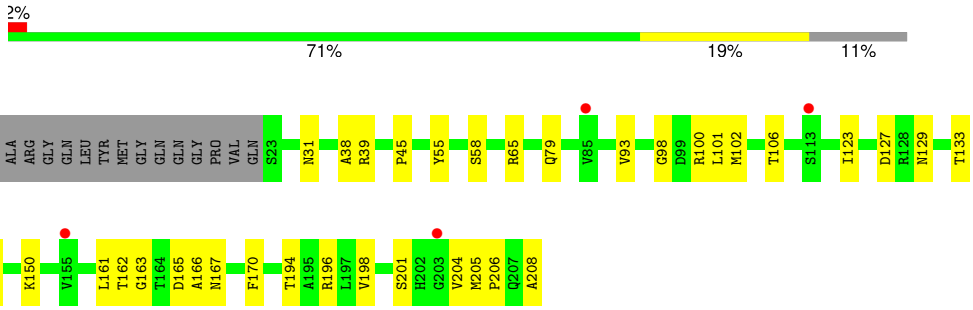
• Molecule 1: coat protein

Chain AE:



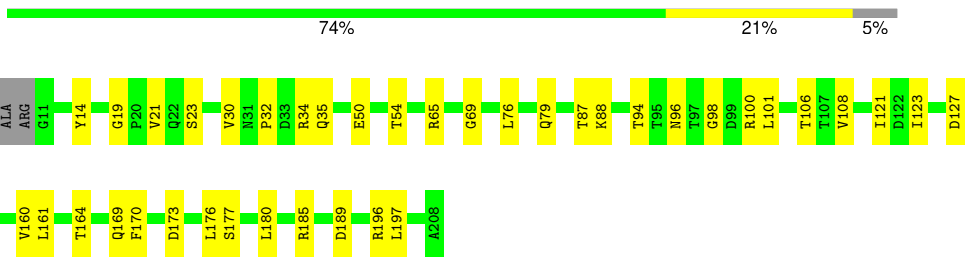
• Molecule 1: coat protein

Chain AF:



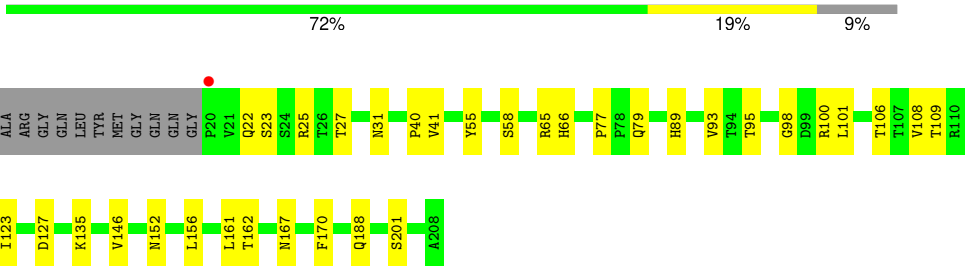
• Molecule 1: coat protein

Chain AG:



• Molecule 1: coat protein

Chain AH:

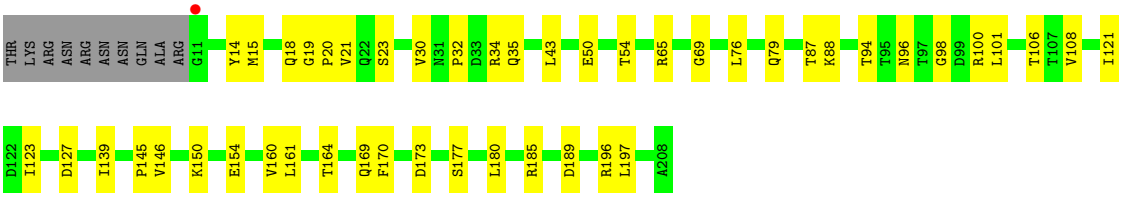


• Molecule 1: coat protein

Chain AI:

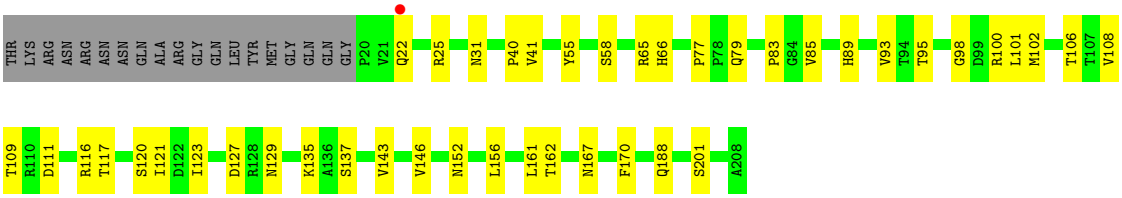
• Molecule 1: coat protein

Chain AJ: 73% 23% 5%



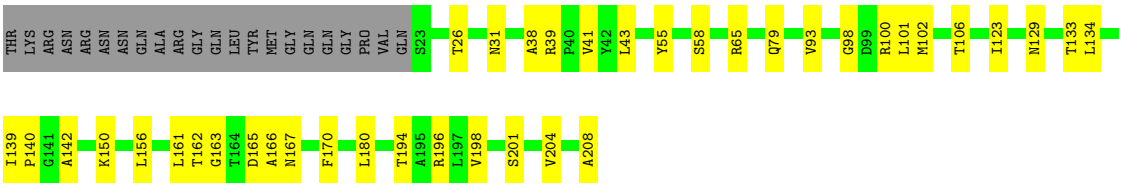
• Molecule 1: coat protein

Chain AK: 70% 21% 9%



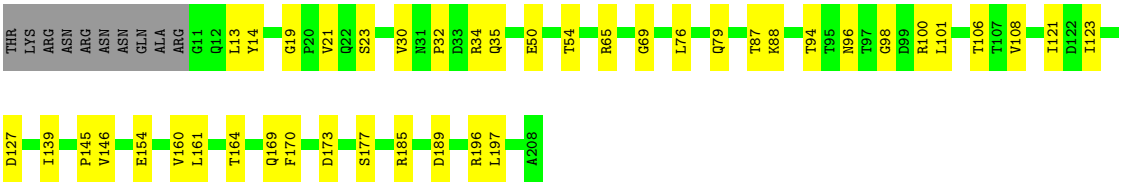
• Molecule 1: coat protein

Chain AL: 71% 19% 11%



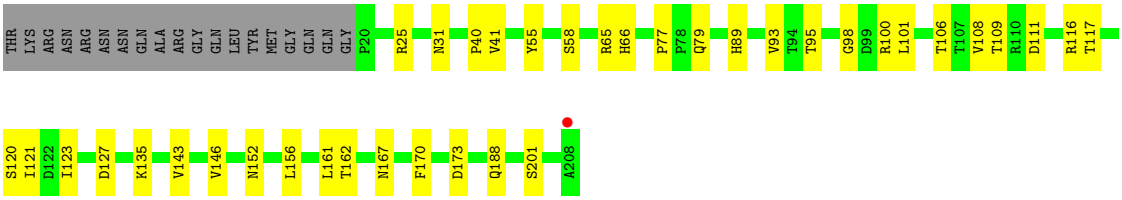
• Molecule 1: coat protein

Chain AM: 75% 20% 5%



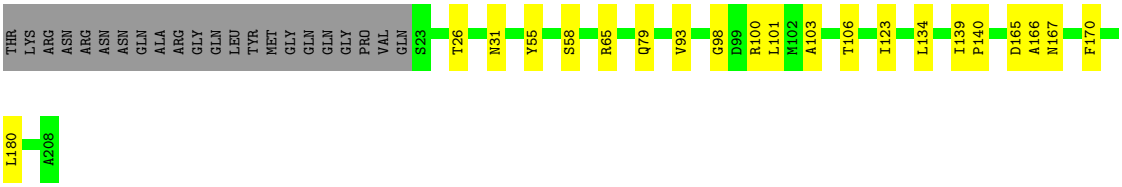
• Molecule 1: coat protein

Chain AN: 73% 18% 9%



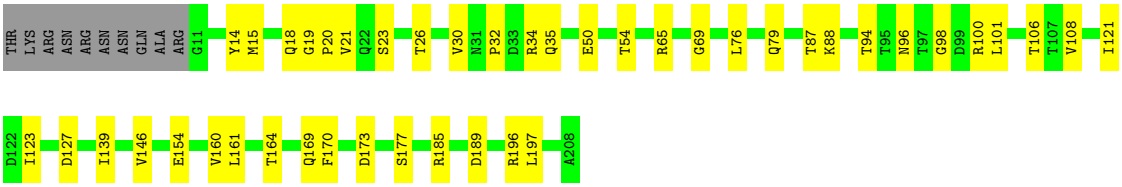
• Molecule 1: coat protein

Chain AO: 79% 10% 11%



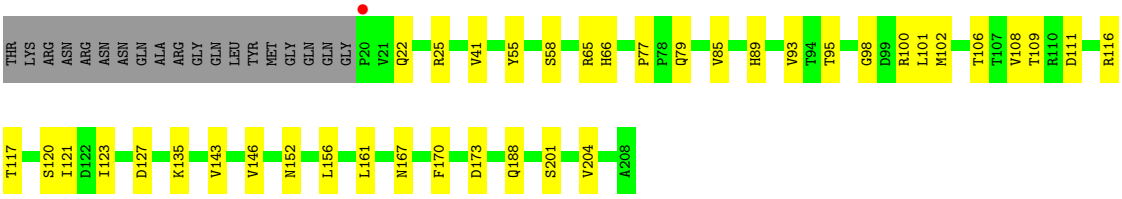
• Molecule 1: coat protein

Chain AP: 74% 21% 5%



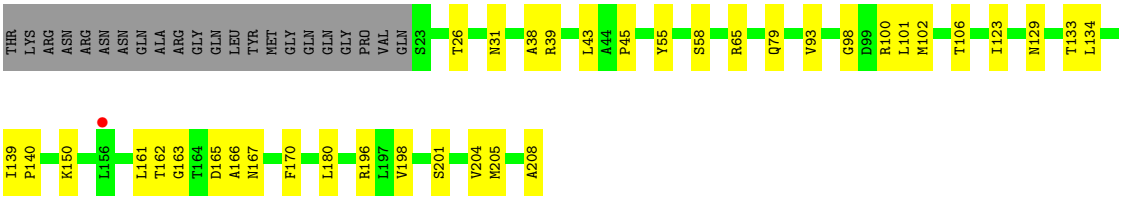
• Molecule 1: coat protein

Chain AQ: 72% 19% 9%



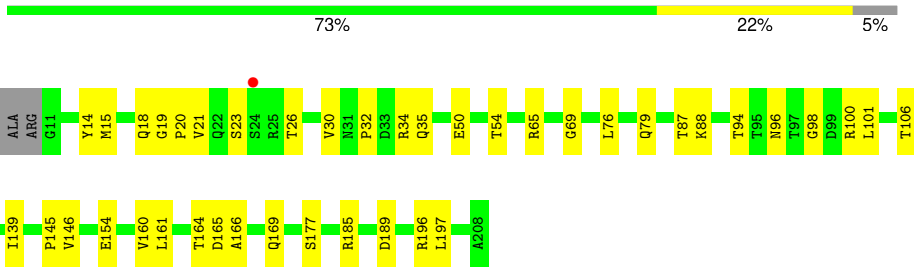
• Molecule 1: coat protein

Chain AR: 72% 18% 11%



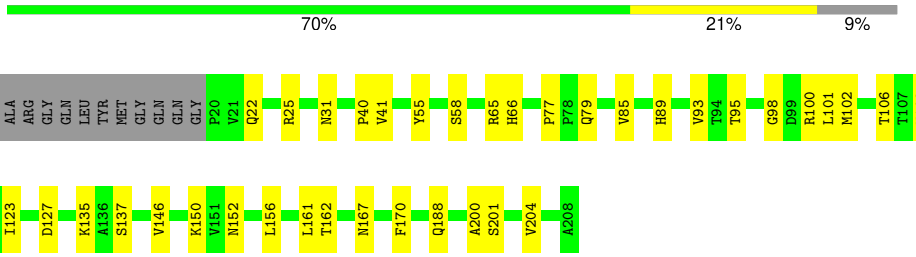
• Molecule 1: coat protein

Chain AS:



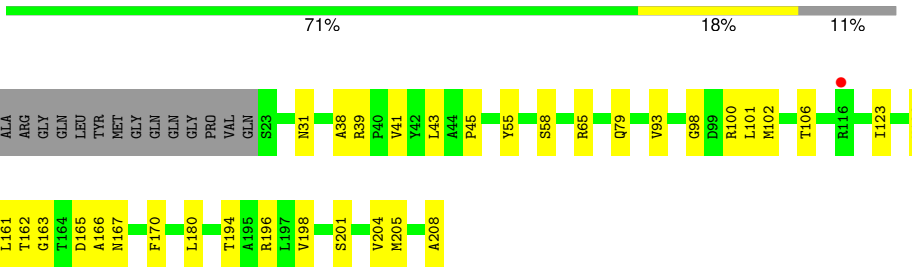
- Molecule 1: coat protein

Chain AT:



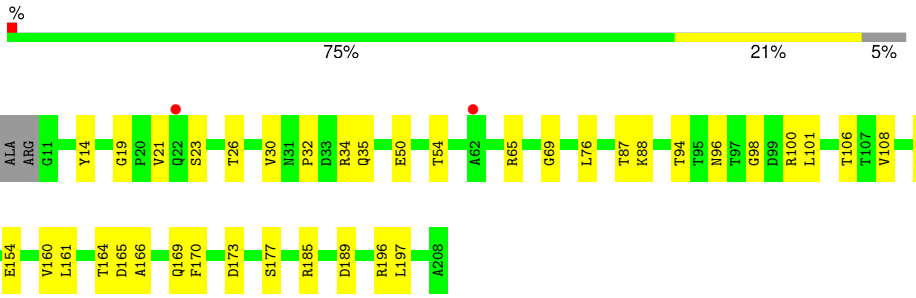
- Molecule 1: coat protein

Chain AU:



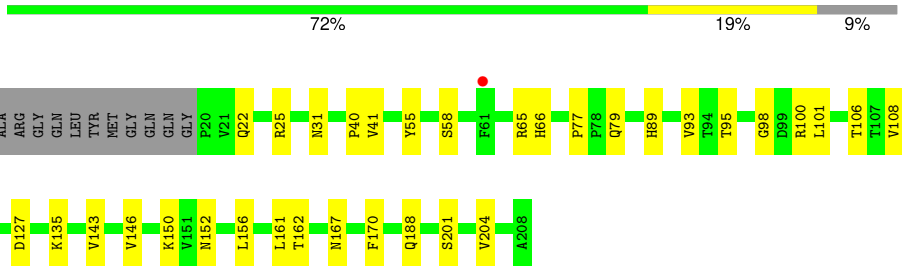
- Molecule 1: coat protein

Chain AV:



- Molecule 1: coat protein

Chain AW:

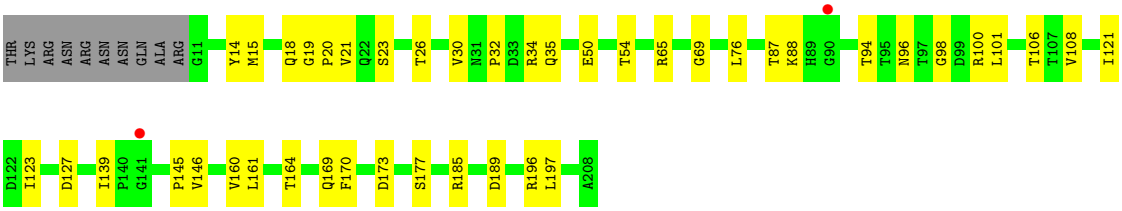


• Molecule 1: coat protein

Chain AX:

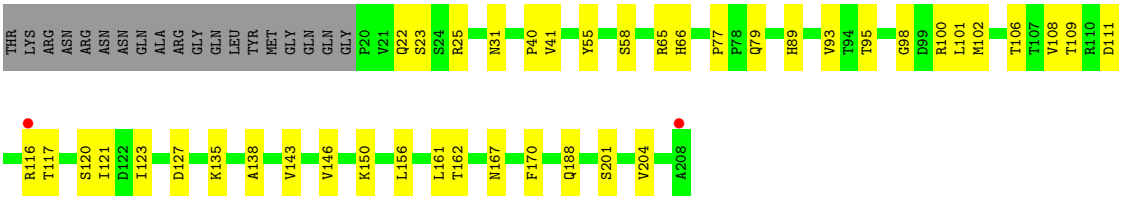
• Molecule 1: coat protein

Chain AY:



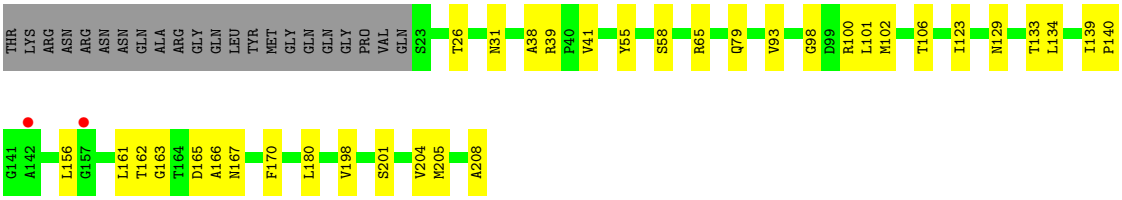
• Molecule 1: coat protein

Chain AZ:



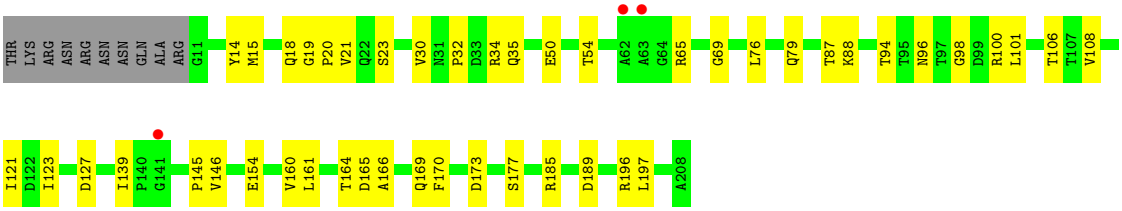
• Molecule 1: coat protein

Chain BA:



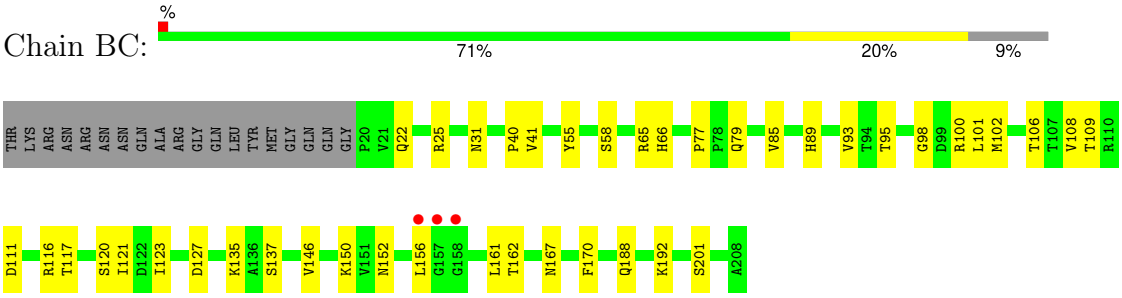
• Molecule 1: coat protein

Chain BB:



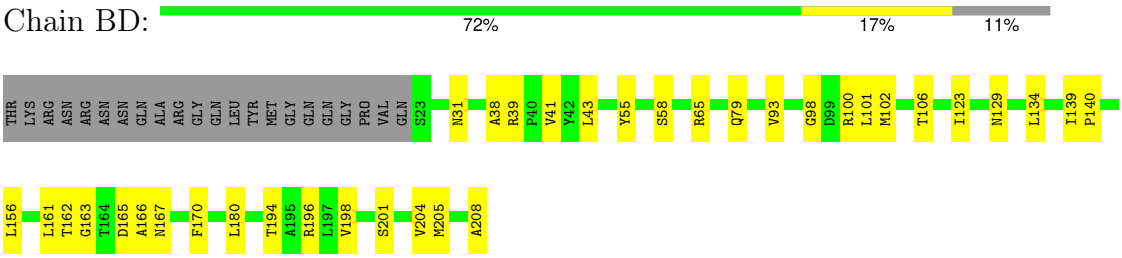
• Molecule 1: coat protein

Chain BC:



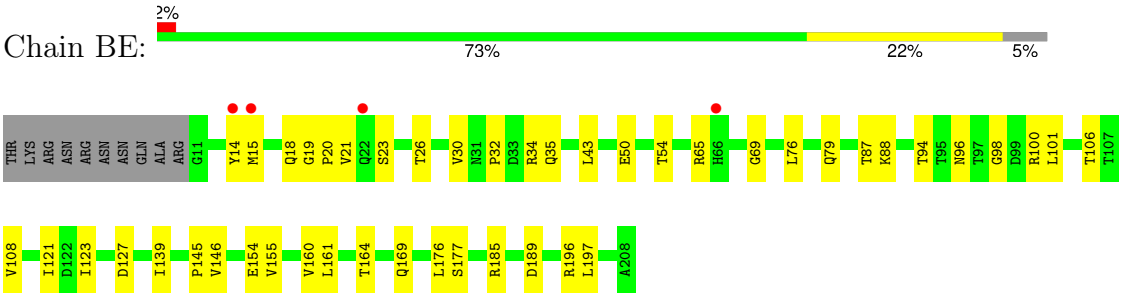
• Molecule 1: coat protein

Chain BD:



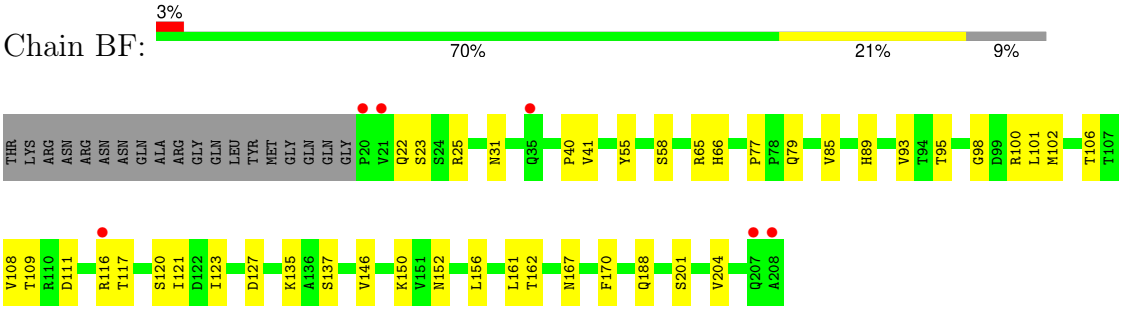
• Molecule 1: coat protein

Chain BE:



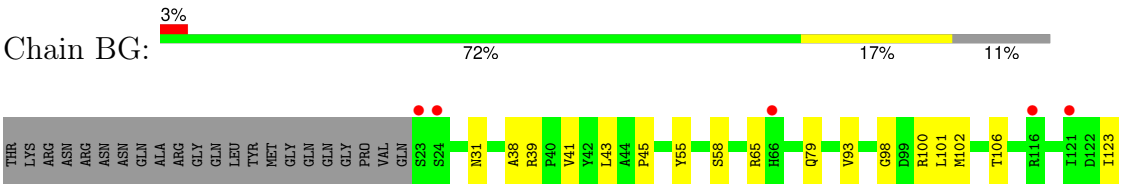
• Molecule 1: coat protein

Chain BF:



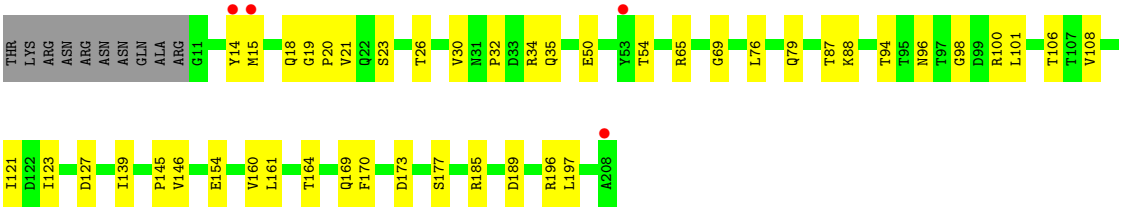
• Molecule 1: coat protein

Chain BG:



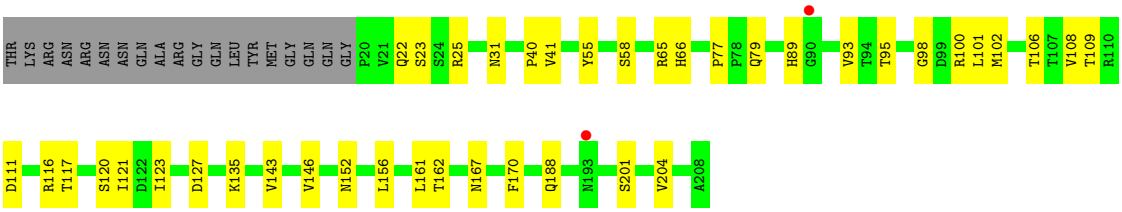
• Molecule 1: coat protein

Chain BH:



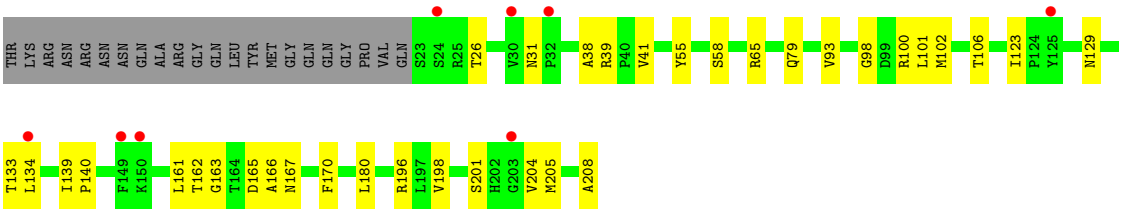
• Molecule 1: coat protein

Chain BI:



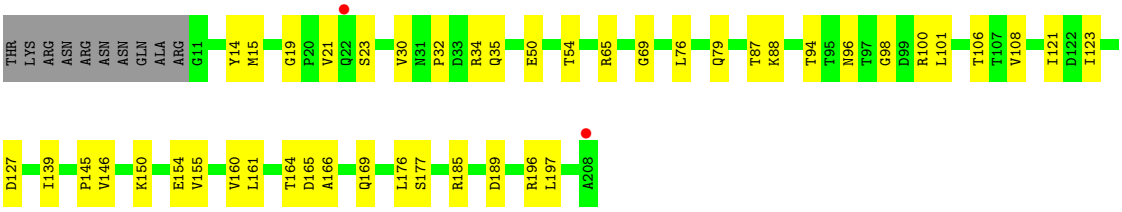
• Molecule 1: coat protein

Chain BJ:



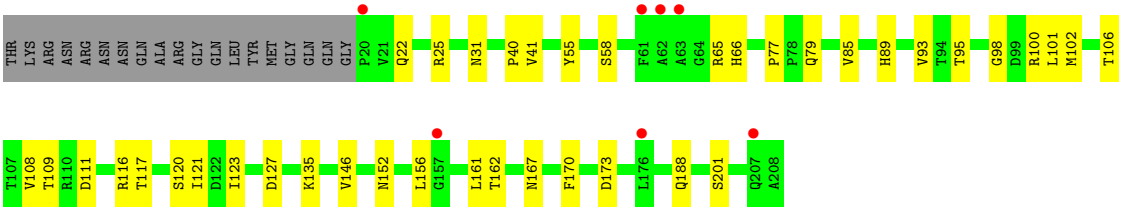
• Molecule 1: coat protein

Chain BK:



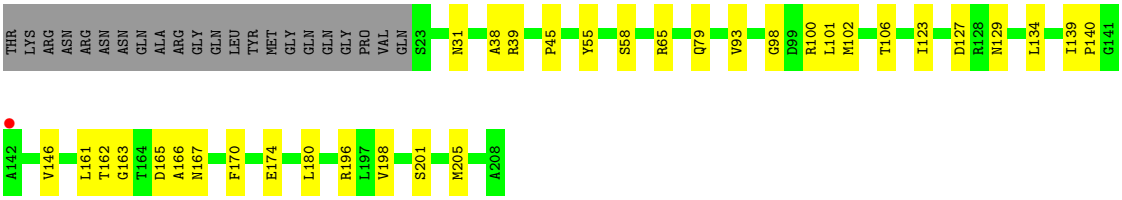
• Molecule 1: coat protein

Chain BL:



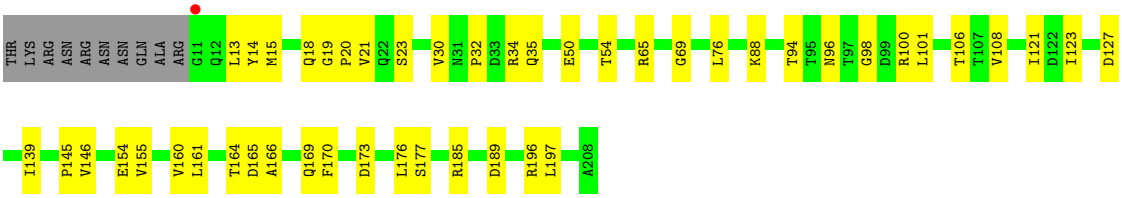
- Molecule 1: coat protein

Chain BM:



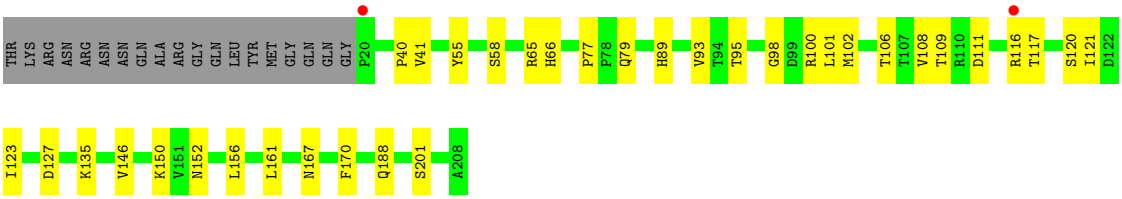
- Molecule 1: coat protein

Chain BN:



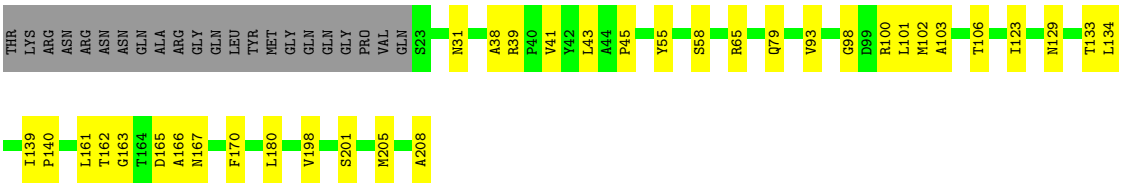
- Molecule 1: coat protein

Chain BO:



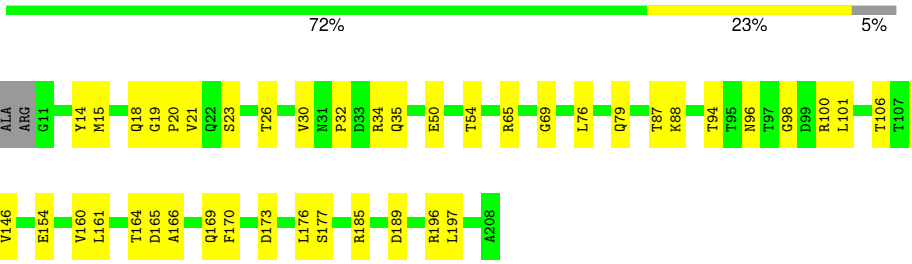
- Molecule 1: coat protein

Chain BP:



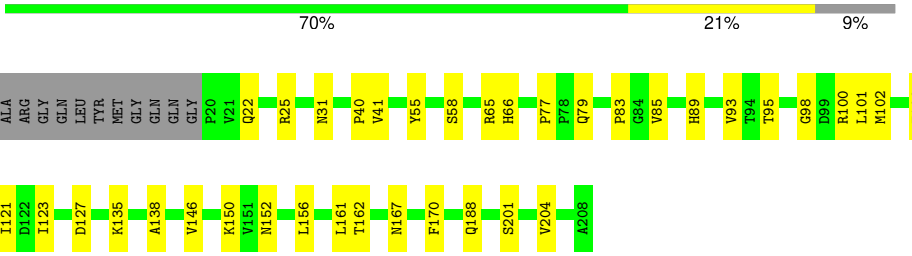
- Molecule 1: coat protein

Chain BQ:



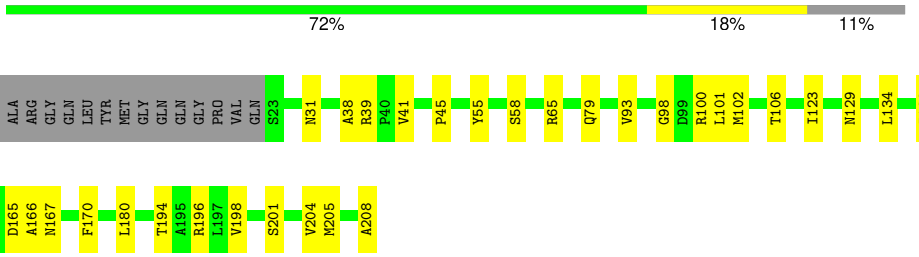
- Molecule 1: coat protein

Chain BR:



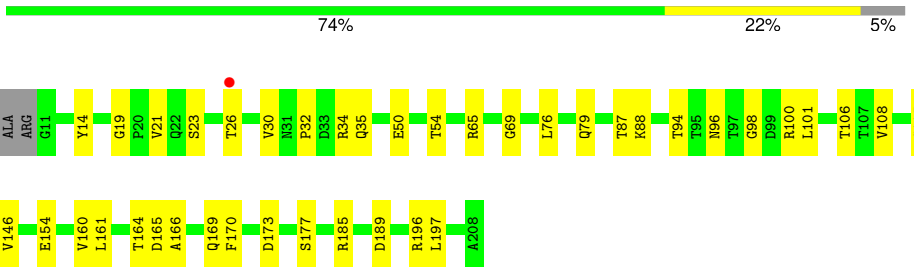
- Molecule 1: coat protein

Chain BS:



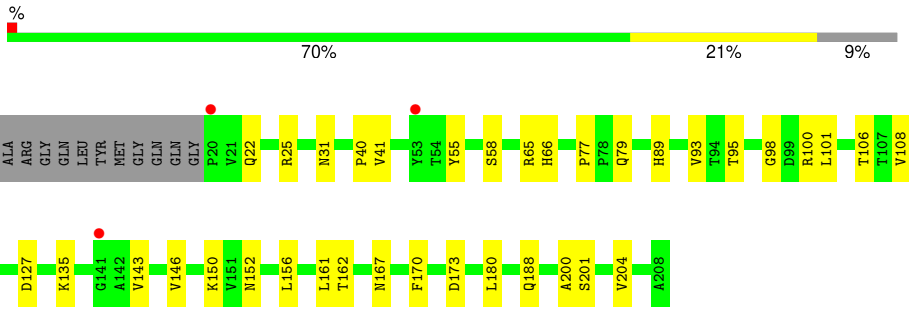
- Molecule 1: coat protein

Chain BT:



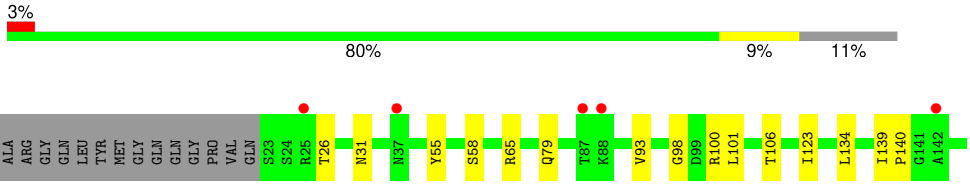
- Molecule 1: coat protein

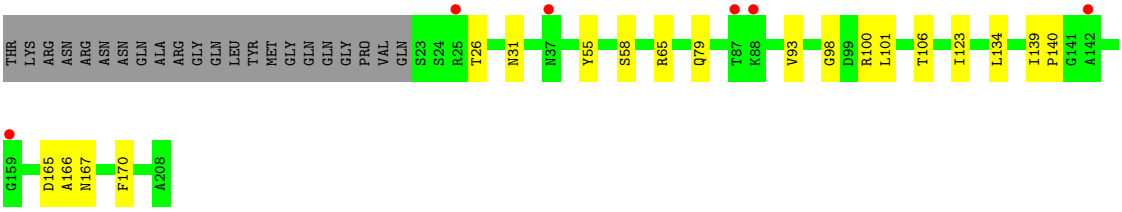
Chain BU:



• Molecule 1: coat protein

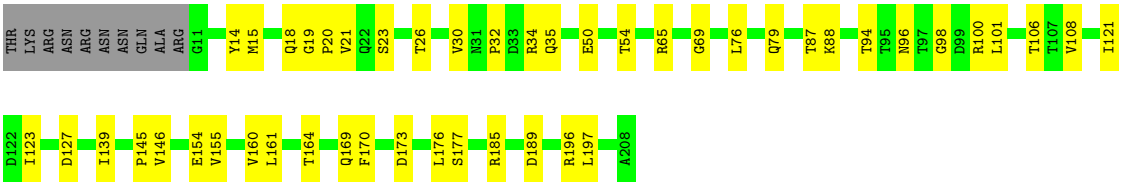
Chain BV:





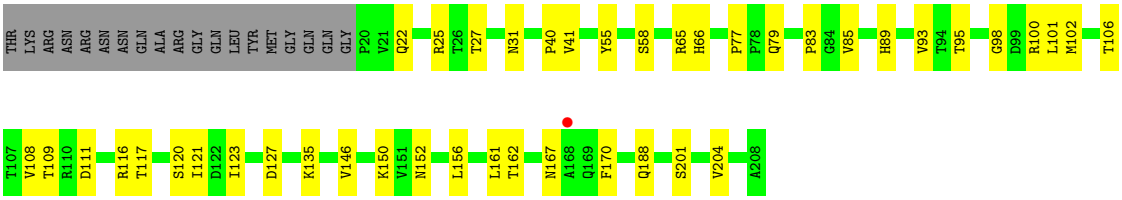
• Molecule 1: coat protein

Chain BW:



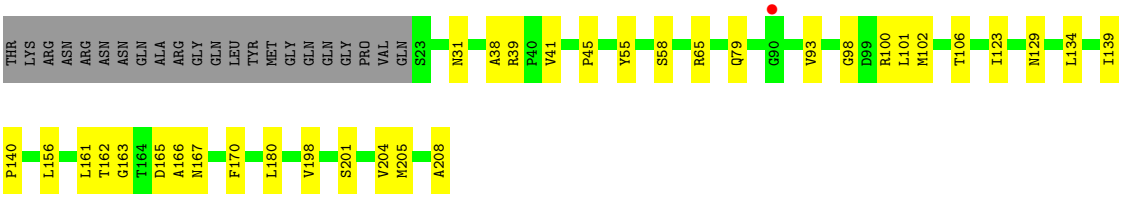
• Molecule 1: coat protein

Chain BX:



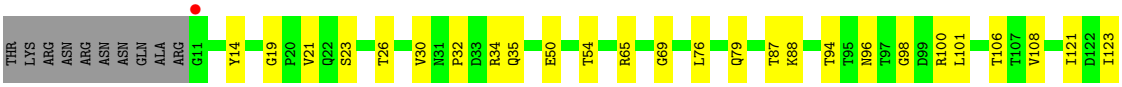
• Molecule 1: coat protein

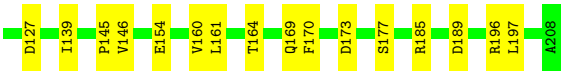
Chain BY:



• Molecule 1: coat protein

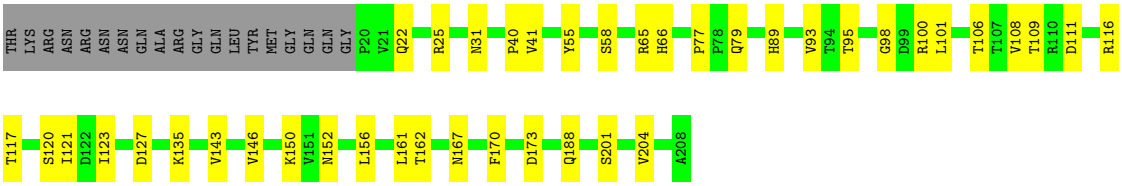
Chain BZ:





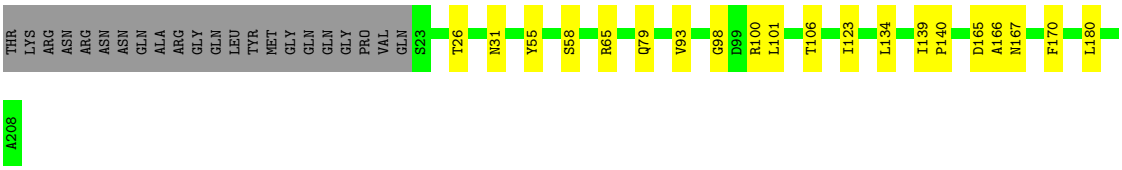
• Molecule 1: coat protein

Chain CA:



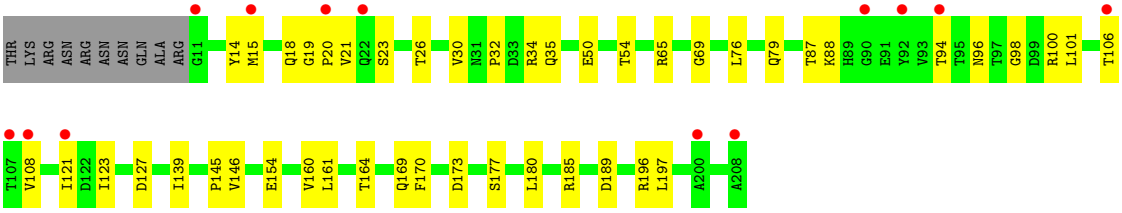
• Molecule 1: coat protein

Chain CB:



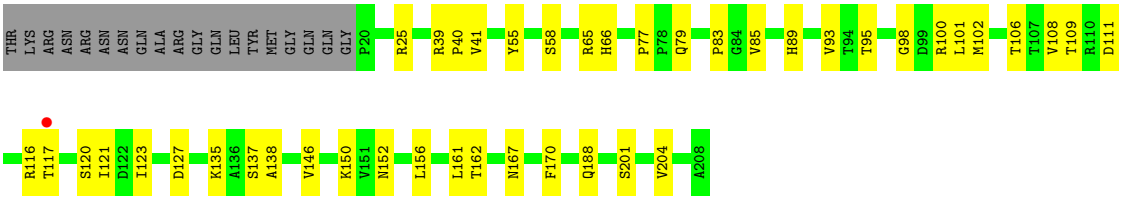
• Molecule 1: coat protein

Chain CC:



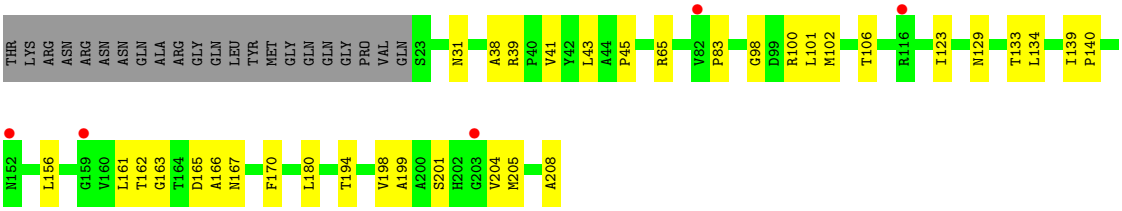
• Molecule 1: coat protein

Chain CD:



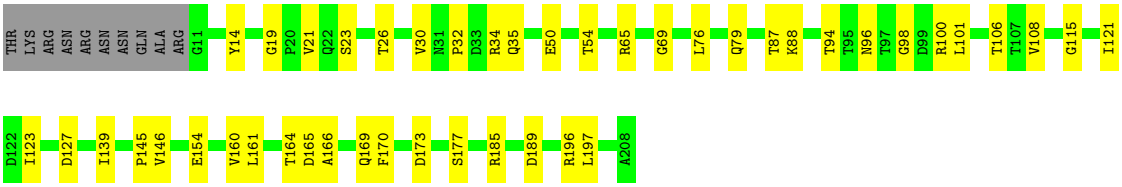
• Molecule 1: coat protein

Chain CE:



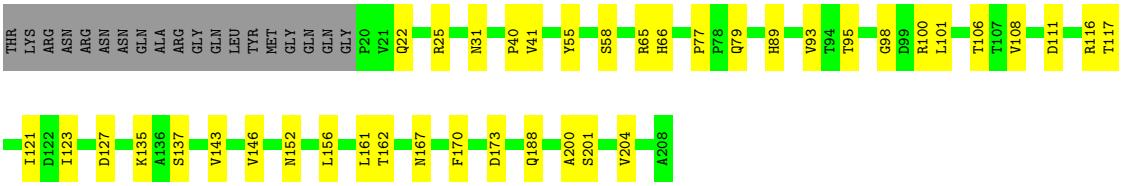
- Molecule 1: coat protein

Chain CF:



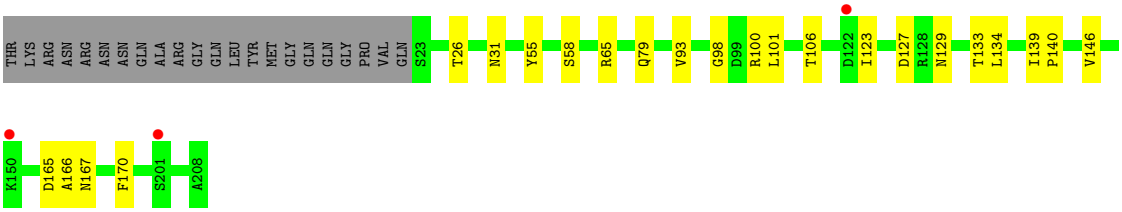
- Molecule 1: coat protein

Chain CG:



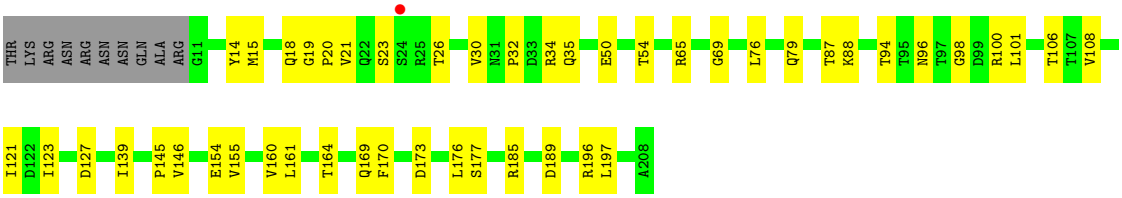
- Molecule 1: coat protein

Chain CH:



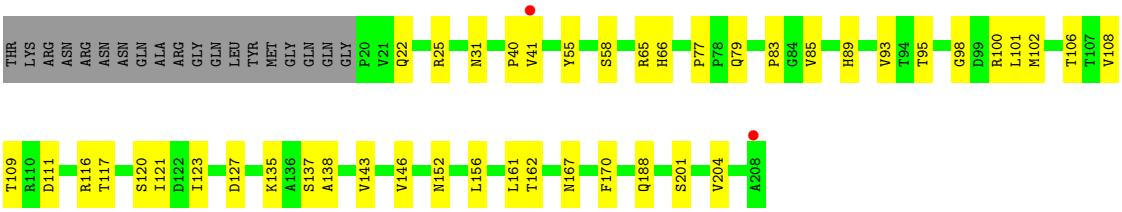
- Molecule 1: coat protein

Chain CI:



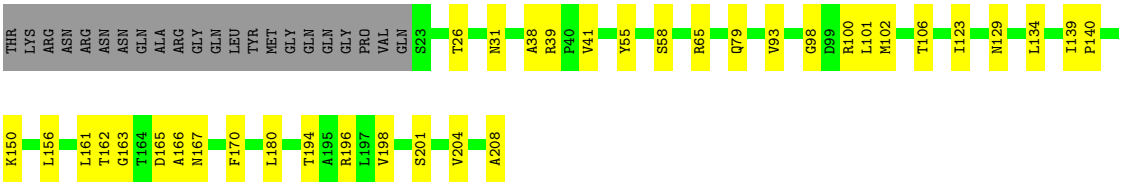
- Molecule 1: coat protein

Chain CJ:



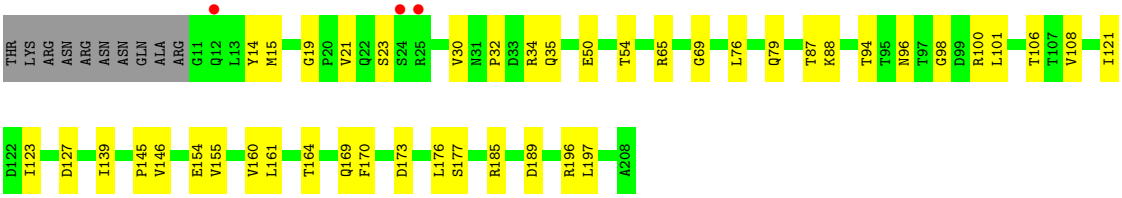
- Molecule 1: coat protein

Chain CK:



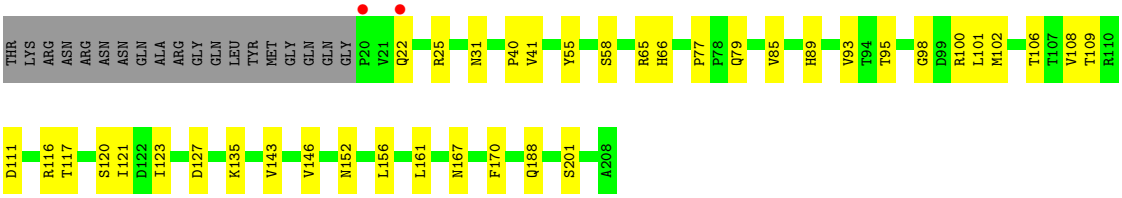
- Molecule 1: coat protein

Chain CL:



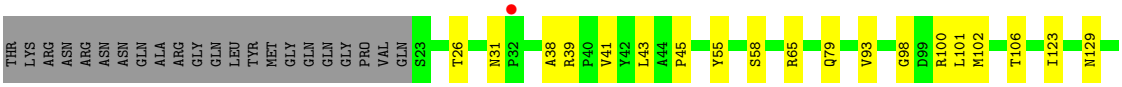
- Molecule 1: coat protein

Chain CM:



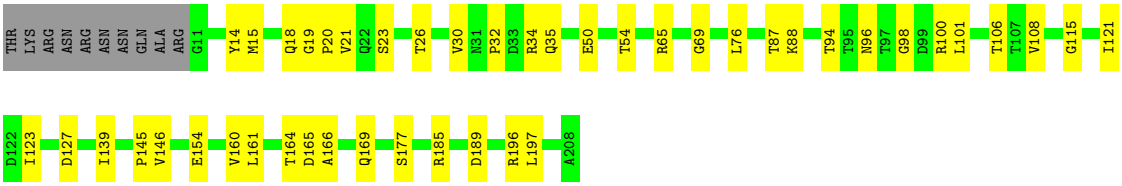
- Molecule 1: coat protein

Chain CN:



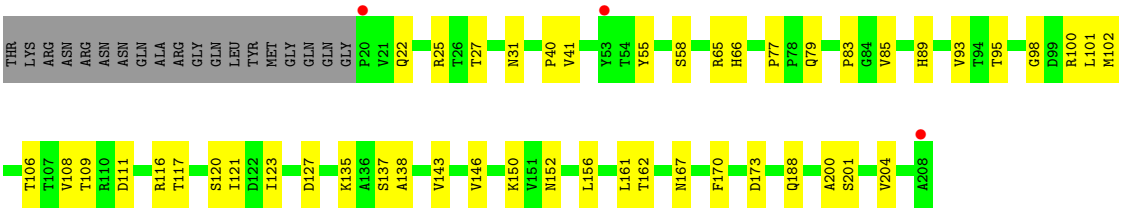
• Molecule 1: coat protein

Chain CO:



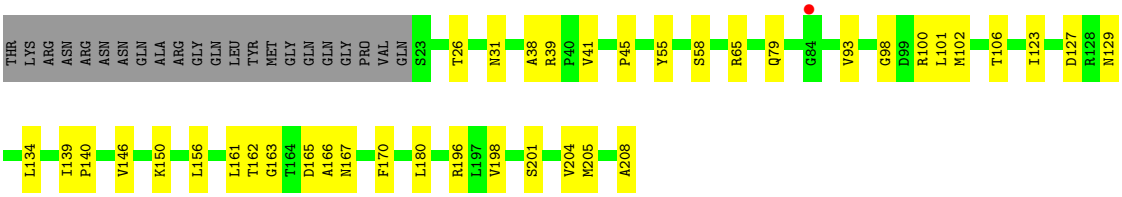
• Molecule 1: coat protein

Chain CP:



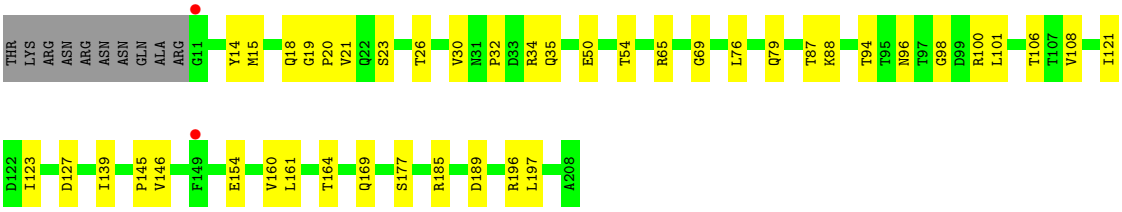
• Molecule 1: coat protein

Chain CQ:



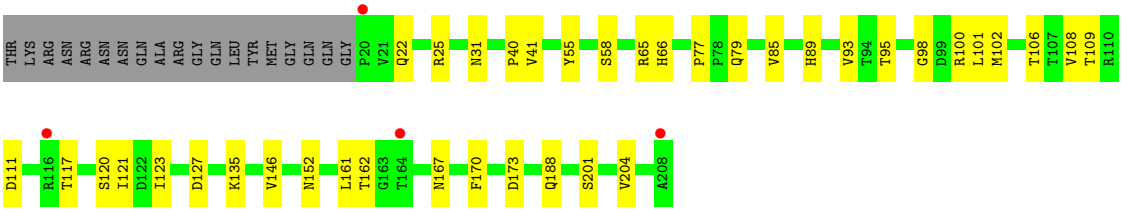
• Molecule 1: coat protein

Chain CR:



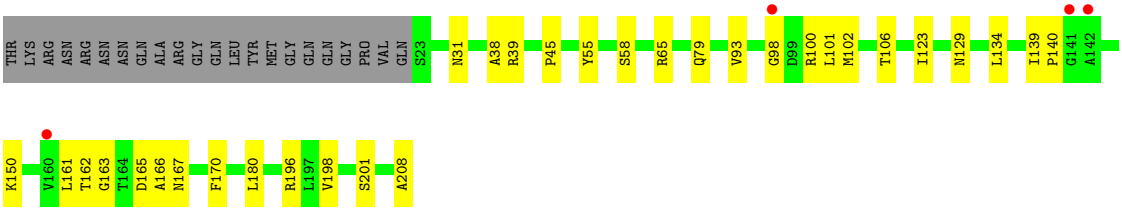
• Molecule 1: coat protein

Chain CS:



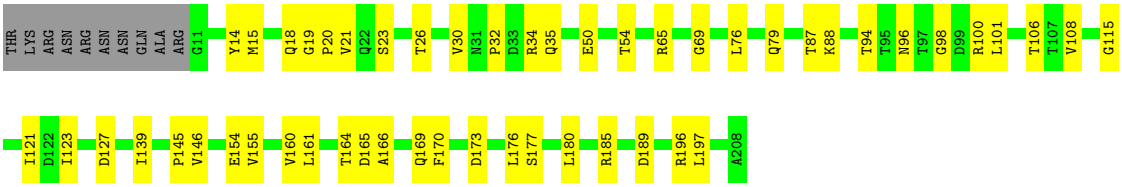
- Molecule 1: coat protein

Chain CT:



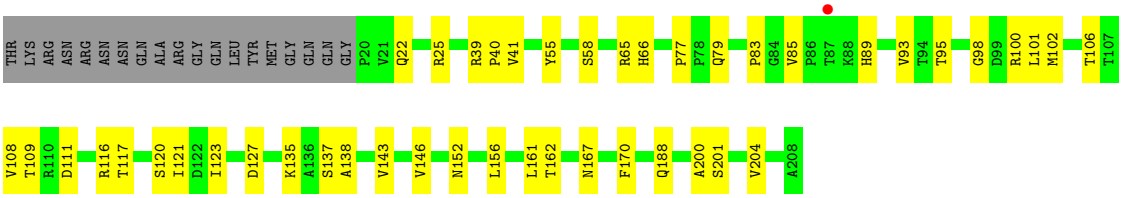
- Molecule 1: coat protein

Chain CU:



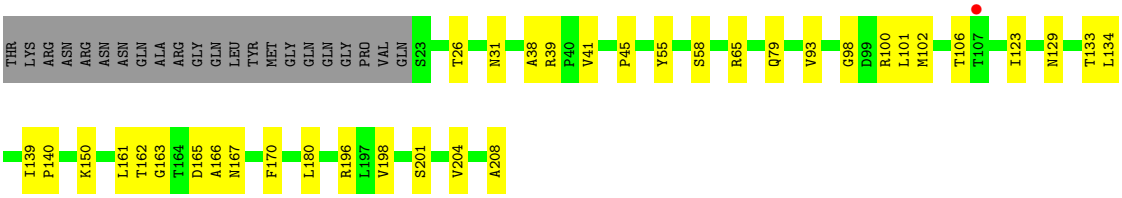
- Molecule 1: coat protein

Chain CV:



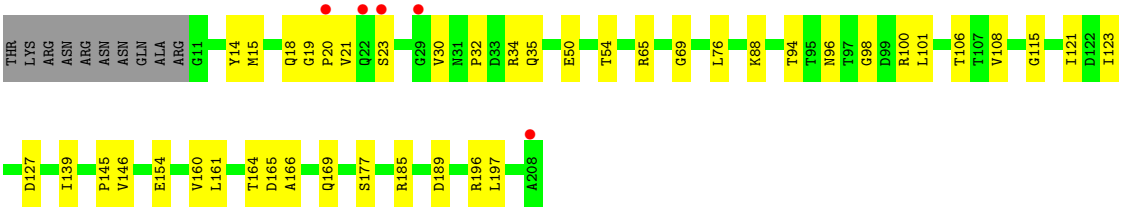
- Molecule 1: coat protein

Chain CW:



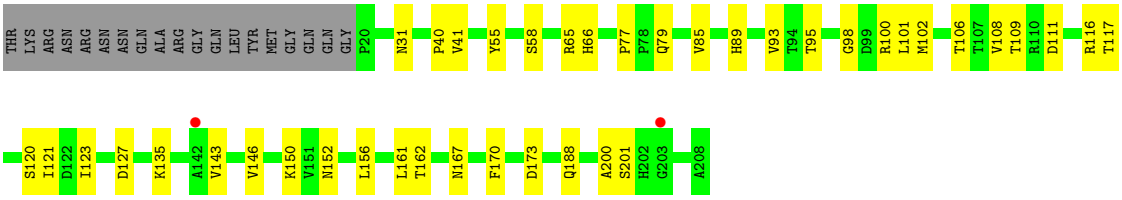
- Molecule 1: coat protein

Chain CX:



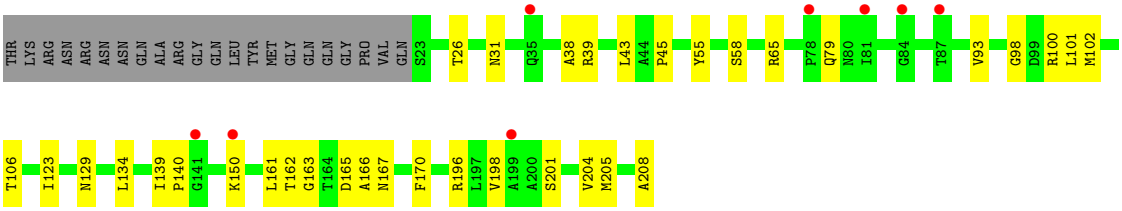
• Molecule 1: coat protein

Chain CY:



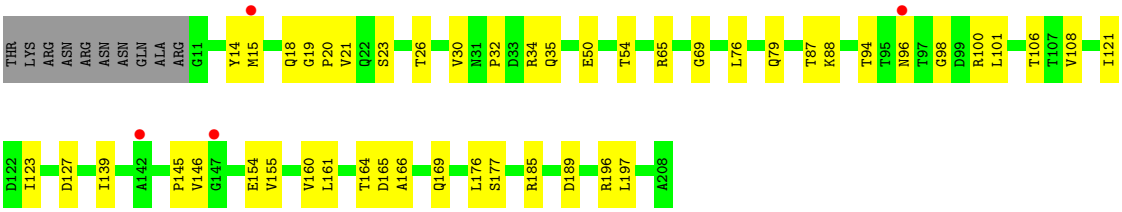
• Molecule 1: coat protein

Chain CZ:



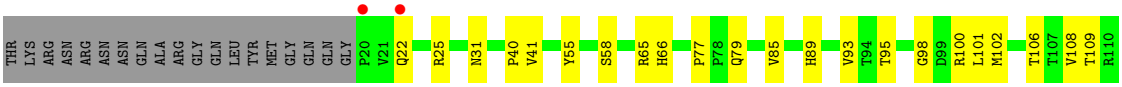
• Molecule 1: coat protein

Chain DA:



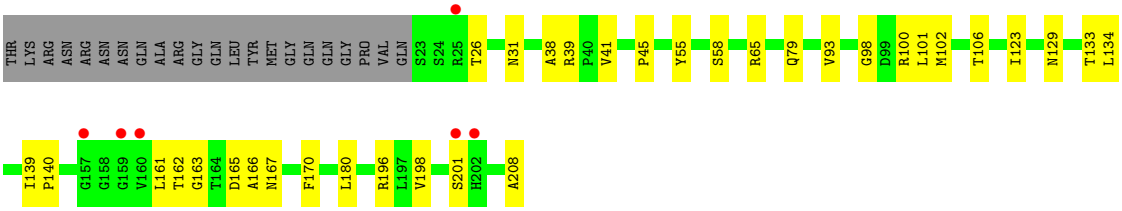
• Molecule 1: coat protein

Chain DB:



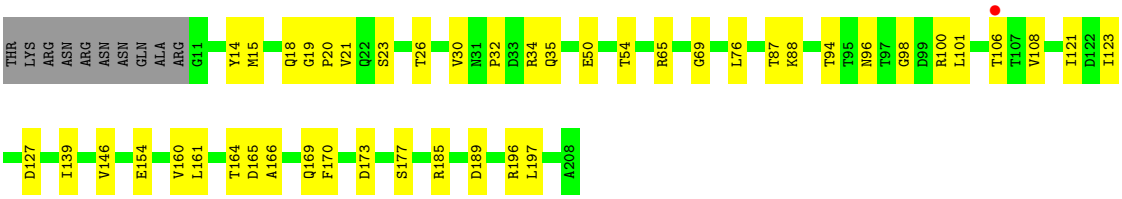
• Molecule 1: coat protein

Chain DC:



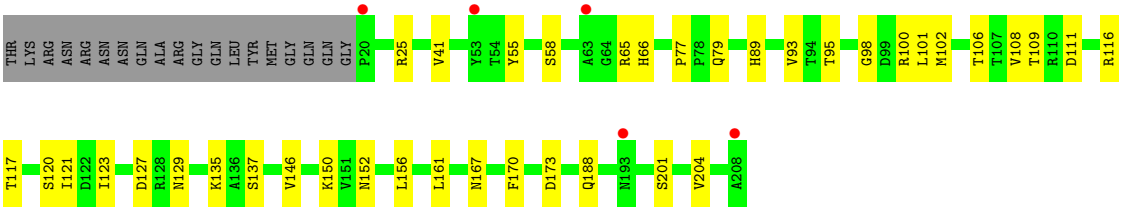
• Molecule 1: coat protein

Chain DD:



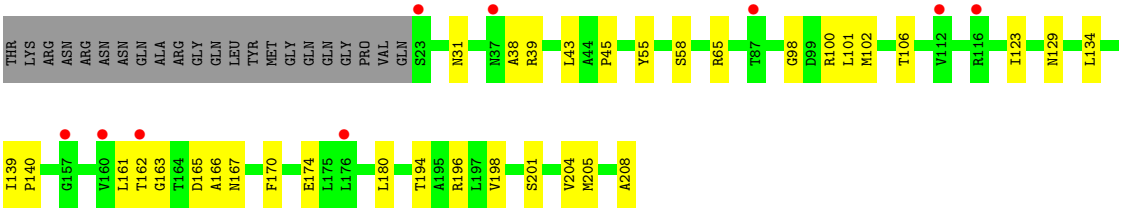
• Molecule 1: coat protein

Chain DE:



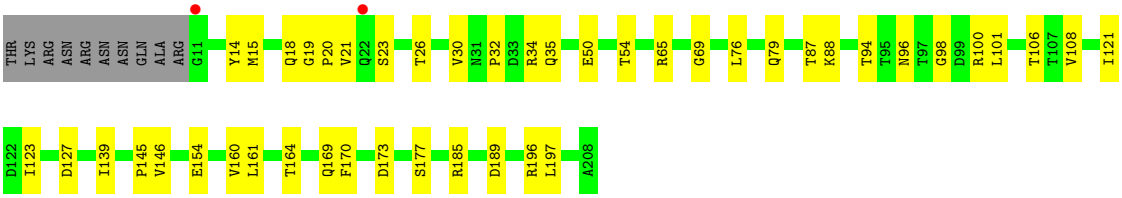
• Molecule 1: coat protein

Chain DF:



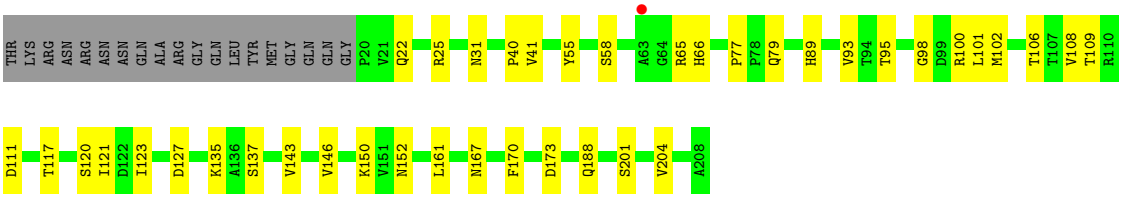
• Molecule 1: coat protein

Chain DG:



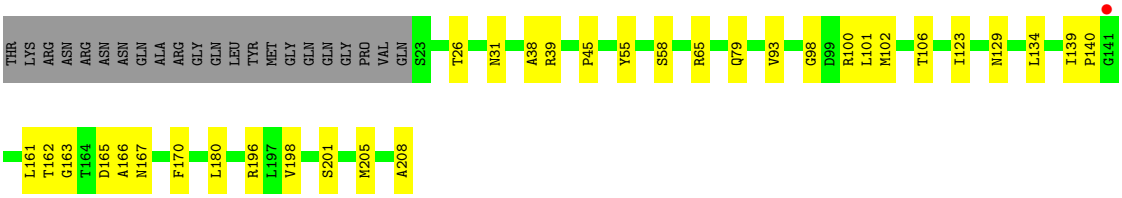
• Molecule 1: coat protein

Chain DH: 72% 19% 9%



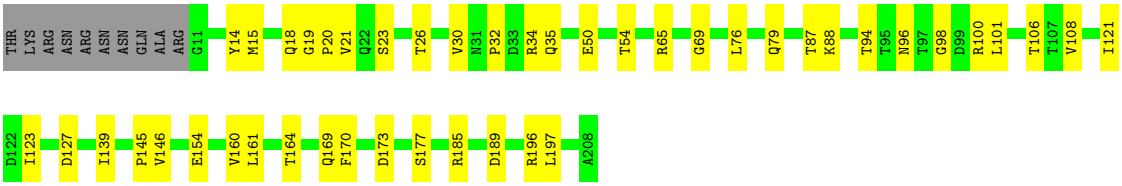
• Molecule 1: coat protein

Chain DI: 74% 16% 11%



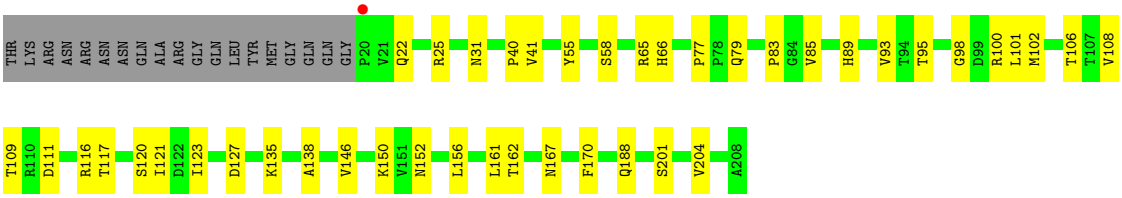
• Molecule 1: coat protein

Chain DJ: 74% 22% 5%



• Molecule 1: coat protein

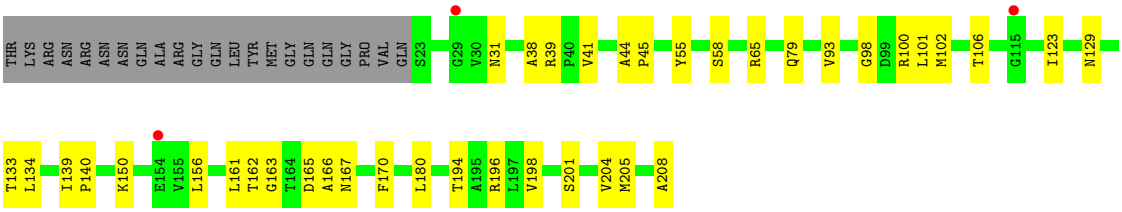
Chain DK: 70% 21% 9%



• Molecule 1: coat protein

Chain DL:

%
71%
19%
11%


THR LYS ARG ASN ARG ASN ASN GLN ALA ARG GLY GLN LEU TYR MET GLY GLN GLN GLY PRO VAL GLN S23 G29 V30 N31 A38 R39 P40 V41 A44 P45 Y55 S58 R65 Q79 V93 G98 D99 R100 L101 M102 T106 G115 I123 N129
T133 L134 I139 P140 K150 E154 V155 L156 L161 T162 G163 T164 D165 A166 N167 F170 L180 T194 A195 R196 L197 V198 S201 V204 M205 A208

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	328.67Å 373.71Å 310.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.33 – 3.30 49.33 – 3.30	Depositor EDS
% Data completeness (in resolution range)	92.6 (49.33-3.30) 94.4 (49.33-3.30)	Depositor EDS
R_{merge}	0.65	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.03 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.265 , 0.267 0.268 , 0.270	Depositor DCC
R_{free} test set	10025 reflections (1.87%)	wwPDB-VP
Wilson B-factor (Å^2)	97.5	Xtriage
Anisotropy	0.183	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 49.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	126960	wwPDB-VP
Average B, all atoms (Å^2)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.55% 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 (i)

5.1 Standard geometry (i)

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	0.33	0/1492	0.54	0/2035
1	AB	0.33	0/1424	0.55	0/1944
1	AC	0.34	0/1400	0.56	0/1911
1	AD	0.33	0/1492	0.54	0/2035
1	AE	0.33	0/1424	0.55	0/1944
1	AF	0.34	0/1400	0.56	0/1911
1	AG	0.33	0/1492	0.54	0/2035
1	AH	0.33	0/1424	0.55	0/1944
1	AI	0.34	0/1400	0.56	0/1911
1	AJ	0.33	0/1492	0.54	0/2035
1	AK	0.33	0/1424	0.55	0/1944
1	AL	0.34	0/1400	0.56	0/1911
1	AM	0.33	0/1492	0.54	0/2035
1	AN	0.34	0/1424	0.55	0/1944
1	AO	0.34	0/1400	0.56	0/1911
1	AP	0.33	0/1492	0.54	0/2035
1	AQ	0.33	0/1424	0.55	0/1944
1	AR	0.34	0/1400	0.56	0/1911
1	AS	0.33	0/1492	0.54	0/2035
1	AT	0.34	0/1424	0.55	0/1944
1	AU	0.34	0/1400	0.56	0/1911
1	AV	0.33	0/1492	0.54	0/2035
1	AW	0.33	0/1424	0.55	0/1944
1	AX	0.34	0/1400	0.56	0/1911
1	AY	0.33	0/1492	0.54	0/2035
1	AZ	0.33	0/1424	0.55	0/1944
1	BA	0.34	0/1400	0.56	0/1911
1	BB	0.33	0/1492	0.54	0/2035
1	BC	0.33	0/1424	0.55	0/1944
1	BD	0.34	0/1400	0.56	0/1911
1	BE	0.33	0/1492	0.54	0/2035
1	BF	0.33	0/1424	0.55	0/1944
1	BG	0.34	0/1400	0.56	0/1911
1	BH	0.33	0/1492	0.54	0/2035

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	BI	0.34	0/1424	0.55	0/1944
1	BJ	0.34	0/1400	0.56	0/1911
1	BK	0.33	0/1492	0.54	0/2035
1	BL	0.33	0/1424	0.55	0/1944
1	BM	0.34	0/1400	0.56	0/1911
1	BN	0.33	0/1492	0.54	0/2035
1	BO	0.33	0/1424	0.55	0/1944
1	BP	0.34	0/1400	0.56	0/1911
1	BQ	0.33	0/1492	0.54	0/2035
1	BR	0.33	0/1424	0.55	0/1944
1	BS	0.34	0/1400	0.56	0/1911
1	BT	0.33	0/1492	0.54	0/2035
1	BU	0.34	0/1424	0.55	0/1944
1	BV	0.34	0/1400	0.56	0/1911
1	BW	0.33	0/1492	0.54	0/2035
1	BX	0.33	0/1424	0.55	0/1944
1	BY	0.34	0/1400	0.56	0/1911
1	BZ	0.33	0/1492	0.54	0/2035
1	CA	0.33	0/1424	0.55	0/1944
1	CB	0.34	0/1400	0.56	0/1911
1	CC	0.33	0/1492	0.54	0/2035
1	CD	0.33	0/1424	0.55	0/1944
1	CE	0.34	0/1400	0.56	0/1911
1	CF	0.33	0/1492	0.54	0/2035
1	CG	0.33	0/1424	0.55	0/1944
1	CH	0.34	0/1400	0.56	0/1911
1	CI	0.33	0/1492	0.54	0/2035
1	CJ	0.33	0/1424	0.55	0/1944
1	CK	0.34	0/1400	0.56	0/1911
1	CL	0.33	0/1492	0.54	0/2035
1	CM	0.34	0/1424	0.55	0/1944
1	CN	0.34	0/1400	0.56	0/1911
1	CO	0.33	0/1492	0.54	0/2035
1	CP	0.33	0/1424	0.55	0/1944
1	CQ	0.34	0/1400	0.56	0/1911
1	CR	0.33	0/1492	0.54	0/2035
1	CS	0.33	0/1424	0.55	0/1944
1	CT	0.34	0/1400	0.56	0/1911
1	CU	0.33	0/1492	0.54	0/2035
1	CV	0.33	0/1424	0.55	0/1944
1	CW	0.34	0/1400	0.56	0/1911
1	CX	0.33	0/1492	0.54	0/2035
1	CY	0.33	0/1424	0.55	0/1944

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	CZ	0.34	0/1400	0.56	0/1911
1	DA	0.33	0/1492	0.54	0/2035
1	DB	0.33	0/1424	0.55	0/1944
1	DC	0.34	0/1400	0.56	0/1911
1	DD	0.33	0/1492	0.54	0/2035
1	DE	0.33	0/1424	0.55	0/1944
1	DF	0.34	0/1400	0.56	0/1911
1	DG	0.33	0/1492	0.54	0/2035
1	DH	0.33	0/1424	0.55	0/1944
1	DI	0.34	0/1400	0.56	0/1911
1	DJ	0.33	0/1492	0.54	0/2035
1	DK	0.33	0/1424	0.55	0/1944
1	DL	0.34	0/1400	0.56	0/1911
All	All	0.33	0/129480	0.55	0/176700

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1463	0	1446	35	0
1	AB	1396	0	1385	32	1
1	AC	1373	0	1360	34	0
1	AD	1463	0	1446	35	0
1	AE	1396	0	1385	39	0
1	AF	1373	0	1360	44	0
1	AG	1463	0	1446	29	0
1	AH	1396	0	1385	28	0
1	AI	1373	0	1360	10	2
1	AJ	1463	0	1446	33	0
1	AK	1396	0	1385	34	0
1	AL	1373	0	1360	43	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AM	1463	0	1446	29	0
1	AN	1396	0	1385	28	0
1	AO	1373	0	1360	14	1
1	AP	1463	0	1446	32	0
1	AQ	1396	0	1385	29	0
1	AR	1373	0	1360	37	0
1	AS	1463	0	1446	33	0
1	AT	1396	0	1385	35	0
1	AU	1373	0	1360	41	0
1	AV	1463	0	1446	31	0
1	AW	1396	0	1385	30	0
1	AX	1373	0	1360	12	2
1	AY	1463	0	1446	31	0
1	AZ	1396	0	1385	34	0
1	BA	1373	0	1360	34	0
1	BB	1463	0	1446	33	0
1	BC	1396	0	1385	33	1
1	BD	1373	0	1360	40	0
1	BE	1463	0	1446	36	0
1	BF	1396	0	1385	34	0
1	BG	1373	0	1360	35	0
1	BH	1463	0	1446	34	0
1	BI	1396	0	1385	34	0
1	BJ	1373	0	1360	36	0
1	BK	1463	0	1446	32	0
1	BL	1396	0	1385	31	0
1	BM	1373	0	1360	32	0
1	BN	1463	0	1446	32	0
1	BO	1396	0	1385	25	0
1	BP	1373	0	1360	35	0
1	BQ	1463	0	1446	34	0
1	BR	1396	0	1385	36	0
1	BS	1373	0	1360	42	0
1	BT	1463	0	1446	31	0
1	BU	1396	0	1385	33	0
1	BV	1373	0	1360	11	1
1	BW	1463	0	1446	34	0
1	BX	1396	0	1385	33	0
1	BY	1373	0	1360	33	0
1	BZ	1463	0	1446	29	0
1	CA	1396	0	1385	32	0
1	CB	1373	0	1360	12	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	CC	1463	0	1446	35	0
1	CD	1396	0	1385	35	0
1	CE	1373	0	1360	42	0
1	CF	1463	0	1446	31	0
1	CG	1396	0	1385	31	0
1	CH	1373	0	1360	13	2
1	CI	1463	0	1446	35	0
1	CJ	1396	0	1385	38	0
1	CK	1373	0	1360	38	0
1	CL	1463	0	1446	31	0
1	CM	1396	0	1385	30	0
1	CN	1373	0	1360	34	0
1	CO	1463	0	1446	33	0
1	CP	1396	0	1385	40	0
1	CQ	1373	0	1360	39	0
1	CR	1463	0	1446	32	0
1	CS	1396	0	1385	32	0
1	CT	1373	0	1360	33	0
1	CU	1463	0	1446	37	0
1	CV	1396	0	1385	38	0
1	CW	1373	0	1360	37	0
1	CX	1463	0	1446	30	0
1	CY	1396	0	1385	31	0
1	CZ	1373	0	1360	37	0
1	DA	1463	0	1446	35	0
1	DB	1396	0	1385	31	0
1	DC	1373	0	1360	35	0
1	DD	1463	0	1446	32	0
1	DE	1396	0	1385	28	0
1	DF	1373	0	1360	33	0
1	DG	1463	0	1446	34	0
1	DH	1396	0	1385	31	0
1	DI	1373	0	1360	33	0
1	DJ	1463	0	1446	34	0
1	DK	1396	0	1385	35	0
1	DL	1373	0	1360	43	0
All	All	126960	0	125730	2072	7

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 8.

The worst 5 of 2072 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:BM:31:ASN:O	1:DF:65:ARG:NH1	2.04	0.90
1:BG:31:ASN:O	1:CZ:65:ARG:NH1	2.04	0.90
1:AL:31:ASN:O	1:CK:65:ARG:NH1	2.05	0.89
1:AL:65:ARG:NH1	1:CK:31:ASN:O	2.09	0.85
1:BP:31:ASN:O	1:DI:65:ARG:NH1	2.09	0.85

The worst 5 of 7 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:AB:60:GLN:OE1	1:BC:192:LYS:NZ[4_556]	1.89	0.31
1:AI:65:ARG:NH1	1:AX:31:ASN:O[2_555]	2.09	0.11
1:BV:31:ASN:O	1:BV:65:ARG:NH1[2_555]	2.13	0.07
1:AO:31:ASN:O	1:AO:65:ARG:NH1[2_555]	2.16	0.04
1:AI:31:ASN:O	1:AX:65:ARG:NH1[2_555]	2.17	0.03

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	196/208 (94%)	191 (97%)	5 (3%)	0	100	100
1	AB	187/208 (90%)	183 (98%)	4 (2%)	0	100	100
1	AC	184/208 (88%)	182 (99%)	2 (1%)	0	100	100
1	AD	196/208 (94%)	191 (97%)	5 (3%)	0	100	100
1	AE	187/208 (90%)	183 (98%)	4 (2%)	0	100	100
1	AF	184/208 (88%)	182 (99%)	2 (1%)	0	100	100
1	AG	196/208 (94%)	191 (97%)	5 (3%)	0	100	100
1	AH	187/208 (90%)	183 (98%)	4 (2%)	0	100	100
1	AI	184/208 (88%)	182 (99%)	2 (1%)	0	100	100
1	AJ	196/208 (94%)	191 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AK	187/208 (90%)	183 (98%)	4 (2%)	0	100	100
1	AL	184/208 (88%)	182 (99%)	2 (1%)	0	100	100
1	AM	196/208 (94%)	191 (97%)	5 (3%)	0	100	100
1	AN	187/208 (90%)	183 (98%)	4 (2%)	0	100	100
1	AO	184/208 (88%)	182 (99%)	2 (1%)	0	100	100
1	AP	196/208 (94%)	191 (97%)	5 (3%)	0	100	100
1	AQ	187/208 (90%)	183 (98%)	4 (2%)	0	100	100
1	AR	184/208 (88%)	182 (99%)	2 (1%)	0	100	100
1	AS	196/208 (94%)	191 (97%)	5 (3%)	0	100	100
1	AT	187/208 (90%)	183 (98%)	4 (2%)	0	100	100
1	AU	184/208 (88%)	182 (99%)	2 (1%)	0	100	100
1	AV	196/208 (94%)	191 (97%)	5 (3%)	0	100	100
1	AW	187/208 (90%)	183 (98%)	4 (2%)	0	100	100
1	AX	184/208 (88%)	182 (99%)	2 (1%)	0	100	100
1	AY	196/208 (94%)	191 (97%)	5 (3%)	0	100	100
1	AZ	187/208 (90%)	183 (98%)	4 (2%)	0	100	100
1	BA	184/208 (88%)	182 (99%)	2 (1%)	0	100	100
1	BB	196/208 (94%)	191 (97%)	5 (3%)	0	100	100
1	BC	187/208 (90%)	183 (98%)	4 (2%)	0	100	100
1	BD	184/208 (88%)	182 (99%)	2 (1%)	0	100	100
1	BE	196/208 (94%)	191 (97%)	5 (3%)	0	100	100
1	BF	187/208 (90%)	183 (98%)	4 (2%)	0	100	100
1	BG	184/208 (88%)	182 (99%)	2 (1%)	0	100	100
1	BH	196/208 (94%)	191 (97%)	5 (3%)	0	100	100
1	BI	187/208 (90%)	183 (98%)	4 (2%)	0	100	100
1	BJ	184/208 (88%)	182 (99%)	2 (1%)	0	100	100
1	BK	196/208 (94%)	191 (97%)	5 (3%)	0	100	100
1	BL	187/208 (90%)	183 (98%)	4 (2%)	0	100	100
1	BM	184/208 (88%)	182 (99%)	2 (1%)	0	100	100
1	BN	196/208 (94%)	191 (97%)	5 (3%)	0	100	100
1	BO	187/208 (90%)	183 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	BP	184/208 (88%)	182 (99%)	2 (1%)	0	100	100
1	BQ	196/208 (94%)	191 (97%)	5 (3%)	0	100	100
1	BR	187/208 (90%)	183 (98%)	4 (2%)	0	100	100
1	BS	184/208 (88%)	182 (99%)	2 (1%)	0	100	100
1	BT	196/208 (94%)	191 (97%)	5 (3%)	0	100	100
1	BU	187/208 (90%)	183 (98%)	4 (2%)	0	100	100
1	BV	184/208 (88%)	182 (99%)	2 (1%)	0	100	100
1	BW	196/208 (94%)	191 (97%)	5 (3%)	0	100	100
1	BX	187/208 (90%)	183 (98%)	4 (2%)	0	100	100
1	BY	184/208 (88%)	182 (99%)	2 (1%)	0	100	100
1	BZ	196/208 (94%)	191 (97%)	5 (3%)	0	100	100
1	CA	187/208 (90%)	183 (98%)	4 (2%)	0	100	100
1	CB	184/208 (88%)	182 (99%)	2 (1%)	0	100	100
1	CC	196/208 (94%)	191 (97%)	5 (3%)	0	100	100
1	CD	187/208 (90%)	183 (98%)	4 (2%)	0	100	100
1	CE	184/208 (88%)	182 (99%)	2 (1%)	0	100	100
1	CF	196/208 (94%)	191 (97%)	5 (3%)	0	100	100
1	CG	187/208 (90%)	183 (98%)	4 (2%)	0	100	100
1	CH	184/208 (88%)	182 (99%)	2 (1%)	0	100	100
1	CI	196/208 (94%)	191 (97%)	5 (3%)	0	100	100
1	CJ	187/208 (90%)	183 (98%)	4 (2%)	0	100	100
1	CK	184/208 (88%)	182 (99%)	2 (1%)	0	100	100
1	CL	196/208 (94%)	191 (97%)	5 (3%)	0	100	100
1	CM	187/208 (90%)	183 (98%)	4 (2%)	0	100	100
1	CN	184/208 (88%)	182 (99%)	2 (1%)	0	100	100
1	CO	196/208 (94%)	191 (97%)	5 (3%)	0	100	100
1	CP	187/208 (90%)	183 (98%)	4 (2%)	0	100	100
1	CQ	184/208 (88%)	182 (99%)	2 (1%)	0	100	100
1	CR	196/208 (94%)	191 (97%)	5 (3%)	0	100	100
1	CS	187/208 (90%)	183 (98%)	4 (2%)	0	100	100
1	CT	184/208 (88%)	182 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	CU	196/208 (94%)	191 (97%)	5 (3%)	0	100	100
1	CV	187/208 (90%)	183 (98%)	4 (2%)	0	100	100
1	CW	184/208 (88%)	182 (99%)	2 (1%)	0	100	100
1	CX	196/208 (94%)	191 (97%)	5 (3%)	0	100	100
1	CY	187/208 (90%)	183 (98%)	4 (2%)	0	100	100
1	CZ	184/208 (88%)	182 (99%)	2 (1%)	0	100	100
1	DA	196/208 (94%)	191 (97%)	5 (3%)	0	100	100
1	DB	187/208 (90%)	183 (98%)	4 (2%)	0	100	100
1	DC	184/208 (88%)	182 (99%)	2 (1%)	0	100	100
1	DD	196/208 (94%)	191 (97%)	5 (3%)	0	100	100
1	DE	187/208 (90%)	183 (98%)	4 (2%)	0	100	100
1	DF	184/208 (88%)	182 (99%)	2 (1%)	0	100	100
1	DG	196/208 (94%)	191 (97%)	5 (3%)	0	100	100
1	DH	187/208 (90%)	183 (98%)	4 (2%)	0	100	100
1	DI	184/208 (88%)	182 (99%)	2 (1%)	0	100	100
1	DJ	196/208 (94%)	191 (97%)	5 (3%)	0	100	100
1	DK	187/208 (90%)	183 (98%)	4 (2%)	0	100	100
1	DL	184/208 (88%)	182 (99%)	2 (1%)	0	100	100
All	All	17010/18720 (91%)	16680 (98%)	330 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	AA	155/164 (94%)	155 (100%)	0	100	100
1	AB	149/164 (91%)	149 (100%)	0	100	100
1	AC	146/164 (89%)	146 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AD	155/164 (94%)	155 (100%)	0	100	100
1	AE	149/164 (91%)	149 (100%)	0	100	100
1	AF	146/164 (89%)	146 (100%)	0	100	100
1	AG	155/164 (94%)	155 (100%)	0	100	100
1	AH	149/164 (91%)	149 (100%)	0	100	100
1	AI	146/164 (89%)	146 (100%)	0	100	100
1	AJ	155/164 (94%)	155 (100%)	0	100	100
1	AK	149/164 (91%)	149 (100%)	0	100	100
1	AL	146/164 (89%)	146 (100%)	0	100	100
1	AM	155/164 (94%)	155 (100%)	0	100	100
1	AN	149/164 (91%)	149 (100%)	0	100	100
1	AO	146/164 (89%)	146 (100%)	0	100	100
1	AP	155/164 (94%)	155 (100%)	0	100	100
1	AQ	149/164 (91%)	149 (100%)	0	100	100
1	AR	146/164 (89%)	146 (100%)	0	100	100
1	AS	155/164 (94%)	155 (100%)	0	100	100
1	AT	149/164 (91%)	149 (100%)	0	100	100
1	AU	146/164 (89%)	146 (100%)	0	100	100
1	AV	155/164 (94%)	155 (100%)	0	100	100
1	AW	149/164 (91%)	149 (100%)	0	100	100
1	AX	146/164 (89%)	146 (100%)	0	100	100
1	AY	155/164 (94%)	155 (100%)	0	100	100
1	AZ	149/164 (91%)	149 (100%)	0	100	100
1	BA	146/164 (89%)	146 (100%)	0	100	100
1	BB	155/164 (94%)	155 (100%)	0	100	100
1	BC	149/164 (91%)	149 (100%)	0	100	100
1	BD	146/164 (89%)	146 (100%)	0	100	100
1	BE	155/164 (94%)	155 (100%)	0	100	100
1	BF	149/164 (91%)	149 (100%)	0	100	100
1	BG	146/164 (89%)	146 (100%)	0	100	100
1	BH	155/164 (94%)	155 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	BI	149/164 (91%)	149 (100%)	0	100	100
1	BJ	146/164 (89%)	146 (100%)	0	100	100
1	BK	155/164 (94%)	155 (100%)	0	100	100
1	BL	149/164 (91%)	149 (100%)	0	100	100
1	BM	146/164 (89%)	146 (100%)	0	100	100
1	BN	155/164 (94%)	155 (100%)	0	100	100
1	BO	149/164 (91%)	149 (100%)	0	100	100
1	BP	146/164 (89%)	146 (100%)	0	100	100
1	BQ	155/164 (94%)	155 (100%)	0	100	100
1	BR	149/164 (91%)	149 (100%)	0	100	100
1	BS	146/164 (89%)	146 (100%)	0	100	100
1	BT	155/164 (94%)	155 (100%)	0	100	100
1	BU	149/164 (91%)	149 (100%)	0	100	100
1	BV	146/164 (89%)	146 (100%)	0	100	100
1	BW	155/164 (94%)	155 (100%)	0	100	100
1	BX	149/164 (91%)	149 (100%)	0	100	100
1	BY	146/164 (89%)	146 (100%)	0	100	100
1	BZ	155/164 (94%)	155 (100%)	0	100	100
1	CA	149/164 (91%)	149 (100%)	0	100	100
1	CB	146/164 (89%)	146 (100%)	0	100	100
1	CC	155/164 (94%)	155 (100%)	0	100	100
1	CD	149/164 (91%)	149 (100%)	0	100	100
1	CE	146/164 (89%)	146 (100%)	0	100	100
1	CF	155/164 (94%)	155 (100%)	0	100	100
1	CG	149/164 (91%)	149 (100%)	0	100	100
1	CH	146/164 (89%)	146 (100%)	0	100	100
1	CI	155/164 (94%)	155 (100%)	0	100	100
1	CJ	149/164 (91%)	149 (100%)	0	100	100
1	CK	146/164 (89%)	146 (100%)	0	100	100
1	CL	155/164 (94%)	155 (100%)	0	100	100
1	CM	149/164 (91%)	149 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	CN	146/164 (89%)	146 (100%)	0	100	100
1	CO	155/164 (94%)	155 (100%)	0	100	100
1	CP	149/164 (91%)	149 (100%)	0	100	100
1	CQ	146/164 (89%)	146 (100%)	0	100	100
1	CR	155/164 (94%)	155 (100%)	0	100	100
1	CS	149/164 (91%)	149 (100%)	0	100	100
1	CT	146/164 (89%)	146 (100%)	0	100	100
1	CU	155/164 (94%)	155 (100%)	0	100	100
1	CV	149/164 (91%)	149 (100%)	0	100	100
1	CW	146/164 (89%)	146 (100%)	0	100	100
1	CX	155/164 (94%)	155 (100%)	0	100	100
1	CY	149/164 (91%)	149 (100%)	0	100	100
1	CZ	146/164 (89%)	146 (100%)	0	100	100
1	DA	155/164 (94%)	155 (100%)	0	100	100
1	DB	149/164 (91%)	149 (100%)	0	100	100
1	DC	146/164 (89%)	146 (100%)	0	100	100
1	DD	155/164 (94%)	155 (100%)	0	100	100
1	DE	149/164 (91%)	149 (100%)	0	100	100
1	DF	146/164 (89%)	146 (100%)	0	100	100
1	DG	155/164 (94%)	155 (100%)	0	100	100
1	DH	149/164 (91%)	149 (100%)	0	100	100
1	DI	146/164 (89%)	146 (100%)	0	100	100
1	DJ	155/164 (94%)	155 (100%)	0	100	100
1	DK	149/164 (91%)	149 (100%)	0	100	100
1	DL	146/164 (89%)	146 (100%)	0	100	100
All	All	13500/14760 (92%)	13500 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
1	CW	129	ASN

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Mol	Chain	Res	Type
1	DL	129	ASN
1	CZ	129	ASN
1	DF	129	ASN
1	BF	31	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	AA	198/208 (95%)	-0.03	1 (0%)	91	91	67, 89, 121, 184	0
1	AB	189/208 (90%)	-0.15	1 (0%)	91	91	60, 89, 124, 186	0
1	AC	186/208 (89%)	-0.09	1 (0%)	91	91	65, 88, 115, 141	0
1	AD	198/208 (95%)	-0.23	2 (1%)	82	82	67, 89, 121, 184	0
1	AE	189/208 (90%)	-0.14	2 (1%)	80	81	60, 89, 124, 186	0
1	AF	186/208 (89%)	0.10	5 (2%)	54	52	65, 88, 115, 141	0
1	AG	198/208 (95%)	-0.26	0	100	100	67, 89, 121, 184	0
1	AH	189/208 (90%)	-0.16	1 (0%)	91	91	60, 89, 124, 186	0
1	AI	186/208 (89%)	-0.19	1 (0%)	91	91	65, 88, 115, 141	0
1	AJ	198/208 (95%)	-0.13	1 (0%)	91	91	67, 89, 121, 184	0
1	AK	189/208 (90%)	-0.13	1 (0%)	91	91	60, 89, 124, 186	0
1	AL	186/208 (89%)	0.02	0	100	100	65, 88, 115, 141	0
1	AM	198/208 (95%)	-0.21	0	100	100	67, 89, 121, 184	0
1	AN	189/208 (90%)	-0.07	1 (0%)	91	91	60, 89, 124, 186	0
1	AO	186/208 (89%)	-0.13	0	100	100	65, 88, 115, 141	0
1	AP	198/208 (95%)	-0.25	0	100	100	67, 89, 121, 184	0
1	AQ	189/208 (90%)	-0.26	1 (0%)	91	91	60, 89, 124, 186	0
1	AR	186/208 (89%)	-0.17	1 (0%)	91	91	65, 88, 115, 141	0
1	AS	198/208 (95%)	0.01	1 (0%)	91	91	67, 89, 121, 184	0
1	AT	189/208 (90%)	-0.09	0	100	100	60, 89, 124, 186	0
1	AU	186/208 (89%)	-0.00	1 (0%)	91	91	65, 88, 115, 141	0
1	AV	198/208 (95%)	-0.20	2 (1%)	82	82	67, 89, 121, 184	0
1	AW	189/208 (90%)	-0.17	1 (0%)	91	91	60, 89, 124, 186	0
1	AX	186/208 (89%)	-0.11	0	100	100	65, 88, 115, 141	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	AY	198/208 (95%)	-0.06	2 (1%)	82	82	67, 89, 121, 184	0
1	AZ	189/208 (90%)	-0.08	2 (1%)	80	81	60, 89, 124, 186	0
1	BA	186/208 (89%)	-0.00	2 (1%)	80	81	65, 88, 115, 141	0
1	BB	198/208 (95%)	0.03	3 (1%)	73	72	67, 89, 121, 184	0
1	BC	189/208 (90%)	-0.06	3 (1%)	72	70	60, 89, 124, 186	0
1	BD	186/208 (89%)	-0.01	0	100	100	65, 88, 115, 141	0
1	BE	198/208 (95%)	-0.01	4 (2%)	65	64	67, 89, 121, 184	0
1	BF	189/208 (90%)	0.20	6 (3%)	47	46	60, 89, 124, 186	0
1	BG	186/208 (89%)	0.23	7 (3%)	40	37	65, 88, 115, 141	0
1	BH	198/208 (95%)	-0.04	4 (2%)	65	64	67, 89, 121, 184	0
1	BI	189/208 (90%)	-0.00	2 (1%)	80	81	60, 89, 124, 186	0
1	BJ	186/208 (89%)	0.26	8 (4%)	35	34	65, 88, 115, 141	0
1	BK	198/208 (95%)	-0.04	2 (1%)	82	82	67, 89, 121, 184	0
1	BL	189/208 (90%)	0.04	7 (3%)	41	38	60, 89, 124, 186	0
1	BM	186/208 (89%)	0.03	1 (0%)	91	91	65, 88, 115, 141	0
1	BN	198/208 (95%)	-0.21	1 (0%)	91	91	67, 89, 121, 184	0
1	BO	189/208 (90%)	-0.28	2 (1%)	80	81	60, 89, 124, 186	0
1	BP	186/208 (89%)	-0.06	0	100	100	65, 88, 115, 141	0
1	BQ	198/208 (95%)	-0.10	0	100	100	67, 89, 121, 184	0
1	BR	189/208 (90%)	-0.20	0	100	100	60, 89, 124, 186	0
1	BS	186/208 (89%)	-0.21	0	100	100	65, 88, 115, 141	0
1	BT	198/208 (95%)	-0.11	1 (0%)	91	91	67, 89, 121, 184	0
1	BU	189/208 (90%)	-0.15	3 (1%)	72	70	60, 89, 124, 186	0
1	BV	186/208 (89%)	0.25	6 (3%)	47	46	65, 88, 115, 141	0
1	BW	198/208 (95%)	-0.18	0	100	100	67, 89, 121, 184	0
1	BX	189/208 (90%)	-0.24	1 (0%)	91	91	60, 89, 124, 186	0
1	BY	186/208 (89%)	-0.04	1 (0%)	91	91	65, 88, 115, 141	0
1	BZ	198/208 (95%)	-0.06	1 (0%)	91	91	67, 89, 121, 184	0
1	CA	189/208 (90%)	-0.15	0	100	100	60, 89, 124, 186	0
1	CB	186/208 (89%)	-0.07	0	100	100	65, 88, 115, 141	0
1	CC	198/208 (95%)	0.31	13 (6%)	18	18	67, 89, 121, 184	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	CD	189/208 (90%)	-0.09	1 (0%)	91	91	60, 89, 124, 186	0
1	CE	186/208 (89%)	0.05	5 (2%)	54	52	65, 88, 115, 141	0
1	CF	198/208 (95%)	-0.17	0	100	100	67, 89, 121, 184	0
1	CG	189/208 (90%)	-0.18	0	100	100	60, 89, 124, 186	0
1	CH	186/208 (89%)	0.10	3 (1%)	72	70	65, 88, 115, 141	0
1	CI	198/208 (95%)	0.03	1 (0%)	91	91	67, 89, 121, 184	0
1	CJ	189/208 (90%)	0.03	2 (1%)	80	81	60, 89, 124, 186	0
1	CK	186/208 (89%)	-0.05	0	100	100	65, 88, 115, 141	0
1	CL	198/208 (95%)	-0.15	3 (1%)	73	72	67, 89, 121, 184	0
1	CM	189/208 (90%)	-0.21	2 (1%)	80	81	60, 89, 124, 186	0
1	CN	186/208 (89%)	-0.12	2 (1%)	80	81	65, 88, 115, 141	0
1	CO	198/208 (95%)	-0.20	0	100	100	67, 89, 121, 184	0
1	CP	189/208 (90%)	-0.24	3 (1%)	72	70	60, 89, 124, 186	0
1	CQ	186/208 (89%)	0.03	1 (0%)	91	91	65, 88, 115, 141	0
1	CR	198/208 (95%)	-0.06	2 (1%)	82	82	67, 89, 121, 184	0
1	CS	189/208 (90%)	0.10	4 (2%)	63	62	60, 89, 124, 186	0
1	CT	186/208 (89%)	-0.05	4 (2%)	62	60	65, 88, 115, 141	0
1	CU	198/208 (95%)	-0.13	0	100	100	67, 89, 121, 184	0
1	CV	189/208 (90%)	-0.18	1 (0%)	91	91	60, 89, 124, 186	0
1	CW	186/208 (89%)	0.05	1 (0%)	91	91	65, 88, 115, 141	0
1	CX	198/208 (95%)	-0.14	5 (2%)	57	54	67, 89, 121, 184	0
1	CY	189/208 (90%)	-0.07	2 (1%)	80	81	60, 89, 124, 186	0
1	CZ	186/208 (89%)	0.27	8 (4%)	35	34	65, 88, 115, 141	0
1	DA	198/208 (95%)	0.10	4 (2%)	65	64	67, 89, 121, 184	0
1	DB	189/208 (90%)	-0.01	4 (2%)	63	62	60, 89, 124, 186	0
1	DC	186/208 (89%)	0.07	6 (3%)	47	46	65, 88, 115, 141	0
1	DD	198/208 (95%)	-0.11	1 (0%)	91	91	67, 89, 121, 184	0
1	DE	189/208 (90%)	0.07	5 (2%)	56	53	60, 89, 124, 186	0
1	DF	186/208 (89%)	0.16	9 (4%)	30	28	65, 88, 115, 141	0
1	DG	198/208 (95%)	-0.14	2 (1%)	82	82	67, 89, 121, 184	0
1	DH	189/208 (90%)	-0.09	1 (0%)	91	91	60, 89, 124, 186	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	DI	186/208 (89%)	-0.17	1 (0%) 91 91	65, 88, 115, 141	0
1	DJ	198/208 (95%)	-0.11	0 100 100	67, 89, 121, 184	0
1	DK	189/208 (90%)	-0.24	1 (0%) 91 91	60, 89, 124, 186	0
1	DL	186/208 (89%)	-0.08	3 (1%) 72 70	65, 88, 115, 141	0
All	All	17190/18720 (91%)	-0.07	193 (1%) 80 81	60, 89, 120, 186	0

The worst 5 of 193 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AY	141	GLY	7.2
1	BO	20	PRO	6.7
1	BL	20	PRO	6.1
1	DE	208	ALA	5.4
1	AQ	20	PRO	4.6

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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.