



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 10:46 PM UTC

PDB ID : 6DWU / pdb_00006dwu
Title : Crystal structure of complex of BBKI and Bovine Trypsin
Authors : Li, M.; Wlodawer, A.; Gustchina, A.
Deposited on : 2018-06-28
Resolution : 3.96 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

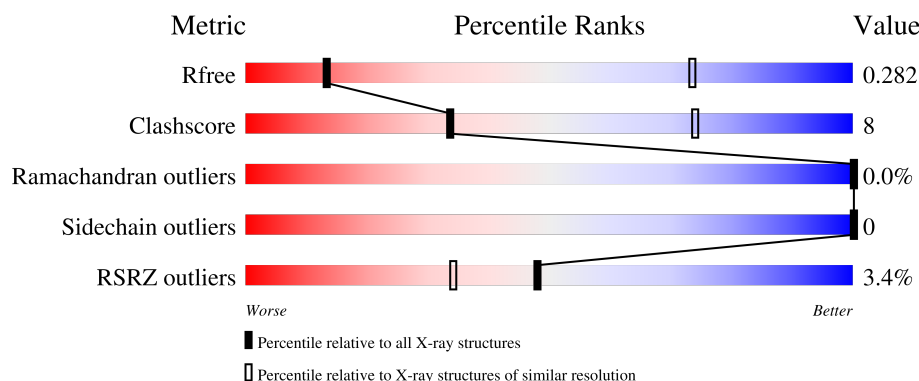
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.96 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



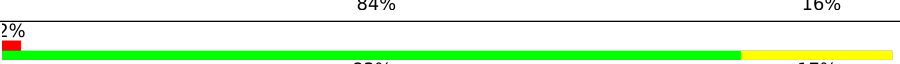
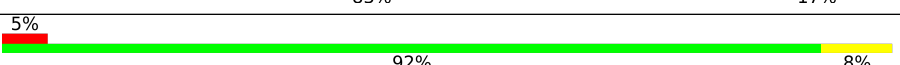
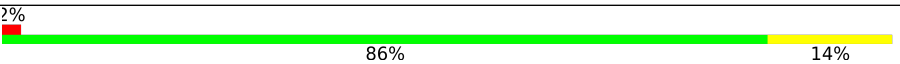
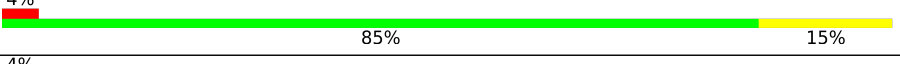
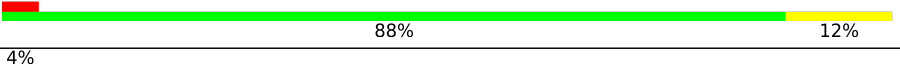
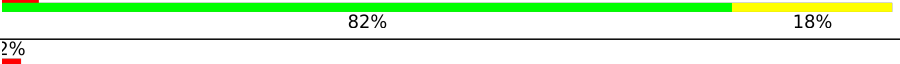
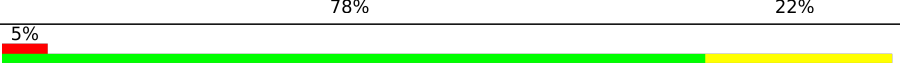
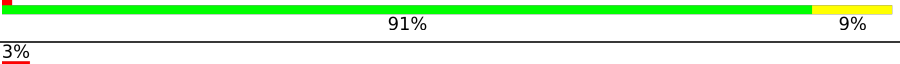
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1046 (4.16-3.76)
Clashscore	190562	1019 (4.14-3.78)
Ramachandran outliers	187476	1031 (4.16-3.76)
Sidechain outliers	187428	1024 (4.16-3.76)
RSRZ outliers	180081	1046 (4.16-3.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AA	223	3% 83% 17%
1	AC	223	4% 80% 20%
1	AE	223	% 83% 17%
1	AG	223	86% 14%
1	AI	223	8% 85% 15%

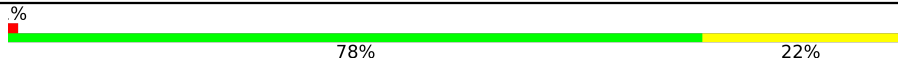
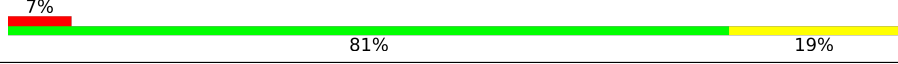
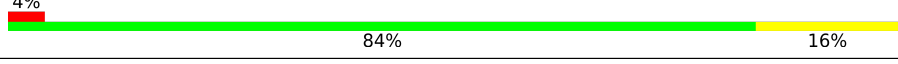
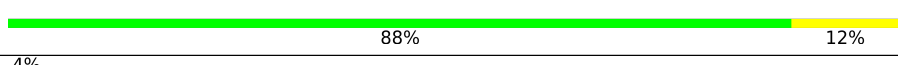
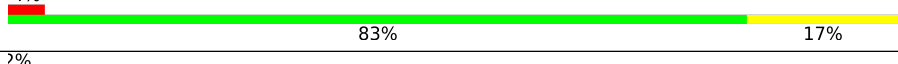
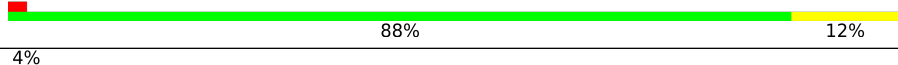
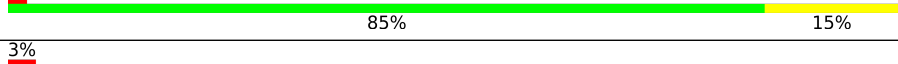
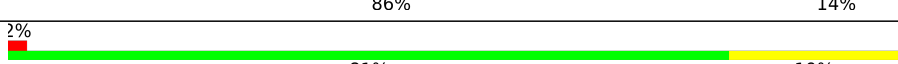
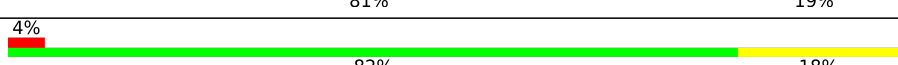
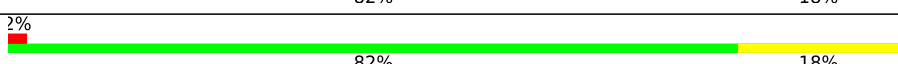
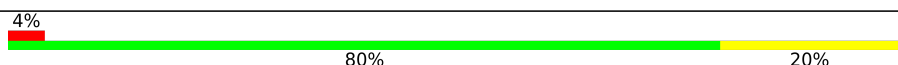
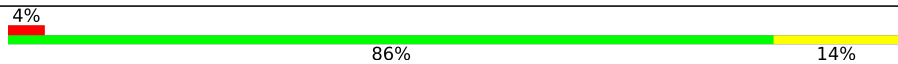
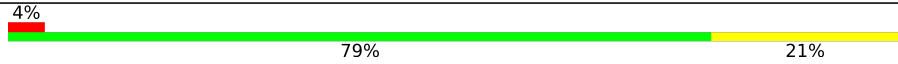
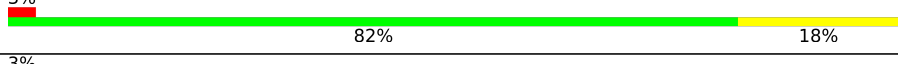
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Mol	Chain	Length	Quality of chain	
1	AK	223		
1	AM	223		
1	AO	223		
1	AQ	223		
1	AS	223		
1	AU	223		
1	BA	223		
1	BC	223		
1	BE	223		
1	BG	223		
1	BI	223		
1	BK	223		
1	BM	223		
1	BO	223		
1	BQ	223		
1	BS	223		
1	BU	223		
1	CA	223		
1	CC	223		
1	CE	223		
1	CG	223		
1	CI	223		
1	CK	223		
1	CM	223		
1	CO	223		

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Mol	Chain	Length	Quality of chain	
1	CQ	223		%
1	CS	223		
1	CU	223		
1	DA	223		
1	DC	223		
1	DE	223		
1	DG	223		
1	DI	223		
1	DK	223		
1	DM	223		
1	DO	223		
1	DQ	223		
1	DS	223		
1	DU	223		
2	AB	163		
2	AD	163		
2	AF	163		
2	AH	163		
2	AJ	163		
2	AL	163		
2	AN	163		
2	AP	163		
2	AR	163		
2	AT	163		
2	AV	163		

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Mol	Chain	Length	Quality of chain
2	BB	163	5% 83% 17%
2	BD	163	3% 72% 28%
2	BF	163	5% 82% 18%
2	BH	163	2% 82% 18%
2	BJ	163	3% 82% 18%
2	BL	163	4% 77% 23%
2	BN	163	0% 85% 15%
2	BP	163	3% 83% 17%
2	BR	163	2% 83% 17%
2	BT	163	4% 83% 17%
2	BV	163	7% 83% 17%
2	CB	163	10% 75% 25%
2	CD	163	11% 68% 32%
2	CF	163	6% 84% 16%
2	CH	163	2% 82% 18%
2	CJ	163	4% 82% 18%
2	CL	163	2% 83% 17%
2	CN	163	2% 85% 15%
2	CP	163	8% 77% 23%
2	CR	163	2% 71% 29%
2	CT	163	2% 80% 20%
2	CV	163	6% 85% 15%
2	DB	163	6% 85% 15%
2	DD	163	7% 86% 13%
2	DF	163	6% 74% 26%

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Mol	Chain	Length	Quality of chain
2	DH	163	2% 81% 19%
2	DJ	163	4% 82% 18%
2	DL	163	4% 78% 22%
2	DN	163	2% 85% 15%
2	DP	163	% 85% 15%
2	DR	163	4% 85% 15%
2	DT	163	6% 79% 21%
2	DV	163	% 81% 19%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 127116 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 Cationic trypsin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	223	Total	C	N	O	S	0	0	0
			1629	1012	279	324	14			
1	AC	223	Total	C	N	O	S	0	0	0
			1629	1012	279	324	14			
1	AE	223	Total	C	N	O	S	0	0	0
			1629	1012	279	324	14			
1	AG	223	Total	C	N	O	S	0	0	0
			1629	1012	279	324	14			
1	AI	223	Total	C	N	O	S	0	0	0
			1629	1012	279	324	14			
1	AK	223	Total	C	N	O	S	0	0	0
			1629	1012	279	324	14			
1	AM	223	Total	C	N	O	S	0	0	0
			1629	1012	279	324	14			
1	AO	223	Total	C	N	O	S	0	0	0
			1629	1012	279	324	14			
1	AQ	223	Total	C	N	O	S	0	0	0
			1629	1012	279	324	14			
1	AS	223	Total	C	N	O	S	0	0	0
			1629	1012	279	324	14			
1	AU	223	Total	C	N	O	S	0	0	0
			1629	1012	279	324	14			
1	BA	223	Total	C	N	O	S	0	0	0
			1629	1012	279	324	14			
1	BC	223	Total	C	N	O	S	0	0	0
			1629	1012	279	324	14			
1	BE	223	Total	C	N	O	S	0	0	0
			1629	1012	279	324	14			
1	BG	223	Total	C	N	O	S	0	0	0
			1629	1012	279	324	14			
1	BI	223	Total	C	N	O	S	0	0	0
			1629	1012	279	324	14			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	BK	223	Total	C	N	O	S	0	0	0
			1629	1012	279	324	14			
1	BM	223	Total	C	N	O	S	0	0	0
			1629	1012	279	324	14			
1	BO	223	Total	C	N	O	S	0	0	0
			1629	1012	279	324	14			
1	BQ	223	Total	C	N	O	S	0	0	0
			1629	1012	279	324	14			
1	BS	223	Total	C	N	O	S	0	0	0
			1629	1012	279	324	14			
1	BU	223	Total	C	N	O	S	0	0	0
			1629	1012	279	324	14			
1	CA	223	Total	C	N	O	S	0	0	0
			1629	1012	279	324	14			
1	CC	223	Total	C	N	O	S	0	0	0
			1629	1012	279	324	14			
1	CE	223	Total	C	N	O	S	0	0	0
			1629	1012	279	324	14			
1	CG	223	Total	C	N	O	S	0	0	0
			1629	1012	279	324	14			
1	CI	223	Total	C	N	O	S	0	0	0
			1629	1012	279	324	14			
1	CK	223	Total	C	N	O	S	0	0	0
			1629	1012	279	324	14			
1	CM	223	Total	C	N	O	S	0	0	0
			1629	1012	279	324	14			
1	CO	223	Total	C	N	O	S	0	0	0
			1629	1012	279	324	14			
1	CQ	223	Total	C	N	O	S	0	0	0
			1629	1012	279	324	14			
1	CS	223	Total	C	N	O	S	0	0	0
			1629	1012	279	324	14			
1	CU	223	Total	C	N	O	S	0	0	0
			1629	1012	279	324	14			
1	DA	223	Total	C	N	O	S	0	0	0
			1629	1012	279	324	14			
1	DC	223	Total	C	N	O	S	0	0	0
			1629	1012	279	324	14			
1	DE	223	Total	C	N	O	S	0	0	0
			1629	1012	279	324	14			
1	DG	223	Total	C	N	O	S	0	0	0
			1629	1012	279	324	14			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	DI	223	Total	C	N	O	S	0	0	0
			1629	1012	279	324	14			
1	DK	223	Total	C	N	O	S	0	0	0
			1629	1012	279	324	14			
1	DM	223	Total	C	N	O	S	0	0	0
			1629	1012	279	324	14			
1	DO	223	Total	C	N	O	S	0	0	0
			1629	1012	279	324	14			
1	DQ	223	Total	C	N	O	S	0	0	0
			1629	1012	279	324	14			
1	DS	223	Total	C	N	O	S	0	0	0
			1629	1012	279	324	14			
1	DU	223	Total	C	N	O	S	0	0	0
			1629	1012	279	324	14			

- Molecule 2 is a protein called Kunitz-type inhibitor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	163	Total	C	N	O	S	0	0	0
			1260	807	217	235	1			
2	AD	163	Total	C	N	O	S	0	0	0
			1260	807	217	235	1			
2	AF	163	Total	C	N	O	S	0	0	0
			1260	807	217	235	1			
2	AH	163	Total	C	N	O	S	0	0	0
			1260	807	217	235	1			
2	AJ	163	Total	C	N	O	S	0	0	0
			1260	807	217	235	1			
2	AL	163	Total	C	N	O	S	0	0	0
			1260	807	217	235	1			
2	AN	163	Total	C	N	O	S	0	0	0
			1260	807	217	235	1			
2	AP	163	Total	C	N	O	S	0	0	0
			1260	807	217	235	1			
2	AR	163	Total	C	N	O	S	0	0	0
			1260	807	217	235	1			
2	AT	163	Total	C	N	O	S	0	0	0
			1260	807	217	235	1			
2	AV	163	Total	C	N	O	S	0	0	0
			1260	807	217	235	1			
2	BB	163	Total	C	N	O	S	0	0	0
			1260	807	217	235	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	BD	163	Total	C	N	O	S	0	0	0
			1260	807	217	235	1			
2	BF	163	Total	C	N	O	S	0	0	0
			1260	807	217	235	1			
2	BH	163	Total	C	N	O	S	0	0	0
			1260	807	217	235	1			
2	BJ	163	Total	C	N	O	S	0	0	0
			1260	807	217	235	1			
2	BL	163	Total	C	N	O	S	0	0	0
			1260	807	217	235	1			
2	BN	163	Total	C	N	O	S	0	0	0
			1260	807	217	235	1			
2	BP	163	Total	C	N	O	S	0	0	0
			1260	807	217	235	1			
2	BR	163	Total	C	N	O	S	0	0	0
			1260	807	217	235	1			
2	BT	163	Total	C	N	O	S	0	0	0
			1260	807	217	235	1			
2	BV	163	Total	C	N	O	S	0	0	0
			1260	807	217	235	1			
2	CB	163	Total	C	N	O	S	0	0	0
			1260	807	217	235	1			
2	CD	163	Total	C	N	O	S	0	0	0
			1260	807	217	235	1			
2	CF	163	Total	C	N	O	S	0	0	0
			1260	807	217	235	1			
2	CH	163	Total	C	N	O	S	0	0	0
			1260	807	217	235	1			
2	CJ	163	Total	C	N	O	S	0	0	0
			1260	807	217	235	1			
2	CL	163	Total	C	N	O	S	0	0	0
			1260	807	217	235	1			
2	CN	163	Total	C	N	O	S	0	0	0
			1260	807	217	235	1			
2	CP	163	Total	C	N	O	S	0	0	0
			1260	807	217	235	1			
2	CR	163	Total	C	N	O	S	0	0	0
			1260	807	217	235	1			
2	CT	163	Total	C	N	O	S	0	0	0
			1260	807	217	235	1			
2	CV	163	Total	C	N	O	S	0	0	0
			1260	807	217	235	1			

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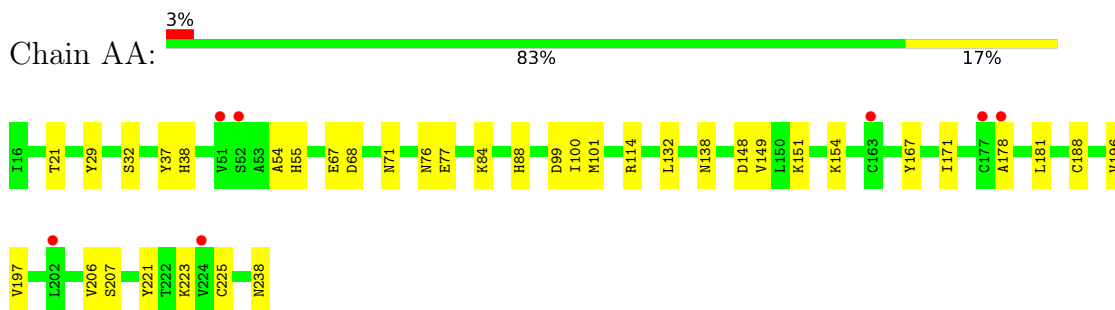
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	DB	163	Total 1260	C 807	N 217	O 235	S 1	0	0	0
2	DD	163	Total 1260	C 807	N 217	O 235	S 1	0	0	0
2	DF	163	Total 1260	C 807	N 217	O 235	S 1	0	0	0
2	DH	163	Total 1260	C 807	N 217	O 235	S 1	0	0	0
2	DJ	163	Total 1260	C 807	N 217	O 235	S 1	0	0	0
2	DL	163	Total 1260	C 807	N 217	O 235	S 1	0	0	0
2	DN	163	Total 1260	C 807	N 217	O 235	S 1	0	0	0
2	DP	163	Total 1260	C 807	N 217	O 235	S 1	0	0	0
2	DR	163	Total 1260	C 807	N 217	O 235	S 1	0	0	0
2	DT	163	Total 1260	C 807	N 217	O 235	S 1	0	0	0
2	DV	163	Total 1260	C 807	N 217	O 235	S 1	0	0	0

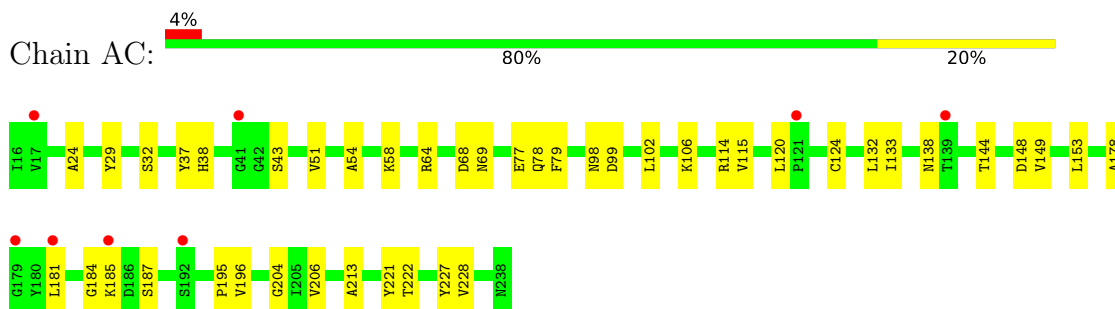
3 Residue-property plots [i](#)

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.

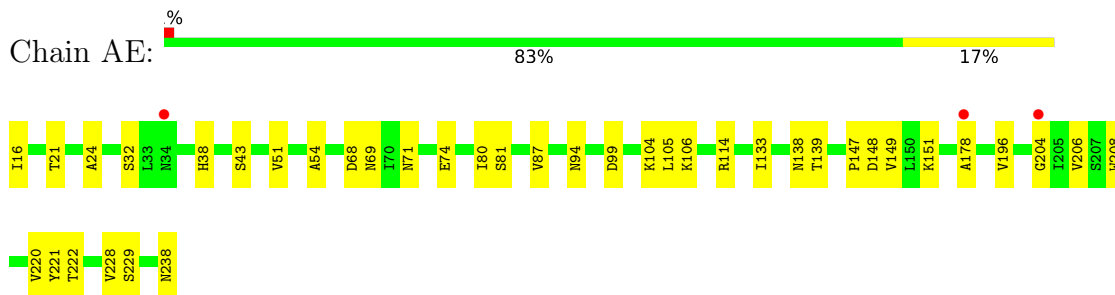
- Molecule 1: Cationic trypsin



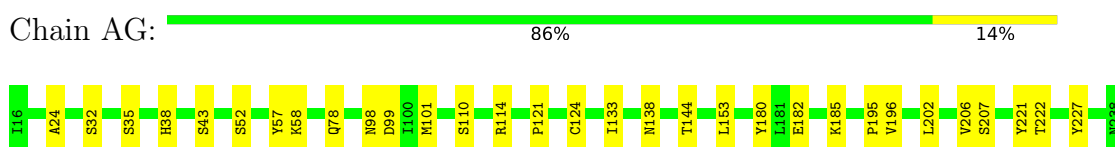
- Molecule 1: Cationic trypsin



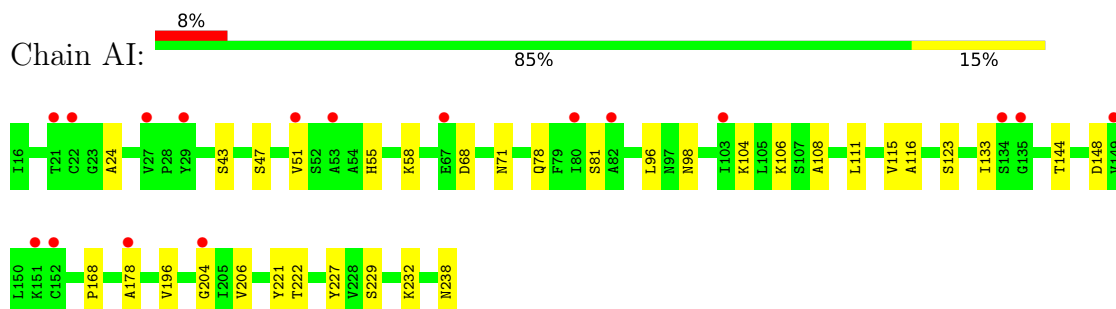
- Molecule 1: Cationic trypsin



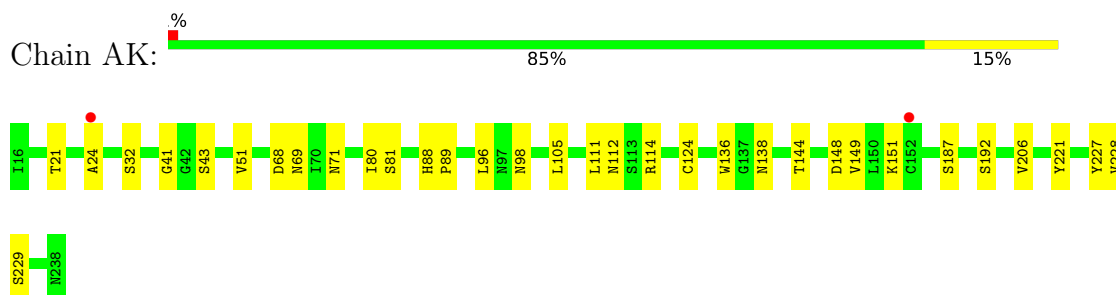
- Molecule 1: Cationic trypsin



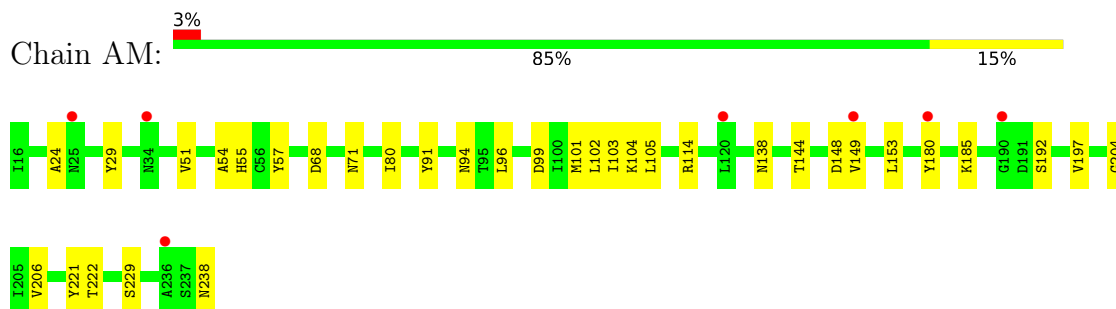
- Molecule 1: Cationic trypsin



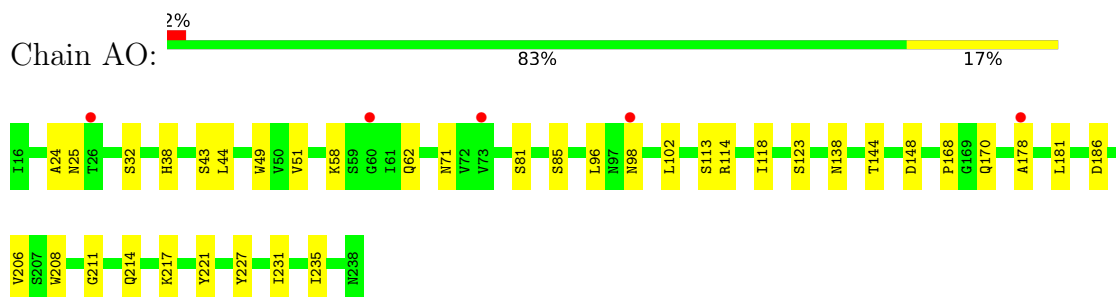
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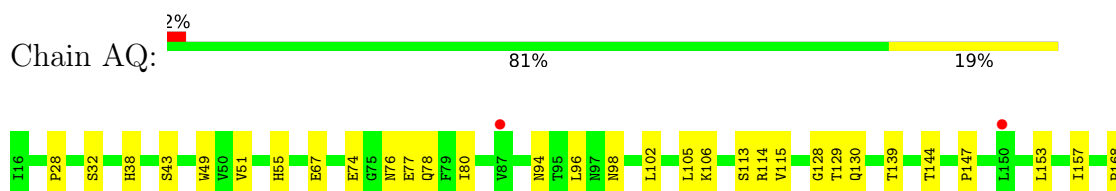
- Molecule 1: Cationic trypsin



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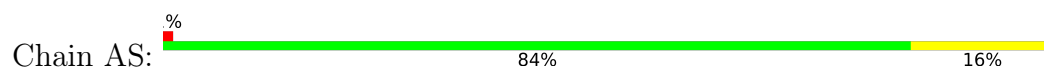


- Molecule 1: Cationic trypsin

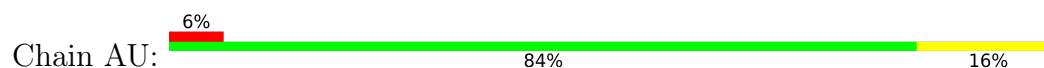




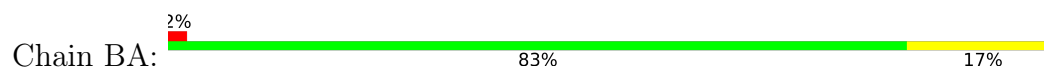
- Molecule 1: Cationic trypsin



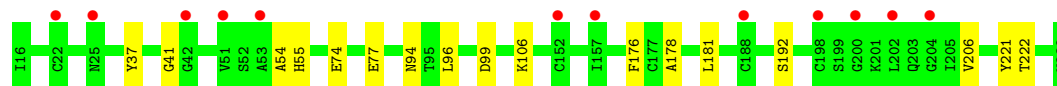
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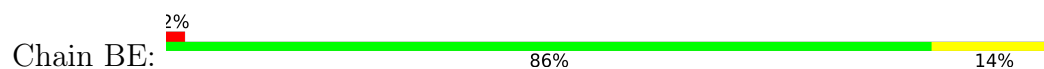
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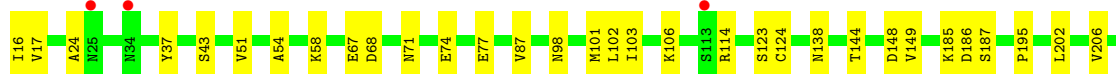
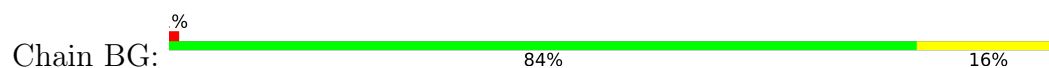


- Molecule 1: Cationic trypsin

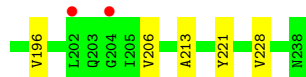
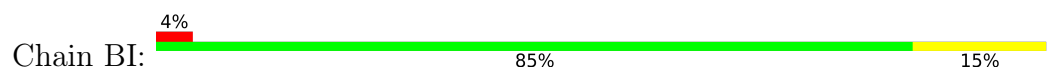




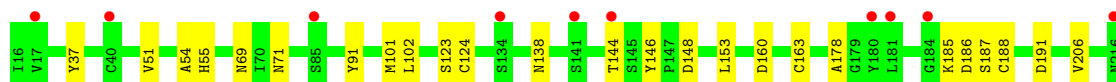
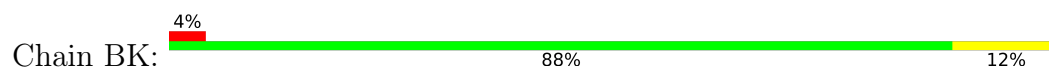
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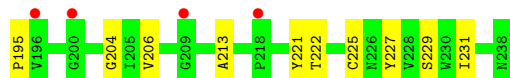
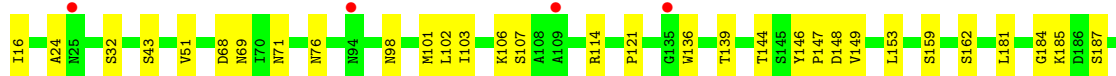
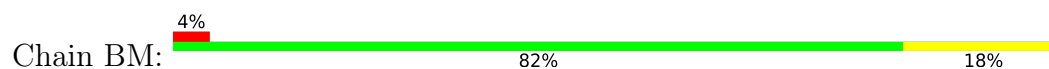
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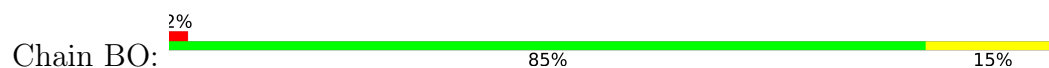
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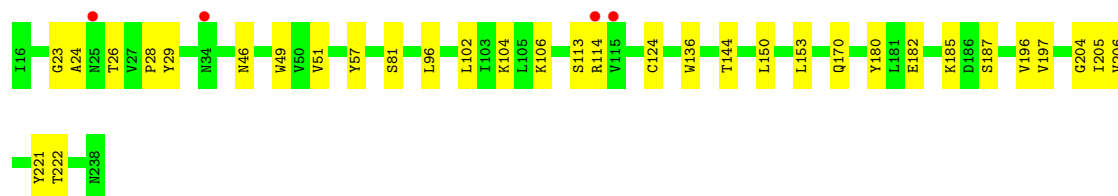


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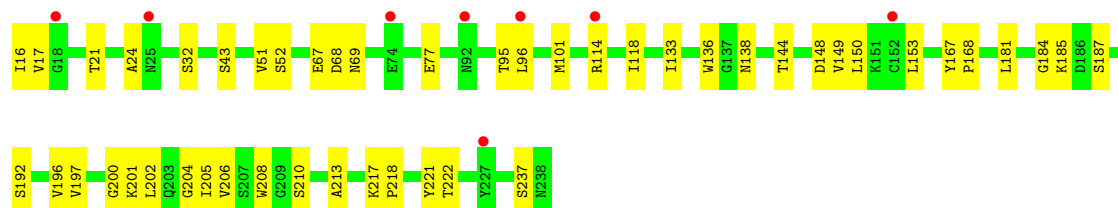
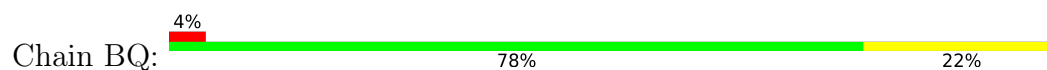


- Molecule 1: Cationic trypsin

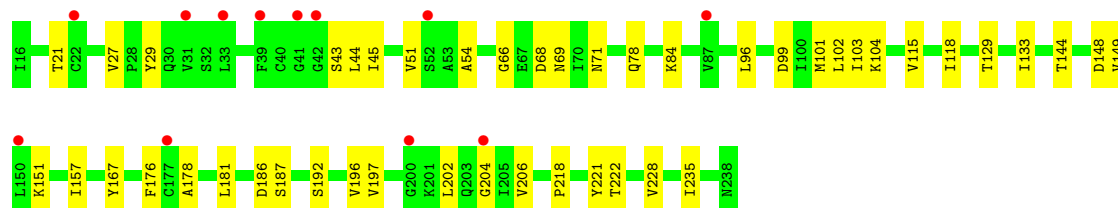
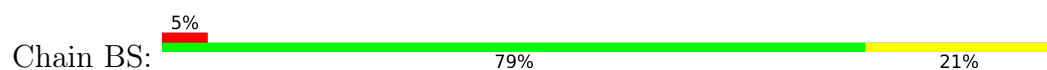




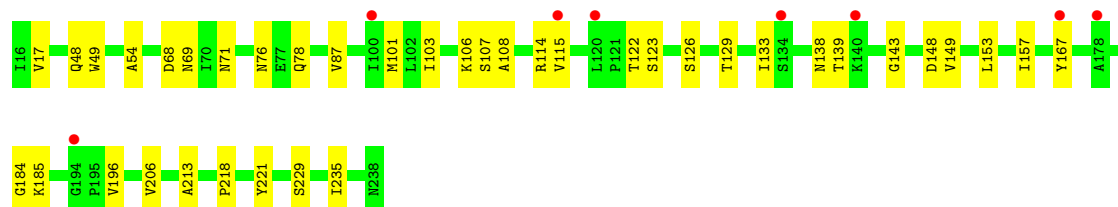
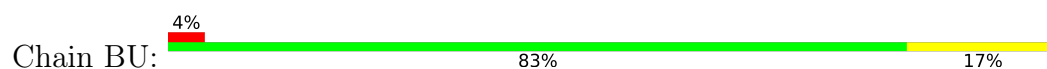
• Molecule 1: Cationic trypsin



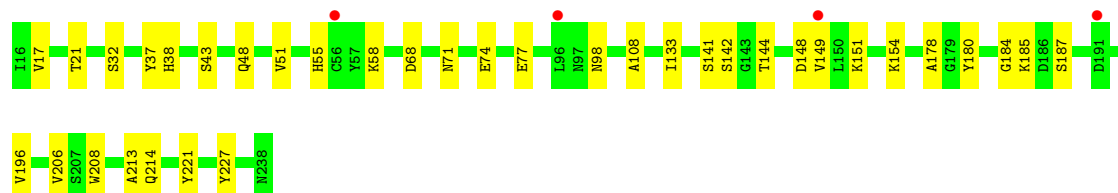
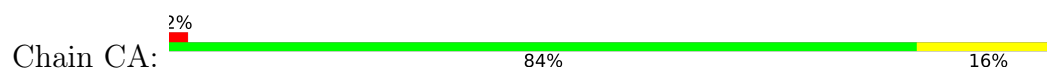
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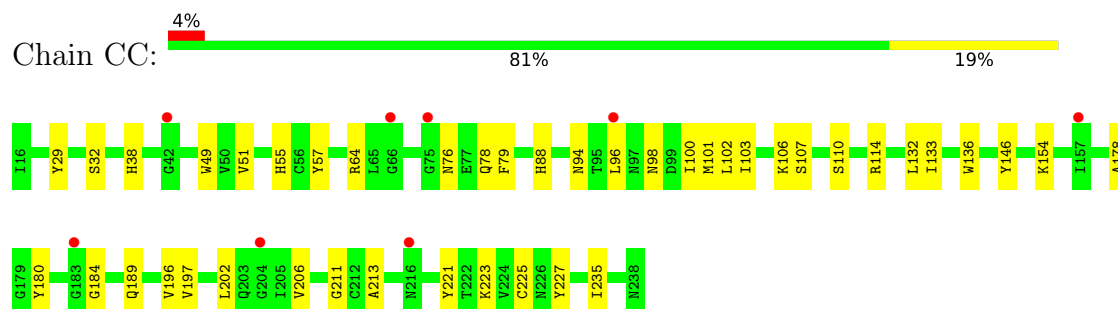
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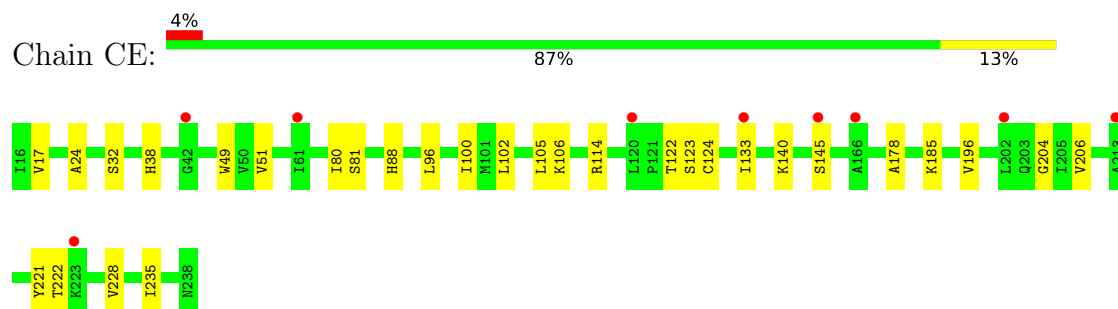
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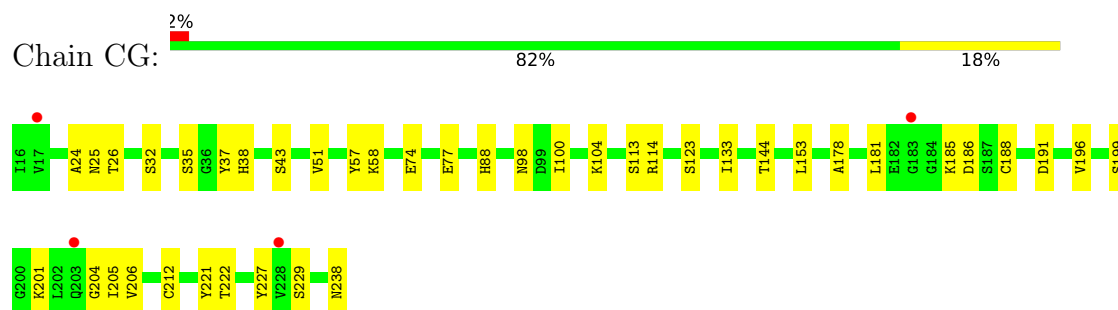
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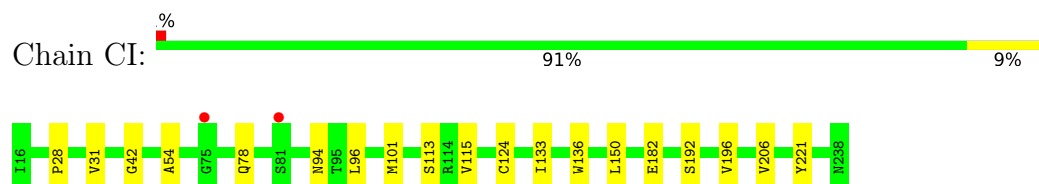
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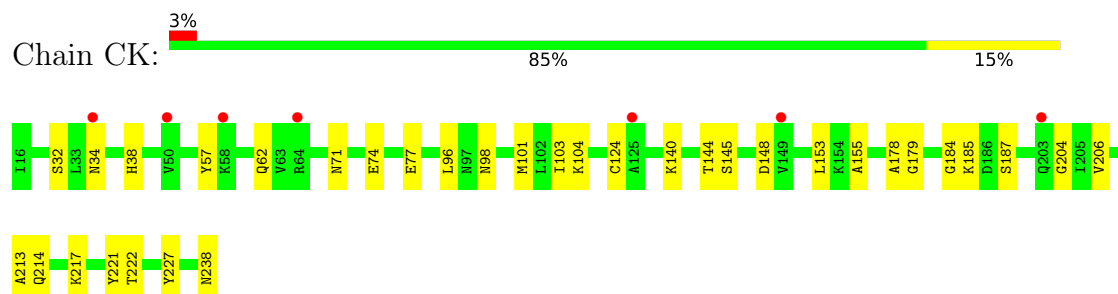
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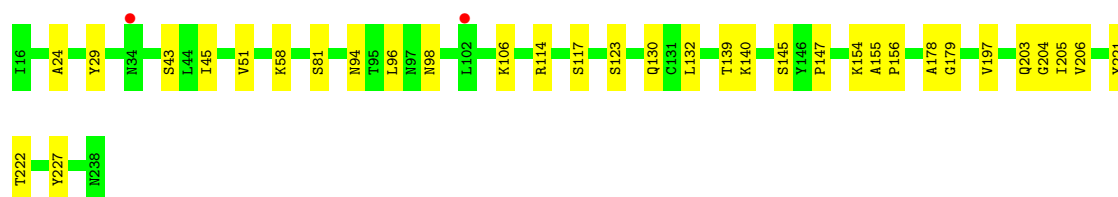
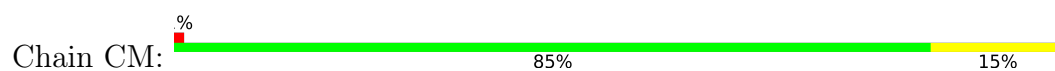
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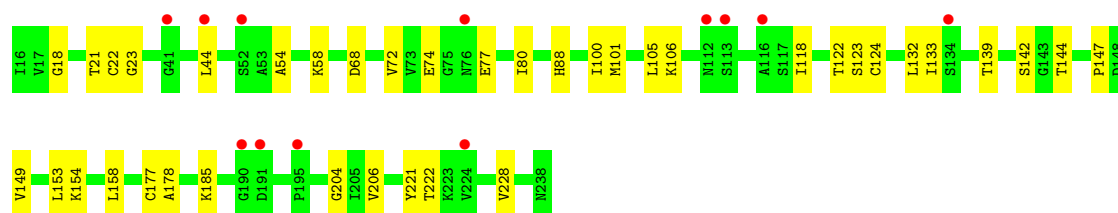
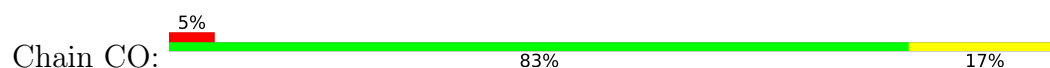
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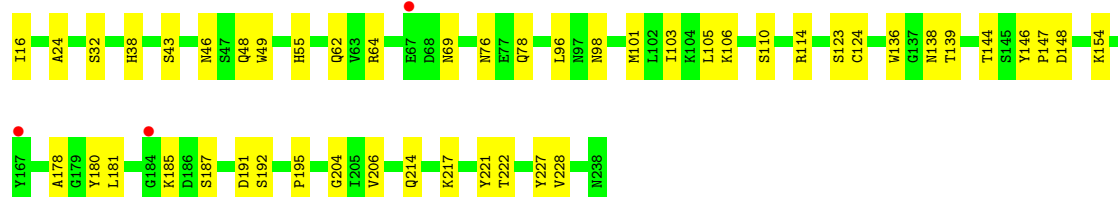
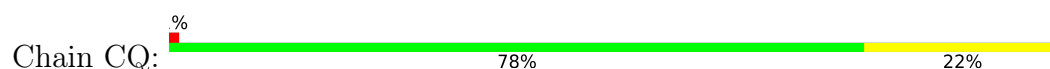
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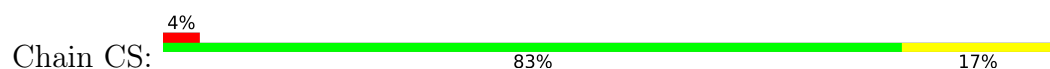
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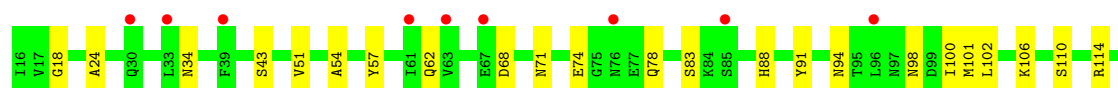
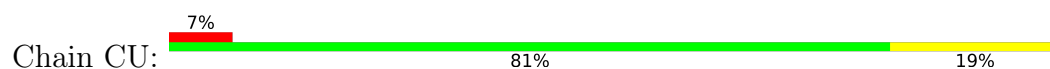
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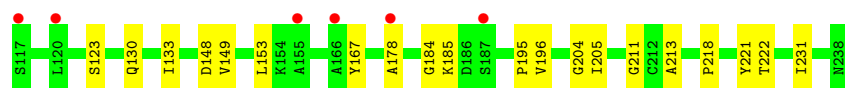


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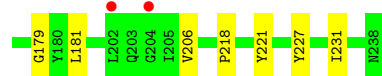
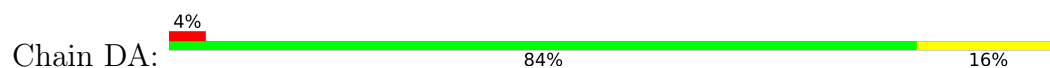


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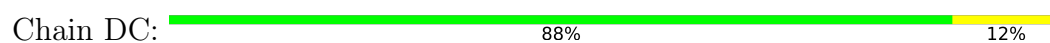




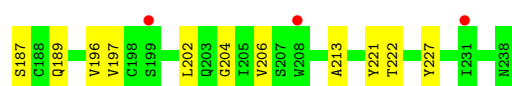
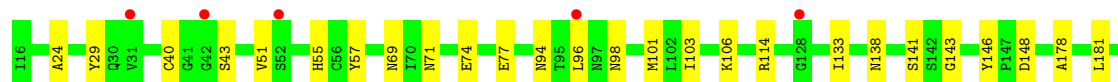
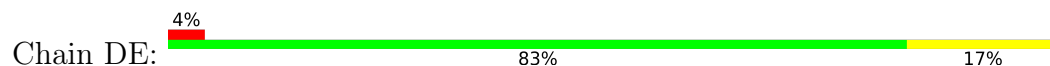
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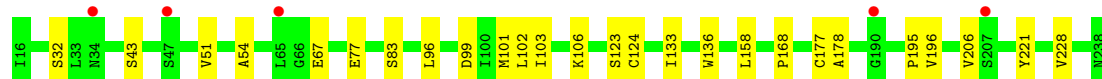
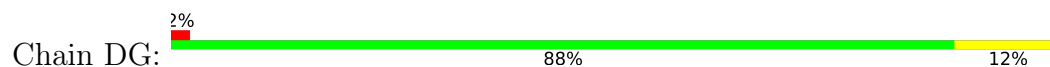
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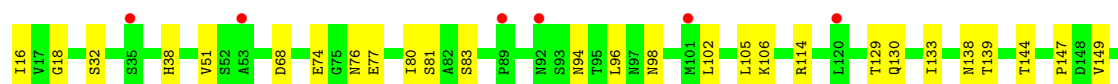
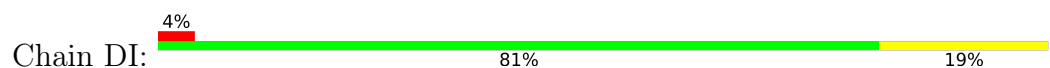
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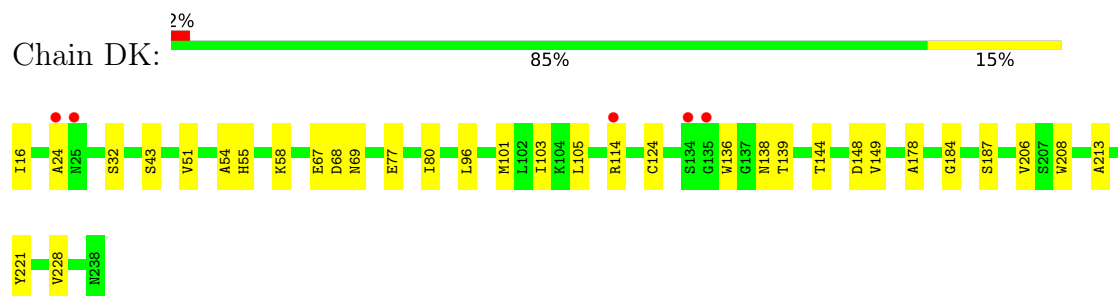
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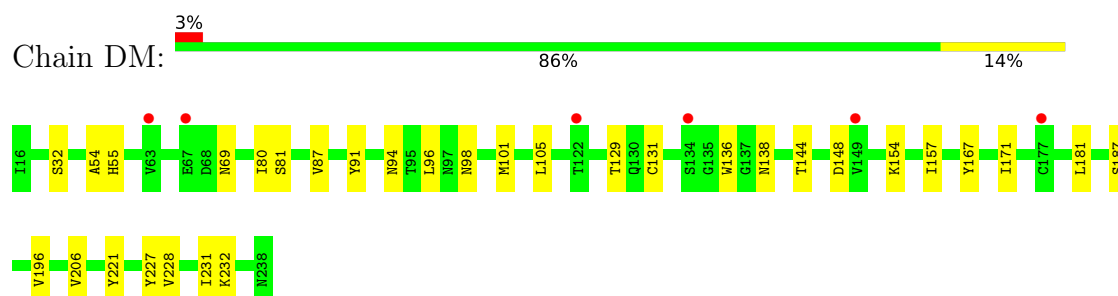
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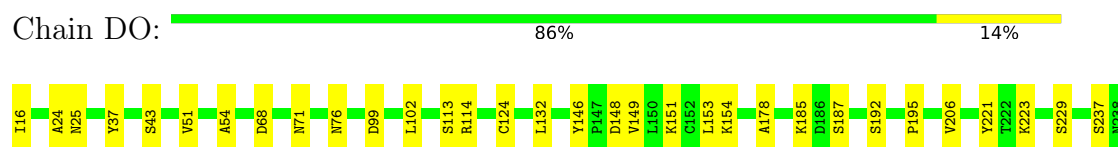
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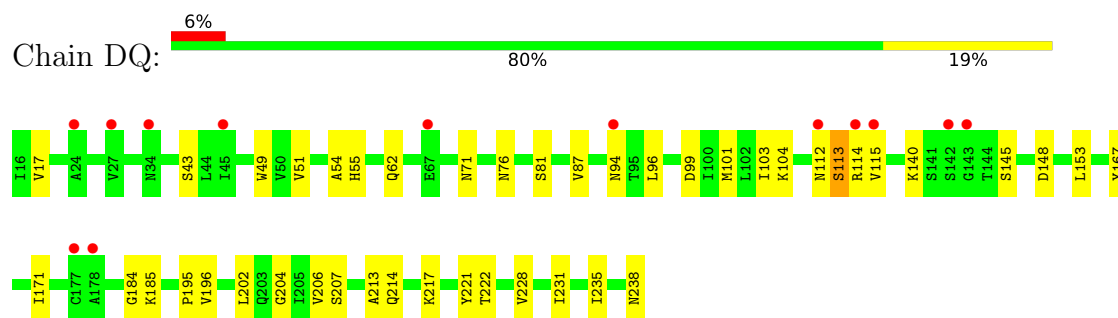
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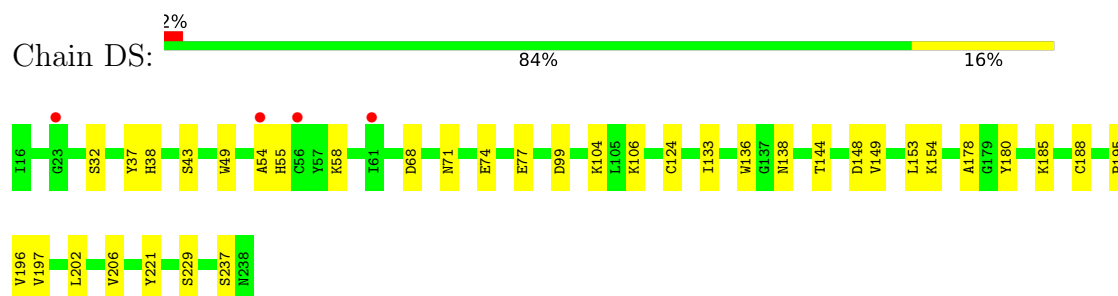
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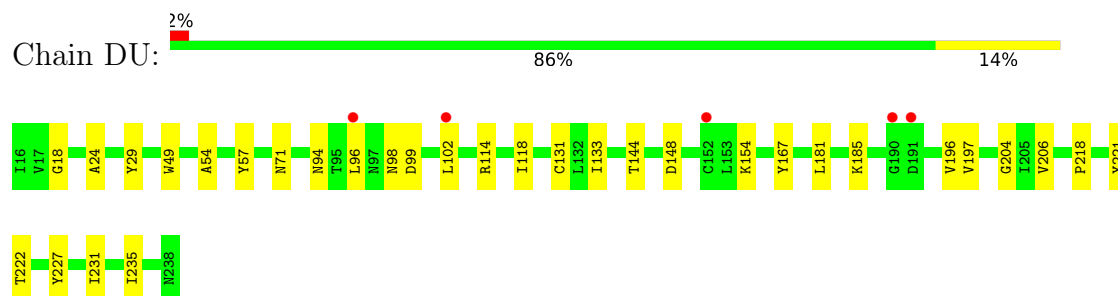
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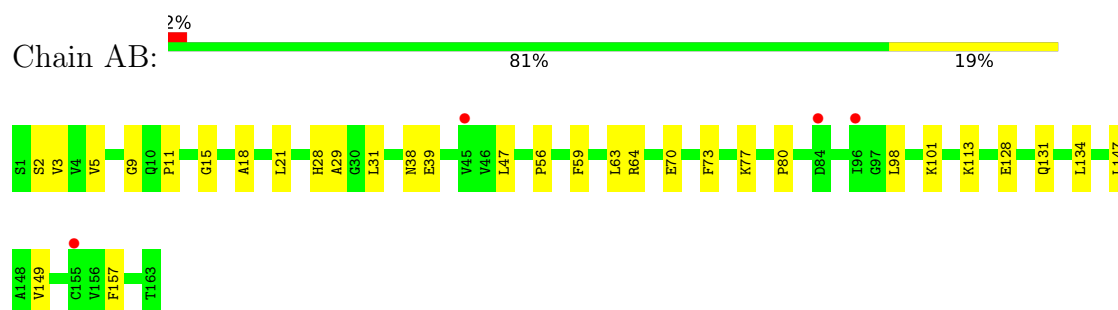
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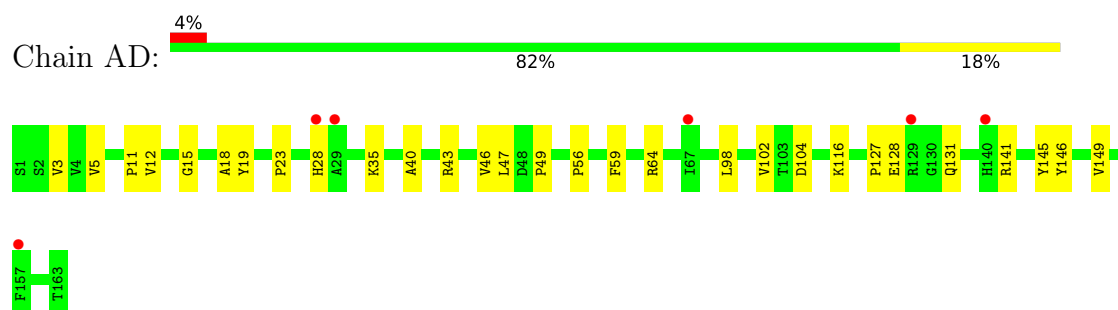
- Molecule 1: Cationic trypsin



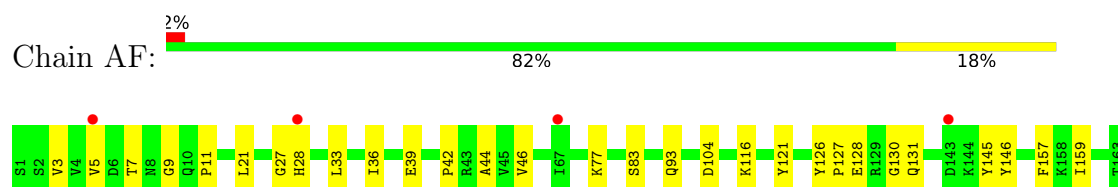
- Molecule 2: Kunitz-type inhibitor



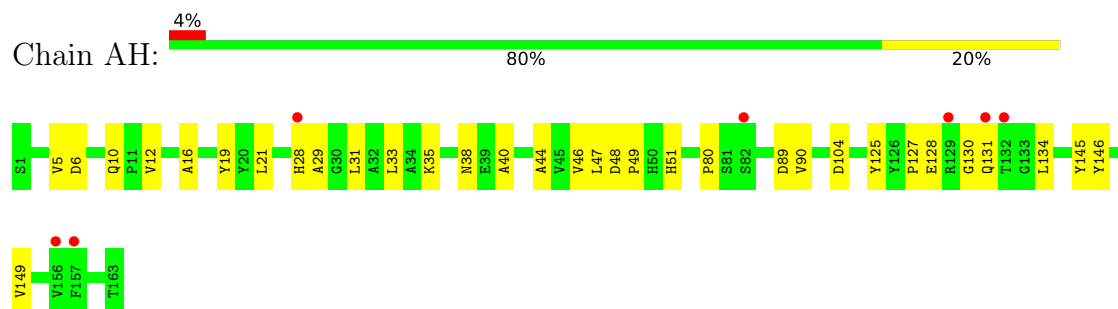
- Molecule 2: Kunitz-type inhibitor



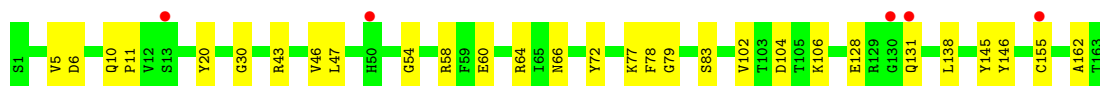
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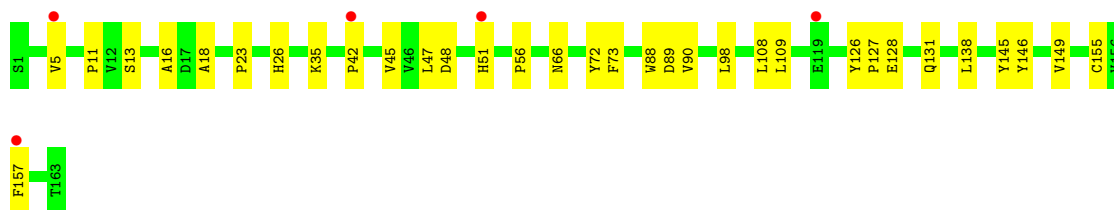
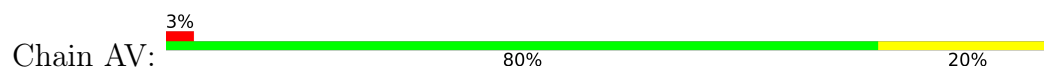
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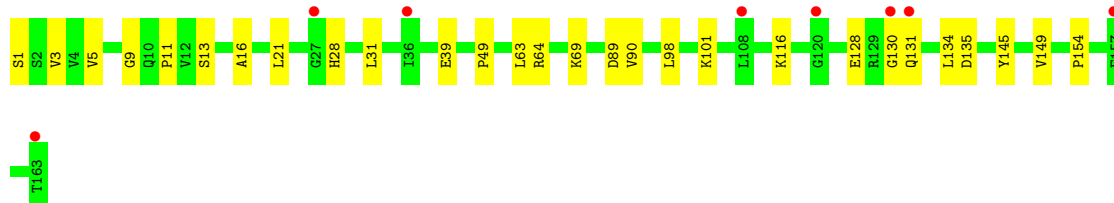
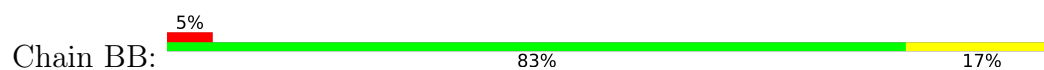
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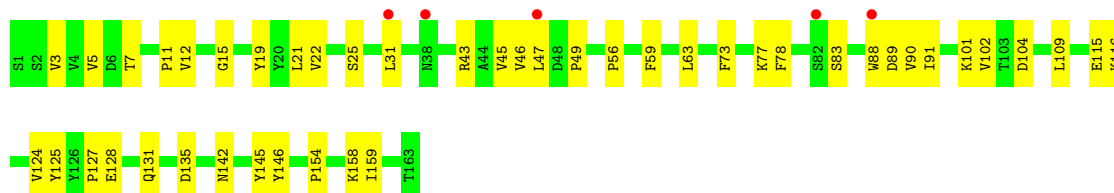
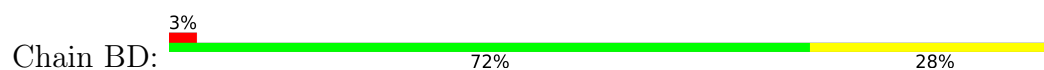
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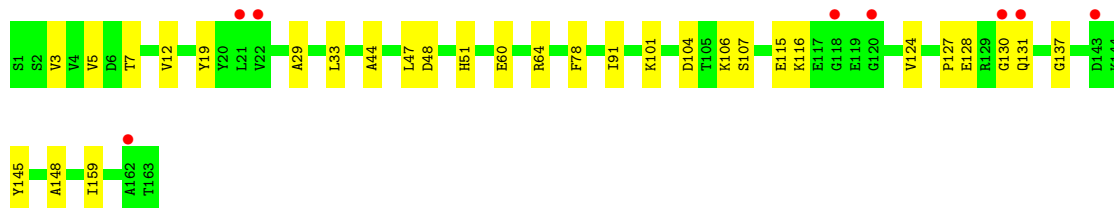
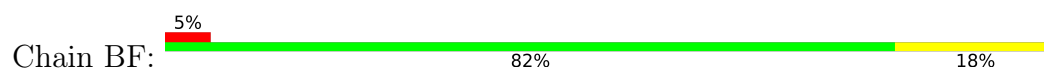
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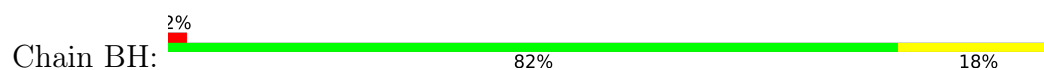
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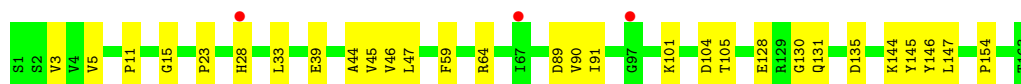


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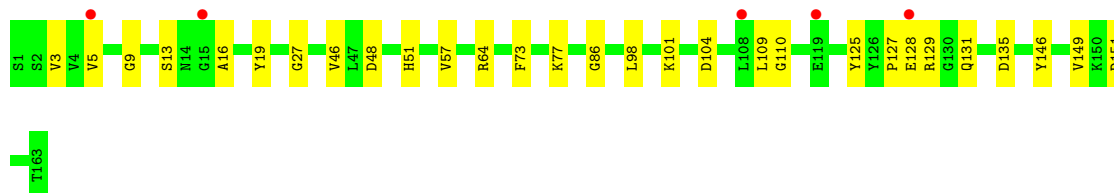
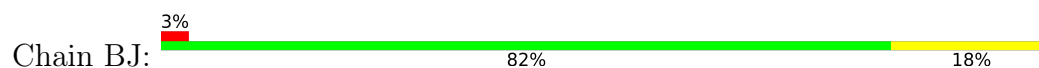


- Molecule 2: Kunitz-type inhibitor

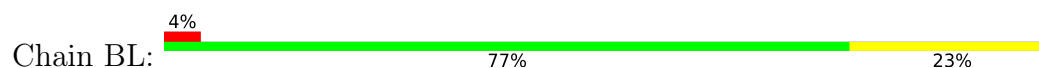




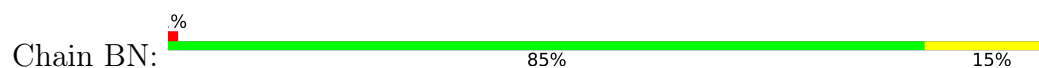
- Molecule 2: Kunitz-type inhibitor



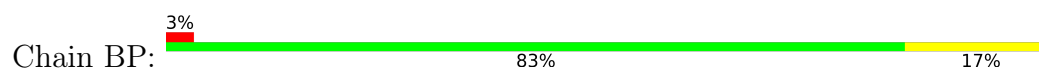
- Molecule 2: Kunitz-type inhibitor



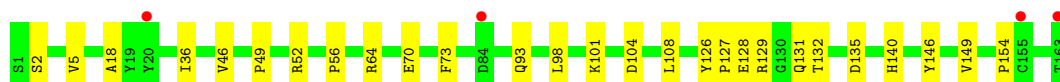
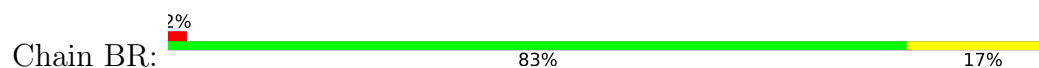
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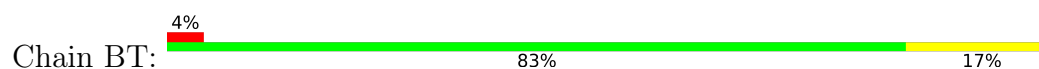
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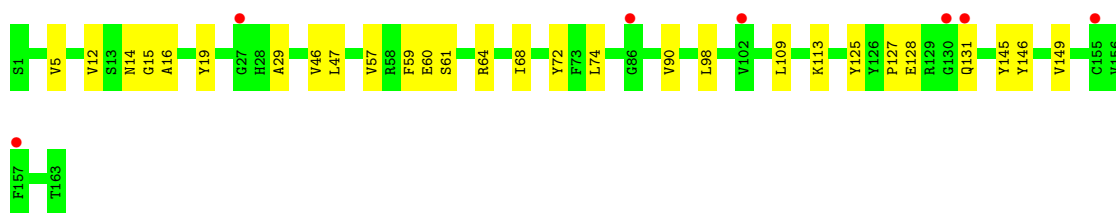


- Molecule 2: Kunitz-type inhibitor

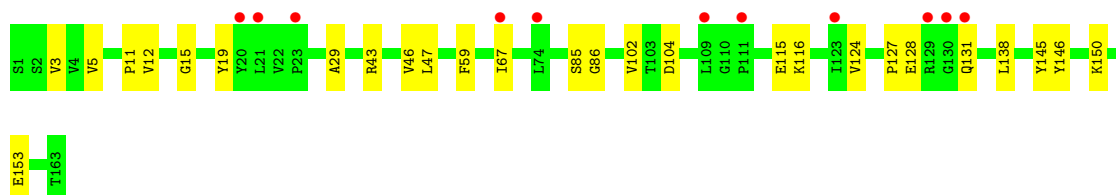
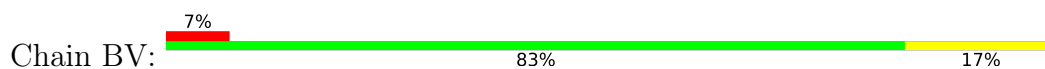


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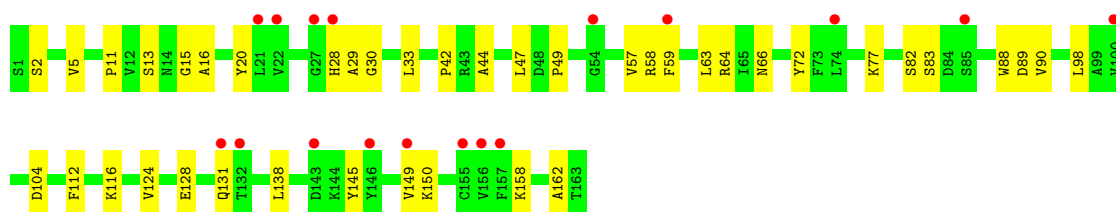
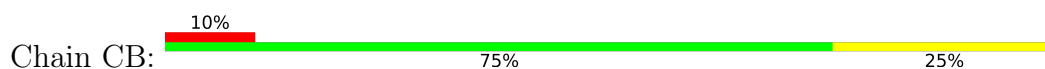




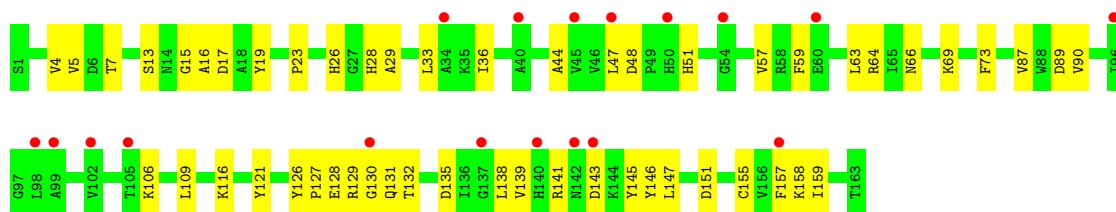
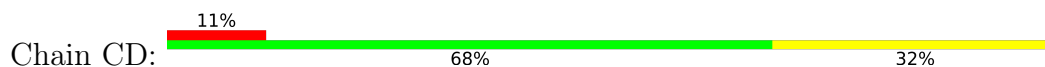
- Molecule 2: Kunitz-type inhibitor



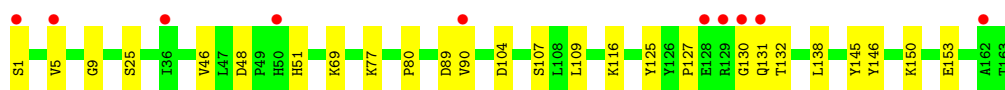
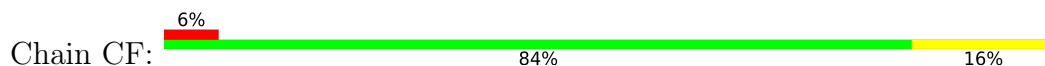
- Molecule 2: Kunitz-type inhibitor



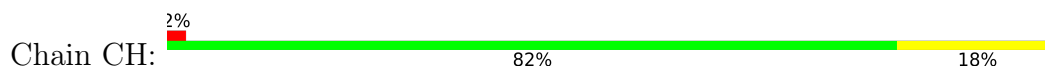
- Molecule 2: Kunitz-type inhibitor



- Molecule 2: Kunitz-type inhibitor

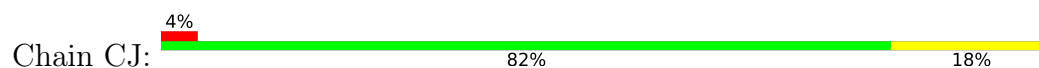


- Molecule 2: Kunitz-type inhibitor

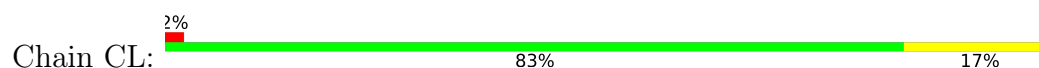




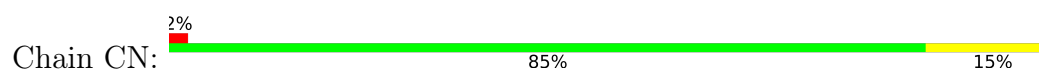
- Molecule 2: Kunitz-type inhibitor



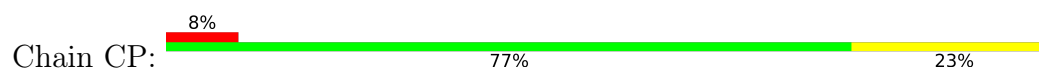
- Molecule 2: Kunitz-type inhibitor



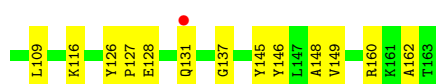
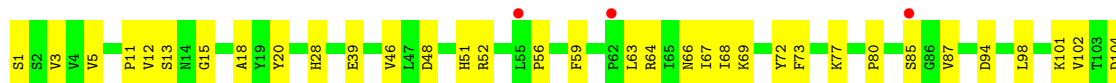
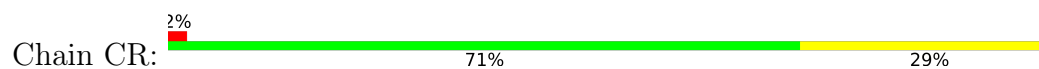
- Molecule 2: Kunitz-type inhibitor



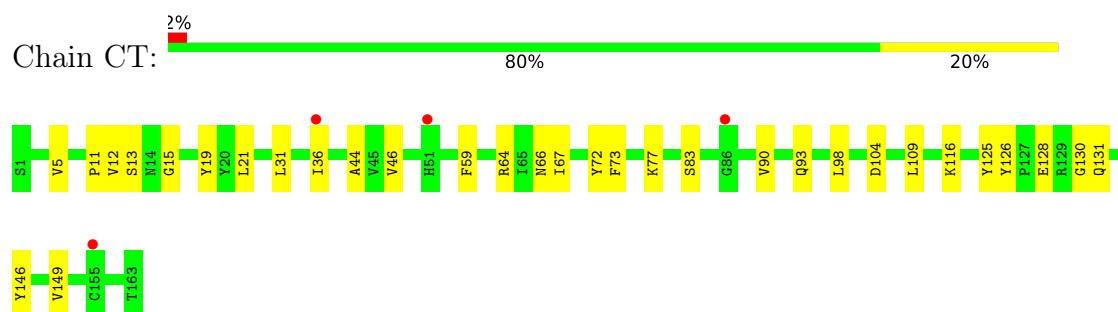
- Molecule 2: Kunitz-type inhibitor



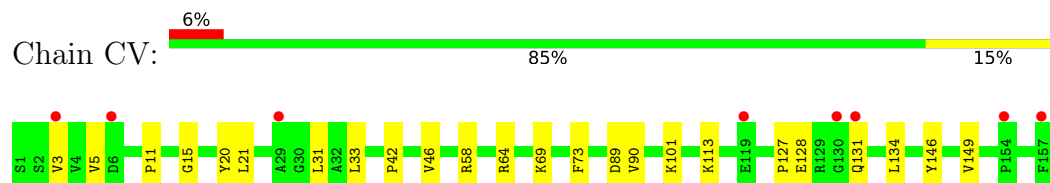
- Molecule 2: Kunitz-type inhibitor



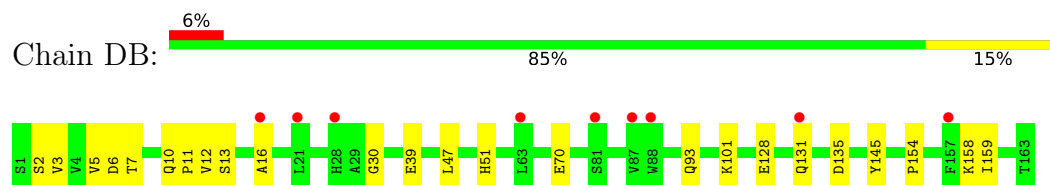
- Molecule 2: Kunitz-type inhibitor



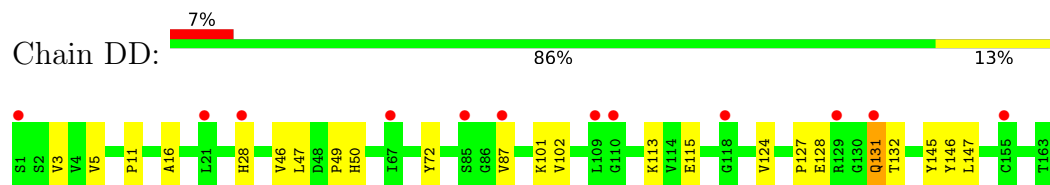
- Molecule 2: Kunitz-type inhibitor



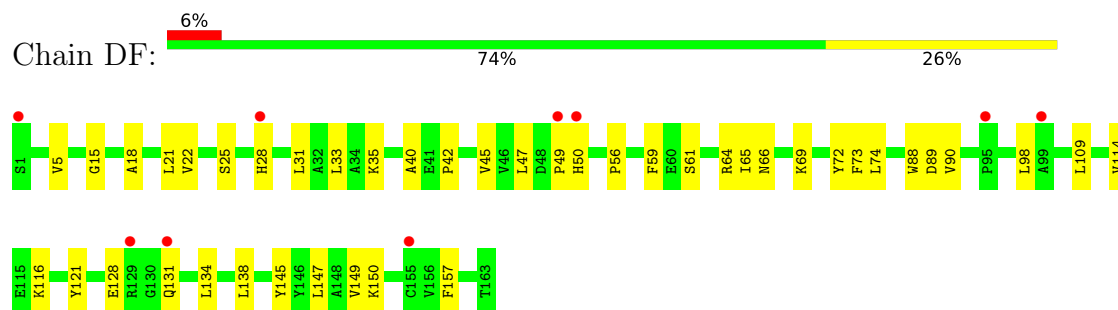
- Molecule 2: Kunitz-type inhibitor



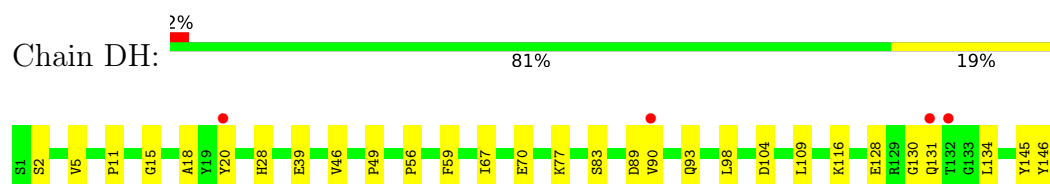
- Molecule 2: Kunitz-type inhibitor



- Molecule 2: Kunitz-type inhibitor

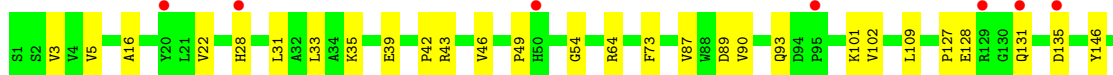
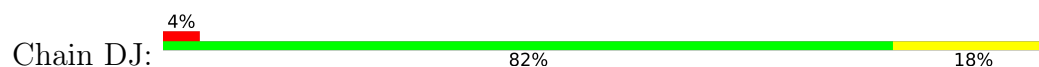


- Molecule 2: Kunitz-type inhibitor



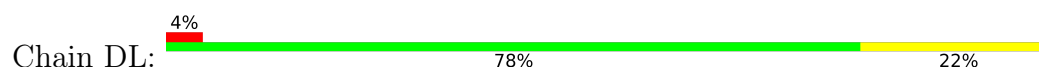
T163

- Molecule 2: Kunitz-type inhibitor



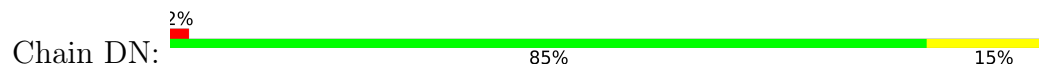
P154 T163

- Molecule 2: Kunitz-type inhibitor



I159 A162 T163

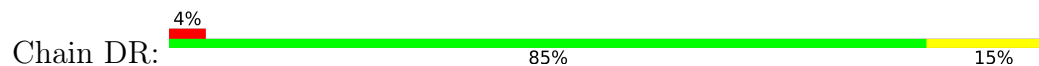
- Molecule 2: Kunitz-type inhibitor



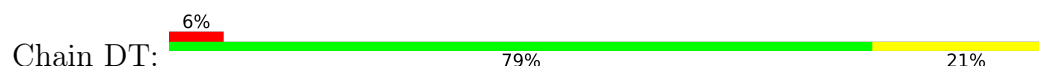
- Molecule 2: Kunitz-type inhibitor

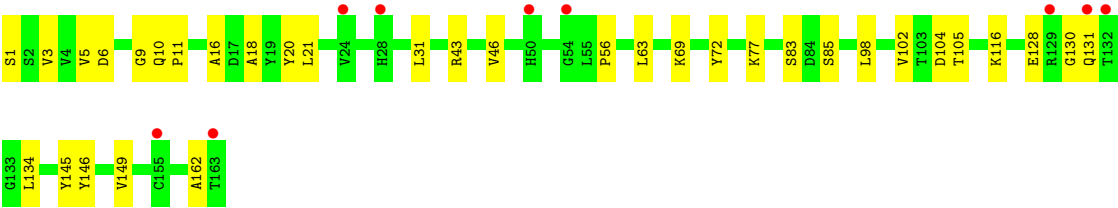


- Molecule 2: Kunitz-type inhibitor

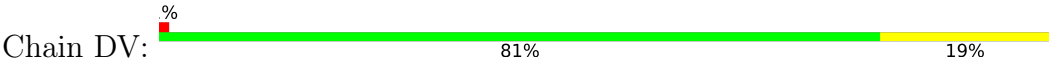


- Molecule 2: Kunitz-type inhibitor





● Molecule 2: Kunitz-type inhibitor



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	137.17Å 483.88Å 137.01Å 90.00° 116.76° 90.00°	Depositor
Resolution (Å)	49.23 – 3.96 49.23 – 3.96	Depositor EDS
% Data completeness (in resolution range)	85.1 (49.23-3.96) 85.8 (49.23-3.96)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.59 (at 4.00Å)	Xtriage
Refinement program	PHENIX (1.12_2829)	Depositor
R, R_{free}	0.226 , 0.281 0.227 , 0.282	Depositor DCC
R_{free} test set	5842 reflections (4.19%)	wwPDB-VP
Wilson B-factor (Å ²)	52.0	Xtriage
Anisotropy	0.368	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 50.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.028 for l,-k,h	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	127116	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.66% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	0.17	0/1660	0.41	0/2250
1	AC	0.16	0/1660	0.40	0/2250
1	AE	0.15	0/1660	0.40	0/2250
1	AG	0.16	0/1660	0.40	0/2250
1	AI	0.17	0/1660	0.44	0/2250
1	AK	0.18	0/1660	0.41	0/2250
1	AM	0.16	0/1660	0.40	0/2250
1	AO	0.15	0/1660	0.39	0/2250
1	AQ	0.17	0/1660	0.44	0/2250
1	AS	0.16	0/1660	0.41	0/2250
1	AU	0.14	0/1660	0.38	0/2250
1	BA	0.16	0/1660	0.40	0/2250
1	BC	0.14	0/1660	0.39	0/2250
1	BE	0.16	0/1660	0.43	0/2250
1	BG	0.17	0/1660	0.42	0/2250
1	BI	0.16	0/1660	0.41	0/2250
1	BK	0.16	0/1660	0.43	0/2250
1	BM	0.17	0/1660	0.46	0/2250
1	BO	0.17	0/1660	0.43	0/2250
1	BQ	0.16	0/1660	0.43	0/2250
1	BS	0.14	0/1660	0.38	0/2250
1	BU	0.15	0/1660	0.40	0/2250
1	CA	0.15	0/1660	0.40	0/2250
1	CC	0.16	0/1660	0.40	0/2250
1	CE	0.17	0/1660	0.44	0/2250
1	CG	0.17	0/1660	0.44	0/2250
1	CI	0.19	0/1660	0.46	0/2250
1	CK	0.19	0/1660	0.43	0/2250
1	CM	0.15	0/1660	0.40	0/2250
1	CO	0.16	0/1660	0.44	0/2250
1	CQ	0.16	0/1660	0.43	0/2250
1	CS	0.15	0/1660	0.41	0/2250
1	CU	0.16	0/1660	0.41	0/2250
1	DA	0.16	0/1660	0.41	0/2250

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	DC	0.17	0/1660	0.40	0/2250
1	DE	0.15	0/1660	0.41	0/2250
1	DG	0.16	0/1660	0.40	0/2250
1	DI	0.17	0/1660	0.43	0/2250
1	DK	0.18	0/1660	0.44	0/2250
1	DM	0.16	0/1660	0.41	0/2250
1	DO	0.18	0/1660	0.44	0/2250
1	DQ	0.17	0/1660	0.40	0/2250
1	DS	0.16	0/1660	0.41	0/2250
1	DU	0.14	0/1660	0.40	0/2250
2	AB	0.17	0/1291	0.50	0/1754
2	AD	0.18	0/1291	0.46	0/1754
2	AF	0.20	0/1291	0.54	0/1754
2	AH	0.20	0/1291	0.54	0/1754
2	AJ	0.19	0/1291	0.48	0/1754
2	AL	0.19	0/1291	0.48	0/1754
2	AN	0.20	0/1291	0.47	0/1754
2	AP	0.18	0/1291	0.46	0/1754
2	AR	0.18	0/1291	0.48	0/1754
2	AT	0.19	0/1291	0.49	0/1754
2	AV	0.17	0/1291	0.47	0/1754
2	BB	0.19	0/1291	0.50	0/1754
2	BD	0.26	0/1291	0.50	0/1754
2	BF	0.17	0/1291	0.43	0/1754
2	BH	0.19	0/1291	0.50	0/1754
2	BJ	0.21	0/1291	0.49	0/1754
2	BL	0.20	0/1291	0.47	0/1754
2	BN	0.19	0/1291	0.48	0/1754
2	BP	0.21	0/1291	0.51	0/1754
2	BR	0.20	0/1291	0.49	0/1754
2	BT	0.15	0/1291	0.43	0/1754
2	BV	0.16	0/1291	0.43	0/1754
2	CB	0.19	0/1291	0.47	0/1754
2	CD	0.20	0/1291	0.52	0/1754
2	CF	0.18	0/1291	0.51	0/1754
2	CH	0.21	0/1291	0.51	0/1754
2	CJ	0.20	0/1291	0.54	0/1754
2	CL	0.20	0/1291	0.48	0/1754
2	CN	0.19	0/1291	0.49	0/1754
2	CP	0.16	0/1291	0.47	0/1754
2	CR	0.19	0/1291	0.48	0/1754
2	CT	0.19	0/1291	0.49	0/1754
2	CV	0.18	0/1291	0.47	0/1754

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	DB	0.18	0/1291	0.49	0/1754
2	DD	0.22	0/1291	0.51	1/1754 (0.1%)
2	DF	0.33	1/1291 (0.1%)	0.61	1/1754 (0.1%)
2	DH	0.21	0/1291	0.46	0/1754
2	DJ	0.25	0/1291	0.48	1/1754 (0.1%)
2	DL	0.21	0/1291	0.51	0/1754
2	DN	0.21	0/1291	0.50	0/1754
2	DP	0.20	0/1291	0.48	0/1754
2	DR	0.20	0/1291	0.49	0/1754
2	DT	0.18	0/1291	0.45	0/1754
2	DV	0.20	0/1291	0.47	0/1754
All	All	0.18	1/129844 (0.0%)	0.45	3/176176 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	DF	22	VAL	CA-C	7.42	1.59	1.53

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	DD	131	GLN	CA-CB-CG	-7.02	100.07	114.10
2	DF	22	VAL	O-C-N	5.87	126.32	120.92
2	DJ	22	VAL	O-C-N	5.35	124.74	121.37

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	1629	0	1588	22	0
1	AC	1629	0	1588	29	1
1	AE	1629	0	1588	26	0
1	AG	1629	0	1588	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AI	1629	0	1588	24	0
1	AK	1629	0	1588	26	0
1	AM	1629	0	1588	21	0
1	AO	1629	0	1588	28	0
1	AQ	1629	0	1588	41	0
1	AS	1629	0	1588	24	0
1	AU	1629	0	1588	25	0
1	BA	1629	0	1588	28	0
1	BC	1629	0	1588	15	0
1	BE	1629	0	1588	23	0
1	BG	1629	0	1588	23	0
1	BI	1629	0	1588	23	0
1	BK	1629	0	1588	21	0
1	BM	1629	0	1588	27	1
1	BO	1629	0	1588	24	0
1	BQ	1629	0	1588	32	0
1	BS	1629	0	1588	33	0
1	BU	1629	0	1588	26	0
1	CA	1629	0	1588	25	0
1	CC	1629	0	1588	32	0
1	CE	1629	0	1588	20	0
1	CG	1629	0	1588	31	0
1	CI	1629	0	1588	13	0
1	CK	1629	0	1588	22	0
1	CM	1629	0	1588	25	0
1	CO	1629	0	1588	33	0
1	CQ	1629	0	1588	36	0
1	CS	1629	0	1588	26	0
1	CU	1629	0	1588	29	1
1	DA	1629	0	1588	20	1
1	DC	1629	0	1588	19	1
1	DE	1629	0	1588	31	0
1	DG	1629	0	1588	17	0
1	DI	1629	0	1588	41	0
1	DK	1629	0	1588	26	0
1	DM	1629	0	1588	25	0
1	DO	1629	0	1588	28	0
1	DQ	1629	0	1588	31	1
1	DS	1629	0	1588	25	0
1	DU	1629	0	1588	21	0
2	AB	1260	0	1265	27	0
2	AD	1260	0	1265	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	AF	1260	0	1265	30	0
2	AH	1260	0	1265	33	0
2	AJ	1260	0	1265	23	0
2	AL	1260	0	1265	32	0
2	AN	1260	0	1265	37	0
2	AP	1260	0	1265	33	0
2	AR	1260	0	1265	30	0
2	AT	1260	0	1265	25	0
2	AV	1260	0	1265	30	1
2	BB	1260	0	1265	28	1
2	BD	1260	0	1265	42	1
2	BF	1260	0	1265	23	0
2	BH	1260	0	1265	26	0
2	BJ	1260	0	1265	34	0
2	BL	1260	0	1265	30	0
2	BN	1260	0	1265	24	0
2	BP	1260	0	1265	27	0
2	BR	1260	0	1265	30	0
2	BT	1260	0	1265	26	0
2	BV	1260	0	1265	18	1
2	CB	1260	0	1265	33	0
2	CD	1260	0	1265	50	0
2	CF	1260	0	1265	22	0
2	CH	1260	0	1265	32	0
2	CJ	1260	0	1265	25	0
2	CL	1260	0	1265	29	1
2	CN	1260	0	1265	29	0
2	CP	1260	0	1265	31	0
2	CR	1260	0	1265	42	0
2	CT	1260	0	1265	28	0
2	CV	1260	0	1265	19	0
2	DB	1260	0	1265	21	0
2	DD	1260	0	1265	22	0
2	DF	1260	0	1265	53	0
2	DH	1260	0	1265	29	0
2	DJ	1260	0	1265	29	0
2	DL	1260	0	1265	39	0
2	DN	1260	0	1265	26	0
2	DP	1260	0	1265	23	0
2	DR	1260	0	1265	23	0
2	DT	1260	0	1265	34	1
2	DV	1260	0	1265	29	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	127116	0	125532	1956	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 1956 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)
2:AL:5:VAL:HG22	2:AN:131:GLN:HG2	1.03	1.03
2:AL:5:VAL:HG22	2:AN:131:GLN:CG	1.91	0.99
2:AL:5:VAL:CG2	2:AN:131:GLN:HG2	1.91	0.99
2:CJ:5:VAL:HG22	2:CL:131:GLN:HG2	1.45	0.97
2:DB:5:VAL:HG12	2:DB:11:PRO:HA	1.50	0.94

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:AC:124:CYS:O	2:AV:145:TYR:OH[2_545]	1.99	0.21
1:DA:124:CYS:O	2:DT:145:TYR:OH[2_646]	2.04	0.16
2:BD:142:ASN:OD1	1:DQ:76:ASN:ND2[1_554]	2.06	0.14
1:CU:74:GLU:O	2:DV:141:ARG:NH2[2_646]	2.09	0.11
1:BM:76:ASN:OD1	2:CL:50:HIS:NE2[1_554]	2.10	0.10

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AA	221/223 (99%)	215 (97%)	6 (3%)	0	100	100
1	AC	221/223 (99%)	216 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AE	221/223 (99%)	215 (97%)	6 (3%)	0	100	100
1	AG	221/223 (99%)	216 (98%)	5 (2%)	0	100	100
1	AI	221/223 (99%)	218 (99%)	3 (1%)	0	100	100
1	AK	221/223 (99%)	217 (98%)	4 (2%)	0	100	100
1	AM	221/223 (99%)	216 (98%)	5 (2%)	0	100	100
1	AO	221/223 (99%)	216 (98%)	5 (2%)	0	100	100
1	AQ	221/223 (99%)	215 (97%)	6 (3%)	0	100	100
1	AS	221/223 (99%)	215 (97%)	6 (3%)	0	100	100
1	AU	221/223 (99%)	216 (98%)	5 (2%)	0	100	100
1	BA	221/223 (99%)	214 (97%)	7 (3%)	0	100	100
1	BC	221/223 (99%)	216 (98%)	5 (2%)	0	100	100
1	BE	221/223 (99%)	216 (98%)	5 (2%)	0	100	100
1	BG	221/223 (99%)	216 (98%)	5 (2%)	0	100	100
1	BI	221/223 (99%)	217 (98%)	4 (2%)	0	100	100
1	BK	221/223 (99%)	217 (98%)	4 (2%)	0	100	100
1	BM	221/223 (99%)	215 (97%)	6 (3%)	0	100	100
1	BO	221/223 (99%)	217 (98%)	4 (2%)	0	100	100
1	BQ	221/223 (99%)	217 (98%)	4 (2%)	0	100	100
1	BS	221/223 (99%)	216 (98%)	5 (2%)	0	100	100
1	BU	221/223 (99%)	217 (98%)	4 (2%)	0	100	100
1	CA	221/223 (99%)	215 (97%)	6 (3%)	0	100	100
1	CC	221/223 (99%)	216 (98%)	5 (2%)	0	100	100
1	CE	221/223 (99%)	217 (98%)	4 (2%)	0	100	100
1	CG	221/223 (99%)	216 (98%)	5 (2%)	0	100	100
1	CI	221/223 (99%)	216 (98%)	5 (2%)	0	100	100
1	CK	221/223 (99%)	218 (99%)	3 (1%)	0	100	100
1	CM	221/223 (99%)	217 (98%)	4 (2%)	0	100	100
1	CO	221/223 (99%)	215 (97%)	5 (2%)	1 (0%)	24	60
1	CQ	221/223 (99%)	214 (97%)	7 (3%)	0	100	100
1	CS	221/223 (99%)	215 (97%)	6 (3%)	0	100	100
1	CU	221/223 (99%)	216 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	DA	221/223 (99%)	214 (97%)	7 (3%)	0	100	100
1	DC	221/223 (99%)	217 (98%)	4 (2%)	0	100	100
1	DE	221/223 (99%)	217 (98%)	4 (2%)	0	100	100
1	DG	221/223 (99%)	216 (98%)	5 (2%)	0	100	100
1	DI	221/223 (99%)	215 (97%)	6 (3%)	0	100	100
1	DK	221/223 (99%)	216 (98%)	5 (2%)	0	100	100
1	DM	221/223 (99%)	216 (98%)	5 (2%)	0	100	100
1	DO	221/223 (99%)	215 (97%)	6 (3%)	0	100	100
1	DQ	221/223 (99%)	214 (97%)	5 (2%)	2 (1%)	14	48
1	DS	221/223 (99%)	217 (98%)	4 (2%)	0	100	100
1	DU	221/223 (99%)	215 (97%)	6 (3%)	0	100	100
2	AB	161/163 (99%)	154 (96%)	7 (4%)	0	100	100
2	AD	161/163 (99%)	152 (94%)	9 (6%)	0	100	100
2	AF	161/163 (99%)	154 (96%)	7 (4%)	0	100	100
2	AH	161/163 (99%)	153 (95%)	8 (5%)	0	100	100
2	AJ	161/163 (99%)	152 (94%)	9 (6%)	0	100	100
2	AL	161/163 (99%)	153 (95%)	8 (5%)	0	100	100
2	AN	161/163 (99%)	153 (95%)	8 (5%)	0	100	100
2	AP	161/163 (99%)	154 (96%)	7 (4%)	0	100	100
2	AR	161/163 (99%)	153 (95%)	8 (5%)	0	100	100
2	AT	161/163 (99%)	153 (95%)	8 (5%)	0	100	100
2	AV	161/163 (99%)	153 (95%)	8 (5%)	0	100	100
2	BB	161/163 (99%)	154 (96%)	7 (4%)	0	100	100
2	BD	161/163 (99%)	154 (96%)	7 (4%)	0	100	100
2	BF	161/163 (99%)	150 (93%)	10 (6%)	1 (1%)	21	56
2	BH	161/163 (99%)	154 (96%)	7 (4%)	0	100	100
2	BJ	161/163 (99%)	153 (95%)	8 (5%)	0	100	100
2	BL	161/163 (99%)	153 (95%)	8 (5%)	0	100	100
2	BN	161/163 (99%)	154 (96%)	7 (4%)	0	100	100
2	BP	161/163 (99%)	154 (96%)	7 (4%)	0	100	100
2	BR	161/163 (99%)	153 (95%)	8 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	BT	161/163 (99%)	154 (96%)	7 (4%)	0	100	100
2	BV	161/163 (99%)	154 (96%)	7 (4%)	0	100	100
2	CB	161/163 (99%)	154 (96%)	7 (4%)	0	100	100
2	CD	161/163 (99%)	154 (96%)	7 (4%)	0	100	100
2	CF	161/163 (99%)	150 (93%)	10 (6%)	1 (1%)	21	56
2	CH	161/163 (99%)	153 (95%)	8 (5%)	0	100	100
2	CJ	161/163 (99%)	153 (95%)	8 (5%)	0	100	100
2	CL	161/163 (99%)	152 (94%)	9 (6%)	0	100	100
2	CN	161/163 (99%)	153 (95%)	8 (5%)	0	100	100
2	CP	161/163 (99%)	154 (96%)	7 (4%)	0	100	100
2	CR	161/163 (99%)	153 (95%)	8 (5%)	0	100	100
2	CT	161/163 (99%)	152 (94%)	9 (6%)	0	100	100
2	CV	161/163 (99%)	152 (94%)	9 (6%)	0	100	100
2	DB	161/163 (99%)	154 (96%)	7 (4%)	0	100	100
2	DD	161/163 (99%)	152 (94%)	9 (6%)	0	100	100
2	DF	161/163 (99%)	152 (94%)	9 (6%)	0	100	100
2	DH	161/163 (99%)	154 (96%)	7 (4%)	0	100	100
2	DJ	161/163 (99%)	152 (94%)	9 (6%)	0	100	100
2	DL	161/163 (99%)	153 (95%)	8 (5%)	0	100	100
2	DN	161/163 (99%)	154 (96%)	7 (4%)	0	100	100
2	DP	161/163 (99%)	153 (95%)	8 (5%)	0	100	100
2	DR	161/163 (99%)	153 (95%)	8 (5%)	0	100	100
2	DT	161/163 (99%)	153 (95%)	8 (5%)	0	100	100
2	DV	161/163 (99%)	154 (96%)	7 (4%)	0	100	100
All	All	16808/16984 (99%)	16235 (97%)	568 (3%)	5 (0%)	100	100

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	BF	107	SER
2	CF	107	SER
1	CO	22	CYS
1	DQ	113	SER
1	DQ	112	ASN

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AA	184/184 (100%)	184 (100%)	0	100	100
1	AC	184/184 (100%)	184 (100%)	0	100	100
1	AE	184/184 (100%)	184 (100%)	0	100	100
1	AG	184/184 (100%)	184 (100%)	0	100	100
1	AI	184/184 (100%)	184 (100%)	0	100	100
1	AK	184/184 (100%)	184 (100%)	0	100	100
1	AM	184/184 (100%)	184 (100%)	0	100	100
1	AO	184/184 (100%)	184 (100%)	0	100	100
1	AQ	184/184 (100%)	184 (100%)	0	100	100
1	AS	184/184 (100%)	184 (100%)	0	100	100
1	AU	184/184 (100%)	184 (100%)	0	100	100
1	BA	184/184 (100%)	184 (100%)	0	100	100
1	BC	184/184 (100%)	184 (100%)	0	100	100
1	BE	184/184 (100%)	184 (100%)	0	100	100
1	BG	184/184 (100%)	184 (100%)	0	100	100
1	BI	184/184 (100%)	184 (100%)	0	100	100
1	BK	184/184 (100%)	184 (100%)	0	100	100
1	BM	184/184 (100%)	184 (100%)	0	100	100
1	BO	184/184 (100%)	184 (100%)	0	100	100
1	BQ	184/184 (100%)	184 (100%)	0	100	100
1	BS	184/184 (100%)	184 (100%)	0	100	100
1	BU	184/184 (100%)	184 (100%)	0	100	100
1	CA	184/184 (100%)	184 (100%)	0	100	100
1	CC	184/184 (100%)	184 (100%)	0	100	100
1	CE	184/184 (100%)	184 (100%)	0	100	100
1	CG	184/184 (100%)	184 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	CI	184/184 (100%)	184 (100%)	0	100	100
1	CK	184/184 (100%)	184 (100%)	0	100	100
1	CM	184/184 (100%)	184 (100%)	0	100	100
1	CO	184/184 (100%)	184 (100%)	0	100	100
1	CQ	184/184 (100%)	184 (100%)	0	100	100
1	CS	184/184 (100%)	184 (100%)	0	100	100
1	CU	184/184 (100%)	184 (100%)	0	100	100
1	DA	184/184 (100%)	184 (100%)	0	100	100
1	DC	184/184 (100%)	184 (100%)	0	100	100
1	DE	184/184 (100%)	184 (100%)	0	100	100
1	DG	184/184 (100%)	184 (100%)	0	100	100
1	DI	184/184 (100%)	184 (100%)	0	100	100
1	DK	184/184 (100%)	184 (100%)	0	100	100
1	DM	184/184 (100%)	184 (100%)	0	100	100
1	DO	184/184 (100%)	184 (100%)	0	100	100
1	DQ	184/184 (100%)	184 (100%)	0	100	100
1	DS	184/184 (100%)	184 (100%)	0	100	100
1	DU	184/184 (100%)	184 (100%)	0	100	100
2	AB	137/137 (100%)	137 (100%)	0	100	100
2	AD	137/137 (100%)	137 (100%)	0	100	100
2	AF	137/137 (100%)	137 (100%)	0	100	100
2	AH	137/137 (100%)	137 (100%)	0	100	100
2	AJ	137/137 (100%)	137 (100%)	0	100	100
2	AL	137/137 (100%)	137 (100%)	0	100	100
2	AN	137/137 (100%)	137 (100%)	0	100	100
2	AP	137/137 (100%)	137 (100%)	0	100	100
2	AR	137/137 (100%)	137 (100%)	0	100	100
2	AT	137/137 (100%)	137 (100%)	0	100	100
2	AV	137/137 (100%)	137 (100%)	0	100	100
2	BB	137/137 (100%)	137 (100%)	0	100	100
2	BD	137/137 (100%)	137 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	BF	137/137 (100%)	137 (100%)	0	100	100
2	BH	137/137 (100%)	137 (100%)	0	100	100
2	BJ	137/137 (100%)	137 (100%)	0	100	100
2	BL	137/137 (100%)	137 (100%)	0	100	100
2	BN	137/137 (100%)	137 (100%)	0	100	100
2	BP	137/137 (100%)	137 (100%)	0	100	100
2	BR	137/137 (100%)	137 (100%)	0	100	100
2	BT	137/137 (100%)	137 (100%)	0	100	100
2	BV	137/137 (100%)	137 (100%)	0	100	100
2	CB	137/137 (100%)	137 (100%)	0	100	100
2	CD	137/137 (100%)	137 (100%)	0	100	100
2	CF	137/137 (100%)	137 (100%)	0	100	100
2	CH	137/137 (100%)	137 (100%)	0	100	100
2	CJ	137/137 (100%)	137 (100%)	0	100	100
2	CL	137/137 (100%)	137 (100%)	0	100	100
2	CN	137/137 (100%)	137 (100%)	0	100	100
2	CP	137/137 (100%)	137 (100%)	0	100	100
2	CR	137/137 (100%)	137 (100%)	0	100	100
2	CT	137/137 (100%)	137 (100%)	0	100	100
2	CV	137/137 (100%)	137 (100%)	0	100	100
2	DB	137/137 (100%)	137 (100%)	0	100	100
2	DD	137/137 (100%)	137 (100%)	0	100	100
2	DF	137/137 (100%)	137 (100%)	0	100	100
2	DH	137/137 (100%)	137 (100%)	0	100	100
2	DJ	137/137 (100%)	137 (100%)	0	100	100
2	DL	137/137 (100%)	137 (100%)	0	100	100
2	DN	137/137 (100%)	137 (100%)	0	100	100
2	DP	137/137 (100%)	137 (100%)	0	100	100
2	DR	137/137 (100%)	137 (100%)	0	100	100
2	DT	137/137 (100%)	137 (100%)	0	100	100
2	DV	137/137 (100%)	137 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	14124/14124 (100%)	14124 (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 145 such sidechains are listed below:

Mol	Chain	Res	Type
1	DE	130	GLN
2	DT	131	GLN
2	DF	92	GLN
1	DM	189	GLN
1	BI	62	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 oligosaccharides 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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	223/223 (100%)	0.48	7 (3%)	51	36	49, 69, 94, 105	0
1	AC	223/223 (100%)	0.79	8 (3%)	46	33	63, 107, 139, 151	0
1	AE	223/223 (100%)	0.44	3 (1%)	75	55	39, 63, 90, 105	0
1	AG	223/223 (100%)	0.38	0	100	100	31, 59, 92, 116	0
1	AI	223/223 (100%)	0.82	17 (7%)	20	19	53, 92, 130, 145	0
1	AK	223/223 (100%)	0.32	2 (0%)	81	62	21, 34, 52, 67	0
1	AM	223/223 (100%)	0.44	7 (3%)	51	36	40, 58, 77, 89	0
1	AO	223/223 (100%)	0.51	5 (2%)	62	44	61, 78, 98, 111	0
1	AQ	223/223 (100%)	0.60	5 (2%)	62	44	43, 72, 94, 105	0
1	AS	223/223 (100%)	0.41	3 (1%)	75	55	51, 67, 87, 98	0
1	AU	223/223 (100%)	0.74	13 (5%)	29	24	82, 115, 141, 149	0
1	BA	223/223 (100%)	0.59	5 (2%)	62	44	68, 85, 101, 114	0
1	BC	223/223 (100%)	0.76	12 (5%)	31	26	87, 114, 141, 160	0
1	BE	223/223 (100%)	0.61	5 (2%)	62	44	55, 82, 109, 121	0
1	BG	223/223 (100%)	0.32	3 (1%)	75	55	26, 39, 57, 67	0
1	BI	223/223 (100%)	0.63	10 (4%)	38	29	47, 73, 100, 112	0
1	BK	223/223 (100%)	0.64	10 (4%)	38	29	46, 83, 119, 141	0
1	BM	223/223 (100%)	0.48	8 (3%)	46	33	44, 60, 74, 81	0
1	BO	223/223 (100%)	0.31	4 (1%)	67	48	33, 47, 60, 67	0
1	BQ	223/223 (100%)	0.50	8 (3%)	46	33	49, 68, 90, 101	0
1	BS	223/223 (100%)	0.73	12 (5%)	31	26	70, 112, 151, 166	0
1	BU	223/223 (100%)	0.58	8 (3%)	46	33	68, 91, 121, 125	0
1	CA	223/223 (100%)	0.67	4 (1%)	67	48	47, 104, 149, 165	0
1	CC	223/223 (100%)	0.67	8 (3%)	46	33	55, 89, 113, 129	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	CE	223/223 (100%)	0.48	9 (4%)	42	31	21, 61, 87, 92	0
1	CG	223/223 (100%)	0.51	4 (1%)	67	48	29, 61, 97, 110	0
1	CI	223/223 (100%)	0.41	2 (0%)	81	62	23, 39, 61, 75	0
1	CK	223/223 (100%)	0.44	7 (3%)	51	36	20, 50, 85, 108	0
1	CM	223/223 (100%)	0.44	2 (0%)	81	62	57, 75, 101, 117	0
1	CO	223/223 (100%)	0.71	12 (5%)	31	26	60, 96, 135, 155	0
1	CQ	223/223 (100%)	0.48	3 (1%)	75	55	42, 65, 88, 94	0
1	CS	223/223 (100%)	0.62	8 (3%)	46	33	63, 94, 126, 137	0
1	CU	223/223 (100%)	0.95	15 (6%)	24	21	80, 119, 151, 166	0
1	DA	223/223 (100%)	0.59	8 (3%)	46	33	49, 81, 120, 136	0
1	DC	223/223 (100%)	0.49	0	100	100	44, 66, 96, 111	0
1	DE	223/223 (100%)	0.65	8 (3%)	46	33	77, 99, 119, 130	0
1	DG	223/223 (100%)	0.48	5 (2%)	62	44	39, 56, 78, 92	0
1	DI	223/223 (100%)	0.67	9 (4%)	42	31	42, 82, 109, 122	0
1	DK	223/223 (100%)	0.33	5 (2%)	62	44	28, 41, 55, 66	0
1	DM	223/223 (100%)	0.49	6 (2%)	56	39	29, 61, 83, 92	0
1	DO	223/223 (100%)	0.40	0	100	100	25, 46, 66, 82	0
1	DQ	223/223 (100%)	0.55	13 (5%)	29	24	43, 73, 101, 118	0
1	DS	223/223 (100%)	0.41	4 (1%)	67	48	25, 51, 81, 96	0
1	DU	223/223 (100%)	0.60	5 (2%)	62	44	66, 95, 125, 141	0
2	AB	163/163 (100%)	0.61	4 (2%)	58	41	42, 72, 110, 134	0
2	AD	163/163 (100%)	0.49	6 (3%)	45	33	39, 64, 87, 114	0
2	AF	163/163 (100%)	0.46	4 (2%)	58	41	22, 42, 67, 91	0
2	AH	163/163 (100%)	0.58	7 (4%)	40	30	24, 39, 66, 82	0
2	AJ	163/163 (100%)	0.45	7 (4%)	40	30	31, 46, 81, 111	0
2	AL	163/163 (100%)	0.51	7 (4%)	40	30	20, 45, 94, 112	0
2	AN	163/163 (100%)	0.44	5 (3%)	51	36	32, 44, 70, 95	0
2	AP	163/163 (100%)	0.59	7 (4%)	40	30	52, 65, 98, 122	0
2	AR	163/163 (100%)	0.53	3 (1%)	67	48	47, 75, 118, 142	0
2	AT	163/163 (100%)	0.44	5 (3%)	51	36	39, 56, 80, 99	0
2	AV	163/163 (100%)	0.60	5 (3%)	51	36	64, 87, 128, 146	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
2	BB	163/163 (100%)	0.58	8 (4%) 35 28	45, 67, 90, 116	0
2	BD	163/163 (100%)	0.63	5 (3%) 51 36	56, 80, 110, 136	0
2	BF	163/163 (100%)	0.78	8 (4%) 35 28	56, 93, 145, 157	0
2	BH	163/163 (100%)	0.54	3 (1%) 67 48	28, 55, 94, 135	0
2	BJ	163/163 (100%)	0.44	5 (3%) 51 36	28, 40, 63, 87	0
2	BL	163/163 (100%)	0.60	6 (3%) 45 33	42, 59, 89, 110	0
2	BN	163/163 (100%)	0.43	1 (0%) 85 70	37, 53, 81, 104	0
2	BP	163/163 (100%)	0.46	5 (3%) 51 36	34, 51, 82, 90	0
2	BR	163/163 (100%)	0.45	4 (2%) 58 41	37, 52, 86, 101	0
2	BT	163/163 (100%)	0.59	7 (4%) 40 30	57, 85, 115, 129	0
2	BV	163/163 (100%)	0.70	11 (6%) 24 21	58, 97, 145, 164	0
2	CB	163/163 (100%)	0.92	17 (10%) 11 13	62, 97, 142, 165	0
2	CD	163/163 (100%)	0.96	18 (11%) 10 13	43, 91, 161, 187	0
2	CF	163/163 (100%)	0.68	10 (6%) 27 23	31, 59, 105, 118	0
2	CH	163/163 (100%)	0.44	3 (1%) 67 48	17, 32, 66, 94	0
2	CJ	163/163 (100%)	0.43	7 (4%) 40 30	16, 36, 80, 107	0
2	CL	163/163 (100%)	0.41	3 (1%) 67 48	16, 33, 66, 81	0
2	CN	163/163 (100%)	0.47	3 (1%) 67 48	46, 60, 77, 93	0
2	CP	163/163 (100%)	0.76	13 (7%) 18 18	71, 109, 152, 162	0
2	CR	163/163 (100%)	0.67	4 (2%) 58 41	39, 78, 120, 138	0
2	CT	163/163 (100%)	0.49	4 (2%) 58 41	32, 57, 94, 121	0
2	CV	163/163 (100%)	0.69	9 (5%) 30 25	51, 87, 130, 144	0
2	DB	163/163 (100%)	0.70	9 (5%) 30 25	53, 87, 138, 157	0
2	DD	163/163 (100%)	0.64	12 (7%) 20 19	40, 62, 99, 118	0
2	DF	163/163 (100%)	0.68	9 (5%) 30 25	66, 88, 130, 147	0
2	DH	163/163 (100%)	0.54	4 (2%) 58 41	37, 52, 85, 112	0
2	DJ	163/163 (100%)	0.48	7 (4%) 40 30	33, 52, 92, 109	0
2	DL	163/163 (100%)	0.44	6 (3%) 45 33	17, 37, 72, 93	0
2	DN	163/163 (100%)	0.45	3 (1%) 67 48	20, 41, 83, 107	0
2	DP	163/163 (100%)	0.45	1 (0%) 85 70	25, 39, 65, 88	0
2	DR	163/163 (100%)	0.55	7 (4%) 40 30	27, 55, 94, 109	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
2	DT	163/163 (100%)	0.57	9 (5%)	30	25	33, 53, 88, 107	0
2	DV	163/163 (100%)	0.48	1 (0%)	85	70	41, 64, 106, 131	0
All	All	16984/16984 (100%)	0.56	574 (3%)	48	34	16, 68, 123, 187	0

The worst 5 of 574 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BI	202	LEU	6.3
1	DE	42	GLY	6.3
2	BF	130	GLY	5.2
1	DI	178	ALA	5.2
2	CL	131	GLN	5.1

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 oligosaccharides 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.