Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 02:49 am BST

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ①) were used in the production of this report:

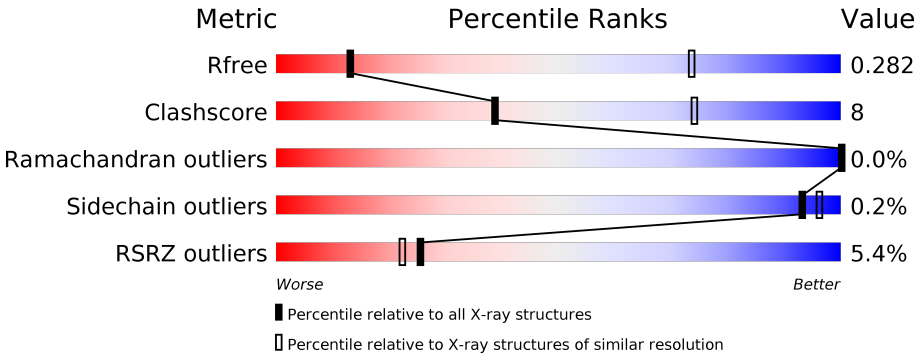
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 3.96 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}	130704	1025 (4.22-3.70)
Clashscore	141614	1085 (4.22-3.70)
Ramachandran outliers	138981	1047 (4.22-3.70)
Sidechain outliers	138945	1039 (4.22-3.70)
RSRZ outliers	127900	1013 (4.28-3.64)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=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	223	3% 83% 17%
1	AC	223	12% 80% 20%
1	AE	223	6% 83% 17%
1	AG	223	4% 87% 13%
1	AI	223	8% 85% 15%
1	AK	223	85% 15%

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Mol	Chain	Length	Quality of chain
1	AM	223	3% 86% 14%
1	AO	223	7% 83% 17%
1	AQ	223	3% 81% 19%
1	AS	223	4% 84% 16%
1	AU	223	20% 85% 15%
1	BA	223	4% 84% 16%
1	BC	223	21% 92% 8%
1	BE	223	9% 87% 13%
1	BG	223	2% 85% 15%
1	BI	223	6% 86% 14%
1	BK	223	6% 87% 13%
1	BM	223	4% 83% 17%
1	BO	223	86% 14%
1	BQ	223	5% 79% 21%
1	BS	223	18% 80% 20%
1	BU	223	7% 84% 16%
1	CA	223	13% 84% 16%
1	CC	223	15% 82% 18%
1	CE	223	4% 87% 13%
1	CG	223	2% 82% 18%
1	CI	223	2% 92% 8%
1	CK	223	2% 84% 16%
1	CM	223	6% 87% 13%
1	CO	223	13% 83% 17%
1	CQ	223	4% 79% 21%

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Mol	Chain	Length	Quality of chain
1	CS	223	17% 83% 17%
1	CU	223	10% 82% 18%
1	DA	223	13% 85% 15%
1	DC	223	% 88% 12%
1	DE	223	20% 84% 16%
1	DG	223	3% 89% 11%
1	DI	223	2% 81% 19%
1	DK	223	2% 86% 14%
1	DM	223	% 86% 14%
1	DO	223	% 85% 15%
1	DQ	223	7% 82% 17%
1	DS	223	2% 84% 16%
1	DU	223	11% 86% 14%
2	AB	163	4% 81% 19%
2	AD	163	4% 82% 18%
2	AF	163	% 83% 17%
2	AH	163	% 79% 21%
2	AJ	163	86% 14%
2	AL	163	% 79% 21%
2	AN	163	% 80% 20%
2	AP	163	3% 80% 20%
2	AR	163	7% 80% 19%
2	AT	163	% 82% 18%
2	AV	163	6% 80% 20%
2	BB	163	% 83% 17%

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Mol	Chain	Length	Quality of chain
2	BD	163	4% 72% 28%
2	BF	163	12% 83% 17%
2	BH	163	3% 82% 18%
2	BJ	163	% 82% 18%
2	BL	163	% 77% 22%
2	BN	163	% 85% 14%
2	BP	163	4% 83% 16%
2	BR	163	% 85% 15%
2	BT	163	2% 83% 17%
2	BV	163	10% 83% 17%
2	CB	163	6% 76% 24%
2	CD	163	9% 68% 32%
2	CF	163	4% 85% 15%
2	CH	163	82% 18%
2	CJ	163	2% 83% 17%
2	CL	163	2% 83% 17%
2	CN	163	85% 15%
2	CP	163	10% 77% 23%
2	CR	163	% 71% 28%
2	CT	163	2% 80% 20%
2	CV	163	7% 84% 16%
2	DB	163	7% 86% 13%
2	DD	163	% 86% 13%
2	DF	163	4% 74% 26%
2	DH	163	% 81% 19%

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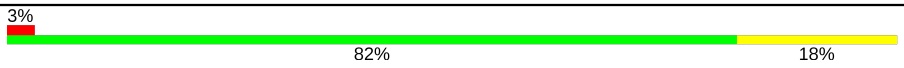
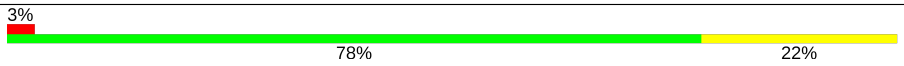
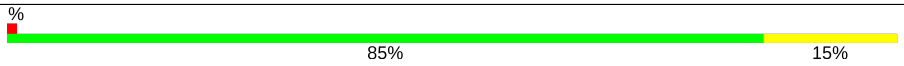
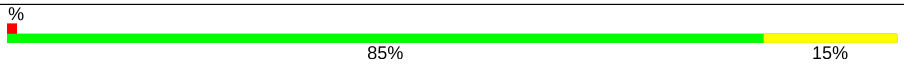
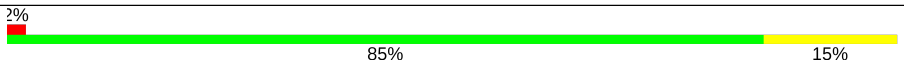
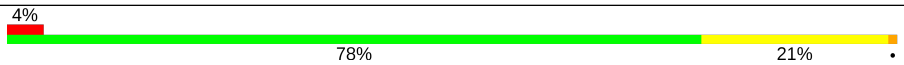
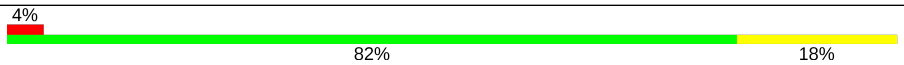
Mol	Chain	Length	Quality of chain
2	DJ	163	
2	DL	163	
2	DN	163	
2	DP	163	
2	DR	163	
2	DT	163	
2	DV	163	

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 inihibitor.

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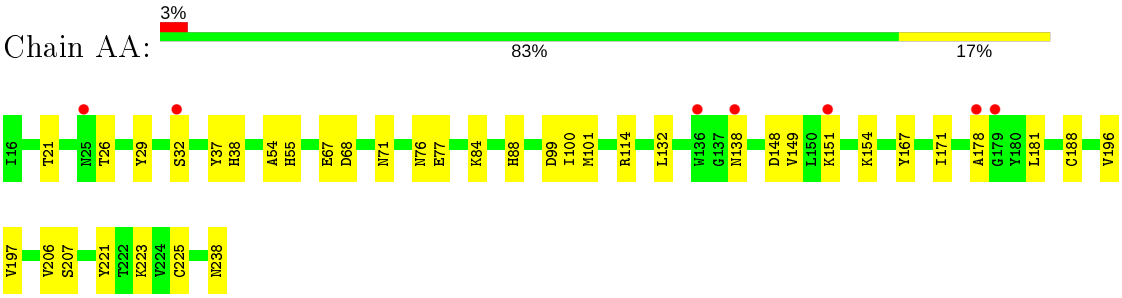
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	DB	163	Total	C	N	O	S	0	0	0
			1260	807	217	235	1			
2	DD	163	Total	C	N	O	S	0	0	0
			1260	807	217	235	1			
2	DF	163	Total	C	N	O	S	0	0	0
			1260	807	217	235	1			
2	DH	163	Total	C	N	O	S	0	0	0
			1260	807	217	235	1			
2	DJ	163	Total	C	N	O	S	0	0	0
			1260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

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

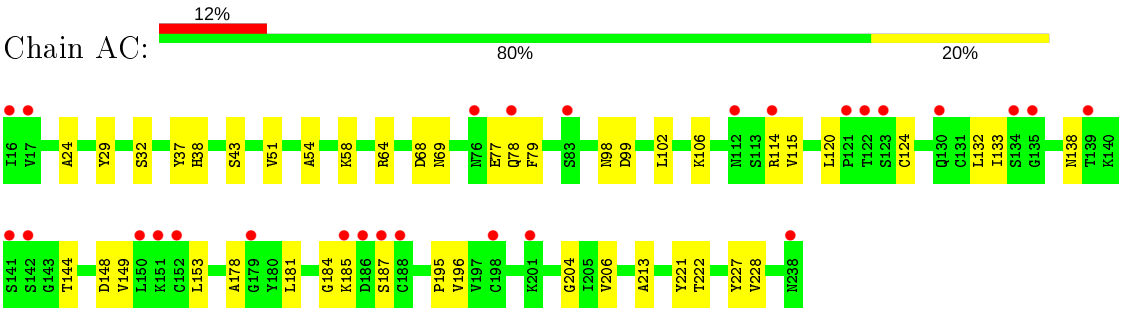
- Molecule 1: Cationic trypsin

Chain AA:



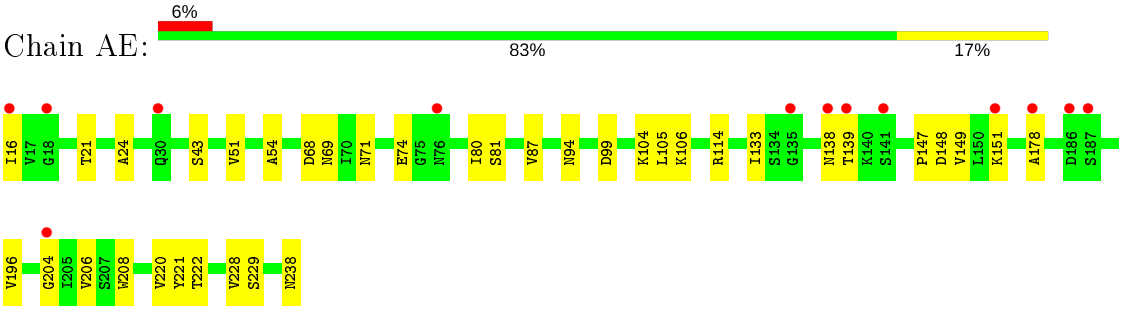
- Molecule 1: Cationic trypsin

Chain AC:



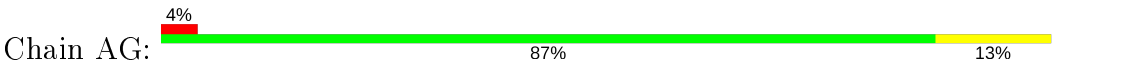
- Molecule 1: Cationic trypsin

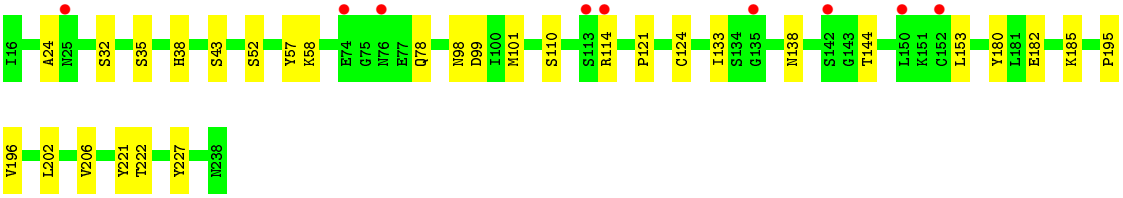
Chain AE:



- Molecule 1: Cationic trypsin

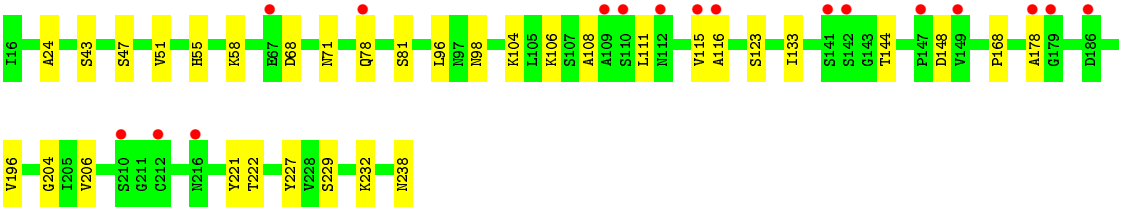
Chain AG:





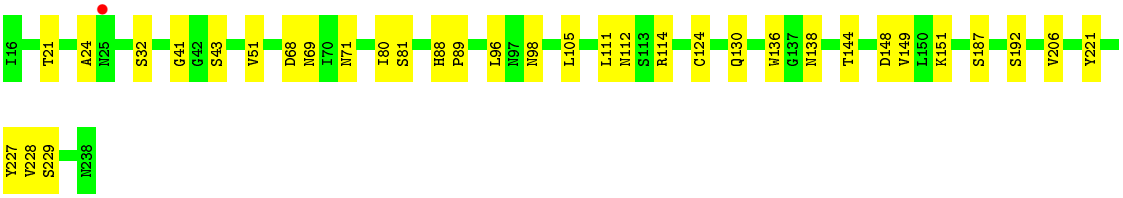
- Molecule 1: Cationic trypsin

Chain AI:



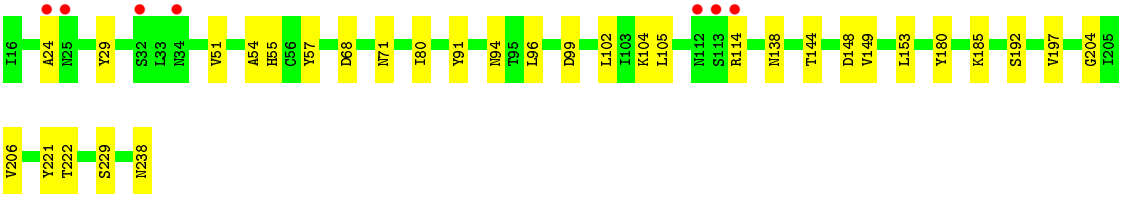
- Molecule 1: Cationic trypsin

Chain AK:



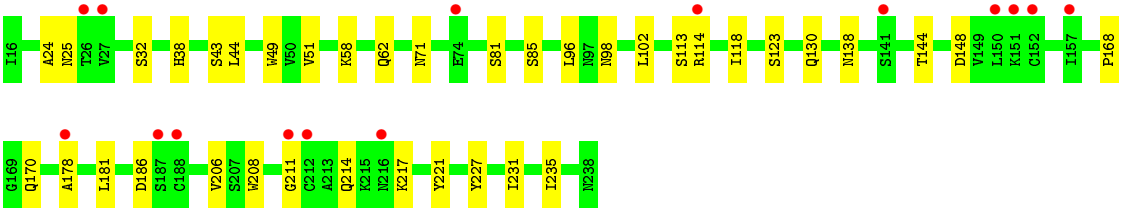
- Molecule 1: Cationic trypsin

Chain AM:



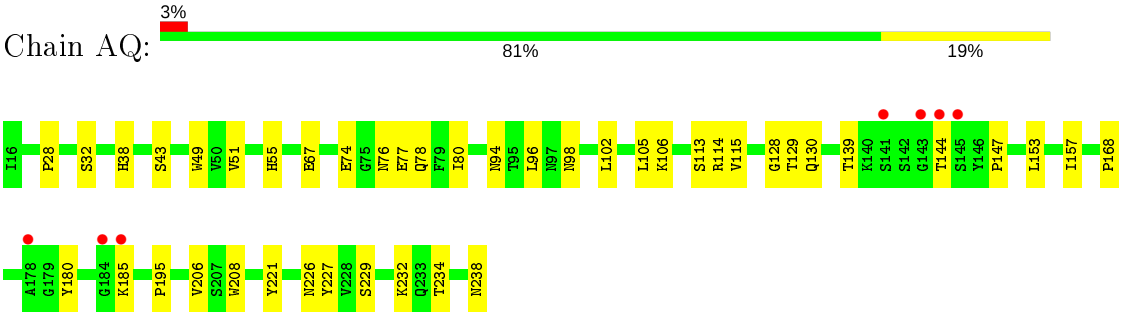
- Molecule 1: Cationic trypsin

Chain AO:



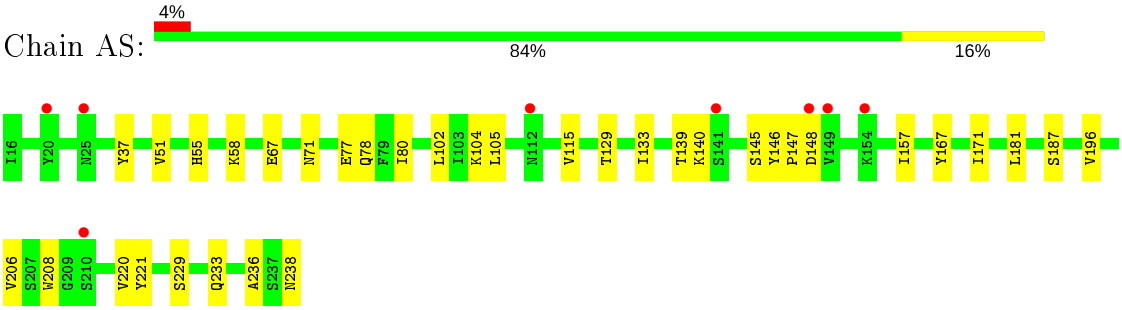
• Molecule 1: Cationic trypsin

Chain AQ:



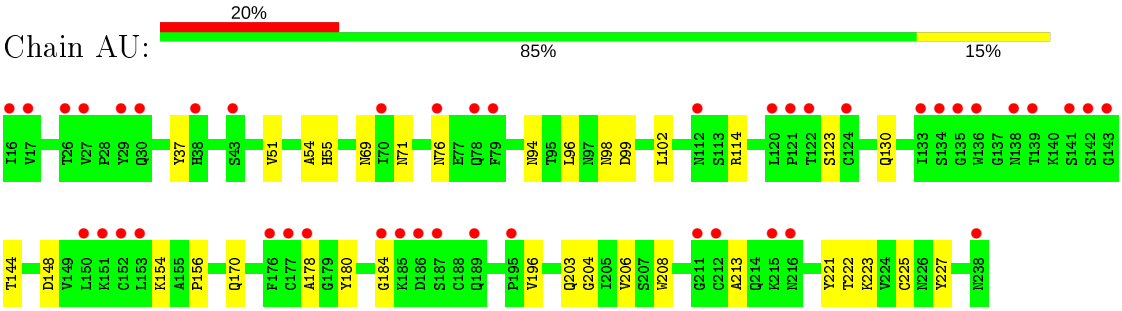
• Molecule 1: Cationic trypsin

Chain AS:



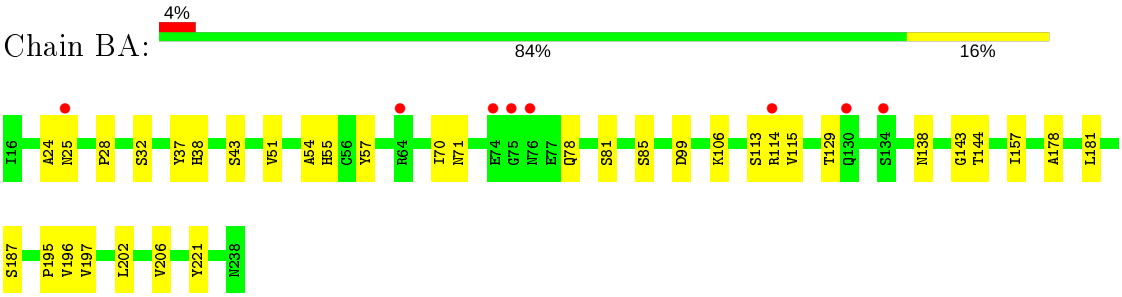
• Molecule 1: Cationic trypsin

Chain AU:



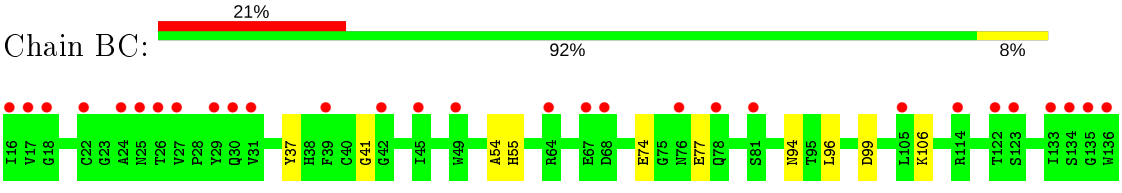
• Molecule 1: Cationic trypsin

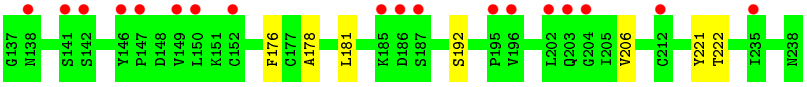
Chain BA:



• Molecule 1: Cationic trypsin

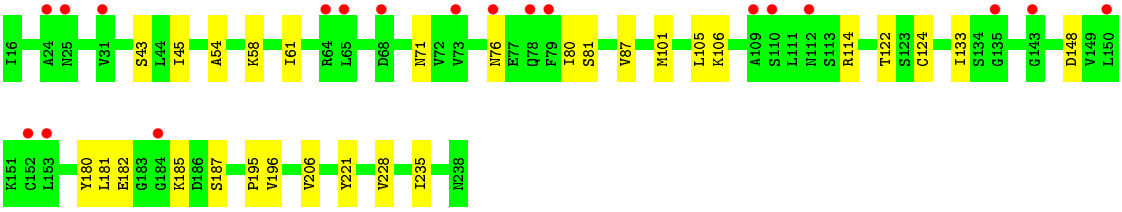
Chain BC:





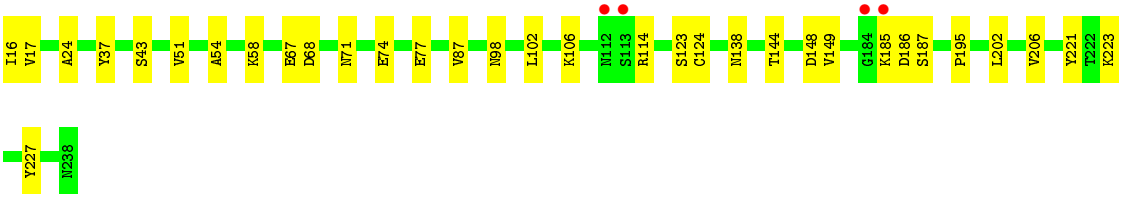
• Molecule 1: Cationic trypsin

Chain BE:



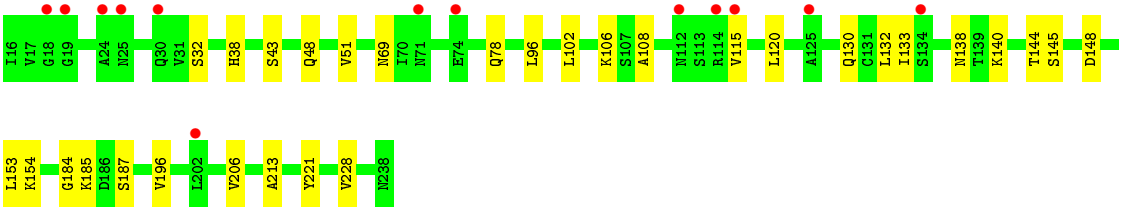
• Molecule 1: Cationic trypsin

Chain BG:



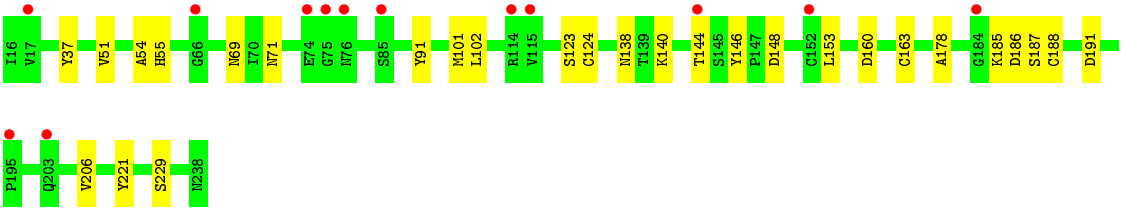
• Molecule 1: Cationic trypsin

Chain BI:



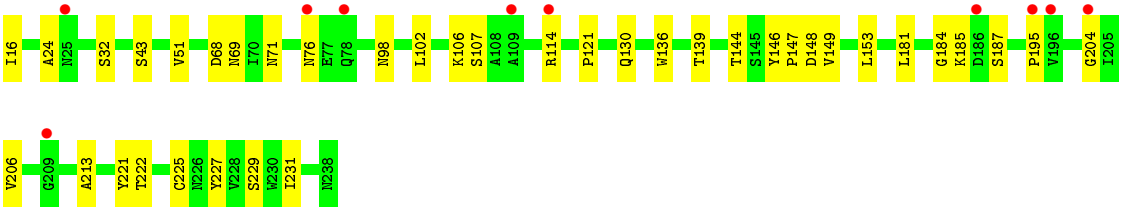
• Molecule 1: Cationic trypsin

Chain BK:



• Molecule 1: Cationic trypsin

Chain BM:

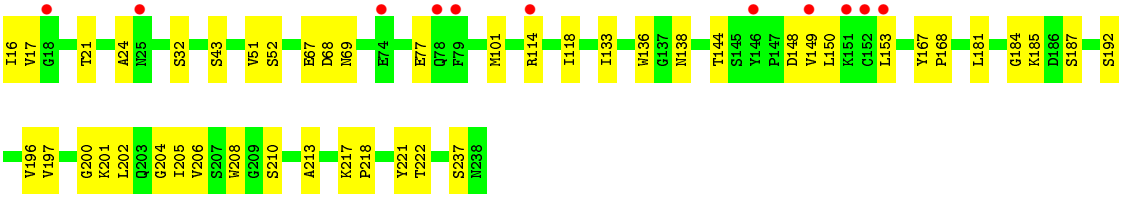


• Molecule 1: Cationic trypsin

Chain BO:

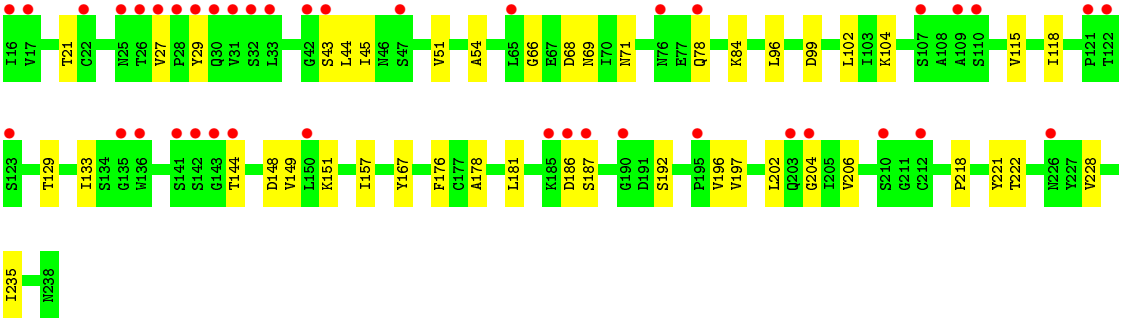
• Molecule 1: Cationic trypsin

Chain BQ:



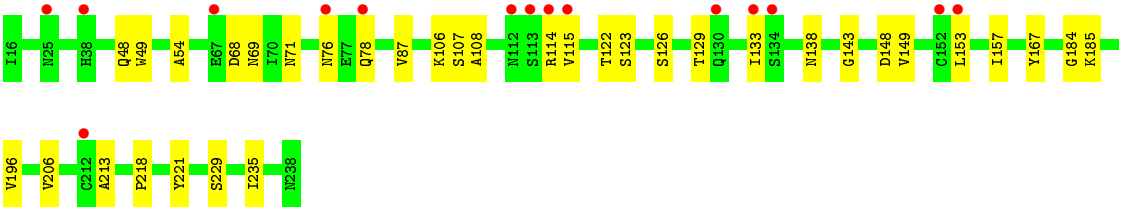
• Molecule 1: Cationic trypsin

Chain BS:



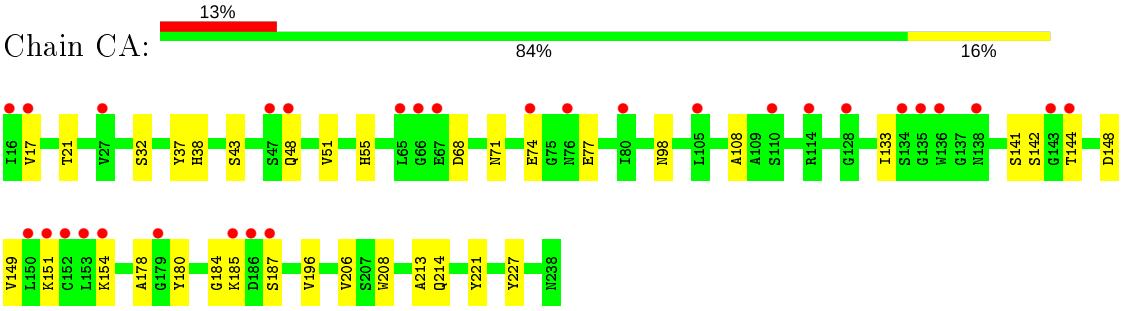
• Molecule 1: Cationic trypsin

Chain BU:



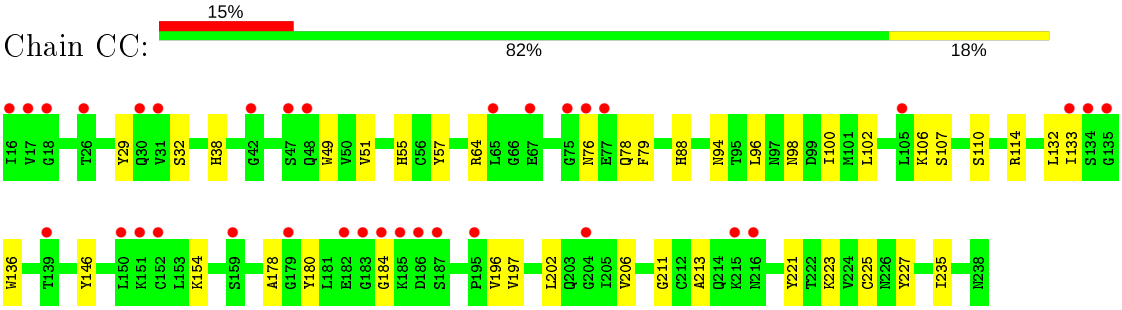
• Molecule 1: Cationic trypsin

Chain CA:



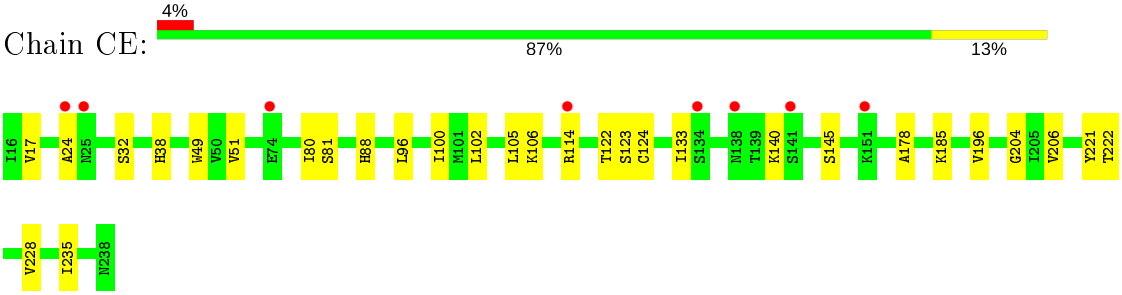
• Molecule 1: Cationic trypsin

Chain CC:



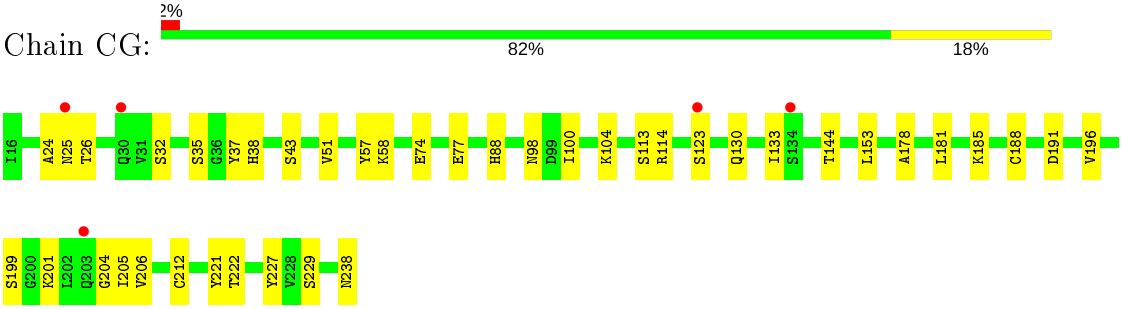
• Molecule 1: Cationic trypsin

Chain CE:



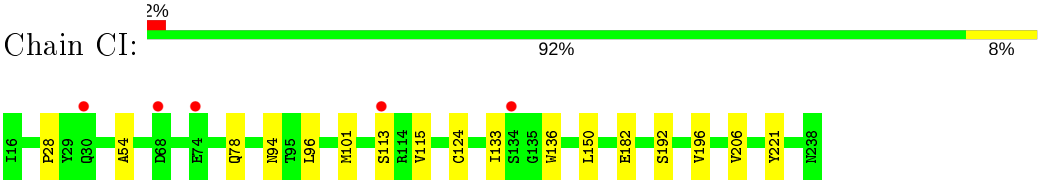
• Molecule 1: Cationic trypsin

Chain CG:



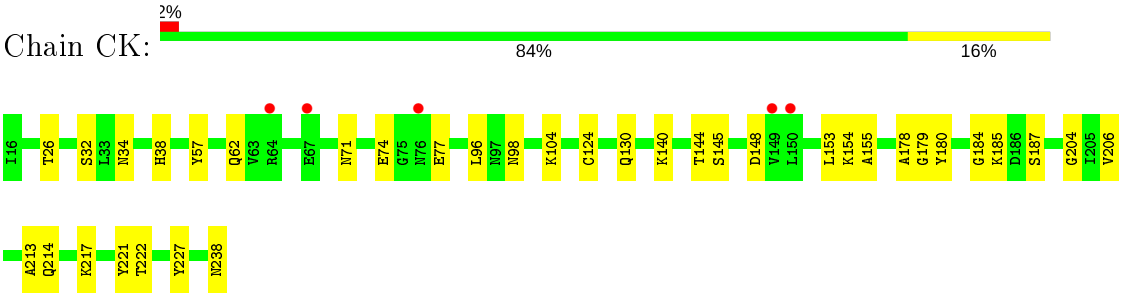
• Molecule 1: Cationic trypsin

Chain CI:



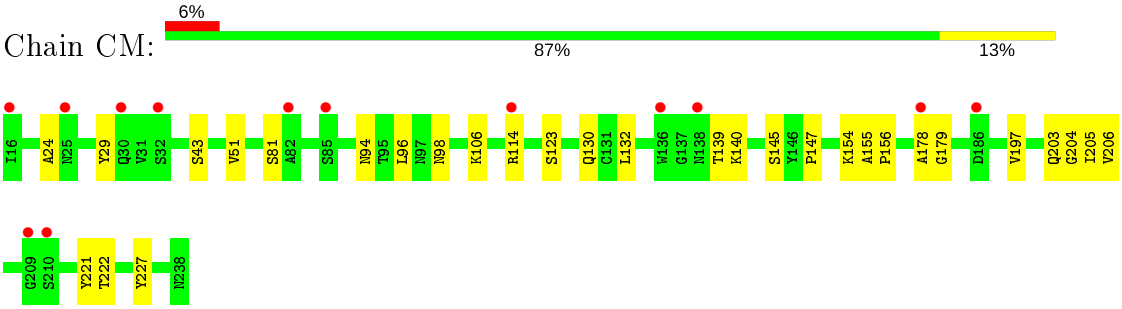
• Molecule 1: Cationic trypsin

Chain CK:



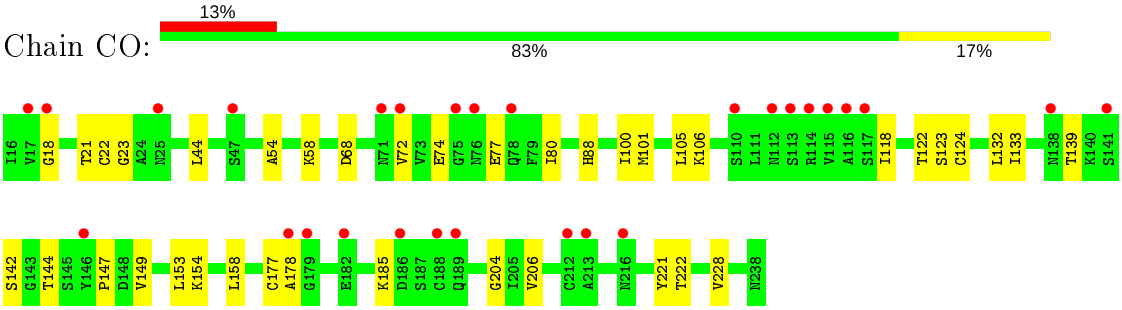
• Molecule 1: Cationic trypsin

Chain CM:



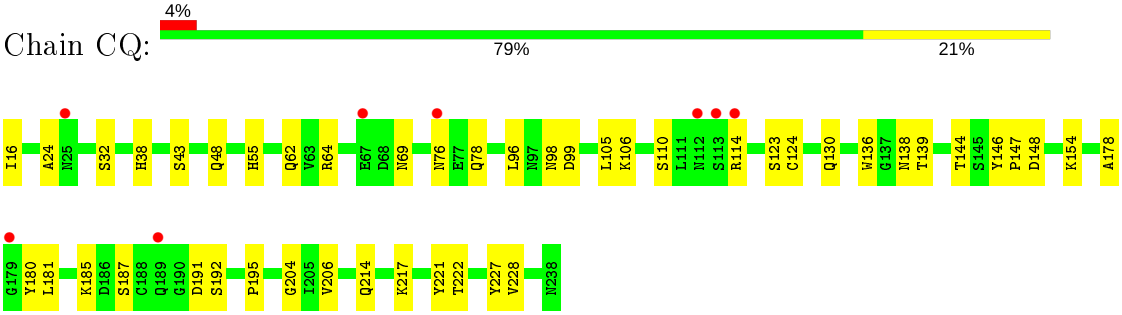
• Molecule 1: Cationic trypsin

Chain CO:



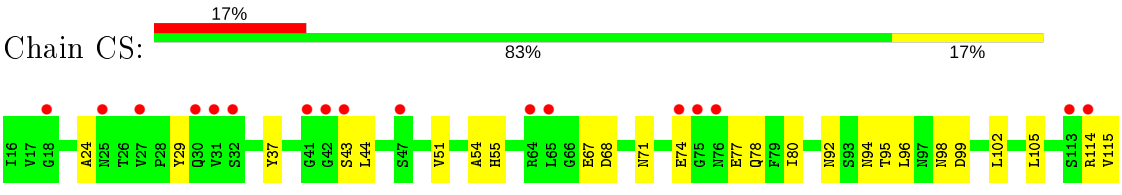
• Molecule 1: Cationic trypsin

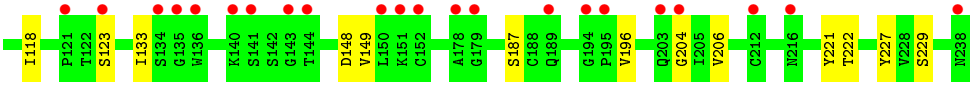
Chain CQ:



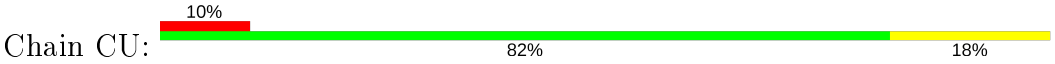
• Molecule 1: Cationic trypsin

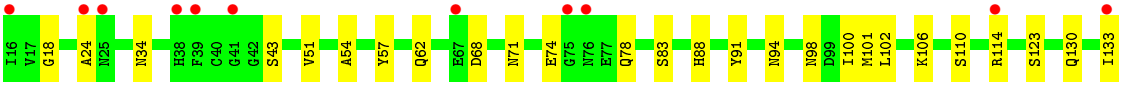
Chain CS:

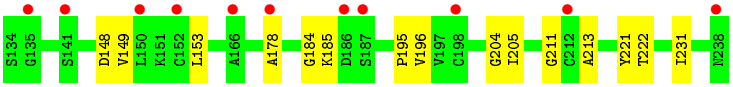




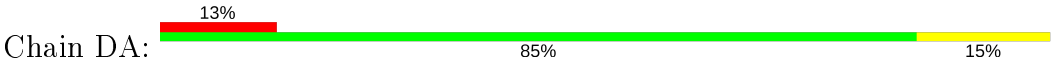
• Molecule 1: Cationic trypsin

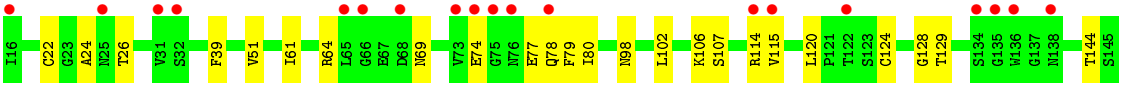


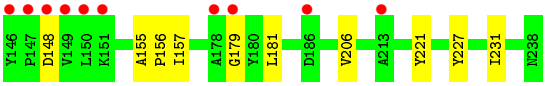




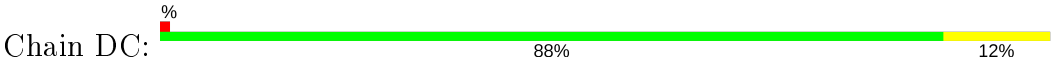
• Molecule 1: Cationic trypsin



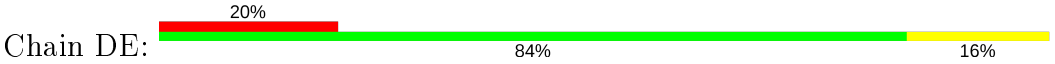


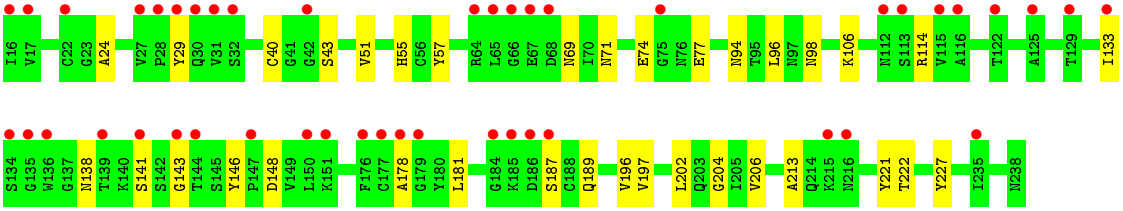


• Molecule 1: Cationic trypsin

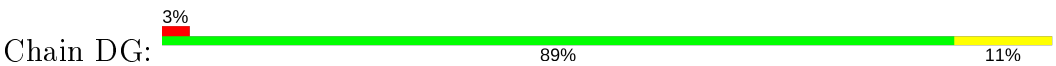


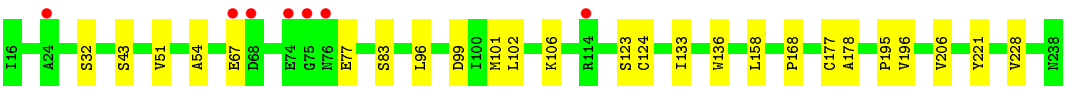
• Molecule 1: Cationic trypsin





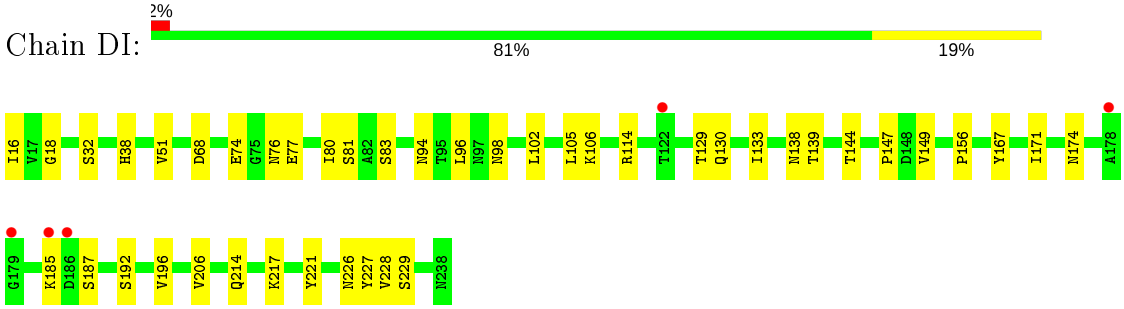
• Molecule 1: Cationic trypsin





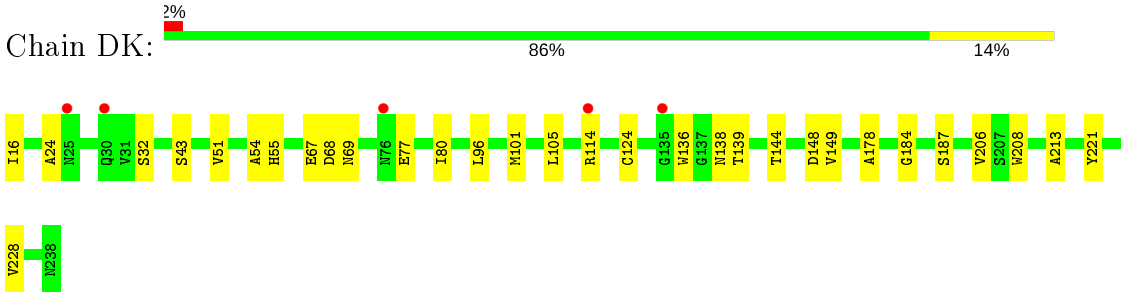
• Molecule 1: Cationic trypsin

Chain DI:



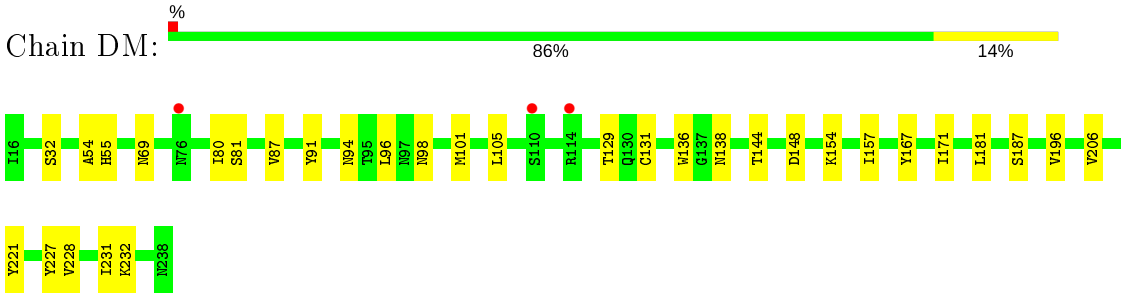
• Molecule 1: Cationic trypsin

Chain DK:



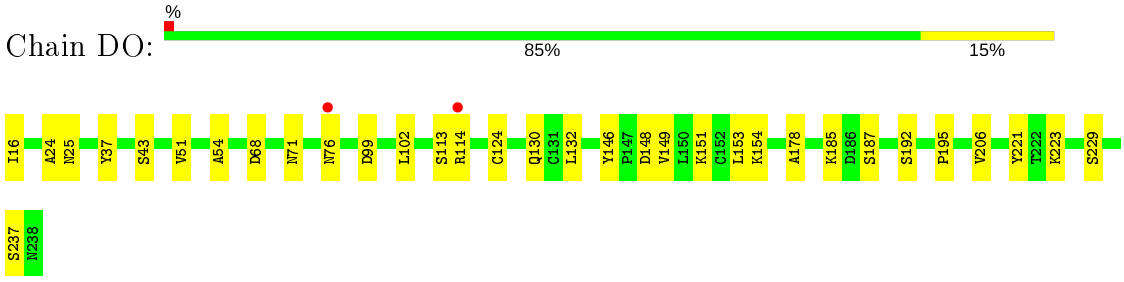
• Molecule 1: Cationic trypsin

Chain DM:



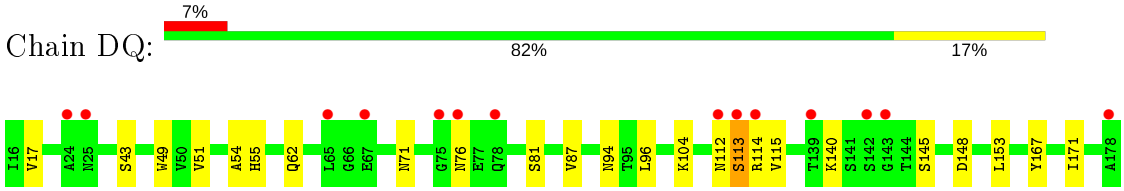
• Molecule 1: Cationic trypsin

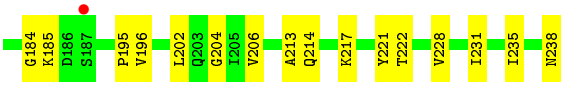
Chain DO:



• Molecule 1: Cationic trypsin

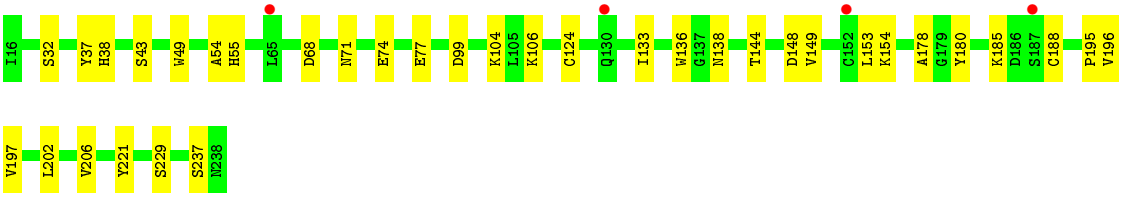
Chain DQ:





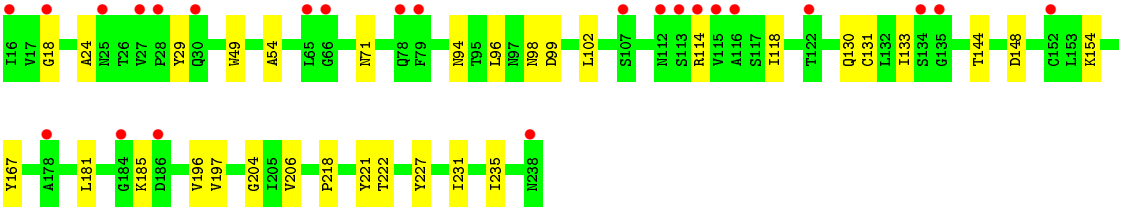
• Molecule 1: Cationic trypsin

Chain DS:



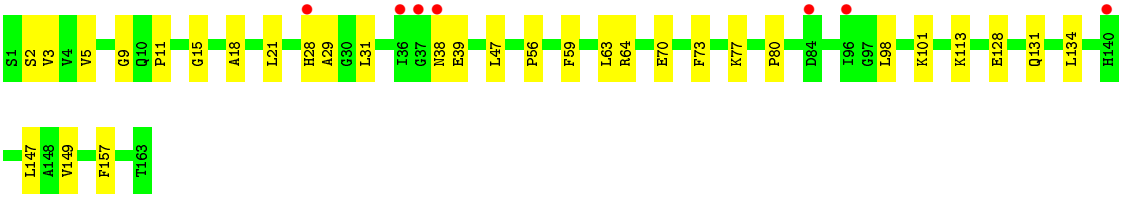
• Molecule 1: Cationic trypsin

Chain DU:



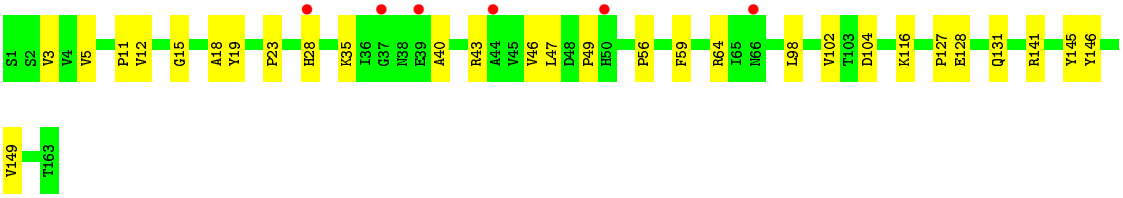
• Molecule 2: Kunitz-type inihibitor

Chain AB:



• Molecule 2: Kunitz-type inihibitor

Chain AD:

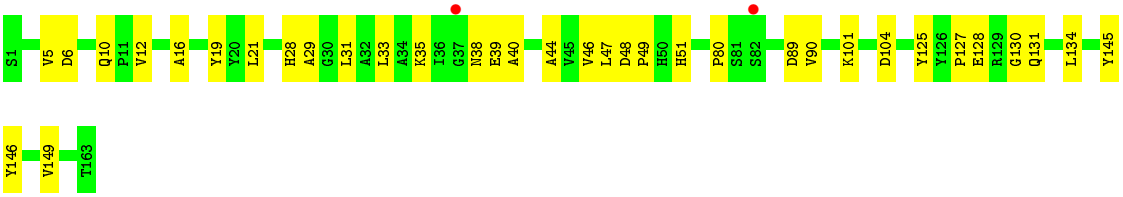


• Molecule 2: Kunitz-type inihibitor

Chain AF:

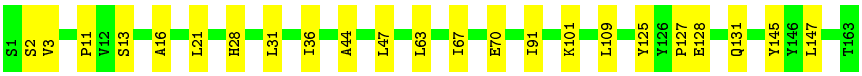
• Molecule 2: Kunitz-type inihibitor

Chain AH:



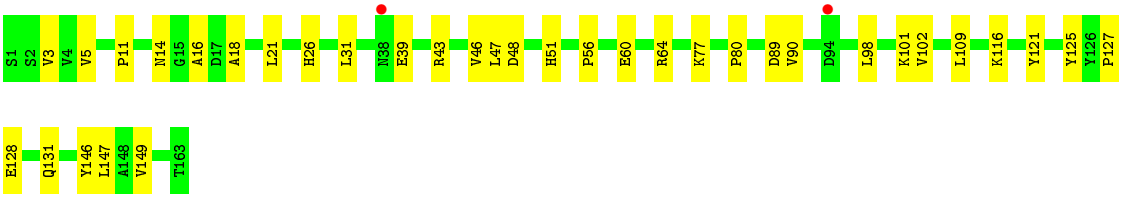
• Molecule 2: Kunitz-type inihibitor

Chain AJ:



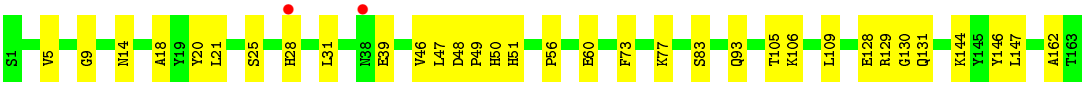
• Molecule 2: Kunitz-type inihibitor

Chain AL:



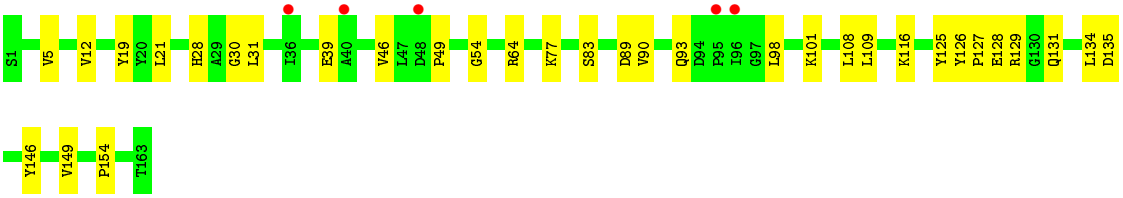
• Molecule 2: Kunitz-type inihibitor

Chain AN:



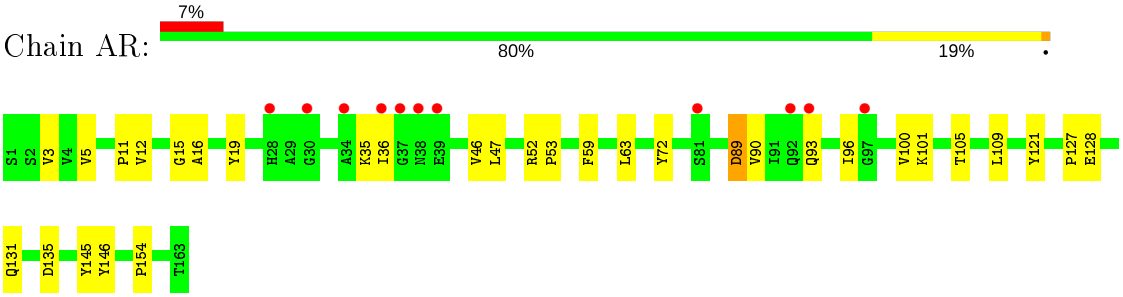
• Molecule 2: Kunitz-type inihibitor

Chain AP:



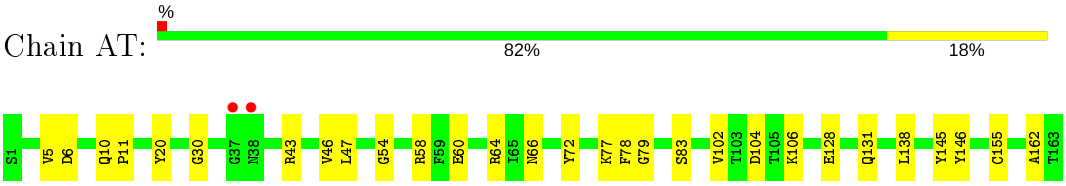
• Molecule 2: Kunitz-type inihibitor

Chain AR:



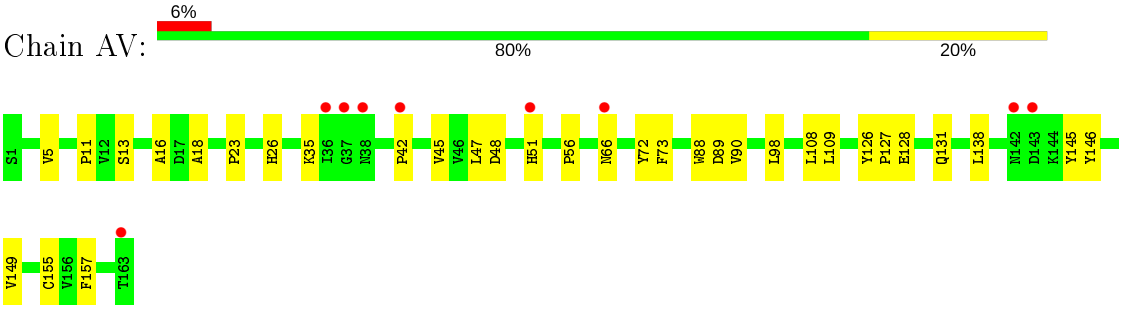
• Molecule 2: Kunitz-type inihibitor

Chain AT:



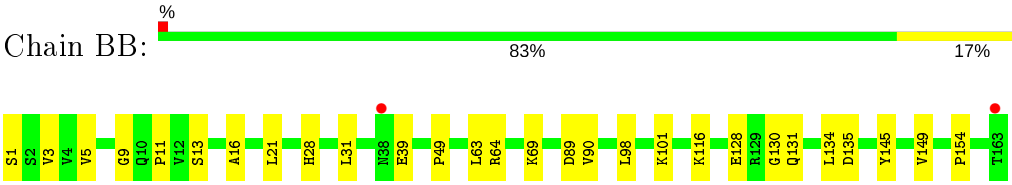
• Molecule 2: Kunitz-type inihibitor

Chain AV:



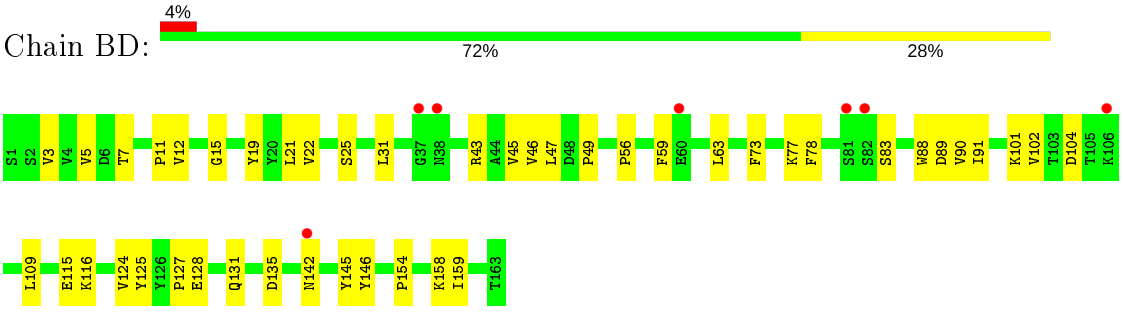
• Molecule 2: Kunitz-type inihibitor

Chain BB:



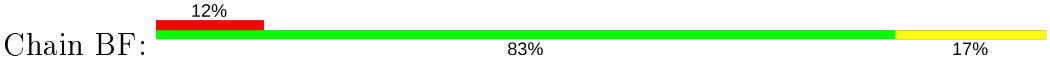
• Molecule 2: Kunitz-type inihibitor

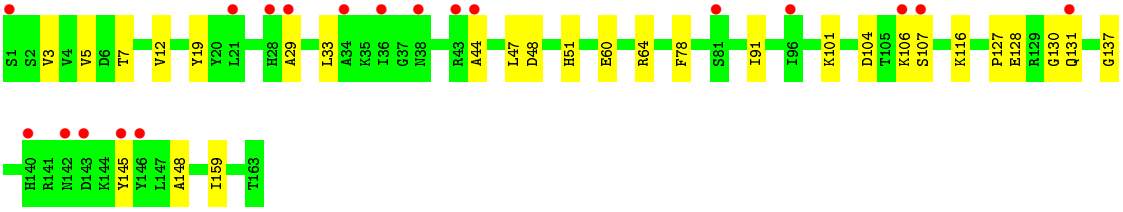
Chain BD:



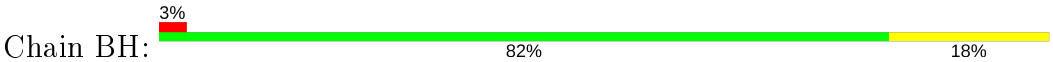
• Molecule 2: Kunitz-type inihibitor

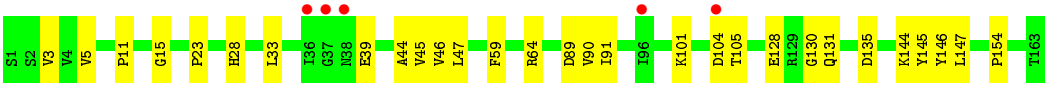
Chain BF:



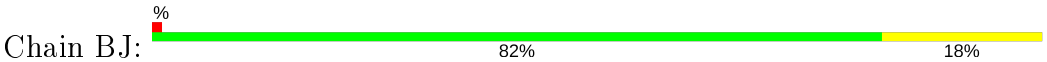


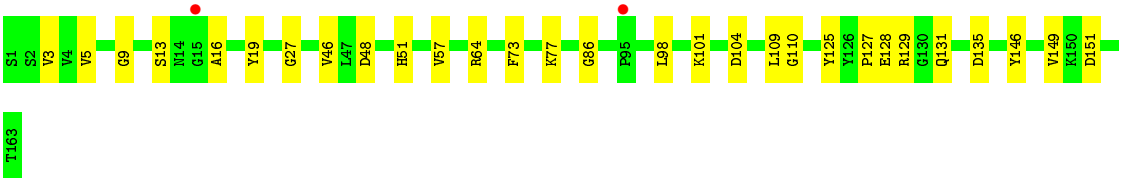
• Molecule 2: Kunitz-type inihibitor



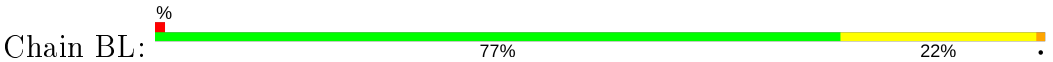


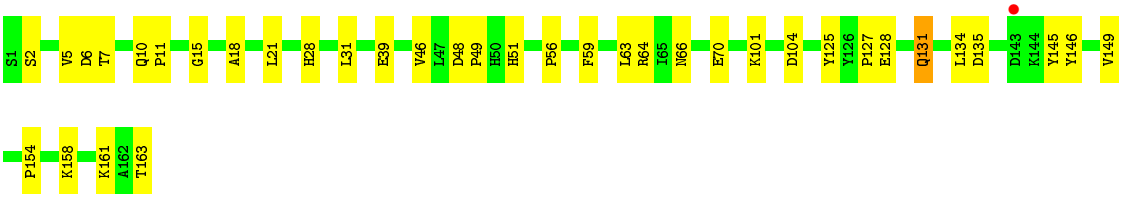
• Molecule 2: Kunitz-type inihibitor





• Molecule 2: Kunitz-type inihibitor





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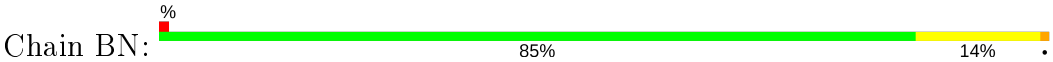
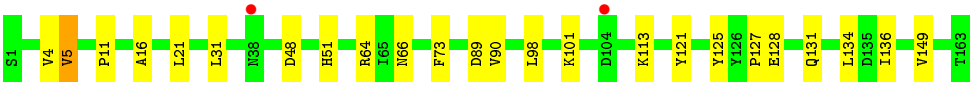
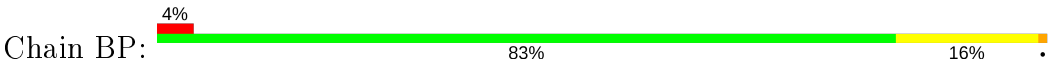
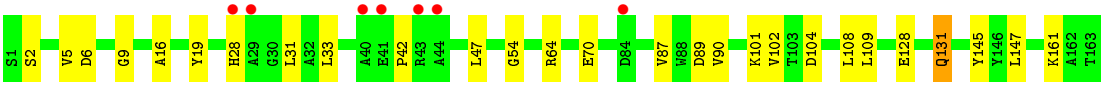




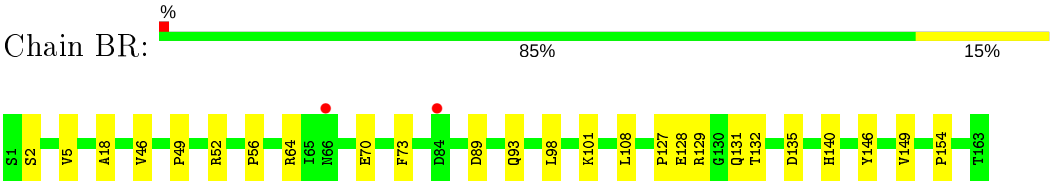
• Molecule 2: Kunitz-type inihibitor





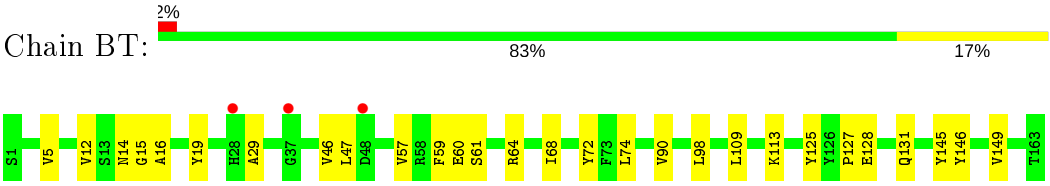
• Molecule 2: Kunitz-type inihibitor

Chain BR:



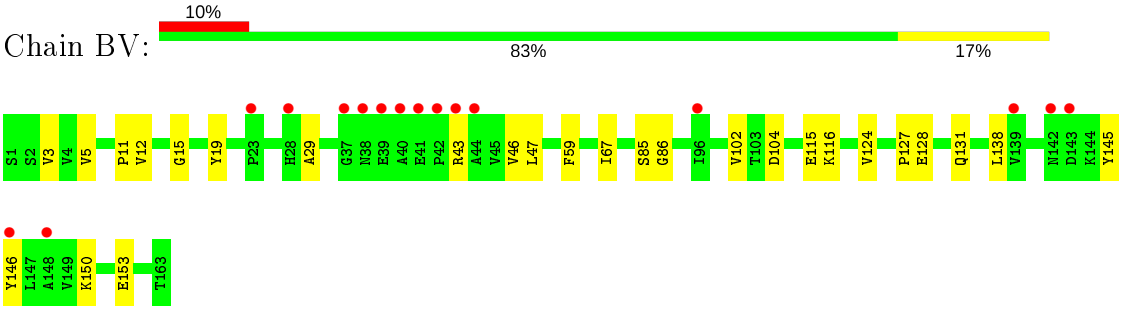
• Molecule 2: Kunitz-type inihibitor

Chain BT:



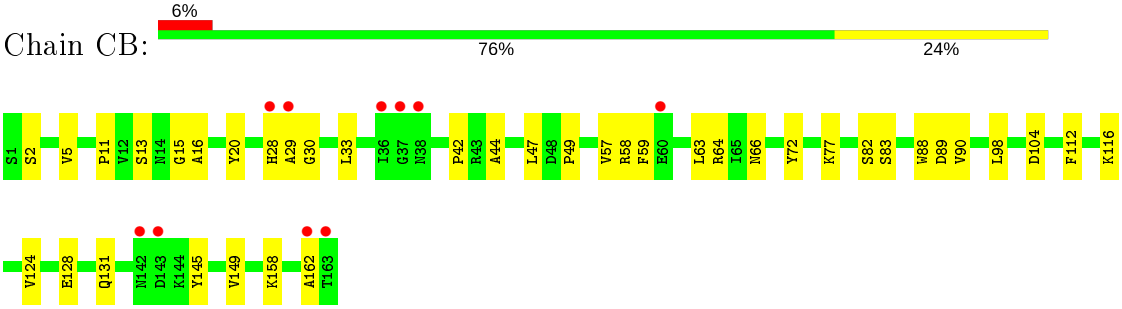
• Molecule 2: Kunitz-type inihibitor

Chain BV:



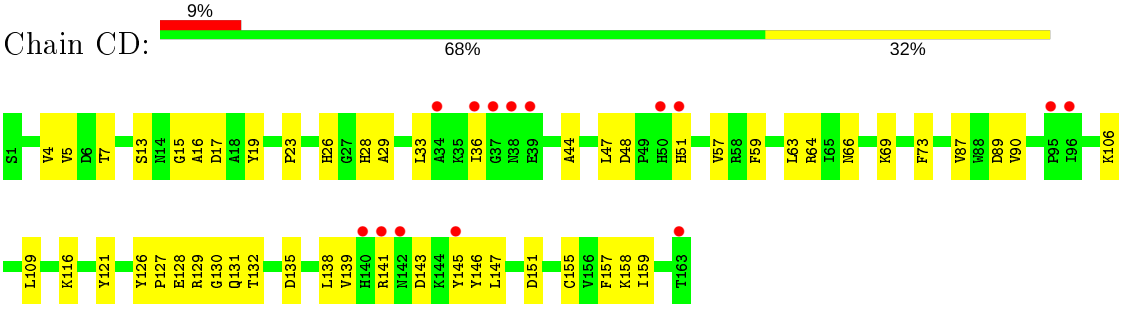
• Molecule 2: Kunitz-type inihibitor

Chain CB:



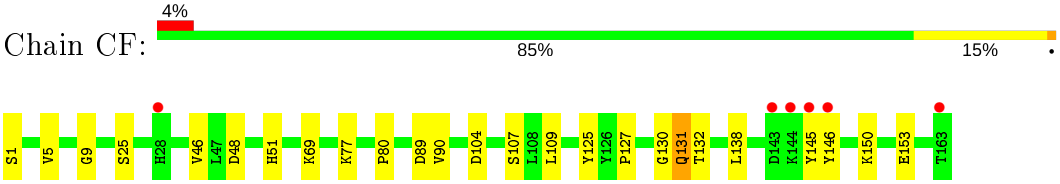
• Molecule 2: Kunitz-type inihibitor

Chain CD:



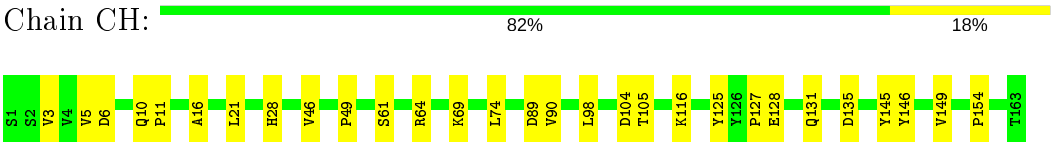
• Molecule 2: Kunitz-type inihibitor

Chain CF:



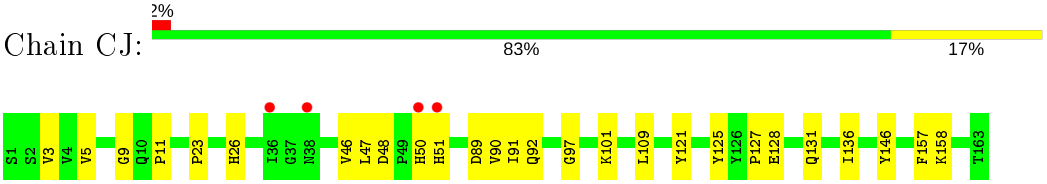
• Molecule 2: Kunitz-type inihibitor

Chain CH:



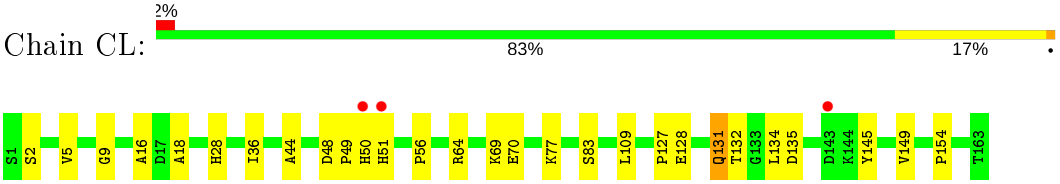
• Molecule 2: Kunitz-type inihibitor

Chain CJ:



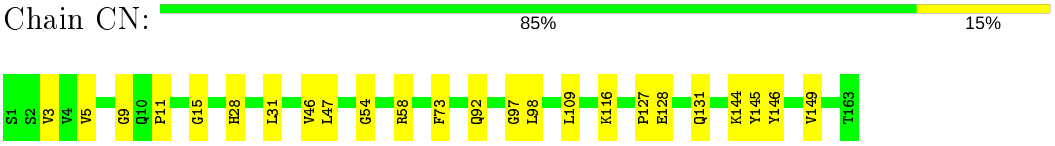
• Molecule 2: Kunitz-type inihibitor

Chain CL:



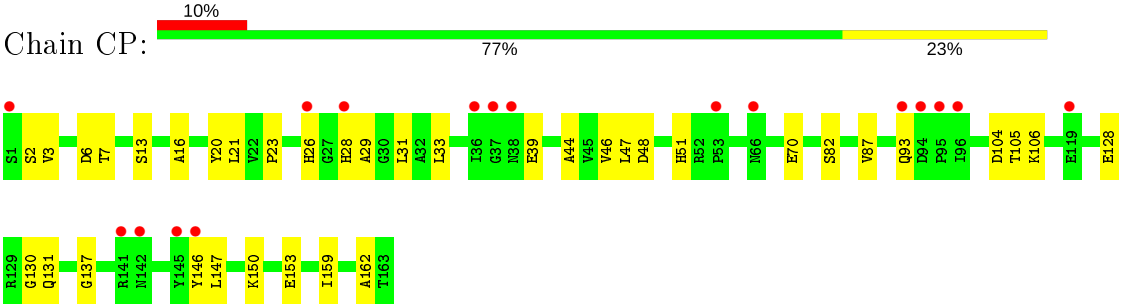
• Molecule 2: Kunitz-type inihibitor

Chain CN:



• Molecule 2: Kunitz-type inihibitor

Chain CP:



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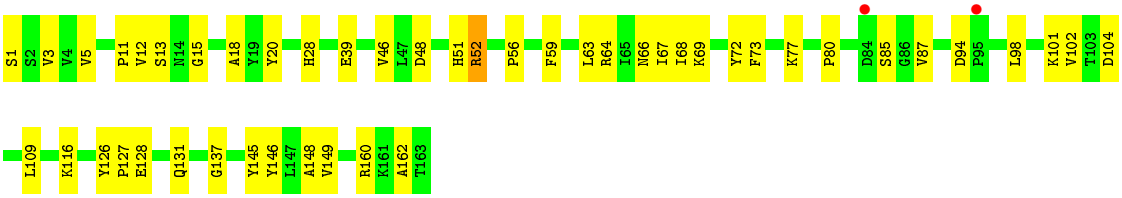

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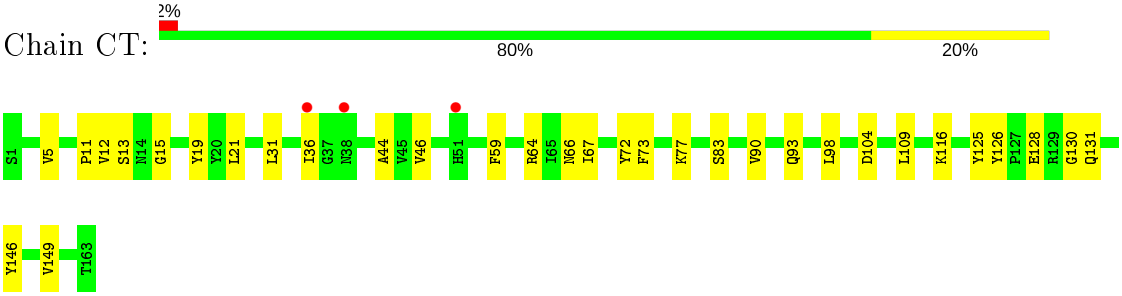

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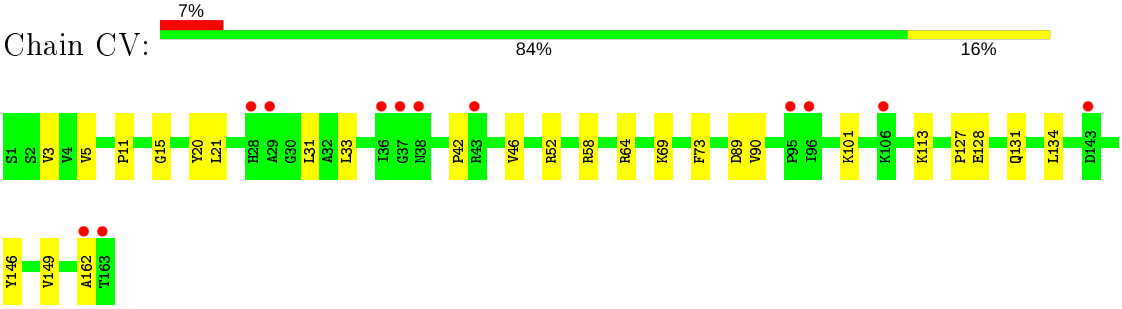

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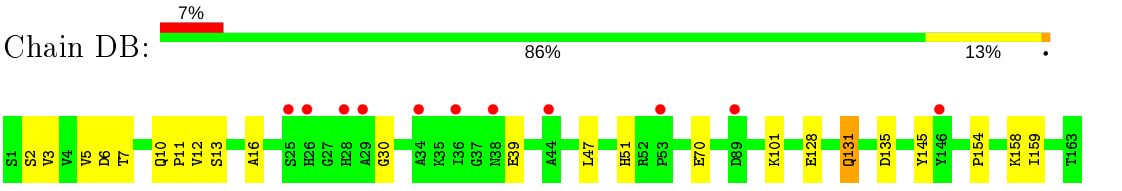

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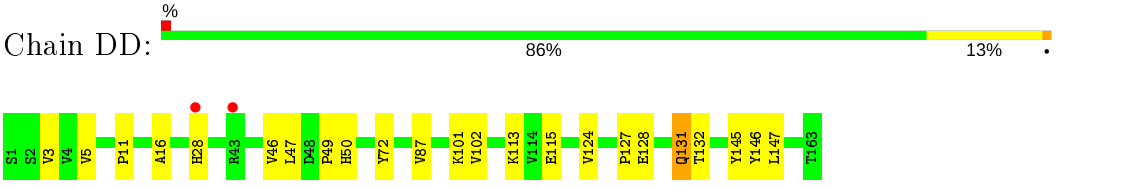
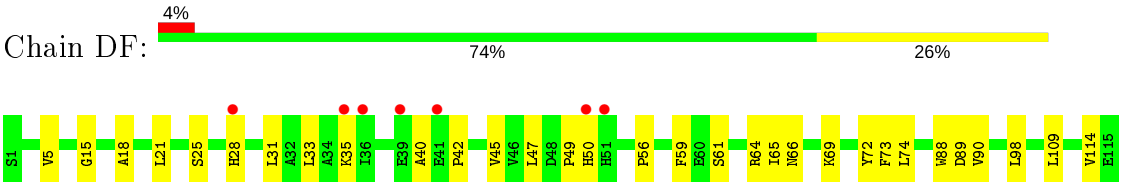
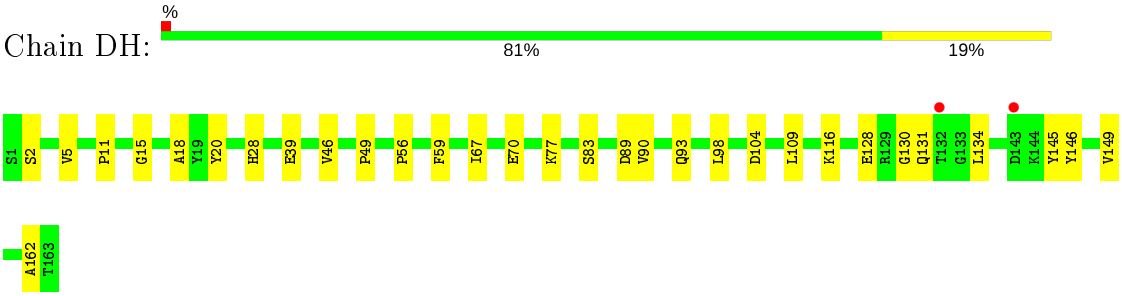


• Molecule 2: Kunitz-type inihibitor



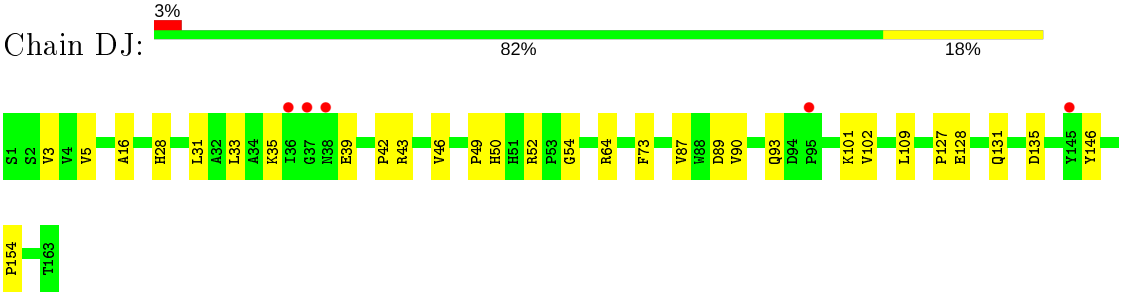
• Molecule 2: Kunitz-type inihibitor

Chain DH:



• Molecule 2: Kunitz-type inihibitor

Chain DJ:



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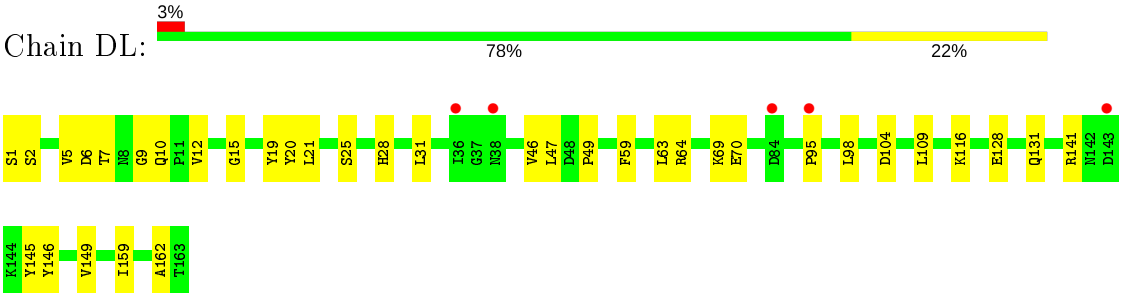
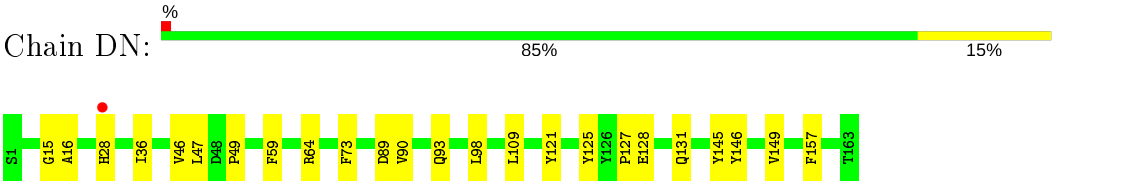
Chain DL:



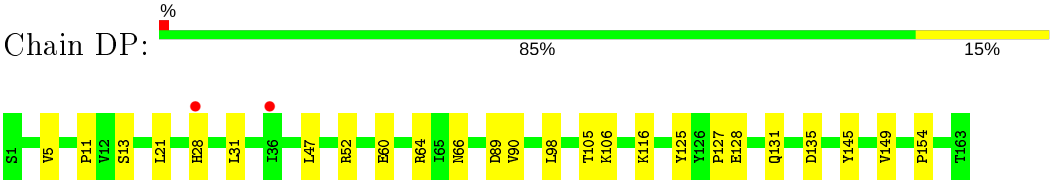
• Molecule 2: Kunitz-type inihibitor

Chain DN:



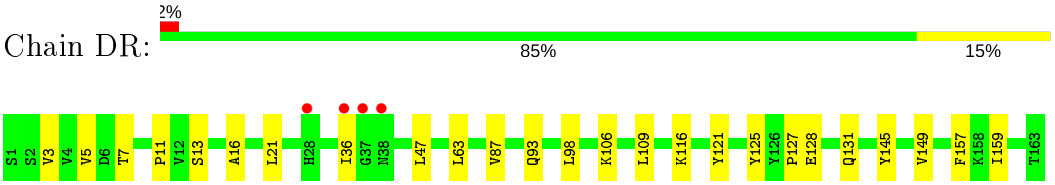
• Molecule 2: Kunitz-type inihibitor

Chain DP:



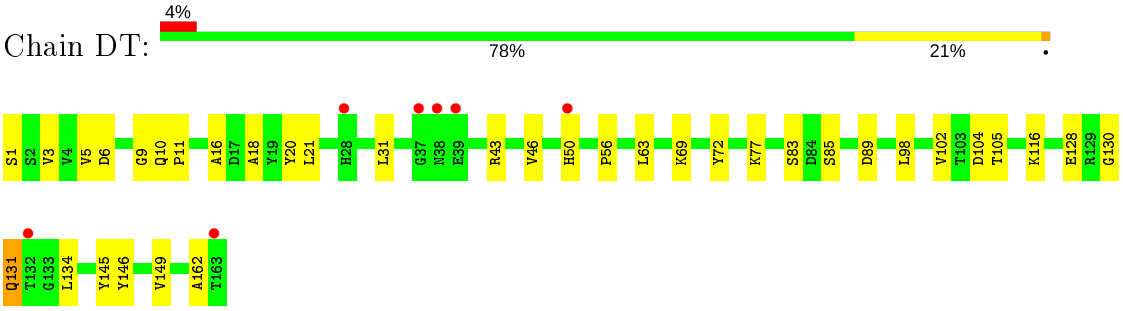
• Molecule 2: Kunitz-type inihibitor

Chain DR:



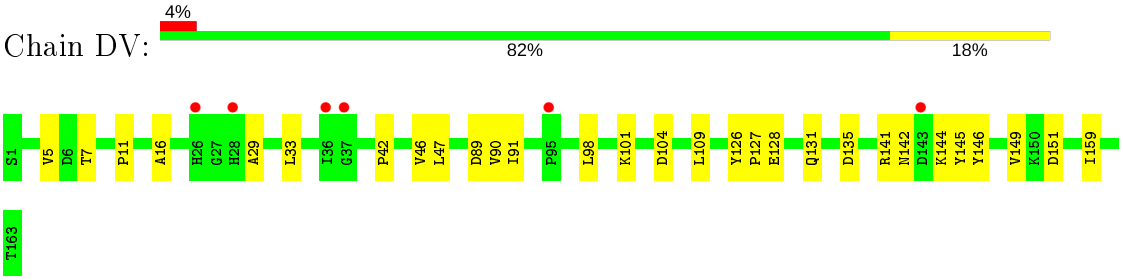
• Molecule 2: Kunitz-type inihibitor

Chain DT:



• Molecule 2: Kunitz-type inihibitor

Chain DV:



4 Data and refinement statistics (i)

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 – 3.94	Depositor EDS
% Data completeness (in resolution range)	85.1 (49.23-3.96) 85.1 (49.23-3.94)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$< I/\sigma(I) >$ [1]	3.59 (at 4.00Å)	Xtriage
Refinement program	PHENIX (1.12_2829)	Depositor
R, R_{free}	0.226 , 0.281 0.226 , 0.282	Depositor DCC
R_{free} test set	5830 reflections (4.92%)	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)	0.24 , 26.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.028 for l,-k,h	Xtriage
F_o,F_c correlation	0.81	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.28	0/1660	0.50	0/2250
1	AC	0.28	0/1660	0.50	0/2250
1	AE	0.28	0/1660	0.50	0/2250
1	AG	0.28	0/1660	0.50	0/2250
1	AI	0.28	0/1660	0.52	0/2250
1	AK	0.29	0/1660	0.50	0/2250
1	AM	0.28	0/1660	0.49	0/2250
1	AO	0.27	0/1660	0.49	0/2250
1	AQ	0.29	0/1660	0.51	0/2250
1	AS	0.28	0/1660	0.49	0/2250
1	AU	0.27	0/1660	0.49	0/2250
1	BA	0.27	0/1660	0.50	0/2250
1	BC	0.27	0/1660	0.49	0/2250
1	BE	0.28	0/1660	0.50	0/2250
1	BG	0.28	0/1660	0.51	0/2250
1	BI	0.27	0/1660	0.50	0/2250
1	BK	0.27	0/1660	0.51	0/2250
1	BM	0.28	0/1660	0.53	0/2250
1	BO	0.28	0/1660	0.50	0/2250
1	BQ	0.28	0/1660	0.51	0/2250
1	BS	0.27	0/1660	0.48	0/2250
1	BU	0.27	0/1660	0.50	0/2250
1	CA	0.28	0/1660	0.50	0/2250
1	CC	0.27	0/1660	0.50	0/2250
1	CE	0.29	0/1660	0.52	0/2250
1	CG	0.30	0/1660	0.50	0/2250
1	CI	0.31	0/1660	0.53	0/2250
1	CK	0.29	0/1660	0.52	0/2250
1	CM	0.28	0/1660	0.50	0/2250
1	CO	0.28	0/1660	0.51	0/2250
1	CQ	0.29	0/1660	0.51	0/2250
1	CS	0.27	0/1660	0.50	0/2250
1	CU	0.27	0/1660	0.49	0/2250
1	DA	0.29	0/1660	0.50	0/2250

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	DC	0.29	0/1660	0.49	0/2250
1	DE	0.27	0/1660	0.49	0/2250
1	DG	0.28	0/1660	0.51	0/2250
1	DI	0.29	0/1660	0.52	0/2250
1	DK	0.30	0/1660	0.53	0/2250
1	DM	0.28	0/1660	0.50	0/2250
1	DO	0.29	0/1660	0.53	0/2250
1	DQ	0.28	0/1660	0.50	0/2250
1	DS	0.28	0/1660	0.50	0/2250
1	DU	0.27	0/1660	0.49	0/2250
2	AB	0.28	0/1291	0.55	0/1754
2	AD	0.29	0/1291	0.53	0/1754
2	AF	0.33	0/1291	0.57	0/1754
2	AH	0.29	0/1291	0.56	0/1754
2	AJ	0.30	0/1291	0.55	0/1754
2	AL	0.31	0/1291	0.52	0/1754
2	AN	0.30	0/1291	0.52	0/1754
2	AP	0.29	0/1291	0.53	0/1754
2	AR	0.28	0/1291	0.53	0/1754
2	AT	0.30	0/1291	0.54	0/1754
2	AV	0.30	0/1291	0.53	0/1754
2	BB	0.29	0/1291	0.55	0/1754
2	BD	0.29	0/1291	0.53	0/1754
2	BF	0.28	0/1291	0.50	0/1754
2	BH	0.30	0/1291	0.55	0/1754
2	BJ	0.30	0/1291	0.53	0/1754
2	BL	0.29	0/1291	0.54	0/1754
2	BN	0.32	0/1291	0.54	1/1754 (0.1%)
2	BP	0.30	0/1291	0.55	0/1754
2	BR	0.31	0/1291	0.55	0/1754
2	BT	0.28	0/1291	0.51	0/1754
2	BV	0.28	0/1291	0.51	0/1754
2	CB	0.30	0/1291	0.53	0/1754
2	CD	0.30	0/1291	0.57	0/1754
2	CF	0.29	0/1291	0.53	0/1754
2	CH	0.31	0/1291	0.55	0/1754
2	CJ	0.31	0/1291	0.56	0/1754
2	CL	0.31	0/1291	0.53	0/1754
2	CN	0.30	0/1291	0.53	0/1754
2	CP	0.28	0/1291	0.51	0/1754
2	CR	0.30	0/1291	0.52	0/1754
2	CT	0.30	0/1291	0.52	0/1754
2	CV	0.27	0/1291	0.51	0/1754

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
2	DB	0.30	0/1291	0.53	0/1754
2	DD	0.32	0/1291	0.56	1/1754 (0.1%)
2	DF	0.34	0/1291	0.57	0/1754
2	DH	0.30	0/1291	0.53	0/1754
2	DJ	0.31	0/1291	0.52	0/1754
2	DL	0.31	0/1291	0.56	0/1754
2	DN	0.30	0/1291	0.55	0/1754
2	DP	0.31	0/1291	0.53	0/1754
2	DR	0.29	0/1291	0.54	0/1754
2	DT	0.29	0/1291	0.53	0/1754
2	DV	0.29	0/1291	0.53	0/1754
All	All	0.29	0/129844	0.52	2/176176 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	DD	131	GLN	CA-CB-CG	-6.06	100.07	113.40
2	BN	5	VAL	CG1-CB-CG2	5.25	119.31	110.90

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	1629	0	1588	23	0
1	AC	1629	0	1588	28	1
1	AE	1629	0	1588	25	0
1	AG	1629	0	1588	20	0
1	AI	1629	0	1588	24	0
1	AK	1629	0	1588	26	0
1	AM	1629	0	1588	20	0
1	AO	1629	0	1588	28	0
1	AQ	1629	0	1588	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AS	1629	0	1588	24	0
1	AU	1629	0	1588	24	0
1	BA	1629	0	1588	27	0
1	BC	1629	0	1588	15	0
1	BE	1629	0	1588	22	0
1	BG	1629	0	1588	22	0
1	BI	1629	0	1588	21	0
1	BK	1629	0	1588	22	0
1	BM	1629	0	1588	25	1
1	BO	1629	0	1588	22	0
1	BQ	1629	0	1588	31	0
1	BS	1629	0	1588	32	0
1	BU	1629	0	1588	24	0
1	CA	1629	0	1588	24	0
1	CC	1629	0	1588	30	0
1	CE	1629	0	1588	20	0
1	CG	1629	0	1588	30	0
1	CI	1629	0	1588	12	0
1	CK	1629	0	1588	23	0
1	CM	1629	0	1588	23	0
1	CO	1629	0	1588	33	0
1	CQ	1629	0	1588	34	0
1	CS	1629	0	1588	26	0
1	CU	1629	0	1588	28	1
1	DA	1629	0	1588	19	1
1	DC	1629	0	1588	20	1
1	DE	1629	0	1588	30	0
1	DG	1629	0	1588	16	0
1	DI	1629	0	1588	41	0
1	DK	1629	0	1588	24	0
1	DM	1629	0	1588	25	0
1	DO	1629	0	1588	28	0
1	DQ	1629	0	1588	29	1
1	DS	1629	0	1588	24	0
1	DU	1629	0	1588	20	0
2	AB	1260	0	1265	27	0
2	AD	1260	0	1265	25	0
2	AF	1260	0	1265	28	0
2	AH	1260	0	1265	34	0
2	AJ	1260	0	1265	23	0
2	AL	1260	0	1265	32	0
2	AN	1260	0	1265	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	AP	1260	0	1265	32	0
2	AR	1260	0	1265	29	0
2	AT	1260	0	1265	25	0
2	AV	1260	0	1265	30	1
2	BB	1260	0	1265	27	1
2	BD	1260	0	1265	40	1
2	BF	1260	0	1265	22	0
2	BH	1260	0	1265	25	0
2	BJ	1260	0	1265	32	0
2	BL	1260	0	1265	29	0
2	BN	1260	0	1265	23	0
2	BP	1260	0	1265	27	0
2	BR	1260	0	1265	27	0
2	BT	1260	0	1265	25	0
2	BV	1260	0	1265	17	1
2	CB	1260	0	1265	32	0
2	CD	1260	0	1265	48	0
2	CF	1260	0	1265	21	0
2	CH	1260	0	1265	29	0
2	CJ	1260	0	1265	24	0
2	CL	1260	0	1265	29	1
2	CN	1260	0	1265	28	0
2	CP	1260	0	1265	29	0
2	CR	1260	0	1265	41	0
2	CT	1260	0	1265	28	0
2	CV	1260	0	1265	18	0
2	DB	1260	0	1265	19	0
2	DD	1260	0	1265	22	0
2	DF	1260	0	1265	53	0
2	DH	1260	0	1265	28	0
2	DJ	1260	0	1265	28	0
2	DL	1260	0	1265	38	0
2	DN	1260	0	1265	24	0
2	DP	1260	0	1265	22	0
2	DR	1260	0	1265	22	0
2	DT	1260	0	1265	33	1
2	DV	1260	0	1265	25	2
All	All	127116	0	125532	1896	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.

All (1896) 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
1:CE:32:SER:HG	1:CE:38:HIS:HD1	0.99	0.98
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
1:AQ:74:GLU:O	2:CD:141:ARG:NH2	2.01	0.93
1:DC:32:SER:HG	1:DC:38:HIS:HD1	1.15	0.93
1:CO:72:VAL:HG22	2:DF:35:LYS:HE3	1.48	0.92
2:AV:127:PRO:HD2	2:AV:131:GLN:NE2	1.84	0.91
1:AC:32:SER:HG	1:AC:38:HIS:HD1	1.16	0.90
2:BJ:27:GLY:HA3	1:BM:229:SER:HB3	1.54	0.89
1:BA:24:ALA:HB1	1:BA:114:ARG:HE	1.38	0.87
1:CU:24:ALA:HB1	1:CU:114:ARG:HE	1.39	0.87
2:AL:5:VAL:HG12	2:AL:11:PRO:HA	1.57	0.87
2:AH:38:ASN:HB3	1:DI:130:GLN:HE21	1.39	0.85
2:AB:28:HIS:HE1	1:AE:229:SER:HB3	1.42	0.85
2:AF:5:VAL:HG22	2:AH:131:GLN:HG2	1.60	0.84
2:CP:28:HIS:HE1	1:CS:229:SER:HB3	1.42	0.82
1:BM:106:LYS:NZ	2:BP:104:ASP:OD1	2.12	0.81
2:DL:28:HIS:CE1	1:DO:229:SER:H	1.97	0.81
1:CM:206:VAL:HA	1:CM:221:TYR:HD1	1.46	0.81
2:BD:47:LEU:HB2	2:BD:145:TYR:HB2	1.61	0.80
2:CH:145:TYR:OH	1:CK:124:CYS:O	2.00	0.80
2:CD:5:VAL:HG22	2:CF:131:GLN:HG2	1.61	0.80
2:DD:5:VAL:HG21	2:DF:131:GLN:NE2	1.97	0.79
1:CC:106:LYS:NZ	2:CF:104:ASP:OD1	2.16	0.79
1:AQ:128:GLY:O	1:CG:25:ASN:ND2	2.16	0.79
2:AF:5:VAL:HG12	2:AF:11:PRO:HA	1.64	0.79
1:CC:32:SER:HG	1:CC:38:HIS:HD1	1.31	0.78
1:AG:182:GLU:HG2	1:BQ:237:SER:HA	1.66	0.78
1:AC:24:ALA:HB1	1:AC:114:ARG:HE	1.50	0.77
1:CK:32:SER:HG	1:CK:38:HIS:HD1	1.28	0.77
1:CU:71:ASN:ND2	1:CU:148:ASP:OD2	2.18	0.77
1:BM:206:VAL:HA	1:BM:221:TYR:HD1	1.49	0.76
2:CT:128:GLU:H	2:CT:131:GLN:NE2	1.84	0.76
2:CL:145:TYR:OH	1:CO:124:CYS:O	2.04	0.76
2:AH:128:GLU:HB2	2:AH:131:GLN:HE22	1.50	0.76
2:DT:128:GLU:HB2	2:DT:131:GLN:HE22	1.50	0.75
1:CG:24:ALA:HB1	1:CG:114:ARG:HH21	1.51	0.75
1:DU:24:ALA:HB1	1:DU:114:ARG:HE	1.51	0.75
1:BC:206:VAL:HA	1:BC:221:TYR:HD1	1.50	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CL:48:ASP:HB3	2:CL:51:HIS:HB2	1.68	0.75
1:AM:96:LEU:HD11	2:AN:109:LEU:HD11	1.69	0.75
2:AL:39:GLU:OE2	2:AL:101:LYS:NZ	2.19	0.74
2:DL:28:HIS:HE1	1:DO:229:SER:H	1.34	0.74
1:DU:206:VAL:HA	1:DU:221:TYR:HD1	1.51	0.74
2:CB:33:LEU:HB3	2:CB:42:PRO:HB2	1.70	0.74
1:DQ:71:ASN:ND2	1:DQ:148:ASP:OD2	2.19	0.74
2:DH:128:GLU:HB2	2:DH:131:GLN:HE22	1.53	0.74
2:DD:128:GLU:H	2:DD:131:GLN:NE2	1.86	0.74
2:DH:145:TYR:OH	1:DK:124:CYS:O	2.06	0.74
1:BE:187:SER:OG	2:BF:64:ARG:NH1	2.20	0.73
1:CQ:76:ASN:HB2	1:CQ:114:ARG:HH11	1.53	0.73
2:BP:128:GLU:H	2:BP:131:GLN:HE22	1.36	0.73
2:BN:5:VAL:HG22	2:BP:131:GLN:HG2	1.70	0.73
2:AD:145:TYR:OH	1:AG:124:CYS:O	2.07	0.72
1:CQ:96:LEU:HD11	2:CR:109:LEU:HD11	1.72	0.72
1:DC:71:ASN:ND2	1:DC:148:ASP:OD2	2.22	0.72
1:CM:24:ALA:HB1	1:CM:114:ARG:HE	1.55	0.71
1:AA:132:LEU:HD13	1:AA:154:LYS:HE2	1.72	0.71
2:DD:5:VAL:HG21	2:DF:131:GLN:HE21	1.54	0.71
2:DV:46:VAL:HG21	2:DV:144:LYS:HD3	1.72	0.71
2:AP:5:VAL:HG11	2:AR:131:GLN:HG2	1.72	0.71
1:CS:206:VAL:HA	1:CS:221:TYR:HD1	1.56	0.71
2:AF:121:TYR:OH	2:AH:131:GLN:OE1	2.09	0.70
1:DE:55:HIS:O	2:DF:72:TYR:OH	2.09	0.70
1:AC:187:SER:OG	2:AD:64:ARG:NH1	2.25	0.70
2:AR:135:ASP:HB3	2:AR:154:PRO:HB3	1.74	0.70
1:AS:187:SER:OG	2:AT:64:ARG:NH1	2.24	0.70
2:AP:28:HIS:HE1	1:AS:229:SER:H	1.37	0.70
2:BH:28:HIS:CD2	1:BK:229:SER:HG	2.10	0.70
1:BQ:24:ALA:HB1	1:BQ:114:ARG:HE	1.56	0.70
2:AP:135:ASP:HB3	2:AP:154:PRO:HB3	1.72	0.70
2:AH:28:HIS:HE1	1:AK:229:SER:HB3	1.56	0.70
1:AO:81:SER:HB2	2:AR:105:THR:HG21	1.73	0.70
1:BS:43:SER:HB2	1:BS:51:VAL:HG22	1.72	0.70
2:CD:29:ALA:HB1	2:CD:47:LEU:HB3	1.74	0.70
2:AH:35:LYS:NZ	1:DI:18:GLY:O	2.24	0.70
1:DO:24:ALA:HB1	1:DO:114:ARG:HE	1.55	0.69
1:BM:206:VAL:HA	1:BM:221:TYR:CD1	2.28	0.69
2:AR:3:VAL:HB	2:AT:128:GLU:HG3	1.74	0.69
2:DR:5:VAL:HG22	2:DT:131:GLN:HG2	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DS:144:THR:HG21	2:DT:16:ALA:HA	1.74	0.69
2:CB:15:GLY:N	2:CB:59:PHE:O	2.26	0.69
2:AH:5:VAL:HG11	2:AJ:131:GLN:HG2	1.75	0.69
1:DQ:81:SER:CB	2:DT:105:THR:HG21	2.23	0.69
1:AA:32:SER:OG	1:AA:38:HIS:ND1	2.20	0.69
1:BU:76:ASN:HB2	1:BU:114:ARG:HH11	1.58	0.69
1:BO:57:TYR:CZ	1:BQ:168:PRO:HB2	2.28	0.68
2:DB:39:GLU:OE2	2:DB:101:LYS:NZ	2.26	0.68
2:AN:5:VAL:HG21	2:AP:131:GLN:HG2	1.73	0.68
1:CS:96:LEU:HD11	2:CT:109:LEU:HD11	1.74	0.68
1:CQ:206:VAL:HA	1:CQ:221:TYR:HD1	1.59	0.68
1:DE:96:LEU:HD11	2:DF:109:LEU:HD11	1.74	0.68
1:CI:28:PRO:HB3	1:CI:113:SER:O	1.94	0.68
2:DD:145:TYR:OH	1:DG:124:CYS:O	2.08	0.68
2:AF:39:GLU:OE2	2:AF:93:GLN:NE2	2.27	0.68
1:BE:106:LYS:NZ	2:BH:104:ASP:OD1	2.20	0.68
1:CO:23:GLY:N	2:DF:50:HIS:HD2	1.91	0.68
2:DF:5:VAL:HG22	2:DH:131:GLN:HG2	1.76	0.68
1:DO:146:TYR:OH	2:DP:66:ASN:OD1	2.10	0.67
1:AM:153:LEU:HD11	1:AM:185:LYS:HD2	1.75	0.67
2:BF:47:LEU:HB2	2:BF:145:TYR:HB2	1.76	0.67
1:BK:153:LEU:HD11	1:BK:185:LYS:HD2	1.75	0.67
2:DH:116:LYS:HG2	1:DI:94:ASN:HD22	1.60	0.67
1:AA:71:ASN:ND2	1:AA:148:ASP:OD2	2.27	0.67
1:DK:187:SER:OG	2:DL:64:ARG:NH1	2.28	0.67
1:CK:71:ASN:ND2	1:CK:148:ASP:OD2	2.27	0.67
1:CQ:206:VAL:HA	1:CQ:221:TYR:CD1	2.30	0.67
2:AL:5:VAL:HG12	2:AL:11:PRO:CA	2.24	0.67
2:CR:46:VAL:HG12	2:CR:146:TYR:HA	1.77	0.67
1:AQ:129:THR:HA	1:CG:113:SER:HB2	1.76	0.67
1:AK:144:THR:HG21	2:AL:16:ALA:HA	1.76	0.66
1:BG:106:LYS:NZ	2:BJ:104:ASP:OD2	2.27	0.66
2:CP:23:PRO:HG3	2:CP:47:LEU:HD13	1.78	0.66
2:DP:127:PRO:HD2	2:DP:131:GLN:NE2	2.11	0.66
2:AH:29:ALA:HB1	2:AH:47:LEU:HB3	1.78	0.66
2:BF:29:ALA:HB1	2:BF:47:LEU:HB3	1.77	0.66
2:BP:128:GLU:HB2	2:BP:131:GLN:OE1	1.96	0.66
2:BV:5:VAL:HG12	2:BV:11:PRO:HA	1.78	0.66
2:CR:48:ASP:HB3	2:CR:51:HIS:HB2	1.77	0.66
1:DE:94:ASN:HD22	2:DF:73:PHE:HE2	1.43	0.66
1:BE:182:GLU:HG2	1:DS:237:SER:HA	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BB:116:LYS:HG2	1:BC:94:ASN:HD22	1.60	0.66
2:CJ:5:VAL:HG22	2:CL:131:GLN:CG	2.25	0.66
1:AM:71:ASN:ND2	1:AM:148:ASP:OD2	2.29	0.66
2:CF:9:GLY:HA2	2:CH:131:GLN:HE22	1.59	0.66
2:DH:46:VAL:HG12	2:DH:146:TYR:HA	1.78	0.66
2:DL:145:TYR:OH	1:DO:124:CYS:O	2.14	0.66
2:BR:128:GLU:H	2:BR:131:GLN:NE2	1.95	0.65
2:CL:49:PRO:HG2	1:CO:123:SER:HB3	1.78	0.65
2:AV:47:LEU:HB2	2:AV:145:TYR:HB2	1.78	0.65
1:CK:155:ALA:HB1	1:CK:179:GLY:HA2	1.78	0.65
1:DO:132:LEU:HD13	1:DO:154:LYS:HE2	1.77	0.65
2:BR:127:PRO:N	2:BR:131:GLN:HE22	1.93	0.65
2:AN:50:HIS:CE1	1:DO:76:ASN:HD21	2.15	0.65
1:DQ:228:VAL:HA	1:DQ:231:ILE:HD12	1.78	0.65
2:AH:40:ALA:O	1:DI:185:LYS:NZ	2.21	0.65
2:AJ:21:LEU:HD12	2:AJ:31:LEU:HD11	1.78	0.65
2:AV:138:LEU:HB3	2:AV:145:TYR:HD1	1.62	0.65
1:DQ:81:SER:HB2	2:DT:105:THR:HG21	1.77	0.65
1:AE:206:VAL:HA	1:AE:221:TYR:HD1	1.61	0.65
1:DI:187:SER:OG	2:DJ:64:ARG:NH1	2.28	0.65
1:AG:32:SER:OG	1:AG:38:HIS:ND1	2.20	0.64
1:AO:71:ASN:ND2	1:AO:148:ASP:OD2	2.30	0.64
2:BR:5:VAL:HG21	2:BT:131:GLN:HB3	1.79	0.64
2:AV:18:ALA:HB1	2:AV:56:PRO:HB2	1.79	0.64
2:DJ:3:VAL:HB	2:DL:128:GLU:HG3	1.79	0.64
1:AI:43:SER:HB2	1:AI:51:VAL:HG22	1.79	0.64
1:CU:130:GLN:HB2	1:DC:25:ASN:HB2	1.79	0.64
2:DV:128:GLU:O	2:DV:131:GLN:HG3	1.97	0.64
1:BS:21:THR:OG1	1:BS:151:LYS:NZ	2.30	0.64
2:CF:77:LYS:NZ	2:CF:80:PRO:O	2.22	0.64
2:AL:127:PRO:HD2	2:AL:131:GLN:NE2	2.13	0.64
2:AJ:47:LEU:HB2	2:AJ:145:TYR:HB2	1.79	0.64
2:BP:5:VAL:HG21	2:BR:131:GLN:HG3	1.78	0.64
2:CN:116:LYS:NZ	2:CP:130:GLY:O	2.19	0.64
2:AF:121:TYR:O	2:AF:157:PHE:N	2.29	0.64
2:AP:46:VAL:HG12	2:AP:146:TYR:HA	1.80	0.63
2:CN:145:TYR:OH	1:CQ:124:CYS:O	2.16	0.63
2:AF:27:GLY:HA3	1:AI:229:SER:HB3	1.80	0.63
1:BU:167:TYR:OH	1:BU:218:PRO:O	2.15	0.63
2:CJ:128:GLU:O	2:CJ:131:GLN:HG3	1.97	0.63
2:CJ:3:VAL:HB	2:CL:128:GLU:HG3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DC:55:HIS:O	2:DD:72:TYR:OH	2.15	0.63
1:DK:67:GLU:HG3	1:DK:77:GLU:HG3	1.79	0.63
2:AF:28:HIS:HD2	1:AI:232:LYS:HD2	1.64	0.63
1:AU:71:ASN:ND2	1:AU:148:ASP:OD2	2.32	0.63
2:BR:18:ALA:HB1	2:BR:56:PRO:HB2	1.81	0.63
2:BL:48:ASP:HB3	2:BL:51:HIS:HB2	1.79	0.63
1:BU:71:ASN:ND2	1:BU:148:ASP:OD2	2.32	0.63
1:AI:206:VAL:HA	1:AI:221:TYR:HD1	1.63	0.63
1:BE:71:ASN:ND2	1:BE:148:ASP:OD2	2.30	0.63
1:BO:187:SER:OG	2:BP:64:ARG:NH1	2.32	0.63
1:AC:206:VAL:HA	1:AC:221:TYR:CD1	2.34	0.63
2:CH:128:GLU:O	2:CH:131:GLN:HG3	1.97	0.63
1:CU:83:SER:HB3	1:CU:106:LYS:HB3	1.81	0.63
2:CR:3:VAL:HB	2:CT:128:GLU:HG3	1.81	0.63
1:DQ:104:LYS:NZ	1:DQ:238:ASN:O	2.25	0.63
1:CS:206:VAL:HA	1:CS:221:TYR:CD1	2.34	0.62
2:AB:39:GLU:OE2	2:AB:101:LYS:NZ	2.30	0.62
2:AP:116:LYS:HG2	1:AQ:94:ASN:HD22	1.64	0.62
2:AH:48:ASP:HB3	2:AH:51:HIS:HB2	1.80	0.62
1:BM:146:TYR:OH	2:BN:66:ASN:OD1	2.12	0.62
2:BV:46:VAL:HG12	2:BV:146:TYR:HA	1.81	0.62
1:AE:43:SER:HB2	1:AE:51:VAL:HG22	1.81	0.62
2:AH:145:TYR:OH	1:AK:124:CYS:O	2.18	0.62
2:BB:1:SER:HA	2:BB:69:LYS:HD3	1.82	0.62
1:BK:187:SER:OG	2:BL:64:ARG:NH1	2.32	0.62
1:CU:78:GLN:OE1	1:CU:110:SER:OG	2.18	0.62
1:DM:187:SER:OG	2:DN:64:ARG:NH1	2.33	0.62
2:CJ:128:GLU:N	2:CJ:131:GLN:OE1	2.33	0.62
1:CS:43:SER:HB2	1:CS:51:VAL:HG22	1.82	0.62
1:DA:39:PHE:HZ	1:DA:61:ILE:HG12	1.65	0.62
1:DE:206:VAL:HA	1:DE:221:TYR:CD1	2.35	0.62
2:DJ:127:PRO:HD2	2:DJ:131:GLN:NE2	2.15	0.62
2:AH:5:VAL:HG21	2:AJ:131:GLN:HG2	1.82	0.62
1:DA:24:ALA:HB1	1:DA:114:ARG:HE	1.64	0.62
1:DE:71:ASN:ND2	1:DE:148:ASP:OD2	2.33	0.62
1:DO:71:ASN:ND2	1:DO:148:ASP:OD2	2.32	0.62
1:AG:24:ALA:HB1	1:AG:114:ARG:HE	1.63	0.62
1:CQ:187:SER:OG	2:CR:64:ARG:NH1	2.31	0.62
1:CC:57:TYR:O	2:CD:69:LYS:NZ	2.25	0.62
2:AL:21:LEU:HD12	2:AL:31:LEU:HD11	1.82	0.61
1:AS:104:LYS:NZ	1:AS:238:ASN:O	2.27	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BV:150:LYS:HG2	2:BV:153:GLU:HB2	1.82	0.61
1:CI:78:GLN:NE2	1:CI:115:VAL:HG21	2.14	0.61
2:CN:128:GLU:O	2:CN:131:GLN:HG3	2.00	0.61
1:CS:24:ALA:HB1	1:CS:114:ARG:HE	1.64	0.61
2:DR:3:VAL:HB	2:DT:128:GLU:HG3	1.82	0.61
2:BD:128:GLU:O	2:BD:131:GLN:HG3	1.99	0.61
1:CA:55:HIS:O	2:CB:72:TYR:OH	2.17	0.61
1:CI:78:GLN:HE22	1:CI:115:VAL:HG21	1.64	0.61
1:CM:206:VAL:HA	1:CM:221:TYR:CD1	2.34	0.61
2:DN:47:LEU:HB2	2:DN:145:TYR:HB2	1.81	0.61
1:DE:187:SER:OG	2:DF:64:ARG:NH1	2.33	0.61
2:BD:5:VAL:HA	2:BD:11:PRO:HA	1.81	0.61
1:BM:153:LEU:HD11	1:BM:185:LYS:HD2	1.81	0.61
2:DF:138:LEU:HB3	2:DF:145:TYR:HD1	1.63	0.61
1:BS:144:THR:HG21	2:BT:16:ALA:HB1	1.81	0.61
2:BJ:3:VAL:HB	2:BL:128:GLU:HG3	1.81	0.61
1:CC:146:TYR:OH	2:CD:66:ASN:OD1	2.15	0.61
2:AH:28:HIS:NE2	1:AK:228:VAL:HB	2.16	0.61
1:BI:96:LEU:HD11	2:BJ:109:LEU:HD11	1.83	0.61
2:BJ:128:GLU:O	2:BJ:131:GLN:HG3	2.00	0.61
2:CP:46:VAL:HG12	2:CP:146:TYR:HA	1.82	0.61
1:CQ:16:ILE:N	1:CQ:191:ASP:OD2	2.34	0.61
2:DD:128:GLU:HB2	2:DD:131:GLN:OE1	1.99	0.61
1:AI:206:VAL:HA	1:AI:221:TYR:CD1	2.35	0.61
2:AV:128:GLU:H	2:AV:131:GLN:HG3	1.66	0.61
2:BH:145:TYR:OH	1:BK:124:CYS:O	2.19	0.61
2:DB:5:VAL:HB	2:DB:10:GLN:O	2.01	0.61
1:CA:142:SER:OG	2:CB:82:SER:OG	2.10	0.61
2:DP:21:LEU:HD12	2:DP:31:LEU:HD11	1.82	0.61
2:BD:22:VAL:HB	2:BD:158:LYS:HB2	1.83	0.60
1:AQ:129:THR:HB	1:AQ:157:ILE:HD12	1.81	0.60
2:DJ:128:GLU:O	2:DJ:131:GLN:HG3	2.01	0.60
2:BB:3:VAL:HB	2:BD:128:GLU:HG3	1.84	0.60
2:BN:98:LEU:HB2	2:BN:149:VAL:HB	1.82	0.60
2:BT:47:LEU:HB2	2:BT:145:TYR:HB2	1.83	0.60
2:DP:145:TYR:OH	1:DS:124:CYS:N	2.33	0.60
1:AK:206:VAL:HA	1:AK:221:TYR:CD1	2.36	0.60
2:BH:15:GLY:N	2:BH:59:PHE:O	2.34	0.60
1:BS:71:ASN:ND2	1:BS:148:ASP:OD2	2.34	0.60
2:CB:145:TYR:OH	1:CE:124:CYS:O	2.18	0.60
2:CN:145:TYR:HE2	1:CQ:123:SER:HB2	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DE:146:TYR:OH	2:DF:66:ASN:OD1	2.18	0.60
2:AB:28:HIS:NE2	1:AE:228:VAL:HB	2.17	0.60
2:DF:121:TYR:O	2:DF:157:PHE:N	2.29	0.60
2:BL:18:ALA:HB1	2:BL:56:PRO:HB2	1.84	0.60
1:CG:57:TYR:O	2:CH:69:LYS:NZ	2.20	0.60
1:DU:71:ASN:ND2	1:DU:148:ASP:OD2	2.34	0.60
1:BS:133:ILE:HG12	1:BS:196:VAL:HG13	1.83	0.60
2:CL:28:HIS:CD2	1:CO:228:VAL:HB	2.37	0.60
1:DO:187:SER:OG	2:DP:64:ARG:NH1	2.35	0.60
2:AB:9:GLY:HA2	2:AD:131:GLN:HE22	1.66	0.59
1:BI:132:LEU:HD13	1:BI:154:LYS:HE2	1.83	0.59
2:BN:4:VAL:HG13	2:BN:121:TYR:CZ	2.37	0.59
1:DC:184:GLY:H	1:DC:213:ALA:HB1	1.67	0.59
1:AI:71:ASN:ND2	1:AI:148:ASP:OD2	2.35	0.59
2:AR:127:PRO:HD2	2:AR:131:GLN:NE2	2.16	0.59
2:BN:5:VAL:HG12	2:BN:11:PRO:HA	1.83	0.59
1:CA:32:SER:OG	1:CA:38:HIS:ND1	2.29	0.59
1:DC:196:VAL:HG21	1:DC:221:TYR:CD1	2.37	0.59
2:DF:21:LEU:HD12	2:DF:31:LEU:HD11	1.84	0.59
2:AR:5:VAL:HG12	2:AR:11:PRO:HA	1.84	0.59
1:BG:58:LYS:HZ1	2:BJ:128:GLU:CD	2.05	0.59
2:BH:3:VAL:HB	2:BJ:128:GLU:HG3	1.84	0.59
2:CR:5:VAL:HG12	2:CR:11:PRO:HA	1.84	0.59
2:DD:46:VAL:HG12	2:DD:146:TYR:HA	1.85	0.59
2:AJ:127:PRO:HD2	2:AJ:131:GLN:NE2	2.17	0.59
1:CG:25:ASN:OD1	1:CG:114:ARG:NE	2.26	0.59
2:CV:46:VAL:HG12	2:CV:146:TYR:HA	1.83	0.59
2:BH:128:GLU:H	2:BH:131:GLN:NE2	2.01	0.59
1:BO:81:SER:HB2	1:BO:106:LYS:HD3	1.84	0.59
1:AQ:130:GLN:HE21	1:CG:26:THR:HA	1.67	0.59
2:BR:131:GLN:HG2	2:BR:132:THR:N	2.18	0.59
1:CK:184:GLY:H	1:CK:213:ALA:HB1	1.67	0.59
1:DA:128:GLY:N	1:DA:157:ILE:O	2.32	0.59
1:AE:71:ASN:ND2	1:AE:148:ASP:OD2	2.35	0.59
2:AN:28:HIS:O	2:AN:49:PRO:HA	2.01	0.59
1:AQ:153:LEU:HD11	1:AQ:185:LYS:HD2	1.85	0.59
2:CF:138:LEU:HD22	2:CF:145:TYR:HB3	1.85	0.59
2:DL:9:GLY:HA2	2:DN:131:GLN:HE22	1.67	0.59
1:AS:133:ILE:HG12	1:AS:196:VAL:HG22	1.85	0.59
1:BK:206:VAL:HA	1:BK:221:TYR:CD1	2.38	0.59
1:BO:205:ILE:HB	1:BO:222:THR:HB	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BE:133:ILE:HG12	1:BE:196:VAL:HG22	1.85	0.58
2:AD:46:VAL:HG12	2:AD:146:TYR:HA	1.85	0.58
1:AE:24:ALA:HB1	1:AE:114:ARG:HE	1.69	0.58
2:BP:28:HIS:NE2	1:BS:228:VAL:HB	2.19	0.58
2:BT:15:GLY:N	2:BT:59:PHE:O	2.37	0.58
2:AV:35:LYS:O	2:AV:146:TYR:OH	2.19	0.58
2:AB:21:LEU:HD12	2:AB:31:LEU:HD11	1.84	0.58
2:AN:128:GLU:C	2:AN:131:GLN:HE22	2.07	0.58
1:BA:106:LYS:NZ	2:BD:104:ASP:OD2	2.33	0.58
1:CG:153:LEU:HD11	1:CG:185:LYS:HD2	1.84	0.58
1:CO:132:LEU:HD13	1:CO:154:LYS:HE2	1.86	0.58
1:BC:96:LEU:HD11	2:BD:109:LEU:HD11	1.85	0.58
1:CA:71:ASN:ND2	1:CA:148:ASP:OD2	2.37	0.58
2:CH:135:ASP:HB3	2:CH:154:PRO:HB3	1.84	0.58
1:DA:206:VAL:HA	1:DA:221:TYR:CD1	2.38	0.58
1:DC:37:TYR:CZ	2:DD:11:PRO:HG2	2.37	0.58
2:AP:39:GLU:OE2	2:AP:101:LYS:NZ	2.26	0.58
1:CG:104:LYS:NZ	1:CG:238:ASN:O	2.27	0.58
1:CO:139:THR:HG23	1:CO:147:PRO:HD3	1.86	0.58
1:BI:153:LEU:HD11	1:BI:185:LYS:HD2	1.86	0.58
2:BL:15:GLY:N	2:BL:59:PHE:O	2.36	0.58
2:DB:47:LEU:HB2	2:DB:145:TYR:HB2	1.86	0.58
2:AV:48:ASP:HB3	2:AV:51:HIS:HB2	1.85	0.58
1:BI:106:LYS:NZ	2:BL:104:ASP:OD1	2.36	0.58
1:AQ:113:SER:HB3	2:CD:143:ASP:HB2	1.86	0.58
1:CI:54:ALA:HA	1:CI:101:MET:HB2	1.86	0.58
2:DB:128:GLU:HB2	2:DB:131:GLN:NE2	2.18	0.58
2:DF:98:LEU:HB2	2:DF:149:VAL:HB	1.86	0.58
2:CP:3:VAL:HB	2:CR:128:GLU:HG3	1.85	0.58
2:AV:5:VAL:HG12	2:AV:11:PRO:HA	1.85	0.57
1:CA:37:TYR:CZ	2:CB:11:PRO:HG2	2.38	0.57
2:CB:77:LYS:HE3	2:CB:83:SER:O	2.04	0.57
1:CM:43:SER:HB2	1:CM:51:VAL:HG22	1.85	0.57
1:CO:74:GLU:N	1:CO:77:GLU:OE1	2.38	0.57
1:BI:153:LEU:HD21	1:BI:185:LYS:HB3	1.85	0.57
2:CR:28:HIS:CE1	2:CR:52:ARG:HD3	2.39	0.57
1:AA:84:LYS:NZ	1:AA:238:ASN:OD1	2.36	0.57
2:BF:7:THR:N	2:BF:159:ILE:O	2.37	0.57
2:CJ:127:PRO:HD2	2:CJ:131:GLN:NE2	2.19	0.57
1:CO:149:VAL:HB	2:DF:50:HIS:CE1	2.39	0.57
2:DV:47:LEU:HB2	2:DV:145:TYR:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AN:21:LEU:HD12	2:AN:31:LEU:HD11	1.85	0.57
2:BF:128:GLU:H	2:BF:131:GLN:NE2	2.03	0.57
1:BQ:153:LEU:HD11	1:BQ:185:LYS:HD2	1.85	0.57
1:CC:96:LEU:HD11	2:CD:109:LEU:HD11	1.85	0.57
2:CR:127:PRO:HD2	2:CR:131:GLN:HE21	1.70	0.57
2:BP:5:VAL:HG21	2:BR:131:GLN:CB	2.35	0.57
1:CI:133:ILE:HG12	1:CI:196:VAL:HG22	1.86	0.57
2:DF:138:LEU:HD22	2:DF:145:TYR:HB3	1.86	0.57
1:AG:206:VAL:HA	1:AG:221:TYR:CD1	2.39	0.57
1:CC:206:VAL:HA	1:CC:221:TYR:CD1	2.39	0.57
1:CK:206:VAL:HA	1:CK:221:TYR:HD1	1.69	0.57
1:DC:153:LEU:HD11	1:DC:185:LYS:HD2	1.85	0.57
1:DE:178:ALA:HB3	1:DE:221:TYR:CE2	2.39	0.57
2:DV:128:GLU:N	2:DV:131:GLN:OE1	2.38	0.57
2:AD:12:VAL:HG13	2:AD:19:TYR:CE1	2.40	0.57
2:AP:28:HIS:CE1	1:AS:229:SER:H	2.20	0.57
2:CH:128:GLU:N	2:CH:131:GLN:OE1	2.37	0.57
2:CT:46:VAL:HG12	2:CT:146:TYR:HA	1.87	0.57
2:DF:33:LEU:HB3	2:DF:42:PRO:HB2	1.87	0.57
1:DK:80:ILE:HG21	1:DK:105:LEU:HB3	1.86	0.57
1:BU:153:LEU:HD11	1:BU:185:LYS:HD2	1.86	0.57
2:CJ:48:ASP:HB3	2:CJ:51:HIS:HB2	1.87	0.57
2:AF:128:GLU:N	2:AF:131:GLN:OE1	2.38	0.57
1:BQ:184:GLY:H	1:BQ:213:ALA:HB1	1.70	0.57
1:CM:140:LYS:HG3	1:CM:145:SER:HB3	1.87	0.57
1:AE:104:LYS:NZ	1:AE:238:ASN:O	2.28	0.56
1:CE:206:VAL:HA	1:CE:221:TYR:CD1	2.40	0.56
1:CK:187:SER:OG	2:CL:64:ARG:NH1	2.38	0.56
1:DE:74:GLU:N	1:DE:77:GLU:OE1	2.38	0.56
2:AD:128:GLU:O	2:AD:131:GLN:HG3	2.05	0.56
2:AF:128:GLU:O	2:AF:131:GLN:HG3	2.05	0.56
1:AM:204:GLY:HA2	1:AM:222:THR:O	2.04	0.56
1:AS:71:ASN:ND2	1:AS:148:ASP:OD2	2.38	0.56
1:BC:206:VAL:HA	1:BC:221:TYR:CD1	2.36	0.56
1:DI:83:SER:HB3	1:DI:106:LYS:HB3	1.88	0.56
2:BT:19:TYR:N	2:BT:57:VAL:O	2.38	0.56
1:CM:94:ASN:HA	2:CN:73:PHE:HE2	1.70	0.56
1:CQ:178:ALA:HB3	1:CQ:221:TYR:CE2	2.41	0.56
2:DN:128:GLU:O	2:DN:131:GLN:HG3	2.05	0.56
2:BB:98:LEU:HB2	2:BB:149:VAL:HB	1.86	0.56
1:BG:37:TYR:CZ	2:BH:11:PRO:HG2	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AG:57:TYR:OH	1:AI:168:PRO:O	2.13	0.56
2:BD:127:PRO:HD2	2:BD:131:GLN:NE2	2.20	0.56
2:CL:18:ALA:HB1	2:CL:56:PRO:HB2	1.87	0.56
1:DO:206:VAL:HA	1:DO:221:TYR:CD1	2.40	0.56
2:DB:3:VAL:HB	2:DD:128:GLU:HG3	1.86	0.56
2:DF:134:LEU:HB3	2:DF:149:VAL:HG13	1.87	0.56
2:DL:128:GLU:H	2:DL:131:GLN:NE2	2.04	0.56
1:DS:206:VAL:HA	1:DS:221:TYR:CD1	2.40	0.56
2:AN:46:VAL:HG12	2:AN:146:TYR:HA	1.87	0.56
1:DG:96:LEU:HD11	2:DH:109:LEU:HD11	1.86	0.56
2:AL:121:TYR:OH	2:AN:131:GLN:HG3	2.05	0.56
1:CA:184:GLY:H	1:CA:213:ALA:HB1	1.71	0.56
1:CU:211:GLY:O	2:CV:64:ARG:NH2	2.38	0.56
2:DL:12:VAL:HG13	2:DL:19:TYR:CE1	2.40	0.56
1:AI:104:LYS:NZ	1:AI:238:ASN:O	2.38	0.56
1:AI:58:LYS:HZ1	2:AL:128:GLU:CD	2.09	0.56
2:CD:23:PRO:HG3	2:CD:47:LEU:HD13	1.88	0.56
2:CF:46:VAL:HG12	2:CF:146:TYR:HA	1.87	0.56
2:DJ:128:GLU:N	2:DJ:131:GLN:OE1	2.39	0.56
1:CK:104:LYS:NZ	1:CK:238:ASN:O	2.31	0.56
2:CP:20:TYR:CE2	2:CP:162:ALA:HA	2.40	0.56
2:DL:47:LEU:HB2	2:DL:145:TYR:HB2	1.86	0.56
1:DS:133:ILE:HG12	1:DS:196:VAL:HG22	1.88	0.56
2:DV:29:ALA:HB1	2:DV:47:LEU:HB3	1.88	0.56
1:BK:186:ASP:OD2	2:BL:64:ARG:NH2	2.32	0.55
2:DD:47:LEU:HG	2:DD:147:LEU:HD11	1.88	0.55
1:BQ:133:ILE:HG12	1:BQ:196:VAL:HG22	1.86	0.55
2:CF:150:LYS:HG2	2:CF:153:GLU:HB2	1.88	0.55
1:AQ:129:THR:HG23	1:CG:113:SER:HA	1.88	0.55
1:DC:51:VAL:HG12	1:DC:102:LEU:HD23	1.87	0.55
1:DS:54:ALA:N	1:DS:99:ASP:OD1	2.38	0.55
1:AO:32:SER:OG	1:AO:38:HIS:ND1	2.24	0.55
1:BM:139:THR:HG23	1:BM:147:PRO:HD3	1.89	0.55
1:CM:139:THR:HG23	1:CM:147:PRO:HD3	1.88	0.55
1:CS:78:GLN:NE2	1:CS:115:VAL:HG21	2.21	0.55
2:BD:89:ASP:OD1	2:BD:90:VAL:N	2.39	0.55
1:CC:154:LYS:O	1:CC:180:TYR:OH	2.23	0.55
2:AP:93:GLN:OE1	2:AP:101:LYS:HD2	2.06	0.55
2:AR:46:VAL:HG12	2:AR:146:TYR:HA	1.87	0.55
1:BG:58:LYS:NZ	2:BJ:128:GLU:OE1	2.39	0.55
1:CE:24:ALA:HB1	1:CE:114:ARG:HE	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CO:144:THR:HG21	2:CP:16:ALA:HA	1.89	0.55
1:BA:144:THR:HG21	2:BB:16:ALA:HA	1.88	0.55
2:BN:128:GLU:O	2:BN:131:GLN:HG3	2.06	0.55
1:BS:96:LEU:HD11	2:BT:109:LEU:HD11	1.89	0.55
2:CN:9:GLY:HA2	2:CP:131:GLN:HE22	1.71	0.55
1:CQ:32:SER:OG	1:CQ:38:HIS:ND1	2.30	0.55
1:DU:144:THR:HG21	2:DV:16:ALA:HB1	1.89	0.55
2:CB:116:LYS:HG2	1:CC:94:ASN:HD22	1.69	0.55
1:DU:167:TYR:OH	1:DU:218:PRO:O	2.17	0.55
2:DV:127:PRO:HD2	2:DV:131:GLN:NE2	2.22	0.55
2:AH:39:GLU:OE2	2:AH:101:LYS:NZ	2.31	0.55
2:BD:77:LYS:HE3	2:BD:83:SER:O	2.07	0.55
2:BJ:128:GLU:N	2:BJ:131:GLN:OE1	2.40	0.55
2:BP:33:LEU:HB3	2:BP:42:PRO:HB2	1.89	0.55
1:BU:184:GLY:H	1:BU:213:ALA:HB1	1.72	0.55
1:CA:184:GLY:N	1:CA:213:ALA:HB1	2.22	0.55
1:CS:94:ASN:HA	2:CT:73:PHE:HE2	1.72	0.55
2:AD:127:PRO:HD2	2:AD:131:GLN:NE2	2.22	0.55
2:BF:137:GLY:N	2:BF:148:ALA:O	2.39	0.55
2:BF:48:ASP:HB3	2:BF:51:HIS:HB2	1.87	0.55
2:CD:126:TYR:HB3	2:CD:128:GLU:O	2.07	0.54
2:CP:47:LEU:HG	2:CP:147:LEU:HD11	1.88	0.54
1:DI:32:SER:OG	1:DI:38:HIS:ND1	2.28	0.54
1:AU:184:GLY:N	1:AU:213:ALA:HB1	2.22	0.54
2:BH:39:GLU:OE2	2:BH:101:LYS:NZ	2.39	0.54
1:CK:96:LEU:HD11	2:CL:109:LEU:HD11	1.88	0.54
1:BU:133:ILE:HG12	1:BU:196:VAL:HG22	1.88	0.54
1:CI:182:GLU:HG2	1:DO:237:SER:HA	1.89	0.54
1:BI:51:VAL:HG12	1:BI:102:LEU:HD23	1.89	0.54
2:CD:4:VAL:HG13	2:CD:121:TYR:CZ	2.42	0.54
2:BB:21:LEU:HD12	2:BB:31:LEU:HD11	1.88	0.54
1:BQ:206:VAL:HA	1:BQ:221:TYR:CD1	2.42	0.54
2:DJ:46:VAL:HG12	2:DJ:146:TYR:HA	1.89	0.54
2:DN:98:LEU:HB2	2:DN:149:VAL:HB	1.89	0.54
2:DP:128:GLU:O	2:DP:131:GLN:HG2	2.07	0.54
2:AT:6:ASP:OD1	2:AT:10:GLN:N	2.32	0.54
2:BB:28:HIS:CD2	1:BE:228:VAL:HB	2.42	0.54
1:CA:206:VAL:HA	1:CA:221:TYR:CD1	2.43	0.54
2:CF:5:VAL:HG11	2:CH:131:GLN:HG2	1.90	0.54
1:CU:196:VAL:HG21	1:CU:221:TYR:CD1	2.43	0.54
2:AJ:36:ILE:HG12	2:AJ:44:ALA:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AQ:106:LYS:NZ	2:AT:104:ASP:OD1	2.37	0.54
1:CI:206:VAL:HA	1:CI:221:TYR:CD1	2.42	0.54
1:CS:187:SER:OG	2:CT:64:ARG:NH1	2.40	0.54
1:AG:98:ASN:HA	1:AG:227:TYR:OH	2.08	0.54
1:BQ:205:ILE:HB	1:BQ:222:THR:HB	1.90	0.54
2:BR:128:GLU:H	2:BR:131:GLN:HE22	1.55	0.54
1:BS:206:VAL:HA	1:BS:221:TYR:CD1	2.42	0.54
2:CL:28:HIS:HD2	1:CO:228:VAL:HB	1.72	0.54
2:CR:20:TYR:N	2:CR:160:ARG:O	2.38	0.54
1:CS:74:GLU:N	1:CS:77:GLU:OE1	2.41	0.54
2:CH:89:ASP:OD1	2:CH:90:VAL:N	2.41	0.54
1:DM:138:ASN:HD21	1:DM:144:THR:HA	1.73	0.54
2:AB:28:HIS:CD2	1:AE:228:VAL:HB	2.42	0.54
1:BA:55:HIS:CE1	2:BB:63:LEU:HD22	2.43	0.54
1:DI:76:ASN:HB2	1:DI:114:ARG:HH11	1.73	0.54
1:AA:206:VAL:HA	1:AA:221:TYR:CD1	2.44	0.53
1:AE:16:ILE:N	1:AE:138:ASN:O	2.42	0.53
2:AF:145:TYR:OH	1:AI:123:SER:HB3	2.07	0.53
2:AT:60:GLU:OE1	2:AT:106:LYS:HD2	2.08	0.53
2:BH:5:VAL:HG21	2:BJ:131:GLN:HB3	1.88	0.53
2:BJ:46:VAL:HG12	2:BJ:146:TYR:HA	1.90	0.53
1:CQ:139:THR:HG23	1:CQ:147:PRO:HD3	1.91	0.53
1:DQ:55:HIS:CE1	2:DR:63:LEU:HD22	2.43	0.53
2:DT:98:LEU:HB2	2:DT:149:VAL:HB	1.90	0.53
2:AB:128:GLU:HB2	2:AB:131:GLN:NE2	2.23	0.53
1:AO:81:SER:CB	2:AR:105:THR:HG21	2.38	0.53
2:BJ:98:LEU:HB2	2:BJ:149:VAL:HB	1.89	0.53
1:BQ:167:TYR:OH	1:BQ:218:PRO:O	2.15	0.53
2:CD:26:HIS:NE2	2:CD:138:LEU:HD13	2.23	0.53
2:CH:127:PRO:HD2	2:CH:131:GLN:NE2	2.24	0.53
1:DE:204:GLY:HA2	1:DE:222:THR:O	2.07	0.53
1:AO:96:LEU:HD11	2:AP:109:LEU:HD11	1.90	0.53
2:BJ:127:PRO:HB2	2:BJ:131:GLN:OE1	2.07	0.53
1:DI:206:VAL:HA	1:DI:221:TYR:CD1	2.44	0.53
2:DL:98:LEU:HB2	2:DL:149:VAL:HB	1.89	0.53
1:DS:32:SER:OG	1:DS:38:HIS:ND1	2.34	0.53
1:BI:206:VAL:HA	1:BI:221:TYR:CD1	2.43	0.53
2:CB:128:GLU:HB2	2:CB:131:GLN:CD	2.29	0.53
2:CD:128:GLU:O	2:CD:131:GLN:HG3	2.08	0.53
1:CM:81:SER:HB3	2:CP:105:THR:HG21	1.90	0.53
1:DE:57:TYR:OH	1:DG:168:PRO:HB2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:DJ:35:LYS:O	2:DJ:146:TYR:OH	2.20	0.53
1:DO:153:LEU:HD11	1:DO:185:LYS:HD2	1.90	0.53
1:AK:187:SER:OG	2:AL:64:ARG:NH1	2.42	0.53
1:AO:25:ASN:HD21	1:AO:113:SER:HB2	1.73	0.53
1:BC:178:ALA:HB3	1:BC:221:TYR:CE2	2.43	0.53
2:BL:145:TYR:OH	1:BO:124:CYS:O	2.25	0.53
1:CA:187:SER:OG	2:CB:64:ARG:NH1	2.39	0.53
2:CD:87:VAL:HG21	2:CD:106:LYS:HB2	1.90	0.53
2:AB:28:HIS:CE1	1:AE:229:SER:HB3	2.32	0.53
1:AK:68:ASP:O	1:AK:149:VAL:HA	2.09	0.53
1:BA:43:SER:HB2	1:BA:51:VAL:HG22	1.90	0.53
2:AF:77:LYS:HE3	2:AF:83:SER:O	2.08	0.53
2:AN:9:GLY:HA2	2:AP:131:GLN:HE22	1.72	0.53
1:AU:170:GLN:HG3	2:AV:108:LEU:HD23	1.90	0.53
1:BE:76:ASN:HB2	1:BE:114:ARG:HH11	1.74	0.53
2:BL:134:LEU:HD13	2:BL:149:VAL:HG11	1.89	0.53
2:BL:28:HIS:O	2:BL:49:PRO:HA	2.09	0.53
1:BQ:187:SER:OG	2:BR:64:ARG:NH1	2.42	0.53
1:CG:204:GLY:HA2	1:CG:222:THR:O	2.08	0.53
1:CK:206:VAL:HA	1:CK:221:TYR:CD1	2.44	0.53
1:DE:24:ALA:HB1	1:DE:114:ARG:HE	1.72	0.53
1:AA:67:GLU:HG3	1:AA:77:GLU:HG2	1.91	0.53
2:AF:46:VAL:HG12	2:AF:146:TYR:HA	1.90	0.53
2:AT:77:LYS:HE3	2:AT:83:SER:O	2.09	0.53
2:BH:28:HIS:NE2	1:BK:229:SER:OG	2.33	0.53
1:CQ:204:GLY:HA2	1:CQ:222:THR:O	2.09	0.53
1:DA:129:THR:O	1:DA:156:PRO:HA	2.09	0.53
1:CO:23:GLY:HA2	2:DF:50:HIS:HA	1.89	0.53
2:DJ:5:VAL:CG2	2:DL:131:GLN:HB3	2.38	0.53
1:AU:130:GLN:OE1	1:AU:156:PRO:HB3	2.09	0.53
1:CA:68:ASP:O	1:CA:149:VAL:HA	2.09	0.53
2:CN:47:LEU:HB2	2:CN:145:TYR:HB2	1.90	0.53
1:AK:24:ALA:HB1	1:AK:114:ARG:HE	1.74	0.53
2:AP:89:ASP:OD1	2:AP:90:VAL:N	2.42	0.53
1:BA:24:ALA:HB1	1:BA:114:ARG:NE	2.18	0.53
1:CC:88:HIS:HB2	1:CC:100:ILE:HG23	1.91	0.53
1:CG:37:TYR:CZ	2:CH:11:PRO:HG2	2.43	0.53
1:DA:69:ASN:HA	1:DA:148:ASP:O	2.09	0.53
1:CO:21:THR:HG23	2:DF:50:HIS:CE1	2.44	0.53
2:AP:21:LEU:HD12	2:AP:31:LEU:HD11	1.91	0.52
2:BD:128:GLU:N	2:BD:131:GLN:OE1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DK:96:LEU:HD11	2:DL:109:LEU:HD11	1.91	0.52
2:DR:128:GLU:O	2:DR:131:GLN:HG3	2.09	0.52
2:AN:5:VAL:HG21	2:AP:131:GLN:CG	2.39	0.52
2:AP:28:HIS:O	2:AP:49:PRO:HA	2.10	0.52
2:AP:98:LEU:HB2	2:AP:149:VAL:HB	1.90	0.52
2:BH:46:VAL:HG21	2:BH:144:LYS:HD3	1.90	0.52
1:BK:146:TYR:OH	2:BL:66:ASN:OD1	2.18	0.52
2:BR:140:HIS:ND1	1:BU:126:SER:OG	2.32	0.52
2:BR:52:ARG:NH1	1:BU:229:SER:HB3	2.24	0.52
2:CN:5:VAL:CG2	2:CP:131:GLN:HB3	2.39	0.52
1:DE:43:SER:HB2	1:DE:51:VAL:HG22	1.91	0.52
1:DM:81:SER:CB	2:DP:105:THR:HG21	2.39	0.52
1:DU:54:ALA:N	1:DU:99:ASP:OD1	2.42	0.52
2:AB:29:ALA:HB1	2:AB:47:LEU:HB3	1.90	0.52
1:CQ:106:LYS:NZ	2:CT:104:ASP:OD1	2.39	0.52
1:DG:206:VAL:HA	1:DG:221:TYR:CD1	2.44	0.52
2:DL:5:VAL:HG11	2:DN:131:GLN:CD	2.30	0.52
2:BP:89:ASP:OD1	2:BP:90:VAL:N	2.40	0.52
1:CA:48:GLN:HG2	1:CA:108:ALA:HA	1.92	0.52
2:CL:135:ASP:HB3	2:CL:154:PRO:HB3	1.91	0.52
2:DN:15:GLY:N	2:DN:59:PHE:O	2.43	0.52
2:DP:5:VAL:HG21	2:DR:131:GLN:HB3	1.91	0.52
1:AE:24:ALA:HB1	1:AE:114:ARG:NE	2.25	0.52
2:AH:80:PRO:HG3	2:BN:51:HIS:CD2	2.44	0.52
1:AQ:113:SER:CB	2:CD:143:ASP:HB2	2.39	0.52
1:AQ:43:SER:HB2	1:AQ:51:VAL:HG22	1.92	0.52
1:AU:51:VAL:HG12	1:AU:102:LEU:HD23	1.90	0.52
2:BB:134:LEU:HD13	2:BB:149:VAL:HG11	1.92	0.52
1:CQ:146:TYR:OH	2:CR:66:ASN:OD1	2.04	0.52
2:CR:77:LYS:NZ	2:CR:80:PRO:O	2.35	0.52
2:DB:5:VAL:HG12	2:DB:11:PRO:CA	2.32	0.52
1:DI:51:VAL:HG12	1:DI:102:LEU:HD23	1.92	0.52
1:DS:71:ASN:ND2	1:DS:148:ASP:OD2	2.42	0.52
2:AB:47:LEU:HG	2:AB:147:LEU:HD11	1.92	0.52
2:BN:48:ASP:HB3	2:BN:51:HIS:HB2	1.91	0.52
2:BT:128:GLU:O	2:BT:131:GLN:HG3	2.10	0.52
2:CD:28:HIS:NE2	1:CG:229:SER:HB3	2.24	0.52
1:CQ:24:ALA:HB1	1:CQ:114:ARG:NE	2.25	0.52
1:DK:68:ASP:O	1:DK:149:VAL:HA	2.10	0.52
1:AG:78:GLN:OE1	1:AG:110:SER:OG	2.27	0.52
1:CK:204:GLY:HA2	1:CK:222:THR:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CO:206:VAL:HA	1:CO:221:TYR:CD1	2.44	0.52
2:CV:5:VAL:HG12	2:CV:11:PRO:HA	1.92	0.52
1:AM:192:SER:HA	1:AM:206:VAL:HG13	1.92	0.52
1:AM:206:VAL:HA	1:AM:221:TYR:CD1	2.45	0.52
2:AT:5:VAL:HG21	2:AV:131:GLN:HG2	1.91	0.52
1:BE:196:VAL:HG21	1:BE:221:TYR:CD1	2.45	0.52
2:CB:2:SER:OG	2:CD:129:ARG:NH1	2.43	0.52
2:CJ:121:TYR:O	2:CJ:157:PHE:N	2.32	0.52
2:DN:125:TYR:CZ	2:DN:127:PRO:HA	2.44	0.52
2:DR:98:LEU:HB2	2:DR:149:VAL:HB	1.92	0.52
1:AK:112:ASN:HA	2:DL:95:PRO:HG3	1.90	0.52
1:CU:57:TYR:O	2:CV:69:LYS:NZ	2.28	0.52
2:CV:21:LEU:HD12	2:CV:31:LEU:HD11	1.90	0.52
2:DR:5:VAL:HG22	2:DT:131:GLN:CG	2.39	0.52
2:AF:127:PRO:HD2	2:AF:131:GLN:NE2	2.25	0.51
2:BH:145:TYR:CE2	1:BK:123:SER:HB2	2.44	0.51
1:CA:133:ILE:HG12	1:CA:196:VAL:HG22	1.91	0.51
1:CU:153:LEU:HD11	1:CU:185:LYS:HD2	1.91	0.51
2:DF:5:VAL:HG22	2:DH:131:GLN:CG	2.40	0.51
2:AR:128:GLU:O	2:AR:131:GLN:HG3	2.10	0.51
2:BD:145:TYR:OH	1:BG:124:CYS:O	2.28	0.51
2:BJ:127:PRO:HD2	2:BJ:131:GLN:NE2	2.25	0.51
1:BS:204:GLY:HA2	1:BS:222:THR:O	2.10	0.51
1:CG:206:VAL:HA	1:CG:221:TYR:CD1	2.45	0.51
2:CR:18:ALA:HB1	2:CR:56:PRO:HB2	1.91	0.51
1:DG:83:SER:HB3	1:DG:106:LYS:HB3	1.92	0.51
1:DI:144:THR:HG21	2:DJ:16:ALA:CB	2.40	0.51
1:DU:133:ILE:HG12	1:DU:196:VAL:HG22	1.93	0.51
1:AQ:96:LEU:HD11	2:AR:109:LEU:HD11	1.92	0.51
1:AU:96:LEU:HD11	2:AV:109:LEU:HD21	1.90	0.51
2:BD:3:VAL:HB	2:BF:128:GLU:HG3	1.92	0.51
2:BN:89:ASP:OD1	2:BN:90:VAL:N	2.43	0.51
1:CU:184:GLY:H	1:CU:213:ALA:HB1	1.76	0.51
2:CV:128:GLU:O	2:CV:131:GLN:HG3	2.10	0.51
2:AN:51:HIS:HD2	1:DO:24:ALA:HB3	1.74	0.51
2:AT:5:VAL:HG21	2:AV:131:GLN:CG	2.41	0.51
2:BL:21:LEU:HD12	2:BL:31:LEU:HD11	1.92	0.51
2:DD:87:VAL:O	2:DD:102:VAL:HA	2.10	0.51
1:DQ:167:TYR:HB2	1:DQ:171:ILE:HD11	1.92	0.51
2:DT:46:VAL:HG12	2:DT:146:TYR:HA	1.92	0.51
1:AM:68:ASP:O	1:AM:149:VAL:HA	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BM:71:ASN:ND2	1:BM:148:ASP:OD2	2.43	0.51
1:BO:24:ALA:HB1	1:BO:114:ARG:NE	2.26	0.51
1:CC:211:GLY:O	2:CD:64:ARG:NH2	2.42	0.51
1:CS:80:ILE:HG21	1:CS:105:LEU:HB3	1.92	0.51
1:CU:184:GLY:N	1:CU:213:ALA:HB1	2.25	0.51
1:DM:196:VAL:HG21	1:DM:221:TYR:CD1	2.46	0.51
1:DM:228:VAL:HA	1:DM:231:ILE:HD12	1.93	0.51
1:AK:71:ASN:ND2	1:AK:148:ASP:OD2	2.43	0.51
2:AP:12:VAL:HG13	2:AP:19:TYR:CE1	2.46	0.51
2:BR:5:VAL:HG11	2:BT:131:GLN:CD	2.31	0.51
1:CE:96:LEU:HD11	2:CF:109:LEU:HD11	1.93	0.51
2:CL:49:PRO:CG	1:CO:123:SER:HB3	2.40	0.51
2:CN:31:LEU:N	2:CN:54:GLY:HA3	2.26	0.51
2:DF:121:TYR:OH	2:DH:131:GLN:OE1	2.21	0.51
1:AO:102:LEU:HD21	1:AO:231:ILE:HG23	1.92	0.51
2:BD:89:ASP:N	2:BD:101:LYS:O	2.44	0.51
2:BP:5:VAL:HG21	2:BR:131:GLN:CG	2.40	0.51
2:CD:147:LEU:HD21	2:CD:157:PHE:HZ	1.75	0.51
1:CK:184:GLY:N	1:CK:213:ALA:HB1	2.26	0.51
1:CQ:138:ASN:HD21	1:CQ:144:THR:HA	1.75	0.51
1:CS:204:GLY:HA2	1:CS:222:THR:O	2.11	0.51
2:AF:116:LYS:NZ	2:AH:130:GLY:O	2.33	0.51
2:AH:5:VAL:HG21	2:AJ:131:GLN:CG	2.40	0.51
1:BA:138:ASN:ND2	1:BA:144:THR:HA	2.26	0.51
2:BJ:135:ASP:HB2	2:BJ:151:ASP:HA	1.93	0.51
2:DV:5:VAL:HG12	2:DV:11:PRO:HA	1.92	0.51
1:AE:54:ALA:N	1:AE:99:ASP:OD1	2.44	0.51
2:AF:145:TYR:CE1	1:AI:123:SER:HB3	2.46	0.51
2:BD:46:VAL:HG12	2:BD:146:TYR:HA	1.92	0.51
1:DK:16:ILE:N	1:DK:138:ASN:O	2.44	0.51
2:DT:5:VAL:HG21	2:DV:131:GLN:CG	2.41	0.51
1:BI:187:SER:OG	2:BJ:64:ARG:NH1	2.37	0.51
2:CJ:26:HIS:CE1	1:CM:123:SER:HB2	2.46	0.51
1:AC:138:ASN:ND2	1:AC:144:THR:HA	2.26	0.50
1:AE:68:ASP:O	1:AE:149:VAL:HA	2.11	0.50
2:AH:46:VAL:HG12	2:AH:146:TYR:HA	1.93	0.50
2:BJ:9:GLY:HA2	2:BL:127:PRO:HG2	1.92	0.50
1:BM:102:LEU:HD11	1:BM:231:ILE:HA	1.92	0.50
2:CN:3:VAL:HB	2:CP:128:GLU:HG3	1.92	0.50
1:CU:34:ASN:O	1:CU:62:GLN:N	2.31	0.50
2:DF:28:HIS:O	2:DF:49:PRO:HA	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BG:16:ILE:HD13	1:BG:187:SER:HA	1.93	0.50
2:BR:98:LEU:HB2	2:BR:149:VAL:HB	1.93	0.50
2:CL:5:VAL:HG21	2:CN:131:GLN:CG	2.40	0.50
1:DE:133:ILE:HG12	1:DE:196:VAL:HG22	1.92	0.50
2:DF:28:HIS:CE1	1:DI:229:SER:HA	2.46	0.50
1:DS:154:LYS:O	1:DS:180:TYR:OH	2.17	0.50
1:DU:131:CYS:O	1:DU:154:LYS:HA	2.11	0.50
1:DU:206:VAL:HA	1:DU:221:TYR:CD1	2.41	0.50
2:DV:91:ILE:HB	2:DV:101:LYS:HD3	1.93	0.50
2:AB:9:GLY:HA2	2:AD:131:GLN:NE2	2.26	0.50
1:AS:78:GLN:NE2	1:AS:115:VAL:HG21	2.26	0.50
1:BA:113:SER:OG	1:BA:114:ARG:N	2.44	0.50
2:BR:46:VAL:HG12	2:BR:146:TYR:HA	1.93	0.50
1:CG:74:GLU:N	1:CG:77:GLU:OE1	2.44	0.50
2:AN:5:VAL:HG11	2:AP:131:GLN:HG2	1.93	0.50
2:AP:128:GLU:O	2:AP:131:GLN:HG3	2.11	0.50
2:DP:135:ASP:HB3	2:DP:154:PRO:HB3	1.94	0.50
2:DP:47:LEU:HB2	2:DP:145:TYR:HB2	1.92	0.50
2:AB:21:LEU:HB3	2:AB:157:PHE:CD1	2.47	0.50
2:AB:5:VAL:HG21	2:AD:131:GLN:CG	2.40	0.50
2:AF:127:PRO:HB2	2:AF:131:GLN:OE1	2.11	0.50
1:AS:51:VAL:HG12	1:AS:102:LEU:HD23	1.93	0.50
2:BT:46:VAL:HG12	2:BT:146:TYR:HA	1.93	0.50
1:CK:178:ALA:HB3	1:CK:221:TYR:CE2	2.47	0.50
1:AQ:206:VAL:HA	1:AQ:221:TYR:CD1	2.47	0.50
2:AV:13:SER:HA	2:AV:66:ASN:O	2.10	0.50
1:BS:54:ALA:N	1:BS:99:ASP:OD1	2.45	0.50
2:CH:46:VAL:HG12	2:CH:146:TYR:HA	1.93	0.50
1:DG:67:GLU:HG3	1:DG:77:GLU:HG3	1.92	0.50
2:DV:135:ASP:HB2	2:DV:151:ASP:HA	1.94	0.50
2:DV:7:THR:N	2:DV:159:ILE:O	2.44	0.50
1:AI:96:LEU:HD11	2:AJ:109:LEU:HD11	1.93	0.50
1:AK:206:VAL:HA	1:AK:221:TYR:HD1	1.76	0.50
1:AS:140:LYS:HG3	1:AS:145:SER:HB3	1.93	0.50
2:AV:126:TYR:HB3	2:AV:128:GLU:O	2.11	0.50
1:AS:58:LYS:HZ1	2:AV:128:GLU:CD	2.14	0.50
1:BK:71:ASN:ND2	1:BK:148:ASP:OD2	2.44	0.50
2:CB:5:VAL:HG11	2:CD:131:GLN:HG2	1.94	0.50
2:CR:137:GLY:N	2:CR:148:ALA:O	2.40	0.50
2:CR:15:GLY:N	2:CR:59:PHE:O	2.44	0.50
2:DL:46:VAL:HG12	2:DL:146:TYR:HA	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DM:206:VAL:HA	1:DM:221:TYR:CD1	2.47	0.50
1:DQ:43:SER:HB2	1:DQ:51:VAL:HG22	1.94	0.50
1:DS:153:LEU:HD11	1:DS:185:LYS:HD2	1.93	0.50
1:AI:133:ILE:HG12	1:AI:196:VAL:HG13	1.93	0.50
1:AI:178:ALA:HB3	1:AI:221:TYR:CE2	2.47	0.50
2:AL:127:PRO:HD2	2:AL:131:GLN:HE22	1.76	0.50
2:AR:35:LYS:O	2:AR:146:TYR:OH	2.19	0.50
2:BD:21:LEU:HD12	2:BD:31:LEU:HD11	1.94	0.50
2:BF:116:LYS:NZ	2:BH:130:GLY:O	2.31	0.50
1:BO:206:VAL:HA	1:BO:221:TYR:CD1	2.46	0.50
2:CJ:158:LYS:NZ	2:CL:132:THR:HG21	2.27	0.50
2:CT:21:LEU:HD12	2:CT:31:LEU:HD11	1.93	0.50
1:BK:55:HIS:HB3	1:BK:91:TYR:OH	2.12	0.50
1:BQ:68:ASP:O	1:BQ:149:VAL:HA	2.12	0.50
1:CG:43:SER:HB2	1:CG:51:VAL:HG22	1.94	0.50
1:CM:123:SER:O	1:CM:203:GLN:NE2	2.26	0.50
2:CN:28:HIS:CD2	1:CQ:228:VAL:HB	2.47	0.50
1:CS:55:HIS:O	2:CT:72:TYR:OH	2.28	0.50
1:DK:138:ASN:ND2	1:DK:144:THR:HA	2.27	0.50
2:AH:128:GLU:HB2	2:AH:131:GLN:NE2	2.23	0.49
1:BG:71:ASN:ND2	1:BG:148:ASP:OD2	2.44	0.49
1:BQ:52:SER:O	1:BQ:101:MET:N	2.44	0.49
2:BR:52:ARG:HH12	1:BU:229:SER:HB3	1.77	0.49
1:CG:98:ASN:HA	1:CG:227:TYR:OH	2.12	0.49
1:CU:18:GLY:HA3	1:CU:185:LYS:HG2	1.94	0.49
2:DF:15:GLY:N	2:DF:59:PHE:O	2.45	0.49
2:DR:21:LEU:HB3	2:DR:157:PHE:CD1	2.46	0.49
2:BT:98:LEU:HB2	2:BT:149:VAL:HB	1.94	0.49
1:CA:144:THR:HG21	2:CB:16:ALA:HA	1.94	0.49
2:CF:48:ASP:HB3	2:CF:51:HIS:HB2	1.94	0.49
2:CT:98:LEU:HB2	2:CT:149:VAL:HB	1.93	0.49
1:DG:54:ALA:N	1:DG:99:ASP:OD1	2.45	0.49
2:DN:127:PRO:HB2	2:DN:131:GLN:OE1	2.12	0.49
2:DR:116:LYS:HD3	2:DT:130:GLY:HA3	1.94	0.49
2:AF:3:VAL:HB	2:AH:128:GLU:HG3	1.94	0.49
1:AM:80:ILE:HG21	1:AM:105:LEU:HB3	1.94	0.49
2:AN:77:LYS:HE3	2:AN:83:SER:O	2.12	0.49
2:AT:138:LEU:HG	2:AT:155:CYS:HB2	1.93	0.49
1:BI:140:LYS:HD2	1:BI:145:SER:HB2	1.95	0.49
2:BN:21:LEU:HD12	2:BN:31:LEU:HD11	1.93	0.49
2:DL:21:LEU:HD12	2:DL:31:LEU:HD11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DO:68:ASP:O	1:DO:149:VAL:HA	2.12	0.49
1:DQ:153:LEU:HD21	1:DQ:185:LYS:HB3	1.94	0.49
2:DR:5:VAL:HA	2:DR:11:PRO:HA	1.93	0.49
2:DV:33:LEU:HB3	2:DV:42:PRO:HB2	1.94	0.49
2:AL:98:LEU:HB2	2:AL:149:VAL:HB	1.94	0.49
1:BS:51:VAL:HG21	1:BS:202:LEU:HD21	1.94	0.49
1:DI:214:GLN:HB2	1:DI:217:LYS:HD2	1.93	0.49
1:DM:32:SER:HB2	1:DM:136:TRP:CZ3	2.47	0.49
2:DP:127:PRO:HD2	2:DP:131:GLN:HE22	1.75	0.49
1:DQ:214:GLN:HB2	1:DQ:217:LYS:HB2	1.94	0.49
2:DR:87:VAL:HG21	2:DR:106:LYS:HB2	1.92	0.49
2:AJ:13:SER:HB2	2:AJ:16:ALA:HB3	1.93	0.49
2:AR:47:LEU:HB2	2:AR:145:TYR:HB2	1.94	0.49
2:BD:49:PRO:HG2	1:BG:123:SER:HB3	1.94	0.49
2:CR:126:TYR:HB3	2:CR:128:GLU:O	2.12	0.49
2:CR:127:PRO:HB2	2:CR:131:GLN:HE22	1.77	0.49
1:AA:181:LEU:H	1:AA:181:LEU:HD22	1.78	0.49
2:AP:126:TYR:HB3	2:AP:128:GLU:O	2.12	0.49
1:AU:69:ASN:HA	1:AU:148:ASP:O	2.12	0.49
1:BO:144:THR:HG21	2:BP:16:ALA:HA	1.94	0.49
1:CC:32:SER:OG	1:CC:38:HIS:ND1	2.32	0.49
2:CD:13:SER:HB2	2:CD:16:ALA:HB3	1.94	0.49
2:CD:158:LYS:NZ	2:CF:132:THR:HG21	2.27	0.49
2:CH:116:LYS:HG2	1:CI:94:ASN:HD22	1.78	0.49
2:CP:21:LEU:HD12	2:CP:31:LEU:HD11	1.95	0.49
1:CQ:154:LYS:O	1:CQ:180:TYR:OH	2.28	0.49
1:CQ:78:GLN:HE22	1:CQ:110:SER:H	1.60	0.49
1:BQ:21:THR:HB	2:DD:50:HIS:CD2	2.48	0.49
1:AU:206:VAL:HA	1:AU:221:TYR:CD1	2.48	0.49
2:BR:49:PRO:HG2	1:BU:123:SER:HB3	1.95	0.49
1:BU:69:ASN:HA	1:BU:148:ASP:O	2.12	0.49
1:CA:208:TRP:HB3	2:CB:63:LEU:HD23	1.94	0.49
2:CP:48:ASP:HB3	2:CP:51:HIS:HB2	1.94	0.49
2:CV:33:LEU:HB3	2:CV:42:PRO:HB2	1.94	0.49
1:DA:22:CYS:HB3	1:DA:26:THR:OG1	2.13	0.49
2:DB:135:ASP:HB3	2:DB:154:PRO:HB3	1.94	0.49
2:DJ:89:ASP:OD1	2:DJ:90:VAL:N	2.42	0.49
2:AL:128:GLU:O	2:AL:131:GLN:HG3	2.13	0.49
1:CA:74:GLU:N	1:CA:77:GLU:OE1	2.45	0.49
1:CM:205:ILE:HB	1:CM:222:THR:HB	1.94	0.49
2:CP:150:LYS:HG2	2:CP:153:GLU:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CR:1:SER:HA	2:CR:69:LYS:HD3	1.94	0.49
2:CR:20:TYR:CE2	2:CR:162:ALA:HA	2.48	0.49
2:DH:18:ALA:HB1	2:DH:56:PRO:HB2	1.95	0.49
1:DO:43:SER:HB2	1:DO:51:VAL:HG22	1.95	0.49
2:BD:135:ASP:HB3	2:BD:154:PRO:HB3	1.94	0.49
1:BC:106:LYS:NZ	2:BF:104:ASP:OD1	2.41	0.49
1:CO:204:GLY:HA2	1:CO:222:THR:O	2.13	0.49
1:CQ:69:ASN:HA	1:CQ:148:ASP:O	2.13	0.49
2:AF:128:GLU:H	2:AF:131:GLN:CD	2.16	0.49
2:AF:21:LEU:HB3	2:AF:157:PHE:CD1	2.47	0.49
2:AL:127:PRO:HB2	2:AL:131:GLN:OE1	2.12	0.49
2:AP:116:LYS:HG2	1:AQ:94:ASN:ND2	2.27	0.49
2:BD:5:VAL:HG13	2:BF:131:GLN:OE1	2.12	0.49
1:CG:188:CYS:N	1:CG:191:ASP:OD2	2.45	0.49
1:CM:98:ASN:HA	1:CM:227:TYR:OH	2.12	0.49
2:DF:25:SER:HA	1:DI:226:ASN:OD1	2.13	0.49
1:DG:54:ALA:HA	1:DG:101:MET:HB2	1.95	0.49
2:DL:15:GLY:N	2:DL:59:PHE:O	2.46	0.49
1:AI:98:ASN:HA	1:AI:227:TYR:OH	2.13	0.48
2:AP:127:PRO:HB2	2:AP:131:GLN:OE1	2.13	0.48
1:AQ:139:THR:HG23	1:AQ:147:PRO:HD3	1.95	0.48
1:AQ:76:ASN:HB2	1:AQ:114:ARG:HH11	1.77	0.48
2:BT:127:PRO:HB2	2:BT:131:GLN:OE1	2.13	0.48
2:CB:49:PRO:HB3	1:CE:122:THR:O	2.13	0.48
1:CO:149:VAL:HB	2:DF:50:HIS:ND1	2.28	0.48
1:DK:206:VAL:HA	1:DK:221:TYR:CD1	2.48	0.48
1:DK:24:ALA:HB1	1:DK:114:ARG:HH21	1.78	0.48
1:DI:106:LYS:NZ	2:DL:104:ASP:OD2	2.46	0.48
2:DN:121:TYR:N	2:DN:157:PHE:O	2.41	0.48
1:DQ:153:LEU:HD11	1:DQ:185:LYS:HD2	1.94	0.48
2:DR:121:TYR:OH	2:DT:131:GLN:OE1	2.30	0.48
2:DT:85:SER:HA	2:DT:104:ASP:HA	1.95	0.48
2:BT:5:VAL:HG21	2:BV:131:GLN:NE2	2.28	0.48
2:BV:85:SER:HA	2:BV:104:ASP:HA	1.94	0.48
1:DI:74:GLU:N	1:DI:77:GLU:OE1	2.45	0.48
1:AC:206:VAL:HA	1:AC:221:TYR:HD1	1.75	0.48
1:AE:21:THR:OG1	1:AE:151:LYS:NZ	2.45	0.48
1:AS:146:TYR:OH	2:AT:66:ASN:OD1	2.15	0.48
1:BA:206:VAL:HA	1:BA:221:TYR:CD1	2.48	0.48
2:BP:47:LEU:HG	2:BP:147:LEU:HD11	1.94	0.48
2:BV:11:PRO:HB2	2:BV:67:ILE:HG22	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CB:89:ASP:OD1	2:CB:90:VAL:N	2.45	0.48
2:CH:98:LEU:HB2	2:CH:149:VAL:HB	1.94	0.48
1:CK:214:GLN:HB2	1:CK:217:LYS:HB2	1.94	0.48
2:CN:145:TYR:CE2	1:CQ:123:SER:HB2	2.47	0.48
1:DA:106:LYS:HG3	1:DA:107:SER:N	2.28	0.48
1:DG:133:ILE:HG12	1:DG:196:VAL:HG22	1.95	0.48
2:DF:116:LYS:NZ	2:DH:130:GLY:O	2.42	0.48
1:DQ:206:VAL:HA	1:DQ:221:TYR:CD1	2.48	0.48
1:AK:98:ASN:HA	1:AK:227:TYR:OH	2.13	0.48
1:AM:29:TYR:CZ	1:AM:197:VAL:HG21	2.49	0.48
1:BO:29:TYR:CZ	1:BO:197:VAL:HG21	2.49	0.48
2:CF:125:TYR:CZ	2:CF:127:PRO:HA	2.48	0.48
2:CL:9:GLY:HA2	2:CN:131:GLN:HE22	1.77	0.48
2:DP:125:TYR:CE2	2:DP:127:PRO:HG3	2.48	0.48
2:AT:77:LYS:NZ	2:AT:78:PHE:O	2.40	0.48
1:BE:81:SER:HB3	2:BH:105:THR:HG21	1.96	0.48
2:BN:5:VAL:HG22	2:BP:131:GLN:CG	2.41	0.48
1:CK:74:GLU:N	1:CK:77:GLU:OE1	2.46	0.48
2:CR:5:VAL:HG21	2:CT:131:GLN:NE2	2.28	0.48
2:CT:12:VAL:HG13	2:CT:19:TYR:CE1	2.49	0.48
2:CV:3:VAL:HG11	2:CV:11:PRO:HB3	1.96	0.48
2:DD:49:PRO:HG2	1:DG:123:SER:HB3	1.94	0.48
2:DR:127:PRO:HB2	2:DR:131:GLN:OE1	2.13	0.48
1:AE:204:GLY:HA2	1:AE:222:THR:O	2.14	0.48
2:AH:89:ASP:OD1	2:AH:90:VAL:N	2.45	0.48
2:AJ:125:TYR:CE2	2:AJ:127:PRO:HG3	2.48	0.48
1:BE:206:VAL:HA	1:BE:221:TYR:CD1	2.49	0.48
1:BS:84:LYS:HB2	1:BS:104:LYS:HB3	1.95	0.48
2:CD:138:LEU:HD22	2:CD:145:TYR:HB3	1.94	0.48
2:CD:48:ASP:HB3	2:CD:51:HIS:HB2	1.94	0.48
1:CK:144:THR:HG21	2:CL:16:ALA:HA	1.94	0.48
1:AC:69:ASN:HA	1:AC:148:ASP:O	2.13	0.48
2:AD:141:ARG:HB3	2:AD:146:TYR:CE2	2.49	0.48
2:AH:28:HIS:O	2:AH:49:PRO:HA	2.14	0.48
1:AI:47:SER:HB2	1:AI:108:ALA:HB1	1.96	0.48
2:AJ:127:PRO:HB2	2:AJ:131:GLN:OE1	2.13	0.48
2:AT:46:VAL:HG12	2:AT:146:TYR:HA	1.95	0.48
1:BI:78:GLN:NE2	1:BI:115:VAL:HG21	2.28	0.48
1:BO:170:GLN:HG3	2:BP:108:LEU:HD23	1.95	0.48
2:CD:138:LEU:HD21	2:CD:155:CYS:SG	2.54	0.48
2:DB:6:ASP:HA	2:DB:159:ILE:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DK:43:SER:HB2	1:DK:51:VAL:HG22	1.96	0.48
1:DU:96:LEU:HD11	2:DV:109:LEU:HD11	1.94	0.48
1:AC:78:GLN:NE2	1:AC:115:VAL:HG21	2.29	0.48
1:AG:180:TYR:HB3	1:AG:182:GLU:OE1	2.14	0.48
2:AR:90:VAL:HG22	2:AR:100:VAL:HG22	1.95	0.48
1:AU:98:ASN:HA	1:AU:227:TYR:OH	2.14	0.48
2:CD:4:VAL:HA	2:CD:121:TYR:OH	2.14	0.48
2:CR:5:VAL:CG2	2:CT:131:GLN:HB3	2.44	0.48
1:DE:106:LYS:NZ	2:DH:104:ASP:OD1	2.46	0.48
1:DI:80:ILE:HG21	1:DI:105:LEU:HB3	1.96	0.48
2:AB:134:LEU:HD13	2:AB:149:VAL:HG11	1.96	0.48
1:AK:32:SER:HB2	1:AK:136:TRP:CZ3	2.49	0.48
1:AO:49:TRP:CD2	1:AO:235:ILE:HG12	2.49	0.48
1:BO:196:VAL:HB	1:BO:204:GLY:HA3	1.95	0.48
1:CE:81:SER:HB3	2:CH:105:THR:HG21	1.96	0.48
2:CJ:89:ASP:OD1	2:CJ:90:VAL:N	2.44	0.48
2:CR:94:ASP:HB2	2:DF:40:ALA:HB2	1.95	0.48
2:CV:127:PRO:HD2	2:CV:131:GLN:NE2	2.29	0.48
1:CO:68:ASP:OD2	2:DF:50:HIS:HB3	2.14	0.48
2:DF:61:SER:HB2	2:DF:74:LEU:HD23	1.96	0.48
2:DH:39:GLU:OE2	2:DH:93:GLN:NE2	2.44	0.48
2:DL:20:TYR:CE2	2:DL:162:ALA:HA	2.48	0.48
2:AF:36:ILE:HG12	2:AF:44:ALA:HB2	1.96	0.48
1:AI:111:LEU:HD22	1:AI:116:ALA:HA	1.94	0.48
2:AJ:11:PRO:HB2	2:AJ:67:ILE:HG22	1.96	0.48
2:AT:5:VAL:HG11	2:AV:131:GLN:HG2	1.95	0.48
2:BD:91:ILE:HB	2:BD:101:LYS:HD3	1.95	0.48
2:BJ:5:VAL:HG22	2:BL:131:GLN:CD	2.34	0.48
1:CM:24:ALA:HB1	1:CM:114:ARG:NE	2.27	0.48
2:DH:15:GLY:N	2:DH:59:PHE:O	2.47	0.48
1:DI:68:ASP:O	1:DI:149:VAL:HA	2.14	0.48
1:DK:96:LEU:HD23	2:DL:63:LEU:HD21	1.96	0.48
1:AO:24:ALA:HB1	1:AO:114:ARG:NE	2.28	0.47
1:AU:178:ALA:HB3	1:AU:221:TYR:CE2	2.49	0.47
2:BB:13:SER:HB2	2:BB:16:ALA:HB3	1.96	0.47
1:CM:204:GLY:HA2	1:CM:222:THR:O	2.14	0.47
1:CS:54:ALA:N	1:CS:99:ASP:OD1	2.47	0.47
1:CU:51:VAL:HG12	1:CU:102:LEU:HD23	1.96	0.47
1:DI:96:LEU:HD11	2:DJ:109:LEU:HD11	1.95	0.47
2:DL:25:SER:O	1:DO:223:LYS:HE2	2.14	0.47
1:AC:133:ILE:HG12	1:AC:196:VAL:HG13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AE:69:ASN:H	1:AE:74:GLU:CD	2.17	0.47
2:AP:77:LYS:HE3	2:AP:83:SER:O	2.14	0.47
1:AU:204:GLY:HA2	1:AU:222:THR:O	2.14	0.47
1:BS:167:TYR:OH	1:BS:218:PRO:O	2.22	0.47
1:BS:176:PHE:CZ	1:BS:221:TYR:HB2	2.50	0.47
1:CO:178:ALA:HB3	1:CO:221:TYR:CE2	2.49	0.47
1:DC:58:LYS:NZ	2:DF:128:GLU:OE2	2.43	0.47
2:DJ:127:PRO:HB2	2:DJ:131:GLN:OE1	2.14	0.47
2:DL:2:SER:HB2	2:DL:70:GLU:OE2	2.15	0.47
1:DM:80:ILE:HG21	1:DM:105:LEU:HB3	1.95	0.47
1:DQ:76:ASN:CB	1:DQ:114:ARG:HD2	2.44	0.47
1:AM:94:ASN:HA	2:AN:73:PHE:HE2	1.79	0.47
2:CT:5:VAL:HG21	2:CV:131:GLN:HB3	1.95	0.47
1:CU:54:ALA:HA	1:CU:101:MET:HB2	1.96	0.47
2:DF:89:ASP:OD1	2:DF:90:VAL:N	2.44	0.47
1:DO:192:SER:HA	1:DO:206:VAL:HG13	1.96	0.47
1:DO:37:TYR:CZ	2:DP:11:PRO:HG2	2.49	0.47
2:AB:2:SER:HB2	2:AB:70:GLU:OE2	2.14	0.47
2:AD:28:HIS:O	2:AD:49:PRO:HA	2.14	0.47
2:AD:43:ARG:O	2:AD:102:VAL:HG22	2.15	0.47
1:AG:206:VAL:HA	1:AG:221:TYR:HD1	1.78	0.47
2:AF:9:GLY:HA2	2:AH:127:PRO:HG2	1.96	0.47
2:AH:6:ASP:OD2	2:AH:10:GLN:HB2	2.15	0.47
1:AO:206:VAL:HA	1:AO:221:TYR:CD1	2.49	0.47
2:AT:6:ASP:OD2	2:AT:10:GLN:HB2	2.15	0.47
1:BG:17:VAL:O	1:BG:185:LYS:HA	2.15	0.47
1:BU:196:VAL:HG21	1:BU:221:TYR:CD1	2.49	0.47
2:CN:15:GLY:O	2:CN:58:ARG:NH1	2.45	0.47
1:CS:44:LEU:O	1:CS:118:ILE:HG22	2.14	0.47
2:CT:116:LYS:HG2	1:CU:94:ASN:HD22	1.78	0.47
2:CR:145:TYR:CE2	1:CU:123:SER:HB2	2.48	0.47
1:DA:78:GLN:NE2	1:DA:115:VAL:HG21	2.30	0.47
2:DB:2:SER:O	2:DB:70:GLU:HG3	2.15	0.47
2:DJ:31:LEU:N	2:DJ:54:GLY:HA3	2.28	0.47
1:DS:74:GLU:N	1:DS:77:GLU:OE1	2.48	0.47
2:DT:9:GLY:HA2	2:DV:131:GLN:HE22	1.79	0.47
1:BA:25:ASN:HD22	1:BA:114:ARG:HG3	1.79	0.47
1:BU:76:ASN:HB2	1:BU:114:ARG:NH1	2.26	0.47
1:CC:98:ASN:HA	1:CC:227:TYR:OH	2.14	0.47
2:CJ:127:PRO:HB2	2:CJ:131:GLN:OE1	2.14	0.47
1:CM:96:LEU:HD11	2:CN:109:LEU:HD11	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AL:26:HIS:ND1	1:AO:123:SER:HB2	2.30	0.47
1:AO:43:SER:HB2	1:AO:51:VAL:HG22	1.94	0.47
2:BB:5:VAL:HG21	2:BD:131:GLN:CG	2.44	0.47
1:CE:106:LYS:NZ	2:CH:104:ASP:OD1	2.42	0.47
1:CO:18:GLY:HA3	1:CO:185:LYS:HG2	1.97	0.47
1:DE:98:ASN:HA	1:DE:227:TYR:OH	2.15	0.47
1:CO:72:VAL:HG11	2:DF:42:PRO:HB3	1.96	0.47
1:DK:138:ASN:HD21	1:DK:144:THR:HA	1.78	0.47
1:DU:18:GLY:HA3	1:DU:185:LYS:HG2	1.96	0.47
1:AA:68:ASP:O	1:AA:149:VAL:HA	2.15	0.47
1:AC:64:ARG:HD3	1:AC:79:PHE:CZ	2.50	0.47
1:AI:24:ALA:HA	1:AI:68:ASP:HB2	1.97	0.47
2:AL:46:VAL:HG12	2:AL:146:TYR:HA	1.97	0.47
2:BB:145:TYR:OH	1:BE:124:CYS:O	2.33	0.47
2:BJ:128:GLU:H	2:BJ:131:GLN:CD	2.18	0.47
1:BM:24:ALA:HB1	1:BM:114:ARG:HE	1.79	0.47
1:CC:178:ALA:HB3	1:CC:221:TYR:CE2	2.49	0.47
2:CH:90:VAL:HB	2:CH:125:TYR:CZ	2.50	0.47
2:CF:5:VAL:HG21	2:CH:131:GLN:CG	2.45	0.47
2:CN:46:VAL:HG21	2:CN:144:LYS:HD3	1.97	0.47
1:CS:71:ASN:ND2	1:CS:148:ASP:OD2	2.48	0.47
2:DD:28:HIS:CD2	1:DG:228:VAL:HB	2.49	0.47
1:DM:54:ALA:HB1	1:DM:87:VAL:HG13	1.95	0.47
1:DO:54:ALA:N	1:DO:99:ASP:OD1	2.47	0.47
2:DP:28:HIS:HB3	2:DP:52:ARG:HD2	1.95	0.47
2:DT:77:LYS:HE3	2:DT:83:SER:O	2.14	0.47
1:DU:98:ASN:OD1	1:DU:227:TYR:OH	2.28	0.47
1:AQ:28:PRO:HB3	1:AQ:113:SER:O	2.15	0.47
2:BB:89:ASP:OD1	2:BB:90:VAL:N	2.46	0.47
1:BC:41:GLY:N	1:BC:192:SER:O	2.38	0.47
2:BB:9:GLY:HA2	2:BD:131:GLN:HE22	1.79	0.47
1:BQ:138:ASN:ND2	1:BQ:144:THR:HA	2.29	0.47
2:CB:16:ALA:O	2:CB:58:ARG:NH1	2.47	0.47
2:CD:7:THR:N	2:CD:159:ILE:O	2.46	0.47
2:DN:121:TYR:O	2:DN:157:PHE:N	2.36	0.47
1:AA:138:ASN:HB3	1:AA:188:CYS:SG	2.55	0.47
2:AD:104:ASP:N	2:AD:104:ASP:OD2	2.40	0.47
2:AL:43:ARG:O	2:AL:102:VAL:HG22	2.15	0.47
1:AM:138:ASN:ND2	1:AM:144:THR:HA	2.30	0.47
1:AS:129:THR:HB	1:AS:157:ILE:HD12	1.96	0.47
2:AT:20:TYR:CE2	2:AT:162:ALA:HA	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CG:205:ILE:HB	1:CG:222:THR:HB	1.97	0.47
2:CH:61:SER:HB2	2:CH:74:LEU:HD23	1.97	0.47
2:CJ:9:GLY:HA2	2:CL:127:PRO:HG2	1.97	0.47
2:CR:98:LEU:HB2	2:CR:149:VAL:HB	1.97	0.47
1:DI:133:ILE:HG12	1:DI:196:VAL:HG13	1.95	0.47
2:DN:28:HIS:O	2:DN:49:PRO:HA	2.15	0.47
1:DQ:184:GLY:H	1:DQ:213:ALA:HB1	1.80	0.47
2:AJ:3:VAL:HB	2:AL:128:GLU:HG3	1.97	0.47
2:AL:48:ASP:HB3	2:AL:51:HIS:HB2	1.97	0.47
1:AM:54:ALA:N	1:AM:99:ASP:OD1	2.48	0.47
2:AN:128:GLU:O	2:AN:131:GLN:NE2	2.48	0.47
2:BL:125:TYR:CZ	2:BL:127:PRO:HA	2.50	0.47
2:BP:5:VAL:HG21	2:BR:131:GLN:HB2	1.96	0.47
2:BR:2:SER:HB2	2:BR:70:GLU:OE2	2.15	0.47
1:BS:78:GLN:NE2	1:BS:115:VAL:HG21	2.29	0.47
2:BV:128:GLU:O	2:BV:131:GLN:HG3	2.14	0.47
1:CC:184:GLY:H	1:CC:213:ALA:HB1	1.80	0.47
1:CC:51:VAL:HG12	1:CC:102:LEU:HD23	1.96	0.47
2:CF:1:SER:HA	2:CF:69:LYS:HD3	1.97	0.47
2:CJ:128:GLU:H	2:CJ:131:GLN:CD	2.17	0.47
1:DS:43:SER:OG	1:DS:195:PRO:HB3	2.15	0.47
2:DV:98:LEU:HB2	2:DV:149:VAL:HB	1.96	0.47
2:AP:134:LEU:HD13	2:AP:149:VAL:HG11	1.97	0.47
1:AS:206:VAL:HA	1:AS:221:TYR:CD1	2.50	0.47
1:AS:196:VAL:HG21	1:AS:221:TYR:CD1	2.50	0.47
2:CN:127:PRO:HB2	2:CN:131:GLN:OE1	2.15	0.47
2:AD:127:PRO:HB2	2:AD:131:GLN:OE1	2.15	0.46
2:AH:134:LEU:HB3	2:AH:149:VAL:HG13	1.97	0.46
1:AM:180:TYR:CE2	1:AM:185:LYS:HE3	2.50	0.46
1:BS:196:VAL:HG21	1:BS:221:TYR:CD1	2.50	0.46
1:CC:94:ASN:HA	2:CD:73:PHE:HE2	1.79	0.46
2:CF:9:GLY:HA2	2:CH:131:GLN:NE2	2.28	0.46
2:CP:87:VAL:HG21	2:CP:106:LYS:HB2	1.97	0.46
1:DM:167:TYR:HB2	1:DM:171:ILE:HD11	1.96	0.46
1:DQ:96:LEU:CD1	2:DR:109:LEU:HD11	2.46	0.46
1:AK:43:SER:HB2	1:AK:51:VAL:HG22	1.97	0.46
1:AQ:144:THR:HG21	2:AR:16:ALA:HB1	1.97	0.46
1:BA:43:SER:OG	1:BA:195:PRO:HB3	2.16	0.46
2:BF:128:GLU:HB2	2:BF:131:GLN:OE1	2.15	0.46
2:BP:31:LEU:N	2:BP:54:GLY:HA3	2.31	0.46
2:CP:7:THR:N	2:CP:159:ILE:O	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:DD:5:VAL:HG22	2:DF:131:GLN:HB3	1.97	0.46
2:DJ:31:LEU:H	2:DJ:54:GLY:HA3	1.80	0.46
2:DL:5:VAL:HG21	2:DN:131:GLN:HB3	1.96	0.46
2:DN:128:GLU:H	2:DN:131:GLN:HG3	1.80	0.46
1:DO:24:ALA:HB1	1:DO:114:ARG:NE	2.27	0.46
1:DS:206:VAL:HA	1:DS:221:TYR:HD1	1.79	0.46
2:AH:12:VAL:HG13	2:AH:19:TYR:CE1	2.50	0.46
2:AN:48:ASP:OD2	1:DO:25:ASN:ND2	2.29	0.46
2:AR:121:TYR:OH	2:AT:131:GLN:HG2	2.16	0.46
1:AQ:55:HIS:O	2:AR:72:TYR:OH	2.33	0.46
2:BB:28:HIS:HD2	1:BE:228:VAL:HB	1.80	0.46
1:BE:133:ILE:HD13	1:BE:221:TYR:CE1	2.50	0.46
2:BL:5:VAL:HG11	2:BN:131:GLN:CD	2.36	0.46
1:CA:98:ASN:HA	1:CA:227:TYR:OH	2.14	0.46
2:CH:5:VAL:HG21	2:CJ:131:GLN:HB3	1.96	0.46
1:CK:34:ASN:O	1:CK:62:GLN:N	2.25	0.46
2:DL:116:LYS:HG2	1:DM:94:ASN:HD22	1.80	0.46
2:AN:28:HIS:NE2	1:AQ:232:LYS:HD2	2.30	0.46
1:AQ:208:TRP:HB3	2:AR:63:LEU:HD23	1.97	0.46
2:AV:89:ASP:OD1	2:AV:90:VAL:N	2.48	0.46
1:BA:37:TYR:CZ	2:BB:11:PRO:HG2	2.51	0.46
2:BD:125:TYR:CZ	2:BD:127:PRO:HA	2.51	0.46
2:BJ:48:ASP:HB3	2:BJ:51:HIS:HB2	1.97	0.46
2:CD:89:ASP:OD1	2:CD:90:VAL:N	2.48	0.46
2:CV:15:GLY:O	2:CV:58:ARG:NH1	2.45	0.46
2:DB:158:LYS:NZ	2:DD:132:THR:HG21	2.30	0.46
1:DC:184:GLY:N	1:DC:213:ALA:HB1	2.31	0.46
1:DI:106:LYS:HZ1	2:DL:104:ASP:CG	2.17	0.46
2:DJ:28:HIS:NE2	1:DM:228:VAL:HG12	2.30	0.46
1:AA:167:TYR:HB2	1:AA:171:ILE:HD11	1.97	0.46
1:AQ:32:SER:OG	1:AQ:38:HIS:ND1	2.39	0.46
2:AT:43:ARG:O	2:AT:102:VAL:HG22	2.14	0.46
1:AU:123:SER:O	1:AU:203:GLN:NE2	2.40	0.46
1:BA:78:GLN:NE2	1:BA:115:VAL:HG21	2.30	0.46
2:BH:45:VAL:HG12	2:BH:147:LEU:HD13	1.98	0.46
2:BJ:128:GLU:HG2	2:BJ:131:GLN:OE1	2.14	0.46
1:CC:49:TRP:CD2	1:CC:235:ILE:HG12	2.50	0.46
2:CF:5:VAL:HG21	2:CH:131:GLN:CB	2.46	0.46
2:DF:138:LEU:O	2:DF:150:LYS:NZ	2.33	0.46
1:DQ:196:VAL:HG21	1:DQ:221:TYR:CD1	2.51	0.46
1:AC:51:VAL:HG12	1:AC:102:LEU:HD23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AC:58:LYS:NZ	2:AF:128:GLU:OE2	2.48	0.46
1:AO:51:VAL:HG12	1:AO:102:LEU:HD23	1.97	0.46
2:AR:127:PRO:HB2	2:AR:131:GLN:OE1	2.15	0.46
2:BB:128:GLU:HB2	2:BB:131:GLN:CD	2.36	0.46
1:BQ:67:GLU:HG3	1:BQ:77:GLU:HG3	1.97	0.46
2:BR:135:ASP:HB3	2:BR:154:PRO:HB3	1.98	0.46
2:BR:73:PHE:HZ	2:BR:129:ARG:O	1.99	0.46
1:BS:206:VAL:HA	1:BS:221:TYR:HD1	1.80	0.46
2:BV:15:GLY:N	2:BV:59:PHE:O	2.49	0.46
2:CN:46:VAL:HG12	2:CN:146:TYR:HA	1.97	0.46
1:CQ:55:HIS:ND1	2:CR:63:LEU:HD22	2.30	0.46
2:AH:33:LEU:HA	2:AH:44:ALA:O	2.15	0.46
1:AK:81:SER:HB3	2:AN:105:THR:HG21	1.98	0.46
2:BH:89:ASP:OD1	2:BH:90:VAL:N	2.44	0.46
1:CC:32:SER:HB2	1:CC:136:TRP:CZ3	2.51	0.46
2:CR:128:GLU:O	2:CR:131:GLN:HG2	2.15	0.46
1:DE:138:ASN:ND2	1:DE:143:GLY:O	2.48	0.46
1:DE:94:ASN:HA	2:DF:73:PHE:CE2	2.51	0.46
2:DR:116:LYS:NZ	2:DT:130:GLY:O	2.46	0.46
1:AG:133:ILE:HG12	1:AG:196:VAL:HG22	1.98	0.46
1:AI:204:GLY:HA2	1:AI:222:THR:O	2.16	0.46
2:AL:125:TYR:CE2	2:AL:127:PRO:HG3	2.50	0.46
1:AO:211:GLY:O	2:AP:64:ARG:NH2	2.41	0.46
1:BE:180:TYR:CD2	1:BE:185:LYS:HB2	2.51	0.46
1:BU:48:GLN:HG2	1:BU:108:ALA:HA	1.96	0.46
1:CA:141:SER:HB2	1:CA:214:GLN:HE22	1.81	0.46
2:CB:49:PRO:HG2	1:CE:123:SER:HB3	1.98	0.46
1:CO:23:GLY:N	2:DF:50:HIS:CD2	2.79	0.46
2:DH:28:HIS:O	2:DH:49:PRO:HA	2.16	0.46
1:DI:167:TYR:HB2	1:DI:171:ILE:HD11	1.97	0.46
2:DJ:135:ASP:HB3	2:DJ:154:PRO:HB3	1.98	0.46
1:DK:208:TRP:HB3	2:DL:63:LEU:HD23	1.97	0.46
1:DQ:49:TRP:CD2	1:DQ:235:ILE:HG12	2.51	0.46
2:DP:28:HIS:CE1	1:DS:229:SER:HG	2.27	0.46
1:AO:98:ASN:HA	1:AO:227:TYR:OH	2.16	0.46
1:AQ:67:GLU:HG3	1:AQ:77:GLU:HG3	1.98	0.46
2:AR:36:ILE:HG23	2:AR:96:ILE:HG12	1.97	0.46
2:AV:98:LEU:HB2	2:AV:149:VAL:HB	1.98	0.46
1:BA:28:PRO:HB3	1:BA:113:SER:O	2.15	0.46
1:BM:76:ASN:HB2	1:BM:114:ARG:NH1	2.30	0.46
1:BQ:43:SER:HB2	1:BQ:51:VAL:HG22	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BV:138:LEU:HD22	2:BV:145:TYR:HB3	1.97	0.46
1:CC:133:ILE:HG12	1:CC:196:VAL:HG22	1.96	0.46
1:CC:55:HIS:CE1	2:CD:63:LEU:HD22	2.50	0.46
1:CG:178:ALA:HB3	1:CG:221:TYR:CE2	2.51	0.46
1:DA:120:LEU:HD11	1:DA:231:ILE:HG21	1.98	0.46
1:DM:54:ALA:HA	1:DM:101:MET:HB2	1.98	0.46
2:DV:126:TYR:HB3	2:DV:128:GLU:O	2.15	0.46
1:AG:43:SER:OG	1:AG:195:PRO:HB3	2.16	0.46
1:AK:21:THR:OG1	1:AK:151:LYS:NZ	2.48	0.46
1:BA:54:ALA:N	1:BA:99:ASP:OD1	2.49	0.46
1:BG:68:ASP:O	1:BG:149:VAL:HA	2.16	0.46
1:BI:32:SER:OG	1:BI:38:HIS:ND1	2.39	0.46
1:BK:160:ASP:HA	1:BK:163:CYS:HB3	1.98	0.46
2:BN:134:LEU:HD13	2:BN:149:VAL:HG11	1.98	0.46
1:BQ:133:ILE:HD13	1:BQ:221:TYR:CZ	2.51	0.46
1:BS:66:GLY:HA3	1:BS:115:VAL:HG22	1.98	0.46
1:BU:138:ASN:ND2	1:BU:143:GLY:O	2.40	0.46
2:CD:47:LEU:HB2	2:CD:145:TYR:HB2	1.97	0.46
1:CG:133:ILE:HG12	1:CG:196:VAL:HG13	1.98	0.46
2:CT:36:ILE:HD12	2:CT:93:GLN:OE1	2.16	0.46
1:CU:43:SER:OG	1:CU:195:PRO:HB3	2.16	0.46
1:DC:24:ALA:HB1	1:DC:114:ARG:HE	1.81	0.46
2:DD:127:PRO:HB2	2:DD:131:GLN:HE22	1.80	0.46
1:DS:32:SER:HB2	1:DS:136:TRP:CZ3	2.51	0.46
1:AE:206:VAL:HA	1:AE:221:TYR:CD1	2.45	0.45
1:BA:187:SER:OG	2:BB:64:ARG:NH1	2.47	0.45
1:BE:80:ILE:HG21	1:BE:105:LEU:HB3	1.98	0.45
1:BG:206:VAL:HA	1:BG:221:TYR:CD1	2.51	0.45
1:BK:69:ASN:HA	1:BK:148:ASP:O	2.17	0.45
1:CE:80:ILE:HG21	1:CE:105:LEU:HB3	1.98	0.45
2:DT:3:VAL:HB	2:DV:128:GLU:HG3	1.97	0.45
1:AC:24:ALA:O	1:AC:114:ARG:HG2	2.17	0.45
1:AE:80:ILE:HG21	1:AE:105:LEU:HB3	1.98	0.45
1:AI:144:THR:HG21	2:AJ:16:ALA:HB1	1.98	0.45
1:AK:41:GLY:N	1:AK:192:SER:O	2.41	0.45
2:AH:28:HIS:CE1	1:AK:229:SER:HB3	2.43	0.45
2:AV:23:PRO:HG2	2:AV:26:HIS:O	2.17	0.45
1:BE:45:ILE:HD11	1:BE:235:ILE:HD11	1.98	0.45
1:BM:144:THR:HG21	2:BN:16:ALA:CB	2.46	0.45
1:BQ:181:LEU:H	1:BQ:181:LEU:HD22	1.82	0.45
2:CR:145:TYR:OH	1:CU:123:SER:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DC:144:THR:HG21	2:DD:16:ALA:HA	1.98	0.45
1:DQ:54:ALA:HB1	1:DQ:87:VAL:HG13	1.97	0.45
1:AA:76:ASN:HB2	1:AA:114:ARG:HH11	1.81	0.45
1:AC:37:TYR:CZ	2:AD:11:PRO:HG2	2.51	0.45
1:AE:81:SER:HB2	1:AE:106:LYS:HD3	1.98	0.45
1:AE:139:THR:HG23	1:AE:147:PRO:HD3	1.97	0.45
2:AN:128:GLU:CA	2:AN:131:GLN:HE22	2.30	0.45
2:AP:125:TYR:CE2	2:AP:127:PRO:HG3	2.51	0.45
1:AQ:153:LEU:HD21	1:AQ:185:LYS:HB3	1.98	0.45
2:BF:5:VAL:CG2	2:BH:131:GLN:HB3	2.47	0.45
1:CC:197:VAL:HG22	1:CC:202:LEU:HA	1.97	0.45
2:CD:127:PRO:HD2	2:CD:131:GLN:NE2	2.31	0.45
1:CS:37:TYR:CZ	2:CT:11:PRO:HG2	2.52	0.45
1:DC:206:VAL:HA	1:DC:221:TYR:CD1	2.50	0.45
1:DE:206:VAL:HA	1:DE:221:TYR:HD1	1.79	0.45
1:DO:43:SER:OG	1:DO:195:PRO:HB3	2.16	0.45
2:DR:36:ILE:HD12	2:DR:93:GLN:OE1	2.17	0.45
2:AL:3:VAL:HB	2:AN:128:GLU:HG3	1.98	0.45
2:AN:144:LYS:NZ	1:DO:113:SER:HB2	2.31	0.45
1:AQ:80:ILE:HG21	1:AQ:105:LEU:HB3	1.97	0.45
1:AQ:180:TYR:CD2	1:AQ:185:LYS:HB2	2.52	0.45
2:BD:127:PRO:HB2	2:BD:131:GLN:OE1	2.16	0.45
1:BK:188:CYS:N	1:BK:191:ASP:OD2	2.41	0.45
1:BK:55:HIS:CE1	2:BL:63:LEU:HD22	2.51	0.45
1:BM:69:ASN:HA	1:BM:148:ASP:O	2.16	0.45
2:BN:73:PHE:CZ	2:BN:113:LYS:HE3	2.51	0.45
2:BT:14:ASN:HA	2:BT:68:ILE:HD11	1.99	0.45
1:BU:206:VAL:HA	1:BU:221:TYR:CD1	2.52	0.45
2:CB:28:HIS:HD2	1:CE:228:VAL:HB	1.81	0.45
2:CP:26:HIS:ND1	1:CS:123:SER:HB2	2.31	0.45
1:CS:98:ASN:HA	1:CS:227:TYR:OH	2.15	0.45
2:DF:116:LYS:HD3	2:DH:130:GLY:CA	2.47	0.45
1:AC:54:ALA:N	1:AC:99:ASP:OD1	2.49	0.45
2:BF:3:VAL:HB	2:BH:128:GLU:HG3	1.97	0.45
2:CJ:125:TYR:HB2	2:CJ:136:ILE:HD11	1.98	0.45
1:CO:158:LEU:HD12	1:CO:177:CYS:HB3	1.99	0.45
2:CP:6:ASP:HA	2:CP:159:ILE:HB	1.97	0.45
1:DK:178:ALA:HB3	1:DK:221:TYR:CE2	2.50	0.45
1:DM:69:ASN:HA	1:DM:148:ASP:O	2.17	0.45
2:DT:6:ASP:OD1	2:DT:10:GLN:N	2.39	0.45
2:AD:3:VAL:HB	2:AF:128:GLU:HG3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AJ:36:ILE:CG1	2:AJ:44:ALA:HB2	2.45	0.45
1:AM:57:TYR:OH	1:AO:168:PRO:HB2	2.16	0.45
1:AO:44:LEU:O	1:AO:118:ILE:HG22	2.17	0.45
2:AV:138:LEU:HG	2:AV:155:CYS:HB2	1.98	0.45
1:BI:138:ASN:HD21	1:BI:144:THR:HA	1.81	0.45
1:CA:21:THR:OG1	1:CA:151:LYS:NZ	2.36	0.45
1:CM:29:TYR:CZ	1:CM:197:VAL:HG21	2.51	0.45
2:CV:89:ASP:OD1	2:CV:90:VAL:N	2.50	0.45
2:DH:77:LYS:HE3	2:DH:83:SER:O	2.17	0.45
1:AA:21:THR:OG1	1:AA:151:LYS:NZ	2.45	0.45
2:AB:18:ALA:HB1	2:AB:56:PRO:HB2	1.97	0.45
1:AE:178:ALA:HB3	1:AE:221:TYR:CE2	2.52	0.45
2:AJ:2:SER:HB2	2:AJ:70:GLU:OE2	2.17	0.45
2:AN:128:GLU:HB2	2:AN:131:GLN:HE22	1.81	0.45
2:AV:23:PRO:HA	2:AV:157:PHE:HA	1.98	0.45
2:BB:135:ASP:HB3	2:BB:154:PRO:HB3	1.99	0.45
2:BB:134:LEU:HB3	2:BB:149:VAL:HG13	1.98	0.45
1:BC:176:PHE:CZ	1:BC:221:TYR:HB2	2.52	0.45
2:BJ:73:PHE:HB3	2:BJ:110:GLY:O	2.16	0.45
2:BV:3:VAL:HG11	2:BV:11:PRO:HB3	1.98	0.45
2:CN:92:GLN:HE22	2:CN:97:GLY:HA2	1.82	0.45
1:CS:133:ILE:HG12	1:CS:196:VAL:HG22	1.98	0.45
2:CV:134:LEU:HB3	2:CV:149:VAL:HG13	1.97	0.45
2:CV:20:TYR:CE2	2:CV:162:ALA:HA	2.51	0.45
2:DH:116:LYS:HG2	1:DI:94:ASN:ND2	2.29	0.45
2:BD:7:THR:HG23	2:BD:159:ILE:O	2.16	0.45
1:BE:181:LEU:HD22	1:BE:181:LEU:H	1.82	0.45
2:BH:91:ILE:HB	2:BH:101:LYS:HD3	1.97	0.45
1:BI:196:VAL:HG21	1:BI:221:TYR:CD1	2.52	0.45
2:BT:12:VAL:O	2:BT:68:ILE:HG12	2.17	0.45
2:BR:49:PRO:HB3	1:BU:122:THR:O	2.17	0.45
1:CM:155:ALA:HB1	1:CM:179:GLY:HA2	1.98	0.45
2:CR:13:SER:HA	2:CR:66:ASN:O	2.17	0.45
2:DF:28:HIS:HE1	1:DI:229:SER:HA	1.81	0.45
1:DK:69:ASN:HA	1:DK:148:ASP:O	2.17	0.45
1:DS:55:HIS:O	2:DT:72:TYR:OH	2.34	0.45
1:DS:106:LYS:NZ	2:DV:104:ASP:OD2	2.49	0.45
1:AI:81:SER:O	1:AI:106:LYS:HG2	2.17	0.45
1:AK:111:LEU:O	2:DL:141:ARG:NH2	2.50	0.45
1:AK:24:ALA:HB1	1:AK:114:ARG:NE	2.32	0.45
1:AU:76:ASN:HB2	1:AU:114:ARG:HH11	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AU:94:ASN:HD22	2:AV:73:PHE:HE2	1.64	0.45
2:BD:12:VAL:HG13	2:BD:19:TYR:CE1	2.52	0.45
1:CE:49:TRP:CD2	1:CE:235:ILE:HG12	2.52	0.45
1:CO:206:VAL:HA	1:CO:221:TYR:HD1	1.82	0.45
1:CQ:214:GLN:HB2	1:CQ:217:LYS:HD2	1.98	0.45
2:DJ:87:VAL:O	2:DJ:102:VAL:HA	2.16	0.45
1:DM:138:ASN:ND2	1:DM:144:THR:HA	2.32	0.45
2:AB:5:VAL:HG21	2:AD:131:GLN:HG2	1.98	0.45
1:AM:104:LYS:NZ	1:AM:238:ASN:O	2.45	0.45
1:AS:37:TYR:CZ	2:AT:11:PRO:HG2	2.52	0.45
1:BC:54:ALA:N	1:BC:99:ASP:OD1	2.49	0.45
1:BC:55:HIS:CD2	2:BD:63:LEU:HD22	2.52	0.45
2:CD:28:HIS:CE1	1:CG:229:SER:HB3	2.51	0.45
2:CF:89:ASP:OD1	2:CF:90:VAL:N	2.45	0.45
1:CS:67:GLU:HG2	1:CS:77:GLU:OE2	2.17	0.45
2:CT:77:LYS:HE3	2:CT:83:SER:O	2.17	0.45
2:DH:2:SER:HB2	2:DH:70:GLU:OE2	2.17	0.45
1:DS:138:ASN:HB3	1:DS:188:CYS:SG	2.57	0.45
1:AA:54:ALA:HA	1:AA:101:MET:HB2	1.99	0.44
2:BD:25:SER:O	1:BG:223:LYS:HE2	2.17	0.44
2:BR:131:GLN:HG2	2:BR:132:THR:O	2.16	0.44
1:BS:178:ALA:HB3	1:BS:221:TYR:CE2	2.52	0.44
1:CI:96:LEU:HD11	2:CJ:109:LEU:HD11	1.98	0.44
1:CK:153:LEU:HD11	1:CK:185:LYS:HD2	1.98	0.44
2:CL:77:LYS:HE3	2:CL:83:SER:O	2.18	0.44
1:CO:142:SER:OG	2:CP:82:SER:OG	2.18	0.44
1:CU:68:ASP:O	1:CU:149:VAL:HA	2.17	0.44
1:DM:144:THR:HG21	2:DN:16:ALA:HB1	1.99	0.44
1:DM:181:LEU:HD22	1:DM:181:LEU:H	1.82	0.44
2:DP:128:GLU:N	2:DP:131:GLN:OE1	2.39	0.44
2:DP:98:LEU:HB2	2:DP:149:VAL:HB	1.99	0.44
1:AU:196:VAL:HG21	1:AU:221:TYR:CD1	2.52	0.44
1:BO:49:TRP:CH2	1:BO:104:LYS:HB2	2.52	0.44
1:BQ:184:GLY:N	1:BQ:213:ALA:HB1	2.31	0.44
1:CG:88:HIS:HB2	1:CG:100:ILE:HG23	1.98	0.44
2:CJ:91:ILE:HB	2:CJ:101:LYS:HD3	1.99	0.44
2:CL:5:VAL:HG21	2:CN:131:GLN:HB3	1.99	0.44
1:CM:106:LYS:NZ	2:CP:104:ASP:OD1	2.42	0.44
1:CQ:48:GLN:HA	1:CQ:105:LEU:HD12	1.99	0.44
2:AB:38:ASN:HD21	1:DC:182:GLU:HB3	1.82	0.44
2:AH:21:LEU:HD12	2:AH:31:LEU:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BI:184:GLY:H	1:BI:213:ALA:HB1	1.82	0.44
1:BK:37:TYR:CZ	2:BL:11:PRO:HG2	2.52	0.44
2:BL:39:GLU:OE2	2:BL:101:LYS:NZ	2.50	0.44
2:CR:116:LYS:NZ	2:CT:130:GLY:O	2.30	0.44
1:DC:76:ASN:HB2	1:DC:114:ARG:HH11	1.82	0.44
1:DQ:43:SER:OG	1:DQ:195:PRO:HB3	2.16	0.44
1:AG:52:SER:O	1:AG:101:MET:N	2.45	0.44
1:AI:78:GLN:NE2	1:AI:115:VAL:HG21	2.32	0.44
2:AV:128:GLU:O	2:AV:131:GLN:HG3	2.17	0.44
1:BK:138:ASN:ND2	1:BK:144:THR:HA	2.33	0.44
1:BO:153:LEU:HD11	1:BO:185:LYS:HD2	1.99	0.44
1:BQ:192:SER:HA	1:BQ:206:VAL:HG13	1.99	0.44
2:CB:33:LEU:HA	2:CB:44:ALA:O	2.17	0.44
2:CD:116:LYS:HD3	2:CF:130:GLY:HA3	1.99	0.44
2:CD:135:ASP:HB2	2:CD:151:ASP:HA	1.98	0.44
2:CD:36:ILE:HG12	2:CD:44:ALA:HB2	1.99	0.44
1:CM:94:ASN:HA	2:CN:73:PHE:CE2	2.52	0.44
1:BK:140:LYS:HZ1	2:DJ:50:HIS:CG	2.35	0.44
2:DR:47:LEU:HB2	2:DR:145:TYR:HB2	2.00	0.44
1:DU:204:GLY:HA2	1:DU:222:THR:O	2.16	0.44
2:AB:15:GLY:N	2:AB:59:PHE:O	2.51	0.44
2:AD:18:ALA:HB1	2:AD:56:PRO:HB2	2.00	0.44
1:AG:121:PRO:HD3	1:AG:202:LEU:O	2.18	0.44
1:AK:80:ILE:HG21	1:AK:105:LEU:HB3	1.99	0.44
2:AL:77:LYS:NZ	2:AL:80:PRO:O	2.48	0.44
2:BJ:77:LYS:HA	2:BJ:86:GLY:O	2.18	0.44
1:BM:68:ASP:O	1:BM:149:VAL:HA	2.16	0.44
1:CG:133:ILE:HG12	1:CG:196:VAL:HG22	2.00	0.44
2:DB:13:SER:HB2	2:DB:16:ALA:HB3	2.00	0.44
1:DG:178:ALA:HB3	1:DG:221:TYR:CE2	2.53	0.44
2:DN:89:ASP:OD1	2:DN:90:VAL:N	2.50	0.44
2:DT:128:GLU:HB2	2:DT:131:GLN:NE2	2.27	0.44
2:AB:77:LYS:NZ	2:AB:80:PRO:O	2.42	0.44
1:AC:120:LEU:HD13	1:AC:228:VAL:HG13	2.00	0.44
2:AB:3:VAL:HB	2:AD:128:GLU:HG3	1.98	0.44
1:AE:133:ILE:HG12	1:AE:196:VAL:HG22	2.00	0.44
2:AN:144:LYS:HZ1	1:DO:113:SER:HB2	1.82	0.44
2:AN:47:LEU:HG	2:AN:147:LEU:HD11	2.00	0.44
1:AO:178:ALA:HB3	1:AO:221:TYR:CE2	2.53	0.44
2:AR:5:VAL:CG1	2:AT:131:GLN:HE22	2.31	0.44
1:AU:55:HIS:O	2:AV:72:TYR:OH	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BC:74:GLU:N	1:BC:77:GLU:OE1	2.51	0.44
1:BG:51:VAL:HG21	1:BG:202:LEU:HD21	2.00	0.44
2:BH:46:VAL:HG12	2:BH:146:TYR:HA	1.99	0.44
2:CH:127:PRO:HB2	2:CH:131:GLN:OE1	2.18	0.44
1:CK:140:LYS:HD2	1:CK:145:SER:HB2	2.00	0.44
1:CQ:98:ASN:HA	1:CQ:227:TYR:OH	2.16	0.44
2:DH:134:LEU:HB3	2:DH:149:VAL:HG13	2.00	0.44
1:DI:144:THR:HG21	2:DJ:16:ALA:HB1	1.99	0.44
1:DK:55:HIS:CE1	2:DL:63:LEU:HD22	2.53	0.44
2:DT:1:SER:HA	2:DT:69:LYS:HD3	1.99	0.44
2:DT:20:TYR:CE2	2:DT:162:ALA:HA	2.53	0.44
2:DV:46:VAL:HG12	2:DV:146:TYR:HA	2.00	0.44
2:DV:89:ASP:OD1	2:DV:90:VAL:N	2.46	0.44
1:AU:184:GLY:H	1:AU:213:ALA:HB1	1.83	0.44
2:AV:138:LEU:HD11	2:AV:155:CYS:SG	2.57	0.44
2:BL:6:ASP:OD1	2:BL:10:GLN:N	2.46	0.44
2:BR:93:GLN:OE1	2:BR:101:LYS:HD2	2.18	0.44
2:BV:86:GLY:HA2	2:BV:102:VAL:HB	2.00	0.44
2:CB:29:ALA:HB1	2:CB:47:LEU:HB3	2.00	0.44
1:AK:151:LYS:NZ	2:CJ:50:HIS:HB3	2.32	0.44
2:CN:5:VAL:HA	2:CN:11:PRO:HA	1.99	0.44
1:DK:184:GLY:N	1:DK:213:ALA:HB1	2.33	0.44
1:DQ:55:HIS:ND1	2:DR:63:LEU:HD22	2.32	0.44
1:AA:223:LYS:HG2	1:AA:225:CYS:SG	2.58	0.44
1:AC:29:TYR:OH	1:AC:132:LEU:HD23	2.18	0.44
2:AL:3:VAL:HG11	2:AL:11:PRO:HB3	2.00	0.44
2:AL:47:LEU:HG	2:AL:147:LEU:HD11	1.99	0.44
2:AT:128:GLU:H	2:AT:131:GLN:HE21	1.64	0.44
2:BP:47:LEU:HB2	2:BP:145:TYR:HB2	2.00	0.44
1:BS:27:VAL:HG13	1:BS:29:TYR:CZ	2.52	0.44
1:CA:178:ALA:HB3	1:CA:221:TYR:CE2	2.52	0.44
1:CQ:181:LEU:H	1:CQ:181:LEU:HD22	1.83	0.44
2:CT:5:VAL:HG11	2:CV:131:GLN:CD	2.38	0.44
1:CU:178:ALA:HB3	1:CU:221:TYR:CE2	2.52	0.44
2:DD:72:TYR:O	2:DD:113:LYS:HG2	2.17	0.44
1:DG:158:LEU:HD12	1:DG:177:CYS:HB3	2.00	0.44
2:DT:5:VAL:HG21	2:DV:131:GLN:CB	2.47	0.44
1:AC:184:GLY:H	1:AC:213:ALA:HB1	1.83	0.44
2:AN:39:GLU:OE2	2:AN:93:GLN:NE2	2.46	0.44
1:BA:197:VAL:HG22	1:BA:202:LEU:HA	2.00	0.44
1:BA:196:VAL:HG21	1:BA:221:TYR:CD1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BH:33:LEU:HA	2:BH:44:ALA:O	2.17	0.44
1:BI:43:SER:HB2	1:BI:51:VAL:HG22	2.00	0.44
1:BM:16:ILE:HD13	1:BM:187:SER:HA	2.00	0.44
2:BN:4:VAL:HG13	2:BN:121:TYR:CE2	2.53	0.44
2:CB:57:VAL:HG11	2:CB:88:TRP:CZ2	2.52	0.44
1:CQ:32:SER:HB2	1:CQ:136:TRP:CZ3	2.53	0.44
1:CQ:180:TYR:CD2	1:CQ:185:LYS:HB2	2.53	0.44
1:CQ:24:ALA:HB1	1:CQ:114:ARG:HE	1.82	0.44
2:DD:3:VAL:HB	2:DF:128:GLU:HG3	1.99	0.44
2:DL:5:VAL:HG11	2:DN:131:GLN:OE1	2.18	0.44
1:AO:138:ASN:ND2	1:AO:144:THR:HA	2.33	0.43
1:AU:208:TRP:CZ3	2:AV:108:LEU:HD21	2.53	0.43
2:BD:43:ARG:O	2:BD:102:VAL:HG22	2.17	0.43
1:BQ:208:TRP:CZ3	2:BR:108:LEU:HD21	2.53	0.43
1:BS:192:SER:HA	1:BS:206:VAL:HG13	2.00	0.43
1:BS:45:ILE:HD11	1:BS:235:ILE:HD11	2.00	0.43
1:BU:129:THR:HB	1:BU:157:ILE:HD12	1.99	0.43
2:CB:13:SER:HA	2:CB:66:ASN:O	2.17	0.43
1:CM:178:ALA:HB3	1:CM:221:TYR:CE2	2.53	0.43
2:CP:137:GLY:HA3	2:CP:150:LYS:HB3	1.99	0.43
1:DE:133:ILE:HD13	1:DE:221:TYR:CE1	2.53	0.43
1:AK:138:ASN:ND2	1:AK:144:THR:HA	2.33	0.43
1:AK:96:LEU:HD11	2:AL:109:LEU:HD11	1.99	0.43
1:AQ:76:ASN:CB	1:AQ:114:ARG:HH11	2.31	0.43
2:BF:7:THR:HG23	2:BF:159:ILE:O	2.18	0.43
1:CC:64:ARG:HD3	1:CC:79:PHE:CZ	2.53	0.43
2:CP:39:GLU:OE2	2:CP:93:GLN:NE2	2.37	0.43
2:CR:87:VAL:O	2:CR:102:VAL:HA	2.18	0.43
2:CT:15:GLY:N	2:CT:59:PHE:O	2.51	0.43
2:DT:5:VAL:HG21	2:DV:131:GLN:HB3	2.00	0.43
2:BJ:13:SER:OG	2:BJ:16:ALA:HB3	2.18	0.43
1:BO:204:GLY:HA2	1:BO:222:THR:O	2.18	0.43
1:BS:44:LEU:O	1:BS:118:ILE:HG22	2.18	0.43
2:CL:134:LEU:HD13	2:CL:149:VAL:HG11	2.00	0.43
1:CQ:62:GLN:OE1	1:CQ:64:ARG:NE	2.39	0.43
2:DB:30:GLY:HA3	2:DB:51:HIS:O	2.17	0.43
2:AD:35:LYS:HE2	2:AD:40:ALA:O	2.19	0.43
1:AU:154:LYS:O	1:AU:180:TYR:OH	2.21	0.43
2:BF:127:PRO:HB2	2:BF:131:GLN:HE22	1.82	0.43
1:BK:54:ALA:HA	1:BK:101:MET:HB2	2.01	0.43
2:BL:161:LYS:HG2	2:BL:163:THR:H	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BO:180:TYR:HB3	1:BO:182:GLU:OE1	2.18	0.43
2:BP:9:GLY:HA2	2:BR:131:GLN:OE1	2.19	0.43
1:BS:78:GLN:HE21	1:BS:115:VAL:HG21	1.84	0.43
1:CA:196:VAL:HG21	1:CA:221:TYR:CD1	2.52	0.43
2:CB:98:LEU:HB2	2:CB:149:VAL:HB	1.99	0.43
1:CK:98:ASN:HA	1:CK:227:TYR:OH	2.18	0.43
2:CL:28:HIS:O	2:CL:49:PRO:HA	2.18	0.43
2:CR:39:GLU:OE2	2:CR:101:LYS:NZ	2.51	0.43
1:DE:51:VAL:HG21	1:DE:202:LEU:HD21	2.00	0.43
1:DI:106:LYS:NZ	2:DL:104:ASP:OD1	2.47	0.43
1:DU:49:TRP:CE2	1:DU:235:ILE:HG12	2.54	0.43
1:DU:29:TYR:CZ	1:DU:197:VAL:HG21	2.53	0.43
1:AK:88:HIS:CG	1:AK:89:PRO:HD2	2.53	0.43
1:AS:208:TRP:CH2	1:AS:220:VAL:HG21	2.53	0.43
2:BF:33:LEU:HD21	2:BF:78:PHE:HE2	1.83	0.43
1:BG:24:ALA:HB1	1:BG:114:ARG:HH21	1.83	0.43
1:BI:120:LEU:HD13	1:BI:228:VAL:HG13	2.01	0.43
2:BL:5:VAL:HG11	2:BN:131:GLN:OE1	2.18	0.43
1:BO:23:GLY:O	1:BO:26:THR:OG1	2.37	0.43
1:BQ:118:ILE:HD11	1:BQ:200:GLY:O	2.18	0.43
1:CI:192:SER:HA	1:CI:206:VAL:HG13	2.01	0.43
1:CM:132:LEU:HD13	1:CM:154:LYS:HE2	2.01	0.43
1:DE:189:GLN:NE2	2:DF:64:ARG:HA	2.33	0.43
2:DF:28:HIS:NE2	1:DI:228:VAL:HG12	2.34	0.43
1:DS:49:TRP:CH2	1:DS:104:LYS:HB2	2.54	0.43
1:BA:81:SER:HB2	1:BA:106:LYS:HD3	2.01	0.43
2:BL:7:THR:HG22	2:BL:158:LYS:HD3	2.01	0.43
1:BS:68:ASP:O	1:BS:149:VAL:HA	2.19	0.43
1:BU:54:ALA:HB1	1:BU:87:VAL:HG13	2.00	0.43
2:CD:15:GLY:N	2:CD:59:PHE:O	2.51	0.43
2:CD:36:ILE:CG1	2:CD:44:ALA:HB2	2.49	0.43
2:CD:19:TYR:N	2:CD:57:VAL:O	2.49	0.43
2:CN:5:VAL:HG21	2:CP:131:GLN:HB3	2.01	0.43
2:CV:89:ASP:N	2:CV:101:LYS:O	2.47	0.43
1:DM:55:HIS:HB3	1:DM:91:TYR:OH	2.18	0.43
1:DQ:51:VAL:HG21	1:DQ:202:LEU:HD21	2.00	0.43
1:AA:37:TYR:CZ	2:AB:11:PRO:HG2	2.54	0.43
1:AS:80:ILE:HG21	1:AS:105:LEU:HB3	1.99	0.43
1:BA:57:TYR:HE2	1:BA:85:SER:HB2	1.83	0.43
1:BG:51:VAL:HG12	1:BG:102:LEU:HD23	2.00	0.43
1:BK:178:ALA:HB3	1:BK:221:TYR:CE2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BV:127:PRO:HD2	2:BV:131:GLN:NE2	2.33	0.43
1:CK:57:TYR:O	2:CL:69:LYS:NZ	2.32	0.43
2:CT:128:GLU:N	2:CT:131:GLN:NE2	2.61	0.43
1:CU:91:TYR:HA	1:CU:98:ASN:HB2	2.01	0.43
1:DE:141:SER:HB3	1:DE:213:ALA:HB3	2.00	0.43
1:DM:129:THR:HB	1:DM:157:ILE:HD12	2.01	0.43
2:DT:116:LYS:HE2	1:DU:94:ASN:HD21	1.84	0.43
1:AG:35:SER:OG	1:AG:58:LYS:HE3	2.19	0.43
2:AJ:128:GLU:O	2:AJ:131:GLN:HG3	2.18	0.43
2:BB:5:VAL:HG21	2:BD:131:GLN:CB	2.49	0.43
2:BB:49:PRO:HB3	1:BE:122:THR:O	2.18	0.43
1:BM:187:SER:OG	2:BN:64:ARG:NH1	2.50	0.43
2:BV:115:GLU:CD	2:BV:124:VAL:HG21	2.40	0.43
1:CC:223:LYS:HG2	1:CC:225:CYS:SG	2.59	0.43
1:CE:88:HIS:HB2	1:CE:100:ILE:HG23	1.98	0.43
1:DC:178:ALA:HB3	1:DC:221:TYR:CE2	2.54	0.43
2:DJ:5:VAL:HG21	2:DL:131:GLN:HB3	2.00	0.43
2:DL:1:SER:HA	2:DL:69:LYS:HD3	2.00	0.43
1:AC:153:LEU:HD11	1:AC:185:LYS:HD2	2.00	0.43
2:AL:18:ALA:HB1	2:AL:56:PRO:HB2	2.01	0.43
2:BD:15:GLY:N	2:BD:59:PHE:O	2.51	0.43
2:BJ:73:PHE:HZ	2:BJ:129:ARG:O	2.02	0.43
2:BT:90:VAL:HB	2:BT:125:TYR:CZ	2.53	0.43
1:BU:68:ASP:O	1:BU:149:VAL:HA	2.18	0.43
2:CH:6:ASP:OD2	2:CH:10:GLN:HB2	2.19	0.43
2:CF:25:SER:O	1:CI:124:CYS:SG	2.77	0.43
1:DG:32:SER:HB2	1:DG:136:TRP:CZ3	2.54	0.43
2:DH:98:LEU:HB2	2:DH:149:VAL:HB	2.00	0.43
1:DI:138:ASN:ND2	1:DI:144:THR:HA	2.33	0.43
1:DO:178:ALA:HB3	1:DO:221:TYR:CE2	2.53	0.43
2:AF:7:THR:N	2:AF:159:ILE:O	2.51	0.43
2:AH:31:LEU:HD23	2:AH:31:LEU:HA	1.86	0.43
1:AO:214:GLN:HB2	1:AO:217:LYS:HD2	2.01	0.43
2:AP:127:PRO:HD2	2:AP:131:GLN:NE2	2.34	0.43
1:AU:54:ALA:N	1:AU:99:ASP:OD1	2.51	0.43
2:BB:128:GLU:HB2	2:BB:131:GLN:NE2	2.33	0.43
1:BE:58:LYS:HB3	1:BE:61:ILE:HD11	2.01	0.43
1:BG:186:ASP:OD2	2:BH:64:ARG:NH2	2.42	0.43
2:BJ:101:LYS:HE2	2:BJ:101:LYS:HB3	1.92	0.43
2:BL:128:GLU:H	2:BL:131:GLN:HE22	1.66	0.43
1:BQ:204:GLY:HA2	1:BQ:222:THR:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BU:78:GLN:NE2	1:BU:115:VAL:HG21	2.34	0.43
2:CR:73:PHE:HB2	2:CR:109:LEU:HD22	2.01	0.43
1:DA:206:VAL:HA	1:DA:221:TYR:HD1	1.82	0.43
1:DG:43:SER:OG	1:DG:195:PRO:HB3	2.19	0.43
2:DJ:33:LEU:HB3	2:DJ:42:PRO:HB2	2.01	0.43
2:DL:116:LYS:HG2	1:DM:94:ASN:ND2	2.33	0.43
1:AC:77:GLU:HB3	1:AC:79:PHE:CE1	2.54	0.42
1:AG:78:GLN:HE22	1:AG:110:SER:H	1.67	0.42
1:AG:153:LEU:HD11	1:AG:185:LYS:HD2	2.01	0.42
2:AT:47:LEU:HB2	2:AT:145:TYR:HB2	2.01	0.42
2:BD:45:VAL:HG11	2:BD:88:TRP:CZ2	2.54	0.42
1:BM:184:GLY:H	1:BM:213:ALA:HB1	1.81	0.42
1:BM:43:SER:OG	1:BM:195:PRO:HB3	2.19	0.42
2:BN:90:VAL:HB	2:BN:125:TYR:CZ	2.54	0.42
2:BP:2:SER:HB2	2:BP:70:GLU:OE2	2.19	0.42
1:BQ:16:ILE:HD13	1:BQ:187:SER:HA	2.00	0.42
2:CB:30:GLY:O	2:CB:47:LEU:HA	2.19	0.42
2:CL:49:PRO:HB3	1:CO:122:THR:O	2.19	0.42
2:DN:36:ILE:HD12	2:DN:93:GLN:OE1	2.18	0.42
1:AC:181:LEU:H	1:AC:181:LEU:HD22	1.84	0.42
1:AU:37:TYR:CZ	2:AV:11:PRO:HG2	2.54	0.42
1:BQ:136:TRP:CZ2	1:BQ:150:LEU:HD13	2.54	0.42
2:BV:43:ARG:O	2:BV:102:VAL:HG22	2.18	0.42
2:CB:20:TYR:CE2	2:CB:162:ALA:HA	2.54	0.42
2:CP:29:ALA:HB1	2:CP:47:LEU:HB3	1.99	0.42
1:CQ:99:ASP:HB3	1:CQ:222:THR:HG1	1.84	0.42
1:CQ:55:HIS:O	2:CR:72:TYR:OH	2.30	0.42
2:DP:89:ASP:OD1	2:DP:90:VAL:N	2.50	0.42
1:DS:37:TYR:CE2	2:DT:11:PRO:HG2	2.54	0.42
2:AF:33:LEU:HB3	2:AF:42:PRO:HB2	2.01	0.42
2:AR:5:VAL:HG13	2:AT:131:GLN:OE1	2.18	0.42
1:BA:178:ALA:HB3	1:BA:221:TYR:CE2	2.53	0.42
2:BT:127:PRO:HD2	2:BT:131:GLN:NE2	2.35	0.42
2:CB:158:LYS:HE2	2:CD:132:THR:HG21	2.01	0.42
2:CD:145:TYR:HE2	1:CG:123:SER:HB2	1.84	0.42
2:CF:5:VAL:HG21	2:CH:131:GLN:HG2	2.00	0.42
1:CG:212:CYS:HA	2:CH:64:ARG:NH2	2.34	0.42
1:DA:98:ASN:HA	1:DA:227:TYR:OH	2.19	0.42
1:DQ:76:ASN:CG	1:DQ:114:ARG:HD2	2.40	0.42
2:AD:23:PRO:HG3	2:AD:47:LEU:HD13	2.02	0.42
2:AF:126:TYR:HB3	2:AF:128:GLU:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BG:74:GLU:N	1:BG:77:GLU:OE1	2.53	0.42
2:BH:5:VAL:HG21	2:BJ:131:GLN:CB	2.50	0.42
1:BO:196:VAL:HB	1:BO:204:GLY:CA	2.49	0.42
1:AQ:113:SER:OG	2:CD:143:ASP:HB2	2.18	0.42
1:CE:178:ALA:HB3	1:CE:221:TYR:CE2	2.54	0.42
1:DG:51:VAL:HG12	1:DG:102:LEU:CD2	2.49	0.42
1:DS:197:VAL:HG22	1:DS:202:LEU:HA	2.01	0.42
1:AC:43:SER:HB2	1:AC:51:VAL:HG22	2.02	0.42
1:AM:180:TYR:CD2	1:AM:185:LYS:HB2	2.53	0.42
1:CG:144:THR:HG21	2:CH:16:ALA:HA	2.00	0.42
1:CM:130:GLN:OE1	1:CM:156:PRO:HB3	2.19	0.42
2:DF:74:LEU:HD12	2:DF:114:VAL:HG23	2.02	0.42
2:DL:6:ASP:OD2	2:DL:10:GLN:HB2	2.19	0.42
1:DQ:204:GLY:HA2	1:DQ:222:THR:O	2.20	0.42
2:DT:21:LEU:HD12	2:DT:31:LEU:HD11	2.01	0.42
1:AC:68:ASP:O	1:AC:149:VAL:HA	2.18	0.42
1:AE:54:ALA:HB1	1:AE:87:VAL:HG13	2.02	0.42
1:AK:69:ASN:HA	1:AK:148:ASP:O	2.20	0.42
1:AS:67:GLU:CG	1:AS:77:GLU:HG3	2.50	0.42
2:BB:39:GLU:OE2	2:BB:101:LYS:NZ	2.50	0.42
1:BC:99:ASP:HB3	1:BC:222:THR:OG1	2.20	0.42
2:BF:33:LEU:HA	2:BF:44:ALA:O	2.20	0.42
1:BM:106:LYS:HG3	1:BM:107:SER:N	2.34	0.42
2:CL:128:GLU:H	2:CL:131:GLN:HE22	1.67	0.42
2:CR:128:GLU:HB2	2:CR:131:GLN:OE1	2.20	0.42
1:DA:181:LEU:HD22	1:DA:181:LEU:H	1.84	0.42
2:DF:45:VAL:HG11	2:DF:88:TRP:CZ2	2.54	0.42
1:DI:76:ASN:CB	1:DI:114:ARG:HH11	2.33	0.42
2:DP:90:VAL:HB	2:DP:125:TYR:CZ	2.55	0.42
1:DS:55:HIS:CG	2:DT:63:LEU:HD22	2.55	0.42
2:DV:7:THR:HG23	2:DV:159:ILE:O	2.19	0.42
1:AG:138:ASN:ND2	1:AG:144:THR:HA	2.34	0.42
1:AG:144:THR:HG21	2:AH:16:ALA:HA	2.02	0.42
1:AM:55:HIS:HB3	1:AM:91:TYR:OH	2.19	0.42
1:AQ:98:ASN:HA	1:AQ:227:TYR:OH	2.20	0.42
1:AS:233:GLN:O	1:AS:236:ALA:HB3	2.20	0.42
2:BD:116:LYS:HD3	2:BF:130:GLY:O	2.19	0.42
1:BO:51:VAL:HG12	1:BO:102:LEU:HD23	2.01	0.42
1:BQ:69:ASN:OD1	1:BQ:148:ASP:HB3	2.20	0.42
1:BS:69:ASN:HA	1:BS:148:ASP:O	2.19	0.42
1:BU:184:GLY:N	1:BU:213:ALA:HB1	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CG:199:SER:O	1:CG:201:LYS:HG2	2.20	0.42
1:CU:205:ILE:HB	1:CU:222:THR:HB	2.02	0.42
1:DI:98:ASN:HA	1:DI:227:TYR:OH	2.20	0.42
2:DJ:43:ARG:O	2:DJ:101:LYS:HA	2.20	0.42
1:DO:206:VAL:HA	1:DO:221:TYR:HD1	1.81	0.42
1:DQ:113:SER:C	1:DQ:115:VAL:H	2.23	0.42
1:AC:106:LYS:NZ	2:AF:104:ASP:OD2	2.47	0.42
2:AJ:91:ILE:HB	2:AJ:101:LYS:HD3	2.01	0.42
2:AN:25:SER:HA	1:AQ:226:ASN:OD1	2.20	0.42
2:AT:30:GLY:HA3	2:AT:54:GLY:HA3	2.02	0.42
1:AS:55:HIS:O	2:AT:72:TYR:OH	2.37	0.42
2:AT:58:ARG:NE	2:AT:79:GLY:O	2.34	0.42
2:BH:23:PRO:HG3	2:BH:47:LEU:HD13	2.02	0.42
1:BI:69:ASN:HA	1:BI:148:ASP:O	2.20	0.42
1:BK:206:VAL:HA	1:BK:221:TYR:HD1	1.83	0.42
2:CD:138:LEU:HA	2:CD:138:LEU:HD23	1.82	0.42
2:CL:5:VAL:HG21	2:CN:131:GLN:CB	2.50	0.42
2:DB:128:GLU:H	2:DB:131:GLN:CD	2.23	0.42
1:DE:24:ALA:HB1	1:DE:114:ARG:NE	2.35	0.42
2:DF:18:ALA:HB1	2:DF:56:PRO:HB2	2.02	0.42
2:DJ:5:VAL:HG11	2:DL:131:GLN:HE22	1.85	0.42
1:DK:54:ALA:HA	1:DK:101:MET:HB2	2.02	0.42
1:AC:204:GLY:HA2	1:AC:222:THR:O	2.19	0.42
1:AU:206:VAL:HA	1:AU:221:TYR:HD1	1.84	0.42
2:BJ:125:TYR:CE2	2:BJ:127:PRO:HG3	2.55	0.42
1:BM:98:ASN:HA	1:BM:227:TYR:OH	2.20	0.42
2:BP:19:TYR:CD2	2:BP:161:LYS:HA	2.54	0.42
1:BQ:210:SER:HB3	1:BQ:217:LYS:HD3	2.01	0.42
1:BS:51:VAL:HG12	1:BS:102:LEU:HD23	2.00	0.42
2:BT:5:VAL:HG11	2:BV:131:GLN:OE1	2.20	0.42
1:BS:187:SER:OG	2:BT:64:ARG:NH1	2.53	0.42
1:CA:17:VAL:O	1:CA:185:LYS:HA	2.20	0.42
2:CD:139:VAL:HB	2:CD:146:TYR:HB2	2.01	0.42
1:CE:140:LYS:HD2	1:CE:145:SER:HB2	2.01	0.42
2:CJ:125:TYR:CE2	2:CJ:127:PRO:HG3	2.54	0.42
1:CO:58:LYS:HZ1	2:CR:128:GLU:CD	2.23	0.42
2:CP:2:SER:O	2:CP:70:GLU:HG3	2.20	0.42
2:CR:85:SER:HA	2:CR:104:ASP:HA	2.01	0.42
2:DB:6:ASP:OD1	2:DB:10:GLN:N	2.48	0.42
1:DI:174:ASN:HA	1:DI:226:ASN:HD22	1.85	0.42
2:DT:116:LYS:HG2	1:DU:94:ASN:HD22	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AH:38:ASN:OD1	1:DI:130:GLN:HG2	2.19	0.42
1:AM:24:ALA:HB1	1:AM:114:ARG:HE	1.84	0.42
2:AL:116:LYS:NZ	2:AN:130:GLY:O	2.43	0.42
2:AN:18:ALA:HB1	2:AN:56:PRO:HB2	2.02	0.42
1:AU:144:THR:HG21	2:AV:16:ALA:HB1	2.01	0.42
2:BB:116:LYS:HG2	1:BC:94:ASN:ND2	2.31	0.42
2:BL:135:ASP:HB3	2:BL:154:PRO:HB3	2.02	0.42
2:CB:28:HIS:CD2	1:CE:228:VAL:HB	2.55	0.42
2:CJ:3:VAL:HG11	2:CJ:11:PRO:HB3	2.01	0.42
1:CS:68:ASP:O	1:CS:149:VAL:HA	2.20	0.42
1:CS:92:ASN:HB3	1:CS:95:THR:OG1	2.19	0.42
2:CR:145:TYR:HE2	1:CU:123:SER:HB2	1.84	0.42
1:CU:88:HIS:HB2	1:CU:100:ILE:HG23	2.02	0.42
1:DA:144:THR:HG21	2:DB:16:ALA:CB	2.49	0.42
2:DD:115:GLU:CD	2:DD:124:VAL:HG21	2.40	0.42
1:DI:139:THR:HG23	1:DI:147:PRO:HD3	2.02	0.42
1:DU:29:TYR:CG	1:DU:118:ILE:HB	2.55	0.42
1:AA:196:VAL:HG21	1:AA:221:TYR:CD1	2.54	0.41
1:AA:178:ALA:HB3	1:AA:221:TYR:CE2	2.55	0.41
2:AD:5:VAL:HG11	2:AF:131:GLN:OE1	2.20	0.41
2:AN:14:ASN:OD1	2:AN:60:GLU:HA	2.20	0.41
1:AQ:180:TYR:HD2	1:AQ:185:LYS:HB2	1.83	0.41
1:AS:181:LEU:H	1:AS:181:LEU:HD22	1.85	0.41
2:BF:12:VAL:HG13	2:BF:19:TYR:CE1	2.54	0.41
2:BL:46:VAL:HG12	2:BL:146:TYR:HA	2.01	0.41
2:BN:136:ILE:HA	2:BN:136:ILE:HD13	1.94	0.41
1:BO:136:TRP:CH2	1:BO:150:LEU:HD13	2.55	0.41
2:BV:12:VAL:HG13	2:BV:19:TYR:CE1	2.55	0.41
2:CB:116:LYS:NZ	2:CD:130:GLY:O	2.37	0.41
1:CG:32:SER:OG	1:CG:38:HIS:ND1	2.32	0.41
1:DO:51:VAL:HG12	1:DO:102:LEU:HD23	2.02	0.41
1:DQ:140:LYS:HD2	1:DQ:145:SER:HB2	2.02	0.41
1:DQ:96:LEU:HD11	2:DR:109:LEU:HD11	2.02	0.41
1:AA:55:HIS:CE1	2:AB:63:LEU:HD22	2.55	0.41
1:AA:188:CYS:O	2:AB:64:ARG:HB3	2.20	0.41
2:AP:134:LEU:HB3	2:AP:149:VAL:HG13	2.01	0.41
1:AO:58:LYS:NZ	2:AR:128:GLU:OE2	2.53	0.41
2:AV:35:LYS:HG3	2:AV:42:PRO:HB3	2.02	0.41
1:BA:129:THR:HB	1:BA:157:ILE:HD12	2.01	0.41
1:BG:98:ASN:HA	1:BG:227:TYR:OH	2.20	0.41
2:BH:135:ASP:HB3	2:BH:154:PRO:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BL:2:SER:HB2	2:BL:70:GLU:OE2	2.21	0.41
2:BN:127:PRO:HB2	2:BN:131:GLN:OE1	2.20	0.41
2:CD:73:PHE:HB2	2:CD:109:LEU:HD22	2.01	0.41
1:CE:17:VAL:O	1:CE:185:LYS:HA	2.20	0.41
2:CJ:46:VAL:HG12	2:CJ:146:TYR:HA	2.02	0.41
2:CN:98:LEU:HB2	2:CN:149:VAL:HB	2.02	0.41
2:CP:33:LEU:HA	2:CP:44:ALA:O	2.20	0.41
1:CO:106:LYS:NZ	2:CR:104:ASP:OD2	2.52	0.41
1:CS:51:VAL:HG12	1:CS:102:LEU:CD2	2.50	0.41
2:CV:128:GLU:N	2:CV:131:GLN:OE1	2.52	0.41
2:DH:5:VAL:HG21	2:DJ:131:GLN:HB3	2.02	0.41
2:DN:46:VAL:HG12	2:DN:146:TYR:HA	2.03	0.41
2:DR:7:THR:N	2:DR:159:ILE:O	2.51	0.41
2:AN:109:LEU:HB2	2:AN:129:ARG:HE	1.84	0.41
1:AO:170:GLN:OE1	2:AP:129:ARG:NH2	2.52	0.41
2:AR:36:ILE:HG23	2:AR:96:ILE:CG1	2.50	0.41
2:BD:125:TYR:CE2	2:BD:127:PRO:HG3	2.55	0.41
1:BE:54:ALA:HA	1:BE:101:MET:HB2	2.02	0.41
1:BS:181:LEU:H	1:BS:181:LEU:HD22	1.85	0.41
1:CO:44:LEU:O	1:CO:118:ILE:HG22	2.20	0.41
1:CQ:192:SER:HA	1:CQ:206:VAL:HG13	2.02	0.41
2:DD:101:LYS:HE2	2:DD:101:LYS:HB3	1.87	0.41
2:DF:138:LEU:HD13	2:DF:145:TYR:CD1	2.55	0.41
2:DP:13:SER:HA	2:DP:66:ASN:O	2.20	0.41
2:DP:60:GLU:OE1	2:DP:106:LYS:HD2	2.20	0.41
1:DU:181:LEU:H	1:DU:181:LEU:HD22	1.84	0.41
1:DU:102:LEU:HD21	1:DU:231:ILE:HG23	2.02	0.41
1:AC:43:SER:OG	1:AC:195:PRO:HB3	2.20	0.41
2:AH:125:TYR:CZ	2:AH:127:PRO:HA	2.55	0.41
2:BF:91:ILE:HB	2:BF:101:LYS:HD3	2.01	0.41
1:BK:51:VAL:HG12	1:BK:102:LEU:HD23	2.03	0.41
1:BQ:17:VAL:O	1:BQ:185:LYS:HA	2.20	0.41
2:BT:29:ALA:HB1	2:BT:47:LEU:HB3	2.02	0.41
2:CB:112:PHE:HA	2:CB:124:VAL:O	2.20	0.41
1:CC:133:ILE:HG12	1:CC:196:VAL:HG13	2.03	0.41
1:CC:184:GLY:N	1:CC:213:ALA:HB1	2.35	0.41
2:CD:13:SER:OG	2:CD:17:ASP:N	2.49	0.41
2:CT:13:SER:HA	2:CT:66:ASN:O	2.20	0.41
1:DA:155:ALA:HB1	1:DA:179:GLY:HA2	2.03	0.41
2:DB:5:VAL:HA	2:DB:12:VAL:HG23	2.01	0.41
2:DL:5:VAL:HG21	2:DN:131:GLN:NE2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:DT:18:ALA:HB1	2:DT:56:PRO:HB2	2.02	0.41
2:AB:73:PHE:CZ	2:AB:113:LYS:HE3	2.56	0.41
1:AO:186:ASP:CG	2:AP:64:ARG:HH12	2.23	0.41
2:AR:36:ILE:HD12	2:AR:93:GLN:OE1	2.19	0.41
2:BD:56:PRO:O	2:BD:78:PHE:HD1	2.04	0.41
2:BF:60:GLU:OE1	2:BF:106:LYS:NZ	2.48	0.41
1:BM:181:LEU:HD22	1:BM:181:LEU:H	1.85	0.41
1:CE:133:ILE:HG12	1:CE:196:VAL:HG22	2.02	0.41
1:CE:204:GLY:HA2	1:CE:222:THR:O	2.20	0.41
1:DE:181:LEU:HD22	1:DE:181:LEU:H	1.85	0.41
1:DM:98:ASN:HA	1:DM:227:TYR:OH	2.20	0.41
1:DQ:62:GLN:HA	1:DQ:81:SER:HA	2.02	0.41
1:AC:178:ALA:HB3	1:AC:221:TYR:CE2	2.55	0.41
1:AO:208:TRP:CZ3	2:AP:108:LEU:HD21	2.55	0.41
1:AQ:49:TRP:CZ3	1:AQ:102:LEU:HB3	2.56	0.41
2:AR:127:PRO:HD2	2:AR:131:GLN:HE22	1.82	0.41
2:AR:52:ARG:HA	2:AR:53:PRO:HA	1.89	0.41
1:BE:43:SER:OG	1:BE:195:PRO:HB3	2.21	0.41
1:BG:54:ALA:HB1	1:BG:87:VAL:HG13	2.01	0.41
1:BI:48:GLN:HG2	1:BI:108:ALA:HA	2.03	0.41
1:BM:51:VAL:HG12	1:BM:102:LEU:HD23	2.01	0.41
2:BT:15:GLY:HA2	2:BT:60:GLU:HG2	2.03	0.41
2:BT:61:SER:HB2	2:BT:74:LEU:HD23	2.02	0.41
1:CA:17:VAL:HG12	1:CA:184:GLY:O	2.20	0.41
1:CC:78:GLN:NE2	1:CC:110:SER:OG	2.54	0.41
1:CO:80:ILE:HG21	1:CO:105:LEU:HB3	2.02	0.41
2:CP:7:THR:HG23	2:CP:159:ILE:O	2.21	0.41
1:CS:29:TYR:CE2	1:CS:118:ILE:HD13	2.55	0.41
2:CT:126:TYR:HB3	2:CT:128:GLU:O	2.20	0.41
2:DF:116:LYS:HD3	2:DH:130:GLY:HA3	2.02	0.41
1:AG:99:ASP:HB3	1:AG:222:THR:OG1	2.21	0.41
1:AQ:43:SER:OG	1:AQ:195:PRO:HB3	2.20	0.41
2:AR:15:GLY:N	2:AR:59:PHE:O	2.54	0.41
2:AR:89:ASP:O	2:AR:101:LYS:N	2.38	0.41
1:BA:138:ASN:ND2	1:BA:143:GLY:O	2.54	0.41
1:BC:37:TYR:CZ	2:BD:11:PRO:HG2	2.56	0.41
1:BG:138:ASN:ND2	1:BG:144:THR:HA	2.36	0.41
2:BJ:19:TYR:N	2:BJ:57:VAL:O	2.48	0.41
2:BJ:5:VAL:HG22	2:BL:131:GLN:HG2	2.02	0.41
2:BP:87:VAL:O	2:BP:102:VAL:HA	2.21	0.41
1:BQ:51:VAL:HG21	1:BQ:202:LEU:HD21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CI:136:TRP:CZ2	1:CI:150:LEU:HD13	2.55	0.41
2:CJ:92:GLN:HE22	2:CJ:97:GLY:HA2	1.84	0.41
1:CK:154:LYS:O	1:CK:180:TYR:OH	2.36	0.41
1:CQ:43:SER:OG	1:CQ:195:PRO:HB3	2.20	0.41
2:CR:11:PRO:HB2	2:CR:67:ILE:HG22	2.03	0.41
1:CU:204:GLY:HA2	1:CU:222:THR:O	2.21	0.41
1:DC:138:ASN:HB3	1:DC:188:CYS:SG	2.61	0.41
2:DF:47:LEU:HG	2:DF:147:LEU:HD11	2.03	0.41
1:DI:192:SER:HA	1:DI:206:VAL:HG13	2.03	0.41
1:DM:131:CYS:O	1:DM:154:LYS:HA	2.20	0.41
2:DN:127:PRO:HD2	2:DN:131:GLN:NE2	2.35	0.41
1:AE:208:TRP:CH2	1:AE:220:VAL:HG21	2.55	0.41
2:AR:12:VAL:HG13	2:AR:19:TYR:CE1	2.55	0.41
2:AV:45:VAL:HG11	2:AV:88:TRP:CZ2	2.55	0.41
2:BB:5:VAL:HG21	2:BD:131:GLN:HB3	2.02	0.41
1:BC:181:LEU:H	1:BC:181:LEU:HD22	1.85	0.41
2:BL:145:TYR:OH	1:BO:124:CYS:N	2.53	0.41
2:BP:5:VAL:HG11	2:BR:131:GLN:HB2	2.03	0.41
1:BQ:32:SER:HB2	1:BQ:136:TRP:CZ3	2.56	0.41
1:BS:29:TYR:CZ	1:BS:197:VAL:HG21	2.54	0.41
2:BT:128:GLU:N	2:BT:131:GLN:OE1	2.53	0.41
2:BT:128:GLU:H	2:BT:131:GLN:CD	2.24	0.41
2:CB:104:ASP:N	2:CB:104:ASP:OD2	2.53	0.41
2:CF:104:ASP:N	2:CF:104:ASP:OD2	2.54	0.41
2:CH:3:VAL:HG11	2:CH:11:PRO:HB3	2.02	0.41
2:CL:2:SER:O	2:CL:70:GLU:HG3	2.20	0.41
1:CM:94:ASN:HD22	2:CN:73:PHE:HE2	1.69	0.41
2:CT:90:VAL:HB	2:CT:125:TYR:CZ	2.56	0.41
1:CU:102:LEU:HD21	1:CU:231:ILE:HG23	2.03	0.41
1:DE:40:CYS:SG	2:DF:65:ILE:HD12	2.60	0.41
2:DT:134:LEU:HD13	2:DT:149:VAL:HG11	2.01	0.41
2:AD:116:LYS:HG2	1:AE:94:ASN:ND2	2.35	0.41
1:AI:96:LEU:CD1	2:AJ:109:LEU:HD11	2.50	0.41
2:AL:89:ASP:OD1	2:AL:90:VAL:N	2.53	0.41
1:BA:32:SER:OG	1:BA:38:HIS:ND1	2.38	0.41
2:BD:142:ASN:ND2	2:BD:146:TYR:OH	2.52	0.41
2:BJ:131:GLN:HB3	2:BJ:131:GLN:HE21	1.59	0.41
1:BM:32:SER:HB2	1:BM:136:TRP:CZ3	2.56	0.41
2:BN:131:GLN:HE21	2:BN:131:GLN:HB3	1.60	0.41
1:BS:186:ASP:OD2	2:BT:64:ARG:NH2	2.44	0.41
1:BU:106:LYS:HG3	1:BU:107:SER:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:43:SER:HB2	1:CA:51:VAL:HG22	2.02	0.41
2:CB:116:LYS:HE2	1:CC:94:ASN:HD21	1.86	0.41
2:CD:33:LEU:HA	2:CD:44:ALA:O	2.21	0.41
1:CK:26:THR:H	1:CK:26:THR:HG1	1.63	0.41
2:CL:36:ILE:CG1	2:CL:44:ALA:HB2	2.51	0.41
1:CO:88:HIS:HB2	1:CO:100:ILE:HG23	2.02	0.41
2:CP:13:SER:HB2	2:CP:16:ALA:HB3	2.03	0.41
1:CU:133:ILE:HG12	1:CU:196:VAL:HG22	2.03	0.41
2:DH:134:LEU:HD13	2:DH:149:VAL:HG11	2.03	0.41
2:DJ:39:GLU:OE2	2:DJ:93:GLN:NE2	2.49	0.41
1:DI:94:ASN:OD1	2:DJ:73:PHE:HE2	2.03	0.41
1:DK:16:ILE:O	1:DK:139:THR:HA	2.21	0.41
1:DQ:17:VAL:O	1:DQ:185:LYS:HA	2.21	0.41
2:DT:43:ARG:O	2:DT:102:VAL:HG22	2.21	0.41
1:AC:98:ASN:HA	1:AC:227:TYR:OH	2.21	0.41
1:AO:181:LEU:HD22	1:AO:181:LEU:H	1.86	0.41
1:AS:167:TYR:HB2	1:AS:171:ILE:HD11	2.02	0.41
2:BD:115:GLU:CD	2:BD:124:VAL:HG21	2.41	0.41
1:BO:28:PRO:HB3	1:BO:113:SER:O	2.20	0.41
1:BU:49:TRP:CD2	1:BU:235:ILE:HG12	2.56	0.41
2:CD:128:GLU:N	2:CD:131:GLN:OE1	2.52	0.41
1:CE:51:VAL:HG12	1:CE:102:LEU:HD23	2.02	0.41
2:CN:127:PRO:HD2	2:CN:131:GLN:NE2	2.35	0.41
2:DB:2:SER:HB2	2:DB:70:GLU:OE2	2.20	0.41
1:DI:16:ILE:HD13	1:DI:187:SER:HA	2.03	0.41
1:DM:96:LEU:HD11	2:DN:109:LEU:HD11	2.03	0.41
2:DV:142:ASN:ND2	2:DV:146:TYR:OH	2.51	0.41
1:AA:99:ASP:OD2	1:AA:207:SER:OG	2.29	0.41
2:AD:98:LEU:HB2	2:AD:149:VAL:HB	2.03	0.41
1:AO:62:GLN:HA	1:AO:81:SER:HA	2.02	0.41
1:AQ:80:ILE:CG2	1:AQ:105:LEU:HB3	2.51	0.41
1:AQ:78:GLN:NE2	1:AQ:115:VAL:HG21	2.36	0.41
1:BA:181:LEU:HD22	1:BA:181:LEU:H	1.86	0.41
1:BM:204:GLY:HA2	1:BM:222:THR:O	2.21	0.41
2:BN:101:LYS:HB3	2:BN:101:LYS:HE2	1.95	0.41
2:BP:101:LYS:HE2	2:BP:101:LYS:HB3	1.83	0.41
2:BP:6:ASP:OD1	2:BP:9:GLY:N	2.54	0.41
1:BS:129:THR:HB	1:BS:157:ILE:HD12	2.02	0.41
1:CC:76:ASN:HB2	1:CC:114:ARG:HH11	1.85	0.41
1:DE:29:TYR:CZ	1:DE:197:VAL:HG21	2.56	0.41
2:DH:20:TYR:CE2	2:DH:162:ALA:HA	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DI:206:VAL:HA	1:DI:221:TYR:HD1	1.85	0.41
1:DK:32:SER:HB2	1:DK:136:TRP:CZ3	2.56	0.41
2:DN:131:GLN:HE21	2:DN:131:GLN:HB3	1.62	0.41
2:DP:116:LYS:HG2	1:DQ:94:ASN:HD21	1.86	0.41
1:DS:68:ASP:O	1:DS:149:VAL:HA	2.20	0.41
1:AA:26:THR:HG1	1:AA:26:THR:H	1.59	0.40
2:AH:104:ASP:OD2	2:AH:104:ASP:N	2.52	0.40
1:AS:67:GLU:HG2	1:AS:77:GLU:HG3	2.02	0.40
1:BI:144:THR:HG21	2:BJ:16:ALA:HB1	2.03	0.40
2:BT:72:TYR:O	2:BT:113:LYS:HG2	2.20	0.40
1:CA:154:LYS:O	1:CA:180:TYR:OH	2.33	0.40
2:CJ:23:PRO:HG3	2:CJ:47:LEU:HD13	2.02	0.40
2:CT:11:PRO:HB2	2:CT:67:ILE:HG22	2.03	0.40
2:DB:7:THR:N	2:DB:159:ILE:O	2.54	0.40
1:DE:69:ASN:HA	1:DE:148:ASP:O	2.21	0.40
2:DH:11:PRO:HB2	2:DH:67:ILE:HG22	2.03	0.40
1:DK:184:GLY:H	1:DK:213:ALA:HB1	1.85	0.40
2:DJ:28:HIS:CE1	1:DM:232:LYS:HD2	2.56	0.40
2:DR:13:SER:HB2	2:DR:16:ALA:HB3	2.03	0.40
1:AA:29:TYR:CZ	1:AA:197:VAL:HG21	2.56	0.40
1:AI:55:HIS:CE1	2:AJ:63:LEU:HD22	2.56	0.40
2:AJ:131:GLN:HE21	2:AJ:131:GLN:HB3	1.59	0.40
2:AN:60:GLU:OE1	2:AN:106:LYS:NZ	2.48	0.40
1:AQ:76:ASN:HB2	1:AQ:114:ARG:NH1	2.36	0.40
1:AS:139:THR:HG23	1:AS:147:PRO:HD3	2.03	0.40
1:BA:70:ILE:HG23	1:BA:71:ASN:OD1	2.21	0.40
1:BM:121:PRO:HG2	1:BM:225:CYS:HA	2.03	0.40
1:BQ:197:VAL:HA	1:BQ:201:LYS:O	2.20	0.40
2:BV:29:ALA:HB1	2:BV:47:LEU:HB3	2.03	0.40
1:CG:181:LEU:H	1:CG:181:LEU:HD22	1.85	0.40
2:CL:131:GLN:H	2:CL:131:GLN:CD	2.25	0.40
2:CT:36:ILE:CG1	2:CT:44:ALA:HB2	2.51	0.40
1:DA:74:GLU:HB2	1:DA:77:GLU:OE2	2.21	0.40
1:DC:181:LEU:HD22	1:DC:181:LEU:H	1.86	0.40
1:DE:57:TYR:O	2:DF:69:LYS:NZ	2.26	0.40
1:DE:189:GLN:HE21	2:DF:64:ARG:HA	1.85	0.40
2:DH:28:HIS:CD2	1:DK:228:VAL:HB	2.56	0.40
1:DS:178:ALA:HB3	1:DS:221:TYR:CE2	2.56	0.40
2:AJ:47:LEU:HG	2:AJ:147:LEU:HD11	2.03	0.40
2:AL:89:ASP:N	2:AL:101:LYS:O	2.52	0.40
2:AJ:28:HIS:CD2	1:AM:229:SER:H	2.39	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AN:20:TYR:CE2	2:AN:162:ALA:HA	2.57	0.40
1:AU:223:LYS:HG2	1:AU:225:CYS:SG	2.61	0.40
1:BI:138:ASN:ND2	1:BI:144:THR:HA	2.35	0.40
1:CC:106:LYS:HG3	1:CC:107:SER:N	2.37	0.40
1:CC:29:TYR:OH	1:CC:132:LEU:HD23	2.22	0.40
1:CG:35:SER:OG	1:CG:58:LYS:HE3	2.22	0.40
2:CH:21:LEU:HD23	2:CH:21:LEU:HA	1.75	0.40
2:CH:28:HIS:O	2:CH:49:PRO:HA	2.21	0.40
2:CR:12:VAL:O	2:CR:68:ILE:HG12	2.22	0.40
1:DA:80:ILE:HG23	1:DA:106:LYS:HE2	2.03	0.40
1:DC:58:LYS:HZ1	2:DF:128:GLU:CD	2.23	0.40
2:DH:89:ASP:OD1	2:DH:90:VAL:N	2.51	0.40
1:DI:129:THR:O	1:DI:156:PRO:HA	2.21	0.40
1:DI:81:SER:HB2	1:DI:106:LYS:NZ	2.36	0.40
2:DJ:28:HIS:O	2:DJ:49:PRO:HA	2.22	0.40
2:DL:28:HIS:O	2:DL:49:PRO:HA	2.21	0.40
2:DR:125:TYR:CZ	2:DR:127:PRO:HA	2.56	0.40
1:AA:88:HIS:HB2	1:AA:100:ILE:HG23	2.03	0.40
2:AB:134:LEU:HB3	2:AB:149:VAL:HG13	2.04	0.40
2:AD:15:GLY:N	2:AD:59:PHE:O	2.54	0.40
2:AP:30:GLY:HA3	2:AP:54:GLY:H	1.85	0.40
1:BG:67:GLU:HG3	1:BG:77:GLU:HG3	2.03	0.40
2:BP:128:GLU:N	2:BP:131:GLN:HE22	2.12	0.40
2:CR:116:LYS:HD3	2:CT:130:GLY:CA	2.52	0.40
1:CS:78:GLN:HE21	1:CS:115:VAL:HG21	1.86	0.40
2:CV:73:PHE:CZ	2:CV:113:LYS:HE3	2.57	0.40
1:DA:51:VAL:HG12	1:DA:102:LEU:HD23	2.03	0.40
1:DA:64:ARG:HD3	1:DA:79:PHE:CZ	2.56	0.40
2:DH:28:HIS:HD2	1:DK:228:VAL:HB	1.86	0.40
1:DI:81:SER:HB2	1:DI:106:LYS:HZ3	1.86	0.40
1:DI:133:ILE:HG12	1:DI:196:VAL:HG22	2.02	0.40
2:DL:7:THR:HG23	2:DL:159:ILE:O	2.22	0.40
2:DT:131:GLN:HE21	2:DT:131:GLN:HB2	1.73	0.40
2:AB:98:LEU:HB2	2:AB:149:VAL:HB	2.04	0.40
2:AL:14:ASN:OD1	2:AL:60:GLU:HA	2.22	0.40
1:AM:51:VAL:HG12	1:AM:102:LEU:HD23	2.03	0.40
2:AN:28:HIS:NE2	1:AQ:229:SER:HA	2.36	0.40
1:AO:24:ALA:HB1	1:AO:114:ARG:HE	1.86	0.40
1:AO:85:SER:O	1:AQ:168:PRO:HB3	2.21	0.40
1:AQ:234:THR:O	1:AQ:238:ASN:ND2	2.29	0.40
1:BA:55:HIS:ND1	2:BB:63:LEU:HD22	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BD:73:PHE:HB2	2:BD:109:LEU:HD22	2.02	0.40
1:BE:54:ALA:HB1	1:BE:87:VAL:HG13	2.04	0.40
1:BG:43:SER:OG	1:BG:195:PRO:HB3	2.21	0.40
1:BI:133:ILE:HG12	1:BI:196:VAL:HG13	2.04	0.40
1:BO:96:LEU:HD11	2:BP:109:LEU:HD11	2.04	0.40
1:CO:54:ALA:HA	1:CO:101:MET:HB2	2.03	0.40
1:CO:133:ILE:O	1:CO:153:LEU:N	2.52	0.40
1:DM:94:ASN:OD1	2:DN:73:PHE:HE2	2.04	0.40
1:DO:16:ILE:HB	1:DO:151:LYS:HB2	2.04	0.40

All (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
2:BB:130:GLY:O	2:BV:116:LYS:NZ[2_655]	2.18	0.02
1:DC:124:CYS:O	2:DV:145:TYR:OH[2_646]	2.18	0.02

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	221/223 (99%)	215 (97%)	6 (3%)	0	100	100
1	AC	221/223 (99%)	216 (98%)	5 (2%)	0	100	100
1	AE	221/223 (99%)	215 (97%)	6 (3%)	0	100	100
1	AG	221/223 (99%)	216 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	29	66
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
1	DA	221/223 (99%)	214 (97%)	7 (3%)	0	100	100
1	DC	221/223 (99%)	217 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	17	54
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%)	25	63
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
2	BT	161/163 (99%)	154 (96%)	7 (4%)	0	100	100
2	BV	161/163 (99%)	154 (96%)	7 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	25	63
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 (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	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%)	183 (100%)	1 (0%)	88	93
1	AM	184/184 (100%)	184 (100%)	0	100	100
1	AO	184/184 (100%)	183 (100%)	1 (0%)	88	93
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%)	183 (100%)	1 (0%)	88	93
1	BK	184/184 (100%)	184 (100%)	0	100	100
1	BM	184/184 (100%)	183 (100%)	1 (0%)	88	93
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%)	183 (100%)	1 (0%)	88	93

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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%)	183 (100%)	1 (0%)	88 93
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%)	183 (100%)	1 (0%)	88 93
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%)	183 (100%)	1 (0%)	88 93
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%)	183 (100%)	1 (0%)	88 93
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%)	136 (99%)	1 (1%)	84 90
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%)	136 (99%)	1 (1%)	84 90
2	BN	137/137 (100%)	137 (100%)	0	100 100
2	BP	137/137 (100%)	136 (99%)	1 (1%)	84 90
2	BR	137/137 (100%)	136 (99%)	1 (1%)	84 90
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%)	136 (99%)	1 (1%)	84 90
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%)	136 (99%)	1 (1%)	84 90
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%)	136 (99%)	1 (1%)	84 90
2	CT	137/137 (100%)	137 (100%)	0	100 100
2	CV	137/137 (100%)	136 (99%)	1 (1%)	84 90
2	DB	137/137 (100%)	136 (99%)	1 (1%)	84 90
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%)	136 (99%)	1 (1%)	84 90
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%)	134 (98%)	3 (2%)	52 71
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%)	14102 (100%)	22 (0%)	93 96

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AK	130	GLN
1	AO	130	GLN
2	AR	89	ASP
1	BI	130	GLN
2	BL	131	GLN
1	BM	130	GLN
2	BP	131	GLN
2	BR	89	ASP
2	CF	131	GLN
1	CG	130	GLN
1	CK	130	GLN
2	CL	131	GLN
1	CQ	130	GLN
2	CR	52	ARG
2	CV	52	ARG
2	DB	131	GLN
2	DJ	52	ARG
1	DO	130	GLN
2	DT	50	HIS
2	DT	89	ASP
2	DT	131	GLN
1	DU	130	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
2	AF	28	HIS
2	AF	140	HIS
2	AH	131	GLN
2	AN	131	GLN
2	AP	28	HIS
1	AQ	94	ASN
1	AQ	130	GLN
1	BA	25	ASN
1	BE	94	ASN
2	BF	131	GLN

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Mol	Chain	Res	Type
2	BL	131	GLN
1	BM	25	ASN
2	BP	131	GLN
2	BR	131	GLN
1	CC	94	ASN
1	CE	34	ASN
2	CF	131	GLN
1	CI	94	ASN
2	CP	28	HIS
2	CR	51	HIS
2	CR	131	GLN
1	DC	25	ASN
2	DD	50	HIS
2	DD	131	GLN
2	DF	50	HIS
1	DI	130	GLN
1	DO	76	ASN
1	DQ	78	GLN
2	DT	131	GLN
1	DU	94	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	AA	223/223 (100%)	0.27	7 (3%) 49 38	49, 69, 94, 105	0
1	AC	223/223 (100%)	0.68	27 (12%) 4 5	63, 107, 139, 151	0
1	AE	223/223 (100%)	0.40	13 (5%) 23 19	39, 63, 90, 105	0
1	AG	223/223 (100%)	0.19	9 (4%) 38 31	31, 59, 92, 116	0
1	AI	223/223 (100%)	0.44	17 (7%) 13 11	53, 92, 130, 145	0
1	AK	223/223 (100%)	-0.19	1 (0%) 92 87	21, 34, 52, 67	0
1	AM	223/223 (100%)	0.20	7 (3%) 49 38	40, 58, 77, 89	0
1	AO	223/223 (100%)	0.36	15 (6%) 17 14	61, 78, 98, 111	0
1	AQ	223/223 (100%)	0.27	7 (3%) 49 38	43, 72, 94, 105	0
1	AS	223/223 (100%)	0.23	8 (3%) 42 34	51, 67, 87, 98	0
1	AU	223/223 (100%)	0.96	44 (19%) 1 1	82, 115, 141, 149	0
1	BA	223/223 (100%)	0.41	8 (3%) 42 34	68, 85, 101, 114	0
1	BC	223/223 (100%)	1.08	47 (21%) 1 1	87, 114, 141, 160	0
1	BE	223/223 (100%)	0.53	19 (8%) 10 9	55, 82, 109, 121	0
1	BG	223/223 (100%)	-0.13	4 (1%) 68 59	26, 39, 57, 67	0
1	BI	223/223 (100%)	0.55	13 (5%) 23 19	47, 73, 100, 112	0
1	BK	223/223 (100%)	0.36	13 (5%) 23 19	46, 83, 119, 141	0
1	BM	223/223 (100%)	0.22	10 (4%) 33 27	44, 60, 74, 81	0
1	BO	223/223 (100%)	-0.11	0 100 100	33, 47, 60, 67	0
1	BQ	223/223 (100%)	0.40	11 (4%) 29 25	49, 68, 90, 101	0
1	BS	223/223 (100%)	0.90	41 (18%) 1 1	70, 112, 151, 166	0
1	BU	223/223 (100%)	0.40	15 (6%) 17 14	68, 91, 121, 125	0
1	CA	223/223 (100%)	0.66	30 (13%) 3 3	47, 104, 149, 165	0
1	CC	223/223 (100%)	0.76	34 (15%) 2 2	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%)	0.22	8 (3%) 42 34	21, 61, 87, 92	0
1	CG	223/223 (100%)	0.07	5 (2%) 62 52	29, 61, 97, 110	0
1	CI	223/223 (100%)	0.04	5 (2%) 62 52	23, 39, 61, 75	0
1	CK	223/223 (100%)	0.03	5 (2%) 62 52	20, 50, 85, 108	0
1	CM	223/223 (100%)	0.44	13 (5%) 23 19	57, 75, 101, 117	0
1	CO	223/223 (100%)	0.64	28 (12%) 3 5	60, 96, 135, 155	0
1	CQ	223/223 (100%)	0.17	8 (3%) 42 34	42, 65, 88, 94	0
1	CS	223/223 (100%)	0.83	39 (17%) 1 2	63, 94, 126, 137	0
1	CU	223/223 (100%)	0.72	22 (9%) 7 7	80, 119, 151, 166	0
1	DA	223/223 (100%)	0.55	29 (13%) 3 4	49, 81, 120, 136	0
1	DC	223/223 (100%)	0.13	3 (1%) 77 68	44, 66, 96, 111	0
1	DE	223/223 (100%)	1.06	45 (20%) 1 1	77, 99, 119, 130	0
1	DG	223/223 (100%)	0.18	7 (3%) 49 38	39, 56, 78, 92	0
1	DI	223/223 (100%)	0.31	5 (2%) 62 52	42, 82, 109, 122	0
1	DK	223/223 (100%)	0.00	5 (2%) 62 52	28, 41, 55, 66	0
1	DM	223/223 (100%)	0.14	3 (1%) 77 68	29, 61, 83, 92	0
1	DO	223/223 (100%)	0.02	2 (0%) 84 77	25, 46, 66, 82	0
1	DQ	223/223 (100%)	0.17	15 (6%) 17 14	43, 73, 101, 118	0
1	DS	223/223 (100%)	0.10	4 (1%) 68 59	25, 51, 81, 96	0
1	DU	223/223 (100%)	0.73	24 (10%) 5 5	66, 95, 125, 141	0
2	AB	163/163 (100%)	0.27	7 (4%) 35 29	42, 72, 110, 134	0
2	AD	163/163 (100%)	0.15	6 (3%) 41 32	39, 64, 87, 114	0
2	AF	163/163 (100%)	-0.08	1 (0%) 89 84	22, 42, 67, 91	0
2	AH	163/163 (100%)	-0.13	2 (1%) 79 70	24, 39, 66, 82	0
2	AJ	163/163 (100%)	-0.16	0 100 100	31, 46, 81, 111	0
2	AL	163/163 (100%)	-0.03	2 (1%) 79 70	20, 45, 94, 112	0
2	AN	163/163 (100%)	-0.17	2 (1%) 79 70	32, 44, 70, 95	0
2	AP	163/163 (100%)	0.19	5 (3%) 49 38	52, 65, 98, 122	0
2	AR	163/163 (100%)	0.41	11 (6%) 17 14	47, 75, 118, 142	0
2	AT	163/163 (100%)	-0.08	2 (1%) 79 70	39, 56, 80, 99	0
2	AV	163/163 (100%)	0.40	9 (5%) 25 22	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%)	0.01	2 (1%) 79 70	45, 67, 90, 116	0
2	BD	163/163 (100%)	0.29	7 (4%) 35 29	56, 80, 110, 136	0
2	BF	163/163 (100%)	0.69	19 (11%) 4 5	56, 93, 145, 157	0
2	BH	163/163 (100%)	0.04	5 (3%) 49 38	28, 55, 94, 135	0
2	BJ	163/163 (100%)	-0.17	2 (1%) 79 70	28, 40, 63, 87	0
2	BL	163/163 (100%)	-0.05	1 (0%) 89 84	42, 59, 89, 110	0
2	BN	163/163 (100%)	-0.01	2 (1%) 79 70	37, 53, 81, 104	0
2	BP	163/163 (100%)	0.12	7 (4%) 35 29	34, 51, 82, 90	0
2	BR	163/163 (100%)	-0.19	2 (1%) 79 70	37, 52, 86, 101	0
2	BT	163/163 (100%)	0.31	3 (1%) 68 59	57, 85, 115, 129	0
2	BV	163/163 (100%)	0.62	16 (9%) 7 7	58, 97, 145, 164	0
2	CB	163/163 (100%)	0.37	10 (6%) 21 17	62, 97, 142, 165	0
2	CD	163/163 (100%)	0.58	14 (8%) 10 9	43, 91, 161, 187	0
2	CF	163/163 (100%)	0.08	6 (3%) 41 32	31, 59, 105, 118	0
2	CH	163/163 (100%)	-0.25	0 100 100	17, 32, 66, 94	0
2	CJ	163/163 (100%)	-0.20	4 (2%) 57 47	16, 36, 80, 107	0
2	CL	163/163 (100%)	-0.19	3 (1%) 68 59	16, 33, 66, 81	0
2	CN	163/163 (100%)	0.04	0 100 100	46, 60, 77, 93	0
2	CP	163/163 (100%)	0.68	17 (10%) 6 6	71, 109, 152, 162	0
2	CR	163/163 (100%)	0.11	2 (1%) 79 70	39, 78, 120, 138	0
2	CT	163/163 (100%)	0.05	3 (1%) 68 59	32, 57, 94, 121	0
2	CV	163/163 (100%)	0.44	12 (7%) 14 12	51, 87, 130, 144	0
2	DB	163/163 (100%)	0.51	11 (6%) 17 14	53, 87, 138, 157	0
2	DD	163/163 (100%)	0.07	2 (1%) 79 70	40, 62, 99, 118	0
2	DF	163/163 (100%)	0.32	7 (4%) 35 29	66, 88, 130, 147	0
2	DH	163/163 (100%)	0.02	2 (1%) 79 70	37, 52, 85, 112	0
2	DJ	163/163 (100%)	0.04	5 (3%) 49 38	33, 52, 92, 109	0
2	DL	163/163 (100%)	-0.12	5 (3%) 49 38	17, 37, 72, 93	0
2	DN	163/163 (100%)	-0.24	1 (0%) 89 84	20, 41, 83, 107	0
2	DP	163/163 (100%)	-0.13	2 (1%) 79 70	25, 39, 65, 88	0
2	DR	163/163 (100%)	0.13	4 (2%) 57 47	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%)	-0.01	7 (4%) 35 29	33, 53, 88, 107	0
2	DV	163/163 (100%)	0.15	6 (3%) 41 32	41, 64, 106, 131	0
All	All	16984/16984 (100%)	0.26	911 (5%) 25 22	16, 68, 123, 187	0

All (911) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AM	25	ASN	6.8
1	CO	76	ASN	6.4
1	CS	135	GLY	6.3
1	BC	25	ASN	6.2
1	DE	134	SER	6.1
2	BD	38	ASN	6.1
1	DE	16	ILE	5.7
2	AR	38	ASN	5.7
1	AU	134	SER	5.5
2	AT	37	GLY	5.5
1	CU	76	ASN	5.5
2	CD	34	ALA	5.4
1	CO	186	ASP	5.2
1	BU	134	SER	5.1
2	AR	37	GLY	5.1
1	BS	30	GLN	5.1
2	BF	96	ILE	5.1
1	CU	187	SER	5.0
1	BC	105	LEU	4.9
1	AC	134	SER	4.9
1	BQ	74	GLU	4.8
1	BC	17	VAL	4.8
2	CD	96	ILE	4.7
2	CB	37	GLY	4.7
2	DV	36	ILE	4.7
1	BC	31	VAL	4.7
1	BS	42	GLY	4.7
2	AB	37	GLY	4.7
2	BF	143	ASP	4.6
1	DE	30	GLN	4.6
2	DV	37	GLY	4.5
1	CC	186	ASP	4.5
2	CB	143	ASP	4.5
1	BC	141	SER	4.5

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Mol	Chain	Res	Type	RSRZ
2	DJ	37	GLY	4.5
1	DE	136	TRP	4.5
1	AC	187	SER	4.4
1	AS	25	ASN	4.4
1	CS	42	GLY	4.4
2	BV	143	ASP	4.4
1	AU	16	ILE	4.4
2	BD	37	GLY	4.4
1	CC	216	ASN	4.4
1	AC	114	ARG	4.4
1	BS	150	LEU	4.4
1	BS	31	VAL	4.4
1	BS	107	SER	4.4
1	DE	150	LEU	4.4
1	AM	113	SER	4.4
1	AC	76	ASN	4.3
1	CC	42	GLY	4.3
1	DE	184	GLY	4.3
1	AM	114	ARG	4.3
1	DE	27	VAL	4.3
2	BF	140	HIS	4.3
1	BE	135	GLY	4.2
1	CS	151	LYS	4.2
1	DA	134	SER	4.2
2	CV	38	ASN	4.2
1	AU	185	LYS	4.1
1	BI	202	LEU	4.1
2	CP	146	TYR	4.1
1	CC	18	GLY	4.1
2	CP	93	GLN	4.1
1	AO	178	ALA	4.1
1	CO	112	ASN	4.1
1	DI	179	GLY	4.1
1	CA	179	GLY	4.1
1	BS	203	GLN	4.0
1	AS	141	SER	4.0
1	CS	178	ALA	4.0
1	CA	114	ARG	4.0
1	DE	151	LYS	4.0
2	AR	39	GLU	4.0
2	CP	28	HIS	4.0
1	CU	25	ASN	4.0

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Mol	Chain	Res	Type	RSRZ
2	BB	163	THR	4.0
2	BF	81	SER	4.0
2	CP	36	ILE	3.9
1	AI	178	ALA	3.9
1	CS	114	ARG	3.9
1	CA	48	GLN	3.9
1	BC	134	SER	3.9
2	DF	35	LYS	3.9
2	CP	38	ASN	3.9
1	CQ	67	GLU	3.9
1	BS	204	GLY	3.9
1	CA	134	SER	3.9
2	BV	38	ASN	3.8
1	CS	30	GLN	3.8
1	DQ	75	GLY	3.8
1	BK	144	THR	3.8
1	DI	178	ALA	3.8
2	DL	38	ASN	3.8
1	AU	135	GLY	3.8
1	DQ	76	ASN	3.8
1	AU	133	ILE	3.8
2	BF	28	HIS	3.7
1	BQ	152	CYS	3.7
2	CP	26	HIS	3.7
1	CA	187	SER	3.7
1	DE	42	GLY	3.7
1	BQ	25	ASN	3.7
1	DE	135	GLY	3.7
1	BC	186	ASP	3.7
1	AU	150	LEU	3.7
2	CP	96	ILE	3.7
1	DQ	24	ALA	3.7
2	CT	36	ILE	3.7
1	AU	216	ASN	3.7
1	AU	186	ASP	3.6
1	DA	114	ARG	3.6
2	AV	36	ILE	3.6
1	CO	75	GLY	3.6
1	DA	135	GLY	3.6
2	BF	145	TYR	3.6
2	BF	142	ASN	3.6
1	CA	76	ASN	3.6

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Mol	Chain	Res	Type	RSRZ
1	DU	114	ARG	3.6
1	AC	135	GLY	3.6
1	CA	150	LEU	3.6
2	DB	28	HIS	3.6
1	DU	122	THR	3.6
2	CB	29	ALA	3.5
1	AU	151	LYS	3.5
2	CV	36	ILE	3.5
1	DQ	114	ARG	3.5
2	AV	37	GLY	3.5
2	AB	96	ILE	3.5
1	AU	78	GLN	3.5
2	BD	142	ASN	3.5
1	CA	66	GLY	3.5
2	BV	142	ASN	3.5
2	AN	38	ASN	3.5
1	DE	31	VAL	3.5
1	CO	179	GLY	3.5
1	CS	134	SER	3.5
1	BM	25	ASN	3.4
2	DB	26	HIS	3.5
2	AL	38	ASN	3.4
1	BC	24	ALA	3.4
2	DF	39	GLU	3.4
1	AE	138	ASN	3.4
1	BI	30	GLN	3.4
1	AE	178	ALA	3.4
1	DA	16	ILE	3.4
1	AU	187	SER	3.4
1	DQ	113	SER	3.4
1	CC	204	GLY	3.4
2	CD	95	PRO	3.4
1	BC	26	THR	3.4
2	CL	143	ASP	3.4
2	BF	34	ALA	3.4
1	CO	113	SER	3.4
1	DQ	187	SER	3.4
1	AU	38	HIS	3.4
1	AU	141	SER	3.4
1	CC	65	LEU	3.4
1	DE	29	TYR	3.4
1	AI	149	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	DU	115	VAL	3.4
1	BC	150	LEU	3.4
1	DE	186	ASP	3.4
1	BK	74	GLU	3.3
1	CS	113	SER	3.3
2	AD	28	HIS	3.3
1	AC	122	THR	3.3
1	DG	74	GLU	3.3
1	BE	65	LEU	3.3
1	BK	76	ASN	3.3
1	AU	29	TYR	3.3
1	AI	110	SER	3.3
1	BC	187	SER	3.3
1	BI	71	ASN	3.3
1	BC	136	TRP	3.3
2	CV	28	HIS	3.3
1	CA	16	ILE	3.3
1	CA	135	GLY	3.3
1	AU	184	GLY	3.3
2	BD	82	SER	3.3
1	CQ	112	ASN	3.3
1	DG	76	ASN	3.3
1	DK	114	ARG	3.3
1	AU	178	ALA	3.3
2	DJ	36	ILE	3.2
1	BS	25	ASN	3.2
1	CU	238	ASN	3.2
2	AR	36	ILE	3.2
1	AI	109	ALA	3.2
1	CK	76	ASN	3.2
1	AI	116	ALA	3.2
1	DU	134	SER	3.2
1	CU	41	GLY	3.2
1	DE	28	PRO	3.2
1	BC	202	LEU	3.2
1	DC	113	SER	3.2
2	DN	28	HIS	3.2
2	CV	37	GLY	3.2
1	BE	150	LEU	3.2
1	BC	18	GLY	3.2
1	DE	187	SER	3.2
2	CD	50	HIS	3.2

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Mol	Chain	Res	Type	RSRZ
1	DA	138	ASN	3.2
1	DK	76	ASN	3.2
1	AU	30	GLN	3.2
1	AQ	144	THR	3.2
2	BP	29	ALA	3.2
1	AU	138	ASN	3.2
1	DU	25	ASN	3.2
1	CI	74	GLU	3.2
1	AC	188	CYS	3.2
1	DA	151	LYS	3.2
2	DB	29	ALA	3.2
2	BF	146	TYR	3.2
1	DE	179	GLY	3.2
1	AU	122	THR	3.2
1	CC	30	GLN	3.1
2	AR	34	ALA	3.1
1	CS	47	SER	3.1
1	DA	179	GLY	3.1
2	CV	95	PRO	3.1
1	AI	179	GLY	3.1
1	CC	183	GLY	3.1
1	BS	43	SER	3.1
1	CA	186	ASP	3.1
1	DE	66	GLY	3.1
1	CO	182	GLU	3.1
2	AN	28	HIS	3.1
1	AU	153	LEU	3.1
1	AC	186	ASP	3.1
1	AU	124	CYS	3.1
2	BT	48	ASP	3.1
1	CO	47	SER	3.1
1	DU	28	PRO	3.1
1	BU	78	GLN	3.1
2	DF	50	HIS	3.1
1	BI	74	GLU	3.1
1	AU	121	PRO	3.1
2	DF	28	HIS	3.1
2	AB	38	ASN	3.1
1	BE	78	GLN	3.1
1	DA	74	GLU	3.1
2	CD	36	ILE	3.1
1	CO	116	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	CO	117	SER	3.1
2	AV	38	ASN	3.0
1	CC	185	LYS	3.0
1	DU	66	GLY	3.0
2	AV	42	PRO	3.0
1	BS	22	CYS	3.0
2	CP	95	PRO	3.0
1	CC	134	SER	3.0
1	DE	144	THR	3.0
1	CS	121	PRO	3.0
1	AM	34	ASN	3.0
1	AO	114	ARG	3.0
1	CS	64	ARG	3.0
2	AR	81	SER	3.0
1	BI	24	ALA	3.0
1	BK	195	PRO	3.0
1	BM	114	ARG	3.0
1	DG	68	ASP	3.0
1	AC	141	SER	3.0
1	AC	179	GLY	3.0
2	DJ	95	PRO	3.0
1	BS	76	ASN	3.0
2	DT	28	HIS	3.0
1	BS	32	SER	3.0
1	DE	64	ARG	3.0
1	CS	27	VAL	3.0
2	BV	39	GLU	3.0
1	AC	121	PRO	2.9
2	DL	95	PRO	2.9
1	DG	114	ARG	2.9
1	AC	17	VAL	2.9
1	BI	25	ASN	2.9
1	BU	76	ASN	2.9
2	DR	36	ILE	2.9
1	CC	26	THR	2.9
1	AE	18	GLY	2.9
1	AU	212	CYS	2.9
2	BH	38	ASN	2.9
1	AC	139	THR	2.9
1	DU	135	GLY	2.9
1	AI	142	SER	2.9
1	BC	68	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
2	DF	41	GLU	2.9
1	CA	110	SER	2.9
1	BM	209	GLY	2.9
1	CU	186	ASP	2.9
1	CS	18	GLY	2.9
2	AB	36	ILE	2.9
1	BU	133	ILE	2.9
1	CU	166	ALA	2.9
1	DA	213	ALA	2.9
1	AU	120	LEU	2.9
1	DA	136	TRP	2.9
2	DT	163	THR	2.9
1	AK	25	ASN	2.9
1	BC	16	ILE	2.9
1	CC	187	SER	2.9
2	CJ	38	ASN	2.9
1	AG	76	ASN	2.9
2	CV	162	ALA	2.9
2	CF	146	TYR	2.9
1	CK	150	LEU	2.9
2	CF	28	HIS	2.9
2	DD	28	HIS	2.9
2	CP	94	ASP	2.9
1	BC	64	ARG	2.9
1	AI	141	SER	2.9
1	BC	114	ARG	2.9
1	AC	238	ASN	2.9
2	BF	29	ALA	2.9
2	CB	163	THR	2.9
1	CS	31	VAL	2.9
2	BV	43	ARG	2.9
1	AU	70	ILE	2.8
1	BM	186	ASP	2.8
1	CM	30	GLN	2.8
1	AG	150	LEU	2.8
1	AU	143	GLY	2.8
1	BC	30	GLN	2.8
2	AP	48	ASP	2.8
1	CS	32	SER	2.8
1	DE	178	ALA	2.8
1	AI	112	ASN	2.8
1	CO	71	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
1	AC	150	LEU	2.8
1	AE	16	ILE	2.8
1	CE	25	ASN	2.8
1	DA	186	ASP	2.8
2	CB	36	ILE	2.8
1	CQ	114	ARG	2.8
1	CS	74	GLU	2.8
1	AO	27	VAL	2.8
2	AP	96	ILE	2.8
2	AP	95	PRO	2.8
1	DE	125	ALA	2.8
1	CS	212	CYS	2.8
1	CC	151	LYS	2.8
1	AE	30	GLN	2.8
1	BC	133	ILE	2.8
2	BV	96	ILE	2.8
2	AT	38	ASN	2.8
1	DA	75	GLY	2.8
2	DR	38	ASN	2.8
2	DB	38	ASN	2.8
2	AF	28	HIS	2.8
1	AU	112	ASN	2.8
1	DE	216	ASN	2.8
1	DG	75	GLY	2.8
2	BH	36	ILE	2.8
1	AC	151	LYS	2.8
1	DS	152	CYS	2.8
2	AB	28	HIS	2.7
1	CO	114	ARG	2.7
1	DS	187	SER	2.7
2	CJ	51	HIS	2.7
2	BV	41	GLU	2.7
1	AQ	184	GLY	2.7
1	BC	42	GLY	2.7
1	DU	178	ALA	2.7
1	DA	149	VAL	2.7
2	DD	43	ARG	2.7
1	CA	47	SER	2.7
1	CO	188	CYS	2.7
1	CQ	25	ASN	2.7
2	BD	81	SER	2.7
2	BV	40	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
2	BV	44	ALA	2.7
1	AI	186	ASP	2.7
1	DA	148	ASP	2.7
2	CB	28	HIS	2.7
2	CD	140	HIS	2.7
2	DF	51	HIS	2.7
1	CC	67	GLU	2.7
2	CF	143	ASP	2.7
2	DB	53	PRO	2.7
1	CU	135	GLY	2.7
2	AP	36	ILE	2.7
1	DA	76	ASN	2.7
1	AO	187	SER	2.7
2	CP	53	PRO	2.7
1	CS	203	GLN	2.7
1	AU	152	CYS	2.7
1	DM	110	SER	2.7
1	DC	30	GLN	2.7
2	CF	145	TYR	2.7
1	BK	66	GLY	2.7
2	CV	29	ALA	2.7
1	CM	178	ALA	2.7
2	BB	38	ASN	2.7
1	BC	135	GLY	2.7
1	BC	204	GLY	2.7
2	BN	38	ASN	2.7
1	DU	186	ASP	2.6
1	BK	152	CYS	2.6
2	BH	37	GLY	2.6
2	CP	37	GLY	2.6
1	AI	67	GLU	2.6
2	BF	38	ASN	2.6
1	BC	212	CYS	2.6
1	CG	30	GLN	2.6
2	BP	84	ASP	2.6
1	BE	64	ARG	2.6
1	AU	195	PRO	2.6
1	BU	114	ARG	2.6
1	CO	189	GLN	2.6
1	CS	41	GLY	2.6
1	BQ	146	TYR	2.6
2	DT	39	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	BS	65	LEU	2.6
1	CM	32	SER	2.6
1	BC	149	VAL	2.6
1	CG	25	ASN	2.6
1	CM	114	ARG	2.6
1	CS	25	ASN	2.6
1	CO	17	VAL	2.6
1	CC	195	PRO	2.6
1	CM	85	SER	2.6
1	CO	115	VAL	2.6
1	DE	139	THR	2.6
2	BF	36	ILE	2.6
1	AI	78	GLN	2.6
1	BI	115	VAL	2.6
1	BC	67	GLU	2.6
1	BS	210	SER	2.6
1	CC	159	SER	2.6
2	AV	66	ASN	2.6
1	AU	176	PHE	2.6
1	CQ	76	ASN	2.6
1	DQ	25	ASN	2.6
2	BP	28	HIS	2.6
1	BC	146	TYR	2.6
1	BS	212	CYS	2.6
1	DE	122	THR	2.6
1	BI	114	ARG	2.6
2	CV	43	ARG	2.6
1	AO	150	LEU	2.6
1	AO	216	ASN	2.6
1	DU	27	VAL	2.6
2	DR	37	GLY	2.6
1	CC	139	THR	2.6
1	DE	235	ILE	2.6
1	AC	83	SER	2.6
1	AS	210	SER	2.6
1	CC	179	GLY	2.6
1	AS	148	ASP	2.6
1	CC	182	GLU	2.6
1	CS	189	GLN	2.6
2	BV	146	TYR	2.6
1	BE	31	VAL	2.6
1	BC	78	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	BK	203	GLN	2.6
1	BS	28	PRO	2.5
1	AG	113	SER	2.5
1	BU	153	LEU	2.5
1	CA	185	LYS	2.5
1	AA	25	ASN	2.5
2	AL	94	ASP	2.5
2	DR	28	HIS	2.5
1	BE	24	ALA	2.5
1	AQ	185	LYS	2.5
1	BG	185	LYS	2.5
2	BJ	95	PRO	2.5
1	AQ	178	ALA	2.5
1	CO	138	ASN	2.5
1	CU	38	HIS	2.5
1	DU	152	CYS	2.5
2	BT	28	HIS	2.5
2	DF	36	ILE	2.5
1	CA	128	GLY	2.5
2	AR	30	GLY	2.5
1	CO	25	ASN	2.5
1	CA	27	VAL	2.5
1	AA	32	SER	2.5
1	BK	114	ARG	2.5
2	AD	39	GLU	2.5
1	BC	45	ILE	2.5
1	CC	76	ASN	2.5
1	DI	122	THR	2.5
1	DQ	178	ALA	2.5
1	AI	115	VAL	2.5
1	BQ	78	GLN	2.5
1	CA	67	GLU	2.5
1	AA	151	LYS	2.5
1	BE	110	SER	2.5
1	CC	75	GLY	2.5
1	BC	196	VAL	2.5
1	BS	195	PRO	2.5
1	DU	116	ALA	2.5
1	DE	115	VAL	2.5
1	DU	30	GLN	2.5
1	CS	216	ASN	2.5
1	AQ	145	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	AU	142	SER	2.5
1	CI	134	SER	2.5
1	CU	16	ILE	2.5
2	DT	50	HIS	2.5
1	BI	112	ASN	2.5
1	DC	112	ASN	2.5
2	CB	142	ASN	2.5
1	BK	85	SER	2.5
1	AO	212	CYS	2.5
1	BU	25	ASN	2.5
1	CS	76	ASN	2.5
1	BS	29	TYR	2.5
1	CM	209	GLY	2.5
2	AB	84	ASP	2.5
1	CQ	113	SER	2.5
1	AG	114	ARG	2.5
1	BC	22	CYS	2.5
2	BV	42	PRO	2.5
1	BK	75	GLY	2.5
1	DU	184	GLY	2.5
1	DE	185	LYS	2.5
1	CA	136	TRP	2.5
1	CM	210	SER	2.4
1	AC	16	ILE	2.4
1	CC	152	CYS	2.4
1	BS	185	LYS	2.4
1	AM	24	ALA	2.4
1	CO	141	SER	2.4
2	DJ	38	ASN	2.4
1	CM	136	TRP	2.4
1	DM	114	ARG	2.4
1	AO	141	SER	2.4
1	CS	238	ASN	2.4
1	BU	115	VAL	2.4
2	AD	50	HIS	2.4
1	BS	109	ALA	2.4
1	CS	195	PRO	2.4
1	DE	113	SER	2.4
1	AG	74	GLU	2.4
2	CB	60	GLU	2.4
1	CS	65	LEU	2.4
1	DA	122	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	DU	238	ASN	2.4
2	BP	41	GLU	2.4
2	DB	36	ILE	2.4
1	AG	152	CYS	2.4
1	BE	152	CYS	2.4
1	DA	78	GLN	2.4
1	AE	186	ASP	2.4
1	BS	186	ASP	2.4
2	BN	104	ASP	2.4
1	BU	67	GLU	2.4
1	AM	112	ASN	2.4
1	BM	195	PRO	2.4
2	BV	28	HIS	2.4
1	CS	150	LEU	2.4
1	AU	238	ASN	2.4
1	BS	33	LEU	2.4
1	DS	130	GLN	2.4
2	AR	28	HIS	2.4
2	AV	51	HIS	2.4
1	CS	136	TRP	2.4
1	AC	201	LYS	2.4
1	BE	184	GLY	2.4
1	AC	112	ASN	2.4
2	BF	43	ARG	2.4
1	AC	152	CYS	2.4
1	BC	152	CYS	2.4
1	DU	16	ILE	2.4
1	AO	211	GLY	2.4
1	BQ	153	LEU	2.4
1	DO	114	ARG	2.4
1	AG	25	ASN	2.4
1	BG	184	GLY	2.4
1	BI	18	GLY	2.4
1	CS	143	GLY	2.4
2	AH	82	SER	2.4
1	CK	149	VAL	2.4
2	CT	38	ASN	2.4
1	CO	178	ALA	2.4
2	AV	143	ASP	2.4
2	DB	25	SER	2.4
1	BA	25	ASN	2.4
1	CU	133	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	CK	64	ARG	2.4
1	AU	17	VAL	2.4
1	BM	109	ALA	2.4
1	BM	196	VAL	2.4
2	BF	44	ALA	2.4
1	BG	113	SER	2.4
2	BF	107	SER	2.4
1	AO	26	THR	2.4
1	AU	79	PHE	2.4
1	BE	79	PHE	2.4
1	CA	144	THR	2.4
1	BC	49	TRP	2.3
1	AU	76	ASN	2.3
1	BI	19	GLY	2.3
1	CM	138	ASN	2.3
1	DE	65	LEU	2.3
1	DE	116	ALA	2.3
2	DV	26	HIS	2.3
1	AE	187	SER	2.3
1	CI	113	SER	2.3
1	CS	123	SER	2.3
1	AC	130	GLN	2.3
1	CC	48	GLN	2.3
1	AU	177	CYS	2.3
1	DU	112	ASN	2.3
2	CJ	36	ILE	2.3
1	AS	149	VAL	2.3
2	AP	40	ALA	2.3
1	DE	133	ILE	2.3
1	BS	123	SER	2.3
1	BS	144	THR	2.3
2	CV	106	LYS	2.3
1	AO	188	CYS	2.3
1	CM	25	ASN	2.3
2	CD	38	ASN	2.3
1	AE	141	SER	2.3
1	BK	184	GLY	2.3
1	DE	141	SER	2.3
2	BD	106	LYS	2.3
1	BE	25	ASN	2.3
1	DK	25	ASN	2.3
1	BS	187	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	CE	141	SER	2.3
1	CO	110	SER	2.3
2	AH	37	GLY	2.3
2	CD	37	GLY	2.3
2	CV	143	ASP	2.3
2	BR	66	ASN	2.3
2	BT	37	GLY	2.3
1	BA	74	GLU	2.3
1	BQ	18	GLY	2.3
1	BU	212	CYS	2.3
1	AU	43	SER	2.3
1	CA	138	ASN	2.3
2	CD	141	ARG	2.3
2	CV	96	ILE	2.3
1	CC	105	LEU	2.3
1	BM	204	GLY	2.3
1	AI	212	CYS	2.3
1	AG	142	SER	2.3
2	CP	141	ARG	2.3
1	DA	147	PRO	2.3
2	BV	23	PRO	2.3
1	CA	152	CYS	2.3
1	CO	212	CYS	2.3
1	AI	216	ASN	2.3
1	BS	47	SER	2.3
1	CS	75	GLY	2.3
1	CU	39	PHE	2.3
1	DG	24	ALA	2.3
2	DV	28	HIS	2.3
1	CC	215	LYS	2.3
1	BC	142	SER	2.3
2	AD	66	ASN	2.3
1	BE	143	GLY	2.3
2	DL	84	ASP	2.3
2	DL	143	ASP	2.3
1	CU	150	LEU	2.3
1	AU	189	GLN	2.3
1	BM	78	GLN	2.3
1	CU	67	GLU	2.3
1	CS	194	GLY	2.3
1	DE	143	GLY	2.3
2	CP	66	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	CE	151	LYS	2.3
1	BU	38	HIS	2.3
1	DE	17	VAL	2.3
2	CL	50	HIS	2.3
1	BA	76	ASN	2.3
2	AR	97	GLY	2.3
1	BE	68	ASP	2.3
1	CC	150	LEU	2.3
2	BH	104	ASP	2.3
1	AA	138	ASN	2.2
1	BC	27	VAL	2.2
1	CO	72	VAL	2.2
1	BQ	114	ARG	2.2
1	CM	186	ASP	2.2
1	CC	77	GLU	2.2
1	CA	105	LEU	2.2
1	DA	115	VAL	2.2
1	DQ	112	ASN	2.2
1	AU	139	THR	2.2
1	AE	204	GLY	2.2
1	BA	130	GLN	2.2
1	CA	17	VAL	2.2
1	DE	177	CYS	2.2
2	DB	34	ALA	2.2
2	DL	36	ILE	2.2
1	CE	134	SER	2.2
1	AU	211	GLY	2.2
1	CA	65	LEU	2.2
1	CI	30	GLN	2.2
1	CO	78	GLN	2.2
2	DT	37	GLY	2.2
1	CE	114	ARG	2.2
2	CF	144	LYS	2.2
1	AS	112	ASN	2.2
1	CU	75	GLY	2.2
1	CS	144	THR	2.2
1	DE	68	ASP	2.2
1	AU	136	TRP	2.2
1	BA	75	GLY	2.2
2	AD	37	GLY	2.2
1	BI	134	SER	2.2
1	CU	141	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	BE	153	LEU	2.2
1	BK	17	VAL	2.2
1	AC	78	GLN	2.2
1	AE	151	LYS	2.2
1	BG	112	ASN	2.2
1	CO	146	TYR	2.2
2	CP	145	TYR	2.2
2	DV	143	ASP	2.2
1	DQ	67	GLU	2.2
1	BQ	151	LYS	2.2
1	DK	30	GLN	2.2
1	BC	29	TYR	2.2
1	CO	216	ASN	2.2
1	AC	123	SER	2.2
1	AG	135	GLY	2.2
1	AO	151	LYS	2.2
1	DA	32	SER	2.2
1	DQ	143	GLY	2.2
1	CU	178	ALA	2.2
1	DA	178	ALA	2.2
1	AS	20	TYR	2.2
2	AR	93	GLN	2.2
1	AE	135	GLY	2.2
1	DE	129	THR	2.2
1	DK	135	GLY	2.2
2	BH	96	ILE	2.2
2	DH	132	THR	2.2
1	AM	32	SER	2.2
1	BA	134	SER	2.2
1	CO	213	ALA	2.2
1	DQ	142	SER	2.2
2	CP	1	SER	2.2
1	BA	114	ARG	2.2
1	BQ	149	VAL	2.2
2	BF	21	LEU	2.2
1	BC	122	THR	2.2
1	BC	138	ASN	2.2
1	BS	26	THR	2.2
1	CQ	179	GLY	2.2
1	DA	25	ASN	2.2
1	DE	32	SER	2.2
1	BK	115	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	BC	147	PRO	2.2
1	BS	135	GLY	2.2
1	CS	179	GLY	2.2
1	DG	67	GLU	2.2
1	DE	112	ASN	2.2
1	AI	210	SER	2.2
1	CU	152	CYS	2.2
1	CA	151	LYS	2.2
1	DS	65	LEU	2.2
1	BQ	79	PHE	2.2
1	BS	121	PRO	2.2
2	CD	39	GLU	2.2
1	BS	226	ASN	2.2
1	AC	185	LYS	2.2
1	AS	154	LYS	2.2
1	CE	74	GLU	2.2
1	AC	142	SER	2.1
1	BS	141	SER	2.1
1	DA	150	LEU	2.1
1	DO	76	ASN	2.1
2	AV	142	ASN	2.1
2	CF	163	THR	2.1
1	BU	152	CYS	2.1
1	CC	31	VAL	2.1
1	DA	65	LEU	2.1
1	DI	186	ASP	2.1
2	BF	1	SER	2.1
2	DT	132	THR	2.1
1	AQ	143	GLY	2.1
1	BS	190	GLY	2.1
1	DU	78	GLN	2.1
2	BP	40	ALA	2.1
2	BV	139	VAL	2.1
1	CM	16	ILE	2.1
1	AC	198	CYS	2.1
1	AO	152	CYS	2.1
1	BC	76	ASN	2.1
1	CO	18	GLY	2.1
2	CP	142	ASN	2.1
2	DB	146	TYR	2.1
1	CE	138	ASN	2.1
1	BS	27	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	DU	65	LEU	2.1
2	DJ	145	TYR	2.1
1	CC	133	ILE	2.1
1	CC	184	GLY	2.1
1	BS	122	THR	2.1
1	BU	130	GLN	2.1
1	CA	153	LEU	2.1
1	CI	68	ASP	2.1
1	DE	22	CYS	2.1
2	DB	44	ALA	2.1
2	CR	95	PRO	2.1
1	AO	74	GLU	2.1
1	BS	136	TRP	2.1
2	BV	37	GLY	2.1
1	AU	26	THR	2.1
1	BC	203	GLN	2.1
1	DA	68	ASP	2.1
1	DQ	65	LEU	2.1
1	BC	195	PRO	2.1
1	CU	114	ARG	2.1
2	AB	140	HIS	2.1
2	CB	162	ALA	2.1
1	AE	139	THR	2.1
2	BL	143	ASP	2.1
2	CV	163	THR	2.1
1	BE	76	ASN	2.1
2	CB	38	ASN	2.1
1	DE	75	GLY	2.1
1	DU	18	GLY	2.1
2	BP	43	ARG	2.1
1	AO	157	ILE	2.1
1	CC	47	SER	2.1
2	BF	131	GLN	2.1
2	AV	163	THR	2.1
2	BR	84	ASP	2.1
2	CD	163	THR	2.1
2	DB	89	ASP	2.1
2	CD	142	ASN	2.1
1	AA	136	TRP	2.1
1	DA	31	VAL	2.1
1	DE	176	PHE	2.1
2	AD	44	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
2	BP	44	ALA	2.1
1	BC	81	SER	2.1
1	BS	16	ILE	2.1
1	DQ	78	GLN	2.1
1	DU	113	SER	2.1
2	CT	51	HIS	2.1
2	CP	119	GLU	2.1
1	CM	82	ALA	2.1
1	DI	185	LYS	2.1
2	CD	145	TYR	2.1
1	CG	134	SER	2.1
1	CC	17	VAL	2.1
1	CC	135	GLY	2.1
1	BI	125	ALA	2.1
1	DU	79	PHE	2.1
2	DT	38	ASN	2.1
1	AU	215	LYS	2.1
1	DE	215	LYS	2.1
1	CA	74	GLU	2.1
1	CS	141	SER	2.1
1	DU	107	SER	2.1
2	CJ	50	HIS	2.1
2	CL	51	HIS	2.1
1	BC	185	LYS	2.1
1	AU	27	VAL	2.1
1	BS	143	GLY	2.1
1	CG	123	SER	2.1
1	CK	67	GLU	2.1
1	CS	152	CYS	2.1
1	CU	24	ALA	2.1
1	BS	17	VAL	2.1
1	DA	73	VAL	2.1
1	DE	67	GLU	2.1
2	BD	60	GLU	2.1
1	AQ	141	SER	2.0
1	CA	154	LYS	2.0
1	CS	43	SER	2.0
2	DP	28	HIS	2.0
1	CC	16	ILE	2.0
2	CR	84	ASP	2.0
1	AE	76	ASN	2.0
1	CG	203	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
2	BJ	15	GLY	2.0
1	BE	109	ALA	2.0
1	BS	142	SER	2.0
2	BV	148	ALA	2.0
1	CU	198	CYS	2.0
1	DA	146	TYR	2.0
1	BE	73	VAL	2.0
1	BU	112	ASN	2.0
1	CA	143	GLY	2.0
1	CS	140	LYS	2.0
1	DM	76	ASN	2.0
2	BF	106	LYS	2.0
1	CU	212	CYS	2.0
2	AR	92	GLN	2.0
1	CE	24	ALA	2.0
1	DE	147	PRO	2.0
2	DP	36	ILE	2.0
1	BU	113	SER	2.0
1	DQ	139	THR	2.0
1	BS	78	GLN	2.0
1	CA	80	ILE	2.0
2	DV	95	PRO	2.0
1	AA	179	GLY	2.0
1	DA	66	GLY	2.0
1	AA	178	ALA	2.0
1	BA	64	ARG	2.0
1	BC	39	PHE	2.0
1	BE	112	ASN	2.0
1	BM	76	ASN	2.0
1	BC	123	SER	2.0
1	BC	235	ILE	2.0
1	CQ	189	GLN	2.0
2	DH	143	ASP	2.0
1	AI	147	PRO	2.0
1	BS	110	SER	2.0
1	CS	204	GLY	2.0
2	CD	51	HIS	2.0

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.