Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 10:51 PM UTC

PDB ID	:	6YFS / pdb_00006yfs
Title	:	Virus-like particle of bacteriophage PQ-465
Authors	:	Rumnieks, J.; Kalnins, G.; Sisovs, M.; Lieknina, I.; Tars, K.
Deposited on	:	2020-03-26
Resolution	:	3.50 Å(reported)

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

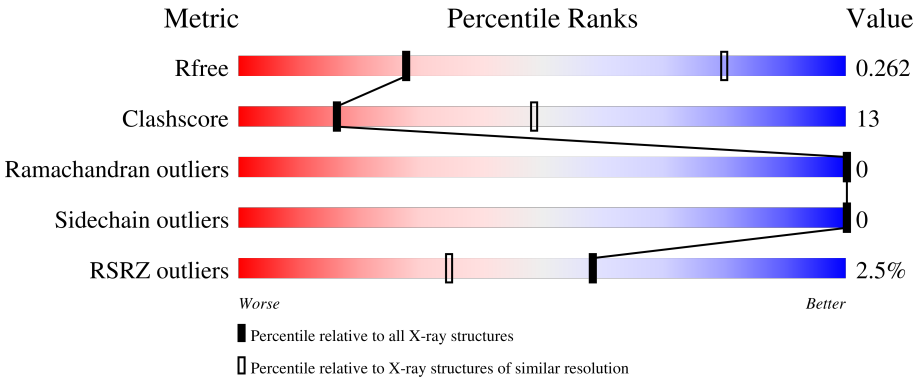
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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

Mol	Chain	Length	Quality of chain
1	AA	126	67% 33%
1	AB	126	2% 69% 29%
1	AC	126	4% 64% 34%
1	AD	126	% 67% 33%
1	AE	126	2% 71% 27%

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Mol	Chain	Length	Quality of chain
1	AF	126	2% 78% 21%
1	AG	126	2% 65% 34%
1	AH	126	% 70% 29%
1	AI	126	2% 72% 26%
1	AJ	126	3% 67% 33%
1	AK	126	3% 70% 29%
1	AL	126	67% 31%
1	AM	126	4% 66% 33%
1	AN	126	71% 27%
1	AO	126	% 60% 38%
1	AP	126	5% 66% 33%
1	AQ	126	2% 70% 29%
1	AR	126	3% 69% 29%
1	AS	126	66% 33%
1	AT	126	2% 71% 27%
1	AU	126	4% 67% 32%
1	AV	126	5% 65% 34%
1	AW	126	2% 68% 30%
1	AX	126	% 60% 38%
1	AY	126	8% 64% 35%
1	AZ	126	6% 68% 30%
1	BA	126	% 71% 28%
1	BB	126	2% 65% 34%
1	BC	126	71% 28%
1	BD	126	3% 65% 33%

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Mol	Chain	Length	Quality of chain
1	BE	126	64% 35%
1	BF	126	69% 29%
1	BG	126	67% 31%
1	BH	126	63% 36%
1	BI	126	70% 29%
1	BJ	126	63% 36%
1	BK	126	66% 33%
1	BL	126	71% 28%
1	BM	126	76% 22%
1	BN	126	4% 63% 36%
1	BO	126	3% 72% 26%
1	BP	126	74% 25%
1	BQ	126	63% 36%
1	BR	126	71% 28%
1	BS	126	4% 67% 32%
1	BT	126	5% 65% 34%
1	BU	126	70% 29%
1	BV	126	59% 40%
1	BW	126	6% 63% 36%
1	BX	126	68% 30%
1	BY	126	3% 68% 30%
1	BZ	126	65% 34%
1	CA	126	71% 28%
1	CB	126	66% 33%
1	CC	126	5% 66% 33%

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Mol	Chain	Length	Quality of chain
1	CD	126	3% 72% 26%
1	CE	126	4% 77% 21%
1	CF	126	5% 65% 34%
1	CG	126	% 70% 29%
1	CH	126	2% 59% 40%
1	CI	126	6% 66% 33%
1	CJ	126	4% 71% 28%
1	CK	126	5% 78% 21%
1	CL	126	2% 64% 35%
1	CM	126	2% 73% 25%
1	CN	126	% 72% 26%
1	CO	126	% 66% 33%
1	CP	126	4% 71% 28%
1	CQ	126	7% 63% 35%
1	CR	126	2% 65% 34%
1	CS	126	3% 68% 30%
1	CT	126	2% 68% 30%
1	CU	126	2% 66% 33%
1	CV	126	3% 71% 27%
1	CW	126	2% 78% 21%
1	CX	126	6% 65% 34%
1	CY	126	4% 71% 27%
1	CZ	126	4% 77% 21%
1	DA	126	2% 67% 32%
1	DB	126	3% 67% 31%

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Mol	Chain	Length	Quality of chain
1	DC	126	4% 78% 21%
1	DD	126	3% 65% 34%
1	DE	126	2% 71% 27%
1	DF	126	% 78% 21%
1	DG	126	% 67% 32%
1	DH	126	% 71% 27%
1	DI	126	3% 77% 21%
1	DJ	126	% 64% 35%
1	DK	126	2% 72% 26%
1	DL	126	4% 78% 21%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 84900 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called coat protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	125	Total	C	N	O	S	0	0	0
			946	586	173	184	3			
1	AB	124	Total	C	N	O	S	0	0	0
			942	584	172	183	3			
1	AC	124	Total	C	N	O	S	0	0	0
			942	584	172	183	3			
1	AD	125	Total	C	N	O	S	0	0	0
			946	586	173	184	3			
1	AE	124	Total	C	N	O	S	0	0	0
			942	584	172	183	3			
1	AF	124	Total	C	N	O	S	0	0	0
			942	584	172	183	3			
1	AG	125	Total	C	N	O	S	0	0	0
			946	586	173	184	3			
1	AH	124	Total	C	N	O	S	0	0	0
			942	584	172	183	3			
1	AI	124	Total	C	N	O	S	0	0	0
			942	584	172	183	3			
1	AJ	125	Total	C	N	O	S	0	0	0
			946	586	173	184	3			
1	AK	124	Total	C	N	O	S	0	0	0
			942	584	172	183	3			
1	AL	124	Total	C	N	O	S	0	0	0
			942	584	172	183	3			
1	AM	125	Total	C	N	O	S	0	0	0
			946	586	173	184	3			
1	AN	124	Total	C	N	O	S	0	0	0
			942	584	172	183	3			
1	AO	124	Total	C	N	O	S	0	0	0
			942	584	172	183	3			
1	AP	125	Total	C	N	O	S	0	0	0
			946	586	173	184	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AQ	124	Total	C	N	O	S	0	0	0
			942	584	172	183	3			
1	AR	124	Total	C	N	O	S	0	0	0
			942	584	172	183	3			
1	AS	125	Total	C	N	O	S	0	0	0
			946	586	173	184	3			
1	AT	124	Total	C	N	O	S	0	0	0
			942	584	172	183	3			
1	AU	124	Total	C	N	O	S	0	0	0
			942	584	172	183	3			
1	AV	125	Total	C	N	O	S	0	0	0
			946	586	173	184	3			
1	AW	124	Total	C	N	O	S	0	0	0
			942	584	172	183	3			
1	AX	124	Total	C	N	O	S	0	0	0
			942	584	172	183	3			
1	AY	125	Total	C	N	O	S	0	0	0
			946	586	173	184	3			
1	AZ	124	Total	C	N	O	S	0	0	0
			942	584	172	183	3			
1	BA	124	Total	C	N	O	S	0	0	0
			942	584	172	183	3			
1	BB	125	Total	C	N	O	S	0	0	0
			946	586	173	184	3			
1	BC	124	Total	C	N	O	S	0	0	0
			942	584	172	183	3			
1	BD	124	Total	C	N	O	S	0	0	0
			942	584	172	183	3			
1	BE	125	Total	C	N	O	S	0	0	0
			946	586	173	184	3			
1	BF	124	Total	C	N	O	S	0	0	0
			942	584	172	183	3			
1	BG	124	Total	C	N	O	S	0	0	0
			942	584	172	183	3			
1	BH	125	Total	C	N	O	S	0	0	0
			946	586	173	184	3			
1	BI	124	Total	C	N	O	S	0	0	0
			942	584	172	183	3			
1	BJ	124	Total	C	N	O	S	0	0	0
			942	584	172	183	3			
1	BK	125	Total	C	N	O	S	0	0	0
			946	586	173	184	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	BL	124	Total	C	N	O	S	0	0	0
			942	584	172	183	3			
1	BM	124	Total	C	N	O	S	0	0	0
			942	584	172	183	3			
1	BN	125	Total	C	N	O	S	0	0	0
			946	586	173	184	3			
1	BO	124	Total	C	N	O	S	0	0	0
			942	584	172	183	3			
1	BP	124	Total	C	N	O	S	0	0	0
			942	584	172	183	3			
1	BQ	125	Total	C	N	O	S	0	0	0
			946	586	173	184	3			
1	BR	124	Total	C	N	O	S	0	0	0
			942	584	172	183	3			
1	BS	124	Total	C	N	O	S	0	0	0
			942	584	172	183	3			
1	BT	125	Total	C	N	O	S	0	0	0
			946	586	173	184	3			
1	BU	124	Total	C	N	O	S	0	0	0
			942	584	172	183	3			
1	BV	124	Total	C	N	O	S	0	0	0
			942	584	172	183	3			
1	BW	125	Total	C	N	O	S	0	0	0
			946	586	173	184	3			
1	BX	124	Total	C	N	O	S	0	0	0
			942	584	172	183	3			
1	BY	124	Total	C	N	O	S	0	0	0
			942	584	172	183	3			
1	BZ	125	Total	C	N	O	S	0	0	0
			946	586	173	184	3			
1	CA	124	Total	C	N	O	S	0	0	0
			942	584	172	183	3			
1	CB	124	Total	C	N	O	S	0	0	0
			942	584	172	183	3			
1	CC	125	Total	C	N	O	S	0	0	0
			946	586	173	184	3			
1	CD	124	Total	C	N	O	S	0	0	0
			942	584	172	183	3			
1	CE	124	Total	C	N	O	S	0	0	0
			942	584	172	183	3			
1	CF	125	Total	C	N	O	S	0	0	0
			946	586	173	184	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	CG	124	Total	C	N	O	S	0	0	0
			942	584	172	183	3			
1	CH	124	Total	C	N	O	S	0	0	0
			942	584	172	183	3			
1	CI	125	Total	C	N	O	S	0	0	0
			946	586	173	184	3			
1	CJ	124	Total	C	N	O	S	0	0	0
			942	584	172	183	3			
1	CK	124	Total	C	N	O	S	0	0	0
			942	584	172	183	3			
1	CL	125	Total	C	N	O	S	0	0	0
			946	586	173	184	3			
1	CM	124	Total	C	N	O	S	0	0	0
			942	584	172	183	3			
1	CN	124	Total	C	N	O	S	0	0	0
			942	584	172	183	3			
1	CO	125	Total	C	N	O	S	0	0	0
			946	586	173	184	3			
1	CP	124	Total	C	N	O	S	0	0	0
			942	584	172	183	3			
1	CQ	124	Total	C	N	O	S	0	0	0
			942	584	172	183	3			
1	CR	125	Total	C	N	O	S	0	0	0
			946	586	173	184	3			
1	CS	124	Total	C	N	O	S	0	0	0
			942	584	172	183	3			
1	CT	124	Total	C	N	O	S	0	0	0
			942	584	172	183	3			
1	CU	125	Total	C	N	O	S	0	0	0
			946	586	173	184	3			
1	CV	124	Total	C	N	O	S	0	0	0
			942	584	172	183	3			
1	CW	124	Total	C	N	O	S	0	0	0
			942	584	172	183	3			
1	CX	125	Total	C	N	O	S	0	0	0
			946	586	173	184	3			
1	CY	124	Total	C	N	O	S	0	0	0
			942	584	172	183	3			
1	CZ	124	Total	C	N	O	S	0	0	0
			942	584	172	183	3			
1	DA	125	Total	C	N	O	S	0	0	0
			946	586	173	184	3			

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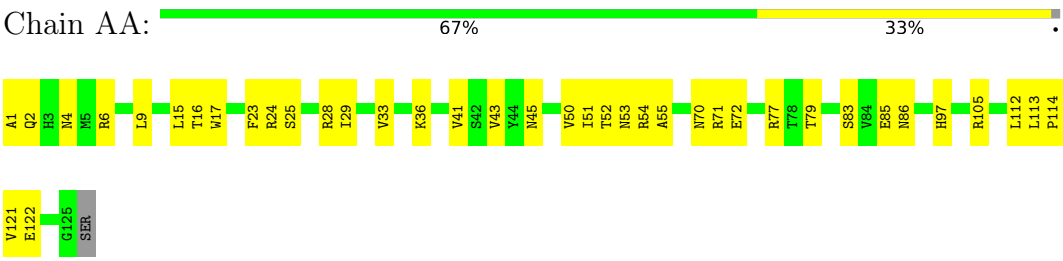
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	DB	124	Total	C	N	O	S	0	0	0
			942	584	172	183	3			
1	DC	124	Total	C	N	O	S	0	0	0
			942	584	172	183	3			
1	DD	125	Total	C	N	O	S	0	0	0
			946	586	173	184	3			
1	DE	124	Total	C	N	O	S	0	0	0
			942	584	172	183	3			
1	DF	124	Total	C	N	O	S	0	0	0
			942	584	172	183	3			
1	DG	125	Total	C	N	O	S	0	0	0
			946	586	173	184	3			
1	DH	124	Total	C	N	O	S	0	0	0
			942	584	172	183	3			
1	DI	124	Total	C	N	O	S	0	0	0
			942	584	172	183	3			
1	DJ	125	Total	C	N	O	S	0	0	0
			946	586	173	184	3			
1	DK	124	Total	C	N	O	S	0	0	0
			942	584	172	183	3			
1	DL	124	Total	C	N	O	S	0	0	0
			942	584	172	183	3			

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

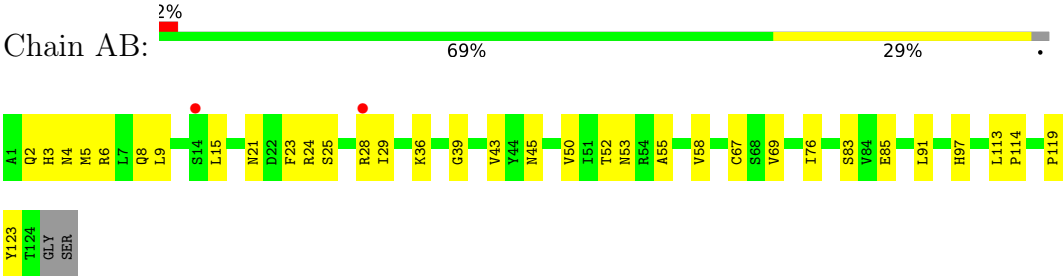
• Molecule 1: coat protein

Chain AA:



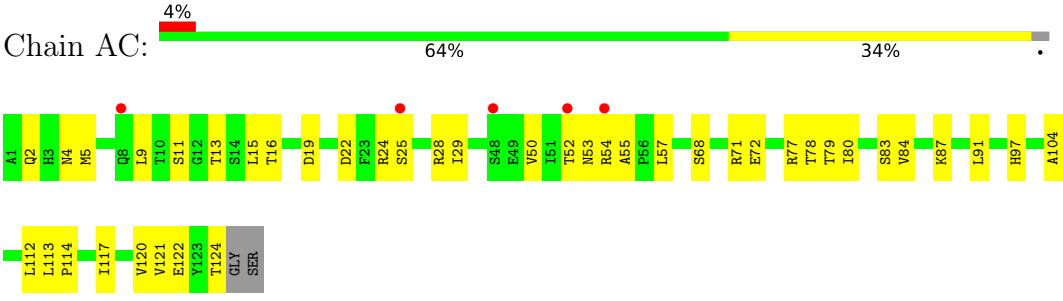
• Molecule 1: coat protein

Chain AB:



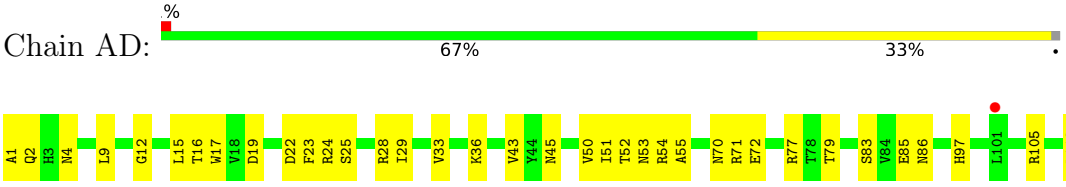
• Molecule 1: coat protein

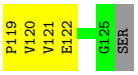
Chain AC:



• Molecule 1: coat protein

Chain AD:



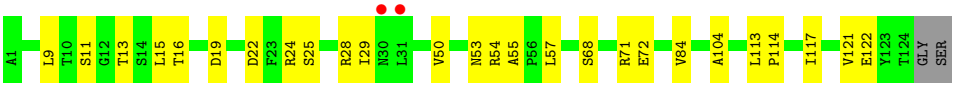


• Molecule 1: coat protein

Chain AE:

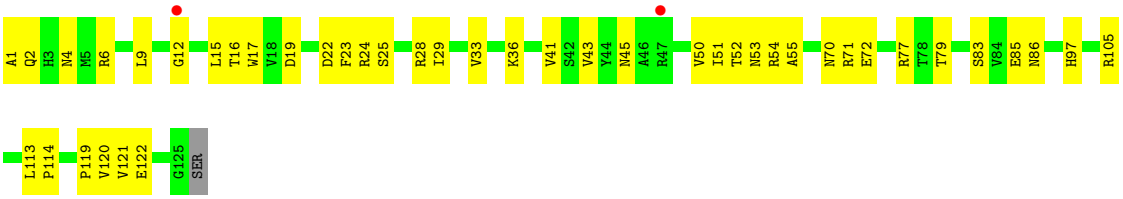
• Molecule 1: coat protein

Chain AF:



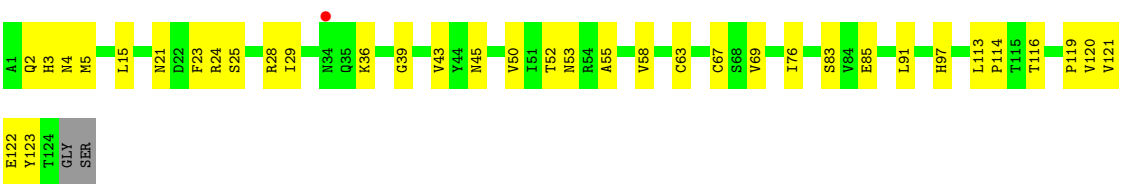
• Molecule 1: coat protein

Chain AG:



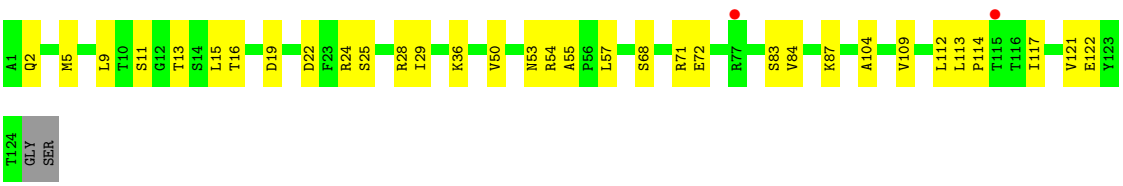
• Molecule 1: coat protein

Chain AH:



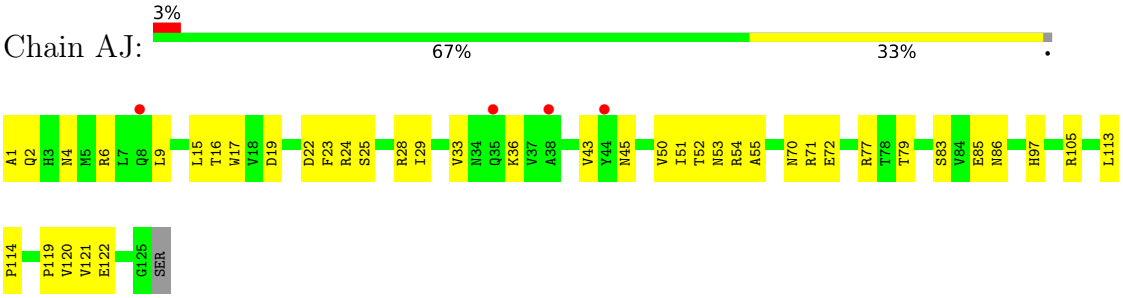
• Molecule 1: coat protein

Chain AI:



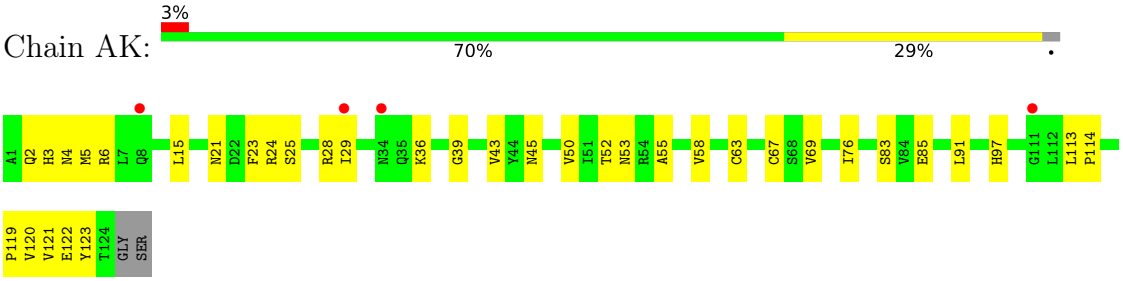
• Molecule 1: coat protein

Chain AJ:



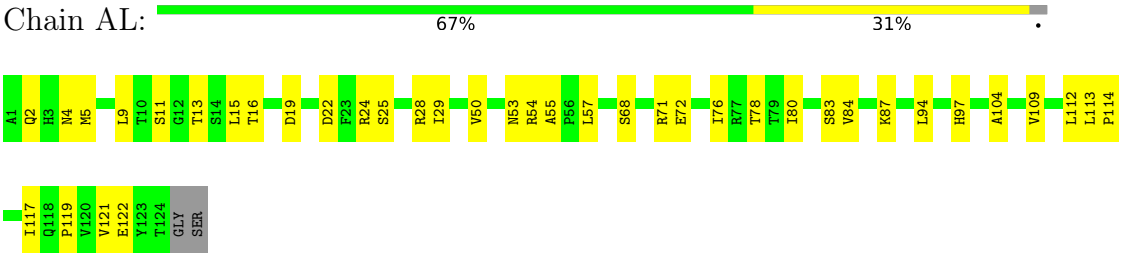
• Molecule 1: coat protein

Chain AK:



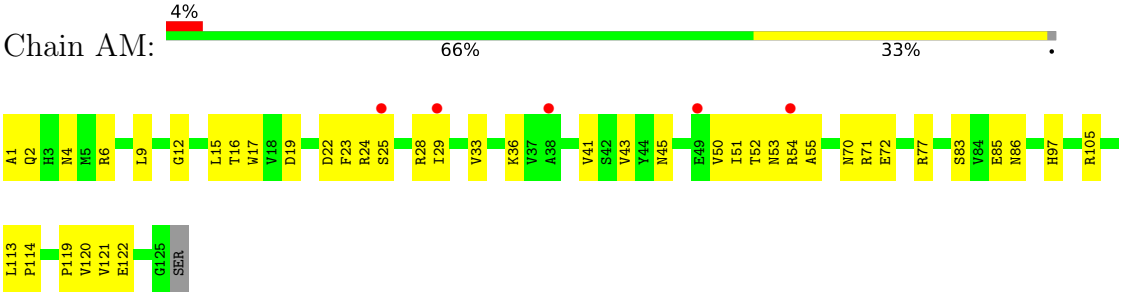
• Molecule 1: coat protein

Chain AL:



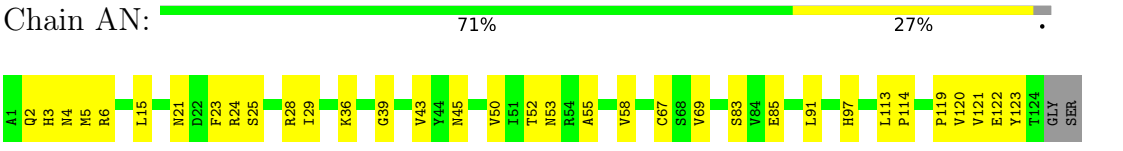
• Molecule 1: coat protein

Chain AM:



• Molecule 1: coat protein

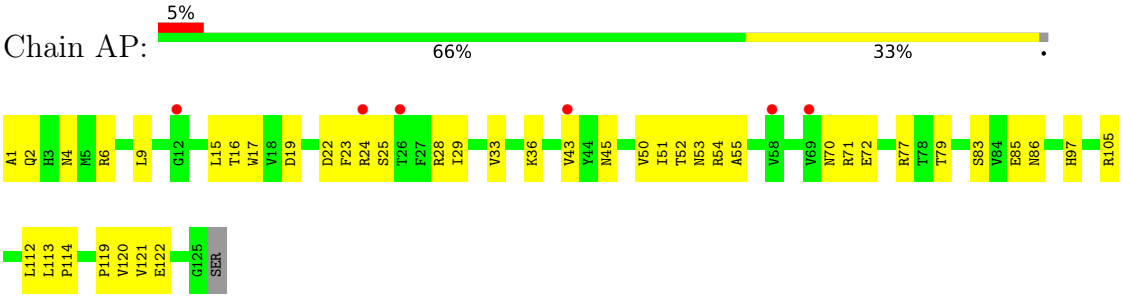
Chain AN:



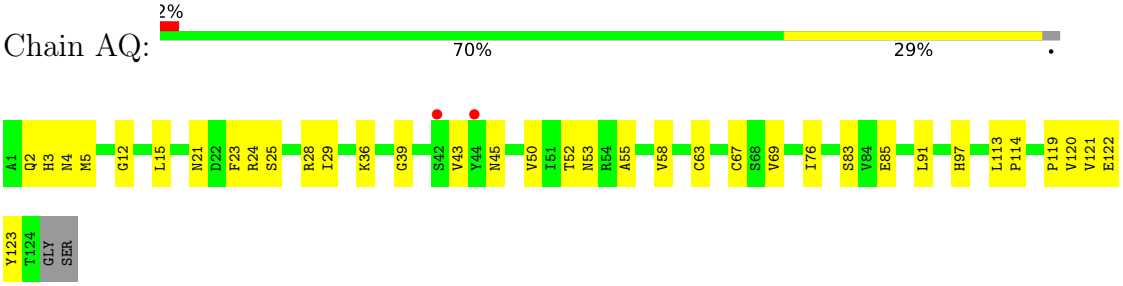
• Molecule 1: coat protein

Chain AO:

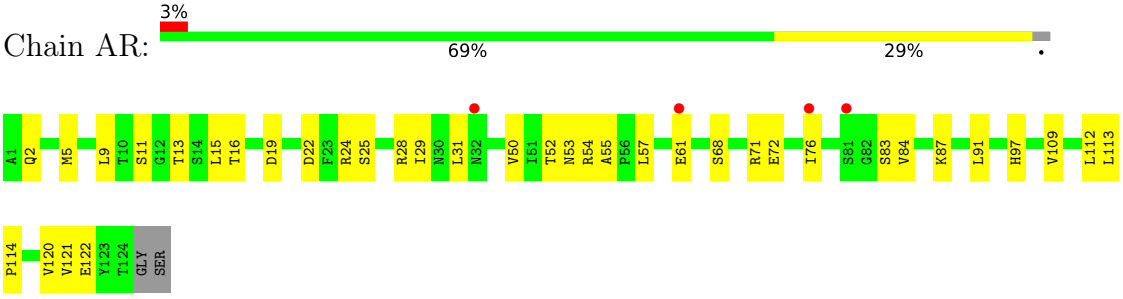
• Molecule 1: coat protein



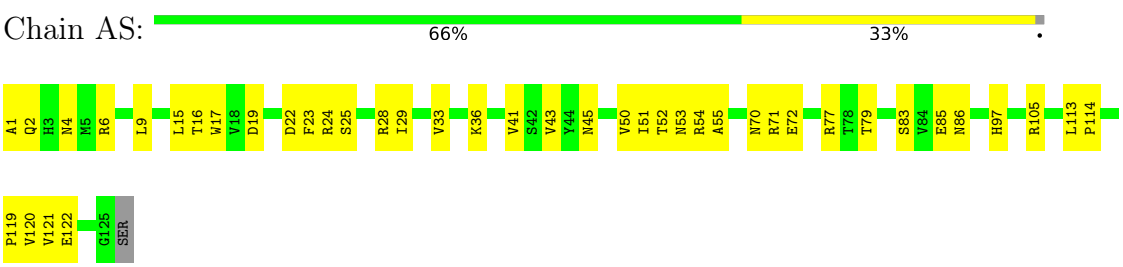
• Molecule 1: coat protein



• Molecule 1: coat protein

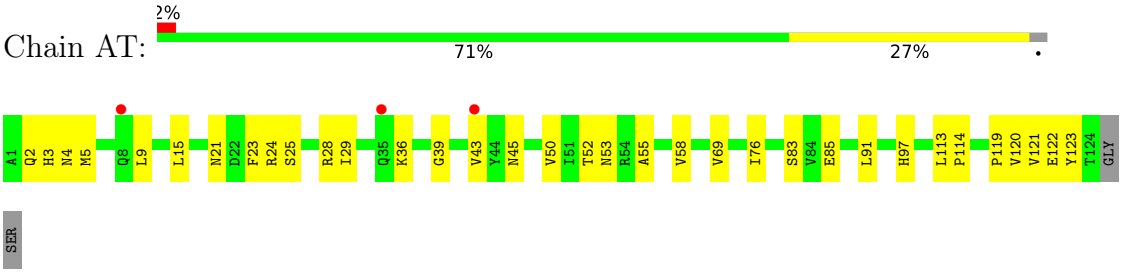


• Molecule 1: coat protein



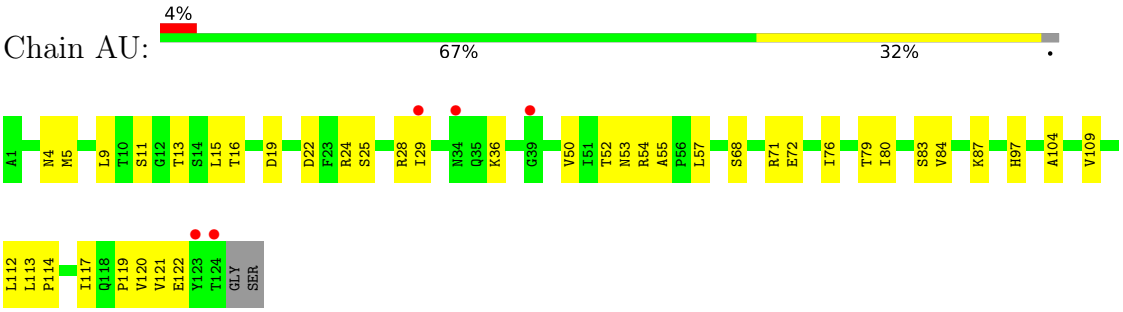
• Molecule 1: coat protein

Chain AT:



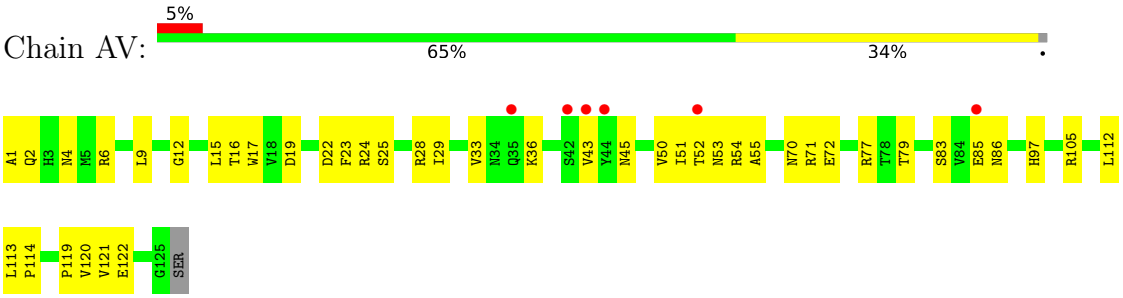
• Molecule 1: coat protein

Chain AU:



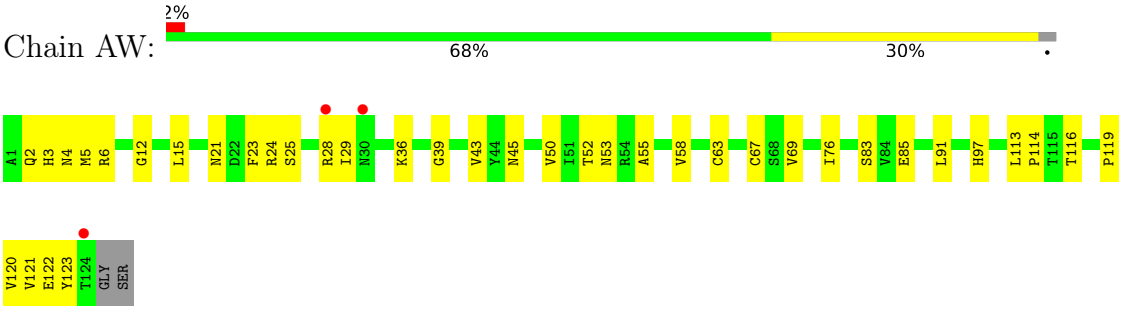
• Molecule 1: coat protein

Chain AV:



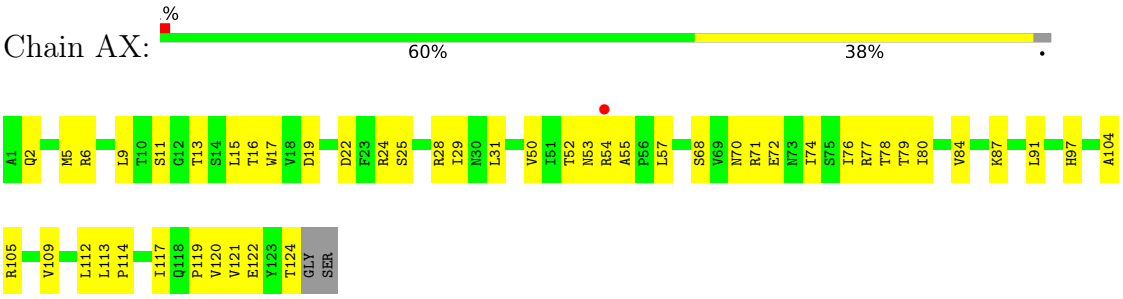
• Molecule 1: coat protein

Chain AW:



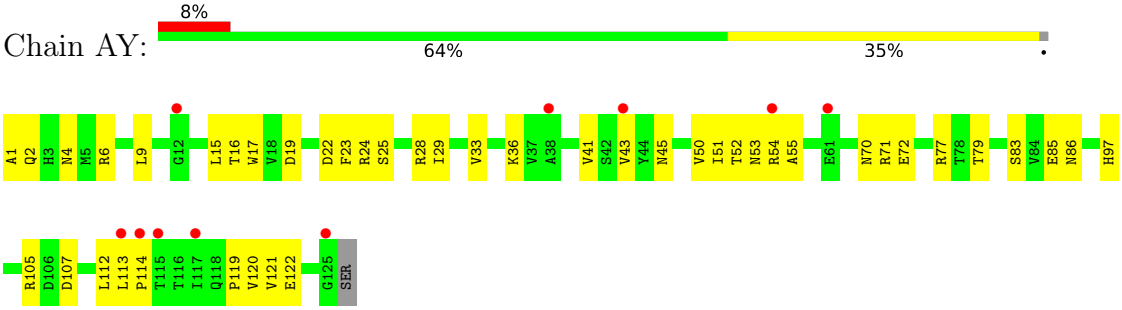
• Molecule 1: coat protein

Chain AX:



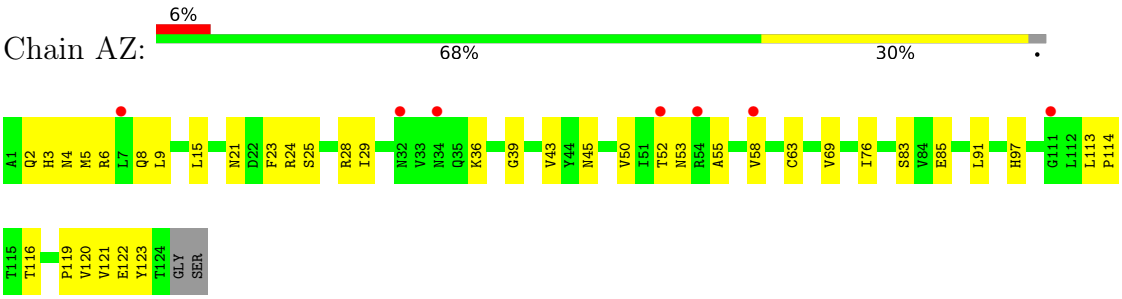
• Molecule 1: coat protein

Chain AY:



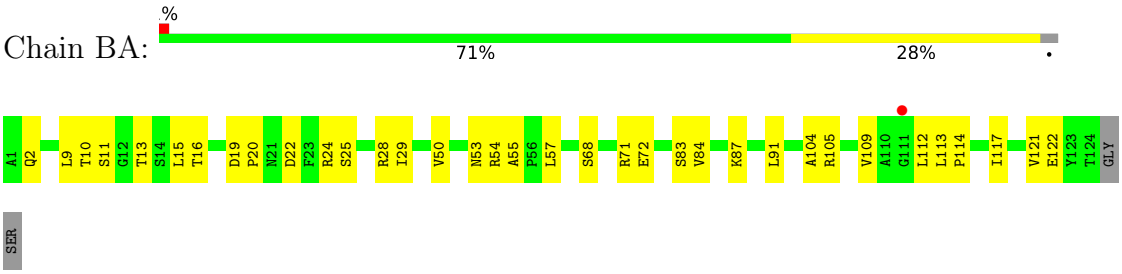
• Molecule 1: coat protein

Chain AZ:



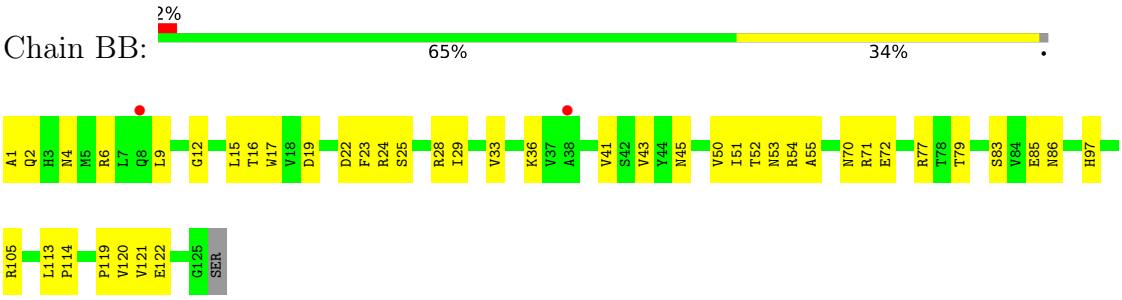
• Molecule 1: coat protein

Chain BA:



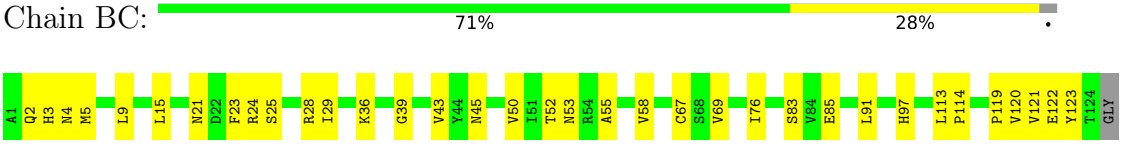
• Molecule 1: coat protein

Chain BB:



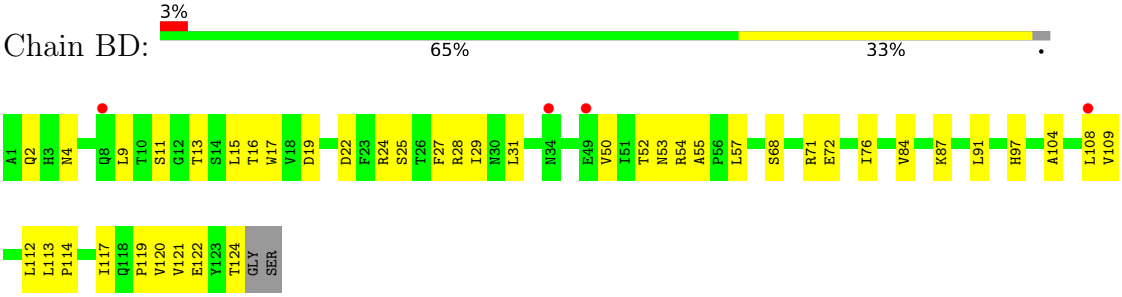
• Molecule 1: coat protein

Chain BC:



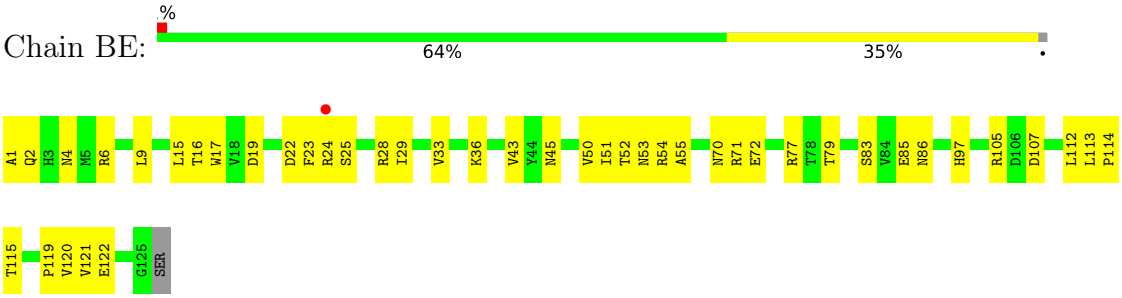
• Molecule 1: coat protein

Chain BD:



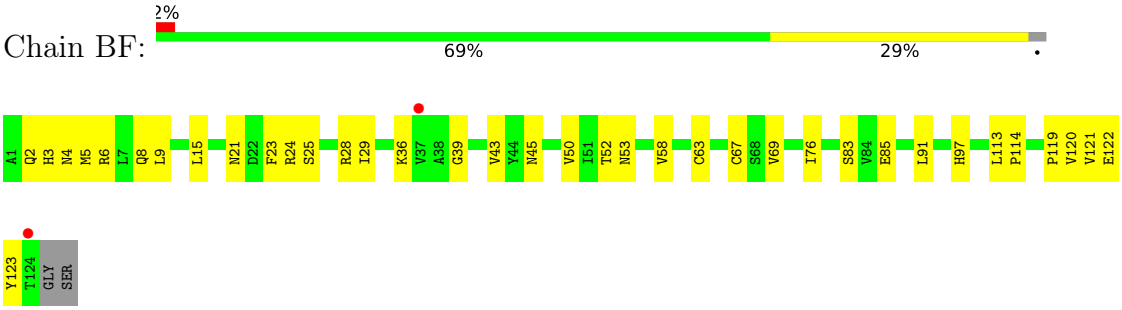
• Molecule 1: coat protein

Chain BE:



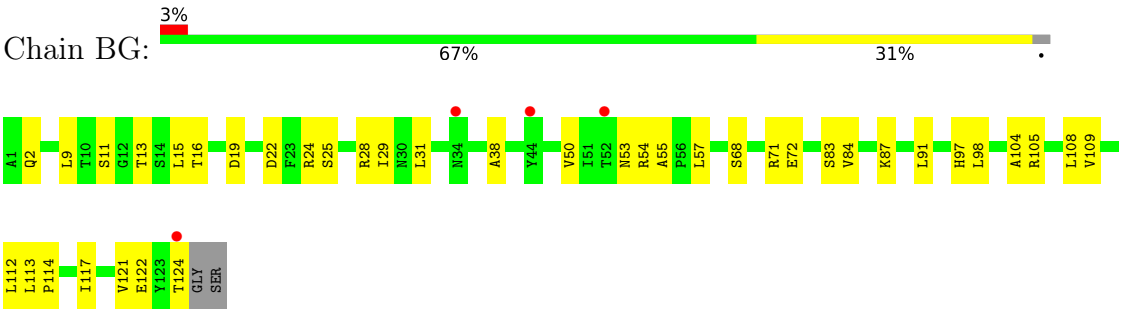
• Molecule 1: coat protein

Chain BF:



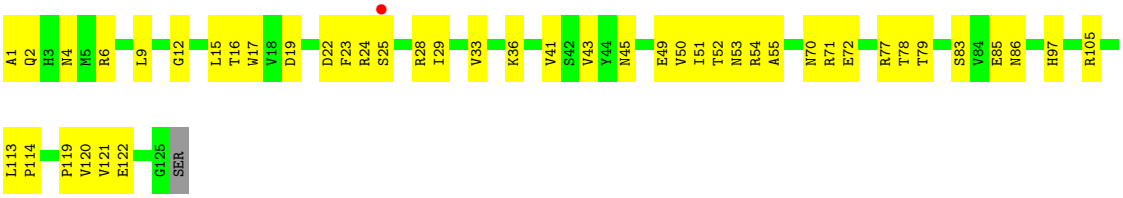
• Molecule 1: coat protein

Chain BG:



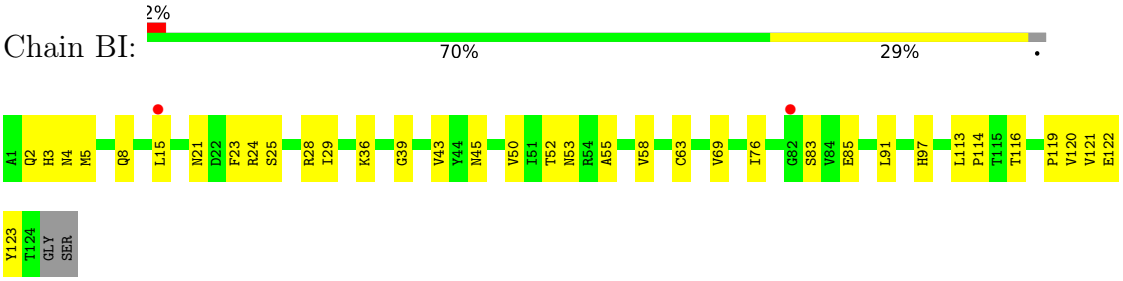
• Molecule 1: coat protein

Chain BH:



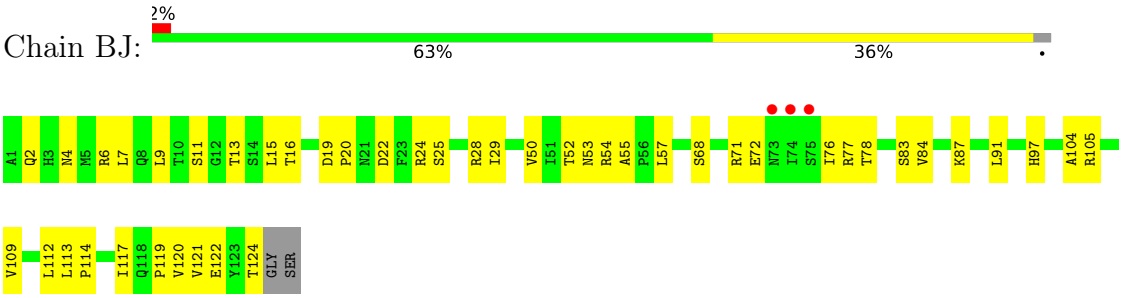
• Molecule 1: coat protein

Chain BI:



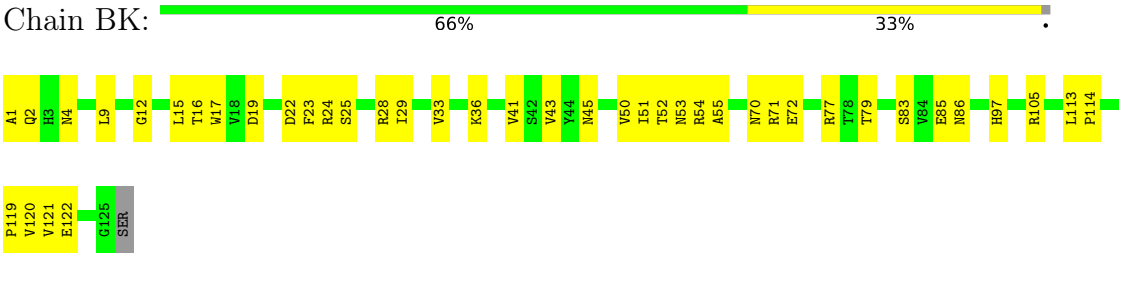
• Molecule 1: coat protein

Chain BJ:



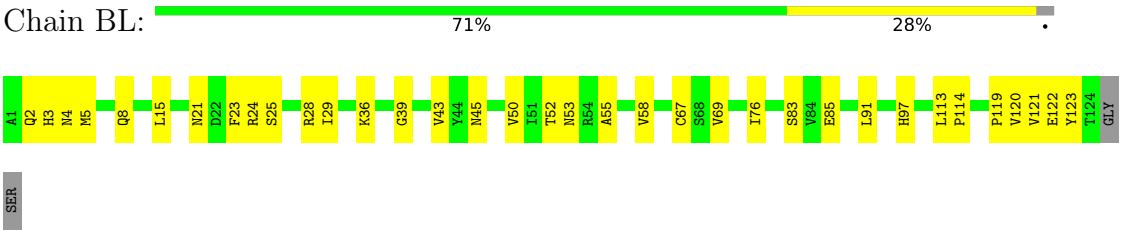
• Molecule 1: coat protein

Chain BK:



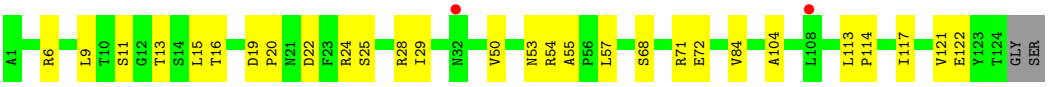
• Molecule 1: coat protein

Chain BL:



• Molecule 1: coat protein

Chain BM:



• Molecule 1: coat protein

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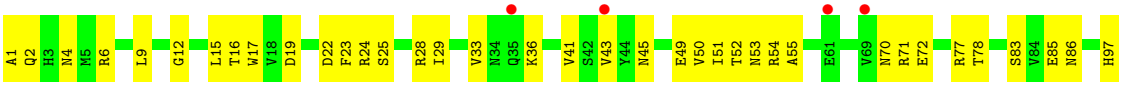
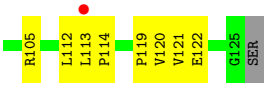


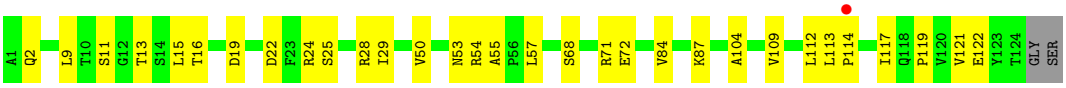


• Molecule 1: coat protein

Chain BO:

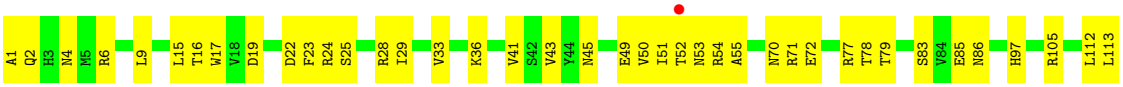
• Molecule 1: coat protein

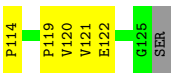
Chain BP:



• Molecule 1: coat protein

Chain BQ:



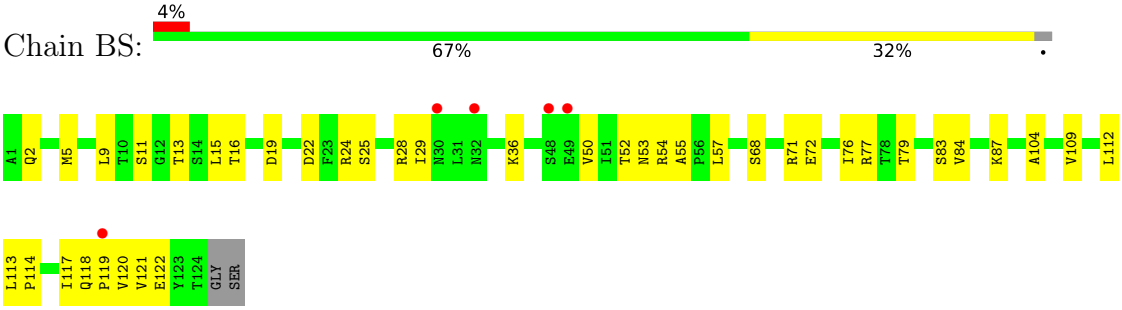


• Molecule 1: coat protein

Chain BR:

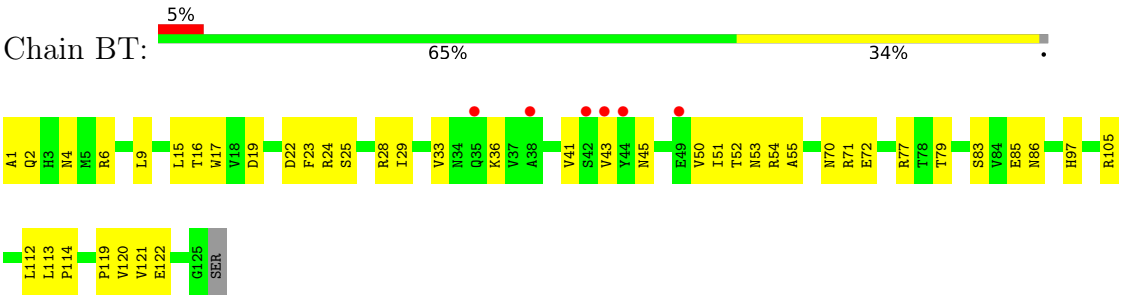
• Molecule 1: coat protein

Chain BS:



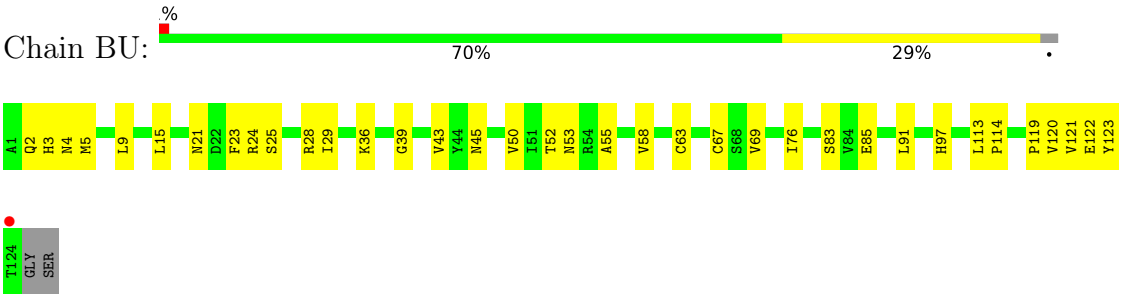
• Molecule 1: coat protein

Chain BT:



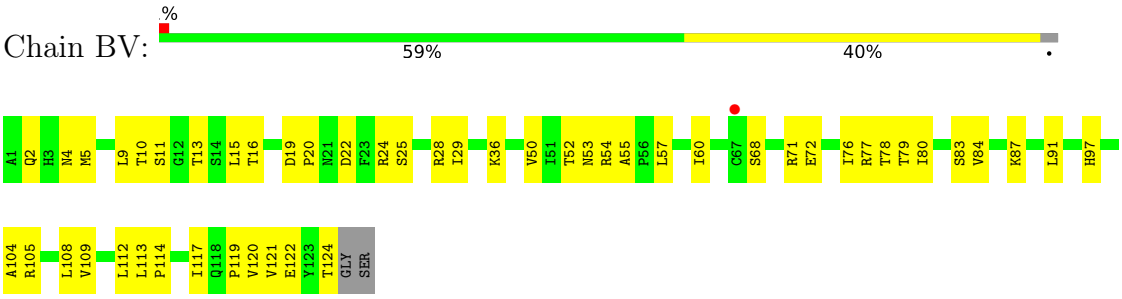
• Molecule 1: coat protein

Chain BU:



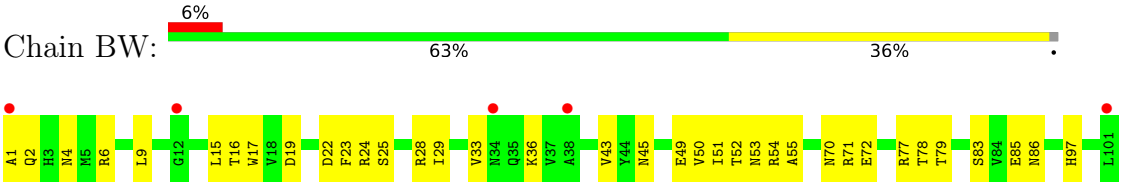
• Molecule 1: coat protein

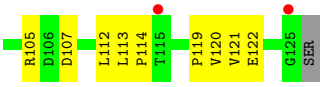
Chain BV:



• Molecule 1: coat protein

Chain BW:



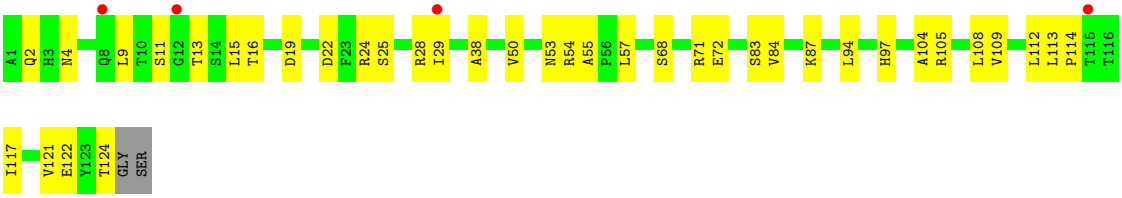


• Molecule 1: coat protein

Chain BX:

• Molecule 1: coat protein

Chain BY:

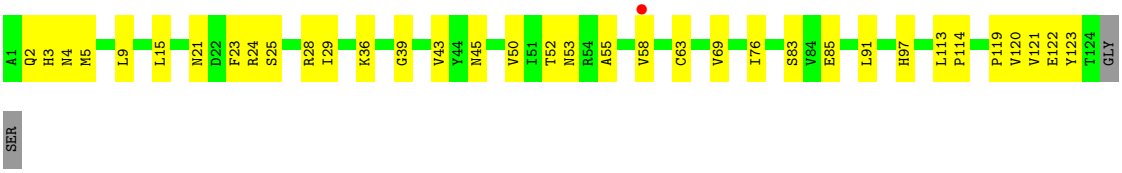


• Molecule 1: coat protein

Chain BZ:

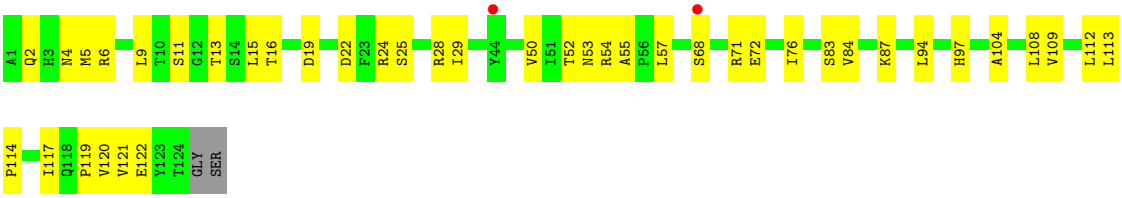
• Molecule 1: coat protein

Chain CA:

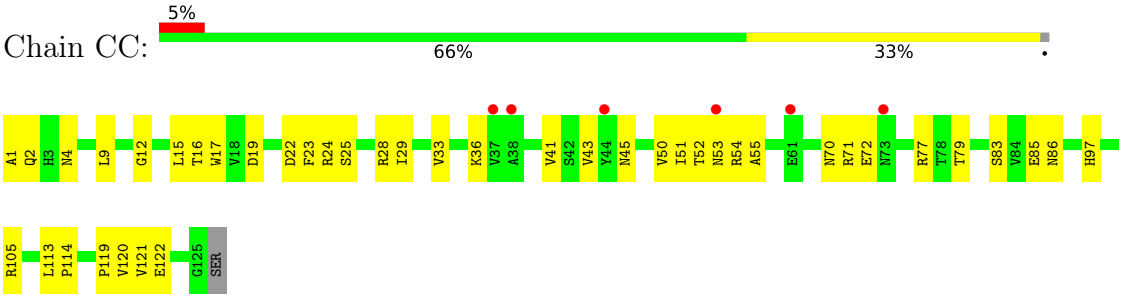


• Molecule 1: coat protein

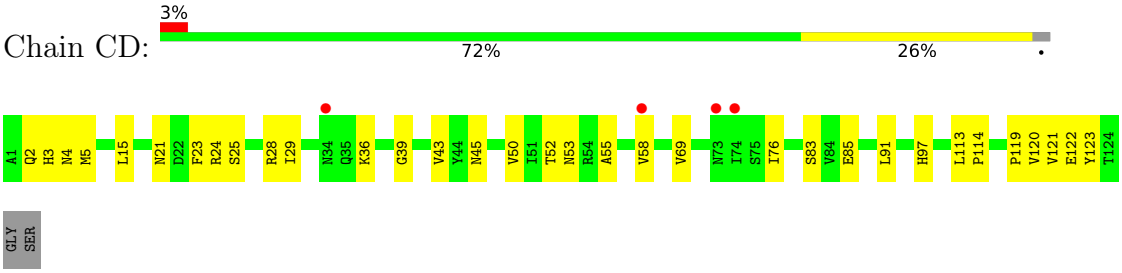
Chain CB:



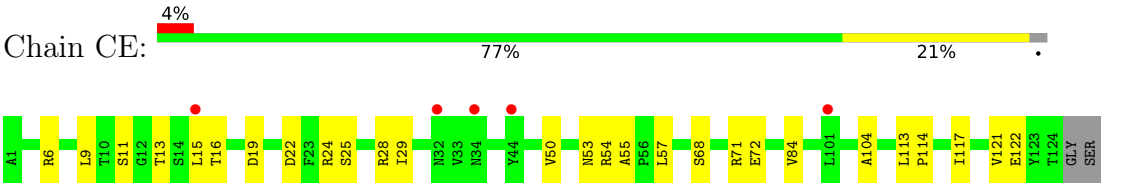
• Molecule 1: coat protein



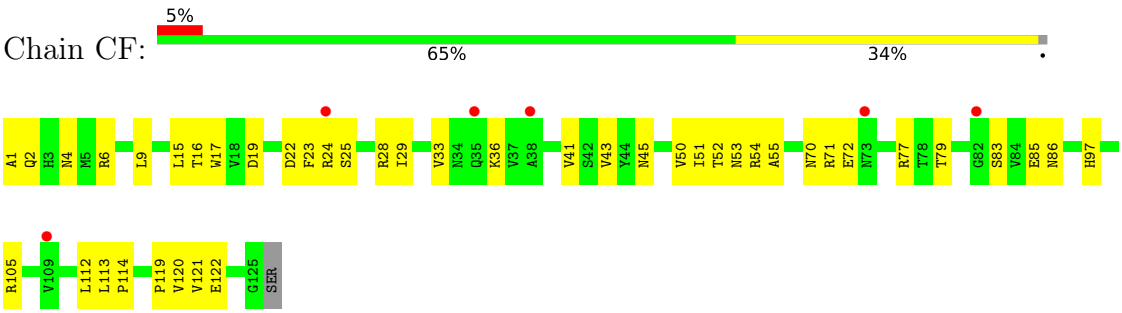
• Molecule 1: coat protein



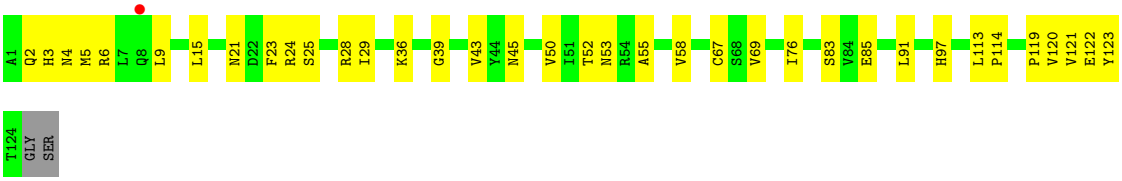
• Molecule 1: coat protein



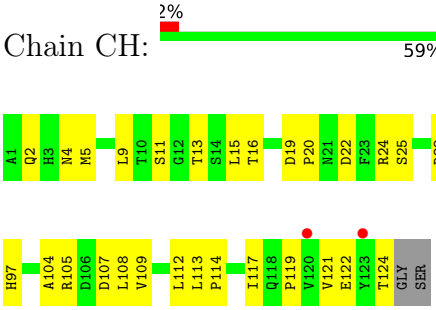
• Molecule 1: coat protein

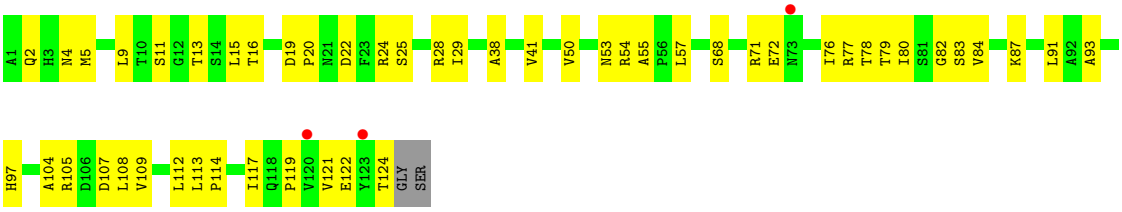


• Molecule 1: coat protein

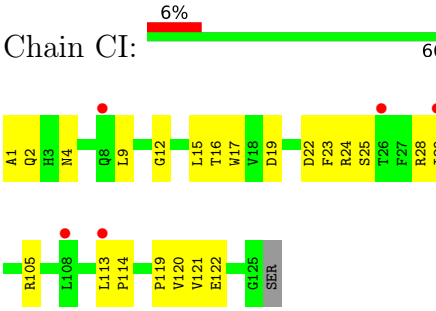


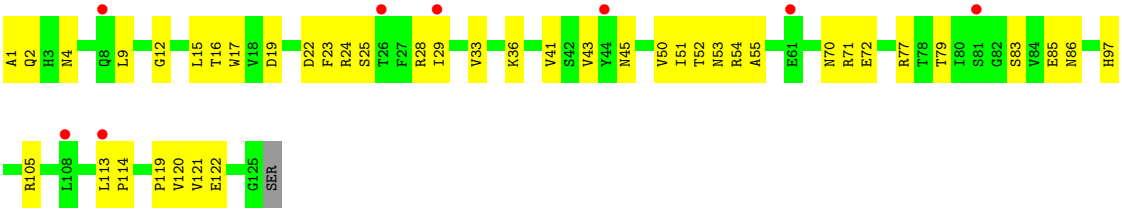
• Molecule 1: coat protein



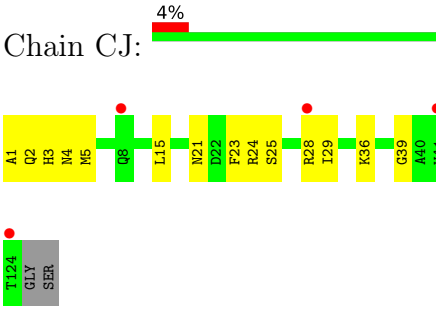


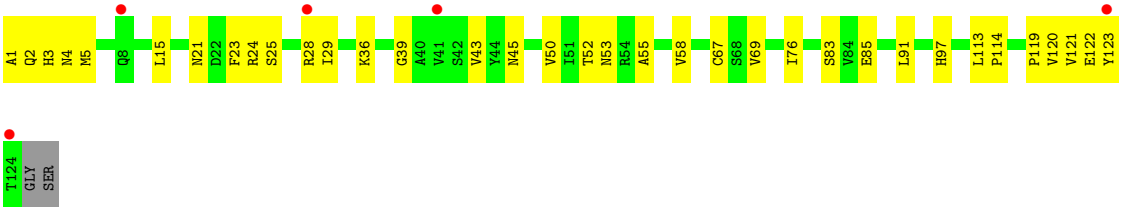
• Molecule 1: coat protein



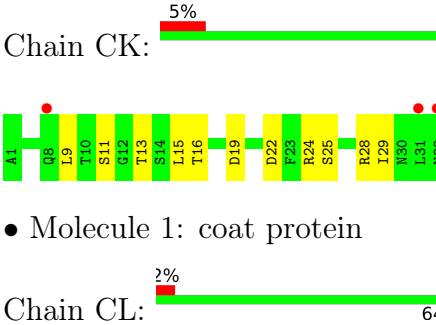


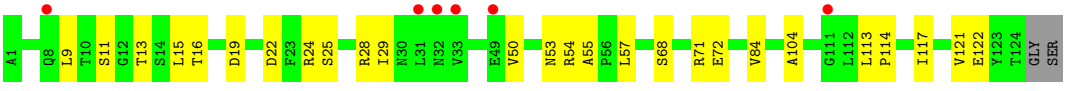
• Molecule 1: coat protein



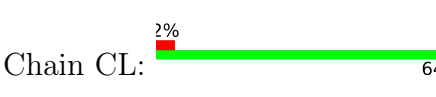


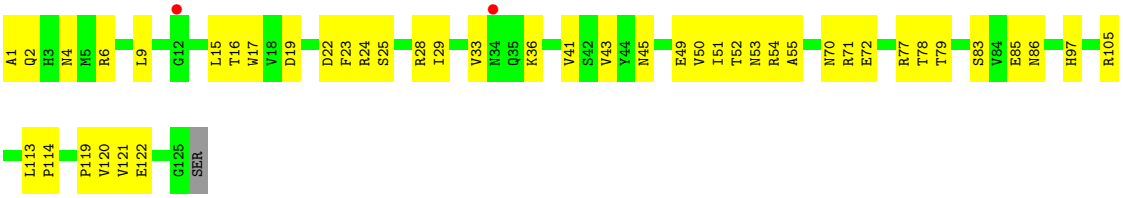
• Molecule 1: coat protein



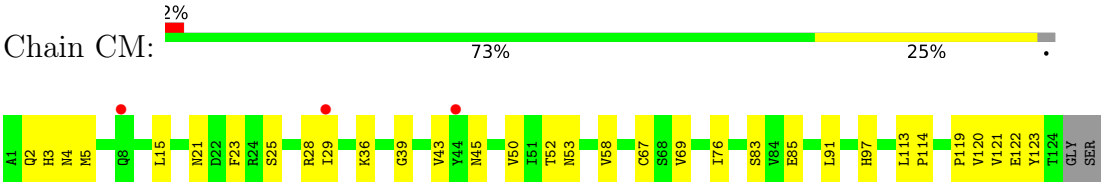


• Molecule 1: coat protein

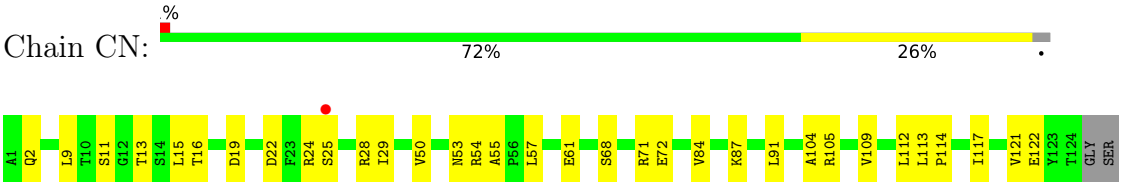




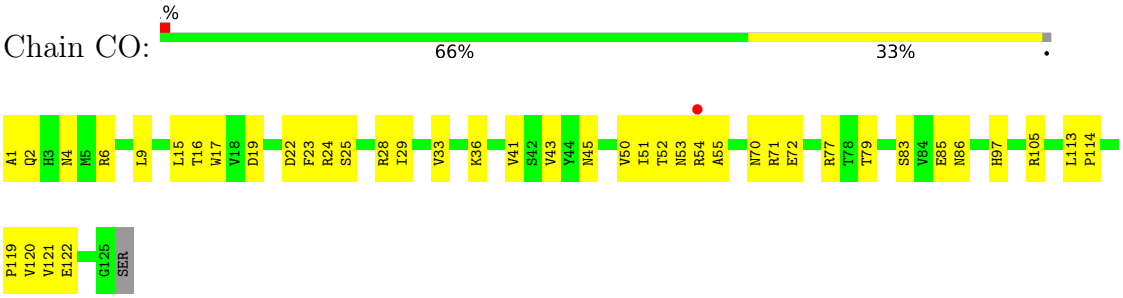
• Molecule 1: coat protein



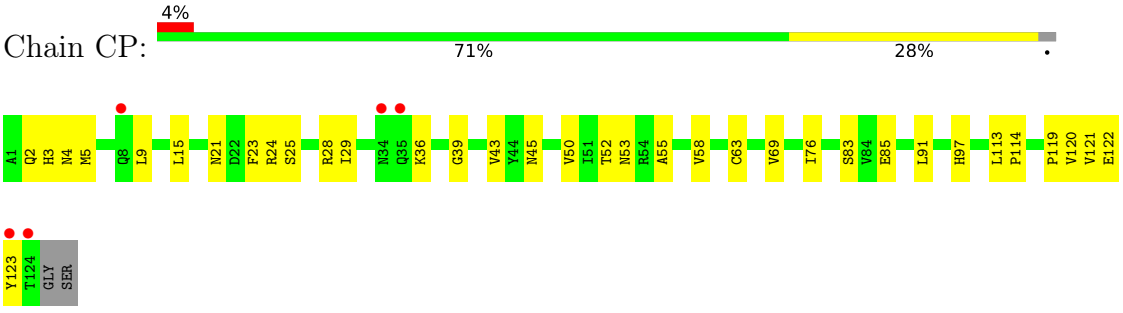
• Molecule 1: coat protein



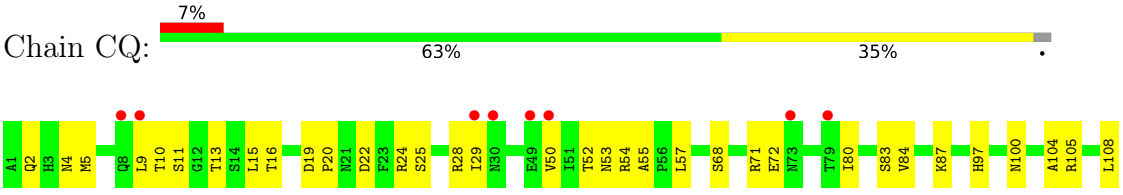
• Molecule 1: coat protein



• Molecule 1: coat protein

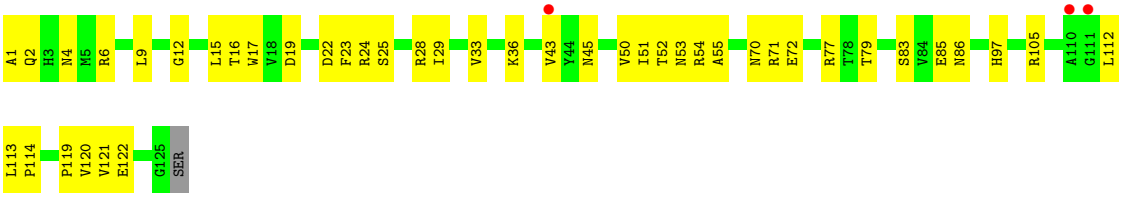


• Molecule 1: coat protein



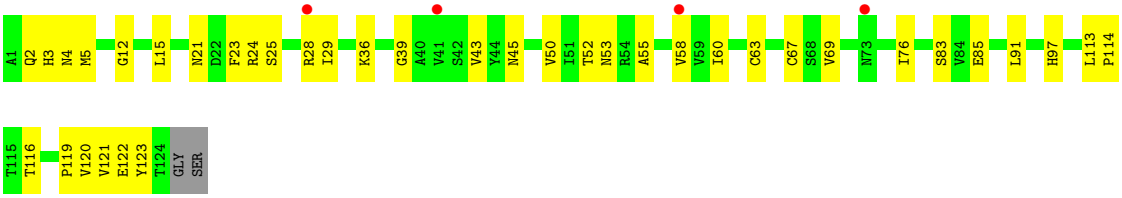
• Molecule 1: coat protein

Chain CR:



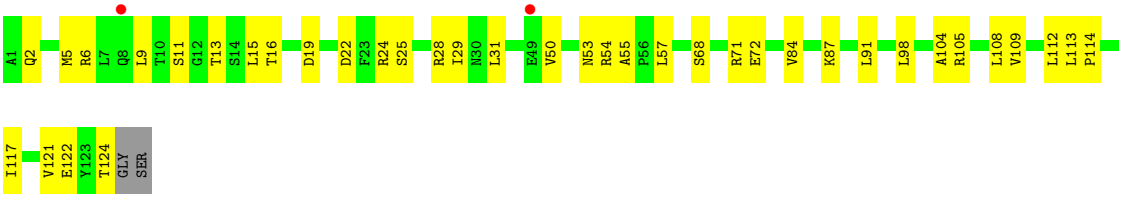
• Molecule 1: coat protein

Chain CS:



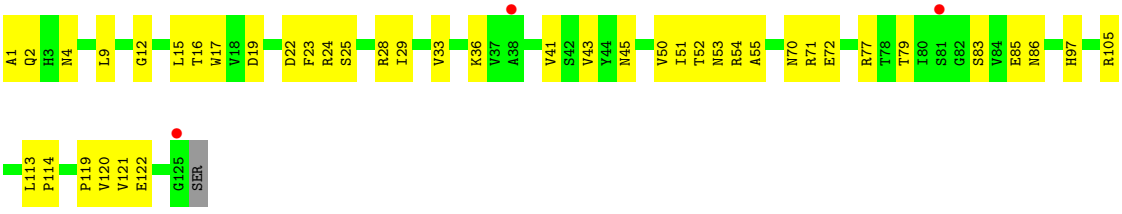
• Molecule 1: coat protein

Chain CT:



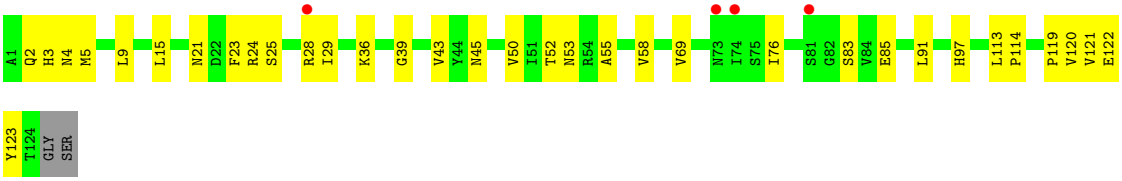
• Molecule 1: coat protein

Chain CU:

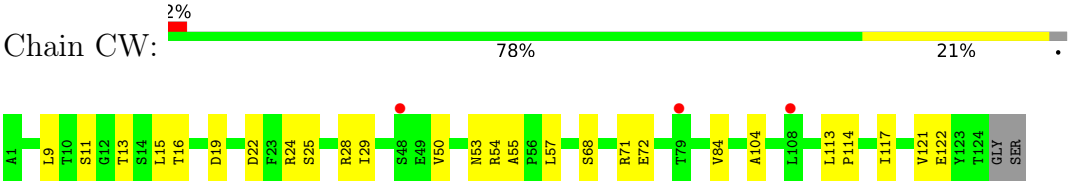


• Molecule 1: coat protein

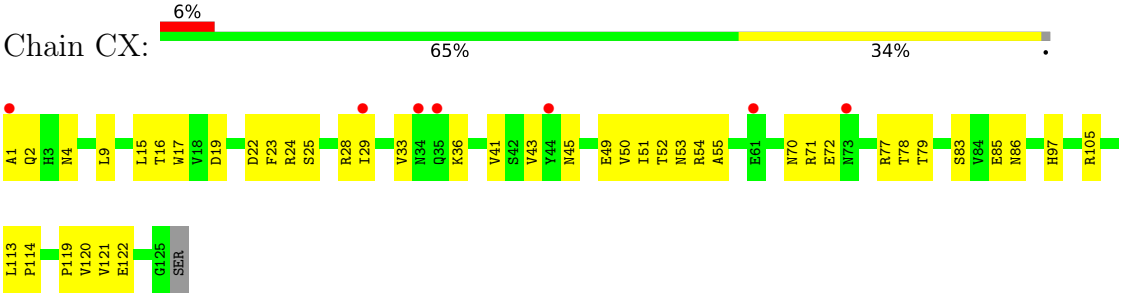
Chain CV:



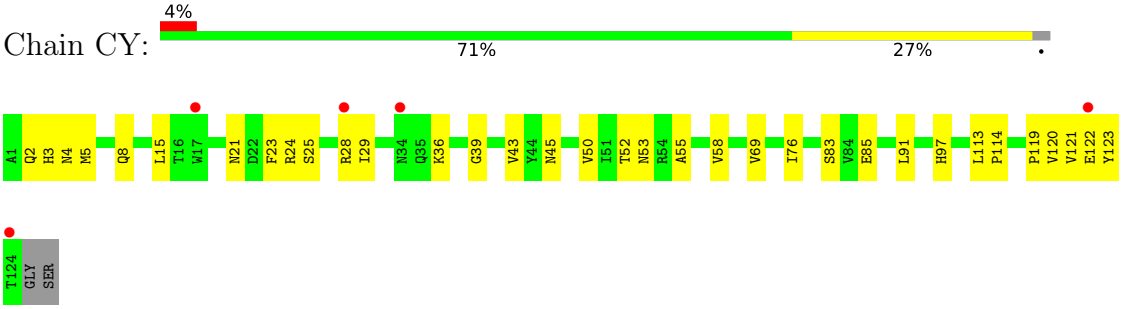
• Molecule 1: coat protein



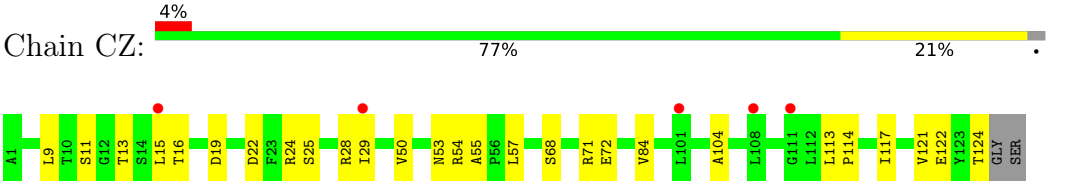
• Molecule 1: coat protein



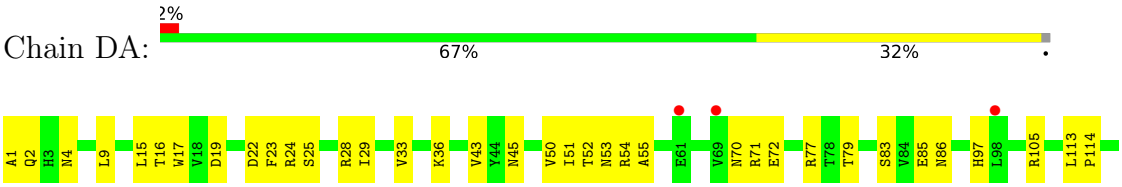
• Molecule 1: coat protein

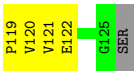


• Molecule 1: coat protein



• Molecule 1: coat protein



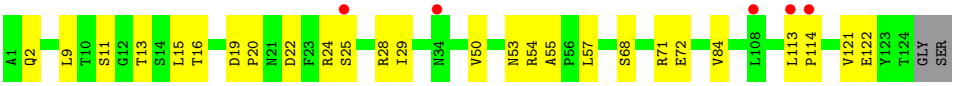


• Molecule 1: coat protein

Chain DB:

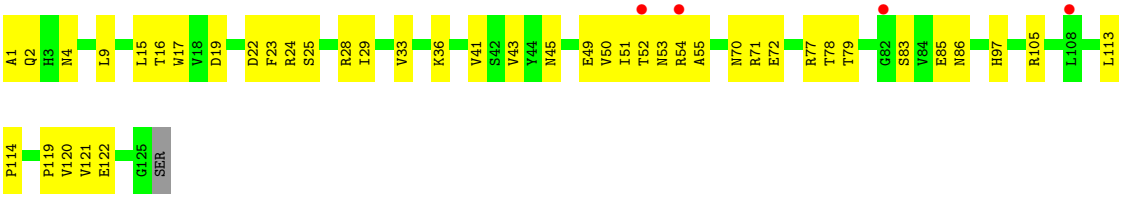
• Molecule 1: coat protein

Chain DC:



• Molecule 1: coat protein

Chain DD:

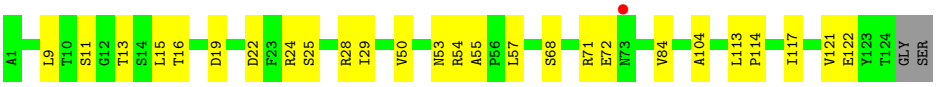


• Molecule 1: coat protein

Chain DE:

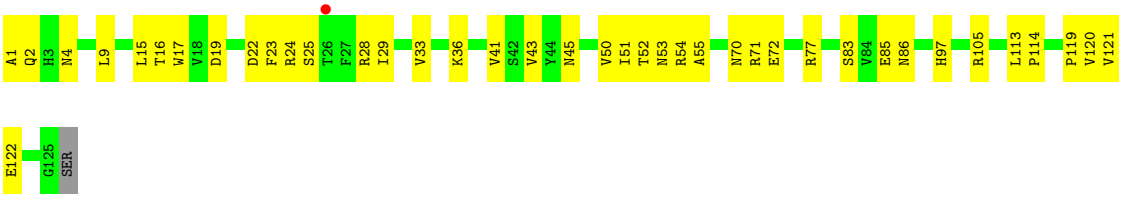
• Molecule 1: coat protein

Chain DF:

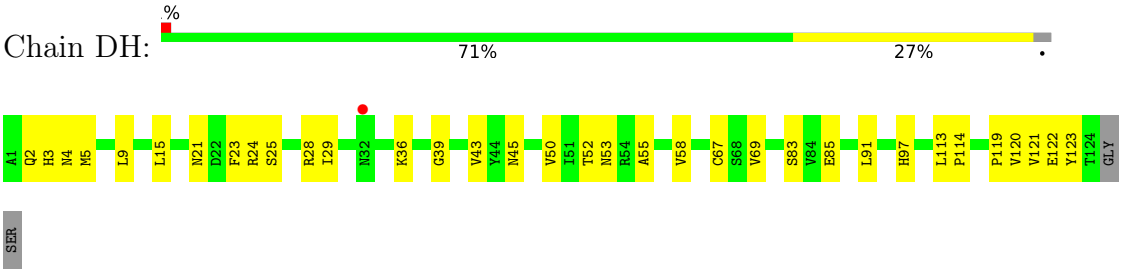


• Molecule 1: coat protein

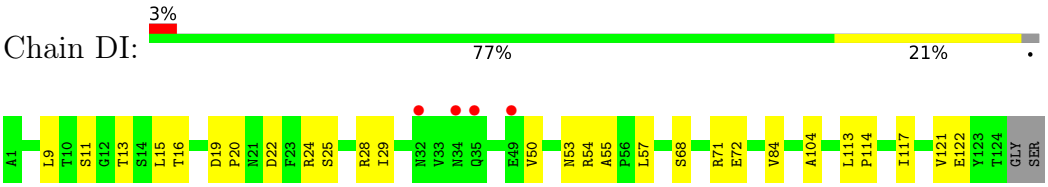
Chain DG:



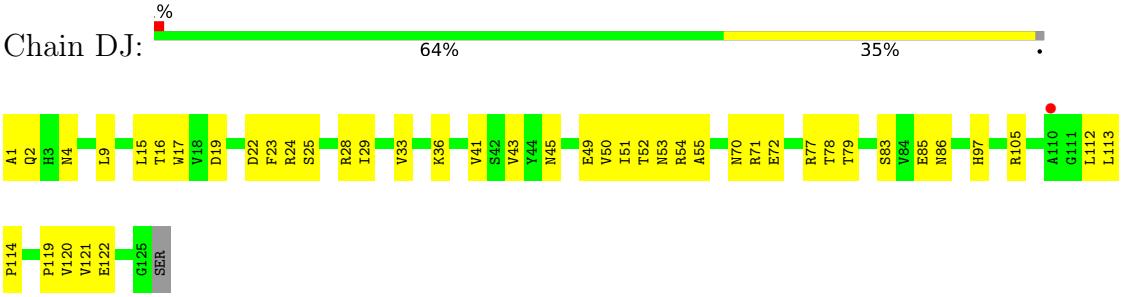
• Molecule 1: coat protein



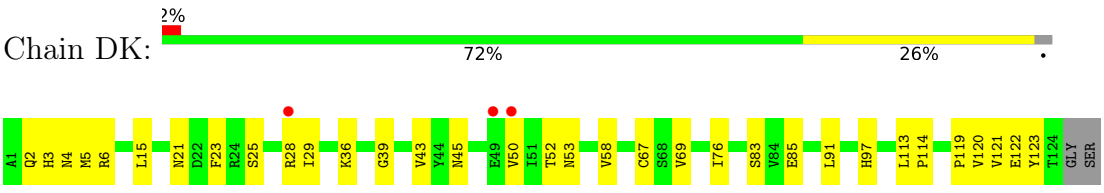
• Molecule 1: coat protein



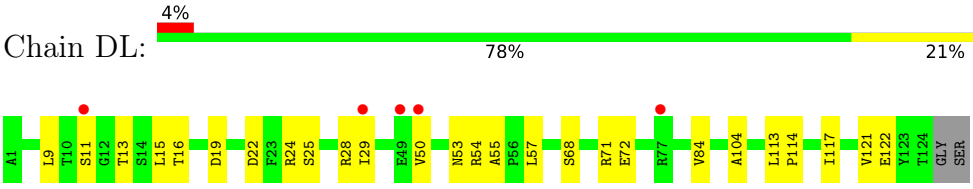
• Molecule 1: coat protein



• Molecule 1: coat protein



• Molecule 1: coat protein



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	453.15Å 309.76Å 294.60Å 90.00° 130.08° 90.00°	Depositor
Resolution (Å)	49.34 – 3.50 49.34 – 3.50	Depositor EDS
% Data completeness (in resolution range)	91.5 (49.34-3.50) 97.2 (49.34-3.50)	Depositor EDS
R_{merge}	0.47	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.96 (at 3.48Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.252 , 0.259 0.256 , 0.262	Depositor DCC
R_{free} test set	9928 reflections (2.60%)	wwPDB-VP
Wilson B-factor (Å^2)	142.1	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 96.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.36$, $< L^2 > = 0.20$	Xtriage
Estimated twinning fraction	0.098 for -h+k-l,-l,-k 0.094 for -h-k-l,l,k 0.110 for -h-2*l,-k,l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	84900	wwPDB-VP
Average B, all atoms (Å^2)	120.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.58% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	AA	0.18	0/958	0.46	0/1308
1	AB	0.19	0/954	0.49	0/1303
1	AC	0.20	0/954	0.44	0/1303
1	AD	0.19	0/958	0.46	0/1308
1	AE	0.19	0/954	0.49	0/1303
1	AF	0.20	0/954	0.44	0/1303
1	AG	0.18	0/958	0.46	0/1308
1	AH	0.19	0/954	0.49	0/1303
1	AI	0.20	0/954	0.44	0/1303
1	AJ	0.18	0/958	0.46	0/1308
1	AK	0.19	0/954	0.49	0/1303
1	AL	0.20	0/954	0.44	0/1303
1	AM	0.19	0/958	0.46	0/1308
1	AN	0.19	0/954	0.49	0/1303
1	AO	0.20	0/954	0.44	0/1303
1	AP	0.19	0/958	0.46	0/1308
1	AQ	0.19	0/954	0.49	0/1303
1	AR	0.20	0/954	0.44	0/1303
1	AS	0.19	0/958	0.46	0/1308
1	AT	0.19	0/954	0.49	0/1303
1	AU	0.20	0/954	0.44	0/1303
1	AV	0.18	0/958	0.46	0/1308
1	AW	0.19	0/954	0.49	0/1303
1	AX	0.20	0/954	0.44	0/1303
1	AY	0.19	0/958	0.46	0/1308
1	AZ	0.19	0/954	0.49	0/1303
1	BA	0.20	0/954	0.44	0/1303
1	BB	0.19	0/958	0.46	0/1308
1	BC	0.19	0/954	0.49	0/1303
1	BD	0.20	0/954	0.44	0/1303
1	BE	0.19	0/958	0.46	0/1308
1	BF	0.19	0/954	0.49	0/1303
1	BG	0.20	0/954	0.44	0/1303
1	BH	0.19	0/958	0.46	0/1308

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	BI	0.19	0/954	0.49	0/1303
1	BJ	0.20	0/954	0.44	0/1303
1	BK	0.19	0/958	0.46	0/1308
1	BL	0.19	0/954	0.49	0/1303
1	BM	0.20	0/954	0.44	0/1303
1	BN	0.19	0/958	0.46	0/1308
1	BO	0.19	0/954	0.49	0/1303
1	BP	0.20	0/954	0.44	0/1303
1	BQ	0.19	0/958	0.46	0/1308
1	BR	0.19	0/954	0.49	0/1303
1	BS	0.20	0/954	0.44	0/1303
1	BT	0.19	0/958	0.46	0/1308
1	BU	0.19	0/954	0.49	0/1303
1	BV	0.20	0/954	0.44	0/1303
1	BW	0.19	0/958	0.46	0/1308
1	BX	0.19	0/954	0.49	0/1303
1	BY	0.20	0/954	0.44	0/1303
1	BZ	0.19	0/958	0.46	0/1308
1	CA	0.19	0/954	0.49	0/1303
1	CB	0.20	0/954	0.44	0/1303
1	CC	0.19	0/958	0.46	0/1308
1	CD	0.19	0/954	0.49	0/1303
1	CE	0.20	0/954	0.44	0/1303
1	CF	0.19	0/958	0.46	0/1308
1	CG	0.19	0/954	0.49	0/1303
1	CH	0.20	0/954	0.44	0/1303
1	CI	0.19	0/958	0.46	0/1308
1	CJ	0.19	0/954	0.49	0/1303
1	CK	0.20	0/954	0.44	0/1303
1	CL	0.18	0/958	0.46	0/1308
1	CM	0.19	0/954	0.49	0/1303
1	CN	0.20	0/954	0.44	0/1303
1	CO	0.19	0/958	0.46	0/1308
1	CP	0.19	0/954	0.49	0/1303
1	CQ	0.20	0/954	0.44	0/1303
1	CR	0.19	0/958	0.46	0/1308
1	CS	0.19	0/954	0.49	0/1303
1	CT	0.20	0/954	0.44	0/1303
1	CU	0.19	0/958	0.46	0/1308
1	CV	0.19	0/954	0.49	0/1303
1	CW	0.20	0/954	0.44	0/1303
1	CX	0.19	0/958	0.46	0/1308
1	CY	0.19	0/954	0.49	0/1303

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	CZ	0.20	0/954	0.44	0/1303
1	DA	0.19	0/958	0.46	0/1308
1	DB	0.19	0/954	0.49	0/1303
1	DC	0.20	0/954	0.44	0/1303
1	DD	0.19	0/958	0.46	0/1308
1	DE	0.19	0/954	0.49	0/1303
1	DF	0.20	0/954	0.44	0/1303
1	DG	0.19	0/958	0.46	0/1308
1	DH	0.19	0/954	0.49	0/1303
1	DI	0.20	0/954	0.44	0/1303
1	DJ	0.18	0/958	0.46	0/1308
1	DK	0.19	0/954	0.49	0/1303
1	DL	0.20	0/954	0.44	0/1303
All	All	0.19	0/85980	0.46	0/117420

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	946	0	956	37	0
1	AB	942	0	953	37	0
1	AC	942	0	953	38	0
1	AD	946	0	957	36	0
1	AE	942	0	953	33	0
1	AF	942	0	954	17	0
1	AG	946	0	956	39	0
1	AH	942	0	953	34	0
1	AI	942	0	953	24	0
1	AJ	946	0	956	35	0
1	AK	942	0	953	34	0
1	AL	942	0	953	35	0

Continued on next page...

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AM	946	0	956	38	0
1	AN	942	0	953	32	0
1	AO	942	0	953	48	0
1	AP	946	0	956	36	0
1	AQ	942	0	953	35	0
1	AR	942	0	953	37	1
1	AS	946	0	956	37	0
1	AT	942	0	953	34	0
1	AU	942	0	953	35	0
1	AV	946	0	956	40	0
1	AW	942	0	953	40	0
1	AX	942	0	953	61	0
1	AY	946	0	956	41	0
1	AZ	942	0	953	39	0
1	BA	942	0	953	28	0
1	BB	946	0	956	39	0
1	BC	942	0	953	35	0
1	BD	942	0	953	37	0
1	BE	946	0	956	39	0
1	BF	942	0	953	38	0
1	BG	942	0	953	35	0
1	BH	946	0	956	40	0
1	BI	942	0	953	38	0
1	BJ	942	0	953	42	0
1	BK	946	0	957	39	0
1	BL	942	0	953	37	0
1	BM	942	0	954	20	0
1	BN	946	0	956	39	0
1	BO	942	0	953	33	0
1	BP	942	0	953	25	0
1	BQ	946	0	956	38	0
1	BR	942	0	953	35	0
1	BS	942	0	953	36	0
1	BT	946	0	956	38	0
1	BU	942	0	953	37	0
1	BV	942	0	953	50	0
1	BW	946	0	956	39	0
1	BX	942	0	953	39	0
1	BY	942	0	953	38	0
1	BZ	946	0	956	39	0
1	CA	942	0	953	35	0
1	CB	942	0	953	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	CC	946	0	957	39	0
1	CD	942	0	953	34	0
1	CE	942	0	954	18	0
1	CF	946	0	956	39	0
1	CG	942	0	953	36	0
1	CH	942	0	953	61	0
1	CI	946	0	957	38	0
1	CJ	942	0	953	31	0
1	CK	942	0	954	17	0
1	CL	946	0	956	39	0
1	CM	942	0	953	31	0
1	CN	942	0	953	26	1
1	CO	946	0	956	36	0
1	CP	942	0	953	35	0
1	CQ	942	0	953	40	0
1	CR	946	0	956	38	0
1	CS	942	0	953	38	0
1	CT	942	0	953	36	0
1	CU	946	0	957	38	0
1	CV	942	0	953	34	0
1	CW	942	0	954	16	0
1	CX	946	0	957	38	0
1	CY	942	0	953	34	0
1	CZ	942	0	954	17	1
1	DA	946	0	957	34	0
1	DB	942	0	953	39	0
1	DC	942	0	954	17	1
1	DD	946	0	957	38	0
1	DE	942	0	953	34	0
1	DF	942	0	954	16	0
1	DG	946	0	957	36	0
1	DH	942	0	953	32	0
1	DI	942	0	954	18	0
1	DJ	946	0	957	39	0
1	DK	942	0	953	31	0
1	DL	942	0	954	17	0
All	All	84900	0	85880	2239	2

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 13.

All (2239) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AZ:23:PHE:HE2	1:BK:33:VAL:HG11	1.09	1.09
1:AX:112:LEU:HD13	1:CF:6:ARG:HD3	1.25	1.08
1:BX:23:PHE:HE2	1:CC:33:VAL:HG11	1.07	1.08
1:AX:2:GLN:OE1	1:CH:124:THR:OG1	1.76	1.01
1:BF:23:PHE:HE2	1:BH:33:VAL:HG11	1.22	1.01
1:AA:6:ARG:HD3	1:BJ:112:LEU:HD13	1.43	0.98
1:AO:112:LEU:HD13	1:BT:6:ARG:HD3	1.46	0.97
1:BX:23:PHE:CE2	1:CC:33:VAL:HG11	1.99	0.97
1:CD:23:PHE:HE2	1:CX:33:VAL:HG11	1.30	0.97
1:CL:33:VAL:HG11	1:CY:23:PHE:HE2	1.30	0.96
1:BD:112:LEU:HD13	1:CO:6:ARG:HD3	1.48	0.96
1:AZ:23:PHE:CE2	1:BK:33:VAL:HG11	2.01	0.96
1:AM:33:VAL:HG11	1:CP:23:PHE:HE2	1.33	0.94
1:AT:23:PHE:HE2	1:BB:33:VAL:HG11	1.32	0.92
1:BG:109:VAL:HG12	1:CT:87:LYS:HB2	1.50	0.92
1:BU:23:PHE:HE2	1:BZ:33:VAL:HG11	1.35	0.91
1:BL:23:PHE:HE2	1:DD:33:VAL:HG11	1.35	0.89
1:AR:112:LEU:HD13	1:BW:6:ARG:HD3	1.52	0.89
1:AR:109:VAL:HG12	1:BY:87:LYS:HB2	1.54	0.88
1:AS:6:ARG:HD3	1:CB:112:LEU:HD13	1.54	0.87
1:CA:23:PHE:HE2	1:CU:33:VAL:HG11	1.39	0.87
1:AB:23:PHE:HE2	1:AV:33:VAL:HG11	1.37	0.87
1:BI:23:PHE:HE2	1:DJ:33:VAL:HG11	1.40	0.86
1:BE:6:ARG:HD3	1:CT:112:LEU:HD13	1.55	0.86
1:AY:6:ARG:HD3	1:CN:112:LEU:HD13	1.58	0.86
1:BF:23:PHE:CE2	1:BH:33:VAL:HG11	2.13	0.82
1:AP:6:ARG:HD3	1:BY:112:LEU:HD13	1.60	0.81
1:BR:23:PHE:HE2	1:CF:33:VAL:HG11	1.45	0.81
1:AR:57:LEU:HD11	1:AR:71:ARG:HH21	1.46	0.81
1:BO:23:PHE:HE2	1:DG:33:VAL:HG11	1.45	0.81
1:CQ:57:LEU:HD11	1:CQ:71:ARG:HH21	1.46	0.81
1:CT:57:LEU:HD11	1:CT:71:ARG:HH21	1.46	0.81
1:AR:87:LYS:HB2	1:BY:109:VAL:HG12	1.62	0.81
1:BG:57:LEU:HD11	1:BG:71:ARG:HH21	1.46	0.81
1:AC:57:LEU:HD11	1:AC:71:ARG:HH21	1.46	0.81
1:AU:57:LEU:HD11	1:AU:71:ARG:HH21	1.46	0.81
1:BG:87:LYS:HB2	1:CT:109:VAL:HG12	1.62	0.81
1:BD:57:LEU:HD11	1:BD:71:ARG:HH21	1.46	0.81
1:DC:57:LEU:HD11	1:DC:71:ARG:HH21	1.46	0.81
1:AO:2:GLN:OE1	1:BV:124:THR:OG1	1.98	0.81
1:CE:57:LEU:HD11	1:CE:71:ARG:HH21	1.46	0.81
1:AI:57:LEU:HD11	1:AI:71:ARG:HH21	1.46	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CZ:57:LEU:HD11	1:CZ:71:ARG:HH21	1.46	0.81
1:AF:57:LEU:HD11	1:AF:71:ARG:HH21	1.46	0.80
1:BA:57:LEU:HD11	1:BA:71:ARG:HH21	1.46	0.80
1:BY:57:LEU:HD11	1:BY:71:ARG:HH21	1.46	0.80
1:DL:57:LEU:HD11	1:DL:71:ARG:HH21	1.46	0.80
1:CI:33:VAL:HG11	1:CV:23:PHE:HE2	1.43	0.80
1:AL:57:LEU:HD11	1:AL:71:ARG:HH21	1.46	0.80
1:BJ:57:LEU:HD11	1:BJ:71:ARG:HH21	1.46	0.80
1:CB:57:LEU:HD11	1:CB:71:ARG:HH21	1.46	0.80
1:DI:57:LEU:HD11	1:DI:71:ARG:HH21	1.46	0.80
1:BV:57:LEU:HD11	1:BV:71:ARG:HH21	1.46	0.80
1:CH:57:LEU:HD11	1:CH:71:ARG:HH21	1.46	0.80
1:BM:57:LEU:HD11	1:BM:71:ARG:HH21	1.46	0.80
1:CK:57:LEU:HD11	1:CK:71:ARG:HH21	1.46	0.79
1:BS:57:LEU:HD11	1:BS:71:ARG:HH21	1.46	0.79
1:DF:57:LEU:HD11	1:DF:71:ARG:HH21	1.46	0.79
1:AC:112:LEU:HD13	1:BH:6:ARG:HD3	1.64	0.79
1:AX:57:LEU:HD11	1:AX:71:ARG:HH21	1.46	0.79
1:CW:57:LEU:HD11	1:CW:71:ARG:HH21	1.46	0.79
1:BP:57:LEU:HD11	1:BP:71:ARG:HH21	1.46	0.79
1:AO:57:LEU:HD11	1:AO:71:ARG:HH21	1.46	0.79
1:CN:57:LEU:HD11	1:CN:71:ARG:HH21	1.46	0.79
1:AJ:6:ARG:HD3	1:BS:112:LEU:HD13	1.63	0.78
1:BA:109:VAL:HG12	1:CN:87:LYS:HB2	1.65	0.78
1:BD:2:GLN:OE1	1:CQ:124:THR:OG1	2.02	0.78
1:BA:87:LYS:HB2	1:CN:109:VAL:HG12	1.66	0.78
1:AG:6:ARG:HD3	1:BP:112:LEU:HD13	1.65	0.78
1:AV:6:ARG:HD3	1:CH:112:LEU:HD13	1.66	0.77
1:AX:87:LYS:HB2	1:CH:109:VAL:HG12	1.66	0.77
1:CD:23:PHE:CE2	1:CX:33:VAL:HG11	2.19	0.76
1:BH:121:VAL:HG12	1:BH:122:GLU:HG3	1.68	0.76
1:AG:33:VAL:HG11	1:DB:23:PHE:HE2	1.50	0.76
1:BT:121:VAL:HG12	1:BT:122:GLU:HG3	1.68	0.76
1:CC:121:VAL:HG12	1:CC:122:GLU:HG3	1.68	0.76
1:AG:121:VAL:HG12	1:AG:122:GLU:HG3	1.68	0.76
1:AJ:121:VAL:HG12	1:AJ:122:GLU:HG3	1.68	0.76
1:AP:121:VAL:HG12	1:AP:122:GLU:HG3	1.68	0.75
1:CO:121:VAL:HG12	1:CO:122:GLU:HG3	1.68	0.75
1:BZ:121:VAL:HG12	1:BZ:122:GLU:HG3	1.68	0.75
1:AA:121:VAL:HG12	1:AA:122:GLU:HG3	1.68	0.75
1:BE:121:VAL:HG12	1:BE:122:GLU:HG3	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BK:121:VAL:HG12	1:BK:122:GLU:HG3	1.68	0.75
1:CF:121:VAL:HG12	1:CF:122:GLU:HG3	1.68	0.75
1:DA:121:VAL:HG12	1:DA:122:GLU:HG3	1.68	0.75
1:AM:121:VAL:HG12	1:AM:122:GLU:HG3	1.68	0.75
1:BB:121:VAL:HG12	1:BB:122:GLU:HG3	1.68	0.75
1:AL:121:VAL:HG12	1:AL:122:GLU:HG3	1.69	0.74
1:AS:121:VAL:HG12	1:AS:122:GLU:HG3	1.68	0.74
1:BN:121:VAL:HG12	1:BN:122:GLU:HG3	1.68	0.74
1:AU:121:VAL:HG12	1:AU:122:GLU:HG3	1.70	0.74
1:AO:121:VAL:HG12	1:AO:122:GLU:HG3	1.69	0.74
1:AV:121:VAL:HG12	1:AV:122:GLU:HG3	1.68	0.74
1:DJ:121:VAL:HG12	1:DJ:122:GLU:HG3	1.68	0.74
1:AR:121:VAL:HG12	1:AR:122:GLU:HG3	1.69	0.74
1:AY:121:VAL:HG12	1:AY:122:GLU:HG3	1.68	0.74
1:BA:112:LEU:HD13	1:CL:6:ARG:HD3	1.68	0.74
1:CR:121:VAL:HG12	1:CR:122:GLU:HG3	1.68	0.74
1:DF:121:VAL:HG12	1:DF:122:GLU:HG3	1.69	0.74
1:CN:121:VAL:HG12	1:CN:122:GLU:HG3	1.70	0.74
1:CW:121:VAL:HG12	1:CW:122:GLU:HG3	1.70	0.74
1:AD:121:VAL:HG12	1:AD:122:GLU:HG3	1.68	0.74
1:AF:121:VAL:HG12	1:AF:122:GLU:HG3	1.69	0.74
1:BQ:121:VAL:HG12	1:BQ:122:GLU:HG3	1.68	0.74
1:CU:121:VAL:HG12	1:CU:122:GLU:HG3	1.68	0.74
1:DG:121:VAL:HG12	1:DG:122:GLU:HG3	1.68	0.74
1:AX:121:VAL:HG12	1:AX:122:GLU:HG3	1.69	0.74
1:CQ:121:VAL:HG12	1:CQ:122:GLU:HG3	1.69	0.74
1:DI:121:VAL:HG12	1:DI:122:GLU:HG3	1.69	0.74
1:BM:121:VAL:HG12	1:BM:122:GLU:HG3	1.69	0.74
1:BV:121:VAL:HG12	1:BV:122:GLU:HG3	1.69	0.74
1:CT:121:VAL:HG12	1:CT:122:GLU:HG3	1.69	0.74
1:CX:121:VAL:HG12	1:CX:122:GLU:HG3	1.68	0.74
1:AI:121:VAL:HG12	1:AI:122:GLU:HG3	1.69	0.74
1:CE:121:VAL:HG12	1:CE:122:GLU:HG3	1.69	0.74
1:DD:121:VAL:HG12	1:DD:122:GLU:HG3	1.68	0.74
1:AM:6:ARG:HD3	1:BV:112:LEU:HD13	1.69	0.73
1:BD:121:VAL:HG12	1:BD:122:GLU:HG3	1.69	0.73
1:BS:121:VAL:HG12	1:BS:122:GLU:HG3	1.69	0.73
1:CH:121:VAL:HG12	1:CH:122:GLU:HG3	1.69	0.73
1:AA:33:VAL:HG11	1:DE:23:PHE:HE2	1.52	0.73
1:BJ:121:VAL:HG12	1:BJ:122:GLU:HG3	1.69	0.73
1:BP:121:VAL:HG12	1:BP:122:GLU:HG3	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BW:121:VAL:HG12	1:BW:122:GLU:HG3	1.68	0.73
1:CL:121:VAL:HG12	1:CL:122:GLU:HG3	1.68	0.73
1:CI:121:VAL:HG12	1:CI:122:GLU:HG3	1.68	0.73
1:DC:121:VAL:HG12	1:DC:122:GLU:HG3	1.70	0.73
1:DL:121:VAL:HG12	1:DL:122:GLU:HG3	1.69	0.73
1:BA:121:VAL:HG12	1:BA:122:GLU:HG3	1.70	0.73
1:BG:121:VAL:HG12	1:BG:122:GLU:HG3	1.70	0.73
1:AU:112:LEU:HD13	1:BZ:6:ARG:HD3	1.71	0.72
1:AZ:24:ARG:NH1	1:BK:85:GLU:OE2	2.22	0.72
1:CK:121:VAL:HG12	1:CK:122:GLU:HG3	1.69	0.72
1:AC:121:VAL:HG12	1:AC:122:GLU:HG3	1.69	0.72
1:AN:23:PHE:HE2	1:BQ:33:VAL:HG11	1.54	0.72
1:AX:91:LEU:HD22	1:CH:105:ARG:NH2	2.04	0.72
1:BC:23:PHE:HE2	1:BN:33:VAL:HG11	1.54	0.72
1:BY:121:VAL:HG12	1:BY:122:GLU:HG3	1.69	0.71
1:CZ:121:VAL:HG12	1:CZ:122:GLU:HG3	1.69	0.71
1:AP:33:VAL:HG11	1:CJ:23:PHE:HE2	1.56	0.71
1:CB:121:VAL:HG12	1:CB:122:GLU:HG3	1.70	0.71
1:AC:124:THR:OG1	1:BJ:2:GLN:OE1	2.07	0.71
1:AL:112:LEU:HD13	1:BQ:6:ARG:HD3	1.72	0.71
1:AC:109:VAL:HG12	1:BJ:87:LYS:HB2	1.71	0.70
1:AW:23:PHE:HE2	1:AY:33:VAL:HG11	1.55	0.70
1:AB:67:CYS:HA	1:AW:63:CYS:HB2	1.74	0.70
1:BX:24:ARG:NH1	1:CC:85:GLU:OE2	2.25	0.70
1:AK:23:PHE:HE2	1:BW:33:VAL:HG11	1.56	0.69
1:AP:36:LYS:HD2	1:AP:45:ASN:HB2	1.75	0.69
1:CF:36:LYS:HD2	1:CF:45:ASN:HB2	1.75	0.69
1:CU:36:LYS:HD2	1:CU:45:ASN:HB2	1.75	0.69
1:CI:36:LYS:HD2	1:CI:45:ASN:HB2	1.75	0.69
1:AD:36:LYS:HD2	1:AD:45:ASN:HB2	1.75	0.69
1:DG:36:LYS:HD2	1:DG:45:ASN:HB2	1.75	0.69
1:AJ:33:VAL:HG11	1:CM:23:PHE:HE2	1.58	0.69
1:AM:36:LYS:HD2	1:AM:45:ASN:HB2	1.75	0.69
1:AV:36:LYS:HD2	1:AV:45:ASN:HB2	1.75	0.69
1:AX:72:GLU:OE2	1:CH:83:SER:N	2.25	0.69
1:BK:36:LYS:HD2	1:BK:45:ASN:HB2	1.75	0.69
1:BN:36:LYS:HD2	1:BN:45:ASN:HB2	1.75	0.69
1:CL:36:LYS:HD2	1:CL:45:ASN:HB2	1.75	0.69
1:AJ:36:LYS:HD2	1:AJ:45:ASN:HB2	1.75	0.69
1:BT:36:LYS:HD2	1:BT:45:ASN:HB2	1.75	0.69
1:CR:36:LYS:HD2	1:CR:45:ASN:HB2	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CX:36:LYS:HD2	1:CX:45:ASN:HB2	1.75	0.69
1:DA:36:LYS:HD2	1:DA:45:ASN:HB2	1.75	0.69
1:AG:36:LYS:HD2	1:AG:45:ASN:HB2	1.75	0.69
1:BW:36:LYS:HD2	1:BW:45:ASN:HB2	1.75	0.69
1:AS:36:LYS:HD2	1:AS:45:ASN:HB2	1.75	0.69
1:CO:36:LYS:HD2	1:CO:45:ASN:HB2	1.75	0.69
1:AX:109:VAL:HG12	1:CH:87:LYS:HB2	1.74	0.68
1:AY:4:ASN:HB3	1:AZ:120:VAL:HG12	1.76	0.68
1:BK:4:ASN:HB3	1:BL:120:VAL:HG12	1.76	0.68
1:DD:4:ASN:HB3	1:DE:120:VAL:HG12	1.76	0.68
1:BW:4:ASN:HB3	1:BX:120:VAL:HG12	1.75	0.68
1:DJ:4:ASN:HB3	1:DK:120:VAL:HG12	1.76	0.68
1:BH:9:LEU:HB2	1:BH:16:THR:HB	1.76	0.68
1:BQ:9:LEU:HB2	1:BQ:16:THR:HB	1.76	0.68
1:CC:4:ASN:HB3	1:CD:120:VAL:HG12	1.76	0.68
1:CF:9:LEU:HB2	1:CF:16:THR:HB	1.76	0.68
1:CO:4:ASN:HB3	1:CP:120:VAL:HG12	1.76	0.68
1:AY:9:LEU:HB2	1:AY:16:THR:HB	1.75	0.68
1:BT:4:ASN:HB3	1:BU:120:VAL:HG12	1.76	0.68
1:BZ:4:ASN:HB3	1:CA:120:VAL:HG12	1.76	0.68
1:BZ:9:LEU:HB2	1:BZ:16:THR:HB	1.76	0.68
1:DC:20:PRO:HB3	1:DJ:112:LEU:HD21	1.74	0.68
1:AA:9:LEU:HB2	1:AA:16:THR:HB	1.76	0.68
1:AS:4:ASN:HB3	1:AT:120:VAL:HG12	1.76	0.68
1:BZ:36:LYS:HD2	1:BZ:45:ASN:HB2	1.75	0.68
1:CL:4:ASN:HB3	1:CM:120:VAL:HG12	1.76	0.68
1:CU:9:LEU:HB2	1:CU:16:THR:HB	1.76	0.68
1:AL:87:LYS:HB2	1:BS:109:VAL:HG12	1.74	0.68
1:AT:23:PHE:CE2	1:BB:33:VAL:HG11	2.23	0.68
1:BB:9:LEU:HB2	1:BB:16:THR:HB	1.76	0.68
1:BK:9:LEU:HB2	1:BK:16:THR:HB	1.76	0.68
1:CL:9:LEU:HB2	1:CL:16:THR:HB	1.76	0.68
1:AD:4:ASN:HB3	1:AE:120:VAL:HG12	1.76	0.68
1:BB:36:LYS:HD2	1:BB:45:ASN:HB2	1.75	0.68
1:CX:4:ASN:HB3	1:CY:120:VAL:HG12	1.76	0.68
1:DJ:36:LYS:HD2	1:DJ:45:ASN:HB2	1.75	0.68
1:BE:9:LEU:HB2	1:BE:16:THR:HB	1.76	0.68
1:CC:36:LYS:HD2	1:CC:45:ASN:HB2	1.75	0.68
1:AA:36:LYS:HD2	1:AA:45:ASN:HB2	1.75	0.67
1:BB:4:ASN:HB3	1:BC:120:VAL:HG12	1.76	0.67
1:BW:9:LEU:HB2	1:BW:16:THR:HB	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DD:36:LYS:HD2	1:DD:45:ASN:HB2	1.75	0.67
1:DG:9:LEU:HB2	1:DG:16:THR:HB	1.76	0.67
1:AD:9:LEU:HB2	1:AD:16:THR:HB	1.76	0.67
1:AJ:9:LEU:HB2	1:AJ:16:THR:HB	1.76	0.67
1:AM:9:LEU:HB2	1:AM:16:THR:HB	1.76	0.67
1:CX:9:LEU:HB2	1:CX:16:THR:HB	1.76	0.67
1:AI:109:VAL:HG12	1:BP:87:LYS:HB2	1.75	0.67
1:AJ:4:ASN:HB3	1:AK:120:VAL:HG12	1.76	0.67
1:AP:9:LEU:HB2	1:AP:16:THR:HB	1.76	0.67
1:CI:4:ASN:HB3	1:CJ:120:VAL:HG12	1.76	0.67
1:CR:4:ASN:HB3	1:CS:120:VAL:HG12	1.76	0.67
1:DA:9:LEU:HB2	1:DA:16:THR:HB	1.76	0.67
1:AI:9:LEU:HB2	1:AI:16:THR:HB	1.77	0.67
1:AY:36:LYS:HD2	1:AY:45:ASN:HB2	1.75	0.67
1:AZ:9:LEU:HD22	1:BK:12:GLY:HA3	1.76	0.67
1:BJ:9:LEU:HB2	1:BJ:16:THR:HB	1.77	0.67
1:BN:9:LEU:HB2	1:BN:16:THR:HB	1.76	0.67
1:CC:9:LEU:HB2	1:CC:16:THR:HB	1.76	0.67
1:DC:9:LEU:HB2	1:DC:16:THR:HB	1.77	0.67
1:AL:9:LEU:HB2	1:AL:16:THR:HB	1.77	0.67
1:BQ:36:LYS:HD2	1:BQ:45:ASN:HB2	1.75	0.67
1:CR:9:LEU:HB2	1:CR:16:THR:HB	1.76	0.67
1:DF:9:LEU:HB2	1:DF:16:THR:HB	1.77	0.67
1:AG:4:ASN:HB3	1:AH:120:VAL:HG12	1.76	0.67
1:AG:9:LEU:HB2	1:AG:16:THR:HB	1.76	0.67
1:AM:4:ASN:HB3	1:AN:120:VAL:HG12	1.76	0.67
1:AX:5:MET:CG	1:CH:121:VAL:HG23	2.25	0.67
1:BA:9:LEU:HB2	1:BA:16:THR:HB	1.77	0.67
1:BN:4:ASN:HB3	1:BO:120:VAL:HG12	1.76	0.67
1:BT:9:LEU:HB2	1:BT:16:THR:HB	1.76	0.67
1:CQ:9:LEU:HB2	1:CQ:16:THR:HB	1.77	0.67
1:DD:9:LEU:HB2	1:DD:16:THR:HB	1.76	0.67
1:AA:4:ASN:HB3	1:AB:120:VAL:HG12	1.76	0.67
1:CT:9:LEU:HB2	1:CT:16:THR:HB	1.77	0.67
1:DJ:9:LEU:HB2	1:DJ:16:THR:HB	1.76	0.67
1:DL:9:LEU:HB2	1:DL:16:THR:HB	1.77	0.67
1:AS:9:LEU:HB2	1:AS:16:THR:HB	1.76	0.67
1:AV:4:ASN:HB3	1:AW:120:VAL:HG12	1.76	0.67
1:AV:9:LEU:HB2	1:AV:16:THR:HB	1.76	0.67
1:BE:36:LYS:HD2	1:BE:45:ASN:HB2	1.75	0.67
1:CI:9:LEU:HB2	1:CI:16:THR:HB	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BE:4:ASN:HB3	1:BF:120:VAL:HG12	1.76	0.67
1:BH:36:LYS:HD2	1:BH:45:ASN:HB2	1.75	0.67
1:BM:9:LEU:HB2	1:BM:16:THR:HB	1.77	0.67
1:BY:9:LEU:HB2	1:BY:16:THR:HB	1.77	0.67
1:CO:9:LEU:HB2	1:CO:16:THR:HB	1.76	0.67
1:AP:4:ASN:HB3	1:AQ:120:VAL:HG12	1.76	0.66
1:AU:9:LEU:HB2	1:AU:16:THR:HB	1.77	0.66
1:AW:29:ILE:HG12	1:AW:50:VAL:HG22	1.78	0.66
1:BL:29:ILE:HG12	1:BL:50:VAL:HG22	1.78	0.66
1:DA:4:ASN:HB3	1:DB:120:VAL:HG12	1.75	0.66
1:AL:109:VAL:HG12	1:BS:87:LYS:HB2	1.77	0.66
1:AQ:29:ILE:HG12	1:AQ:50:VAL:HG22	1.78	0.66
1:BD:9:LEU:HB2	1:BD:16:THR:HB	1.77	0.66
1:CU:4:ASN:HB3	1:CV:120:VAL:HG12	1.76	0.66
1:CV:29:ILE:HG12	1:CV:50:VAL:HG22	1.78	0.66
1:AX:17:TRP:CD2	1:CH:119:PRO:HG3	2.31	0.66
1:BU:29:ILE:HG12	1:BU:50:VAL:HG22	1.78	0.66
1:DB:29:ILE:HG12	1:DB:50:VAL:HG22	1.78	0.66
1:AL:2:GLN:HA	1:BS:121:VAL:O	1.95	0.66
1:CG:29:ILE:HG12	1:CG:50:VAL:HG22	1.78	0.66
1:CM:29:ILE:HG12	1:CM:50:VAL:HG22	1.78	0.66
1:DG:4:ASN:HB3	1:DH:120:VAL:HG12	1.76	0.66
1:CJ:29:ILE:HG12	1:CJ:50:VAL:HG22	1.78	0.66
1:CZ:9:LEU:HB2	1:CZ:16:THR:HB	1.77	0.66
1:AT:29:ILE:HG12	1:AT:50:VAL:HG22	1.78	0.66
1:CK:9:LEU:HB2	1:CK:16:THR:HB	1.77	0.66
1:CN:9:LEU:HB2	1:CN:16:THR:HB	1.77	0.66
1:CY:29:ILE:HG12	1:CY:50:VAL:HG22	1.78	0.66
1:AX:5:MET:HG3	1:CH:121:VAL:HG23	1.78	0.66
1:BH:4:ASN:HB3	1:BI:120:VAL:HG12	1.76	0.66
1:BO:29:ILE:HG12	1:BO:50:VAL:HG22	1.78	0.66
1:BR:29:ILE:HG12	1:BR:50:VAL:HG22	1.78	0.66
1:BS:9:LEU:HB2	1:BS:16:THR:HB	1.77	0.66
1:BP:9:LEU:HB2	1:BP:16:THR:HB	1.77	0.66
1:BX:29:ILE:HG12	1:BX:50:VAL:HG22	1.78	0.66
1:AU:109:VAL:HG12	1:CB:87:LYS:HB2	1.78	0.66
1:BQ:4:ASN:HB3	1:BR:120:VAL:HG12	1.75	0.66
1:DE:29:ILE:HG12	1:DE:50:VAL:HG22	1.78	0.66
1:CE:9:LEU:HB2	1:CE:16:THR:HB	1.77	0.65
1:AB:29:ILE:HG12	1:AB:50:VAL:HG22	1.78	0.65
1:AK:29:ILE:HG12	1:AK:50:VAL:HG22	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AO:9:LEU:HB2	1:AO:16:THR:HB	1.77	0.65
1:AR:9:LEU:HB2	1:AR:16:THR:HB	1.77	0.65
1:BB:1:ALA:N	1:BC:122:GLU:OE1	2.23	0.65
1:BF:29:ILE:HG12	1:BF:50:VAL:HG22	1.78	0.65
1:CH:9:LEU:HB2	1:CH:16:THR:HB	1.77	0.65
1:CF:4:ASN:HB3	1:CG:120:VAL:HG12	1.76	0.65
1:DI:9:LEU:HB2	1:DI:16:THR:HB	1.77	0.65
1:AC:9:LEU:HB2	1:AC:16:THR:HB	1.77	0.65
1:AE:29:ILE:HG12	1:AE:50:VAL:HG22	1.78	0.65
1:AM:33:VAL:HG11	1:CP:23:PHE:CE2	2.25	0.65
1:BG:9:LEU:HB2	1:BG:16:THR:HB	1.77	0.65
1:CB:9:LEU:HB2	1:CB:16:THR:HB	1.77	0.65
1:CL:33:VAL:HG11	1:CY:23:PHE:CE2	2.21	0.65
1:CW:9:LEU:HB2	1:CW:16:THR:HB	1.77	0.65
1:DH:29:ILE:HG12	1:DH:50:VAL:HG22	1.78	0.65
1:AQ:23:PHE:HE2	1:BT:33:VAL:HG11	1.60	0.65
1:AX:9:LEU:HB2	1:AX:16:THR:HB	1.77	0.65
1:AZ:29:ILE:HG12	1:AZ:50:VAL:HG22	1.78	0.65
1:AF:9:LEU:HB2	1:AF:16:THR:HB	1.77	0.65
1:BV:9:LEU:HB2	1:BV:16:THR:HB	1.77	0.65
1:CD:29:ILE:HG12	1:CD:50:VAL:HG22	1.78	0.65
1:CP:29:ILE:HG12	1:CP:50:VAL:HG22	1.78	0.65
1:AE:23:PHE:HE2	1:AS:33:VAL:HG11	1.62	0.65
1:AH:29:ILE:HG12	1:AH:50:VAL:HG22	1.78	0.65
1:CA:29:ILE:HG12	1:CA:50:VAL:HG22	1.78	0.64
1:AZ:69:VAL:HB	1:BK:41:VAL:HG11	1.78	0.64
1:BI:29:ILE:HG12	1:BI:50:VAL:HG22	1.78	0.64
1:CS:29:ILE:HG12	1:CS:50:VAL:HG22	1.78	0.64
1:AN:29:ILE:HG12	1:AN:50:VAL:HG22	1.78	0.64
1:BB:4:ASN:HA	1:BC:120:VAL:HA	1.80	0.64
1:BG:124:THR:OG1	1:CT:2:GLN:OE1	2.11	0.64
1:BK:29:ILE:HG12	1:BK:50:VAL:HG22	1.80	0.64
1:DD:1:ALA:N	1:DE:122:GLU:OE1	2.23	0.64
1:AP:4:ASN:HA	1:AQ:120:VAL:HA	1.80	0.64
1:AX:31:LEU:HD12	1:CH:108:LEU:HD23	1.80	0.64
1:BW:29:ILE:HG12	1:BW:50:VAL:HG22	1.80	0.64
1:DG:4:ASN:HA	1:DH:120:VAL:HA	1.80	0.64
1:DJ:4:ASN:HA	1:DK:120:VAL:HA	1.80	0.64
1:DJ:29:ILE:HG12	1:DJ:50:VAL:HG22	1.80	0.64
1:AM:4:ASN:HA	1:AN:120:VAL:HA	1.80	0.64
1:AY:29:ILE:HG12	1:AY:50:VAL:HG22	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BC:29:ILE:HG12	1:BC:50:VAL:HG22	1.78	0.64
1:CO:29:ILE:HG12	1:CO:50:VAL:HG22	1.80	0.64
1:DD:29:ILE:HG12	1:DD:50:VAL:HG22	1.80	0.64
1:AS:29:ILE:HG12	1:AS:50:VAL:HG22	1.80	0.64
1:AX:50:VAL:HG12	1:CH:97:HIS:CE1	2.33	0.64
1:AY:4:ASN:HA	1:AZ:120:VAL:HA	1.80	0.64
1:BT:29:ILE:HG12	1:BT:50:VAL:HG22	1.80	0.64
1:BW:4:ASN:HA	1:BX:120:VAL:HA	1.80	0.64
1:CC:29:ILE:HG12	1:CC:50:VAL:HG22	1.80	0.64
1:CF:4:ASN:HA	1:CG:120:VAL:HA	1.80	0.64
1:CO:4:ASN:HA	1:CP:120:VAL:HA	1.80	0.64
1:AP:1:ALA:N	1:AQ:122:GLU:OE1	2.23	0.64
1:BB:6:ARG:HD3	1:CQ:112:LEU:HD13	1.80	0.64
1:BZ:29:ILE:HG12	1:BZ:50:VAL:HG22	1.80	0.64
1:BE:4:ASN:HA	1:BF:120:VAL:HA	1.80	0.64
1:CG:67:CYS:HA	1:CS:63:CYS:HB2	1.79	0.64
1:CL:29:ILE:HG12	1:CL:50:VAL:HG22	1.80	0.64
1:DK:29:ILE:HG12	1:DK:50:VAL:HG22	1.78	0.64
1:AA:4:ASN:HA	1:AB:120:VAL:HA	1.80	0.63
1:AD:4:ASN:HA	1:AE:120:VAL:HA	1.80	0.63
1:AG:4:ASN:HA	1:AH:120:VAL:HA	1.80	0.63
1:AX:71:ARG:O	1:CH:38:ALA:HB1	1.99	0.63
1:BT:4:ASN:HA	1:BU:120:VAL:HA	1.80	0.63
1:CU:1:ALA:N	1:CV:122:GLU:OE1	2.23	0.63
1:BZ:4:ASN:HA	1:CA:120:VAL:HA	1.80	0.63
1:CX:29:ILE:HG12	1:CX:50:VAL:HG22	1.80	0.63
1:DD:4:ASN:HA	1:DE:120:VAL:HA	1.80	0.63
1:AJ:1:ALA:N	1:AK:122:GLU:OE1	2.23	0.63
1:AJ:4:ASN:HA	1:AK:120:VAL:HA	1.80	0.63
1:CI:29:ILE:HG12	1:CI:50:VAL:HG22	1.80	0.63
1:AA:29:ILE:HG12	1:AA:50:VAL:HG22	1.80	0.63
1:AD:29:ILE:HG12	1:AD:50:VAL:HG22	1.80	0.63
1:AG:29:ILE:HG12	1:AG:50:VAL:HG22	1.80	0.63
1:AJ:29:ILE:HG12	1:AJ:50:VAL:HG22	1.80	0.63
1:BX:69:VAL:HB	1:CC:41:VAL:HG11	1.79	0.63
1:AB:9:LEU:HD22	1:AV:12:GLY:HA3	1.79	0.63
1:AM:29:ILE:HG12	1:AM:50:VAL:HG22	1.80	0.63
1:AV:4:ASN:HA	1:AW:120:VAL:HA	1.80	0.63
1:BB:29:ILE:HG12	1:BB:50:VAL:HG22	1.80	0.63
1:BZ:1:ALA:N	1:CA:122:GLU:OE1	2.23	0.63
1:DA:4:ASN:HA	1:DB:120:VAL:HA	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AH:23:PHE:HE2	1:BE:33:VAL:HG11	1.63	0.63
1:AV:29:ILE:HG12	1:AV:50:VAL:HG22	1.80	0.63
1:BE:29:ILE:HG12	1:BE:50:VAL:HG22	1.80	0.63
1:CR:29:ILE:HG12	1:CR:50:VAL:HG22	1.80	0.63
1:BG:112:LEU:HD13	1:CR:6:ARG:HD3	1.80	0.62
1:BR:69:VAL:HB	1:CF:41:VAL:HG11	1.80	0.62
1:BN:29:ILE:HG12	1:BN:50:VAL:HG22	1.80	0.62
1:CJ:113:LEU:HD12	1:CJ:114:PRO:HD2	1.82	0.62
1:AB:113:LEU:HD12	1:AB:114:PRO:HD2	1.82	0.62
1:AD:33:VAL:HG11	1:DH:23:PHE:HE2	1.64	0.62
1:AK:113:LEU:HD12	1:AK:114:PRO:HD2	1.82	0.62
1:AS:4:ASN:HA	1:AT:120:VAL:HA	1.80	0.62
1:AT:113:LEU:HD12	1:AT:114:PRO:HD2	1.82	0.62
1:BL:23:PHE:CE2	1:DD:33:VAL:HG11	2.25	0.62
1:BN:4:ASN:HA	1:BO:120:VAL:HA	1.80	0.62
1:BQ:4:ASN:HA	1:BR:120:VAL:HA	1.80	0.62
1:BR:113:LEU:HD12	1:BR:114:PRO:HD2	1.82	0.62
1:CC:4:ASN:HA	1:CD:120:VAL:HA	1.80	0.62
1:CI:4:ASN:HA	1:CJ:120:VAL:HA	1.80	0.62
1:CX:4:ASN:HA	1:CY:120:VAL:HA	1.80	0.62
1:BK:97:HIS:HB2	1:BL:52:THR:HG21	1.82	0.62
1:BO:113:LEU:HD12	1:BO:114:PRO:HD2	1.81	0.62
1:BT:97:HIS:HB2	1:BU:52:THR:HG21	1.82	0.62
1:BW:97:HIS:HB2	1:BX:52:THR:HG21	1.82	0.62
1:CL:4:ASN:HA	1:CM:120:VAL:HA	1.80	0.62
1:CY:113:LEU:HD12	1:CY:114:PRO:HD2	1.82	0.62
1:DA:1:ALA:N	1:DB:122:GLU:OE1	2.23	0.62
1:AA:97:HIS:HB2	1:AB:52:THR:HG21	1.82	0.62
1:AP:29:ILE:HG12	1:AP:50:VAL:HG22	1.80	0.62
1:BC:113:LEU:HD12	1:BC:114:PRO:HD2	1.82	0.62
1:BD:87:LYS:HB2	1:CQ:109:VAL:HG12	1.81	0.62
1:BF:113:LEU:HD12	1:BF:114:PRO:HD2	1.82	0.62
1:BG:91:LEU:HD22	1:CT:105:ARG:NH2	2.14	0.62
1:BK:4:ASN:HA	1:BL:120:VAL:HA	1.80	0.62
1:CG:9:LEU:HD22	1:CR:12:GLY:HA3	1.81	0.62
1:CG:113:LEU:HD12	1:CG:114:PRO:HD2	1.82	0.62
1:CR:1:ALA:N	1:CS:122:GLU:OE1	2.23	0.62
1:CR:4:ASN:HA	1:CS:120:VAL:HA	1.80	0.62
1:AM:97:HIS:HB2	1:AN:52:THR:HG21	1.82	0.62
1:AP:97:HIS:HB2	1:AQ:52:THR:HG21	1.82	0.62
1:AY:97:HIS:HB2	1:AZ:52:THR:HG21	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BH:4:ASN:HA	1:BI:120:VAL:HA	1.80	0.62
1:BH:29:ILE:HG12	1:BH:50:VAL:HG22	1.80	0.62
1:BU:9:LEU:HD22	1:BZ:12:GLY:HA3	1.81	0.62
1:DH:113:LEU:HD12	1:DH:114:PRO:HD2	1.82	0.62
1:AD:97:HIS:HB2	1:AE:52:THR:HG21	1.82	0.62
1:AN:113:LEU:HD12	1:AN:114:PRO:HD2	1.82	0.62
1:BL:113:LEU:HD12	1:BL:114:PRO:HD2	1.82	0.62
1:CU:29:ILE:HG12	1:CU:50:VAL:HG22	1.80	0.62
1:BB:97:HIS:HB2	1:BC:52:THR:HG21	1.82	0.62
1:BI:113:LEU:HD12	1:BI:114:PRO:HD2	1.82	0.62
1:BQ:97:HIS:HB2	1:BR:52:THR:HG21	1.82	0.62
1:BX:113:LEU:HD12	1:BX:114:PRO:HD2	1.82	0.62
1:CI:1:ALA:N	1:CJ:122:GLU:OE1	2.23	0.62
1:DA:29:ILE:HG12	1:DA:50:VAL:HG22	1.80	0.62
1:DJ:1:ALA:N	1:DK:122:GLU:OE1	2.23	0.62
1:AW:113:LEU:HD12	1:AW:114:PRO:HD2	1.82	0.62
1:BZ:97:HIS:HB2	1:CA:52:THR:HG21	1.82	0.62
1:CP:113:LEU:HD12	1:CP:114:PRO:HD2	1.82	0.62
1:CU:4:ASN:HA	1:CV:120:VAL:HA	1.80	0.62
1:DB:113:LEU:HD12	1:DB:114:PRO:HD2	1.82	0.62
1:AG:97:HIS:HB2	1:AH:52:THR:HG21	1.82	0.61
1:CC:97:HIS:HB2	1:CD:52:THR:HG21	1.82	0.61
1:CF:29:ILE:HG12	1:CF:50:VAL:HG22	1.80	0.61
1:DE:113:LEU:HD12	1:DE:114:PRO:HD2	1.82	0.61
1:DG:29:ILE:HG12	1:DG:50:VAL:HG22	1.80	0.61
1:DJ:97:HIS:HB2	1:DK:52:THR:HG21	1.82	0.61
1:AA:1:ALA:N	1:AB:122:GLU:OE1	2.23	0.61
1:AE:113:LEU:HD12	1:AE:114:PRO:HD2	1.82	0.61
1:AQ:113:LEU:HD12	1:AQ:114:PRO:HD2	1.82	0.61
1:CX:1:ALA:N	1:CY:122:GLU:OE1	2.23	0.61
1:BQ:29:ILE:HG12	1:BQ:50:VAL:HG22	1.80	0.61
1:CA:113:LEU:HD12	1:CA:114:PRO:HD2	1.82	0.61
1:AI:112:LEU:HD13	1:BN:6:ARG:HD3	1.82	0.61
1:CO:97:HIS:HB2	1:CP:52:THR:HG21	1.82	0.61
1:CR:97:HIS:HB2	1:CS:52:THR:HG21	1.82	0.61
1:BN:1:ALA:N	1:BO:122:GLU:OE1	2.23	0.61
1:BU:113:LEU:HD12	1:BU:114:PRO:HD2	1.82	0.61
1:CU:97:HIS:HB2	1:CV:52:THR:HG21	1.82	0.61
1:DD:97:HIS:HB2	1:DE:52:THR:HG21	1.82	0.61
1:CO:1:ALA:N	1:CP:122:GLU:OE1	2.23	0.61
1:AR:72:GLU:OE2	1:BY:83:SER:N	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AV:97:HIS:HB2	1:AW:52:THR:HG21	1.82	0.61
1:AZ:113:LEU:HD12	1:AZ:114:PRO:HD2	1.81	0.61
1:CV:113:LEU:HD12	1:CV:114:PRO:HD2	1.82	0.61
1:CX:97:HIS:HB2	1:CY:52:THR:HG21	1.82	0.61
1:BW:1:ALA:N	1:BX:122:GLU:OE1	2.23	0.61
1:AI:87:LYS:HB2	1:BP:109:VAL:HG12	1.82	0.61
1:AK:67:CYS:HA	1:BX:63:CYS:HB2	1.82	0.61
1:BI:69:VAL:HB	1:DJ:41:VAL:HG11	1.83	0.61
1:DG:1:ALA:N	1:DH:122:GLU:OE1	2.23	0.61
1:AH:113:LEU:HD12	1:AH:114:PRO:HD2	1.82	0.60
1:AJ:70:ASN:HD22	1:AK:39:GLY:HA3	1.66	0.60
1:AJ:97:HIS:HB2	1:AK:52:THR:HG21	1.82	0.60
1:AS:97:HIS:HB2	1:AT:52:THR:HG21	1.82	0.60
1:CC:70:ASN:HD22	1:CD:39:GLY:HA3	1.66	0.60
1:CF:70:ASN:HD22	1:CG:39:GLY:HA3	1.66	0.60
1:CI:97:HIS:HB2	1:CJ:52:THR:HG21	1.82	0.60
1:DA:97:HIS:HB2	1:DB:52:THR:HG21	1.82	0.60
1:AA:70:ASN:HD22	1:AB:39:GLY:HA3	1.66	0.60
1:BE:97:HIS:HB2	1:BF:52:THR:HG21	1.82	0.60
1:BH:70:ASN:HD22	1:BI:39:GLY:HA3	1.66	0.60
1:BK:70:ASN:HD22	1:BL:39:GLY:HA3	1.66	0.60
1:BX:36:LYS:HD2	1:BX:45:ASN:HD22	1.67	0.60
1:CF:1:ALA:N	1:CG:122:GLU:OE1	2.23	0.60
1:AX:124:THR:OG1	1:CH:2:GLN:OE1	2.10	0.60
1:CO:33:VAL:HG11	1:CS:23:PHE:HE2	1.65	0.60
1:BO:36:LYS:HD2	1:BO:45:ASN:HD22	1.67	0.60
1:BT:70:ASN:HD22	1:BU:39:GLY:HA3	1.66	0.60
1:CF:97:HIS:HB2	1:CG:52:THR:HG21	1.82	0.60
1:CM:113:LEU:HD12	1:CM:114:PRO:HD2	1.82	0.60
1:AM:70:ASN:HD22	1:AN:39:GLY:HA3	1.66	0.60
1:BH:97:HIS:HB2	1:BI:52:THR:HG21	1.82	0.60
1:BU:36:LYS:HD2	1:BU:45:ASN:HD22	1.67	0.60
1:CD:36:LYS:HD2	1:CD:45:ASN:HD22	1.67	0.60
1:CS:113:LEU:HD12	1:CS:114:PRO:HD2	1.82	0.60
1:CV:36:LYS:HD2	1:CV:45:ASN:HD22	1.67	0.60
1:DH:36:LYS:HD2	1:DH:45:ASN:HD22	1.67	0.60
1:DJ:70:ASN:HD22	1:DK:39:GLY:HA3	1.66	0.60
1:CU:70:ASN:HD22	1:CV:39:GLY:HA3	1.66	0.60
1:DK:36:LYS:HD2	1:DK:45:ASN:HD22	1.67	0.60
1:AV:70:ASN:HD22	1:AW:39:GLY:HA3	1.66	0.60
1:BE:70:ASN:HD22	1:BF:39:GLY:HA3	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BN:97:HIS:HB2	1:BO:52:THR:HG21	1.82	0.60
1:BR:36:LYS:HD2	1:BR:45:ASN:HD22	1.67	0.60
1:CM:36:LYS:HD2	1:CM:45:ASN:HD22	1.67	0.60
1:CR:70:ASN:HD22	1:CS:39:GLY:HA3	1.66	0.60
1:DG:70:ASN:HD22	1:DH:39:GLY:HA3	1.66	0.60
1:DK:113:LEU:HD12	1:DK:114:PRO:HD2	1.82	0.60
1:AB:36:LYS:HD2	1:AB:45:ASN:HD22	1.67	0.60
1:AK:36:LYS:HD2	1:AK:45:ASN:HD22	1.67	0.60
1:AL:83:SER:N	1:BS:72:GLU:OE2	2.32	0.60
1:AY:1:ALA:N	1:AZ:122:GLU:OE1	2.23	0.60
1:BC:36:LYS:HD2	1:BC:45:ASN:HD22	1.67	0.60
1:BX:9:LEU:HD22	1:CC:12:GLY:HA3	1.83	0.60
1:CO:70:ASN:HD22	1:CP:39:GLY:HA3	1.66	0.60
1:DA:70:ASN:HD22	1:DB:39:GLY:HA3	1.66	0.60
1:DB:36:LYS:HD2	1:DB:45:ASN:HD22	1.67	0.60
1:DE:36:LYS:HD2	1:DE:45:ASN:HD22	1.67	0.60
1:AP:70:ASN:HD22	1:AQ:39:GLY:HA3	1.66	0.60
1:CD:113:LEU:HD12	1:CD:114:PRO:HD2	1.82	0.60
1:CL:97:HIS:HB2	1:CM:52:THR:HG21	1.82	0.60
1:AQ:36:LYS:HD2	1:AQ:45:ASN:HD22	1.67	0.60
1:CA:36:LYS:HD2	1:CA:45:ASN:HD22	1.67	0.60
1:CL:70:ASN:HD22	1:CM:39:GLY:HA3	1.66	0.60
1:AZ:36:LYS:HD2	1:AZ:45:ASN:HD22	1.67	0.59
1:CJ:36:LYS:HD2	1:CJ:45:ASN:HD22	1.67	0.59
1:AB:45:ASN:HA	1:AB:83:SER:HA	1.85	0.59
1:AS:1:ALA:N	1:AT:122:GLU:OE1	2.23	0.59
1:BF:45:ASN:HA	1:BF:83:SER:HA	1.84	0.59
1:CC:1:ALA:N	1:CD:122:GLU:OE1	2.23	0.59
1:DE:45:ASN:HA	1:DE:83:SER:HA	1.85	0.59
1:DG:97:HIS:HB2	1:DH:52:THR:HG21	1.82	0.59
1:DH:45:ASN:HA	1:DH:83:SER:HA	1.85	0.59
1:AE:36:LYS:HD2	1:AE:45:ASN:HD22	1.67	0.59
1:AH:36:LYS:HD2	1:AH:45:ASN:HD22	1.67	0.59
1:AN:36:LYS:HD2	1:AN:45:ASN:HD22	1.67	0.59
1:BC:45:ASN:HA	1:BC:83:SER:HA	1.85	0.59
1:BI:23:PHE:CE2	1:DJ:33:VAL:HG11	2.31	0.59
1:BI:36:LYS:HD2	1:BI:45:ASN:HD22	1.67	0.59
1:BQ:70:ASN:HD22	1:BR:39:GLY:HA3	1.66	0.59
1:BZ:70:ASN:HD22	1:CA:39:GLY:HA3	1.66	0.59
1:CM:45:ASN:HA	1:CM:83:SER:HA	1.84	0.59
1:AS:70:ASN:HD22	1:AT:39:GLY:HA3	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AW:45:ASN:HA	1:AW:83:SER:HA	1.84	0.59
1:BL:36:LYS:HD2	1:BL:45:ASN:HD22	1.67	0.59
1:BN:70:ASN:HD22	1:BO:39:GLY:HA3	1.66	0.59
1:CJ:45:ASN:HA	1:CJ:83:SER:HA	1.84	0.59
1:CX:70:ASN:HD22	1:CY:39:GLY:HA3	1.66	0.59
1:DK:45:ASN:HA	1:DK:83:SER:HA	1.85	0.59
1:CI:70:ASN:HD22	1:CJ:39:GLY:HA3	1.66	0.59
1:CS:45:ASN:HA	1:CS:83:SER:HA	1.85	0.59
1:CY:45:ASN:HA	1:CY:83:SER:HA	1.85	0.59
1:AW:36:LYS:HD2	1:AW:45:ASN:HD22	1.67	0.59
1:AY:70:ASN:HD22	1:AZ:39:GLY:HA3	1.66	0.59
1:BF:36:LYS:HD2	1:BF:45:ASN:HD22	1.67	0.59
1:CP:45:ASN:HA	1:CP:83:SER:HA	1.85	0.59
1:AV:6:ARG:NH1	1:CH:107:ASP:OD1	2.29	0.59
1:AX:17:TRP:CE3	1:CH:119:PRO:HG3	2.38	0.59
1:BQ:1:ALA:N	1:BR:122:GLU:OE1	2.23	0.59
1:BR:45:ASN:HA	1:BR:83:SER:HA	1.85	0.59
1:DD:70:ASN:HD22	1:DE:39:GLY:HA3	1.66	0.59
1:AG:70:ASN:HD22	1:AH:39:GLY:HA3	1.66	0.59
1:AH:63:CYS:HB2	1:DB:67:CYS:HA	1.85	0.59
1:AM:1:ALA:N	1:AN:122:GLU:OE1	2.23	0.59
1:AD:1:ALA:N	1:AE:122:GLU:OE1	2.23	0.59
1:AH:45:ASN:HA	1:AH:83:SER:HA	1.85	0.59
1:BH:1:ALA:N	1:BI:122:GLU:OE1	2.23	0.59
1:CS:36:LYS:HD2	1:CS:45:ASN:HD22	1.67	0.59
1:AO:120:VAL:HA	1:BV:4:ASN:HA	1.85	0.59
1:BB:70:ASN:HD22	1:BC:39:GLY:HA3	1.67	0.59
1:BW:70:ASN:HD22	1:BX:39:GLY:HA3	1.66	0.59
1:CD:69:VAL:HB	1:CX:41:VAL:HG11	1.84	0.59
1:CP:36:LYS:HD2	1:CP:45:ASN:HD22	1.67	0.59
1:AD:70:ASN:HD22	1:AE:39:GLY:HA3	1.66	0.58
1:AT:45:ASN:HA	1:AT:83:SER:HA	1.85	0.58
1:BI:45:ASN:HA	1:BI:83:SER:HA	1.85	0.58
1:BO:45:ASN:HA	1:BO:83:SER:HA	1.84	0.58
1:CA:45:ASN:HA	1:CA:83:SER:HA	1.85	0.58
1:CG:36:LYS:HD2	1:CG:45:ASN:HD22	1.67	0.58
1:AT:36:LYS:HD2	1:AT:45:ASN:HD22	1.67	0.58
1:BU:45:ASN:HA	1:BU:83:SER:HA	1.84	0.58
1:CG:45:ASN:HA	1:CG:83:SER:HA	1.84	0.58
1:AX:105:ARG:NH2	1:CH:91:LEU:HD22	2.19	0.58
1:BX:45:ASN:HA	1:BX:83:SER:HA	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BL:45:ASN:HA	1:BL:83:SER:HA	1.85	0.58
1:CD:45:ASN:HA	1:CD:83:SER:HA	1.85	0.58
1:CY:36:LYS:HD2	1:CY:45:ASN:HD22	1.67	0.58
1:CV:45:ASN:HA	1:CV:83:SER:HA	1.84	0.58
1:DB:45:ASN:HA	1:DB:83:SER:HA	1.84	0.58
1:AE:45:ASN:HA	1:AE:83:SER:HA	1.85	0.58
1:AN:45:ASN:HA	1:AN:83:SER:HA	1.84	0.58
1:CA:69:VAL:HB	1:CU:41:VAL:HG11	1.86	0.58
1:CQ:10:THR:O	1:CS:12:GLY:N	2.29	0.58
1:AQ:45:ASN:HA	1:AQ:83:SER:HA	1.85	0.58
1:AK:45:ASN:HA	1:AK:83:SER:HA	1.85	0.58
1:AZ:45:ASN:HA	1:AZ:83:SER:HA	1.84	0.58
1:AM:120:VAL:HA	1:AN:4:ASN:HA	1.87	0.57
1:AG:120:VAL:HA	1:AH:4:ASN:HA	1.87	0.57
1:AO:124:THR:OG1	1:BV:2:GLN:OE1	2.17	0.57
1:AY:120:VAL:HA	1:AZ:4:ASN:HA	1.86	0.57
1:BT:1:ALA:N	1:BU:122:GLU:OE1	2.23	0.57
1:DD:120:VAL:HA	1:DE:4:ASN:HA	1.87	0.57
1:BE:120:VAL:HA	1:BF:4:ASN:HA	1.87	0.57
1:BQ:120:VAL:HA	1:BR:4:ASN:HA	1.87	0.57
1:AM:85:GLU:OE2	1:CP:24:ARG:NH1	2.38	0.57
1:AR:2:GLN:OE1	1:BY:124:THR:OG1	2.19	0.57
1:CI:120:VAL:HA	1:CJ:4:ASN:HA	1.87	0.57
1:AO:87:LYS:HB2	1:BV:109:VAL:HG12	1.86	0.57
1:AC:87:LYS:HB2	1:BJ:109:VAL:HG12	1.86	0.57
1:CU:120:VAL:HA	1:CV:4:ASN:HA	1.87	0.57
1:AJ:120:VAL:HA	1:AK:4:ASN:HA	1.87	0.57
1:BB:120:VAL:HA	1:BC:4:ASN:HA	1.87	0.57
1:AV:1:ALA:N	1:AW:122:GLU:OE1	2.23	0.57
1:CX:120:VAL:HA	1:CY:4:ASN:HA	1.86	0.57
1:AV:121:VAL:O	1:AW:2:GLN:HA	2.05	0.57
1:BB:121:VAL:O	1:BC:2:GLN:HA	2.05	0.57
1:BD:52:THR:HG21	1:CQ:97:HIS:HB2	1.85	0.57
1:BG:105:ARG:NH2	1:CT:91:LEU:HD22	2.20	0.57
1:CC:120:VAL:HA	1:CD:4:ASN:HA	1.87	0.57
1:CO:120:VAL:HA	1:CP:4:ASN:HA	1.86	0.57
1:AG:121:VAL:O	1:AH:2:GLN:HA	2.05	0.57
1:AR:91:LEU:HD22	1:BY:105:ARG:NH2	2.20	0.57
1:AV:120:VAL:HA	1:AW:4:ASN:HA	1.86	0.57
1:BK:120:VAL:HA	1:BL:4:ASN:HA	1.86	0.57
1:BT:120:VAL:HA	1:BU:4:ASN:HA	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CQ:20:PRO:HB3	1:CR:112:LEU:HD21	1.87	0.57
1:BE:121:VAL:O	1:BF:2:GLN:HA	2.05	0.56
1:BW:119:PRO:HG2	1:BX:5:MET:HB2	1.88	0.56
1:CL:121:VAL:O	1:CM:2:GLN:HA	2.05	0.56
1:CR:120:VAL:HA	1:CS:4:ASN:HA	1.86	0.56
1:AO:52:THR:HG21	1:BV:97:HIS:HB2	1.87	0.56
1:BH:120:VAL:HA	1:BI:4:ASN:HA	1.86	0.56
1:CL:120:VAL:HA	1:CM:4:ASN:HA	1.87	0.56
1:DA:120:VAL:HA	1:DB:4:ASN:HA	1.87	0.56
1:AD:120:VAL:HA	1:AE:4:ASN:HA	1.87	0.56
1:AX:52:THR:HG21	1:CH:97:HIS:HB2	1.88	0.56
1:AX:72:GLU:CD	1:CH:83:SER:HB2	2.31	0.56
1:AY:121:VAL:O	1:AZ:2:GLN:HA	2.05	0.56
1:BE:1:ALA:N	1:BF:122:GLU:OE1	2.23	0.56
1:BG:109:VAL:HG12	1:CT:87:LYS:CB	2.29	0.56
1:BT:121:VAL:O	1:BU:2:GLN:HA	2.05	0.56
1:CR:119:PRO:HG2	1:CS:5:MET:HB2	1.88	0.56
1:DA:119:PRO:HG2	1:DB:5:MET:HB2	1.88	0.56
1:DJ:120:VAL:HA	1:DK:4:ASN:HA	1.87	0.56
1:AA:120:VAL:HA	1:AB:4:ASN:HA	1.86	0.56
1:AD:121:VAL:O	1:AE:2:GLN:HA	2.05	0.56
1:CR:121:VAL:O	1:CS:2:GLN:HA	2.05	0.56
1:CU:119:PRO:HG2	1:CV:5:MET:HB2	1.88	0.56
1:DG:121:VAL:O	1:DH:2:GLN:HA	2.05	0.56
1:BH:119:PRO:HG2	1:BI:5:MET:HB2	1.88	0.56
1:BK:121:VAL:O	1:BL:2:GLN:HA	2.05	0.56
1:BN:121:VAL:O	1:BO:2:GLN:HA	2.05	0.56
1:BQ:121:VAL:O	1:BR:2:GLN:HA	2.05	0.56
1:BU:24:ARG:NH1	1:BZ:85:GLU:OE2	2.38	0.56
1:BW:120:VAL:HA	1:BX:4:ASN:HA	1.86	0.56
1:CX:119:PRO:HG2	1:CY:5:MET:HB2	1.88	0.56
1:DJ:121:VAL:O	1:DK:2:GLN:HA	2.05	0.56
1:AD:119:PRO:HG2	1:AE:5:MET:HB2	1.88	0.56
1:CC:119:PRO:HG2	1:CD:5:MET:HB2	1.88	0.56
1:CL:1:ALA:N	1:CM:122:GLU:OE1	2.23	0.56
1:AB:24:ARG:NH1	1:AV:85:GLU:OE2	2.39	0.56
1:AS:120:VAL:HA	1:AT:4:ASN:HA	1.87	0.56
1:AV:119:PRO:HG2	1:AW:5:MET:HB2	1.88	0.56
1:BB:113:LEU:HD12	1:BB:114:PRO:HD2	1.88	0.56
1:BD:119:PRO:HG2	1:CQ:5:MET:HB2	1.86	0.56
1:CC:121:VAL:O	1:CD:2:GLN:HA	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DD:121:VAL:O	1:DE:2:GLN:HA	2.05	0.56
1:AG:119:PRO:HG2	1:AH:5:MET:HB2	1.88	0.56
1:AP:113:LEU:HD12	1:AP:114:PRO:HD2	1.88	0.56
1:AP:120:VAL:HA	1:AQ:4:ASN:HA	1.87	0.56
1:AT:24:ARG:NH1	1:BB:85:GLU:OE2	2.39	0.56
1:AX:120:VAL:HA	1:CH:4:ASN:HA	1.87	0.56
1:BH:121:VAL:O	1:BI:2:GLN:HA	2.05	0.56
1:BN:120:VAL:HA	1:BO:4:ASN:HA	1.86	0.56
1:BW:113:LEU:HD12	1:BW:114:PRO:HD2	1.88	0.56
1:BZ:119:PRO:HG2	1:CA:5:MET:HB2	1.88	0.56
1:CF:113:LEU:HD12	1:CF:114:PRO:HD2	1.88	0.56
1:CF:120:VAL:HA	1:CG:4:ASN:HA	1.87	0.56
1:CI:121:VAL:O	1:CJ:2:GLN:HA	2.05	0.56
1:CU:121:VAL:O	1:CV:2:GLN:HA	2.05	0.56
1:CX:121:VAL:O	1:CY:2:GLN:HA	2.05	0.56
1:DA:121:VAL:O	1:DB:2:GLN:HA	2.05	0.56
1:AS:119:PRO:HG2	1:AT:5:MET:HB2	1.88	0.56
1:BZ:121:VAL:O	1:CA:2:GLN:HA	2.05	0.56
1:CC:113:LEU:HD12	1:CC:114:PRO:HD2	1.88	0.56
1:CO:119:PRO:HG2	1:CP:5:MET:HB2	1.88	0.56
1:CO:121:VAL:O	1:CP:2:GLN:HA	2.05	0.56
1:AM:121:VAL:O	1:AN:2:GLN:HA	2.05	0.56
1:AV:113:LEU:HD12	1:AV:114:PRO:HD2	1.88	0.56
1:AY:112:LEU:HD13	1:BM:6:ARG:HD3	1.88	0.56
1:BT:119:PRO:HG2	1:BU:5:MET:HB2	1.88	0.56
1:BZ:120:VAL:HA	1:CA:4:ASN:HA	1.87	0.56
1:DG:113:LEU:HD12	1:DG:114:PRO:HD2	1.88	0.56
1:DG:120:VAL:HA	1:DH:4:ASN:HA	1.86	0.56
1:AA:121:VAL:O	1:AB:2:GLN:HA	2.05	0.55
1:AM:113:LEU:HD12	1:AM:114:PRO:HD2	1.88	0.55
1:BD:120:VAL:HA	1:CQ:4:ASN:HA	1.88	0.55
1:BN:113:LEU:HD12	1:BN:114:PRO:HD2	1.88	0.55
1:CF:121:VAL:O	1:CG:2:GLN:HA	2.05	0.55
1:DJ:113:LEU:HD12	1:DJ:114:PRO:HD2	1.88	0.55
1:DJ:119:PRO:HG2	1:DK:5:MET:HB2	1.88	0.55
1:AA:119:PRO:HG2	1:AB:5:MET:HB2	1.88	0.55
1:AJ:121:VAL:O	1:AK:2:GLN:HA	2.05	0.55
1:AS:121:VAL:O	1:AT:2:GLN:HA	2.05	0.55
1:BZ:113:LEU:HD12	1:BZ:114:PRO:HD2	1.88	0.55
1:CL:119:PRO:HG2	1:CM:5:MET:HB2	1.88	0.55
1:AA:113:LEU:HD12	1:AA:114:PRO:HD2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AU:5:MET:HB2	1:CB:119:PRO:HG2	1.87	0.55
1:AY:113:LEU:HD12	1:AY:114:PRO:HD2	1.88	0.55
1:BK:119:PRO:HG2	1:BL:5:MET:HB2	1.88	0.55
1:BT:113:LEU:HD12	1:BT:114:PRO:HD2	1.88	0.55
1:BW:121:VAL:O	1:BX:2:GLN:HA	2.05	0.55
1:CF:119:PRO:HG2	1:CG:5:MET:HB2	1.88	0.55
1:AG:113:LEU:HD12	1:AG:114:PRO:HD2	1.88	0.55
1:AN:23:PHE:HD1	1:AN:23:PHE:H	1.55	0.55
1:BK:113:LEU:HD12	1:BK:114:PRO:HD2	1.88	0.55
1:BQ:113:LEU:HD12	1:BQ:114:PRO:HD2	1.88	0.55
1:CA:23:PHE:HD1	1:CA:23:PHE:H	1.55	0.55
1:CG:23:PHE:HD1	1:CG:23:PHE:H	1.55	0.55
1:DG:119:PRO:HG2	1:DH:5:MET:HB2	1.88	0.55
1:AD:113:LEU:HD12	1:AD:114:PRO:HD2	1.88	0.55
1:AQ:23:PHE:HD1	1:AQ:23:PHE:H	1.55	0.55
1:AS:113:LEU:HD12	1:AS:114:PRO:HD2	1.88	0.55
1:CL:113:LEU:HD12	1:CL:114:PRO:HD2	1.88	0.55
1:CR:113:LEU:HD12	1:CR:114:PRO:HD2	1.88	0.55
1:DD:113:LEU:HD12	1:DD:114:PRO:HD2	1.88	0.55
1:AU:52:THR:HG21	1:CB:97:HIS:HB2	1.88	0.55
1:CY:23:PHE:H	1:CY:23:PHE:HD1	1.55	0.55
1:AC:83:SER:N	1:BJ:72:GLU:OE2	2.39	0.55
1:AR:121:VAL:O	1:BY:2:GLN:HA	2.06	0.55
1:BB:119:PRO:HG2	1:BC:5:MET:HB2	1.88	0.55
1:BG:121:VAL:HG23	1:CT:5:MET:HG3	1.89	0.55
1:BH:113:LEU:HD12	1:BH:114:PRO:HD2	1.88	0.55
1:BL:23:PHE:H	1:BL:23:PHE:HD1	1.55	0.55
1:DE:23:PHE:HD1	1:DE:23:PHE:H	1.55	0.55
1:AJ:119:PRO:HG2	1:AK:5:MET:HB2	1.88	0.55
1:AO:72:GLU:OE2	1:BV:83:SER:N	2.40	0.55
1:AP:121:VAL:O	1:AQ:2:GLN:HA	2.05	0.55
1:BN:119:PRO:HG2	1:BO:5:MET:HB2	1.88	0.55
1:BX:23:PHE:HD1	1:BX:23:PHE:H	1.55	0.55
1:CU:113:LEU:HD12	1:CU:114:PRO:HD2	1.88	0.55
1:AJ:113:LEU:HD12	1:AJ:114:PRO:HD2	1.88	0.55
1:BD:109:VAL:HG12	1:CQ:87:LYS:HB2	1.89	0.55
1:BQ:119:PRO:HG2	1:BR:5:MET:HB2	1.88	0.55
1:CS:23:PHE:HD1	1:CS:23:PHE:H	1.55	0.55
1:AB:23:PHE:H	1:AB:23:PHE:HD1	1.55	0.54
1:BI:23:PHE:H	1:BI:23:PHE:HD1	1.55	0.54
1:AW:23:PHE:HD1	1:AW:23:PHE:H	1.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AY:119:PRO:HG2	1:AZ:5:MET:HB2	1.88	0.54
1:AZ:23:PHE:HD1	1:AZ:23:PHE:H	1.55	0.54
1:BU:23:PHE:HD1	1:BU:23:PHE:H	1.55	0.54
1:CD:23:PHE:HD1	1:CD:23:PHE:H	1.55	0.54
1:DA:113:LEU:HD12	1:DA:114:PRO:HD2	1.88	0.54
1:AA:43:VAL:HB	1:AA:85:GLU:HG3	1.90	0.54
1:CI:119:PRO:HG2	1:CJ:5:MET:HB2	1.88	0.54
1:DD:119:PRO:HG2	1:DE:5:MET:HB2	1.88	0.54
1:AM:119:PRO:HG2	1:AN:5:MET:HB2	1.88	0.54
1:BG:109:VAL:CG1	1:CT:87:LYS:HB2	2.30	0.54
1:DD:43:VAL:HB	1:DD:85:GLU:HG3	1.90	0.54
1:AG:1:ALA:N	1:AH:122:GLU:OE1	2.23	0.54
1:BC:23:PHE:HD1	1:BC:23:PHE:H	1.55	0.54
1:BD:72:GLU:OE2	1:CQ:83:SER:N	2.38	0.54
1:BE:113:LEU:HD12	1:BE:114:PRO:HD2	1.88	0.54
1:BF:8:GLN:HE21	1:BI:113:LEU:HB3	1.73	0.54
1:BW:43:VAL:HB	1:BW:85:GLU:HG3	1.90	0.54
1:CI:113:LEU:HD12	1:CI:114:PRO:HD2	1.88	0.54
1:DH:23:PHE:HD1	1:DH:23:PHE:H	1.55	0.54
1:AS:43:VAL:HB	1:AS:85:GLU:HG3	1.90	0.54
1:BE:119:PRO:HG2	1:BF:5:MET:HB2	1.88	0.54
1:BQ:120:VAL:HG23	1:BR:4:ASN:HA	1.90	0.54
1:BT:43:VAL:HB	1:BT:85:GLU:HG3	1.90	0.54
1:CN:24:ARG:HB3	1:CN:55:ALA:HB3	1.90	0.54
1:CR:43:VAL:HB	1:CR:85:GLU:HG3	1.90	0.54
1:AK:23:PHE:HD1	1:AK:23:PHE:H	1.55	0.54
1:AR:109:VAL:CG1	1:BY:87:LYS:HB2	2.34	0.54
1:AX:24:ARG:HB3	1:AX:55:ALA:HB3	1.90	0.54
1:CO:43:VAL:HB	1:CO:85:GLU:HG3	1.90	0.54
1:CO:113:LEU:HD12	1:CO:114:PRO:HD2	1.88	0.54
1:CU:43:VAL:HB	1:CU:85:GLU:HG3	1.90	0.54
1:DK:23:PHE:HD1	1:DK:23:PHE:H	1.55	0.54
1:AP:119:PRO:HG2	1:AQ:5:MET:HB2	1.88	0.54
1:BK:43:VAL:HB	1:BK:85:GLU:HG3	1.90	0.54
1:BL:69:VAL:HB	1:DD:41:VAL:HG11	1.90	0.54
1:BZ:43:VAL:HB	1:BZ:85:GLU:HG3	1.90	0.54
1:CI:43:VAL:HB	1:CI:85:GLU:HG3	1.90	0.54
1:CJ:23:PHE:HD1	1:CJ:23:PHE:H	1.55	0.54
1:CM:23:PHE:HD1	1:CM:23:PHE:H	1.55	0.54
1:CW:24:ARG:HB3	1:CW:55:ALA:HB3	1.90	0.54
1:AD:43:VAL:HB	1:AD:85:GLU:HG3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AM:120:VAL:HG23	1:AN:4:ASN:HA	1.90	0.54
1:CF:120:VAL:HG23	1:CG:4:ASN:HA	1.90	0.54
1:AP:43:VAL:HB	1:AP:85:GLU:HG3	1.90	0.54
1:BE:43:VAL:HB	1:BE:85:GLU:HG3	1.90	0.54
1:BH:43:VAL:HB	1:BH:85:GLU:HG3	1.90	0.54
1:BK:120:VAL:HG23	1:BL:4:ASN:HA	1.90	0.54
1:BW:120:VAL:HG23	1:BX:4:ASN:HA	1.90	0.54
1:CC:43:VAL:HB	1:CC:85:GLU:HG3	1.90	0.54
1:CX:120:VAL:HG23	1:CY:4:ASN:HA	1.90	0.54
1:DA:43:VAL:HB	1:DA:85:GLU:HG3	1.90	0.54
1:DA:120:VAL:HG23	1:DB:4:ASN:HA	1.90	0.54
1:DJ:43:VAL:HB	1:DJ:85:GLU:HG3	1.90	0.54
1:AA:120:VAL:HG23	1:AB:4:ASN:HA	1.90	0.53
1:AC:4:ASN:HA	1:BJ:120:VAL:HA	1.91	0.53
1:AC:52:THR:HG21	1:BJ:97:HIS:HB2	1.89	0.53
1:AF:24:ARG:HB3	1:AF:55:ALA:HB3	1.90	0.53
1:AL:24:ARG:HB3	1:AL:55:ALA:HB3	1.90	0.53
1:AO:91:LEU:HD22	1:BV:105:ARG:NH2	2.24	0.53
1:BR:23:PHE:H	1:BR:23:PHE:HD1	1.55	0.53
1:BS:24:ARG:HB3	1:BS:55:ALA:HB3	1.90	0.53
1:BU:23:PHE:CE2	1:BZ:33:VAL:HG11	2.27	0.53
1:BV:24:ARG:HB3	1:BV:55:ALA:HB3	1.90	0.53
1:CV:23:PHE:H	1:CV:23:PHE:HD1	1.55	0.53
1:CZ:24:ARG:HB3	1:CZ:55:ALA:HB3	1.90	0.53
1:AC:24:ARG:HB3	1:AC:55:ALA:HB3	1.90	0.53
1:AJ:120:VAL:HG23	1:AK:4:ASN:HA	1.90	0.53
1:AV:120:VAL:HG23	1:AW:4:ASN:HA	1.90	0.53
1:CB:24:ARG:HB3	1:CB:55:ALA:HB3	1.90	0.53
1:CL:43:VAL:HB	1:CL:85:GLU:HG3	1.90	0.53
1:CT:24:ARG:HB3	1:CT:55:ALA:HB3	1.90	0.53
1:DI:24:ARG:HB3	1:DI:55:ALA:HB3	1.90	0.53
1:AR:24:ARG:HB3	1:AR:55:ALA:HB3	1.90	0.53
1:AY:120:VAL:HG23	1:AZ:4:ASN:HA	1.90	0.53
1:BF:23:PHE:HD1	1:BF:23:PHE:H	1.55	0.53
1:BY:24:ARG:HB3	1:BY:55:ALA:HB3	1.90	0.53
1:AH:23:PHE:H	1:AH:23:PHE:HD1	1.55	0.53
1:CX:113:LEU:HD12	1:CX:114:PRO:HD2	1.88	0.53
1:DG:120:VAL:HG23	1:DH:4:ASN:HA	1.90	0.53
1:AO:119:PRO:HG2	1:BV:5:MET:HB2	1.89	0.53
1:BO:23:PHE:H	1:BO:23:PHE:HD1	1.55	0.53
1:CI:120:VAL:HG23	1:CJ:4:ASN:HA	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DJ:120:VAL:HG23	1:DK:4:ASN:HA	1.90	0.53
1:AI:24:ARG:HB3	1:AI:55:ALA:HB3	1.90	0.53
1:AO:24:ARG:HB3	1:AO:55:ALA:HB3	1.90	0.53
1:AS:120:VAL:HG23	1:AT:4:ASN:HA	1.90	0.53
1:BB:43:VAL:HB	1:BB:85:GLU:HG3	1.90	0.53
1:BO:23:PHE:CE2	1:DG:33:VAL:HG11	2.36	0.53
1:CI:41:VAL:HG11	1:CV:69:VAL:HB	1.91	0.53
1:CP:23:PHE:HD1	1:CP:23:PHE:H	1.55	0.53
1:CX:43:VAL:HB	1:CX:85:GLU:HG3	1.90	0.53
1:DB:23:PHE:H	1:DB:23:PHE:HD1	1.55	0.53
1:AD:120:VAL:HG23	1:AE:4:ASN:HA	1.90	0.53
1:BE:120:VAL:HG23	1:BF:4:ASN:HA	1.90	0.53
1:DD:120:VAL:HG23	1:DE:4:ASN:HA	1.90	0.53
1:AE:23:PHE:H	1:AE:23:PHE:HD1	1.55	0.53
1:AI:121:VAL:O	1:BP:2:GLN:HA	2.09	0.53
1:AV:43:VAL:HB	1:AV:85:GLU:HG3	1.90	0.53
1:BQ:43:VAL:HB	1:BQ:85:GLU:HG3	1.90	0.53
1:CA:24:ARG:NH1	1:CU:85:GLU:OE2	2.41	0.53
1:DF:24:ARG:HB3	1:DF:55:ALA:HB3	1.90	0.53
1:AM:43:VAL:HB	1:AM:85:GLU:HG3	1.90	0.53
1:AO:72:GLU:HG3	1:BV:36:LYS:HZ1	1.74	0.53
1:BO:69:VAL:HB	1:DG:41:VAL:HG11	1.90	0.53
1:CE:24:ARG:HB3	1:CE:55:ALA:HB3	1.90	0.53
1:CQ:24:ARG:HB3	1:CQ:55:ALA:HB3	1.90	0.53
1:CU:120:VAL:HG23	1:CV:4:ASN:HA	1.90	0.53
1:DG:43:VAL:HB	1:DG:85:GLU:HG3	1.90	0.53
1:DL:24:ARG:HB3	1:DL:55:ALA:HB3	1.90	0.53
1:AL:4:ASN:ND2	1:BS:118:GLN:NE2	2.57	0.53
1:AU:87:LYS:HB2	1:CB:109:VAL:HG12	1.91	0.53
1:AY:43:VAL:HB	1:AY:85:GLU:HG3	1.90	0.53
1:AY:52:THR:HG21	1:AZ:97:HIS:HB2	1.91	0.53
1:CG:67:CYS:CB	1:CS:63:CYS:SG	2.96	0.53
1:DJ:52:THR:HG21	1:DK:97:HIS:HB2	1.92	0.53
1:AG:120:VAL:HG23	1:AH:4:ASN:HA	1.90	0.52
1:AJ:43:VAL:HB	1:AJ:85:GLU:HG3	1.90	0.52
1:AP:52:THR:HG21	1:AQ:97:HIS:HB2	1.92	0.52
1:BB:120:VAL:HG23	1:BC:4:ASN:HA	1.90	0.52
1:AC:2:GLN:OE1	1:BJ:124:THR:OG1	2.19	0.52
1:AP:120:VAL:HG23	1:AQ:4:ASN:HA	1.90	0.52
1:BN:120:VAL:HG23	1:BO:4:ASN:HA	1.90	0.52
1:DC:24:ARG:HB3	1:DC:55:ALA:HB3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DG:52:THR:HG21	1:DH:97:HIS:HB2	1.91	0.52
1:BA:24:ARG:HB3	1:BA:55:ALA:HB3	1.90	0.52
1:BE:52:THR:HG21	1:BF:97:HIS:HB2	1.92	0.52
1:BK:1:ALA:N	1:BL:122:GLU:OE1	2.23	0.52
1:BZ:120:VAL:HG23	1:CA:4:ASN:HA	1.90	0.52
1:CK:24:ARG:HB3	1:CK:55:ALA:HB3	1.90	0.52
1:CL:120:VAL:HG23	1:CM:4:ASN:HA	1.90	0.52
1:CO:120:VAL:HG23	1:CP:4:ASN:HA	1.90	0.52
1:AO:76:ILE:HG12	1:BV:80:ILE:HG12	1.91	0.52
1:BB:52:THR:HG21	1:BC:97:HIS:HB2	1.92	0.52
1:BJ:24:ARG:HB3	1:BJ:55:ALA:HB3	1.90	0.52
1:BK:52:THR:HG21	1:BL:97:HIS:HB2	1.92	0.52
1:BN:43:VAL:HB	1:BN:85:GLU:HG3	1.90	0.52
1:AX:97:HIS:CE1	1:CH:50:VAL:HG12	2.45	0.52
1:BH:52:THR:HG21	1:BI:97:HIS:HB2	1.91	0.52
1:CO:52:THR:HG21	1:CP:97:HIS:HB2	1.92	0.52
1:AU:83:SER:N	1:CB:72:GLU:OE2	2.43	0.52
1:BA:105:ARG:NH2	1:CN:91:LEU:HD22	2.25	0.52
1:BG:24:ARG:HB3	1:BG:55:ALA:HB3	1.90	0.52
1:BM:24:ARG:HB3	1:BM:55:ALA:HB3	1.90	0.52
1:BN:52:THR:HG21	1:BO:97:HIS:HB2	1.92	0.52
1:BQ:52:THR:HG21	1:BR:97:HIS:HB2	1.91	0.52
1:CH:24:ARG:HB3	1:CH:55:ALA:HB3	1.90	0.52
1:AG:43:VAL:HB	1:AG:85:GLU:HG3	1.90	0.52
1:AT:23:PHE:HD1	1:AT:23:PHE:H	1.55	0.52
1:AU:24:ARG:HB3	1:AU:55:ALA:HB3	1.90	0.52
1:BH:120:VAL:HG23	1:BI:4:ASN:HA	1.90	0.52
1:BN:112:LEU:HD21	1:DI:20:PRO:HB3	1.91	0.52
1:AC:91:LEU:HD22	1:BJ:105:ARG:NH2	2.23	0.52
1:CF:43:VAL:HB	1:CF:85:GLU:HG3	1.90	0.52
1:AE:63:CYS:HB2	1:DH:67:CYS:HA	1.91	0.52
1:AS:52:THR:HG21	1:AT:97:HIS:HB2	1.92	0.52
1:BT:120:VAL:HG23	1:BU:4:ASN:HA	1.90	0.52
1:CC:120:VAL:HG23	1:CD:4:ASN:HA	1.90	0.52
1:CX:52:THR:HG21	1:CY:97:HIS:HB2	1.91	0.52
1:AX:76:ILE:HG12	1:CH:80:ILE:HG12	1.91	0.52
1:CG:23:PHE:HE2	1:CR:33:VAL:HG11	1.75	0.52
1:AI:5:MET:HB2	1:BP:119:PRO:HG2	1.91	0.51
1:AJ:52:THR:HG21	1:AK:97:HIS:HB2	1.92	0.51
1:AX:70:ASN:OD1	1:CH:41:VAL:HG23	2.10	0.51
1:BP:24:ARG:HB3	1:BP:55:ALA:HB3	1.90	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:23:PHE:CE2	1:CU:33:VAL:HG11	2.31	0.51
1:CR:52:THR:HG21	1:CS:97:HIS:HB2	1.92	0.51
1:CR:120:VAL:HG23	1:CS:4:ASN:HA	1.90	0.51
1:AA:52:THR:HG21	1:AB:97:HIS:HB2	1.92	0.51
1:AG:52:THR:HG21	1:AH:97:HIS:HB2	1.92	0.51
1:AR:15:LEU:O	1:AR:28:ARG:HA	2.11	0.51
1:AV:52:THR:HG21	1:AW:97:HIS:HB2	1.92	0.51
1:BA:25:SER:CB	1:BA:54:ARG:HG2	2.41	0.51
1:BV:25:SER:CB	1:BV:54:ARG:HG2	2.41	0.51
1:CB:25:SER:CB	1:CB:54:ARG:HG2	2.41	0.51
1:CQ:25:SER:CB	1:CQ:54:ARG:HG2	2.41	0.51
1:DL:25:SER:CB	1:DL:54:ARG:HG2	2.41	0.51
1:AS:15:LEU:O	1:AS:28:ARG:HA	2.11	0.51
1:AS:24:ARG:NH1	1:AS:71:ARG:HH11	2.09	0.51
1:AT:69:VAL:HB	1:BB:41:VAL:HG11	1.92	0.51
1:CK:25:SER:CB	1:CK:54:ARG:HG2	2.41	0.51
1:CT:15:LEU:O	1:CT:28:ARG:HA	2.11	0.51
1:AC:25:SER:CB	1:AC:54:ARG:HG2	2.41	0.51
1:AL:25:SER:CB	1:AL:54:ARG:HG2	2.41	0.51
1:AM:12:GLY:HA3	1:CP:9:LEU:HD22	1.92	0.51
1:AM:15:LEU:O	1:AM:28:ARG:HA	2.11	0.51
1:AU:15:LEU:O	1:AU:28:ARG:HA	2.11	0.51
1:BD:24:ARG:HB3	1:BD:55:ALA:HB3	1.90	0.51
1:BE:24:ARG:NH1	1:BE:71:ARG:HH11	2.09	0.51
1:BF:24:ARG:NH1	1:BH:85:GLU:OE2	2.42	0.51
1:BG:15:LEU:O	1:BG:28:ARG:HA	2.11	0.51
1:BH:24:ARG:NH1	1:BH:71:ARG:HH11	2.09	0.51
1:BQ:15:LEU:O	1:BQ:28:ARG:HA	2.11	0.51
1:BS:15:LEU:O	1:BS:28:ARG:HA	2.11	0.51
1:BT:15:LEU:O	1:BT:28:ARG:HA	2.11	0.51
1:CL:52:THR:HG21	1:CM:97:HIS:HB2	1.91	0.51
1:CW:15:LEU:O	1:CW:28:ARG:HA	2.11	0.51
1:AA:24:ARG:NH1	1:AA:71:ARG:HH11	2.09	0.51
1:BB:15:LEU:O	1:BB:28:ARG:HA	2.11	0.51
1:BB:24:ARG:NH1	1:BB:71:ARG:HH11	2.09	0.51
1:BR:23:PHE:CE2	1:CF:33:VAL:HG11	2.35	0.51
1:BY:15:LEU:O	1:BY:28:ARG:HA	2.11	0.51
1:CF:52:THR:HG21	1:CG:97:HIS:HB2	1.92	0.51
1:CI:85:GLU:OE2	1:CV:24:ARG:NH1	2.43	0.51
1:DA:15:LEU:O	1:DA:28:ARG:HA	2.11	0.51
1:AD:15:LEU:O	1:AD:28:ARG:HA	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AG:15:LEU:O	1:AG:28:ARG:HA	2.11	0.51
1:AU:121:VAL:O	1:CB:2:GLN:HA	2.11	0.51
1:AV:24:ARG:NH1	1:AV:71:ARG:HH11	2.09	0.51
1:AX:25:SER:CB	1:AX:54:ARG:HG2	2.41	0.51
1:BI:24:ARG:NH1	1:DJ:85:GLU:OE2	2.43	0.51
1:BN:15:LEU:O	1:BN:28:ARG:HA	2.11	0.51
1:BS:25:SER:CB	1:BS:54:ARG:HG2	2.41	0.51
1:BZ:52:THR:HG21	1:CA:97:HIS:HB2	1.92	0.51
1:CE:25:SER:CB	1:CE:54:ARG:HG2	2.41	0.51
1:CQ:15:LEU:O	1:CQ:28:ARG:HA	2.11	0.51
1:CU:15:LEU:O	1:CU:28:ARG:HA	2.11	0.51
1:CU:52:THR:HG21	1:CV:97:HIS:HB2	1.91	0.51
1:DD:52:THR:HG21	1:DE:97:HIS:HB2	1.91	0.51
1:DG:24:ARG:NH1	1:DG:71:ARG:HH11	2.09	0.51
1:DI:15:LEU:O	1:DI:28:ARG:HA	2.11	0.51
1:DJ:15:LEU:O	1:DJ:28:ARG:HA	2.11	0.51
1:AD:52:THR:HG21	1:AE:97:HIS:HB2	1.92	0.51
1:AI:15:LEU:O	1:AI:28:ARG:HA	2.11	0.51
1:AM:24:ARG:NH1	1:AM:71:ARG:HH11	2.09	0.51
1:AM:52:THR:HG21	1:AN:97:HIS:HB2	1.92	0.51
1:AO:25:SER:CB	1:AO:54:ARG:HG2	2.41	0.51
1:AZ:8:GLN:HE21	1:BL:113:LEU:HB3	1.76	0.51
1:BG:25:SER:CB	1:BG:54:ARG:HG2	2.41	0.51
1:CB:15:LEU:O	1:CB:28:ARG:HA	2.11	0.51
1:CL:24:ARG:NH1	1:CL:71:ARG:HH11	2.09	0.51
1:CO:15:LEU:O	1:CO:28:ARG:HA	2.11	0.51
1:CR:24:ARG:NH1	1:CR:71:ARG:HH11	2.09	0.51
1:CW:25:SER:CB	1:CW:54:ARG:HG2	2.41	0.51
1:DA:24:ARG:NH1	1:DA:71:ARG:HH11	2.09	0.51
1:DA:52:THR:HG21	1:DB:97:HIS:HB2	1.92	0.51
1:DC:25:SER:CB	1:DC:54:ARG:HG2	2.41	0.51
1:AD:24:ARG:NH1	1:AD:71:ARG:HH11	2.09	0.51
1:AI:25:SER:CB	1:AI:54:ARG:HG2	2.41	0.51
1:AP:15:LEU:O	1:AP:28:ARG:HA	2.11	0.51
1:AR:52:THR:HG21	1:BY:97:HIS:HB2	1.91	0.51
1:AU:4:ASN:HA	1:CB:120:VAL:HA	1.93	0.51
1:AX:15:LEU:O	1:AX:28:ARG:HA	2.11	0.51
1:AY:24:ARG:NH1	1:AY:71:ARG:HH11	2.09	0.51
1:BF:9:LEU:HD22	1:BH:12:GLY:HA3	1.93	0.51
1:BQ:24:ARG:NH1	1:BQ:71:ARG:HH11	2.09	0.51
1:CI:52:THR:HG21	1:CJ:97:HIS:HB2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CK:15:LEU:O	1:CK:28:ARG:HA	2.11	0.51
1:CL:15:LEU:O	1:CL:28:ARG:HA	2.11	0.51
1:CR:15:LEU:O	1:CR:28:ARG:HA	2.11	0.51
1:CX:24:ARG:NH1	1:CX:71:ARG:HH11	2.09	0.51
1:DL:15:LEU:O	1:DL:28:ARG:HA	2.11	0.51
1:AJ:24:ARG:NH1	1:AJ:71:ARG:HH11	2.09	0.51
1:AQ:69:VAL:HB	1:BT:41:VAL:HG11	1.93	0.51
1:BT:52:THR:HG21	1:BU:97:HIS:HB2	1.91	0.51
1:CC:24:ARG:NH1	1:CC:71:ARG:HH11	2.09	0.51
1:CE:15:LEU:O	1:CE:28:ARG:HA	2.11	0.51
1:CH:25:SER:CB	1:CH:54:ARG:HG2	2.41	0.51
1:CN:15:LEU:O	1:CN:28:ARG:HA	2.11	0.51
1:CN:25:SER:CB	1:CN:54:ARG:HG2	2.41	0.51
1:DI:25:SER:CB	1:DI:54:ARG:HG2	2.41	0.51
1:AA:15:LEU:O	1:AA:28:ARG:HA	2.11	0.50
1:AG:24:ARG:NH1	1:AG:71:ARG:HH11	2.09	0.50
1:AG:51:ILE:HG12	1:AG:77:ARG:HG2	1.93	0.50
1:AR:25:SER:CB	1:AR:54:ARG:HG2	2.41	0.50
1:AX:5:MET:HG2	1:CH:121:VAL:HG23	1.93	0.50
1:BA:15:LEU:O	1:BA:28:ARG:HA	2.11	0.50
1:BK:24:ARG:NH1	1:BK:71:ARG:HH11	2.09	0.50
1:BP:25:SER:CB	1:BP:54:ARG:HG2	2.41	0.50
1:CO:24:ARG:NH1	1:CO:71:ARG:HH11	2.09	0.50
1:DJ:24:ARG:NH1	1:DJ:71:ARG:HH11	2.09	0.50
1:AF:25:SER:CB	1:AF:54:ARG:HG2	2.41	0.50
1:AM:51:ILE:HG12	1:AM:77:ARG:HG2	1.94	0.50
1:AU:11:SER:C	1:AU:13:THR:H	2.20	0.50
1:BE:112:LEU:HD11	1:BJ:20:PRO:HB3	1.93	0.50
1:BM:25:SER:CB	1:BM:54:ARG:HG2	2.41	0.50
1:BN:24:ARG:NH1	1:BN:71:ARG:HH11	2.09	0.50
1:BN:51:ILE:HG12	1:BN:77:ARG:HG2	1.94	0.50
1:BV:15:LEU:O	1:BV:28:ARG:HA	2.11	0.50
1:BW:52:THR:HG21	1:BX:97:HIS:HB2	1.92	0.50
1:DF:11:SER:C	1:DF:13:THR:H	2.20	0.50
1:DF:15:LEU:O	1:DF:28:ARG:HA	2.11	0.50
1:AD:51:ILE:HG12	1:AD:77:ARG:HG2	1.93	0.50
1:BM:15:LEU:O	1:BM:28:ARG:HA	2.11	0.50
1:BZ:15:LEU:O	1:BZ:28:ARG:HA	2.11	0.50
1:CC:15:LEU:O	1:CC:28:ARG:HA	2.11	0.50
1:CI:15:LEU:O	1:CI:28:ARG:HA	2.11	0.50
1:CX:15:LEU:O	1:CX:28:ARG:HA	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DB:116:THR:HG21	1:DK:6:ARG:HD2	1.93	0.50
1:DC:15:LEU:O	1:DC:28:ARG:HA	2.11	0.50
1:AA:51:ILE:HG12	1:AA:77:ARG:HG2	1.94	0.50
1:AC:11:SER:C	1:AC:13:THR:H	2.20	0.50
1:AL:15:LEU:O	1:AL:28:ARG:HA	2.11	0.50
1:AP:24:ARG:NH1	1:AP:71:ARG:HH11	2.09	0.50
1:AX:50:VAL:O	1:CH:97:HIS:HE1	1.93	0.50
1:BB:51:ILE:HG12	1:BB:77:ARG:HG2	1.93	0.50
1:BE:51:ILE:HG12	1:BE:77:ARG:HG2	1.94	0.50
1:BK:15:LEU:O	1:BK:28:ARG:HA	2.11	0.50
1:CF:15:LEU:O	1:CF:28:ARG:HA	2.11	0.50
1:CF:24:ARG:NH1	1:CF:71:ARG:HH11	2.09	0.50
1:CF:51:ILE:HG12	1:CF:77:ARG:HG2	1.93	0.50
1:CK:11:SER:C	1:CK:13:THR:H	2.20	0.50
1:CN:11:SER:C	1:CN:13:THR:H	2.20	0.50
1:CU:51:ILE:HG12	1:CU:77:ARG:HG2	1.94	0.50
1:DD:24:ARG:NH1	1:DD:71:ARG:HH11	2.09	0.50
1:DG:51:ILE:HG12	1:DG:77:ARG:HG2	1.94	0.50
1:AB:23:PHE:CE2	1:AV:33:VAL:HG11	2.30	0.50
1:AC:15:LEU:O	1:AC:28:ARG:HA	2.11	0.50
1:AJ:15:LEU:O	1:AJ:28:ARG:HA	2.11	0.50
1:AO:15:LEU:O	1:AO:28:ARG:HA	2.11	0.50
1:AU:25:SER:CB	1:AU:54:ARG:HG2	2.41	0.50
1:AX:87:LYS:HB2	1:CH:109:VAL:CG1	2.40	0.50
1:AX:121:VAL:O	1:CH:2:GLN:HA	2.11	0.50
1:BD:25:SER:CB	1:BD:54:ARG:HG2	2.41	0.50
1:BE:15:LEU:O	1:BE:28:ARG:HA	2.11	0.50
1:BF:36:LYS:HD2	1:BF:45:ASN:ND2	2.27	0.50
1:BH:15:LEU:O	1:BH:28:ARG:HA	2.11	0.50
1:BY:25:SER:CB	1:BY:54:ARG:HG2	2.41	0.50
1:CH:15:LEU:O	1:CH:28:ARG:HA	2.11	0.50
1:CY:36:LYS:HD2	1:CY:45:ASN:ND2	2.27	0.50
1:AV:15:LEU:O	1:AV:28:ARG:HA	2.11	0.50
1:BJ:11:SER:C	1:BJ:13:THR:H	2.20	0.50
1:BP:11:SER:C	1:BP:13:THR:H	2.20	0.50
1:BP:15:LEU:O	1:BP:28:ARG:HA	2.11	0.50
1:BW:51:ILE:HG12	1:BW:77:ARG:HG2	1.94	0.50
1:CC:52:THR:HG21	1:CD:97:HIS:HB2	1.92	0.50
1:CT:11:SER:C	1:CT:13:THR:H	2.20	0.50
1:DD:15:LEU:O	1:DD:28:ARG:HA	2.11	0.50
1:DF:25:SER:CB	1:DF:54:ARG:HG2	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BD:11:SER:C	1:BD:13:THR:H	2.20	0.50
1:BW:15:LEU:O	1:BW:28:ARG:HA	2.11	0.50
1:CE:11:SER:C	1:CE:13:THR:H	2.20	0.50
1:CG:36:LYS:HD2	1:CG:45:ASN:ND2	2.27	0.50
1:CT:25:SER:CB	1:CT:54:ARG:HG2	2.41	0.50
1:CX:51:ILE:HG12	1:CX:77:ARG:HG2	1.94	0.50
1:DG:15:LEU:O	1:DG:28:ARG:HA	2.11	0.50
1:AF:11:SER:C	1:AF:13:THR:H	2.20	0.50
1:AO:105:ARG:NH2	1:BV:91:LEU:HD22	2.26	0.50
1:AO:109:VAL:HG12	1:BV:87:LYS:HB2	1.93	0.50
1:AP:51:ILE:HG12	1:AP:77:ARG:HG2	1.93	0.50
1:BI:36:LYS:HD2	1:BI:45:ASN:ND2	2.27	0.50
1:BM:11:SER:C	1:BM:13:THR:H	2.20	0.50
1:BO:36:LYS:HD2	1:BO:45:ASN:ND2	2.27	0.50
1:BY:11:SER:C	1:BY:13:THR:H	2.20	0.50
1:BZ:24:ARG:NH1	1:BZ:71:ARG:HH11	2.09	0.50
1:CZ:15:LEU:O	1:CZ:28:ARG:HA	2.11	0.50
1:DI:11:SER:C	1:DI:13:THR:H	2.20	0.50
1:AO:97:HIS:HB2	1:BV:52:THR:HG21	1.93	0.50
1:AX:11:SER:C	1:AX:13:THR:H	2.20	0.50
1:AY:15:LEU:O	1:AY:28:ARG:HA	2.11	0.50
1:BJ:25:SER:CB	1:BJ:54:ARG:HG2	2.41	0.50
1:BW:24:ARG:NH1	1:BW:71:ARG:HH11	2.09	0.50
1:CZ:11:SER:C	1:CZ:13:THR:H	2.20	0.50
1:CZ:25:SER:CB	1:CZ:54:ARG:HG2	2.41	0.50
1:AI:11:SER:C	1:AI:13:THR:H	2.20	0.49
1:AO:113:LEU:HD12	1:AO:114:PRO:HD2	1.94	0.49
1:AR:11:SER:C	1:AR:13:THR:H	2.20	0.49
1:AX:76:ILE:HG23	1:CH:80:ILE:HG12	1.94	0.49
1:AY:107:ASP:OD1	1:BM:6:ARG:NH1	2.44	0.49
1:BD:15:LEU:O	1:BD:28:ARG:HA	2.11	0.49
1:BG:11:SER:C	1:BG:13:THR:H	2.20	0.49
1:BQ:51:ILE:HG12	1:BQ:77:ARG:HG2	1.93	0.49
1:CI:24:ARG:NH1	1:CI:71:ARG:HH11	2.09	0.49
1:AF:15:LEU:O	1:AF:28:ARG:HA	2.11	0.49
1:AG:12:GLY:HA3	1:DB:9:LEU:HD22	1.94	0.49
1:AX:113:LEU:HD12	1:AX:114:PRO:HD2	1.94	0.49
1:BC:36:LYS:HD2	1:BC:45:ASN:ND2	2.27	0.49
1:BJ:15:LEU:O	1:BJ:28:ARG:HA	2.11	0.49
1:CI:51:ILE:HG12	1:CI:77:ARG:HG2	1.93	0.49
1:CK:113:LEU:HD12	1:CK:114:PRO:HD2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CM:36:LYS:HD2	1:CM:45:ASN:ND2	2.27	0.49
1:AA:41:VAL:HG11	1:DE:69:VAL:HB	1.95	0.49
1:AC:113:LEU:HD12	1:AC:114:PRO:HD2	1.94	0.49
1:AI:2:GLN:HA	1:BP:121:VAL:O	2.11	0.49
1:AW:36:LYS:HD2	1:AW:45:ASN:ND2	2.27	0.49
1:AW:67:CYS:HA	1:AZ:63:CYS:HB2	1.94	0.49
1:BH:51:ILE:HG12	1:BH:77:ARG:HG2	1.93	0.49
1:CO:51:ILE:HG12	1:CO:77:ARG:HG2	1.94	0.49
1:CU:24:ARG:NH1	1:CU:71:ARG:HH11	2.09	0.49
1:DC:113:LEU:HD12	1:DC:114:PRO:HD2	1.94	0.49
1:DE:36:LYS:HD2	1:DE:45:ASN:ND2	2.27	0.49
1:AH:36:LYS:HD2	1:AH:45:ASN:ND2	2.27	0.49
1:AI:83:SER:N	1:BP:72:GLU:OE2	2.45	0.49
1:AL:113:LEU:HD12	1:AL:114:PRO:HD2	1.94	0.49
1:AN:36:LYS:HD2	1:AN:45:ASN:ND2	2.27	0.49
1:AS:51:ILE:HG12	1:AS:77:ARG:HG2	1.94	0.49
1:AW:69:VAL:HB	1:AY:41:VAL:HG11	1.94	0.49
1:AX:72:GLU:OE2	1:CH:83:SER:HB2	2.12	0.49
1:BG:113:LEU:HD12	1:BG:114:PRO:HD2	1.94	0.49
1:BQ:17:TRP:CD2	1:BR:119:PRO:HG2	2.48	0.49
1:BZ:51:ILE:HG12	1:BZ:77:ARG:HG2	1.94	0.49
1:CF:17:TRP:CD2	1:CG:119:PRO:HG2	2.48	0.49
1:CM:25:SER:HA	1:CM:53:ASN:O	2.13	0.49
1:CQ:11:SER:C	1:CQ:13:THR:H	2.20	0.49
1:CW:113:LEU:HD12	1:CW:114:PRO:HD2	1.95	0.49
1:AE:36:LYS:HD2	1:AE:45:ASN:ND2	2.27	0.49
1:AO:72:GLU:CG	1:BV:36:LYS:HZ1	2.26	0.49
1:AQ:36:LYS:HD2	1:AQ:45:ASN:ND2	2.27	0.49
1:AR:50:VAL:HG12	1:BY:97:HIS:CE1	2.48	0.49
1:AS:17:TRP:CD2	1:AT:119:PRO:HG2	2.48	0.49
1:BA:113:LEU:HD12	1:BA:114:PRO:HD2	1.94	0.49
1:BL:25:SER:HA	1:BL:53:ASN:O	2.13	0.49
1:BR:36:LYS:HD2	1:BR:45:ASN:ND2	2.27	0.49
1:BZ:17:TRP:CD2	1:CA:119:PRO:HG2	2.48	0.49
1:CA:25:SER:HA	1:CA:53:ASN:O	2.13	0.49
1:CH:113:LEU:HD12	1:CH:114:PRO:HD2	1.94	0.49
1:CL:51:ILE:HG12	1:CL:77:ARG:HG2	1.94	0.49
1:CP:25:SER:HA	1:CP:53:ASN:O	2.13	0.49
1:CR:51:ILE:HG12	1:CR:77:ARG:HG2	1.94	0.49
1:CZ:113:LEU:HD12	1:CZ:114:PRO:HD2	1.95	0.49
1:AD:17:TRP:CD2	1:AE:119:PRO:HG2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AM:41:VAL:HG11	1:CP:69:VAL:HB	1.94	0.49
1:AP:24:ARG:HH11	1:AP:71:ARG:HH11	1.61	0.49
1:AX:77:ARG:O	1:CH:78:THR:HA	2.13	0.49
1:BH:17:TRP:CD2	1:BI:119:PRO:HG2	2.48	0.49
1:BP:113:LEU:HD12	1:BP:114:PRO:HD2	1.94	0.49
1:CF:112:LEU:HD13	1:CT:6:ARG:HD3	1.95	0.49
1:CJ:25:SER:HA	1:CJ:53:ASN:O	2.13	0.49
1:CO:24:ARG:HH11	1:CO:71:ARG:HH11	1.61	0.49
1:DA:17:TRP:CD2	1:DB:119:PRO:HG2	2.48	0.49
1:DJ:17:TRP:CD2	1:DK:119:PRO:HG2	2.48	0.49
1:AJ:51:ILE:HG12	1:AJ:77:ARG:HG2	1.94	0.49
1:AP:17:TRP:CD2	1:AQ:119:PRO:HG2	2.48	0.49
1:AT:25:SER:HA	1:AT:53:ASN:O	2.13	0.49
1:AY:51:ILE:HG12	1:AY:77:ARG:HG2	1.93	0.49
1:BA:2:GLN:HA	1:CN:121:VAL:O	2.11	0.49
1:BR:24:ARG:NH1	1:CF:85:GLU:OE2	2.45	0.49
1:BT:17:TRP:CD2	1:BU:119:PRO:HG2	2.48	0.49
1:BT:24:ARG:HH11	1:BT:71:ARG:HH11	1.61	0.49
1:BU:36:LYS:HD2	1:BU:45:ASN:ND2	2.27	0.49
1:CP:36:LYS:HD2	1:CP:45:ASN:ND2	2.27	0.49
1:DD:17:TRP:CD2	1:DE:119:PRO:HG2	2.48	0.49
1:DD:24:ARG:HH11	1:DD:71:ARG:HH11	1.61	0.49
1:AA:17:TRP:CD2	1:AB:119:PRO:HG2	2.48	0.49
1:AD:24:ARG:HH11	1:AD:71:ARG:HH11	1.61	0.49
1:AG:17:TRP:CD2	1:AH:119:PRO:HG2	2.48	0.49
1:AK:25:SER:HA	1:AK:53:ASN:O	2.13	0.49
1:AT:36:LYS:HD2	1:AT:45:ASN:ND2	2.27	0.49
1:AV:51:ILE:HG12	1:AV:77:ARG:HG2	1.94	0.49
1:AY:17:TRP:CD2	1:AZ:119:PRO:HG2	2.48	0.49
1:BA:11:SER:C	1:BA:13:THR:H	2.20	0.49
1:BE:24:ARG:HH11	1:BE:71:ARG:HH11	1.61	0.49
1:BM:113:LEU:HD12	1:BM:114:PRO:HD2	1.94	0.49
1:BS:113:LEU:HD12	1:BS:114:PRO:HD2	1.94	0.49
1:CC:24:ARG:HH11	1:CC:71:ARG:HH11	1.61	0.49
1:CS:36:LYS:HD2	1:CS:45:ASN:ND2	2.27	0.49
1:DA:51:ILE:HG12	1:DA:77:ARG:HG2	1.93	0.49
1:DB:25:SER:HA	1:DB:53:ASN:O	2.13	0.49
1:AW:25:SER:HA	1:AW:53:ASN:O	2.13	0.49
1:BF:25:SER:HA	1:BF:53:ASN:O	2.13	0.49
1:BR:25:SER:HA	1:BR:53:ASN:O	2.13	0.49
1:CF:24:ARG:HH11	1:CF:71:ARG:HH11	1.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CS:25:SER:HA	1:CS:53:ASN:O	2.13	0.49
1:CV:25:SER:HA	1:CV:53:ASN:O	2.13	0.49
1:DH:25:SER:HA	1:DH:53:ASN:O	2.13	0.49
1:DJ:51:ILE:HG12	1:DJ:77:ARG:HG2	1.94	0.49
1:DL:11:SER:C	1:DL:13:THR:H	2.20	0.49
1:AA:24:ARG:HH11	1:AA:71:ARG:HH11	1.61	0.49
1:AB:25:SER:HA	1:AB:53:ASN:O	2.13	0.49
1:AL:11:SER:C	1:AL:13:THR:H	2.20	0.49
1:BE:17:TRP:CD2	1:BF:119:PRO:HG2	2.48	0.49
1:BJ:113:LEU:HD12	1:BJ:114:PRO:HD2	1.94	0.49
1:BL:36:LYS:HD2	1:BL:45:ASN:ND2	2.27	0.49
1:BS:11:SER:C	1:BS:13:THR:H	2.20	0.49
1:BX:25:SER:HA	1:BX:53:ASN:O	2.13	0.49
1:CH:11:SER:C	1:CH:13:THR:H	2.20	0.49
1:CQ:113:LEU:HD12	1:CQ:114:PRO:HD2	1.94	0.49
1:CT:113:LEU:HD12	1:CT:114:PRO:HD2	1.94	0.49
1:CU:17:TRP:CD2	1:CV:119:PRO:HG2	2.48	0.49
1:CX:24:ARG:HH11	1:CX:71:ARG:HH11	1.61	0.49
1:AG:24:ARG:HH11	1:AG:71:ARG:HH11	1.61	0.48
1:AM:17:TRP:CD2	1:AN:119:PRO:HG2	2.48	0.48
1:AM:45:ASN:HA	1:AM:83:SER:HA	1.95	0.48
1:AP:86:ASN:ND2	1:AQ:58:VAL:HA	2.28	0.48
1:AQ:15:LEU:O	1:AQ:28:ARG:HA	2.13	0.48
1:AR:50:VAL:O	1:BY:97:HIS:HE1	1.96	0.48
1:AV:86:ASN:ND2	1:AW:58:VAL:HA	2.28	0.48
1:AX:54:ARG:HD2	1:CH:93:ALA:HB2	1.93	0.48
1:BN:17:TRP:CD2	1:BO:119:PRO:HG2	2.48	0.48
1:BT:51:ILE:HG12	1:BT:77:ARG:HG2	1.93	0.48
1:BY:113:LEU:HD12	1:BY:114:PRO:HD2	1.94	0.48
1:CO:17:TRP:CD2	1:CP:119:PRO:HG2	2.48	0.48
1:CW:11:SER:C	1:CW:13:THR:H	2.20	0.48
1:DG:17:TRP:CD2	1:DH:119:PRO:HG2	2.48	0.48
1:DH:15:LEU:O	1:DH:28:ARG:HA	2.14	0.48
1:DK:25:SER:HA	1:DK:53:ASN:O	2.13	0.48
1:AD:86:ASN:ND2	1:AE:58:VAL:HA	2.28	0.48
1:AI:113:LEU:HD12	1:AI:114:PRO:HD2	1.94	0.48
1:AZ:9:LEU:HD13	1:BK:12:GLY:N	2.28	0.48
1:BC:15:LEU:O	1:BC:28:ARG:HA	2.13	0.48
1:BI:15:LEU:O	1:BI:28:ARG:HA	2.14	0.48
1:BO:15:LEU:O	1:BO:28:ARG:HA	2.14	0.48
1:BV:11:SER:C	1:BV:13:THR:H	2.20	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CC:51:ILE:HG12	1:CC:77:ARG:HG2	1.93	0.48
1:CI:17:TRP:CD2	1:CJ:119:PRO:HG2	2.48	0.48
1:CI:24:ARG:HH11	1:CI:71:ARG:HH11	1.61	0.48
1:CN:113:LEU:HD12	1:CN:114:PRO:HD2	1.95	0.48
1:CS:15:LEU:O	1:CS:28:ARG:HA	2.14	0.48
1:DD:45:ASN:HA	1:DD:83:SER:HA	1.96	0.48
1:DF:113:LEU:HD12	1:DF:114:PRO:HD2	1.94	0.48
1:AE:15:LEU:O	1:AE:28:ARG:HA	2.14	0.48
1:AE:25:SER:HA	1:AE:53:ASN:O	2.13	0.48
1:AH:25:SER:HA	1:AH:53:ASN:O	2.13	0.48
1:AO:11:SER:C	1:AO:13:THR:H	2.20	0.48
1:AY:86:ASN:ND2	1:AZ:58:VAL:HA	2.29	0.48
1:AZ:25:SER:HA	1:AZ:53:ASN:O	2.13	0.48
1:BG:87:LYS:HB2	1:CT:109:VAL:CG1	2.37	0.48
1:BH:24:ARG:HH11	1:BH:71:ARG:HH11	1.61	0.48
1:BK:45:ASN:HA	1:BK:83:SER:HA	1.96	0.48
1:BL:15:LEU:O	1:BL:28:ARG:HA	2.14	0.48
1:BR:15:LEU:O	1:BR:28:ARG:HA	2.14	0.48
1:BT:24:ARG:NH1	1:BT:71:ARG:HH11	2.09	0.48
1:BV:113:LEU:HD12	1:BV:114:PRO:HD2	1.94	0.48
1:BZ:45:ASN:HA	1:BZ:83:SER:HA	1.96	0.48
1:CD:25:SER:HA	1:CD:53:ASN:O	2.13	0.48
1:CG:25:SER:HA	1:CG:53:ASN:O	2.13	0.48
1:CM:15:LEU:O	1:CM:28:ARG:HA	2.14	0.48
1:CX:86:ASN:ND2	1:CY:58:VAL:HA	2.29	0.48
1:CY:25:SER:HA	1:CY:53:ASN:O	2.13	0.48
1:DD:86:ASN:ND2	1:DE:58:VAL:HA	2.28	0.48
1:DH:36:LYS:HD2	1:DH:45:ASN:ND2	2.27	0.48
1:AA:86:ASN:ND2	1:AB:58:VAL:HA	2.28	0.48
1:AC:80:ILE:HG12	1:BJ:76:ILE:HG12	1.95	0.48
1:AN:15:LEU:O	1:AN:28:ARG:HA	2.13	0.48
1:AQ:25:SER:HA	1:AQ:53:ASN:O	2.13	0.48
1:AZ:36:LYS:HD2	1:AZ:45:ASN:ND2	2.27	0.48
1:BB:17:TRP:CD2	1:BC:119:PRO:HG2	2.48	0.48
1:BD:113:LEU:HD12	1:BD:114:PRO:HD2	1.94	0.48
1:BG:108:LEU:HD23	1:CT:31:LEU:HD12	1.95	0.48
1:BK:17:TRP:CD2	1:BL:119:PRO:HG2	2.48	0.48
1:BK:51:ILE:HG12	1:BK:77:ARG:HG2	1.94	0.48
1:CI:33:VAL:HG11	1:CV:23:PHE:CE2	2.35	0.48
1:CR:45:ASN:HA	1:CR:83:SER:HA	1.96	0.48
1:DA:45:ASN:HA	1:DA:83:SER:HA	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DC:11:SER:C	1:DC:13:THR:H	2.20	0.48
1:DD:51:ILE:HG12	1:DD:77:ARG:HG2	1.93	0.48
1:DG:86:ASN:ND2	1:DH:58:VAL:HA	2.28	0.48
1:AM:24:ARG:HH11	1:AM:71:ARG:HH11	1.61	0.48
1:AN:25:SER:HA	1:AN:53:ASN:O	2.13	0.48
1:AR:113:LEU:HD12	1:AR:114:PRO:HD2	1.94	0.48
1:AT:15:LEU:O	1:AT:28:ARG:HA	2.14	0.48
1:AU:113:LEU:HD12	1:AU:114:PRO:HD2	1.94	0.48
1:AV:45:ASN:HA	1:AV:83:SER:HA	1.96	0.48
1:BB:86:ASN:ND2	1:BC:58:VAL:HA	2.28	0.48
1:BC:25:SER:HA	1:BC:53:ASN:O	2.13	0.48
1:BH:86:ASN:ND2	1:BI:58:VAL:HA	2.28	0.48
1:BW:86:ASN:ND2	1:BX:58:VAL:HA	2.28	0.48
1:CA:15:LEU:O	1:CA:28:ARG:HA	2.14	0.48
1:CA:36:LYS:HD2	1:CA:45:ASN:ND2	2.27	0.48
1:CB:11:SER:C	1:CB:13:THR:H	2.20	0.48
1:CJ:36:LYS:HD2	1:CJ:45:ASN:ND2	2.27	0.48
1:CL:45:ASN:HA	1:CL:83:SER:HA	1.96	0.48
1:CL:86:ASN:ND2	1:CM:58:VAL:HA	2.28	0.48
1:CR:17:TRP:CD2	1:CS:119:PRO:HG2	2.48	0.48
1:CX:17:TRP:CD2	1:CY:119:PRO:HG2	2.48	0.48
1:DJ:86:ASN:ND2	1:DK:58:VAL:HA	2.28	0.48
1:AA:45:ASN:HA	1:AA:83:SER:HA	1.96	0.48
1:AU:120:VAL:HA	1:CB:4:ASN:HA	1.94	0.48
1:AV:17:TRP:CD2	1:AW:119:PRO:HG2	2.48	0.48
1:BN:24:ARG:HH11	1:BN:71:ARG:HH11	1.61	0.48
1:CC:86:ASN:ND2	1:CD:58:VAL:HA	2.29	0.48
1:CO:45:ASN:HA	1:CO:83:SER:HA	1.95	0.48
1:DE:25:SER:HA	1:DE:53:ASN:O	2.13	0.48
1:DJ:24:ARG:HH11	1:DJ:71:ARG:HH11	1.61	0.48
1:DK:36:LYS:HD2	1:DK:45:ASN:ND2	2.27	0.48
1:AD:12:GLY:HA3	1:DH:9:LEU:HD22	1.95	0.48
1:AH:15:LEU:O	1:AH:28:ARG:HA	2.13	0.48
1:AL:5:MET:HB2	1:BS:119:PRO:HG2	1.94	0.48
1:BE:86:ASN:ND2	1:BF:58:VAL:HA	2.28	0.48
1:BH:45:ASN:HA	1:BH:83:SER:HA	1.96	0.48
1:BQ:24:ARG:HH11	1:BQ:71:ARG:HH11	1.61	0.48
1:BU:15:LEU:O	1:BU:28:ARG:HA	2.14	0.48
1:BX:36:LYS:HD2	1:BX:45:ASN:ND2	2.27	0.48
1:CE:113:LEU:HD12	1:CE:114:PRO:HD2	1.94	0.48
1:CR:86:ASN:ND2	1:CS:58:VAL:HA	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AB:15:LEU:O	1:AB:28:ARG:HA	2.14	0.48
1:AG:86:ASN:ND2	1:AH:58:VAL:HA	2.28	0.48
1:AJ:17:TRP:CD2	1:AK:119:PRO:HG2	2.48	0.48
1:AJ:24:ARG:HH11	1:AJ:71:ARG:HH11	1.61	0.48
1:BO:25:SER:HA	1:BO:53:ASN:O	2.13	0.48
1:CB:113:LEU:HD12	1:CB:114:PRO:HD2	1.94	0.48
1:CF:86:ASN:ND2	1:CG:58:VAL:HA	2.28	0.48
1:CI:45:ASN:HA	1:CI:83:SER:HA	1.96	0.48
1:CI:86:ASN:ND2	1:CJ:58:VAL:HA	2.29	0.48
1:DL:113:LEU:HD12	1:DL:114:PRO:HD2	1.94	0.48
1:AC:120:VAL:HA	1:BJ:4:ASN:HA	1.96	0.48
1:AF:113:LEU:HD12	1:AF:114:PRO:HD2	1.94	0.48
1:AJ:45:ASN:HA	1:AJ:83:SER:HA	1.96	0.48
1:AK:36:LYS:HD2	1:AK:45:ASN:ND2	2.27	0.48
1:AS:86:ASN:ND2	1:AT:58:VAL:HA	2.28	0.48
1:BI:25:SER:HA	1:BI:53:ASN:O	2.13	0.48
1:BZ:24:ARG:HH11	1:BZ:71:ARG:HH11	1.61	0.48
1:BZ:86:ASN:ND2	1:CA:58:VAL:HA	2.28	0.48
1:CL:17:TRP:CD2	1:CM:119:PRO:HG2	2.48	0.48
1:CU:45:ASN:HA	1:CU:83:SER:HA	1.96	0.48
1:DA:86:ASN:ND2	1:DB:58:VAL:HA	2.28	0.48
1:DB:36:LYS:HD2	1:DB:45:ASN:ND2	2.27	0.48
1:DI:113:LEU:HD12	1:DI:114:PRO:HD2	1.94	0.48
1:DK:15:LEU:O	1:DK:28:ARG:HA	2.14	0.48
1:AB:36:LYS:HD2	1:AB:45:ASN:ND2	2.27	0.48
1:AL:121:VAL:O	1:BS:2:GLN:HA	2.13	0.48
1:AR:71:ARG:O	1:BY:38:ALA:HB1	2.14	0.48
1:AZ:15:LEU:O	1:AZ:28:ARG:HA	2.14	0.48
1:BA:83:SER:N	1:CN:72:GLU:OE2	2.47	0.48
1:BA:91:LEU:HD22	1:CN:105:ARG:NH2	2.29	0.48
1:BB:24:ARG:HH11	1:BB:71:ARG:HH11	1.61	0.48
1:BQ:86:ASN:ND2	1:BR:58:VAL:HA	2.28	0.48
1:BX:15:LEU:O	1:BX:28:ARG:HA	2.14	0.48
1:CP:15:LEU:O	1:CP:28:ARG:HA	2.14	0.48
1:DB:15:LEU:O	1:DB:28:ARG:HA	2.14	0.48
1:DE:15:LEU:O	1:DE:28:ARG:HA	2.14	0.48
1:AC:97:HIS:HB2	1:BJ:52:THR:HG21	1.96	0.47
1:AV:24:ARG:HH11	1:AV:71:ARG:HH11	1.61	0.47
1:BQ:45:ASN:HA	1:BQ:83:SER:HA	1.96	0.47
1:BW:17:TRP:CD2	1:BX:119:PRO:HG2	2.48	0.47
1:AJ:86:ASN:ND2	1:AK:58:VAL:HA	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BK:24:ARG:HH11	1:BK:71:ARG:HH11	1.61	0.47
1:CD:36:LYS:HD2	1:CD:45:ASN:ND2	2.27	0.47
1:CG:15:LEU:O	1:CG:28:ARG:HA	2.14	0.47
1:CV:15:LEU:O	1:CV:28:ARG:HA	2.14	0.47
1:CV:36:LYS:HD2	1:CV:45:ASN:ND2	2.27	0.47
1:CY:15:LEU:O	1:CY:28:ARG:HA	2.14	0.47
1:AL:4:ASN:HB2	1:BS:119:PRO:O	2.13	0.47
1:AO:121:VAL:O	1:BV:2:GLN:HA	2.13	0.47
1:AQ:67:CYS:HA	1:BU:63:CYS:HB2	1.95	0.47
1:AS:24:ARG:HH11	1:AS:71:ARG:HH11	1.61	0.47
1:CC:17:TRP:CD2	1:CD:119:PRO:HG2	2.48	0.47
1:CL:24:ARG:HH11	1:CL:71:ARG:HH11	1.61	0.47
1:CO:86:ASN:ND2	1:CP:58:VAL:HA	2.28	0.47
1:CR:24:ARG:HH11	1:CR:71:ARG:HH11	1.61	0.47
1:CU:24:ARG:HH11	1:CU:71:ARG:HH11	1.61	0.47
1:AB:8:GLN:HE21	1:AW:113:LEU:HB3	1.79	0.47
1:AG:45:ASN:HA	1:AG:83:SER:HA	1.96	0.47
1:AK:15:LEU:O	1:AK:28:ARG:HA	2.14	0.47
1:AM:86:ASN:ND2	1:AN:58:VAL:HA	2.29	0.47
1:AO:4:ASN:HA	1:BV:120:VAL:HA	1.94	0.47
1:BE:107:ASP:OD1	1:BJ:6:ARG:NH1	2.41	0.47
1:BU:25:SER:HA	1:BU:53:ASN:O	2.13	0.47
1:CU:86:ASN:ND2	1:CV:58:VAL:HA	2.29	0.47
1:AO:108:LEU:HD21	1:BV:29:ILE:CG2	2.45	0.47
1:AW:15:LEU:O	1:AW:28:ARG:HA	2.14	0.47
1:BF:69:VAL:HB	1:BH:41:VAL:HG11	1.95	0.47
1:CJ:15:LEU:O	1:CJ:28:ARG:HA	2.14	0.47
1:DC:20:PRO:CB	1:DJ:112:LEU:HD21	2.41	0.47
1:BT:86:ASN:ND2	1:BU:58:VAL:HA	2.28	0.47
1:CC:45:ASN:HA	1:CC:83:SER:HA	1.96	0.47
1:AG:41:VAL:HG11	1:DB:69:VAL:HB	1.97	0.47
1:AG:85:GLU:OE2	1:DB:24:ARG:NH1	2.46	0.47
1:AO:120:VAL:HG22	1:BV:4:ASN:HB3	1.96	0.47
1:BB:45:ASN:HA	1:BB:83:SER:HA	1.96	0.47
1:BD:97:HIS:HB2	1:CQ:52:THR:HG21	1.97	0.47
1:BF:15:LEU:O	1:BF:28:ARG:HA	2.14	0.47
1:BN:45:ASN:HA	1:BN:83:SER:HA	1.96	0.47
1:BN:86:ASN:ND2	1:BO:58:VAL:HA	2.29	0.47
1:BT:45:ASN:HA	1:BT:83:SER:HA	1.96	0.47
1:BW:24:ARG:HH11	1:BW:71:ARG:HH11	1.61	0.47
1:BW:45:ASN:HA	1:BW:83:SER:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CF:45:ASN:HA	1:CF:83:SER:HA	1.96	0.47
1:CX:45:ASN:HA	1:CX:83:SER:HA	1.96	0.47
1:CZ:25:SER:HA	1:CZ:53:ASN:O	2.15	0.47
1:AO:25:SER:HA	1:AO:53:ASN:O	2.15	0.47
1:AO:77:ARG:O	1:BV:78:THR:HA	2.14	0.47
1:AX:31:LEU:HD12	1:CH:108:LEU:CD2	2.43	0.47
1:BG:2:GLN:OE1	1:CT:124:THR:OG1	2.24	0.47
1:BK:86:ASN:ND2	1:BL:58:VAL:HA	2.28	0.47
1:CD:15:LEU:O	1:CD:28:ARG:HA	2.14	0.47
1:CL:85:GLU:OE2	1:CY:24:ARG:NH1	2.47	0.47
1:DG:45:ASN:HA	1:DG:83:SER:HA	1.96	0.47
1:DL:25:SER:HA	1:DL:53:ASN:O	2.15	0.47
1:AI:25:SER:HA	1:AI:53:ASN:O	2.15	0.47
1:AU:25:SER:HA	1:AU:53:ASN:O	2.15	0.47
1:AY:45:ASN:HA	1:AY:83:SER:HA	1.96	0.47
1:BP:25:SER:HA	1:BP:53:ASN:O	2.15	0.47
1:BV:25:SER:HA	1:BV:53:ASN:O	2.15	0.47
1:CK:25:SER:HA	1:CK:53:ASN:O	2.15	0.47
1:DC:25:SER:HA	1:DC:53:ASN:O	2.15	0.47
1:DI:25:SER:HA	1:DI:53:ASN:O	2.15	0.47
1:DJ:45:ASN:HA	1:DJ:83:SER:HA	1.96	0.47
1:AC:25:SER:HA	1:AC:53:ASN:O	2.15	0.47
1:AD:45:ASN:HA	1:AD:83:SER:HA	1.96	0.47
1:BG:25:SER:HB2	1:BG:54:ARG:HG2	1.98	0.47
1:BO:24:ARG:NH1	1:DG:85:GLU:OE2	2.48	0.47
1:BS:25:SER:HA	1:BS:53:ASN:O	2.15	0.47
1:CT:25:SER:HA	1:CT:53:ASN:O	2.15	0.47
1:DB:63:CYS:HB2	1:DK:67:CYS:HA	1.96	0.47
1:DG:24:ARG:HH11	1:DG:71:ARG:HH11	1.61	0.47
1:AC:5:MET:HB2	1:BJ:119:PRO:HG2	1.96	0.46
1:AS:45:ASN:HA	1:AS:83:SER:HA	1.96	0.46
1:AY:24:ARG:HH11	1:AY:71:ARG:HH11	1.61	0.46
1:BD:25:SER:HB2	1:BD:54:ARG:HG2	1.98	0.46
1:BL:24:ARG:NH1	1:DD:85:GLU:OE2	2.47	0.46
1:BY:25:SER:HA	1:BY:53:ASN:O	2.15	0.46
1:AL:97:HIS:HB2	1:BS:52:THR:HG21	1.97	0.46
1:BB:25:SER:HA	1:BB:53:ASN:O	2.16	0.46
1:BE:25:SER:HA	1:BE:53:ASN:O	2.16	0.46
1:BJ:25:SER:HB2	1:BJ:54:ARG:HG2	1.98	0.46
1:BX:9:LEU:HD13	1:CC:12:GLY:N	2.30	0.46
1:BZ:25:SER:HA	1:BZ:53:ASN:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CW:25:SER:HB2	1:CW:54:ARG:HG2	1.98	0.46
1:AN:67:CYS:HA	1:BR:63:CYS:HB2	1.97	0.46
1:AP:45:ASN:HA	1:AP:83:SER:HA	1.96	0.46
1:AR:87:LYS:HB2	1:BY:109:VAL:CG1	2.39	0.46
1:AX:25:SER:HA	1:AX:53:ASN:O	2.15	0.46
1:CB:25:SER:HB2	1:CB:54:ARG:HG2	1.98	0.46
1:CE:25:SER:HB2	1:CE:54:ARG:HG2	1.98	0.46
1:CK:25:SER:HB2	1:CK:54:ARG:HG2	1.98	0.46
1:CL:25:SER:HA	1:CL:53:ASN:O	2.16	0.46
1:CO:41:VAL:HG11	1:CS:69:VAL:HB	1.97	0.46
1:CU:25:SER:HA	1:CU:53:ASN:O	2.16	0.46
1:AG:25:SER:HA	1:AG:53:ASN:O	2.16	0.46
1:AM:23:PHE:HE2	1:AO:84:VAL:HG11	1.81	0.46
1:AP:25:SER:HA	1:AP:53:ASN:O	2.16	0.46
1:BE:45:ASN:HA	1:BE:83:SER:HA	1.96	0.46
1:CB:25:SER:HA	1:CB:53:ASN:O	2.15	0.46
1:CR:25:SER:HA	1:CR:53:ASN:O	2.16	0.46
1:CW:25:SER:HA	1:CW:53:ASN:O	2.15	0.46
1:DL:25:SER:HB2	1:DL:54:ARG:HG2	1.98	0.46
1:AA:25:SER:HA	1:AA:53:ASN:O	2.16	0.46
1:AF:25:SER:HA	1:AF:53:ASN:O	2.15	0.46
1:AP:112:LEU:HD21	1:BV:20:PRO:HB3	1.97	0.46
1:AX:70:ASN:CG	1:CH:41:VAL:HG23	2.40	0.46
1:BS:25:SER:HB2	1:BS:54:ARG:HG2	1.98	0.46
1:DC:25:SER:HB2	1:DC:54:ARG:HG2	1.98	0.46
1:DF:25:SER:HA	1:DF:53:ASN:O	2.15	0.46
1:AD:23:PHE:HE2	1:AF:84:VAL:HG11	1.81	0.46
1:AE:69:VAL:HB	1:AS:41:VAL:HG11	1.97	0.46
1:AJ:23:PHE:HE2	1:AL:84:VAL:HG11	1.81	0.46
1:AT:9:LEU:HD22	1:BB:12:GLY:HA3	1.96	0.46
1:BK:25:SER:HA	1:BK:53:ASN:O	2.16	0.46
1:CO:25:SER:HA	1:CO:53:ASN:O	2.16	0.46
1:DA:24:ARG:HH11	1:DA:71:ARG:HH11	1.61	0.46
1:AA:112:LEU:HD13	1:AX:6:ARG:HD3	1.97	0.46
1:AC:105:ARG:NH2	1:BJ:91:LEU:HD22	2.31	0.46
1:AL:25:SER:HA	1:AL:53:ASN:O	2.15	0.46
1:AR:25:SER:HB2	1:AR:54:ARG:HG2	1.98	0.46
1:AX:25:SER:HB2	1:AX:54:ARG:HG2	1.98	0.46
1:AY:25:SER:HA	1:AY:53:ASN:O	2.16	0.46
1:BD:108:LEU:HD21	1:CQ:29:ILE:HG21	1.98	0.46
1:BJ:25:SER:HA	1:BJ:53:ASN:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BP:25:SER:HB2	1:BP:54:ARG:HG2	1.98	0.46
1:BQ:112:LEU:HD21	1:CH:20:PRO:HB3	1.98	0.46
1:BV:25:SER:HB2	1:BV:54:ARG:HG2	1.98	0.46
1:CD:24:ARG:NH1	1:CX:85:GLU:OE2	2.48	0.46
1:CH:25:SER:HA	1:CH:53:ASN:O	2.15	0.46
1:CN:25:SER:HA	1:CN:53:ASN:O	2.15	0.46
1:CQ:25:SER:HA	1:CQ:53:ASN:O	2.15	0.46
1:DI:25:SER:HB2	1:DI:54:ARG:HG2	1.98	0.46
1:DJ:25:SER:HA	1:DJ:53:ASN:O	2.16	0.46
1:AG:23:PHE:HE2	1:AI:84:VAL:HG11	1.81	0.46
1:AL:25:SER:HB2	1:AL:54:ARG:HG2	1.98	0.46
1:BN:25:SER:HA	1:BN:53:ASN:O	2.16	0.46
1:BQ:25:SER:HA	1:BQ:53:ASN:O	2.16	0.46
1:BX:8:GLN:HE21	1:CD:113:LEU:HB3	1.80	0.46
1:BY:25:SER:HB2	1:BY:54:ARG:HG2	1.98	0.46
1:BZ:23:PHE:HE2	1:CB:84:VAL:HG11	1.81	0.46
1:CC:23:PHE:HE2	1:CE:84:VAL:HG11	1.81	0.46
1:CI:23:PHE:HE2	1:CK:84:VAL:HG11	1.81	0.46
1:DD:23:PHE:HE2	1:DF:84:VAL:HG11	1.81	0.46
1:DG:23:PHE:HE2	1:DI:84:VAL:HG11	1.81	0.46
1:AC:25:SER:HB2	1:AC:54:ARG:HG2	1.98	0.46
1:AX:109:VAL:CG1	1:CH:87:LYS:HB2	2.43	0.46
1:BK:23:PHE:HE2	1:BM:84:VAL:HG11	1.81	0.46
1:BN:23:PHE:HE2	1:BP:84:VAL:HG11	1.81	0.46
1:BW:25:SER:HA	1:BW:53:ASN:O	2.16	0.46
1:BY:57:LEU:HD21	1:BY:68:SER:HB2	1.98	0.46
1:CE:25:SER:HA	1:CE:53:ASN:O	2.15	0.46
1:CE:57:LEU:HD21	1:CE:68:SER:HB2	1.98	0.46
1:CL:41:VAL:HG11	1:CY:69:VAL:HB	1.98	0.46
1:CU:23:PHE:HE2	1:CW:84:VAL:HG11	1.81	0.46
1:AV:23:PHE:HE2	1:AX:84:VAL:HG11	1.81	0.46
1:AX:57:LEU:HD21	1:AX:68:SER:HB2	1.98	0.46
1:BE:23:PHE:HE2	1:BG:84:VAL:HG11	1.81	0.46
1:BG:87:LYS:CB	1:CT:109:VAL:HG12	2.41	0.46
1:BH:23:PHE:HE2	1:BJ:84:VAL:HG11	1.81	0.46
1:BT:25:SER:HA	1:BT:53:ASN:O	2.16	0.46
1:BW:23:PHE:HE2	1:BY:84:VAL:HG11	1.81	0.46
1:CF:23:PHE:HE2	1:CH:84:VAL:HG11	1.81	0.46
1:CN:57:LEU:HD21	1:CN:68:SER:HB2	1.98	0.46
1:AO:17:TRP:CD2	1:BV:119:PRO:HG3	2.51	0.45
1:AO:57:LEU:HD21	1:AO:68:SER:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AO:76:ILE:HA	1:BV:79:THR:O	2.16	0.45
1:AS:25:SER:HA	1:AS:53:ASN:O	2.16	0.45
1:BA:25:SER:HA	1:BA:53:ASN:O	2.15	0.45
1:BF:6:ARG:HD2	1:BI:116:THR:CG2	2.46	0.45
1:BG:25:SER:HA	1:BG:53:ASN:O	2.15	0.45
1:CL:23:PHE:HE2	1:CN:84:VAL:HG11	1.81	0.45
1:CO:23:PHE:HE2	1:CQ:84:VAL:HG11	1.81	0.45
1:CQ:57:LEU:HD21	1:CQ:68:SER:HB2	1.98	0.45
1:AV:25:SER:HA	1:AV:53:ASN:O	2.16	0.45
1:BB:23:PHE:HE2	1:BD:84:VAL:HG11	1.81	0.45
1:BM:25:SER:HA	1:BM:53:ASN:O	2.15	0.45
1:BP:57:LEU:HD21	1:BP:68:SER:HB2	1.98	0.45
1:BT:23:PHE:HE2	1:BV:84:VAL:HG11	1.81	0.45
1:CR:23:PHE:HE2	1:CT:84:VAL:HG11	1.81	0.45
1:CW:57:LEU:HD21	1:CW:68:SER:HB2	1.98	0.45
1:DA:33:VAL:HG11	1:DK:23:PHE:HE2	1.81	0.45
1:AM:25:SER:HA	1:AM:53:ASN:O	2.16	0.45
1:AO:108:LEU:HD21	1:BV:29:ILE:HG21	1.97	0.45
1:AR:25:SER:HA	1:AR:53:ASN:O	2.15	0.45
1:BM:57:LEU:HD21	1:BM:68:SER:HB2	1.98	0.45
1:CZ:57:LEU:HD21	1:CZ:68:SER:HB2	1.98	0.45
1:DA:23:PHE:HE2	1:DC:84:VAL:HG11	1.81	0.45
1:DF:25:SER:HB2	1:DF:54:ARG:HG2	1.98	0.45
1:AD:25:SER:HA	1:AD:53:ASN:O	2.16	0.45
1:AF:57:LEU:HD21	1:AF:68:SER:HB2	1.98	0.45
1:AH:116:THR:HG21	1:DB:6:ARG:HD2	1.99	0.45
1:AQ:12:GLY:N	1:BV:10:THR:O	2.39	0.45
1:AR:31:LEU:HD12	1:BY:108:LEU:HD23	1.98	0.45
1:AY:2:GLN:OE1	1:AZ:123:TYR:HA	2.17	0.45
1:BA:25:SER:HB2	1:BA:54:ARG:HG2	1.98	0.45
1:BD:17:TRP:CE3	1:CQ:119:PRO:HG3	2.52	0.45
1:BF:67:CYS:HA	1:BI:63:CYS:HB2	1.98	0.45
1:BG:98:LEU:HD22	1:CT:98:LEU:HD22	1.99	0.45
1:BK:2:GLN:OE1	1:BL:123:TYR:HA	2.17	0.45
1:BM:25:SER:HB2	1:BM:54:ARG:HG2	1.98	0.45
1:CI:2:GLN:OE1	1:CJ:123:TYR:HA	2.17	0.45
1:CK:57:LEU:HD21	1:CK:68:SER:HB2	1.99	0.45
1:DA:25:SER:HA	1:DA:53:ASN:O	2.16	0.45
1:DD:25:SER:HA	1:DD:53:ASN:O	2.16	0.45
1:DG:25:SER:HA	1:DG:53:ASN:O	2.16	0.45
1:AC:57:LEU:HD21	1:AC:68:SER:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AU:97:HIS:HB2	1:CB:52:THR:HG21	1.99	0.45
1:AW:12:GLY:N	1:BA:10:THR:O	2.36	0.45
1:BA:57:LEU:HD21	1:BA:68:SER:HB2	1.98	0.45
1:BD:25:SER:HA	1:BD:53:ASN:O	2.15	0.45
1:BP:29:ILE:HG12	1:BP:50:VAL:HG22	1.99	0.45
1:CH:57:LEU:HD21	1:CH:68:SER:HB2	1.98	0.45
1:DA:2:GLN:OE1	1:DB:123:TYR:HA	2.17	0.45
1:AJ:2:GLN:OE1	1:AK:123:TYR:HA	2.17	0.45
1:AL:57:LEU:HD21	1:AL:68:SER:HB2	1.98	0.45
1:AN:6:ARG:HD2	1:BR:116:THR:HG21	1.98	0.45
1:AV:2:GLN:OE1	1:AW:123:TYR:HA	2.17	0.45
1:BB:2:GLN:OE1	1:BC:123:TYR:HA	2.17	0.45
1:BC:9:LEU:HD22	1:BN:12:GLY:HA3	1.98	0.45
1:BD:108:LEU:HD21	1:CQ:29:ILE:CG2	2.47	0.45
1:BE:115:THR:HG21	1:BJ:7:LEU:HB3	1.99	0.45
1:BG:121:VAL:HG23	1:CT:5:MET:CG	2.47	0.45
1:BH:25:SER:HA	1:BH:53:ASN:O	2.16	0.45
1:BN:2:GLN:OE1	1:BO:123:TYR:HA	2.17	0.45
1:BV:57:LEU:HD21	1:BV:68:SER:HB2	1.98	0.45
1:CI:25:SER:HA	1:CI:53:ASN:O	2.16	0.45
1:CK:29:ILE:HG12	1:CK:50:VAL:HG22	1.99	0.45
1:CX:23:PHE:HE2	1:CZ:84:VAL:HG11	1.81	0.45
1:CZ:25:SER:HB2	1:CZ:54:ARG:HG2	1.98	0.45
1:CZ:29:ILE:HG12	1:CZ:50:VAL:HG22	1.99	0.45
1:AD:2:GLN:OE1	1:AE:123:TYR:HA	2.17	0.45
1:AO:31:LEU:HD12	1:BV:108:LEU:HD23	1.99	0.45
1:AQ:121:VAL:HG12	1:AQ:122:GLU:HG3	1.99	0.45
1:AU:29:ILE:CG2	1:CB:108:LEU:HD21	2.47	0.45
1:AU:29:ILE:HG21	1:CB:108:LEU:HD21	1.99	0.45
1:BC:24:ARG:NH1	1:BN:85:GLU:OE2	2.49	0.45
1:BD:76:ILE:HG12	1:CQ:80:ILE:HG12	1.98	0.45
1:BG:57:LEU:HD21	1:BG:68:SER:HB2	1.98	0.45
1:BJ:57:LEU:HD21	1:BJ:68:SER:HB2	1.98	0.45
1:BQ:23:PHE:HE2	1:BS:84:VAL:HG11	1.81	0.45
1:BT:2:GLN:OE1	1:BU:123:TYR:HA	2.17	0.45
1:CE:29:ILE:HG12	1:CE:50:VAL:HG22	1.99	0.45
1:CF:2:GLN:OE1	1:CG:123:TYR:HA	2.17	0.45
1:CH:25:SER:HB2	1:CH:54:ARG:HG2	1.98	0.45
1:CL:2:GLN:OE1	1:CM:123:TYR:HA	2.17	0.45
1:CU:2:GLN:OE1	1:CV:123:TYR:HA	2.17	0.45
1:AA:23:PHE:HE2	1:AC:84:VAL:HG11	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AD:25:SER:CB	1:AD:54:ARG:HG2	2.47	0.45
1:AF:25:SER:HB2	1:AF:54:ARG:HG2	1.98	0.45
1:AF:29:ILE:HG12	1:AF:50:VAL:HG22	1.99	0.45
1:AS:25:SER:CB	1:AS:54:ARG:HG2	2.47	0.45
1:AY:25:SER:CB	1:AY:54:ARG:HG2	2.47	0.45
1:BU:121:VAL:HG12	1:BU:122:GLU:HG3	1.99	0.45
1:CS:121:VAL:HG12	1:CS:122:GLU:HG3	1.99	0.45
1:CT:57:LEU:HD21	1:CT:68:SER:HB2	1.98	0.45
1:DJ:2:GLN:OE1	1:DK:123:TYR:HA	2.17	0.45
1:DJ:23:PHE:HE2	1:DL:84:VAL:HG11	1.81	0.45
1:AA:2:GLN:OE1	1:AB:123:TYR:HA	2.17	0.45
1:AI:25:SER:HB2	1:AI:54:ARG:HG2	1.98	0.45
1:AJ:25:SER:HA	1:AJ:53:ASN:O	2.16	0.45
1:AU:57:LEU:HD21	1:AU:68:SER:HB2	1.98	0.45
1:AW:6:ARG:HD2	1:AZ:116:THR:HG21	1.99	0.45
1:BL:121:VAL:HG12	1:BL:122:GLU:HG3	1.99	0.45
1:BS:29:ILE:HG12	1:BS:50:VAL:HG22	1.99	0.45
1:BS:57:LEU:HD21	1:BS:68:SER:HB2	1.98	0.45
1:BW:2:GLN:OE1	1:BX:123:TYR:HA	2.17	0.45
1:BW:25:SER:CB	1:BW:54:ARG:HG2	2.47	0.45
1:BZ:25:SER:CB	1:BZ:54:ARG:HG2	2.47	0.45
1:CD:121:VAL:HG12	1:CD:122:GLU:HG3	1.99	0.45
1:CF:25:SER:HA	1:CF:53:ASN:O	2.16	0.45
1:CN:25:SER:HB2	1:CN:54:ARG:HG2	1.98	0.45
1:CQ:25:SER:HB2	1:CQ:54:ARG:HG2	1.98	0.45
1:CR:2:GLN:OE1	1:CS:123:TYR:HA	2.17	0.45
1:CX:2:GLN:OE1	1:CY:123:TYR:HA	2.17	0.45
1:DA:25:SER:CB	1:DA:54:ARG:HG2	2.47	0.45
1:DI:29:ILE:HG12	1:DI:50:VAL:HG22	1.99	0.45
1:AO:41:VAL:HG21	1:BV:60:ILE:HD12	1.99	0.45
1:AP:23:PHE:HE2	1:AR:84:VAL:HG11	1.81	0.45
1:AS:2:GLN:OE1	1:AT:123:TYR:HA	2.17	0.45
1:AU:25:SER:HB2	1:AU:54:ARG:HG2	1.98	0.45
1:AY:23:PHE:HE2	1:BA:84:VAL:HG11	1.81	0.45
1:BF:121:VAL:HG12	1:BF:122:GLU:HG3	1.99	0.45
1:BH:25:SER:CB	1:BH:54:ARG:HG2	2.47	0.45
1:BV:29:ILE:HG12	1:BV:50:VAL:HG22	1.99	0.45
1:CC:2:GLN:OE1	1:CD:123:TYR:HA	2.17	0.45
1:CP:121:VAL:HG12	1:CP:122:GLU:HG3	1.99	0.45
1:CX:25:SER:HA	1:CX:53:ASN:O	2.16	0.45
1:DC:29:ILE:HG12	1:DC:50:VAL:HG22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DD:25:SER:CB	1:DD:54:ARG:HG2	2.47	0.45
1:DF:57:LEU:HD21	1:DF:68:SER:HB2	1.98	0.45
1:AE:121:VAL:HG12	1:AE:122:GLU:HG3	1.99	0.44
1:AG:25:SER:CB	1:AG:54:ARG:HG2	2.47	0.44
1:AM:2:GLN:OE1	1:AN:123:TYR:HA	2.17	0.44
1:AO:78:THR:HA	1:BV:77:ARG:O	2.17	0.44
1:AS:23:PHE:HE2	1:AU:84:VAL:HG11	1.81	0.44
1:BB:25:SER:CB	1:BB:54:ARG:HG2	2.47	0.44
1:BD:91:LEU:HD22	1:CQ:105:ARG:NH2	2.32	0.44
1:BI:121:VAL:HG12	1:BI:122:GLU:HG3	1.99	0.44
1:CB:57:LEU:HD21	1:CB:68:SER:HB2	1.98	0.44
1:DB:121:VAL:HG12	1:DB:122:GLU:HG3	1.99	0.44
1:DL:29:ILE:HG12	1:DL:50:VAL:HG22	1.99	0.44
1:AI:29:ILE:HG12	1:AI:50:VAL:HG22	1.99	0.44
1:AO:29:ILE:HG12	1:AO:50:VAL:HG22	1.99	0.44
1:AP:25:SER:CB	1:AP:54:ARG:HG2	2.47	0.44
1:AV:112:LEU:HD21	1:BA:20:PRO:HB3	1.99	0.44
1:BA:29:ILE:HG12	1:BA:50:VAL:HG22	1.99	0.44
1:BC:67:CYS:HA	1:BO:63:CYS:HB2	1.98	0.44
1:BD:57:LEU:HD21	1:BD:68:SER:HB2	1.98	0.44
1:BE:2:GLN:OE1	1:BF:123:TYR:HA	2.17	0.44
1:BG:29:ILE:HG12	1:BG:50:VAL:HG22	1.99	0.44
1:BL:67:CYS:HA	1:DE:63:CYS:HB2	1.99	0.44
1:BQ:2:GLN:OE1	1:BR:123:TYR:HA	2.17	0.44
1:BU:67:CYS:HA	1:CA:63:CYS:HB2	1.99	0.44
1:BZ:2:GLN:OE1	1:CA:123:TYR:HA	2.17	0.44
1:CB:29:ILE:HG12	1:CB:50:VAL:HG22	1.99	0.44
1:DC:57:LEU:HD21	1:DC:68:SER:HB2	1.98	0.44
1:DI:57:LEU:HD21	1:DI:68:SER:HB2	1.98	0.44
1:AC:77:ARG:O	1:BJ:78:THR:HA	2.18	0.44
1:AG:2:GLN:OE1	1:AH:123:TYR:HA	2.17	0.44
1:AO:25:SER:HB2	1:AO:54:ARG:HG2	1.98	0.44
1:AO:36:LYS:HZ1	1:BV:72:GLU:HG3	1.82	0.44
1:AZ:121:VAL:HG12	1:AZ:122:GLU:HG3	1.99	0.44
1:BC:121:VAL:HG12	1:BC:122:GLU:HG3	1.99	0.44
1:BH:2:GLN:OE1	1:BI:123:TYR:HA	2.17	0.44
1:BJ:29:ILE:HG12	1:BJ:50:VAL:HG22	1.99	0.44
1:CC:25:SER:CB	1:CC:54:ARG:HG2	2.47	0.44
1:CX:25:SER:CB	1:CX:54:ARG:HG2	2.47	0.44
1:AA:25:SER:CB	1:AA:54:ARG:HG2	2.47	0.44
1:AJ:25:SER:CB	1:AJ:54:ARG:HG2	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AM:25:SER:CB	1:AM:54:ARG:HG2	2.47	0.44
1:AP:2:GLN:OE1	1:AQ:123:TYR:HA	2.17	0.44
1:BD:31:LEU:HD12	1:CQ:108:LEU:HD23	1.99	0.44
1:BE:25:SER:CB	1:BE:54:ARG:HG2	2.47	0.44
1:BQ:25:SER:CB	1:BQ:54:ARG:HG2	2.47	0.44
1:BY:29:ILE:HG12	1:BY:50:VAL:HG22	1.99	0.44
1:CR:25:SER:CB	1:CR:54:ARG:HG2	2.47	0.44
1:CT:25:SER:HB2	1:CT:54:ARG:HG2	1.98	0.44
1:CV:121:VAL:HG12	1:CV:122:GLU:HG3	1.99	0.44
1:AI:57:LEU:HD21	1:AI:68:SER:HB2	1.98	0.44
1:AR:57:LEU:HD21	1:AR:68:SER:HB2	1.98	0.44
1:AX:120:VAL:HG22	1:CH:4:ASN:HB3	2.00	0.44
1:BC:69:VAL:HB	1:BN:41:VAL:HG11	1.99	0.44
1:BK:25:SER:CB	1:BK:54:ARG:HG2	2.47	0.44
1:CA:9:LEU:HD22	1:CU:12:GLY:HA3	1.98	0.44
1:CC:25:SER:HA	1:CC:53:ASN:O	2.16	0.44
1:CG:6:ARG:HD2	1:CS:116:THR:HG21	1.99	0.44
1:DG:25:SER:CB	1:DG:54:ARG:HG2	2.47	0.44
1:AD:85:GLU:OE2	1:DH:24:ARG:NH1	2.51	0.44
1:AL:29:ILE:HG12	1:AL:50:VAL:HG22	1.99	0.44
1:AU:36:LYS:HZ1	1:CB:72:GLU:HG3	1.82	0.44
1:AV:25:SER:CB	1:AV:54:ARG:HG2	2.47	0.44
1:BN:25:SER:CB	1:BN:54:ARG:HG2	2.47	0.44
1:BT:25:SER:CB	1:BT:54:ARG:HG2	2.47	0.44
1:CG:9:LEU:HD22	1:CR:12:GLY:CA	2.46	0.44
1:CI:25:SER:CB	1:CI:54:ARG:HG2	2.47	0.44
1:AC:29:ILE:HG12	1:AC:50:VAL:HG22	1.99	0.44
1:AR:29:ILE:HG12	1:AR:50:VAL:HG22	1.99	0.44
1:AU:29:ILE:HG12	1:AU:50:VAL:HG22	1.99	0.44
1:CA:121:VAL:HG12	1:CA:122:GLU:HG3	1.99	0.44
1:CL:25:SER:CB	1:CL:54:ARG:HG2	2.47	0.44
1:CO:2:GLN:OE1	1:CP:123:TYR:HA	2.17	0.44
1:CO:25:SER:CB	1:CO:54:ARG:HG2	2.47	0.44
1:CT:29:ILE:HG12	1:CT:50:VAL:HG22	1.99	0.44
1:CW:29:ILE:HG12	1:CW:50:VAL:HG22	1.99	0.44
1:AB:121:VAL:HG12	1:AB:122:GLU:HG3	1.99	0.44
1:AC:19:ASP:HB3	1:AC:22:ASP:O	2.18	0.44
1:AC:121:VAL:O	1:BJ:2:GLN:HA	2.17	0.44
1:AU:19:ASP:HB3	1:AU:22:ASP:O	2.18	0.44
1:BA:19:ASP:HB3	1:BA:22:ASP:O	2.18	0.44
1:BO:121:VAL:HG12	1:BO:122:GLU:HG3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BY:19:ASP:HB3	1:BY:22:ASP:O	2.18	0.44
1:CG:121:VAL:HG12	1:CG:122:GLU:HG3	1.99	0.44
1:CW:19:ASP:HB3	1:CW:22:ASP:O	2.18	0.44
1:DG:2:GLN:OE1	1:DH:123:TYR:HA	2.17	0.44
1:DL:57:LEU:HD21	1:DL:68:SER:HB2	1.98	0.44
1:AC:79:THR:O	1:BJ:76:ILE:HA	2.17	0.44
1:AT:121:VAL:HG12	1:AT:122:GLU:HG3	1.99	0.44
1:AX:87:LYS:CB	1:CH:109:VAL:HG12	2.42	0.44
1:BD:120:VAL:HG22	1:CQ:4:ASN:HB3	1.99	0.44
1:CB:19:ASP:HB3	1:CB:22:ASP:O	2.18	0.44
1:CJ:121:VAL:HG12	1:CJ:122:GLU:HG3	1.99	0.44
1:CN:29:ILE:HG12	1:CN:50:VAL:HG22	1.99	0.44
1:DK:121:VAL:HG12	1:DK:122:GLU:HG3	1.99	0.44
1:AC:78:THR:HA	1:BJ:77:ARG:O	2.18	0.43
1:AH:121:VAL:HG12	1:AH:122:GLU:HG3	1.99	0.43
1:AX:17:TRP:CD2	1:CH:119:PRO:CG	3.01	0.43
1:AX:19:ASP:HB3	1:AX:22:ASP:O	2.18	0.43
1:AX:29:ILE:HG12	1:AX:50:VAL:HG22	1.99	0.43
1:CQ:29:ILE:HG12	1:CQ:50:VAL:HG22	1.99	0.43
1:CU:25:SER:CB	1:CU:54:ARG:HG2	2.47	0.43
1:DI:19:ASP:HB3	1:DI:22:ASP:O	2.18	0.43
1:DJ:25:SER:CB	1:DJ:54:ARG:HG2	2.47	0.43
1:AL:72:GLU:OE2	1:BS:83:SER:N	2.51	0.43
1:BG:97:HIS:CE1	1:CT:50:VAL:HG12	2.53	0.43
1:CH:19:ASP:HB3	1:CH:22:ASP:O	2.18	0.43
1:CI:2:GLN:HG3	1:CI:2:GLN:O	2.19	0.43
1:CY:121:VAL:HG12	1:CY:122:GLU:HG3	1.99	0.43
1:AA:85:GLU:OE2	1:DE:24:ARG:NH1	2.51	0.43
1:AB:6:ARG:HD2	1:AW:116:THR:HG21	2.00	0.43
1:AQ:24:ARG:NH1	1:BT:85:GLU:OE2	2.49	0.43
1:AW:24:ARG:NH1	1:AY:85:GLU:OE2	2.51	0.43
1:BD:121:VAL:O	1:CQ:2:GLN:HA	2.17	0.43
1:BN:2:GLN:HG3	1:BN:2:GLN:O	2.19	0.43
1:CF:25:SER:CB	1:CF:54:ARG:HG2	2.47	0.43
1:DB:69:VAL:HG12	1:DB:69:VAL:O	2.19	0.43
1:DF:55:ALA:HA	1:DF:72:GLU:O	2.19	0.43
1:AE:69:VAL:HG12	1:AE:69:VAL:O	2.19	0.43
1:AG:105:ARG:HH11	1:AH:91:LEU:HD22	1.84	0.43
1:AK:121:VAL:HG12	1:AK:122:GLU:HG3	1.99	0.43
1:AX:74:ILE:HG22	1:CH:82:GLY:HA2	2.01	0.43
1:BA:55:ALA:HA	1:BA:72:GLU:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BD:19:ASP:HB3	1:BD:22:ASP:O	2.18	0.43
1:BG:19:ASP:HB3	1:BG:22:ASP:O	2.18	0.43
1:BH:2:GLN:HG3	1:BH:2:GLN:O	2.19	0.43
1:BI:69:VAL:O	1:BI:69:VAL:HG12	2.19	0.43
1:CA:69:VAL:O	1:CA:69:VAL:HG12	2.19	0.43
1:CS:69:VAL:O	1:CS:69:VAL:HG12	2.19	0.43
1:CZ:19:ASP:HB3	1:CZ:22:ASP:O	2.18	0.43
1:DC:19:ASP:HB3	1:DC:22:ASP:O	2.18	0.43
1:DD:2:GLN:OE1	1:DE:123:TYR:HA	2.17	0.43
1:DE:121:VAL:HG12	1:DE:122:GLU:HG3	1.99	0.43
1:DF:29:ILE:HG12	1:DF:50:VAL:HG22	1.99	0.43
1:AL:19:ASP:HB3	1:AL:22:ASP:O	2.18	0.43
1:AX:78:THR:HA	1:CH:77:ARG:O	2.18	0.43
1:BG:31:LEU:HD12	1:CT:108:LEU:HD23	2.00	0.43
1:BQ:105:ARG:HH11	1:BR:91:LEU:HD22	1.84	0.43
1:BR:121:VAL:HG12	1:BR:122:GLU:HG3	1.99	0.43
1:BU:69:VAL:HB	1:BZ:41:VAL:HG11	2.00	0.43
1:BW:112:LEU:HD13	1:CE:6:ARG:HD3	2.00	0.43
1:CB:55:ALA:HA	1:CB:72:GLU:O	2.19	0.43
1:CI:105:ARG:HH11	1:CJ:91:LEU:HD22	1.84	0.43
1:CJ:69:VAL:O	1:CJ:69:VAL:HG12	2.19	0.43
1:CM:121:VAL:HG12	1:CM:122:GLU:HG3	1.99	0.43
1:CO:105:ARG:HH11	1:CP:91:LEU:HD22	1.84	0.43
1:CR:2:GLN:HG3	1:CR:2:GLN:O	2.19	0.43
1:CT:19:ASP:HB3	1:CT:22:ASP:O	2.18	0.43
1:DH:121:VAL:HG12	1:DH:122:GLU:HG3	1.99	0.43
1:DJ:2:GLN:O	1:DJ:2:GLN:HG3	2.19	0.43
1:AJ:2:GLN:O	1:AJ:2:GLN:HG3	2.19	0.43
1:AN:121:VAL:HG12	1:AN:122:GLU:HG3	1.99	0.43
1:AO:55:ALA:HA	1:AO:72:GLU:O	2.19	0.43
1:AR:72:GLU:OE2	1:BY:83:SER:HB2	2.18	0.43
1:AW:43:VAL:HB	1:AW:85:GLU:OE1	2.19	0.43
1:BJ:55:ALA:HA	1:BJ:72:GLU:O	2.19	0.43
1:BM:55:ALA:HA	1:BM:72:GLU:O	2.19	0.43
1:BP:19:ASP:HB3	1:BP:22:ASP:O	2.18	0.43
1:BW:2:GLN:O	1:BW:2:GLN:HG3	2.19	0.43
1:BX:121:VAL:HG12	1:BX:122:GLU:HG3	1.99	0.43
1:CD:69:VAL:O	1:CD:69:VAL:HG12	2.19	0.43
1:CH:55:ALA:HA	1:CH:72:GLU:O	2.19	0.43
1:CO:2:GLN:HG3	1:CO:2:GLN:O	2.19	0.43
1:DD:2:GLN:O	1:DD:2:GLN:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DH:43:VAL:HB	1:DH:85:GLU:OE1	2.19	0.43
1:AC:55:ALA:HA	1:AC:72:GLU:O	2.19	0.43
1:AI:55:ALA:HA	1:AI:72:GLU:O	2.19	0.43
1:AK:69:VAL:O	1:AK:69:VAL:HG12	2.19	0.43
1:AL:72:GLU:HG3	1:BS:36:LYS:HZ1	1.84	0.43
1:AO:19:ASP:HB3	1:AO:22:ASP:O	2.18	0.43
1:AO:79:THR:O	1:BV:76:ILE:HA	2.19	0.43
1:AS:105:ARG:HH11	1:AT:91:LEU:HD22	1.84	0.43
1:AV:2:GLN:HG3	1:AV:2:GLN:O	2.19	0.43
1:BA:121:VAL:O	1:CN:2:GLN:HA	2.19	0.43
1:BD:17:TRP:CD2	1:CQ:119:PRO:HG3	2.53	0.43
1:BI:43:VAL:HB	1:BI:85:GLU:OE1	2.19	0.43
1:BJ:19:ASP:HB3	1:BJ:22:ASP:O	2.18	0.43
1:BL:43:VAL:HB	1:BL:85:GLU:OE1	2.19	0.43
1:BQ:2:GLN:HG3	1:BQ:2:GLN:O	2.19	0.43
1:BV:55:ALA:HA	1:BV:72:GLU:O	2.19	0.43
1:CP:69:VAL:O	1:CP:69:VAL:HG12	2.19	0.43
1:CY:69:VAL:O	1:CY:69:VAL:HG12	2.19	0.43
1:AB:43:VAL:HB	1:AB:85:GLU:OE1	2.19	0.43
1:AB:69:VAL:O	1:AB:69:VAL:HG12	2.19	0.43
1:AF:55:ALA:HA	1:AF:72:GLU:O	2.19	0.43
1:AH:113:LEU:HB3	1:DB:8:GLN:HE21	1.84	0.43
1:AQ:43:VAL:HB	1:AQ:85:GLU:OE1	2.19	0.43
1:AQ:69:VAL:O	1:AQ:69:VAL:HG12	2.19	0.43
1:AR:87:LYS:CB	1:BY:109:VAL:HG12	2.42	0.43
1:AT:69:VAL:O	1:AT:69:VAL:HG12	2.19	0.43
1:AU:80:ILE:HG12	1:CB:76:ILE:HG12	2.00	0.43
1:AX:55:ALA:HA	1:AX:72:GLU:O	2.19	0.43
1:BS:55:ALA:HA	1:BS:72:GLU:O	2.19	0.43
1:BX:69:VAL:O	1:BX:69:VAL:HG12	2.19	0.43
1:CC:105:ARG:HH11	1:CD:91:LEU:HD22	1.84	0.43
1:CE:19:ASP:HB3	1:CE:22:ASP:O	2.18	0.43
1:CN:19:ASP:HB3	1:CN:22:ASP:O	2.18	0.43
1:CP:43:VAL:HB	1:CP:85:GLU:OE1	2.19	0.43
1:DA:105:ARG:HH11	1:DB:91:LEU:HD22	1.84	0.43
1:AJ:105:ARG:HH11	1:AK:91:LEU:HD22	1.84	0.43
1:AM:105:ARG:HH11	1:AN:91:LEU:HD22	1.84	0.43
1:AR:19:ASP:HB3	1:AR:22:ASP:O	2.18	0.43
1:AW:121:VAL:HG12	1:AW:122:GLU:HG3	1.99	0.43
1:AZ:69:VAL:O	1:AZ:69:VAL:HG12	2.19	0.43
1:BC:43:VAL:HB	1:BC:85:GLU:OE1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BD:29:ILE:HG12	1:BD:50:VAL:HG22	1.99	0.43
1:BD:55:ALA:HA	1:BD:72:GLU:O	2.19	0.43
1:BK:2:GLN:HG3	1:BK:2:GLN:O	2.19	0.43
1:BO:69:VAL:O	1:BO:69:VAL:HG12	2.19	0.43
1:BZ:2:GLN:O	1:BZ:2:GLN:HG3	2.19	0.43
1:CH:29:ILE:HG12	1:CH:50:VAL:HG22	1.99	0.43
1:CZ:55:ALA:HA	1:CZ:72:GLU:O	2.19	0.43
1:DA:2:GLN:HG3	1:DA:2:GLN:O	2.19	0.43
1:DH:69:VAL:O	1:DH:69:VAL:HG12	2.19	0.43
1:AA:2:GLN:HG3	1:AA:2:GLN:O	2.19	0.43
1:AN:69:VAL:O	1:AN:69:VAL:HG12	2.19	0.43
1:AU:119:PRO:HG2	1:CB:5:MET:HB2	2.01	0.43
1:AY:105:ARG:HH11	1:AZ:91:LEU:HD22	1.84	0.43
1:BF:43:VAL:HB	1:BF:85:GLU:OE1	2.19	0.43
1:BU:69:VAL:HG12	1:BU:69:VAL:O	2.19	0.43
1:BV:19:ASP:HB3	1:BV:22:ASP:O	2.18	0.43
1:BW:105:ARG:HH11	1:BX:91:LEU:HD22	1.84	0.43
1:CC:2:GLN:HG3	1:CC:2:GLN:O	2.19	0.43
1:CE:55:ALA:HA	1:CE:72:GLU:O	2.19	0.43
1:CK:55:ALA:HA	1:CK:72:GLU:O	2.19	0.43
1:CL:2:GLN:HG3	1:CL:2:GLN:O	2.19	0.43
1:CT:55:ALA:HA	1:CT:72:GLU:O	2.19	0.43
1:CV:43:VAL:HB	1:CV:85:GLU:OE1	2.19	0.43
1:DB:43:VAL:HB	1:DB:85:GLU:OE1	2.19	0.43
1:AK:6:ARG:HD2	1:BX:116:THR:HG21	2.01	0.42
1:BD:4:ASN:HA	1:CQ:120:VAL:HA	2.01	0.42
1:BM:19:ASP:HB3	1:BM:22:ASP:O	2.18	0.42
1:BM:29:ILE:HG12	1:BM:50:VAL:HG22	1.99	0.42
1:BR:43:VAL:HB	1:BR:85:GLU:OE1	2.19	0.42
1:BT:2:GLN:HG3	1:BT:2:GLN:O	2.19	0.42
1:BW:122:GLU:OE1	1:BX:1:ALA:N	2.40	0.42
1:CD:43:VAL:HB	1:CD:85:GLU:OE1	2.19	0.42
1:CL:105:ARG:HH11	1:CM:91:LEU:HD22	1.84	0.42
1:CM:113:LEU:HB3	1:CY:8:GLN:HE21	1.84	0.42
1:CU:2:GLN:HG3	1:CU:2:GLN:O	2.19	0.42
1:CU:55:ALA:HA	1:CU:72:GLU:O	2.20	0.42
1:CU:105:ARG:HH11	1:CV:91:LEU:HD22	1.84	0.42
1:CV:69:VAL:O	1:CV:69:VAL:HG12	2.19	0.42
1:DF:19:ASP:HB3	1:DF:22:ASP:O	2.18	0.42
1:DG:2:GLN:O	1:DG:2:GLN:HG3	2.19	0.42
1:DG:55:ALA:HA	1:DG:72:GLU:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DL:19:ASP:HB3	1:DL:22:ASP:O	2.18	0.42
1:DL:55:ALA:HA	1:DL:72:GLU:O	2.19	0.42
1:AA:105:ARG:HH11	1:AB:91:LEU:HD22	1.84	0.42
1:AL:78:THR:HA	1:BS:77:ARG:O	2.18	0.42
1:AM:2:GLN:O	1:AM:2:GLN:HG3	2.19	0.42
1:AP:2:GLN:O	1:AP:2:GLN:HG3	2.19	0.42
1:AW:69:VAL:O	1:AW:69:VAL:HG12	2.19	0.42
1:AY:2:GLN:HG3	1:AY:2:GLN:O	2.19	0.42
1:BE:2:GLN:HG3	1:BE:2:GLN:O	2.19	0.42
1:BG:83:SER:N	1:CT:72:GLU:OE2	2.53	0.42
1:BP:55:ALA:HA	1:BP:72:GLU:O	2.19	0.42
1:CK:19:ASP:HB3	1:CK:22:ASP:O	2.18	0.42
1:CM:43:VAL:HB	1:CM:85:GLU:OE1	2.19	0.42
1:CM:69:VAL:O	1:CM:69:VAL:HG12	2.19	0.42
1:DE:69:VAL:O	1:DE:69:VAL:HG12	2.19	0.42
1:AD:2:GLN:HG3	1:AD:2:GLN:O	2.19	0.42
1:AP:55:ALA:HA	1:AP:72:GLU:O	2.19	0.42
1:AX:71:ARG:C	1:CH:38:ALA:HB1	2.44	0.42
1:AZ:43:VAL:HB	1:AZ:85:GLU:OE1	2.19	0.42
1:BH:105:ARG:HH11	1:BI:91:LEU:HD22	1.84	0.42
1:BR:69:VAL:HG12	1:BR:69:VAL:O	2.19	0.42
1:BT:55:ALA:HA	1:BT:72:GLU:O	2.19	0.42
1:CF:2:GLN:HG3	1:CF:2:GLN:O	2.19	0.42
1:CF:105:ARG:HH11	1:CG:91:LEU:HD22	1.84	0.42
1:CJ:43:VAL:HB	1:CJ:85:GLU:OE1	2.19	0.42
1:CQ:19:ASP:HB3	1:CQ:22:ASP:O	2.18	0.42
1:CQ:55:ALA:HA	1:CQ:72:GLU:O	2.19	0.42
1:AD:105:ARG:HH11	1:AE:91:LEU:HD22	1.84	0.42
1:AR:97:HIS:CE1	1:BY:50:VAL:HG12	2.54	0.42
1:BL:69:VAL:O	1:BL:69:VAL:HG12	2.19	0.42
1:BN:105:ARG:HH11	1:BO:91:LEU:HD22	1.84	0.42
1:BT:112:LEU:HD13	1:CB:6:ARG:HD3	2.02	0.42
1:CH:104:ALA:HB2	1:CH:117:ILE:HD13	2.02	0.42
1:CI:55:ALA:HA	1:CI:72:GLU:O	2.19	0.42
1:CQ:104:ALA:HB2	1:CQ:117:ILE:HD13	2.02	0.42
1:CX:105:ARG:HH11	1:CY:91:LEU:HD22	1.84	0.42
1:CY:43:VAL:HB	1:CY:85:GLU:OE1	2.19	0.42
1:DD:105:ARG:HH11	1:DE:91:LEU:HD22	1.84	0.42
1:AE:43:VAL:HB	1:AE:85:GLU:OE1	2.19	0.42
1:AF:19:ASP:HB3	1:AF:22:ASP:O	2.18	0.42
1:AI:19:ASP:HB3	1:AI:22:ASP:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AS:2:GLN:HG3	1:AS:2:GLN:O	2.19	0.42
1:AT:43:VAL:HB	1:AT:85:GLU:OE1	2.19	0.42
1:AU:55:ALA:HA	1:AU:72:GLU:O	2.19	0.42
1:AV:55:ALA:HA	1:AV:72:GLU:O	2.19	0.42
1:AX:79:THR:O	1:CH:76:ILE:HA	2.20	0.42
1:BD:104:ALA:HB2	1:BD:117:ILE:HD13	2.02	0.42
1:BF:6:ARG:HD2	1:BI:116:THR:HG21	2.00	0.42
1:BW:55:ALA:HA	1:BW:72:GLU:O	2.19	0.42
1:CF:55:ALA:HA	1:CF:72:GLU:O	2.19	0.42
1:CN:55:ALA:HA	1:CN:72:GLU:O	2.19	0.42
1:CS:43:VAL:HB	1:CS:85:GLU:OE1	2.19	0.42
1:DD:55:ALA:HA	1:DD:72:GLU:O	2.20	0.42
1:DI:104:ALA:HB2	1:DI:117:ILE:HD13	2.02	0.42
1:DJ:55:ALA:HA	1:DJ:72:GLU:O	2.19	0.42
1:AG:33:VAL:HG11	1:DB:23:PHE:CE2	2.41	0.42
1:AX:2:GLN:HA	1:CH:122:GLU:HB2	2.01	0.42
1:BC:69:VAL:O	1:BC:69:VAL:HG12	2.19	0.42
1:BS:19:ASP:HB3	1:BS:22:ASP:O	2.18	0.42
1:BZ:55:ALA:HA	1:BZ:72:GLU:O	2.20	0.42
1:DA:55:ALA:HA	1:DA:72:GLU:O	2.19	0.42
1:DJ:105:ARG:HH11	1:DK:91:LEU:HD22	1.84	0.42
1:AK:43:VAL:HB	1:AK:85:GLU:OE1	2.19	0.42
1:AM:55:ALA:HA	1:AM:72:GLU:O	2.19	0.42
1:AR:55:ALA:HA	1:AR:72:GLU:O	2.19	0.42
1:AR:120:VAL:HA	1:BY:4:ASN:HA	2.01	0.42
1:BB:2:GLN:HG3	1:BB:2:GLN:O	2.19	0.42
1:BB:55:ALA:HA	1:BB:72:GLU:O	2.20	0.42
1:BE:55:ALA:HA	1:BE:72:GLU:O	2.19	0.42
1:BO:43:VAL:HB	1:BO:85:GLU:OE1	2.19	0.42
1:BW:107:ASP:OD1	1:CE:6:ARG:NH1	2.49	0.42
1:BX:43:VAL:HB	1:BX:85:GLU:OE1	2.19	0.42
1:CB:104:ALA:HB2	1:CB:117:ILE:HD13	2.02	0.42
1:CC:55:ALA:HA	1:CC:72:GLU:O	2.19	0.42
1:CI:12:GLY:HA3	1:CV:9:LEU:HD22	2.00	0.42
1:CL:55:ALA:HA	1:CL:72:GLU:O	2.19	0.42
1:DC:55:ALA:HA	1:DC:72:GLU:O	2.19	0.42
1:DK:69:VAL:O	1:DK:69:VAL:HG12	2.19	0.42
1:AH:67:CYS:HA	1:BF:63:CYS:HB2	2.00	0.42
1:AI:104:ALA:HB2	1:AI:117:ILE:HD13	2.02	0.42
1:AJ:72:GLU:HG3	1:AK:36:LYS:HE2	2.02	0.42
1:AO:80:ILE:HG12	1:BV:76:ILE:HG12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AR:5:MET:HG3	1:BY:121:VAL:HG23	2.00	0.42
1:CO:55:ALA:HA	1:CO:72:GLU:O	2.19	0.42
1:CW:55:ALA:HA	1:CW:72:GLU:O	2.19	0.42
1:CX:2:GLN:HG3	1:CX:2:GLN:O	2.19	0.42
1:CX:55:ALA:HA	1:CX:72:GLU:O	2.19	0.42
1:DE:43:VAL:HB	1:DE:85:GLU:OE1	2.19	0.42
1:DG:105:ARG:HH11	1:DH:91:LEU:HD22	1.84	0.42
1:AA:55:ALA:HA	1:AA:72:GLU:O	2.19	0.42
1:AB:24:ARG:HB3	1:AB:55:ALA:HB3	2.02	0.42
1:AH:69:VAL:HG12	1:AH:69:VAL:O	2.19	0.42
1:AL:55:ALA:HA	1:AL:72:GLU:O	2.19	0.42
1:BE:105:ARG:HH11	1:BF:91:LEU:HD22	1.84	0.42
1:BG:38:ALA:HB1	1:CT:71:ARG:O	2.20	0.42
1:BN:55:ALA:HA	1:BN:72:GLU:O	2.20	0.42
1:BT:105:ARG:HH11	1:BU:91:LEU:HD22	1.84	0.42
1:BU:24:ARG:HB3	1:BU:55:ALA:HB3	2.02	0.42
1:BY:55:ALA:HA	1:BY:72:GLU:O	2.19	0.42
1:CL:72:GLU:HG3	1:CM:36:LYS:HE2	2.02	0.42
1:DF:104:ALA:HB2	1:DF:117:ILE:HD13	2.02	0.42
1:DI:55:ALA:HA	1:DI:72:GLU:O	2.19	0.42
1:DL:104:ALA:HB2	1:DL:117:ILE:HD13	2.02	0.42
1:AA:72:GLU:HG3	1:AB:36:LYS:HE2	2.02	0.42
1:AH:3:HIS:CE1	1:AH:21:ASN:HD22	2.38	0.42
1:AH:43:VAL:HB	1:AH:85:GLU:OE1	2.19	0.42
1:AI:36:LYS:HZ1	1:BP:72:GLU:HG3	1.84	0.42
1:AN:24:ARG:HB3	1:AN:55:ALA:HB3	2.02	0.42
1:AN:43:VAL:HB	1:AN:85:GLU:OE1	2.19	0.42
1:AV:105:ARG:HH11	1:AW:91:LEU:HD22	1.84	0.42
1:BC:24:ARG:HB3	1:BC:55:ALA:HB3	2.02	0.42
1:BG:55:ALA:HA	1:BG:72:GLU:O	2.19	0.42
1:BN:72:GLU:HG3	1:BO:36:LYS:HE2	2.02	0.42
1:BS:104:ALA:HB2	1:BS:117:ILE:HD13	2.02	0.42
1:BU:43:VAL:HB	1:BU:85:GLU:OE1	2.19	0.42
1:CA:24:ARG:HB3	1:CA:55:ALA:HB3	2.02	0.42
1:CC:72:GLU:HG3	1:CD:36:LYS:HE2	2.02	0.42
1:CG:69:VAL:O	1:CG:69:VAL:HG12	2.19	0.42
1:CS:3:HIS:CE1	1:CS:21:ASN:HD22	2.38	0.42
1:CW:104:ALA:HB2	1:CW:117:ILE:HD13	2.02	0.42
1:CZ:104:ALA:HB2	1:CZ:117:ILE:HD13	2.02	0.42
1:DE:24:ARG:HB3	1:DE:55:ALA:HB3	2.02	0.42
1:DK:43:VAL:HB	1:DK:85:GLU:OE1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AE:3:HIS:CE1	1:AE:21:ASN:HD22	2.38	0.41
1:AJ:19:ASP:HB3	1:AJ:22:ASP:O	2.20	0.41
1:AR:83:SER:N	1:BY:72:GLU:OE2	2.52	0.41
1:AY:72:GLU:HG3	1:AZ:36:LYS:HE2	2.02	0.41
1:BF:69:VAL:O	1:BF:69:VAL:HG12	2.19	0.41
1:BH:55:ALA:HA	1:BH:72:GLU:O	2.20	0.41
1:BJ:104:ALA:HB2	1:BJ:117:ILE:HD13	2.02	0.41
1:BK:105:ARG:HH11	1:BL:91:LEU:HD22	1.84	0.41
1:BM:104:ALA:HB2	1:BM:117:ILE:HD13	2.02	0.41
1:BN:19:ASP:HB3	1:BN:22:ASP:O	2.20	0.41
1:BO:3:HIS:CE1	1:BO:21:ASN:HD22	2.38	0.41
1:BZ:105:ARG:HH11	1:CA:91:LEU:HD22	1.84	0.41
1:CA:43:VAL:HB	1:CA:85:GLU:OE1	2.19	0.41
1:CD:24:ARG:HB3	1:CD:55:ALA:HB3	2.02	0.41
1:CF:72:GLU:HG3	1:CG:36:LYS:HE2	2.02	0.41
1:CO:19:ASP:HB3	1:CO:22:ASP:O	2.21	0.41
1:CU:72:GLU:HG3	1:CV:36:LYS:HE2	2.02	0.41
1:CV:24:ARG:HB3	1:CV:55:ALA:HB3	2.02	0.41
1:DD:19:ASP:HB3	1:DD:22:ASP:O	2.20	0.41
1:DH:3:HIS:CE1	1:DH:21:ASN:HD22	2.38	0.41
1:AB:6:ARG:HD2	1:AW:116:THR:CG2	2.51	0.41
1:AD:19:ASP:HB3	1:AD:22:ASP:O	2.20	0.41
1:AD:55:ALA:HA	1:AD:72:GLU:O	2.20	0.41
1:AD:72:GLU:HG3	1:AE:36:LYS:HE2	2.02	0.41
1:AG:2:GLN:HG3	1:AG:2:GLN:O	2.19	0.41
1:BB:105:ARG:HH11	1:BC:91:LEU:HD22	1.84	0.41
1:BQ:19:ASP:HB3	1:BQ:22:ASP:O	2.20	0.41
1:BX:3:HIS:CE1	1:BX:21:ASN:HD22	2.38	0.41
1:CI:122:GLU:OE1	1:CJ:1:ALA:N	2.40	0.41
1:CO:72:GLU:HG3	1:CP:36:LYS:HE2	2.02	0.41
1:CY:3:HIS:CE1	1:CY:21:ASN:HD22	2.38	0.41
1:DH:24:ARG:HB3	1:DH:55:ALA:HB3	2.02	0.41
1:AE:24:ARG:HB3	1:AE:55:ALA:HB3	2.02	0.41
1:AL:72:GLU:CG	1:BS:36:LYS:HZ1	2.34	0.41
1:AO:17:TRP:CE3	1:BV:119:PRO:HG3	2.55	0.41
1:AP:19:ASP:HB3	1:AP:22:ASP:O	2.21	0.41
1:AQ:3:HIS:CE1	1:AQ:21:ASN:HD22	2.38	0.41
1:AU:104:ALA:HB2	1:AU:117:ILE:HD13	2.02	0.41
1:BB:72:GLU:HG3	1:BC:36:LYS:HE2	2.02	0.41
1:BI:3:HIS:CE1	1:BI:21:ASN:HD22	2.38	0.41
1:BK:55:ALA:HA	1:BK:72:GLU:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CC:19:ASP:HB3	1:CC:22:ASP:O	2.21	0.41
1:CD:3:HIS:CE1	1:CD:21:ASN:HD22	2.38	0.41
1:CJ:3:HIS:CE1	1:CJ:21:ASN:HD22	2.38	0.41
1:CP:24:ARG:HB3	1:CP:55:ALA:HB3	2.02	0.41
1:CX:72:GLU:HG3	1:CY:36:LYS:HE2	2.02	0.41
1:DB:3:HIS:CE1	1:DB:21:ASN:HD22	2.38	0.41
1:AG:72:GLU:HG3	1:AH:36:LYS:HE2	2.02	0.41
1:AJ:55:ALA:HA	1:AJ:72:GLU:O	2.19	0.41
1:AL:76:ILE:HA	1:BS:79:THR:O	2.20	0.41
1:AM:19:ASP:HB3	1:AM:22:ASP:O	2.21	0.41
1:AQ:24:ARG:HB3	1:AQ:55:ALA:HB3	2.02	0.41
1:AX:76:ILE:HA	1:CH:79:THR:O	2.21	0.41
1:BE:72:GLU:HG3	1:BF:36:LYS:HE2	2.02	0.41
1:BQ:55:ALA:HA	1:BQ:72:GLU:O	2.19	0.41
1:BV:104:ALA:HB2	1:BV:117:ILE:HD13	2.02	0.41
1:CG:24:ARG:HB3	1:CG:55:ALA:HB3	2.02	0.41
1:CG:43:VAL:HB	1:CG:85:GLU:OE1	2.19	0.41
1:DG:19:ASP:HB3	1:DG:22:ASP:O	2.21	0.41
1:AC:97:HIS:CE1	1:BJ:50:VAL:HG12	2.56	0.41
1:AE:24:ARG:NH1	1:AS:85:GLU:OE2	2.52	0.41
1:AF:104:ALA:HB2	1:AF:117:ILE:HD13	2.02	0.41
1:AK:3:HIS:CE1	1:AK:21:ASN:HD22	2.38	0.41
1:AN:3:HIS:CE1	1:AN:21:ASN:HD22	2.38	0.41
1:AN:69:VAL:HB	1:BQ:41:VAL:HG11	2.02	0.41
1:AR:76:ILE:HD13	1:BY:94:LEU:HA	2.03	0.41
1:AU:79:THR:O	1:CB:76:ILE:HA	2.20	0.41
1:AW:3:HIS:CE1	1:AW:21:ASN:HD22	2.38	0.41
1:AY:55:ALA:HA	1:AY:72:GLU:O	2.20	0.41
1:AZ:3:HIS:CE1	1:AZ:21:ASN:HD22	2.38	0.41
1:BA:104:ALA:HB2	1:BA:117:ILE:HD13	2.02	0.41
1:BW:19:ASP:HB3	1:BW:22:ASP:O	2.21	0.41
1:CF:19:ASP:HB3	1:CF:22:ASP:O	2.21	0.41
1:CP:63:CYS:HB2	1:CS:67:CYS:HA	2.01	0.41
1:DK:3:HIS:CE1	1:DK:21:ASN:HD22	2.38	0.41
1:AA:79:THR:O	1:AB:76:ILE:HA	2.21	0.41
1:AB:3:HIS:CE1	1:AB:21:ASN:HD22	2.38	0.41
1:AG:19:ASP:HB3	1:AG:22:ASP:O	2.21	0.41
1:AK:24:ARG:HB3	1:AK:55:ALA:HB3	2.02	0.41
1:AL:94:LEU:HA	1:BS:76:ILE:HD13	2.03	0.41
1:AO:41:VAL:HG11	1:BV:60:ILE:HD11	2.03	0.41
1:AS:19:ASP:HB3	1:AS:22:ASP:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AT:3:HIS:CE1	1:AT:21:ASN:HD22	2.38	0.41
1:AW:24:ARG:HB3	1:AW:55:ALA:HB3	2.02	0.41
1:BB:19:ASP:HB3	1:BB:22:ASP:O	2.20	0.41
1:BK:72:GLU:HG3	1:BL:36:LYS:HE2	2.02	0.41
1:BT:19:ASP:HB3	1:BT:22:ASP:O	2.21	0.41
1:CG:69:VAL:CG2	1:CS:60:ILE:HD13	2.50	0.41
1:CN:104:ALA:HB2	1:CN:117:ILE:HD13	2.02	0.41
1:CR:19:ASP:HB3	1:CR:22:ASP:O	2.21	0.41
1:CR:105:ARG:HH11	1:CS:91:LEU:HD22	1.84	0.41
1:DA:19:ASP:HB3	1:DA:22:ASP:O	2.20	0.41
1:DA:79:THR:O	1:DB:76:ILE:HA	2.21	0.41
1:AC:4:ASN:HB3	1:BJ:120:VAL:HG22	2.01	0.41
1:AG:55:ALA:HA	1:AG:72:GLU:O	2.19	0.41
1:AL:104:ALA:HB2	1:AL:117:ILE:HD13	2.02	0.41
1:AP:72:GLU:HG3	1:AQ:36:LYS:HE2	2.02	0.41
1:AU:76:ILE:HD13	1:CB:94:LEU:HA	2.02	0.41
1:AX:104:ALA:HB2	1:AX:117:ILE:HD13	2.02	0.41
1:AZ:24:ARG:HB3	1:AZ:55:ALA:HB3	2.02	0.41
1:BE:112:LEU:HD13	1:BJ:6:ARG:HD3	2.01	0.41
1:BG:104:ALA:HB2	1:BG:117:ILE:HD13	2.02	0.41
1:BT:72:GLU:HG3	1:BU:36:LYS:HE2	2.02	0.41
1:CA:3:HIS:CE1	1:CA:21:ASN:HD22	2.38	0.41
1:CF:79:THR:O	1:CG:76:ILE:HA	2.21	0.41
1:CG:3:HIS:CE1	1:CG:21:ASN:HD22	2.38	0.41
1:CI:19:ASP:HB3	1:CI:22:ASP:O	2.20	0.41
1:CI:79:THR:O	1:CJ:76:ILE:HA	2.21	0.41
1:CM:3:HIS:CE1	1:CM:21:ASN:HD22	2.38	0.41
1:CT:104:ALA:HB2	1:CT:117:ILE:HD13	2.02	0.41
1:DJ:19:ASP:HB3	1:DJ:22:ASP:O	2.20	0.41
1:AT:24:ARG:HB3	1:AT:55:ALA:HB3	2.02	0.41
1:AV:72:GLU:HG3	1:AW:36:LYS:HE2	2.02	0.41
1:BH:72:GLU:HG3	1:BI:36:LYS:HE2	2.02	0.41
1:BH:79:THR:O	1:BI:76:ILE:HA	2.21	0.41
1:BK:19:ASP:HB3	1:BK:22:ASP:O	2.21	0.41
1:BL:3:HIS:CE1	1:BL:21:ASN:HD22	2.38	0.41
1:BR:3:HIS:CE1	1:BR:21:ASN:HD22	2.38	0.41
1:CE:104:ALA:HB2	1:CE:117:ILE:HD13	2.02	0.41
1:CL:79:THR:O	1:CM:76:ILE:HA	2.21	0.41
1:CO:79:THR:O	1:CP:76:ILE:HA	2.21	0.41
1:CU:79:THR:O	1:CV:76:ILE:HA	2.21	0.41
1:CX:19:ASP:HB3	1:CX:22:ASP:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DG:72:GLU:HG3	1:DH:36:LYS:HE2	2.02	0.41
1:AD:79:THR:O	1:AE:76:ILE:HA	2.21	0.41
1:AP:79:THR:O	1:AQ:76:ILE:HA	2.21	0.41
1:AP:105:ARG:HH11	1:AQ:91:LEU:HD22	1.84	0.41
1:AR:22:ASP:OD2	1:AR:24:ARG:HB2	2.21	0.41
1:AS:55:ALA:HA	1:AS:72:GLU:O	2.19	0.41
1:AU:72:GLU:OE2	1:CB:83:SER:N	2.53	0.41
1:AX:80:ILE:HG12	1:CH:76:ILE:HG23	2.03	0.41
1:BA:87:LYS:HB2	1:CN:109:VAL:CG1	2.45	0.41
1:BE:19:ASP:HB3	1:BE:22:ASP:O	2.21	0.41
1:BL:8:GLN:HE21	1:DE:113:LEU:HB3	1.86	0.41
1:BP:104:ALA:HB2	1:BP:117:ILE:HD13	2.02	0.41
1:BW:72:GLU:HG3	1:BX:36:LYS:HE2	2.02	0.41
1:BY:104:ALA:HB2	1:BY:117:ILE:HD13	2.02	0.41
1:BZ:19:ASP:HB3	1:BZ:22:ASP:O	2.20	0.41
1:CK:22:ASP:OD2	1:CK:24:ARG:HB2	2.21	0.41
1:CR:55:ALA:HA	1:CR:72:GLU:O	2.19	0.41
1:CV:3:HIS:CE1	1:CV:21:ASN:HD22	2.38	0.41
1:CX:79:THR:O	1:CY:76:ILE:HA	2.21	0.41
1:CY:24:ARG:HB3	1:CY:55:ALA:HB3	2.02	0.41
1:DB:24:ARG:HB3	1:DB:55:ALA:HB3	2.02	0.41
1:AC:104:ALA:HB2	1:AC:117:ILE:HD13	2.02	0.41
1:AO:104:ALA:HB2	1:AO:117:ILE:HD13	2.02	0.41
1:AU:22:ASP:OD2	1:AU:24:ARG:HB2	2.21	0.41
1:AW:23:PHE:CE2	1:AY:33:VAL:HG11	2.45	0.41
1:AX:119:PRO:HG2	1:CH:5:MET:HB2	2.03	0.41
1:AZ:6:ARG:NH2	1:BL:113:LEU:O	2.54	0.41
1:BF:3:HIS:CE1	1:BF:21:ASN:HD22	2.38	0.41
1:BL:24:ARG:HB3	1:BL:55:ALA:HB3	2.02	0.41
1:BU:23:PHE:CD1	1:BU:23:PHE:N	2.89	0.41
1:BX:24:ARG:HB3	1:BX:55:ALA:HB3	2.02	0.41
1:BZ:79:THR:O	1:CA:76:ILE:HA	2.21	0.41
1:CK:104:ALA:HB2	1:CK:117:ILE:HD13	2.02	0.41
1:CS:23:PHE:CD1	1:CS:23:PHE:N	2.89	0.41
1:CU:19:ASP:HB3	1:CU:22:ASP:O	2.21	0.41
1:DA:72:GLU:HG3	1:DB:36:LYS:HE2	2.02	0.41
1:DD:79:THR:O	1:DE:76:ILE:HA	2.21	0.41
1:DI:22:ASP:OD2	1:DI:24:ARG:HB2	2.21	0.41
1:DJ:79:THR:O	1:DK:76:ILE:HA	2.21	0.41
1:AC:72:GLU:OE2	1:BJ:83:SER:N	2.53	0.40
1:AL:80:ILE:HG12	1:BS:76:ILE:HG12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AQ:63:CYS:HB2	1:CJ:67:CYS:HA	2.03	0.40
1:AY:79:THR:O	1:AZ:76:ILE:HA	2.21	0.40
1:BA:22:ASP:OD2	1:BA:24:ARG:HB2	2.21	0.40
1:BC:23:PHE:CD1	1:BC:23:PHE:N	2.89	0.40
1:BD:124:THR:OG1	1:CQ:2:GLN:OE1	2.31	0.40
1:BP:22:ASP:OD2	1:BP:24:ARG:HB2	2.21	0.40
1:BR:24:ARG:HB3	1:BR:55:ALA:HB3	2.02	0.40
1:BS:22:ASP:OD2	1:BS:24:ARG:HB2	2.21	0.40
1:BY:22:ASP:OD2	1:BY:24:ARG:HB2	2.21	0.40
1:BZ:72:GLU:HG3	1:CA:36:LYS:HE2	2.02	0.40
1:CQ:22:ASP:OD2	1:CQ:24:ARG:HB2	2.21	0.40
1:AL:4:ASN:HA	1:BS:120:VAL:HA	2.03	0.40
1:AL:119:PRO:HG2	1:BS:5:MET:HB2	2.03	0.40
1:AS:72:GLU:HG3	1:AT:36:LYS:HE2	2.02	0.40
1:AX:22:ASP:OD2	1:AX:24:ARG:HB2	2.22	0.40
1:BH:19:ASP:HB3	1:BH:22:ASP:O	2.21	0.40
1:BI:24:ARG:HB3	1:BI:55:ALA:HB3	2.02	0.40
1:BK:79:THR:O	1:BL:76:ILE:HA	2.21	0.40
1:BW:49:GLU:HA	1:BW:78:THR:O	2.22	0.40
1:CL:19:ASP:HB3	1:CL:22:ASP:O	2.21	0.40
1:CP:3:HIS:CE1	1:CP:21:ASN:HD22	2.38	0.40
1:CS:24:ARG:HB3	1:CS:55:ALA:HB3	2.02	0.40
1:CZ:22:ASP:OD2	1:CZ:24:ARG:HB2	2.21	0.40
1:DL:22:ASP:OD2	1:DL:24:ARG:HB2	2.21	0.40
1:AF:22:ASP:OD2	1:AF:24:ARG:HB2	2.21	0.40
1:AK:23:PHE:CD1	1:AK:23:PHE:N	2.89	0.40
1:AM:72:GLU:HG3	1:AN:36:LYS:HE2	2.02	0.40
1:AV:79:THR:O	1:AW:76:ILE:HA	2.21	0.40
1:BB:79:THR:O	1:BC:76:ILE:HA	2.21	0.40
1:BC:3:HIS:CE1	1:BC:21:ASN:HD22	2.38	0.40
1:BO:24:ARG:HB3	1:BO:55:ALA:HB3	2.02	0.40
1:BT:79:THR:O	1:BU:76:ILE:HA	2.21	0.40
1:BW:79:THR:O	1:BX:76:ILE:HA	2.21	0.40
1:CJ:24:ARG:HB3	1:CJ:55:ALA:HB3	2.02	0.40
1:CN:22:ASP:OD2	1:CN:24:ARG:HB2	2.21	0.40
1:DD:72:GLU:HG3	1:DE:36:LYS:HE2	2.02	0.40
1:DE:3:HIS:CE1	1:DE:21:ASN:HD22	2.38	0.40
1:DJ:49:GLU:HA	1:DJ:78:THR:O	2.22	0.40
1:AO:22:ASP:OD2	1:AO:24:ARG:HB2	2.21	0.40
1:AS:79:THR:O	1:AT:76:ILE:HA	2.21	0.40
1:AV:19:ASP:HB3	1:AV:22:ASP:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AY:19:ASP:HB3	1:AY:22:ASP:O	2.21	0.40
1:BD:27:PHE:CZ	1:CQ:100:ASN:HB3	2.57	0.40
1:BH:49:GLU:HA	1:BH:78:THR:O	2.22	0.40
1:BM:22:ASP:OD2	1:BM:24:ARG:HB2	2.21	0.40
1:BN:49:GLU:HA	1:BN:78:THR:O	2.22	0.40
1:BQ:49:GLU:HA	1:BQ:78:THR:O	2.22	0.40
1:BQ:72:GLU:HG3	1:BR:36:LYS:HE2	2.02	0.40
1:CC:79:THR:O	1:CD:76:ILE:HA	2.21	0.40
1:CL:49:GLU:HA	1:CL:78:THR:O	2.22	0.40
1:CR:72:GLU:HG3	1:CS:36:LYS:HE2	2.02	0.40
1:AC:2:GLN:HA	1:BJ:121:VAL:O	2.22	0.40
1:AG:79:THR:O	1:AH:76:ILE:HA	2.21	0.40
1:AH:24:ARG:HB3	1:AH:55:ALA:HB3	2.02	0.40
1:AJ:79:THR:O	1:AK:76:ILE:HA	2.21	0.40
1:AK:63:CYS:HB2	1:CM:67:CYS:HA	2.02	0.40
1:AY:112:LEU:HD11	1:BM:20:PRO:HB3	2.04	0.40
1:BE:79:THR:O	1:BF:76:ILE:HA	2.21	0.40
1:BI:8:GLN:HE21	1:DK:113:LEU:HB3	1.87	0.40
1:BQ:79:THR:O	1:BR:76:ILE:HA	2.21	0.40
1:BU:3:HIS:CE1	1:BU:21:ASN:HD22	2.38	0.40
1:BV:22:ASP:OD2	1:BV:24:ARG:HB2	2.21	0.40
1:CR:79:THR:O	1:CS:76:ILE:HA	2.21	0.40
1:CX:49:GLU:HA	1:CX:78:THR:O	2.22	0.40
1:DD:49:GLU:HA	1:DD:78:THR:O	2.22	0.40

All (2) 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:AR:61:GLU:OE2	1:CN:61:GLU:OE1[4_546]	2.16	0.04
1:CZ:124:THR:OG1	1:DC:2:GLN:OE1[2_555]	2.17	0.03

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AA	123/126 (98%)	121 (98%)	2 (2%)	0	100	100
1	AB	122/126 (97%)	119 (98%)	3 (2%)	0	100	100
1	AC	122/126 (97%)	120 (98%)	2 (2%)	0	100	100
1	AD	123/126 (98%)	121 (98%)	2 (2%)	0	100	100
1	AE	122/126 (97%)	119 (98%)	3 (2%)	0	100	100
1	AF	122/126 (97%)	120 (98%)	2 (2%)	0	100	100
1	AG	123/126 (98%)	121 (98%)	2 (2%)	0	100	100
1	AH	122/126 (97%)	119 (98%)	3 (2%)	0	100	100
1	AI	122/126 (97%)	120 (98%)	2 (2%)	0	100	100
1	AJ	123/126 (98%)	121 (98%)	2 (2%)	0	100	100
1	AK	122/126 (97%)	119 (98%)	3 (2%)	0	100	100
1	AL	122/126 (97%)	120 (98%)	2 (2%)	0	100	100
1	AM	123/126 (98%)	121 (98%)	2 (2%)	0	100	100
1	AN	122/126 (97%)	119 (98%)	3 (2%)	0	100	100
1	AO	122/126 (97%)	120 (98%)	2 (2%)	0	100	100
1	AP	123/126 (98%)	121 (98%)	2 (2%)	0	100	100
1	AQ	122/126 (97%)	119 (98%)	3 (2%)	0	100	100
1	AR	122/126 (97%)	120 (98%)	2 (2%)	0	100	100
1	AS	123/126 (98%)	121 (98%)	2 (2%)	0	100	100
1	AT	122/126 (97%)	119 (98%)	3 (2%)	0	100	100
1	AU	122/126 (97%)	120 (98%)	2 (2%)	0	100	100
1	AV	123/126 (98%)	121 (98%)	2 (2%)	0	100	100
1	AW	122/126 (97%)	119 (98%)	3 (2%)	0	100	100
1	AX	122/126 (97%)	120 (98%)	2 (2%)	0	100	100
1	AY	123/126 (98%)	121 (98%)	2 (2%)	0	100	100
1	AZ	122/126 (97%)	119 (98%)	3 (2%)	0	100	100
1	BA	122/126 (97%)	120 (98%)	2 (2%)	0	100	100
1	BB	123/126 (98%)	121 (98%)	2 (2%)	0	100	100
1	BC	122/126 (97%)	119 (98%)	3 (2%)	0	100	100
1	BD	122/126 (97%)	120 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	BE	123/126 (98%)	121 (98%)	2 (2%)	0	100	100
1	BF	122/126 (97%)	119 (98%)	3 (2%)	0	100	100
1	BG	122/126 (97%)	120 (98%)	2 (2%)	0	100	100
1	BH	123/126 (98%)	121 (98%)	2 (2%)	0	100	100
1	BI	122/126 (97%)	119 (98%)	3 (2%)	0	100	100
1	BJ	122/126 (97%)	120 (98%)	2 (2%)	0	100	100
1	BK	123/126 (98%)	121 (98%)	2 (2%)	0	100	100
1	BL	122/126 (97%)	119 (98%)	3 (2%)	0	100	100
1	BM	122/126 (97%)	120 (98%)	2 (2%)	0	100	100
1	BN	123/126 (98%)	121 (98%)	2 (2%)	0	100	100
1	BO	122/126 (97%)	119 (98%)	3 (2%)	0	100	100
1	BP	122/126 (97%)	120 (98%)	2 (2%)	0	100	100
1	BQ	123/126 (98%)	121 (98%)	2 (2%)	0	100	100
1	BR	122/126 (97%)	119 (98%)	3 (2%)	0	100	100
1	BS	122/126 (97%)	120 (98%)	2 (2%)	0	100	100
1	BT	123/126 (98%)	121 (98%)	2 (2%)	0	100	100
1	BU	122/126 (97%)	119 (98%)	3 (2%)	0	100	100
1	BV	122/126 (97%)	120 (98%)	2 (2%)	0	100	100
1	BW	123/126 (98%)	121 (98%)	2 (2%)	0	100	100
1	BX	122/126 (97%)	119 (98%)	3 (2%)	0	100	100
1	BY	122/126 (97%)	120 (98%)	2 (2%)	0	100	100
1	BZ	123/126 (98%)	121 (98%)	2 (2%)	0	100	100
1	CA	122/126 (97%)	119 (98%)	3 (2%)	0	100	100
1	CB	122/126 (97%)	120 (98%)	2 (2%)	0	100	100
1	CC	123/126 (98%)	121 (98%)	2 (2%)	0	100	100
1	CD	122/126 (97%)	119 (98%)	3 (2%)	0	100	100
1	CE	122/126 (97%)	120 (98%)	2 (2%)	0	100	100
1	CF	123/126 (98%)	121 (98%)	2 (2%)	0	100	100
1	CG	122/126 (97%)	119 (98%)	3 (2%)	0	100	100
1	CH	122/126 (97%)	120 (98%)	2 (2%)	0	100	100
1	CI	123/126 (98%)	121 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	CJ	122/126 (97%)	119 (98%)	3 (2%)	0	100	100
1	CK	122/126 (97%)	120 (98%)	2 (2%)	0	100	100
1	CL	123/126 (98%)	121 (98%)	2 (2%)	0	100	100
1	CM	122/126 (97%)	119 (98%)	3 (2%)	0	100	100
1	CN	122/126 (97%)	120 (98%)	2 (2%)	0	100	100
1	CO	123/126 (98%)	121 (98%)	2 (2%)	0	100	100
1	CP	122/126 (97%)	119 (98%)	3 (2%)	0	100	100
1	CQ	122/126 (97%)	120 (98%)	2 (2%)	0	100	100
1	CR	123/126 (98%)	121 (98%)	2 (2%)	0	100	100
1	CS	122/126 (97%)	119 (98%)	3 (2%)	0	100	100
1	CT	122/126 (97%)	120 (98%)	2 (2%)	0	100	100
1	CU	123/126 (98%)	121 (98%)	2 (2%)	0	100	100
1	CV	122/126 (97%)	119 (98%)	3 (2%)	0	100	100
1	CW	122/126 (97%)	120 (98%)	2 (2%)	0	100	100
1	CX	123/126 (98%)	121 (98%)	2 (2%)	0	100	100
1	CY	122/126 (97%)	119 (98%)	3 (2%)	0	100	100
1	CZ	122/126 (97%)	120 (98%)	2 (2%)	0	100	100
1	DA	123/126 (98%)	121 (98%)	2 (2%)	0	100	100
1	DB	122/126 (97%)	119 (98%)	3 (2%)	0	100	100
1	DC	122/126 (97%)	120 (98%)	2 (2%)	0	100	100
1	DD	123/126 (98%)	121 (98%)	2 (2%)	0	100	100
1	DE	122/126 (97%)	119 (98%)	3 (2%)	0	100	100
1	DF	122/126 (97%)	120 (98%)	2 (2%)	0	100	100
1	DG	123/126 (98%)	121 (98%)	2 (2%)	0	100	100
1	DH	122/126 (97%)	119 (98%)	3 (2%)	0	100	100
1	DI	122/126 (97%)	120 (98%)	2 (2%)	0	100	100
1	DJ	123/126 (98%)	121 (98%)	2 (2%)	0	100	100
1	DK	122/126 (97%)	119 (98%)	3 (2%)	0	100	100
1	DL	122/126 (97%)	120 (98%)	2 (2%)	0	100	100
All	All	11010/11340 (97%)	10800 (98%)	210 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AA	106/107 (99%)	106 (100%)	0	100	100
1	AB	106/107 (99%)	106 (100%)	0	100	100
1	AC	106/107 (99%)	106 (100%)	0	100	100
1	AD	106/107 (99%)	106 (100%)	0	100	100
1	AE	106/107 (99%)	106 (100%)	0	100	100
1	AF	106/107 (99%)	106 (100%)	0	100	100
1	AG	106/107 (99%)	106 (100%)	0	100	100
1	AH	106/107 (99%)	106 (100%)	0	100	100
1	AI	106/107 (99%)	106 (100%)	0	100	100
1	AJ	106/107 (99%)	106 (100%)	0	100	100
1	AK	106/107 (99%)	106 (100%)	0	100	100
1	AL	106/107 (99%)	106 (100%)	0	100	100
1	AM	106/107 (99%)	106 (100%)	0	100	100
1	AN	106/107 (99%)	106 (100%)	0	100	100
1	AO	106/107 (99%)	106 (100%)	0	100	100
1	AP	106/107 (99%)	106 (100%)	0	100	100
1	AQ	106/107 (99%)	106 (100%)	0	100	100
1	AR	106/107 (99%)	106 (100%)	0	100	100
1	AS	106/107 (99%)	106 (100%)	0	100	100
1	AT	106/107 (99%)	106 (100%)	0	100	100
1	AU	106/107 (99%)	106 (100%)	0	100	100
1	AV	106/107 (99%)	106 (100%)	0	100	100
1	AW	106/107 (99%)	106 (100%)	0	100	100
1	AX	106/107 (99%)	106 (100%)	0	100	100
1	AY	106/107 (99%)	106 (100%)	0	100	100
1	AZ	106/107 (99%)	106 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	BA	106/107 (99%)	106 (100%)	0	100	100
1	BB	106/107 (99%)	106 (100%)	0	100	100
1	BC	106/107 (99%)	106 (100%)	0	100	100
1	BD	106/107 (99%)	106 (100%)	0	100	100
1	BE	106/107 (99%)	106 (100%)	0	100	100
1	BF	106/107 (99%)	106 (100%)	0	100	100
1	BG	106/107 (99%)	106 (100%)	0	100	100
1	BH	106/107 (99%)	106 (100%)	0	100	100
1	BI	106/107 (99%)	106 (100%)	0	100	100
1	BJ	106/107 (99%)	106 (100%)	0	100	100
1	BK	106/107 (99%)	106 (100%)	0	100	100
1	BL	106/107 (99%)	106 (100%)	0	100	100
1	BM	106/107 (99%)	106 (100%)	0	100	100
1	BN	106/107 (99%)	106 (100%)	0	100	100
1	BO	106/107 (99%)	106 (100%)	0	100	100
1	BP	106/107 (99%)	106 (100%)	0	100	100
1	BQ	106/107 (99%)	106 (100%)	0	100	100
1	BR	106/107 (99%)	106 (100%)	0	100	100
1	BS	106/107 (99%)	106 (100%)	0	100	100
1	BT	106/107 (99%)	106 (100%)	0	100	100
1	BU	106/107 (99%)	106 (100%)	0	100	100
1	BV	106/107 (99%)	106 (100%)	0	100	100
1	BW	106/107 (99%)	106 (100%)	0	100	100
1	BX	106/107 (99%)	106 (100%)	0	100	100
1	BY	106/107 (99%)	106 (100%)	0	100	100
1	BZ	106/107 (99%)	106 (100%)	0	100	100
1	CA	106/107 (99%)	106 (100%)	0	100	100
1	CB	106/107 (99%)	106 (100%)	0	100	100
1	CC	106/107 (99%)	106 (100%)	0	100	100
1	CD	106/107 (99%)	106 (100%)	0	100	100
1	CE	106/107 (99%)	106 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	CF	106/107 (99%)	106 (100%)	0	100	100
1	CG	106/107 (99%)	106 (100%)	0	100	100
1	CH	106/107 (99%)	106 (100%)	0	100	100
1	CI	106/107 (99%)	106 (100%)	0	100	100
1	CJ	106/107 (99%)	106 (100%)	0	100	100
1	CK	106/107 (99%)	106 (100%)	0	100	100
1	CL	106/107 (99%)	106 (100%)	0	100	100
1	CM	106/107 (99%)	106 (100%)	0	100	100
1	CN	106/107 (99%)	106 (100%)	0	100	100
1	CO	106/107 (99%)	106 (100%)	0	100	100
1	CP	106/107 (99%)	106 (100%)	0	100	100
1	CQ	106/107 (99%)	106 (100%)	0	100	100
1	CR	106/107 (99%)	106 (100%)	0	100	100
1	CS	106/107 (99%)	106 (100%)	0	100	100
1	CT	106/107 (99%)	106 (100%)	0	100	100
1	CU	106/107 (99%)	106 (100%)	0	100	100
1	CV	106/107 (99%)	106 (100%)	0	100	100
1	CW	106/107 (99%)	106 (100%)	0	100	100
1	CX	106/107 (99%)	106 (100%)	0	100	100
1	CY	106/107 (99%)	106 (100%)	0	100	100
1	CZ	106/107 (99%)	106 (100%)	0	100	100
1	DA	106/107 (99%)	106 (100%)	0	100	100
1	DB	106/107 (99%)	106 (100%)	0	100	100
1	DC	106/107 (99%)	106 (100%)	0	100	100
1	DD	106/107 (99%)	106 (100%)	0	100	100
1	DE	106/107 (99%)	106 (100%)	0	100	100
1	DF	106/107 (99%)	106 (100%)	0	100	100
1	DG	106/107 (99%)	106 (100%)	0	100	100
1	DH	106/107 (99%)	106 (100%)	0	100	100
1	DI	106/107 (99%)	106 (100%)	0	100	100
1	DJ	106/107 (99%)	106 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	DK	106/107 (99%)	106 (100%)	0	100	100
1	DL	106/107 (99%)	106 (100%)	0	100	100
All	All	9540/9630 (99%)	9540 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (136) such sidechains are listed below:

Mol	Chain	Res	Type
1	AA	8	GLN
1	AA	86	ASN
1	AB	8	GLN
1	AB	21	ASN
1	AB	118	GLN
1	AD	86	ASN
1	AE	21	ASN
1	AE	118	GLN
1	AG	86	ASN
1	AH	21	ASN
1	AH	118	GLN
1	AI	118	GLN
1	AJ	86	ASN
1	AK	21	ASN
1	AK	118	GLN
1	AL	4	ASN
1	AL	118	GLN
1	AM	8	GLN
1	AM	86	ASN
1	AN	8	GLN
1	AN	21	ASN
1	AN	118	GLN
1	AP	8	GLN
1	AP	86	ASN
1	AQ	21	ASN
1	AQ	118	GLN
1	AS	8	GLN
1	AS	86	ASN
1	AT	21	ASN
1	AT	118	GLN
1	AV	8	GLN
1	AV	86	ASN

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Mol	Chain	Res	Type
1	AW	8	GLN
1	AW	21	ASN
1	AW	118	GLN
1	AY	8	GLN
1	AY	86	ASN
1	AZ	8	GLN
1	AZ	21	ASN
1	AZ	118	GLN
1	BB	8	GLN
1	BB	86	ASN
1	BC	8	GLN
1	BC	21	ASN
1	BC	118	GLN
1	BE	8	GLN
1	BE	86	ASN
1	BF	8	GLN
1	BF	21	ASN
1	BF	118	GLN
1	BH	8	GLN
1	BH	86	ASN
1	BI	8	GLN
1	BI	21	ASN
1	BI	118	GLN
1	BK	8	GLN
1	BK	86	ASN
1	BL	8	GLN
1	BL	21	ASN
1	BL	118	GLN
1	BN	8	GLN
1	BN	86	ASN
1	BN	100	ASN
1	BO	21	ASN
1	BO	118	GLN
1	BP	118	GLN
1	BQ	8	GLN
1	BQ	86	ASN
1	BR	21	ASN
1	BR	118	GLN
1	BS	118	GLN
1	BT	86	ASN
1	BU	8	GLN
1	BU	21	ASN

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Mol	Chain	Res	Type
1	BU	118	GLN
1	BW	8	GLN
1	BW	86	ASN
1	BX	8	GLN
1	BX	21	ASN
1	BX	118	GLN
1	BZ	8	GLN
1	BZ	86	ASN
1	CA	8	GLN
1	CA	21	ASN
1	CA	118	GLN
1	CC	86	ASN
1	CD	8	GLN
1	CD	21	ASN
1	CD	118	GLN
1	CF	8	GLN
1	CF	32	ASN
1	CF	86	ASN
1	CG	21	ASN
1	CG	118	GLN
1	CI	8	GLN
1	CI	86	ASN
1	CJ	21	ASN
1	CJ	118	GLN
1	CL	8	GLN
1	CL	86	ASN
1	CM	21	ASN
1	CM	118	GLN
1	CO	8	GLN
1	CO	86	ASN
1	CP	8	GLN
1	CP	21	ASN
1	CP	118	GLN
1	CR	8	GLN
1	CR	86	ASN
1	CS	21	ASN
1	CS	118	GLN
1	CU	86	ASN
1	CV	21	ASN
1	CV	118	GLN
1	CX	8	GLN
1	CX	86	ASN

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Mol	Chain	Res	Type
1	CY	8	GLN
1	CY	21	ASN
1	CY	118	GLN
1	DA	8	GLN
1	DA	86	ASN
1	DB	8	GLN
1	DB	21	ASN
1	DB	118	GLN
1	DD	8	GLN
1	DD	86	ASN
1	DE	21	ASN
1	DE	118	GLN
1	DG	8	GLN
1	DG	86	ASN
1	DH	21	ASN
1	DH	118	GLN
1	DJ	8	GLN
1	DJ	86	ASN
1	DK	21	ASN
1	DK	118	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	125/126 (99%)	0.17	0 100 100	80, 119, 153, 190	0
1	AB	124/126 (98%)	0.16	2 (1%) 70 45	78, 117, 144, 167	0
1	AC	124/126 (98%)	0.24	5 (4%) 42 23	83, 121, 153, 187	0
1	AD	125/126 (99%)	0.10	1 (0%) 82 60	80, 119, 153, 190	0
1	AE	124/126 (98%)	0.17	3 (2%) 59 35	78, 117, 144, 167	0
1	AF	124/126 (98%)	0.18	2 (1%) 70 45	83, 121, 153, 187	0
1	AG	125/126 (99%)	0.16	2 (1%) 70 45	80, 119, 153, 190	0
1	AH	124/126 (98%)	0.11	1 (0%) 82 60	78, 117, 144, 167	0
1	AI	124/126 (98%)	0.09	2 (1%) 70 45	83, 121, 153, 187	0
1	AJ	125/126 (99%)	0.07	4 (3%) 50 29	80, 119, 153, 190	0
1	AK	124/126 (98%)	0.02	4 (3%) 50 29	78, 117, 144, 167	0
1	AL	124/126 (98%)	-0.08	0 100 100	83, 121, 153, 187	0
1	AM	125/126 (99%)	0.23	5 (4%) 42 23	80, 119, 153, 190	0
1	AN	124/126 (98%)	0.08	0 100 100	78, 117, 144, 167	0
1	AO	124/126 (98%)	0.08	1 (0%) 82 60	83, 121, 153, 187	0
1	AP	125/126 (99%)	0.29	6 (4%) 35 19	80, 119, 153, 190	0
1	AQ	124/126 (98%)	0.22	2 (1%) 70 45	78, 117, 144, 167	0
1	AR	124/126 (98%)	0.29	4 (3%) 50 29	83, 121, 153, 187	0
1	AS	125/126 (99%)	0.04	0 100 100	80, 119, 153, 190	0
1	AT	124/126 (98%)	0.11	3 (2%) 59 35	78, 117, 144, 167	0
1	AU	124/126 (98%)	0.30	5 (4%) 42 23	83, 121, 153, 187	0
1	AV	125/126 (99%)	0.16	6 (4%) 35 19	80, 119, 153, 190	0
1	AW	124/126 (98%)	0.12	3 (2%) 59 35	78, 117, 144, 167	0
1	AX	124/126 (98%)	0.03	1 (0%) 82 60	83, 121, 153, 187	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	AY	125/126 (99%)	0.46	10 (8%) 18 12	80, 119, 153, 190	0
1	AZ	124/126 (98%)	0.25	7 (5%) 30 17	78, 117, 144, 167	0
1	BA	124/126 (98%)	0.08	1 (0%) 82 60	83, 121, 153, 187	0
1	BB	125/126 (99%)	0.25	2 (1%) 70 45	80, 119, 153, 190	0
1	BC	124/126 (98%)	-0.01	0 100 100	78, 117, 144, 167	0
1	BD	124/126 (98%)	0.22	4 (3%) 50 29	83, 121, 153, 187	0
1	BE	125/126 (99%)	0.12	1 (0%) 82 60	80, 119, 153, 190	0
1	BF	124/126 (98%)	0.10	2 (1%) 70 45	78, 117, 144, 167	0
1	BG	124/126 (98%)	0.13	4 (3%) 50 29	83, 121, 153, 187	0
1	BH	125/126 (99%)	0.07	1 (0%) 82 60	80, 119, 153, 190	0
1	BI	124/126 (98%)	-0.01	2 (1%) 70 45	78, 117, 144, 167	0
1	BJ	124/126 (98%)	0.28	3 (2%) 59 35	83, 121, 153, 187	0
1	BK	125/126 (99%)	-0.01	0 100 100	80, 119, 153, 190	0
1	BL	124/126 (98%)	-0.04	0 100 100	78, 117, 144, 167	0
1	BM	124/126 (98%)	0.17	2 (1%) 70 45	83, 121, 153, 187	0
1	BN	125/126 (99%)	-0.01	5 (4%) 42 23	80, 119, 153, 190	0
1	BO	124/126 (98%)	0.13	4 (3%) 50 29	78, 117, 144, 167	0
1	BP	124/126 (98%)	0.10	1 (0%) 82 60	83, 121, 153, 187	0
1	BQ	125/126 (99%)	0.00	1 (0%) 82 60	80, 119, 153, 190	0
1	BR	124/126 (98%)	0.16	2 (1%) 70 45	78, 117, 144, 167	0
1	BS	124/126 (98%)	0.09	5 (4%) 42 23	83, 121, 153, 187	0
1	BT	125/126 (99%)	0.24	6 (4%) 35 19	80, 119, 153, 190	0
1	BU	124/126 (98%)	0.04	1 (0%) 82 60	78, 117, 144, 167	0
1	BV	124/126 (98%)	0.09	1 (0%) 82 60	83, 121, 153, 187	0
1	BW	125/126 (99%)	0.29	7 (5%) 30 17	80, 119, 153, 190	0
1	BX	124/126 (98%)	0.14	1 (0%) 82 60	78, 117, 144, 167	0
1	BY	124/126 (98%)	0.50	4 (3%) 50 29	83, 121, 153, 187	0
1	BZ	125/126 (99%)	0.15	3 (2%) 59 35	80, 119, 153, 190	0
1	CA	124/126 (98%)	0.04	1 (0%) 82 60	78, 117, 144, 167	0
1	CB	124/126 (98%)	0.19	2 (1%) 70 45	83, 121, 153, 187	0
1	CC	125/126 (99%)	0.25	6 (4%) 35 19	80, 119, 153, 190	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	CD	124/126 (98%)	0.18	4 (3%)	50	29	78, 117, 144, 167	0
1	CE	124/126 (98%)	0.34	5 (4%)	42	23	83, 121, 153, 187	0
1	CF	125/126 (99%)	0.28	6 (4%)	35	19	80, 119, 153, 190	0
1	CG	124/126 (98%)	0.01	1 (0%)	82	60	78, 117, 144, 167	0
1	CH	124/126 (98%)	0.23	3 (2%)	59	35	83, 121, 153, 187	0
1	CI	125/126 (99%)	0.45	8 (6%)	25	15	80, 119, 153, 190	0
1	CJ	124/126 (98%)	0.49	5 (4%)	42	23	78, 117, 144, 167	0
1	CK	124/126 (98%)	0.39	6 (4%)	35	19	83, 121, 153, 187	0
1	CL	125/126 (99%)	0.14	2 (1%)	70	45	80, 119, 153, 190	0
1	CM	124/126 (98%)	0.17	3 (2%)	59	35	78, 117, 144, 167	0
1	CN	124/126 (98%)	0.16	1 (0%)	82	60	83, 121, 153, 187	0
1	CO	125/126 (99%)	0.08	1 (0%)	82	60	80, 119, 153, 190	0
1	CP	124/126 (98%)	0.27	5 (4%)	42	23	78, 117, 144, 167	0
1	CQ	124/126 (98%)	0.33	9 (7%)	21	13	83, 121, 153, 187	0
1	CR	125/126 (99%)	0.33	3 (2%)	59	35	80, 119, 153, 190	0
1	CS	124/126 (98%)	0.19	4 (3%)	50	29	78, 117, 144, 167	0
1	CT	124/126 (98%)	0.16	2 (1%)	70	45	83, 121, 153, 187	0
1	CU	125/126 (99%)	0.21	3 (2%)	59	35	80, 119, 153, 190	0
1	CV	124/126 (98%)	0.22	4 (3%)	50	29	78, 117, 144, 167	0
1	CW	124/126 (98%)	0.16	3 (2%)	59	35	83, 121, 153, 187	0
1	CX	125/126 (99%)	0.29	7 (5%)	30	17	80, 119, 153, 190	0
1	CY	124/126 (98%)	0.39	5 (4%)	42	23	78, 117, 144, 167	0
1	CZ	124/126 (98%)	0.33	5 (4%)	42	23	83, 121, 153, 187	0
1	DA	125/126 (99%)	0.11	3 (2%)	59	35	80, 119, 153, 190	0
1	DB	124/126 (98%)	0.17	4 (3%)	50	29	78, 117, 144, 167	0
1	DC	124/126 (98%)	0.29	5 (4%)	42	23	83, 121, 153, 187	0
1	DD	125/126 (99%)	0.16	4 (3%)	50	29	80, 119, 153, 190	0
1	DE	124/126 (98%)	0.08	2 (1%)	70	45	78, 117, 144, 167	0
1	DF	124/126 (98%)	0.06	1 (0%)	82	60	83, 121, 153, 187	0
1	DG	125/126 (99%)	0.09	1 (0%)	82	60	80, 119, 153, 190	0
1	DH	124/126 (98%)	0.10	1 (0%)	82	60	78, 117, 144, 167	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	DI	124/126 (98%)	0.15	4 (3%) 50 29	83, 121, 153, 187	0
1	DJ	125/126 (99%)	0.03	1 (0%) 82 60	80, 119, 153, 190	0
1	DK	124/126 (98%)	0.19	3 (2%) 59 35	78, 117, 144, 167	0
1	DL	124/126 (98%)	0.14	5 (4%) 42 23	83, 121, 153, 187	0
All	All	11190/11340 (98%)	0.17	280 (2%) 58 35	78, 120, 150, 190	0

All (280) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	CY	124	THR	5.6
1	CR	43	VAL	4.9
1	BT	38	ALA	4.6
1	CI	8	GLN	4.1
1	AP	24	ARG	4.1
1	CE	32	ASN	4.0
1	CQ	29	ILE	4.0
1	CZ	111	GLY	3.9
1	CC	38	ALA	3.9
1	BT	43	VAL	3.9
1	CS	58	VAL	3.8
1	AU	124	THR	3.7
1	DC	108	LEU	3.7
1	CM	44	TYR	3.7
1	DK	50	VAL	3.7
1	BB	38	ALA	3.7
1	AT	8	GLN	3.7
1	BZ	8	GLN	3.6
1	AP	26	THR	3.6
1	AG	47	ARG	3.5
1	AT	35	GLN	3.5
1	AV	43	VAL	3.4
1	CG	8	GLN	3.4
1	AJ	44	TYR	3.4
1	AV	44	TYR	3.4
1	BT	35	GLN	3.4
1	CJ	124	THR	3.4
1	CX	44	TYR	3.3
1	AE	29	ILE	3.3
1	CB	44	TYR	3.2
1	AY	115	THR	3.2
1	DK	28	ARG	3.2

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Mol	Chain	Res	Type	RSRZ
1	CW	108	LEU	3.2
1	BR	50	VAL	3.2
1	DL	29	ILE	3.2
1	CJ	28	ARG	3.2
1	DE	28	ARG	3.2
1	CM	8	GLN	3.2
1	AM	38	ALA	3.1
1	BD	49	GLU	3.1
1	AE	28	ARG	3.1
1	AU	123	TYR	3.1
1	CF	73	ASN	3.1
1	CL	34	ASN	3.1
1	CU	38	ALA	3.1
1	AQ	42	SER	3.1
1	DC	114	PRO	3.1
1	CV	73	ASN	3.1
1	DH	32	ASN	3.1
1	BX	8	GLN	3.1
1	BG	34	ASN	3.0
1	AJ	8	GLN	3.0
1	AP	12	GLY	3.0
1	CQ	49	GLU	3.0
1	BP	114	PRO	3.0
1	BW	34	ASN	3.0
1	CK	31	LEU	3.0
1	BD	8	GLN	3.0
1	AY	38	ALA	3.0
1	CI	26	THR	3.0
1	BS	49	GLU	2.9
1	AY	114	PRO	2.9
1	BT	42	SER	2.9
1	CZ	29	ILE	2.9
1	CD	58	VAL	2.9
1	DB	82	GLY	2.9
1	BQ	52	THR	2.9
1	AR	76	ILE	2.9
1	CP	124	THR	2.8
1	AV	85	GLU	2.8
1	CC	73	ASN	2.8
1	CQ	73	ASN	2.8
1	CR	111	GLY	2.8
1	CH	123	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
1	CP	8	GLN	2.8
1	CY	28	ARG	2.8
1	BD	34	ASN	2.8
1	CE	44	TYR	2.8
1	CU	81	SER	2.8
1	DC	34	ASN	2.8
1	CL	12	GLY	2.7
1	BI	15	LEU	2.7
1	AM	25	SER	2.7
1	AR	61	GLU	2.7
1	BY	115	THR	2.7
1	CI	61	GLU	2.7
1	AU	34	ASN	2.7
1	CD	73	ASN	2.7
1	CF	38	ALA	2.7
1	CJ	8	GLN	2.7
1	AK	29	ILE	2.7
1	CQ	50	VAL	2.7
1	BY	8	GLN	2.7
1	AM	29	ILE	2.7
1	BH	25	SER	2.7
1	AY	113	LEU	2.7
1	CZ	15	LEU	2.7
1	CT	49	GLU	2.7
1	BF	37	VAL	2.7
1	AV	52	THR	2.6
1	BS	30	ASN	2.6
1	BZ	73	ASN	2.6
1	AQ	44	TYR	2.6
1	BJ	73	ASN	2.6
1	AU	39	GLY	2.6
1	AP	58	VAL	2.6
1	DB	28	ARG	2.6
1	AR	32	ASN	2.6
1	BW	125	GLY	2.6
1	CX	73	ASN	2.6
1	DC	113	LEU	2.6
1	CB	68	SER	2.6
1	CK	111	GLY	2.6
1	CU	125	GLY	2.6
1	CO	54	ARG	2.6
1	CS	28	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	AC	52	THR	2.6
1	CQ	79	THR	2.6
1	BN	35	GLN	2.5
1	DI	32	ASN	2.5
1	DL	50	VAL	2.5
1	DC	25	SER	2.5
1	CI	44	TYR	2.5
1	AM	54	ARG	2.5
1	CZ	108	LEU	2.5
1	BB	8	GLN	2.5
1	CX	61	GLU	2.5
1	AD	101	LEU	2.5
1	CJ	123	TYR	2.5
1	DD	82	GLY	2.5
1	AJ	35	GLN	2.5
1	BW	1	ALA	2.5
1	AZ	34	ASN	2.5
1	BF	124	THR	2.5
1	BG	124	THR	2.5
1	DD	52	THR	2.5
1	AW	28	ARG	2.5
1	CZ	101	LEU	2.5
1	AZ	32	ASN	2.4
1	AY	125	GLY	2.4
1	BO	58	VAL	2.4
1	CR	110	ALA	2.4
1	AZ	52	THR	2.4
1	BG	52	THR	2.4
1	BZ	26	THR	2.4
1	AZ	58	VAL	2.4
1	BN	69	VAL	2.4
1	CV	28	ARG	2.4
1	DD	54	ARG	2.4
1	BJ	75	SER	2.4
1	BN	43	VAL	2.4
1	CA	58	VAL	2.4
1	BE	24	ARG	2.4
1	DL	49	GLU	2.4
1	BO	21	ASN	2.4
1	BT	44	TYR	2.4
1	CI	29	ILE	2.4
1	DI	35	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	BD	108	LEU	2.4
1	DK	49	GLU	2.4
1	AP	69	VAL	2.4
1	BV	67	CYS	2.4
1	AG	12	GLY	2.3
1	AJ	38	ALA	2.3
1	AF	31	LEU	2.3
1	AV	35	GLN	2.3
1	BM	108	LEU	2.3
1	CV	81	SER	2.3
1	AI	115	THR	2.3
1	CD	34	ASN	2.3
1	BO	15	LEU	2.3
1	AC	8	GLN	2.3
1	CP	35	GLN	2.3
1	CS	41	VAL	2.3
1	CV	74	ILE	2.3
1	BM	32	ASN	2.3
1	DB	34	ASN	2.3
1	CF	35	GLN	2.3
1	AC	48	SER	2.3
1	AO	78	THR	2.3
1	CQ	30	ASN	2.3
1	CY	34	ASN	2.3
1	DA	61	GLU	2.3
1	BY	29	ILE	2.3
1	BA	111	GLY	2.3
1	BW	12	GLY	2.3
1	BW	115	THR	2.3
1	AR	81	SER	2.3
1	CQ	123	TYR	2.3
1	CX	35	GLN	2.3
1	AP	43	VAL	2.3
1	CK	49	GLU	2.2
1	AY	117	ILE	2.2
1	AY	12	GLY	2.2
1	CE	101	LEU	2.2
1	AV	42	SER	2.2
1	AH	34	ASN	2.2
1	CT	8	GLN	2.2
1	BT	49	GLU	2.2
1	BS	119	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	BN	113	LEU	2.2
1	DJ	110	ALA	2.2
1	CC	44	TYR	2.2
1	AY	43	VAL	2.2
1	AW	30	ASN	2.2
1	DI	49	GLU	2.2
1	CX	1	ALA	2.2
1	AC	25	SER	2.2
1	BR	48	SER	2.2
1	BS	48	SER	2.2
1	CH	120	VAL	2.2
1	CK	33	VAL	2.2
1	CP	123	TYR	2.2
1	CX	29	ILE	2.2
1	CI	113	LEU	2.2
1	DA	98	LEU	2.2
1	DB	98	LEU	2.2
1	DD	108	LEU	2.2
1	AB	28	ARG	2.2
1	CY	17	TRP	2.2
1	AW	124	THR	2.1
1	CW	79	THR	2.1
1	DA	69	VAL	2.1
1	CD	74	ILE	2.1
1	AB	14	SER	2.1
1	CI	81	SER	2.1
1	AM	49	GLU	2.1
1	AY	61	GLU	2.1
1	AT	43	VAL	2.1
1	CJ	41	VAL	2.1
1	CM	29	ILE	2.1
1	CQ	9	LEU	2.1
1	CQ	8	GLN	2.1
1	DL	77	ARG	2.1
1	CY	122	GLU	2.1
1	AF	30	ASN	2.1
1	BO	17	TRP	2.1
1	AE	15	LEU	2.1
1	BU	124	THR	2.1
1	BN	61	GLU	2.1
1	BY	12	GLY	2.1
1	CN	25	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	AK	34	ASN	2.1
1	BS	32	ASN	2.1
1	CX	34	ASN	2.1
1	AI	77	ARG	2.1
1	AZ	54	ARG	2.1
1	AZ	111	GLY	2.1
1	CF	82	GLY	2.1
1	CC	61	GLU	2.1
1	DE	68	SER	2.1
1	CF	109	VAL	2.1
1	AY	54	ARG	2.1
1	BJ	74	ILE	2.1
1	CI	108	LEU	2.1
1	AK	8	GLN	2.1
1	BI	82	GLY	2.1
1	CW	48	SER	2.0
1	AU	29	ILE	2.0
1	CF	24	ARG	2.0
1	CP	34	ASN	2.0
1	CS	73	ASN	2.0
1	DF	73	ASN	2.0
1	BG	44	TYR	2.0
1	AK	111	GLY	2.0
1	CK	8	GLN	2.0
1	AX	54	ARG	2.0
1	DL	11	SER	2.0
1	CC	53	ASN	2.0
1	CE	34	ASN	2.0
1	CH	73	ASN	2.0
1	CK	32	ASN	2.0
1	DI	34	ASN	2.0
1	BW	38	ALA	2.0
1	DG	26	THR	2.0
1	AC	54	ARG	2.0
1	CC	37	VAL	2.0
1	AZ	7	LEU	2.0
1	BW	101	LEU	2.0
1	CE	15	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.