Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2022 – 04:25 pm GMT

PDB ID	:	6YFQ
Title	:	Virus-like particle of bacteriophage NT-214
Authors	:	Rumnieks, J.; Kalnins, G.; Sisovs, M.; Lieknina, I.; Tars, K.
Deposited on	:	2020-03-26
Resolution	:	3.80 Å(reported)

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

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

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

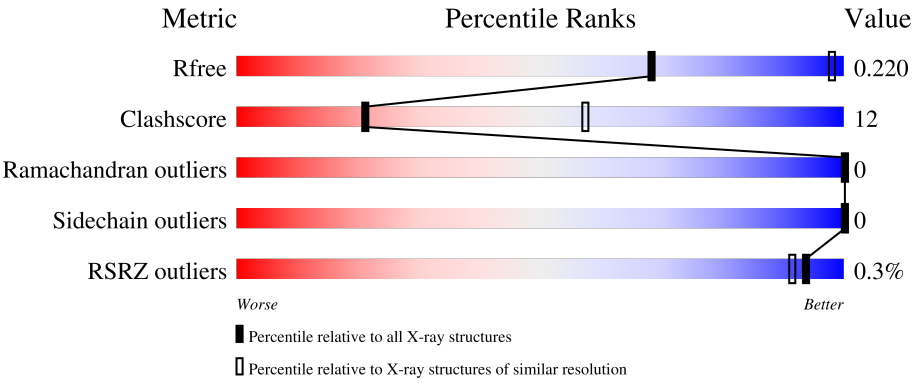
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.26
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

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 3.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1212 (4.00-3.60)
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)
RSRZ outliers	127900	1121 (4.00-3.60)

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	135	73% 27%
1	AB	135	70% 30%
1	AC	135	71% 29%
1	AD	135	% 75% 25%
1	AE	135	69% 31%

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Mol	Chain	Length	Quality of chain
1	AF	135	65% 35%
1	AG	135	% 74% 26%
1	AH	135	70% 30%
1	AI	135	67% 33%
1	AJ	135	% 72% 28%
1	AK	135	69% 31%
1	AL	135	% 76% 24%
1	AM	135	% 72% 28%
1	AN	135	73% 27%
1	AO	135	74% 26%
1	AP	135	2% 72% 28%
1	AQ	135	72% 28%
1	AR	135	70% 30%
1	AS	135	% 79% 21%
1	AT	135	67% 33%
1	AU	135	70% 30%
1	AV	135	% 79% 21%
1	AW	135	70% 30%
1	AX	135	69% 31%
1	AY	135	% 72% 28%
1	AZ	135	% 75% 25%
1	BA	135	70% 30%
1	BB	135	% 72% 28%
1	BC	135	77% 23%
1	BD	135	70% 30%

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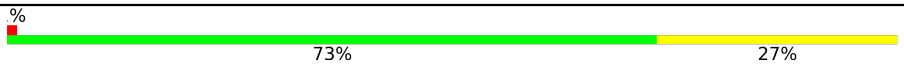
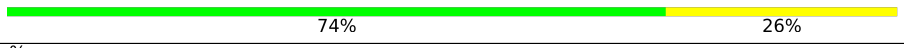
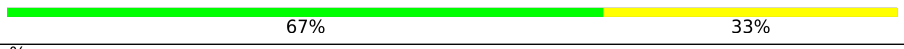
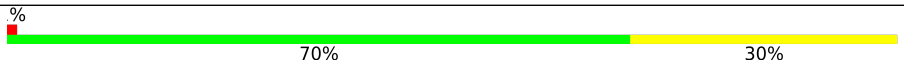
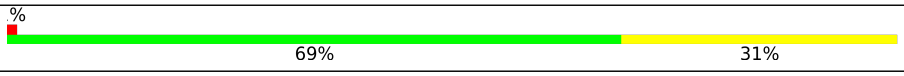
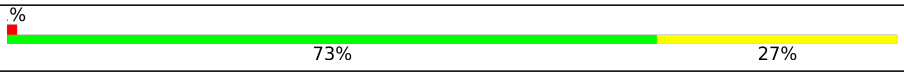
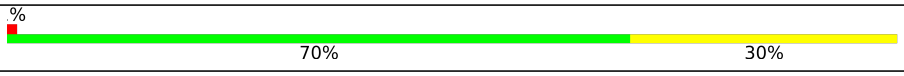
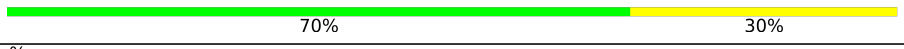
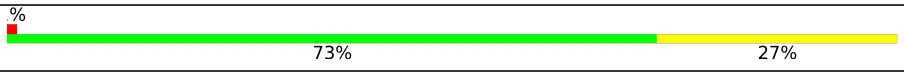
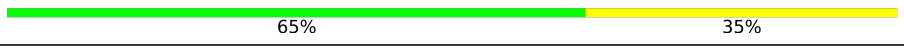
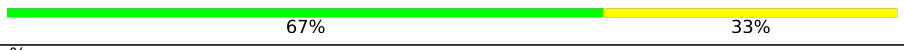
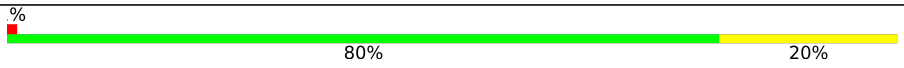
Mol	Chain	Length	Quality of chain
1	BE	135	
1	BF	135	
1	BG	135	
1	BH	135	
1	BI	135	
1	BJ	135	
1	BK	135	
1	BL	135	
1	BM	135	
1	BN	135	
1	BO	135	
1	BP	135	
1	BQ	135	
1	BR	135	
1	BS	135	
1	BT	135	
1	BU	135	
1	BV	135	
1	BW	135	
1	BX	135	
1	BY	135	
1	BZ	135	
1	CA	135	
1	CB	135	
1	CC	135	

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Mol	Chain	Length	Quality of chain
1	CD	135	67% 33%
1	CE	135	65% 35%
1	CF	135	% 75% 25%
1	CG	135	71% 29%
1	CH	135	68% 32%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 61200 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	135	Total	C	N	O	S	0	0	0
			1020	649	170	195	6			
1	AB	135	Total	C	N	O	S	0	0	0
			1020	649	170	195	6			
1	AC	135	Total	C	N	O	S	0	0	0
			1020	649	170	195	6			
1	AD	135	Total	C	N	O	S	0	0	0
			1020	649	170	195	6			
1	AE	135	Total	C	N	O	S	0	0	0
			1020	649	170	195	6			
1	AF	135	Total	C	N	O	S	0	0	0
			1020	649	170	195	6			
1	AG	135	Total	C	N	O	S	0	0	0
			1020	649	170	195	6			
1	AH	135	Total	C	N	O	S	0	0	0
			1020	649	170	195	6			
1	AI	135	Total	C	N	O	S	0	0	0
			1020	649	170	195	6			
1	AJ	135	Total	C	N	O	S	0	0	0
			1020	649	170	195	6			
1	AK	135	Total	C	N	O	S	0	0	0
			1020	649	170	195	6			
1	AL	135	Total	C	N	O	S	0	0	0
			1020	649	170	195	6			
1	AM	135	Total	C	N	O	S	0	0	0
			1020	649	170	195	6			
1	AN	135	Total	C	N	O	S	0	0	0
			1020	649	170	195	6			
1	AO	135	Total	C	N	O	S	0	0	0
			1020	649	170	195	6			
1	AP	135	Total	C	N	O	S	0	0	0
			1020	649	170	195	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AQ	135	Total	C	N	O	S	0	0	0
			1020	649	170	195	6			
1	AR	135	Total	C	N	O	S	0	0	0
			1020	649	170	195	6			
1	AS	135	Total	C	N	O	S	0	0	0
			1020	649	170	195	6			
1	AT	135	Total	C	N	O	S	0	0	0
			1020	649	170	195	6			
1	AU	135	Total	C	N	O	S	0	0	0
			1020	649	170	195	6			
1	AV	135	Total	C	N	O	S	0	0	0
			1020	649	170	195	6			
1	AW	135	Total	C	N	O	S	0	0	0
			1020	649	170	195	6			
1	AX	135	Total	C	N	O	S	0	0	0
			1020	649	170	195	6			
1	AY	135	Total	C	N	O	S	0	0	0
			1020	649	170	195	6			
1	AZ	135	Total	C	N	O	S	0	0	0
			1020	649	170	195	6			
1	BA	135	Total	C	N	O	S	0	0	0
			1020	649	170	195	6			
1	BB	135	Total	C	N	O	S	0	0	0
			1020	649	170	195	6			
1	BC	135	Total	C	N	O	S	0	0	0
			1020	649	170	195	6			
1	BD	135	Total	C	N	O	S	0	0	0
			1020	649	170	195	6			
1	BE	135	Total	C	N	O	S	0	0	0
			1020	649	170	195	6			
1	BF	135	Total	C	N	O	S	0	0	0
			1020	649	170	195	6			
1	BG	135	Total	C	N	O	S	0	0	0
			1020	649	170	195	6			
1	BH	135	Total	C	N	O	S	0	0	0
			1020	649	170	195	6			
1	BI	135	Total	C	N	O	S	0	0	0
			1020	649	170	195	6			
1	BJ	135	Total	C	N	O	S	0	0	0
			1020	649	170	195	6			
1	BK	135	Total	C	N	O	S	0	0	0
			1020	649	170	195	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	BL	135	Total	C	N	O	S	0	0	0
			1020	649	170	195	6			
1	BM	135	Total	C	N	O	S	0	0	0
			1020	649	170	195	6			
1	BN	135	Total	C	N	O	S	0	0	0
			1020	649	170	195	6			
1	BO	135	Total	C	N	O	S	0	0	0
			1020	649	170	195	6			
1	BP	135	Total	C	N	O	S	0	0	0
			1020	649	170	195	6			
1	BQ	135	Total	C	N	O	S	0	0	0
			1020	649	170	195	6			
1	BR	135	Total	C	N	O	S	0	0	0
			1020	649	170	195	6			
1	BS	135	Total	C	N	O	S	0	0	0
			1020	649	170	195	6			
1	BT	135	Total	C	N	O	S	0	0	0
			1020	649	170	195	6			
1	BU	135	Total	C	N	O	S	0	0	0
			1020	649	170	195	6			
1	BV	135	Total	C	N	O	S	0	0	0
			1020	649	170	195	6			
1	BW	135	Total	C	N	O	S	0	0	0
			1020	649	170	195	6			
1	BX	135	Total	C	N	O	S	0	0	0
			1020	649	170	195	6			
1	BY	135	Total	C	N	O	S	0	0	0
			1020	649	170	195	6			
1	BZ	135	Total	C	N	O	S	0	0	0
			1020	649	170	195	6			
1	CA	135	Total	C	N	O	S	0	0	0
			1020	649	170	195	6			
1	CB	135	Total	C	N	O	S	0	0	0
			1020	649	170	195	6			
1	CC	135	Total	C	N	O	S	0	0	0
			1020	649	170	195	6			
1	CD	135	Total	C	N	O	S	0	0	0
			1020	649	170	195	6			
1	CE	135	Total	C	N	O	S	0	0	0
			1020	649	170	195	6			
1	CF	135	Total	C	N	O	S	0	0	0
			1020	649	170	195	6			

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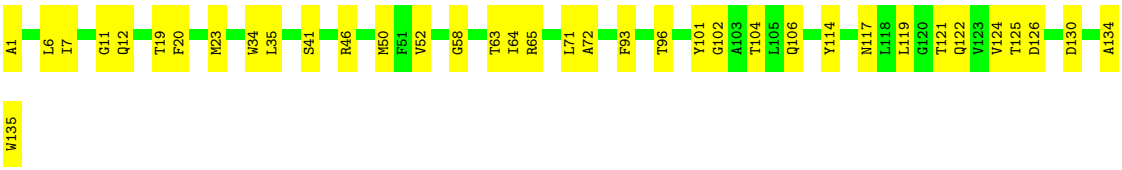
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	CG	135	Total	C	N	O	S	0	0	0
			1020	649	170	195	6			
1	CH	135	Total	C	N	O	S	0	0	0
			1020	649	170	195	6			

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.

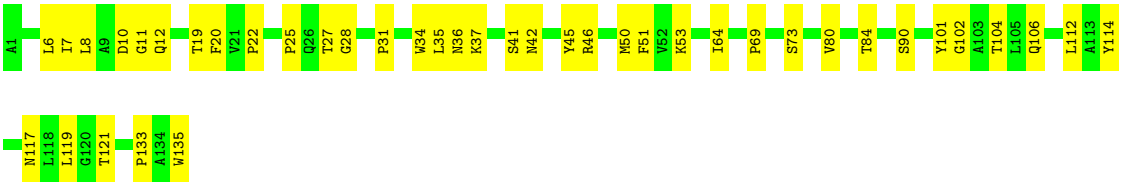
• Molecule 1: coat protein

Chain AA:



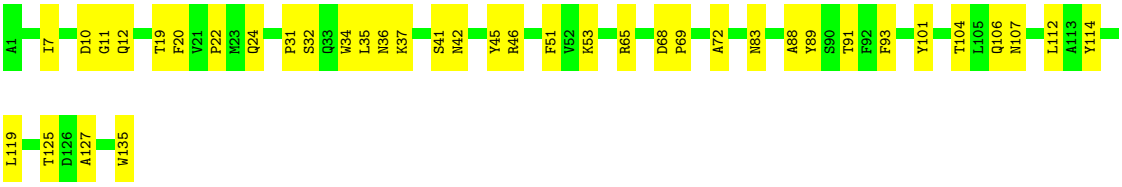
• Molecule 1: coat protein

Chain AB:



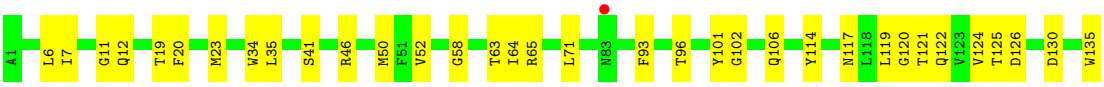
• Molecule 1: coat protein

Chain AC:



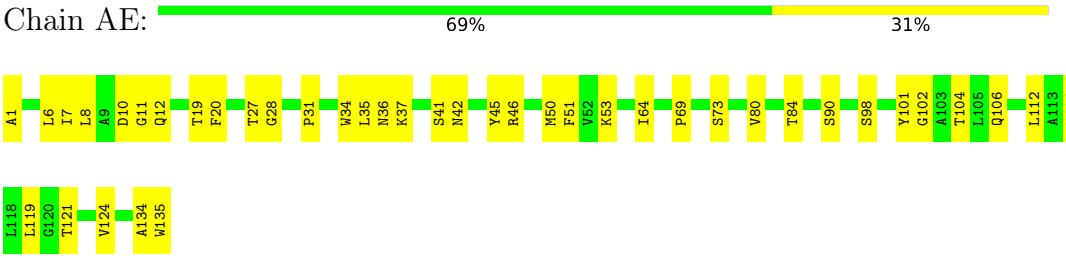
• Molecule 1: coat protein

Chain AD:



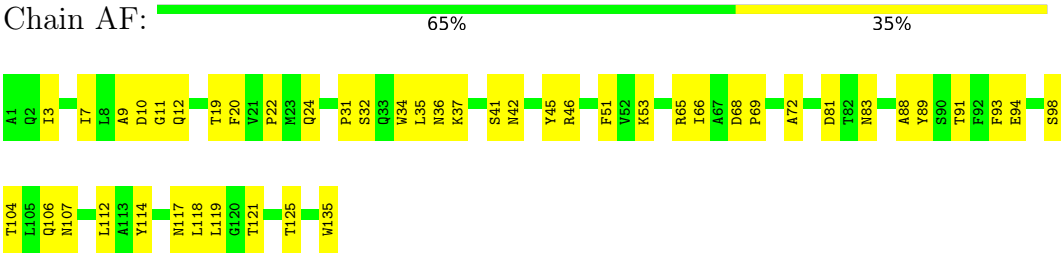
• Molecule 1: coat protein

Chain AE:



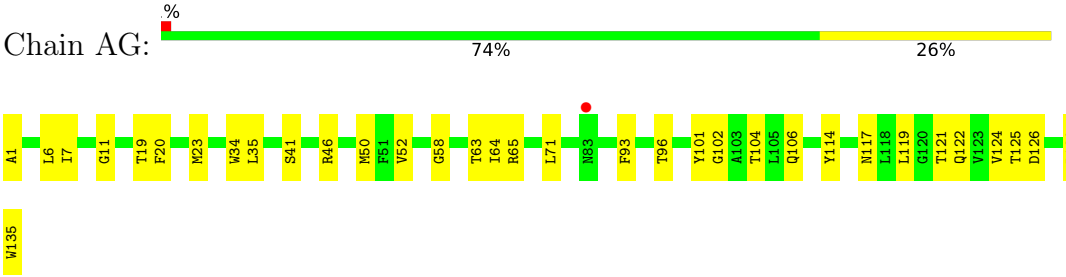
• Molecule 1: coat protein

Chain AF:



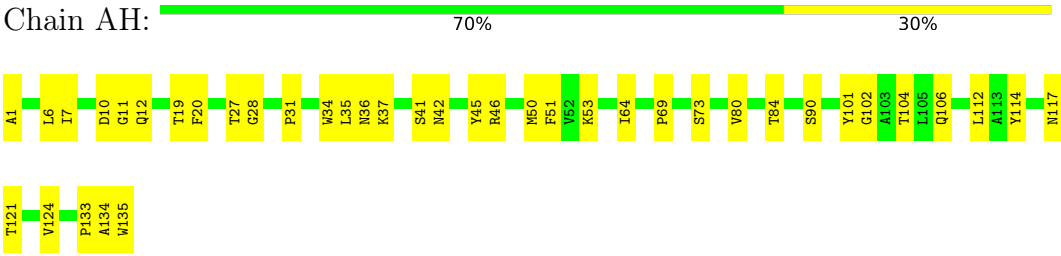
• Molecule 1: coat protein

Chain AG:



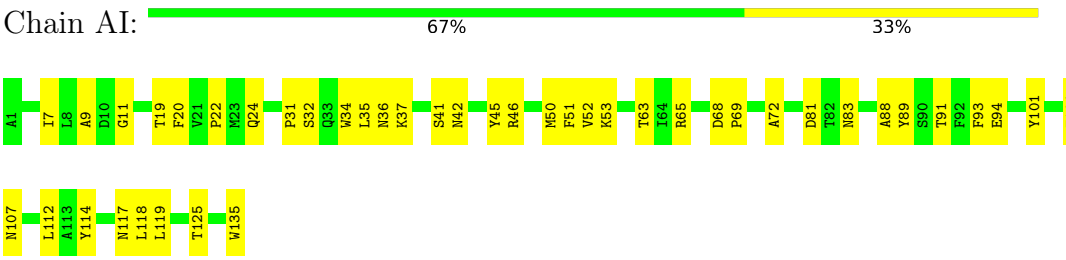
• Molecule 1: coat protein

Chain AH:



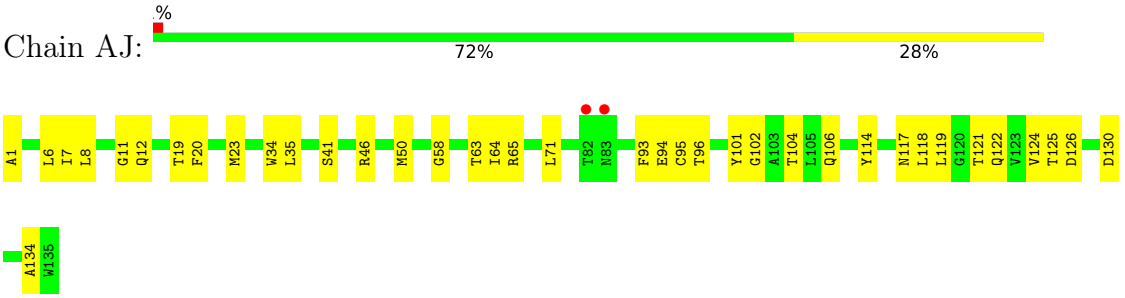
• Molecule 1: coat protein

Chain AI:



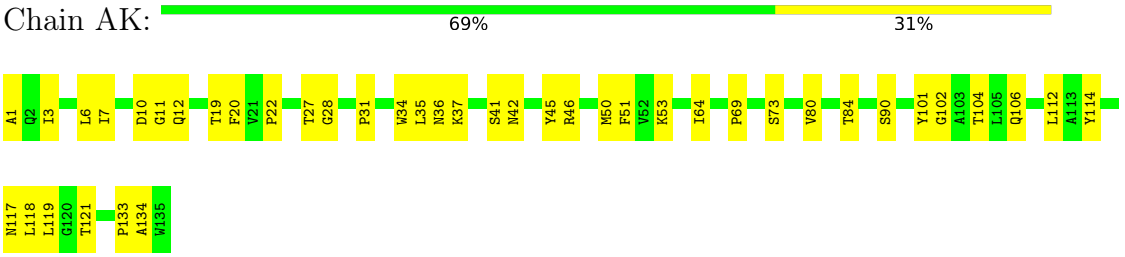
• Molecule 1: coat protein

Chain AJ:



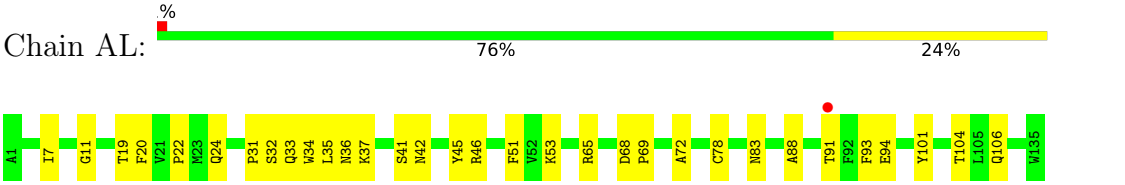
• Molecule 1: coat protein

Chain AK:



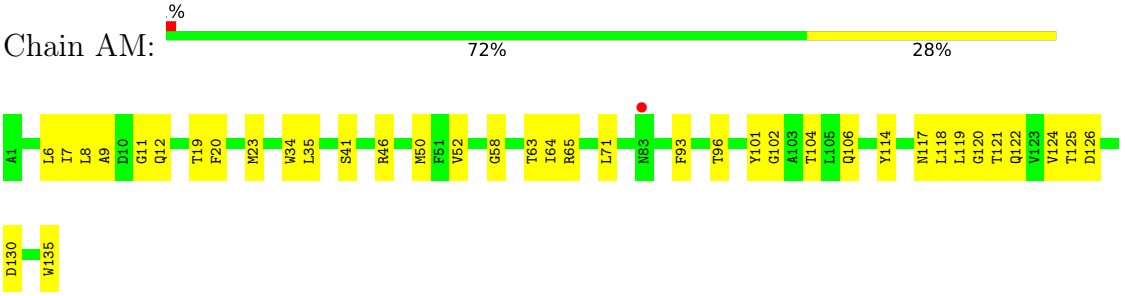
• Molecule 1: coat protein

Chain AL:



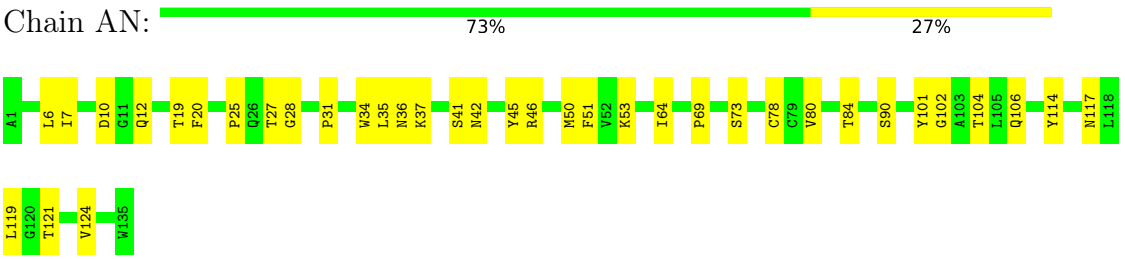
• Molecule 1: coat protein

Chain AM:



• Molecule 1: coat protein

Chain AN:

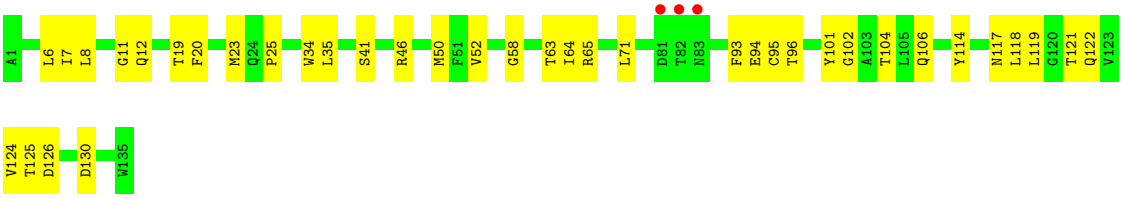


• Molecule 1: coat protein

Chain AO:

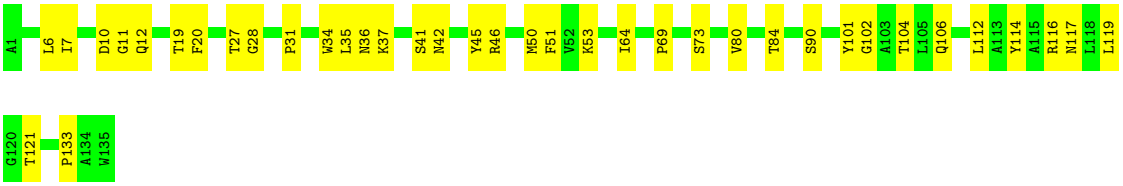
• Molecule 1: coat protein

Chain AP:



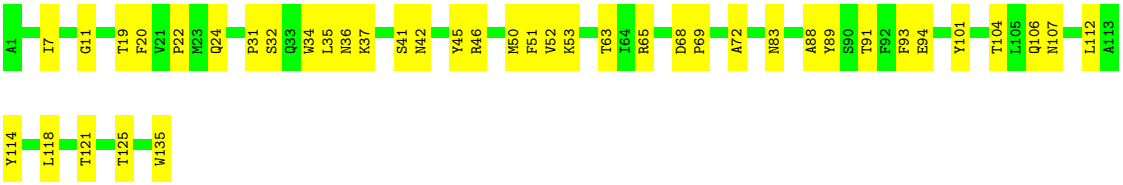
• Molecule 1: coat protein

Chain AQ:



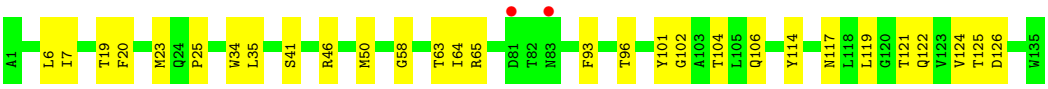
• Molecule 1: coat protein

Chain AR:



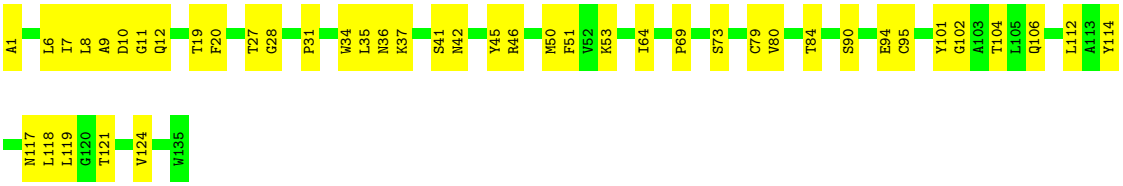
• Molecule 1: coat protein

Chain AS:



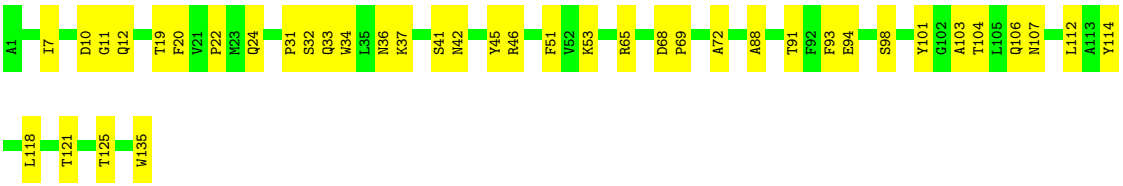
• Molecule 1: coat protein

Chain AT:



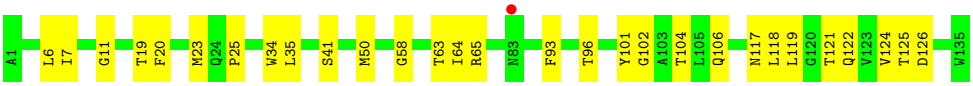
• Molecule 1: coat protein

Chain AU:



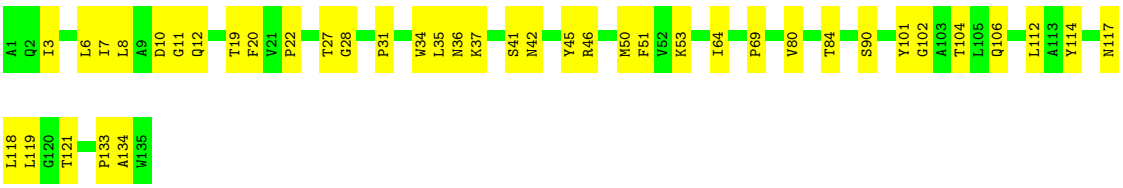
• Molecule 1: coat protein

Chain AV:



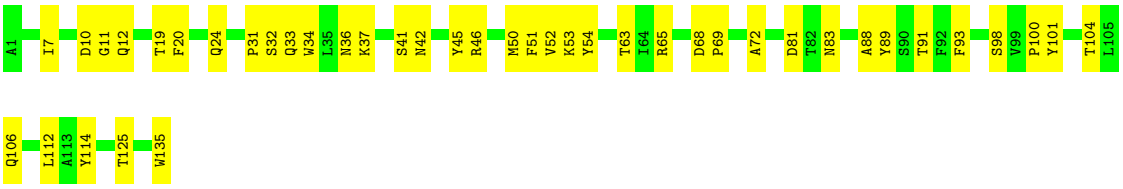
• Molecule 1: coat protein

Chain AW:



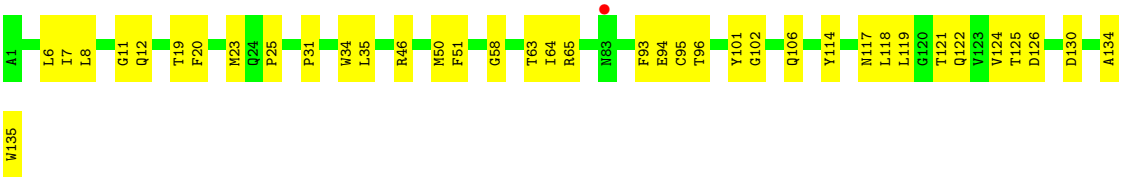
• Molecule 1: coat protein

Chain AX:



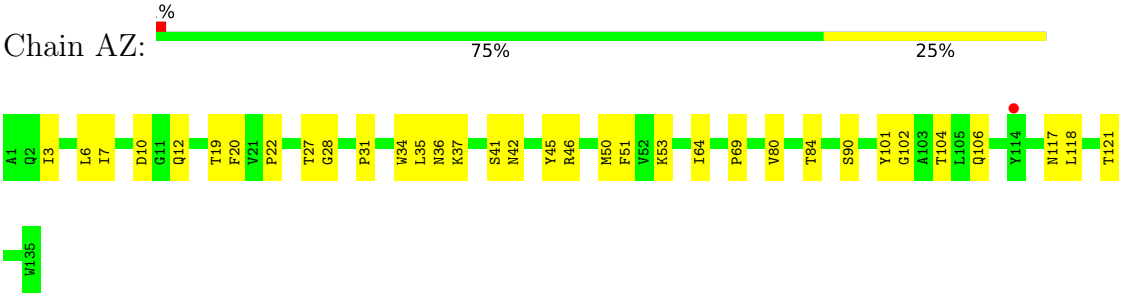
• Molecule 1: coat protein

Chain AY:



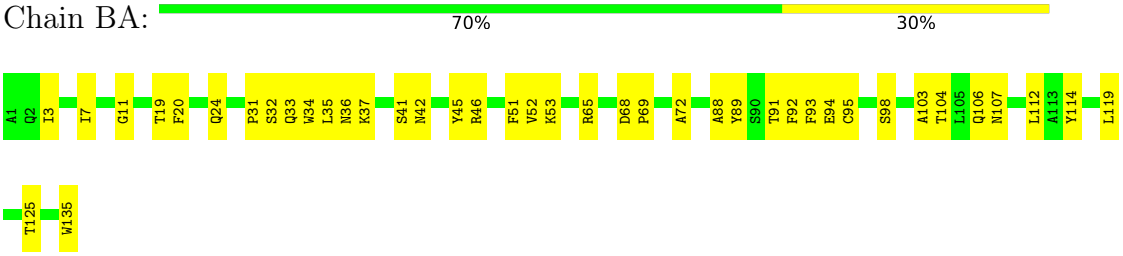
• Molecule 1: coat protein

Chain AZ:



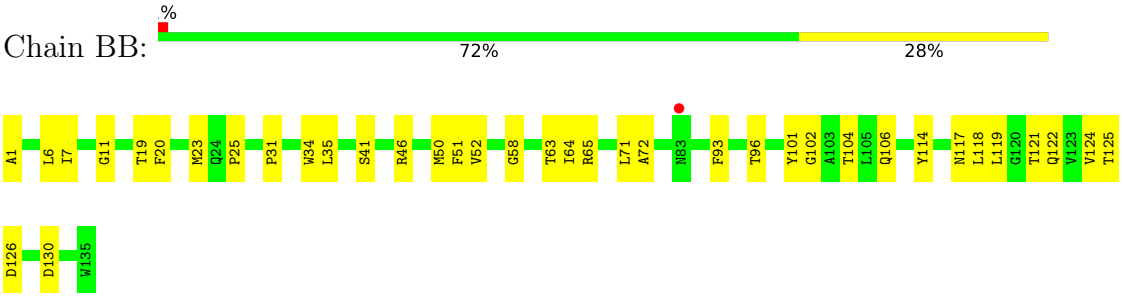
• Molecule 1: coat protein

Chain BA:



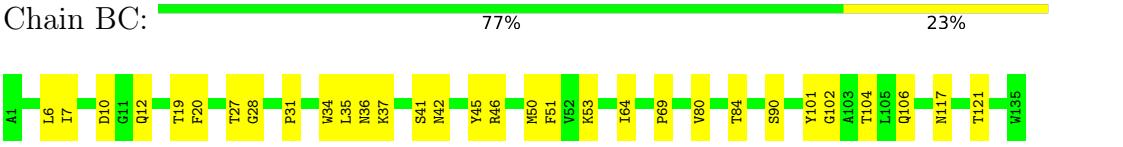
• Molecule 1: coat protein

Chain BB:



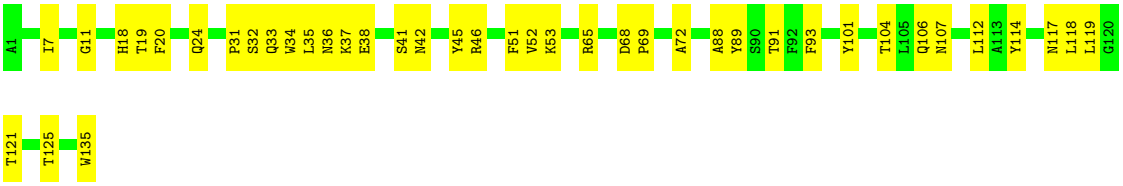
• Molecule 1: coat protein

Chain BC:



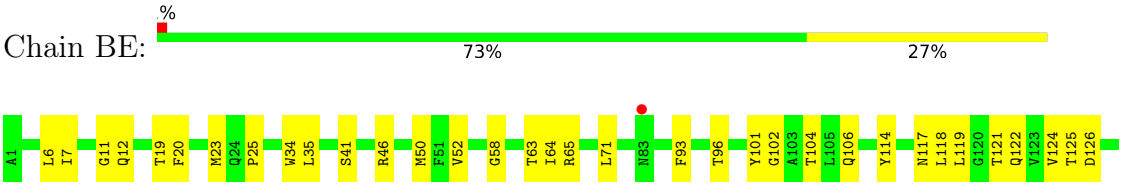
• Molecule 1: coat protein

Chain BD:



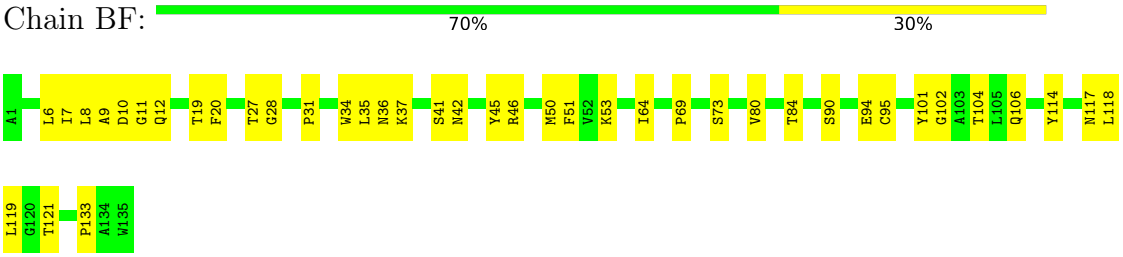
• Molecule 1: coat protein

Chain BE:



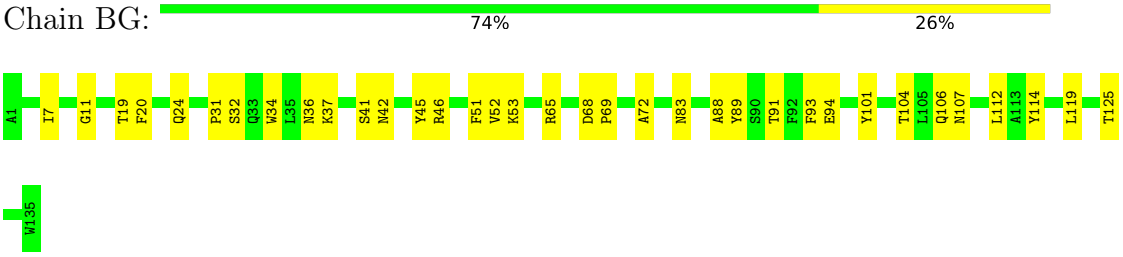
• Molecule 1: coat protein

Chain BF:



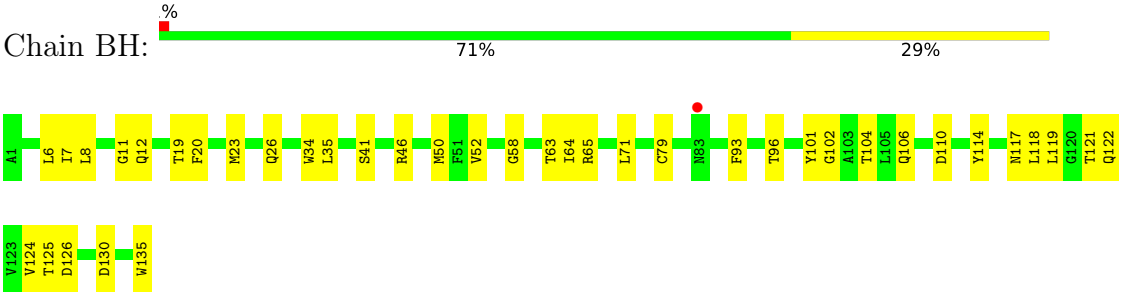
• Molecule 1: coat protein

Chain BG:



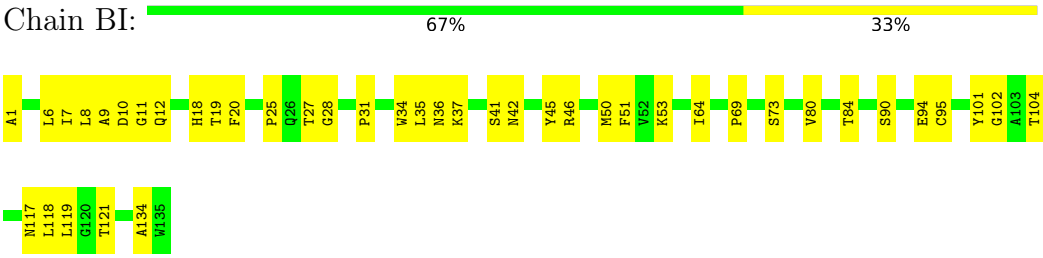
• Molecule 1: coat protein

Chain BH:



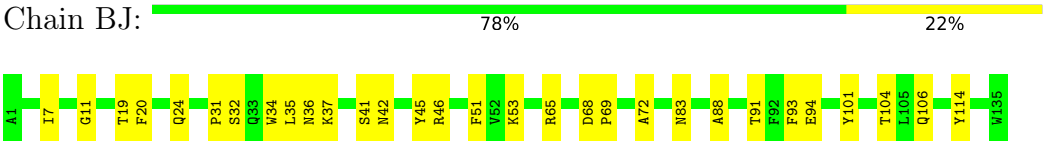
• Molecule 1: coat protein

Chain BI:



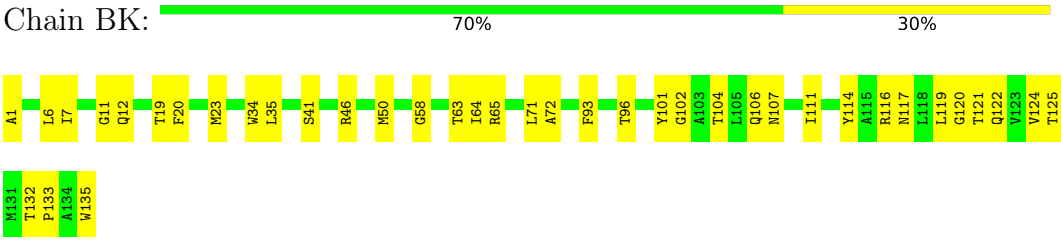
• Molecule 1: coat protein

Chain BJ:



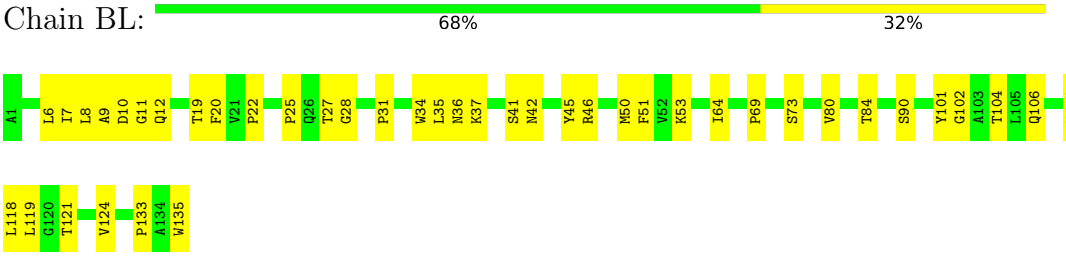
• Molecule 1: coat protein

Chain BK:



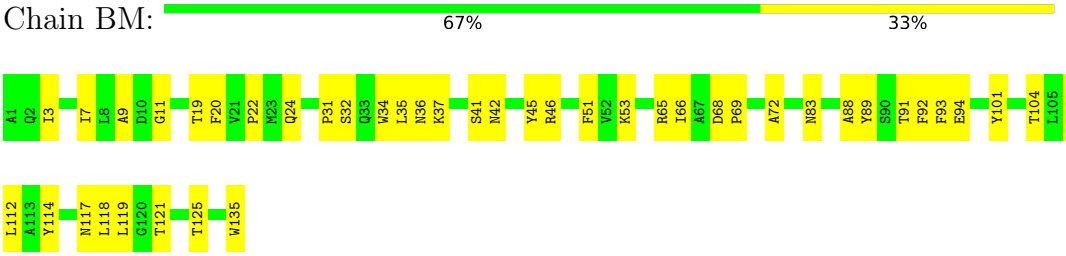
• Molecule 1: coat protein

Chain BL:



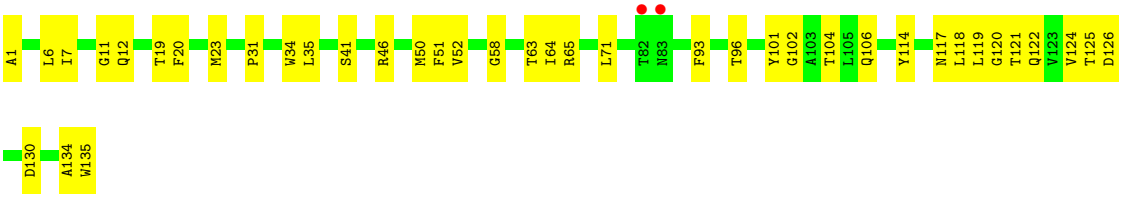
• Molecule 1: coat protein

Chain BM:



• Molecule 1: coat protein

Chain BN:

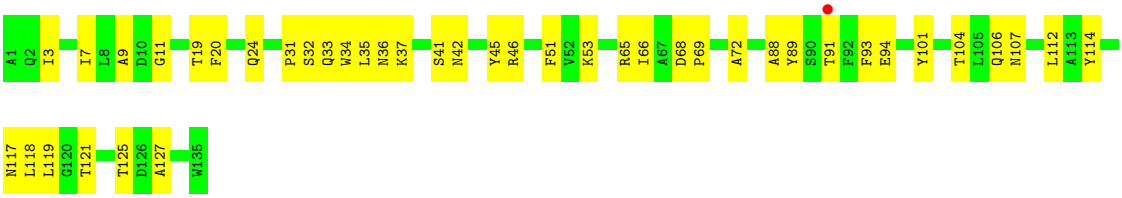


• Molecule 1: coat protein

Chain BO:

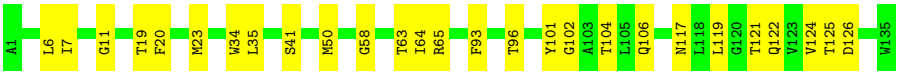
• Molecule 1: coat protein

Chain BP:



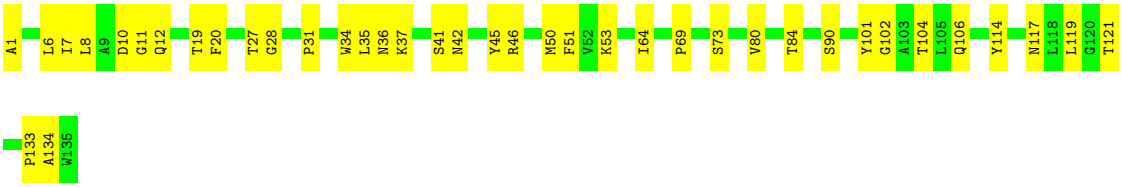
• Molecule 1: coat protein

Chain BQ:



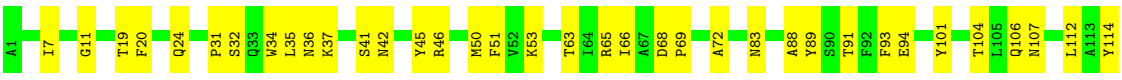
• Molecule 1: coat protein

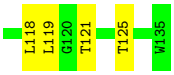
Chain BR:



• Molecule 1: coat protein

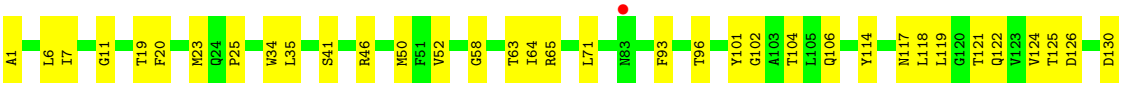
Chain BS:





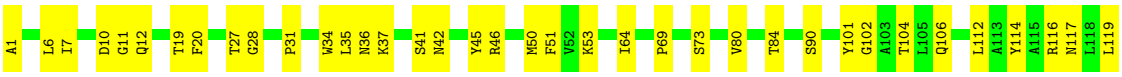
• Molecule 1: coat protein

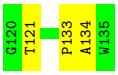
Chain BT:



• Molecule 1: coat protein

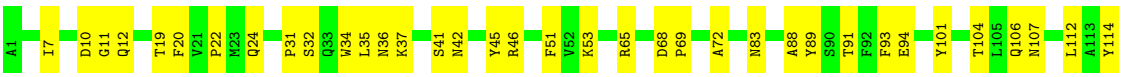
Chain BU:

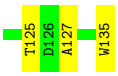




• Molecule 1: coat protein

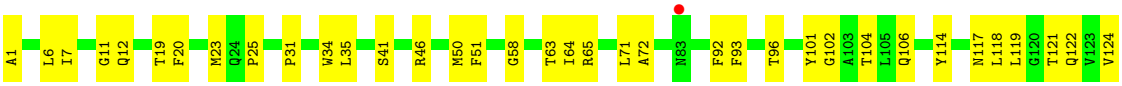
Chain BV:





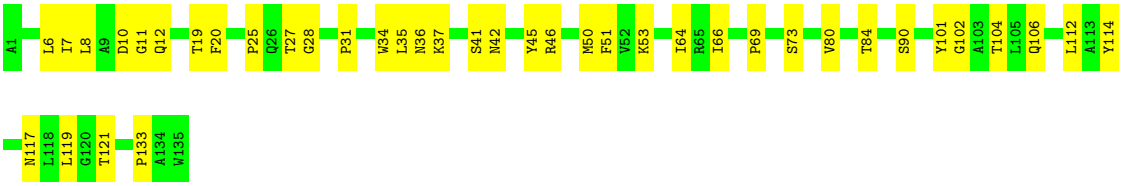
• Molecule 1: coat protein

Chain BW:



• Molecule 1: coat protein

Chain BX:

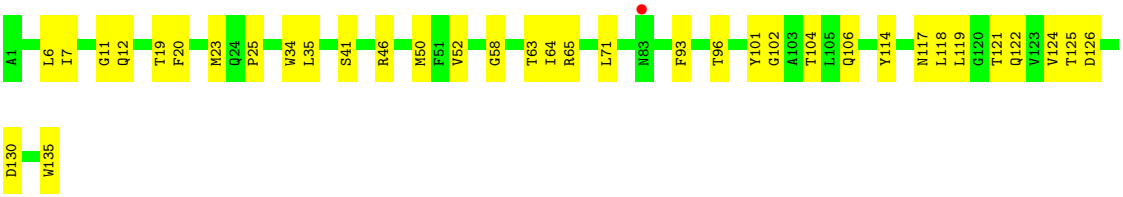


• Molecule 1: coat protein

Chain BY:

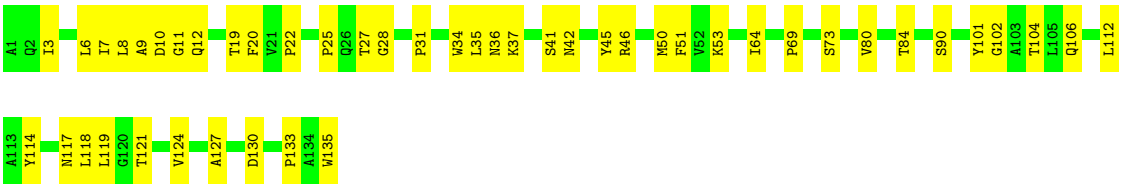
• Molecule 1: coat protein

Chain BZ:



• Molecule 1: coat protein

Chain CA:

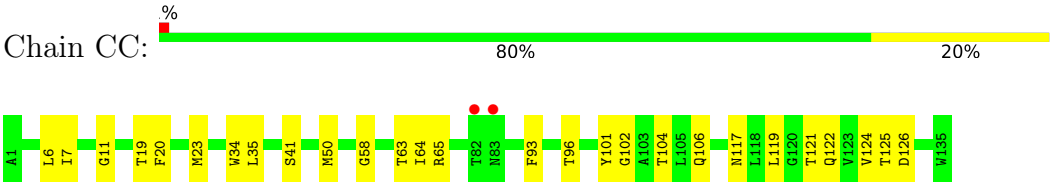


• Molecule 1: coat protein

Chain CB:

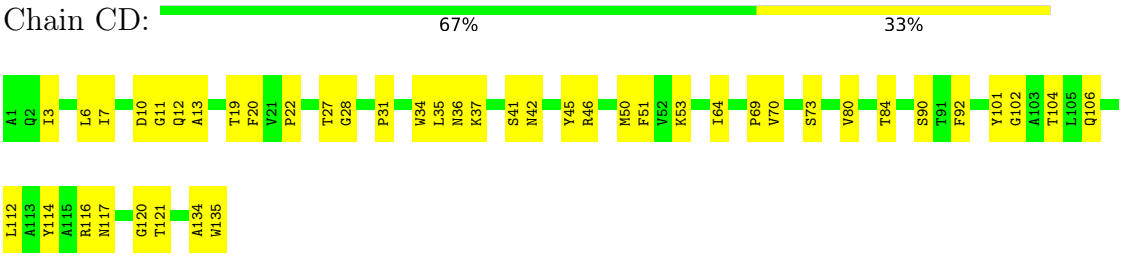
• Molecule 1: coat protein

Chain CC:



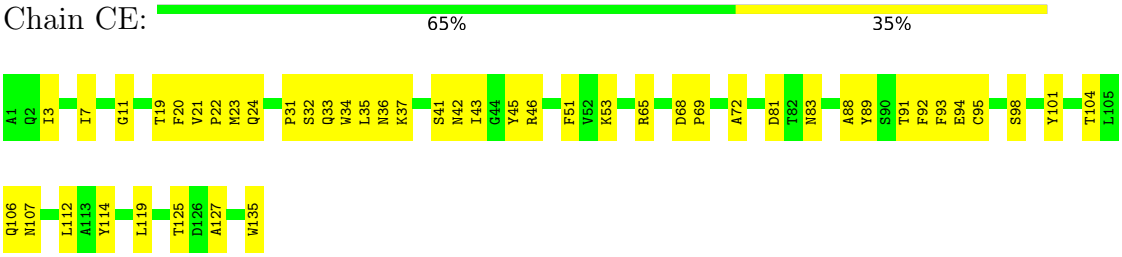
• Molecule 1: coat protein

Chain CD:



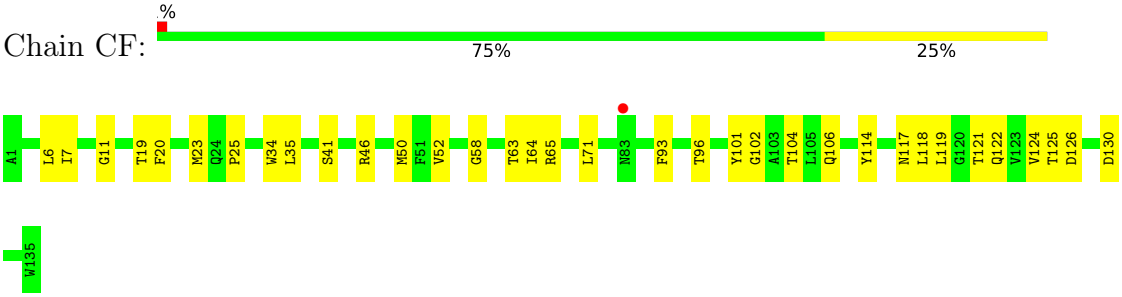
• Molecule 1: coat protein

Chain CE:



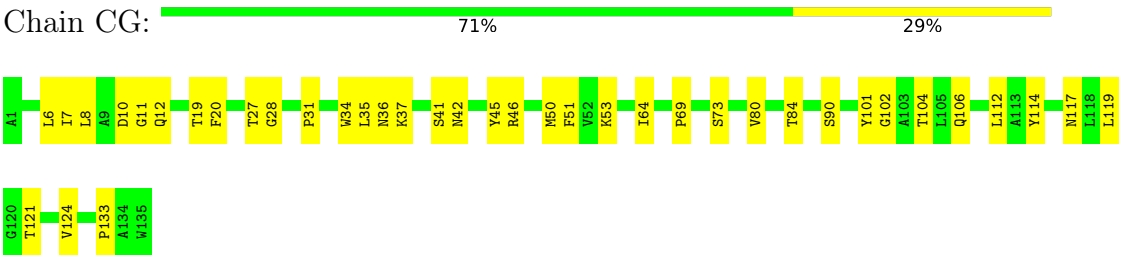
• Molecule 1: coat protein

Chain CF:



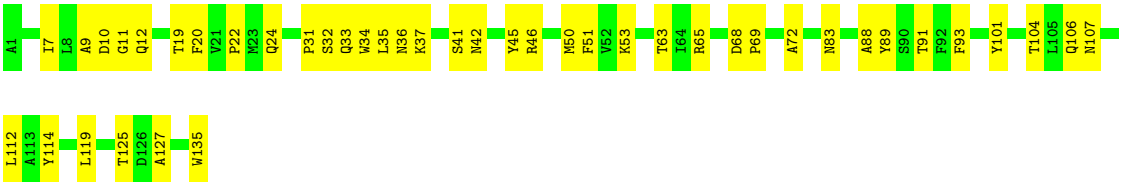
• Molecule 1: coat protein

Chain CG:



• Molecule 1: coat protein

Chain CH:


A1
I7
L8
A9
D10
G11
Q12
T19
F20
V21
P22
M23
Q24
P31
S32
Q33
W34
L35
N36
K37
S41
N42
Y45
R46
M50
F51
V52
K53
T63
I64
R65
D68
P69
A72
N83
A88
Y89
S90
T91
F92
F93
Y101
T104
L105
Q106
N107
L112
A113
Y114
L119
T125
D126
A127
W135

4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	341.90Å 341.90Å 1253.64Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.95 – 3.80 49.96 – 3.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.95-3.80) 100.0 (49.96-3.80)	Depositor EDS
R_{merge}	0.60	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.98 (at 3.77Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.220 , 0.222 0.219 , 0.220	Depositor DCC
R_{free} test set	5000 reflections (1.81%)	wwPDB-VP
Wilson B-factor (Å^2)	152.0	Xtriage
Anisotropy	0.136	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	61200	wwPDB-VP
Average B, all atoms (Å^2)	135.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.40% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	AA	0.31	0/1043	0.52	0/1428
1	AB	0.31	0/1043	0.53	0/1428
1	AC	0.32	0/1043	0.53	0/1428
1	AD	0.31	0/1043	0.52	0/1428
1	AE	0.31	0/1043	0.53	0/1428
1	AF	0.32	0/1043	0.53	0/1428
1	AG	0.31	0/1043	0.52	0/1428
1	AH	0.31	0/1043	0.53	0/1428
1	AI	0.32	0/1043	0.53	0/1428
1	AJ	0.31	0/1043	0.52	0/1428
1	AK	0.31	0/1043	0.53	0/1428
1	AL	0.32	0/1043	0.53	0/1428
1	AM	0.31	0/1043	0.52	0/1428
1	AN	0.31	0/1043	0.53	0/1428
1	AO	0.32	0/1043	0.53	0/1428
1	AP	0.31	0/1043	0.52	0/1428
1	AQ	0.31	0/1043	0.53	0/1428
1	AR	0.32	0/1043	0.53	0/1428
1	AS	0.32	0/1043	0.52	0/1428
1	AT	0.31	0/1043	0.53	0/1428
1	AU	0.32	0/1043	0.53	0/1428
1	AV	0.32	0/1043	0.52	0/1428
1	AW	0.31	0/1043	0.53	0/1428
1	AX	0.32	0/1043	0.53	0/1428
1	AY	0.31	0/1043	0.52	0/1428
1	AZ	0.31	0/1043	0.53	0/1428
1	BA	0.32	0/1043	0.53	0/1428
1	BB	0.31	0/1043	0.52	0/1428
1	BC	0.31	0/1043	0.53	0/1428
1	BD	0.32	0/1043	0.53	0/1428
1	BE	0.32	0/1043	0.52	0/1428
1	BF	0.31	0/1043	0.53	0/1428
1	BG	0.32	0/1043	0.53	0/1428
1	BH	0.31	0/1043	0.52	0/1428

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	BI	0.31	0/1043	0.53	0/1428
1	BJ	0.32	0/1043	0.53	0/1428
1	BK	0.32	0/1043	0.52	0/1428
1	BL	0.31	0/1043	0.53	0/1428
1	BM	0.32	0/1043	0.53	0/1428
1	BN	0.31	0/1043	0.52	0/1428
1	BO	0.31	0/1043	0.53	0/1428
1	BP	0.32	0/1043	0.53	0/1428
1	BQ	0.31	0/1043	0.52	0/1428
1	BR	0.31	0/1043	0.53	0/1428
1	BS	0.32	0/1043	0.53	0/1428
1	BT	0.31	0/1043	0.52	0/1428
1	BU	0.31	0/1043	0.53	0/1428
1	BV	0.32	0/1043	0.53	0/1428
1	BW	0.32	0/1043	0.52	0/1428
1	BX	0.31	0/1043	0.53	0/1428
1	BY	0.32	0/1043	0.53	0/1428
1	BZ	0.31	0/1043	0.52	0/1428
1	CA	0.31	0/1043	0.53	0/1428
1	CB	0.32	0/1043	0.53	0/1428
1	CC	0.32	0/1043	0.52	0/1428
1	CD	0.31	0/1043	0.53	0/1428
1	CE	0.32	0/1043	0.53	0/1428
1	CF	0.32	0/1043	0.52	0/1428
1	CG	0.31	0/1043	0.53	0/1428
1	CH	0.32	0/1043	0.53	0/1428
All	All	0.32	0/62580	0.53	0/85680

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	1020	0	1017	32	0
1	AB	1020	0	1017	39	0
1	AC	1020	0	1017	32	0
1	AD	1020	0	1017	29	0
1	AE	1020	0	1017	38	0
1	AF	1020	0	1017	41	0
1	AG	1020	0	1017	31	0
1	AH	1020	0	1017	38	0
1	AI	1020	0	1017	37	0
1	AJ	1020	0	1018	35	0
1	AK	1020	0	1017	38	0
1	AL	1020	0	1018	22	4
1	AM	1020	0	1017	33	1
1	AN	1020	0	1018	26	4
1	AO	1020	0	1018	28	0
1	AP	1020	0	1017	34	0
1	AQ	1020	0	1017	34	0
1	AR	1020	0	1017	32	0
1	AS	1020	0	1018	17	3
1	AT	1020	0	1018	41	1
1	AU	1020	0	1017	32	0
1	AV	1020	0	1018	18	2
1	AW	1020	0	1018	35	0
1	AX	1020	0	1017	36	0
1	AY	1020	0	1017	34	0
1	AZ	1020	0	1018	26	1
1	BA	1020	0	1018	34	0
1	BB	1020	0	1017	30	0
1	BC	1020	0	1018	24	1
1	BD	1020	0	1018	33	0
1	BE	1020	0	1017	32	0
1	BF	1020	0	1017	38	0
1	BG	1020	0	1017	28	0
1	BH	1020	0	1018	38	1
1	BI	1020	0	1017	44	0
1	BJ	1020	0	1018	20	3
1	BK	1020	0	1017	36	0
1	BL	1020	0	1017	43	0
1	BM	1020	0	1017	40	0
1	BN	1020	0	1017	33	0
1	BO	1020	0	1018	25	2
1	BP	1020	0	1018	36	0
1	BQ	1020	0	1018	16	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	BR	1020	0	1018	34	0
1	BS	1020	0	1017	31	0
1	BT	1020	0	1017	30	0
1	BU	1020	0	1017	36	0
1	BV	1020	0	1017	32	0
1	BW	1020	0	1017	34	0
1	BX	1020	0	1017	35	0
1	BY	1020	0	1017	34	0
1	BZ	1020	0	1017	32	0
1	CA	1020	0	1017	48	0
1	CB	1020	0	1017	39	0
1	CC	1020	0	1018	16	1
1	CD	1020	0	1018	40	1
1	CE	1020	0	1017	44	0
1	CF	1020	0	1017	30	0
1	CG	1020	0	1017	37	0
1	CH	1020	0	1017	36	0
All	All	61200	0	61040	1476	13

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 12.

All (1476) 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:AX:106:GLN:NE2	1:CB:11:GLY:O	1.99	0.94
1:AM:46:ARG:NH1	1:BL:114:TYR:OH	2.02	0.93
1:BH:46:ARG:NH1	1:CA:114:TYR:OH	2.06	0.88
1:AM:114:TYR:OH	1:BL:46:ARG:NH1	2.06	0.88
1:AP:46:ARG:NH1	1:BF:114:TYR:OH	2.07	0.87
1:AA:46:ARG:NH1	1:AH:114:TYR:OH	2.08	0.86
1:BK:11:GLY:O	1:CD:106:GLN:NE2	2.07	0.85
1:BH:114:TYR:OH	1:CA:46:ARG:NH1	2.09	0.85
1:AB:114:TYR:OH	1:BZ:46:ARG:NH1	2.09	0.85
1:AU:106:GLN:NE2	1:BY:11:GLY:O	2.12	0.83
1:AX:112:LEU:HD21	1:CB:125:THR:HG22	1.61	0.82
1:AA:114:TYR:OH	1:AH:46:ARG:NH1	2.12	0.82
1:BR:114:TYR:OH	1:BT:46:ARG:NH1	2.13	0.82
1:AB:46:ARG:NH1	1:BZ:114:TYR:OH	2.14	0.81
1:AD:11:GLY:O	1:AQ:106:GLN:NE2	2.13	0.81
1:AU:11:GLY:O	1:BY:106:GLN:NE2	2.14	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AP:114:TYR:OH	1:BF:46:ARG:NH1	2.13	0.81
1:BX:114:TYR:OH	1:CF:46:ARG:NH1	2.14	0.81
1:AE:114:TYR:OH	1:BW:46:ARG:NH1	2.14	0.80
1:AX:11:GLY:O	1:CB:106:GLN:NE2	2.14	0.80
1:AJ:46:ARG:NH1	1:BI:114:TYR:OH	2.14	0.80
1:BN:11:GLY:O	1:BU:106:GLN:NE2	2.14	0.80
1:BD:112:LEU:HD21	1:CH:125:THR:HG22	1.64	0.80
1:AC:11:GLY:O	1:BG:106:GLN:NE2	2.16	0.79
1:AE:106:GLN:NE2	1:BW:11:GLY:O	2.16	0.79
1:AC:125:THR:HG22	1:BG:112:LEU:HD21	1.63	0.79
1:BD:46:ARG:NH1	1:CH:114:TYR:OH	2.16	0.78
1:AI:46:ARG:NH1	1:BP:114:TYR:OH	2.16	0.78
1:BK:114:TYR:OH	1:CD:46:ARG:NH1	2.16	0.78
1:BA:106:GLN:NE2	1:CE:11:GLY:O	2.17	0.78
1:BE:46:ARG:NH1	1:CG:114:TYR:OH	2.17	0.77
1:AR:106:GLN:NE2	1:BV:11:GLY:O	2.17	0.77
1:BD:106:GLN:NE2	1:CH:11:GLY:O	2.17	0.77
1:AC:112:LEU:HD21	1:BG:125:THR:HG22	1.66	0.77
1:AX:46:ARG:NH1	1:CB:114:TYR:OH	2.18	0.77
1:AA:11:GLY:O	1:AH:106:GLN:NE2	2.18	0.77
1:AC:106:GLN:NE2	1:BG:11:GLY:O	2.18	0.76
1:AO:112:LEU:HD21	1:BS:125:THR:HG22	1.67	0.76
1:BE:11:GLY:O	1:CG:106:GLN:NE2	2.19	0.76
1:BK:46:ARG:NH1	1:CD:114:TYR:OH	2.18	0.76
1:AD:106:GLN:NE2	1:AQ:11:GLY:O	2.18	0.76
1:AO:125:THR:HG22	1:BS:112:LEU:HD21	1.66	0.76
1:AR:112:LEU:HD21	1:BV:125:THR:HG22	1.68	0.76
1:AT:114:TYR:OH	1:AY:46:ARG:NH1	2.19	0.76
1:AJ:114:TYR:OH	1:BI:46:ARG:NH1	2.19	0.75
1:BA:46:ARG:NH1	1:CE:114:TYR:OH	2.19	0.75
1:AR:11:GLY:O	1:BV:106:GLN:NE2	2.20	0.75
1:AT:106:GLN:NE2	1:AY:11:GLY:O	2.19	0.75
1:AU:125:THR:HG22	1:BY:112:LEU:HD21	1.68	0.75
1:AI:114:TYR:OH	1:BP:46:ARG:NH1	2.20	0.75
1:AW:114:TYR:OH	1:BB:46:ARG:NH1	2.20	0.74
1:AB:106:GLN:NE2	1:BZ:11:GLY:O	2.20	0.74
1:AG:46:ARG:NH1	1:AK:114:TYR:OH	2.21	0.74
1:BN:106:GLN:NE2	1:BU:11:GLY:O	2.21	0.74
1:AI:112:LEU:HD21	1:BP:125:THR:HG22	1.70	0.74
1:AT:11:GLY:O	1:AY:106:GLN:NE2	2.20	0.74
1:BN:46:ARG:NH1	1:BU:114:TYR:OH	2.21	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BX:46:ARG:NH1	1:CF:114:TYR:OH	2.21	0.73
1:AG:11:GLY:O	1:AK:106:GLN:NE2	2.22	0.73
1:AT:46:ARG:NH1	1:AY:114:TYR:OH	2.21	0.73
1:BH:11:GLY:O	1:CA:106:GLN:NE2	2.22	0.73
1:AR:46:ARG:NH1	1:BV:114:TYR:OH	2.22	0.73
1:BA:114:TYR:OH	1:CE:46:ARG:NH1	2.22	0.73
1:BE:114:TYR:OH	1:CG:46:ARG:NH1	2.22	0.73
1:BK:135:TRP:CE3	1:CE:22:PRO:HG2	2.23	0.73
1:BH:102:GLY:O	1:CA:73:SER:OG	2.07	0.73
1:BR:46:ARG:NH1	1:BT:114:TYR:OH	2.22	0.73
1:AF:46:ARG:NH1	1:BM:114:TYR:OH	2.22	0.72
1:AO:11:GLY:O	1:BS:106:GLN:NE2	2.22	0.72
1:AE:46:ARG:NH1	1:BW:114:TYR:OH	2.22	0.72
1:AR:125:THR:HG22	1:BV:112:LEU:HD21	1.71	0.72
1:AF:83:ASN:ND2	1:BW:71:LEU:O	2.23	0.72
1:AF:114:TYR:OH	1:BM:46:ARG:NH1	2.23	0.72
1:AT:73:SER:OG	1:AY:102:GLY:O	2.07	0.72
1:CA:80:VAL:HA	1:CA:84:THR:HG21	1.73	0.71
1:AQ:80:VAL:HA	1:AQ:84:THR:HG21	1.73	0.71
1:BX:80:VAL:HA	1:BX:84:THR:HG21	1.73	0.71
1:AZ:80:VAL:HA	1:AZ:84:THR:HG21	1.73	0.71
1:AK:80:VAL:HA	1:AK:84:THR:HG21	1.73	0.71
1:AN:80:VAL:HA	1:AN:84:THR:HG21	1.73	0.71
1:AF:125:THR:HG22	1:BM:112:LEU:HD21	1.72	0.71
1:AB:80:VAL:HA	1:AB:84:THR:HG21	1.73	0.71
1:AW:80:VAL:HA	1:AW:84:THR:HG21	1.73	0.71
1:AE:80:VAL:HA	1:AE:84:THR:HG21	1.73	0.71
1:CD:80:VAL:HA	1:CD:84:THR:HG21	1.73	0.70
1:AU:112:LEU:HD21	1:BY:125:THR:HG22	1.73	0.70
1:AW:46:ARG:NH1	1:BB:114:TYR:OH	2.24	0.70
1:AR:114:TYR:OH	1:BV:46:ARG:NH1	2.23	0.70
1:AT:80:VAL:HA	1:AT:84:THR:HG21	1.73	0.70
1:AH:80:VAL:HA	1:AH:84:THR:HG21	1.73	0.70
1:BU:80:VAL:HA	1:BU:84:THR:HG21	1.73	0.70
1:AJ:11:GLY:O	1:BI:106:GLN:NE2	2.25	0.70
1:AV:25:PRO:HG3	1:CB:135:TRP:CD1	2.26	0.70
1:AF:112:LEU:HD21	1:BM:125:THR:HG22	1.71	0.70
1:AG:114:TYR:OH	1:AK:46:ARG:NH1	2.24	0.70
1:BD:114:TYR:OH	1:CH:46:ARG:NH1	2.25	0.70
1:BN:114:TYR:OH	1:BU:46:ARG:NH1	2.25	0.70
1:BR:80:VAL:HA	1:BR:84:THR:HG21	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BH:106:GLN:NE2	1:CA:11:GLY:O	2.25	0.69
1:BC:80:VAL:HA	1:BC:84:THR:HG21	1.73	0.69
1:AW:106:GLN:NE2	1:BB:11:GLY:O	2.25	0.69
1:BI:80:VAL:HA	1:BI:84:THR:HG21	1.73	0.69
1:AO:114:TYR:OH	1:BS:46:ARG:NH1	2.25	0.69
1:BL:80:VAL:HA	1:BL:84:THR:HG21	1.73	0.69
1:CG:80:VAL:HA	1:CG:84:THR:HG21	1.73	0.69
1:BE:106:GLN:NE2	1:CG:11:GLY:O	2.25	0.69
1:BF:80:VAL:HA	1:BF:84:THR:HG21	1.73	0.69
1:BO:80:VAL:HA	1:BO:84:THR:HG21	1.73	0.69
1:BA:112:LEU:HD21	1:CE:125:THR:HG22	1.75	0.69
1:AO:46:ARG:NH1	1:BS:114:TYR:OH	2.26	0.69
1:BD:11:GLY:O	1:CH:106:GLN:NE2	2.26	0.69
1:AA:71:LEU:O	1:AI:83:ASN:ND2	2.26	0.68
1:AE:11:GLY:O	1:BW:106:GLN:NE2	2.26	0.68
1:BA:11:GLY:O	1:CE:106:GLN:NE2	2.26	0.68
1:AI:125:THR:HG22	1:BP:112:LEU:HD21	1.76	0.68
1:AD:46:ARG:NH1	1:AQ:114:TYR:OH	2.26	0.68
1:AM:11:GLY:O	1:BL:106:GLN:NE2	2.28	0.67
1:BK:106:GLN:NE2	1:CD:11:GLY:O	2.25	0.67
1:AO:106:GLN:NE2	1:BS:11:GLY:O	2.28	0.67
1:BD:125:THR:HG22	1:CH:112:LEU:HD21	1.76	0.67
1:AJ:106:GLN:NE2	1:BI:11:GLY:O	2.28	0.67
1:AJ:102:GLY:O	1:BI:73:SER:OG	2.13	0.66
1:BK:71:LEU:O	1:CE:83:ASN:ND2	2.28	0.66
1:BX:106:GLN:NE2	1:CF:11:GLY:O	2.28	0.66
1:AK:31:PRO:HB3	1:AK:51:PHE:HB2	1.78	0.66
1:CD:31:PRO:HB3	1:CD:51:PHE:HB2	1.78	0.66
1:BR:106:GLN:NE2	1:BT:11:GLY:O	2.28	0.65
1:BC:31:PRO:HB3	1:BC:51:PHE:HB2	1.79	0.65
1:BF:31:PRO:HB3	1:BF:51:PHE:HB2	1.78	0.65
1:BL:31:PRO:HB3	1:BL:51:PHE:HB2	1.78	0.65
1:BX:31:PRO:HB3	1:BX:51:PHE:HB2	1.78	0.65
1:AC:114:TYR:OH	1:BG:46:ARG:NH1	2.29	0.65
1:AW:31:PRO:HB3	1:AW:51:PHE:HB2	1.78	0.65
1:BA:125:THR:HG22	1:CE:112:LEU:HD21	1.78	0.65
1:BR:31:PRO:HB3	1:BR:51:PHE:HB2	1.78	0.65
1:BI:31:PRO:HB3	1:BI:51:PHE:HB2	1.78	0.65
1:CA:31:PRO:HB3	1:CA:51:PHE:HB2	1.78	0.65
1:AQ:31:PRO:HB3	1:AQ:51:PHE:HB2	1.78	0.65
1:AZ:31:PRO:HB3	1:AZ:51:PHE:HB2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CG:31:PRO:HB3	1:CG:51:PHE:HB2	1.78	0.65
1:AD:114:TYR:OH	1:AQ:46:ARG:NH1	2.30	0.65
1:AF:106:GLN:NE2	1:BM:11:GLY:O	2.30	0.65
1:AP:11:GLY:O	1:BF:106:GLN:NE2	2.30	0.65
1:AS:23:MET:HG3	1:AS:35:LEU:HD12	1.79	0.65
1:AU:114:TYR:OH	1:BY:46:ARG:NH1	2.29	0.65
1:AI:106:GLN:NE2	1:BP:11:GLY:O	2.29	0.65
1:AH:31:PRO:HB3	1:AH:51:PHE:HB2	1.78	0.64
1:AS:7:ILE:HG12	1:AS:19:THR:HG22	1.80	0.64
1:AV:7:ILE:HG12	1:AV:19:THR:HG22	1.80	0.64
1:BQ:23:MET:HG3	1:BQ:35:LEU:HD12	1.79	0.64
1:AA:23:MET:HG3	1:AA:35:LEU:HD12	1.79	0.64
1:BH:7:ILE:HG12	1:BH:19:THR:HG22	1.80	0.64
1:BT:23:MET:HG3	1:BT:35:LEU:HD12	1.79	0.64
1:AI:11:GLY:O	1:BP:106:GLN:NE2	2.30	0.64
1:AT:31:PRO:HB3	1:AT:51:PHE:HB2	1.78	0.64
1:AN:31:PRO:HB3	1:AN:51:PHE:HB2	1.78	0.64
1:AY:7:ILE:HG12	1:AY:19:THR:HG22	1.80	0.64
1:AJ:7:ILE:HG12	1:AJ:19:THR:HG22	1.80	0.64
1:AM:23:MET:HG3	1:AM:35:LEU:HD12	1.79	0.64
1:BN:23:MET:HG3	1:BN:35:LEU:HD12	1.79	0.64
1:BO:31:PRO:HB3	1:BO:51:PHE:HB2	1.78	0.64
1:AD:23:MET:HG3	1:AD:35:LEU:HD12	1.79	0.64
1:BB:23:MET:HG3	1:BB:35:LEU:HD12	1.79	0.64
1:AM:7:ILE:HG12	1:AM:19:THR:HG22	1.80	0.64
1:BW:7:ILE:HG12	1:BW:19:THR:HG22	1.80	0.63
1:AB:11:GLY:O	1:BZ:106:GLN:NE2	2.30	0.63
1:AE:31:PRO:HB3	1:AE:51:PHE:HB2	1.78	0.63
1:AP:7:ILE:HG12	1:AP:19:THR:HG22	1.80	0.63
1:BU:31:PRO:HB3	1:BU:51:PHE:HB2	1.78	0.63
1:CC:7:ILE:HG12	1:CC:19:THR:HG22	1.80	0.63
1:CC:23:MET:HG3	1:CC:35:LEU:HD12	1.79	0.63
1:AB:31:PRO:HB3	1:AB:51:PHE:HB2	1.78	0.63
1:AG:7:ILE:HG12	1:AG:19:THR:HG22	1.80	0.63
1:BK:7:ILE:HG12	1:BK:19:THR:HG22	1.80	0.63
1:BZ:7:ILE:HG12	1:BZ:19:THR:HG22	1.80	0.63
1:CF:23:MET:HG3	1:CF:35:LEU:HD12	1.79	0.63
1:AC:46:ARG:NH1	1:BG:114:TYR:OH	2.31	0.63
1:BB:7:ILE:HG12	1:BB:19:THR:HG22	1.80	0.63
1:CF:7:ILE:HG12	1:CF:19:THR:HG22	1.80	0.63
1:AG:23:MET:HG3	1:AG:35:LEU:HD12	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BT:7:ILE:HG12	1:BT:19:THR:HG22	1.80	0.63
1:BW:23:MET:HG3	1:BW:35:LEU:HD12	1.79	0.63
1:BZ:23:MET:HG3	1:BZ:35:LEU:HD12	1.79	0.63
1:AG:106:GLN:NE2	1:AK:11:GLY:O	2.30	0.63
1:AU:46:ARG:NH1	1:BY:114:TYR:OH	2.32	0.63
1:BK:23:MET:HG3	1:BK:35:LEU:HD12	1.79	0.63
1:AA:7:ILE:HG12	1:AA:19:THR:HG22	1.80	0.63
1:BH:23:MET:HG3	1:BH:35:LEU:HD12	1.79	0.63
1:AP:23:MET:HG3	1:AP:35:LEU:HD12	1.79	0.63
1:AX:114:TYR:OH	1:CB:46:ARG:NH1	2.32	0.63
1:BE:7:ILE:HG12	1:BE:19:THR:HG22	1.80	0.62
1:BE:23:MET:HG3	1:BE:35:LEU:HD12	1.79	0.62
1:BN:7:ILE:HG12	1:BN:19:THR:HG22	1.80	0.62
1:AY:23:MET:HG3	1:AY:35:LEU:HD12	1.79	0.62
1:AV:23:MET:HG3	1:AV:35:LEU:HD12	1.79	0.62
1:AJ:23:MET:HG3	1:AJ:35:LEU:HD12	1.79	0.62
1:CB:72:ALA:HB2	1:CB:88:ALA:HB2	1.82	0.62
1:AO:72:ALA:HB2	1:AO:88:ALA:HB2	1.82	0.62
1:AX:52:VAL:HG21	1:CB:127:ALA:HB1	1.81	0.62
1:CE:72:ALA:HB2	1:CE:88:ALA:HB2	1.82	0.62
1:AD:7:ILE:HG12	1:AD:19:THR:HG22	1.80	0.62
1:BG:72:ALA:HB2	1:BG:88:ALA:HB2	1.82	0.62
1:BQ:7:ILE:HG12	1:BQ:19:THR:HG22	1.80	0.62
1:BY:72:ALA:HB2	1:BY:88:ALA:HB2	1.82	0.62
1:CH:72:ALA:HB2	1:CH:88:ALA:HB2	1.82	0.62
1:AA:106:GLN:NE2	1:AH:11:GLY:O	2.30	0.61
1:AC:72:ALA:HB2	1:AC:88:ALA:HB2	1.82	0.61
1:BP:72:ALA:HB2	1:BP:88:ALA:HB2	1.82	0.61
1:AR:72:ALA:HB2	1:AR:88:ALA:HB2	1.82	0.61
1:AF:37:LYS:HE3	1:BW:130:ASP:O	2.00	0.61
1:AL:72:ALA:HB2	1:AL:88:ALA:HB2	1.82	0.61
1:BJ:72:ALA:HB2	1:BJ:88:ALA:HB2	1.82	0.61
1:AX:125:THR:HG22	1:CB:112:LEU:HD21	1.81	0.61
1:BD:72:ALA:HB2	1:BD:88:ALA:HB2	1.82	0.61
1:AX:72:ALA:HB2	1:AX:88:ALA:HB2	1.82	0.61
1:BS:83:ASN:ND2	1:BT:71:LEU:O	2.33	0.61
1:AF:72:ALA:HB2	1:AF:88:ALA:HB2	1.82	0.61
1:BC:102:GLY:HA2	1:BD:41:SER:HB3	1.84	0.60
1:BI:102:GLY:HA2	1:BJ:41:SER:HB3	1.84	0.60
1:AN:102:GLY:HA2	1:AO:41:SER:HB3	1.84	0.60
1:AT:102:GLY:HA2	1:AU:41:SER:HB3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BK:135:TRP:CD2	1:CE:22:PRO:HG2	2.37	0.60
1:AQ:102:GLY:HA2	1:AR:41:SER:HB3	1.84	0.60
1:AZ:102:GLY:HA2	1:BA:41:SER:HB3	1.84	0.60
1:BS:72:ALA:HB2	1:BS:88:ALA:HB2	1.82	0.60
1:AB:102:GLY:HA2	1:AC:41:SER:HB3	1.84	0.60
1:AU:72:ALA:HB2	1:AU:88:ALA:HB2	1.82	0.60
1:AW:102:GLY:HA2	1:AX:41:SER:HB3	1.84	0.60
1:BA:72:ALA:HB2	1:BA:88:ALA:HB2	1.82	0.60
1:AE:37:LYS:HA	1:AE:45:TYR:CD1	2.37	0.60
1:AF:11:GLY:O	1:BM:106:GLN:NE2	2.34	0.60
1:BR:37:LYS:HA	1:BR:45:TYR:CD1	2.37	0.60
1:CD:102:GLY:HA2	1:CE:41:SER:HB3	1.84	0.60
1:AI:72:ALA:HB2	1:AI:88:ALA:HB2	1.82	0.60
1:BM:72:ALA:HB2	1:BM:88:ALA:HB2	1.82	0.60
1:BX:37:LYS:HA	1:BX:45:TYR:CD1	2.37	0.60
1:CD:37:LYS:HA	1:CD:45:TYR:CD1	2.37	0.60
1:AW:37:LYS:HA	1:AW:45:TYR:CD1	2.37	0.60
1:AX:83:ASN:ND2	1:BB:71:LEU:O	2.34	0.60
1:AK:37:LYS:HA	1:AK:45:TYR:CD1	2.37	0.59
1:AQ:37:LYS:HA	1:AQ:45:TYR:CD1	2.37	0.59
1:AT:37:LYS:HA	1:AT:45:TYR:CD1	2.37	0.59
1:AZ:37:LYS:HA	1:AZ:45:TYR:CD1	2.37	0.59
1:BF:37:LYS:HA	1:BF:45:TYR:CD1	2.37	0.59
1:BH:114:TYR:HH	1:CA:46:ARG:NH1	1.99	0.59
1:BL:37:LYS:HA	1:BL:45:TYR:CD1	2.37	0.59
1:BU:37:LYS:HA	1:BU:45:TYR:CD1	2.37	0.59
1:BV:72:ALA:HB2	1:BV:88:ALA:HB2	1.82	0.59
1:AN:37:LYS:HA	1:AN:45:TYR:CD1	2.37	0.59
1:BU:102:GLY:HA2	1:BV:41:SER:HB3	1.83	0.59
1:AC:83:ASN:ND2	1:BZ:71:LEU:O	2.35	0.59
1:BF:102:GLY:HA2	1:BG:41:SER:HB3	1.84	0.59
1:AB:37:LYS:HA	1:AB:45:TYR:CD1	2.37	0.59
1:AH:37:LYS:HA	1:AH:45:TYR:CD1	2.37	0.59
1:CG:102:GLY:HA2	1:CH:41:SER:HB3	1.84	0.59
1:AH:102:GLY:HA2	1:AI:41:SER:HB3	1.84	0.59
1:BO:37:LYS:HA	1:BO:45:TYR:CD1	2.37	0.59
1:AM:12:GLN:HG2	1:BL:106:GLN:NE2	2.18	0.59
1:BC:37:LYS:HA	1:BC:45:TYR:CD1	2.37	0.59
1:BI:37:LYS:HA	1:BI:45:TYR:CD1	2.37	0.59
1:AP:102:GLY:O	1:BF:73:SER:OG	2.21	0.59
1:BX:11:GLY:O	1:CF:106:GLN:NE2	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:37:LYS:HA	1:CA:45:TYR:CD1	2.37	0.59
1:AI:89:TYR:OH	1:BP:107:ASN:ND2	2.36	0.58
1:BO:102:GLY:HA2	1:BP:41:SER:HB3	1.84	0.58
1:CG:37:LYS:HA	1:CG:45:TYR:CD1	2.37	0.58
1:AA:130:ASP:O	1:AI:37:LYS:HE3	2.04	0.58
1:AK:102:GLY:HA2	1:AL:41:SER:HB3	1.84	0.58
1:BL:102:GLY:HA2	1:BM:41:SER:HB3	1.84	0.58
1:BR:102:GLY:HA2	1:BS:41:SER:HB3	1.84	0.58
1:CA:102:GLY:HA2	1:CB:41:SER:HB3	1.84	0.58
1:AC:104:THR:HG22	1:AC:106:GLN:H	1.69	0.58
1:AO:104:THR:HG22	1:AO:106:GLN:H	1.69	0.58
1:BJ:104:THR:HG22	1:BJ:106:GLN:H	1.69	0.58
1:AE:102:GLY:HA2	1:AF:41:SER:HB3	1.84	0.58
1:BV:104:THR:HG22	1:BV:106:GLN:H	1.69	0.58
1:CH:104:THR:HG22	1:CH:106:GLN:H	1.69	0.58
1:BP:104:THR:HG22	1:BP:106:GLN:H	1.69	0.58
1:AF:119:LEU:HD12	1:BM:119:LEU:HD12	1.86	0.58
1:CE:104:THR:HG22	1:CE:106:GLN:H	1.69	0.58
1:BH:20:PHE:HB3	1:BH:34:TRP:HB3	1.86	0.58
1:BT:20:PHE:HB3	1:BT:34:TRP:HB3	1.86	0.58
1:BX:102:GLY:HA2	1:BY:41:SER:HB3	1.84	0.58
1:AF:104:THR:HG22	1:AF:106:GLN:H	1.69	0.58
1:BA:104:THR:HG22	1:BA:106:GLN:H	1.69	0.58
1:BD:104:THR:HG22	1:BD:106:GLN:H	1.69	0.58
1:BN:20:PHE:HB3	1:BN:34:TRP:HB3	1.86	0.58
1:AP:106:GLN:NE2	1:BF:11:GLY:O	2.36	0.57
1:AX:104:THR:HG22	1:AX:106:GLN:H	1.69	0.57
1:AY:20:PHE:HB3	1:AY:34:TRP:HB3	1.86	0.57
1:BK:20:PHE:HB3	1:BK:34:TRP:HB3	1.86	0.57
1:BR:11:GLY:O	1:BT:106:GLN:NE2	2.35	0.57
1:AG:20:PHE:HB3	1:AG:34:TRP:HB3	1.86	0.57
1:AA:135:TRP:CE3	1:AI:22:PRO:HG2	2.39	0.57
1:AI:104:THR:HG22	1:AI:106:GLN:H	1.69	0.57
1:AU:104:THR:HG22	1:AU:106:GLN:H	1.69	0.57
1:BB:20:PHE:HB3	1:BB:34:TRP:HB3	1.86	0.57
1:BC:7:ILE:HG12	1:BC:19:THR:HG22	1.87	0.57
1:AB:7:ILE:HG12	1:AB:19:THR:HG22	1.87	0.57
1:AP:20:PHE:HB3	1:AP:34:TRP:HB3	1.86	0.57
1:BE:20:PHE:HB3	1:BE:34:TRP:HB3	1.86	0.57
1:BE:102:GLY:O	1:CG:73:SER:OG	2.23	0.57
1:BM:104:THR:HG22	1:BM:106:GLN:H	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BQ:20:PHE:HB3	1:BQ:34:TRP:HB3	1.86	0.57
1:CC:20:PHE:HB3	1:CC:34:TRP:HB3	1.86	0.57
1:AF:89:TYR:OH	1:BM:107:ASN:ND2	2.37	0.57
1:AN:7:ILE:HG12	1:AN:19:THR:HG22	1.87	0.57
1:AW:7:ILE:HG12	1:AW:19:THR:HG22	1.87	0.57
1:BS:104:THR:HG22	1:BS:106:GLN:H	1.69	0.57
1:AR:104:THR:HG22	1:AR:106:GLN:H	1.69	0.57
1:BL:7:ILE:HG12	1:BL:19:THR:HG22	1.87	0.57
1:BO:7:ILE:HG12	1:BO:19:THR:HG22	1.87	0.57
1:BX:7:ILE:HG12	1:BX:19:THR:HG22	1.87	0.57
1:AS:20:PHE:HB3	1:AS:34:TRP:HB3	1.86	0.57
1:AA:20:PHE:HB3	1:AA:34:TRP:HB3	1.86	0.57
1:AE:134:ALA:HA	1:BW:1:ALA:O	2.05	0.57
1:BG:104:THR:HG22	1:BG:106:GLN:H	1.69	0.57
1:CB:104:THR:HG22	1:CB:106:GLN:H	1.69	0.57
1:AD:20:PHE:HB3	1:AD:34:TRP:HB3	1.86	0.56
1:AM:20:PHE:HB3	1:AM:34:TRP:HB3	1.86	0.56
1:BF:7:ILE:HG12	1:BF:19:THR:HG22	1.87	0.56
1:BI:7:ILE:HG12	1:BI:19:THR:HG22	1.87	0.56
1:BY:104:THR:HG22	1:BY:106:GLN:H	1.69	0.56
1:AE:7:ILE:HG12	1:AE:19:THR:HG22	1.87	0.56
1:BD:89:TYR:OH	1:CH:107:ASN:ND2	2.38	0.56
1:AJ:20:PHE:HB3	1:AJ:34:TRP:HB3	1.86	0.56
1:AK:7:ILE:HG12	1:AK:19:THR:HG22	1.87	0.56
1:AL:104:THR:HG22	1:AL:106:GLN:H	1.69	0.56
1:AZ:7:ILE:HG12	1:AZ:19:THR:HG22	1.87	0.56
1:AV:20:PHE:HB3	1:AV:34:TRP:HB3	1.86	0.56
1:AW:11:GLY:O	1:BB:106:GLN:NE2	2.38	0.56
1:BU:7:ILE:HG12	1:BU:19:THR:HG22	1.87	0.56
1:AG:71:LEU:O	1:AL:83:ASN:ND2	2.39	0.56
1:BZ:20:PHE:HB3	1:BZ:34:TRP:HB3	1.86	0.56
1:AT:7:ILE:HG12	1:AT:19:THR:HG22	1.87	0.56
1:BW:20:PHE:HB3	1:BW:34:TRP:HB3	1.86	0.56
1:CF:20:PHE:HB3	1:CF:34:TRP:HB3	1.86	0.56
1:CG:7:ILE:HG12	1:CG:19:THR:HG22	1.87	0.56
1:BR:7:ILE:HG12	1:BR:19:THR:HG22	1.87	0.56
1:AA:102:GLY:O	1:AH:73:SER:OG	2.23	0.55
1:BX:119:LEU:HD12	1:CF:119:LEU:HD12	1.88	0.55
1:CA:7:ILE:HG12	1:CA:19:THR:HG22	1.87	0.55
1:AH:36:ASN:HB3	1:AH:46:ARG:H	1.71	0.55
1:AH:7:ILE:HG12	1:AH:19:THR:HG22	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AQ:36:ASN:HB3	1:AQ:46:ARG:H	1.71	0.55
1:AW:36:ASN:HB3	1:AW:46:ARG:H	1.71	0.55
1:BK:102:GLY:O	1:CD:73:SER:OG	2.24	0.55
1:BO:36:ASN:HB3	1:BO:46:ARG:H	1.72	0.55
1:AJ:46:ARG:HH12	1:BI:114:TYR:HH	1.55	0.55
1:AK:36:ASN:HB3	1:AK:46:ARG:H	1.71	0.55
1:AQ:7:ILE:HG12	1:AQ:19:THR:HG22	1.87	0.55
1:AT:36:ASN:HB3	1:AT:46:ARG:H	1.71	0.55
1:CD:7:ILE:HG12	1:CD:19:THR:HG22	1.87	0.55
1:AI:119:LEU:HD12	1:BP:119:LEU:HD12	1.89	0.55
1:BC:27:THR:HG22	1:BC:28:GLY:H	1.72	0.55
1:BC:36:ASN:HB3	1:BC:46:ARG:H	1.71	0.55
1:BK:125:THR:HG22	1:CD:112:LEU:HD21	1.88	0.55
1:CG:36:ASN:HB3	1:CG:46:ARG:H	1.72	0.55
1:AE:27:THR:HG22	1:AE:28:GLY:H	1.72	0.55
1:AF:107:ASN:ND2	1:BM:89:TYR:OH	2.40	0.55
1:AN:36:ASN:HB3	1:AN:46:ARG:H	1.72	0.55
1:BU:36:ASN:HB3	1:BU:46:ARG:H	1.72	0.55
1:BX:36:ASN:HB3	1:BX:46:ARG:H	1.72	0.55
1:AH:27:THR:HG22	1:AH:28:GLY:H	1.72	0.55
1:AZ:36:ASN:HB3	1:AZ:46:ARG:H	1.71	0.55
1:BO:27:THR:HG22	1:BO:28:GLY:H	1.72	0.55
1:AW:27:THR:HG22	1:AW:28:GLY:H	1.72	0.55
1:BL:36:ASN:HB3	1:BL:46:ARG:H	1.71	0.55
1:CB:51:PHE:HE2	1:CB:53:LYS:HB2	1.72	0.55
1:AC:37:LYS:HE3	1:BZ:130:ASP:O	2.07	0.55
1:AE:36:ASN:HB3	1:AE:46:ARG:H	1.71	0.55
1:CG:27:THR:HG22	1:CG:28:GLY:H	1.72	0.55
1:AZ:27:THR:HG22	1:AZ:28:GLY:H	1.72	0.54
1:BJ:51:PHE:HE2	1:BJ:53:LYS:HB2	1.72	0.54
1:BN:102:GLY:O	1:BU:73:SER:OG	2.25	0.54
1:AF:135:TRP:OXT	1:BM:3:ILE:N	2.36	0.54
1:AL:51:PHE:HE2	1:AL:53:LYS:HB2	1.72	0.54
1:BF:36:ASN:HB3	1:BF:46:ARG:H	1.71	0.54
1:BY:51:PHE:HE2	1:BY:53:LYS:HB2	1.72	0.54
1:CA:36:ASN:HB3	1:CA:46:ARG:H	1.72	0.54
1:AC:51:PHE:HE2	1:AC:53:LYS:HB2	1.72	0.54
1:AI:107:ASN:ND2	1:BP:89:TYR:OH	2.40	0.54
1:BE:71:LEU:O	1:CH:83:ASN:ND2	2.41	0.54
1:CA:27:THR:HG22	1:CA:28:GLY:H	1.72	0.54
1:CD:27:THR:HG22	1:CD:28:GLY:H	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CD:36:ASN:HB3	1:CD:46:ARG:H	1.72	0.54
1:BG:51:PHE:HE2	1:BG:53:LYS:HB2	1.72	0.54
1:BP:51:PHE:HE2	1:BP:53:LYS:HB2	1.72	0.54
1:BU:27:THR:HG22	1:BU:28:GLY:H	1.72	0.54
1:BV:51:PHE:HE2	1:BV:53:LYS:HB2	1.72	0.54
1:CH:51:PHE:HE2	1:CH:53:LYS:HB2	1.72	0.54
1:AN:27:THR:HG22	1:AN:28:GLY:H	1.72	0.54
1:AO:51:PHE:HE2	1:AO:53:LYS:HB2	1.72	0.54
1:AT:27:THR:HG22	1:AT:28:GLY:H	1.72	0.54
1:BA:51:PHE:HE2	1:BA:53:LYS:HB2	1.72	0.54
1:BA:98:SER:HB2	1:CE:92:PHE:HB2	1.88	0.54
1:BI:36:ASN:HB3	1:BI:46:ARG:H	1.71	0.54
1:AX:51:PHE:HE2	1:AX:53:LYS:HB2	1.72	0.54
1:BR:104:THR:HG22	1:BR:106:GLN:H	1.73	0.54
1:AP:71:LEU:O	1:BG:83:ASN:ND2	2.41	0.54
1:BN:71:LEU:O	1:BV:83:ASN:ND2	2.40	0.54
1:AB:36:ASN:HB3	1:AB:46:ARG:H	1.71	0.54
1:AB:106:GLN:NE2	1:BZ:12:GLN:HG2	2.23	0.54
1:AE:104:THR:HG22	1:AE:106:GLN:H	1.73	0.54
1:AM:52:VAL:HB	1:BL:133:PRO:HB3	1.89	0.54
1:AN:104:THR:HG22	1:AN:106:GLN:H	1.73	0.54
1:AR:51:PHE:HE2	1:AR:53:LYS:HB2	1.72	0.54
1:BF:27:THR:HG22	1:BF:28:GLY:H	1.72	0.54
1:BR:27:THR:HG22	1:BR:28:GLY:H	1.72	0.54
1:AB:27:THR:HG22	1:AB:28:GLY:H	1.72	0.54
1:BK:133:PRO:HD3	1:CE:23:MET:SD	2.47	0.54
1:BO:104:THR:HG22	1:BO:106:GLN:H	1.73	0.54
1:CD:104:THR:HG22	1:CD:106:GLN:H	1.73	0.54
1:AK:104:THR:HG22	1:AK:106:GLN:H	1.73	0.54
1:BA:89:TYR:OH	1:CE:107:ASN:ND2	2.40	0.54
1:AD:102:GLY:O	1:AQ:73:SER:OG	2.26	0.53
1:AK:27:THR:HG22	1:AK:28:GLY:H	1.72	0.53
1:AQ:27:THR:HG22	1:AQ:28:GLY:H	1.72	0.53
1:AQ:104:THR:HG22	1:AQ:106:GLN:H	1.73	0.53
1:AU:51:PHE:HE2	1:AU:53:LYS:HB2	1.72	0.53
1:BR:36:ASN:HB3	1:BR:46:ARG:H	1.71	0.53
1:BS:51:PHE:HE2	1:BS:53:LYS:HB2	1.72	0.53
1:BU:104:THR:HG22	1:BU:106:GLN:H	1.73	0.53
1:BX:104:THR:HG22	1:BX:106:GLN:H	1.73	0.53
1:AD:125:THR:HG22	1:AQ:112:LEU:HD21	1.90	0.53
1:AP:130:ASP:O	1:BG:37:LYS:HE3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BF:104:THR:HG22	1:BF:106:GLN:H	1.73	0.53
1:BM:51:PHE:HE2	1:BM:53:LYS:HB2	1.72	0.53
1:BX:27:THR:HG22	1:BX:28:GLY:H	1.72	0.53
1:AT:104:THR:HG22	1:AT:106:GLN:H	1.73	0.53
1:BI:27:THR:HG22	1:BI:28:GLY:H	1.72	0.53
1:CE:51:PHE:HE2	1:CE:53:LYS:HB2	1.72	0.53
1:AF:51:PHE:HE2	1:AF:53:LYS:HB2	1.72	0.53
1:BX:133:PRO:HB3	1:CF:52:VAL:HB	1.91	0.53
1:CA:104:THR:HG22	1:CA:106:GLN:H	1.73	0.53
1:AH:104:THR:HG22	1:AH:106:GLN:H	1.73	0.53
1:AM:106:GLN:NE2	1:BL:11:GLY:O	2.39	0.53
1:AS:6:LEU:HB3	1:AS:20:PHE:HB2	1.91	0.53
1:AV:6:LEU:HB3	1:AV:20:PHE:HB2	1.91	0.53
1:BB:25:PRO:HG3	1:CH:135:TRP:CD1	2.44	0.53
1:BI:104:THR:HG22	1:BI:106:GLN:H	1.73	0.53
1:AJ:118:LEU:HD13	1:BI:8:LEU:HD11	1.90	0.53
1:AP:118:LEU:HD13	1:BF:8:LEU:HD11	1.91	0.53
1:BL:27:THR:HG22	1:BL:28:GLY:H	1.72	0.53
1:BY:7:ILE:HG12	1:BY:19:THR:HG22	1.91	0.53
1:CG:104:THR:HG22	1:CG:106:GLN:H	1.73	0.53
1:BD:51:PHE:HE2	1:BD:53:LYS:HB2	1.72	0.53
1:AK:50:MET:HG3	1:AK:64:ILE:HG12	1.91	0.53
1:AZ:50:MET:HG3	1:AZ:64:ILE:HG12	1.91	0.53
1:BC:104:THR:HG22	1:BC:106:GLN:H	1.73	0.53
1:BL:104:THR:HG22	1:BL:106:GLN:H	1.73	0.53
1:AA:6:LEU:HB3	1:AA:20:PHE:HB2	1.91	0.53
1:AB:104:THR:HG22	1:AB:106:GLN:H	1.73	0.53
1:AH:50:MET:HG3	1:AH:64:ILE:HG12	1.91	0.53
1:AO:107:ASN:ND2	1:BS:89:TYR:OH	2.42	0.53
1:AW:104:THR:HG22	1:AW:106:GLN:H	1.73	0.53
1:BM:7:ILE:HG12	1:BM:19:THR:HG22	1.91	0.53
1:BT:6:LEU:HB3	1:BT:20:PHE:HB2	1.91	0.53
1:CH:7:ILE:HG12	1:CH:19:THR:HG22	1.91	0.53
1:AB:73:SER:OG	1:BZ:102:GLY:O	2.27	0.52
1:BE:6:LEU:HB3	1:BE:20:PHE:HB2	1.91	0.52
1:BH:135:TRP:CE3	1:CB:22:PRO:HG2	2.44	0.52
1:BX:50:MET:HG3	1:BX:64:ILE:HG12	1.91	0.52
1:AD:58:GLY:H	1:AD:101:TYR:HB3	1.75	0.52
1:AI:51:PHE:HE2	1:AI:53:LYS:HB2	1.72	0.52
1:AO:7:ILE:HG12	1:AO:19:THR:HG22	1.91	0.52
1:BF:50:MET:HG3	1:BF:64:ILE:HG12	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BJ:7:ILE:HG12	1:BJ:19:THR:HG22	1.91	0.52
1:BQ:6:LEU:HB3	1:BQ:20:PHE:HB2	1.91	0.52
1:AE:73:SER:OG	1:BW:102:GLY:O	2.27	0.52
1:AQ:50:MET:HG3	1:AQ:64:ILE:HG12	1.92	0.52
1:AX:52:VAL:CG2	1:CB:127:ALA:HB1	2.39	0.52
1:AY:6:LEU:HB3	1:AY:20:PHE:HB2	1.91	0.52
1:BG:7:ILE:HG12	1:BG:19:THR:HG22	1.91	0.52
1:BK:132:THR:HG23	1:CE:21:VAL:HG11	1.92	0.52
1:BL:50:MET:HG3	1:BL:64:ILE:HG12	1.91	0.52
1:BY:83:ASN:ND2	1:CF:71:LEU:O	2.42	0.52
1:AV:58:GLY:H	1:AV:101:TYR:HB3	1.75	0.52
1:BH:58:GLY:H	1:BH:101:TYR:HB3	1.75	0.52
1:BI:50:MET:HG3	1:BI:64:ILE:HG12	1.92	0.52
1:BZ:6:LEU:HB3	1:BZ:20:PHE:HB2	1.91	0.52
1:CA:50:MET:HG3	1:CA:64:ILE:HG12	1.91	0.52
1:AE:69:PRO:HA	1:AE:90:SER:HB3	1.92	0.52
1:AX:7:ILE:HG12	1:AX:19:THR:HG22	1.91	0.52
1:BK:107:ASN:CG	1:CD:70:VAL:HG11	2.30	0.52
1:BK:130:ASP:O	1:CE:37:LYS:HE3	2.09	0.52
1:BP:7:ILE:HG12	1:BP:19:THR:HG22	1.91	0.52
1:BU:50:MET:HG3	1:BU:64:ILE:HG12	1.92	0.52
1:CF:58:GLY:H	1:CF:101:TYR:HB3	1.75	0.52
1:AM:6:LEU:HB3	1:AM:20:PHE:HB2	1.91	0.52
1:AP:6:LEU:HB3	1:AP:20:PHE:HB2	1.91	0.52
1:AR:7:ILE:HG12	1:AR:19:THR:HG22	1.91	0.52
1:AS:58:GLY:H	1:AS:101:TYR:HB3	1.75	0.52
1:BL:69:PRO:HA	1:BL:90:SER:HB3	1.92	0.52
1:BQ:58:GLY:H	1:BQ:101:TYR:HB3	1.75	0.52
1:BR:50:MET:HG3	1:BR:64:ILE:HG12	1.91	0.52
1:AQ:69:PRO:HA	1:AQ:90:SER:HB3	1.92	0.52
1:AW:50:MET:HG3	1:AW:64:ILE:HG12	1.91	0.52
1:AY:58:GLY:H	1:AY:101:TYR:HB3	1.75	0.52
1:BI:69:PRO:HA	1:BI:90:SER:HB3	1.92	0.52
1:BW:58:GLY:H	1:BW:101:TYR:HB3	1.75	0.52
1:AJ:46:ARG:NH1	1:BI:114:TYR:HH	2.05	0.52
1:AM:130:ASP:O	1:BM:37:LYS:HE3	2.10	0.52
1:AZ:104:THR:HG22	1:AZ:106:GLN:H	1.73	0.52
1:BW:6:LEU:HB3	1:BW:20:PHE:HB2	1.91	0.52
1:BZ:58:GLY:H	1:BZ:101:TYR:HB3	1.75	0.52
1:CG:69:PRO:HA	1:CG:90:SER:HB3	1.92	0.52
1:AP:58:GLY:H	1:AP:101:TYR:HB3	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BD:52:VAL:HG21	1:CH:127:ALA:HB1	1.91	0.52
1:BH:12:GLN:HG2	1:CA:106:GLN:NE2	2.25	0.52
1:CB:7:ILE:HG12	1:CB:19:THR:HG22	1.91	0.52
1:CC:58:GLY:H	1:CC:101:TYR:HB3	1.75	0.52
1:CE:7:ILE:HG12	1:CE:19:THR:HG22	1.91	0.52
1:AX:20:PHE:HB3	1:AX:34:TRP:HB3	1.92	0.52
1:BE:58:GLY:H	1:BE:101:TYR:HB3	1.75	0.52
1:BO:50:MET:HG3	1:BO:64:ILE:HG12	1.91	0.52
1:BV:20:PHE:HB3	1:BV:34:TRP:HB3	1.93	0.52
1:CF:6:LEU:HB3	1:CF:20:PHE:HB2	1.91	0.52
1:AF:20:PHE:HB3	1:AF:34:TRP:HB3	1.93	0.51
1:AH:69:PRO:HA	1:AH:90:SER:HB3	1.92	0.51
1:AI:7:ILE:HG12	1:AI:19:THR:HG22	1.91	0.51
1:AL:20:PHE:HB3	1:AL:34:TRP:HB3	1.93	0.51
1:AM:71:LEU:O	1:BM:83:ASN:ND2	2.43	0.51
1:AU:20:PHE:HB3	1:AU:34:TRP:HB3	1.93	0.51
1:BK:1:ALA:O	1:CD:134:ALA:HA	2.10	0.51
1:BS:7:ILE:HG12	1:BS:19:THR:HG22	1.91	0.51
1:CC:6:LEU:HB3	1:CC:20:PHE:HB2	1.91	0.51
1:AB:50:MET:HG3	1:AB:64:ILE:HG12	1.91	0.51
1:AC:7:ILE:HG12	1:AC:19:THR:HG22	1.91	0.51
1:AJ:58:GLY:H	1:AJ:101:TYR:HB3	1.75	0.51
1:AP:114:TYR:HH	1:BF:46:ARG:NH1	2.08	0.51
1:AT:69:PRO:HA	1:AT:90:SER:HB3	1.92	0.51
1:AX:135:TRP:CD1	1:BZ:25:PRO:HG3	2.45	0.51
1:BG:20:PHE:HB3	1:BG:34:TRP:HB3	1.93	0.51
1:BH:6:LEU:HB3	1:BH:20:PHE:HB2	1.91	0.51
1:BV:7:ILE:HG12	1:BV:19:THR:HG22	1.91	0.51
1:CE:20:PHE:HB3	1:CE:34:TRP:HB3	1.93	0.51
1:AD:6:LEU:HB3	1:AD:20:PHE:HB2	1.91	0.51
1:AD:52:VAL:HB	1:AQ:133:PRO:HB3	1.91	0.51
1:AG:58:GLY:H	1:AG:101:TYR:HB3	1.75	0.51
1:AJ:6:LEU:HB3	1:AJ:20:PHE:HB2	1.91	0.51
1:AJ:130:ASP:O	1:BJ:37:LYS:HE3	2.10	0.51
1:AL:7:ILE:HG12	1:AL:19:THR:HG22	1.91	0.51
1:BA:103:ALA:HA	1:CE:89:TYR:CE1	2.46	0.51
1:BH:46:ARG:NH1	1:CA:114:TYR:HH	2.08	0.51
1:BX:69:PRO:HA	1:BX:90:SER:HB3	1.92	0.51
1:BY:20:PHE:HB3	1:BY:34:TRP:HB3	1.92	0.51
1:AB:69:PRO:HA	1:AB:90:SER:HB3	1.92	0.51
1:AN:69:PRO:HA	1:AN:90:SER:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AR:20:PHE:HB3	1:AR:34:TRP:HB3	1.93	0.51
1:BB:6:LEU:HB3	1:BB:20:PHE:HB2	1.91	0.51
1:BD:7:ILE:HG12	1:BD:19:THR:HG22	1.91	0.51
1:BJ:20:PHE:HB3	1:BJ:34:TRP:HB3	1.93	0.51
1:AE:50:MET:HG3	1:AE:64:ILE:HG12	1.92	0.51
1:AT:50:MET:HG3	1:AT:64:ILE:HG12	1.92	0.51
1:AZ:69:PRO:HA	1:AZ:90:SER:HB3	1.92	0.51
1:BO:69:PRO:HA	1:BO:90:SER:HB3	1.92	0.51
1:AM:58:GLY:H	1:AM:101:TYR:HB3	1.75	0.51
1:BC:50:MET:HG3	1:BC:64:ILE:HG12	1.92	0.51
1:BM:20:PHE:HB3	1:BM:34:TRP:HB3	1.93	0.51
1:BN:58:GLY:H	1:BN:101:TYR:HB3	1.75	0.51
1:BR:119:LEU:HD12	1:BT:119:LEU:HD12	1.92	0.51
1:CD:50:MET:HG3	1:CD:64:ILE:HG12	1.91	0.51
1:AU:7:ILE:HG12	1:AU:19:THR:HG22	1.91	0.51
1:BA:7:ILE:HG12	1:BA:19:THR:HG22	1.91	0.51
1:BC:69:PRO:HA	1:BC:90:SER:HB3	1.92	0.51
1:BF:69:PRO:HA	1:BF:90:SER:HB3	1.92	0.51
1:BN:6:LEU:HB3	1:BN:20:PHE:HB2	1.91	0.51
1:CG:50:MET:HG3	1:CG:64:ILE:HG12	1.92	0.51
1:BK:6:LEU:HB3	1:BK:20:PHE:HB2	1.91	0.51
1:BR:69:PRO:HA	1:BR:90:SER:HB3	1.92	0.51
1:CA:69:PRO:HA	1:CA:90:SER:HB3	1.92	0.51
1:AC:20:PHE:HB3	1:AC:34:TRP:HB3	1.93	0.51
1:AF:7:ILE:HG12	1:AF:19:THR:HG22	1.91	0.51
1:AW:119:LEU:HD12	1:BB:119:LEU:HD12	1.91	0.51
1:BF:20:PHE:HB3	1:BF:34:TRP:HB3	1.93	0.51
1:BH:46:ARG:HH12	1:CA:114:TYR:HH	1.58	0.51
1:BL:25:PRO:HD3	1:CD:135:TRP:HB2	1.93	0.51
1:AJ:102:GLY:HA2	1:AK:41:SER:CB	2.41	0.51
1:AK:20:PHE:HB3	1:AK:34:TRP:HB3	1.93	0.51
1:AS:102:GLY:HA2	1:AT:41:SER:CB	2.41	0.51
1:BI:20:PHE:HB3	1:BI:34:TRP:HB3	1.93	0.51
1:BT:58:GLY:H	1:BT:101:TYR:HB3	1.75	0.51
1:CG:20:PHE:HB3	1:CG:34:TRP:HB3	1.93	0.51
1:AE:1:ALA:O	1:BW:134:ALA:HA	2.11	0.50
1:BN:102:GLY:HA2	1:BO:41:SER:CB	2.41	0.50
1:BS:20:PHE:HB3	1:BS:34:TRP:HB3	1.93	0.50
1:BX:20:PHE:HB3	1:BX:34:TRP:HB3	1.93	0.50
1:BZ:102:GLY:HA2	1:CA:41:SER:CB	2.41	0.50
1:AA:58:GLY:H	1:AA:101:TYR:HB3	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AG:119:LEU:HD12	1:AK:119:LEU:HD12	1.93	0.50
1:AM:102:GLY:HA2	1:AN:41:SER:CB	2.41	0.50
1:AV:102:GLY:HA2	1:AW:41:SER:CB	2.41	0.50
1:AY:102:GLY:HA2	1:AZ:41:SER:CB	2.41	0.50
1:BA:20:PHE:HB3	1:BA:34:TRP:HB3	1.92	0.50
1:BU:69:PRO:HA	1:BU:90:SER:HB3	1.92	0.50
1:BW:102:GLY:HA2	1:BX:41:SER:CB	2.41	0.50
1:AA:102:GLY:HA2	1:AB:41:SER:CB	2.41	0.50
1:AG:6:LEU:HB3	1:AG:20:PHE:HB2	1.91	0.50
1:BB:102:GLY:HA2	1:BC:41:SER:CB	2.41	0.50
1:BE:102:GLY:HA2	1:BF:41:SER:CB	2.41	0.50
1:BL:20:PHE:HB3	1:BL:34:TRP:HB3	1.93	0.50
1:CC:102:GLY:HA2	1:CD:41:SER:CB	2.41	0.50
1:CD:69:PRO:HA	1:CD:90:SER:HB3	1.92	0.50
1:CH:20:PHE:HB3	1:CH:34:TRP:HB3	1.93	0.50
1:AD:119:LEU:HD12	1:AQ:119:LEU:HD12	1.94	0.50
1:AF:81:ASP:HB3	1:BW:72:ALA:HB1	1.93	0.50
1:BK:58:GLY:H	1:BK:101:TYR:HB3	1.75	0.50
1:BQ:102:GLY:HA2	1:BR:41:SER:CB	2.41	0.50
1:AE:98:SER:HB2	1:BW:92:PHE:HB2	1.93	0.50
1:AF:3:ILE:N	1:BM:135:TRP:OXT	2.39	0.50
1:AK:69:PRO:HA	1:AK:90:SER:HB3	1.92	0.50
1:AN:50:MET:HG3	1:AN:64:ILE:HG12	1.91	0.50
1:AO:20:PHE:HB3	1:AO:34:TRP:HB3	1.93	0.50
1:AP:25:PRO:HG3	1:BV:135:TRP:CD1	2.46	0.50
1:AW:69:PRO:HA	1:AW:90:SER:HB3	1.92	0.50
1:CD:20:PHE:HB3	1:CD:34:TRP:HB3	1.93	0.50
1:AC:22:PRO:HG2	1:BZ:135:TRP:CE3	2.47	0.50
1:AD:102:GLY:HA2	1:AE:41:SER:CB	2.41	0.50
1:AM:102:GLY:O	1:BL:73:SER:OG	2.30	0.50
1:AZ:20:PHE:HB3	1:AZ:34:TRP:HB3	1.93	0.50
1:BB:58:GLY:H	1:BB:101:TYR:HB3	1.75	0.50
1:BU:20:PHE:HB3	1:BU:34:TRP:HB3	1.93	0.50
1:AB:20:PHE:HB3	1:AB:34:TRP:HB3	1.93	0.50
1:AN:20:PHE:HB3	1:AN:34:TRP:HB3	1.93	0.50
1:AP:119:LEU:HA	1:AP:124:VAL:HG11	1.94	0.50
1:AI:20:PHE:HB3	1:AI:34:TRP:HB3	1.92	0.50
1:BC:20:PHE:HB3	1:BC:34:TRP:HB3	1.93	0.50
1:BK:119:LEU:HA	1:BK:124:VAL:HG11	1.94	0.50
1:BN:125:THR:HG22	1:BU:112:LEU:HD21	1.93	0.50
1:BO:20:PHE:HB3	1:BO:34:TRP:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:114:TYR:HH	1:AH:46:ARG:NH1	2.08	0.50
1:AH:20:PHE:HB3	1:AH:34:TRP:HB3	1.93	0.50
1:AW:20:PHE:HB3	1:AW:34:TRP:HB3	1.93	0.50
1:CB:20:PHE:HB3	1:CB:34:TRP:HB3	1.93	0.50
1:BK:102:GLY:HA2	1:BL:41:SER:CB	2.41	0.49
1:BR:20:PHE:HB3	1:BR:34:TRP:HB3	1.93	0.49
1:AE:106:GLN:NE2	1:BW:12:GLN:HG2	2.27	0.49
1:AX:100:PRO:HD2	1:CB:91:THR:HG22	1.93	0.49
1:BD:20:PHE:HB3	1:BD:34:TRP:HB3	1.93	0.49
1:BP:20:PHE:HB3	1:BP:34:TRP:HB3	1.92	0.49
1:BT:102:GLY:HA2	1:BU:41:SER:CB	2.41	0.49
1:CA:20:PHE:HB3	1:CA:34:TRP:HB3	1.93	0.49
1:AJ:114:TYR:HH	1:BI:46:ARG:NH1	2.10	0.49
1:AM:119:LEU:HA	1:AM:124:VAL:HG11	1.94	0.49
1:AY:119:LEU:HA	1:AY:124:VAL:HG11	1.94	0.49
1:BE:119:LEU:HA	1:BE:124:VAL:HG11	1.94	0.49
1:BH:102:GLY:HA2	1:BI:41:SER:CB	2.41	0.49
1:BH:119:LEU:HA	1:BH:124:VAL:HG11	1.94	0.49
1:AG:102:GLY:HA2	1:AH:41:SER:CB	2.41	0.49
1:AT:20:PHE:HB3	1:AT:34:TRP:HB3	1.93	0.49
1:CF:102:GLY:HA2	1:CG:41:SER:CB	2.41	0.49
1:AA:119:LEU:HA	1:AA:124:VAL:HG11	1.94	0.49
1:AE:20:PHE:HB3	1:AE:34:TRP:HB3	1.93	0.49
1:AP:102:GLY:HA2	1:AQ:41:SER:CB	2.41	0.49
1:AQ:20:PHE:HB3	1:AQ:34:TRP:HB3	1.93	0.49
1:AR:89:TYR:OH	1:BV:107:ASN:ND2	2.46	0.49
1:BN:135:TRP:CE3	1:BV:22:PRO:HG2	2.48	0.49
1:AG:119:LEU:HA	1:AG:124:VAL:HG11	1.94	0.49
1:AV:119:LEU:HA	1:AV:124:VAL:HG11	1.94	0.49
1:AZ:10:ASP:OD2	1:AZ:12:GLN:NE2	2.46	0.49
1:BB:119:LEU:HA	1:BB:124:VAL:HG11	1.94	0.49
1:BE:130:ASP:O	1:CH:37:LYS:HE3	2.13	0.49
1:BT:119:LEU:HA	1:BT:124:VAL:HG11	1.94	0.49
1:AJ:119:LEU:HA	1:AJ:124:VAL:HG11	1.94	0.49
1:AJ:119:LEU:HD12	1:BI:119:LEU:HD12	1.94	0.49
1:BH:130:ASP:O	1:CB:37:LYS:HE3	2.12	0.49
1:CF:119:LEU:HA	1:CF:124:VAL:HG11	1.94	0.49
1:AG:102:GLY:O	1:AK:73:SER:OG	2.31	0.49
1:AJ:95:CYS:HA	1:BI:94:GLU:O	2.12	0.49
1:BS:37:LYS:HE3	1:BT:130:ASP:O	2.12	0.49
1:BZ:119:LEU:HA	1:BZ:124:VAL:HG11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AO:89:TYR:OH	1:BS:107:ASN:ND2	2.46	0.48
1:BN:119:LEU:HA	1:BN:124:VAL:HG11	1.94	0.48
1:BO:37:LYS:HA	1:BO:45:TYR:CE1	2.48	0.48
1:BX:8:LEU:HD11	1:CF:118:LEU:HD13	1.95	0.48
1:CC:119:LEU:HA	1:CC:124:VAL:HG11	1.94	0.48
1:AB:133:PRO:HB3	1:BZ:52:VAL:HB	1.94	0.48
1:AD:119:LEU:HA	1:AD:124:VAL:HG11	1.94	0.48
1:AQ:37:LYS:HA	1:AQ:45:TYR:CE1	2.48	0.48
1:BL:37:LYS:HA	1:BL:45:TYR:CE1	2.48	0.48
1:CF:122:GLN:O	1:CF:126:ASP:HB2	2.14	0.48
1:AK:37:LYS:HA	1:AK:45:TYR:CE1	2.48	0.48
1:AS:122:GLN:O	1:AS:126:ASP:HB2	2.14	0.48
1:AZ:37:LYS:HA	1:AZ:45:TYR:CE1	2.48	0.48
1:BK:122:GLN:O	1:BK:126:ASP:HB2	2.14	0.48
1:CC:122:GLN:O	1:CC:126:ASP:HB2	2.14	0.48
1:AE:37:LYS:HA	1:AE:45:TYR:CE1	2.48	0.48
1:AT:37:LYS:HA	1:AT:45:TYR:CE1	2.48	0.48
1:BC:37:LYS:HA	1:BC:45:TYR:CE1	2.48	0.48
1:BK:111:ILE:HD11	1:CD:92:PHE:C	2.33	0.48
1:BN:52:VAL:HB	1:BU:133:PRO:HB3	1.94	0.48
1:BN:122:GLN:O	1:BN:126:ASP:HB2	2.14	0.48
1:BW:119:LEU:HA	1:BW:124:VAL:HG11	1.94	0.48
1:CG:37:LYS:HA	1:CG:45:TYR:CE1	2.48	0.48
1:AB:37:LYS:HA	1:AB:45:TYR:CE1	2.48	0.48
1:AP:122:GLN:O	1:AP:126:ASP:HB2	2.14	0.48
1:BR:8:LEU:HD11	1:BT:118:LEU:HD13	1.94	0.48
1:BX:37:LYS:HA	1:BX:45:TYR:CE1	2.49	0.48
1:CA:37:LYS:HA	1:CA:45:TYR:CE1	2.48	0.48
1:CG:10:ASP:OD2	1:CG:12:GLN:NE2	2.46	0.48
1:AJ:94:GLU:O	1:BI:95:CYS:HA	2.14	0.48
1:BH:122:GLN:O	1:BH:126:ASP:HB2	2.14	0.48
1:BL:6:LEU:HB3	1:BL:20:PHE:HB2	1.96	0.48
1:BQ:119:LEU:HA	1:BQ:124:VAL:HG11	1.94	0.48
1:BR:37:LYS:HA	1:BR:45:TYR:CE1	2.49	0.48
1:BT:122:GLN:O	1:BT:126:ASP:HB2	2.14	0.48
1:BW:122:GLN:O	1:BW:126:ASP:HB2	2.14	0.48
1:AB:25:PRO:HD3	1:AH:135:TRP:HB2	1.94	0.48
1:AG:122:GLN:O	1:AG:126:ASP:HB2	2.14	0.48
1:AT:10:ASP:OD2	1:AT:12:GLN:NE2	2.46	0.48
1:AT:46:ARG:NH1	1:AY:114:TYR:HH	2.11	0.48
1:BF:6:LEU:HB3	1:BF:20:PHE:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BX:101:TYR:HA	1:BY:42:ASN:HB2	1.96	0.48
1:CD:10:ASP:OD2	1:CD:12:GLN:NE2	2.46	0.48
1:AB:10:ASP:OD2	1:AB:12:GLN:NE2	2.46	0.48
1:AB:101:TYR:HA	1:AC:42:ASN:HB2	1.96	0.48
1:AH:37:LYS:HA	1:AH:45:TYR:CE1	2.48	0.48
1:AM:118:LEU:HD13	1:BL:8:LEU:HD11	1.95	0.48
1:AT:101:TYR:HA	1:AU:42:ASN:HB2	1.96	0.48
1:AX:89:TYR:OH	1:CB:107:ASN:ND2	2.46	0.48
1:AZ:101:TYR:HA	1:BA:42:ASN:HB2	1.96	0.48
1:BB:122:GLN:O	1:BB:126:ASP:HB2	2.14	0.48
1:BE:52:VAL:HB	1:CG:133:PRO:HB3	1.96	0.48
1:BE:117:ASN:O	1:BE:121:THR:HG23	2.14	0.48
1:BQ:122:GLN:O	1:BQ:126:ASP:HB2	2.14	0.48
1:BR:73:SER:OG	1:BT:102:GLY:O	2.32	0.48
1:BU:10:ASP:OD2	1:BU:12:GLN:NE2	2.46	0.48
1:AN:6:LEU:HB3	1:AN:20:PHE:HB2	1.96	0.48
1:AN:69:PRO:HA	1:AN:90:SER:CB	2.44	0.48
1:AY:117:ASN:O	1:AY:121:THR:HG23	2.14	0.48
1:BA:52:VAL:HG21	1:CE:127:ALA:HB1	1.96	0.48
1:BB:117:ASN:O	1:BB:121:THR:HG23	2.14	0.48
1:BZ:122:GLN:O	1:BZ:126:ASP:HB2	2.14	0.48
1:CA:10:ASP:OD2	1:CA:12:GLN:NE2	2.46	0.48
1:AB:6:LEU:HB3	1:AB:20:PHE:HB2	1.96	0.47
1:BF:37:LYS:HA	1:BF:45:TYR:CE1	2.48	0.47
1:BI:37:LYS:HA	1:BI:45:TYR:CE1	2.48	0.47
1:BK:117:ASN:O	1:BK:121:THR:HG23	2.14	0.47
1:BR:6:LEU:HB3	1:BR:20:PHE:HB2	1.96	0.47
1:AA:122:GLN:O	1:AA:126:ASP:HB2	2.14	0.47
1:AB:46:ARG:NH1	1:BZ:114:TYR:HH	2.11	0.47
1:AD:71:LEU:O	1:AR:83:ASN:ND2	2.47	0.47
1:AJ:117:ASN:O	1:AJ:121:THR:HG23	2.14	0.47
1:AN:101:TYR:HA	1:AO:42:ASN:HB2	1.96	0.47
1:AQ:69:PRO:HA	1:AQ:90:SER:CB	2.44	0.47
1:AQ:101:TYR:HA	1:AR:42:ASN:HB2	1.96	0.47
1:AR:135:TRP:CD1	1:BT:25:PRO:HG3	2.49	0.47
1:AW:37:LYS:HA	1:AW:45:TYR:CE1	2.48	0.47
1:AW:134:ALA:HA	1:BB:1:ALA:O	2.14	0.47
1:BC:69:PRO:HA	1:BC:90:SER:CB	2.44	0.47
1:BE:119:LEU:HD12	1:CG:119:LEU:HD12	1.97	0.47
1:BW:117:ASN:O	1:BW:121:THR:HG23	2.14	0.47
1:CD:37:LYS:HA	1:CD:45:TYR:CE1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CG:6:LEU:HB3	1:CG:20:PHE:HB2	1.96	0.47
1:AH:10:ASP:OD2	1:AH:12:GLN:NE2	2.46	0.47
1:AM:122:GLN:O	1:AM:126:ASP:HB2	2.14	0.47
1:AV:122:GLN:O	1:AV:126:ASP:HB2	2.14	0.47
1:BC:6:LEU:HB3	1:BC:20:PHE:HB2	1.96	0.47
1:BI:10:ASP:OD2	1:BI:12:GLN:NE2	2.46	0.47
1:CG:69:PRO:HA	1:CG:90:SER:CB	2.44	0.47
1:AH:101:TYR:HA	1:AI:42:ASN:HB2	1.96	0.47
1:AQ:10:ASP:OD2	1:AQ:12:GLN:NE2	2.46	0.47
1:AQ:51:PHE:HE2	1:AQ:53:LYS:HB2	1.80	0.47
1:AV:117:ASN:O	1:AV:121:THR:HG23	2.14	0.47
1:BX:69:PRO:HA	1:BX:90:SER:CB	2.44	0.47
1:AG:125:THR:HG22	1:AK:112:LEU:HD21	1.95	0.47
1:AK:10:ASP:OD2	1:AK:12:GLN:NE2	2.46	0.47
1:AN:51:PHE:HE2	1:AN:53:LYS:HB2	1.80	0.47
1:AO:119:LEU:HD12	1:BS:119:LEU:HD12	1.97	0.47
1:AP:117:ASN:O	1:AP:121:THR:HG23	2.14	0.47
1:AS:119:LEU:HA	1:AS:124:VAL:HG11	1.94	0.47
1:AZ:69:PRO:HA	1:AZ:90:SER:CB	2.44	0.47
1:BF:51:PHE:HE2	1:BF:53:LYS:HB2	1.80	0.47
1:BH:52:VAL:HB	1:CA:133:PRO:HB3	1.96	0.47
1:BI:101:TYR:HA	1:BJ:42:ASN:HB2	1.96	0.47
1:BL:69:PRO:HA	1:BL:90:SER:CB	2.44	0.47
1:BN:117:ASN:O	1:BN:121:THR:HG23	2.14	0.47
1:BU:69:PRO:HA	1:BU:90:SER:CB	2.44	0.47
1:CA:101:TYR:HA	1:CB:42:ASN:HB2	1.96	0.47
1:CF:117:ASN:O	1:CF:121:THR:HG23	2.14	0.47
1:AE:51:PHE:HE2	1:AE:53:LYS:HB2	1.80	0.47
1:AJ:122:GLN:O	1:AJ:126:ASP:HB2	2.14	0.47
1:AM:114:TYR:HH	1:BL:46:ARG:NH1	2.07	0.47
1:AN:37:LYS:HA	1:AN:45:TYR:CE1	2.48	0.47
1:BC:51:PHE:HE2	1:BC:53:LYS:HB2	1.80	0.47
1:BE:122:GLN:O	1:BE:126:ASP:HB2	2.14	0.47
1:BR:69:PRO:HA	1:BR:90:SER:CB	2.44	0.47
1:AE:101:TYR:HA	1:AF:42:ASN:HB2	1.96	0.47
1:AG:52:VAL:HB	1:AK:133:PRO:HB3	1.97	0.47
1:AK:6:LEU:HB3	1:AK:20:PHE:HB2	1.96	0.47
1:AK:101:TYR:HA	1:AL:42:ASN:HB2	1.96	0.47
1:AP:119:LEU:HD12	1:BF:119:LEU:HD12	1.95	0.47
1:AS:117:ASN:O	1:AS:121:THR:HG23	2.14	0.47
1:AY:122:GLN:O	1:AY:126:ASP:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BF:69:PRO:HA	1:BF:90:SER:CB	2.44	0.47
1:BH:63:THR:HG22	1:BH:96:THR:HG22	1.97	0.47
1:BH:117:ASN:O	1:BH:121:THR:HG23	2.14	0.47
1:BI:69:PRO:HA	1:BI:90:SER:CB	2.44	0.47
1:BL:101:TYR:HA	1:BM:42:ASN:HB2	1.96	0.47
1:BO:69:PRO:HA	1:BO:90:SER:CB	2.44	0.47
1:BR:101:TYR:HA	1:BS:42:ASN:HB2	1.96	0.47
1:BU:37:LYS:HA	1:BU:45:TYR:CE1	2.48	0.47
1:BU:51:PHE:HE2	1:BU:53:LYS:HB2	1.80	0.47
1:BZ:117:ASN:O	1:BZ:121:THR:HG23	2.14	0.47
1:CA:6:LEU:HB3	1:CA:20:PHE:HB2	1.96	0.47
1:CC:117:ASN:O	1:CC:121:THR:HG23	2.14	0.47
1:AA:117:ASN:O	1:AA:121:THR:HG23	2.14	0.47
1:AD:122:GLN:O	1:AD:126:ASP:HB2	2.14	0.47
1:AE:69:PRO:HA	1:AE:90:SER:CB	2.44	0.47
1:AM:63:THR:HG22	1:AM:96:THR:HG22	1.97	0.47
1:AW:101:TYR:HA	1:AX:42:ASN:HB2	1.96	0.47
1:BC:10:ASP:OD2	1:BC:12:GLN:NE2	2.46	0.47
1:BG:65:ARG:HA	1:BG:93:PHE:O	2.15	0.47
1:BN:130:ASP:O	1:BV:37:LYS:HE3	2.15	0.47
1:AF:65:ARG:HA	1:AF:93:PHE:O	2.15	0.47
1:AJ:12:GLN:HG2	1:BI:106:GLN:NE2	2.29	0.47
1:AK:69:PRO:HA	1:AK:90:SER:CB	2.44	0.47
1:AM:117:ASN:O	1:AM:121:THR:HG23	2.14	0.47
1:AW:51:PHE:HE2	1:AW:53:LYS:HB2	1.80	0.47
1:CD:6:LEU:HB3	1:CD:20:PHE:HB2	1.96	0.47
1:CD:101:TYR:HA	1:CE:42:ASN:HB2	1.96	0.47
1:AB:51:PHE:HE2	1:AB:53:LYS:HB2	1.80	0.47
1:AR:107:ASN:ND2	1:BV:89:TYR:OH	2.48	0.47
1:BC:101:TYR:HA	1:BD:42:ASN:HB2	1.96	0.47
1:BL:51:PHE:HE2	1:BL:53:LYS:HB2	1.80	0.47
1:CD:69:PRO:HA	1:CD:90:SER:CB	2.44	0.47
1:CD:117:ASN:O	1:CD:121:THR:HG23	2.15	0.47
1:CE:65:ARG:HA	1:CE:93:PHE:O	2.15	0.47
1:CG:117:ASN:O	1:CG:121:THR:HG23	2.15	0.47
1:AA:63:THR:HG22	1:AA:96:THR:HG22	1.97	0.46
1:AB:69:PRO:HA	1:AB:90:SER:CB	2.44	0.46
1:AU:65:ARG:HA	1:AU:93:PHE:O	2.15	0.46
1:BF:117:ASN:O	1:BF:121:THR:HG23	2.16	0.46
1:BO:51:PHE:HE2	1:BO:53:LYS:HB2	1.80	0.46
1:BU:6:LEU:HB3	1:BU:20:PHE:HB2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BU:101:TYR:HA	1:BV:42:ASN:HB2	1.96	0.46
1:CG:51:PHE:HE2	1:CG:53:LYS:HB2	1.80	0.46
1:CH:65:ARG:HA	1:CH:93:PHE:O	2.15	0.46
1:AG:117:ASN:O	1:AG:121:THR:HG23	2.14	0.46
1:AL:65:ARG:HA	1:AL:93:PHE:O	2.15	0.46
1:AT:69:PRO:HA	1:AT:90:SER:CB	2.44	0.46
1:AT:119:LEU:HD12	1:AY:119:LEU:HD12	1.96	0.46
1:AV:63:THR:HG22	1:AV:96:THR:HG22	1.97	0.46
1:AZ:6:LEU:HB3	1:AZ:20:PHE:HB2	1.96	0.46
1:BE:63:THR:HG22	1:BE:96:THR:HG22	1.97	0.46
1:BI:6:LEU:HB3	1:BI:20:PHE:HB2	1.96	0.46
1:BI:51:PHE:HE2	1:BI:53:LYS:HB2	1.80	0.46
1:BO:101:TYR:HA	1:BP:42:ASN:HB2	1.96	0.46
1:BR:10:ASP:OD2	1:BR:12:GLN:NE2	2.46	0.46
1:BR:117:ASN:O	1:BR:121:THR:HG23	2.15	0.46
1:BS:65:ARG:HA	1:BS:93:PHE:O	2.15	0.46
1:BX:51:PHE:HE2	1:BX:53:LYS:HB2	1.80	0.46
1:AD:135:TRP:CE3	1:AR:22:PRO:HG2	2.51	0.46
1:AK:51:PHE:HE2	1:AK:53:LYS:HB2	1.80	0.46
1:AM:119:LEU:HD12	1:BL:119:LEU:HD12	1.97	0.46
1:AW:6:LEU:HB3	1:AW:20:PHE:HB2	1.96	0.46
1:AW:69:PRO:HA	1:AW:90:SER:CB	2.44	0.46
1:BB:63:THR:HG22	1:BB:96:THR:HG22	1.97	0.46
1:BK:63:THR:HG22	1:BK:96:THR:HG22	1.97	0.46
1:BL:22:PRO:HG2	1:CD:135:TRP:CH2	2.51	0.46
1:BT:117:ASN:O	1:BT:121:THR:HG23	2.14	0.46
1:AH:51:PHE:HE2	1:AH:53:LYS:HB2	1.80	0.46
1:AH:117:ASN:O	1:AH:121:THR:HG23	2.15	0.46
1:AO:31:PRO:HB3	1:AO:51:PHE:HB2	1.98	0.46
1:AQ:6:LEU:HB3	1:AQ:20:PHE:HB2	1.96	0.46
1:AR:65:ARG:HA	1:AR:93:PHE:O	2.15	0.46
1:AT:6:LEU:HB3	1:AT:20:PHE:HB2	1.96	0.46
1:AZ:117:ASN:O	1:AZ:121:THR:HG23	2.16	0.46
1:BA:31:PRO:HB3	1:BA:51:PHE:HB2	1.98	0.46
1:BD:65:ARG:HA	1:BD:93:PHE:O	2.15	0.46
1:BH:52:VAL:HG21	1:CA:127:ALA:HB1	1.96	0.46
1:BL:117:ASN:O	1:BL:121:THR:HG23	2.16	0.46
1:BO:6:LEU:HB3	1:BO:20:PHE:HB2	1.96	0.46
1:CH:31:PRO:HB3	1:CH:51:PHE:HB2	1.98	0.46
1:AD:63:THR:HG22	1:AD:96:THR:HG22	1.97	0.46
1:AE:114:TYR:HH	1:BW:46:ARG:NH1	2.12	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AT:51:PHE:HE2	1:AT:53:LYS:HB2	1.80	0.46
1:BD:31:PRO:HB3	1:BD:51:PHE:HB2	1.98	0.46
1:BG:68:ASP:HB3	1:BG:91:THR:OG1	2.16	0.46
1:BL:10:ASP:OD2	1:BL:12:GLN:NE2	2.46	0.46
1:BO:10:ASP:OD2	1:BO:12:GLN:NE2	2.46	0.46
1:BR:51:PHE:HE2	1:BR:53:LYS:HB2	1.80	0.46
1:BU:117:ASN:O	1:BU:121:THR:HG23	2.16	0.46
1:BY:65:ARG:HA	1:BY:93:PHE:O	2.15	0.46
1:AA:12:GLN:HG2	1:AH:106:GLN:NE2	2.29	0.46
1:AH:6:LEU:HB3	1:AH:20:PHE:HB2	1.96	0.46
1:AH:69:PRO:HA	1:AH:90:SER:CB	2.44	0.46
1:BA:107:ASN:ND2	1:CE:89:TYR:OH	2.48	0.46
1:BC:117:ASN:O	1:BC:121:THR:HG23	2.16	0.46
1:BJ:31:PRO:HB3	1:BJ:51:PHE:HB2	1.98	0.46
1:BO:117:ASN:O	1:BO:121:THR:HG23	2.16	0.46
1:BX:6:LEU:HB3	1:BX:20:PHE:HB2	1.96	0.46
1:BX:117:ASN:O	1:BX:121:THR:HG23	2.15	0.46
1:CG:101:TYR:HA	1:CH:42:ASN:HB2	1.96	0.46
1:AB:117:ASN:O	1:AB:121:THR:HG23	2.16	0.46
1:AC:65:ARG:HA	1:AC:93:PHE:O	2.15	0.46
1:AC:68:ASP:HB3	1:AC:91:THR:OG1	2.16	0.46
1:AI:135:TRP:OXT	1:BP:3:ILE:N	2.45	0.46
1:AJ:63:THR:HG22	1:AJ:96:THR:HG22	1.97	0.46
1:AO:65:ARG:HA	1:AO:93:PHE:O	2.15	0.46
1:AY:63:THR:HG22	1:AY:96:THR:HG22	1.97	0.46
1:AZ:51:PHE:HE2	1:AZ:53:LYS:HB2	1.80	0.46
1:BD:68:ASP:HB3	1:BD:91:THR:OG1	2.16	0.46
1:BJ:65:ARG:HA	1:BJ:93:PHE:O	2.15	0.46
1:BV:68:ASP:HB3	1:BV:91:THR:OG1	2.16	0.46
1:CA:69:PRO:HA	1:CA:90:SER:CB	2.44	0.46
1:AA:1:ALA:O	1:AH:134:ALA:HA	2.16	0.46
1:AF:68:ASP:HB3	1:AF:91:THR:OG1	2.16	0.46
1:AI:65:ARG:HA	1:AI:93:PHE:O	2.15	0.46
1:AK:117:ASN:O	1:AK:121:THR:HG23	2.16	0.46
1:AX:68:ASP:HB3	1:AX:91:THR:OG1	2.16	0.46
1:BA:68:ASP:HB3	1:BA:91:THR:OG1	2.16	0.46
1:BA:135:TRP:OXT	1:CE:3:ILE:N	2.43	0.46
1:BF:101:TYR:HA	1:BG:42:ASN:HB2	1.96	0.46
1:BM:68:ASP:HB3	1:BM:91:THR:OG1	2.16	0.46
1:BQ:63:THR:HG22	1:BQ:96:THR:HG22	1.97	0.46
1:BV:65:ARG:HA	1:BV:93:PHE:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CE:68:ASP:HB3	1:CE:91:THR:OG1	2.16	0.46
1:AC:31:PRO:HB3	1:AC:51:PHE:HB2	1.98	0.46
1:AD:117:ASN:O	1:AD:121:THR:HG23	2.14	0.46
1:AE:10:ASP:OD2	1:AE:12:GLN:NE2	2.46	0.46
1:AL:31:PRO:HB3	1:AL:51:PHE:HB2	1.98	0.46
1:AP:63:THR:HG22	1:AP:96:THR:HG22	1.97	0.46
1:AW:112:LEU:HD21	1:BB:125:THR:HG22	1.98	0.46
1:BN:63:THR:HG22	1:BN:96:THR:HG22	1.97	0.46
1:BW:63:THR:HG22	1:BW:96:THR:HG22	1.97	0.46
1:BY:68:ASP:HB3	1:BY:91:THR:OG1	2.16	0.46
1:CA:51:PHE:HE2	1:CA:53:LYS:HB2	1.80	0.46
1:CB:65:ARG:HA	1:CB:93:PHE:O	2.15	0.46
1:AE:6:LEU:HB3	1:AE:20:PHE:HB2	1.96	0.46
1:AX:65:ARG:HA	1:AX:93:PHE:O	2.15	0.46
1:BH:26:GLN:NE2	1:CA:133:PRO:HB2	2.31	0.46
1:BI:117:ASN:O	1:BI:121:THR:HG23	2.16	0.46
1:BQ:117:ASN:O	1:BQ:121:THR:HG23	2.14	0.46
1:BX:10:ASP:OD2	1:BX:12:GLN:NE2	2.46	0.46
1:CB:68:ASP:HB3	1:CB:91:THR:OG1	2.16	0.46
1:AQ:117:ASN:O	1:AQ:121:THR:HG23	2.16	0.45
1:AT:117:ASN:O	1:AT:121:THR:HG23	2.16	0.45
1:AU:37:LYS:HE3	1:AY:130:ASP:O	2.15	0.45
1:CC:63:THR:HG22	1:CC:96:THR:HG22	1.97	0.45
1:AC:107:ASN:ND2	1:BG:89:TYR:OH	2.49	0.45
1:AI:68:ASP:HB3	1:AI:91:THR:OG1	2.16	0.45
1:BA:65:ARG:HA	1:BA:93:PHE:O	2.15	0.45
1:BD:119:LEU:HD12	1:CH:119:LEU:HD12	1.98	0.45
1:BI:25:PRO:HD3	1:CA:135:TRP:HB2	1.97	0.45
1:BJ:68:ASP:HB3	1:BJ:91:THR:OG1	2.16	0.45
1:AS:63:THR:HG22	1:AS:96:THR:HG22	1.97	0.45
1:AU:68:ASP:HB3	1:AU:91:THR:OG1	2.16	0.45
1:AW:117:ASN:O	1:AW:121:THR:HG23	2.16	0.45
1:BN:119:LEU:HD12	1:BU:119:LEU:HD12	1.98	0.45
1:BP:68:ASP:HB3	1:BP:91:THR:OG1	2.16	0.45
1:BT:63:THR:HG22	1:BT:96:THR:HG22	1.97	0.45
1:AF:9:ALA:O	1:BM:117:ASN:ND2	2.50	0.45
1:AI:46:ARG:HG2	1:AI:69:PRO:HD2	1.99	0.45
1:AN:117:ASN:O	1:AN:121:THR:HG23	2.16	0.45
1:BM:65:ARG:HA	1:BM:93:PHE:O	2.15	0.45
1:BP:65:ARG:HA	1:BP:93:PHE:O	2.15	0.45
1:BX:73:SER:OG	1:CF:102:GLY:O	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:117:ASN:O	1:CA:121:THR:HG23	2.15	0.45
1:AE:117:ASN:O	1:AE:121:THR:HG23	2.15	0.45
1:AI:117:ASN:ND2	1:BP:9:ALA:O	2.50	0.45
1:AL:68:ASP:HB3	1:AL:91:THR:OG1	2.16	0.45
1:AN:10:ASP:OD2	1:AN:12:GLN:NE2	2.46	0.45
1:AR:52:VAL:HG21	1:BV:127:ALA:HB1	1.99	0.45
1:AT:112:LEU:HD21	1:AY:125:THR:HG22	1.98	0.45
1:AU:46:ARG:HG2	1:AU:69:PRO:HD2	1.99	0.45
1:BG:31:PRO:HB3	1:BG:51:PHE:HB2	1.98	0.45
1:BP:31:PRO:HB3	1:BP:51:PHE:HB2	1.98	0.45
1:BY:46:ARG:HG2	1:BY:69:PRO:HD2	1.99	0.45
1:AC:46:ARG:HG2	1:AC:69:PRO:HD2	1.99	0.45
1:AM:117:ASN:ND2	1:BL:9:ALA:O	2.50	0.45
1:AR:31:PRO:HB3	1:AR:51:PHE:HB2	1.98	0.45
1:AX:31:PRO:HB3	1:AX:51:PHE:HB2	1.98	0.45
1:BG:46:ARG:HG2	1:BG:69:PRO:HD2	1.99	0.45
1:BR:133:PRO:HB3	1:BT:52:VAL:HB	1.98	0.45
1:BS:31:PRO:HB3	1:BS:51:PHE:HB2	1.98	0.45
1:CD:51:PHE:HE2	1:CD:53:LYS:HB2	1.80	0.45
1:AC:24:GLN:O	1:AC:32:SER:HA	2.17	0.45
1:AF:46:ARG:HG2	1:AF:69:PRO:HD2	1.99	0.45
1:AF:66:ILE:HD11	1:BM:118:LEU:CD2	2.46	0.45
1:AG:63:THR:HG22	1:AG:96:THR:HG22	1.97	0.45
1:AP:12:GLN:HG2	1:BF:106:GLN:NE2	2.31	0.45
1:AR:68:ASP:HB3	1:AR:91:THR:OG1	2.16	0.45
1:AU:24:GLN:O	1:AU:32:SER:HA	2.17	0.45
1:BA:24:GLN:O	1:BA:32:SER:HA	2.17	0.45
1:BS:68:ASP:HB3	1:BS:91:THR:OG1	2.16	0.45
1:CF:63:THR:HG22	1:CF:96:THR:HG22	1.97	0.45
1:AC:119:LEU:HD12	1:BG:119:LEU:HD12	1.99	0.45
1:AD:114:TYR:HH	1:AQ:46:ARG:NH1	2.15	0.45
1:AL:46:ARG:HG2	1:AL:69:PRO:HD2	1.99	0.45
1:AW:133:PRO:HB3	1:BB:52:VAL:HB	1.99	0.45
1:BD:24:GLN:O	1:BD:32:SER:HA	2.17	0.45
1:BD:46:ARG:HG2	1:BD:69:PRO:HD2	1.99	0.45
1:BP:24:GLN:O	1:BP:32:SER:HA	2.17	0.45
1:AM:135:TRP:CE3	1:BM:22:PRO:HG2	2.51	0.45
1:AP:95:CYS:HA	1:BF:94:GLU:O	2.17	0.45
1:AR:46:ARG:HG2	1:AR:69:PRO:HD2	1.99	0.45
1:AX:46:ARG:HG2	1:AX:69:PRO:HD2	1.99	0.45
1:BE:135:TRP:CE3	1:CH:22:PRO:HG2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BJ:24:GLN:O	1:BJ:32:SER:HA	2.17	0.45
1:BZ:63:THR:HG22	1:BZ:96:THR:HG22	1.97	0.45
1:CH:46:ARG:HG2	1:CH:69:PRO:HD2	1.99	0.45
1:AF:31:PRO:HB3	1:AF:51:PHE:HB2	1.98	0.45
1:AI:9:ALA:O	1:BP:117:ASN:ND2	2.50	0.45
1:AU:31:PRO:HB3	1:AU:51:PHE:HB2	1.98	0.45
1:AU:135:TRP:CD1	1:BW:25:PRO:HG3	2.52	0.45
1:BG:24:GLN:O	1:BG:32:SER:HA	2.17	0.45
1:AJ:71:LEU:O	1:BJ:83:ASN:ND2	2.51	0.44
1:AO:46:ARG:HG2	1:AO:69:PRO:HD2	1.99	0.44
1:AO:68:ASP:HB3	1:AO:91:THR:OG1	2.16	0.44
1:AX:24:GLN:O	1:AX:32:SER:HA	2.17	0.44
1:BE:125:THR:HG22	1:CG:112:LEU:HD21	1.98	0.44
1:BQ:50:MET:HG3	1:BQ:64:ILE:HG12	2.00	0.44
1:BS:24:GLN:O	1:BS:32:SER:HA	2.17	0.44
1:CH:68:ASP:HB3	1:CH:91:THR:OG1	2.16	0.44
1:AB:135:TRP:HB2	1:CA:25:PRO:HD3	1.99	0.44
1:AJ:50:MET:HG3	1:AJ:64:ILE:HG12	2.00	0.44
1:AX:37:LYS:HE3	1:BB:130:ASP:O	2.16	0.44
1:BD:107:ASN:ND2	1:CH:89:TYR:OH	2.51	0.44
1:BM:24:GLN:O	1:BM:32:SER:HA	2.17	0.44
1:BM:31:PRO:HB3	1:BM:51:PHE:HB2	1.98	0.44
1:BN:50:MET:HG3	1:BN:64:ILE:HG12	2.00	0.44
1:BY:31:PRO:HB3	1:BY:51:PHE:HB2	1.98	0.44
1:CB:24:GLN:O	1:CB:32:SER:HA	2.17	0.44
1:CE:31:PRO:HB3	1:CE:51:PHE:HB2	1.98	0.44
1:AM:9:ALA:HB3	1:BL:117:ASN:ND2	2.32	0.44
1:BW:50:MET:HG3	1:BW:64:ILE:HG12	2.00	0.44
1:AI:24:GLN:O	1:AI:32:SER:HA	2.17	0.44
1:AL:24:GLN:O	1:AL:32:SER:HA	2.17	0.44
1:AX:54:TYR:HD1	1:CB:131:MET:HG3	1.82	0.44
1:BK:12:GLN:HG2	1:CD:106:GLN:NE2	2.32	0.44
1:BK:72:ALA:HB1	1:CE:81:ASP:HB3	1.98	0.44
1:BT:50:MET:HG3	1:BT:64:ILE:HG12	2.00	0.44
1:BV:31:PRO:HB3	1:BV:51:PHE:HB2	1.98	0.44
1:CB:46:ARG:HG2	1:CB:69:PRO:HD2	1.99	0.44
1:AM:50:MET:HG3	1:AM:64:ILE:HG12	2.00	0.44
1:AO:24:GLN:O	1:AO:32:SER:HA	2.17	0.44
1:AU:22:PRO:HG2	1:AY:135:TRP:CE3	2.53	0.44
1:BE:46:ARG:NH1	1:CG:114:TYR:HH	2.15	0.44
1:BE:50:MET:HG3	1:BE:64:ILE:HG12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CE:24:GLN:O	1:CE:32:SER:HA	2.17	0.44
1:AF:24:GLN:O	1:AF:32:SER:HA	2.17	0.44
1:AG:130:ASP:O	1:AL:37:LYS:HE3	2.18	0.44
1:BA:46:ARG:HG2	1:BA:69:PRO:HD2	1.99	0.44
1:BF:10:ASP:OD2	1:BF:12:GLN:NE2	2.46	0.44
1:BS:46:ARG:HG2	1:BS:69:PRO:HD2	1.99	0.44
1:BY:24:GLN:O	1:BY:32:SER:HA	2.17	0.44
1:CB:31:PRO:HB3	1:CB:51:PHE:HB2	1.98	0.44
1:CE:46:ARG:HG2	1:CE:69:PRO:HD2	1.99	0.44
1:AI:31:PRO:HB3	1:AI:51:PHE:HB2	1.98	0.44
1:AJ:8:LEU:HD11	1:BI:118:LEU:HD13	2.00	0.44
1:AS:25:PRO:HG3	1:BY:135:TRP:CD1	2.53	0.44
1:AT:106:GLN:NE2	1:AY:12:GLN:HG2	2.32	0.44
1:CC:50:MET:HG3	1:CC:64:ILE:HG12	2.00	0.44
1:AH:27:THR:HG22	1:AH:28:GLY:N	2.33	0.44
1:AP:50:MET:HG3	1:AP:64:ILE:HG12	2.00	0.44
1:AW:10:ASP:OD2	1:AW:12:GLN:NE2	2.46	0.44
1:BH:50:MET:HG3	1:BH:64:ILE:HG12	2.00	0.44
1:BR:27:THR:HG22	1:BR:28:GLY:N	2.33	0.44
1:CE:36:ASN:HB2	1:CE:46:ARG:HB2	2.00	0.44
1:CH:24:GLN:O	1:CH:32:SER:HA	2.17	0.44
1:AD:50:MET:HG3	1:AD:64:ILE:HG12	1.99	0.44
1:AF:22:PRO:HG2	1:BW:135:TRP:CE3	2.53	0.44
1:BA:36:ASN:HB2	1:BA:46:ARG:HB2	2.00	0.44
1:BG:36:ASN:HB2	1:BG:46:ARG:HB2	2.00	0.44
1:BL:27:THR:HG22	1:BL:28:GLY:N	2.33	0.44
1:AA:46:ARG:HH12	1:AH:114:TYR:HH	1.66	0.43
1:AI:36:ASN:HB2	1:AI:46:ARG:HB2	2.00	0.43
1:AN:27:THR:HG22	1:AN:28:GLY:N	2.33	0.43
1:AV:50:MET:HG3	1:AV:64:ILE:HG12	2.00	0.43
1:BE:114:TYR:HH	1:CG:46:ARG:NH1	2.16	0.43
1:BM:36:ASN:HB2	1:BM:46:ARG:HB2	2.00	0.43
1:BV:46:ARG:HG2	1:BV:69:PRO:HD2	1.99	0.43
1:CA:27:THR:HG22	1:CA:28:GLY:N	2.33	0.43
1:CF:50:MET:HG3	1:CF:64:ILE:HG12	2.00	0.43
1:AA:50:MET:HG3	1:AA:64:ILE:HG12	2.00	0.43
1:AY:50:MET:HG3	1:AY:64:ILE:HG12	2.00	0.43
1:BM:46:ARG:HG2	1:BM:69:PRO:HD2	1.99	0.43
1:BV:24:GLN:O	1:BV:32:SER:HA	2.17	0.43
1:BY:37:LYS:HE3	1:CF:130:ASP:O	2.18	0.43
1:BZ:50:MET:HG3	1:BZ:64:ILE:HG12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CH:36:ASN:HB2	1:CH:46:ARG:HB2	2.00	0.43
1:AJ:134:ALA:HA	1:BI:1:ALA:O	2.18	0.43
1:AP:8:LEU:HD11	1:BF:118:LEU:HD13	2.01	0.43
1:AR:24:GLN:O	1:AR:32:SER:HA	2.17	0.43
1:AR:36:ASN:HB2	1:AR:46:ARG:HB2	2.00	0.43
1:AT:8:LEU:HD11	1:AY:118:LEU:HD13	2.01	0.43
1:BD:52:VAL:CG2	1:CH:127:ALA:HB1	2.48	0.43
1:BK:50:MET:HG3	1:BK:64:ILE:HG12	2.00	0.43
1:CB:36:ASN:HB2	1:CB:46:ARG:HB2	2.00	0.43
1:AA:72:ALA:HB1	1:AI:81:ASP:HB3	1.99	0.43
1:AU:36:ASN:HB2	1:AU:46:ARG:HB2	2.00	0.43
1:AD:130:ASP:O	1:AR:37:LYS:HE3	2.19	0.43
1:AT:94:GLU:O	1:AY:95:CYS:HA	2.19	0.43
1:BP:46:ARG:HG2	1:BP:69:PRO:HD2	1.99	0.43
1:BI:27:THR:HG22	1:BI:28:GLY:N	2.33	0.43
1:BJ:46:ARG:HG2	1:BJ:69:PRO:HD2	1.99	0.43
1:AY:25:PRO:HG3	1:CE:135:TRP:CD1	2.54	0.43
1:BD:36:ASN:HB2	1:BD:46:ARG:HB2	2.00	0.43
1:BF:27:THR:HG22	1:BF:28:GLY:N	2.33	0.43
1:AF:117:ASN:ND2	1:BM:9:ALA:O	2.52	0.43
1:AZ:27:THR:HG22	1:AZ:28:GLY:N	2.33	0.43
1:BD:18:HIS:ND1	1:BD:38:GLU:OE2	2.43	0.43
1:BO:27:THR:HG22	1:BO:28:GLY:N	2.33	0.43
1:BP:36:ASN:HB2	1:BP:46:ARG:HB2	2.00	0.43
1:AG:50:MET:HG3	1:AG:64:ILE:HG12	2.00	0.43
1:BH:71:LEU:O	1:CB:83:ASN:ND2	2.52	0.43
1:BH:117:ASN:ND2	1:CA:9:ALA:HB3	2.34	0.43
1:BH:119:LEU:HD12	1:CA:119:LEU:HD12	2.01	0.43
1:BP:37:LYS:HA	1:BP:45:TYR:CD1	2.54	0.43
1:BX:27:THR:HG22	1:BX:28:GLY:N	2.33	0.43
1:BY:36:ASN:HB2	1:BY:46:ARG:HB2	2.00	0.43
1:AU:37:LYS:HA	1:AU:45:TYR:CD1	2.54	0.43
1:AU:103:ALA:HA	1:BY:89:TYR:CE1	2.54	0.43
1:BD:37:LYS:HA	1:BD:45:TYR:CD1	2.54	0.43
1:BV:36:ASN:HB2	1:BV:46:ARG:HB2	2.00	0.43
1:BX:102:GLY:HA2	1:BY:41:SER:CB	2.49	0.43
1:CD:27:THR:HG22	1:CD:28:GLY:N	2.33	0.43
1:AB:27:THR:HG22	1:AB:28:GLY:N	2.33	0.42
1:AC:89:TYR:OH	1:BG:107:ASN:ND2	2.52	0.42
1:AE:27:THR:HG22	1:AE:28:GLY:N	2.33	0.42
1:AI:52:VAL:HG21	1:BP:127:ALA:HB1	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AQ:27:THR:HG22	1:AQ:28:GLY:N	2.33	0.42
1:AW:102:GLY:HA2	1:AX:41:SER:CB	2.49	0.42
1:AX:36:ASN:HB2	1:AX:46:ARG:HB2	2.00	0.42
1:BS:37:LYS:HA	1:BS:45:TYR:CD1	2.54	0.42
1:AC:36:ASN:HB2	1:AC:46:ARG:HB2	2.00	0.42
1:AC:37:LYS:HA	1:AC:45:TYR:CD1	2.54	0.42
1:AG:46:ARG:NH1	1:AK:114:TYR:HH	2.16	0.42
1:AG:135:TRP:CE3	1:AL:22:PRO:HG2	2.54	0.42
1:AN:36:ASN:HB2	1:AN:46:ARG:HB2	2.02	0.42
1:AR:37:LYS:HA	1:AR:45:TYR:CD1	2.54	0.42
1:AX:98:SER:HB2	1:CB:92:PHE:HB2	2.01	0.42
1:AZ:35:LEU:HD22	1:AZ:45:TYR:HB3	2.02	0.42
1:BA:37:LYS:HA	1:BA:45:TYR:CD1	2.54	0.42
1:BC:35:LEU:HD22	1:BC:45:TYR:HB3	2.01	0.42
1:BO:35:LEU:HD22	1:BO:45:TYR:HB3	2.01	0.42
1:BO:102:GLY:HA2	1:BP:41:SER:CB	2.49	0.42
1:BR:46:ARG:NH1	1:BT:114:TYR:HH	2.17	0.42
1:BS:36:ASN:HB2	1:BS:46:ARG:HB2	2.00	0.42
1:BY:37:LYS:HA	1:BY:45:TYR:CD1	2.54	0.42
1:AA:125:THR:HG22	1:AH:112:LEU:HD21	2.01	0.42
1:AK:27:THR:HG22	1:AK:28:GLY:N	2.33	0.42
1:AK:118:LEU:HD12	1:AK:118:LEU:HA	1.85	0.42
1:AO:37:LYS:HA	1:AO:45:TYR:CD1	2.54	0.42
1:AS:50:MET:HG3	1:AS:64:ILE:HG12	2.00	0.42
1:AT:1:ALA:O	1:AY:134:ALA:HA	2.19	0.42
1:AZ:102:GLY:HA2	1:BA:41:SER:CB	2.49	0.42
1:BB:50:MET:HG3	1:BB:64:ILE:HG12	2.00	0.42
1:BL:118:LEU:HD12	1:BL:118:LEU:HA	1.85	0.42
1:BX:36:ASN:HB2	1:BX:46:ARG:HB2	2.02	0.42
1:CH:37:LYS:HA	1:CH:45:TYR:CD1	2.54	0.42
1:AG:46:ARG:HH12	1:AK:114:TYR:HH	1.68	0.42
1:BA:95:CYS:HA	1:CE:95:CYS:HA	2.01	0.42
1:BF:35:LEU:HD22	1:BF:45:TYR:HB3	2.02	0.42
1:BI:35:LEU:HD22	1:BI:45:TYR:HB3	2.01	0.42
1:BJ:37:LYS:HA	1:BJ:45:TYR:CD1	2.54	0.42
1:BL:102:GLY:HA2	1:BM:41:SER:CB	2.49	0.42
1:BR:1:ALA:O	1:BT:134:ALA:HA	2.19	0.42
1:CA:35:LEU:HD22	1:CA:45:TYR:HB3	2.02	0.42
1:CA:102:GLY:HA2	1:CB:41:SER:CB	2.49	0.42
1:AB:35:LEU:HD22	1:AB:45:TYR:HB3	2.02	0.42
1:AG:104:THR:HG22	1:AG:106:GLN:H	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AI:37:LYS:HA	1:AI:45:TYR:CD1	2.54	0.42
1:AM:104:THR:HG22	1:AM:106:GLN:H	1.85	0.42
1:AN:25:PRO:HD3	1:BL:135:TRP:HB2	2.01	0.42
1:AW:36:ASN:HB2	1:AW:46:ARG:HB2	2.02	0.42
1:BU:27:THR:HG22	1:BU:28:GLY:N	2.33	0.42
1:CC:104:THR:HG22	1:CC:106:GLN:H	1.85	0.42
1:AE:36:ASN:HB2	1:AE:46:ARG:HB2	2.02	0.42
1:AO:36:ASN:HB2	1:AO:46:ARG:HB2	2.00	0.42
1:AS:104:THR:HG22	1:AS:106:GLN:H	1.85	0.42
1:AT:36:ASN:HB2	1:AT:46:ARG:HB2	2.02	0.42
1:AW:118:LEU:HD12	1:AW:118:LEU:HA	1.85	0.42
1:BA:92:PHE:HB2	1:CE:98:SER:HB2	2.00	0.42
1:BB:65:ARG:HA	1:BB:93:PHE:O	2.20	0.42
1:BC:27:THR:HG22	1:BC:28:GLY:N	2.33	0.42
1:BE:104:THR:HG22	1:BE:106:GLN:H	1.85	0.42
1:BG:37:LYS:HA	1:BG:45:TYR:CD1	2.54	0.42
1:BJ:36:ASN:HB2	1:BJ:46:ARG:HB2	2.00	0.42
1:BK:104:THR:HG22	1:BK:106:GLN:H	1.85	0.42
1:BR:35:LEU:HD22	1:BR:45:TYR:HB3	2.02	0.42
1:BW:104:THR:HG22	1:BW:106:GLN:H	1.85	0.42
1:CF:104:THR:HG22	1:CF:106:GLN:H	1.85	0.42
1:AB:36:ASN:HB2	1:AB:46:ARG:HB2	2.02	0.42
1:AE:35:LEU:HD22	1:AE:45:TYR:HB3	2.02	0.42
1:AF:66:ILE:HD11	1:BM:118:LEU:HD22	2.02	0.42
1:AG:1:ALA:O	1:AK:134:ALA:HA	2.19	0.42
1:AJ:117:ASN:ND2	1:BI:9:ALA:HB3	2.34	0.42
1:AK:36:ASN:HB2	1:AK:46:ARG:HB2	2.02	0.42
1:AK:102:GLY:HA2	1:AL:41:SER:CB	2.49	0.42
1:BL:35:LEU:HD22	1:BL:45:TYR:HB3	2.01	0.42
1:BT:101:TYR:HA	1:BU:42:ASN:HB2	2.02	0.42
1:AF:36:ASN:HB2	1:AF:46:ARG:HB2	2.00	0.42
1:AG:65:ARG:HA	1:AG:93:PHE:O	2.20	0.42
1:AI:118:LEU:CD2	1:BP:66:ILE:HD11	2.49	0.42
1:AM:12:GLN:HG2	1:BL:106:GLN:HE21	1.83	0.42
1:AS:65:ARG:HA	1:AS:93:PHE:O	2.20	0.42
1:AV:101:TYR:HA	1:AW:42:ASN:HB2	2.02	0.42
1:AW:27:THR:HG22	1:AW:28:GLY:N	2.33	0.42
1:BN:101:TYR:HA	1:BO:42:ASN:HB2	2.02	0.42
1:AJ:104:THR:HG22	1:AJ:106:GLN:H	1.85	0.42
1:AL:37:LYS:HA	1:AL:45:TYR:CD1	2.54	0.42
1:AP:65:ARG:HA	1:AP:93:PHE:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AT:27:THR:HG22	1:AT:28:GLY:N	2.33	0.42
1:AV:65:ARG:HA	1:AV:93:PHE:O	2.20	0.42
1:AY:101:TYR:HA	1:AZ:42:ASN:HB2	2.02	0.42
1:AZ:118:LEU:HA	1:AZ:118:LEU:HD12	1.85	0.42
1:BE:12:GLN:HG2	1:CG:106:GLN:NE2	2.34	0.42
1:BH:118:LEU:HD13	1:CA:8:LEU:HD11	2.01	0.42
1:BM:37:LYS:HA	1:BM:45:TYR:CD1	2.54	0.42
1:BU:35:LEU:HD22	1:BU:45:TYR:HB3	2.02	0.42
1:BZ:101:TYR:HA	1:CA:42:ASN:HB2	2.02	0.42
1:CF:65:ARG:HA	1:CF:93:PHE:O	2.20	0.42
1:AB:22:PRO:HG2	1:AH:135:TRP:CH2	2.55	0.42
1:AF:37:LYS:HA	1:AF:45:TYR:CD1	2.54	0.42
1:AG:134:ALA:HA	1:AK:1:ALA:O	2.20	0.42
1:AQ:35:LEU:HD22	1:AQ:45:TYR:HB3	2.02	0.42
1:AV:118:LEU:HD12	1:AV:118:LEU:HA	1.87	0.42
1:BB:101:TYR:HA	1:BC:42:ASN:HB2	2.02	0.42
1:BF:36:ASN:HB2	1:BF:46:ARG:HB2	2.02	0.42
1:BH:65:ARG:HA	1:BH:93:PHE:O	2.20	0.42
1:BK:65:ARG:HA	1:BK:93:PHE:O	2.20	0.42
1:BQ:101:TYR:HA	1:BR:42:ASN:HB2	2.02	0.42
1:BX:35:LEU:HD22	1:BX:45:TYR:HB3	2.02	0.42
1:BZ:65:ARG:HA	1:BZ:93:PHE:O	2.20	0.42
1:BZ:104:THR:HG22	1:BZ:106:GLN:H	1.85	0.42
1:CC:65:ARG:HA	1:CC:93:PHE:O	2.20	0.42
1:AA:104:THR:HG22	1:AA:106:GLN:H	1.85	0.41
1:AC:135:TRP:CD1	1:BE:25:PRO:HG3	2.55	0.41
1:AH:35:LEU:HD22	1:AH:45:TYR:HB3	2.02	0.41
1:AO:118:LEU:HD22	1:BS:66:ILE:HD11	2.02	0.41
1:AS:41:SER:HB3	1:AU:101:TYR:OH	2.20	0.41
1:AU:107:ASN:ND2	1:BY:89:TYR:OH	2.53	0.41
1:AX:37:LYS:HA	1:AX:45:TYR:CD1	2.54	0.41
1:BM:51:PHE:CE2	1:BM:53:LYS:HB2	2.55	0.41
1:BR:134:ALA:HA	1:BT:1:ALA:O	2.19	0.41
1:CB:18:HIS:ND1	1:CB:38:GLU:OE2	2.43	0.41
1:CD:35:LEU:HD22	1:CD:45:TYR:HB3	2.02	0.41
1:AD:65:ARG:HA	1:AD:93:PHE:O	2.20	0.41
1:AD:120:GLY:HA2	1:AQ:116:ARG:NH2	2.34	0.41
1:AL:36:ASN:HB2	1:AL:46:ARG:HB2	2.00	0.41
1:BC:102:GLY:HA2	1:BD:41:SER:CB	2.49	0.41
1:BQ:65:ARG:HA	1:BQ:93:PHE:O	2.20	0.41
1:CB:37:LYS:HA	1:CB:45:TYR:CD1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CG:35:LEU:HD22	1:CG:45:TYR:HB3	2.02	0.41
1:AB:112:LEU:HD21	1:BZ:125:THR:HG22	2.02	0.41
1:AF:118:LEU:CD2	1:BM:66:ILE:HD11	2.50	0.41
1:AG:41:SER:HB3	1:AI:101:TYR:OH	2.20	0.41
1:AJ:65:ARG:HA	1:AJ:93:PHE:O	2.20	0.41
1:BD:117:ASN:ND2	1:CH:9:ALA:HB3	2.35	0.41
1:BV:37:LYS:HA	1:BV:45:TYR:CD1	2.54	0.41
1:BV:51:PHE:CE2	1:BV:53:LYS:HB2	2.55	0.41
1:BW:41:SER:HB3	1:BY:101:TYR:OH	2.21	0.41
1:BW:65:ARG:HA	1:BW:93:PHE:O	2.20	0.41
1:CE:37:LYS:HA	1:CE:45:TYR:CD1	2.54	0.41
1:AE:112:LEU:HD21	1:BW:125:THR:HG22	2.02	0.41
1:AN:102:GLY:HA2	1:AO:41:SER:CB	2.49	0.41
1:BE:65:ARG:HA	1:BE:93:PHE:O	2.20	0.41
1:BH:110:ASP:OD1	1:CA:10:ASP:HB2	2.19	0.41
1:BN:12:GLN:HG2	1:BU:106:GLN:NE2	2.36	0.41
1:BN:104:THR:HG22	1:BN:106:GLN:H	1.85	0.41
1:BN:120:GLY:HA2	1:BU:116:ARG:NH2	2.35	0.41
1:BP:20:PHE:HA	1:BP:35:LEU:O	2.21	0.41
1:BQ:104:THR:HG22	1:BQ:106:GLN:H	1.85	0.41
1:BR:36:ASN:HB2	1:BR:46:ARG:HB2	2.02	0.41
1:CA:36:ASN:HB2	1:CA:46:ARG:HB2	2.02	0.41
1:CB:20:PHE:HA	1:CB:35:LEU:O	2.21	0.41
1:CC:101:TYR:HA	1:CD:42:ASN:HB2	2.02	0.41
1:AA:52:VAL:HB	1:AH:133:PRO:HB3	2.02	0.41
1:AB:8:LEU:HD11	1:BZ:118:LEU:HD13	2.02	0.41
1:AB:114:TYR:HH	1:BZ:46:ARG:HH12	1.66	0.41
1:AC:127:ALA:HB1	1:BG:52:VAL:HG21	2.02	0.41
1:AF:20:PHE:HA	1:AF:35:LEU:O	2.21	0.41
1:AM:41:SER:HB3	1:AO:101:TYR:OH	2.21	0.41
1:AR:20:PHE:HA	1:AR:35:LEU:O	2.21	0.41
1:AW:8:LEU:HD11	1:BB:118:LEU:HD13	2.01	0.41
1:AY:65:ARG:HA	1:AY:93:PHE:O	2.20	0.41
1:BA:20:PHE:HA	1:BA:35:LEU:O	2.21	0.41
1:BD:20:PHE:HA	1:BD:35:LEU:O	2.21	0.41
1:BH:41:SER:HB3	1:BJ:101:TYR:OH	2.21	0.41
1:BI:36:ASN:HB2	1:BI:46:ARG:HB2	2.02	0.41
1:BI:37:LYS:HE2	1:CA:130:ASP:O	2.20	0.41
1:BI:102:GLY:HA2	1:BJ:41:SER:CB	2.49	0.41
1:BO:36:ASN:HB2	1:BO:46:ARG:HB2	2.02	0.41
1:BT:121:THR:O	1:BT:125:THR:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CE:20:PHE:HA	1:CE:35:LEU:O	2.21	0.41
1:AA:134:ALA:HA	1:AH:1:ALA:O	2.21	0.41
1:AD:41:SER:HB3	1:AF:101:TYR:OH	2.21	0.41
1:AD:101:TYR:HA	1:AE:42:ASN:HB2	2.02	0.41
1:AE:8:LEU:HD11	1:BW:118:LEU:HD13	2.03	0.41
1:AH:36:ASN:HB2	1:AH:46:ARG:HB2	2.02	0.41
1:AJ:41:SER:HB3	1:AL:101:TYR:OH	2.20	0.41
1:AM:121:THR:O	1:AM:125:THR:HG23	2.21	0.41
1:AP:121:THR:O	1:AP:125:THR:HG23	2.21	0.41
1:AW:35:LEU:HD22	1:AW:45:TYR:HB3	2.02	0.41
1:BE:118:LEU:HD13	1:CG:8:LEU:HD11	2.03	0.41
1:BH:8:LEU:HD11	1:CA:118:LEU:HD13	2.03	0.41
1:BK:41:SER:HB3	1:BM:101:TYR:OH	2.20	0.41
1:BN:65:ARG:HA	1:BN:93:PHE:O	2.20	0.41
1:BT:65:ARG:HA	1:BT:93:PHE:O	2.20	0.41
1:BU:36:ASN:HB2	1:BU:46:ARG:HB2	2.02	0.41
1:BV:20:PHE:HA	1:BV:35:LEU:O	2.21	0.41
1:AJ:101:TYR:HA	1:AK:42:ASN:HB2	2.02	0.41
1:AP:94:GLU:O	1:BF:95:CYS:HA	2.20	0.41
1:AT:35:LEU:HD22	1:AT:45:TYR:HB3	2.02	0.41
1:AV:121:THR:O	1:AV:125:THR:HG23	2.21	0.41
1:AX:24:GLN:HB3	1:AX:33:GLN:HG2	2.03	0.41
1:AY:121:THR:O	1:AY:125:THR:HG23	2.21	0.41
1:AZ:36:ASN:HB2	1:AZ:46:ARG:HB2	2.02	0.41
1:BB:104:THR:HG22	1:BB:106:GLN:H	1.85	0.41
1:BB:121:THR:O	1:BB:125:THR:HG23	2.21	0.41
1:BK:101:TYR:HA	1:BL:42:ASN:HB2	2.02	0.41
1:BL:36:ASN:HB2	1:BL:46:ARG:HB2	2.02	0.41
1:BX:112:LEU:HD21	1:CF:125:THR:HG22	2.03	0.41
1:CC:41:SER:HB3	1:CE:101:TYR:OH	2.20	0.41
1:CH:20:PHE:HA	1:CH:35:LEU:O	2.21	0.41
1:AA:65:ARG:HA	1:AA:93:PHE:O	2.20	0.41
1:AB:102:GLY:HA2	1:AC:41:SER:CB	2.49	0.41
1:AN:35:LEU:HD22	1:AN:45:TYR:HB3	2.02	0.41
1:AP:104:THR:HG22	1:AP:106:GLN:H	1.85	0.41
1:AS:101:TYR:HA	1:AT:42:ASN:HB2	2.02	0.41
1:AU:10:ASP:OD2	1:AU:12:GLN:NE2	2.54	0.41
1:AV:104:THR:HG22	1:AV:106:GLN:H	1.85	0.41
1:AX:81:ASP:HB3	1:BB:72:ALA:HB1	2.03	0.41
1:BC:36:ASN:HB2	1:BC:46:ARG:HB2	2.02	0.41
1:BD:118:LEU:HA	1:BD:121:THR:HG23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BH:101:TYR:HA	1:BI:42:ASN:HB2	2.02	0.41
1:BH:104:THR:HG22	1:BH:106:GLN:H	1.85	0.41
1:BZ:121:THR:O	1:BZ:125:THR:HG23	2.21	0.41
1:CG:36:ASN:HB2	1:CG:46:ARG:HB2	2.02	0.41
1:AA:101:TYR:HA	1:AB:42:ASN:HB2	2.02	0.41
1:AB:119:LEU:HD12	1:BZ:119:LEU:HD12	2.01	0.41
1:AE:135:TRP:HB2	1:BX:25:PRO:HD3	2.02	0.41
1:AF:98:SER:HB2	1:BM:92:PHE:HB2	2.02	0.41
1:AG:101:TYR:HA	1:AH:42:ASN:HB2	2.02	0.41
1:AG:121:THR:O	1:AG:125:THR:HG23	2.21	0.41
1:AI:65:ARG:HB3	1:AI:94:GLU:HG2	2.03	0.41
1:AJ:121:THR:O	1:AJ:125:THR:HG23	2.21	0.41
1:AK:35:LEU:HD22	1:AK:45:TYR:HB3	2.02	0.41
1:AM:8:LEU:HD11	1:BL:118:LEU:HD13	2.03	0.41
1:AM:65:ARG:HA	1:AM:93:PHE:O	2.20	0.41
1:AP:117:ASN:ND2	1:BF:9:ALA:HB3	2.36	0.41
1:AQ:36:ASN:HB2	1:AQ:46:ARG:HB2	2.02	0.41
1:AR:118:LEU:HA	1:AR:121:THR:HG23	2.03	0.41
1:AT:95:CYS:HA	1:AY:94:GLU:O	2.20	0.41
1:AT:102:GLY:HA2	1:AU:41:SER:CB	2.49	0.41
1:AT:118:LEU:HD13	1:AY:8:LEU:HD11	2.03	0.41
1:AU:24:GLN:HB3	1:AU:33:GLN:HG2	2.03	0.41
1:AV:41:SER:HB3	1:AX:101:TYR:OH	2.20	0.41
1:AX:10:ASP:OD2	1:AX:12:GLN:NE2	2.54	0.41
1:AX:112:LEU:CD2	1:CB:125:THR:HG22	2.42	0.41
1:BA:119:LEU:HD12	1:CE:119:LEU:HD12	2.02	0.41
1:BB:41:SER:HB3	1:BD:101:TYR:OH	2.20	0.41
1:BD:24:GLN:HB3	1:BD:33:GLN:HG2	2.03	0.41
1:BE:41:SER:HB3	1:BG:101:TYR:OH	2.21	0.41
1:BK:119:LEU:HA	1:BK:119:LEU:HD23	1.95	0.41
1:BL:119:LEU:HA	1:BL:124:VAL:HG11	2.03	0.41
1:BM:20:PHE:HA	1:BM:35:LEU:O	2.21	0.41
1:BN:121:THR:O	1:BN:125:THR:HG23	2.21	0.41
1:BN:134:ALA:HA	1:BU:1:ALA:O	2.21	0.41
1:BS:118:LEU:HA	1:BS:121:THR:HG23	2.03	0.41
1:BV:65:ARG:HB3	1:BV:94:GLU:HG2	2.03	0.41
1:BW:121:THR:O	1:BW:125:THR:HG23	2.21	0.41
1:BY:10:ASP:OD2	1:BY:12:GLN:NE2	2.54	0.41
1:CB:10:ASP:OD2	1:CB:12:GLN:NE2	2.54	0.41
1:CB:24:GLN:HB3	1:CB:33:GLN:HG2	2.03	0.41
1:CE:24:GLN:HB3	1:CE:33:GLN:HG2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CF:41:SER:HB3	1:CH:101:TYR:OH	2.20	0.41
1:CG:27:THR:HG22	1:CG:28:GLY:N	2.33	0.41
1:AC:10:ASP:OD2	1:AC:12:GLN:NE2	2.54	0.41
1:AE:102:GLY:HA2	1:AF:41:SER:CB	2.49	0.41
1:AJ:1:ALA:O	1:BI:134:ALA:HA	2.21	0.41
1:AL:20:PHE:HA	1:AL:35:LEU:O	2.21	0.41
1:AN:119:LEU:HA	1:AN:124:VAL:HG11	2.03	0.41
1:AP:101:TYR:HA	1:AQ:42:ASN:HB2	2.02	0.41
1:AR:65:ARG:HB3	1:AR:94:GLU:HG2	2.03	0.41
1:AS:121:THR:O	1:AS:125:THR:HG23	2.21	0.41
1:AU:118:LEU:HA	1:AU:121:THR:HG23	2.03	0.41
1:BA:65:ARG:HB3	1:BA:94:GLU:HG2	2.03	0.41
1:BE:101:TYR:HA	1:BF:42:ASN:HB2	2.02	0.41
1:BG:65:ARG:HB3	1:BG:94:GLU:HG2	2.03	0.41
1:BN:118:LEU:HD12	1:BN:118:LEU:HA	1.87	0.41
1:BO:119:LEU:HA	1:BO:124:VAL:HG11	2.03	0.41
1:BS:20:PHE:HA	1:BS:35:LEU:O	2.21	0.41
1:BY:51:PHE:CE2	1:BY:53:LYS:HB2	2.55	0.41
1:CB:65:ARG:HB3	1:CB:94:GLU:HG2	2.03	0.41
1:CF:121:THR:O	1:CF:125:THR:HG23	2.21	0.41
1:CG:119:LEU:HA	1:CG:124:VAL:HG11	2.03	0.41
1:AH:119:LEU:HA	1:AH:124:VAL:HG11	2.03	0.40
1:AL:65:ARG:HB3	1:AL:94:GLU:HG2	2.03	0.40
1:AP:117:ASN:ND2	1:BF:9:ALA:O	2.54	0.40
1:AU:65:ARG:HB3	1:AU:94:GLU:HG2	2.03	0.40
1:BA:24:GLN:HB3	1:BA:33:GLN:HG2	2.03	0.40
1:BE:46:ARG:HH12	1:CG:114:TYR:HH	1.66	0.40
1:BJ:20:PHE:HA	1:BJ:35:LEU:O	2.21	0.40
1:BM:118:LEU:HA	1:BM:121:THR:HG23	2.03	0.40
1:BP:118:LEU:HA	1:BP:121:THR:HG23	2.03	0.40
1:BT:41:SER:HB3	1:BV:101:TYR:OH	2.21	0.40
1:BW:101:TYR:HA	1:BX:42:ASN:HB2	2.02	0.40
1:BX:66:ILE:HD11	1:CF:118:LEU:CD2	2.50	0.40
1:BY:118:LEU:HA	1:BY:121:THR:HG23	2.03	0.40
1:BZ:41:SER:HB3	1:CB:101:TYR:OH	2.21	0.40
1:CA:119:LEU:HA	1:CA:124:VAL:HG11	2.03	0.40
1:CC:121:THR:O	1:CC:125:THR:HG23	2.21	0.40
1:CD:36:ASN:HB2	1:CD:46:ARG:HB2	2.02	0.40
1:CD:102:GLY:HA2	1:CE:41:SER:CB	2.49	0.40
1:CE:65:ARG:HB3	1:CE:94:GLU:HG2	2.03	0.40
1:CF:101:TYR:HA	1:CG:42:ASN:HB2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CH:10:ASP:OD2	1:CH:12:GLN:NE2	2.54	0.40
1:CH:24:GLN:HB3	1:CH:33:GLN:HG2	2.03	0.40
1:AC:20:PHE:HA	1:AC:35:LEU:O	2.21	0.40
1:AD:12:GLN:HG2	1:AQ:106:GLN:NE2	2.37	0.40
1:AE:119:LEU:HA	1:AE:124:VAL:HG11	2.03	0.40
1:AK:3:ILE:HG12	1:AK:22:PRO:HB3	2.04	0.40
1:AL:24:GLN:HB3	1:AL:33:GLN:HG2	2.03	0.40
1:AO:10:ASP:OD2	1:AO:12:GLN:NE2	2.54	0.40
1:BD:135:TRP:CD1	1:CF:25:PRO:HG3	2.55	0.40
1:BJ:65:ARG:HB3	1:BJ:94:GLU:HG2	2.03	0.40
1:BK:120:GLY:HA2	1:CD:116:ARG:NH2	2.35	0.40
1:BP:51:PHE:CE2	1:BP:53:LYS:HB2	2.55	0.40
1:BQ:41:SER:HB3	1:BS:101:TYR:OH	2.21	0.40
1:BT:104:THR:HG22	1:BT:106:GLN:H	1.85	0.40
1:BV:10:ASP:OD2	1:BV:12:GLN:NE2	2.54	0.40
1:BY:24:GLN:HB3	1:BY:33:GLN:HG2	2.03	0.40
1:CD:3:ILE:HG12	1:CD:22:PRO:HB3	2.04	0.40
1:AA:121:THR:O	1:AA:125:THR:HG23	2.21	0.40
1:AF:65:ARG:HB3	1:AF:94:GLU:HG2	2.03	0.40
1:AI:117:ASN:ND2	1:BP:9:ALA:HB3	2.36	0.40
1:AR:50:MET:HA	1:AR:63:THR:O	2.22	0.40
1:AT:119:LEU:HA	1:AT:124:VAL:HG11	2.03	0.40
1:AU:98:SER:HB2	1:BY:92:PHE:HB2	2.03	0.40
1:AZ:3:ILE:HG12	1:AZ:22:PRO:HB3	2.04	0.40
1:BH:117:ASN:HD21	1:CA:9:ALA:HB3	1.86	0.40
1:BK:116:ARG:NH2	1:CD:120:GLY:HA2	2.36	0.40
1:BN:31:PRO:HB3	1:BN:51:PHE:HB2	2.04	0.40
1:BN:41:SER:HB3	1:BP:101:TYR:OH	2.21	0.40
1:BS:65:ARG:HB3	1:BS:94:GLU:HG2	2.03	0.40
1:BY:50:MET:HA	1:BY:63:THR:O	2.22	0.40
1:CB:118:LEU:HA	1:CB:121:THR:HG23	2.03	0.40
1:CH:50:MET:HA	1:CH:63:THR:O	2.22	0.40
1:AA:41:SER:HB3	1:AC:101:TYR:OH	2.21	0.40
1:AD:121:THR:O	1:AD:125:THR:HG23	2.21	0.40
1:AF:118:LEU:HA	1:AF:121:THR:HG23	2.03	0.40
1:AI:20:PHE:HA	1:AI:35:LEU:O	2.21	0.40
1:AW:3:ILE:HG12	1:AW:22:PRO:HB3	2.04	0.40
1:AX:50:MET:HA	1:AX:63:THR:O	2.22	0.40
1:AY:31:PRO:HB3	1:AY:51:PHE:HB2	2.04	0.40
1:BA:3:ILE:N	1:CE:135:TRP:OXT	2.48	0.40
1:BB:31:PRO:HB3	1:BB:51:PHE:HB2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BH:121:THR:O	1:BH:125:THR:HG23	2.21	0.40
1:BK:121:THR:O	1:BK:125:THR:HG23	2.21	0.40
1:BM:65:ARG:HB3	1:BM:94:GLU:HG2	2.03	0.40
1:BP:24:GLN:HB3	1:BP:33:GLN:HG2	2.03	0.40
1:BQ:121:THR:O	1:BQ:125:THR:HG23	2.21	0.40
1:BW:31:PRO:HB3	1:BW:51:PHE:HB2	2.04	0.40
1:CA:3:ILE:HG12	1:CA:22:PRO:HB3	2.04	0.40
1:CF:118:LEU:HD12	1:CF:118:LEU:HA	1.87	0.40
1:CH:51:PHE:CE2	1:CH:53:LYS:HB2	2.55	0.40
1:AF:10:ASP:OD2	1:AF:12:GLN:NE2	2.54	0.40
1:AI:50:MET:HA	1:AI:63:THR:O	2.22	0.40
1:AM:101:TYR:HA	1:AN:42:ASN:HB2	2.02	0.40
1:AO:119:LEU:HD23	1:AO:119:LEU:HA	1.92	0.40
1:AP:41:SER:HB3	1:AR:101:TYR:OH	2.20	0.40
1:AP:52:VAL:HB	1:BF:133:PRO:HB3	2.03	0.40
1:AT:9:ALA:HB3	1:AY:117:ASN:ND2	2.37	0.40
1:AT:106:GLN:HE22	1:AY:12:GLN:HA	1.86	0.40
1:BH:125:THR:HG22	1:CA:112:LEU:HD21	2.04	0.40
1:BI:18:HIS:CE1	1:BI:46:ARG:HH12	2.40	0.40
1:BN:1:ALA:O	1:BU:134:ALA:HA	2.21	0.40
1:BP:65:ARG:HB3	1:BP:94:GLU:HG2	2.03	0.40
1:BS:50:MET:HA	1:BS:63:THR:O	2.22	0.40
1:BU:51:PHE:CE2	1:BU:53:LYS:HB2	2.57	0.40
1:BY:20:PHE:HA	1:BY:35:LEU:O	2.21	0.40
1:CD:101:TYR:CD1	1:CE:43:ILE:HD11	2.57	0.40

All (13) 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:AL:78:CYS:SG	1:BH:79:CYS:SG[3_555]	1.55	0.65
1:AN:78:CYS:SG	1:AT:79:CYS:SG[3_555]	1.76	0.44
1:AN:73:SER:OG	1:AS:102:GLY:O[3_555]	1.83	0.37
1:AN:114:TYR:OH	1:AS:46:ARG:NH1[3_555]	1.95	0.25
1:AN:46:ARG:NH1	1:AS:114:TYR:OH[3_555]	2.00	0.20
1:AL:106:GLN:NE2	1:BJ:11:GLY:O[3_555]	2.01	0.19
1:AZ:106:GLN:NE2	1:CC:11:GLY:O[2_555]	2.10	0.10
1:AV:11:GLY:O	1:BO:106:GLN:NE2[2_555]	2.12	0.08
1:BC:106:GLN:NE2	1:BQ:11:GLY:O[2_555]	2.12	0.08
1:AL:46:ARG:NH1	1:BJ:114:TYR:OH[3_555]	2.14	0.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AL:11:GLY:O	1:BJ:106:GLN:NE2[3_555]	2.15	0.05
1:AV:106:GLN:NE2	1:BO:11:GLY:O[2_555]	2.16	0.04
1:AM:120:GLY:O	1:CD:13:ALA:CB[12_555]	2.19	0.01

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	133/135 (98%)	131 (98%)	2 (2%)	0	100	100
1	AB	133/135 (98%)	130 (98%)	3 (2%)	0	100	100
1	AC	133/135 (98%)	132 (99%)	1 (1%)	0	100	100
1	AD	133/135 (98%)	131 (98%)	2 (2%)	0	100	100
1	AE	133/135 (98%)	130 (98%)	3 (2%)	0	100	100
1	AF	133/135 (98%)	132 (99%)	1 (1%)	0	100	100
1	AG	133/135 (98%)	131 (98%)	2 (2%)	0	100	100
1	AH	133/135 (98%)	130 (98%)	3 (2%)	0	100	100
1	AI	133/135 (98%)	132 (99%)	1 (1%)	0	100	100
1	AJ	133/135 (98%)	131 (98%)	2 (2%)	0	100	100
1	AK	133/135 (98%)	130 (98%)	3 (2%)	0	100	100
1	AL	133/135 (98%)	132 (99%)	1 (1%)	0	100	100
1	AM	133/135 (98%)	131 (98%)	2 (2%)	0	100	100
1	AN	133/135 (98%)	130 (98%)	3 (2%)	0	100	100
1	AO	133/135 (98%)	132 (99%)	1 (1%)	0	100	100
1	AP	133/135 (98%)	131 (98%)	2 (2%)	0	100	100
1	AQ	133/135 (98%)	130 (98%)	3 (2%)	0	100	100
1	AR	133/135 (98%)	132 (99%)	1 (1%)	0	100	100
1	AS	133/135 (98%)	131 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AT	133/135 (98%)	130 (98%)	3 (2%)	0	100	100
1	AU	133/135 (98%)	132 (99%)	1 (1%)	0	100	100
1	AV	133/135 (98%)	131 (98%)	2 (2%)	0	100	100
1	AW	133/135 (98%)	130 (98%)	3 (2%)	0	100	100
1	AX	133/135 (98%)	132 (99%)	1 (1%)	0	100	100
1	AY	133/135 (98%)	131 (98%)	2 (2%)	0	100	100
1	AZ	133/135 (98%)	130 (98%)	3 (2%)	0	100	100
1	BA	133/135 (98%)	132 (99%)	1 (1%)	0	100	100
1	BB	133/135 (98%)	131 (98%)	2 (2%)	0	100	100
1	BC	133/135 (98%)	130 (98%)	3 (2%)	0	100	100
1	BD	133/135 (98%)	132 (99%)	1 (1%)	0	100	100
1	BE	133/135 (98%)	131 (98%)	2 (2%)	0	100	100
1	BF	133/135 (98%)	130 (98%)	3 (2%)	0	100	100
1	BG	133/135 (98%)	132 (99%)	1 (1%)	0	100	100
1	BH	133/135 (98%)	131 (98%)	2 (2%)	0	100	100
1	BI	133/135 (98%)	130 (98%)	3 (2%)	0	100	100
1	BJ	133/135 (98%)	132 (99%)	1 (1%)	0	100	100
1	BK	133/135 (98%)	131 (98%)	2 (2%)	0	100	100
1	BL	133/135 (98%)	130 (98%)	3 (2%)	0	100	100
1	BM	133/135 (98%)	132 (99%)	1 (1%)	0	100	100
1	BN	133/135 (98%)	131 (98%)	2 (2%)	0	100	100
1	BO	133/135 (98%)	130 (98%)	3 (2%)	0	100	100
1	BP	133/135 (98%)	132 (99%)	1 (1%)	0	100	100
1	BQ	133/135 (98%)	131 (98%)	2 (2%)	0	100	100
1	BR	133/135 (98%)	130 (98%)	3 (2%)	0	100	100
1	BS	133/135 (98%)	132 (99%)	1 (1%)	0	100	100
1	BT	133/135 (98%)	131 (98%)	2 (2%)	0	100	100
1	BU	133/135 (98%)	130 (98%)	3 (2%)	0	100	100
1	BV	133/135 (98%)	132 (99%)	1 (1%)	0	100	100
1	BW	133/135 (98%)	131 (98%)	2 (2%)	0	100	100
1	BX	133/135 (98%)	130 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	BY	133/135 (98%)	132 (99%)	1 (1%)	0	100	100
1	BZ	133/135 (98%)	131 (98%)	2 (2%)	0	100	100
1	CA	133/135 (98%)	130 (98%)	3 (2%)	0	100	100
1	CB	133/135 (98%)	132 (99%)	1 (1%)	0	100	100
1	CC	133/135 (98%)	131 (98%)	2 (2%)	0	100	100
1	CD	133/135 (98%)	130 (98%)	3 (2%)	0	100	100
1	CE	133/135 (98%)	132 (99%)	1 (1%)	0	100	100
1	CF	133/135 (98%)	131 (98%)	2 (2%)	0	100	100
1	CG	133/135 (98%)	130 (98%)	3 (2%)	0	100	100
1	CH	133/135 (98%)	132 (99%)	1 (1%)	0	100	100
All	All	7980/8100 (98%)	7860 (98%)	120 (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	112/112 (100%)	112 (100%)	0	100	100
1	AB	112/112 (100%)	112 (100%)	0	100	100
1	AC	112/112 (100%)	112 (100%)	0	100	100
1	AD	112/112 (100%)	112 (100%)	0	100	100
1	AE	112/112 (100%)	112 (100%)	0	100	100
1	AF	112/112 (100%)	112 (100%)	0	100	100
1	AG	112/112 (100%)	112 (100%)	0	100	100
1	AH	112/112 (100%)	112 (100%)	0	100	100
1	AI	112/112 (100%)	112 (100%)	0	100	100
1	AJ	112/112 (100%)	112 (100%)	0	100	100
1	AK	112/112 (100%)	112 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AL	112/112 (100%)	112 (100%)	0	100	100
1	AM	112/112 (100%)	112 (100%)	0	100	100
1	AN	112/112 (100%)	112 (100%)	0	100	100
1	AO	112/112 (100%)	112 (100%)	0	100	100
1	AP	112/112 (100%)	112 (100%)	0	100	100
1	AQ	112/112 (100%)	112 (100%)	0	100	100
1	AR	112/112 (100%)	112 (100%)	0	100	100
1	AS	112/112 (100%)	112 (100%)	0	100	100
1	AT	112/112 (100%)	112 (100%)	0	100	100
1	AU	112/112 (100%)	112 (100%)	0	100	100
1	AV	112/112 (100%)	112 (100%)	0	100	100
1	AW	112/112 (100%)	112 (100%)	0	100	100
1	AX	112/112 (100%)	112 (100%)	0	100	100
1	AY	112/112 (100%)	112 (100%)	0	100	100
1	AZ	112/112 (100%)	112 (100%)	0	100	100
1	BA	112/112 (100%)	112 (100%)	0	100	100
1	BB	112/112 (100%)	112 (100%)	0	100	100
1	BC	112/112 (100%)	112 (100%)	0	100	100
1	BD	112/112 (100%)	112 (100%)	0	100	100
1	BE	112/112 (100%)	112 (100%)	0	100	100
1	BF	112/112 (100%)	112 (100%)	0	100	100
1	BG	112/112 (100%)	112 (100%)	0	100	100
1	BH	112/112 (100%)	112 (100%)	0	100	100
1	BI	112/112 (100%)	112 (100%)	0	100	100
1	BJ	112/112 (100%)	112 (100%)	0	100	100
1	BK	112/112 (100%)	112 (100%)	0	100	100
1	BL	112/112 (100%)	112 (100%)	0	100	100
1	BM	112/112 (100%)	112 (100%)	0	100	100
1	BN	112/112 (100%)	112 (100%)	0	100	100
1	BO	112/112 (100%)	112 (100%)	0	100	100
1	BP	112/112 (100%)	112 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	BQ	112/112 (100%)	112 (100%)	0	100	100
1	BR	112/112 (100%)	112 (100%)	0	100	100
1	BS	112/112 (100%)	112 (100%)	0	100	100
1	BT	112/112 (100%)	112 (100%)	0	100	100
1	BU	112/112 (100%)	112 (100%)	0	100	100
1	BV	112/112 (100%)	112 (100%)	0	100	100
1	BW	112/112 (100%)	112 (100%)	0	100	100
1	BX	112/112 (100%)	112 (100%)	0	100	100
1	BY	112/112 (100%)	112 (100%)	0	100	100
1	BZ	112/112 (100%)	112 (100%)	0	100	100
1	CA	112/112 (100%)	112 (100%)	0	100	100
1	CB	112/112 (100%)	112 (100%)	0	100	100
1	CC	112/112 (100%)	112 (100%)	0	100	100
1	CD	112/112 (100%)	112 (100%)	0	100	100
1	CE	112/112 (100%)	112 (100%)	0	100	100
1	CF	112/112 (100%)	112 (100%)	0	100	100
1	CG	112/112 (100%)	112 (100%)	0	100	100
1	CH	112/112 (100%)	112 (100%)	0	100	100
All	All	6720/6720 (100%)	6720 (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 (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	AA	117	ASN
1	AB	106	GLN
1	AC	107	ASN
1	AE	106	GLN
1	AF	107	ASN
1	AH	106	GLN
1	AI	107	ASN
1	AI	117	ASN
1	AK	106	GLN
1	AM	117	ASN

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Mol	Chain	Res	Type
1	AO	107	ASN
1	AQ	106	GLN
1	AR	107	ASN
1	AR	117	ASN
1	AT	106	GLN
1	AU	107	ASN
1	AW	106	GLN
1	AX	107	ASN
1	AX	117	ASN
1	BA	107	ASN
1	BA	117	ASN
1	BD	107	ASN
1	BD	117	ASN
1	BF	106	GLN
1	BG	107	ASN
1	BH	117	ASN
1	BI	106	GLN
1	BL	106	GLN
1	BL	117	ASN
1	BM	107	ASN
1	BP	107	ASN
1	BR	106	GLN
1	BS	107	ASN
1	BS	117	ASN
1	BU	106	GLN
1	BV	107	ASN
1	BV	117	ASN
1	BX	106	GLN
1	BY	107	ASN
1	BZ	117	ASN
1	CA	106	GLN
1	CB	107	ASN
1	CD	106	GLN
1	CE	107	ASN
1	CE	117	ASN
1	CG	106	GLN
1	CH	107	ASN
1	CH	117	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

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	135/135 (100%)	-0.41	0 100 100	87, 131, 205, 282	0
1	AB	135/135 (100%)	-0.36	0 100 100	92, 130, 161, 181	0
1	AC	135/135 (100%)	-0.20	0 100 100	97, 138, 196, 233	0
1	AD	135/135 (100%)	-0.34	1 (0%) 87 83	87, 131, 205, 282	0
1	AE	135/135 (100%)	-0.39	0 100 100	92, 130, 161, 181	0
1	AF	135/135 (100%)	-0.27	0 100 100	97, 138, 196, 233	0
1	AG	135/135 (100%)	-0.30	1 (0%) 87 83	87, 131, 205, 282	0
1	AH	135/135 (100%)	-0.37	0 100 100	92, 130, 161, 181	0
1	AI	135/135 (100%)	-0.26	0 100 100	97, 138, 196, 233	0
1	AJ	135/135 (100%)	-0.01	2 (1%) 73 66	87, 131, 205, 282	0
1	AK	135/135 (100%)	-0.42	0 100 100	92, 130, 161, 181	0
1	AL	135/135 (100%)	-0.15	1 (0%) 87 83	97, 138, 196, 233	0
1	AM	135/135 (100%)	-0.10	1 (0%) 87 83	87, 131, 205, 282	0
1	AN	135/135 (100%)	-0.35	0 100 100	92, 130, 161, 181	0
1	AO	135/135 (100%)	-0.16	0 100 100	97, 138, 196, 233	0
1	AP	135/135 (100%)	-0.32	3 (2%) 62 54	87, 131, 205, 282	0
1	AQ	135/135 (100%)	-0.44	0 100 100	92, 130, 161, 181	0
1	AR	135/135 (100%)	-0.33	0 100 100	97, 138, 196, 233	0
1	AS	135/135 (100%)	-0.25	2 (1%) 73 66	87, 131, 205, 282	0
1	AT	135/135 (100%)	-0.26	0 100 100	92, 130, 161, 181	0
1	AU	135/135 (100%)	-0.21	0 100 100	97, 138, 196, 233	0
1	AV	135/135 (100%)	-0.29	1 (0%) 87 83	87, 131, 205, 282	0
1	AW	135/135 (100%)	-0.34	0 100 100	92, 130, 161, 181	0
1	AX	135/135 (100%)	-0.32	0 100 100	97, 138, 196, 233	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	AY	135/135 (100%)	-0.28	1 (0%) 87 83	87, 131, 205, 282	0
1	AZ	135/135 (100%)	-0.28	1 (0%) 87 83	92, 130, 161, 181	0
1	BA	135/135 (100%)	-0.15	0 100 100	97, 138, 196, 233	0
1	BB	135/135 (100%)	-0.42	1 (0%) 87 83	87, 131, 205, 282	0
1	BC	135/135 (100%)	-0.51	0 100 100	92, 130, 161, 181	0
1	BD	135/135 (100%)	-0.27	0 100 100	97, 138, 196, 233	0
1	BE	135/135 (100%)	-0.47	1 (0%) 87 83	87, 131, 205, 282	0
1	BF	135/135 (100%)	-0.53	0 100 100	92, 130, 161, 181	0
1	BG	135/135 (100%)	-0.35	0 100 100	97, 138, 196, 233	0
1	BH	135/135 (100%)	-0.22	1 (0%) 87 83	87, 131, 205, 282	0
1	BI	135/135 (100%)	-0.33	0 100 100	92, 130, 161, 181	0
1	BJ	135/135 (100%)	-0.23	0 100 100	97, 138, 196, 233	0
1	BK	135/135 (100%)	-0.28	0 100 100	87, 131, 205, 282	0
1	BL	135/135 (100%)	-0.24	0 100 100	92, 130, 161, 181	0
1	BM	135/135 (100%)	-0.29	0 100 100	97, 138, 196, 233	0
1	BN	135/135 (100%)	-0.34	2 (1%) 73 66	87, 131, 205, 282	0
1	BO	135/135 (100%)	-0.44	0 100 100	92, 130, 161, 181	0
1	BP	135/135 (100%)	-0.07	1 (0%) 87 83	97, 138, 196, 233	0
1	BQ	135/135 (100%)	-0.44	0 100 100	87, 131, 205, 282	0
1	BR	135/135 (100%)	-0.51	0 100 100	92, 130, 161, 181	0
1	BS	135/135 (100%)	-0.32	0 100 100	97, 138, 196, 233	0
1	BT	135/135 (100%)	-0.36	1 (0%) 87 83	87, 131, 205, 282	0
1	BU	135/135 (100%)	-0.50	0 100 100	92, 130, 161, 181	0
1	BV	135/135 (100%)	-0.37	0 100 100	97, 138, 196, 233	0
1	BW	135/135 (100%)	-0.21	1 (0%) 87 83	87, 131, 205, 282	0
1	BX	135/135 (100%)	-0.60	0 100 100	92, 130, 161, 181	0
1	BY	135/135 (100%)	-0.19	0 100 100	97, 138, 196, 233	0
1	BZ	135/135 (100%)	-0.24	1 (0%) 87 83	87, 131, 205, 282	0
1	CA	135/135 (100%)	-0.20	0 100 100	92, 130, 161, 181	0
1	CB	135/135 (100%)	-0.27	0 100 100	97, 138, 196, 233	0
1	CC	135/135 (100%)	-0.13	2 (1%) 73 66	87, 131, 205, 282	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	CD	135/135 (100%)	-0.27	0 100 100	92, 130, 161, 181	0
1	CE	135/135 (100%)	-0.27	0 100 100	97, 138, 196, 233	0
1	CF	135/135 (100%)	-0.37	1 (0%) 87 83	87, 131, 205, 282	0
1	CG	135/135 (100%)	-0.41	0 100 100	92, 130, 161, 181	0
1	CH	135/135 (100%)	-0.38	0 100 100	97, 138, 196, 233	0
All	All	8100/8100 (100%)	-0.31	26 (0%) 94 91	87, 133, 181, 282	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AP	83	ASN	6.2
1	AJ	83	ASN	5.9
1	AS	83	ASN	5.2
1	BN	83	ASN	4.9
1	CC	83	ASN	4.1
1	BZ	83	ASN	3.9
1	AJ	82	THR	3.6
1	BB	83	ASN	3.5
1	BW	83	ASN	3.4
1	AD	83	ASN	3.3
1	BT	83	ASN	3.2
1	AM	83	ASN	3.2
1	AY	83	ASN	3.1
1	AG	83	ASN	3.0
1	AP	82	THR	2.8
1	BH	83	ASN	2.7
1	CF	83	ASN	2.6
1	AP	81	ASP	2.6
1	BN	82	THR	2.4
1	BP	91	THR	2.3
1	BE	83	ASN	2.2
1	AV	83	ASN	2.2
1	CC	82	THR	2.1
1	AZ	114	TYR	2.1
1	AS	81	ASP	2.0
1	AL	91	THR	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 monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.