Full wwPDB X-ray Structure Validation Report ⓘ

Feb 10, 2022 – 09:04 am GMT

PDB ID	:	6YFL
Title	:	Virus-like particle of bacteriophage ESE020
Authors	:	Rumnieks, J.; Kalnins, G.; Sisovs, M.; Lieknina, I.; Tars, K.
Deposited on	:	2020-03-26
Resolution	:	3.30 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:

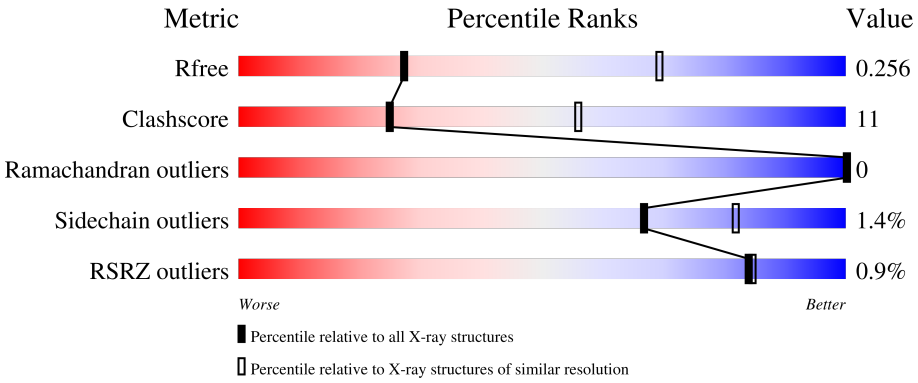
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.26
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 3.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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

Mol	Chain	Length	Quality of chain
1	AA	153	4% 70% 22% 8%
1	AB	153	% 69% 31%
1	AC	153	2% 75% 25%
1	AD	153	70% 22% 8%
1	AE	153	% 69% 31%

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Mol	Chain	Length	Quality of chain
1	AF	153	76% 24%
1	AG	153	67% 25% 8%
1	AH	153	71% 29%
1	AI	153	82% 18%
1	AJ	153	72% 20% 8%
1	AK	153	65% 35%
1	AL	153	73% 27%
1	AM	153	75% 17% 8%
1	AN	153	70% 30%
1	AO	153	75% 25%
1	AP	153	69% 24% 8%
1	AQ	153	5% 72% 28%
1	AR	153	72% 28%
1	AS	153	70% 22% 8%
1	AT	153	76% 24%
1	AU	153	76% 24%
1	AV	153	6% 71% 22% 8%
1	AW	153	72% 28%
1	AX	153	6% 71% 29%
1	AY	153	67% 25% 8%
1	AZ	153	59% 41%
1	BA	153	70% 30%
1	BB	153	68% 24% 8%
1	BC	153	67% 33%
1	BD	153	71% 29%

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Mol	Chain	Length	Quality of chain
1	BE	153	69% 23% 8%
1	BF	153	78% 22%
1	BG	153	75% 25%
1	BH	153	65% 27% 8%
1	BI	153	67% 33%
1	BJ	153	76% 24%
1	BK	153	78% 14% 8%
1	BL	153	70% 30%
1	BM	153	71% 29%
1	BN	153	69% 24% 8%
1	BO	153	77% 23%
1	BP	153	75% 25%
1	BQ	153	71% 21% 8%
1	BR	153	75% 25%
1	BS	153	74% 26%
1	BT	153	79% 13% 8%
1	BU	153	73% 27%
1	BV	153	76% 24%
1	BW	153	67% 25% 8%
1	BX	153	67% 33%
1	BY	153	73% 27%
1	BZ	153	75% 17% 8%
1	CA	153	69% 31%
1	CB	153	71% 29%
1	CC	153	60% 32% 8%

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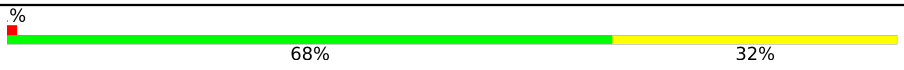
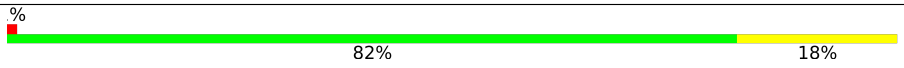
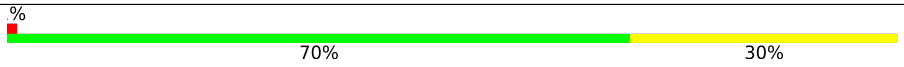
Mol	Chain	Length	Quality of chain
1	CD	153	
1	CE	153	
1	CF	153	
1	CG	153	
1	CH	153	

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 63520 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	141	Total	C	N	O	S	0	0	0
			1004	628	172	202	2			
1	AB	153	Total	C	N	O	S	0	0	0
			1086	678	187	219	2			
1	AC	153	Total	C	N	O	S	0	0	0
			1086	678	187	219	2			
1	AD	141	Total	C	N	O	S	0	0	0
			1004	628	172	202	2			
1	AE	153	Total	C	N	O	S	0	0	0
			1086	678	187	219	2			
1	AF	153	Total	C	N	O	S	0	0	0
			1086	678	187	219	2			
1	AG	141	Total	C	N	O	S	0	0	0
			1004	628	172	202	2			
1	AH	153	Total	C	N	O	S	0	0	0
			1086	678	187	219	2			
1	AI	153	Total	C	N	O	S	0	0	0
			1086	678	187	219	2			
1	AJ	141	Total	C	N	O	S	0	0	0
			1004	628	172	202	2			
1	AK	153	Total	C	N	O	S	0	0	0
			1086	678	187	219	2			
1	AL	153	Total	C	N	O	S	0	0	0
			1086	678	187	219	2			
1	AM	141	Total	C	N	O	S	0	0	0
			1004	628	172	202	2			
1	AN	153	Total	C	N	O	S	0	0	0
			1086	678	187	219	2			
1	AO	153	Total	C	N	O	S	0	0	0
			1086	678	187	219	2			
1	AP	141	Total	C	N	O	S	0	0	0
			1004	628	172	202	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AQ	153	Total	C	N	O	S	0	0	0
			1086	678	187	219	2			
1	AR	153	Total	C	N	O	S	0	0	0
			1086	678	187	219	2			
1	AS	141	Total	C	N	O	S	0	0	0
			1004	628	172	202	2			
1	AT	153	Total	C	N	O	S	0	0	0
			1086	678	187	219	2			
1	AU	153	Total	C	N	O	S	0	0	0
			1086	678	187	219	2			
1	AV	141	Total	C	N	O	S	0	0	0
			1004	628	172	202	2			
1	AW	153	Total	C	N	O	S	0	0	0
			1086	678	187	219	2			
1	AX	153	Total	C	N	O	S	0	0	0
			1086	678	187	219	2			
1	AY	141	Total	C	N	O	S	0	0	0
			1004	628	172	202	2			
1	AZ	153	Total	C	N	O	S	0	0	0
			1086	678	187	219	2			
1	BA	153	Total	C	N	O	S	0	0	0
			1086	678	187	219	2			
1	BB	141	Total	C	N	O	S	0	0	0
			1004	628	172	202	2			
1	BC	153	Total	C	N	O	S	0	0	0
			1086	678	187	219	2			
1	BD	153	Total	C	N	O	S	0	0	0
			1086	678	187	219	2			
1	BE	141	Total	C	N	O	S	0	0	0
			1004	628	172	202	2			
1	BF	153	Total	C	N	O	S	0	0	0
			1086	678	187	219	2			
1	BG	153	Total	C	N	O	S	0	0	0
			1086	678	187	219	2			
1	BH	141	Total	C	N	O	S	0	0	0
			1004	628	172	202	2			
1	BI	153	Total	C	N	O	S	0	0	0
			1086	678	187	219	2			
1	BJ	153	Total	C	N	O	S	0	0	0
			1086	678	187	219	2			
1	BK	141	Total	C	N	O	S	0	0	0
			1004	628	172	202	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	BL	153	Total	C	N	O	S	0	0	0
			1086	678	187	219	2			
1	BM	153	Total	C	N	O	S	0	0	0
			1086	678	187	219	2			
1	BN	141	Total	C	N	O	S	0	0	0
			1004	628	172	202	2			
1	BO	153	Total	C	N	O	S	0	0	0
			1086	678	187	219	2			
1	BP	153	Total	C	N	O	S	0	0	0
			1086	678	187	219	2			
1	BQ	141	Total	C	N	O	S	0	0	0
			1004	628	172	202	2			
1	BR	153	Total	C	N	O	S	0	0	0
			1086	678	187	219	2			
1	BS	153	Total	C	N	O	S	0	0	0
			1086	678	187	219	2			
1	BT	141	Total	C	N	O	S	0	0	0
			1004	628	172	202	2			
1	BU	153	Total	C	N	O	S	0	0	0
			1086	678	187	219	2			
1	BV	153	Total	C	N	O	S	0	0	0
			1086	678	187	219	2			
1	BW	141	Total	C	N	O	S	0	0	0
			1004	628	172	202	2			
1	BX	153	Total	C	N	O	S	0	0	0
			1086	678	187	219	2			
1	BY	153	Total	C	N	O	S	0	0	0
			1086	678	187	219	2			
1	BZ	141	Total	C	N	O	S	0	0	0
			1004	628	172	202	2			
1	CA	153	Total	C	N	O	S	0	0	0
			1086	678	187	219	2			
1	CB	153	Total	C	N	O	S	0	0	0
			1086	678	187	219	2			
1	CC	141	Total	C	N	O	S	0	0	0
			1004	628	172	202	2			
1	CD	153	Total	C	N	O	S	0	0	0
			1086	678	187	219	2			
1	CE	153	Total	C	N	O	S	0	0	0
			1086	678	187	219	2			
1	CF	141	Total	C	N	O	S	0	0	0
			1004	628	172	202	2			

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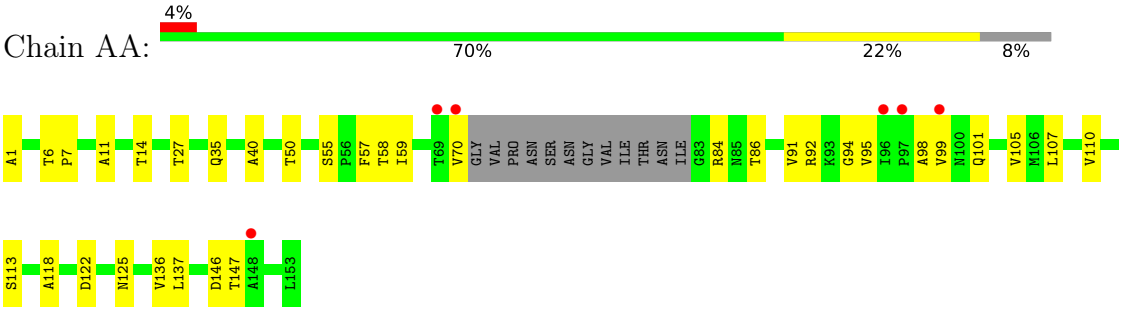
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	CG	153	Total	C	N	O	S	0	0	0
			1086	678	187	219	2			
1	CH	153	Total	C	N	O	S	0	0	0
			1086	678	187	219	2			

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.

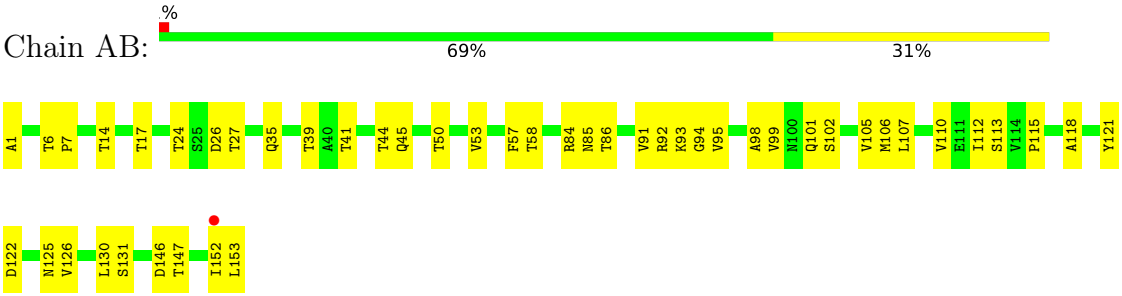
- Molecule 1: coat protein

Chain AA:



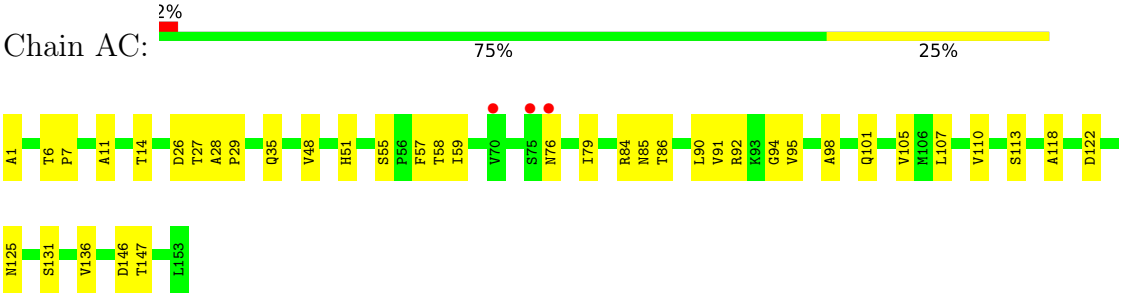
- Molecule 1: coat protein

Chain AB:



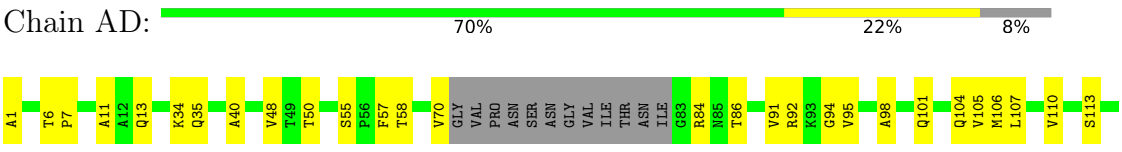
- Molecule 1: coat protein

Chain AC:



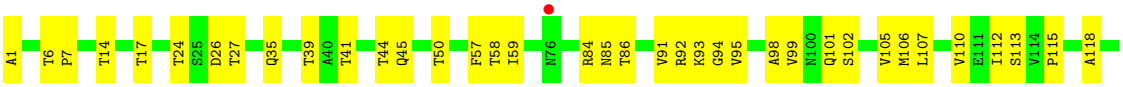
- Molecule 1: coat protein

Chain AD:



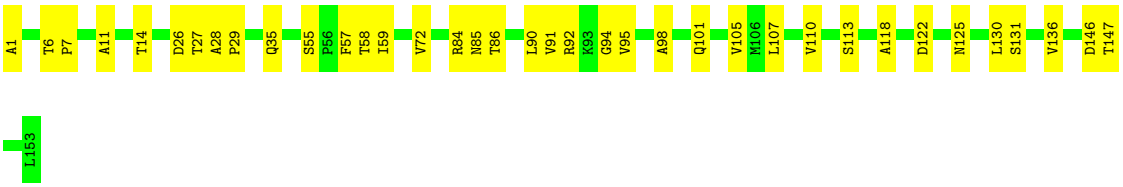
• Molecule 1: coat protein

Chain AE:



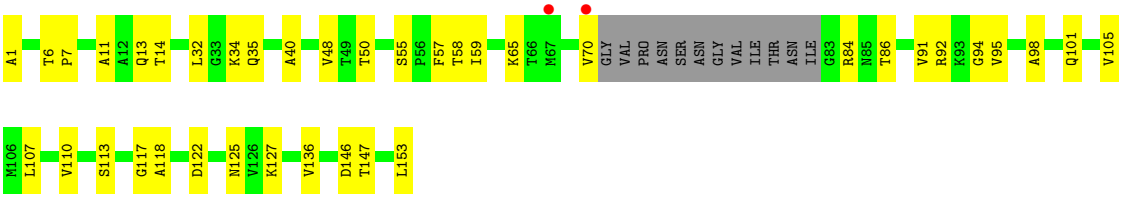
• Molecule 1: coat protein

Chain AF:



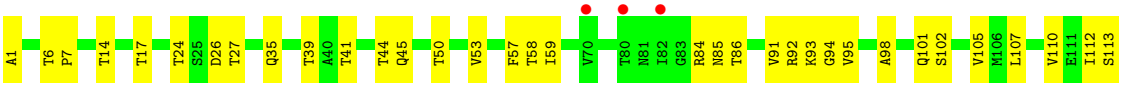
• Molecule 1: coat protein

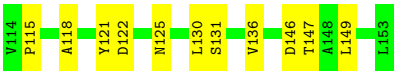
Chain AG:



• Molecule 1: coat protein

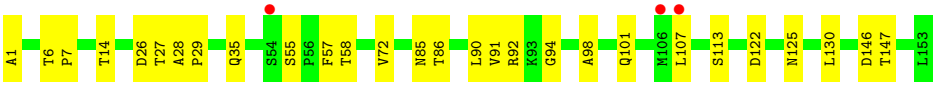
Chain AH:





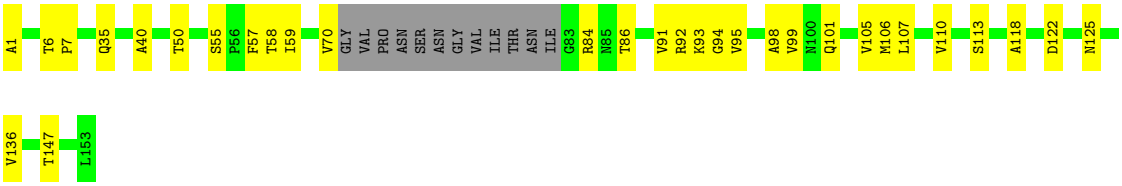
• Molecule 1: coat protein

Chain AI:



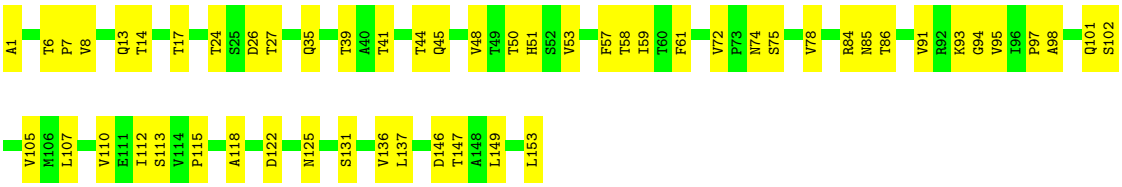
• Molecule 1: coat protein

Chain AJ:



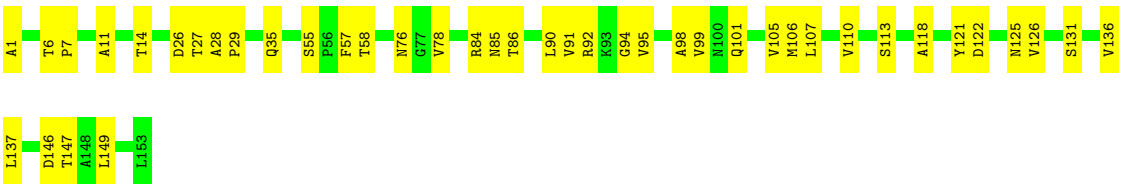
• Molecule 1: coat protein

Chain AK:



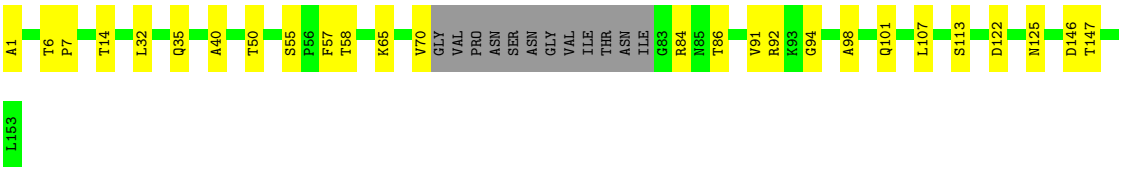
• Molecule 1: coat protein

Chain AL:



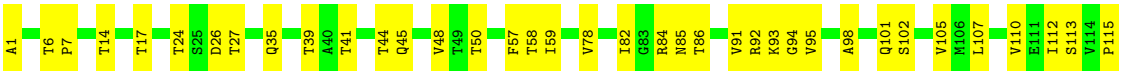
• Molecule 1: coat protein

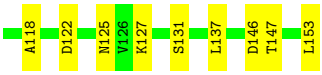
Chain AM:



• Molecule 1: coat protein

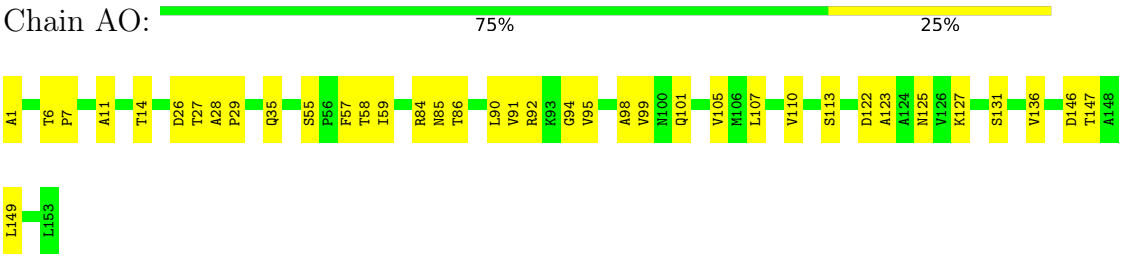
Chain AN:





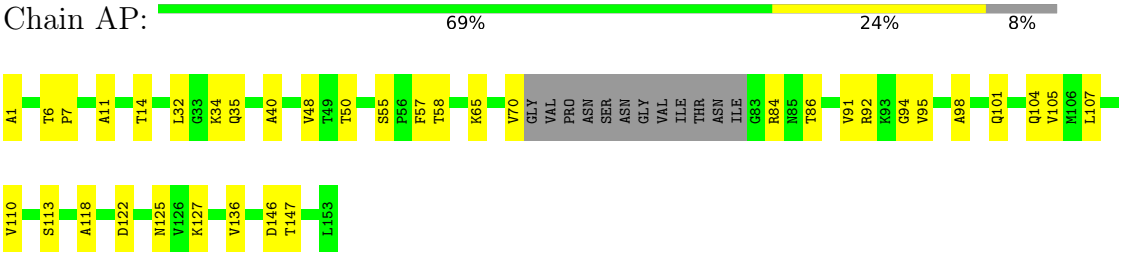
• Molecule 1: coat protein

Chain AO:



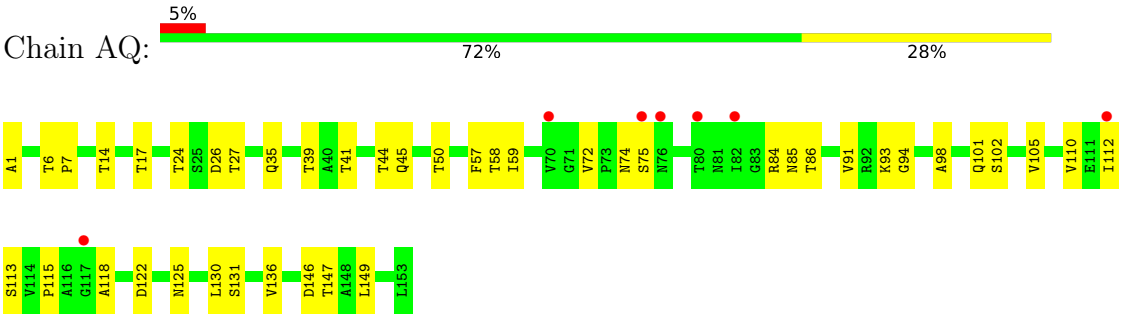
• Molecule 1: coat protein

Chain AP:



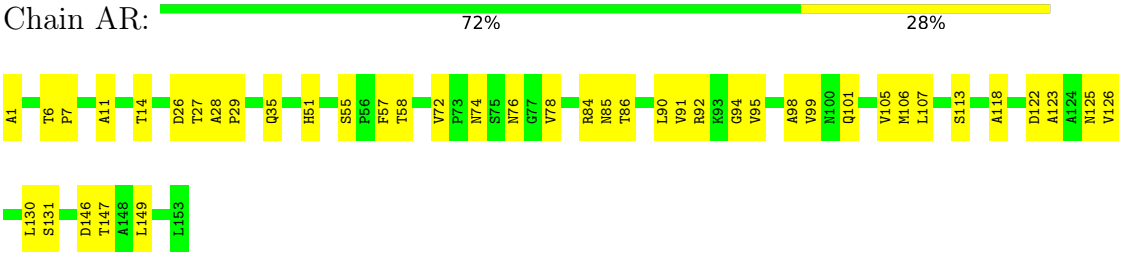
• Molecule 1: coat protein

Chain AQ:



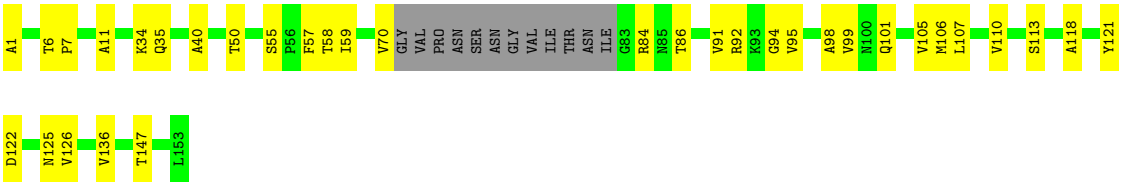
• Molecule 1: coat protein

Chain AR:



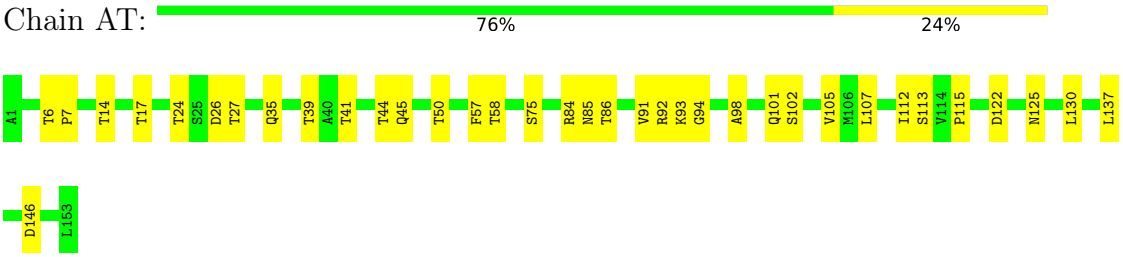
• Molecule 1: coat protein

Chain AS:



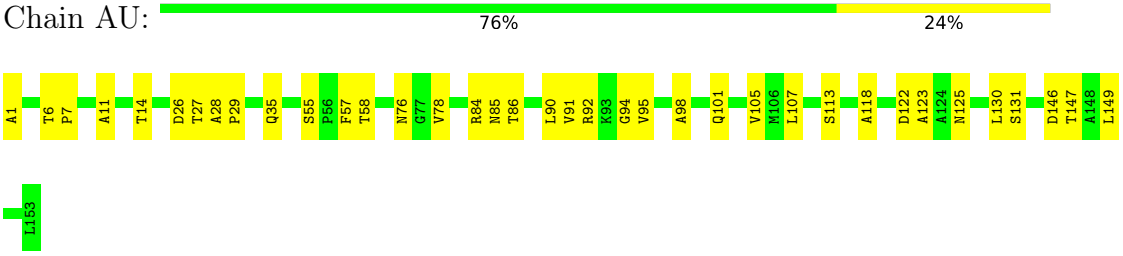
• Molecule 1: coat protein

Chain AT:



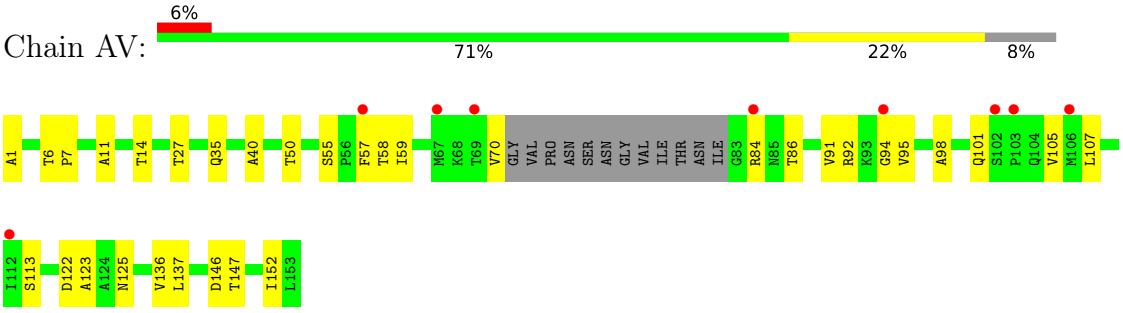
• Molecule 1: coat protein

Chain AU:



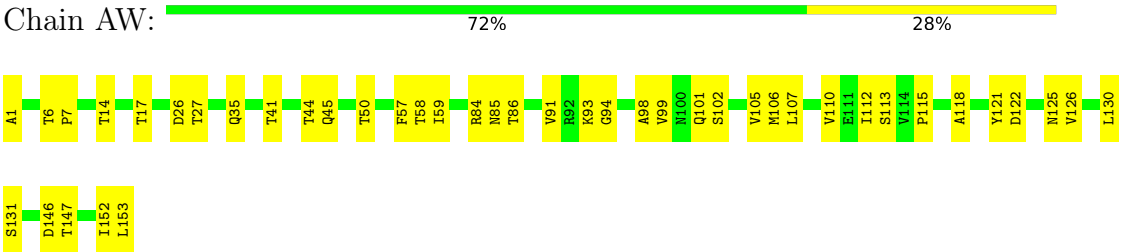
• Molecule 1: coat protein

Chain AV:



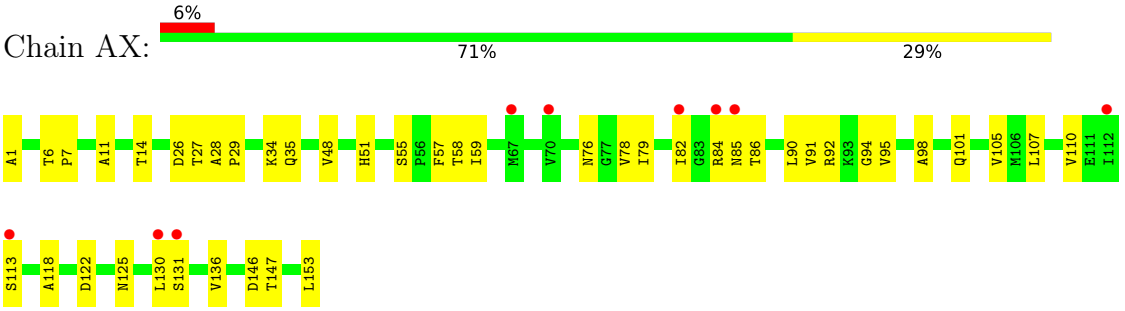
• Molecule 1: coat protein

Chain AW:



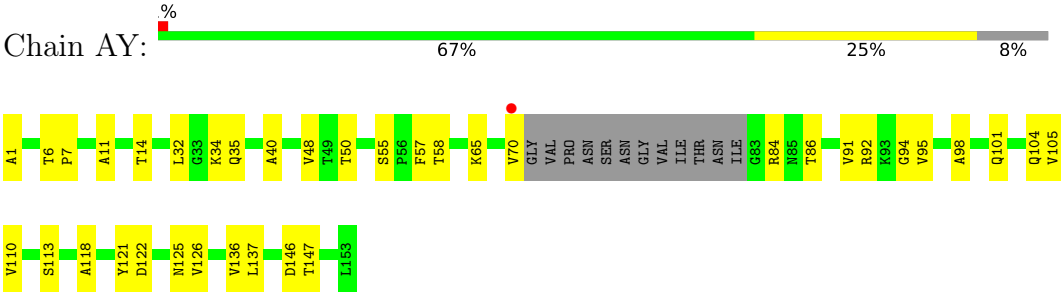
• Molecule 1: coat protein

Chain AX:



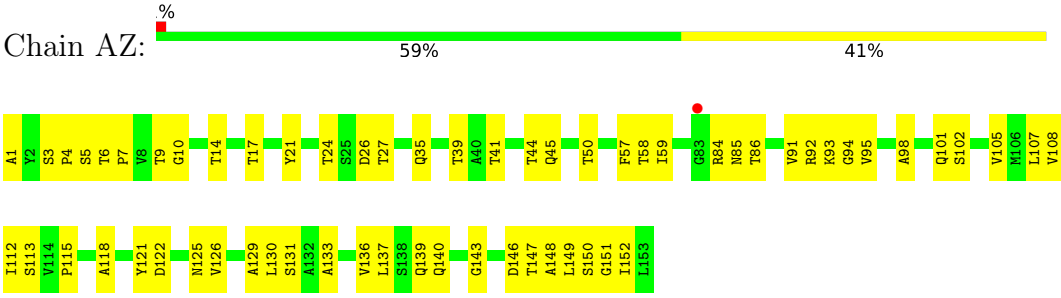
• Molecule 1: coat protein

Chain AY:



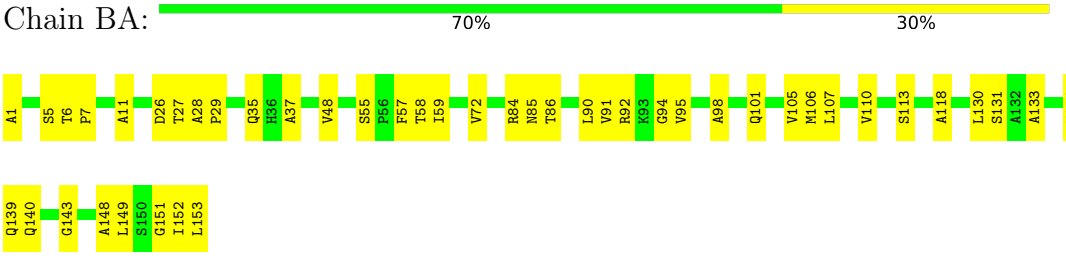
• Molecule 1: coat protein

Chain AZ:



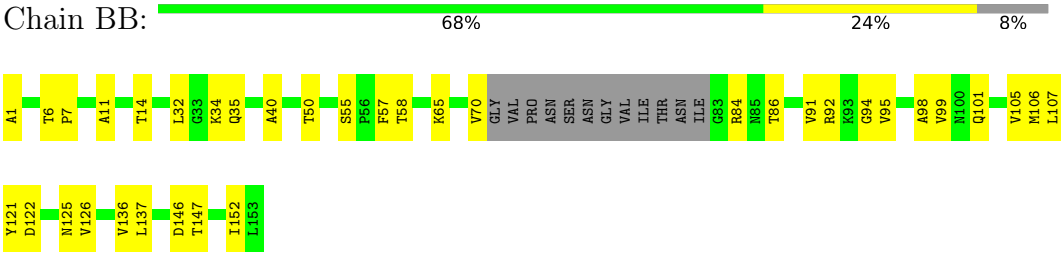
• Molecule 1: coat protein

Chain BA:



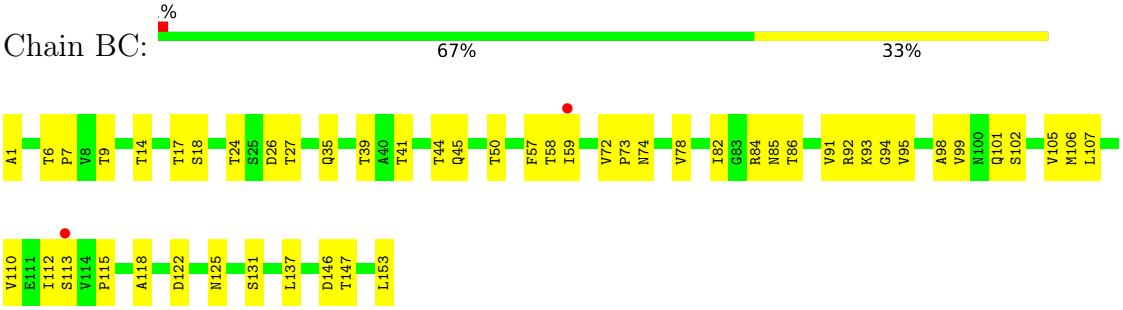
• Molecule 1: coat protein

Chain BB:



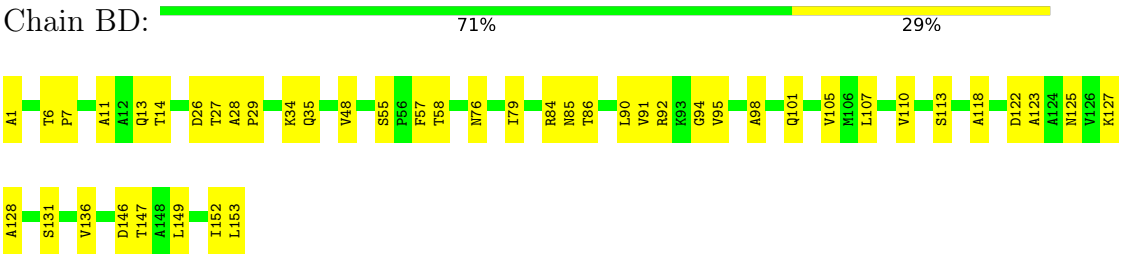
• Molecule 1: coat protein

Chain BC:



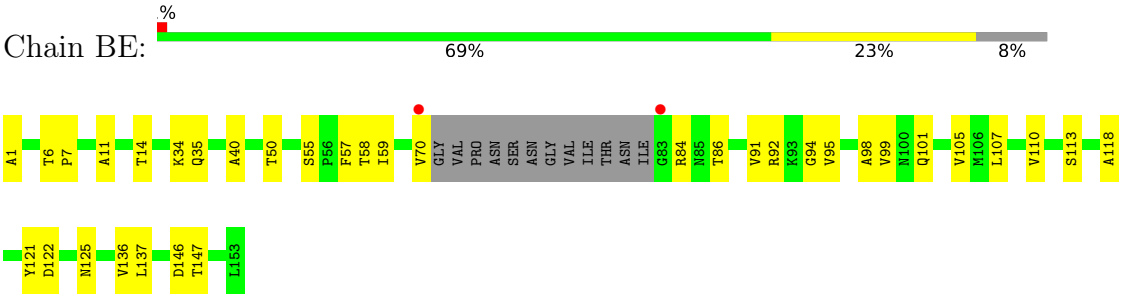
• Molecule 1: coat protein

Chain BD:



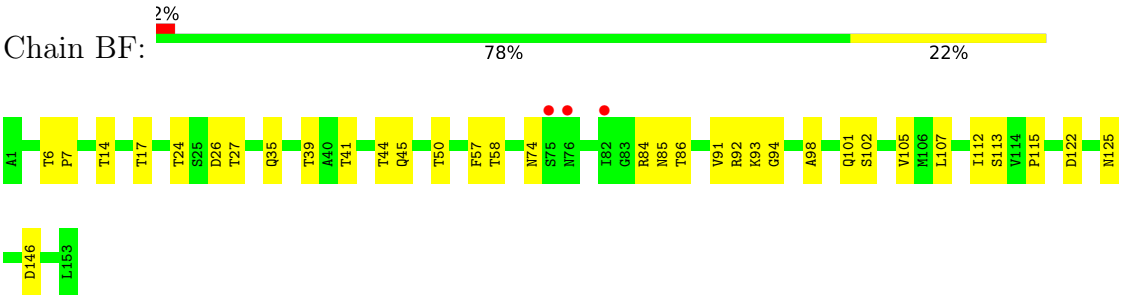
• Molecule 1: coat protein

Chain BE:



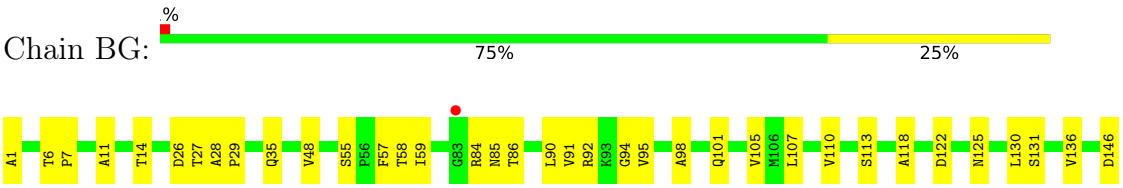
• Molecule 1: coat protein

Chain BF:



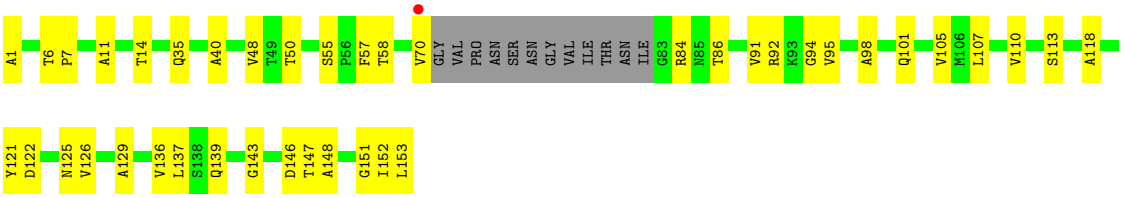
• Molecule 1: coat protein

Chain BG:



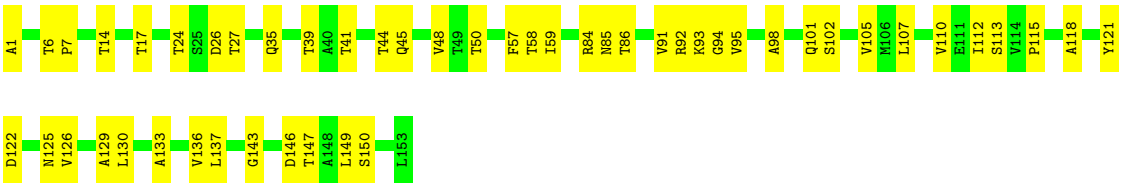
• Molecule 1: coat protein

Chain BH:



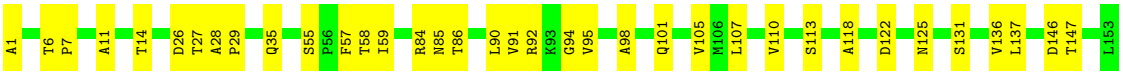
• Molecule 1: coat protein

Chain BI:



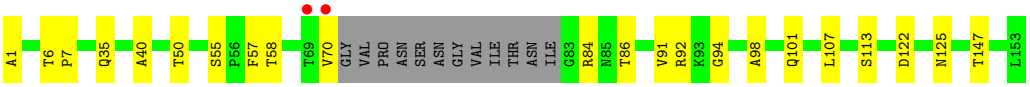
• Molecule 1: coat protein

Chain BJ:



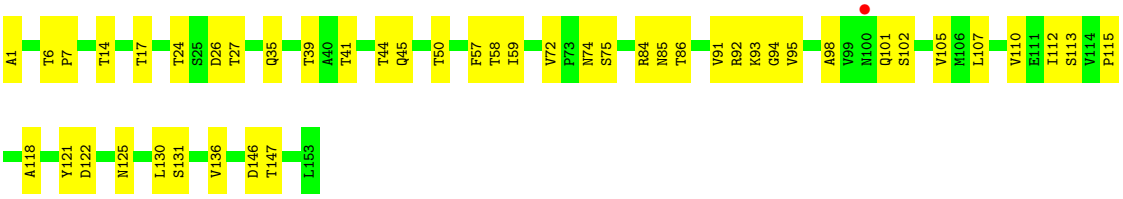
• Molecule 1: coat protein

Chain BK:



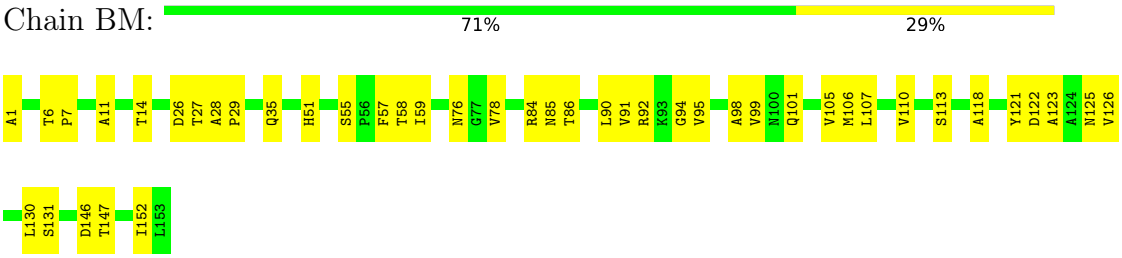
• Molecule 1: coat protein

Chain BL:



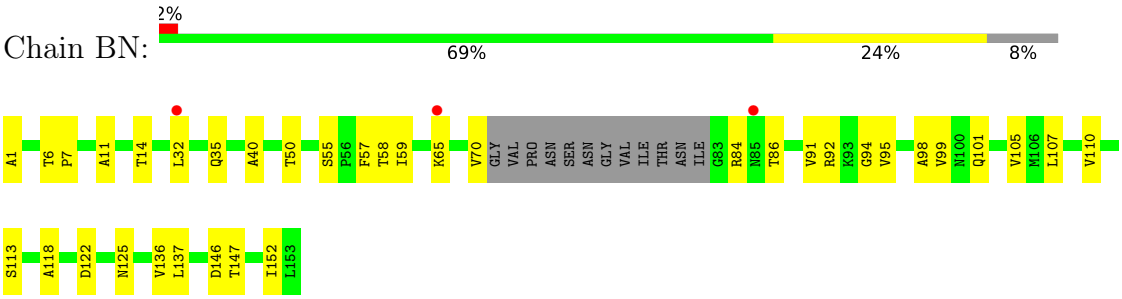
• Molecule 1: coat protein

Chain BM:



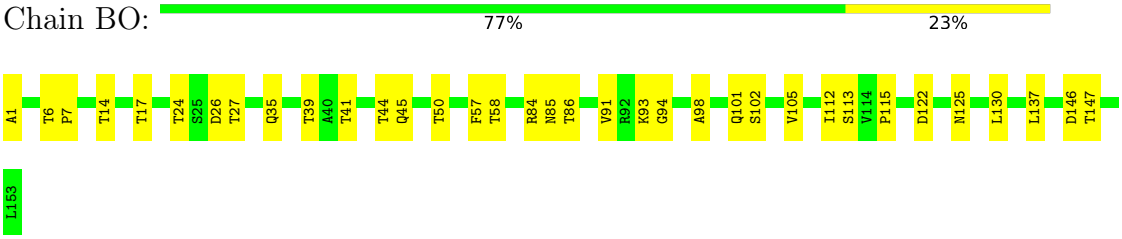
• Molecule 1: coat protein

Chain BN:



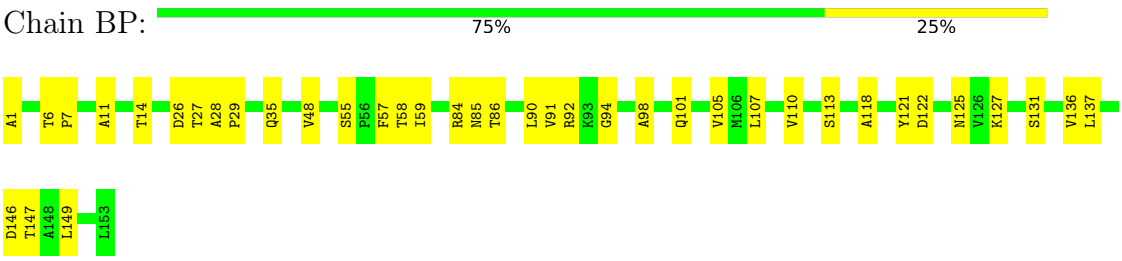
• Molecule 1: coat protein

Chain BO:



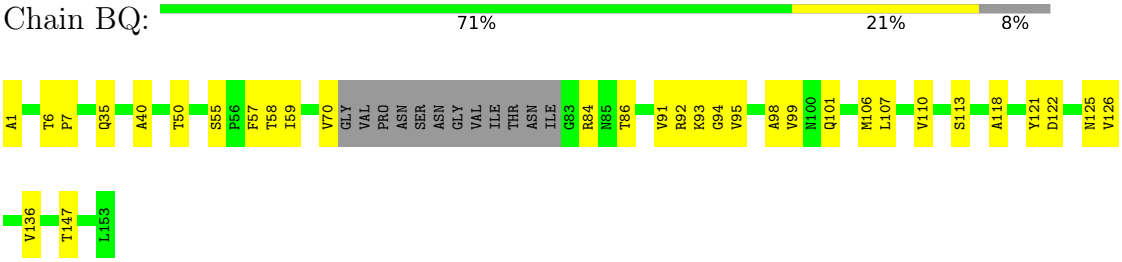
• Molecule 1: coat protein

Chain BP:



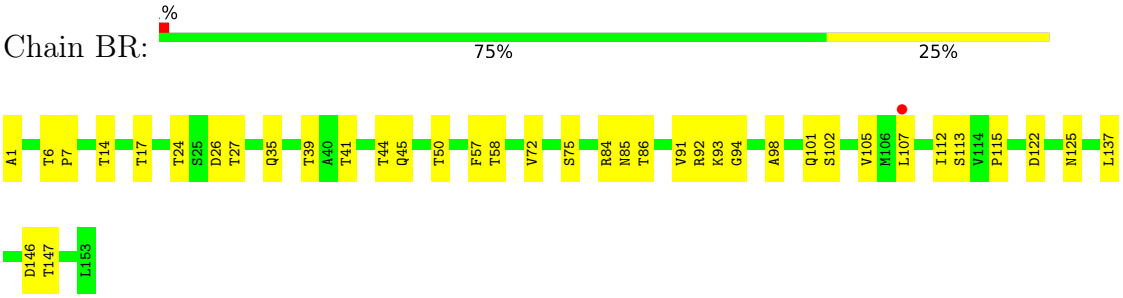
• Molecule 1: coat protein

Chain BQ:



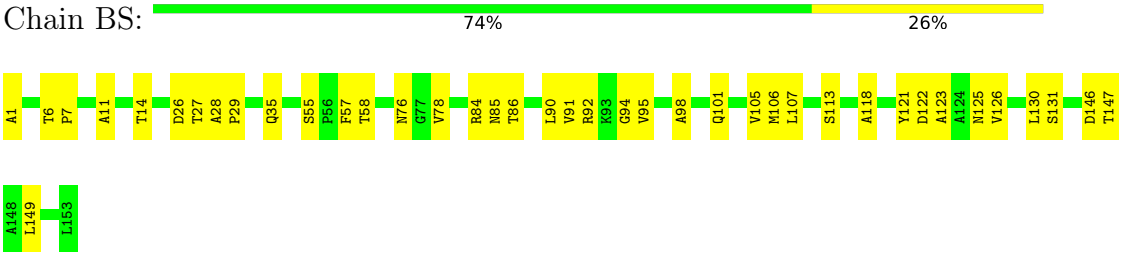
• Molecule 1: coat protein

Chain BR:



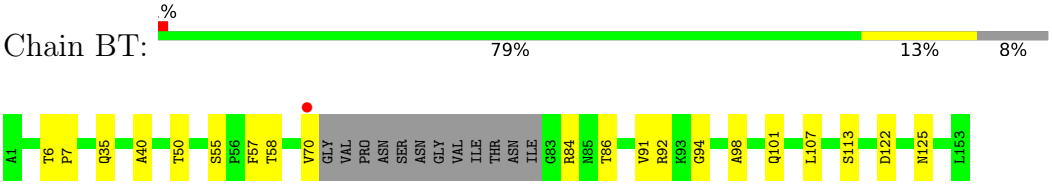
• Molecule 1: coat protein

Chain BS:



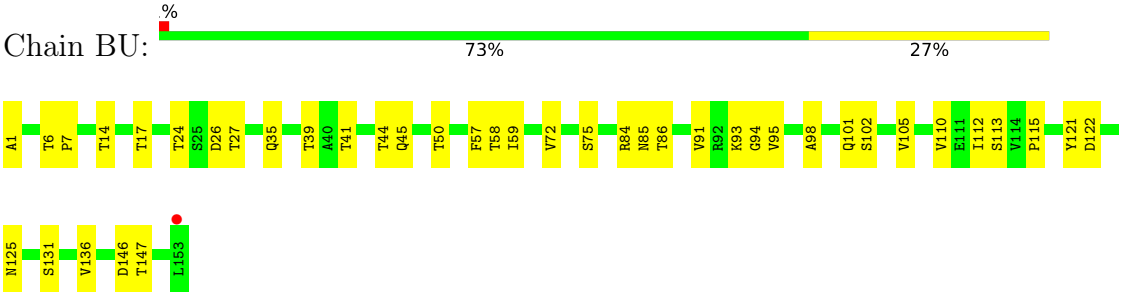
• Molecule 1: coat protein

Chain BT:



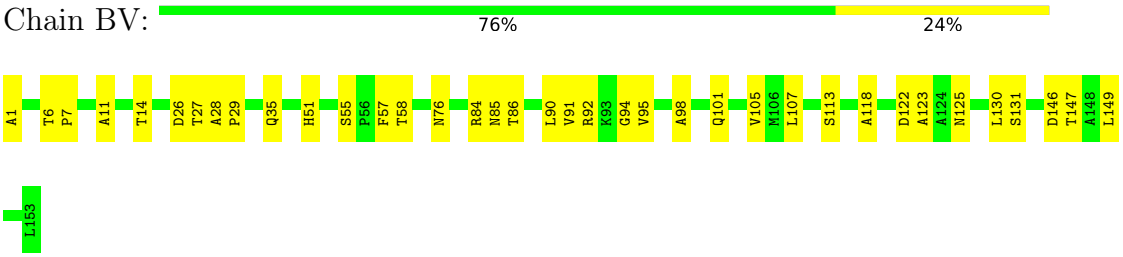
• Molecule 1: coat protein

Chain BU:



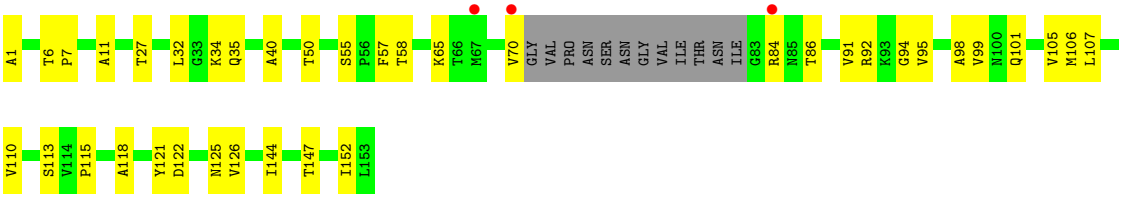
• Molecule 1: coat protein

Chain BV:



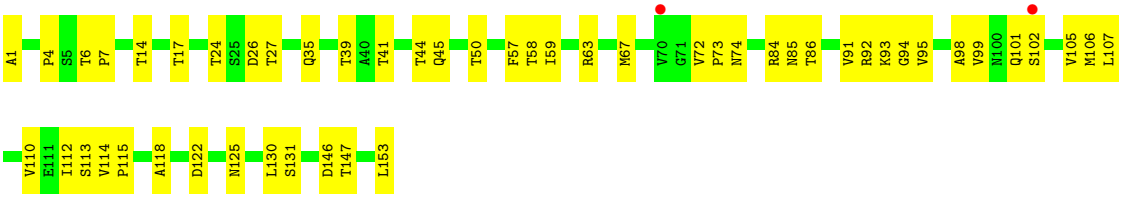
• Molecule 1: coat protein

Chain BW:



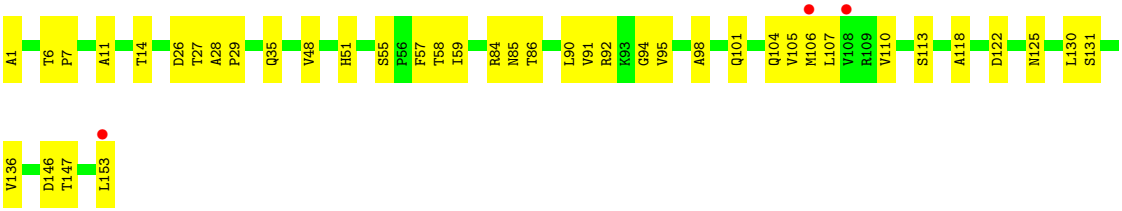
• Molecule 1: coat protein

Chain BX:



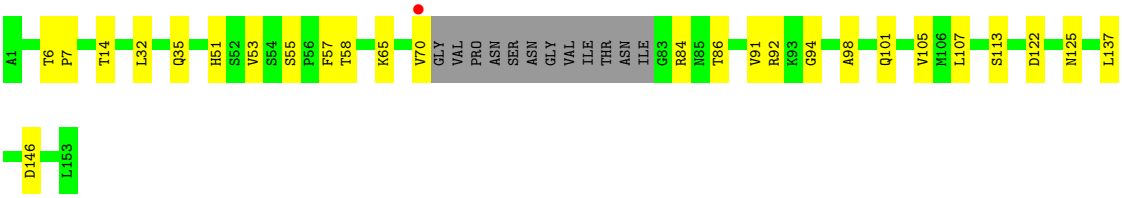
• Molecule 1: coat protein

Chain BY:



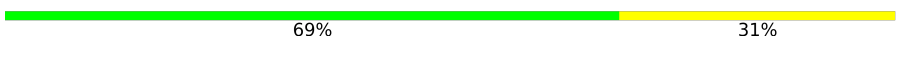
• Molecule 1: coat protein

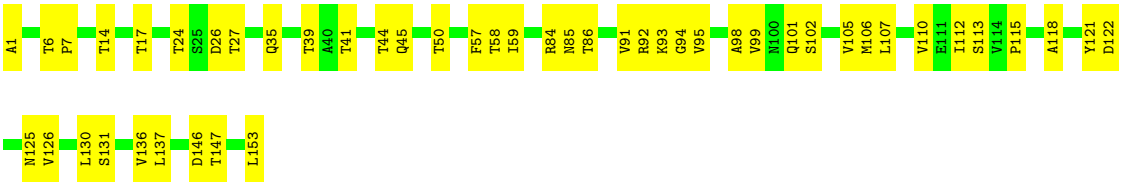
Chain BZ:



• Molecule 1: coat protein

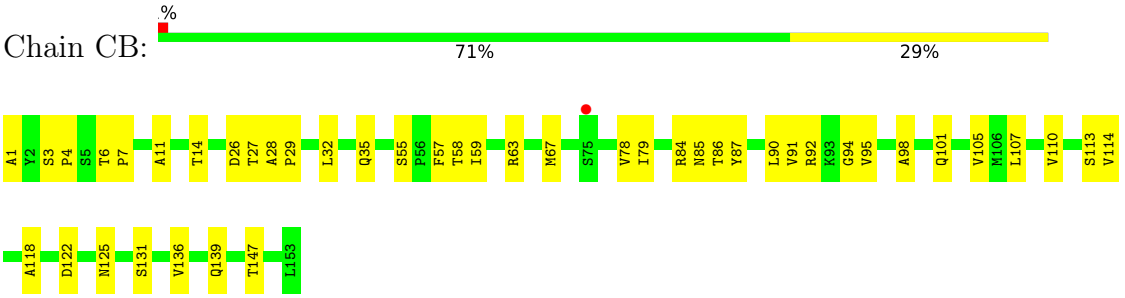
Chain CA:





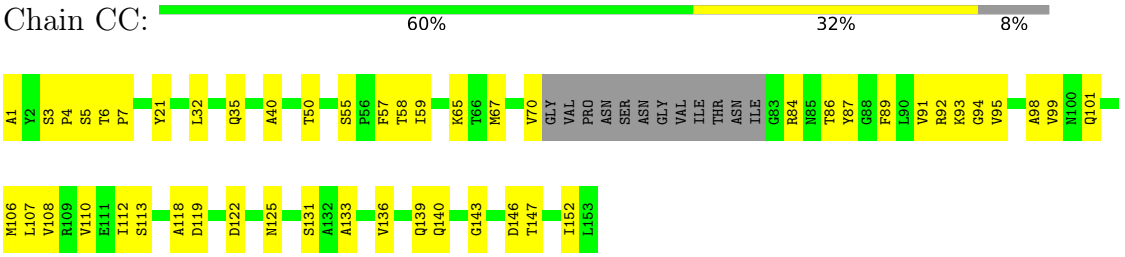
• Molecule 1: coat protein

Chain CB:



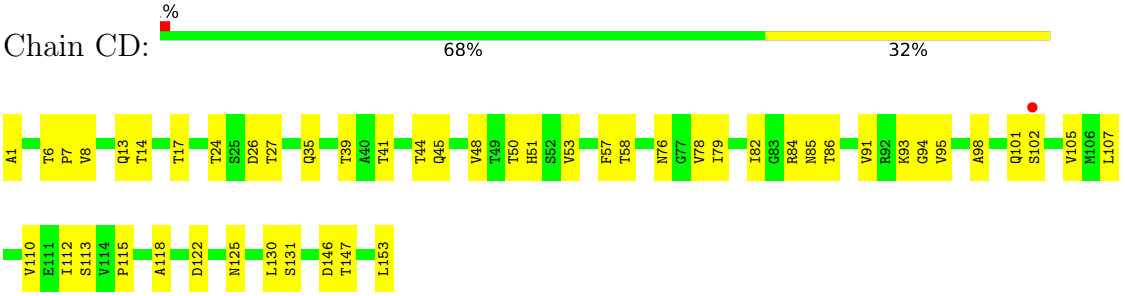
• Molecule 1: coat protein

Chain CC:



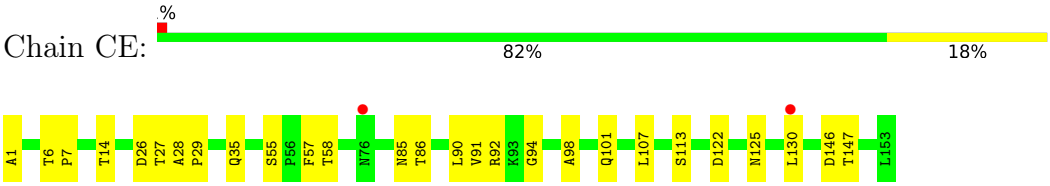
• Molecule 1: coat protein

Chain CD:



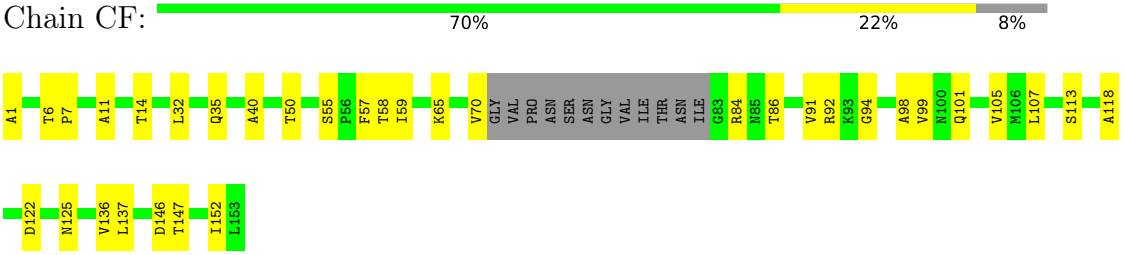
• Molecule 1: coat protein

Chain CE:



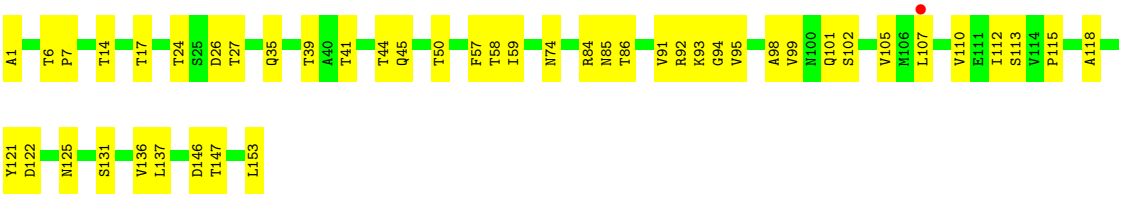
• Molecule 1: coat protein

Chain CF:



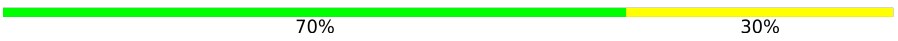
• Molecule 1: coat protein

Chain CG:



• Molecule 1: coat protein

Chain CH:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	419.73Å 419.73Å 761.14Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	97.45 – 3.30 97.45 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.1 (97.45-3.30) 99.4 (97.45-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.42	Depositor
$< I/\sigma(I) >$ [1]	1.30 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.248 , 0.251 0.254 , 0.256	Depositor DCC
R_{free} test set	10000 reflections (2.63%)	wwPDB-VP
Wilson B-factor (Å^2)	67.4	Xtriage
Anisotropy	0.251	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	0.86	EDS
Total number of atoms	63520	wwPDB-VP
Average B, all atoms (Å^2)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.16% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	AA	0.30	0/1021	0.53	0/1396
1	AB	0.32	0/1105	0.55	0/1514
1	AC	0.31	0/1105	0.54	0/1514
1	AD	0.30	0/1021	0.53	0/1396
1	AE	0.32	0/1105	0.55	0/1514
1	AF	0.31	0/1105	0.54	0/1514
1	AG	0.30	0/1021	0.53	0/1396
1	AH	0.32	0/1105	0.55	0/1514
1	AI	0.31	0/1105	0.54	0/1514
1	AJ	0.30	0/1021	0.53	0/1396
1	AK	0.32	0/1105	0.55	0/1514
1	AL	0.31	0/1105	0.54	0/1514
1	AM	0.30	0/1021	0.53	0/1396
1	AN	0.32	0/1105	0.55	0/1514
1	AO	0.31	0/1105	0.54	0/1514
1	AP	0.30	0/1021	0.53	0/1396
1	AQ	0.32	0/1105	0.55	0/1514
1	AR	0.31	0/1105	0.54	0/1514
1	AS	0.30	0/1021	0.53	0/1396
1	AT	0.32	0/1105	0.55	0/1514
1	AU	0.31	0/1105	0.54	0/1514
1	AV	0.30	0/1021	0.53	0/1396
1	AW	0.32	0/1105	0.55	0/1514
1	AX	0.31	0/1105	0.54	0/1514
1	AY	0.30	0/1021	0.53	0/1396
1	AZ	0.32	0/1105	0.55	0/1514
1	BA	0.31	0/1105	0.54	0/1514
1	BB	0.30	0/1021	0.53	0/1396
1	BC	0.32	0/1105	0.55	0/1514
1	BD	0.31	0/1105	0.54	0/1514
1	BE	0.30	0/1021	0.53	0/1396
1	BF	0.32	0/1105	0.55	0/1514
1	BG	0.31	0/1105	0.54	0/1514
1	BH	0.30	0/1021	0.53	0/1396

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	BI	0.32	0/1105	0.55	0/1514
1	BJ	0.31	0/1105	0.54	0/1514
1	BK	0.30	0/1021	0.53	0/1396
1	BL	0.32	0/1105	0.55	0/1514
1	BM	0.31	0/1105	0.54	0/1514
1	BN	0.30	0/1021	0.53	0/1396
1	BO	0.32	0/1105	0.55	0/1514
1	BP	0.31	0/1105	0.54	0/1514
1	BQ	0.30	0/1021	0.53	0/1396
1	BR	0.32	0/1105	0.55	0/1514
1	BS	0.31	0/1105	0.54	0/1514
1	BT	0.30	0/1021	0.53	0/1396
1	BU	0.32	0/1105	0.55	0/1514
1	BV	0.31	0/1105	0.54	0/1514
1	BW	0.30	0/1021	0.53	0/1396
1	BX	0.32	0/1105	0.55	0/1514
1	BY	0.31	0/1105	0.54	0/1514
1	BZ	0.30	0/1021	0.53	0/1396
1	CA	0.32	0/1105	0.55	0/1514
1	CB	0.31	0/1105	0.54	0/1514
1	CC	0.30	0/1021	0.53	0/1396
1	CD	0.32	0/1105	0.55	0/1514
1	CE	0.31	0/1105	0.54	0/1514
1	CF	0.30	0/1021	0.53	0/1396
1	CG	0.32	0/1105	0.55	0/1514
1	CH	0.31	0/1105	0.54	0/1514
All	All	0.31	0/64620	0.54	0/88480

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	1004	0	1019	25	0
1	AB	1086	0	1103	38	0
1	AC	1086	0	1103	29	0
1	AD	1004	0	1019	30	0
1	AE	1086	0	1103	39	0
1	AF	1086	0	1103	26	0
1	AG	1004	0	1019	36	0
1	AH	1086	0	1103	33	0
1	AI	1086	0	1103	14	2
1	AJ	1004	0	1019	30	0
1	AK	1086	0	1103	48	0
1	AL	1086	0	1103	37	0
1	AM	1004	0	1019	13	3
1	AN	1086	0	1103	39	0
1	AO	1086	0	1103	29	0
1	AP	1004	0	1019	33	0
1	AQ	1086	0	1103	31	0
1	AR	1086	0	1103	35	0
1	AS	1004	0	1019	30	0
1	AT	1086	0	1103	21	1
1	AU	1086	0	1103	27	0
1	AV	1004	0	1019	23	0
1	AW	1086	0	1103	37	0
1	AX	1086	0	1103	40	0
1	AY	1004	0	1019	32	0
1	AZ	1086	0	1103	74	1
1	BA	1086	0	1103	43	0
1	BB	1004	0	1019	33	0
1	BC	1086	0	1103	42	1
1	BD	1086	0	1103	46	0
1	BE	1004	0	1019	29	0
1	BF	1086	0	1103	19	2
1	BG	1086	0	1103	29	0
1	BH	1004	0	1019	35	0
1	BI	1086	0	1103	42	0
1	BJ	1086	0	1103	24	0
1	BK	1004	0	1019	11	3
1	BL	1086	0	1103	35	0
1	BM	1086	0	1103	39	0
1	BN	1004	0	1019	27	0
1	BO	1086	0	1103	19	3
1	BP	1086	0	1103	28	0
1	BQ	1004	0	1019	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	BR	1086	0	1103	21	3
1	BS	1086	0	1103	32	0
1	BT	1004	0	1019	11	1
1	BU	1086	0	1103	29	0
1	BV	1086	0	1103	27	0
1	BW	1004	0	1019	32	0
1	BX	1086	0	1103	47	0
1	BY	1086	0	1103	36	0
1	BZ	1004	0	1019	14	2
1	CA	1086	0	1103	39	0
1	CB	1086	0	1103	39	1
1	CC	1004	0	1019	62	0
1	CD	1086	0	1103	48	0
1	CE	1086	0	1103	13	2
1	CF	1004	0	1019	23	0
1	CG	1086	0	1103	37	0
1	CH	1086	0	1103	49	0
All	All	63520	0	64500	1383	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 11.

All (1383) 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:AP:84:ARG:NH1	1:CD:105:VAL:O	1.85	1.08
1:AG:84:ARG:NH1	1:AK:105:VAL:O	1.91	1.02
1:AZ:1:ALA:N	1:CC:147:THR:OG1	2.01	0.93
1:AB:147:THR:OG1	1:BW:1:ALA:N	2.02	0.93
1:AE:1:ALA:N	1:BQ:147:THR:OG1	2.05	0.89
1:AW:147:THR:OG1	1:BB:1:ALA:N	2.06	0.89
1:AY:1:ALA:N	1:BC:147:THR:OG1	2.07	0.88
1:AZ:139:GLN:OE1	1:CC:4:PRO:HA	1.76	0.86
1:AD:105:VAL:O	1:AN:84:ARG:NH1	2.09	0.85
1:AS:147:THR:OG1	1:CA:1:ALA:N	2.10	0.85
1:AX:84:ARG:NH1	1:BY:105:VAL:O	2.11	0.84
1:AZ:105:VAL:O	1:CC:84:ARG:NH1	2.10	0.84
1:BE:84:ARG:NH1	1:CG:105:VAL:O	2.09	0.84
1:AL:1:ALA:N	1:BM:147:THR:OG1	2.11	0.84
1:AP:147:THR:OG1	1:CD:1:ALA:N	2.11	0.83
1:CH:98:ALA:HB3	1:CH:101:GLN:HG2	1.61	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:98:ALA:HB3	1:BA:101:GLN:HG2	1.61	0.83
1:AZ:149:LEU:O	1:CD:53:VAL:HG23	1.78	0.83
1:BD:98:ALA:HB3	1:BD:101:GLN:HG2	1.61	0.83
1:AJ:84:ARG:NH1	1:BI:105:VAL:O	2.11	0.82
1:BP:98:ALA:HB3	1:BP:101:GLN:HG2	1.61	0.82
1:AB:1:ALA:N	1:BW:147:THR:OG1	2.12	0.82
1:AL:98:ALA:HB3	1:AL:101:GLN:HG2	1.61	0.82
1:AZ:136:VAL:HG21	1:CC:59:ILE:HD13	1.60	0.82
1:CB:98:ALA:HB3	1:CB:101:GLN:HG2	1.61	0.82
1:AC:98:ALA:HB3	1:AC:101:GLN:HG2	1.61	0.82
1:BH:1:ALA:N	1:BX:147:THR:OG1	2.11	0.82
1:BY:98:ALA:HB3	1:BY:101:GLN:HG2	1.61	0.82
1:BD:131:SER:HB2	1:CH:11:ALA:O	1.78	0.82
1:BS:98:ALA:HB3	1:BS:101:GLN:HG2	1.61	0.82
1:BJ:98:ALA:HB3	1:BJ:101:GLN:HG2	1.61	0.82
1:AJ:147:THR:OG1	1:BI:1:ALA:N	2.13	0.81
1:AP:105:VAL:O	1:CD:84:ARG:NH1	2.13	0.81
1:AS:1:ALA:N	1:CA:147:THR:OG1	2.12	0.81
1:AY:84:ARG:NH1	1:BC:105:VAL:O	2.13	0.81
1:AO:98:ALA:HB3	1:AO:101:GLN:HG2	1.61	0.81
1:BD:84:ARG:NH1	1:CH:105:VAL:O	2.13	0.81
1:BV:98:ALA:HB3	1:BV:101:GLN:HG2	1.61	0.81
1:AF:98:ALA:HB3	1:AF:101:GLN:HG2	1.61	0.81
1:AU:98:ALA:HB3	1:AU:101:GLN:HG2	1.61	0.81
1:BP:55:SER:HB2	1:BP:94:GLY:HA3	1.63	0.81
1:BG:98:ALA:HB3	1:BG:101:GLN:HG2	1.61	0.81
1:BY:55:SER:HB2	1:BY:94:GLY:HA3	1.63	0.81
1:AC:55:SER:HB2	1:AC:94:GLY:HA3	1.63	0.81
1:AD:84:ARG:NH1	1:AN:105:VAL:O	2.13	0.81
1:AI:98:ALA:HB3	1:AI:101:GLN:HG2	1.61	0.81
1:BD:55:SER:HB2	1:BD:94:GLY:HA3	1.63	0.81
1:AX:98:ALA:HB3	1:AX:101:GLN:HG2	1.61	0.81
1:BM:98:ALA:HB3	1:BM:101:GLN:HG2	1.61	0.81
1:AL:55:SER:HB2	1:AL:94:GLY:HA3	1.63	0.80
1:AR:55:SER:HB2	1:AR:94:GLY:HA3	1.63	0.80
1:BA:105:VAL:O	1:CB:84:ARG:NH1	2.14	0.80
1:AR:98:ALA:HB3	1:AR:101:GLN:HG2	1.61	0.80
1:CF:55:SER:HB2	1:CF:94:GLY:HA3	1.64	0.80
1:BA:55:SER:HB2	1:BA:94:GLY:HA3	1.63	0.80
1:BS:55:SER:HB2	1:BS:94:GLY:HA3	1.63	0.80
1:AS:55:SER:HB2	1:AS:94:GLY:HA3	1.64	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AM:55:SER:HB2	1:AM:94:GLY:HA3	1.64	0.80
1:CC:55:SER:HB2	1:CC:94:GLY:HA3	1.64	0.80
1:CE:98:ALA:HB3	1:CE:101:GLN:HG2	1.61	0.80
1:AI:55:SER:HB2	1:AI:94:GLY:HA3	1.63	0.80
1:AX:55:SER:HB2	1:AX:94:GLY:HA3	1.63	0.80
1:BQ:55:SER:HB2	1:BQ:94:GLY:HA3	1.64	0.80
1:AD:55:SER:HB2	1:AD:94:GLY:HA3	1.64	0.80
1:AE:147:THR:OG1	1:BQ:1:ALA:N	2.15	0.80
1:BM:55:SER:HB2	1:BM:94:GLY:HA3	1.63	0.80
1:AF:55:SER:HB2	1:AF:94:GLY:HA3	1.63	0.79
1:AJ:55:SER:HB2	1:AJ:94:GLY:HA3	1.64	0.79
1:AP:55:SER:HB2	1:AP:94:GLY:HA3	1.64	0.79
1:BD:105:VAL:O	1:CH:84:ARG:NH1	2.15	0.79
1:BT:55:SER:HB2	1:BT:94:GLY:HA3	1.64	0.79
1:BV:55:SER:HB2	1:BV:94:GLY:HA3	1.63	0.79
1:BE:147:THR:OG1	1:CG:1:ALA:N	2.16	0.79
1:BZ:55:SER:HB2	1:BZ:94:GLY:HA3	1.64	0.79
1:CB:55:SER:HB2	1:CB:94:GLY:HA3	1.63	0.79
1:AB:105:VAL:O	1:BW:84:ARG:NH1	2.14	0.79
1:BJ:55:SER:HB2	1:BJ:94:GLY:HA3	1.63	0.79
1:CH:55:SER:HB2	1:CH:94:GLY:HA3	1.63	0.79
1:BE:1:ALA:N	1:CG:147:THR:OG1	2.15	0.79
1:BN:55:SER:HB2	1:BN:94:GLY:HA3	1.64	0.79
1:BG:55:SER:HB2	1:BG:94:GLY:HA3	1.63	0.79
1:AG:55:SER:HB2	1:AG:94:GLY:HA3	1.64	0.79
1:AA:55:SER:HB2	1:AA:94:GLY:HA3	1.64	0.79
1:CE:55:SER:HB2	1:CE:94:GLY:HA3	1.63	0.79
1:AO:55:SER:HB2	1:AO:94:GLY:HA3	1.63	0.78
1:AV:55:SER:HB2	1:AV:94:GLY:HA3	1.64	0.78
1:AU:55:SER:HB2	1:AU:94:GLY:HA3	1.63	0.78
1:BB:55:SER:HB2	1:BB:94:GLY:HA3	1.64	0.78
1:BE:55:SER:HB2	1:BE:94:GLY:HA3	1.64	0.78
1:AZ:143:GLY:HA3	1:CC:1:ALA:O	1.84	0.78
1:BK:55:SER:HB2	1:BK:94:GLY:HA3	1.64	0.78
1:BD:11:ALA:O	1:CH:131:SER:HB2	1.83	0.78
1:AP:1:ALA:N	1:CD:147:THR:OG1	2.17	0.77
1:AY:105:VAL:O	1:BC:84:ARG:NH1	2.17	0.77
1:AY:55:SER:HB2	1:AY:94:GLY:HA3	1.64	0.77
1:BW:55:SER:HB2	1:BW:94:GLY:HA3	1.64	0.77
1:AD:1:ALA:N	1:AN:147:THR:OG1	2.17	0.77
1:BH:55:SER:HB2	1:BH:94:GLY:HA3	1.64	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AC:84:ARG:NH1	1:BG:105:VAL:O	2.18	0.76
1:AX:105:VAL:O	1:BY:84:ARG:NH1	2.18	0.76
1:AD:11:ALA:O	1:AN:131:SER:HB2	1.85	0.76
1:BH:136:VAL:HG21	1:BX:59:ILE:HD13	1.68	0.75
1:AR:72:VAL:HB	1:CD:78:VAL:HG22	1.68	0.74
1:AL:147:THR:OG1	1:BM:1:ALA:N	2.18	0.74
1:AR:1:ALA:N	1:BS:147:THR:OG1	2.19	0.74
1:AR:147:THR:OG1	1:BS:1:ALA:N	2.21	0.73
1:AX:147:THR:OG1	1:BY:1:ALA:N	2.20	0.73
1:BA:151:GLY:HA2	1:CB:67:MET:HE1	1.70	0.73
1:AG:105:VAL:O	1:AK:84:ARG:NH1	2.21	0.73
1:AG:70:VAL:HG13	1:AH:102:SER:HB2	1.71	0.73
1:AM:70:VAL:HG13	1:AN:102:SER:HB2	1.71	0.72
1:AP:70:VAL:HG13	1:AQ:102:SER:HB2	1.71	0.72
1:BZ:70:VAL:HG13	1:CA:102:SER:HB2	1.71	0.72
1:AX:1:ALA:N	1:BY:147:THR:OG1	2.20	0.72
1:AZ:95:VAL:HG11	1:CC:118:ALA:HB1	1.72	0.72
1:BN:70:VAL:HG13	1:BO:102:SER:HB2	1.71	0.72
1:BQ:70:VAL:HG13	1:BR:102:SER:HB2	1.71	0.72
1:AA:70:VAL:HG13	1:AB:102:SER:HB2	1.71	0.72
1:BW:70:VAL:HG13	1:BX:102:SER:HB2	1.71	0.72
1:CF:70:VAL:HG13	1:CG:102:SER:HB2	1.71	0.72
1:AV:70:VAL:HG13	1:AW:102:SER:HB2	1.71	0.72
1:BK:70:VAL:HG13	1:BL:102:SER:HB2	1.71	0.72
1:BH:105:VAL:O	1:BX:84:ARG:NH1	2.23	0.71
1:AU:1:ALA:N	1:BV:147:THR:OG1	2.24	0.71
1:BB:70:VAL:HG13	1:BC:102:SER:HB2	1.71	0.71
1:AW:1:ALA:N	1:BB:147:THR:OG1	2.21	0.71
1:AD:70:VAL:HG13	1:AE:102:SER:HB2	1.71	0.71
1:AA:136:VAL:HG21	1:AH:59:ILE:HD13	1.73	0.71
1:AY:70:VAL:HG13	1:AZ:102:SER:HB2	1.71	0.71
1:AZ:121:TYR:CE1	1:CC:99:VAL:HA	2.25	0.71
1:BN:98:ALA:HB3	1:BN:101:GLN:HG2	1.73	0.71
1:AG:98:ALA:HB3	1:AG:101:GLN:HG2	1.73	0.70
1:AJ:70:VAL:HG13	1:AK:102:SER:HB2	1.71	0.70
1:AP:11:ALA:O	1:CD:131:SER:HB2	1.90	0.70
1:BB:98:ALA:HB3	1:BB:101:GLN:HG2	1.73	0.70
1:BE:70:VAL:HG13	1:BF:102:SER:HB2	1.71	0.70
1:CC:70:VAL:HG13	1:CD:102:SER:HB2	1.71	0.70
1:BQ:98:ALA:HB3	1:BQ:101:GLN:HG2	1.73	0.70
1:BZ:98:ALA:HB3	1:BZ:101:GLN:HG2	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AO:131:SER:HB2	1:BP:11:ALA:O	1.90	0.70
1:AP:98:ALA:HB3	1:AP:101:GLN:HG2	1.73	0.70
1:AS:70:VAL:HG13	1:AT:102:SER:HB2	1.71	0.70
1:AS:98:ALA:HB3	1:AS:101:GLN:HG2	1.73	0.70
1:AA:98:ALA:HB3	1:AA:101:GLN:HG2	1.73	0.70
1:AY:98:ALA:HB3	1:AY:101:GLN:HG2	1.73	0.70
1:BT:70:VAL:HG13	1:BU:102:SER:HB2	1.71	0.70
1:CC:98:ALA:HB3	1:CC:101:GLN:HG2	1.73	0.70
1:AD:98:ALA:HB3	1:AD:101:GLN:HG2	1.73	0.70
1:AG:147:THR:OG1	1:AK:1:ALA:N	2.21	0.70
1:AO:84:ARG:NH1	1:BP:105:VAL:O	2.25	0.69
1:AY:11:ALA:O	1:BC:131:SER:HB2	1.91	0.69
1:BH:70:VAL:HG13	1:BI:102:SER:HB2	1.71	0.69
1:AM:98:ALA:HB3	1:AM:101:GLN:HG2	1.73	0.69
1:AZ:129:ALA:HB2	1:CC:93:LYS:CB	2.22	0.69
1:BW:98:ALA:HB3	1:BW:101:GLN:HG2	1.73	0.69
1:AL:105:VAL:O	1:BM:84:ARG:NH1	2.24	0.69
1:AU:147:THR:OG1	1:BV:1:ALA:N	2.25	0.69
1:AJ:98:ALA:HB3	1:AJ:101:GLN:HG2	1.73	0.69
1:AS:84:ARG:NH1	1:CA:105:VAL:O	2.23	0.69
1:BH:98:ALA:HB3	1:BH:101:GLN:HG2	1.73	0.69
1:BT:98:ALA:HB3	1:BT:101:GLN:HG2	1.73	0.69
1:AV:98:ALA:HB3	1:AV:101:GLN:HG2	1.73	0.69
1:BK:98:ALA:HB3	1:BK:101:GLN:HG2	1.73	0.68
1:BE:98:ALA:HB3	1:BE:101:GLN:HG2	1.73	0.68
1:CF:98:ALA:HB3	1:CF:101:GLN:HG2	1.73	0.68
1:BH:11:ALA:O	1:BX:131:SER:HB2	1.94	0.68
1:AC:147:THR:OG1	1:BG:1:ALA:N	2.26	0.68
1:AS:99:VAL:HA	1:CA:121:TYR:CE1	2.29	0.67
1:AU:11:ALA:O	1:BV:131:SER:HB2	1.93	0.67
1:AX:118:ALA:HB1	1:BY:95:VAL:HG11	1.76	0.67
1:AP:125:ASN:OD1	1:CD:48:VAL:HA	1.95	0.67
1:AZ:140:GLN:NE2	1:CC:3:SER:O	2.27	0.67
1:AP:118:ALA:HB1	1:CD:95:VAL:HG11	1.77	0.67
1:AY:147:THR:OG1	1:BC:1:ALA:N	2.26	0.67
1:AG:125:ASN:OD1	1:AK:48:VAL:HA	1.94	0.67
1:AR:105:VAL:O	1:BS:84:ARG:NH1	2.26	0.67
1:AU:131:SER:HB2	1:BV:11:ALA:O	1.95	0.67
1:BH:137:LEU:HD11	1:BX:110:VAL:HG21	1.77	0.67
1:AG:34:LYS:HD2	1:AK:153:LEU:HB3	1.77	0.67
1:AB:131:SER:HB2	1:BW:11:ALA:O	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AE:84:ARG:HG2	1:AE:115:PRO:HA	1.78	0.66
1:AK:84:ARG:HG2	1:AK:115:PRO:HA	1.78	0.66
1:BF:84:ARG:HG2	1:BF:115:PRO:HA	1.78	0.66
1:BL:147:THR:OG1	1:BN:1:ALA:N	2.27	0.66
1:BL:84:ARG:HG2	1:BL:115:PRO:HA	1.78	0.66
1:AZ:121:TYR:CZ	1:CC:99:VAL:HA	2.30	0.66
1:AZ:84:ARG:HG2	1:AZ:115:PRO:HA	1.78	0.66
1:CD:84:ARG:HG2	1:CD:115:PRO:HA	1.78	0.66
1:AT:84:ARG:HG2	1:AT:115:PRO:HA	1.78	0.66
1:AH:84:ARG:HG2	1:AH:115:PRO:HA	1.78	0.66
1:BI:84:ARG:HG2	1:BI:115:PRO:HA	1.78	0.66
1:BR:84:ARG:HG2	1:BR:115:PRO:HA	1.78	0.66
1:AQ:84:ARG:HG2	1:AQ:115:PRO:HA	1.78	0.65
1:AX:11:ALA:O	1:BY:131:SER:HB2	1.96	0.65
1:AZ:137:LEU:HD11	1:CC:110:VAL:HG21	1.78	0.65
1:BD:147:THR:OG1	1:CH:1:ALA:N	2.26	0.65
1:AC:1:ALA:N	1:BG:147:THR:OG1	2.27	0.65
1:CA:84:ARG:HG2	1:CA:115:PRO:HA	1.78	0.65
1:AB:84:ARG:HG2	1:AB:115:PRO:HA	1.78	0.65
1:AS:99:VAL:HA	1:CA:121:TYR:CZ	2.32	0.65
1:BC:41:THR:HB	1:BC:45:GLN:HE21	1.62	0.65
1:BX:84:ARG:HG2	1:BX:115:PRO:HA	1.78	0.65
1:AR:11:ALA:O	1:BS:131:SER:HB2	1.95	0.65
1:BU:84:ARG:HG2	1:BU:115:PRO:HA	1.78	0.65
1:BA:1:ALA:N	1:CB:147:THR:OG1	2.30	0.65
1:BI:41:THR:HB	1:BI:45:GLN:HE21	1.62	0.65
1:CG:41:THR:HB	1:CG:45:GLN:HE21	1.62	0.65
1:AL:11:ALA:O	1:BM:131:SER:HB2	1.97	0.65
1:BC:84:ARG:HG2	1:BC:115:PRO:HA	1.78	0.65
1:BX:41:THR:HB	1:BX:45:GLN:HE21	1.62	0.65
1:AA:1:ALA:N	1:AH:147:THR:OG1	2.29	0.65
1:AB:41:THR:HB	1:AB:45:GLN:HE21	1.62	0.65
1:BO:84:ARG:HG2	1:BO:115:PRO:HA	1.78	0.65
1:AX:131:SER:HB2	1:BY:11:ALA:O	1.96	0.65
1:BA:11:ALA:O	1:CB:131:SER:HB2	1.96	0.65
1:BL:1:ALA:N	1:BN:147:THR:OG1	2.27	0.65
1:AE:41:THR:HB	1:AE:45:GLN:HE21	1.62	0.64
1:AT:41:THR:HB	1:AT:45:GLN:HE21	1.62	0.64
1:AZ:41:THR:HB	1:AZ:45:GLN:HE21	1.62	0.64
1:BL:41:THR:HB	1:BL:45:GLN:HE21	1.62	0.64
1:AG:1:ALA:N	1:AK:147:THR:OG1	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AJ:1:ALA:N	1:BI:147:THR:OG1	2.29	0.64
1:AW:99:VAL:HA	1:BB:121:TYR:CE1	2.32	0.64
1:BU:147:THR:OG1	1:CF:1:ALA:N	2.30	0.64
1:CD:41:THR:HB	1:CD:45:GLN:HE21	1.62	0.64
1:AW:84:ARG:HG2	1:AW:115:PRO:HA	1.78	0.64
1:CA:41:THR:HB	1:CA:45:GLN:HE21	1.62	0.64
1:CG:84:ARG:HG2	1:CG:115:PRO:HA	1.78	0.64
1:AQ:41:THR:HB	1:AQ:45:GLN:HE21	1.62	0.64
1:AB:107:LEU:HB3	1:BW:113:SER:OG	1.98	0.64
1:AZ:126:VAL:HA	1:CC:106:MET:SD	2.38	0.64
1:AZ:133:ALA:HB2	1:CC:91:VAL:HG21	1.78	0.64
1:BU:41:THR:HB	1:BU:45:GLN:HE21	1.62	0.64
1:AK:41:THR:HB	1:AK:45:GLN:HE21	1.62	0.64
1:AN:84:ARG:HG2	1:AN:115:PRO:HA	1.78	0.64
1:AP:95:VAL:HG11	1:CD:118:ALA:HB1	1.80	0.64
1:AU:84:ARG:NH1	1:BV:105:VAL:O	2.31	0.64
1:AW:131:SER:HB2	1:BB:11:ALA:O	1.97	0.64
1:AH:41:THR:HB	1:AH:45:GLN:HE21	1.62	0.63
1:AQ:131:SER:HB2	1:AV:11:ALA:O	1.97	0.63
1:AU:105:VAL:O	1:BV:84:ARG:NH1	2.32	0.63
1:BA:136:VAL:HG21	1:CB:59:ILE:HD13	1.80	0.63
1:AE:121:TYR:CE1	1:BQ:99:VAL:HA	2.33	0.63
1:BF:41:THR:HB	1:BF:45:GLN:HE21	1.62	0.63
1:AD:95:VAL:HG11	1:AN:118:ALA:HB1	1.81	0.63
1:AI:35:GLN:HE21	1:AI:58:THR:HB	1.64	0.63
1:BD:35:GLN:HE21	1:BD:58:THR:HB	1.64	0.63
1:BP:35:GLN:HE21	1:BP:58:THR:HB	1.64	0.63
1:BV:35:GLN:HE21	1:BV:58:THR:HB	1.64	0.63
1:AW:106:MET:SD	1:BB:126:VAL:HA	2.38	0.63
1:BM:35:GLN:HE21	1:BM:58:THR:HB	1.64	0.63
1:CH:35:GLN:HE21	1:CH:58:THR:HB	1.64	0.63
1:AJ:59:ILE:HD13	1:BI:136:VAL:HG21	1.81	0.63
1:AR:131:SER:HB2	1:BS:11:ALA:O	1.98	0.63
1:AU:35:GLN:HE21	1:AU:58:THR:HB	1.64	0.63
1:BQ:35:GLN:HE21	1:BQ:58:THR:HB	1.64	0.63
1:AL:35:GLN:HE21	1:AL:58:THR:HB	1.64	0.63
1:AN:41:THR:HB	1:AN:45:GLN:HE21	1.62	0.63
1:AV:35:GLN:HE21	1:AV:58:THR:HB	1.64	0.63
1:AW:41:THR:HB	1:AW:45:GLN:HE21	1.62	0.63
1:BR:41:THR:HB	1:BR:45:GLN:HE21	1.62	0.63
1:AJ:118:ALA:HB1	1:BI:95:VAL:HG11	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:35:GLN:HE21	1:BA:58:THR:HB	1.64	0.63
1:BO:41:THR:HB	1:BO:45:GLN:HE21	1.62	0.63
1:AR:35:GLN:HE21	1:AR:58:THR:HB	1.64	0.63
1:BW:35:GLN:HE21	1:BW:58:THR:HB	1.64	0.63
1:CC:35:GLN:HE21	1:CC:58:THR:HB	1.64	0.63
1:CF:35:GLN:HE21	1:CF:58:THR:HB	1.64	0.63
1:AC:105:VAL:O	1:BG:84:ARG:NH1	2.31	0.62
1:AF:35:GLN:HE21	1:AF:58:THR:HB	1.64	0.62
1:AK:35:GLN:HE21	1:AK:58:THR:HB	1.64	0.62
1:AM:35:GLN:HE21	1:AM:58:THR:HB	1.64	0.62
1:BG:35:GLN:HE21	1:BG:58:THR:HB	1.64	0.62
1:BI:35:GLN:HE21	1:BI:58:THR:HB	1.64	0.62
1:AA:147:THR:OG1	1:AH:1:ALA:N	2.32	0.62
1:AD:48:VAL:HA	1:AN:125:ASN:OD1	1.98	0.62
1:AF:147:THR:OG1	1:BJ:1:ALA:N	2.31	0.62
1:AG:35:GLN:HE21	1:AG:58:THR:HB	1.64	0.62
1:AH:35:GLN:HE21	1:AH:58:THR:HB	1.65	0.62
1:AZ:21:TYR:HE2	1:CC:131:SER:HG	1.47	0.62
1:BR:35:GLN:HE21	1:BR:58:THR:HB	1.64	0.62
1:BU:35:GLN:HE21	1:BU:58:THR:HB	1.65	0.62
1:AO:35:GLN:HE21	1:AO:58:THR:HB	1.64	0.62
1:AQ:35:GLN:HE21	1:AQ:58:THR:HB	1.64	0.62
1:BX:35:GLN:HE21	1:BX:58:THR:HB	1.65	0.62
1:BZ:35:GLN:HE21	1:BZ:58:THR:HB	1.64	0.62
1:CA:35:GLN:HE21	1:CA:58:THR:HB	1.65	0.62
1:AG:11:ALA:O	1:AK:131:SER:HB2	1.98	0.62
1:AY:95:VAL:HG11	1:BC:118:ALA:HB1	1.82	0.62
1:AZ:126:VAL:HG13	1:CC:106:MET:SD	2.39	0.62
1:BC:35:GLN:HE21	1:BC:58:THR:HB	1.65	0.62
1:BF:35:GLN:HE21	1:BF:58:THR:HB	1.64	0.62
1:AD:35:GLN:HE21	1:AD:58:THR:HB	1.64	0.62
1:AD:147:THR:OG1	1:AN:1:ALA:N	2.31	0.62
1:AW:35:GLN:HE21	1:AW:58:THR:HB	1.64	0.62
1:BL:35:GLN:HE21	1:BL:58:THR:HB	1.65	0.62
1:BS:35:GLN:HE21	1:BS:58:THR:HB	1.64	0.62
1:AA:35:GLN:HE21	1:AA:58:THR:HB	1.64	0.62
1:AC:131:SER:HB2	1:BG:11:ALA:O	1.99	0.62
1:AG:118:ALA:HB1	1:AK:95:VAL:HG11	1.80	0.62
1:CB:35:GLN:HE21	1:CB:58:THR:HB	1.64	0.62
1:AB:35:GLN:HE21	1:AB:58:THR:HB	1.64	0.62
1:AE:98:ALA:HB3	1:AE:101:GLN:HB2	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AS:35:GLN:HE21	1:AS:58:THR:HB	1.64	0.62
1:BX:98:ALA:HB3	1:BX:101:GLN:HB2	1.82	0.62
1:CG:98:ALA:HB3	1:CG:101:GLN:HB2	1.82	0.62
1:AN:35:GLN:HE21	1:AN:58:THR:HB	1.64	0.62
1:CG:35:GLN:HE21	1:CG:58:THR:HB	1.64	0.62
1:AB:98:ALA:HB3	1:AB:101:GLN:HB2	1.82	0.61
1:BO:98:ALA:HB3	1:BO:101:GLN:HB2	1.82	0.61
1:CE:35:GLN:HE21	1:CE:58:THR:HB	1.64	0.61
1:AN:98:ALA:HB3	1:AN:101:GLN:HB2	1.82	0.61
1:AO:105:VAL:O	1:BP:84:ARG:NH1	2.32	0.61
1:AQ:147:THR:OG1	1:AV:1:ALA:N	2.33	0.61
1:AT:35:GLN:HE21	1:AT:58:THR:HB	1.64	0.61
1:AW:98:ALA:HB3	1:AW:101:GLN:HB2	1.82	0.61
1:AE:35:GLN:HE21	1:AE:58:THR:HB	1.65	0.61
1:BH:35:GLN:HE21	1:BH:58:THR:HB	1.64	0.61
1:AO:11:ALA:O	1:BP:131:SER:HB2	2.00	0.61
1:AP:35:GLN:HE21	1:AP:58:THR:HB	1.64	0.61
1:AT:98:ALA:HB3	1:AT:101:GLN:HB2	1.82	0.61
1:AZ:35:GLN:HE21	1:AZ:58:THR:HB	1.65	0.61
1:BJ:35:GLN:HE21	1:BJ:58:THR:HB	1.64	0.61
1:BK:35:GLN:HE21	1:BK:58:THR:HB	1.64	0.61
1:BO:35:GLN:HE21	1:BO:58:THR:HB	1.64	0.61
1:AQ:98:ALA:HB3	1:AQ:101:GLN:HB2	1.82	0.61
1:AZ:98:ALA:HB3	1:AZ:101:GLN:HB2	1.82	0.61
1:BE:11:ALA:O	1:CG:131:SER:HB2	2.01	0.61
1:BE:105:VAL:O	1:CG:84:ARG:NH1	2.34	0.61
1:BY:35:GLN:HE21	1:BY:58:THR:HB	1.64	0.61
1:AC:35:GLN:HE21	1:AC:58:THR:HB	1.64	0.61
1:AE:41:THR:HB	1:AE:45:GLN:NE2	2.16	0.61
1:AZ:1:ALA:O	1:CC:143:GLY:HA3	2.01	0.61
1:AZ:140:GLN:OE1	1:CC:3:SER:N	2.23	0.61
1:BU:41:THR:HB	1:BU:45:GLN:NE2	2.16	0.61
1:CD:41:THR:HB	1:CD:45:GLN:NE2	2.16	0.61
1:AO:147:THR:OG1	1:BP:1:ALA:N	2.29	0.61
1:AY:118:ALA:HB1	1:BC:95:VAL:HG11	1.82	0.61
1:BI:41:THR:HB	1:BI:45:GLN:NE2	2.16	0.61
1:CD:35:GLN:HE21	1:CD:58:THR:HB	1.64	0.61
1:BB:35:GLN:HE21	1:BB:58:THR:HB	1.64	0.61
1:BE:35:GLN:HE21	1:BE:58:THR:HB	1.64	0.61
1:AY:35:GLN:HE21	1:AY:58:THR:HB	1.64	0.61
1:BT:35:GLN:HE21	1:BT:58:THR:HB	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AE:105:VAL:O	1:BQ:84:ARG:NH1	2.26	0.61
1:AH:98:ALA:HB3	1:AH:101:GLN:HB2	1.82	0.61
1:AN:41:THR:HB	1:AN:45:GLN:NE2	2.16	0.61
1:AQ:41:THR:HB	1:AQ:45:GLN:NE2	2.16	0.61
1:AZ:5:SER:HB2	1:CC:139:GLN:NE2	2.16	0.61
1:BX:41:THR:HB	1:BX:45:GLN:NE2	2.16	0.61
1:CA:41:THR:HB	1:CA:45:GLN:NE2	2.16	0.61
1:AB:41:THR:HB	1:AB:45:GLN:NE2	2.16	0.60
1:AJ:35:GLN:HE21	1:AJ:58:THR:HB	1.64	0.60
1:AT:41:THR:HB	1:AT:45:GLN:NE2	2.16	0.60
1:BL:98:ALA:HB3	1:BL:101:GLN:HB2	1.82	0.60
1:BR:98:ALA:HB3	1:BR:101:GLN:HB2	1.82	0.60
1:AH:41:THR:HB	1:AH:45:GLN:NE2	2.16	0.60
1:BN:35:GLN:HE21	1:BN:58:THR:HB	1.64	0.60
1:CA:98:ALA:HB3	1:CA:101:GLN:HB2	1.82	0.60
1:AK:98:ALA:HB3	1:AK:101:GLN:HB2	1.82	0.60
1:AW:41:THR:HB	1:AW:45:GLN:NE2	2.16	0.60
1:BO:41:THR:HB	1:BO:45:GLN:NE2	2.16	0.60
1:CG:41:THR:HB	1:CG:45:GLN:NE2	2.16	0.60
1:AZ:41:THR:HB	1:AZ:45:GLN:NE2	2.16	0.60
1:BC:41:THR:HB	1:BC:45:GLN:NE2	2.16	0.60
1:BL:41:THR:HB	1:BL:45:GLN:NE2	2.16	0.60
1:AZ:133:ALA:CB	1:CC:91:VAL:HG21	2.31	0.60
1:CD:98:ALA:HB3	1:CD:101:GLN:HB2	1.82	0.60
1:BF:41:THR:HB	1:BF:45:GLN:NE2	2.16	0.60
1:BR:41:THR:HB	1:BR:45:GLN:NE2	2.16	0.60
1:AR:84:ARG:NH1	1:BS:105:VAL:O	2.34	0.60
1:BC:98:ALA:HB3	1:BC:101:GLN:HB2	1.82	0.60
1:BF:98:ALA:HB3	1:BF:101:GLN:HB2	1.82	0.60
1:BA:137:LEU:HD11	1:CB:110:VAL:HG21	1.84	0.60
1:BI:98:ALA:HB3	1:BI:101:GLN:HB2	1.82	0.60
1:BN:6:THR:HB	1:BN:7:PRO:HD3	1.84	0.60
1:BU:98:ALA:HB3	1:BU:101:GLN:HB2	1.82	0.60
1:AA:59:ILE:HD13	1:AH:136:VAL:HG21	1.84	0.59
1:AX:35:GLN:HE21	1:AX:58:THR:HB	1.64	0.59
1:AF:72:VAL:HB	1:AN:78:VAL:HG22	1.84	0.59
1:BH:6:THR:HB	1:BH:7:PRO:HD3	1.84	0.59
1:BH:139:GLN:OE1	1:BX:4:PRO:HA	2.02	0.59
1:AL:84:ARG:NH1	1:BM:105:VAL:O	2.35	0.59
1:AP:6:THR:HB	1:AP:7:PRO:HD3	1.84	0.59
1:AF:84:ARG:NH1	1:BJ:105:VAL:O	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BQ:6:THR:HB	1:BQ:7:PRO:HD3	1.85	0.59
1:BU:1:ALA:N	1:CF:147:THR:OG1	2.33	0.59
1:BZ:6:THR:HB	1:BZ:7:PRO:HD3	1.84	0.59
1:AC:118:ALA:HB1	1:BG:95:VAL:HG11	1.83	0.59
1:AK:41:THR:HB	1:AK:45:GLN:NE2	2.16	0.59
1:BD:1:ALA:N	1:CH:147:THR:OG1	2.30	0.59
1:AL:76:ASN:HD21	1:BL:75:SER:HA	1.68	0.59
1:BH:95:VAL:HG11	1:BX:118:ALA:HB1	1.84	0.59
1:BK:6:THR:HB	1:BK:7:PRO:HD3	1.84	0.59
1:BT:6:THR:HB	1:BT:7:PRO:HD3	1.84	0.59
1:BE:6:THR:HB	1:BE:7:PRO:HD3	1.84	0.59
1:AZ:110:VAL:HG22	1:CC:110:VAL:HG22	1.83	0.59
1:BU:59:ILE:HD13	1:CF:136:VAL:HG21	1.85	0.59
1:BW:6:THR:HB	1:BW:7:PRO:HD3	1.84	0.59
1:AF:1:ALA:N	1:BJ:147:THR:OG1	2.35	0.59
1:AS:6:THR:HB	1:AS:7:PRO:HD3	1.84	0.59
1:CC:6:THR:HB	1:CC:7:PRO:HD3	1.84	0.59
1:AC:11:ALA:O	1:BG:131:SER:HB2	2.01	0.58
1:AM:6:THR:HB	1:AM:7:PRO:HD3	1.84	0.58
1:AN:6:THR:HB	1:AN:7:PRO:HD3	1.85	0.58
1:AQ:59:ILE:HD13	1:AV:136:VAL:HG21	1.85	0.58
1:AX:110:VAL:HG22	1:BY:110:VAL:HG22	1.84	0.58
1:AZ:5:SER:HB2	1:CC:139:GLN:HE22	1.66	0.58
1:CA:6:THR:HB	1:CA:7:PRO:HD3	1.85	0.58
1:AH:6:THR:HB	1:AH:7:PRO:HD3	1.85	0.58
1:AT:6:THR:HB	1:AT:7:PRO:HD3	1.85	0.58
1:AZ:59:ILE:HD13	1:CC:136:VAL:HG21	1.85	0.58
1:AE:6:THR:HB	1:AE:7:PRO:HD3	1.85	0.58
1:AP:34:LYS:HD2	1:CD:153:LEU:HB3	1.85	0.58
1:BL:59:ILE:HD13	1:BN:136:VAL:HG21	1.85	0.58
1:BA:48:VAL:HA	1:CB:125:ASN:OD1	2.03	0.58
1:BF:6:THR:HB	1:BF:7:PRO:HD3	1.85	0.58
1:BJ:6:THR:HB	1:BJ:7:PRO:HD3	1.86	0.58
1:AD:6:THR:HB	1:AD:7:PRO:HD3	1.84	0.58
1:AI:6:THR:HB	1:AI:7:PRO:HD3	1.86	0.58
1:BB:6:THR:HB	1:BB:7:PRO:HD3	1.84	0.58
1:BV:6:THR:HB	1:BV:7:PRO:HD3	1.86	0.58
1:BY:6:THR:HB	1:BY:7:PRO:HD3	1.86	0.58
1:AL:6:THR:HB	1:AL:7:PRO:HD3	1.86	0.58
1:AL:78:VAL:HG11	1:BL:72:VAL:HG11	1.86	0.58
1:BL:6:THR:HB	1:BL:7:PRO:HD3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AC:6:THR:HB	1:AC:7:PRO:HD3	1.86	0.58
1:AK:6:THR:HB	1:AK:7:PRO:HD3	1.85	0.58
1:AV:6:THR:HB	1:AV:7:PRO:HD3	1.84	0.58
1:BC:6:THR:HB	1:BC:7:PRO:HD3	1.85	0.58
1:CF:6:THR:HB	1:CF:7:PRO:HD3	1.84	0.58
1:CG:6:THR:HB	1:CG:7:PRO:HD3	1.85	0.58
1:CH:6:THR:HB	1:CH:7:PRO:HD3	1.86	0.58
1:AG:6:THR:HB	1:AG:7:PRO:HD3	1.84	0.58
1:AR:6:THR:HB	1:AR:7:PRO:HD3	1.86	0.58
1:AY:6:THR:HB	1:AY:7:PRO:HD3	1.84	0.58
1:BU:6:THR:HB	1:BU:7:PRO:HD3	1.85	0.58
1:AB:95:VAL:HG11	1:BW:118:ALA:HB1	1.86	0.58
1:AE:126:VAL:HA	1:BQ:106:MET:SD	2.44	0.58
1:AJ:6:THR:HB	1:AJ:7:PRO:HD3	1.84	0.58
1:BD:6:THR:HB	1:BD:7:PRO:HD3	1.86	0.58
1:BO:6:THR:HB	1:BO:7:PRO:HD3	1.86	0.58
1:BP:6:THR:HB	1:BP:7:PRO:HD3	1.86	0.58
1:CB:6:THR:HB	1:CB:7:PRO:HD3	1.86	0.58
1:AA:6:THR:HB	1:AA:7:PRO:HD3	1.84	0.58
1:AE:121:TYR:CZ	1:BQ:99:VAL:HA	2.39	0.58
1:AO:6:THR:HB	1:AO:7:PRO:HD3	1.86	0.58
1:AU:6:THR:HB	1:AU:7:PRO:HD3	1.86	0.57
1:BA:95:VAL:HG11	1:CB:118:ALA:HB1	1.86	0.57
1:AP:110:VAL:HG22	1:CD:110:VAL:HG22	1.86	0.57
1:AY:136:VAL:HG21	1:BC:59:ILE:HD13	1.85	0.57
1:CD:6:THR:HB	1:CD:7:PRO:HD3	1.85	0.57
1:AZ:5:SER:N	1:CC:139:GLN:OE1	2.37	0.57
1:BG:6:THR:HB	1:BG:7:PRO:HD3	1.86	0.57
1:BR:6:THR:HB	1:BR:7:PRO:HD3	1.86	0.57
1:AZ:6:THR:HB	1:AZ:7:PRO:HD3	1.86	0.57
1:CE:6:THR:HB	1:CE:7:PRO:HD3	1.86	0.57
1:AW:6:THR:HB	1:AW:7:PRO:HD3	1.85	0.57
1:BA:6:THR:HB	1:BA:7:PRO:HD3	1.86	0.57
1:BA:149:LEU:O	1:BZ:53:VAL:HG23	2.04	0.57
1:AQ:6:THR:HB	1:AQ:7:PRO:HD3	1.85	0.57
1:AB:6:THR:HB	1:AB:7:PRO:HD3	1.85	0.57
1:BI:6:THR:HB	1:BI:7:PRO:HD3	1.85	0.57
1:BL:105:VAL:O	1:BN:84:ARG:NH1	2.30	0.57
1:BS:6:THR:HB	1:BS:7:PRO:HD3	1.86	0.57
1:AC:59:ILE:HD13	1:BG:136:VAL:HG21	1.87	0.57
1:AP:113:SER:OG	1:CD:107:LEU:HB3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AZ:129:ALA:HB2	1:CC:93:LYS:HB2	1.84	0.57
1:BX:6:THR:HB	1:BX:7:PRO:HD3	1.85	0.57
1:AX:79:ILE:HG13	1:BY:101:GLN:NE2	2.19	0.57
1:BM:6:THR:HB	1:BM:7:PRO:HD3	1.86	0.57
1:AZ:137:LEU:HG	1:CC:89:PHE:CE2	2.40	0.56
1:BD:125:ASN:OD1	1:CH:48:VAL:HA	2.04	0.56
1:BE:147:THR:HG1	1:CG:1:ALA:H3	1.51	0.56
1:AA:84:ARG:NH1	1:AH:105:VAL:O	2.34	0.56
1:AG:110:VAL:HG22	1:AK:110:VAL:HG22	1.85	0.56
1:AJ:95:VAL:HG11	1:BI:118:ALA:HB1	1.87	0.56
1:AK:53:VAL:HG23	1:BI:149:LEU:O	2.05	0.56
1:AX:6:THR:HB	1:AX:7:PRO:HD3	1.86	0.56
1:AX:125:ASN:OD1	1:BY:48:VAL:HA	2.04	0.56
1:AE:118:ALA:HB1	1:BQ:95:VAL:HG11	1.86	0.56
1:AF:59:ILE:HD13	1:BJ:136:VAL:HG21	1.87	0.56
1:AZ:17:THR:HB	1:AZ:44:THR:HB	1.88	0.56
1:BA:101:GLN:HE22	1:CB:78:VAL:HA	1.70	0.56
1:AF:131:SER:HB2	1:BJ:11:ALA:O	2.05	0.56
1:AZ:118:ALA:HB1	1:CC:95:VAL:HG11	1.87	0.56
1:BU:136:VAL:HG21	1:CF:59:ILE:HD13	1.88	0.56
1:AE:17:THR:HB	1:AE:44:THR:HB	1.88	0.56
1:AF:6:THR:HB	1:AF:7:PRO:HD3	1.86	0.56
1:BE:118:ALA:HB1	1:CG:95:VAL:HG11	1.88	0.56
1:BI:17:THR:HB	1:BI:44:THR:HB	1.88	0.56
1:BO:17:THR:HB	1:BO:44:THR:HB	1.88	0.56
1:AT:17:THR:HB	1:AT:44:THR:HB	1.88	0.56
1:AW:17:THR:HB	1:AW:44:THR:HB	1.88	0.56
1:AE:59:ILE:HD13	1:BQ:136:VAL:HG21	1.88	0.56
1:AP:104:GLN:HG3	1:CD:82:ILE:HG21	1.86	0.56
1:AY:34:LYS:HD2	1:BC:153:LEU:HB3	1.88	0.56
1:BC:17:THR:HB	1:BC:44:THR:HB	1.88	0.56
1:BU:131:SER:HB2	1:CF:11:ALA:O	2.05	0.56
1:CD:17:THR:HB	1:CD:44:THR:HB	1.88	0.56
1:BH:126:VAL:HA	1:BX:106:MET:SD	2.46	0.56
1:BL:131:SER:HB2	1:BN:11:ALA:O	2.06	0.56
1:CA:17:THR:HB	1:CA:44:THR:HB	1.88	0.56
1:AZ:3:SER:O	1:CC:140:GLN:NE2	2.39	0.55
1:BA:152:ILE:HD11	1:BZ:51:HIS:CD2	2.41	0.55
1:BU:17:THR:HB	1:BU:44:THR:HB	1.88	0.55
1:AB:17:THR:HB	1:AB:44:THR:HB	1.88	0.55
1:BL:17:THR:HB	1:BL:44:THR:HB	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BX:17:THR:HB	1:BX:44:THR:HB	1.88	0.55
1:AS:122:ASP:OD2	1:AS:125:ASN:ND2	2.39	0.55
1:AX:95:VAL:HG11	1:BY:118:ALA:HB1	1.87	0.55
1:AK:72:VAL:HG11	1:BM:78:VAL:HG11	1.89	0.55
1:AL:121:TYR:CE1	1:BM:99:VAL:HA	2.42	0.55
1:AQ:17:THR:HB	1:AQ:44:THR:HB	1.88	0.55
1:AS:121:TYR:CE1	1:CA:99:VAL:HA	2.41	0.55
1:AH:17:THR:HB	1:AH:44:THR:HB	1.88	0.55
1:AY:110:VAL:HG22	1:BC:110:VAL:HG22	1.88	0.55
1:AD:118:ALA:HB1	1:AN:95:VAL:HG11	1.89	0.55
1:AG:59:ILE:HD13	1:AK:136:VAL:HG21	1.89	0.55
1:AW:99:VAL:HA	1:BB:121:TYR:CZ	2.41	0.55
1:BR:17:THR:HB	1:BR:44:THR:HB	1.88	0.55
1:BU:105:VAL:O	1:CF:84:ARG:NH1	2.32	0.55
1:AK:17:THR:HB	1:AK:44:THR:HB	1.88	0.55
1:AB:99:VAL:HA	1:BW:121:TYR:CE1	2.41	0.55
1:AD:136:VAL:HG21	1:AN:59:ILE:HD13	1.87	0.55
1:BH:152:ILE:HD11	1:BY:51:HIS:CD2	2.41	0.55
1:AL:131:SER:HB2	1:BM:11:ALA:O	2.07	0.54
1:AN:17:THR:HB	1:AN:44:THR:HB	1.88	0.54
1:BX:63:ARG:HH11	1:BX:67:MET:HE1	1.72	0.54
1:CG:17:THR:HB	1:CG:44:THR:HB	1.88	0.54
1:AS:136:VAL:HG21	1:CA:59:ILE:HD13	1.88	0.54
1:BD:131:SER:HB3	1:CH:13:GLN:CG	2.38	0.54
1:AB:113:SER:OG	1:BW:107:LEU:HB3	2.07	0.54
1:BD:152:ILE:O	1:CH:1:ALA:N	2.40	0.54
1:AQ:84:ARG:NH1	1:AV:105:VAL:O	2.40	0.54
1:BF:17:THR:HB	1:BF:44:THR:HB	1.88	0.54
1:BH:122:ASP:OD2	1:BH:125:ASN:ND2	2.39	0.54
1:AM:122:ASP:OD2	1:AM:125:ASN:ND2	2.39	0.54
1:AD:122:ASP:OD2	1:AD:125:ASN:ND2	2.39	0.54
1:AF:105:VAL:O	1:BJ:84:ARG:NH1	2.41	0.54
1:AQ:72:VAL:HG11	1:BS:78:VAL:HG11	1.90	0.54
1:AQ:105:VAL:O	1:AV:84:ARG:NH1	2.32	0.54
1:BA:139:GLN:OE1	1:CB:4:PRO:HA	2.08	0.54
1:BX:14:THR:OG1	1:BX:146:ASP:OD1	2.23	0.54
1:AG:122:ASP:OD2	1:AG:125:ASN:ND2	2.39	0.54
1:AP:48:VAL:HA	1:CD:125:ASN:OD1	2.06	0.54
1:AJ:110:VAL:HG22	1:BI:110:VAL:HG22	1.90	0.54
1:AU:149:LEU:HD13	1:BV:123:ALA:HB1	1.90	0.53
1:BE:34:LYS:HD2	1:CG:153:LEU:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AC:110:VAL:HG22	1:BG:110:VAL:HG22	1.91	0.53
1:AL:107:LEU:HB3	1:BM:113:SER:OG	2.09	0.53
1:AR:95:VAL:HG11	1:BS:118:ALA:HB1	1.91	0.53
1:AY:48:VAL:HA	1:BC:125:ASN:OD1	2.08	0.53
1:BT:122:ASP:OD2	1:BT:125:ASN:ND2	2.39	0.53
1:AS:95:VAL:HG11	1:CA:118:ALA:HB1	1.90	0.53
1:AQ:1:ALA:N	1:AV:147:THR:OG1	2.39	0.53
1:BN:122:ASP:OD2	1:BN:125:ASN:ND2	2.39	0.53
1:AP:122:ASP:OD2	1:AP:125:ASN:ND2	2.39	0.53
1:BR:122:ASP:OD2	1:BR:125:ASN:ND2	2.40	0.53
1:AD:110:VAL:HG22	1:AN:110:VAL:HG22	1.91	0.53
1:AJ:122:ASP:OD2	1:AJ:125:ASN:ND2	2.39	0.53
1:AX:113:SER:OG	1:BY:107:LEU:HB3	2.09	0.53
1:BB:122:ASP:OD2	1:BB:125:ASN:ND2	2.39	0.53
1:AB:106:MET:SD	1:BW:126:VAL:HA	2.49	0.53
1:AX:48:VAL:HA	1:BY:125:ASN:OD1	2.08	0.53
1:BD:48:VAL:HA	1:CH:125:ASN:OD1	2.08	0.52
1:BI:122:ASP:OD2	1:BI:125:ASN:ND2	2.40	0.52
1:CF:122:ASP:OD2	1:CF:125:ASN:ND2	2.39	0.52
1:AJ:136:VAL:HG21	1:BI:59:ILE:HD13	1.91	0.52
1:AT:14:THR:OG1	1:AT:146:ASP:OD1	2.23	0.52
1:AW:59:ILE:HD13	1:BB:136:VAL:HG21	1.90	0.52
1:AZ:150:SER:O	1:CD:51:HIS:NE2	2.37	0.52
1:BC:14:THR:OG1	1:BC:146:ASP:OD1	2.23	0.52
1:BE:95:VAL:HG11	1:CG:118:ALA:HB1	1.91	0.52
1:BH:48:VAL:HA	1:BX:125:ASN:OD1	2.09	0.52
1:AA:95:VAL:HG11	1:AH:118:ALA:HB1	1.92	0.52
1:BC:122:ASP:OD2	1:BC:125:ASN:ND2	2.40	0.52
1:AZ:151:GLY:HA2	1:CC:67:MET:HE3	1.90	0.52
1:AF:11:ALA:O	1:BJ:131:SER:HB2	2.09	0.52
1:AS:121:TYR:CZ	1:CA:99:VAL:HA	2.45	0.52
1:BL:122:ASP:OD2	1:BL:125:ASN:ND2	2.40	0.52
1:AZ:133:ALA:CA	1:CC:91:VAL:HG21	2.40	0.52
1:BD:92:ARG:HG2	1:BD:107:LEU:HD13	1.92	0.52
1:BP:92:ARG:HG2	1:BP:107:LEU:HD13	1.92	0.52
1:CG:122:ASP:OD2	1:CG:125:ASN:ND2	2.40	0.52
1:AB:84:ARG:NH1	1:BW:105:VAL:O	2.43	0.52
1:AE:113:SER:OG	1:BQ:107:LEU:HB3	2.09	0.52
1:BL:136:VAL:HG21	1:BN:59:ILE:HD13	1.92	0.52
1:BR:14:THR:OG1	1:BR:146:ASP:OD1	2.23	0.52
1:BV:92:ARG:HG2	1:BV:107:LEU:HD13	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BY:92:ARG:HG2	1:BY:107:LEU:HD13	1.92	0.52
1:AV:122:ASP:OD2	1:AV:125:ASN:ND2	2.39	0.52
1:AZ:107:LEU:HB3	1:CC:113:SER:OG	2.10	0.52
1:BS:92:ARG:HG2	1:BS:107:LEU:HD13	1.92	0.52
1:AB:153:LEU:HB3	1:BW:34:LYS:HD2	1.91	0.52
1:AR:92:ARG:HG2	1:AR:107:LEU:HD13	1.92	0.52
1:AE:14:THR:OG1	1:AE:146:ASP:OD1	2.23	0.51
1:AE:122:ASP:OD2	1:AE:125:ASN:ND2	2.40	0.51
1:AI:92:ARG:HG2	1:AI:107:LEU:HD13	1.92	0.51
1:AP:107:LEU:HB3	1:CD:113:SER:OG	2.10	0.51
1:AW:121:TYR:CZ	1:BB:99:VAL:HA	2.44	0.51
1:BM:92:ARG:HG2	1:BM:107:LEU:HD13	1.92	0.51
1:BQ:122:ASP:OD2	1:BQ:125:ASN:ND2	2.39	0.51
1:CE:92:ARG:HG2	1:CE:107:LEU:HD13	1.92	0.51
1:AE:126:VAL:HG13	1:BQ:106:MET:SD	2.50	0.51
1:AL:92:ARG:HG2	1:AL:107:LEU:HD13	1.92	0.51
1:AO:1:ALA:N	1:BP:147:THR:OG1	2.37	0.51
1:AX:92:ARG:HG2	1:AX:107:LEU:HD13	1.92	0.51
1:AA:122:ASP:OD2	1:AA:125:ASN:ND2	2.39	0.51
1:AL:95:VAL:HG11	1:BM:118:ALA:HB1	1.90	0.51
1:BG:92:ARG:HG2	1:BG:107:LEU:HD13	1.92	0.51
1:BJ:92:ARG:HG2	1:BJ:107:LEU:HD13	1.92	0.51
1:AD:34:LYS:HD2	1:AN:153:LEU:HB3	1.93	0.51
1:AE:107:LEU:HB3	1:BQ:113:SER:OG	2.11	0.51
1:AU:92:ARG:HG2	1:AU:107:LEU:HD13	1.92	0.51
1:AE:136:VAL:HG21	1:BQ:59:ILE:HD13	1.90	0.51
1:AO:92:ARG:HG2	1:AO:107:LEU:HD13	1.92	0.51
1:AP:101:GLN:HG3	1:CD:79:ILE:HD12	1.92	0.51
1:AS:11:ALA:O	1:CA:131:SER:HB2	2.11	0.51
1:AF:136:VAL:HG21	1:BJ:59:ILE:HD13	1.91	0.51
1:AP:101:GLN:NE2	1:CD:79:ILE:HG13	2.26	0.51
1:BD:13:GLN:CG	1:CH:131:SER:HB3	2.41	0.51
1:BE:110:VAL:HG22	1:CG:110:VAL:HG22	1.92	0.51
1:CE:14:THR:OG1	1:CE:146:ASP:OD1	2.24	0.51
1:CH:92:ARG:HG2	1:CH:107:LEU:HD13	1.92	0.51
1:AC:92:ARG:HG2	1:AC:107:LEU:HD13	1.92	0.51
1:AK:14:THR:OG1	1:AK:146:ASP:OD1	2.23	0.51
1:BA:98:ALA:HB2	1:CB:79:ILE:HD12	1.93	0.51
1:BC:74:ASN:O	1:CH:76:ASN:ND2	2.43	0.51
1:AL:113:SER:OG	1:BM:107:LEU:HB3	2.10	0.51
1:AA:105:VAL:O	1:AH:84:ARG:NH1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AK:122:ASP:OD2	1:AK:125:ASN:ND2	2.40	0.50
1:AS:107:LEU:HB3	1:CA:113:SER:OG	2.11	0.50
1:AW:126:VAL:HA	1:BB:106:MET:SD	2.52	0.50
1:CC:122:ASP:OD2	1:CC:125:ASN:ND2	2.39	0.50
1:BD:123:ALA:HB1	1:CH:149:LEU:HD13	1.92	0.50
1:BE:113:SER:OG	1:CG:107:LEU:HB3	2.11	0.50
1:BH:151:GLY:HA2	1:BX:67:MET:HE3	1.93	0.50
1:CA:122:ASP:OD2	1:CA:125:ASN:ND2	2.40	0.50
1:AB:122:ASP:OD2	1:AB:125:ASN:ND2	2.40	0.50
1:CB:92:ARG:HG2	1:CB:107:LEU:HD13	1.92	0.50
1:AC:125:ASN:OD1	1:BG:48:VAL:HA	2.12	0.50
1:AF:92:ARG:HG2	1:AF:107:LEU:HD13	1.92	0.50
1:AT:122:ASP:OD2	1:AT:125:ASN:ND2	2.40	0.50
1:BA:151:GLY:HA2	1:CB:67:MET:CE	2.40	0.50
1:BE:122:ASP:OD2	1:BE:125:ASN:ND2	2.39	0.50
1:CB:122:ASP:OD2	1:CB:125:ASN:ND2	2.41	0.50
1:AY:113:SER:OG	1:BC:107:LEU:HB3	2.11	0.50
1:AZ:147:THR:OG1	1:CC:1:ALA:N	2.44	0.50
1:CD:122:ASP:OD2	1:CD:125:ASN:ND2	2.40	0.50
1:AL:118:ALA:HB1	1:BM:95:VAL:HG11	1.92	0.50
1:AH:53:VAL:HG23	1:AK:149:LEU:O	2.11	0.50
1:AR:51:HIS:CD2	1:AV:152:ILE:HD11	2.47	0.50
1:AR:107:LEU:HB3	1:BS:113:SER:OG	2.12	0.50
1:AR:123:ALA:HB1	1:BS:149:LEU:HD13	1.92	0.50
1:AZ:133:ALA:HA	1:CC:91:VAL:HG21	1.92	0.50
1:BA:92:ARG:HG2	1:BA:107:LEU:HD13	1.92	0.50
1:BD:1:ALA:N	1:CH:152:ILE:O	2.45	0.50
1:BF:14:THR:OG1	1:BF:146:ASP:OD1	2.23	0.50
1:BK:122:ASP:OD2	1:BK:125:ASN:ND2	2.39	0.50
1:BO:122:ASP:OD2	1:BO:125:ASN:ND2	2.40	0.50
1:BW:122:ASP:OD2	1:BW:125:ASN:ND2	2.39	0.50
1:AG:153:LEU:HD22	1:AK:61:PHE:CD2	2.46	0.50
1:BA:106:MET:HG3	1:CB:113:SER:O	2.12	0.50
1:BH:143:GLY:HA3	1:BX:1:ALA:O	2.11	0.50
1:AC:14:THR:OG1	1:AC:146:ASP:OD1	2.25	0.50
1:BD:127:LYS:HG3	1:CH:149:LEU:HD11	1.93	0.50
1:BH:153:LEU:HD21	1:BX:63:ARG:HB3	1.93	0.50
1:BP:122:ASP:OD2	1:BP:125:ASN:ND2	2.41	0.49
1:AL:76:ASN:ND2	1:BL:74:ASN:O	2.45	0.49
1:AN:122:ASP:OD2	1:AN:125:ASN:ND2	2.40	0.49
1:AU:123:ALA:HB1	1:BV:149:LEU:HD13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:143:GLY:HA3	1:CB:1:ALA:O	2.12	0.49
1:BF:122:ASP:OD2	1:BF:125:ASN:ND2	2.40	0.49
1:CG:14:THR:OG1	1:CG:146:ASP:OD1	2.23	0.49
1:AB:126:VAL:HA	1:BW:106:MET:SD	2.52	0.49
1:AJ:110:VAL:HG21	1:BI:137:LEU:HD11	1.94	0.49
1:AL:126:VAL:HG13	1:BM:106:MET:SD	2.52	0.49
1:AY:122:ASP:OD2	1:AY:125:ASN:ND2	2.39	0.49
1:BD:95:VAL:HG11	1:CH:118:ALA:HB1	1.95	0.49
1:BU:122:ASP:OD2	1:BU:125:ASN:ND2	2.40	0.49
1:AA:11:ALA:O	1:AH:131:SER:HB2	2.12	0.49
1:BL:14:THR:OG1	1:BL:146:ASP:OD1	2.23	0.49
1:AD:137:LEU:HD11	1:AN:110:VAL:HG21	1.95	0.49
1:AG:34:LYS:HG3	1:AK:153:LEU:HD13	1.93	0.49
1:AQ:136:VAL:HG21	1:AV:59:ILE:HD13	1.95	0.49
1:AS:59:ILE:HD13	1:CA:136:VAL:HG21	1.95	0.49
1:BL:84:ARG:NH1	1:BN:105:VAL:O	2.46	0.49
1:CD:58:THR:O	1:CD:91:VAL:HA	2.13	0.49
1:AW:105:VAL:O	1:BB:84:ARG:NH1	2.38	0.49
1:BA:148:ALA:HA	1:CB:87:TYR:CE2	2.47	0.49
1:BX:58:THR:O	1:BX:91:VAL:HA	2.13	0.49
1:AO:59:ILE:HD13	1:BP:136:VAL:HG21	1.93	0.49
1:AB:106:MET:SD	1:BW:126:VAL:HG13	2.52	0.49
1:AH:122:ASP:OD2	1:AH:125:ASN:ND2	2.40	0.49
1:AK:58:THR:O	1:AK:91:VAL:HA	2.13	0.49
1:AZ:58:THR:O	1:AZ:91:VAL:HA	2.13	0.49
1:BL:58:THR:O	1:BL:91:VAL:HA	2.13	0.49
1:CH:122:ASP:OD2	1:CH:125:ASN:ND2	2.41	0.49
1:AI:72:VAL:HB	1:AK:78:VAL:HG22	1.95	0.48
1:AS:110:VAL:HG22	1:CA:110:VAL:HG22	1.94	0.48
1:BA:37:ALA:HB3	1:CC:152:ILE:HD13	1.95	0.48
1:BC:58:THR:O	1:BC:91:VAL:HA	2.13	0.48
1:BF:58:THR:O	1:BF:91:VAL:HA	2.13	0.48
1:CA:58:THR:O	1:CA:91:VAL:HA	2.13	0.48
1:AB:41:THR:HG23	1:AB:50:THR:HG22	1.96	0.48
1:AR:122:ASP:OD2	1:AR:125:ASN:ND2	2.41	0.48
1:BR:58:THR:O	1:BR:91:VAL:HA	2.13	0.48
1:BU:58:THR:O	1:BU:91:VAL:HA	2.13	0.48
1:AE:58:THR:O	1:AE:91:VAL:HA	2.13	0.48
1:AS:105:VAL:O	1:CA:84:ARG:NH1	2.46	0.48
1:AF:118:ALA:HB1	1:BJ:95:VAL:HG11	1.96	0.48
1:AN:58:THR:O	1:AN:91:VAL:HA	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AR:76:ASN:HD21	1:BR:75:SER:HA	1.79	0.48
1:AV:14:THR:OG1	1:AV:146:ASP:OD1	2.26	0.48
1:AY:137:LEU:HD11	1:BC:110:VAL:HG21	1.94	0.48
1:BI:58:THR:O	1:BI:91:VAL:HA	2.13	0.48
1:BU:41:THR:HG23	1:BU:50:THR:HG22	1.96	0.48
1:CA:41:THR:HG23	1:CA:50:THR:HG22	1.96	0.48
1:AE:41:THR:HG23	1:AE:50:THR:HG22	1.96	0.48
1:AG:48:VAL:HA	1:AK:125:ASN:OD1	2.13	0.48
1:BD:131:SER:HB3	1:CH:13:GLN:HG3	1.95	0.48
1:BU:14:THR:OG1	1:BU:146:ASP:OD1	2.23	0.48
1:CF:14:THR:OG1	1:CF:146:ASP:OD1	2.26	0.48
1:AG:95:VAL:HG11	1:AK:118:ALA:HB1	1.95	0.48
1:AP:14:THR:OG1	1:AP:146:ASP:OD1	2.26	0.48
1:AS:113:SER:OG	1:CA:107:LEU:HB3	2.13	0.48
1:AT:58:THR:O	1:AT:91:VAL:HA	2.13	0.48
1:BL:41:THR:HG23	1:BL:50:THR:HG22	1.96	0.48
1:AB:58:THR:O	1:AB:91:VAL:HA	2.13	0.48
1:AL:121:TYR:CZ	1:BM:99:VAL:HA	2.49	0.48
1:AQ:58:THR:O	1:AQ:91:VAL:HA	2.13	0.48
1:AW:41:THR:HG23	1:AW:50:THR:HG22	1.96	0.48
1:AW:110:VAL:HG21	1:BB:137:LEU:HD11	1.95	0.48
1:AZ:95:VAL:HG11	1:CC:118:ALA:CB	2.42	0.48
1:AZ:152:ILE:HG23	1:CD:26:ASP:OD1	2.14	0.48
1:BI:41:THR:HG23	1:BI:50:THR:HG22	1.96	0.48
1:BS:122:ASP:OD2	1:BS:125:ASN:ND2	2.41	0.48
1:BZ:122:ASP:OD2	1:BZ:125:ASN:ND2	2.39	0.48
1:CD:41:THR:HG23	1:CD:50:THR:HG22	1.96	0.48
1:AA:110:VAL:HG22	1:AH:110:VAL:HG22	1.96	0.48
1:AE:110:VAL:HG22	1:BQ:110:VAL:HG22	1.95	0.48
1:AJ:113:SER:OG	1:BI:107:LEU:HB3	2.13	0.48
1:AX:59:ILE:HD13	1:BY:136:VAL:HG21	1.95	0.48
1:AY:107:LEU:HB3	1:BC:113:SER:OG	2.13	0.48
1:BE:136:VAL:HG21	1:CG:59:ILE:HD13	1.95	0.48
1:BV:51:HIS:CD2	1:CF:152:ILE:HD11	2.49	0.48
1:AZ:139:GLN:OE1	1:CC:4:PRO:CA	2.55	0.48
1:BA:5:SER:HB2	1:CB:139:GLN:HE22	1.79	0.48
1:CD:14:THR:OG1	1:CD:146:ASP:OD1	2.23	0.48
1:CE:122:ASP:OD2	1:CE:125:ASN:ND2	2.41	0.48
1:AN:14:THR:OG1	1:AN:146:ASP:OD1	2.23	0.48
1:AS:34:LYS:HD2	1:CA:153:LEU:HB3	1.95	0.48
1:AW:58:THR:O	1:AW:91:VAL:HA	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AZ:91:VAL:HG21	1:CC:133:ALA:HB2	1.96	0.48
1:AZ:152:ILE:HG23	1:CD:26:ASP:HA	1.95	0.48
1:AB:14:THR:OG1	1:AB:146:ASP:OD1	2.23	0.47
1:AE:95:VAL:HG11	1:BQ:118:ALA:HB1	1.95	0.47
1:AH:58:THR:O	1:AH:91:VAL:HA	2.13	0.47
1:AV:27:THR:OG1	1:BY:153:LEU:HB3	2.14	0.47
1:AZ:122:ASP:OD2	1:AZ:125:ASN:ND2	2.40	0.47
1:BC:41:THR:HG23	1:BC:50:THR:HG22	1.96	0.47
1:BD:149:LEU:HD11	1:CH:127:LYS:HG3	1.95	0.47
1:BL:118:ALA:HB1	1:BN:95:VAL:HG11	1.96	0.47
1:AH:41:THR:HG23	1:AH:50:THR:HG22	1.96	0.47
1:AI:122:ASP:OD2	1:AI:125:ASN:ND2	2.41	0.47
1:AL:14:THR:OG1	1:AL:146:ASP:OD1	2.24	0.47
1:AY:14:THR:OG1	1:AY:146:ASP:OD1	2.26	0.47
1:AZ:41:THR:HG23	1:AZ:50:THR:HG22	1.96	0.47
1:AC:122:ASP:OD2	1:AC:125:ASN:ND2	2.41	0.47
1:AK:41:THR:HG23	1:AK:50:THR:HG22	1.96	0.47
1:AZ:10:GLY:HA3	1:CC:131:SER:OG	2.14	0.47
1:BD:101:GLN:NE2	1:CH:79:ILE:HG13	2.29	0.47
1:AT:41:THR:HG23	1:AT:50:THR:HG22	1.96	0.47
1:CG:58:THR:O	1:CG:91:VAL:HA	2.13	0.47
1:AI:14:THR:OG1	1:AI:146:ASP:OD1	2.25	0.47
1:AO:26:ASP:OD1	1:AO:27:THR:N	2.48	0.47
1:AX:14:THR:OG1	1:AX:146:ASP:OD1	2.25	0.47
1:AX:76:ASN:ND2	1:BX:74:ASN:O	2.48	0.47
1:AZ:4:PRO:HA	1:CC:139:GLN:OE1	2.15	0.47
1:BA:84:ARG:NH1	1:CB:105:VAL:O	2.48	0.47
1:BF:41:THR:HG23	1:BF:50:THR:HG22	1.96	0.47
1:AN:41:THR:HG23	1:AN:50:THR:HG22	1.96	0.47
1:BA:153:LEU:HB2	1:CB:63:ARG:HD3	1.95	0.47
1:BC:72:VAL:CG1	1:CH:78:VAL:HG11	2.44	0.47
1:BG:122:ASP:OD2	1:BG:125:ASN:ND2	2.41	0.47
1:BO:41:THR:HG23	1:BO:50:THR:HG22	1.96	0.47
1:BO:58:THR:O	1:BO:91:VAL:HA	2.13	0.47
1:AC:136:VAL:HG21	1:BG:59:ILE:HD13	1.97	0.47
1:AL:122:ASP:OD2	1:AL:125:ASN:ND2	2.41	0.47
1:AQ:41:THR:HG23	1:AQ:50:THR:HG22	1.96	0.47
1:AW:106:MET:SD	1:BB:126:VAL:HG13	2.55	0.47
1:AZ:149:LEU:HD22	1:CC:119:ASP:O	2.15	0.47
1:BA:26:ASP:OD1	1:BA:27:THR:N	2.48	0.47
1:BG:26:ASP:OD1	1:BG:27:THR:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BO:14:THR:OG1	1:BO:146:ASP:OD1	2.23	0.47
1:BU:121:TYR:CZ	1:CF:99:VAL:HA	2.50	0.47
1:BX:41:THR:HG23	1:BX:50:THR:HG22	1.96	0.47
1:BX:122:ASP:OD2	1:BX:125:ASN:ND2	2.40	0.47
1:BY:122:ASP:OD2	1:BY:125:ASN:ND2	2.41	0.47
1:CA:14:THR:OG1	1:CA:146:ASP:OD1	2.23	0.47
1:AF:58:THR:O	1:AF:91:VAL:HA	2.15	0.47
1:AL:26:ASP:OD1	1:AL:27:THR:N	2.48	0.47
1:AU:58:THR:O	1:AU:91:VAL:HA	2.15	0.47
1:AX:1:ALA:H2	1:BY:147:THR:HG1	1.59	0.47
1:AX:82:ILE:HG21	1:BY:104:GLN:HG3	1.96	0.47
1:BG:58:THR:O	1:BG:91:VAL:HA	2.15	0.47
1:BH:148:ALA:HB1	1:BX:114:VAL:HG21	1.96	0.47
1:BP:26:ASP:OD1	1:BP:27:THR:N	2.48	0.47
1:BS:14:THR:OG1	1:BS:146:ASP:OD1	2.24	0.47
1:CE:26:ASP:OD1	1:CE:27:THR:N	2.48	0.47
1:CG:41:THR:HG23	1:CG:50:THR:HG22	1.96	0.47
1:AE:106:MET:SD	1:BQ:126:VAL:HA	2.55	0.47
1:AU:78:VAL:HG11	1:BU:72:VAL:HG11	1.97	0.47
1:AW:113:SER:OG	1:BB:107:LEU:HB3	2.15	0.47
1:BA:58:THR:O	1:BA:91:VAL:HA	2.15	0.47
1:BD:26:ASP:OD1	1:BD:27:THR:N	2.48	0.47
1:BE:59:ILE:HD13	1:CG:136:VAL:HG21	1.97	0.47
1:BE:99:VAL:HA	1:CG:121:TYR:CZ	2.50	0.47
1:BH:126:VAL:HG13	1:BX:106:MET:SD	2.55	0.47
1:AG:117:GLY:HA3	1:AK:97:PRO:O	2.16	0.47
1:AZ:130:LEU:HD23	1:CC:108:VAL:HG21	1.97	0.47
1:BD:58:THR:O	1:BD:91:VAL:HA	2.15	0.47
1:AB:121:TYR:CZ	1:BW:99:VAL:HA	2.51	0.46
1:AC:58:THR:O	1:AC:91:VAL:HA	2.15	0.46
1:AG:14:THR:OG1	1:AG:146:ASP:OD1	2.26	0.46
1:AJ:99:VAL:HA	1:BI:121:TYR:CE1	2.50	0.46
1:AS:106:MET:SD	1:CA:126:VAL:HA	2.55	0.46
1:AX:107:LEU:HB3	1:BY:113:SER:OG	2.15	0.46
1:BE:107:LEU:HB3	1:CG:113:SER:OG	2.16	0.46
1:CB:26:ASP:OD1	1:CB:27:THR:N	2.48	0.46
1:CB:58:THR:O	1:CB:91:VAL:HA	2.15	0.46
1:AL:58:THR:O	1:AL:91:VAL:HA	2.15	0.46
1:AR:58:THR:O	1:AR:91:VAL:HA	2.15	0.46
1:AW:14:THR:OG1	1:AW:146:ASP:OD1	2.23	0.46
1:AW:122:ASP:OD2	1:AW:125:ASN:ND2	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AX:58:THR:O	1:AX:91:VAL:HA	2.15	0.46
1:BH:121:TYR:CE1	1:BX:99:VAL:HA	2.51	0.46
1:BJ:58:THR:O	1:BJ:91:VAL:HA	2.15	0.46
1:AI:26:ASP:OD1	1:AI:27:THR:N	2.48	0.46
1:AU:26:ASP:OD1	1:AU:27:THR:N	2.48	0.46
1:AX:51:HIS:CD2	1:BB:152:ILE:HD11	2.50	0.46
1:BD:13:GLN:HG3	1:CH:131:SER:HB3	1.97	0.46
1:BR:41:THR:HG23	1:BR:50:THR:HG22	1.96	0.46
1:BV:26:ASP:OD1	1:BV:27:THR:N	2.48	0.46
1:BV:122:ASP:OD2	1:BV:125:ASN:ND2	2.41	0.46
1:BY:58:THR:O	1:BY:91:VAL:HA	2.15	0.46
1:AO:58:THR:O	1:AO:91:VAL:HA	2.15	0.46
1:AU:122:ASP:OD2	1:AU:125:ASN:ND2	2.41	0.46
1:AX:78:VAL:HG11	1:BX:72:VAL:CG1	2.45	0.46
1:BD:149:LEU:HD13	1:CH:123:ALA:HB1	1.97	0.46
1:BP:14:THR:OG1	1:BP:146:ASP:OD1	2.25	0.46
1:CE:58:THR:O	1:CE:91:VAL:HA	2.15	0.46
1:CH:58:THR:O	1:CH:91:VAL:HA	2.15	0.46
1:AW:107:LEU:HB3	1:BB:113:SER:OG	2.15	0.46
1:BJ:14:THR:OG1	1:BJ:146:ASP:OD1	2.25	0.46
1:BJ:26:ASP:OD1	1:BJ:27:THR:N	2.48	0.46
1:AF:26:ASP:OD1	1:AF:27:THR:N	2.48	0.46
1:AX:26:ASP:OD1	1:AX:27:THR:N	2.48	0.46
1:AL:110:VAL:HG22	1:BM:110:VAL:HG22	1.98	0.46
1:AQ:122:ASP:OD2	1:AQ:125:ASN:ND2	2.40	0.46
1:BM:58:THR:O	1:BM:91:VAL:HA	2.15	0.46
1:BS:26:ASP:OD1	1:BS:27:THR:N	2.48	0.46
1:BS:58:THR:O	1:BS:91:VAL:HA	2.15	0.46
1:AF:14:THR:OG1	1:AF:146:ASP:OD1	2.25	0.46
1:AK:75:SER:HA	1:BM:76:ASN:HD21	1.80	0.46
1:AL:136:VAL:HG21	1:BM:59:ILE:HD13	1.98	0.46
1:AO:125:ASN:OD1	1:BP:48:VAL:HA	2.16	0.46
1:BV:58:THR:O	1:BV:91:VAL:HA	2.15	0.46
1:BY:26:ASP:OD1	1:BY:27:THR:N	2.48	0.46
1:CH:26:ASP:OD1	1:CH:27:THR:N	2.48	0.46
1:AO:123:ALA:HB1	1:BP:149:LEU:HD13	1.98	0.45
1:AZ:136:VAL:CG2	1:CC:59:ILE:HD13	2.39	0.45
1:BJ:122:ASP:OD2	1:BJ:125:ASN:ND2	2.41	0.45
1:AB:152:ILE:O	1:BW:1:ALA:N	2.49	0.45
1:AL:126:VAL:HA	1:BM:106:MET:SD	2.57	0.45
1:AP:127:LYS:O	1:CD:13:GLN:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AR:72:VAL:CB	1:CD:78:VAL:HG22	2.42	0.45
1:AU:14:THR:OG1	1:AU:146:ASP:OD1	2.24	0.45
1:AW:152:ILE:O	1:BB:1:ALA:N	2.50	0.45
1:AZ:110:VAL:HG22	1:CC:110:VAL:HG13	1.98	0.45
1:BA:153:LEU:CD2	1:CB:32:LEU:O	2.64	0.45
1:BP:58:THR:O	1:BP:91:VAL:HA	2.15	0.45
1:CD:130:LEU:HD23	1:CD:130:LEU:HA	1.85	0.45
1:AG:58:THR:O	1:AG:91:VAL:HA	2.17	0.45
1:AJ:99:VAL:HA	1:BI:121:TYR:CZ	2.51	0.45
1:AJ:106:MET:SD	1:BI:126:VAL:HA	2.56	0.45
1:AU:118:ALA:HB1	1:BV:95:VAL:HG11	1.97	0.45
1:BM:130:LEU:HD23	1:BM:130:LEU:HA	1.81	0.45
1:BT:58:THR:O	1:BT:91:VAL:HA	2.17	0.45
1:AI:58:THR:O	1:AI:91:VAL:HA	2.15	0.45
1:AO:122:ASP:OD2	1:AO:125:ASN:ND2	2.41	0.45
1:AP:58:THR:O	1:AP:91:VAL:HA	2.17	0.45
1:AR:149:LEU:HD13	1:BS:123:ALA:HB1	1.99	0.45
1:AX:130:LEU:HD23	1:AX:130:LEU:HA	1.81	0.45
1:BE:58:THR:O	1:BE:91:VAL:HA	2.17	0.45
1:BK:58:THR:O	1:BK:91:VAL:HA	2.17	0.45
1:AA:58:THR:O	1:AA:91:VAL:HA	2.17	0.45
1:AD:104:GLN:HG3	1:AN:82:ILE:HG21	1.98	0.45
1:AG:136:VAL:CG2	1:AK:8:VAL:HG11	2.47	0.45
1:AX:113:SER:O	1:BY:106:MET:HG3	2.17	0.45
1:BA:90:LEU:HD21	1:BA:92:ARG:HG3	1.99	0.45
1:BH:110:VAL:HG22	1:BX:110:VAL:HG22	1.99	0.45
1:BN:58:THR:O	1:BN:91:VAL:HA	2.17	0.45
1:CA:130:LEU:HD23	1:CA:130:LEU:HA	1.85	0.45
1:BA:118:ALA:HB1	1:CB:95:VAL:HG11	1.98	0.45
1:BG:90:LEU:HD21	1:BG:92:ARG:HG3	1.99	0.45
1:BM:26:ASP:OD1	1:BM:27:THR:N	2.48	0.45
1:BY:90:LEU:HD21	1:BY:92:ARG:HG3	1.99	0.45
1:AD:58:THR:O	1:AD:91:VAL:HA	2.17	0.45
1:AR:26:ASP:OD1	1:AR:27:THR:N	2.48	0.45
1:AY:58:THR:O	1:AY:91:VAL:HA	2.17	0.45
1:BA:72:VAL:HB	1:BC:78:VAL:HG22	1.98	0.45
1:BV:90:LEU:HD21	1:BV:92:ARG:HG3	1.99	0.45
1:AF:90:LEU:HD21	1:AF:92:ARG:HG3	1.99	0.45
1:AH:14:THR:OG1	1:AH:146:ASP:OD1	2.23	0.45
1:AL:99:VAL:HA	1:BM:121:TYR:CE1	2.52	0.45
1:AM:58:THR:O	1:AM:91:VAL:HA	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AS:58:THR:O	1:AS:91:VAL:HA	2.17	0.45
1:AV:58:THR:O	1:AV:91:VAL:HA	2.17	0.45
1:AX:78:VAL:HG21	1:BX:73:PRO:HG2	1.99	0.45
1:BD:122:ASP:OD2	1:BD:125:ASN:ND2	2.41	0.45
1:BU:84:ARG:NH1	1:CF:105:VAL:O	2.50	0.45
1:CC:58:THR:O	1:CC:91:VAL:HA	2.17	0.45
1:BB:58:THR:O	1:BB:91:VAL:HA	2.17	0.45
1:BC:93:LYS:NZ	1:BC:94:GLY:O	2.50	0.45
1:BS:90:LEU:HD21	1:BS:92:ARG:HG3	1.99	0.45
1:AA:137:LEU:HD11	1:AH:110:VAL:HG21	1.99	0.45
1:AE:130:LEU:HD23	1:AE:130:LEU:HA	1.85	0.45
1:AL:90:LEU:HD21	1:AL:92:ARG:HG3	1.99	0.45
1:AW:93:LYS:NZ	1:AW:94:GLY:O	2.50	0.45
1:BB:14:THR:OG1	1:BB:146:ASP:OD1	2.26	0.45
1:BM:14:THR:OG1	1:BM:146:ASP:OD1	2.24	0.45
1:BP:90:LEU:HD21	1:BP:92:ARG:HG3	1.99	0.45
1:AC:79:ILE:HG13	1:BG:101:GLN:NE2	2.32	0.44
1:AI:90:LEU:HD21	1:AI:92:ARG:HG3	1.99	0.44
1:AJ:58:THR:O	1:AJ:91:VAL:HA	2.17	0.44
1:AO:14:THR:OG1	1:AO:146:ASP:OD1	2.25	0.44
1:AW:121:TYR:CE1	1:BB:99:VAL:HA	2.52	0.44
1:AZ:93:LYS:NZ	1:AZ:94:GLY:O	2.50	0.44
1:BD:153:LEU:HG	1:CH:34:LYS:HD2	1.97	0.44
1:BE:99:VAL:HA	1:CG:121:TYR:CE1	2.52	0.44
1:BI:93:LYS:NZ	1:BI:94:GLY:O	2.50	0.44
1:AJ:105:VAL:O	1:BI:84:ARG:NH1	2.50	0.44
1:AK:93:LYS:NZ	1:AK:94:GLY:O	2.50	0.44
1:BD:90:LEU:HD21	1:BD:92:ARG:HG3	1.99	0.44
1:AE:133:ALA:HB2	1:BQ:91:VAL:HG21	1.99	0.44
1:AJ:91:VAL:HG21	1:BI:133:ALA:HB2	1.99	0.44
1:AQ:110:VAL:HG21	1:AV:137:LEU:HD11	1.98	0.44
1:BD:127:LYS:O	1:CH:13:GLN:HG3	2.17	0.44
1:BD:131:SER:HB3	1:CH:13:GLN:HG2	1.98	0.44
1:BJ:90:LEU:HD21	1:BJ:92:ARG:HG3	1.99	0.44
1:CB:90:LEU:HD21	1:CB:92:ARG:HG3	1.99	0.44
1:CH:14:THR:OG1	1:CH:146:ASP:OD1	2.25	0.44
1:AW:130:LEU:HD23	1:AW:130:LEU:HA	1.85	0.44
1:AZ:21:TYR:HE2	1:CC:131:SER:OG	2.00	0.44
1:BQ:58:THR:O	1:BQ:91:VAL:HA	2.17	0.44
1:CF:58:THR:O	1:CF:91:VAL:HA	2.17	0.44
1:AR:90:LEU:HD21	1:AR:92:ARG:HG3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:140:GLN:NE2	1:CB:3:SER:O	2.50	0.44
1:BD:118:ALA:HB1	1:CH:95:VAL:HG11	1.99	0.44
1:BH:129:ALA:HB2	1:BX:93:LYS:CB	2.48	0.44
1:BH:147:THR:OG1	1:BX:1:ALA:N	2.49	0.44
1:BU:86:THR:HA	1:BU:112:ILE:O	2.18	0.44
1:CD:93:LYS:NZ	1:CD:94:GLY:O	2.50	0.44
1:AB:93:LYS:NZ	1:AB:94:GLY:O	2.50	0.44
1:AD:95:VAL:HG11	1:AN:118:ALA:CB	2.47	0.44
1:AH:93:LYS:NZ	1:AH:94:GLY:O	2.50	0.44
1:AO:95:VAL:HG11	1:BP:118:ALA:HB1	1.99	0.44
1:AP:34:LYS:HG3	1:CD:153:LEU:HD13	1.99	0.44
1:AR:113:SER:OG	1:BS:107:LEU:HB3	2.17	0.44
1:AR:126:VAL:HA	1:BS:106:MET:SD	2.58	0.44
1:AX:90:LEU:HD21	1:AX:92:ARG:HG3	1.99	0.44
1:BI:86:THR:HA	1:BI:112:ILE:O	2.18	0.44
1:BM:86:THR:HG22	1:BM:113:SER:CB	2.48	0.44
1:BM:90:LEU:HD21	1:BM:92:ARG:HG3	1.99	0.44
1:BO:130:LEU:HD23	1:BO:130:LEU:HA	1.85	0.44
1:BX:86:THR:HA	1:BX:112:ILE:O	2.18	0.44
1:AB:86:THR:HA	1:AB:112:ILE:O	2.18	0.44
1:AB:118:ALA:HB1	1:BW:95:VAL:HG11	1.98	0.44
1:AC:90:LEU:HD21	1:AC:92:ARG:HG3	1.99	0.44
1:AC:113:SER:OG	1:BG:107:LEU:HB3	2.17	0.44
1:AE:93:LYS:NZ	1:AE:94:GLY:O	2.50	0.44
1:AO:86:THR:HG22	1:AO:113:SER:CB	2.48	0.44
1:AQ:93:LYS:NZ	1:AQ:94:GLY:O	2.50	0.44
1:AR:118:ALA:HB1	1:BS:95:VAL:HG11	2.00	0.44
1:AU:113:SER:OG	1:BV:107:LEU:HB3	2.18	0.44
1:AZ:139:GLN:OE1	1:CC:5:SER:N	2.48	0.44
1:BH:14:THR:OG1	1:BH:146:ASP:OD1	2.26	0.44
1:BH:58:THR:O	1:BH:91:VAL:HA	2.17	0.44
1:BM:122:ASP:OD2	1:BM:125:ASN:ND2	2.41	0.44
1:BS:130:LEU:HD23	1:BS:130:LEU:HA	1.81	0.44
1:AE:86:THR:HA	1:AE:112:ILE:O	2.18	0.44
1:AF:95:VAL:HG11	1:BJ:118:ALA:HB1	1.99	0.44
1:AO:90:LEU:HD21	1:AO:92:ARG:HG3	1.99	0.44
1:AT:86:THR:HA	1:AT:112:ILE:O	2.18	0.44
1:AU:90:LEU:HD21	1:AU:92:ARG:HG3	1.99	0.44
1:BF:86:THR:HA	1:BF:112:ILE:O	2.18	0.44
1:BJ:86:THR:HG22	1:BJ:113:SER:CB	2.48	0.44
1:BR:93:LYS:NZ	1:BR:94:GLY:O	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BW:58:THR:O	1:BW:91:VAL:HA	2.17	0.44
1:AC:28:ALA:HB1	1:AC:29:PRO:HD2	2.00	0.44
1:AC:95:VAL:HG11	1:BG:118:ALA:HB1	2.00	0.44
1:AL:86:THR:HG22	1:AL:113:SER:CB	2.48	0.44
1:AP:98:ALA:HB3	1:AP:101:GLN:CG	2.47	0.44
1:AP:136:VAL:CG2	1:CD:8:VAL:HG11	2.47	0.44
1:AW:84:ARG:NH1	1:BB:105:VAL:O	2.51	0.44
1:AX:122:ASP:OD2	1:AX:125:ASN:ND2	2.41	0.44
1:AY:126:VAL:HG13	1:BC:106:MET:SD	2.58	0.44
1:BV:14:THR:OG1	1:BV:146:ASP:OD1	2.25	0.44
1:BZ:58:THR:O	1:BZ:91:VAL:HA	2.17	0.44
1:CA:86:THR:HA	1:CA:112:ILE:O	2.18	0.44
1:CE:90:LEU:HD21	1:CE:92:ARG:HG3	1.99	0.44
1:CH:90:LEU:HD21	1:CH:92:ARG:HG3	1.99	0.44
1:AE:99:VAL:HA	1:BQ:121:TYR:CE1	2.53	0.43
1:AK:74:ASN:O	1:BM:76:ASN:ND2	2.51	0.43
1:AW:86:THR:HA	1:AW:112:ILE:O	2.18	0.43
1:AZ:149:LEU:C	1:CD:53:VAL:HG23	2.39	0.43
1:BA:28:ALA:HB1	1:BA:29:PRO:HD2	2.00	0.43
1:BD:107:LEU:HB3	1:CH:113:SER:OG	2.18	0.43
1:BF:93:LYS:NZ	1:BF:94:GLY:O	2.50	0.43
1:BR:86:THR:HA	1:BR:112:ILE:O	2.18	0.43
1:AC:26:ASP:OD1	1:AC:27:THR:N	2.48	0.43
1:AF:86:THR:HG22	1:AF:113:SER:CB	2.48	0.43
1:AF:122:ASP:OD2	1:AF:125:ASN:ND2	2.41	0.43
1:AN:86:THR:HA	1:AN:112:ILE:O	2.18	0.43
1:AN:137:LEU:HD23	1:AN:137:LEU:HA	1.89	0.43
1:AR:78:VAL:HG11	1:BR:72:VAL:HG11	2.00	0.43
1:AR:86:THR:HG22	1:AR:113:SER:CB	2.48	0.43
1:AZ:108:VAL:HG22	1:CC:112:ILE:HG23	1.99	0.43
1:BA:86:THR:HG22	1:BA:113:SER:CB	2.48	0.43
1:BA:110:VAL:HG22	1:CB:110:VAL:HG22	2.00	0.43
1:BD:14:THR:OG1	1:BD:146:ASP:OD1	2.24	0.43
1:BD:128:ALA:HA	1:CH:16:PHE:HE2	1.83	0.43
1:BG:86:THR:HG22	1:BG:113:SER:CB	2.48	0.43
1:BK:98:ALA:HB3	1:BK:101:GLN:CG	2.47	0.43
1:BL:93:LYS:NZ	1:BL:94:GLY:O	2.50	0.43
1:BL:95:VAL:HG11	1:BN:118:ALA:HB1	2.00	0.43
1:BL:121:TYR:CZ	1:BN:99:VAL:HA	2.53	0.43
1:BU:93:LYS:NZ	1:BU:94:GLY:O	2.50	0.43
1:BV:86:THR:HG22	1:BV:113:SER:CB	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CD:86:THR:HA	1:CD:112:ILE:O	2.18	0.43
1:CE:28:ALA:HB1	1:CE:29:PRO:HD2	2.00	0.43
1:AA:14:THR:OG1	1:AA:146:ASP:OD1	2.26	0.43
1:AO:136:VAL:HG21	1:BP:59:ILE:HD13	1.99	0.43
1:AU:86:THR:HG22	1:AU:113:SER:CB	2.48	0.43
1:AZ:152:ILE:HG12	1:CD:26:ASP:OD2	2.19	0.43
1:BG:28:ALA:HB1	1:BG:29:PRO:HD2	2.00	0.43
1:BJ:28:ALA:HB1	1:BJ:29:PRO:HD2	2.00	0.43
1:BO:93:LYS:NZ	1:BO:94:GLY:O	2.50	0.43
1:BP:86:THR:HG22	1:BP:113:SER:CB	2.48	0.43
1:AD:107:LEU:HB3	1:AN:113:SER:OG	2.18	0.43
1:AJ:93:LYS:CB	1:BI:129:ALA:HB2	2.48	0.43
1:AZ:86:THR:HA	1:AZ:112:ILE:O	2.18	0.43
1:BY:86:THR:HG22	1:BY:113:SER:CB	2.48	0.43
1:AF:28:ALA:HB1	1:AF:29:PRO:HD2	2.00	0.43
1:AG:113:SER:OG	1:AK:107:LEU:HB3	2.18	0.43
1:BZ:137:LEU:HD23	1:BZ:137:LEU:HA	1.89	0.43
1:CB:86:THR:HG22	1:CB:113:SER:CB	2.48	0.43
1:CH:86:THR:HG22	1:CH:113:SER:CB	2.48	0.43
1:AE:129:ALA:HB2	1:BQ:93:LYS:CB	2.48	0.43
1:AQ:75:SER:HA	1:BS:76:ASN:HD21	1.83	0.43
1:AU:76:ASN:HD21	1:BU:75:SER:HA	1.82	0.43
1:AZ:1:ALA:HB3	1:CC:146:ASP:HB2	2.00	0.43
1:AZ:152:ILE:HG12	1:CD:26:ASP:CG	2.38	0.43
1:BC:86:THR:HA	1:BC:112:ILE:O	2.18	0.43
1:BD:110:VAL:HG22	1:CH:110:VAL:HG22	2.00	0.43
1:BE:137:LEU:HD23	1:BE:137:LEU:HA	1.89	0.43
1:BS:28:ALA:HB1	1:BS:29:PRO:HD2	2.00	0.43
1:AA:98:ALA:HB3	1:AA:101:GLN:CG	2.47	0.43
1:AA:118:ALA:HB1	1:AH:95:VAL:HG11	2.01	0.43
1:AL:28:ALA:HB1	1:AL:29:PRO:HD2	2.00	0.43
1:BC:72:VAL:HG11	1:CH:78:VAL:HG11	2.01	0.43
1:BC:73:PRO:HG2	1:CH:78:VAL:HG21	2.01	0.43
1:BL:86:THR:HA	1:BL:112:ILE:O	2.18	0.43
1:BM:28:ALA:HB1	1:BM:29:PRO:HD2	2.00	0.43
1:BS:86:THR:HG22	1:BS:113:SER:CB	2.48	0.43
1:BU:95:VAL:HG11	1:CF:118:ALA:HB1	2.01	0.43
1:BY:28:ALA:HB1	1:BY:29:PRO:HD2	2.00	0.43
1:AI:86:THR:HG22	1:AI:113:SER:CB	2.48	0.43
1:AL:1:ALA:N	1:BM:152:ILE:O	2.52	0.43
1:BD:28:ALA:HB1	1:BD:29:PRO:HD2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BD:86:THR:HG22	1:BD:113:SER:CB	2.48	0.43
1:BI:130:LEU:HD23	1:BI:130:LEU:HA	1.85	0.43
1:CG:93:LYS:NZ	1:CG:94:GLY:O	2.50	0.43
1:AH:130:LEU:HD23	1:AH:130:LEU:HA	1.85	0.43
1:AI:130:LEU:HA	1:AI:130:LEU:HD23	1.81	0.43
1:AM:14:THR:OG1	1:AM:146:ASP:OD1	2.26	0.43
1:AO:110:VAL:HG22	1:BP:110:VAL:HG22	2.01	0.43
1:AX:86:THR:HG22	1:AX:113:SER:CB	2.48	0.43
1:BA:95:VAL:HG11	1:CB:118:ALA:CB	2.48	0.43
1:BA:133:ALA:HB2	1:CB:91:VAL:HG21	2.00	0.43
1:BV:28:ALA:HB1	1:BV:29:PRO:HD2	2.00	0.43
1:AF:110:VAL:HG21	1:BJ:137:LEU:HD11	2.00	0.43
1:AL:106:MET:SD	1:BM:126:VAL:HG13	2.59	0.43
1:BH:95:VAL:HG11	1:BX:118:ALA:CB	2.47	0.43
1:BZ:14:THR:OG1	1:BZ:146:ASP:OD1	2.26	0.43
1:AG:136:VAL:HG21	1:AK:59:ILE:HD13	2.01	0.42
1:AS:126:VAL:HA	1:CA:106:MET:SD	2.59	0.42
1:AT:26:ASP:OD1	1:AT:27:THR:N	2.52	0.42
1:AT:137:LEU:HD23	1:AT:137:LEU:HA	1.88	0.42
1:BH:118:ALA:HB1	1:BX:95:VAL:HG11	2.00	0.42
1:BN:92:ARG:HG2	1:BN:107:LEU:HD13	2.01	0.42
1:CH:28:ALA:HB1	1:CH:29:PRO:HD2	2.00	0.42
1:AA:99:VAL:HA	1:AH:121:TYR:CZ	2.54	0.42
1:AB:86:THR:HG22	1:AB:113:SER:CB	2.50	0.42
1:AC:86:THR:HG22	1:AC:113:SER:CB	2.48	0.42
1:AG:110:VAL:HG21	1:AK:137:LEU:HD11	2.00	0.42
1:AK:26:ASP:OD1	1:AK:27:THR:N	2.52	0.42
1:AL:149:LEU:HD13	1:BM:123:ALA:HB1	2.01	0.42
1:AM:98:ALA:HB3	1:AM:101:GLN:CG	2.47	0.42
1:AQ:86:THR:HA	1:AQ:112:ILE:O	2.18	0.42
1:AQ:118:ALA:HB1	1:AV:95:VAL:HG11	2.01	0.42
1:AZ:137:LEU:HD21	1:CC:89:PHE:CD2	2.54	0.42
1:BA:131:SER:HB2	1:CB:11:ALA:O	2.19	0.42
1:BL:26:ASP:OD1	1:BL:27:THR:N	2.52	0.42
1:BT:98:ALA:HB3	1:BT:101:GLN:CG	2.47	0.42
1:CE:86:THR:HG22	1:CE:113:SER:CB	2.48	0.42
1:CG:86:THR:HA	1:CG:112:ILE:O	2.18	0.42
1:AB:130:LEU:HD13	1:BW:144:ILE:HG22	2.01	0.42
1:AG:13:GLN:CG	1:AK:131:SER:HB3	2.49	0.42
1:AJ:1:ALA:O	1:BI:143:GLY:HA3	2.18	0.42
1:AO:28:ALA:HB1	1:AO:29:PRO:HD2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BC:86:THR:HG22	1:BC:113:SER:CB	2.50	0.42
1:BI:26:ASP:OD1	1:BI:27:THR:N	2.52	0.42
1:BI:137:LEU:HD23	1:BI:137:LEU:HA	1.88	0.42
1:BL:130:LEU:HA	1:BL:130:LEU:HD23	1.85	0.42
1:BN:98:ALA:HB3	1:BN:101:GLN:CG	2.47	0.42
1:BU:26:ASP:OD1	1:BU:27:THR:N	2.52	0.42
1:CD:26:ASP:OD1	1:CD:27:THR:N	2.53	0.42
1:CD:86:THR:HG22	1:CD:113:SER:CB	2.50	0.42
1:AG:92:ARG:HG2	1:AG:107:LEU:HD13	2.01	0.42
1:AH:86:THR:HA	1:AH:112:ILE:O	2.18	0.42
1:AK:72:VAL:CG1	1:BM:78:VAL:HG11	2.50	0.42
1:AS:118:ALA:HB1	1:CA:95:VAL:HG11	2.01	0.42
1:AU:28:ALA:HB1	1:AU:29:PRO:HD2	2.00	0.42
1:AW:153:LEU:HB3	1:BB:34:LYS:HD2	2.00	0.42
1:BF:26:ASP:OD1	1:BF:27:THR:N	2.52	0.42
1:BF:86:THR:HG22	1:BF:113:SER:CB	2.50	0.42
1:BL:86:THR:HG22	1:BL:113:SER:CB	2.50	0.42
1:BO:26:ASP:OD1	1:BO:27:THR:N	2.52	0.42
1:BO:86:THR:HG22	1:BO:113:SER:CB	2.50	0.42
1:BP:28:ALA:HB1	1:BP:29:PRO:HD2	2.00	0.42
1:BY:14:THR:OG1	1:BY:146:ASP:OD1	2.24	0.42
1:CC:98:ALA:HB3	1:CC:101:GLN:CG	2.47	0.42
1:CF:92:ARG:HG2	1:CF:107:LEU:HD13	2.01	0.42
1:AA:92:ARG:HG2	1:AA:107:LEU:HD13	2.01	0.42
1:BH:92:ARG:HG2	1:BH:107:LEU:HD13	2.01	0.42
1:BK:92:ARG:HG2	1:BK:107:LEU:HD13	2.01	0.42
1:BO:86:THR:HA	1:BO:112:ILE:O	2.18	0.42
1:BR:86:THR:HG22	1:BR:113:SER:CB	2.50	0.42
1:BX:130:LEU:HD23	1:BX:130:LEU:HA	1.85	0.42
1:CC:92:ARG:HG2	1:CC:107:LEU:HD13	2.01	0.42
1:AD:92:ARG:HG2	1:AD:107:LEU:HD13	2.01	0.42
1:AG:127:LYS:O	1:AK:13:GLN:HG3	2.20	0.42
1:AN:26:ASP:OD1	1:AN:27:THR:N	2.53	0.42
1:AQ:26:ASP:OD1	1:AQ:27:THR:N	2.52	0.42
1:AQ:86:THR:HG22	1:AQ:113:SER:CB	2.50	0.42
1:AS:92:ARG:HG2	1:AS:107:LEU:HD13	2.01	0.42
1:AV:92:ARG:HG2	1:AV:107:LEU:HD13	2.01	0.42
1:AX:28:ALA:HB1	1:AX:29:PRO:HD2	2.00	0.42
1:AX:136:VAL:HG21	1:BY:59:ILE:HD13	2.01	0.42
1:BC:26:ASP:OD1	1:BC:27:THR:N	2.52	0.42
1:BD:136:VAL:HG22	1:CH:8:VAL:HG11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BL:110:VAL:HG22	1:BN:110:VAL:HG22	2.01	0.42
1:BT:92:ARG:HG2	1:BT:107:LEU:HD13	2.01	0.42
1:CB:28:ALA:HB1	1:CB:29:PRO:HD2	2.00	0.42
1:AG:98:ALA:HB3	1:AG:101:GLN:CG	2.47	0.42
1:AH:26:ASP:OD1	1:AH:27:THR:N	2.52	0.42
1:AR:28:ALA:HB1	1:AR:29:PRO:HD2	2.00	0.42
1:AT:75:SER:HA	1:BV:76:ASN:HD21	1.84	0.42
1:BD:79:ILE:HG13	1:CH:101:GLN:NE2	2.35	0.42
1:BE:14:THR:OG1	1:BE:146:ASP:OD1	2.26	0.42
1:AM:92:ARG:HG2	1:AM:107:LEU:HD13	2.01	0.42
1:AP:92:ARG:HG2	1:AP:107:LEU:HD13	2.01	0.42
1:BI:86:THR:HG22	1:BI:113:SER:CB	2.50	0.42
1:BT:86:THR:HG22	1:BT:113:SER:CB	2.50	0.42
1:BU:86:THR:HG22	1:BU:113:SER:CB	2.50	0.42
1:BW:92:ARG:HG2	1:BW:107:LEU:HD13	2.01	0.42
1:CA:86:THR:HG22	1:CA:113:SER:CB	2.50	0.42
1:AD:86:THR:HG22	1:AD:113:SER:CB	2.50	0.42
1:AE:26:ASP:OD1	1:AE:27:THR:N	2.52	0.42
1:AJ:106:MET:SD	1:BI:126:VAL:HG13	2.60	0.42
1:AK:86:THR:HA	1:AK:112:ILE:O	2.18	0.42
1:AK:86:THR:HG22	1:AK:113:SER:CB	2.50	0.42
1:AN:86:THR:HG22	1:AN:113:SER:CB	2.50	0.42
1:AN:93:LYS:NZ	1:AN:94:GLY:O	2.50	0.42
1:AW:26:ASP:OD1	1:AW:27:THR:N	2.52	0.42
1:AW:86:THR:HG22	1:AW:113:SER:CB	2.50	0.42
1:AY:1:ALA:H3	1:BC:147:THR:HG1	1.55	0.42
1:AZ:86:THR:HG22	1:AZ:113:SER:CB	2.50	0.42
1:BE:92:ARG:HG2	1:BE:107:LEU:HD13	2.01	0.42
1:BM:51:HIS:CD2	1:BN:152:ILE:HD11	2.55	0.42
1:BX:26:ASP:OD1	1:BX:27:THR:N	2.52	0.42
1:CA:93:LYS:NZ	1:CA:94:GLY:O	2.50	0.42
1:CA:137:LEU:HD23	1:CA:137:LEU:HA	1.88	0.42
1:AA:86:THR:HG22	1:AA:113:SER:CB	2.50	0.42
1:AB:110:VAL:HG22	1:BW:110:VAL:HG22	2.01	0.42
1:AE:137:LEU:HD11	1:BQ:110:VAL:HG21	2.02	0.42
1:AI:28:ALA:HB1	1:AI:29:PRO:HD2	2.00	0.42
1:AL:137:LEU:HD11	1:BM:110:VAL:HG21	2.02	0.42
1:AS:86:THR:HG22	1:AS:113:SER:CB	2.50	0.42
1:AV:86:THR:HG22	1:AV:113:SER:CB	2.50	0.42
1:AX:118:ALA:CB	1:BY:95:VAL:HG11	2.47	0.42
1:BA:5:SER:HB2	1:CB:139:GLN:NE2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AD:125:ASN:OD1	1:AN:48:VAL:HA	2.20	0.41
1:AJ:40:ALA:HA	1:AJ:50:THR:HG21	2.02	0.41
1:AJ:92:ARG:HG2	1:AJ:107:LEU:HD13	2.01	0.41
1:AM:40:ALA:HA	1:AM:50:THR:HG21	2.02	0.41
1:AZ:24:THR:CG2	1:AZ:39:THR:HB	2.51	0.41
1:AZ:148:ALA:HA	1:CC:87:TYR:CE2	2.55	0.41
1:BB:40:ALA:HA	1:BB:50:THR:HG21	2.02	0.41
1:BC:137:LEU:HD23	1:BC:137:LEU:HA	1.88	0.41
1:BD:113:SER:OG	1:CH:107:LEU:HB3	2.20	0.41
1:BH:84:ARG:NH1	1:BX:105:VAL:O	2.45	0.41
1:BL:24:THR:CG2	1:BL:39:THR:HB	2.50	0.41
1:AB:24:THR:CG2	1:AB:39:THR:HB	2.51	0.41
1:AF:110:VAL:HG22	1:BJ:110:VAL:HG22	2.02	0.41
1:AJ:107:LEU:HB3	1:BI:113:SER:OG	2.21	0.41
1:AO:127:LYS:HG3	1:BP:149:LEU:HD11	2.02	0.41
1:AP:40:ALA:HA	1:AP:50:THR:HG21	2.02	0.41
1:AT:24:THR:CG2	1:AT:39:THR:HB	2.51	0.41
1:AU:107:LEU:HB3	1:BV:113:SER:OG	2.20	0.41
1:AZ:131:SER:OG	1:CC:21:TYR:CE2	2.73	0.41
1:BB:86:THR:HG22	1:BB:113:SER:CB	2.50	0.41
1:BF:24:THR:CG2	1:BF:39:THR:HB	2.51	0.41
1:BU:24:THR:CG2	1:BU:39:THR:HB	2.51	0.41
1:BZ:86:THR:HG22	1:BZ:113:SER:CB	2.50	0.41
1:BZ:92:ARG:HG2	1:BZ:107:LEU:HD13	2.01	0.41
1:CD:24:THR:CG2	1:CD:39:THR:HB	2.51	0.41
1:CG:86:THR:HG22	1:CG:113:SER:CB	2.50	0.41
1:AE:86:THR:HG22	1:AE:113:SER:CB	2.50	0.41
1:AE:106:MET:SD	1:BQ:126:VAL:HG13	2.59	0.41
1:AL:78:VAL:HG11	1:BL:72:VAL:CG1	2.48	0.41
1:AS:98:ALA:HB3	1:AS:101:GLN:CG	2.47	0.41
1:AX:153:LEU:HB3	1:BW:27:THR:OG1	2.21	0.41
1:AY:86:THR:HG22	1:AY:113:SER:CB	2.50	0.41
1:BQ:86:THR:HG22	1:BQ:113:SER:CB	2.50	0.41
1:BR:26:ASP:OD1	1:BR:27:THR:N	2.52	0.41
1:AA:40:ALA:HA	1:AA:50:THR:HG21	2.02	0.41
1:AB:53:VAL:HG23	1:AH:149:LEU:O	2.21	0.41
1:AD:113:SER:OG	1:AN:107:LEU:HB3	2.20	0.41
1:AG:136:VAL:HG22	1:AK:8:VAL:HG11	2.02	0.41
1:AM:86:THR:HG22	1:AM:113:SER:CB	2.50	0.41
1:AY:40:ALA:HA	1:AY:50:THR:HG21	2.02	0.41
1:AZ:14:THR:OG1	1:AZ:146:ASP:OD1	2.23	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AZ:26:ASP:OD1	1:AZ:27:THR:N	2.52	0.41
1:BA:130:LEU:HD23	1:BA:130:LEU:HA	1.81	0.41
1:BE:121:TYR:CE1	1:CG:99:VAL:HA	2.55	0.41
1:BI:92:ARG:HG2	1:BI:107:LEU:HD13	2.03	0.41
1:BO:24:THR:CG2	1:BO:39:THR:HB	2.51	0.41
1:BQ:40:ALA:HA	1:BQ:50:THR:HG21	2.02	0.41
1:BR:24:THR:CG2	1:BR:39:THR:HB	2.50	0.41
1:BX:86:THR:HG22	1:BX:113:SER:CB	2.50	0.41
1:CA:26:ASP:OD1	1:CA:27:THR:N	2.52	0.41
1:CC:86:THR:HG22	1:CC:113:SER:CB	2.50	0.41
1:CG:26:ASP:OD1	1:CG:27:THR:N	2.52	0.41
1:CG:137:LEU:HD23	1:CG:137:LEU:HA	1.89	0.41
1:AA:27:THR:OG1	1:BG:153:LEU:HB3	2.20	0.41
1:AG:86:THR:HG22	1:AG:113:SER:CB	2.50	0.41
1:AH:86:THR:HG22	1:AH:113:SER:CB	2.50	0.41
1:AJ:86:THR:HG22	1:AJ:113:SER:CB	2.50	0.41
1:AT:130:LEU:HD23	1:AT:130:LEU:HA	1.85	0.41
1:AV:40:ALA:HA	1:AV:50:THR:HG21	2.02	0.41
1:BH:40:ALA:HA	1:BH:50:THR:HG21	2.02	0.41
1:BQ:98:ALA:HB3	1:BQ:101:GLN:CG	2.47	0.41
1:CA:24:THR:CG2	1:CA:39:THR:HB	2.50	0.41
1:CA:92:ARG:HG2	1:CA:107:LEU:HD13	2.03	0.41
1:AD:13:GLN:HG3	1:AN:127:LYS:O	2.21	0.41
1:AG:40:ALA:HA	1:AG:50:THR:HG21	2.02	0.41
1:AH:24:THR:CG2	1:AH:39:THR:HB	2.50	0.41
1:AP:86:THR:HG22	1:AP:113:SER:CB	2.50	0.41
1:AP:118:ALA:CB	1:CD:95:VAL:HG11	2.48	0.41
1:AT:86:THR:HG22	1:AT:113:SER:CB	2.50	0.41
1:AT:93:LYS:NZ	1:AT:94:GLY:O	2.50	0.41
1:AX:78:VAL:HG11	1:BX:72:VAL:HG11	2.02	0.41
1:AY:92:ARG:HG2	1:AY:107:LEU:HD13	2.01	0.41
1:BB:92:ARG:HG2	1:BB:107:LEU:HD13	2.01	0.41
1:BE:40:ALA:HA	1:BE:50:THR:HG21	2.02	0.41
1:BG:14:THR:OG1	1:BG:146:ASP:OD1	2.25	0.41
1:BI:24:THR:CG2	1:BI:39:THR:HB	2.51	0.41
1:BK:86:THR:HG22	1:BK:113:SER:CB	2.50	0.41
1:BN:86:THR:HG22	1:BN:113:SER:CB	2.50	0.41
1:AC:76:ASN:ND2	1:BF:74:ASN:O	2.53	0.41
1:AQ:130:LEU:HD23	1:AQ:130:LEU:HA	1.85	0.41
1:AR:126:VAL:HG13	1:BS:106:MET:SD	2.61	0.41
1:AU:95:VAL:HG11	1:BV:118:ALA:HB1	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BC:24:THR:CG2	1:BC:39:THR:HB	2.51	0.41
1:BD:13:GLN:HG2	1:CH:131:SER:HB3	2.02	0.41
1:BF:92:ARG:HG2	1:BF:107:LEU:HD13	2.03	0.41
1:BH:86:THR:HG22	1:BH:113:SER:CB	2.50	0.41
1:BL:92:ARG:HG2	1:BL:107:LEU:HD13	2.03	0.41
1:BN:40:ALA:HA	1:BN:50:THR:HG21	2.02	0.41
1:CC:40:ALA:HA	1:CC:50:THR:HG21	2.02	0.41
1:CF:40:ALA:HA	1:CF:50:THR:HG21	2.02	0.41
1:AE:92:ARG:HG2	1:AE:107:LEU:HD13	2.03	0.41
1:AN:92:ARG:HG2	1:AN:107:LEU:HD13	2.03	0.41
1:AR:106:MET:SD	1:BS:126:VAL:HG13	2.60	0.41
1:AY:98:ALA:HB3	1:AY:101:GLN:CG	2.47	0.41
1:BB:137:LEU:HD23	1:BB:137:LEU:HA	1.89	0.41
1:BE:86:THR:HG22	1:BE:113:SER:CB	2.50	0.41
1:BH:151:GLY:CA	1:BX:67:MET:HE3	2.50	0.41
1:BW:86:THR:HG22	1:BW:113:SER:CB	2.50	0.41
1:AB:106:MET:HA	1:BW:115:PRO:HD3	2.03	0.41
1:AD:106:MET:HG3	1:AN:113:SER:O	2.20	0.41
1:AE:24:THR:CG2	1:AE:39:THR:HB	2.51	0.41
1:AG:153:LEU:HD22	1:AK:61:PHE:HD2	1.86	0.41
1:AJ:125:ASN:OD1	1:BI:48:VAL:HA	2.21	0.41
1:AK:24:THR:CG2	1:AK:39:THR:HB	2.51	0.41
1:AO:55:SER:O	1:AO:55:SER:OG	2.39	0.41
1:AR:14:THR:OG1	1:AR:146:ASP:OD1	2.24	0.41
1:AS:40:ALA:HA	1:AS:50:THR:HG21	2.02	0.41
1:AW:118:ALA:HB1	1:BB:95:VAL:HG11	2.02	0.41
1:AW:153:LEU:HD23	1:AW:153:LEU:HA	1.90	0.41
1:AY:121:TYR:CE1	1:BC:99:VAL:HA	2.55	0.41
1:AZ:130:LEU:HD23	1:AZ:130:LEU:HA	1.85	0.41
1:BD:34:LYS:HD2	1:CH:153:LEU:HG	2.03	0.41
1:BQ:92:ARG:HG2	1:BQ:107:LEU:HD13	2.01	0.41
1:BR:137:LEU:HD23	1:BR:137:LEU:HA	1.88	0.41
1:CF:86:THR:HG22	1:CF:113:SER:CB	2.50	0.41
1:AQ:24:THR:CG2	1:AQ:39:THR:HB	2.51	0.41
1:AZ:92:ARG:HG2	1:AZ:107:LEU:HD13	2.03	0.41
1:BI:14:THR:OG1	1:BI:146:ASP:OD1	2.23	0.41
1:BN:32:LEU:CD1	1:BN:65:LYS:HG2	2.51	0.41
1:BN:55:SER:O	1:BN:55:SER:OG	2.39	0.41
1:BO:137:LEU:HD23	1:BO:137:LEU:HA	1.88	0.41
1:BW:32:LEU:CD1	1:BW:65:LYS:HG2	2.51	0.41
1:AB:26:ASP:OD1	1:AB:27:THR:N	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AC:51:HIS:CD2	1:BW:152:ILE:HD11	2.56	0.40
1:AF:130:LEU:HD23	1:AF:130:LEU:HA	1.82	0.40
1:AO:149:LEU:HD11	1:BP:127:LYS:HG3	2.03	0.40
1:AP:32:LEU:CD1	1:AP:65:LYS:HG2	2.52	0.40
1:AQ:74:ASN:O	1:BS:76:ASN:ND2	2.54	0.40
1:AR:74:ASN:HA	1:CD:76:ASN:O	2.21	0.40
1:AR:99:VAL:HA	1:BS:121:TYR:CE1	2.56	0.40
1:AY:137:LEU:HD23	1:AY:137:LEU:HA	1.89	0.40
1:BN:14:THR:OG1	1:BN:146:ASP:OD1	2.26	0.40
1:BR:92:ARG:HG2	1:BR:107:LEU:HD13	2.03	0.40
1:BW:40:ALA:HA	1:BW:50:THR:HG21	2.02	0.40
1:BX:153:LEU:HD23	1:BX:153:LEU:HA	1.90	0.40
1:CC:32:LEU:CD1	1:CC:65:LYS:HG2	2.51	0.40
1:CE:130:LEU:HD23	1:CE:130:LEU:HA	1.81	0.40
1:AB:92:ARG:HG2	1:AB:107:LEU:HD13	2.03	0.40
1:AC:48:VAL:HA	1:BG:125:ASN:OD1	2.21	0.40
1:AD:137:LEU:HD23	1:AD:137:LEU:HA	1.89	0.40
1:AM:32:LEU:CD1	1:AM:65:LYS:HG2	2.51	0.40
1:AO:99:VAL:HA	1:BP:121:TYR:CE1	2.56	0.40
1:AT:92:ARG:HG2	1:AT:107:LEU:HD13	2.03	0.40
1:AU:130:LEU:HD23	1:AU:130:LEU:HA	1.81	0.40
1:BH:55:SER:O	1:BH:55:SER:OG	2.39	0.40
1:AH:92:ARG:HG2	1:AH:107:LEU:HD13	2.03	0.40
1:AN:24:THR:CG2	1:AN:39:THR:HB	2.50	0.40
1:AQ:14:THR:OG1	1:AQ:146:ASP:OD1	2.23	0.40
1:BC:92:ARG:HG2	1:BC:107:LEU:HD13	2.03	0.40
1:BD:76:ASN:ND2	1:CG:74:ASN:O	2.54	0.40
1:BD:136:VAL:CG2	1:CH:8:VAL:HG11	2.51	0.40
1:BG:130:LEU:HA	1:BG:130:LEU:HD23	1.82	0.40
1:BK:40:ALA:HA	1:BK:50:THR:HG21	2.02	0.40
1:BU:110:VAL:HG21	1:CF:137:LEU:HD11	2.03	0.40
1:BX:93:LYS:NZ	1:BX:94:GLY:O	2.50	0.40
1:BY:130:LEU:HA	1:BY:130:LEU:HD23	1.82	0.40
1:BZ:32:LEU:CD1	1:BZ:65:LYS:HG2	2.51	0.40
1:CF:32:LEU:CD1	1:CF:65:LYS:HG2	2.52	0.40
1:AK:51:HIS:NE2	1:BI:150:SER:O	2.53	0.40
1:AO:110:VAL:HG21	1:BP:137:LEU:HD11	2.02	0.40
1:AQ:149:LEU:HD13	1:AV:123:ALA:HB1	2.03	0.40
1:AX:34:LYS:HD2	1:BY:153:LEU:HG	2.02	0.40
1:AY:104:GLN:HG3	1:BC:82:ILE:HG21	2.02	0.40
1:BA:59:ILE:HD13	1:CB:136:VAL:HG21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BB:32:LEU:CD1	1:BB:65:LYS:HG2	2.51	0.40
1:BL:110:VAL:HG21	1:BN:137:LEU:HD11	2.03	0.40
1:BX:24:THR:CG2	1:BX:39:THR:HB	2.51	0.40
1:BX:92:ARG:HG2	1:BX:107:LEU:HD13	2.03	0.40
1:CG:24:THR:CG2	1:CG:39:THR:HB	2.51	0.40
1:CG:92:ARG:HG2	1:CG:107:LEU:HD13	2.03	0.40
1:AD:40:ALA:HA	1:AD:50:THR:HG21	2.02	0.40
1:AG:32:LEU:CD1	1:AG:65:LYS:HG2	2.52	0.40
1:AR:130:LEU:HD23	1:AR:130:LEU:HA	1.81	0.40
1:AY:32:LEU:CD1	1:AY:65:LYS:HG2	2.52	0.40
1:BA:148:ALA:HB1	1:CB:114:VAL:HG21	2.02	0.40
1:BT:40:ALA:HA	1:BT:50:THR:HG21	2.02	0.40
1:BV:130:LEU:HD23	1:BV:130:LEU:HA	1.82	0.40
1:CC:55:SER:O	1:CC:55:SER:OG	2.39	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:AI:147:THR:OG1	1:CE:1:ALA:N[3_555]	1.94	0.26
1:BC:9:THR:OG1	1:BC:18:SER:OG[10_455]	1.95	0.25
1:BK:84:ARG:NH1	1:BR:105:VAL:O[3_555]	2.02	0.18
1:AI:1:ALA:N	1:CE:147:THR:OG1[3_555]	2.09	0.11
1:AT:105:VAL:O	1:BT:84:ARG:NH1[2_555]	2.12	0.08
1:BF:84:ARG:NH1	1:BZ:105:VAL:O[3_555]	2.12	0.08
1:AM:84:ARG:NH1	1:BO:105:VAL:O[2_555]	2.15	0.05
1:AM:147:THR:OG1	1:BO:1:ALA:N[2_555]	2.15	0.05
1:AZ:9:THR:CG2	1:CB:14:THR:O[10_455]	2.16	0.04
1:BK:147:THR:OG1	1:BR:1:ALA:N[3_555]	2.17	0.03
1:BK:1:ALA:N	1:BR:147:THR:OG1[3_555]	2.18	0.02
1:AM:1:ALA:N	1:BO:147:THR:OG1[2_555]	2.19	0.01
1:BF:105:VAL:O	1:BZ:84:ARG:NH1[3_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	137/153 (90%)	135 (98%)	2 (2%)	0	100	100
1	AB	151/153 (99%)	147 (97%)	4 (3%)	0	100	100
1	AC	151/153 (99%)	149 (99%)	2 (1%)	0	100	100
1	AD	137/153 (90%)	135 (98%)	2 (2%)	0	100	100
1	AE	151/153 (99%)	147 (97%)	4 (3%)	0	100	100
1	AF	151/153 (99%)	149 (99%)	2 (1%)	0	100	100
1	AG	137/153 (90%)	135 (98%)	2 (2%)	0	100	100
1	AH	151/153 (99%)	147 (97%)	4 (3%)	0	100	100
1	AI	151/153 (99%)	149 (99%)	2 (1%)	0	100	100
1	AJ	137/153 (90%)	135 (98%)	2 (2%)	0	100	100
1	AK	151/153 (99%)	147 (97%)	4 (3%)	0	100	100
1	AL	151/153 (99%)	149 (99%)	2 (1%)	0	100	100
1	AM	137/153 (90%)	135 (98%)	2 (2%)	0	100	100
1	AN	151/153 (99%)	147 (97%)	4 (3%)	0	100	100
1	AO	151/153 (99%)	149 (99%)	2 (1%)	0	100	100
1	AP	137/153 (90%)	135 (98%)	2 (2%)	0	100	100
1	AQ	151/153 (99%)	147 (97%)	4 (3%)	0	100	100
1	AR	151/153 (99%)	149 (99%)	2 (1%)	0	100	100
1	AS	137/153 (90%)	135 (98%)	2 (2%)	0	100	100
1	AT	151/153 (99%)	148 (98%)	3 (2%)	0	100	100
1	AU	151/153 (99%)	149 (99%)	2 (1%)	0	100	100
1	AV	137/153 (90%)	135 (98%)	2 (2%)	0	100	100
1	AW	151/153 (99%)	147 (97%)	4 (3%)	0	100	100
1	AX	151/153 (99%)	149 (99%)	2 (1%)	0	100	100
1	AY	137/153 (90%)	135 (98%)	2 (2%)	0	100	100
1	AZ	151/153 (99%)	148 (98%)	3 (2%)	0	100	100
1	BA	151/153 (99%)	149 (99%)	2 (1%)	0	100	100
1	BB	137/153 (90%)	135 (98%)	2 (2%)	0	100	100
1	BC	151/153 (99%)	147 (97%)	4 (3%)	0	100	100
1	BD	151/153 (99%)	149 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	BE	137/153 (90%)	135 (98%)	2 (2%)	0	100	100
1	BF	151/153 (99%)	147 (97%)	4 (3%)	0	100	100
1	BG	151/153 (99%)	149 (99%)	2 (1%)	0	100	100
1	BH	137/153 (90%)	135 (98%)	2 (2%)	0	100	100
1	BI	151/153 (99%)	148 (98%)	3 (2%)	0	100	100
1	BJ	151/153 (99%)	149 (99%)	2 (1%)	0	100	100
1	BK	137/153 (90%)	135 (98%)	2 (2%)	0	100	100
1	BL	151/153 (99%)	147 (97%)	4 (3%)	0	100	100
1	BM	151/153 (99%)	149 (99%)	2 (1%)	0	100	100
1	BN	137/153 (90%)	135 (98%)	2 (2%)	0	100	100
1	BO	151/153 (99%)	148 (98%)	3 (2%)	0	100	100
1	BP	151/153 (99%)	149 (99%)	2 (1%)	0	100	100
1	BQ	137/153 (90%)	135 (98%)	2 (2%)	0	100	100
1	BR	151/153 (99%)	147 (97%)	4 (3%)	0	100	100
1	BS	151/153 (99%)	149 (99%)	2 (1%)	0	100	100
1	BT	137/153 (90%)	135 (98%)	2 (2%)	0	100	100
1	BU	151/153 (99%)	148 (98%)	3 (2%)	0	100	100
1	BV	151/153 (99%)	149 (99%)	2 (1%)	0	100	100
1	BW	137/153 (90%)	135 (98%)	2 (2%)	0	100	100
1	BX	151/153 (99%)	148 (98%)	3 (2%)	0	100	100
1	BY	151/153 (99%)	149 (99%)	2 (1%)	0	100	100
1	BZ	137/153 (90%)	135 (98%)	2 (2%)	0	100	100
1	CA	151/153 (99%)	147 (97%)	4 (3%)	0	100	100
1	CB	151/153 (99%)	149 (99%)	2 (1%)	0	100	100
1	CC	137/153 (90%)	135 (98%)	2 (2%)	0	100	100
1	CD	151/153 (99%)	147 (97%)	4 (3%)	0	100	100
1	CE	151/153 (99%)	149 (99%)	2 (1%)	0	100	100
1	CF	137/153 (90%)	135 (98%)	2 (2%)	0	100	100
1	CG	151/153 (99%)	147 (97%)	4 (3%)	0	100	100
1	CH	151/153 (99%)	149 (99%)	2 (1%)	0	100	100
All	All	8780/9180 (96%)	8626 (98%)	154 (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	109/119 (92%)	108 (99%)	1 (1%)	78	87
1	AB	119/119 (100%)	117 (98%)	2 (2%)	60	78
1	AC	119/119 (100%)	117 (98%)	2 (2%)	60	78
1	AD	109/119 (92%)	108 (99%)	1 (1%)	78	87
1	AE	119/119 (100%)	117 (98%)	2 (2%)	60	78
1	AF	119/119 (100%)	117 (98%)	2 (2%)	60	78
1	AG	109/119 (92%)	108 (99%)	1 (1%)	78	87
1	AH	119/119 (100%)	117 (98%)	2 (2%)	60	78
1	AI	119/119 (100%)	117 (98%)	2 (2%)	60	78
1	AJ	109/119 (92%)	108 (99%)	1 (1%)	78	87
1	AK	119/119 (100%)	117 (98%)	2 (2%)	60	78
1	AL	119/119 (100%)	117 (98%)	2 (2%)	60	78
1	AM	109/119 (92%)	108 (99%)	1 (1%)	78	87
1	AN	119/119 (100%)	117 (98%)	2 (2%)	60	78
1	AO	119/119 (100%)	117 (98%)	2 (2%)	60	78
1	AP	109/119 (92%)	108 (99%)	1 (1%)	78	87
1	AQ	119/119 (100%)	117 (98%)	2 (2%)	60	78
1	AR	119/119 (100%)	117 (98%)	2 (2%)	60	78
1	AS	109/119 (92%)	108 (99%)	1 (1%)	78	87
1	AT	119/119 (100%)	117 (98%)	2 (2%)	60	78
1	AU	119/119 (100%)	117 (98%)	2 (2%)	60	78
1	AV	109/119 (92%)	108 (99%)	1 (1%)	78	87
1	AW	119/119 (100%)	117 (98%)	2 (2%)	60	78
1	AX	119/119 (100%)	117 (98%)	2 (2%)	60	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AY	109/119 (92%)	108 (99%)	1 (1%)	78	87
1	AZ	119/119 (100%)	117 (98%)	2 (2%)	60	78
1	BA	119/119 (100%)	117 (98%)	2 (2%)	60	78
1	BB	109/119 (92%)	108 (99%)	1 (1%)	78	87
1	BC	119/119 (100%)	117 (98%)	2 (2%)	60	78
1	BD	119/119 (100%)	117 (98%)	2 (2%)	60	78
1	BE	109/119 (92%)	108 (99%)	1 (1%)	78	87
1	BF	119/119 (100%)	117 (98%)	2 (2%)	60	78
1	BG	119/119 (100%)	117 (98%)	2 (2%)	60	78
1	BH	109/119 (92%)	108 (99%)	1 (1%)	78	87
1	BI	119/119 (100%)	117 (98%)	2 (2%)	60	78
1	BJ	119/119 (100%)	117 (98%)	2 (2%)	60	78
1	BK	109/119 (92%)	108 (99%)	1 (1%)	78	87
1	BL	119/119 (100%)	117 (98%)	2 (2%)	60	78
1	BM	119/119 (100%)	117 (98%)	2 (2%)	60	78
1	BN	109/119 (92%)	108 (99%)	1 (1%)	78	87
1	BO	119/119 (100%)	117 (98%)	2 (2%)	60	78
1	BP	119/119 (100%)	117 (98%)	2 (2%)	60	78
1	BQ	109/119 (92%)	108 (99%)	1 (1%)	78	87
1	BR	119/119 (100%)	117 (98%)	2 (2%)	60	78
1	BS	119/119 (100%)	117 (98%)	2 (2%)	60	78
1	BT	109/119 (92%)	108 (99%)	1 (1%)	78	87
1	BU	119/119 (100%)	117 (98%)	2 (2%)	60	78
1	BV	119/119 (100%)	117 (98%)	2 (2%)	60	78
1	BW	109/119 (92%)	108 (99%)	1 (1%)	78	87
1	BX	119/119 (100%)	117 (98%)	2 (2%)	60	78
1	BY	119/119 (100%)	117 (98%)	2 (2%)	60	78
1	BZ	109/119 (92%)	108 (99%)	1 (1%)	78	87
1	CA	119/119 (100%)	117 (98%)	2 (2%)	60	78
1	CB	119/119 (100%)	117 (98%)	2 (2%)	60	78
1	CC	109/119 (92%)	108 (99%)	1 (1%)	78	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	CD	119/119 (100%)	117 (98%)	2 (2%)	60 78
1	CE	119/119 (100%)	117 (98%)	2 (2%)	60 78
1	CF	109/119 (92%)	108 (99%)	1 (1%)	78 87
1	CG	119/119 (100%)	117 (98%)	2 (2%)	60 78
1	CH	119/119 (100%)	117 (98%)	2 (2%)	60 78
All	All	6940/7140 (97%)	6840 (99%)	100 (1%)	67 82

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AA	57	PHE
1	AB	57	PHE
1	AB	85	ASN
1	AC	57	PHE
1	AC	85	ASN
1	AD	57	PHE
1	AE	57	PHE
1	AE	85	ASN
1	AF	57	PHE
1	AF	85	ASN
1	AG	57	PHE
1	AH	57	PHE
1	AH	85	ASN
1	AI	57	PHE
1	AI	85	ASN
1	AJ	57	PHE
1	AK	57	PHE
1	AK	85	ASN
1	AL	57	PHE
1	AL	85	ASN
1	AM	57	PHE
1	AN	57	PHE
1	AN	85	ASN
1	AO	57	PHE
1	AO	85	ASN
1	AP	57	PHE
1	AQ	57	PHE
1	AQ	85	ASN
1	AR	57	PHE
1	AR	85	ASN

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Mol	Chain	Res	Type
1	AS	57	PHE
1	AT	57	PHE
1	AT	85	ASN
1	AU	57	PHE
1	AU	85	ASN
1	AV	57	PHE
1	AW	57	PHE
1	AW	85	ASN
1	AX	57	PHE
1	AX	85	ASN
1	AY	57	PHE
1	AZ	57	PHE
1	AZ	85	ASN
1	BA	57	PHE
1	BA	85	ASN
1	BB	57	PHE
1	BC	57	PHE
1	BC	85	ASN
1	BD	57	PHE
1	BD	85	ASN
1	BE	57	PHE
1	BF	57	PHE
1	BF	85	ASN
1	BG	57	PHE
1	BG	85	ASN
1	BH	57	PHE
1	BI	57	PHE
1	BI	85	ASN
1	BJ	57	PHE
1	BJ	85	ASN
1	BK	57	PHE
1	BL	57	PHE
1	BL	85	ASN
1	BM	57	PHE
1	BM	85	ASN
1	BN	57	PHE
1	BO	57	PHE
1	BO	85	ASN
1	BP	57	PHE
1	BP	85	ASN
1	BQ	57	PHE
1	BR	57	PHE

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Mol	Chain	Res	Type
1	BR	85	ASN
1	BS	57	PHE
1	BS	85	ASN
1	BT	57	PHE
1	BU	57	PHE
1	BU	85	ASN
1	BV	57	PHE
1	BV	85	ASN
1	BW	57	PHE
1	BX	57	PHE
1	BX	85	ASN
1	BY	57	PHE
1	BY	85	ASN
1	BZ	57	PHE
1	CA	57	PHE
1	CA	85	ASN
1	CB	57	PHE
1	CB	85	ASN
1	CC	57	PHE
1	CD	57	PHE
1	CD	85	ASN
1	CE	57	PHE
1	CE	85	ASN
1	CF	57	PHE
1	CG	57	PHE
1	CG	85	ASN
1	CH	57	PHE
1	CH	85	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	AC	76	ASN
1	AL	76	ASN
1	AR	76	ASN
1	AU	76	ASN
1	AX	101	GLN
1	BA	101	GLN
1	BD	101	GLN
1	BG	76	ASN
1	BG	101	GLN
1	BJ	76	ASN

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Mol	Chain	Res	Type
1	BM	76	ASN
1	BP	76	ASN
1	BS	76	ASN
1	BV	76	ASN
1	CH	101	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no 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	141/153 (92%)	0.19	6 (4%) 35 34	48, 70, 90, 111	0
1	AB	153/153 (100%)	0.17	1 (0%) 87 88	49, 70, 97, 108	0
1	AC	153/153 (100%)	-0.12	3 (1%) 65 64	48, 72, 95, 110	0
1	AD	141/153 (92%)	0.07	0 100 100	48, 70, 90, 111	0
1	AE	153/153 (100%)	-0.07	1 (0%) 87 88	49, 70, 97, 108	0
1	AF	153/153 (100%)	-0.05	0 100 100	48, 72, 95, 110	0
1	AG	141/153 (92%)	0.02	2 (1%) 75 75	48, 70, 90, 111	0
1	AH	153/153 (100%)	0.20	3 (1%) 65 64	49, 70, 97, 108	0
1	AI	153/153 (100%)	0.33	3 (1%) 65 64	48, 72, 95, 110	0
1	AJ	141/153 (92%)	0.17	0 100 100	48, 70, 90, 111	0
1	AK	153/153 (100%)	-0.05	0 100 100	49, 70, 97, 108	0
1	AL	153/153 (100%)	-0.14	0 100 100	48, 72, 95, 110	0
1	AM	141/153 (92%)	0.07	0 100 100	48, 70, 90, 111	0
1	AN	153/153 (100%)	-0.02	0 100 100	49, 70, 97, 108	0
1	AO	153/153 (100%)	-0.08	0 100 100	48, 72, 95, 110	0
1	AP	141/153 (92%)	0.13	0 100 100	48, 70, 90, 111	0
1	AQ	153/153 (100%)	0.34	7 (4%) 32 30	49, 70, 97, 108	0
1	AR	153/153 (100%)	-0.12	0 100 100	48, 72, 95, 110	0
1	AS	141/153 (92%)	0.05	0 100 100	48, 70, 90, 111	0
1	AT	153/153 (100%)	0.00	0 100 100	49, 70, 97, 108	0
1	AU	153/153 (100%)	-0.06	0 100 100	48, 72, 95, 110	0
1	AV	141/153 (92%)	0.42	9 (6%) 19 19	48, 70, 90, 111	0
1	AW	153/153 (100%)	0.01	0 100 100	49, 70, 97, 108	0
1	AX	153/153 (100%)	0.42	9 (5%) 22 22	48, 72, 95, 110	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	AY	141/153 (92%)	0.19	1 (0%) 87 88	48, 70, 90, 111	0
1	AZ	153/153 (100%)	0.38	1 (0%) 87 88	49, 70, 97, 108	0
1	BA	153/153 (100%)	0.27	0 100 100	48, 72, 95, 110	0
1	BB	141/153 (92%)	-0.06	0 100 100	48, 70, 90, 111	0
1	BC	153/153 (100%)	0.29	2 (1%) 77 77	49, 70, 97, 108	0
1	BD	153/153 (100%)	0.04	0 100 100	48, 72, 95, 110	0
1	BE	141/153 (92%)	0.04	2 (1%) 75 75	48, 70, 90, 111	0
1	BF	153/153 (100%)	0.11	3 (1%) 65 64	49, 70, 97, 108	0
1	BG	153/153 (100%)	-0.18	1 (0%) 87 88	48, 72, 95, 110	0
1	BH	141/153 (92%)	0.12	1 (0%) 87 88	48, 70, 90, 111	0
1	BI	153/153 (100%)	0.14	0 100 100	49, 70, 97, 108	0
1	BJ	153/153 (100%)	0.17	0 100 100	48, 72, 95, 110	0
1	BK	141/153 (92%)	0.17	2 (1%) 75 75	48, 70, 90, 111	0
1	BL	153/153 (100%)	0.28	1 (0%) 87 88	49, 70, 97, 108	0
1	BM	153/153 (100%)	-0.06	0 100 100	48, 72, 95, 110	0
1	BN	141/153 (92%)	0.22	3 (2%) 63 62	48, 70, 90, 111	0
1	BO	153/153 (100%)	0.02	0 100 100	49, 70, 97, 108	0
1	BP	153/153 (100%)	-0.05	0 100 100	48, 72, 95, 110	0
1	BQ	141/153 (92%)	0.01	0 100 100	48, 70, 90, 111	0
1	BR	153/153 (100%)	0.25	1 (0%) 87 88	49, 70, 97, 108	0
1	BS	153/153 (100%)	-0.12	0 100 100	48, 72, 95, 110	0
1	BT	141/153 (92%)	0.12	1 (0%) 87 88	48, 70, 90, 111	0
1	BU	153/153 (100%)	0.19	1 (0%) 87 88	49, 70, 97, 108	0
1	BV	153/153 (100%)	-0.07	0 100 100	48, 72, 95, 110	0
1	BW	141/153 (92%)	0.20	3 (2%) 63 62	48, 70, 90, 111	0
1	BX	153/153 (100%)	0.23	2 (1%) 77 77	49, 70, 97, 108	0
1	BY	153/153 (100%)	0.22	3 (1%) 65 64	48, 72, 95, 110	0
1	BZ	141/153 (92%)	-0.01	1 (0%) 87 88	48, 70, 90, 111	0
1	CA	153/153 (100%)	0.08	0 100 100	49, 70, 97, 108	0
1	CB	153/153 (100%)	0.25	1 (0%) 87 88	48, 72, 95, 110	0
1	CC	141/153 (92%)	0.29	0 100 100	48, 70, 90, 111	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	CD	153/153 (100%)	0.33	1 (0%) 87 88	49, 70, 97, 108	0
1	CE	153/153 (100%)	0.33	2 (1%) 77 77	48, 72, 95, 110	0
1	CF	141/153 (92%)	0.28	0 100 100	48, 70, 90, 111	0
1	CG	153/153 (100%)	0.18	1 (0%) 87 88	49, 70, 97, 108	0
1	CH	153/153 (100%)	-0.01	0 100 100	48, 72, 95, 110	0
All	All	8940/9180 (97%)	0.11	78 (0%) 84 84	48, 71, 97, 111	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BK	70	VAL	4.4
1	BW	84	ARG	3.2
1	AI	106	MET	3.2
1	BE	70	VAL	3.1
1	AV	69	THR	2.9
1	AC	76	ASN	2.8
1	BF	76	ASN	2.8
1	BN	32	LEU	2.8
1	CE	130	LEU	2.8
1	BF	75	SER	2.7
1	AX	131	SER	2.7
1	BH	70	VAL	2.6
1	AQ	82	ILE	2.6
1	CB	75	SER	2.6
1	BX	102	SER	2.6
1	BZ	70	VAL	2.6
1	AX	113	SER	2.6
1	AG	70	VAL	2.5
1	AY	70	VAL	2.5
1	AQ	75	SER	2.5
1	BT	70	VAL	2.5
1	AA	69	THR	2.5
1	AH	70	VAL	2.5
1	AX	82	ILE	2.4
1	CE	76	ASN	2.4
1	AV	106	MET	2.4
1	AI	54	SER	2.4
1	AQ	112	ILE	2.4
1	BF	82	ILE	2.4
1	AE	76	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	AQ	76	ASN	2.4
1	AB	152	ILE	2.4
1	AX	84	ARG	2.4
1	BL	100	ASN	2.4
1	AX	112	ILE	2.3
1	AA	148	ALA	2.3
1	BN	85	ASN	2.3
1	AX	70	VAL	2.3
1	AV	84	ARG	2.3
1	AG	67	MET	2.3
1	AQ	80	THR	2.3
1	AQ	70	VAL	2.3
1	CG	107	LEU	2.3
1	BK	69	THR	2.3
1	AQ	117	GLY	2.2
1	BW	67	MET	2.2
1	BY	106	MET	2.2
1	BC	113	SER	2.2
1	AH	82	ILE	2.2
1	AI	107	LEU	2.2
1	AV	67	MET	2.2
1	BX	70	VAL	2.2
1	CD	102	SER	2.1
1	AX	130	LEU	2.1
1	BY	153	LEU	2.1
1	AC	70	VAL	2.1
1	AZ	83	GLY	2.1
1	AA	99	VAL	2.1
1	BC	59	ILE	2.1
1	AV	94	GLY	2.1
1	AA	97	PRO	2.1
1	AV	112	ILE	2.1
1	BY	108	VAL	2.1
1	AH	80	THR	2.1
1	BG	83	GLY	2.1
1	AX	67	MET	2.1
1	AV	103	PRO	2.1
1	AA	70	VAL	2.0
1	AC	75	SER	2.0
1	AV	102	SER	2.0
1	BE	83	GLY	2.0
1	AX	85	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
1	BW	70	VAL	2.0
1	AA	96	ILE	2.0
1	BR	107	LEU	2.0
1	AV	57	PHE	2.0
1	BN	65	LYS	2.0
1	BU	153	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no 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.