Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:40 PM GMT

PDB ID	:	1GAV
Title	:	BACTERIOPHAGE GA PROTEIN CAPSID
Authors	:	Tars, K.; Bundule, M.; Liljas, L.
Deposited on	:	1997-01-28
Resolution	:	3.40 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

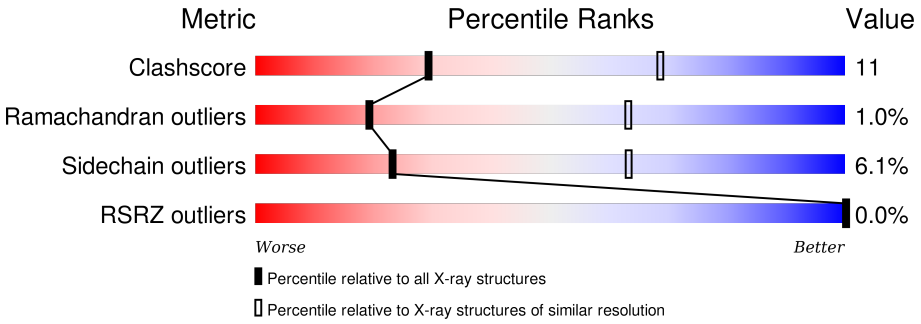
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 3.40 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))
Clashscore	102246	1611 (3.50-3.30)
Ramachandran outliers	100387	1571 (3.50-3.30)
Sidechain outliers	100360	1571 (3.50-3.30)
RSRZ outliers	91569	1485 (3.50-3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	0	129	80% 17% ·
1	1	129	73% 23% ·
1	2	129	69% 29% ·
1	3	129	67% 29% 5%
1	4	129	75% 22% ·
1	5	129	70% 29% ·
1	6	129	67% 29% ·

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Mol	Chain	Length	Quality of chain
1	7	129	81% 16%
1	8	129	70% 29%
1	9	129	67% 28% 5%
1	A	129	70% 29%
1	B	129	67% 28% 5%
1	C	129	78% 19%
1	D	129	68% 30%
1	E	129	67% 29% 5%
1	F	129	73% 24%
1	G	129	68% 30%
1	H	129	65% 30% 5%
1	I	129	75% 21%
1	J	129	69% 29%
1	K	129	67% 29% 5%
1	L	129	% 80% 17%
1	M	129	70% 29%
1	N	129	66% 30%
1	O	129	79% 18%
1	P	129	67% 31%
1	Q	129	66% 30%
1	R	129	73% 24%
1	S	129	68% 30%
1	T	129	66% 29% 5%
1	U	129	75% 21%
1	V	129	70% 29%

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Mol	Chain	Length	Quality of chain
1	W	129	67% 28% 5%
1	X	129	81% 16%
1	Y	129	69% 29%
1	Z	129	66% 29% 5%
1	a	129	96%
1	b	129	92% 8%
1	c	129	94% 5%
1	d	129	96%
1	e	129	92% 8%
1	f	129	94% 5%
1	g	129	96%
1	h	129	92% 8%
1	i	129	94% 5%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 43335 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 BACTERIOPHAGE GA PROTEIN CAPSID.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	129	Total	C	N	O	0	0	0
			963	612	164	187			
1	B	129	Total	C	N	O	0	0	0
			963	612	164	187			
1	C	129	Total	C	N	O	0	0	0
			963	612	164	187			
1	D	129	Total	C	N	O	0	0	0
			963	612	164	187			
1	E	129	Total	C	N	O	0	0	0
			963	612	164	187			
1	F	129	Total	C	N	O	0	0	0
			963	612	164	187			
1	G	129	Total	C	N	O	0	0	0
			963	612	164	187			
1	H	129	Total	C	N	O	0	0	0
			963	612	164	187			
1	I	129	Total	C	N	O	0	0	0
			963	612	164	187			
1	J	129	Total	C	N	O	0	0	0
			963	612	164	187			
1	K	129	Total	C	N	O	0	0	0
			963	612	164	187			
1	L	129	Total	C	N	O	0	0	0
			963	612	164	187			
1	M	129	Total	C	N	O	0	0	0
			963	612	164	187			
1	N	129	Total	C	N	O	0	0	0
			963	612	164	187			
1	O	129	Total	C	N	O	0	0	0
			963	612	164	187			
1	P	129	Total	C	N	O	0	0	0
			963	612	164	187			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	Q	129	Total	C	N	O	0	0	0
			963	612	164	187			
1	R	129	Total	C	N	O	0	0	0
			963	612	164	187			
1	S	129	Total	C	N	O	0	0	0
			963	612	164	187			
1	T	129	Total	C	N	O	0	0	0
			963	612	164	187			
1	U	129	Total	C	N	O	0	0	0
			963	612	164	187			
1	V	129	Total	C	N	O	0	0	0
			963	612	164	187			
1	W	129	Total	C	N	O	0	0	0
			963	612	164	187			
1	X	129	Total	C	N	O	0	0	0
			963	612	164	187			
1	Y	129	Total	C	N	O	0	0	0
			963	612	164	187			
1	Z	129	Total	C	N	O	0	0	0
			963	612	164	187			
1	1	129	Total	C	N	O	0	0	0
			963	612	164	187			
1	2	129	Total	C	N	O	0	0	0
			963	612	164	187			
1	3	129	Total	C	N	O	0	0	0
			963	612	164	187			
1	4	129	Total	C	N	O	0	0	0
			963	612	164	187			
1	5	129	Total	C	N	O	0	0	0
			963	612	164	187			
1	6	129	Total	C	N	O	0	0	0
			963	612	164	187			
1	7	129	Total	C	N	O	0	0	0
			963	612	164	187			
1	8	129	Total	C	N	O	0	0	0
			963	612	164	187			
1	9	129	Total	C	N	O	0	0	0
			963	612	164	187			
1	0	129	Total	C	N	O	0	0	0
			963	612	164	187			
1	a	129	Total	C	N	O	0	0	0
			963	612	164	187			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	b	129	Total	C	N	O	0	0	0
			963	612	164	187			
1	c	129	Total	C	N	O	0	0	0
			963	612	164	187			
1	d	129	Total	C	N	O	0	0	0
			963	612	164	187			
1	e	129	Total	C	N	O	0	0	0
			963	612	164	187			
1	f	129	Total	C	N	O	0	0	0
			963	612	164	187			
1	g	129	Total	C	N	O	0	0	0
			963	612	164	187			
1	h	129	Total	C	N	O	0	0	0
			963	612	164	187			
1	i	129	Total	C	N	O	0	0	0
			963	612	164	187			

There are 90 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	59	THR	ALA	VARIANT	UNP P07234
A	79	VAL	GLY	VARIANT	UNP P07234
B	59	THR	ALA	VARIANT	UNP P07234
B	79	VAL	GLY	VARIANT	UNP P07234
C	59	THR	ALA	VARIANT	UNP P07234
C	79	VAL	GLY	VARIANT	UNP P07234
D	59	THR	ALA	VARIANT	UNP P07234
D	79	VAL	GLY	VARIANT	UNP P07234
E	59	THR	ALA	VARIANT	UNP P07234
E	79	VAL	GLY	VARIANT	UNP P07234
F	59	THR	ALA	VARIANT	UNP P07234
F	79	VAL	GLY	VARIANT	UNP P07234
G	59	THR	ALA	VARIANT	UNP P07234
G	79	VAL	GLY	VARIANT	UNP P07234
H	59	THR	ALA	VARIANT	UNP P07234
H	79	VAL	GLY	VARIANT	UNP P07234
I	59	THR	ALA	VARIANT	UNP P07234
I	79	VAL	GLY	VARIANT	UNP P07234
J	59	THR	ALA	VARIANT	UNP P07234
J	79	VAL	GLY	VARIANT	UNP P07234
K	59	THR	ALA	VARIANT	UNP P07234
K	79	VAL	GLY	VARIANT	UNP P07234
L	59	THR	ALA	VARIANT	UNP P07234

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Chain	Residue	Modelled	Actual	Comment	Reference
L	79	VAL	GLY	VARIANT	UNP P07234
M	59	THR	ALA	VARIANT	UNP P07234
M	79	VAL	GLY	VARIANT	UNP P07234
N	59	THR	ALA	VARIANT	UNP P07234
N	79	VAL	GLY	VARIANT	UNP P07234
O	59	THR	ALA	VARIANT	UNP P07234
O	79	VAL	GLY	VARIANT	UNP P07234
P	59	THR	ALA	VARIANT	UNP P07234
P	79	VAL	GLY	VARIANT	UNP P07234
Q	59	THR	ALA	VARIANT	UNP P07234
Q	79	VAL	GLY	VARIANT	UNP P07234
R	59	THR	ALA	VARIANT	UNP P07234
R	79	VAL	GLY	VARIANT	UNP P07234
S	59	THR	ALA	VARIANT	UNP P07234
S	79	VAL	GLY	VARIANT	UNP P07234
T	59	THR	ALA	VARIANT	UNP P07234
T	79	VAL	GLY	VARIANT	UNP P07234
U	59	THR	ALA	VARIANT	UNP P07234
U	79	VAL	GLY	VARIANT	UNP P07234
V	59	THR	ALA	VARIANT	UNP P07234
V	79	VAL	GLY	VARIANT	UNP P07234
W	59	THR	ALA	VARIANT	UNP P07234
W	79	VAL	GLY	VARIANT	UNP P07234
X	59	THR	ALA	VARIANT	UNP P07234
X	79	VAL	GLY	VARIANT	UNP P07234
Y	59	THR	ALA	VARIANT	UNP P07234
Y	79	VAL	GLY	VARIANT	UNP P07234
Z	59	THR	ALA	VARIANT	UNP P07234
Z	79	VAL	GLY	VARIANT	UNP P07234
1	59	THR	ALA	VARIANT	UNP P07234
1	79	VAL	GLY	VARIANT	UNP P07234
2	59	THR	ALA	VARIANT	UNP P07234
2	79	VAL	GLY	VARIANT	UNP P07234
3	59	THR	ALA	VARIANT	UNP P07234
3	79	VAL	GLY	VARIANT	UNP P07234
4	59	THR	ALA	VARIANT	UNP P07234
4	79	VAL	GLY	VARIANT	UNP P07234
5	59	THR	ALA	VARIANT	UNP P07234
5	79	VAL	GLY	VARIANT	UNP P07234
6	59	THR	ALA	VARIANT	UNP P07234
6	79	VAL	GLY	VARIANT	UNP P07234
7	59	THR	ALA	VARIANT	UNP P07234

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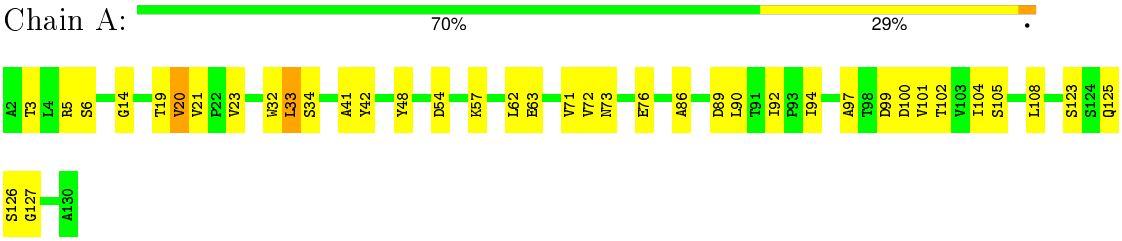
Chain	Residue	Modelled	Actual	Comment	Reference
7	79	VAL	GLY	VARIANT	UNP P07234
8	59	THR	ALA	VARIANT	UNP P07234
8	79	VAL	GLY	VARIANT	UNP P07234
9	59	THR	ALA	VARIANT	UNP P07234
9	79	VAL	GLY	VARIANT	UNP P07234
0	59	THR	ALA	VARIANT	UNP P07234
0	79	VAL	GLY	VARIANT	UNP P07234
a	59	THR	ALA	VARIANT	UNP P07234
a	79	VAL	GLY	VARIANT	UNP P07234
b	59	THR	ALA	VARIANT	UNP P07234
b	79	VAL	GLY	VARIANT	UNP P07234
c	59	THR	ALA	VARIANT	UNP P07234
c	79	VAL	GLY	VARIANT	UNP P07234
d	59	THR	ALA	VARIANT	UNP P07234
d	79	VAL	GLY	VARIANT	UNP P07234
e	59	THR	ALA	VARIANT	UNP P07234
e	79	VAL	GLY	VARIANT	UNP P07234
f	59	THR	ALA	VARIANT	UNP P07234
f	79	VAL	GLY	VARIANT	UNP P07234
g	59	THR	ALA	VARIANT	UNP P07234
g	79	VAL	GLY	VARIANT	UNP P07234
h	59	THR	ALA	VARIANT	UNP P07234
h	79	VAL	GLY	VARIANT	UNP P07234
i	59	THR	ALA	VARIANT	UNP P07234
i	79	VAL	GLY	VARIANT	UNP P07234

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

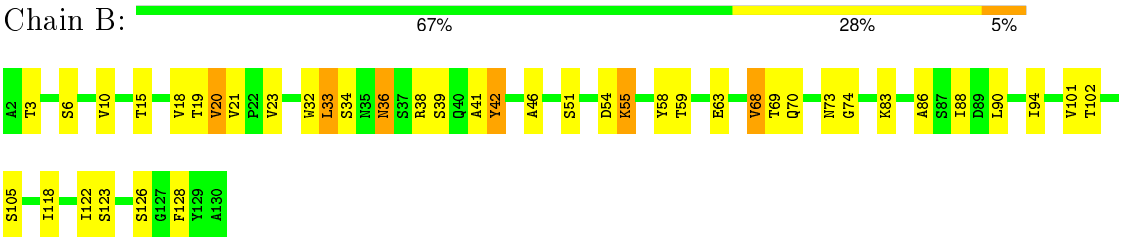
- Molecule 1: BACTERIOPHAGE GA PROTEIN CAPSID

Chain A:



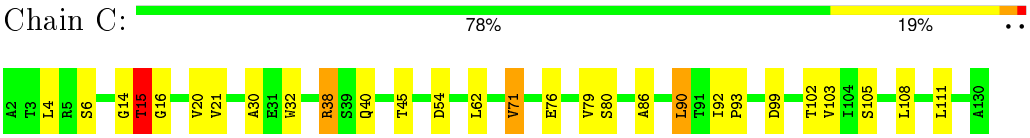
- Molecule 1: BACTERIOPHAGE GA PROTEIN CAPSID

Chain B:



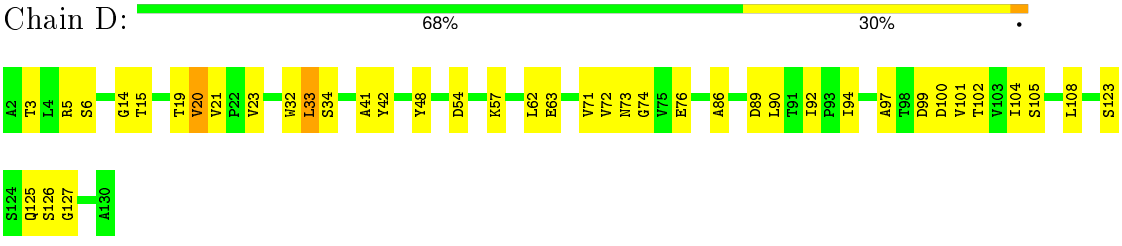
- Molecule 1: BACTERIOPHAGE GA PROTEIN CAPSID

Chain C:



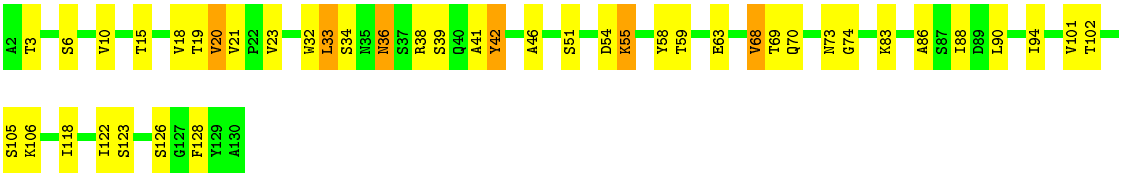
- Molecule 1: BACTERIOPHAGE GA PROTEIN CAPSID

Chain D:



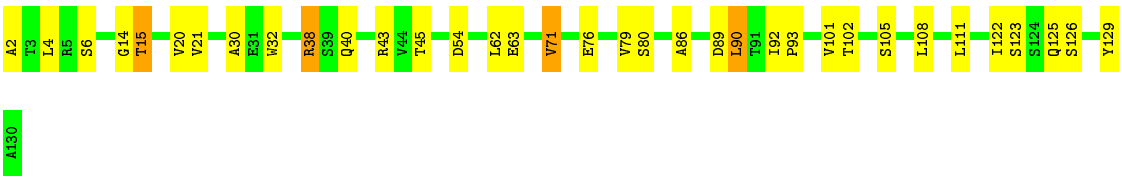
- Molecule 1: BACTERIOPHAGE GA PROTEIN CAPSID

Chain E:



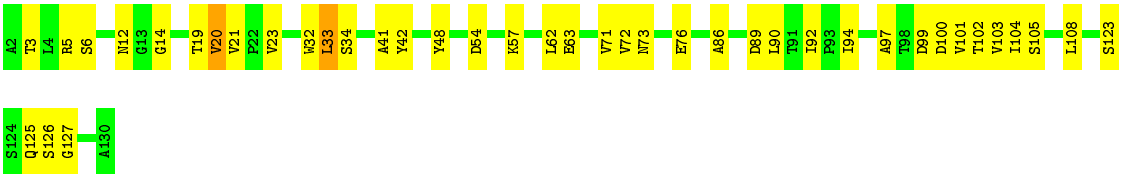
• Molecule 1: BACTERIOPHAGE GA PROTEIN CAPSID

Chain F:



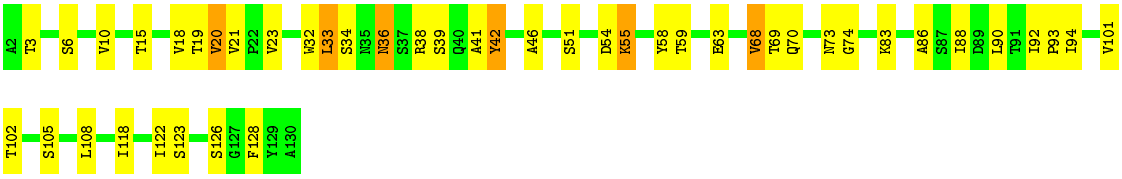
• Molecule 1: BACTERIOPHAGE GA PROTEIN CAPSID

Chain G:



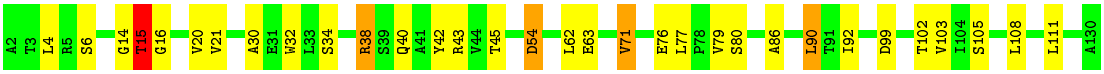
• Molecule 1: BACTERIOPHAGE GA PROTEIN CAPSID

Chain H:



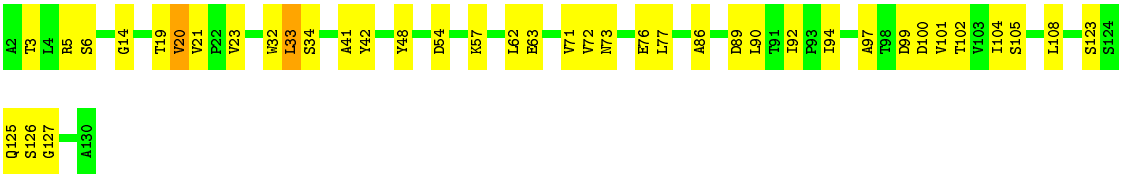
• Molecule 1: BACTERIOPHAGE GA PROTEIN CAPSID

Chain I:



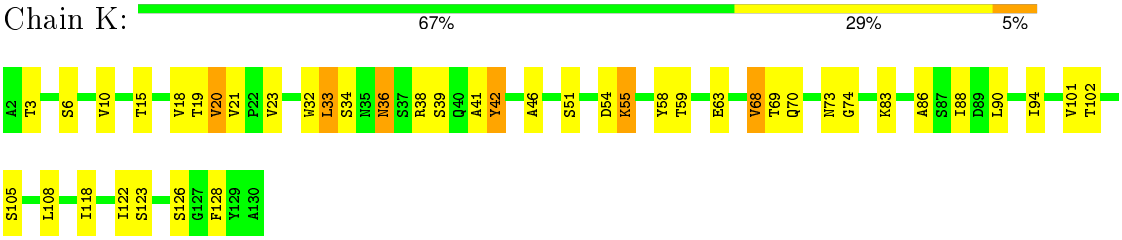
• Molecule 1: BACTERIOPHAGE GA PROTEIN CAPSID

Chain J:



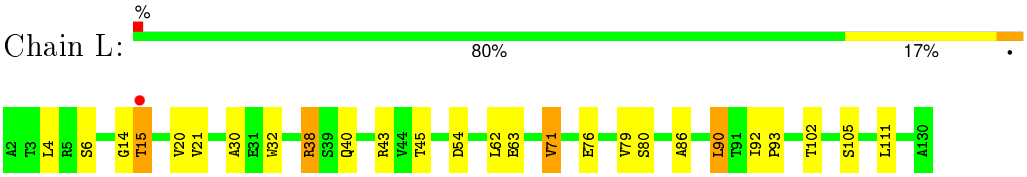
• Molecule 1: BACTERIOPHAGE GA PROTEIN CAPSID

Chain K:



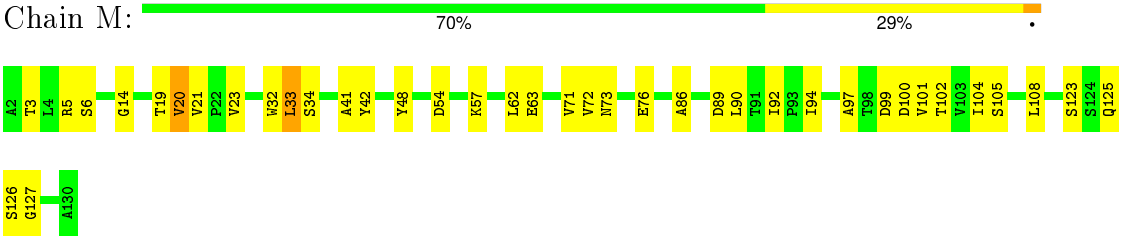
• Molecule 1: BACTERIOPHAGE GA PROTEIN CAPSID

Chain L:



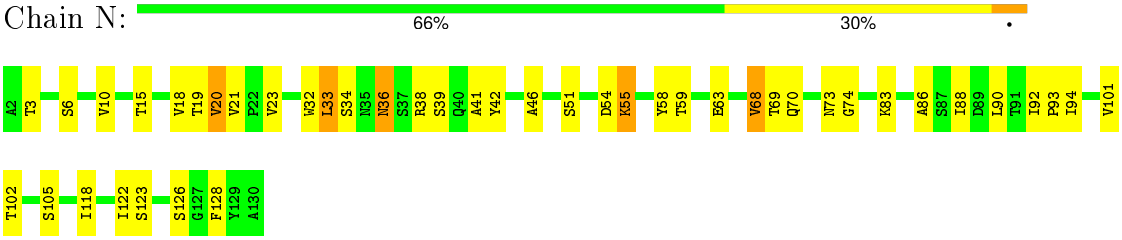
• Molecule 1: BACTERIOPHAGE GA PROTEIN CAPSID

Chain M:



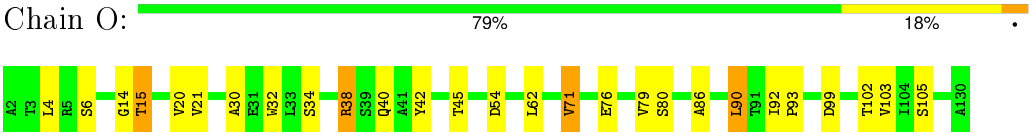
• Molecule 1: BACTERIOPHAGE GA PROTEIN CAPSID

Chain N:



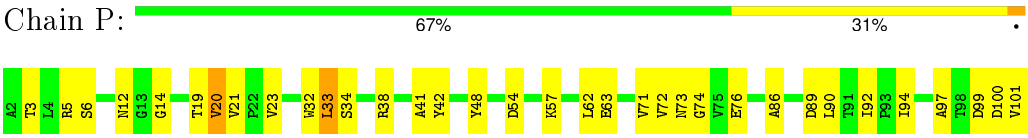
• Molecule 1: BACTERIOPHAGE GA PROTEIN CAPSID

Chain O:



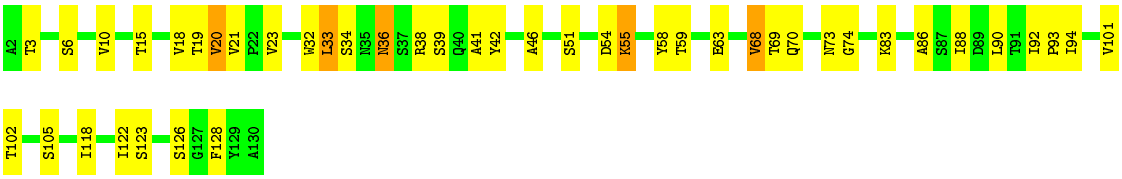
• Molecule 1: BACTERIOPHAGE GA PROTEIN CAPSID

Chain P:



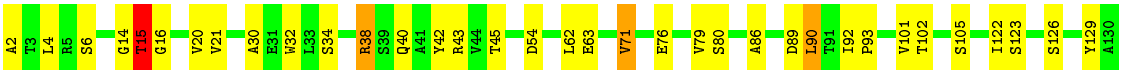
• Molecule 1: BACTERIOPHAGE GA PROTEIN CAPSID

Chain Q:



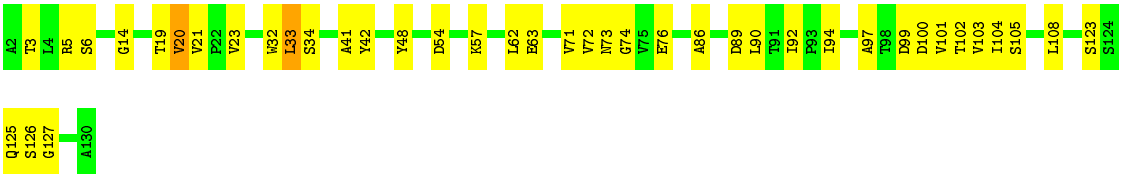
• Molecule 1: BACTERIOPHAGE GA PROTEIN CAPSID

Chain R:



• Molecule 1: BACTERIOPHAGE GA PROTEIN CAPSID

Chain S:

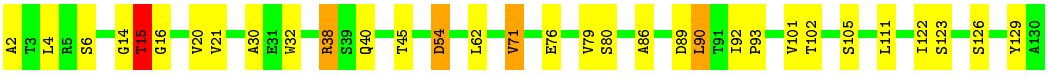


• Molecule 1: BACTERIOPHAGE GA PROTEIN CAPSID

Chain T:

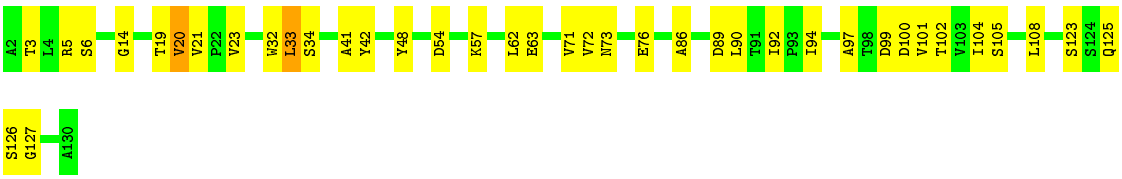
• Molecule 1: BACTERIOPHAGE GA PROTEIN CAPSID

Chain U:



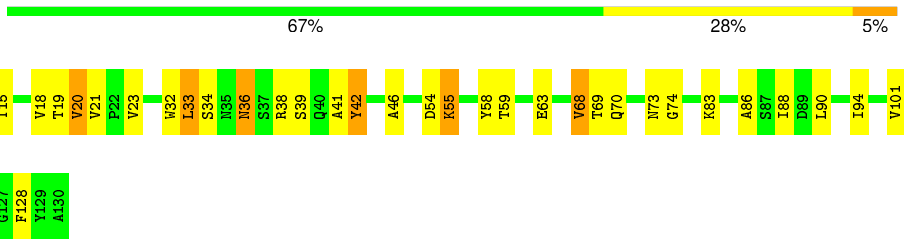
• Molecule 1: BACTERIOPHAGE GA PROTEIN CAPSID

Chain V:



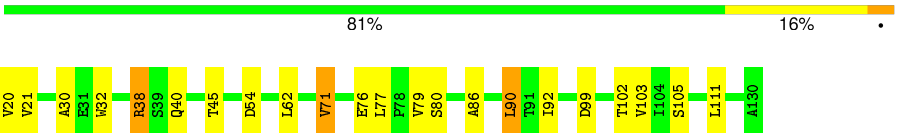
• Molecule 1: BACTERIOPHAGE GA PROTEIN CAPSID

Chain W:



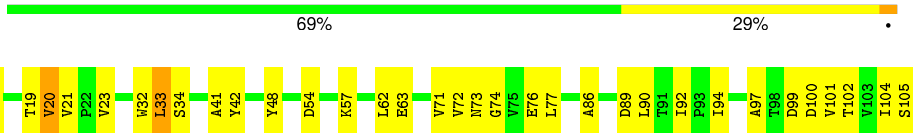
• Molecule 1: BACTERIOPHAGE GA PROTEIN CAPSID

Chain X:



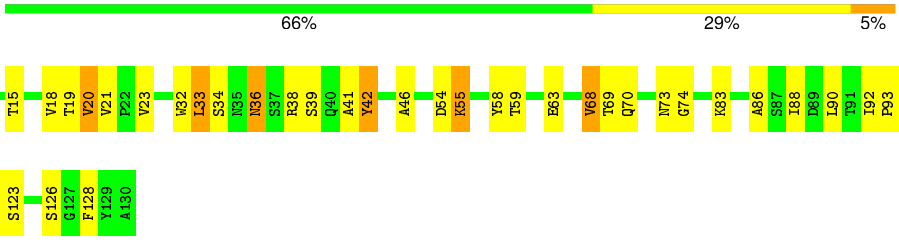
• Molecule 1: BACTERIOPHAGE GA PROTEIN CAPSID

Chain Y:



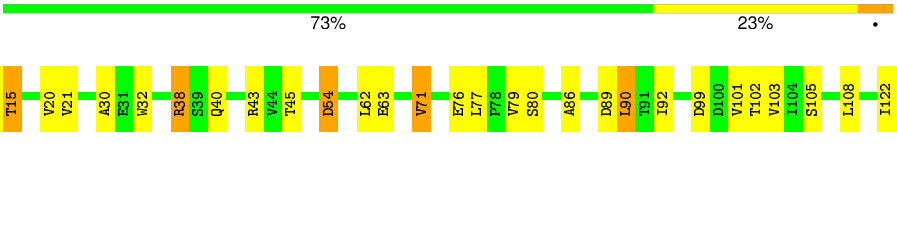
• Molecule 1: BACTERIOPHAGE GA PROTEIN CAPSID

Chain Z:



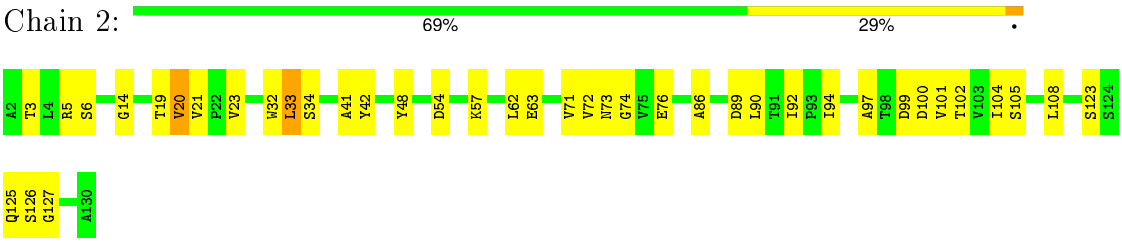
• Molecule 1: BACTERIOPHAGE GA PROTEIN CAPSID

Chain 1:



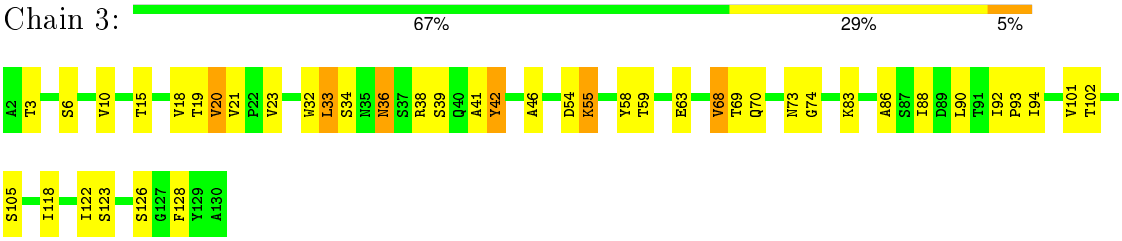
• Molecule 1: BACTERIOPHAGE GA PROTEIN CAPSID

Chain 2:



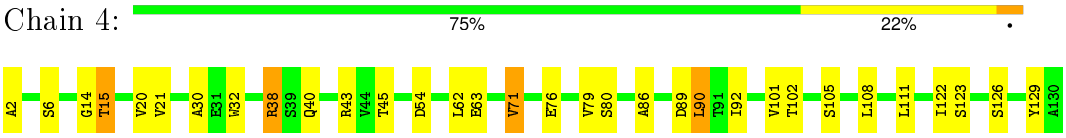
• Molecule 1: BACTERIOPHAGE GA PROTEIN CAPSID

Chain 3:



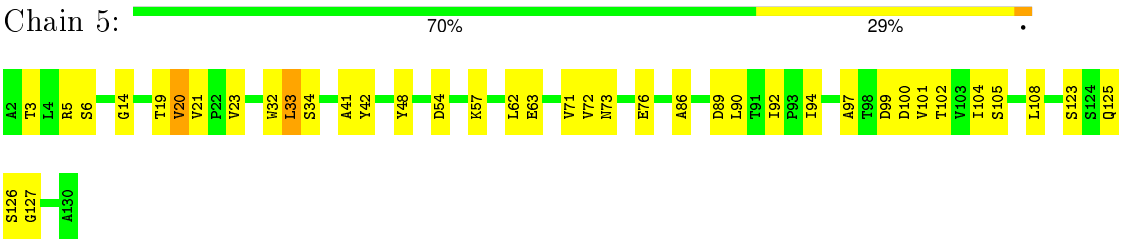
• Molecule 1: BACTERIOPHAGE GA PROTEIN CAPSID

Chain 4:



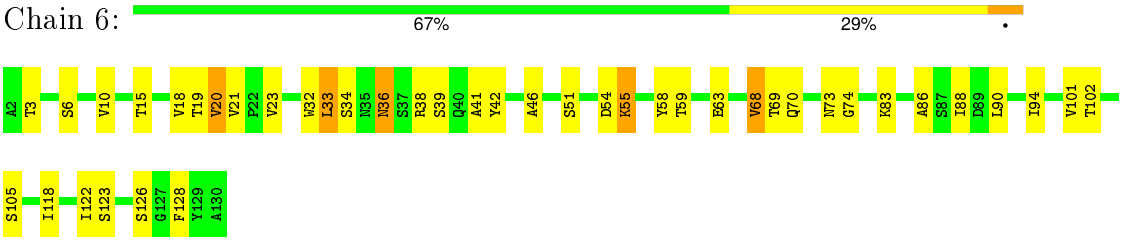
• Molecule 1: BACTERIOPHAGE GA PROTEIN CAPSID

Chain 5:



• Molecule 1: BACTERIOPHAGE GA PROTEIN CAPSID

Chain 6:

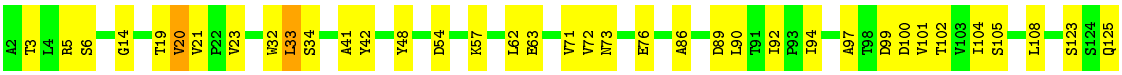


• Molecule 1: BACTERIOPHAGE GA PROTEIN CAPSID

Chain 7:

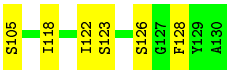
• Molecule 1: BACTERIOPHAGE GA PROTEIN CAPSID

Chain 8:



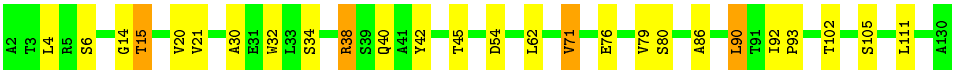
• Molecule 1: BACTERIOPHAGE GA PROTEIN CAPSID

Chain 9:



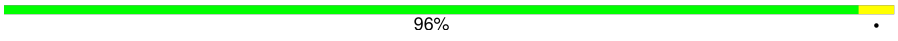
• Molecule 1: BACTERIOPHAGE GA PROTEIN CAPSID

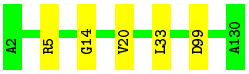
Chain 0:



• Molecule 1: BACTERIOPHAGE GA PROTEIN CAPSID

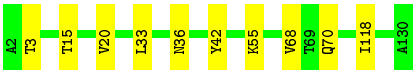
Chain a:





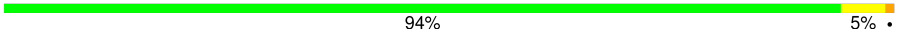
• Molecule 1: BACTERIOPHAGE GA PROTEIN CAPSID

Chain b:



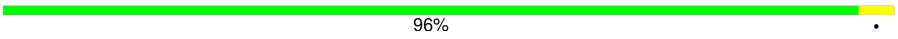
• Molecule 1: BACTERIOPHAGE GA PROTEIN CAPSID

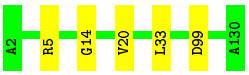
Chain c:



• Molecule 1: BACTERIOPHAGE GA PROTEIN CAPSID

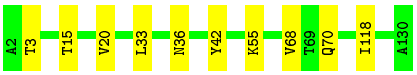
Chain d:





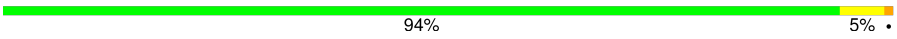
- Molecule 1: BACTERIOPHAGE GA PROTEIN CAPSID

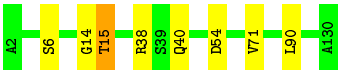
Chain e:



- Molecule 1: BACTERIOPHAGE GA PROTEIN CAPSID

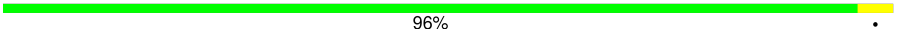
Chain f:

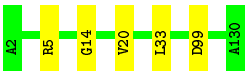




- Molecule 1: BACTERIOPHAGE GA PROTEIN CAPSID

Chain g:



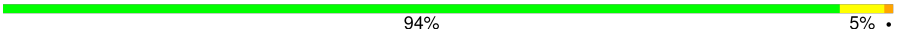


- Molecule 1: BACTERIOPHAGE GA PROTEIN CAPSID

Chain h:

- Molecule 1: BACTERIOPHAGE GA PROTEIN CAPSID

Chain i:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	272.70Å 293.50Å 339.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.40 49.31 – 3.39	Depositor EDS
% Data completeness (in resolution range)	66.0 (30.00-3.40) 65.4 (49.31-3.39)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.02 (at 3.40Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.279 , (Not available) 0.245 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	46.8	Xtriage
Anisotropy	0.124	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 58.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Outliers	4 of 122583 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	43335	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.55% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	0	0.82	0/980	0.84	0/1336
1	1	0.82	0/980	0.84	0/1336
1	2	0.82	0/980	0.87	0/1336
1	3	0.88	0/980	0.90	1/1336 (0.1%)
1	4	0.82	0/980	0.84	0/1336
1	5	0.82	0/980	0.87	0/1336
1	6	0.88	0/980	0.90	1/1336 (0.1%)
1	7	0.82	0/980	0.84	0/1336
1	8	0.82	0/980	0.87	0/1336
1	9	0.88	0/980	0.90	1/1336 (0.1%)
1	A	0.82	0/980	0.87	0/1336
1	B	0.88	0/980	0.90	1/1336 (0.1%)
1	C	0.82	0/980	0.84	0/1336
1	D	0.82	0/980	0.87	0/1336
1	E	0.88	0/980	0.90	1/1336 (0.1%)
1	F	0.82	0/980	0.84	0/1336
1	G	0.82	0/980	0.87	0/1336
1	H	0.88	0/980	0.90	1/1336 (0.1%)
1	I	0.82	0/980	0.84	0/1336
1	J	0.82	0/980	0.87	0/1336
1	K	0.88	0/980	0.90	1/1336 (0.1%)
1	L	0.82	0/980	0.84	0/1336
1	M	0.82	0/980	0.87	0/1336
1	N	0.88	0/980	0.90	1/1336 (0.1%)
1	O	0.82	0/980	0.84	0/1336
1	P	0.82	0/980	0.87	0/1336
1	Q	0.88	0/980	0.90	1/1336 (0.1%)
1	R	0.82	0/980	0.84	0/1336
1	S	0.82	0/980	0.87	0/1336
1	T	0.88	0/980	0.90	1/1336 (0.1%)
1	U	0.82	0/980	0.84	0/1336
1	V	0.82	0/980	0.87	0/1336
1	W	0.88	0/980	0.90	1/1336 (0.1%)
1	X	0.82	0/980	0.84	0/1336

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	Y	0.82	0/980	0.87	0/1336
1	Z	0.88	0/980	0.90	1/1336 (0.1%)
1	a	0.82	0/980	0.87	0/1336
1	b	0.88	0/980	0.90	1/1336 (0.1%)
1	c	0.82	0/980	0.84	0/1336
1	d	0.82	0/980	0.87	0/1336
1	e	0.88	0/980	0.90	1/1336 (0.1%)
1	f	0.82	0/980	0.84	0/1336
1	g	0.82	0/980	0.87	0/1336
1	h	0.88	0/980	0.90	1/1336 (0.1%)
1	i	0.82	0/980	0.84	0/1336
All	All	0.84	0/44100	0.87	15/60120 (0.0%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Q	42	TYR	N-CA-C	-5.65	95.74	111.00
1	T	42	TYR	N-CA-C	-5.65	95.74	111.00
1	Z	42	TYR	N-CA-C	-5.65	95.74	111.00
1	E	42	TYR	N-CA-C	-5.65	95.75	111.00
1	K	42	TYR	N-CA-C	-5.65	95.75	111.00
1	3	42	TYR	N-CA-C	-5.65	95.75	111.00
1	6	42	TYR	N-CA-C	-5.65	95.75	111.00
1	b	42	TYR	N-CA-C	-5.65	95.75	111.00
1	e	42	TYR	N-CA-C	-5.65	95.75	111.00
1	B	42	TYR	N-CA-C	-5.65	95.75	111.00
1	H	42	TYR	N-CA-C	-5.65	95.75	111.00
1	9	42	TYR	N-CA-C	-5.65	95.75	111.00
1	N	42	TYR	N-CA-C	-5.64	95.78	111.00
1	W	42	TYR	N-CA-C	-5.64	95.78	111.00
1	h	42	TYR	N-CA-C	-5.64	95.78	111.00

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	0	963	0	976	18	0
1	1	963	0	976	38	0
1	2	963	0	976	35	0
1	3	963	0	976	37	0
1	4	963	0	976	35	0
1	5	963	0	976	31	0
1	6	963	0	976	35	0
1	7	963	0	976	18	0
1	8	963	0	976	31	0
1	9	963	0	976	35	0
1	A	963	0	976	39	0
1	B	963	0	976	51	0
1	C	963	0	976	21	0
1	D	963	0	976	47	2
1	E	963	0	976	51	0
1	F	963	0	976	59	0
1	G	963	0	976	41	0
1	H	963	0	976	51	0
1	I	963	0	976	25	0
1	J	963	0	976	32	0
1	K	963	0	976	38	0
1	L	963	0	976	19	0
1	M	963	0	976	31	0
1	N	963	0	976	36	0
1	O	963	0	976	18	0
1	P	963	0	976	37	0
1	Q	963	0	976	38	0
1	R	963	0	976	38	0
1	S	963	0	976	36	0
1	T	963	0	976	38	0
1	U	963	0	976	36	0
1	V	963	0	976	31	2
1	W	963	0	976	36	0
1	X	963	0	976	17	0
1	Y	963	0	976	35	0
1	Z	963	0	976	37	0
1	a	963	0	976	0	0
1	b	963	0	976	0	0
1	c	963	0	976	0	0
1	d	963	0	976	0	0
1	e	963	0	976	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	f	963	0	976	0	0
1	g	963	0	976	0	0
1	h	963	0	976	0	0
1	i	963	0	976	0	0
All	All	43335	0	43920	987	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (987) 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:U:101:VAL:HG12	1:4:123:SER:HA	1.42	1.01
1:F:123:SER:HA	1:R:101:VAL:HG12	95.48	1.00
1:F:101:VAL:HG12	1:1:123:SER:HA	1.42	1.00
1:F:101:VAL:HG12	1:R:123:SER:HA	58.93	1.00
1:F:123:SER:HA	1:1:101:VAL:HG12	1.42	0.99
1:U:123:SER:HA	1:4:101:VAL:HG12	1.42	0.97
1:R:20:VAL:CG1	1:R:32:TRP:HB3	1.99	0.93
1:0:20:VAL:CG1	1:0:32:TRP:HB3	2.00	0.92
1:O:20:VAL:CG1	1:O:32:TRP:HB3	2.00	0.92
1:L:20:VAL:CG1	1:L:32:TRP:HB3	2.00	0.92
1:4:20:VAL:CG1	1:4:32:TRP:HB3	2.00	0.92
1:U:20:VAL:CG1	1:U:32:TRP:HB3	1.99	0.92
1:I:20:VAL:CG1	1:I:32:TRP:HB3	2.00	0.92
1:7:20:VAL:CG1	1:7:32:TRP:HB3	2.00	0.92
1:C:20:VAL:CG1	1:C:32:TRP:HB3	2.00	0.92
1:F:20:VAL:CG1	1:F:32:TRP:HB3	2.00	0.92
1:1:20:VAL:CG1	1:1:32:TRP:HB3	1.99	0.91
1:X:20:VAL:CG1	1:X:32:TRP:HB3	2.00	0.91
1:G:71:VAL:HG12	1:G:76:GLU:HB3	1.62	0.81
1:X:20:VAL:HG12	1:X:32:TRP:HB3	1.63	0.81
1:E:20:VAL:HG13	1:E:32:TRP:HB3	1.62	0.81
1:D:71:VAL:HG12	1:D:76:GLU:HB3	1.62	0.81
1:4:20:VAL:HG12	1:4:32:TRP:HB3	1.63	0.81
1:6:20:VAL:HG13	1:6:32:TRP:HB3	1.62	0.81
1:M:71:VAL:HG12	1:M:76:GLU:HB3	1.63	0.81
1:K:20:VAL:HG13	1:K:32:TRP:HB3	1.62	0.81
1:Q:20:VAL:HG13	1:Q:32:TRP:HB3	1.62	0.81
1:2:71:VAL:HG12	1:2:76:GLU:HB3	1.62	0.81
1:9:20:VAL:HG13	1:9:32:TRP:HB3	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:7:20:VAL:HG12	1:7:32:TRP:HB3	1.63	0.81
1:B:20:VAL:HG13	1:B:32:TRP:HB3	1.62	0.81
1:T:20:VAL:HG13	1:T:32:TRP:HB3	1.62	0.81
1:S:71:VAL:HG12	1:S:76:GLU:HB3	1.62	0.81
1:P:71:VAL:HG12	1:P:76:GLU:HB3	1.62	0.80
1:A:71:VAL:HG12	1:A:76:GLU:HB3	1.62	0.80
1:C:20:VAL:HG12	1:C:32:TRP:HB3	1.62	0.80
1:Z:20:VAL:HG13	1:Z:32:TRP:HB3	1.62	0.80
1:W:20:VAL:HG13	1:W:32:TRP:HB3	1.62	0.80
1:F:20:VAL:HG12	1:F:32:TRP:HB3	1.63	0.80
1:L:20:VAL:HG12	1:L:32:TRP:HB3	1.63	0.80
1:J:71:VAL:HG12	1:J:76:GLU:HB3	1.62	0.80
1:8:71:VAL:HG12	1:8:76:GLU:HB3	1.62	0.80
1:3:20:VAL:HG13	1:3:32:TRP:HB3	1.62	0.80
1:V:71:VAL:HG12	1:V:76:GLU:HB3	1.63	0.80
1:N:20:VAL:HG13	1:N:32:TRP:HB3	1.62	0.80
1:H:20:VAL:HG13	1:H:32:TRP:HB3	1.62	0.80
1:I:20:VAL:HG12	1:I:32:TRP:HB3	1.62	0.79
1:Y:71:VAL:HG12	1:Y:76:GLU:HB3	1.62	0.79
1:5:71:VAL:HG12	1:5:76:GLU:HB3	1.62	0.79
1:1:20:VAL:HG12	1:1:32:TRP:HB3	1.62	0.79
1:O:20:VAL:HG12	1:O:32:TRP:HB3	1.63	0.78
1:R:20:VAL:HG12	1:R:32:TRP:HB3	1.62	0.78
1:0:20:VAL:HG12	1:0:32:TRP:HB3	1.62	0.78
1:U:20:VAL:HG12	1:U:32:TRP:HB3	1.62	0.78
1:N:123:SER:HA	1:Y:101:VAL:HG12	1.68	0.76
1:Q:63:GLU:HB3	1:Q:83:LYS:HE2	1.68	0.76
1:E:63:GLU:HB3	1:E:83:LYS:HE2	1.68	0.76
1:D:101:VAL:HG12	1:Z:123:SER:HA	96.25	0.76
1:3:123:SER:HA	1:8:101:VAL:HG12	1.68	0.76
1:W:63:GLU:HB3	1:W:83:LYS:HE2	1.68	0.76
1:A:101:VAL:HG12	1:E:123:SER:HA	139.14	0.76
1:H:123:SER:HA	1:5:101:VAL:HG12	1.68	0.76
1:B:123:SER:HA	1:V:101:VAL:HG12	146.58	0.75
1:H:63:GLU:HB3	1:H:83:LYS:HE2	1.68	0.75
1:D:101:VAL:HG12	1:T:123:SER:HA	1.68	0.75
1:9:63:GLU:HB3	1:9:83:LYS:HE2	1.68	0.75
1:Z:63:GLU:HB3	1:Z:83:LYS:HE2	1.68	0.75
1:P:101:VAL:HG12	1:W:123:SER:HA	1.68	0.75
1:B:63:GLU:HB3	1:B:83:LYS:HE2	1.68	0.75
1:H:123:SER:HA	1:S:101:VAL:HG12	53.02	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:123:SER:HA	1:G:101:VAL:HG12	1.68	0.74
1:Q:123:SER:HA	1:2:101:VAL:HG12	1.68	0.74
1:3:63:GLU:HB3	1:3:83:LYS:HE2	1.68	0.74
1:K:63:GLU:HB3	1:K:83:LYS:HE2	1.68	0.74
1:6:63:GLU:HB3	1:6:83:LYS:HE2	1.68	0.74
1:N:63:GLU:HB3	1:N:83:LYS:HE2	1.68	0.74
1:G:101:VAL:HG12	1:6:123:SER:HA	53.50	0.74
1:T:63:GLU:HB3	1:T:83:LYS:HE2	1.68	0.73
1:A:101:VAL:HG12	1:9:123:SER:HA	142.74	0.73
1:B:123:SER:HA	1:J:101:VAL:HG12	1.68	0.73
1:F:2:ALA:N	1:1:129:TYR:CE1	2.57	0.73
1:B:126:SER:HA	1:W:23:VAL:HG13	141.61	0.73
1:K:123:SER:HA	1:M:101:VAL:HG12	1.68	0.73
1:F:129:TYR:CE1	1:R:2:ALA:N	91.61	0.73
1:U:129:TYR:CE1	1:4:2:ALA:N	2.57	0.73
1:F:2:ALA:N	1:R:129:TYR:CE1	77.17	0.72
1:B:126:SER:HA	1:K:23:VAL:HG13	1.71	0.72
1:U:2:ALA:N	1:4:129:TYR:CE1	2.57	0.72
1:E:126:SER:HA	1:H:23:VAL:HG13	1.71	0.72
1:B:23:VAL:HG13	1:E:126:SER:HA	146.88	0.72
1:K:126:SER:HA	1:N:23:VAL:HG13	1.71	0.72
1:Q:126:SER:HA	1:3:23:VAL:HG13	1.71	0.72
1:B:23:VAL:HG13	1:9:126:SER:HA	143.13	0.72
1:Q:23:VAL:HG13	1:W:126:SER:HA	1.71	0.72
1:F:129:TYR:CE1	1:1:2:ALA:N	2.57	0.72
1:E:23:VAL:HG13	1:T:126:SER:HA	1.71	0.72
1:H:23:VAL:HG13	1:6:126:SER:HA	58.74	0.72
1:H:126:SER:HA	1:T:23:VAL:HG13	59.71	0.71
1:N:126:SER:HA	1:Z:23:VAL:HG13	1.71	0.71
1:E:23:VAL:HG13	1:Z:126:SER:HA	95.20	0.71
1:H:126:SER:HA	1:6:23:VAL:HG13	1.71	0.71
1:3:126:SER:HA	1:9:23:VAL:HG13	1.71	0.70
1:C:102:THR:O	1:C:105:SER:HB3	1.91	0.70
1:4:102:THR:O	1:4:105:SER:HB3	1.91	0.70
1:7:102:THR:O	1:7:105:SER:HB3	1.91	0.70
1:X:102:THR:O	1:X:105:SER:HB3	1.91	0.70
1:I:102:THR:O	1:I:105:SER:HB3	1.91	0.70
1:R:102:THR:O	1:R:105:SER:HB3	1.91	0.70
1:L:102:THR:O	1:L:105:SER:HB3	1.91	0.70
1:F:102:THR:O	1:F:105:SER:HB3	1.91	0.70
1:O:102:THR:O	1:O:105:SER:HB3	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:102:THR:O	1:U:105:SER:HB3	1.91	0.69
1:F:126:SER:HA	1:Y:23:VAL:HG12	1.74	0.69
1:0:102:THR:O	1:0:105:SER:HB3	1.91	0.69
1:F:126:SER:HA	1:P:23:VAL:HG12	94.56	0.69
1:1:102:THR:O	1:1:105:SER:HB3	1.91	0.69
1:U:126:SER:HA	1:2:23:VAL:HG12	1.74	0.69
1:D:23:VAL:HG12	1:R:126:SER:HA	64.90	0.69
1:S:23:VAL:HG12	1:4:126:SER:HA	1.74	0.68
1:P:102:THR:O	1:P:105:SER:HB3	1.94	0.68
1:2:102:THR:O	1:2:105:SER:HB3	1.94	0.68
1:M:102:THR:O	1:M:105:SER:HB3	1.94	0.68
1:A:102:THR:O	1:A:105:SER:HB3	1.94	0.68
1:S:23:VAL:HG21	1:S:33:LEU:HB2	1.76	0.68
1:V:102:THR:O	1:V:105:SER:HB3	1.94	0.68
1:D:102:THR:O	1:D:105:SER:HB3	1.94	0.68
1:U:122:ILE:O	1:4:101:VAL:CG1	2.42	0.68
1:G:102:THR:O	1:G:105:SER:HB3	1.94	0.68
1:S:102:THR:O	1:S:105:SER:HB3	1.94	0.68
1:5:102:THR:O	1:5:105:SER:HB3	1.94	0.68
1:D:23:VAL:HG12	1:1:126:SER:HA	1.74	0.68
1:Y:102:THR:O	1:Y:105:SER:HB3	1.94	0.68
1:2:23:VAL:HG21	1:2:33:LEU:HB2	1.76	0.68
1:F:101:VAL:CG1	1:1:122:ILE:O	2.42	0.68
1:A:23:VAL:HG21	1:A:33:LEU:HB2	1.76	0.68
1:Y:20:VAL:HG13	1:Y:32:TRP:HB3	1.76	0.67
1:P:23:VAL:HG21	1:P:33:LEU:HB2	1.76	0.67
1:D:23:VAL:HG21	1:D:33:LEU:HB2	1.76	0.67
1:5:23:VAL:HG21	1:5:33:LEU:HB2	1.76	0.67
1:V:20:VAL:HG13	1:V:32:TRP:HB3	1.77	0.67
1:F:122:ILE:O	1:R:101:VAL:CG1	93.88	0.67
1:F:101:VAL:CG1	1:R:122:ILE:O	58.20	0.67
1:V:23:VAL:HG21	1:V:33:LEU:HB2	1.76	0.67
1:2:20:VAL:HG13	1:2:32:TRP:HB3	1.77	0.67
1:G:23:VAL:HG21	1:G:33:LEU:HB2	1.76	0.67
1:U:101:VAL:CG1	1:4:122:ILE:O	2.42	0.67
1:T:68:VAL:O	1:T:69:THR:HB	1.95	0.67
1:K:68:VAL:O	1:K:69:THR:HB	1.95	0.67
1:3:68:VAL:O	1:3:69:THR:HB	1.95	0.67
1:Y:23:VAL:HG21	1:Y:33:LEU:HB2	1.76	0.67
1:M:20:VAL:HG13	1:M:32:TRP:HB3	1.77	0.67
1:F:122:ILE:O	1:1:101:VAL:CG1	2.42	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:102:THR:O	1:J:105:SER:HB3	1.94	0.67
1:D:20:VAL:HG13	1:D:32:TRP:HB3	1.77	0.67
1:Z:68:VAL:O	1:Z:69:THR:HB	1.95	0.67
1:8:102:THR:O	1:8:105:SER:HB3	1.94	0.67
1:D:62:LEU:HB3	1:D:86:ALA:HB3	1.77	0.67
1:Q:68:VAL:O	1:Q:69:THR:HB	1.95	0.67
1:B:68:VAL:O	1:B:69:THR:HB	1.95	0.67
1:E:68:VAL:O	1:E:69:THR:HB	1.95	0.66
1:S:62:LEU:HB3	1:S:86:ALA:HB3	1.77	0.66
1:G:20:VAL:HG13	1:G:32:TRP:HB3	1.77	0.66
1:M:62:LEU:HB3	1:M:86:ALA:HB3	1.77	0.66
1:J:23:VAL:HG21	1:J:33:LEU:HB2	1.76	0.66
1:5:20:VAL:HG13	1:5:32:TRP:HB3	1.77	0.66
1:A:62:LEU:HB3	1:A:86:ALA:HB3	1.77	0.66
1:H:68:VAL:O	1:H:69:THR:HB	1.95	0.66
1:2:62:LEU:HB3	1:2:86:ALA:HB3	1.77	0.66
1:M:23:VAL:HG21	1:M:33:LEU:HB2	1.76	0.66
1:A:20:VAL:HG13	1:A:32:TRP:HB3	1.77	0.66
1:W:68:VAL:O	1:W:69:THR:HB	1.95	0.66
1:8:23:VAL:HG21	1:8:33:LEU:HB2	1.76	0.66
1:G:62:LEU:HB3	1:G:86:ALA:HB3	1.77	0.66
1:J:20:VAL:HG13	1:J:32:TRP:HB3	1.77	0.66
1:F:123:SER:HA	1:R:101:VAL:CG1	95.60	0.66
1:N:68:VAL:O	1:N:69:THR:HB	1.95	0.65
1:6:68:VAL:O	1:6:69:THR:HB	1.95	0.65
1:P:62:LEU:HB3	1:P:86:ALA:HB3	1.77	0.65
1:5:62:LEU:HB3	1:5:86:ALA:HB3	1.77	0.65
1:8:20:VAL:HG13	1:8:32:TRP:HB3	1.77	0.65
1:Y:62:LEU:HB3	1:Y:86:ALA:HB3	1.77	0.65
1:V:62:LEU:HB3	1:V:86:ALA:HB3	1.77	0.65
1:P:20:VAL:HG13	1:P:32:TRP:HB3	1.76	0.65
1:9:68:VAL:O	1:9:69:THR:HB	1.95	0.65
1:S:20:VAL:HG13	1:S:32:TRP:HB3	1.76	0.65
1:A:6:SER:HB3	1:A:21:VAL:HG12	1.79	0.65
1:8:62:LEU:HB3	1:8:86:ALA:HB3	1.77	0.65
1:5:6:SER:HB3	1:5:21:VAL:HG12	1.79	0.65
1:P:6:SER:HB3	1:P:21:VAL:HG12	1.79	0.65
1:Y:6:SER:HB3	1:Y:21:VAL:HG12	1.79	0.64
1:G:6:SER:HB3	1:G:21:VAL:HG12	1.79	0.64
1:S:6:SER:HB3	1:S:21:VAL:HG12	1.79	0.64
1:J:62:LEU:HB3	1:J:86:ALA:HB3	1.77	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:6:SER:HB3	1:D:21:VAL:HG12	1.79	0.64
1:U:101:VAL:CG1	1:4:123:SER:HA	2.23	0.63
1:J:6:SER:HB3	1:J:21:VAL:HG12	1.79	0.63
1:V:6:SER:HB3	1:V:21:VAL:HG12	1.79	0.63
1:F:101:VAL:CG1	1:R:123:SER:HA	58.61	0.63
1:2:6:SER:HB3	1:2:21:VAL:HG12	1.79	0.63
1:M:6:SER:HB3	1:M:21:VAL:HG12	1.79	0.63
1:U:123:SER:HA	1:4:101:VAL:CG1	2.23	0.62
1:F:123:SER:HA	1:1:101:VAL:CG1	2.23	0.62
1:8:6:SER:HB3	1:8:21:VAL:HG12	1.79	0.62
1:F:101:VAL:CG1	1:1:123:SER:HA	2.23	0.62
1:6:33:LEU:HD22	1:6:41:ALA:HB1	1.83	0.61
1:D:23:VAL:CG1	1:R:126:SER:HA	64.77	0.61
1:F:126:SER:HA	1:Y:23:VAL:CG1	2.31	0.61
1:T:33:LEU:HD22	1:T:41:ALA:HB1	1.83	0.61
1:B:101:VAL:CG1	1:J:123:SER:HA	2.31	0.61
1:H:101:VAL:CG1	1:5:123:SER:HA	2.31	0.61
1:K:101:VAL:CG1	1:M:123:SER:HA	2.31	0.61
1:0:79:VAL:HG12	1:0:80:SER:N	2.16	0.60
1:I:79:VAL:HG12	1:I:80:SER:N	2.16	0.60
1:4:71:VAL:HG12	1:4:76:GLU:HB3	1.83	0.60
1:N:101:VAL:CG1	1:Y:123:SER:HA	2.31	0.60
1:4:79:VAL:HG12	1:4:80:SER:N	2.16	0.60
1:B:33:LEU:HD22	1:B:41:ALA:HB1	1.83	0.60
1:I:71:VAL:HG12	1:I:76:GLU:HB3	1.83	0.60
1:R:79:VAL:HG12	1:R:80:SER:N	2.16	0.60
1:L:79:VAL:HG12	1:L:80:SER:N	2.16	0.60
1:H:101:VAL:CG1	1:S:123:SER:HA	92.77	0.60
1:E:101:VAL:CG1	1:G:123:SER:HA	2.31	0.60
1:D:23:VAL:CG1	1:1:126:SER:HA	2.31	0.60
1:O:79:VAL:HG12	1:O:80:SER:N	2.17	0.60
1:R:71:VAL:HG12	1:R:76:GLU:HB3	1.83	0.60
1:3:33:LEU:HD22	1:3:41:ALA:HB1	1.83	0.60
1:Q:33:LEU:HD22	1:Q:41:ALA:HB1	1.83	0.60
1:U:126:SER:HA	1:2:23:VAL:CG1	2.31	0.60
1:Q:101:VAL:CG1	1:2:123:SER:HA	2.31	0.60
1:F:79:VAL:HG12	1:F:80:SER:N	2.16	0.60
1:9:33:LEU:HD22	1:9:41:ALA:HB1	1.83	0.60
1:G:123:SER:HA	1:6:101:VAL:CG1	93.15	0.60
1:7:71:VAL:HG12	1:7:76:GLU:HB3	1.84	0.60
1:X:79:VAL:HG12	1:X:80:SER:N	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:7:79:VAL:HG12	1:7:80:SER:N	2.16	0.60
1:E:33:LEU:HD22	1:E:41:ALA:HB1	1.83	0.60
1:1:79:VAL:HG12	1:1:80:SER:N	2.16	0.60
1:W:33:LEU:HD22	1:W:41:ALA:HB1	1.83	0.60
1:Z:33:LEU:HD22	1:Z:41:ALA:HB1	1.83	0.60
1:S:23:VAL:CG1	1:4:126:SER:HA	2.31	0.60
1:F:71:VAL:HG12	1:F:76:GLU:HB3	1.83	0.60
1:K:33:LEU:HD22	1:K:41:ALA:HB1	1.83	0.60
1:F:126:SER:HA	1:P:23:VAL:CG1	95.28	0.60
1:U:71:VAL:HG12	1:U:76:GLU:HB3	1.83	0.60
1:C:79:VAL:HG12	1:C:80:SER:N	2.16	0.60
1:P:123:SER:HA	1:W:101:VAL:CG1	2.31	0.60
1:D:123:SER:HA	1:Z:101:VAL:CG1	57.57	0.60
1:N:33:LEU:HD22	1:N:41:ALA:HB1	1.83	0.59
1:C:71:VAL:HG12	1:C:76:GLU:HB3	1.83	0.59
1:0:71:VAL:HG12	1:0:76:GLU:HB3	1.83	0.59
1:H:33:LEU:HD22	1:H:41:ALA:HB1	1.83	0.59
1:A:123:SER:HA	1:9:101:VAL:CG1	139.47	0.59
1:D:123:SER:HA	1:T:101:VAL:CG1	2.31	0.59
1:U:79:VAL:HG12	1:U:80:SER:N	2.16	0.59
1:3:101:VAL:CG1	1:8:123:SER:HA	2.31	0.59
1:A:123:SER:HA	1:E:101:VAL:CG1	117.18	0.59
1:O:71:VAL:HG12	1:O:76:GLU:HB3	1.84	0.59
1:B:101:VAL:CG1	1:V:123:SER:HA	148.14	0.59
1:L:71:VAL:HG12	1:L:76:GLU:HB3	1.84	0.59
1:X:71:VAL:HG12	1:X:76:GLU:HB3	1.84	0.59
1:D:123:SER:HA	1:Z:101:VAL:HG13	58.48	0.58
1:K:101:VAL:HG13	1:M:123:SER:HA	1.85	0.58
1:B:123:SER:HA	1:V:101:VAL:CG1	145.89	0.58
1:G:123:SER:HA	1:6:101:VAL:HG13	92.35	0.58
1:A:123:SER:HA	1:9:101:VAL:HG13	138.61	0.58
1:1:71:VAL:HG12	1:1:76:GLU:HB3	1.83	0.58
1:Q:123:SER:HA	1:2:101:VAL:CG1	2.34	0.58
1:B:101:VAL:HG13	1:J:123:SER:HA	1.85	0.58
1:3:123:SER:HA	1:8:101:VAL:CG1	2.34	0.58
1:N:123:SER:HA	1:Y:101:VAL:CG1	2.33	0.58
1:H:101:VAL:HG13	1:S:123:SER:HA	91.83	0.58
1:E:101:VAL:HG13	1:G:123:SER:HA	1.85	0.58
1:P:101:VAL:CG1	1:W:123:SER:HA	2.33	0.58
1:H:54:ASP:HA	1:H:94:ILE:HD13	1.86	0.58
1:9:54:ASP:HA	1:9:94:ILE:HD13	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:54:ASP:HA	1:3:94:ILE:HD13	1.86	0.58
1:Q:101:VAL:HG13	1:2:123:SER:HA	1.86	0.57
1:N:54:ASP:HA	1:N:94:ILE:HD13	1.86	0.57
1:B:54:ASP:HA	1:B:94:ILE:HD13	1.86	0.57
1:D:101:VAL:CG1	1:Z:123:SER:HA	96.52	0.57
1:G:101:VAL:CG1	1:6:123:SER:HA	52.69	0.57
1:H:101:VAL:HG13	1:5:123:SER:HA	1.85	0.57
1:P:123:SER:HA	1:W:101:VAL:HG13	1.86	0.57
1:D:123:SER:HA	1:T:101:VAL:HG13	1.86	0.57
1:6:54:ASP:HA	1:6:94:ILE:HD13	1.86	0.57
1:B:123:SER:HA	1:J:101:VAL:CG1	2.34	0.57
1:B:101:VAL:HG13	1:V:123:SER:HA	148.31	0.57
1:3:101:VAL:HG13	1:8:123:SER:HA	1.85	0.57
1:Z:54:ASP:HA	1:Z:94:ILE:HD13	1.86	0.57
1:A:101:VAL:CG1	1:9:123:SER:HA	143.04	0.57
1:K:123:SER:HA	1:M:101:VAL:CG1	2.34	0.57
1:E:54:ASP:HA	1:E:94:ILE:HD13	1.86	0.57
1:4:71:VAL:CG1	1:4:76:GLU:HB3	2.35	0.57
1:U:71:VAL:CG1	1:U:76:GLU:HB3	2.35	0.57
1:N:101:VAL:HG13	1:Y:123:SER:HA	1.86	0.57
1:I:71:VAL:CG1	1:I:76:GLU:HB3	2.35	0.57
1:C:71:VAL:CG1	1:C:76:GLU:HB3	2.35	0.57
1:T:54:ASP:HA	1:T:94:ILE:HD13	1.86	0.57
1:A:101:VAL:CG1	1:E:123:SER:HA	138.69	0.57
1:D:101:VAL:CG1	1:T:123:SER:HA	2.34	0.56
1:F:71:VAL:CG1	1:F:76:GLU:HB3	2.35	0.56
1:L:71:VAL:CG1	1:L:76:GLU:HB3	2.35	0.56
1:H:123:SER:HA	1:5:101:VAL:CG1	2.34	0.56
1:1:71:VAL:CG1	1:1:76:GLU:HB3	2.35	0.56
1:R:71:VAL:CG1	1:R:76:GLU:HB3	2.35	0.56
1:7:71:VAL:CG1	1:7:76:GLU:HB3	2.35	0.56
1:X:71:VAL:CG1	1:X:76:GLU:HB3	2.35	0.56
1:K:54:ASP:HA	1:K:94:ILE:HD13	1.86	0.56
1:W:54:ASP:HA	1:W:94:ILE:HD13	1.86	0.56
1:Q:54:ASP:HA	1:Q:94:ILE:HD13	1.86	0.56
1:B:68:VAL:HG21	1:W:73:ASN:HB3	143.09	0.56
1:F:122:ILE:O	1:R:101:VAL:HG11	94.45	0.56
1:C:79:VAL:HG12	1:C:80:SER:H	1.71	0.56
1:0:71:VAL:CG1	1:0:76:GLU:HB3	2.35	0.56
1:E:73:ASN:HB3	1:Z:68:VAL:HG21	114.54	0.56
1:B:68:VAL:HG21	1:K:73:ASN:HB3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:ASN:HB3	1:E:68:VAL:HG21	140.62	0.56
1:A:123:SER:HA	1:E:101:VAL:HG13	117.70	0.56
1:U:79:VAL:HG12	1:U:80:SER:H	1.71	0.56
1:E:68:VAL:HG21	1:H:73:ASN:HB3	1.88	0.56
1:E:123:SER:HA	1:G:101:VAL:CG1	2.34	0.56
1:E:73:ASN:HB3	1:T:68:VAL:HG21	1.88	0.56
1:K:68:VAL:HG21	1:N:73:ASN:HB3	1.88	0.56
1:B:73:ASN:HB3	1:9:68:VAL:HG21	143.73	0.56
1:D:94:ILE:HG13	1:E:39:SER:HB3	1.89	0.56
1:8:94:ILE:HG13	1:9:39:SER:HB3	1.88	0.56
1:R:79:VAL:HG12	1:R:80:SER:H	1.71	0.55
1:X:79:VAL:HG12	1:X:80:SER:H	1.71	0.55
1:7:79:VAL:HG12	1:7:80:SER:H	1.71	0.55
1:5:94:ILE:HG13	1:6:39:SER:HB3	1.88	0.55
1:U:122:ILE:O	1:4:101:VAL:HG11	2.06	0.55
1:H:68:VAL:HG21	1:T:73:ASN:HB3	32.54	0.55
1:0:79:VAL:HG12	1:0:80:SER:H	1.71	0.55
1:S:94:ILE:HG13	1:T:39:SER:HB3	1.89	0.55
1:V:94:ILE:HG13	1:W:39:SER:HB3	1.89	0.55
1:F:101:VAL:HG11	1:1:122:ILE:O	2.06	0.55
1:I:79:VAL:HG12	1:I:80:SER:H	1.71	0.55
1:U:101:VAL:HG11	1:4:122:ILE:O	2.06	0.55
1:Q:73:ASN:HB3	1:W:68:VAL:HG21	1.88	0.55
1:L:79:VAL:HG12	1:L:80:SER:H	1.71	0.55
1:F:122:ILE:O	1:1:101:VAL:HG11	2.06	0.55
1:H:73:ASN:HB3	1:6:68:VAL:HG21	31.47	0.55
1:4:79:VAL:HG12	1:4:80:SER:H	1.71	0.55
1:Y:94:ILE:HG13	1:Z:39:SER:HB3	1.89	0.55
1:J:94:ILE:HG13	1:K:39:SER:HB3	1.88	0.55
1:Q:68:VAL:HG21	1:3:73:ASN:HB3	1.88	0.55
1:H:68:VAL:HG21	1:6:73:ASN:HB3	1.88	0.55
1:O:71:VAL:CG1	1:O:76:GLU:HB3	2.35	0.55
1:N:68:VAL:HG21	1:Z:73:ASN:HB3	1.88	0.55
1:F:101:VAL:HG11	1:R:122:ILE:O	58.83	0.54
1:I:21:VAL:O	1:I:32:TRP:HA	2.08	0.54
1:H:123:SER:HA	1:S:101:VAL:CG1	52.53	0.54
1:M:94:ILE:HG13	1:N:39:SER:HB3	1.89	0.54
1:A:94:ILE:HG13	1:B:39:SER:HB3	1.88	0.54
1:1:79:VAL:HG12	1:1:80:SER:H	1.71	0.54
1:B:102:THR:O	1:B:105:SER:HB3	2.08	0.54
1:W:102:THR:O	1:W:105:SER:HB3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:21:VAL:O	1:O:32:TRP:HA	2.08	0.54
1:7:21:VAL:O	1:7:32:TRP:HA	2.08	0.54
1:X:21:VAL:O	1:X:32:TRP:HA	2.08	0.54
1:3:68:VAL:HG21	1:9:73:ASN:HB3	1.88	0.54
1:O:79:VAL:HG12	1:O:80:SER:H	1.71	0.54
1:G:94:ILE:HG13	1:H:39:SER:HB3	1.88	0.54
1:9:102:THR:O	1:9:105:SER:HB3	2.08	0.54
1:6:102:THR:O	1:6:105:SER:HB3	2.08	0.54
1:U:21:VAL:O	1:U:32:TRP:HA	2.08	0.54
1:F:79:VAL:HG12	1:F:80:SER:H	1.71	0.54
1:Q:102:THR:O	1:Q:105:SER:HB3	2.08	0.54
1:K:102:THR:O	1:K:105:SER:HB3	2.08	0.54
1:E:102:THR:O	1:E:105:SER:HB3	2.08	0.54
1:T:102:THR:O	1:T:105:SER:HB3	2.08	0.54
1:H:102:THR:O	1:H:105:SER:HB3	2.08	0.54
1:R:21:VAL:O	1:R:32:TRP:HA	2.08	0.54
1:C:21:VAL:O	1:C:32:TRP:HA	2.08	0.54
1:3:102:THR:O	1:3:105:SER:HB3	2.08	0.54
1:L:21:VAL:O	1:L:32:TRP:HA	2.08	0.54
1:F:21:VAL:O	1:F:32:TRP:HA	2.08	0.54
1:P:94:ILE:HG13	1:Q:39:SER:HB3	1.89	0.54
1:0:21:VAL:O	1:0:32:TRP:HA	2.08	0.53
1:1:21:VAL:O	1:1:32:TRP:HA	2.08	0.53
1:N:102:THR:O	1:N:105:SER:HB3	2.08	0.53
1:2:94:ILE:HG13	1:3:39:SER:HB3	1.89	0.53
1:Z:102:THR:O	1:Z:105:SER:HB3	2.08	0.53
1:4:21:VAL:O	1:4:32:TRP:HA	2.08	0.53
1:E:21:VAL:O	1:E:32:TRP:HA	2.10	0.52
1:K:21:VAL:O	1:K:32:TRP:HA	2.10	0.52
1:T:21:VAL:O	1:T:32:TRP:HA	2.09	0.52
1:3:21:VAL:O	1:3:32:TRP:HA	2.10	0.52
1:Z:21:VAL:O	1:Z:32:TRP:HA	2.09	0.52
1:Q:21:VAL:O	1:Q:32:TRP:HA	2.09	0.52
1:N:21:VAL:O	1:N:32:TRP:HA	2.10	0.52
1:H:21:VAL:O	1:H:32:TRP:HA	2.10	0.52
1:A:71:VAL:CG1	1:A:76:GLU:HB3	2.38	0.52
1:D:3:THR:OG1	1:Z:128:PHE:HA	85.10	0.52
1:P:3:THR:OG1	1:W:128:PHE:HA	2.10	0.52
1:K:128:PHE:HA	1:M:3:THR:OG1	2.10	0.52
1:W:21:VAL:O	1:W:32:TRP:HA	2.10	0.52
1:B:128:PHE:HA	1:J:3:THR:OG1	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:21:VAL:O	1:B:32:TRP:HA	2.10	0.52
1:H:128:PHE:HA	1:S:3:THR:OG1	71.60	0.52
1:D:3:THR:OG1	1:T:128:PHE:HA	2.10	0.51
1:B:128:PHE:HA	1:V:3:THR:OG1	144.61	0.51
1:7:38:ARG:N	1:7:38:ARG:HD3	2.25	0.51
1:Z:68:VAL:O	1:Z:69:THR:CB	2.59	0.51
1:B:68:VAL:O	1:B:69:THR:CB	2.59	0.51
1:G:3:THR:OG1	1:6:128:PHE:HA	71.50	0.51
1:P:71:VAL:CG1	1:P:76:GLU:HB3	2.39	0.51
1:H:128:PHE:HA	1:5:3:THR:OG1	2.10	0.51
1:F:38:ARG:N	1:F:38:ARG:HD3	2.25	0.51
1:A:3:THR:OG1	1:9:128:PHE:HA	143.31	0.51
1:E:128:PHE:HA	1:G:3:THR:OG1	2.10	0.51
1:9:21:VAL:O	1:9:32:TRP:HA	2.10	0.51
1:Q:68:VAL:O	1:Q:69:THR:CB	2.59	0.51
1:Q:128:PHE:HA	1:2:3:THR:OG1	2.10	0.51
1:C:38:ARG:N	1:C:38:ARG:HD3	2.25	0.51
1:T:68:VAL:O	1:T:69:THR:CB	2.59	0.51
1:9:68:VAL:O	1:9:69:THR:CB	2.59	0.51
1:R:38:ARG:N	1:R:38:ARG:HD3	2.25	0.51
1:G:71:VAL:CG1	1:G:76:GLU:HB3	2.38	0.51
1:6:21:VAL:O	1:6:32:TRP:HA	2.10	0.51
1:5:71:VAL:CG1	1:5:76:GLU:HB3	2.38	0.51
1:6:68:VAL:O	1:6:69:THR:CB	2.59	0.51
1:3:128:PHE:HA	1:8:3:THR:OG1	2.10	0.51
1:E:68:VAL:O	1:E:69:THR:CB	2.59	0.51
1:H:68:VAL:O	1:H:69:THR:CB	2.59	0.51
1:4:38:ARG:HD3	1:4:38:ARG:N	2.25	0.51
1:6:34:SER:OG	1:6:36:ASN:ND2	2.44	0.51
1:B:34:SER:OG	1:B:36:ASN:ND2	2.44	0.51
1:3:68:VAL:O	1:3:69:THR:CB	2.59	0.51
1:A:3:THR:OG1	1:E:128:PHE:HA	148.65	0.51
1:3:34:SER:OG	1:3:36:ASN:ND2	2.44	0.51
1:N:34:SER:OG	1:N:36:ASN:ND2	2.44	0.51
1:0:38:ARG:N	1:0:38:ARG:HD3	2.25	0.50
1:9:34:SER:OG	1:9:36:ASN:ND2	2.44	0.50
1:1:38:ARG:N	1:1:38:ARG:HD3	2.25	0.50
1:N:128:PHE:HA	1:Y:3:THR:OG1	2.10	0.50
1:O:38:ARG:N	1:O:38:ARG:HD3	2.25	0.50
1:U:38:ARG:HD3	1:U:38:ARG:N	2.25	0.50
1:I:38:ARG:N	1:I:38:ARG:HD3	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:38:ARG:N	1:L:38:ARG:HD3	2.25	0.50
1:K:34:SER:OG	1:K:36:ASN:ND2	2.44	0.50
1:H:34:SER:OG	1:H:36:ASN:ND2	2.44	0.50
1:X:38:ARG:N	1:X:38:ARG:HD3	2.25	0.50
1:T:34:SER:OG	1:T:36:ASN:ND2	2.44	0.50
1:D:71:VAL:CG1	1:D:76:GLU:HB3	2.39	0.50
1:E:34:SER:OG	1:E:36:ASN:ND2	2.44	0.50
1:Q:34:SER:OG	1:Q:36:ASN:ND2	2.44	0.50
1:2:71:VAL:CG1	1:2:76:GLU:HB3	2.39	0.50
1:W:34:SER:OG	1:W:36:ASN:ND2	2.44	0.50
1:K:6:SER:HB3	1:K:21:VAL:HG12	1.94	0.50
1:W:6:SER:HB3	1:W:21:VAL:HG12	1.94	0.50
1:H:6:SER:HB3	1:H:21:VAL:HG12	1.94	0.50
1:9:6:SER:HB3	1:9:21:VAL:HG12	1.94	0.50
1:K:68:VAL:O	1:K:69:THR:CB	2.59	0.50
1:N:68:VAL:O	1:N:69:THR:CB	2.59	0.50
1:Y:33:LEU:HD22	1:Y:41:ALA:HB1	1.94	0.49
1:S:33:LEU:HD22	1:S:41:ALA:HB1	1.94	0.49
1:Z:34:SER:OG	1:Z:36:ASN:ND2	2.44	0.49
1:V:33:LEU:HD22	1:V:41:ALA:HB1	1.94	0.49
1:G:33:LEU:HD22	1:G:41:ALA:HB1	1.94	0.49
1:P:33:LEU:HD22	1:P:41:ALA:HB1	1.94	0.49
1:J:33:LEU:HD22	1:J:41:ALA:HB1	1.94	0.49
1:B:6:SER:HB3	1:B:21:VAL:HG12	1.94	0.49
1:J:92:ILE:HG12	1:J:104:ILE:HD13	1.95	0.49
1:M:71:VAL:CG1	1:M:76:GLU:HB3	2.39	0.49
1:2:92:ILE:HG12	1:2:104:ILE:HD13	1.95	0.49
1:E:6:SER:HB3	1:E:21:VAL:HG12	1.94	0.49
1:T:6:SER:HB3	1:T:21:VAL:HG12	1.94	0.49
1:D:92:ILE:HG12	1:D:104:ILE:HD13	1.95	0.49
1:D:33:LEU:HD22	1:D:41:ALA:HB1	1.94	0.49
1:8:33:LEU:HD22	1:8:41:ALA:HB1	1.94	0.49
1:S:71:VAL:CG1	1:S:76:GLU:HB3	2.39	0.49
1:Z:6:SER:HB3	1:Z:21:VAL:HG12	1.94	0.49
1:P:92:ILE:HG12	1:P:104:ILE:HD13	1.95	0.49
1:A:33:LEU:HD22	1:A:41:ALA:HB1	1.94	0.49
1:6:6:SER:HB3	1:6:21:VAL:HG12	1.94	0.49
1:8:92:ILE:HG12	1:8:104:ILE:HD13	1.95	0.48
1:5:92:ILE:HG12	1:5:104:ILE:HD13	1.95	0.48
1:V:92:ILE:HG12	1:V:104:ILE:HD13	1.95	0.48
1:M:92:ILE:HG12	1:M:104:ILE:HD13	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:54:ASP:C	1:N:55:LYS:HD2	2.34	0.48
1:Z:54:ASP:C	1:Z:55:LYS:HD2	2.34	0.48
1:N:6:SER:HB3	1:N:21:VAL:HG12	1.94	0.48
1:9:54:ASP:C	1:9:55:LYS:HD2	2.34	0.48
1:G:92:ILE:HG12	1:G:104:ILE:HD13	1.95	0.48
1:S:92:ILE:HG12	1:S:104:ILE:HD13	1.95	0.48
1:H:54:ASP:C	1:H:55:LYS:HD2	2.34	0.48
1:W:54:ASP:C	1:W:55:LYS:HD2	2.34	0.48
1:2:33:LEU:HD22	1:2:41:ALA:HB1	1.94	0.48
1:Q:54:ASP:C	1:Q:55:LYS:HD2	2.34	0.48
1:Q:6:SER:HB3	1:Q:21:VAL:HG12	1.94	0.48
1:A:92:ILE:HG12	1:A:104:ILE:HD13	1.95	0.48
1:5:33:LEU:HD22	1:5:41:ALA:HB1	1.94	0.48
1:M:33:LEU:HD22	1:M:41:ALA:HB1	1.94	0.48
1:B:54:ASP:C	1:B:55:LYS:HD2	2.34	0.48
1:T:54:ASP:C	1:T:55:LYS:HD2	2.34	0.48
1:Z:10:VAL:HB	1:Z:18:VAL:HB	1.96	0.48
1:J:71:VAL:CG1	1:J:76:GLU:HB3	2.38	0.47
1:3:6:SER:HB3	1:3:21:VAL:HG12	1.94	0.47
1:8:33:LEU:HD23	1:8:33:LEU:HA	1.60	0.47
1:6:54:ASP:C	1:6:55:LYS:HD2	2.34	0.47
1:K:10:VAL:HB	1:K:18:VAL:HB	1.96	0.47
1:9:10:VAL:HB	1:9:18:VAL:HB	1.96	0.47
1:H:10:VAL:HB	1:H:18:VAL:HB	1.96	0.47
1:Y:92:ILE:HG12	1:Y:104:ILE:HD13	1.95	0.47
1:K:54:ASP:C	1:K:55:LYS:HD2	2.34	0.47
1:T:10:VAL:HB	1:T:18:VAL:HB	1.96	0.47
1:Z:23:VAL:HG21	1:Z:33:LEU:HB2	1.97	0.47
1:W:68:VAL:O	1:W:69:THR:CB	2.59	0.47
1:3:54:ASP:C	1:3:55:LYS:HD2	2.34	0.47
1:B:86:ALA:HA	1:J:89:ASP:O	2.15	0.47
1:E:86:ALA:HA	1:G:89:ASP:O	2.15	0.47
1:1:4:LEU:HA	1:1:4:LEU:HD12	1.74	0.47
1:E:54:ASP:C	1:E:55:LYS:HD2	2.34	0.47
1:Q:10:VAL:HB	1:Q:18:VAL:HB	1.96	0.47
1:E:10:VAL:HB	1:E:18:VAL:HB	1.96	0.47
1:O:4:LEU:HD12	1:O:4:LEU:HA	1.74	0.47
1:9:19:THR:HG22	1:9:20:VAL:N	2.30	0.47
1:Z:19:THR:HG22	1:Z:20:VAL:N	2.30	0.47
1:Y:71:VAL:CG1	1:Y:76:GLU:HB3	2.39	0.47
1:K:23:VAL:HG21	1:K:33:LEU:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:23:VAL:HG21	1:B:33:LEU:HB2	1.97	0.47
1:A:89:ASP:O	1:9:86:ALA:HA	128.28	0.47
1:P:89:ASP:O	1:W:86:ALA:HA	2.15	0.47
1:D:89:ASP:O	1:T:86:ALA:HA	2.15	0.47
1:6:10:VAL:HB	1:6:18:VAL:HB	1.96	0.47
1:Q:86:ALA:HA	1:2:89:ASP:O	2.15	0.47
1:N:86:ALA:HA	1:Y:89:ASP:O	2.15	0.47
1:T:19:THR:HG22	1:T:20:VAL:N	2.30	0.47
1:E:23:VAL:HG21	1:E:33:LEU:HB2	1.97	0.47
1:U:126:SER:OG	1:2:23:VAL:HG13	2.15	0.47
1:3:10:VAL:HB	1:3:18:VAL:HB	1.96	0.47
1:8:71:VAL:CG1	1:8:76:GLU:HB3	2.38	0.47
1:W:23:VAL:HG21	1:W:33:LEU:HB2	1.97	0.47
1:3:54:ASP:OD1	1:3:54:ASP:N	2.48	0.47
1:A:89:ASP:O	1:E:86:ALA:HA	118.74	0.47
1:H:88:ILE:HD12	1:H:88:ILE:N	2.30	0.47
1:6:19:THR:HG22	1:6:20:VAL:N	2.30	0.47
1:F:126:SER:OG	1:Y:23:VAL:HG13	2.15	0.47
1:Z:54:ASP:OD1	1:Z:54:ASP:N	2.48	0.47
1:I:62:LEU:HB3	1:I:86:ALA:HB3	1.97	0.47
1:C:90:LEU:HD13	1:C:92:ILE:HD11	1.97	0.47
1:1:90:LEU:HD13	1:1:92:ILE:HD11	1.97	0.47
1:X:90:LEU:HD13	1:X:92:ILE:HD11	1.97	0.47
1:B:88:ILE:N	1:B:88:ILE:HD12	2.30	0.47
1:6:88:ILE:N	1:6:88:ILE:HD12	2.30	0.47
1:M:108:LEU:HD23	1:M:108:LEU:HA	1.73	0.47
1:E:19:THR:HG22	1:E:20:VAL:N	2.30	0.46
1:W:19:THR:HG22	1:W:20:VAL:N	2.30	0.46
1:3:19:THR:HG22	1:3:20:VAL:N	2.30	0.46
1:N:23:VAL:HG21	1:N:33:LEU:HB2	1.97	0.46
1:D:23:VAL:HG13	1:R:126:SER:OG	65.59	0.46
1:A:19:THR:HG22	1:A:20:VAL:N	2.30	0.46
1:B:86:ALA:HA	1:V:89:ASP:O	133.27	0.46
1:U:62:LEU:HB3	1:U:86:ALA:HB3	1.97	0.46
1:4:62:LEU:HB3	1:4:86:ALA:HB3	1.97	0.46
1:N:10:VAL:HB	1:N:18:VAL:HB	1.96	0.46
1:N:88:ILE:HD12	1:N:88:ILE:N	2.30	0.46
1:T:23:VAL:HG21	1:T:33:LEU:HB2	1.97	0.46
1:D:19:THR:HG22	1:D:20:VAL:N	2.30	0.46
1:G:19:THR:HG22	1:G:20:VAL:N	2.30	0.46
1:P:19:THR:HG22	1:P:20:VAL:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:9:54:ASP:N	1:9:54:ASP:OD1	2.48	0.46
1:B:54:ASP:N	1:B:54:ASP:OD1	2.48	0.46
1:L:62:LEU:HB3	1:L:86:ALA:HB3	1.97	0.46
1:K:86:ALA:HA	1:M:89:ASP:O	2.15	0.46
1:3:86:ALA:HA	1:8:89:ASP:O	2.15	0.46
1:E:88:ILE:HD12	1:E:88:ILE:N	2.30	0.46
1:H:19:THR:HG22	1:H:20:VAL:N	2.30	0.46
1:P:33:LEU:HD23	1:P:33:LEU:HA	1.60	0.46
1:S:23:VAL:HG13	1:4:126:SER:OG	2.15	0.46
1:M:19:THR:HG22	1:M:20:VAL:N	2.30	0.46
1:S:19:THR:HG22	1:S:20:VAL:N	2.30	0.46
1:H:54:ASP:OD1	1:H:54:ASP:N	2.48	0.46
1:N:54:ASP:OD1	1:N:54:ASP:N	2.48	0.46
1:E:54:ASP:OD1	1:E:54:ASP:N	2.48	0.46
1:A:97:ALA:O	1:A:100:ASP:HB2	2.16	0.46
1:T:88:ILE:N	1:T:88:ILE:HD12	2.30	0.46
1:W:88:ILE:HD12	1:W:88:ILE:N	2.30	0.46
1:O:62:LEU:HB3	1:O:86:ALA:HB3	1.97	0.46
1:Y:19:THR:HG22	1:Y:20:VAL:N	2.30	0.46
1:5:19:THR:HG22	1:5:20:VAL:N	2.30	0.46
1:D:89:ASP:O	1:Z:86:ALA:HA	80.28	0.46
1:D:97:ALA:O	1:D:100:ASP:HB2	2.16	0.46
1:C:62:LEU:HB3	1:C:86:ALA:HB3	1.97	0.46
1:B:10:VAL:HB	1:B:18:VAL:HB	1.96	0.46
1:V:101:VAL:O	1:V:104:ILE:HB	2.16	0.46
1:J:19:THR:HG22	1:J:20:VAL:N	2.30	0.46
1:Q:54:ASP:N	1:Q:54:ASP:OD1	2.48	0.46
1:J:97:ALA:O	1:J:100:ASP:HB2	2.16	0.46
1:U:90:LEU:HD13	1:U:92:ILE:HD11	1.97	0.46
1:R:90:LEU:HD13	1:R:92:ILE:HD11	1.97	0.46
1:3:88:ILE:N	1:3:88:ILE:HD12	2.30	0.46
1:H:86:ALA:HA	1:S:89:ASP:O	53.97	0.46
1:M:101:VAL:O	1:M:104:ILE:HB	2.16	0.46
1:2:19:THR:HG22	1:2:20:VAL:N	2.30	0.46
1:G:89:ASP:O	1:6:86:ALA:HA	53.02	0.46
1:K:88:ILE:HD12	1:K:88:ILE:N	2.30	0.46
1:K:19:THR:HG22	1:K:20:VAL:N	2.30	0.46
1:B:19:THR:HG22	1:B:20:VAL:N	2.30	0.46
1:N:19:THR:HG22	1:N:20:VAL:N	2.30	0.46
1:A:101:VAL:O	1:A:104:ILE:HB	2.16	0.46
1:3:23:VAL:HG21	1:3:33:LEU:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:23:VAL:HG13	1:1:126:SER:OG	2.15	0.46
1:K:54:ASP:N	1:K:54:ASP:OD1	2.48	0.46
1:H:86:ALA:HA	1:5:89:ASP:O	2.15	0.46
1:1:62:LEU:HB3	1:1:86:ALA:HB3	1.97	0.46
1:G:97:ALA:O	1:G:100:ASP:HB2	2.16	0.46
1:Q:88:ILE:HD12	1:Q:88:ILE:N	2.30	0.46
1:8:101:VAL:O	1:8:104:ILE:HB	2.16	0.46
1:5:101:VAL:O	1:5:104:ILE:HB	2.16	0.46
1:V:19:THR:HG22	1:V:20:VAL:N	2.30	0.46
1:J:33:LEU:HA	1:J:33:LEU:HD23	1.60	0.46
1:F:90:LEU:HD13	1:F:92:ILE:HD11	1.97	0.46
1:W:10:VAL:HB	1:W:18:VAL:HB	1.96	0.46
1:Y:97:ALA:O	1:Y:100:ASP:HB2	2.16	0.46
1:3:92:ILE:HA	1:3:93:PRO:HD2	1.84	0.46
1:8:97:ALA:O	1:8:100:ASP:HB2	2.16	0.46
1:9:88:ILE:N	1:9:88:ILE:HD12	2.30	0.46
1:Q:19:THR:HG22	1:Q:20:VAL:N	2.30	0.46
1:H:23:VAL:HG21	1:H:33:LEU:HB2	1.97	0.46
1:6:23:VAL:HG21	1:6:33:LEU:HB2	1.97	0.46
1:6:54:ASP:N	1:6:54:ASP:OD1	2.48	0.46
1:W:54:ASP:OD1	1:W:54:ASP:N	2.48	0.46
1:4:90:LEU:HD13	1:4:92:ILE:HD11	1.97	0.46
1:D:101:VAL:O	1:D:104:ILE:HB	2.16	0.45
1:G:62:LEU:HD12	1:G:63:GLU:H	1.82	0.45
1:V:97:ALA:O	1:V:100:ASP:HB2	2.16	0.45
1:P:97:ALA:O	1:P:100:ASP:HB2	2.16	0.45
1:7:90:LEU:HD13	1:7:92:ILE:HD11	1.97	0.45
1:X:62:LEU:HB3	1:X:86:ALA:HB3	1.97	0.45
1:C:30:ALA:O	1:C:45:THR:HA	2.17	0.45
1:F:62:LEU:HB3	1:F:86:ALA:HB3	1.97	0.45
1:Z:88:ILE:N	1:Z:88:ILE:HD12	2.30	0.45
1:I:111:LEU:HA	1:I:111:LEU:HD12	1.79	0.45
1:G:101:VAL:O	1:G:104:ILE:HB	2.16	0.45
1:Q:23:VAL:HG21	1:Q:33:LEU:HB2	1.97	0.45
1:9:23:VAL:HG21	1:9:33:LEU:HB2	1.97	0.45
1:M:62:LEU:HD12	1:M:63:GLU:H	1.82	0.45
1:T:54:ASP:N	1:T:54:ASP:OD1	2.48	0.45
1:F:30:ALA:O	1:F:45:THR:HA	2.17	0.45
1:0:30:ALA:O	1:0:45:THR:HA	2.17	0.45
1:7:30:ALA:O	1:7:45:THR:HA	2.17	0.45
1:R:62:LEU:HB3	1:R:86:ALA:HB3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:30:ALA:O	1:U:45:THR:HA	2.17	0.45
1:L:90:LEU:HD13	1:L:92:ILE:HD11	1.97	0.45
1:2:108:LEU:HA	1:2:108:LEU:HD23	1.73	0.45
1:2:101:VAL:O	1:2:104:ILE:HB	2.16	0.45
1:8:62:LEU:HD12	1:8:63:GLU:H	1.82	0.45
1:5:62:LEU:HD12	1:5:63:GLU:H	1.82	0.45
1:8:19:THR:HG22	1:8:20:VAL:N	2.30	0.45
1:2:97:ALA:O	1:2:100:ASP:HB2	2.16	0.45
1:1:30:ALA:O	1:1:45:THR:HA	2.17	0.45
1:I:90:LEU:HD13	1:I:92:ILE:HD11	1.97	0.45
1:4:30:ALA:O	1:4:45:THR:HA	2.17	0.45
1:Q:92:ILE:HA	1:Q:93:PRO:HD2	1.84	0.45
1:4:111:LEU:HD12	1:4:111:LEU:HA	1.79	0.45
1:V:71:VAL:CG1	1:V:76:GLU:HB3	2.39	0.45
1:6:33:LEU:HD23	1:6:33:LEU:HA	1.83	0.45
1:K:58:TYR:HB2	1:K:90:LEU:HB3	1.99	0.45
1:I:30:ALA:O	1:I:45:THR:HA	2.17	0.45
1:7:62:LEU:HB3	1:7:86:ALA:HB3	1.97	0.45
1:C:108:LEU:HA	1:C:108:LEU:HD23	1.78	0.45
1:4:108:LEU:HA	1:4:108:LEU:HD23	1.78	0.45
1:0:62:LEU:HB3	1:0:86:ALA:HB3	1.97	0.45
1:P:101:VAL:O	1:P:104:ILE:HB	2.16	0.45
1:F:126:SER:OG	1:P:23:VAL:HG13	95.95	0.45
1:0:90:LEU:HD13	1:0:92:ILE:HD11	1.97	0.45
1:R:30:ALA:O	1:R:45:THR:HA	2.17	0.45
1:J:101:VAL:O	1:J:104:ILE:HB	2.16	0.45
1:B:33:LEU:HD23	1:B:33:LEU:HA	1.82	0.45
1:H:58:TYR:HB2	1:H:90:LEU:HB3	1.99	0.45
1:I:15:THR:HB	1:I:16:GLY:H	1.68	0.45
1:O:30:ALA:O	1:O:45:THR:HA	2.17	0.45
1:S:101:VAL:O	1:S:104:ILE:HB	2.16	0.45
1:Y:33:LEU:HA	1:Y:33:LEU:HD23	1.60	0.45
1:D:33:LEU:HA	1:D:33:LEU:HD23	1.60	0.45
1:P:62:LEU:HD12	1:P:63:GLU:H	1.82	0.45
1:T:58:TYR:HB2	1:T:90:LEU:HB3	1.99	0.45
1:J:57:LYS:HA	1:J:90:LEU:O	2.17	0.45
1:Y:57:LYS:HA	1:Y:90:LEU:O	2.17	0.45
1:C:15:THR:HB	1:C:16:GLY:H	1.68	0.45
1:M:97:ALA:O	1:M:100:ASP:HB2	2.16	0.45
1:E:58:TYR:HB2	1:E:90:LEU:HB3	1.99	0.45
1:5:57:LYS:HA	1:5:90:LEU:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:58:TYR:HB2	1:Z:90:LEU:HB3	1.99	0.45
1:J:108:LEU:HA	1:J:108:LEU:HD23	1.73	0.45
1:G:57:LYS:HA	1:G:90:LEU:O	2.17	0.45
1:Y:101:VAL:O	1:Y:104:ILE:HB	2.16	0.45
1:A:62:LEU:HD12	1:A:63:GLU:H	1.82	0.45
1:2:62:LEU:HD12	1:2:63:GLU:H	1.81	0.45
1:Y:62:LEU:HD12	1:Y:63:GLU:H	1.82	0.45
1:S:97:ALA:O	1:S:100:ASP:HB2	2.16	0.45
1:B:58:TYR:HB2	1:B:90:LEU:HB3	1.99	0.45
1:K:33:LEU:HD23	1:K:33:LEU:HA	1.83	0.44
1:L:30:ALA:O	1:L:45:THR:HA	2.17	0.44
1:5:97:ALA:O	1:5:100:ASP:HB2	2.16	0.44
1:P:108:LEU:HA	1:P:108:LEU:HD23	1.73	0.44
1:F:108:LEU:HA	1:F:108:LEU:HD23	1.78	0.44
1:A:33:LEU:HA	1:A:33:LEU:HD23	1.60	0.44
1:D:62:LEU:HD12	1:D:63:GLU:H	1.81	0.44
1:J:62:LEU:HD12	1:J:63:GLU:H	1.82	0.44
1:D:125:GLN:O	1:1:38:ARG:NH2	57.95	0.44
1:Q:58:TYR:HB2	1:Q:90:LEU:HB3	1.99	0.44
1:X:30:ALA:O	1:X:45:THR:HA	2.17	0.44
1:F:2:ALA:N	1:R:129:TYR:HE1	77.49	0.44
1:T:33:LEU:HD23	1:T:33:LEU:HA	1.82	0.44
1:O:90:LEU:HD13	1:O:92:ILE:HD11	1.97	0.44
1:2:33:LEU:HD23	1:2:33:LEU:HA	1.60	0.44
1:F:89:ASP:O	1:1:86:ALA:HA	2.18	0.44
1:D:57:LYS:HA	1:D:90:LEU:O	2.17	0.44
1:M:72:VAL:HG12	1:M:73:ASN:ND2	2.33	0.44
1:S:62:LEU:HD12	1:S:63:GLU:H	1.82	0.44
1:V:62:LEU:HD12	1:V:63:GLU:H	1.82	0.44
1:N:92:ILE:HA	1:N:93:PRO:HD2	1.84	0.44
1:P:12:ASN:HD22	1:W:106:LYS:HZ3	1.66	0.44
1:S:57:LYS:HA	1:S:90:LEU:O	2.17	0.44
1:Y:72:VAL:HG12	1:Y:73:ASN:ND2	2.33	0.44
1:G:72:VAL:HG12	1:G:73:ASN:ND2	2.33	0.44
1:F:4:LEU:HA	1:F:4:LEU:HD12	1.74	0.44
1:C:38:ARG:NH2	1:J:125:GLN:O	2.50	0.44
1:F:86:ALA:HA	1:1:89:ASP:O	2.18	0.44
1:8:57:LYS:HA	1:8:90:LEU:O	2.17	0.44
1:D:72:VAL:HG12	1:D:73:ASN:ND2	2.33	0.44
1:U:111:LEU:HA	1:U:111:LEU:HD12	1.79	0.44
1:F:111:LEU:HA	1:F:111:LEU:HD12	1.79	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:89:ASP:O	1:R:86:ALA:HA	61.47	0.44
1:0:92:ILE:HA	1:0:93:PRO:HD3	1.87	0.44
1:2:57:LYS:HA	1:2:90:LEU:O	2.17	0.44
1:V:72:VAL:HG12	1:V:73:ASN:ND2	2.33	0.44
1:J:72:VAL:HG12	1:J:73:ASN:ND2	2.33	0.44
1:5:72:VAL:HG12	1:5:73:ASN:ND2	2.33	0.44
1:U:89:ASP:O	1:4:86:ALA:HA	2.18	0.44
1:R:92:ILE:HA	1:R:93:PRO:HD3	1.87	0.44
1:W:58:TYR:HB2	1:W:90:LEU:HB3	1.99	0.44
1:M:57:LYS:HA	1:M:90:LEU:O	2.17	0.44
1:G:33:LEU:HD23	1:G:33:LEU:HA	1.60	0.43
1:V:54:ASP:HA	1:V:94:ILE:HD13	2.00	0.43
1:8:72:VAL:HG12	1:8:73:ASN:ND2	2.33	0.43
1:U:15:THR:HB	1:U:16:GLY:H	1.69	0.43
1:3:58:TYR:HB2	1:3:90:LEU:HB3	1.99	0.43
1:V:57:LYS:HA	1:V:90:LEU:O	2.17	0.43
1:A:54:ASP:HA	1:A:94:ILE:HD13	2.00	0.43
1:P:57:LYS:HA	1:P:90:LEU:O	2.17	0.43
1:A:57:LYS:HA	1:A:90:LEU:O	2.17	0.43
1:G:108:LEU:HD23	1:G:108:LEU:HA	1.73	0.43
1:Q:33:LEU:HA	1:Q:33:LEU:HD23	1.82	0.43
1:S:33:LEU:HD23	1:S:33:LEU:HA	1.60	0.43
1:D:54:ASP:HA	1:D:94:ILE:HD13	2.00	0.43
1:C:38:ARG:NH2	1:V:125:GLN:O	142.03	0.43
1:O:92:ILE:HA	1:O:93:PRO:HD3	1.87	0.43
1:R:34:SER:HG	1:R:42:TYR:H	1.67	0.43
1:0:34:SER:HG	1:0:42:TYR:H	1.67	0.43
1:9:58:TYR:HB2	1:9:90:LEU:HB3	1.99	0.43
1:F:129:TYR:HE1	1:1:2:ALA:N	2.14	0.43
1:M:54:ASP:HA	1:M:94:ILE:HD13	2.00	0.43
1:P:54:ASP:HA	1:P:94:ILE:HD13	2.01	0.43
1:A:72:VAL:HG12	1:A:73:ASN:ND2	2.33	0.43
1:M:34:SER:HB3	1:M:42:TYR:HB2	2.01	0.43
1:S:72:VAL:HG12	1:S:73:ASN:ND2	2.33	0.43
1:S:108:LEU:HA	1:S:108:LEU:HD23	1.73	0.43
1:A:101:VAL:HG11	1:9:122:ILE:O	142.22	0.43
1:G:125:GLN:O	1:7:38:ARG:NH2	93.28	0.43
1:I:90:LEU:HA	1:I:90:LEU:HD23	1.83	0.43
1:6:58:TYR:HB2	1:6:90:LEU:HB3	1.99	0.43
1:G:34:SER:HB3	1:G:42:TYR:HB2	2.01	0.43
1:K:122:ILE:O	1:M:101:VAL:HG11	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:8:54:ASP:HA	1:8:94:ILE:HD13	2.00	0.43
1:I:38:ARG:NH2	1:5:125:GLN:O	2.50	0.43
1:I:38:ARG:NH2	1:S:125:GLN:O	93.75	0.43
1:A:34:SER:HB3	1:A:42:TYR:HB2	2.01	0.43
1:5:34:SER:HB3	1:5:42:TYR:HB2	2.01	0.43
1:3:122:ILE:O	1:8:101:VAL:HG11	2.19	0.43
1:O:38:ARG:NH2	1:Y:125:GLN:O	2.50	0.43
1:U:86:ALA:HA	1:4:89:ASP:O	2.18	0.43
1:2:72:VAL:HG12	1:2:73:ASN:ND2	2.33	0.43
1:C:111:LEU:HD12	1:C:111:LEU:HA	1.79	0.43
1:D:101:VAL:HG11	1:Z:122:ILE:O	95.65	0.43
1:D:101:VAL:HG11	1:T:122:ILE:O	2.19	0.43
1:H:122:ILE:O	1:5:101:VAL:HG11	2.19	0.43
1:P:101:VAL:HG11	1:W:122:ILE:O	2.19	0.43
1:3:33:LEU:HA	1:3:33:LEU:HD23	1.83	0.43
1:Z:33:LEU:HA	1:Z:33:LEU:HD23	1.82	0.43
1:5:54:ASP:HA	1:5:94:ILE:HD13	2.00	0.43
1:P:72:VAL:HG12	1:P:73:ASN:ND2	2.33	0.43
1:D:34:SER:HB3	1:D:42:TYR:HB2	2.01	0.43
1:A:101:VAL:HG11	1:E:122:ILE:O	138.59	0.43
1:E:33:LEU:HA	1:E:33:LEU:HD23	1.83	0.43
1:Y:54:ASP:HA	1:Y:94:ILE:HD13	2.01	0.43
1:F:86:ALA:HA	1:R:89:ASP:O	79.84	0.43
1:V:34:SER:HB3	1:V:42:TYR:HB2	2.01	0.43
1:O:34:SER:HG	1:O:42:TYR:H	1.67	0.43
1:0:4:LEU:HA	1:0:4:LEU:HD12	1.74	0.43
1:Y:77:LEU:HA	1:Y:77:LEU:HD23	1.76	0.43
1:E:122:ILE:O	1:G:101:VAL:HG11	2.19	0.42
1:J:54:ASP:HA	1:J:94:ILE:HD13	2.00	0.42
1:P:125:GLN:O	1:X:38:ARG:NH2	2.50	0.42
1:N:58:TYR:HB2	1:N:90:LEU:HB3	1.99	0.42
1:J:34:SER:HB3	1:J:42:TYR:HB2	2.01	0.42
1:H:122:ILE:O	1:S:101:VAL:HG11	52.93	0.42
1:2:54:ASP:HA	1:2:94:ILE:HD13	2.00	0.42
1:U:92:ILE:HA	1:U:93:PRO:HD3	1.87	0.42
1:S:48:TYR:HE2	1:T:38:ARG:HH12	1.67	0.42
1:A:48:TYR:HE2	1:B:38:ARG:HH12	1.68	0.42
1:K:108:LEU:HA	1:K:108:LEU:HD23	1.92	0.42
1:R:15:THR:HB	1:R:16:GLY:H	1.69	0.42
1:8:34:SER:HB3	1:8:42:TYR:HB2	2.01	0.42
1:N:122:ILE:O	1:Y:101:VAL:HG11	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:ILE:O	1:J:101:VAL:HG11	2.19	0.42
1:B:126:SER:HA	1:K:23:VAL:CG1	2.47	0.42
1:D:48:TYR:HE2	1:E:38:ARG:HH12	1.67	0.42
1:C:4:LEU:HD12	1:C:4:LEU:HA	1.74	0.42
1:5:108:LEU:HD23	1:5:108:LEU:HA	1.73	0.42
1:P:48:TYR:HE2	1:Q:38:ARG:HH12	1.67	0.42
1:G:54:ASP:HA	1:G:94:ILE:HD13	2.00	0.42
1:A:125:GLN:O	1:F:38:ARG:NH2	102.95	0.42
1:2:34:SER:HB3	1:2:42:TYR:HB2	2.01	0.42
1:8:108:LEU:HD23	1:8:108:LEU:HA	1.73	0.42
1:Q:122:ILE:O	1:2:101:VAL:HG11	2.19	0.42
1:H:126:SER:HA	1:T:23:VAL:CG1	59.76	0.42
1:Q:46:ALA:HA	1:Q:59:THR:O	2.20	0.42
1:Y:34:SER:HB3	1:Y:42:TYR:HB2	2.01	0.42
1:6:46:ALA:HA	1:6:59:THR:O	2.20	0.42
1:H:46:ALA:HA	1:H:59:THR:O	2.20	0.42
1:Z:108:LEU:HA	1:Z:108:LEU:HD23	1.92	0.42
1:4:90:LEU:HD23	1:4:90:LEU:HA	1.83	0.42
1:K:46:ALA:HA	1:K:59:THR:O	2.20	0.42
1:E:106:LYS:HZ3	1:G:12:ASN:HD22	1.66	0.42
1:M:48:TYR:HE2	1:N:38:ARG:HH12	1.68	0.42
1:7:15:THR:HB	1:7:16:GLY:H	1.68	0.42
1:I:108:LEU:HD23	1:I:108:LEU:HA	1.78	0.42
1:7:111:LEU:HA	1:7:111:LEU:HD12	1.79	0.42
1:B:74:GLY:HA2	1:9:69:THR:HG21	138.65	0.42
1:A:125:GLN:O	1:0:38:ARG:NH2	132.93	0.42
1:T:46:ALA:HA	1:T:59:THR:O	2.20	0.42
1:J:48:TYR:HE2	1:K:38:ARG:HH12	1.67	0.42
1:2:48:TYR:HE2	1:3:38:ARG:HH12	1.67	0.42
1:9:46:ALA:HA	1:9:59:THR:O	2.20	0.42
1:S:34:SER:HB3	1:S:42:TYR:HB2	2.01	0.42
1:G:48:TYR:HE2	1:H:38:ARG:HH12	1.68	0.42
1:E:74:GLY:HA2	1:Z:69:THR:HG21	118.67	0.42
1:D:62:LEU:HD12	1:D:63:GLU:N	2.35	0.42
1:B:69:THR:HG21	1:W:74:GLY:HA2	138.50	0.42
1:S:54:ASP:HA	1:S:94:ILE:HD13	2.01	0.42
1:4:38:ARG:NH2	1:8:125:GLN:O	2.50	0.42
1:A:126:SER:OG	1:A:127:GLY:N	2.53	0.42
1:5:48:TYR:HE2	1:6:38:ARG:HH12	1.67	0.42
1:N:46:ALA:HA	1:N:59:THR:O	2.20	0.42
1:5:126:SER:OG	1:5:127:GLY:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:ILE:O	1:V:101:VAL:HG11	144.64	0.42
1:E:69:THR:HG21	1:H:74:GLY:HA2	2.02	0.42
1:M:62:LEU:HD12	1:M:63:GLU:N	2.35	0.42
1:G:62:LEU:HD12	1:G:63:GLU:N	2.35	0.42
1:1:79:VAL:CG1	1:1:80:SER:N	2.83	0.42
1:F:71:VAL:HG22	1:Y:74:GLY:HA3	2.02	0.42
1:8:126:SER:OG	1:8:127:GLY:N	2.53	0.42
1:P:34:SER:HB3	1:P:42:TYR:HB2	2.01	0.42
1:B:46:ALA:HA	1:B:59:THR:O	2.20	0.42
1:N:33:LEU:HA	1:N:33:LEU:HD23	1.82	0.41
1:S:62:LEU:HD12	1:S:63:GLU:N	2.35	0.41
1:J:62:LEU:HD12	1:J:63:GLU:N	2.35	0.41
1:3:46:ALA:HA	1:3:59:THR:O	2.20	0.41
1:G:126:SER:OG	1:G:127:GLY:N	2.53	0.41
1:Z:46:ALA:HA	1:Z:59:THR:O	2.20	0.41
1:V:108:LEU:HD23	1:V:108:LEU:HA	1.73	0.41
1:D:108:LEU:HA	1:D:108:LEU:HD23	1.73	0.41
1:E:74:GLY:HA2	1:T:69:THR:HG21	2.02	0.41
1:H:69:THR:HG21	1:T:74:GLY:HA2	22.64	0.41
1:F:71:VAL:HG22	1:P:74:GLY:HA3	127.17	0.41
1:C:92:ILE:HA	1:C:93:PRO:HD3	1.87	0.41
1:E:46:ALA:HA	1:E:59:THR:O	2.20	0.41
1:W:46:ALA:HA	1:W:59:THR:O	2.20	0.41
1:D:126:SER:OG	1:D:127:GLY:N	2.53	0.41
1:2:126:SER:OG	1:2:127:GLY:N	2.53	0.41
1:I:34:SER:HG	1:I:42:TYR:H	1.73	0.41
1:Y:126:SER:OG	1:Y:127:GLY:N	2.53	0.41
1:S:126:SER:OG	1:S:127:GLY:N	2.53	0.41
1:5:33:LEU:HA	1:5:33:LEU:HD23	1.60	0.41
1:Q:69:THR:HG21	1:3:74:GLY:HA2	2.02	0.41
1:H:69:THR:HG21	1:6:74:GLY:HA2	2.02	0.41
1:5:62:LEU:HD12	1:5:63:GLU:N	2.35	0.41
1:0:79:VAL:CG1	1:0:80:SER:N	2.83	0.41
1:H:92:ILE:HA	1:H:93:PRO:HD2	1.84	0.41
1:P:126:SER:OG	1:P:127:GLY:N	2.53	0.41
1:U:2:ALA:N	1:4:129:TYR:HE1	2.14	0.41
1:B:23:VAL:CG1	1:E:126:SER:HA	146.76	0.41
1:Q:74:GLY:HA2	1:W:69:THR:HG21	2.02	0.41
1:L:38:ARG:NH2	1:M:125:GLN:O	2.50	0.41
1:J:126:SER:OG	1:J:127:GLY:N	2.53	0.41
1:I:77:LEU:HA	1:I:77:LEU:HD23	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:48:TYR:HE2	1:W:38:ARG:HH12	1.68	0.41
1:F:92:ILE:HA	1:F:93:PRO:HD3	1.87	0.41
1:M:126:SER:OG	1:M:127:GLY:N	2.53	0.41
1:U:129:TYR:HE1	1:4:2:ALA:N	2.14	0.41
1:Q:23:VAL:CG1	1:W:126:SER:HA	2.47	0.41
1:V:33:LEU:HD23	1:V:33:LEU:HA	1.60	0.41
1:A:62:LEU:HD12	1:A:63:GLU:N	2.35	0.41
1:S:74:GLY:HA3	1:4:71:VAL:HG22	2.02	0.41
1:X:79:VAL:CG1	1:X:80:SER:N	2.83	0.41
1:D:125:GLN:O	1:U:38:ARG:NH2	2.50	0.41
1:K:34:SER:HB3	1:K:42:TYR:HB2	2.03	0.41
1:H:34:SER:HB3	1:H:42:TYR:HB2	2.03	0.41
1:E:34:SER:HB3	1:E:42:TYR:HB2	2.03	0.41
1:Z:34:SER:HB3	1:Z:42:TYR:HB2	2.03	0.41
1:F:90:LEU:HD23	1:F:90:LEU:HA	1.83	0.41
1:P:62:LEU:HD12	1:P:63:GLU:N	2.35	0.41
1:F:38:ARG:NH2	1:G:125:GLN:O	2.50	0.41
1:T:34:SER:HB3	1:T:42:TYR:HB2	2.03	0.41
1:L:90:LEU:HD23	1:L:90:LEU:HA	1.83	0.41
1:U:4:LEU:HA	1:U:4:LEU:HD12	1.74	0.41
1:L:4:LEU:HD12	1:L:4:LEU:HA	1.74	0.41
1:X:111:LEU:HA	1:X:111:LEU:HD12	1.79	0.41
1:G:101:VAL:HG11	1:6:122:ILE:O	53.07	0.41
1:3:69:THR:HG21	1:9:74:GLY:HA2	2.02	0.41
1:2:62:LEU:HD12	1:2:63:GLU:N	2.35	0.41
1:N:69:THR:HG21	1:Z:74:GLY:HA2	2.02	0.41
1:L:79:VAL:CG1	1:L:80:SER:N	2.83	0.41
1:U:71:VAL:HG22	1:2:74:GLY:HA3	2.02	0.41
1:R:90:LEU:HD23	1:R:90:LEU:HA	1.83	0.41
1:8:48:TYR:HE2	1:9:38:ARG:HH12	1.68	0.41
1:V:126:SER:OG	1:V:127:GLY:N	2.53	0.41
1:1:108:LEU:HA	1:1:108:LEU:HD23	1.78	0.41
1:B:69:THR:HG21	1:K:74:GLY:HA2	2.02	0.41
1:B:74:GLY:HA2	1:E:69:THR:HG21	137.32	0.41
1:Y:62:LEU:HD12	1:Y:63:GLU:N	2.35	0.41
1:8:62:LEU:HD12	1:8:63:GLU:N	2.35	0.41
1:3:34:SER:HB3	1:3:42:TYR:HB2	2.03	0.41
1:L:92:ILE:HA	1:L:93:PRO:HD3	1.87	0.41
1:R:4:LEU:HA	1:R:4:LEU:HD12	1.74	0.41
1:T:92:ILE:HA	1:T:93:PRO:HD2	1.84	0.41
1:I:4:LEU:HD12	1:I:4:LEU:HA	1.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:54:ASP:N	1:1:54:ASP:OD1	2.54	0.41
1:A:108:LEU:HD23	1:A:108:LEU:HA	1.73	0.41
1:K:69:THR:HG21	1:N:74:GLY:HA2	2.02	0.41
1:H:74:GLY:HA2	1:6:69:THR:HG21	21.72	0.41
1:V:62:LEU:HD12	1:V:63:GLU:N	2.35	0.41
1:O:79:VAL:CG1	1:O:80:SER:N	2.83	0.41
1:D:74:GLY:HA3	1:1:71:VAL:HG22	2.02	0.41
1:R:38:ARG:NH2	1:2:125:GLN:O	2.50	0.41
1:B:34:SER:HB3	1:B:42:TYR:HB2	2.03	0.41
1:J:77:LEU:HA	1:J:77:LEU:HD23	1.77	0.41
1:Q:126:SER:HA	1:3:23:VAL:CG1	2.47	0.40
1:D:74:GLY:HA3	1:R:71:VAL:HG22	18.63	0.40
1:H:108:LEU:HA	1:H:108:LEU:HD23	1.92	0.40
1:I:99:ASP:O	1:I:103:VAL:HG23	2.22	0.40
1:F:101:VAL:HG13	1:1:122:ILE:O	2.21	0.40
1:F:129:TYR:HE1	1:R:2:ALA:N	91.75	0.40
1:I:79:VAL:CG1	1:I:80:SER:N	2.83	0.40
1:B:51:SER:O	1:B:55:LYS:HG2	2.22	0.40
1:E:51:SER:O	1:E:55:LYS:HG2	2.22	0.40
1:K:51:SER:O	1:K:55:LYS:HG2	2.22	0.40
1:W:34:SER:HB3	1:W:42:TYR:HB2	2.03	0.40
1:C:90:LEU:HD23	1:C:90:LEU:HA	1.83	0.40
1:Y:48:TYR:HE2	1:Z:38:ARG:HH12	1.67	0.40
1:X:77:LEU:HD23	1:X:77:LEU:HA	1.86	0.40
1:1:99:ASP:O	1:1:103:VAL:HG23	2.22	0.40
1:9:51:SER:O	1:9:55:LYS:HG2	2.22	0.40
1:I:43:ARG:HB3	1:I:63:GLU:HB2	2.04	0.40
1:X:99:ASP:O	1:X:103:VAL:HG23	2.21	0.40
1:0:111:LEU:HD12	1:0:111:LEU:HA	1.79	0.40
1:1:77:LEU:HD23	1:1:77:LEU:HA	1.86	0.40
1:Z:92:ILE:HA	1:Z:93:PRO:HD2	1.84	0.40
1:M:33:LEU:HD23	1:M:33:LEU:HA	1.60	0.40
1:H:51:SER:O	1:H:55:LYS:HG2	2.22	0.40
1:6:51:SER:O	1:6:55:LYS:HG2	2.22	0.40
1:T:51:SER:O	1:T:55:LYS:HG2	2.22	0.40
1:9:34:SER:HB3	1:9:42:TYR:HB2	2.03	0.40
1:1:43:ARG:HB3	1:1:63:GLU:HB2	2.04	0.40
1:R:43:ARG:HB3	1:R:63:GLU:HB2	2.04	0.40
1:C:99:ASP:O	1:C:103:VAL:HG23	2.22	0.40
1:L:43:ARG:HB3	1:L:63:GLU:HB2	2.04	0.40
1:4:43:ARG:HB3	1:4:63:GLU:HB2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:7:54:ASP:OD1	1:7:54:ASP:N	2.54	0.40
1:L:111:LEU:HA	1:L:111:LEU:HD12	1.79	0.40
1:F:122:ILE:O	1:R:101:VAL:HG13	93.01	0.40
1:F:79:VAL:CG1	1:F:80:SER:N	2.83	0.40
1:N:51:SER:O	1:N:55:LYS:HG2	2.22	0.40
1:Q:51:SER:O	1:Q:55:LYS:HG2	2.22	0.40
1:7:90:LEU:HA	1:7:90:LEU:HD23	1.83	0.40
1:O:99:ASP:O	1:O:103:VAL:HG23	2.21	0.40
1:7:99:ASP:O	1:7:103:VAL:HG23	2.21	0.40
1:F:43:ARG:HB3	1:F:63:GLU:HB2	2.04	0.40
1:F:125:GLN:O	1:P:38:ARG:NH1	96.15	0.40
1:U:54:ASP:OD1	1:U:54:ASP:N	2.54	0.40
1:I:54:ASP:N	1:I:54:ASP:OD1	2.54	0.40
1:S:103:VAL:HG23	1:S:103:VAL:H	1.71	0.40
1:G:103:VAL:HG23	1:G:103:VAL:H	1.71	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:15:THR:CG2	1:V:6:SER:O[8_554]	1.49	0.71
1:D:15:THR:CB	1:V:6:SER:O[8_554]	2.15	0.05

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	0	127/129 (98%)	117 (92%)	8 (6%)	2 (2%)	12	53
1	1	127/129 (98%)	117 (92%)	8 (6%)	2 (2%)	12	53
1	2	127/129 (98%)	111 (87%)	15 (12%)	1 (1%)	24	67
1	3	127/129 (98%)	117 (92%)	9 (7%)	1 (1%)	24	67

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	4	127/129 (98%)	117 (92%)	8 (6%)	2 (2%)	12	53
1	5	127/129 (98%)	111 (87%)	15 (12%)	1 (1%)	24	67
1	6	127/129 (98%)	117 (92%)	9 (7%)	1 (1%)	24	67
1	7	127/129 (98%)	116 (91%)	9 (7%)	2 (2%)	12	53
1	8	127/129 (98%)	111 (87%)	15 (12%)	1 (1%)	24	67
1	9	127/129 (98%)	117 (92%)	9 (7%)	1 (1%)	24	67
1	A	127/129 (98%)	111 (87%)	15 (12%)	1 (1%)	24	67
1	B	127/129 (98%)	117 (92%)	9 (7%)	1 (1%)	24	67
1	C	127/129 (98%)	117 (92%)	8 (6%)	2 (2%)	12	53
1	D	127/129 (98%)	111 (87%)	15 (12%)	1 (1%)	24	67
1	E	127/129 (98%)	117 (92%)	9 (7%)	1 (1%)	24	67
1	F	127/129 (98%)	117 (92%)	8 (6%)	2 (2%)	12	53
1	G	127/129 (98%)	111 (87%)	15 (12%)	1 (1%)	24	67
1	H	127/129 (98%)	117 (92%)	9 (7%)	1 (1%)	24	67
1	I	127/129 (98%)	117 (92%)	8 (6%)	2 (2%)	12	53
1	J	127/129 (98%)	111 (87%)	15 (12%)	1 (1%)	24	67
1	K	127/129 (98%)	117 (92%)	9 (7%)	1 (1%)	24	67
1	L	127/129 (98%)	116 (91%)	9 (7%)	2 (2%)	12	53
1	M	127/129 (98%)	111 (87%)	15 (12%)	1 (1%)	24	67
1	N	127/129 (98%)	117 (92%)	9 (7%)	1 (1%)	24	67
1	O	127/129 (98%)	117 (92%)	8 (6%)	2 (2%)	12	53
1	P	127/129 (98%)	111 (87%)	15 (12%)	1 (1%)	24	67
1	Q	127/129 (98%)	117 (92%)	9 (7%)	1 (1%)	24	67
1	R	127/129 (98%)	117 (92%)	8 (6%)	2 (2%)	12	53
1	S	127/129 (98%)	111 (87%)	15 (12%)	1 (1%)	24	67
1	T	127/129 (98%)	117 (92%)	9 (7%)	1 (1%)	24	67
1	U	127/129 (98%)	117 (92%)	8 (6%)	2 (2%)	12	53
1	V	127/129 (98%)	111 (87%)	15 (12%)	1 (1%)	24	67
1	W	127/129 (98%)	117 (92%)	9 (7%)	1 (1%)	24	67
1	X	127/129 (98%)	117 (92%)	8 (6%)	2 (2%)	12	53
1	Y	127/129 (98%)	111 (87%)	15 (12%)	1 (1%)	24	67

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Z	127/129 (98%)	117 (92%)	9 (7%)	1 (1%)	24	67
1	a	127/129 (98%)	111 (87%)	15 (12%)	1 (1%)	24	67
1	b	127/129 (98%)	117 (92%)	9 (7%)	1 (1%)	24	67
1	c	127/129 (98%)	116 (91%)	9 (7%)	2 (2%)	12	53
1	d	127/129 (98%)	111 (87%)	15 (12%)	1 (1%)	24	67
1	e	127/129 (98%)	117 (92%)	9 (7%)	1 (1%)	24	67
1	f	127/129 (98%)	117 (92%)	8 (6%)	2 (2%)	12	53
1	g	127/129 (98%)	111 (87%)	15 (12%)	1 (1%)	24	67
1	h	127/129 (98%)	117 (92%)	9 (7%)	1 (1%)	24	67
1	i	127/129 (98%)	117 (92%)	8 (6%)	2 (2%)	12	53
All	All	5715/5805 (98%)	5172 (90%)	483 (8%)	60 (1%)	19	63

All (60) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	15	THR
1	C	14	GLY
1	C	15	THR
1	E	15	THR
1	F	14	GLY
1	F	15	THR
1	H	15	THR
1	I	14	GLY
1	I	15	THR
1	K	15	THR
1	L	14	GLY
1	L	15	THR
1	N	15	THR
1	O	14	GLY
1	O	15	THR
1	Q	15	THR
1	R	14	GLY
1	R	15	THR
1	T	15	THR
1	U	14	GLY
1	U	15	THR
1	W	15	THR
1	X	14	GLY

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Mol	Chain	Res	Type
1	X	15	THR
1	Z	15	THR
1	1	14	GLY
1	1	15	THR
1	3	15	THR
1	4	14	GLY
1	4	15	THR
1	6	15	THR
1	7	14	GLY
1	7	15	THR
1	9	15	THR
1	0	14	GLY
1	0	15	THR
1	b	15	THR
1	c	14	GLY
1	c	15	THR
1	e	15	THR
1	f	14	GLY
1	f	15	THR
1	h	15	THR
1	i	14	GLY
1	i	15	THR
1	A	14	GLY
1	D	14	GLY
1	G	14	GLY
1	J	14	GLY
1	M	14	GLY
1	P	14	GLY
1	S	14	GLY
1	V	14	GLY
1	Y	14	GLY
1	2	14	GLY
1	5	14	GLY
1	8	14	GLY
1	a	14	GLY
1	d	14	GLY
1	g	14	GLY

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	0	104/104 (100%)	97 (93%)	7 (7%)	20	60
1	1	104/104 (100%)	97 (93%)	7 (7%)	20	60
1	2	104/104 (100%)	100 (96%)	4 (4%)	40	76
1	3	104/104 (100%)	96 (92%)	8 (8%)	16	53
1	4	104/104 (100%)	97 (93%)	7 (7%)	20	60
1	5	104/104 (100%)	100 (96%)	4 (4%)	40	76
1	6	104/104 (100%)	96 (92%)	8 (8%)	16	53
1	7	104/104 (100%)	97 (93%)	7 (7%)	20	60
1	8	104/104 (100%)	100 (96%)	4 (4%)	40	76
1	9	104/104 (100%)	96 (92%)	8 (8%)	16	53
1	A	104/104 (100%)	100 (96%)	4 (4%)	40	76
1	B	104/104 (100%)	96 (92%)	8 (8%)	16	53
1	C	104/104 (100%)	97 (93%)	7 (7%)	20	60
1	D	104/104 (100%)	100 (96%)	4 (4%)	40	76
1	E	104/104 (100%)	96 (92%)	8 (8%)	16	53
1	F	104/104 (100%)	97 (93%)	7 (7%)	20	60
1	G	104/104 (100%)	100 (96%)	4 (4%)	40	76
1	H	104/104 (100%)	96 (92%)	8 (8%)	16	53
1	I	104/104 (100%)	97 (93%)	7 (7%)	20	60
1	J	104/104 (100%)	100 (96%)	4 (4%)	40	76
1	K	104/104 (100%)	96 (92%)	8 (8%)	16	53
1	L	104/104 (100%)	97 (93%)	7 (7%)	20	60
1	M	104/104 (100%)	100 (96%)	4 (4%)	40	76
1	N	104/104 (100%)	96 (92%)	8 (8%)	16	53
1	O	104/104 (100%)	97 (93%)	7 (7%)	20	60
1	P	104/104 (100%)	100 (96%)	4 (4%)	40	76
1	Q	104/104 (100%)	96 (92%)	8 (8%)	16	53
1	R	104/104 (100%)	97 (93%)	7 (7%)	20	60
1	S	104/104 (100%)	100 (96%)	4 (4%)	40	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	T	104/104 (100%)	96 (92%)	8 (8%)	16 53
1	U	104/104 (100%)	97 (93%)	7 (7%)	20 60
1	V	104/104 (100%)	100 (96%)	4 (4%)	40 76
1	W	104/104 (100%)	96 (92%)	8 (8%)	16 53
1	X	104/104 (100%)	97 (93%)	7 (7%)	20 60
1	Y	104/104 (100%)	100 (96%)	4 (4%)	40 76
1	Z	104/104 (100%)	96 (92%)	8 (8%)	16 53
1	a	104/104 (100%)	100 (96%)	4 (4%)	40 76
1	b	104/104 (100%)	96 (92%)	8 (8%)	16 53
1	c	104/104 (100%)	97 (93%)	7 (7%)	20 60
1	d	104/104 (100%)	100 (96%)	4 (4%)	40 76
1	e	104/104 (100%)	96 (92%)	8 (8%)	16 53
1	f	104/104 (100%)	97 (93%)	7 (7%)	20 60
1	g	104/104 (100%)	100 (96%)	4 (4%)	40 76
1	h	104/104 (100%)	96 (92%)	8 (8%)	16 53
1	i	104/104 (100%)	97 (93%)	7 (7%)	20 60
All	All	4680/4680 (100%)	4395 (94%)	285 (6%)	23 63

All (285) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ARG
1	A	20	VAL
1	A	33	LEU
1	A	99	ASP
1	B	3	THR
1	B	20	VAL
1	B	33	LEU
1	B	36	ASN
1	B	55	LYS
1	B	68	VAL
1	B	70	GLN
1	B	118	ILE
1	C	6	SER
1	C	15	THR
1	C	38	ARG

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Mol	Chain	Res	Type
1	C	40	GLN
1	C	54	ASP
1	C	71	VAL
1	C	90	LEU
1	D	5	ARG
1	D	20	VAL
1	D	33	LEU
1	D	99	ASP
1	E	3	THR
1	E	20	VAL
1	E	33	LEU
1	E	36	ASN
1	E	55	LYS
1	E	68	VAL
1	E	70	GLN
1	E	118	ILE
1	F	6	SER
1	F	15	THR
1	F	38	ARG
1	F	40	GLN
1	F	54	ASP
1	F	71	VAL
1	F	90	LEU
1	G	5	ARG
1	G	20	VAL
1	G	33	LEU
1	G	99	ASP
1	H	3	THR
1	H	20	VAL
1	H	33	LEU
1	H	36	ASN
1	H	55	LYS
1	H	68	VAL
1	H	70	GLN
1	H	118	ILE
1	I	6	SER
1	I	15	THR
1	I	38	ARG
1	I	40	GLN
1	I	54	ASP
1	I	71	VAL
1	I	90	LEU

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Mol	Chain	Res	Type
1	J	5	ARG
1	J	20	VAL
1	J	33	LEU
1	J	99	ASP
1	K	3	THR
1	K	20	VAL
1	K	33	LEU
1	K	36	ASN
1	K	55	LYS
1	K	68	VAL
1	K	70	GLN
1	K	118	ILE
1	L	6	SER
1	L	15	THR
1	L	38	ARG
1	L	40	GLN
1	L	54	ASP
1	L	71	VAL
1	L	90	LEU
1	M	5	ARG
1	M	20	VAL
1	M	33	LEU
1	M	99	ASP
1	N	3	THR
1	N	20	VAL
1	N	33	LEU
1	N	36	ASN
1	N	55	LYS
1	N	68	VAL
1	N	70	GLN
1	N	118	ILE
1	O	6	SER
1	O	15	THR
1	O	38	ARG
1	O	40	GLN
1	O	54	ASP
1	O	71	VAL
1	O	90	LEU
1	P	5	ARG
1	P	20	VAL
1	P	33	LEU
1	P	99	ASP

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Mol	Chain	Res	Type
1	Q	3	THR
1	Q	20	VAL
1	Q	33	LEU
1	Q	36	ASN
1	Q	55	LYS
1	Q	68	VAL
1	Q	70	GLN
1	Q	118	ILE
1	R	6	SER
1	R	15	THR
1	R	38	ARG
1	R	40	GLN
1	R	54	ASP
1	R	71	VAL
1	R	90	LEU
1	S	5	ARG
1	S	20	VAL
1	S	33	LEU
1	S	99	ASP
1	T	3	THR
1	T	20	VAL
1	T	33	LEU
1	T	36	ASN
1	T	55	LYS
1	T	68	VAL
1	T	70	GLN
1	T	118	ILE
1	U	6	SER
1	U	15	THR
1	U	38	ARG
1	U	40	GLN
1	U	54	ASP
1	U	71	VAL
1	U	90	LEU
1	V	5	ARG
1	V	20	VAL
1	V	33	LEU
1	V	99	ASP
1	W	3	THR
1	W	20	VAL
1	W	33	LEU
1	W	36	ASN

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Mol	Chain	Res	Type
1	W	55	LYS
1	W	68	VAL
1	W	70	GLN
1	W	118	ILE
1	X	6	SER
1	X	15	THR
1	X	38	ARG
1	X	40	GLN
1	X	54	ASP
1	X	71	VAL
1	X	90	LEU
1	Y	5	ARG
1	Y	20	VAL
1	Y	33	LEU
1	Y	99	ASP
1	Z	3	THR
1	Z	20	VAL
1	Z	33	LEU
1	Z	36	ASN
1	Z	55	LYS
1	Z	68	VAL
1	Z	70	GLN
1	Z	118	ILE
1	1	6	SER
1	1	15	THR
1	1	38	ARG
1	1	40	GLN
1	1	54	ASP
1	1	71	VAL
1	1	90	LEU
1	2	5	ARG
1	2	20	VAL
1	2	33	LEU
1	2	99	ASP
1	3	3	THR
1	3	20	VAL
1	3	33	LEU
1	3	36	ASN
1	3	55	LYS
1	3	68	VAL
1	3	70	GLN
1	3	118	ILE

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Mol	Chain	Res	Type
1	4	6	SER
1	4	15	THR
1	4	38	ARG
1	4	40	GLN
1	4	54	ASP
1	4	71	VAL
1	4	90	LEU
1	5	5	ARG
1	5	20	VAL
1	5	33	LEU
1	5	99	ASP
1	6	3	THR
1	6	20	VAL
1	6	33	LEU
1	6	36	ASN
1	6	55	LYS
1	6	68	VAL
1	6	70	GLN
1	6	118	ILE
1	7	6	SER
1	7	15	THR
1	7	38	ARG
1	7	40	GLN
1	7	54	ASP
1	7	71	VAL
1	7	90	LEU
1	8	5	ARG
1	8	20	VAL
1	8	33	LEU
1	8	99	ASP
1	9	3	THR
1	9	20	VAL
1	9	33	LEU
1	9	36	ASN
1	9	55	LYS
1	9	68	VAL
1	9	70	GLN
1	9	118	ILE
1	0	6	SER
1	0	15	THR
1	0	38	ARG
1	0	40	GLN

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Mol	Chain	Res	Type
1	0	54	ASP
1	0	71	VAL
1	0	90	LEU
1	a	5	ARG
1	a	20	VAL
1	a	33	LEU
1	a	99	ASP
1	b	3	THR
1	b	20	VAL
1	b	33	LEU
1	b	36	ASN
1	b	55	LYS
1	b	68	VAL
1	b	70	GLN
1	b	118	ILE
1	c	6	SER
1	c	15	THR
1	c	38	ARG
1	c	40	GLN
1	c	54	ASP
1	c	71	VAL
1	c	90	LEU
1	d	5	ARG
1	d	20	VAL
1	d	33	LEU
1	d	99	ASP
1	e	3	THR
1	e	20	VAL
1	e	33	LEU
1	e	36	ASN
1	e	55	LYS
1	e	68	VAL
1	e	70	GLN
1	e	118	ILE
1	f	6	SER
1	f	15	THR
1	f	38	ARG
1	f	40	GLN
1	f	54	ASP
1	f	71	VAL
1	f	90	LEU
1	g	5	ARG

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Mol	Chain	Res	Type
1	g	20	VAL
1	g	33	LEU
1	g	99	ASP
1	h	3	THR
1	h	20	VAL
1	h	33	LEU
1	h	36	ASN
1	h	55	LYS
1	h	68	VAL
1	h	70	GLN
1	h	118	ILE
1	i	6	SER
1	i	15	THR
1	i	38	ARG
1	i	40	GLN
1	i	54	ASP
1	i	71	VAL
1	i	90	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (101) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	36	ASN
1	A	73	ASN
1	B	36	ASN
1	B	70	GLN
1	C	36	ASN
1	C	73	ASN
1	D	12	ASN
1	D	36	ASN
1	D	73	ASN
1	E	36	ASN
1	E	70	GLN
1	F	36	ASN
1	F	73	ASN
1	G	12	ASN
1	G	36	ASN
1	G	73	ASN
1	H	36	ASN
1	H	70	GLN
1	I	36	ASN

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Mol	Chain	Res	Type
1	J	12	ASN
1	J	36	ASN
1	J	73	ASN
1	K	36	ASN
1	K	70	GLN
1	L	36	ASN
1	L	73	ASN
1	M	12	ASN
1	M	36	ASN
1	M	73	ASN
1	N	36	ASN
1	N	70	GLN
1	O	36	ASN
1	O	73	ASN
1	P	12	ASN
1	P	36	ASN
1	P	73	ASN
1	Q	36	ASN
1	Q	70	GLN
1	R	36	ASN
1	R	73	ASN
1	S	12	ASN
1	S	36	ASN
1	S	73	ASN
1	T	36	ASN
1	T	70	GLN
1	U	36	ASN
1	U	73	ASN
1	V	12	ASN
1	V	36	ASN
1	V	73	ASN
1	W	36	ASN
1	W	70	GLN
1	X	36	ASN
1	X	73	ASN
1	Y	12	ASN
1	Y	36	ASN
1	Y	73	ASN
1	Z	36	ASN
1	Z	70	GLN
1	1	36	ASN
1	1	73	ASN

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Mol	Chain	Res	Type
1	2	12	ASN
1	2	36	ASN
1	2	73	ASN
1	3	36	ASN
1	3	70	GLN
1	4	36	ASN
1	4	73	ASN
1	5	12	ASN
1	5	36	ASN
1	5	73	ASN
1	6	36	ASN
1	6	70	GLN
1	7	36	ASN
1	8	12	ASN
1	8	36	ASN
1	8	73	ASN
1	9	36	ASN
1	9	70	GLN
1	0	36	ASN
1	a	12	ASN
1	a	36	ASN
1	a	73	ASN
1	b	36	ASN
1	b	70	GLN
1	c	36	ASN
1	c	73	ASN
1	d	12	ASN
1	d	36	ASN
1	d	73	ASN
1	e	36	ASN
1	e	70	GLN
1	f	36	ASN
1	g	12	ASN
1	g	36	ASN
1	g	73	ASN
1	h	36	ASN
1	h	70	GLN
1	i	36	ASN
1	i	73	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	0	129/129 (100%)	-0.57	0	100	100	4, 19, 52, 83	0
1	1	129/129 (100%)	-0.65	0	100	100	4, 19, 52, 83	0
1	2	129/129 (100%)	-0.59	0	100	100	2, 18, 56, 81	0
1	3	129/129 (100%)	-0.59	0	100	100	3, 15, 50, 77	0
1	4	129/129 (100%)	-0.46	0	100	100	4, 19, 52, 83	0
1	5	129/129 (100%)	-0.60	0	100	100	2, 18, 56, 81	0
1	6	129/129 (100%)	-0.66	0	100	100	3, 15, 50, 77	0
1	7	129/129 (100%)	-0.59	0	100	100	4, 19, 52, 83	0
1	8	129/129 (100%)	-0.57	0	100	100	2, 18, 56, 81	0
1	9	129/129 (100%)	-0.62	0	100	100	3, 15, 50, 77	0
1	A	129/129 (100%)	-0.71	0	100	100	2, 18, 56, 81	0
1	B	129/129 (100%)	-0.78	0	100	100	3, 15, 50, 77	0
1	C	129/129 (100%)	-0.60	0	100	100	4, 19, 52, 83	0
1	D	129/129 (100%)	-0.56	0	100	100	2, 18, 56, 81	0
1	E	129/129 (100%)	-0.67	0	100	100	3, 15, 50, 77	0
1	F	129/129 (100%)	-0.60	0	100	100	4, 19, 52, 83	0
1	G	129/129 (100%)	-0.54	0	100	100	2, 18, 56, 81	0
1	H	129/129 (100%)	-0.68	0	100	100	3, 15, 50, 77	0
1	I	129/129 (100%)	-0.47	0	100	100	4, 19, 52, 83	0
1	J	129/129 (100%)	-0.67	0	100	100	2, 18, 56, 81	0
1	K	129/129 (100%)	-0.66	0	100	100	3, 15, 50, 77	0
1	L	129/129 (100%)	-0.44	1 (0%)	87	83	4, 19, 52, 83	0
1	M	129/129 (100%)	-0.61	0	100	100	2, 18, 56, 81	0
1	N	129/129 (100%)	-0.76	0	100	100	3, 15, 50, 77	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	O	129/129 (100%)	-0.58	0	100	100	4, 19, 52, 83	0
1	P	129/129 (100%)	-0.58	0	100	100	2, 18, 56, 81	0
1	Q	129/129 (100%)	-0.71	0	100	100	3, 15, 50, 77	0
1	R	129/129 (100%)	-0.60	0	100	100	4, 19, 52, 83	0
1	S	129/129 (100%)	-0.62	0	100	100	2, 18, 56, 81	0
1	T	129/129 (100%)	-0.63	0	100	100	3, 15, 50, 77	0
1	U	129/129 (100%)	-0.49	0	100	100	4, 19, 52, 83	0
1	V	129/129 (100%)	-0.58	0	100	100	2, 18, 56, 81	0
1	W	129/129 (100%)	-0.60	0	100	100	3, 15, 50, 77	0
1	X	129/129 (100%)	-0.49	0	100	100	4, 19, 52, 83	0
1	Y	129/129 (100%)	-0.73	0	100	100	2, 18, 56, 81	0
1	Z	129/129 (100%)	-0.63	0	100	100	3, 15, 50, 77	0
1	a	129/129 (100%)	-0.55	0	100	100	2, 18, 56, 81	0
1	b	129/129 (100%)	-0.71	0	100	100	3, 15, 50, 77	0
1	c	129/129 (100%)	-0.55	0	100	100	4, 19, 52, 83	0
1	d	129/129 (100%)	-0.61	0	100	100	2, 18, 56, 81	0
1	e	129/129 (100%)	-0.73	0	100	100	3, 15, 50, 77	0
1	f	129/129 (100%)	-0.45	0	100	100	4, 19, 52, 83	0
1	g	129/129 (100%)	-0.60	0	100	100	2, 18, 56, 81	0
1	h	129/129 (100%)	-0.62	0	100	100	3, 15, 50, 77	0
1	i	129/129 (100%)	-0.58	0	100	100	4, 19, 52, 83	0
All	All	5805/5805 (100%)	-0.61	1 (0%)	100	100	2, 17, 55, 83	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	15	THR	2.6

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.