



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2018 – 10:44 pm GMT

PDB ID : 2FHG
Title : Crystal Structure of Mycobacterial Tuberculosis Proteasome
Authors : Hu, G.; Lin, G.; Wang, M.; Dick, L.; Xu, R.M.; Nathan, C.; Li, H.
Deposited on : 2005-12-23
Resolution : 3.23 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 : trunk30967
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30967

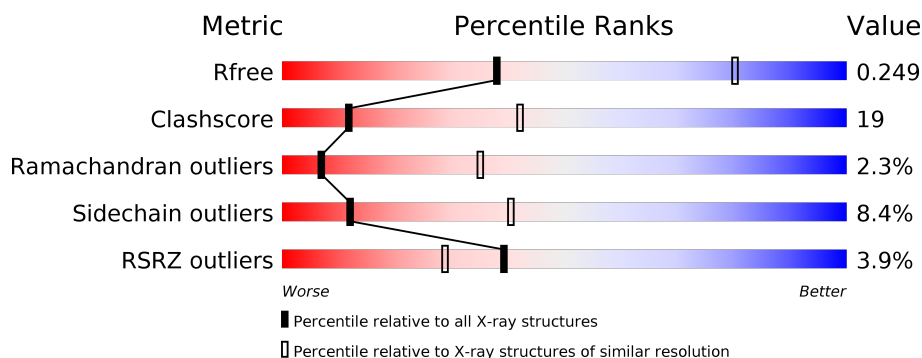
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.23 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}	111664	1379 (3.28-3.20)
Clashscore	122126	1510 (3.28-3.20)
Ramachandran outliers	120053	1485 (3.28-3.20)
Sidechain outliers	120020	1484 (3.28-3.20)
RSRZ outliers	108989	1331 (3.28-3.20)

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 $\leq 5\%$. 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	1	250	<div> <div>8%</div> <div> <div></div> <div>53%</div> <div>31%</div> <div>•</div> <div>12%</div> </div> </div>
1	A	250	<div> <div>2%</div> <div> <div></div> <div>53%</div> <div>32%</div> <div>•</div> <div>12%</div> </div> </div>
1	B	250	<div> <div>2%</div> <div> <div></div> <div>54%</div> <div>30%</div> <div>•</div> <div>12%</div> </div> </div>
1	D	250	<div> <div>6%</div> <div> <div></div> <div>54%</div> <div>31%</div> <div>•</div> <div>12%</div> </div> </div>
1	F	250	<div> <div>4%</div> <div> <div></div> <div>54%</div> <div>30%</div> <div>•</div> <div>12%</div> </div> </div>
1	I	250	<div> <div>5%</div> <div> <div></div> <div>53%</div> <div>31%</div> <div>•</div> <div>12%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	K	250	
1	M	250	
1	O	250	
1	Q	250	
1	S	250	
1	U	250	
1	W	250	
1	Y	250	
2	2	240	
2	C	240	
2	E	240	
2	G	240	
2	H	240	
2	J	240	
2	L	240	
2	N	240	
2	P	240	
2	R	240	
2	T	240	
2	V	240	
2	X	240	
2	Z	240	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 46846 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 20S proteasome, alpha and beta subunits.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	220	Total	C	N	O	S	0	0	0
			1692	1058	309	322	3			
1	B	220	Total	C	N	O	S	0	0	0
			1692	1058	309	322	3			
1	D	220	Total	C	N	O	S	0	0	0
			1692	1058	309	322	3			
1	F	220	Total	C	N	O	S	0	0	0
			1692	1058	309	322	3			
1	I	220	Total	C	N	O	S	0	0	0
			1692	1058	309	322	3			
1	K	220	Total	C	N	O	S	0	0	0
			1692	1058	309	322	3			
1	M	220	Total	C	N	O	S	0	0	0
			1692	1058	309	322	3			
1	O	220	Total	C	N	O	S	0	0	0
			1692	1058	309	322	3			
1	Q	220	Total	C	N	O	S	0	0	0
			1692	1058	309	322	3			
1	S	220	Total	C	N	O	S	0	0	0
			1692	1058	309	322	3			
1	U	220	Total	C	N	O	S	0	0	0
			1692	1058	309	322	3			
1	W	220	Total	C	N	O	S	0	0	0
			1692	1058	309	322	3			
1	Y	220	Total	C	N	O	S	0	0	0
			1692	1058	309	322	3			
1	1	220	Total	C	N	O	S	0	0	0
			1692	1058	309	322	3			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	INITIATING METHIONINE	GB 13881852

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Chain	Residue	Modelled	Actual	Comment	Reference
A	0	ASN	-	CLONING ARTIFACT	GB 13881852
A	1	SER	-	CLONING ARTIFACT	GB 13881852
B	-1	MET	-	INITIATING METHIONINE	GB 13881852
B	0	ASN	-	CLONING ARTIFACT	GB 13881852
B	1	SER	-	CLONING ARTIFACT	GB 13881852
D	-1	MET	-	INITIATING METHIONINE	GB 13881852
D	0	ASN	-	CLONING ARTIFACT	GB 13881852
D	1	SER	-	CLONING ARTIFACT	GB 13881852
F	-1	MET	-	INITIATING METHIONINE	GB 13881852
F	0	ASN	-	CLONING ARTIFACT	GB 13881852
F	1	SER	-	CLONING ARTIFACT	GB 13881852
I	-1	MET	-	INITIATING METHIONINE	GB 13881852
I	0	ASN	-	CLONING ARTIFACT	GB 13881852
I	1	SER	-	CLONING ARTIFACT	GB 13881852
K	-1	MET	-	INITIATING METHIONINE	GB 13881852
K	0	ASN	-	CLONING ARTIFACT	GB 13881852
K	1	SER	-	CLONING ARTIFACT	GB 13881852
M	-1	MET	-	INITIATING METHIONINE	GB 13881852
M	0	ASN	-	CLONING ARTIFACT	GB 13881852
M	1	SER	-	CLONING ARTIFACT	GB 13881852
O	-1	MET	-	INITIATING METHIONINE	GB 13881852
O	0	ASN	-	CLONING ARTIFACT	GB 13881852
O	1	SER	-	CLONING ARTIFACT	GB 13881852
Q	-1	MET	-	INITIATING METHIONINE	GB 13881852
Q	0	ASN	-	CLONING ARTIFACT	GB 13881852
Q	1	SER	-	CLONING ARTIFACT	GB 13881852
S	-1	MET	-	INITIATING METHIONINE	GB 13881852
S	0	ASN	-	CLONING ARTIFACT	GB 13881852
S	1	SER	-	CLONING ARTIFACT	GB 13881852
U	-1	MET	-	INITIATING METHIONINE	GB 13881852
U	0	ASN	-	CLONING ARTIFACT	GB 13881852
U	1	SER	-	CLONING ARTIFACT	GB 13881852
W	-1	MET	-	INITIATING METHIONINE	GB 13881852
W	0	ASN	-	CLONING ARTIFACT	GB 13881852
W	1	SER	-	CLONING ARTIFACT	GB 13881852
Y	-1	MET	-	INITIATING METHIONINE	GB 13881852
Y	0	ASN	-	CLONING ARTIFACT	GB 13881852
Y	1	SER	-	CLONING ARTIFACT	GB 13881852
1	-1	MET	-	INITIATING METHIONINE	GB 13881852
1	0	ASN	-	CLONING ARTIFACT	GB 13881852
1	1	SER	-	CLONING ARTIFACT	GB 13881852

- Molecule 2 is a protein called proteasome, beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	222	Total 1638	C 1027	N 282	O 324	S 5	0	0	0
2	C	222	Total 1638	C 1027	N 282	O 324	S 5	0	0	0
2	E	222	Total 1638	C 1027	N 282	O 324	S 5	0	0	0
2	G	222	Total 1638	C 1027	N 282	O 324	S 5	0	0	0
2	J	222	Total 1638	C 1027	N 282	O 324	S 5	0	0	0
2	L	222	Total 1638	C 1027	N 282	O 324	S 5	0	0	0
2	N	222	Total 1638	C 1027	N 282	O 324	S 5	0	0	0
2	P	222	Total 1638	C 1027	N 282	O 324	S 5	0	0	0
2	R	222	Total 1638	C 1027	N 282	O 324	S 5	0	0	0
2	T	222	Total 1638	C 1027	N 282	O 324	S 5	0	0	0
2	V	222	Total 1638	C 1027	N 282	O 324	S 5	0	0	0
2	X	222	Total 1638	C 1027	N 282	O 324	S 5	0	0	0
2	Z	222	Total 1638	C 1027	N 282	O 324	S 5	0	0	0
2	2	222	Total 1638	C 1027	N 282	O 324	S 5	0	0	0

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	535	HIS	-	EXPRESSION TAG	GB 13881852
H	536	HIS	-	EXPRESSION TAG	GB 13881852
H	537	HIS	-	EXPRESSION TAG	GB 13881852
H	538	HIS	-	EXPRESSION TAG	GB 13881852
H	539	HIS	-	EXPRESSION TAG	GB 13881852
H	540	HIS	-	EXPRESSION TAG	GB 13881852
C	535	HIS	-	EXPRESSION TAG	GB 13881852
C	536	HIS	-	EXPRESSION TAG	GB 13881852
C	537	HIS	-	EXPRESSION TAG	GB 13881852
C	538	HIS	-	EXPRESSION TAG	GB 13881852
C	539	HIS	-	EXPRESSION TAG	GB 13881852
C	540	HIS	-	EXPRESSION TAG	GB 13881852

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Chain	Residue	Modelled	Actual	Comment	Reference
E	535	HIS	-	EXPRESSION TAG	GB 13881852
E	536	HIS	-	EXPRESSION TAG	GB 13881852
E	537	HIS	-	EXPRESSION TAG	GB 13881852
E	538	HIS	-	EXPRESSION TAG	GB 13881852
E	539	HIS	-	EXPRESSION TAG	GB 13881852
E	540	HIS	-	EXPRESSION TAG	GB 13881852
G	535	HIS	-	EXPRESSION TAG	GB 13881852
G	536	HIS	-	EXPRESSION TAG	GB 13881852
G	537	HIS	-	EXPRESSION TAG	GB 13881852
G	538	HIS	-	EXPRESSION TAG	GB 13881852
G	539	HIS	-	EXPRESSION TAG	GB 13881852
G	540	HIS	-	EXPRESSION TAG	GB 13881852
J	535	HIS	-	EXPRESSION TAG	GB 13881852
J	536	HIS	-	EXPRESSION TAG	GB 13881852
J	537	HIS	-	EXPRESSION TAG	GB 13881852
J	538	HIS	-	EXPRESSION TAG	GB 13881852
J	539	HIS	-	EXPRESSION TAG	GB 13881852
J	540	HIS	-	EXPRESSION TAG	GB 13881852
L	535	HIS	-	EXPRESSION TAG	GB 13881852
L	536	HIS	-	EXPRESSION TAG	GB 13881852
L	537	HIS	-	EXPRESSION TAG	GB 13881852
L	538	HIS	-	EXPRESSION TAG	GB 13881852
L	539	HIS	-	EXPRESSION TAG	GB 13881852
L	540	HIS	-	EXPRESSION TAG	GB 13881852
N	535	HIS	-	EXPRESSION TAG	GB 13881852
N	536	HIS	-	EXPRESSION TAG	GB 13881852
N	537	HIS	-	EXPRESSION TAG	GB 13881852
N	538	HIS	-	EXPRESSION TAG	GB 13881852
N	539	HIS	-	EXPRESSION TAG	GB 13881852
N	540	HIS	-	EXPRESSION TAG	GB 13881852
P	535	HIS	-	EXPRESSION TAG	GB 13881852
P	536	HIS	-	EXPRESSION TAG	GB 13881852
P	537	HIS	-	EXPRESSION TAG	GB 13881852
P	538	HIS	-	EXPRESSION TAG	GB 13881852
P	539	HIS	-	EXPRESSION TAG	GB 13881852
P	540	HIS	-	EXPRESSION TAG	GB 13881852
R	535	HIS	-	EXPRESSION TAG	GB 13881852
R	536	HIS	-	EXPRESSION TAG	GB 13881852
R	537	HIS	-	EXPRESSION TAG	GB 13881852
R	538	HIS	-	EXPRESSION TAG	GB 13881852
R	539	HIS	-	EXPRESSION TAG	GB 13881852
R	540	HIS	-	EXPRESSION TAG	GB 13881852

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Chain	Residue	Modelled	Actual	Comment	Reference
T	535	HIS	-	EXPRESSION TAG	GB 13881852
T	536	HIS	-	EXPRESSION TAG	GB 13881852
T	537	HIS	-	EXPRESSION TAG	GB 13881852
T	538	HIS	-	EXPRESSION TAG	GB 13881852
T	539	HIS	-	EXPRESSION TAG	GB 13881852
T	540	HIS	-	EXPRESSION TAG	GB 13881852
V	535	HIS	-	EXPRESSION TAG	GB 13881852
V	536	HIS	-	EXPRESSION TAG	GB 13881852
V	537	HIS	-	EXPRESSION TAG	GB 13881852
V	538	HIS	-	EXPRESSION TAG	GB 13881852
V	539	HIS	-	EXPRESSION TAG	GB 13881852
V	540	HIS	-	EXPRESSION TAG	GB 13881852
X	535	HIS	-	EXPRESSION TAG	GB 13881852
X	536	HIS	-	EXPRESSION TAG	GB 13881852
X	537	HIS	-	EXPRESSION TAG	GB 13881852
X	538	HIS	-	EXPRESSION TAG	GB 13881852
X	539	HIS	-	EXPRESSION TAG	GB 13881852
X	540	HIS	-	EXPRESSION TAG	GB 13881852
Z	535	HIS	-	EXPRESSION TAG	GB 13881852
Z	536	HIS	-	EXPRESSION TAG	GB 13881852
Z	537	HIS	-	EXPRESSION TAG	GB 13881852
Z	538	HIS	-	EXPRESSION TAG	GB 13881852
Z	539	HIS	-	EXPRESSION TAG	GB 13881852
Z	540	HIS	-	EXPRESSION TAG	GB 13881852
2	535	HIS	-	EXPRESSION TAG	GB 13881852
2	536	HIS	-	EXPRESSION TAG	GB 13881852
2	537	HIS	-	EXPRESSION TAG	GB 13881852
2	538	HIS	-	EXPRESSION TAG	GB 13881852
2	539	HIS	-	EXPRESSION TAG	GB 13881852
2	540	HIS	-	EXPRESSION TAG	GB 13881852

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total O 2 2	0	0
3	H	1	Total O 1 1	0	0
3	B	7	Total O 7 7	0	0
3	C	6	Total O 6 6	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	11	Total O 11 11	0	0
3	E	9	Total O 9 9	0	0
3	F	10	Total O 10 10	0	0
3	G	9	Total O 9 9	0	0
3	I	7	Total O 7 7	0	0
3	J	5	Total O 5 5	0	0
3	K	15	Total O 15 15	0	0
3	L	4	Total O 4 4	0	0
3	M	11	Total O 11 11	0	0
3	N	7	Total O 7 7	0	0
3	O	8	Total O 8 8	0	0
3	P	4	Total O 4 4	0	0
3	Q	6	Total O 6 6	0	0
3	R	5	Total O 5 5	0	0
3	S	13	Total O 13 13	0	0
3	T	6	Total O 6 6	0	0
3	U	7	Total O 7 7	0	0
3	V	10	Total O 10 10	0	0
3	W	8	Total O 8 8	0	0
3	X	4	Total O 4 4	0	0
3	Y	12	Total O 12 12	0	0

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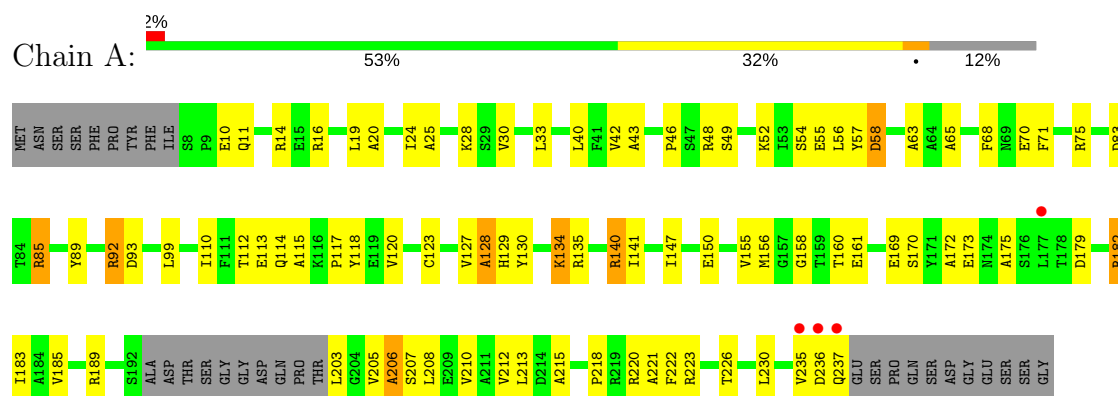
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	Z	7	Total 7	O 7	0	0
3	1	13	Total 13	O 13	0	0
3	2	19	Total 19	O 19	0	0

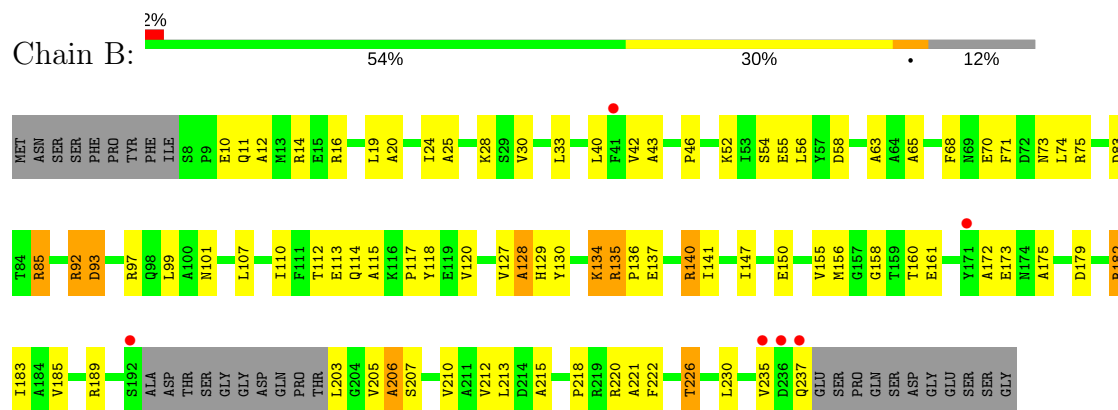
3 Residue-property plots

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

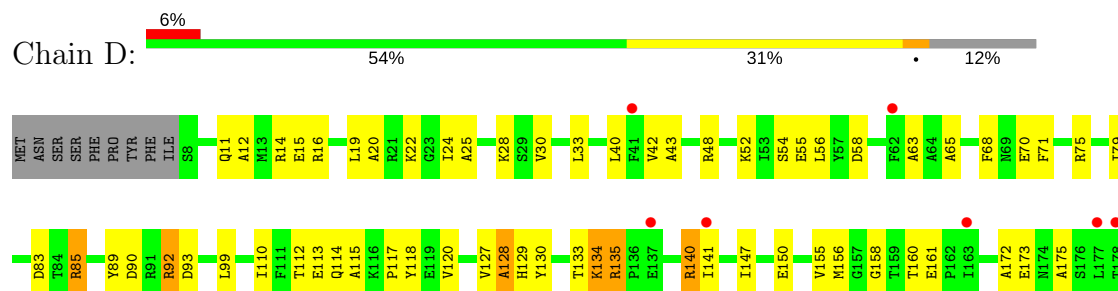
- Molecule 1: 20S proteasome, alpha and beta subunits

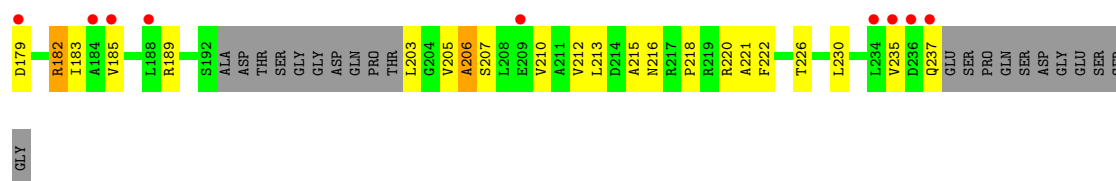


- Molecule 1: 20S proteasome, alpha and beta subunits

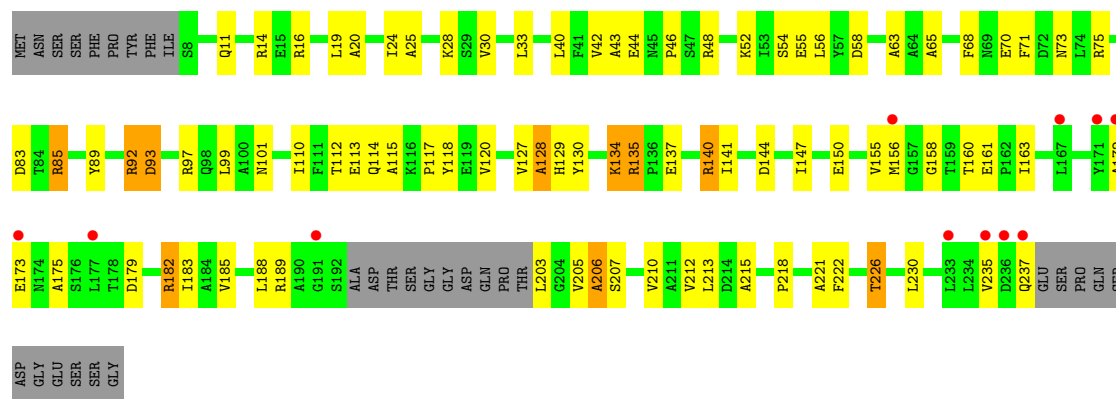


- Molecule 1: 20S proteasome, alpha and beta subunits

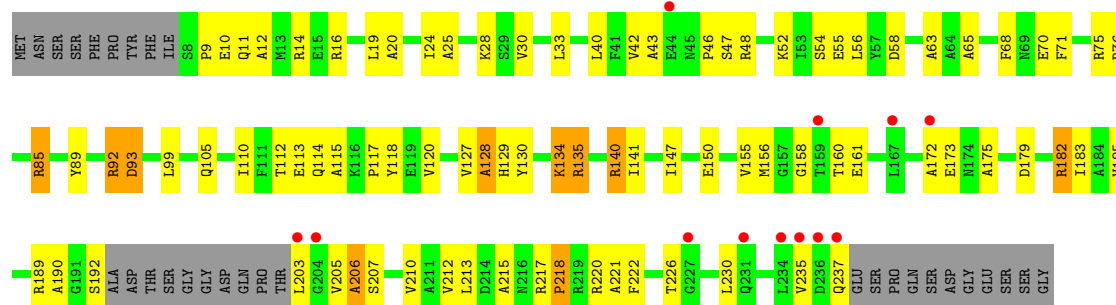




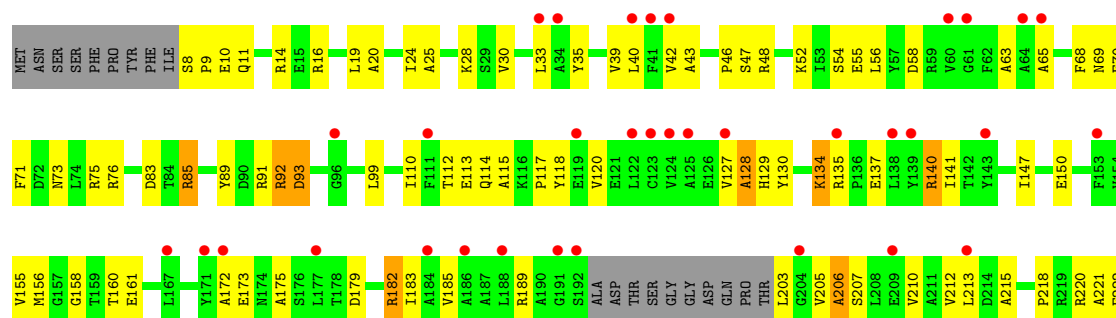
- Molecule 1: 20S proteasome, alpha and beta subunits



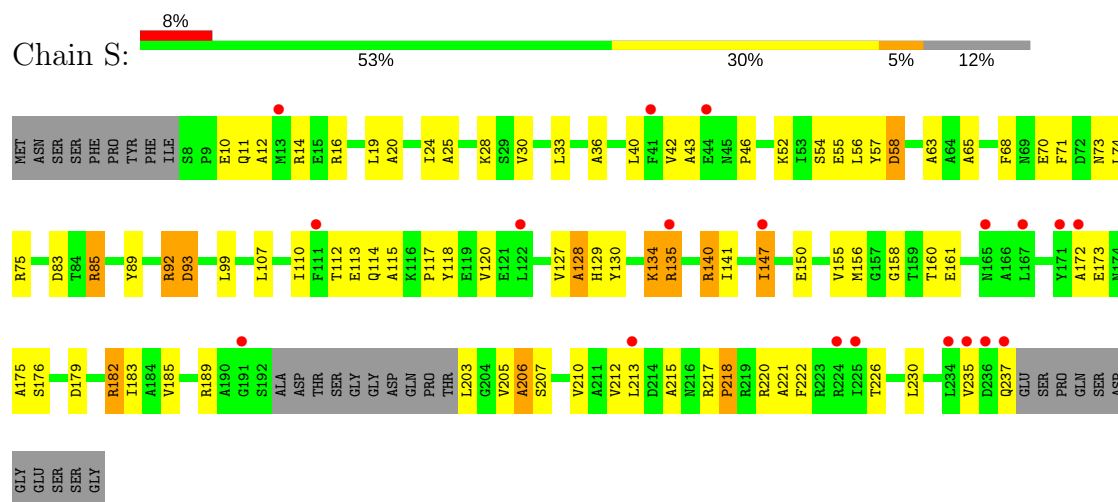
- Molecule 1: 20S proteasome, alpha and beta subunits



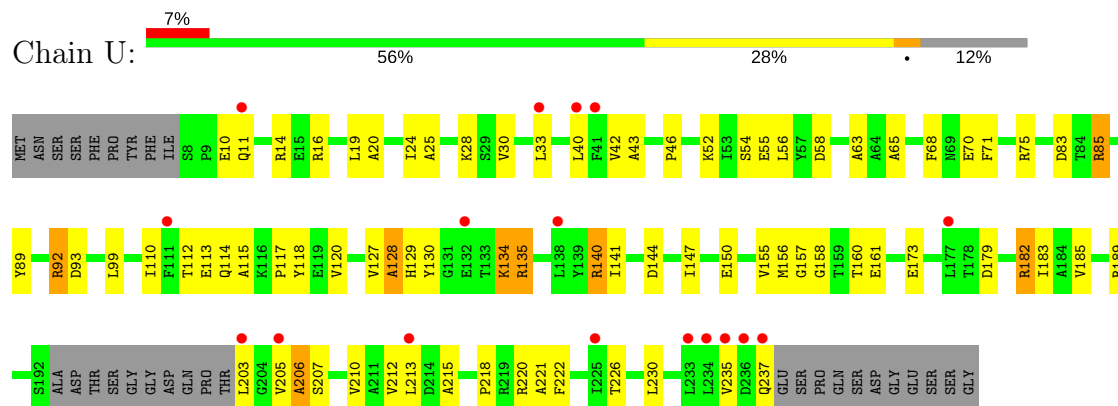
- Molecule 1: 20S proteasome, alpha and beta subunits



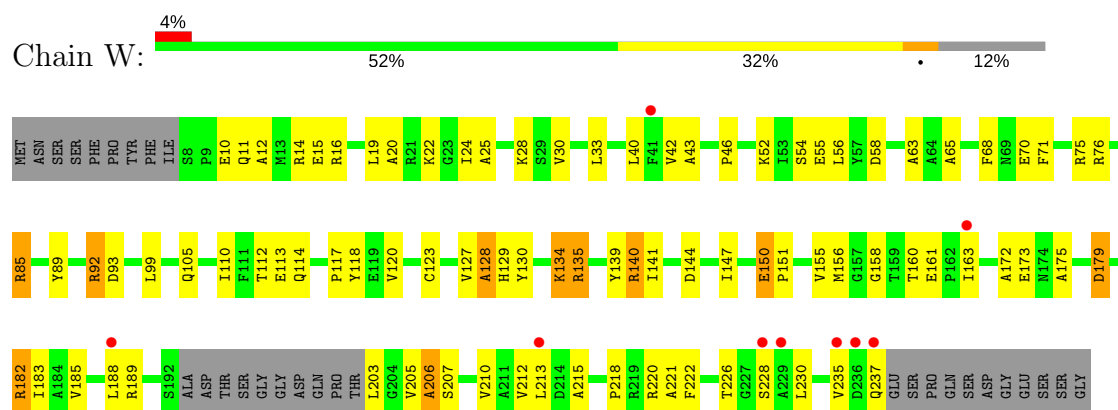
- Molecule 1: 20S proteasome, alpha and beta subunits



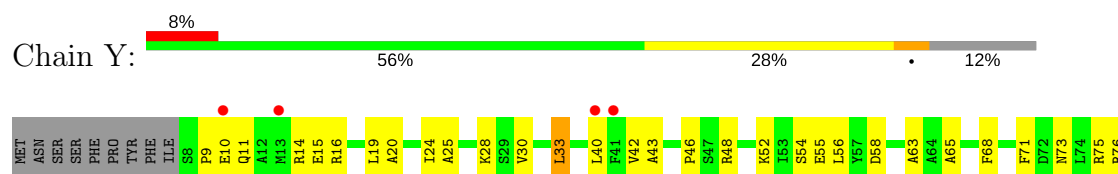
- Molecule 1: 20S proteasome, alpha and beta subunits

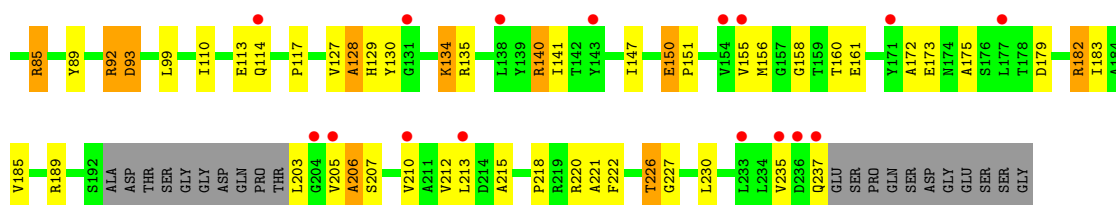


- Molecule 1: 20S proteasome, alpha and beta subunits

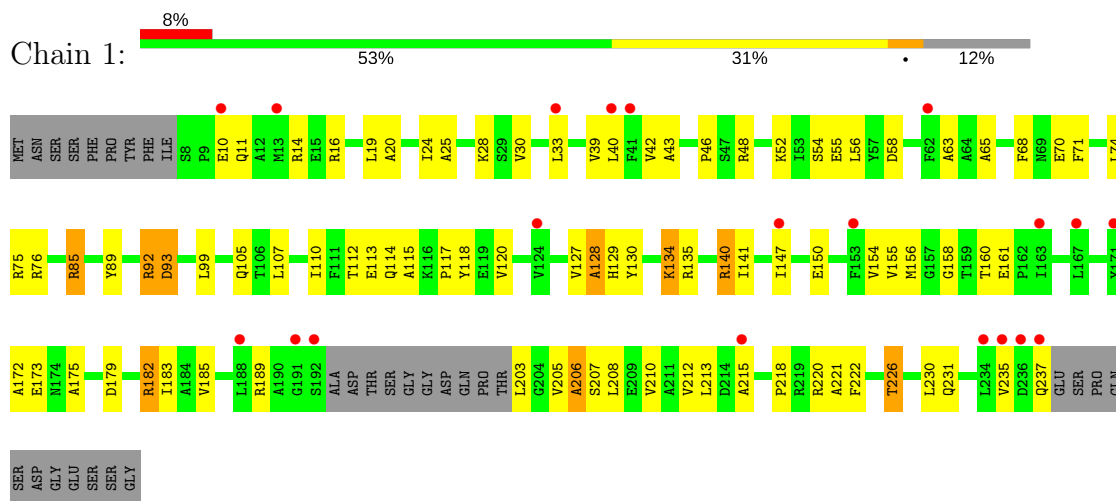


- Molecule 1: 20S proteasome, alpha and beta subunits

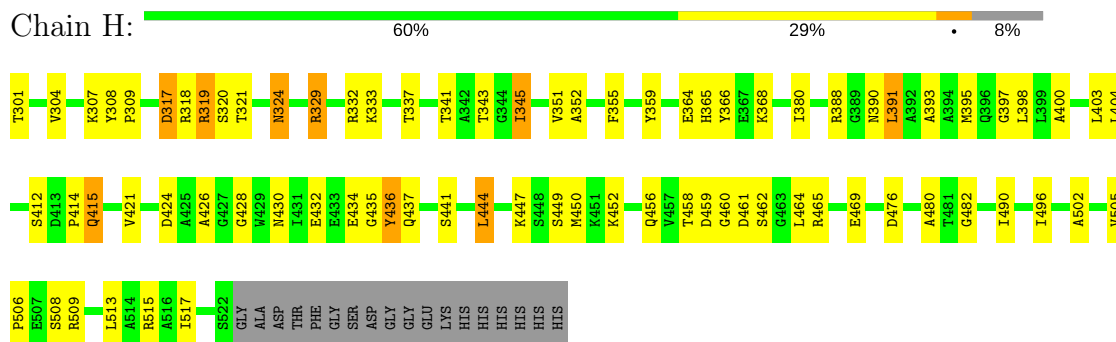




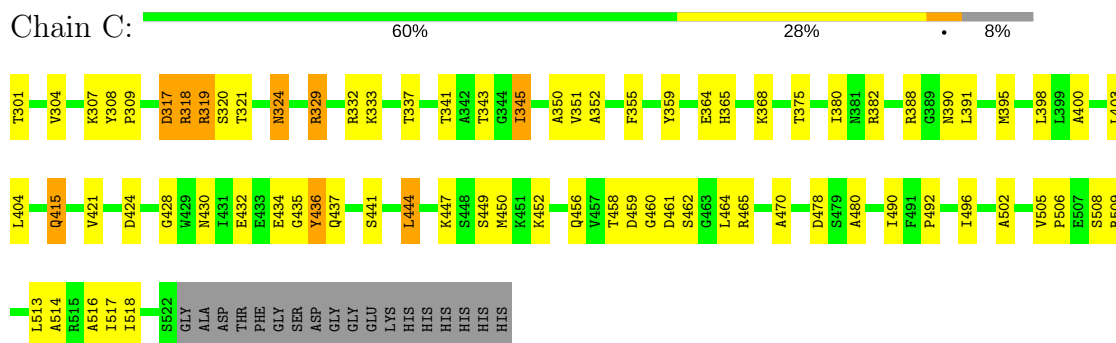
- Molecule 1: 20S proteasome, alpha and beta subunits



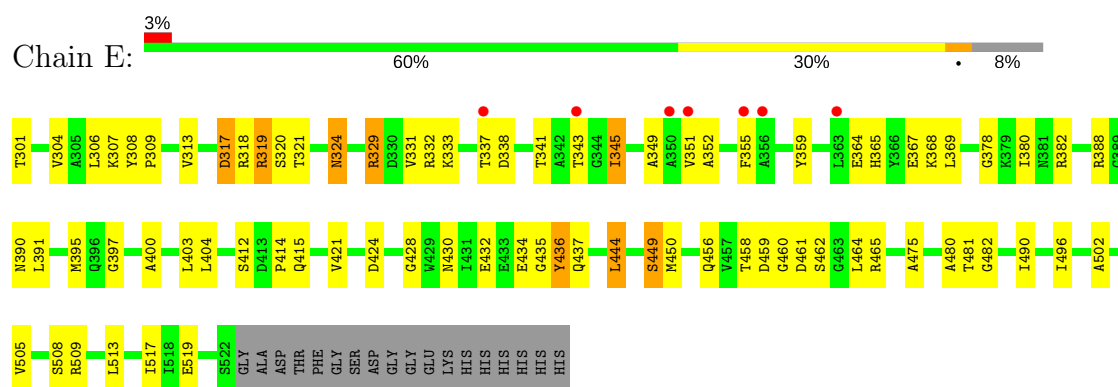
- Molecule 2: proteasome, beta subunit



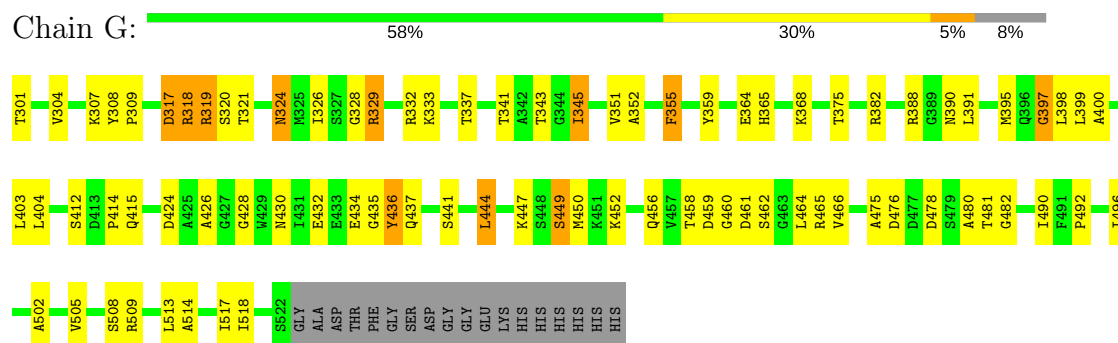
- Molecule 2: proteasome, beta subunit



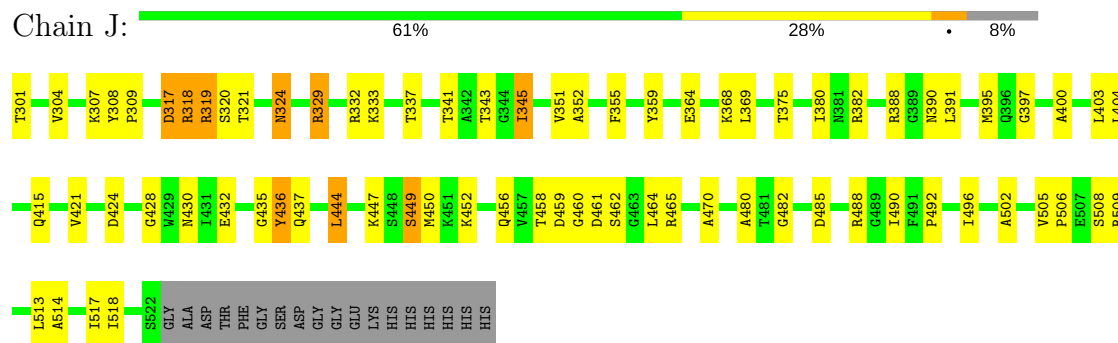
- Molecule 2: proteasome, beta subunit



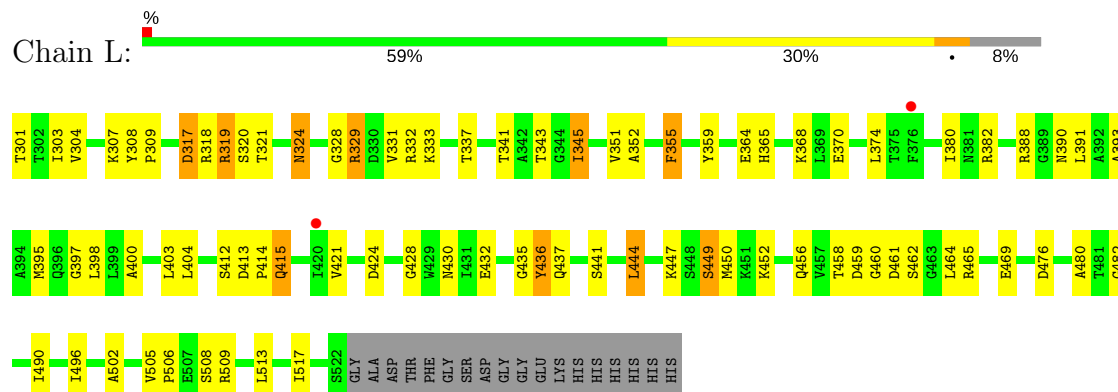
- Molecule 2: proteasome, beta subunit



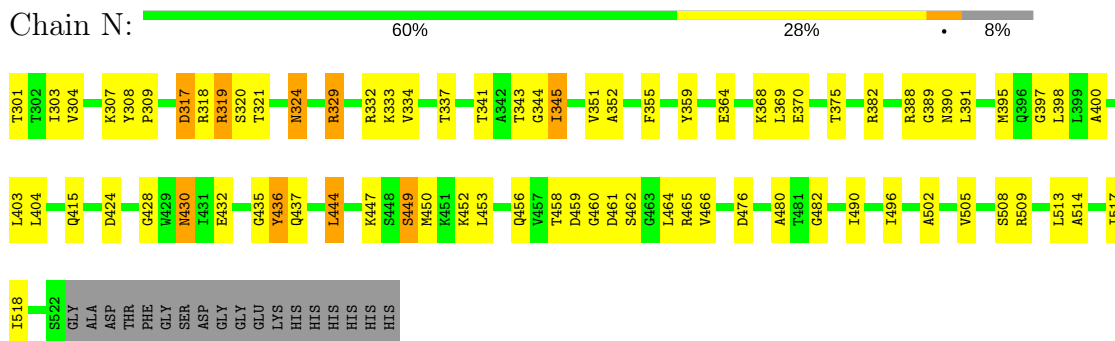
- Molecule 2: proteasome, beta subunit



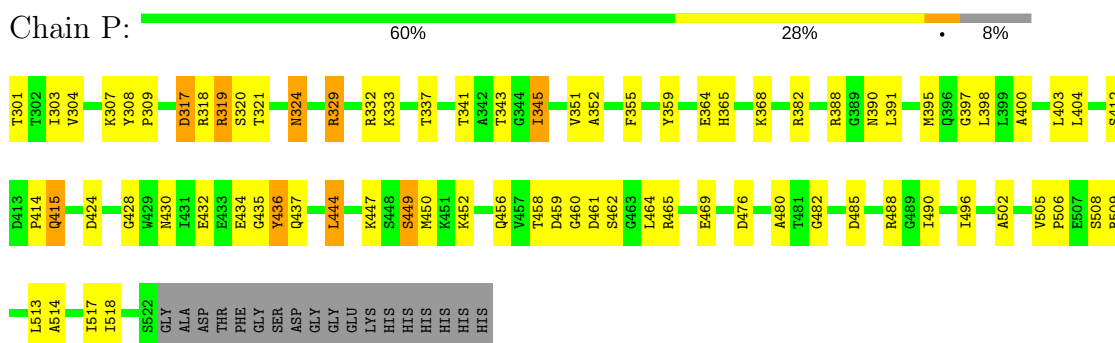
- Molecule 2: proteasome, beta subunit



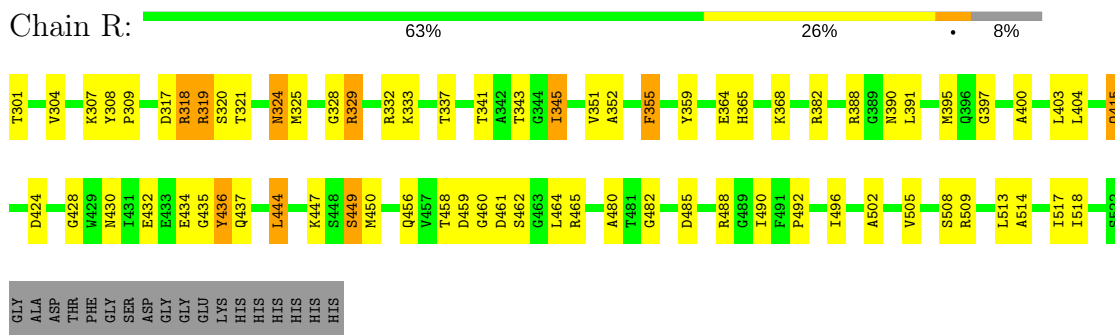
- Molecule 2: proteasome, beta subunit



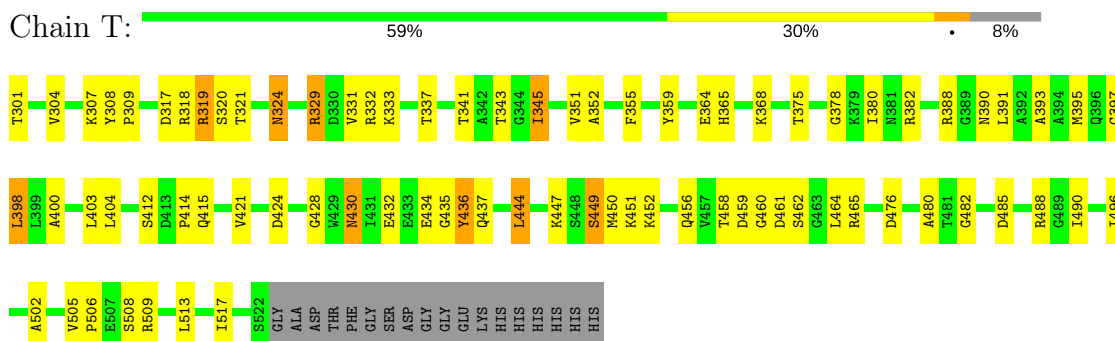
- Molecule 2: proteasome, beta subunit



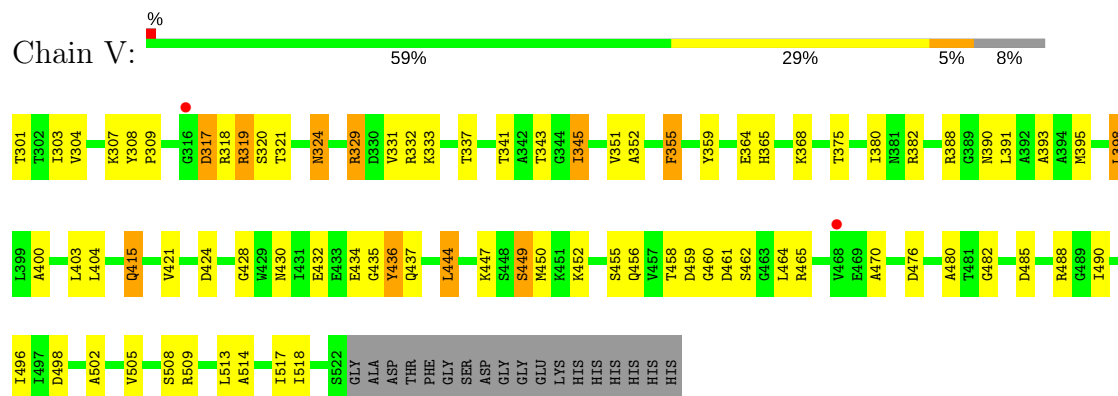
- Molecule 2: proteasome, beta subunit



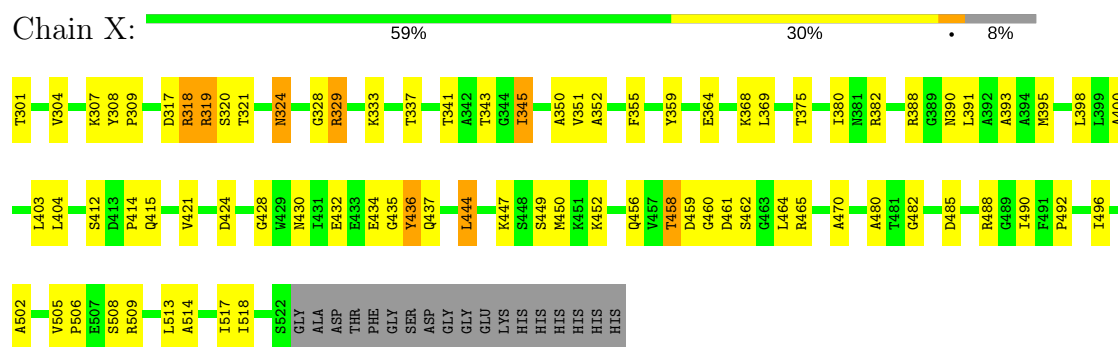
- Molecule 2: proteasome, beta subunit



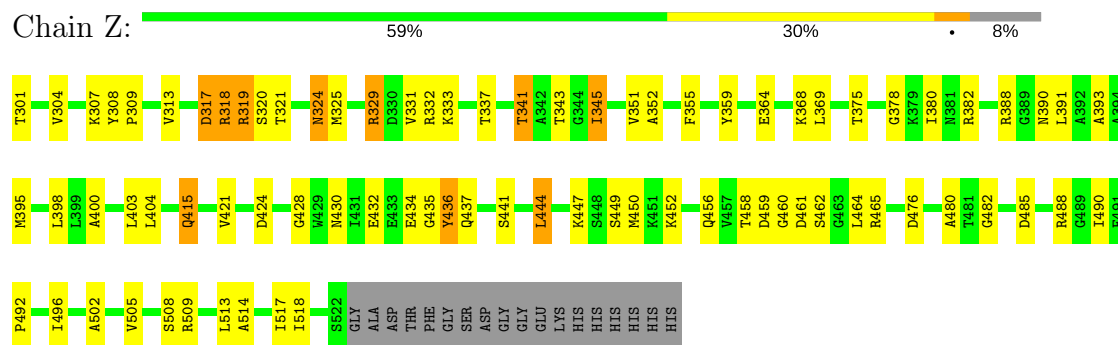
- Molecule 2: proteasome, beta subunit



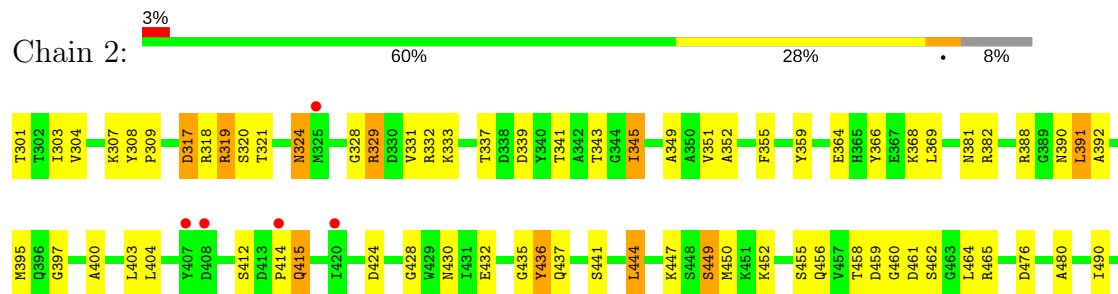
- Molecule 2: proteasome, beta subunit



- Molecule 2: proteasome, beta subunit



- Molecule 2: proteasome, beta subunit





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	173.33Å 113.80Å 200.13Å 90.00° 113.93° 90.00°	Depositor
Resolution (Å)	50.00 – 3.23 49.63 – 3.23	Depositor EDS
% Data completeness (in resolution range)	79.6 (50.00-3.23) 79.6 (49.63-3.23)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.49 (at 3.25Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.243 , 0.266 0.247 , 0.249	Depositor DCC
R_{free} test set	2776 reflections (3.04%)	wwPDB-VP
Wilson B-factor (Å ²)	82.0	Xtriage
Anisotropy	0.332	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 102.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.046 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	46846	wwPDB-VP
Average B, all atoms (Å ²)	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.55% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	1	0.43	0/1717	0.59	0/2320
1	A	0.54	1/1717 (0.1%)	0.63	0/2320
1	B	0.49	0/1717	0.62	0/2320
1	D	0.47	0/1717	0.61	0/2320
1	F	0.45	0/1717	0.60	0/2320
1	I	0.44	0/1717	0.60	0/2320
1	K	0.43	0/1717	0.59	0/2320
1	M	0.45	0/1717	0.60	0/2320
1	O	0.45	0/1717	0.60	0/2320
1	Q	0.44	0/1717	0.59	0/2320
1	S	0.43	0/1717	0.59	0/2320
1	U	0.43	0/1717	0.60	0/2320
1	W	0.47	0/1717	0.61	0/2320
1	Y	0.43	0/1717	0.59	0/2320
2	2	0.42	0/1662	0.61	0/2254
2	C	0.52	0/1662	0.65	0/2254
2	E	0.54	0/1662	0.66	0/2254
2	G	0.48	0/1662	0.65	0/2254
2	H	0.55	0/1662	0.66	0/2254
2	J	0.49	0/1662	0.63	0/2254
2	L	0.51	0/1662	0.65	0/2254
2	N	0.49	0/1662	0.64	0/2254
2	P	0.49	0/1662	0.64	0/2254
2	R	0.50	0/1662	0.65	0/2254
2	T	0.46	0/1662	0.63	0/2254
2	V	0.47	0/1662	0.65	0/2254
2	X	0.49	0/1662	0.64	0/2254
2	Z	0.48	0/1662	0.64	0/2254
All	All	0.47	1/47306 (0.0%)	0.62	0/64036

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	123	CYS	CB-SG	-5.45	1.73	1.81

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	1	1692	0	1688	75	0
1	A	1692	0	1688	77	4
1	B	1692	0	1688	75	0
1	D	1692	0	1688	72	4
1	F	1692	0	1688	80	0
1	I	1692	0	1688	72	2
1	K	1692	0	1688	84	0
1	M	1692	0	1688	88	0
1	O	1692	0	1688	77	0
1	Q	1692	0	1688	68	0
1	S	1692	0	1688	77	0
1	U	1692	0	1688	69	2
1	W	1692	0	1688	77	1
1	Y	1692	0	1688	72	0
2	2	1638	0	1630	67	1
2	C	1638	0	1630	58	0
2	E	1638	0	1630	60	1
2	G	1638	0	1630	67	3
2	H	1638	0	1630	62	0
2	J	1638	0	1630	56	2
2	L	1638	0	1630	68	0
2	N	1638	0	1630	62	1
2	P	1638	0	1630	61	1
2	R	1638	0	1630	54	0
2	T	1638	0	1630	60	0
2	V	1638	0	1630	64	2
2	X	1638	0	1630	59	3
2	Z	1638	0	1630	62	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	1	13	0	0	10	0
3	2	19	0	0	8	0
3	A	2	0	0	2	0
3	B	7	0	0	2	0
3	C	6	0	0	0	0
3	D	11	0	0	3	0
3	E	9	0	0	3	0
3	F	10	0	0	1	0
3	G	9	0	0	3	0
3	H	1	0	0	3	0
3	I	7	0	0	3	0
3	J	5	0	0	0	0
3	K	15	0	0	8	0
3	L	4	0	0	3	0
3	M	11	0	0	5	0
3	N	7	0	0	5	0
3	O	8	0	0	8	0
3	P	4	0	0	0	0
3	Q	6	0	0	2	0
3	R	5	0	0	2	0
3	S	13	0	0	3	0
3	T	6	0	0	4	0
3	U	7	0	0	1	0
3	V	10	0	0	4	0
3	W	8	0	0	3	0
3	X	4	0	0	1	0
3	Y	12	0	0	8	0
3	Z	7	0	0	4	0
All	All	46846	0	46452	1730	14

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 19.

All (1730) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:444:LEU:HD12	2:Z:444:LEU:HD12	1.27	1.15
2:L:444:LEU:HD12	2:P:444:LEU:HD12	1.30	1.13
2:J:452:LYS:HG3	3:Z:190:HOH:O	1.47	1.12
1:K:14:ARG:HG2	3:K:260:HOH:O	1.56	1.06
2:N:444:LEU:HD12	2:V:444:LEU:HD12	1.35	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:444:LEU:HD12	2:R:444:LEU:HD12	1.38	1.04
1:O:49:SER:OG	3:O:255:HOH:O	1.78	1.02
1:Y:33:LEU:HD21	3:Y:254:HOH:O	1.59	1.02
1:D:15:GLU:OE1	1:K:9:PRO:HD2	1.59	1.00
2:L:382:ARG:HD3	1:M:89:TYR:HD1	1.26	0.99
2:N:461:ASP:HB2	3:N:140:HOH:O	1.61	0.99
1:W:14:ARG:HB3	1:W:14:ARG:HH11	1.29	0.98
2:T:430:ASN:HB2	3:T:45:HOH:O	1.62	0.98
2:N:345:ILE:HD13	2:N:352:ALA:HB1	1.46	0.97
1:Y:14:ARG:HB3	1:Y:14:ARG:HH11	1.29	0.97
1:S:14:ARG:HH11	1:S:14:ARG:HB3	1.30	0.97
2:Z:452:LYS:HB2	3:Z:190:HOH:O	1.64	0.97
1:U:14:ARG:HB3	1:U:14:ARG:HH11	1.26	0.97
1:I:14:ARG:HH11	1:I:14:ARG:HB3	1.25	0.96
1:I:14:ARG:HB3	1:I:14:ARG:HH11	1.30	0.96
1:K:14:ARG:HH11	1:K:14:ARG:HB3	1.30	0.96
1:B:93:ASP:O	3:B:252:HOH:O	1.83	0.96
2:L:382:ARG:HD3	1:M:89:TYR:CD1	2.01	0.95
2:H:444:LEU:HD12	2:E:444:LEU:HD12	1.47	0.95
1:Q:14:ARG:HH11	1:Q:14:ARG:HB3	1.32	0.95
1:O:14:ARG:HH11	1:O:14:ARG:HB3	1.27	0.95
1:M:14:ARG:HB3	1:M:14:ARG:HH11	1.29	0.94
1:B:14:ARG:HH11	1:B:14:ARG:HB3	1.30	0.94
2:G:444:LEU:HD12	2:2:444:LEU:HD12	1.48	0.94
1:A:48:ARG:HH22	1:B:135:ARG:HB3	1.28	0.93
1:F:14:ARG:HH11	1:F:14:ARG:HB3	1.31	0.93
2:X:375:THR:OG1	1:Y:93:ASP:OD1	1.86	0.92
1:A:14:ARG:HH11	1:A:14:ARG:HB3	1.32	0.92
1:D:14:ARG:HB3	1:D:14:ARG:HH11	1.35	0.91
2:J:444:LEU:HD12	2:Z:444:LEU:CD1	2.01	0.91
2:C:345:ILE:HD13	2:C:352:ALA:HB1	1.53	0.90
2:G:345:ILE:HD13	2:G:352:ALA:HB1	1.52	0.90
2:L:444:LEU:HD12	2:P:444:LEU:CD1	2.02	0.90
2:R:509:ARG:HG3	3:R:112:HOH:O	1.72	0.89
2:J:444:LEU:CD1	2:Z:444:LEU:HD12	2.02	0.89
2:P:345:ILE:HD13	2:P:352:ALA:HB1	1.54	0.89
2:X:345:ILE:HD13	2:X:352:ALA:HB1	1.54	0.89
2:J:345:ILE:HD13	2:J:352:ALA:HB1	1.56	0.88
1:K:115:ALA:HB3	1:M:112:THR:CG2	2.02	0.88
2:L:444:LEU:CD1	2:P:444:LEU:HD12	2.02	0.88
2:T:345:ILE:HD13	2:T:352:ALA:HB1	1.54	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:444:LEU:HD12	2:V:444:LEU:CD1	2.03	0.87
2:H:345:ILE:HD13	2:H:352:ALA:HB1	1.56	0.87
2:2:345:ILE:HD13	2:2:352:ALA:HB1	1.53	0.87
2:V:308:TYR:OH	3:V:32:HOH:O	1.94	0.86
1:A:11:GLN:HG2	1:A:14:ARG:HH12	1.40	0.86
2:N:444:LEU:CD1	2:V:444:LEU:HD12	2.05	0.86
2:V:345:ILE:HD13	2:V:352:ALA:HB1	1.56	0.86
2:L:345:ILE:HD13	2:L:352:ALA:HB1	1.56	0.86
1:D:83:ASP:OD2	2:E:365:HIS:HD2	1.59	0.86
2:T:444:LEU:HD12	2:X:444:LEU:HD12	1.57	0.86
1:D:11:GLN:HG2	1:D:14:ARG:NH1	1.89	0.85
1:A:11:GLN:HG2	1:A:14:ARG:NH1	1.90	0.85
1:D:92:ARG:HG3	1:D:129:HIS:HE1	1.41	0.85
1:O:92:ARG:HG3	1:O:129:HIS:HE1	1.42	0.85
2:R:345:ILE:HD13	2:R:352:ALA:HB1	1.56	0.84
1:U:92:ARG:HG3	1:U:129:HIS:HE1	1.42	0.84
1:D:11:GLN:HG2	1:D:14:ARG:HH12	1.42	0.84
2:E:345:ILE:HD13	2:E:352:ALA:HB1	1.60	0.84
2:Z:345:ILE:HD13	2:Z:352:ALA:HB1	1.59	0.83
2:V:303:ILE:HG13	3:V:155:HOH:O	1.76	0.83
1:U:11:GLN:HG2	1:U:14:ARG:HH12	1.44	0.83
1:S:11:GLN:HG2	1:S:14:ARG:NH1	1.94	0.82
1:S:92:ARG:HG3	1:S:129:HIS:HE1	1.43	0.82
1:W:11:GLN:HG2	1:W:14:ARG:NH1	1.94	0.82
1:Y:92:ARG:HG3	1:Y:129:HIS:HE1	1.43	0.82
1:K:92:ARG:HG3	1:K:129:HIS:HE1	1.43	0.82
2:P:304:VAL:HG21	2:P:450:MET:CE	2.09	0.82
1:U:11:GLN:HG2	1:U:14:ARG:NH1	1.95	0.82
1:I:92:ARG:HG3	1:I:129:HIS:HE1	1.43	0.82
1:B:92:ARG:HG3	1:B:129:HIS:HE1	1.43	0.82
1:S:11:GLN:HG2	1:S:14:ARG:HH12	1.46	0.81
1:K:115:ALA:HB3	1:M:112:THR:HG22	1.62	0.81
3:Q:254:HOH:O	2:Z:378:GLY:HA3	1.81	0.81
1:A:92:ARG:HG3	1:A:129:HIS:HE1	1.46	0.81
1:1:93:ASP:OD2	3:1:252:HOH:O	1.98	0.81
1:K:11:GLN:HG2	1:K:14:ARG:NH1	1.96	0.81
1:F:11:GLN:HG2	1:F:14:ARG:NH1	1.95	0.80
1:Q:92:ARG:HG3	1:Q:129:HIS:HE1	1.44	0.80
2:N:304:VAL:HG21	2:N:450:MET:CE	2.12	0.80
1:Q:11:GLN:HG2	1:Q:14:ARG:HH12	1.46	0.80
1:W:92:ARG:HG3	1:W:129:HIS:HE1	1.47	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:11:GLN:HG2	1:I:14:ARG:NH1	1.96	0.80
1:M:92:ARG:HG3	1:M:129:HIS:HE1	1.45	0.80
1:O:11:GLN:HG2	1:O:14:ARG:NH1	1.96	0.80
2:2:304:VAL:HG21	2:2:450:MET:CE	2.12	0.80
1:Q:11:GLN:HG2	1:Q:14:ARG:NH1	1.96	0.80
2:L:337:THR:OG1	2:L:343:THR:HG22	1.82	0.79
1:M:11:GLN:HG2	1:M:14:ARG:NH1	1.97	0.79
1:B:55:GLU:HB2	1:B:222:PHE:CD2	2.18	0.79
2:H:304:VAL:HG21	2:H:450:MET:CE	2.11	0.79
2:E:304:VAL:HG21	2:E:450:MET:CE	2.13	0.79
1:O:10:GLU:HA	1:U:19:LEU:HD12	1.65	0.79
1:1:92:ARG:HG3	1:1:129:HIS:HE1	1.48	0.79
1:B:11:GLN:HG2	1:B:14:ARG:NH1	1.97	0.78
1:F:11:GLN:HG2	1:F:14:ARG:HH12	1.47	0.78
1:F:135:ARG:HB3	1:M:48:ARG:HH22	1.48	0.78
1:O:29:SER:O	3:O:252:HOH:O	2.02	0.78
2:G:332:ARG:HD3	3:G:210:HOH:O	1.84	0.78
1:D:92:ARG:HG3	1:D:129:HIS:CE1	2.19	0.78
2:J:304:VAL:HG21	2:J:450:MET:CE	2.15	0.78
1:W:11:GLN:HG2	1:W:14:ARG:HH12	1.47	0.77
1:I:11:GLN:HG2	1:I:14:ARG:HH12	1.50	0.77
2:G:304:VAL:HG21	2:G:450:MET:CE	2.14	0.77
2:G:382:ARG:HD3	1:W:89:TYR:CD1	2.19	0.77
1:O:85:ARG:HH11	1:O:85:ARG:HG2	1.49	0.77
2:E:304:VAL:HG21	2:E:450:MET:HE3	1.65	0.77
1:1:55:GLU:HB2	1:1:222:PHE:CD2	2.20	0.77
1:B:11:GLN:HG2	1:B:14:ARG:HH12	1.50	0.77
1:U:89:TYR:CD1	2:2:382:ARG:HD3	2.19	0.77
1:1:11:GLN:HG2	1:1:14:ARG:NH1	1.99	0.77
1:K:11:GLN:HG2	1:K:14:ARG:HH12	1.47	0.77
2:L:304:VAL:HG21	2:L:450:MET:CE	2.13	0.77
2:P:304:VAL:HG21	2:P:450:MET:HE3	1.65	0.77
1:Y:11:GLN:HG2	1:Y:14:ARG:NH1	1.98	0.77
1:Y:85:ARG:HG2	1:Y:85:ARG:HH11	1.49	0.76
1:K:92:ARG:HG3	1:K:129:HIS:CE1	2.20	0.76
1:O:11:GLN:HG2	1:O:14:ARG:HH12	1.51	0.76
2:L:459:ASP:H	2:L:462:SER:HB3	1.50	0.76
1:F:85:ARG:HH11	1:F:85:ARG:HG2	1.51	0.76
1:I:92:ARG:HG3	1:I:129:HIS:CE1	2.21	0.76
2:H:459:ASP:H	2:H:462:SER:HB3	1.50	0.76
2:V:304:VAL:HG21	2:V:450:MET:CE	2.16	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:304:VAL:HG21	2:L:450:MET:HE3	1.67	0.76
1:A:48:ARG:HH22	1:B:135:ARG:CB	1.98	0.76
1:A:85:ARG:HG2	1:A:85:ARG:HH11	1.51	0.76
1:Q:92:ARG:HG3	1:Q:129:HIS:CE1	2.22	0.75
3:X:157:HOH:O	2:Z:325:MET:HE3	1.86	0.75
1:O:92:ARG:HG3	1:O:129:HIS:CE1	2.20	0.75
1:1:11:GLN:HG2	1:1:14:ARG:HH12	1.52	0.75
1:M:92:ARG:HG3	1:M:129:HIS:CE1	2.22	0.75
1:Q:93:ASP:OD2	3:Q:254:HOH:O	2.05	0.75
2:T:304:VAL:HG21	2:T:450:MET:CE	2.16	0.75
1:U:92:ARG:HG3	1:U:129:HIS:CE1	2.21	0.75
1:W:150:GLU:HG3	3:W:253:HOH:O	1.85	0.75
1:M:11:GLN:HG2	1:M:14:ARG:HH12	1.49	0.75
1:M:85:ARG:HH11	1:M:85:ARG:HG2	1.52	0.75
2:R:424:ASP:HB3	2:R:428:GLY:H	1.52	0.75
1:S:55:GLU:HB2	1:S:222:PHE:CD2	2.22	0.75
2:T:451:LYS:HB3	3:T:79:HOH:O	1.85	0.75
2:G:444:LEU:HD12	2:2:444:LEU:CD1	2.18	0.74
1:S:19:LEU:HD12	1:1:10:GLU:HA	1.68	0.74
1:A:55:GLU:HB2	1:A:222:PHE:CD2	2.22	0.74
2:X:304:VAL:HG21	2:X:450:MET:CE	2.18	0.74
2:2:459:ASP:H	2:2:462:SER:HB3	1.52	0.74
1:A:208:LEU:HB3	3:A:250:HOH:O	1.87	0.74
2:T:459:ASP:H	2:T:462:SER:HB3	1.53	0.74
2:R:459:ASP:H	2:R:462:SER:HB3	1.53	0.74
2:C:304:VAL:HG21	2:C:450:MET:CE	2.17	0.74
1:F:92:ARG:HG3	1:F:129:HIS:HE1	1.51	0.74
2:V:329:ARG:O	2:V:490:ILE:HG21	1.87	0.74
1:Y:11:GLN:HG2	1:Y:14:ARG:HH12	1.52	0.74
1:A:115:ALA:HB3	1:B:112:THR:HG22	1.70	0.74
1:Y:92:ARG:HG3	1:Y:129:HIS:CE1	2.22	0.74
2:Z:424:ASP:HB3	2:Z:428:GLY:H	1.53	0.74
2:G:444:LEU:CD1	2:2:444:LEU:HD12	2.18	0.74
1:B:92:ARG:HG3	1:B:129:HIS:CE1	2.21	0.74
1:Y:55:GLU:HB2	1:Y:222:PHE:CD2	2.23	0.74
1:S:85:ARG:HH11	1:S:85:ARG:HG2	1.53	0.73
1:S:92:ARG:HG3	1:S:129:HIS:CE1	2.22	0.73
1:U:112:THR:CG2	1:1:115:ALA:HB3	2.18	0.73
1:K:55:GLU:HB2	1:K:222:PHE:CD2	2.23	0.73
1:M:55:GLU:HB2	1:M:222:PHE:CD2	2.23	0.73
1:1:206:ALA:HB1	3:1:258:HOH:O	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:459:ASP:H	2:C:462:SER:HB3	1.54	0.73
1:D:15:GLU:OE1	1:K:9:PRO:CD	2.36	0.73
2:Z:304:VAL:HG21	2:Z:450:MET:CE	2.19	0.73
1:S:40:LEU:HA	1:S:212:VAL:HG12	1.69	0.73
1:A:112:THR:CG2	1:O:115:ALA:HB3	2.19	0.73
2:N:337:THR:OG1	2:N:343:THR:HG22	1.88	0.73
2:C:444:LEU:CD1	2:R:444:LEU:HD12	2.17	0.73
1:U:14:ARG:NH1	1:U:14:ARG:HB3	2.01	0.72
1:K:40:LEU:HA	1:K:212:VAL:HG12	1.70	0.72
1:A:92:ARG:HG3	1:A:129:HIS:CE1	2.24	0.72
2:T:319:ARG:HG3	2:T:320:SER:N	2.05	0.72
1:W:92:ARG:HG3	1:W:129:HIS:CE1	2.25	0.72
1:I:55:GLU:HB2	1:I:222:PHE:CD2	2.25	0.72
2:J:424:ASP:HB3	2:J:428:GLY:H	1.55	0.72
2:X:424:ASP:HB3	2:X:428:GLY:H	1.54	0.72
1:I:40:LEU:HA	1:I:212:VAL:HG12	1.71	0.72
1:A:112:THR:HG22	1:O:115:ALA:HB3	1.72	0.72
2:P:337:THR:OG1	2:P:343:THR:HG22	1.89	0.72
2:R:304:VAL:HG21	2:R:450:MET:CE	2.20	0.72
1:I:14:ARG:HB3	1:I:14:ARG:NH1	2.02	0.72
1:B:19:LEU:HD12	1:I:10:GLU:HA	1.72	0.72
1:D:40:LEU:HA	1:D:212:VAL:HG12	1.72	0.72
1:F:55:GLU:HB2	1:F:222:PHE:CD2	2.24	0.72
1:O:40:LEU:HA	1:O:212:VAL:HG12	1.72	0.72
1:W:85:ARG:HH11	1:W:85:ARG:HG2	1.55	0.72
2:C:337:THR:OG1	2:C:343:THR:HG22	1.89	0.72
1:I:85:ARG:HH11	1:I:85:ARG:HG2	1.53	0.71
2:J:382:ARG:HD3	1:S:89:TYR:CD1	2.25	0.71
1:F:112:THR:HG22	1:M:115:ALA:HB3	1.72	0.71
2:V:319:ARG:HG3	2:V:320:SER:N	2.04	0.71
1:F:19:LEU:HD12	1:W:10:GLU:HA	1.72	0.71
2:P:459:ASP:H	2:P:462:SER:HB3	1.55	0.71
1:I:92:ARG:HG3	1:I:129:HIS:CE1	2.25	0.71
1:B:14:ARG:HB3	1:B:14:ARG:NH1	2.06	0.71
2:G:459:ASP:H	2:G:462:SER:HB3	1.55	0.71
1:O:55:GLU:HB2	1:O:222:PHE:CD2	2.25	0.71
1:A:40:LEU:HA	1:A:212:VAL:HG12	1.73	0.71
2:E:382:ARG:HD3	1:K:89:TYR:CD1	2.25	0.71
1:U:89:TYR:HD1	2:2:382:ARG:HD3	1.55	0.71
1:W:40:LEU:HA	1:W:212:VAL:HG12	1.73	0.71
2:E:424:ASP:HB3	2:E:428:GLY:H	1.53	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:304:VAL:HG21	2:G:450:MET:HE3	1.72	0.71
1:U:55:GLU:HB2	1:U:222:PHE:CD2	2.24	0.71
1:D:55:GLU:HB2	1:D:222:PHE:CD2	2.25	0.71
1:F:40:LEU:HA	1:F:212:VAL:HG12	1.72	0.71
2:E:459:ASP:H	2:E:462:SER:HB3	1.55	0.71
2:G:329:ARG:O	2:G:490:ILE:HG21	1.90	0.71
2:T:382:ARG:HD3	1:I:89:TYR:CD1	2.25	0.71
1:Q:85:ARG:HH11	1:Q:85:ARG:HG2	1.55	0.71
2:G:462:SER:O	2:G:465:ARG:HG2	1.92	0.70
2:R:319:ARG:HG3	2:R:320:SER:N	2.06	0.70
2:X:459:ASP:H	2:X:462:SER:HB3	1.53	0.70
2:G:424:ASP:HB3	2:G:428:GLY:H	1.55	0.70
2:C:444:LEU:HD12	2:R:444:LEU:CD1	2.18	0.70
1:W:19:LEU:HD12	1:Y:10:GLU:HA	1.74	0.70
1:F:110:ILE:HG23	1:F:114:GLN:HG3	1.72	0.70
2:P:424:ASP:HB3	2:P:428:GLY:H	1.55	0.70
1:S:14:ARG:NH1	1:S:14:ARG:HB3	2.05	0.70
1:U:40:LEU:HA	1:U:212:VAL:HG12	1.73	0.70
1:U:85:ARG:HG2	1:U:85:ARG:HH11	1.56	0.70
1:W:14:ARG:NH1	1:W:14:ARG:HB3	2.06	0.70
1:F:189:ARG:NH1	3:F:254:HOH:O	2.22	0.70
2:J:329:ARG:O	2:J:490:ILE:HG21	1.91	0.70
2:T:329:ARG:O	2:T:490:ILE:HG21	1.91	0.70
2:P:329:ARG:O	2:P:490:ILE:HG21	1.92	0.69
2:V:337:THR:OG1	2:V:343:THR:HG22	1.92	0.69
1:I:28:LYS:HB2	1:I:52:LYS:NZ	2.07	0.69
1:Q:14:ARG:NH1	1:Q:14:ARG:HB3	2.07	0.69
1:Q:55:GLU:HB2	1:Q:222:PHE:CD2	2.28	0.69
2:2:304:VAL:HG21	2:2:450:MET:HE3	1.73	0.69
1:D:83:ASP:OD2	2:E:365:HIS:CD2	2.43	0.69
2:2:329:ARG:O	2:2:490:ILE:HG21	1.92	0.69
2:V:459:ASP:H	2:V:462:SER:HB3	1.57	0.69
2:G:337:THR:OG1	2:G:343:THR:HG22	1.92	0.69
1:K:14:ARG:HB3	1:K:14:ARG:NH1	2.05	0.69
1:M:76:ARG:NH2	2:N:370:GLU:OE2	2.21	0.69
2:V:498:ASP:HB3	3:V:32:HOH:O	1.93	0.69
2:E:337:THR:OG1	2:E:343:THR:HG22	1.93	0.69
2:N:459:ASP:H	2:N:462:SER:HB3	1.58	0.69
2:V:424:ASP:HB3	2:V:428:GLY:H	1.58	0.69
2:Z:329:ARG:HG2	3:Z:131:HOH:O	1.91	0.69
2:C:319:ARG:HG3	2:C:320:SER:N	2.07	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:424:ASP:HB3	2:H:428:GLY:H	1.55	0.69
1:Q:40:LEU:HA	1:Q:212:VAL:HG12	1.75	0.69
1:Q:89:TYR:CD1	2:Z:382:ARG:HD3	2.28	0.69
2:T:424:ASP:HB3	2:T:428:GLY:H	1.57	0.69
2:Z:459:ASP:H	2:Z:462:SER:HB3	1.58	0.69
2:E:329:ARG:O	2:E:490:ILE:HG21	1.93	0.68
2:J:459:ASP:H	2:J:462:SER:HB3	1.58	0.68
2:X:329:ARG:O	2:X:490:ILE:HG21	1.92	0.68
1:M:14:ARG:HB3	1:M:14:ARG:NH1	2.06	0.68
2:N:304:VAL:HG21	2:N:450:MET:HE3	1.75	0.68
1:F:14:ARG:HB3	1:F:14:ARG:NH1	2.05	0.68
2:G:308:TYR:HB2	2:G:309:PRO:HD2	1.75	0.68
1:I:182:ARG:HD3	1:I:235:VAL:HB	1.75	0.68
2:C:382:ARG:HD3	1:I:89:TYR:CD1	2.27	0.68
2:R:304:VAL:HG21	2:R:450:MET:HE3	1.75	0.68
1:Y:40:LEU:HA	1:Y:212:VAL:HG12	1.75	0.68
1:K:85:ARG:HG2	1:K:85:ARG:HH11	1.58	0.68
2:E:382:ARG:HD3	1:K:89:TYR:HD1	1.58	0.68
2:Z:329:ARG:O	2:Z:490:ILE:HG21	1.93	0.68
1:Q:110:ILE:HG23	1:Q:114:GLN:HG3	1.75	0.68
1:B:115:ALA:HB3	1:I:112:THR:CG2	2.22	0.68
1:I:14:ARG:HB3	1:I:14:ARG:NH1	2.06	0.68
2:X:382:ARG:HD3	1:Y:89:TYR:CD1	2.29	0.68
1:D:85:ARG:HH11	1:D:85:ARG:HG2	1.59	0.68
2:P:319:ARG:HG3	2:P:320:SER:N	2.08	0.68
1:I:85:ARG:HH11	1:I:85:ARG:HG2	1.58	0.68
1:A:110:ILE:HG23	1:A:114:GLN:HG3	1.76	0.68
2:C:424:ASP:HB3	2:C:428:GLY:H	1.58	0.68
1:I:40:LEU:HA	1:I:212:VAL:HG12	1.76	0.68
2:R:329:ARG:O	2:R:490:ILE:HG21	1.93	0.68
1:F:93:ASP:OD1	2:N:375:THR:OG1	2.12	0.68
2:N:424:ASP:HB3	2:N:428:GLY:H	1.58	0.68
2:P:462:SER:O	2:P:465:ARG:HG2	1.94	0.68
1:W:55:GLU:HB2	1:W:222:PHE:CD2	2.28	0.68
1:Y:14:ARG:HB3	1:Y:14:ARG:NH1	2.06	0.68
1:O:14:ARG:HB3	1:O:14:ARG:NH1	2.04	0.68
2:E:319:ARG:HG3	2:E:320:SER:N	2.07	0.67
2:H:337:THR:OG1	2:H:343:THR:HG22	1.94	0.67
2:N:319:ARG:HG3	2:N:320:SER:N	2.09	0.67
1:A:182:ARG:HD3	1:A:235:VAL:HB	1.75	0.67
2:L:329:ARG:O	2:L:490:ILE:HG21	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:329:ARG:O	2:N:490:ILE:HG21	1.94	0.67
2:G:319:ARG:HG3	2:G:320:SER:N	2.09	0.67
2:X:337:THR:OG1	2:X:343:THR:HG22	1.95	0.67
2:C:329:ARG:O	2:C:490:ILE:HG21	1.95	0.67
1:F:92:ARG:HG3	1:F:129:HIS:CE1	2.29	0.67
1:B:40:LEU:HA	1:B:212:VAL:HG12	1.75	0.67
2:J:337:THR:OG1	2:J:343:THR:HG22	1.94	0.67
1:A:189:ARG:CZ	1:A:237:GLN:HB3	2.24	0.67
1:D:110:ILE:HG23	1:D:114:GLN:HG3	1.77	0.67
1:B:85:ARG:HH11	1:B:85:ARG:HG2	1.58	0.67
2:H:319:ARG:HG3	2:H:320:SER:N	2.08	0.67
1:I:110:ILE:HG23	1:I:114:GLN:HG3	1.77	0.67
2:X:319:ARG:HG3	2:X:320:SER:N	2.11	0.66
2:Z:319:ARG:HG3	2:Z:320:SER:N	2.10	0.66
2:Z:436:TYR:H	2:Z:436:TYR:HD1	1.43	0.66
2:H:304:VAL:HG21	2:H:450:MET:HE3	1.76	0.66
1:A:14:ARG:NH1	1:A:14:ARG:HB3	2.09	0.66
1:D:14:ARG:HB3	1:D:14:ARG:NH1	2.08	0.66
1:K:28:LYS:HB2	1:K:52:LYS:NZ	2.10	0.66
1:M:40:LEU:HA	1:M:212:VAL:HG12	1.76	0.66
1:S:115:ALA:HB3	1:I:112:THR:HG22	1.76	0.66
2:J:319:ARG:HG3	2:J:320:SER:N	2.09	0.66
1:Y:227:GLY:O	3:Y:249:HOH:O	2.13	0.66
2:2:424:ASP:HB3	2:2:428:GLY:H	1.60	0.66
2:L:424:ASP:HB3	2:L:428:GLY:H	1.61	0.66
2:L:449:SER:HB2	2:P:452:LYS:NZ	2.11	0.66
2:N:324:ASN:H	2:N:324:ASN:HD22	1.43	0.66
1:U:112:THR:HG22	1:I:115:ALA:HB3	1.78	0.66
1:F:101:ASN:OD1	1:M:68:PHE:HE1	1.79	0.66
1:Y:15:GLU:HB2	3:Y:257:HOH:O	1.95	0.66
2:Z:304:VAL:HG21	2:Z:450:MET:HE3	1.78	0.66
2:H:329:ARG:O	2:H:490:ILE:HG21	1.96	0.65
2:J:436:TYR:H	2:J:436:TYR:HD1	1.44	0.65
1:M:182:ARG:HD3	1:M:235:VAL:HB	1.78	0.65
1:M:30:VAL:O	3:M:256:HOH:O	2.13	0.65
2:T:304:VAL:HG21	2:T:450:MET:HE3	1.77	0.65
1:K:115:ALA:HB3	1:M:112:THR:HG23	1.76	0.65
3:G:124:HOH:O	2:N:430:ASN:HB3	1.96	0.65
2:N:464:LEU:HD12	2:N:496:ILE:HD11	1.78	0.65
2:X:464:LEU:HD12	2:X:496:ILE:HD11	1.77	0.65
2:J:304:VAL:HG21	2:J:450:MET:HE3	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:444:LEU:HD12	2:X:444:LEU:CD1	2.24	0.65
1:F:115:ALA:HB3	1:W:112:THR:CG2	2.26	0.65
1:W:15:GLU:OE1	1:Y:9:PRO:HD2	1.96	0.65
1:F:182:ARG:HD3	1:F:235:VAL:HB	1.78	0.65
2:L:308:TYR:HB2	2:L:309:PRO:HD2	1.79	0.65
2:T:444:LEU:CD1	2:X:444:LEU:HD12	2.25	0.65
1:Y:182:ARG:HD3	1:Y:235:VAL:HB	1.79	0.65
1:U:16:ARG:HE	1:U:117:PRO:HD3	1.61	0.65
2:X:308:TYR:HB2	2:X:309:PRO:HD2	1.79	0.65
1:1:39:VAL:N	3:1:256:HOH:O	2.29	0.65
2:Z:337:THR:OG1	2:Z:343:THR:HG22	1.97	0.65
1:U:189:ARG:CZ	1:U:237:GLN:HB3	2.26	0.65
2:2:308:TYR:HB2	2:2:309:PRO:HD2	1.78	0.64
1:O:110:ILE:HG23	1:O:114:GLN:HG3	1.78	0.64
2:2:337:THR:OG1	2:2:343:THR:HG22	1.97	0.64
1:F:135:ARG:CB	1:M:48:ARG:HH22	2.09	0.64
1:W:189:ARG:CZ	1:W:237:GLN:HB3	2.28	0.64
2:E:308:TYR:HB2	2:E:309:PRO:HD2	1.78	0.64
2:H:515:ARG:NE	3:H:114:HOH:O	2.30	0.64
1:M:56:LEU:HD13	1:M:99:LEU:CD2	2.27	0.64
2:X:304:VAL:HG21	2:X:450:MET:HE3	1.80	0.64
1:1:208:LEU:HB3	3:1:253:HOH:O	1.97	0.64
2:2:319:ARG:HG3	2:2:320:SER:N	2.12	0.64
1:K:182:ARG:HD3	1:K:235:VAL:HB	1.78	0.64
2:V:462:SER:O	2:V:465:ARG:HG2	1.97	0.64
1:S:189:ARG:CZ	1:S:237:GLN:HB3	2.28	0.64
1:S:56:LEU:HD13	1:S:99:LEU:CD2	2.28	0.64
1:B:182:ARG:HD3	1:B:235:VAL:HB	1.78	0.64
2:2:339:ASP:HA	3:2:95:HOH:O	1.97	0.64
1:M:156:MET:HG2	3:M:256:HOH:O	1.99	0.64
1:Q:56:LEU:HD13	1:Q:99:LEU:CD2	2.28	0.64
1:W:110:ILE:HG23	1:W:114:GLN:HG3	1.80	0.64
2:C:464:LEU:HD12	2:C:496:ILE:HD11	1.80	0.63
2:N:303:ILE:HD12	3:N:120:HOH:O	1.96	0.63
2:2:462:SER:O	2:2:465:ARG:HG2	1.99	0.63
2:T:382:ARG:HD3	1:1:89:TYR:HD1	1.63	0.63
2:2:464:LEU:HD12	2:2:496:ILE:HD11	1.79	0.63
1:B:110:ILE:HG23	1:B:114:GLN:HG3	1.79	0.63
2:E:462:SER:O	2:E:465:ARG:HG2	1.99	0.63
1:A:115:ALA:HB3	1:B:112:THR:CG2	2.28	0.63
2:G:382:ARG:HD3	1:W:89:TYR:HD1	1.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:308:TYR:HB2	2:H:309:PRO:HD2	1.79	0.63
2:J:308:TYR:HB2	2:J:309:PRO:HD2	1.80	0.63
1:O:189:ARG:CZ	1:O:237:GLN:HB3	2.28	0.63
1:O:89:TYR:CD1	2:V:382:ARG:HD3	2.32	0.63
2:R:464:LEU:HD12	2:R:496:ILE:HD11	1.79	0.63
1:1:189:ARG:CZ	1:1:237:GLN:HB3	2.29	0.63
1:F:189:ARG:CZ	1:F:237:GLN:HB3	2.28	0.63
2:N:462:SER:O	2:N:465:ARG:HG2	1.99	0.63
1:D:90:ASP:HB3	3:D:249:HOH:O	1.98	0.63
2:J:464:LEU:HD12	2:J:496:ILE:HD11	1.79	0.63
1:M:110:ILE:HG23	1:M:114:GLN:HG3	1.78	0.63
2:V:351:VAL:HB	2:V:400:ALA:HB2	1.81	0.63
1:F:73:ASN:HD22	1:W:105:GLN:CD	2.02	0.63
2:Z:462:SER:O	2:Z:465:ARG:HG2	1.97	0.63
1:B:189:ARG:CZ	1:B:237:GLN:HB3	2.28	0.63
2:R:462:SER:O	2:R:465:ARG:HG2	1.99	0.63
1:S:213:LEU:HA	1:S:221:ALA:O	1.99	0.63
2:V:308:TYR:HB2	2:V:309:PRO:HD2	1.79	0.63
1:W:182:ARG:HD3	1:W:235:VAL:HB	1.79	0.63
1:S:115:ALA:HB3	1:1:112:THR:CG2	2.28	0.63
2:X:462:SER:O	2:X:465:ARG:HG2	1.99	0.63
1:Q:182:ARG:HD3	1:Q:235:VAL:HB	1.82	0.62
1:A:30:VAL:HG22	1:A:43:ALA:HB1	1.79	0.62
1:F:179:ASP:O	1:F:183:ILE:HG12	1.99	0.62
2:P:308:TYR:HB2	2:P:309:PRO:HD2	1.81	0.62
2:R:337:THR:OG1	2:R:343:THR:HG22	1.99	0.62
2:J:462:SER:O	2:J:465:ARG:HG2	1.99	0.62
1:M:179:ASP:O	1:M:183:ILE:HG12	2.00	0.62
1:S:182:ARG:HD3	1:S:235:VAL:HB	1.81	0.62
2:T:308:TYR:HB2	2:T:309:PRO:HD2	1.81	0.62
2:C:308:TYR:HB2	2:C:309:PRO:HD2	1.80	0.62
2:L:462:SER:O	2:L:465:ARG:HG2	1.99	0.62
1:D:112:THR:CG2	1:Q:115:ALA:HB3	2.29	0.62
2:G:449:SER:HB2	2:2:452:LYS:NZ	2.14	0.62
1:M:154:VAL:HG13	3:M:249:HOH:O	1.99	0.62
1:Q:189:ARG:CZ	1:Q:237:GLN:HB3	2.30	0.62
1:S:16:ARG:HE	1:S:117:PRO:HD3	1.64	0.62
1:1:16:ARG:HE	1:1:117:PRO:HD3	1.64	0.62
1:D:28:LYS:HB2	1:D:52:LYS:NZ	2.15	0.62
1:S:28:LYS:HB2	1:S:52:LYS:NZ	2.15	0.62
2:T:462:SER:O	2:T:465:ARG:HG2	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:16:ARG:HE	1:Q:117:PRO:HD3	1.65	0.62
1:O:56:LEU:HD13	1:O:99:LEU:CD2	2.30	0.61
1:U:182:ARG:HD3	1:U:235:VAL:HB	1.82	0.61
1:Y:16:ARG:HE	1:Y:117:PRO:HD3	1.65	0.61
1:M:79:ILE:HD13	2:N:368:LYS:HB3	1.80	0.61
1:Q:10:GLU:HA	1:Y:19:LEU:HD12	1.82	0.61
1:K:16:ARG:HE	1:K:117:PRO:HD3	1.66	0.61
2:L:319:ARG:HG3	2:L:320:SER:N	2.14	0.61
2:R:436:TYR:HD1	2:R:436:TYR:H	1.49	0.61
2:E:461:ASP:OD1	2:E:509:ARG:HD2	2.01	0.61
2:H:452:LYS:NZ	2:E:449:SER:HB2	2.15	0.61
2:T:337:THR:OG1	2:T:343:THR:HG22	1.99	0.61
1:W:179:ASP:O	1:W:183:ILE:HG12	2.00	0.61
2:C:351:VAL:HB	2:C:400:ALA:HB2	1.83	0.61
1:B:115:ALA:HB3	1:I:112:THR:HG22	1.82	0.61
2:V:436:TYR:HD1	2:V:436:TYR:H	1.48	0.61
2:C:304:VAL:HG21	2:C:450:MET:HE3	1.82	0.61
1:D:179:ASP:O	1:D:183:ILE:HG12	2.01	0.61
2:N:344:GLY:HA3	3:N:120:HOH:O	2.00	0.61
1:O:68:PHE:HA	1:O:71:PHE:CE2	2.36	0.61
2:P:351:VAL:HB	2:P:400:ALA:HB2	1.83	0.61
2:R:424:ASP:HB3	2:R:428:GLY:N	2.15	0.61
2:G:464:LEU:HD12	2:G:496:ILE:HD11	1.80	0.61
1:K:110:ILE:HG23	1:K:114:GLN:HG3	1.83	0.61
1:K:189:ARG:CZ	1:K:237:GLN:HB3	2.30	0.61
1:I:182:ARG:HD3	1:I:235:VAL:HB	1.82	0.60
2:2:436:TYR:HD1	2:2:436:TYR:H	1.48	0.60
2:C:462:SER:O	2:C:465:ARG:HG2	2.01	0.60
1:O:30:VAL:HA	3:O:250:HOH:O	2.01	0.60
1:O:83:ASP:OD2	2:P:365:HIS:HD2	1.85	0.60
2:R:325:MET:HE3	3:Z:100:HOH:O	2.01	0.60
1:S:36:ALA:HB3	3:S:252:HOH:O	2.01	0.60
2:H:444:LEU:HD12	2:E:444:LEU:CD1	2.27	0.60
1:Y:189:ARG:CZ	1:Y:237:GLN:HB3	2.30	0.60
2:L:436:TYR:H	2:L:436:TYR:HD1	1.50	0.60
1:Q:68:PHE:HA	1:Q:71:PHE:CE2	2.37	0.60
2:T:436:TYR:H	2:T:436:TYR:HD1	1.49	0.60
1:Y:206:ALA:HB1	3:Y:249:HOH:O	2.02	0.60
2:R:324:ASN:H	2:R:324:ASN:HD22	1.49	0.60
2:J:324:ASN:HD22	2:J:324:ASN:H	1.49	0.60
1:O:213:LEU:HA	1:O:221:ALA:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:308:TYR:HB2	2:Z:309:PRO:HD2	1.84	0.60
2:J:449:SER:HB2	2:Z:452:LYS:NZ	2.17	0.60
1:A:48:ARG:NH2	1:B:135:ARG:HB3	2.08	0.60
2:R:351:VAL:HB	2:R:400:ALA:HB2	1.82	0.60
1:I:179:ASP:O	1:I:183:ILE:HG12	2.02	0.60
1:I:213:LEU:HA	1:I:221:ALA:O	2.02	0.60
1:A:16:ARG:HE	1:A:117:PRO:HD3	1.66	0.60
1:I:48:ARG:HH22	1:S:135:ARG:HB3	1.67	0.60
1:I:179:ASP:O	1:I:183:ILE:HG12	2.02	0.60
2:T:452:LYS:NZ	3:T:79:HOH:O	2.34	0.60
1:A:213:LEU:HA	1:A:221:ALA:O	2.02	0.59
1:I:189:ARG:CZ	1:I:237:GLN:HB3	2.32	0.59
1:K:213:LEU:HA	1:K:221:ALA:O	2.02	0.59
1:F:16:ARG:HE	1:F:117:PRO:HD3	1.67	0.59
1:S:110:ILE:HG23	1:S:114:GLN:HG3	1.83	0.59
1:A:68:PHE:HE1	1:B:101:ASN:OD1	1.83	0.59
2:C:375:THR:OG1	1:I:93:ASP:OD1	2.21	0.59
2:J:461:ASP:OD1	2:J:509:ARG:HD2	2.03	0.59
1:O:16:ARG:HE	1:O:117:PRO:HD3	1.67	0.59
1:A:28:LYS:HB2	1:A:52:LYS:NZ	2.17	0.59
2:H:436:TYR:H	2:H:436:TYR:HD1	1.50	0.59
2:P:324:ASN:HD22	2:P:324:ASN:H	1.48	0.59
1:U:68:PHE:HA	1:U:71:PHE:CE2	2.38	0.59
1:Y:205:VAL:C	1:Y:207:SER:H	2.05	0.59
1:I:28:LYS:HB2	1:I:52:LYS:NZ	2.17	0.59
1:F:213:LEU:HA	1:F:221:ALA:O	2.03	0.59
1:M:16:ARG:HE	1:M:117:PRO:HD3	1.66	0.59
2:N:436:TYR:H	2:N:436:TYR:HD1	1.49	0.59
2:P:464:LEU:HD12	2:P:496:ILE:HD11	1.85	0.59
2:V:304:VAL:HG21	2:V:450:MET:HE3	1.83	0.59
1:A:179:ASP:O	1:A:183:ILE:HG12	2.02	0.59
1:B:213:LEU:HA	1:B:221:ALA:O	2.02	0.59
2:H:444:LEU:CD1	2:E:444:LEU:HD12	2.26	0.59
1:I:56:LEU:HD13	1:I:99:LEU:CD2	2.32	0.59
2:J:351:VAL:HB	2:J:400:ALA:HB2	1.85	0.59
1:D:189:ARG:CZ	1:D:237:GLN:HB3	2.33	0.59
1:D:90:ASP:CB	3:D:249:HOH:O	2.50	0.59
1:O:182:ARG:HD3	1:O:235:VAL:HB	1.83	0.59
1:U:213:LEU:HA	1:U:221:ALA:O	2.02	0.59
1:I:110:ILE:HG23	1:I:114:GLN:HG3	1.83	0.59
2:G:436:TYR:HD1	2:G:436:TYR:H	1.51	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:324:ASN:HD22	2:H:324:ASN:H	1.50	0.59
1:D:19:LEU:HD12	1:K:10:GLU:HA	1.83	0.59
2:N:308:TYR:HB2	2:N:309:PRO:HD2	1.84	0.59
2:G:351:VAL:HB	2:G:400:ALA:HB2	1.85	0.59
2:H:329:ARG:NH2	2:L:476:ASP:O	2.34	0.59
1:I:213:LEU:HA	1:I:221:ALA:O	2.03	0.59
2:L:413:ASP:HA	3:L:73:HOH:O	2.02	0.58
1:M:28:LYS:HB2	1:M:52:LYS:NZ	2.17	0.58
2:R:308:TYR:HB2	2:R:309:PRO:HD2	1.85	0.58
2:Z:351:VAL:HB	2:Z:400:ALA:HB2	1.85	0.58
1:I:16:ARG:HE	1:I:117:PRO:HD3	1.67	0.58
1:F:112:THR:CG2	1:M:115:ALA:HB3	2.32	0.58
1:S:83:ASP:OD2	2:T:365:HIS:HD2	1.86	0.58
2:V:464:LEU:HD12	2:V:496:ILE:HD11	1.85	0.58
2:H:462:SER:O	2:H:465:ARG:HG2	2.03	0.58
2:N:449:SER:HB2	2:V:452:LYS:NZ	2.19	0.58
1:Y:213:LEU:HA	1:Y:221:ALA:O	2.04	0.58
1:D:16:ARG:HE	1:D:117:PRO:HD3	1.68	0.58
1:O:205:VAL:C	1:O:207:SER:H	2.06	0.58
1:O:93:ASP:OD1	2:V:375:THR:OG1	2.21	0.58
2:T:351:VAL:HB	2:T:400:ALA:HB2	1.85	0.58
1:B:16:ARG:HE	1:B:117:PRO:HD3	1.68	0.58
2:G:456:GLN:HE22	2:G:465:ARG:NH1	2.00	0.58
1:I:205:VAL:C	1:I:207:SER:H	2.07	0.58
2:J:375:THR:OG1	1:S:93:ASP:OD1	2.20	0.58
1:K:69:ASN:ND2	3:K:258:HOH:O	2.36	0.58
2:T:464:LEU:HD12	2:T:496:ILE:HD11	1.84	0.58
1:S:56:LEU:HD13	1:S:99:LEU:HD22	1.86	0.58
2:G:375:THR:OG1	1:W:93:ASP:OD1	2.21	0.58
1:B:28:LYS:HB2	1:B:52:LYS:NZ	2.19	0.58
2:C:382:ARG:HD3	1:I:89:TYR:HD1	1.68	0.58
1:K:179:ASP:O	1:K:183:ILE:HG12	2.03	0.58
1:K:205:VAL:C	1:K:207:SER:H	2.07	0.58
1:M:189:ARG:CZ	1:M:237:GLN:HB3	2.33	0.58
1:U:28:LYS:HB2	1:U:52:LYS:NZ	2.18	0.58
1:I:14:ARG:CB	1:I:14:ARG:HH11	2.10	0.58
1:D:182:ARG:HD3	1:D:235:VAL:HB	1.84	0.58
1:U:205:VAL:C	1:U:207:SER:H	2.05	0.58
1:W:16:ARG:HE	1:W:117:PRO:HD3	1.68	0.58
1:Y:179:ASP:O	1:Y:183:ILE:HG12	2.04	0.58
1:A:205:VAL:C	1:A:207:SER:H	2.07	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:464:LEU:HD12	2:L:496:ILE:HD11	1.85	0.58
1:Q:179:ASP:O	1:Q:183:ILE:HG12	2.03	0.58
1:Q:205:VAL:C	1:Q:207:SER:H	2.07	0.58
2:J:364:GLU:HG2	2:J:368:LYS:HE2	1.86	0.57
1:W:205:VAL:C	1:W:207:SER:H	2.06	0.57
1:F:28:LYS:HB2	1:F:52:LYS:NZ	2.19	0.57
2:G:341:THR:CG2	2:G:404:LEU:HD11	2.34	0.57
2:2:351:VAL:HB	2:2:400:ALA:HB2	1.86	0.57
1:B:68:PHE:HA	1:B:71:PHE:CE2	2.39	0.57
2:E:424:ASP:HB3	2:E:428:GLY:N	2.17	0.57
1:Q:30:VAL:HG22	1:Q:43:ALA:HB1	1.86	0.57
2:C:461:ASP:OD1	2:C:509:ARG:HD2	2.04	0.57
1:M:127:VAL:CG2	1:M:215:ALA:HB2	2.35	0.57
1:Y:110:ILE:HG23	1:Y:114:GLN:HG3	1.85	0.57
1:Y:28:LYS:HB2	1:Y:52:LYS:NZ	2.19	0.57
1:A:30:VAL:HG22	1:A:43:ALA:CB	2.34	0.57
2:E:436:TYR:HD1	2:E:436:TYR:H	1.50	0.57
1:O:28:LYS:HB2	1:O:52:LYS:NZ	2.20	0.57
1:W:28:LYS:HB2	1:W:52:LYS:NZ	2.18	0.57
1:D:128:ALA:HB2	1:D:134:LYS:HB3	1.87	0.57
2:L:395:MET:HA	2:L:395:MET:CE	2.34	0.57
2:L:449:SER:HB2	2:P:452:LYS:HZ1	1.69	0.57
1:B:179:ASP:O	1:B:183:ILE:HG12	2.04	0.57
1:F:205:VAL:C	1:F:207:SER:H	2.08	0.57
1:F:89:TYR:CD1	2:N:382:ARG:HD3	2.39	0.57
2:N:351:VAL:HB	2:N:400:ALA:HB2	1.85	0.57
2:T:341:THR:CG2	2:T:404:LEU:HD11	2.34	0.57
1:D:205:VAL:C	1:D:207:SER:H	2.08	0.57
2:E:351:VAL:HB	2:E:400:ALA:HB2	1.85	0.57
2:J:341:THR:CG2	2:J:404:LEU:HD11	2.34	0.57
1:U:179:ASP:O	1:U:183:ILE:HG12	2.04	0.57
2:X:351:VAL:HB	2:X:400:ALA:HB2	1.87	0.57
2:G:424:ASP:HB3	2:G:428:GLY:N	2.19	0.57
1:Q:28:LYS:HB2	1:Q:52:LYS:NZ	2.20	0.57
1:S:179:ASP:O	1:S:183:ILE:HG12	2.04	0.57
2:C:436:TYR:H	2:C:436:TYR:HD1	1.51	0.57
1:I:68:PHE:HA	1:I:71:PHE:CE2	2.40	0.57
1:S:68:PHE:HA	1:S:71:PHE:CE2	2.40	0.57
2:G:341:THR:HG22	2:G:404:LEU:HD11	1.87	0.56
2:R:341:THR:CG2	2:R:404:LEU:HD11	2.35	0.56
1:S:205:VAL:C	1:S:207:SER:H	2.08	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:395:MET:HA	2:2:395:MET:CE	2.35	0.56
1:I:9:PRO:HD3	3:I:249:HOH:O	2.05	0.56
2:L:341:THR:CG2	2:L:404:LEU:HD11	2.35	0.56
1:O:179:ASP:O	1:O:183:ILE:HG12	2.05	0.56
1:F:115:ALA:HB3	1:W:112:THR:HG22	1.86	0.56
2:J:424:ASP:HB3	2:J:428:GLY:N	2.19	0.56
2:N:364:GLU:HG2	2:N:368:LYS:HE2	1.88	0.56
2:T:452:LYS:HG2	3:T:79:HOH:O	2.04	0.56
1:I:205:VAL:C	1:I:207:SER:H	2.08	0.56
1:D:56:LEU:HD13	1:D:99:LEU:CD2	2.35	0.56
2:G:465:ARG:HG3	2:G:466:VAL:N	2.20	0.56
1:K:56:LEU:HD13	1:K:99:LEU:CD2	2.34	0.56
2:L:324:ASN:HD22	2:L:324:ASN:H	1.53	0.56
1:U:30:VAL:HG22	1:U:43:ALA:HB1	1.87	0.56
2:Z:464:LEU:HD12	2:Z:496:ILE:HD11	1.86	0.56
2:H:366:TYR:OH	1:B:93:ASP:HB3	2.06	0.56
2:L:341:THR:HG22	2:L:404:LEU:HD11	1.86	0.56
1:M:30:VAL:HG13	1:M:43:ALA:HB2	1.88	0.56
1:D:48:ARG:HD2	1:K:137:GLU:OE2	2.06	0.56
1:M:205:VAL:C	1:M:207:SER:H	2.08	0.56
1:M:213:LEU:HA	1:M:221:ALA:O	2.05	0.56
1:I:25:ALA:O	1:I:158:GLY:HA2	2.05	0.56
1:K:73:ASN:HD22	1:M:105:GLN:CD	2.09	0.56
1:A:128:ALA:HB2	1:A:134:LYS:HB3	1.88	0.56
1:B:205:VAL:C	1:B:207:SER:H	2.09	0.56
1:D:68:PHE:HA	1:D:71:PHE:CE2	2.40	0.56
2:H:351:VAL:HB	2:H:400:ALA:HB2	1.88	0.56
2:H:424:ASP:HB3	2:H:428:GLY:N	2.21	0.56
2:L:464:LEU:HD11	2:L:505:VAL:HG11	1.87	0.56
1:O:14:ARG:HH11	1:O:14:ARG:CB	2.12	0.56
2:H:461:ASP:OD1	2:H:509:ARG:HD2	2.05	0.56
1:D:22:LYS:HD2	1:K:10:GLU:OE2	2.06	0.56
2:T:449:SER:HB2	2:X:452:LYS:NZ	2.20	0.56
2:V:324:ASN:H	2:V:324:ASN:HD22	1.52	0.56
1:I:30:VAL:HG13	1:I:43:ALA:HB2	1.88	0.56
2:L:456:GLN:HE22	2:L:465:ARG:NH1	2.04	0.56
2:P:395:MET:HA	2:P:395:MET:CE	2.35	0.56
1:I:68:PHE:HA	1:I:71:PHE:CE2	2.40	0.56
2:2:324:ASN:HD22	2:2:324:ASN:H	1.54	0.56
2:H:464:LEU:HD12	2:H:496:ILE:HD11	1.88	0.56
2:L:364:GLU:HG2	2:L:368:LYS:HE2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:68:PHE:HA	1:M:71:PHE:CE2	2.41	0.56
2:P:436:TYR:HD1	2:P:436:TYR:H	1.52	0.56
2:T:424:ASP:HB3	2:T:428:GLY:N	2.20	0.56
1:1:155:VAL:HG12	1:1:160:THR:HG22	1.87	0.55
2:H:337:THR:HG21	2:H:359:TYR:CD2	2.41	0.55
2:P:424:ASP:HB3	2:P:428:GLY:N	2.19	0.55
2:Z:424:ASP:HB3	2:Z:428:GLY:N	2.18	0.55
2:2:341:THR:CG2	2:2:404:LEU:HD11	2.35	0.55
2:V:424:ASP:HB3	2:V:428:GLY:N	2.20	0.55
2:X:436:TYR:H	2:X:436:TYR:HD1	1.52	0.55
2:X:456:GLN:HE22	2:X:465:ARG:NH1	2.04	0.55
1:Y:25:ALA:O	1:Y:158:GLY:HA2	2.06	0.55
2:Z:456:GLN:HE22	2:Z:465:ARG:NH1	2.04	0.55
2:R:341:THR:HG22	2:R:404:LEU:HD11	1.86	0.55
2:T:341:THR:HG22	2:T:404:LEU:HD11	1.88	0.55
1:A:185:VAL:HB	1:A:235:VAL:HG11	1.88	0.55
1:O:42:VAL:HG22	1:O:210:VAL:HG22	1.88	0.55
1:O:25:ALA:O	1:O:158:GLY:HA2	2.06	0.55
1:U:110:ILE:HG23	1:U:114:GLN:HG3	1.89	0.55
1:S:30:VAL:HG22	1:S:43:ALA:HB1	1.88	0.55
2:Z:301:THR:HA	2:Z:333:LYS:NZ	2.21	0.55
2:2:392:ALA:HB3	3:2:136:HOH:O	2.07	0.55
1:A:56:LEU:HD13	1:A:99:LEU:CD2	2.37	0.55
1:Q:213:LEU:HA	1:Q:221:ALA:O	2.06	0.55
1:Q:56:LEU:HD13	1:Q:99:LEU:HD22	1.88	0.55
2:T:395:MET:CE	2:T:395:MET:HA	2.37	0.55
1:U:56:LEU:HD13	1:U:99:LEU:CD2	2.37	0.55
1:1:128:ALA:HB2	1:1:134:LYS:HB3	1.88	0.55
2:C:324:ASN:HD22	2:C:324:ASN:H	1.54	0.55
2:H:341:THR:CG2	2:H:404:LEU:HD11	2.36	0.55
2:L:351:VAL:HB	2:L:400:ALA:HB2	1.87	0.55
1:1:206:ALA:CB	3:1:258:HOH:O	2.51	0.55
1:A:19:LEU:HD12	1:B:10:GLU:HA	1.89	0.55
1:I:226:THR:O	1:I:230:LEU:HB2	2.06	0.55
2:J:513:LEU:O	2:J:517:ILE:HG12	2.07	0.55
1:K:83:ASP:OD2	2:L:365:HIS:HD2	1.90	0.55
1:A:68:PHE:HA	1:A:71:PHE:CE2	2.42	0.55
2:E:341:THR:HG22	2:E:404:LEU:HD11	1.88	0.55
2:E:317:ASP:OD1	2:E:333:LYS:NZ	2.39	0.55
2:H:456:GLN:HE22	2:H:465:ARG:NH1	2.05	0.55
2:L:424:ASP:HB3	2:L:428:GLY:N	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:344:GLY:CA	3:N:120:HOH:O	2.52	0.55
2:N:395:MET:HA	2:N:395:MET:CE	2.37	0.55
1:W:213:LEU:HA	1:W:221:ALA:O	2.07	0.55
1:F:56:LEU:HD13	1:F:99:LEU:CD2	2.37	0.54
2:G:364:GLU:HG2	2:G:368:LYS:HE2	1.87	0.54
1:S:25:ALA:O	1:S:158:GLY:HA2	2.07	0.54
2:Z:324:ASN:H	2:Z:324:ASN:HD22	1.55	0.54
1:B:127:VAL:CG2	1:B:215:ALA:HB2	2.36	0.54
2:C:452:LYS:NZ	2:R:449:SER:HB2	2.21	0.54
1:F:135:ARG:HB3	1:M:48:ARG:NH2	2.21	0.54
2:N:513:LEU:O	2:N:517:ILE:HG12	2.07	0.54
1:Q:93:ASP:OD1	2:Z:375:THR:OG1	2.24	0.54
1:B:56:LEU:HD13	1:B:99:LEU:CD2	2.37	0.54
2:C:395:MET:HA	2:C:395:MET:CE	2.38	0.54
2:E:456:GLN:HE22	2:E:465:ARG:NH1	2.05	0.54
1:F:42:VAL:HG22	1:F:210:VAL:HG22	1.90	0.54
1:F:25:ALA:O	1:F:158:GLY:HA2	2.07	0.54
1:K:128:ALA:HB2	1:K:134:LYS:HB3	1.90	0.54
2:R:513:LEU:O	2:R:517:ILE:HG12	2.07	0.54
2:X:395:MET:HA	2:X:395:MET:CE	2.38	0.54
1:U:42:VAL:HG22	1:U:210:VAL:HG22	1.90	0.54
1:W:56:LEU:HD13	1:W:99:LEU:CD2	2.36	0.54
2:X:301:THR:HA	2:X:333:LYS:NZ	2.21	0.54
1:I:127:VAL:CG2	1:I:215:ALA:HB2	2.38	0.54
1:F:48:ARG:HH22	1:W:135:ARG:HB3	1.73	0.54
1:F:68:PHE:HA	1:F:71:PHE:CE2	2.42	0.54
2:H:513:LEU:O	2:H:517:ILE:HG12	2.07	0.54
1:I:14:ARG:HH11	1:I:14:ARG:CB	2.14	0.54
2:J:341:THR:HG22	2:J:404:LEU:HD11	1.88	0.54
2:R:509:ARG:CG	3:R:112:HOH:O	2.43	0.54
1:Y:155:VAL:HG12	1:Y:160:THR:HG22	1.89	0.54
1:A:185:VAL:HB	1:A:235:VAL:CG1	2.38	0.54
1:I:76:ARG:NH1	2:J:369:LEU:HD22	2.22	0.54
1:W:68:PHE:HA	1:W:71:PHE:CE2	2.43	0.54
1:I:205:VAL:HG12	1:I:206:ALA:N	2.23	0.54
1:I:56:LEU:HD13	1:I:99:LEU:CD2	2.38	0.54
1:D:63:ALA:O	1:D:156:MET:HE1	2.07	0.54
1:I:20:ALA:O	1:I:24:ILE:HG12	2.08	0.54
1:I:30:VAL:HG22	1:I:43:ALA:HB1	1.89	0.54
1:M:128:ALA:HB2	1:M:134:LYS:HB3	1.88	0.54
1:M:30:VAL:HG22	1:M:43:ALA:HB1	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:128:ALA:HB2	1:O:134:LYS:HB3	1.89	0.54
1:D:185:VAL:HB	1:D:235:VAL:CG1	2.38	0.54
1:M:76:ARG:HG2	2:N:369:LEU:HD22	1.90	0.54
2:N:476:ASP:O	2:P:329:ARG:NH2	2.41	0.54
2:Z:464:LEU:HD11	2:Z:505:VAL:HG11	1.90	0.54
2:E:341:THR:CG2	2:E:404:LEU:HD11	2.37	0.54
1:F:30:VAL:HG22	1:F:43:ALA:HB1	1.89	0.54
1:K:76:ARG:NH2	2:L:370:GLU:OE2	2.36	0.54
1:1:42:VAL:HG22	1:1:210:VAL:HG22	1.90	0.54
2:2:381:ASN:HA	3:2:75:HOH:O	2.08	0.54
2:G:395:MET:HA	2:G:395:MET:CE	2.37	0.54
1:I:19:LEU:HD12	1:S:10:GLU:HA	1.90	0.54
1:K:127:VAL:CG2	1:K:215:ALA:HB2	2.38	0.54
1:M:205:VAL:HG12	1:M:206:ALA:N	2.23	0.54
2:N:424:ASP:HB3	2:N:428:GLY:N	2.22	0.54
2:V:395:MET:HA	2:V:395:MET:CE	2.38	0.54
1:D:30:VAL:HG22	1:D:43:ALA:HB1	1.89	0.53
2:E:324:ASN:H	2:E:324:ASN:HD22	1.55	0.53
1:U:127:VAL:CG2	1:U:215:ALA:HB2	2.38	0.53
1:W:140:ARG:HB3	1:W:140:ARG:HH11	1.73	0.53
2:X:424:ASP:HB3	2:X:428:GLY:N	2.21	0.53
1:Y:85:ARG:HG2	1:Y:85:ARG:NH1	2.22	0.53
1:D:213:LEU:HA	1:D:221:ALA:O	2.08	0.53
1:F:128:ALA:HB2	1:F:134:LYS:HB3	1.89	0.53
2:H:364:GLU:HG2	2:H:368:LYS:HE2	1.90	0.53
1:S:185:VAL:HB	1:S:235:VAL:CG1	2.38	0.53
1:I:48:ARG:HA	3:I:250:HOH:O	2.08	0.53
1:K:42:VAL:HG22	1:K:210:VAL:HG22	1.90	0.53
1:M:42:VAL:HG22	1:M:210:VAL:HG22	1.90	0.53
2:T:464:LEU:HD11	2:T:505:VAL:HG11	1.89	0.53
1:D:127:VAL:CG2	1:D:215:ALA:HB2	2.38	0.53
2:G:513:LEU:O	2:G:517:ILE:HG12	2.09	0.53
1:M:226:THR:O	1:M:230:LEU:HB2	2.09	0.53
2:P:341:THR:CG2	2:P:404:LEU:HD11	2.38	0.53
2:R:456:GLN:HE22	2:R:465:ARG:NH1	2.06	0.53
1:S:30:VAL:HG13	1:S:43:ALA:HB2	1.89	0.53
1:U:25:ALA:O	1:U:158:GLY:HA2	2.09	0.53
1:W:230:LEU:HD13	3:W:250:HOH:O	2.07	0.53
2:Z:395:MET:HA	2:Z:395:MET:CE	2.39	0.53
2:E:395:MET:CE	2:E:395:MET:HA	2.39	0.53
1:A:83:ASP:OD2	2:H:365:HIS:HD2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:115:ALA:HB3	1:K:112:THR:HG22	1.90	0.53
2:R:464:LEU:HD11	2:R:505:VAL:HG11	1.89	0.53
1:W:25:ALA:O	1:W:158:GLY:HA2	2.09	0.53
1:F:185:VAL:HB	1:F:235:VAL:CG1	2.39	0.53
2:H:341:THR:HG22	2:H:404:LEU:HD11	1.90	0.53
1:I:128:ALA:HB2	1:I:134:LYS:HB3	1.90	0.53
2:J:395:MET:HA	2:J:395:MET:CE	2.39	0.53
2:L:513:LEU:O	2:L:517:ILE:HG12	2.08	0.53
1:M:56:LEU:HD13	1:M:99:LEU:HD22	1.89	0.53
1:O:20:ALA:O	1:O:24:ILE:HG12	2.08	0.53
2:V:301:THR:HA	2:V:333:LYS:NZ	2.24	0.53
1:Y:68:PHE:HA	1:Y:71:PHE:CE2	2.43	0.53
1:B:25:ALA:O	1:B:158:GLY:HA2	2.09	0.53
1:B:185:VAL:HB	1:B:235:VAL:CG1	2.39	0.53
1:B:30:VAL:HG22	1:B:43:ALA:HB1	1.91	0.53
1:K:68:PHE:HA	1:K:71:PHE:CE2	2.44	0.53
1:W:30:VAL:HG22	1:W:43:ALA:HB1	1.90	0.53
1:M:14:ARG:HH11	1:M:14:ARG:CB	2.13	0.53
2:P:317:ASP:OD1	2:P:333:LYS:NZ	2.41	0.53
2:P:513:LEU:O	2:P:517:ILE:HG12	2.09	0.53
2:T:301:THR:HA	2:T:333:LYS:HZ3	1.74	0.53
2:T:456:GLN:HE22	2:T:465:ARG:NH1	2.06	0.53
1:D:185:VAL:HB	1:D:235:VAL:HG11	1.91	0.53
1:I:56:LEU:HD13	1:I:99:LEU:HD22	1.91	0.53
1:Q:128:ALA:HB2	1:Q:134:LYS:HB3	1.91	0.53
2:T:461:ASP:OD1	2:T:509:ARG:HD2	2.09	0.53
2:X:461:ASP:OD1	2:X:509:ARG:HD2	2.09	0.53
1:Q:89:TYR:HD1	2:Z:382:ARG:HD3	1.74	0.53
1:B:42:VAL:HG22	1:B:210:VAL:HG22	1.91	0.53
1:F:63:ALA:O	1:F:156:MET:HE1	2.09	0.53
1:I:127:VAL:CG2	1:I:215:ALA:HB2	2.39	0.53
1:M:127:VAL:HG21	1:M:215:ALA:HB2	1.91	0.53
2:L:452:LYS:NZ	2:P:449:SER:HB2	2.24	0.53
2:R:461:ASP:OD1	2:R:509:ARG:HD2	2.09	0.53
2:T:449:SER:HB2	2:X:452:LYS:HZ1	1.74	0.53
2:2:341:THR:HG22	2:2:404:LEU:HD11	1.90	0.52
2:2:424:ASP:HB3	2:2:428:GLY:N	2.24	0.52
1:B:30:VAL:HG13	1:B:43:ALA:HB2	1.91	0.52
1:I:140:ARG:HH11	1:I:140:ARG:HB3	1.73	0.52
2:N:324:ASN:H	2:N:324:ASN:ND2	2.06	0.52
1:O:161:GLU:H	1:O:161:GLU:CD	2.13	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:37:GLY:HA3	3:O:256:HOH:O	2.09	0.52
1:I:48:ARG:HH22	1:S:135:ARG:CB	2.22	0.52
2:Z:341:THR:HG22	2:Z:404:LEU:HD11	1.91	0.52
2:Z:364:GLU:HG2	2:Z:368:LYS:HE2	1.90	0.52
1:B:140:ARG:HB3	1:B:140:ARG:HH11	1.74	0.52
1:F:226:THR:O	1:F:230:LEU:HB2	2.08	0.52
1:K:25:ALA:O	1:K:158:GLY:HA2	2.09	0.52
1:O:30:VAL:HG22	1:O:43:ALA:HB1	1.92	0.52
2:G:452:LYS:NZ	2:2:449:SER:HB2	2.24	0.52
2:C:424:ASP:HB3	2:C:428:GLY:N	2.22	0.52
1:D:141:ILE:N	1:D:141:ILE:HD12	2.24	0.52
1:F:20:ALA:O	1:F:24:ILE:HG12	2.09	0.52
1:Q:155:VAL:HG12	1:Q:160:THR:HG22	1.91	0.52
1:Q:185:VAL:HB	1:Q:235:VAL:CG1	2.39	0.52
1:U:14:ARG:CB	1:U:14:ARG:HH11	2.10	0.52
2:V:364:GLU:HG2	2:V:368:LYS:HE2	1.92	0.52
1:Y:14:ARG:HH11	1:Y:14:ARG:CB	2.13	0.52
2:2:364:GLU:HG2	2:2:368:LYS:HE2	1.91	0.52
1:O:85:ARG:NH1	1:O:85:ARG:HG2	2.22	0.52
2:X:513:LEU:O	2:X:517:ILE:HG12	2.10	0.52
1:I:141:ILE:HD12	1:I:141:ILE:N	2.25	0.52
1:K:226:THR:O	1:K:230:LEU:HB2	2.09	0.52
1:M:54:SER:CB	1:M:75:ARG:HD2	2.40	0.52
1:A:89:TYR:CD1	2:P:382:ARG:HD3	2.44	0.52
1:U:205:VAL:HG12	1:U:206:ALA:N	2.25	0.52
2:V:341:THR:CG2	2:V:404:LEU:HD11	2.40	0.52
2:X:341:THR:CG2	2:X:404:LEU:HD11	2.40	0.52
1:F:14:ARG:HH11	1:F:14:ARG:CB	2.14	0.52
1:F:185:VAL:HB	1:F:235:VAL:HG11	1.91	0.52
2:G:449:SER:HB2	2:2:452:LYS:HZ3	1.73	0.52
1:I:25:ALA:O	1:I:158:GLY:HA2	2.10	0.52
2:L:447:LYS:NZ	3:L:61:HOH:O	2.43	0.52
1:S:185:VAL:HB	1:S:235:VAL:HG11	1.90	0.52
1:W:22:LYS:HD2	1:Y:10:GLU:OE2	2.09	0.52
1:1:231:GLN:HG2	3:1:258:HOH:O	2.10	0.52
2:E:464:LEU:HD12	2:E:496:ILE:HD11	1.92	0.52
1:O:56:LEU:HD13	1:O:99:LEU:HD22	1.90	0.52
1:Q:14:ARG:HH11	1:Q:14:ARG:CB	2.15	0.52
1:Q:127:VAL:CG2	1:Q:215:ALA:HB2	2.40	0.52
2:Z:513:LEU:O	2:Z:517:ILE:HG12	2.10	0.52
2:2:455:SER:HB3	3:2:159:HOH:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:464:LEU:HD11	2:2:505:VAL:HG11	1.92	0.52
1:A:205:VAL:HG12	1:A:206:ALA:N	2.24	0.52
1:A:205:VAL:HG12	1:A:206:ALA:H	1.75	0.52
1:A:20:ALA:O	1:A:24:ILE:HG12	2.09	0.52
2:V:464:LEU:HD11	2:V:505:VAL:HG11	1.92	0.52
1:Y:127:VAL:CG2	1:Y:215:ALA:HB2	2.40	0.52
1:1:30:VAL:HG22	1:1:43:ALA:HB1	1.92	0.52
1:A:30:VAL:HG13	1:A:43:ALA:HB2	1.91	0.52
1:B:73:ASN:HD22	1:I:105:GLN:CD	2.13	0.52
2:N:464:LEU:HD11	2:N:505:VAL:HG11	1.92	0.52
1:U:155:VAL:HG12	1:U:160:THR:HG22	1.92	0.52
2:X:321:THR:HG21	2:X:480:ALA:HB1	1.92	0.52
2:C:341:THR:HG22	2:C:404:LEU:HD11	1.91	0.52
1:Q:205:VAL:HG12	1:Q:206:ALA:N	2.25	0.52
1:Q:42:VAL:HG22	1:Q:210:VAL:HG22	1.91	0.52
2:R:337:THR:HG21	2:R:359:TYR:CD2	2.45	0.52
1:S:128:ALA:HB2	1:S:134:LYS:HB3	1.91	0.52
2:T:324:ASN:HD22	2:T:324:ASN:H	1.57	0.52
1:U:20:ALA:O	1:U:24:ILE:HG12	2.10	0.52
1:Y:30:VAL:HG22	1:Y:43:ALA:HB1	1.90	0.52
2:2:307:LYS:N	3:2:14:HOH:O	2.21	0.51
1:A:25:ALA:O	1:A:158:GLY:HA2	2.10	0.51
1:O:30:VAL:HG13	1:O:43:ALA:HB2	1.92	0.51
2:P:324:ASN:N	2:P:324:ASN:HD22	2.06	0.51
2:T:513:LEU:O	2:T:517:ILE:HG12	2.09	0.51
1:Y:128:ALA:HB2	1:Y:134:LYS:HB3	1.90	0.51
1:A:42:VAL:HG22	1:A:210:VAL:HG22	1.92	0.51
2:H:324:ASN:HD22	2:H:324:ASN:N	2.07	0.51
1:I:42:VAL:HG22	1:I:210:VAL:HG22	1.92	0.51
1:1:161:GLU:CD	1:1:161:GLU:H	2.14	0.51
1:1:185:VAL:HB	1:1:235:VAL:CG1	2.40	0.51
1:A:141:ILE:N	1:A:141:ILE:HD12	2.25	0.51
1:B:226:THR:O	1:B:230:LEU:HB2	2.09	0.51
2:C:301:THR:HA	2:C:333:LYS:NZ	2.25	0.51
2:J:301:THR:HA	2:J:333:LYS:NZ	2.25	0.51
1:K:30:VAL:HG22	1:K:43:ALA:HB1	1.91	0.51
2:R:307:LYS:HE2	2:R:435:GLY:HA2	1.92	0.51
1:U:140:ARG:HB3	1:U:140:ARG:HH11	1.75	0.51
2:Z:461:ASP:OD1	2:Z:509:ARG:HD2	2.09	0.51
2:C:364:GLU:HG2	2:C:368:LYS:HE2	1.93	0.51
2:C:456:GLN:HE22	2:C:465:ARG:NH1	2.08	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:452:LYS:HZ1	2:E:449:SER:HB2	1.74	0.51
2:H:301:THR:N	2:H:441:SER:HG	2.09	0.51
2:L:461:ASP:OD1	2:L:509:ARG:HD2	2.10	0.51
1:O:205:VAL:HG12	1:O:206:ALA:N	2.25	0.51
2:V:513:LEU:O	2:V:517:ILE:HG12	2.10	0.51
1:W:128:ALA:HB2	1:W:134:LYS:HB3	1.93	0.51
1:W:161:GLU:H	1:W:161:GLU:CD	2.13	0.51
1:W:226:THR:O	1:W:230:LEU:HB2	2.10	0.51
1:1:141:ILE:HD12	1:1:141:ILE:N	2.26	0.51
1:1:226:THR:O	1:1:230:LEU:HB2	2.10	0.51
1:B:30:VAL:CG2	1:B:65:ALA:HB2	2.41	0.51
1:Q:226:THR:O	1:Q:230:LEU:HB2	2.10	0.51
2:G:464:LEU:HD11	2:G:505:VAL:HG11	1.93	0.51
1:K:91:ARG:HG3	3:K:257:HOH:O	2.10	0.51
1:Y:161:GLU:CD	1:Y:161:GLU:H	2.14	0.51
2:2:513:LEU:O	2:2:517:ILE:HG12	2.11	0.51
1:B:185:VAL:HB	1:B:235:VAL:HG11	1.92	0.51
1:D:42:VAL:HG22	1:D:210:VAL:HG22	1.93	0.51
1:O:112:THR:HG22	1:U:115:ALA:HB3	1.93	0.51
2:C:452:LYS:HZ1	2:R:449:SER:HB2	1.75	0.51
2:X:324:ASN:H	2:X:324:ASN:HD22	1.58	0.51
1:A:127:VAL:CG2	1:A:215:ALA:HB2	2.40	0.51
2:H:395:MET:HA	2:H:395:MET:CE	2.41	0.51
2:N:341:THR:HG22	2:N:404:LEU:HD11	1.92	0.51
1:O:185:VAL:HB	1:O:235:VAL:CG1	2.41	0.51
1:Y:56:LEU:HD13	1:Y:99:LEU:CD2	2.40	0.51
1:1:185:VAL:HB	1:1:235:VAL:HG11	1.93	0.51
1:B:155:VAL:HG12	1:B:160:THR:HG22	1.93	0.51
1:O:127:VAL:CG2	1:O:215:ALA:HB2	2.40	0.51
1:Q:140:ARG:HH11	1:Q:140:ARG:HB3	1.76	0.51
1:Q:25:ALA:O	1:Q:158:GLY:HA2	2.11	0.51
2:R:324:ASN:HD22	2:R:324:ASN:N	2.08	0.51
1:1:20:ALA:O	1:1:24:ILE:HG12	2.10	0.51
1:B:127:VAL:HG21	1:B:215:ALA:HB2	1.93	0.51
2:C:513:LEU:O	2:C:517:ILE:HG12	2.11	0.51
2:H:321:THR:HG21	2:H:480:ALA:HB1	1.93	0.51
1:I:30:VAL:CG2	1:I:65:ALA:HB2	2.40	0.51
1:M:20:ALA:O	1:M:24:ILE:HG12	2.11	0.51
1:S:226:THR:O	1:S:230:LEU:HB2	2.11	0.51
1:S:30:VAL:CG2	1:S:65:ALA:HB2	2.40	0.51
2:V:341:THR:HG22	2:V:404:LEU:HD11	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:127:VAL:CG2	1:W:215:ALA:HB2	2.41	0.50
2:2:317:ASP:OD1	2:2:333:LYS:NZ	2.38	0.50
1:F:30:VAL:HG13	1:F:43:ALA:HB2	1.93	0.50
1:I:127:VAL:HG21	1:I:215:ALA:HB2	1.92	0.50
1:Q:63:ALA:O	1:Q:156:MET:HE1	2.12	0.50
1:Q:185:VAL:HB	1:Q:235:VAL:HG11	1.93	0.50
2:R:301:THR:HA	2:R:333:LYS:NZ	2.26	0.50
2:V:456:GLN:HE22	2:V:465:ARG:NH1	2.09	0.50
1:B:54:SER:CB	1:B:75:ARG:HD2	2.42	0.50
1:S:42:VAL:HG22	1:S:210:VAL:HG22	1.92	0.50
1:W:185:VAL:HB	1:W:235:VAL:CG1	2.42	0.50
1:Y:226:THR:O	1:Y:230:LEU:HB2	2.10	0.50
1:B:128:ALA:HB2	1:B:134:LYS:HB3	1.92	0.50
2:C:464:LEU:HD11	2:C:505:VAL:HG11	1.94	0.50
2:E:517:ILE:HA	3:E:38:HOH:O	2.11	0.50
2:G:461:ASP:OD1	2:G:509:ARG:HD2	2.11	0.50
1:I:115:ALA:HB3	1:S:112:THR:CG2	2.42	0.50
1:O:155:VAL:HG12	1:O:160:THR:HG22	1.93	0.50
2:R:395:MET:CE	2:R:395:MET:HA	2.42	0.50
1:W:205:VAL:HG12	1:W:206:ALA:N	2.26	0.50
1:A:182:ARG:HD3	1:A:235:VAL:CB	2.40	0.50
2:E:464:LEU:HD11	2:E:505:VAL:HG11	1.94	0.50
2:G:301:THR:HA	2:G:333:LYS:NZ	2.26	0.50
2:G:309:PRO:HG3	2:G:458:THR:O	2.12	0.50
1:K:185:VAL:HB	1:K:235:VAL:CG1	2.41	0.50
1:K:30:VAL:HG13	1:K:43:ALA:HB2	1.93	0.50
1:M:25:ALA:O	1:M:158:GLY:HA2	2.12	0.50
1:S:161:GLU:CD	1:S:161:GLU:H	2.15	0.50
1:W:19:LEU:HD12	1:Y:10:GLU:CA	2.42	0.50
2:N:309:PRO:HG3	2:N:458:THR:O	2.12	0.50
1:U:128:ALA:HB2	1:U:134:LYS:HB3	1.93	0.50
1:W:127:VAL:HG21	1:W:215:ALA:HB2	1.94	0.50
1:D:25:ALA:O	1:D:158:GLY:HA2	2.11	0.50
2:E:513:LEU:O	2:E:517:ILE:HG12	2.10	0.50
2:J:309:PRO:HG3	2:J:458:THR:O	2.12	0.50
1:K:161:GLU:H	1:K:161:GLU:CD	2.15	0.50
1:U:85:ARG:NH1	1:U:85:ARG:HG2	2.26	0.50
1:W:141:ILE:HD12	1:W:141:ILE:N	2.26	0.50
2:H:301:THR:HA	2:H:333:LYS:NZ	2.27	0.50
2:H:309:PRO:HG3	2:H:458:THR:O	2.11	0.50
1:K:48:ARG:HH22	1:M:135:ARG:CB	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:341:THR:CG2	2:N:404:LEU:HD11	2.42	0.50
1:O:226:THR:O	1:O:230:LEU:HB2	2.11	0.50
1:U:30:VAL:HG13	1:U:43:ALA:HB2	1.92	0.50
2:V:317:ASP:OD1	2:V:333:LYS:NZ	2.45	0.50
1:A:127:VAL:HG21	1:A:215:ALA:HB2	1.94	0.50
1:B:14:ARG:CB	1:B:14:ARG:HH11	2.13	0.50
1:D:127:VAL:HG21	1:D:215:ALA:HB2	1.94	0.50
1:I:182:ARG:HB2	1:I:182:ARG:NH1	2.26	0.50
1:K:127:VAL:HG11	1:K:213:LEU:HB3	1.93	0.50
2:T:307:LYS:HE2	2:T:435:GLY:HA2	1.94	0.50
1:1:70:GLU:HB3	1:1:118:TYR:CD2	2.47	0.49
1:1:56:LEU:HD13	1:1:99:LEU:HD22	1.94	0.49
1:A:226:THR:O	1:A:230:LEU:HB2	2.12	0.49
2:E:301:THR:HA	2:E:333:LYS:NZ	2.27	0.49
2:L:432:GLU:HG3	2:L:437:GLN:HB2	1.94	0.49
1:M:155:VAL:HG12	1:M:160:THR:HG22	1.94	0.49
2:P:364:GLU:HG2	2:P:368:LYS:HE2	1.93	0.49
1:U:127:VAL:HG21	1:U:215:ALA:HB2	1.94	0.49
1:W:155:VAL:HG12	1:W:160:THR:HG22	1.94	0.49
1:A:63:ALA:O	1:A:156:MET:HE1	2.12	0.49
1:D:161:GLU:H	1:D:161:GLU:CD	2.15	0.49
1:K:30:VAL:CG2	1:K:65:ALA:HB2	2.42	0.49
2:P:324:ASN:ND2	2:P:324:ASN:H	2.10	0.49
2:R:437:GLN:OE1	2:R:447:LYS:HD3	2.12	0.49
2:V:461:ASP:OD1	2:V:509:ARG:HD2	2.13	0.49
1:Y:185:VAL:HB	1:Y:235:VAL:CG1	2.42	0.49
2:Z:341:THR:CG2	2:Z:404:LEU:HD11	2.42	0.49
1:B:161:GLU:H	1:B:161:GLU:CD	2.15	0.49
2:C:380:ILE:HD11	2:C:421:VAL:HG21	1.94	0.49
1:F:85:ARG:NH1	1:F:85:ARG:HG2	2.24	0.49
2:P:341:THR:HG22	2:P:404:LEU:HD11	1.93	0.49
1:1:127:VAL:HG21	1:1:215:ALA:HB2	1.94	0.49
2:C:309:PRO:HG3	2:C:458:THR:O	2.11	0.49
2:C:341:THR:CG2	2:C:404:LEU:HD11	2.41	0.49
1:D:140:ARG:HH11	1:D:140:ARG:HB3	1.76	0.49
1:M:161:GLU:CD	1:M:161:GLU:H	2.14	0.49
1:S:140:ARG:HH11	1:S:140:ARG:HB3	1.76	0.49
2:X:301:THR:HA	2:X:333:LYS:HZ3	1.77	0.49
1:Y:76:ARG:NH1	2:Z:369:LEU:HD22	2.27	0.49
2:Z:309:PRO:HG3	2:Z:458:THR:O	2.12	0.49
2:C:301:THR:HA	2:C:333:LYS:HZ3	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:309:PRO:HG3	2:P:458:THR:O	2.12	0.49
1:Q:30:VAL:HG13	1:Q:43:ALA:HB2	1.93	0.49
1:S:147:ILE:HG22	3:S:251:HOH:O	2.12	0.49
1:U:226:THR:O	1:U:230:LEU:HB2	2.12	0.49
1:W:14:ARG:CB	1:W:14:ARG:HH11	2.14	0.49
1:B:20:ALA:O	1:B:24:ILE:HG12	2.12	0.49
1:D:56:LEU:HD13	1:D:99:LEU:HD22	1.95	0.49
1:F:127:VAL:CG2	1:F:215:ALA:HB2	2.42	0.49
1:I:54:SER:CB	1:I:75:ARG:HD2	2.42	0.49
1:O:185:VAL:HB	1:O:235:VAL:HG11	1.93	0.49
1:W:56:LEU:HD13	1:W:99:LEU:HD22	1.94	0.49
2:H:464:LEU:HD11	2:H:505:VAL:HG11	1.95	0.49
1:I:161:GLU:H	1:I:161:GLU:CD	2.15	0.49
1:I:85:ARG:NH1	1:I:85:ARG:HG2	2.25	0.49
2:P:464:LEU:HD11	2:P:505:VAL:HG11	1.95	0.49
1:Q:20:ALA:O	1:Q:24:ILE:HG12	2.13	0.49
1:S:14:ARG:HH11	1:S:14:ARG:CB	2.13	0.49
1:S:127:VAL:HG11	1:S:213:LEU:HB3	1.95	0.49
1:U:185:VAL:HB	1:U:235:VAL:CG1	2.42	0.49
1:W:185:VAL:HB	1:W:235:VAL:HG11	1.93	0.49
1:W:30:VAL:CG2	1:W:65:ALA:HB2	2.43	0.49
2:X:341:THR:HG22	2:X:404:LEU:HD11	1.94	0.49
2:E:364:GLU:HG2	2:E:368:LYS:HE2	1.95	0.49
1:I:185:VAL:HB	1:I:235:VAL:CG1	2.41	0.49
2:L:307:LYS:HE2	2:L:435:GLY:HA2	1.95	0.49
1:M:71:PHE:HB3	1:M:120:VAL:HG11	1.94	0.49
1:O:30:VAL:CG2	1:O:65:ALA:HB2	2.42	0.49
1:S:20:ALA:O	1:S:24:ILE:HG12	2.13	0.49
1:D:155:VAL:HG12	1:D:160:THR:HG22	1.94	0.49
1:K:140:ARG:HH11	1:K:140:ARG:HB3	1.76	0.49
1:K:71:PHE:HB3	1:K:120:VAL:HG11	1.94	0.49
1:S:85:ARG:NH1	1:S:85:ARG:HG2	2.25	0.49
2:X:329:ARG:NH2	2:2:476:ASP:O	2.45	0.49
1:F:155:VAL:HG12	1:F:160:THR:HG22	1.94	0.49
1:I:155:VAL:HG12	1:I:160:THR:HG22	1.93	0.49
1:I:205:VAL:HG12	1:I:206:ALA:N	2.27	0.49
2:J:464:LEU:HD11	2:J:505:VAL:HG11	1.94	0.49
2:L:393:ALA:HB2	3:L:166:HOH:O	2.13	0.49
2:R:364:GLU:HG2	2:R:368:LYS:HE2	1.95	0.49
1:S:155:VAL:HG12	1:S:160:THR:HG22	1.95	0.49
2:T:301:THR:HA	2:T:333:LYS:NZ	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:SER:CB	1:A:75:ARG:HD2	2.42	0.48
1:D:205:VAL:HG12	1:D:206:ALA:N	2.27	0.48
1:D:54:SER:CB	1:D:75:ARG:HD2	2.43	0.48
1:F:85:ARG:CG	1:F:85:ARG:HH11	2.23	0.48
1:K:155:VAL:HG12	1:K:160:THR:HG22	1.95	0.48
2:N:449:SER:HB2	2:V:452:LYS:HZ1	1.77	0.48
1:O:141:ILE:N	1:O:141:ILE:HD12	2.28	0.48
2:P:301:THR:HA	2:P:333:LYS:NZ	2.28	0.48
2:R:324:ASN:H	2:R:324:ASN:ND2	2.11	0.48
2:X:337:THR:HG21	2:X:359:TYR:CD2	2.48	0.48
2:X:432:GLU:HG3	2:X:437:GLN:HB2	1.95	0.48
1:Y:42:VAL:HG22	1:Y:210:VAL:HG22	1.95	0.48
1:A:172:ALA:HB3	1:A:175:ALA:HB2	1.95	0.48
1:B:56:LEU:HD13	1:B:99:LEU:HD22	1.96	0.48
2:G:324:ASN:H	2:G:324:ASN:HD22	1.59	0.48
2:P:456:GLN:HE22	2:P:465:ARG:NH1	2.10	0.48
1:S:85:ARG:HH11	1:S:85:ARG:CG	2.25	0.48
2:V:485:ASP:OD2	2:V:488:ARG:HB2	2.13	0.48
1:W:151:PRO:HD2	3:W:253:HOH:O	2.12	0.48
2:X:437:GLN:OE1	2:X:447:LYS:HD3	2.13	0.48
1:I:30:VAL:CG2	1:I:65:ALA:HB2	2.43	0.48
2:C:432:GLU:HG3	2:C:437:GLN:HB2	1.95	0.48
1:I:185:VAL:HB	1:I:235:VAL:HG11	1.95	0.48
2:N:461:ASP:OD1	2:N:509:ARG:HD2	2.13	0.48
1:O:89:TYR:HD1	2:V:382:ARG:HD3	1.77	0.48
1:Y:54:SER:CB	1:Y:75:ARG:HD2	2.43	0.48
2:J:382:ARG:HD3	1:S:89:TYR:HD1	1.74	0.48
2:J:436:TYR:CD1	2:J:436:TYR:N	2.81	0.48
1:Q:127:VAL:HG21	1:Q:215:ALA:HB2	1.95	0.48
2:2:337:THR:HG21	2:2:359:TYR:CD2	2.49	0.48
2:C:337:THR:HG21	2:C:359:TYR:CD2	2.49	0.48
1:K:182:ARG:HD3	1:K:235:VAL:CB	2.43	0.48
1:M:28:LYS:HB2	3:M:253:HOH:O	2.14	0.48
1:U:185:VAL:HB	1:U:235:VAL:HG11	1.95	0.48
1:W:20:ALA:O	1:W:24:ILE:HG12	2.13	0.48
1:W:30:VAL:HG13	1:W:43:ALA:HB2	1.95	0.48
2:X:464:LEU:HD11	2:X:505:VAL:HG11	1.95	0.48
1:Y:30:VAL:CG2	1:Y:65:ALA:HB2	2.43	0.48
1:B:141:ILE:N	1:B:141:ILE:HD12	2.29	0.48
1:M:185:VAL:HB	1:M:235:VAL:CG1	2.44	0.48
1:M:127:VAL:HG11	1:M:213:LEU:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:205:VAL:HG12	1:S:206:ALA:N	2.28	0.48
1:Y:140:ARG:HB3	1:Y:140:ARG:HH11	1.77	0.48
2:Z:436:TYR:N	2:Z:436:TYR:CD1	2.81	0.48
2:J:449:SER:HB2	2:Z:452:LYS:HZ1	1.77	0.48
2:2:307:LYS:HE2	2:2:435:GLY:HA2	1.95	0.48
1:F:30:VAL:CG2	1:F:65:ALA:HB2	2.43	0.48
2:J:324:ASN:N	2:J:324:ASN:HD22	2.09	0.48
1:M:182:ARG:HD3	1:M:235:VAL:CB	2.44	0.48
1:O:140:ARG:HH11	1:O:140:ARG:HB3	1.78	0.48
1:1:30:VAL:HG13	1:1:43:ALA:HB2	1.95	0.48
1:B:182:ARG:HD3	1:B:235:VAL:CB	2.44	0.48
2:C:317:ASP:OD1	2:C:333:LYS:NZ	2.46	0.48
1:K:141:ILE:HD12	1:K:141:ILE:N	2.28	0.48
2:L:309:PRO:HG3	2:L:458:THR:O	2.14	0.48
1:B:205:VAL:HG12	1:B:206:ALA:N	2.29	0.48
1:F:140:ARG:HB3	1:F:140:ARG:HH11	1.79	0.48
1:K:54:SER:CB	1:K:75:ARG:HD2	2.43	0.48
2:N:301:THR:HA	2:N:333:LYS:NZ	2.29	0.48
1:Q:161:GLU:H	1:Q:161:GLU:CD	2.18	0.48
2:T:364:GLU:HG2	2:T:368:LYS:HE2	1.96	0.48
1:Y:205:VAL:HG12	1:Y:206:ALA:N	2.29	0.48
2:Z:432:GLU:HG3	2:Z:437:GLN:HB2	1.96	0.48
2:2:456:GLN:HE22	2:2:465:ARG:NH1	2.12	0.47
2:H:391:LEU:CD1	2:C:398:LEU:HD21	2.44	0.47
1:D:20:ALA:O	1:D:24:ILE:HG12	2.14	0.47
2:L:301:THR:HA	2:L:333:LYS:NZ	2.29	0.47
2:L:388:ARG:C	2:L:390:ASN:H	2.17	0.47
1:O:127:VAL:HG21	1:O:215:ALA:HB2	1.96	0.47
1:U:10:GLU:HA	1:1:19:LEU:HD12	1.95	0.47
1:U:83:ASP:OD2	2:V:365:HIS:HD2	1.96	0.47
2:H:436:TYR:N	2:H:436:TYR:HD1	2.12	0.47
1:Q:30:VAL:HG22	1:Q:43:ALA:CB	2.44	0.47
2:X:309:PRO:HG3	2:X:458:THR:O	2.14	0.47
1:Y:127:VAL:HG21	1:Y:215:ALA:HB2	1.95	0.47
1:S:73:ASN:HD22	1:1:105:GLN:CD	2.17	0.47
2:2:349:ALA:HB1	3:2:22:HOH:O	2.14	0.47
2:2:412:SER:HB2	3:2:97:HOH:O	2.14	0.47
1:D:127:VAL:HG11	1:D:213:LEU:HB3	1.96	0.47
2:L:320:SER:HB3	2:L:328:GLY:HA3	1.96	0.47
2:T:321:THR:HG21	2:T:480:ALA:HB1	1.96	0.47
1:U:30:VAL:CG2	1:U:65:ALA:HB2	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:20:ALA:O	1:Y:24:ILE:HG12	2.14	0.47
1:Y:185:VAL:HB	1:Y:235:VAL:HG11	1.96	0.47
1:Y:30:VAL:HG13	1:Y:43:ALA:HB2	1.95	0.47
1:B:172:ALA:HB3	1:B:175:ALA:HB2	1.95	0.47
1:F:48:ARG:HH22	1:W:135:ARG:CB	2.27	0.47
2:H:324:ASN:H	2:H:324:ASN:ND2	2.11	0.47
1:U:161:GLU:CD	1:U:161:GLU:H	2.17	0.47
2:Z:321:THR:HG21	2:Z:480:ALA:HB1	1.95	0.47
2:2:324:ASN:HD22	2:2:324:ASN:N	2.12	0.47
1:A:140:ARG:HH11	1:A:140:ARG:HB3	1.80	0.47
1:B:182:ARG:HB2	1:B:182:ARG:NH1	2.30	0.47
2:C:450:MET:HE3	2:C:470:ALA:CB	2.44	0.47
1:K:20:ALA:O	1:K:24:ILE:HG12	2.14	0.47
2:L:380:ILE:HD11	2:L:421:VAL:HG21	1.97	0.47
1:M:140:ARG:HH11	1:M:140:ARG:HB3	1.79	0.47
2:P:301:THR:HA	2:P:333:LYS:HZ3	1.79	0.47
2:P:514:ALA:O	2:P:518:ILE:HG13	2.15	0.47
1:Q:105:GLN:CD	1:Y:73:ASN:HD22	2.18	0.47
1:1:205:VAL:HG12	1:1:206:ALA:H	1.78	0.47
1:A:85:ARG:NH1	1:A:85:ARG:HG2	2.23	0.47
1:A:99:LEU:HD12	1:A:99:LEU:H	1.80	0.47
1:F:172:ALA:HB3	1:F:175:ALA:HB2	1.95	0.47
2:X:364:GLU:HG2	2:X:368:LYS:HE2	1.96	0.47
2:C:324:ASN:N	2:C:324:ASN:HD22	2.12	0.47
1:D:12:ALA:O	1:D:16:ARG:HG2	2.15	0.47
1:K:185:VAL:HB	1:K:235:VAL:HG11	1.94	0.47
1:K:19:LEU:HD12	1:M:10:GLU:HA	1.97	0.47
2:N:432:GLU:HG3	2:N:437:GLN:HB2	1.96	0.47
1:W:63:ALA:O	1:W:156:MET:HE1	2.14	0.47
2:2:461:ASP:OD1	2:2:509:ARG:HD2	2.14	0.47
1:A:161:GLU:CD	1:A:161:GLU:H	2.17	0.47
1:F:182:ARG:NH1	1:F:182:ARG:HB2	2.29	0.47
2:G:301:THR:N	2:G:441:SER:HG	2.13	0.47
2:H:515:ARG:CD	3:H:114:HOH:O	2.63	0.47
1:I:28:LYS:HB2	1:I:52:LYS:HZ2	1.79	0.47
1:K:205:VAL:HG12	1:K:206:ALA:N	2.29	0.47
2:L:374:LEU:HD22	1:M:93:ASP:OD2	2.15	0.47
2:L:321:THR:HG21	2:L:480:ALA:HB1	1.97	0.47
1:O:85:ARG:HH11	1:O:85:ARG:CG	2.22	0.47
1:U:30:VAL:HG22	1:U:43:ALA:CB	2.45	0.47
2:X:514:ALA:O	2:X:518:ILE:HG13	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:182:ARG:HD3	1:Y:235:VAL:CB	2.45	0.47
1:D:172:ALA:HB3	1:D:175:ALA:HB2	1.97	0.47
2:L:324:ASN:HD22	2:L:324:ASN:N	2.12	0.47
1:S:63:ALA:O	1:S:156:MET:HE1	2.15	0.47
2:V:432:GLU:HG3	2:V:437:GLN:HB2	1.95	0.47
2:T:329:ARG:NH2	2:Z:476:ASP:O	2.46	0.47
2:2:437:GLN:OE1	2:2:447:LYS:HD3	2.14	0.47
2:E:337:THR:HG21	2:E:359:TYR:CD2	2.49	0.47
1:U:54:SER:CB	1:U:75:ARG:HD2	2.44	0.47
1:Y:85:ARG:HH11	1:Y:85:ARG:CG	2.21	0.47
1:I:63:ALA:O	1:I:156:MET:HE1	2.15	0.47
1:F:56:LEU:HD13	1:F:99:LEU:HD22	1.96	0.47
2:H:437:GLN:OE1	2:H:447:LYS:HD3	2.15	0.47
1:K:14:ARG:CB	1:K:14:ARG:HH11	2.13	0.47
1:O:205:VAL:HG12	1:O:206:ALA:H	1.80	0.47
1:S:70:GLU:HB3	1:S:118:TYR:CD2	2.50	0.47
2:T:432:GLU:HG3	2:T:437:GLN:HB2	1.97	0.47
1:W:42:VAL:HG22	1:W:210:VAL:HG22	1.96	0.47
2:2:317:ASP:HB2	3:2:50:HOH:O	2.14	0.46
2:2:432:GLU:HG3	2:2:437:GLN:HB2	1.96	0.46
2:2:496:ILE:O	2:2:502:ALA:HA	2.14	0.46
1:D:30:VAL:HG13	1:D:43:ALA:HB2	1.96	0.46
1:F:127:VAL:HG21	1:F:215:ALA:HB2	1.96	0.46
2:H:436:TYR:CD1	2:H:436:TYR:N	2.82	0.46
1:I:63:ALA:O	1:I:156:MET:HE1	2.16	0.46
1:K:127:VAL:HG21	1:K:215:ALA:HB2	1.96	0.46
1:M:30:VAL:CG2	1:M:65:ALA:HB2	2.44	0.46
2:N:337:THR:HG21	2:N:359:TYR:CD2	2.50	0.46
1:O:43:ALA:HA	3:O:250:HOH:O	2.15	0.46
1:S:30:VAL:HG22	1:S:43:ALA:CB	2.46	0.46
1:Y:129:HIS:HD2	3:Y:251:HOH:O	1.98	0.46
1:Y:56:LEU:HD13	1:Y:99:LEU:HD22	1.97	0.46
1:F:182:ARG:HD3	1:F:235:VAL:CB	2.43	0.46
1:O:63:ALA:O	1:O:156:MET:HE1	2.15	0.46
1:O:70:GLU:HB3	1:O:118:TYR:CD2	2.51	0.46
1:U:157:GLY:N	3:U:250:HOH:O	2.48	0.46
2:Z:337:THR:HG21	2:Z:359:TYR:CD2	2.51	0.46
1:D:226:THR:O	1:D:230:LEU:HB2	2.14	0.46
1:F:161:GLU:H	1:F:161:GLU:CD	2.18	0.46
1:F:205:VAL:HG12	1:F:206:ALA:N	2.30	0.46
2:J:388:ARG:C	2:J:390:ASN:H	2.19	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:47:SER:HA	3:K:256:HOH:O	2.16	0.46
1:M:76:ARG:HG2	2:N:369:LEU:CD2	2.46	0.46
1:Q:127:VAL:HG11	1:Q:213:LEU:HB3	1.97	0.46
2:R:496:ILE:O	2:R:502:ALA:HA	2.15	0.46
2:T:375:THR:N	3:1:252:HOH:O	2.45	0.46
1:U:55:GLU:OE2	1:U:220:ARG:CD	2.64	0.46
2:V:324:ASN:H	2:V:324:ASN:ND2	2.13	0.46
2:V:455:SER:HB3	3:V:51:HOH:O	2.14	0.46
2:V:485:ASP:OD2	2:V:488:ARG:CB	2.64	0.46
1:Y:141:ILE:N	1:Y:141:ILE:HD12	2.30	0.46
1:1:160:THR:HG23	3:1:259:HOH:O	2.14	0.46
1:A:55:GLU:OE2	1:A:220:ARG:CD	2.64	0.46
1:B:85:ARG:HG2	1:B:85:ARG:NH1	2.29	0.46
1:I:28:LYS:HE2	1:I:46:PRO:HD3	1.97	0.46
2:J:324:ASN:ND2	2:J:324:ASN:H	2.11	0.46
1:K:172:ALA:HB3	1:K:175:ALA:HB2	1.97	0.46
2:P:337:THR:HG21	2:P:359:TYR:CD2	2.51	0.46
2:2:436:TYR:CD1	2:2:436:TYR:N	2.84	0.46
1:F:127:VAL:HG11	1:F:213:LEU:HB3	1.98	0.46
2:G:432:GLU:HG3	2:G:437:GLN:HB2	1.97	0.46
2:H:412:SER:O	2:H:414:PRO:HD3	2.16	0.46
1:O:182:ARG:NH1	1:O:182:ARG:HB2	2.30	0.46
2:R:514:ALA:O	2:R:518:ILE:HG13	2.16	0.46
1:S:127:VAL:CG2	1:S:215:ALA:HB2	2.46	0.46
1:W:85:ARG:NH1	1:W:85:ARG:HG2	2.26	0.46
2:G:317:ASP:HB2	3:G:109:HOH:O	2.16	0.46
2:J:496:ILE:O	2:J:502:ALA:HA	2.16	0.46
1:M:205:VAL:HG12	1:M:206:ALA:H	1.80	0.46
1:M:55:GLU:OE2	1:M:220:ARG:CD	2.64	0.46
2:N:514:ALA:O	2:N:518:ILE:HG13	2.15	0.46
1:Q:182:ARG:NH1	1:Q:182:ARG:HB2	2.31	0.46
1:U:127:VAL:HG11	1:U:213:LEU:HB3	1.97	0.46
2:Z:514:ALA:O	2:Z:518:ILE:HG13	2.15	0.46
1:1:140:ARG:HH11	1:1:140:ARG:HB3	1.80	0.46
1:A:48:ARG:HD2	1:B:137:GLU:CD	2.36	0.46
1:M:30:VAL:HG22	1:M:43:ALA:CB	2.46	0.46
1:Q:85:ARG:NH1	1:Q:85:ARG:HG2	2.25	0.46
1:W:28:LYS:HE2	1:W:46:PRO:HD3	1.97	0.46
1:A:48:ARG:HD2	1:B:137:GLU:OE2	2.15	0.46
1:B:55:GLU:OE2	1:B:220:ARG:CD	2.64	0.46
1:K:70:GLU:HB3	1:K:118:TYR:CD2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:301:THR:N	2:L:441:SER:HG	2.14	0.46
1:Q:83:ASP:OD2	2:R:365:HIS:HD2	1.98	0.46
2:R:388:ARG:C	2:R:390:ASN:H	2.19	0.46
2:V:436:TYR:CD1	2:V:436:TYR:N	2.84	0.46
1:Y:172:ALA:HB3	1:Y:175:ALA:HB2	1.98	0.46
2:Z:301:THR:HA	2:Z:333:LYS:HZ3	1.81	0.46
2:2:324:ASN:ND2	2:2:324:ASN:H	2.13	0.46
1:F:137:GLU:CD	1:M:48:ARG:HD2	2.36	0.46
2:L:317:ASP:OD1	2:L:333:LYS:NZ	2.47	0.46
1:S:141:ILE:HD12	1:S:141:ILE:N	2.31	0.46
1:S:172:ALA:HB3	1:S:175:ALA:HB2	1.97	0.46
1:S:30:VAL:HG23	1:S:65:ALA:HB2	1.98	0.46
2:X:388:ARG:C	2:X:390:ASN:H	2.20	0.46
1:Y:30:VAL:HG22	1:Y:43:ALA:CB	2.46	0.46
1:B:83:ASP:OD2	2:C:365:HIS:HD2	1.99	0.46
2:G:301:THR:HA	2:G:333:LYS:HZ2	1.81	0.46
1:K:55:GLU:OE2	1:K:220:ARG:CD	2.63	0.46
1:K:56:LEU:HD13	1:K:99:LEU:HD22	1.98	0.46
2:P:485:ASP:OD2	2:P:488:ARG:HB2	2.16	0.46
1:Q:30:VAL:CG2	1:Q:65:ALA:HB2	2.46	0.46
1:U:182:ARG:HD3	1:U:235:VAL:CB	2.46	0.46
1:W:182:ARG:HD3	1:W:235:VAL:CB	2.46	0.46
2:Z:496:ILE:O	2:Z:502:ALA:HA	2.16	0.46
1:D:30:VAL:CG2	1:D:65:ALA:HB2	2.46	0.45
1:F:137:GLU:OE2	1:M:48:ARG:HD2	2.16	0.45
1:F:54:SER:CB	1:F:75:ARG:HD2	2.46	0.45
2:J:317:ASP:OD1	2:J:333:LYS:NZ	2.49	0.45
2:L:324:ASN:ND2	2:L:324:ASN:H	2.14	0.45
2:L:496:ILE:O	2:L:502:ALA:HA	2.16	0.45
1:Q:70:GLU:HB3	1:Q:118:TYR:CD2	2.51	0.45
2:V:309:PRO:HG3	2:V:458:THR:O	2.16	0.45
1:Y:28:LYS:HE2	1:Y:46:PRO:HD3	1.97	0.45
2:E:388:ARG:C	2:E:390:ASN:H	2.20	0.45
1:F:141:ILE:N	1:F:141:ILE:HD12	2.30	0.45
1:F:30:VAL:HG22	1:F:43:ALA:CB	2.46	0.45
2:J:432:GLU:HG3	2:J:437:GLN:HB2	1.97	0.45
1:D:135:ARG:CB	1:Q:48:ARG:HH22	2.29	0.45
1:U:205:VAL:HG12	1:U:206:ALA:H	1.79	0.45
1:U:56:LEU:HD13	1:U:99:LEU:HD22	1.97	0.45
2:V:307:LYS:HE2	2:V:435:GLY:HA2	1.98	0.45
1:1:172:ALA:HB3	1:1:175:ALA:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:388:ARG:C	2:2:390:ASN:H	2.19	0.45
1:B:127:VAL:HG11	1:B:213:LEU:HB3	1.97	0.45
2:C:437:GLN:OE1	2:C:447:LYS:HD3	2.16	0.45
2:C:496:ILE:O	2:C:502:ALA:HA	2.16	0.45
1:O:127:VAL:HG11	1:O:213:LEU:HB3	1.97	0.45
2:V:309:PRO:O	2:V:415:GLN:HG2	2.16	0.45
1:U:135:ARG:CB	1:1:48:ARG:HH22	2.29	0.45
1:U:135:ARG:HB3	1:1:48:ARG:HH22	1.80	0.45
2:E:432:GLU:HG3	2:E:437:GLN:HB2	1.99	0.45
2:G:307:LYS:HE2	2:G:435:GLY:HA2	1.97	0.45
1:I:71:PHE:HB3	1:I:120:VAL:HG11	1.97	0.45
2:N:301:THR:HG23	2:N:333:LYS:HD3	1.98	0.45
2:2:301:THR:HA	2:2:333:LYS:HZ3	1.82	0.45
2:G:337:THR:HG21	2:G:359:TYR:CD2	2.51	0.45
1:I:182:ARG:HD3	1:I:235:VAL:CB	2.43	0.45
2:L:337:THR:OG1	2:L:343:THR:CG2	2.60	0.45
2:T:437:GLN:OE1	2:T:447:LYS:HD3	2.17	0.45
2:T:309:PRO:HG3	2:T:458:THR:O	2.17	0.45
1:Y:63:ALA:O	1:Y:156:MET:HE1	2.17	0.45
1:A:85:ARG:CG	1:A:85:ARG:HH11	2.25	0.45
1:D:30:VAL:HG22	1:D:43:ALA:CB	2.46	0.45
1:I:30:VAL:HG22	1:I:43:ALA:CB	2.47	0.45
1:S:182:ARG:HB2	1:S:182:ARG:NH1	2.32	0.45
2:V:337:THR:HG21	2:V:359:TYR:CD2	2.52	0.45
1:W:127:VAL:HG11	1:W:213:LEU:HB3	1.99	0.45
1:A:223:ARG:NH1	3:A:249:HOH:O	2.50	0.45
2:E:324:ASN:H	2:E:324:ASN:ND2	2.14	0.45
1:F:115:ALA:HB3	1:W:112:THR:HG23	1.97	0.45
2:L:452:LYS:HZ3	2:P:449:SER:HB2	1.81	0.45
2:R:301:THR:HA	2:R:333:LYS:HZ2	1.81	0.45
2:R:436:TYR:N	2:R:436:TYR:CD1	2.83	0.45
1:S:28:LYS:HE2	1:S:46:PRO:HD3	1.99	0.45
1:S:54:SER:CB	1:S:75:ARG:HD2	2.47	0.45
2:T:324:ASN:ND2	2:T:324:ASN:H	2.15	0.45
2:X:318:ARG:HD2	2:X:492:PRO:HA	1.99	0.45
1:B:70:GLU:HB3	1:B:118:TYR:CD2	2.52	0.45
2:E:436:TYR:CD1	2:E:436:TYR:N	2.85	0.45
2:H:317:ASP:OD1	2:H:333:LYS:NZ	2.47	0.45
2:H:307:LYS:HE2	2:H:435:GLY:HA2	1.99	0.45
1:U:141:ILE:N	1:U:141:ILE:HD12	2.31	0.45
2:Z:317:ASP:OD1	2:Z:333:LYS:NZ	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:182:ARG:NH1	1:1:182:ARG:HB2	2.31	0.45
2:G:496:ILE:O	2:G:502:ALA:HA	2.17	0.45
1:M:141:ILE:N	1:M:141:ILE:HD12	2.32	0.45
2:N:437:GLN:OE1	2:N:447:LYS:HD3	2.17	0.45
1:S:176:SER:HA	3:S:252:HOH:O	2.15	0.45
2:Z:324:ASN:H	2:Z:324:ASN:ND2	2.15	0.45
2:E:307:LYS:HE2	2:E:435:GLY:HA2	1.99	0.45
2:G:320:SER:HB3	2:G:328:GLY:HA3	1.99	0.45
2:P:307:LYS:HE2	2:P:435:GLY:HA2	1.99	0.45
2:P:432:GLU:HG3	2:P:437:GLN:HB2	1.99	0.45
1:Q:205:VAL:HG12	1:Q:206:ALA:H	1.82	0.45
1:Q:54:SER:CB	1:Q:75:ARG:HD2	2.47	0.45
1:U:28:LYS:HE2	1:U:46:PRO:HD3	1.99	0.45
1:Y:182:ARG:NH1	1:Y:182:ARG:HB2	2.32	0.45
1:1:127:VAL:HG11	1:1:213:LEU:HB3	2.00	0.44
1:1:55:GLU:OE2	1:1:220:ARG:CD	2.66	0.44
2:C:324:ASN:ND2	2:C:324:ASN:H	2.14	0.44
1:F:71:PHE:HB3	1:F:120:VAL:HG11	1.99	0.44
2:L:469:GLU:HG3	2:L:517:ILE:HG21	1.98	0.44
1:M:185:VAL:HB	1:M:235:VAL:HG11	1.98	0.44
1:F:97:ARG:HG3	1:M:49:SER:HB2	1.98	0.44
1:Q:182:ARG:HD3	1:Q:235:VAL:CB	2.46	0.44
1:U:182:ARG:HB2	1:U:182:ARG:NH1	2.32	0.44
2:V:324:ASN:N	2:V:324:ASN:HD22	2.12	0.44
2:V:380:ILE:HD11	2:V:421:VAL:HG21	1.99	0.44
1:W:205:VAL:HG12	1:W:206:ALA:H	1.83	0.44
1:1:71:PHE:HB3	1:1:120:VAL:HG11	1.98	0.44
1:1:28:LYS:HE2	1:1:46:PRO:HD3	1.99	0.44
1:B:134:LYS:NZ	3:B:254:HOH:O	2.51	0.44
1:M:28:LYS:HE2	1:M:46:PRO:HD3	2.00	0.44
2:P:496:ILE:O	2:P:502:ALA:HA	2.17	0.44
2:R:432:GLU:HG3	2:R:437:GLN:HB2	1.99	0.44
2:T:436:TYR:N	2:T:436:TYR:HD1	2.15	0.44
2:V:437:GLN:OE1	2:V:447:LYS:HD3	2.16	0.44
2:V:496:ILE:O	2:V:502:ALA:HA	2.18	0.44
1:W:30:VAL:HG22	1:W:43:ALA:CB	2.47	0.44
2:X:485:ASP:OD2	2:X:488:ARG:HB2	2.17	0.44
1:A:182:ARG:HB2	1:A:182:ARG:NH1	2.32	0.44
1:A:56:LEU:HD13	1:A:99:LEU:HD22	1.99	0.44
2:N:307:LYS:HE2	2:N:435:GLY:HA2	1.99	0.44
1:O:172:ALA:HB3	1:O:175:ALA:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:30:VAL:HG22	1:1:43:ALA:CB	2.47	0.44
2:2:321:THR:HG21	2:2:480:ALA:HB1	1.98	0.44
2:H:515:ARG:HD3	3:H:114:HOH:O	2.17	0.44
1:M:63:ALA:O	1:M:156:MET:HE1	2.18	0.44
1:M:182:ARG:HB2	1:M:182:ARG:NH1	2.33	0.44
2:R:309:PRO:HG3	2:R:458:THR:O	2.17	0.44
2:2:320:SER:HB3	2:2:328:GLY:HA3	1.98	0.44
1:A:70:GLU:HB3	1:A:118:TYR:CD2	2.52	0.44
2:L:436:TYR:N	2:L:436:TYR:CD1	2.84	0.44
2:L:437:GLN:OE1	2:L:447:LYS:HD3	2.18	0.44
1:W:172:ALA:HB3	1:W:175:ALA:HB2	1.99	0.44
2:C:436:TYR:CD1	2:C:436:TYR:N	2.85	0.44
1:D:79:ILE:HD12	2:E:369:LEU:HD23	1.99	0.44
2:E:496:ILE:O	2:E:502:ALA:HA	2.18	0.44
2:H:432:GLU:HG3	2:H:437:GLN:HB2	1.99	0.44
2:N:321:THR:HG21	2:N:480:ALA:HB1	1.99	0.44
1:Q:172:ALA:HB3	1:Q:175:ALA:HB2	2.00	0.44
1:S:182:ARG:HD3	1:S:235:VAL:CB	2.46	0.44
1:1:182:ARG:HD3	1:1:235:VAL:CB	2.46	0.44
1:A:57:TYR:O	1:A:58:ASP:C	2.56	0.44
1:M:56:LEU:HD13	1:M:99:LEU:HD23	1.98	0.44
1:M:70:GLU:HB3	1:M:118:TYR:CD2	2.52	0.44
2:P:437:GLN:OE1	2:P:447:LYS:HD3	2.17	0.44
2:T:485:ASP:OD2	2:T:488:ARG:HB2	2.18	0.44
2:T:496:ILE:O	2:T:502:ALA:HA	2.17	0.44
2:V:436:TYR:N	2:V:436:TYR:HD1	2.14	0.44
2:N:452:LYS:NZ	2:V:449:SER:HB2	2.33	0.44
1:W:54:SER:CB	1:W:75:ARG:HD2	2.48	0.44
1:W:85:ARG:HH11	1:W:85:ARG:CG	2.26	0.44
1:Y:28:LYS:HD3	3:Y:258:HOH:O	2.17	0.44
2:Z:485:ASP:OD2	2:Z:488:ARG:HB2	2.18	0.44
2:2:436:TYR:HD1	2:2:436:TYR:N	2.15	0.44
1:B:30:VAL:HG22	1:B:43:ALA:CB	2.48	0.44
1:D:182:ARG:NH1	1:D:182:ARG:HB2	2.33	0.44
1:D:205:VAL:HG12	1:D:206:ALA:H	1.82	0.44
2:H:380:ILE:HD11	2:H:421:VAL:HG21	1.99	0.44
2:P:388:ARG:C	2:P:390:ASN:H	2.20	0.44
2:T:320:SER:HB2	2:T:331:VAL:HG21	2.00	0.44
1:B:30:VAL:HG23	1:B:65:ALA:HB2	2.00	0.44
1:D:70:GLU:HB3	1:D:118:TYR:CD2	2.53	0.44
1:F:70:GLU:HB3	1:F:118:TYR:CD2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:318:ARG:HD2	2:G:492:PRO:HA	2.00	0.44
2:G:412:SER:O	2:G:414:PRO:HD3	2.17	0.44
1:S:83:ASP:OD2	2:T:365:HIS:CD2	2.68	0.44
2:G:452:LYS:HZ1	2:2:449:SER:HB2	1.83	0.43
1:F:83:ASP:OD2	2:G:365:HIS:HD2	2.01	0.43
2:G:437:GLN:OE1	2:G:447:LYS:HD3	2.18	0.43
2:L:412:SER:O	2:L:414:PRO:HD3	2.17	0.43
2:N:436:TYR:CD1	2:N:436:TYR:N	2.85	0.43
1:O:182:ARG:HD3	1:O:235:VAL:CB	2.47	0.43
1:O:31:VAL:N	3:O:250:HOH:O	2.50	0.43
1:W:71:PHE:HB3	1:W:120:VAL:HG11	2.00	0.43
2:E:309:PRO:HG3	2:E:458:THR:O	2.18	0.43
1:F:28:LYS:HE3	1:F:44:GLU:HG3	2.01	0.43
2:G:324:ASN:HD22	2:G:324:ASN:N	2.16	0.43
2:G:436:TYR:N	2:G:436:TYR:CD1	2.86	0.43
2:G:476:ASP:O	2:V:329:ARG:NH2	2.50	0.43
1:I:30:VAL:HG23	1:I:65:ALA:HB2	2.00	0.43
1:K:182:ARG:NH1	1:K:182:ARG:HB2	2.33	0.43
1:K:35:TYR:HE2	3:K:249:HOH:O	2.01	0.43
1:K:93:ASP:OD2	3:K:254:HOH:O	2.21	0.43
2:P:461:ASP:OD1	2:P:509:ARG:HD2	2.17	0.43
2:T:436:TYR:CD1	2:T:436:TYR:N	2.84	0.43
2:V:301:THR:HG23	2:V:333:LYS:HD3	2.00	0.43
2:V:450:MET:HE3	2:V:470:ALA:CB	2.47	0.43
2:X:496:ILE:HG13	2:X:505:VAL:CG2	2.48	0.43
1:Y:150:GLU:HG2	3:Y:253:HOH:O	2.18	0.43
2:2:391:LEU:O	2:2:395:MET:HG2	2.18	0.43
2:E:301:THR:HA	2:E:333:LYS:HZ3	1.83	0.43
2:E:324:ASN:N	2:E:324:ASN:HD22	2.12	0.43
2:G:426:ALA:HB3	2:X:350:ALA:CB	2.49	0.43
2:G:449:SER:HB2	2:2:452:LYS:HZ1	1.83	0.43
2:G:514:ALA:O	2:G:518:ILE:HG13	2.17	0.43
1:I:172:ALA:HB3	1:I:175:ALA:HB2	1.99	0.43
1:I:127:VAL:HG11	1:I:213:LEU:HB3	1.99	0.43
2:J:307:LYS:HE2	2:J:435:GLY:HA2	2.00	0.43
2:N:324:ASN:ND2	2:N:324:ASN:N	2.66	0.43
1:O:28:LYS:HE2	1:O:46:PRO:HD3	2.00	0.43
1:S:71:PHE:HB3	1:S:120:VAL:HG11	2.00	0.43
1:U:70:GLU:HB3	1:U:118:TYR:CD2	2.53	0.43
2:V:388:ARG:C	2:V:390:ASN:H	2.22	0.43
2:X:324:ASN:H	2:X:324:ASN:ND2	2.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:LYS:HE2	1:A:46:PRO:HD3	2.00	0.43
1:D:220:ARG:HH22	2:E:367:GLU:CD	2.22	0.43
1:D:85:ARG:HG2	1:D:85:ARG:NH1	2.29	0.43
1:F:97:ARG:NH1	1:M:49:SER:HB2	2.34	0.43
2:H:476:ASP:O	2:L:329:ARG:NH2	2.52	0.43
1:I:47:SER:HB2	3:I:254:HOH:O	2.18	0.43
1:K:30:VAL:HG22	1:K:43:ALA:CB	2.48	0.43
2:P:301:THR:HG23	2:P:333:LYS:HD3	1.99	0.43
2:R:320:SER:HB3	2:R:328:GLY:HA3	2.01	0.43
1:W:76:ARG:NH1	2:X:369:LEU:HD22	2.34	0.43
1:Y:85:ARG:NH1	1:Y:85:ARG:CG	2.78	0.43
1:1:30:VAL:HG23	1:1:65:ALA:HB2	2.00	0.43
2:H:505:VAL:HA	2:H:506:PRO:HD3	1.89	0.43
1:I:205:VAL:HG12	1:I:206:ALA:H	1.83	0.43
2:J:485:ASP:OD2	2:J:488:ARG:HB2	2.18	0.43
2:L:337:THR:HG21	2:L:359:TYR:CD2	2.53	0.43
1:Q:105:GLN:NE2	1:Y:73:ASN:HD22	2.16	0.43
1:Q:141:ILE:N	1:Q:141:ILE:HD12	2.33	0.43
2:C:505:VAL:HA	2:C:506:PRO:HD3	1.89	0.43
1:D:71:PHE:HB3	1:D:120:VAL:HG11	2.01	0.43
2:E:338:ASP:HB2	3:E:189:HOH:O	2.18	0.43
2:N:496:ILE:O	2:N:502:ALA:HA	2.18	0.43
2:P:412:SER:O	2:P:414:PRO:HD3	2.18	0.43
2:V:301:THR:HA	2:V:333:LYS:HZ3	1.83	0.43
1:W:12:ALA:O	1:W:16:ARG:HG2	2.18	0.43
2:C:388:ARG:C	2:C:390:ASN:H	2.21	0.43
2:C:436:TYR:HD1	2:C:436:TYR:N	2.15	0.43
2:G:321:THR:HG21	2:G:480:ALA:HB1	2.01	0.43
2:L:303:ILE:HD11	2:L:333:LYS:HB3	2.01	0.43
2:N:324:ASN:HD22	2:N:324:ASN:N	2.05	0.43
2:T:324:ASN:HD22	2:T:324:ASN:N	2.13	0.43
1:A:213:LEU:HD12	1:A:222:PHE:HD1	1.84	0.43
1:K:28:LYS:HE2	1:K:46:PRO:HD3	2.00	0.43
1:M:12:ALA:O	1:M:16:ARG:HG2	2.17	0.43
1:W:213:LEU:HD12	1:W:222:PHE:HD1	1.83	0.43
2:Z:437:GLN:OE1	2:Z:447:LYS:HD3	2.19	0.43
1:1:76:ARG:NH1	2:2:369:LEU:HD22	2.33	0.43
2:R:355:PHE:HD1	2:R:355:PHE:HA	1.77	0.43
1:D:89:TYR:CD1	2:R:382:ARG:HD3	2.54	0.43
1:S:205:VAL:HG12	1:S:206:ALA:H	1.84	0.43
1:S:85:ARG:NH1	1:S:85:ARG:CG	2.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:70:GLU:HB3	1:W:118:TYR:CD2	2.53	0.43
2:Z:380:ILE:HD11	2:Z:421:VAL:HG21	2.01	0.43
1:1:54:SER:CB	1:1:75:ARG:HD2	2.49	0.43
2:C:309:PRO:O	2:C:415:GLN:HG2	2.19	0.43
2:E:436:TYR:HD1	2:E:436:TYR:N	2.15	0.43
2:G:388:ARG:C	2:G:390:ASN:H	2.22	0.43
2:H:415:GLN:HE21	2:H:415:GLN:HB3	1.60	0.43
1:I:85:ARG:NH1	1:I:85:ARG:CG	2.82	0.43
1:M:234:LEU:O	3:M:252:HOH:O	2.21	0.43
1:O:83:ASP:OD2	2:P:365:HIS:CD2	2.69	0.43
2:P:321:THR:HG21	2:P:480:ALA:HB1	2.01	0.43
1:Y:213:LEU:HD12	1:Y:222:PHE:HD1	1.84	0.43
1:B:74:LEU:HD11	1:B:107:LEU:HD21	2.01	0.42
2:E:320:SER:HB2	2:E:331:VAL:HG21	2.01	0.42
2:E:412:SER:O	2:E:414:PRO:HD3	2.19	0.42
2:H:388:ARG:C	2:H:390:ASN:H	2.22	0.42
2:L:320:SER:HB2	2:L:331:VAL:HG21	2.00	0.42
1:M:85:ARG:HG2	1:M:85:ARG:NH1	2.24	0.42
1:F:89:TYR:HD1	2:N:382:ARG:HD3	1.82	0.42
2:P:436:TYR:N	2:P:436:TYR:CD1	2.86	0.42
2:2:309:PRO:HG3	2:2:458:THR:O	2.19	0.42
1:A:127:VAL:HG11	1:A:213:LEU:HB3	2.01	0.42
2:G:301:THR:HG23	2:G:333:LYS:HD3	2.00	0.42
2:L:415:GLN:HB3	2:L:415:GLN:HE21	1.61	0.42
1:S:127:VAL:HG21	1:S:215:ALA:HB2	2.00	0.42
1:S:12:ALA:O	1:S:16:ARG:HG2	2.19	0.42
2:T:388:ARG:C	2:T:390:ASN:H	2.22	0.42
1:Y:205:VAL:HG12	1:Y:206:ALA:H	1.84	0.42
1:Y:127:VAL:HG11	1:Y:213:LEU:HB3	2.00	0.42
2:2:505:VAL:HA	2:2:506:PRO:HD3	1.92	0.42
1:D:112:THR:HG23	1:Q:115:ALA:HB3	2.01	0.42
2:E:306:LEU:HB2	2:E:313:VAL:CG1	2.49	0.42
2:J:301:THR:HG23	2:J:333:LYS:HD3	2.01	0.42
2:J:337:THR:HG21	2:J:359:TYR:CD2	2.54	0.42
2:N:388:ARG:C	2:N:390:ASN:H	2.22	0.42
2:X:380:ILE:HD11	2:X:421:VAL:HG21	2.01	0.42
1:Q:135:ARG:HB3	1:Y:48:ARG:HH22	1.83	0.42
2:Z:307:LYS:HE2	2:Z:435:GLY:HA2	2.01	0.42
2:H:426:ALA:HB3	2:C:350:ALA:CB	2.49	0.42
1:D:55:GLU:OE2	1:D:220:ARG:CD	2.67	0.42
2:H:496:ILE:O	2:H:502:ALA:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:12:ALA:O	1:I:16:ARG:HG2	2.18	0.42
2:J:505:VAL:HA	2:J:506:PRO:HD3	1.87	0.42
1:O:205:VAL:C	1:O:207:SER:N	2.73	0.42
1:O:54:SER:CB	1:O:75:ARG:HD2	2.49	0.42
1:S:74:LEU:HD11	1:S:107:LEU:HD21	2.01	0.42
2:T:380:ILE:HD11	2:T:421:VAL:HG21	2.02	0.42
1:U:205:VAL:C	1:U:207:SER:N	2.72	0.42
2:V:320:SER:HB2	2:V:331:VAL:HG21	2.01	0.42
2:Z:324:ASN:N	2:Z:324:ASN:HD22	2.14	0.42
2:2:303:ILE:HD11	2:2:333:LYS:HB3	2.01	0.42
1:B:63:ALA:O	1:B:156:MET:HE1	2.19	0.42
2:C:307:LYS:HE2	2:C:435:GLY:HA2	2.00	0.42
1:K:85:ARG:HG2	1:K:85:ARG:NH1	2.28	0.42
1:O:213:LEU:HD12	1:O:222:PHE:HD1	1.84	0.42
2:P:469:GLU:HG3	2:P:517:ILE:HG21	2.02	0.42
2:P:485:ASP:OD2	2:P:488:ARG:CB	2.67	0.42
1:U:63:ALA:O	1:U:156:MET:HE1	2.19	0.42
1:U:213:LEU:HD12	1:U:222:PHE:HD1	1.84	0.42
2:X:436:TYR:N	2:X:436:TYR:CD1	2.88	0.42
2:Z:301:THR:HG23	2:Z:333:LYS:HD3	2.01	0.42
2:Z:320:SER:HB2	2:Z:331:VAL:HG21	2.02	0.42
1:1:85:ARG:HG2	1:1:85:ARG:NH1	2.29	0.42
2:2:301:THR:HA	2:2:333:LYS:NZ	2.34	0.42
2:2:415:GLN:HE21	2:2:415:GLN:HB3	1.60	0.42
1:B:71:PHE:HB3	1:B:120:VAL:HG11	2.01	0.42
1:O:56:LEU:HD13	1:O:99:LEU:HD23	2.01	0.42
2:P:505:VAL:HA	2:P:506:PRO:HD3	1.90	0.42
2:R:301:THR:HG23	2:R:333:LYS:HD3	2.02	0.42
2:R:485:ASP:OD2	2:R:488:ARG:HB2	2.19	0.42
1:S:56:LEU:HD13	1:S:99:LEU:HD23	2.02	0.42
1:W:55:GLU:OE2	1:W:220:ARG:CD	2.68	0.42
2:Z:388:ARG:C	2:Z:390:ASN:H	2.22	0.42
2:E:378:GLY:HA3	3:K:254:HOH:O	2.19	0.42
2:L:355:PHE:HA	2:L:355:PHE:HD1	1.74	0.42
2:L:505:VAL:HA	2:L:506:PRO:HD3	1.90	0.42
1:Q:28:LYS:HE2	1:Q:46:PRO:HD3	2.00	0.42
2:V:321:THR:HG21	2:V:480:ALA:HB1	2.02	0.42
2:X:393:ALA:HB1	2:X:398:LEU:HB2	2.00	0.42
1:1:182:ARG:HA	1:1:235:VAL:HB	2.02	0.42
2:2:320:SER:HB2	2:2:331:VAL:HG21	2.01	0.42
1:A:14:ARG:CB	1:A:14:ARG:HH11	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:213:LEU:HD12	1:D:222:PHE:HD1	1.85	0.42
2:E:456:GLN:NE2	2:E:465:ARG:NH1	2.68	0.42
2:G:326:ILE:HD12	2:G:326:ILE:H	1.84	0.42
2:H:304:VAL:HG21	2:H:450:MET:HE1	2.00	0.42
2:L:449:SER:HB2	2:P:452:LYS:HZ3	1.83	0.42
2:N:317:ASP:OD1	2:N:333:LYS:NZ	2.52	0.42
1:O:30:VAL:CA	3:O:250:HOH:O	2.65	0.42
2:P:303:ILE:HD11	2:P:333:LYS:HB3	2.02	0.42
1:U:182:ARG:HA	1:U:235:VAL:HB	2.02	0.42
1:U:85:ARG:HH11	1:U:85:ARG:CG	2.29	0.42
2:X:450:MET:HE3	2:X:470:ALA:CB	2.50	0.42
1:Y:151:PRO:HD2	3:Y:250:HOH:O	2.18	0.42
1:A:134:LYS:HE2	1:A:134:LYS:HA	2.01	0.42
1:K:56:LEU:HD13	1:K:99:LEU:HD23	2.00	0.42
2:L:456:GLN:NE2	2:L:465:ARG:NH1	2.67	0.42
1:O:30:VAL:HG22	1:O:43:ALA:CB	2.49	0.42
1:U:71:PHE:HB3	1:U:120:VAL:HG11	2.01	0.42
2:G:329:ARG:NH2	2:V:476:ASP:O	2.52	0.42
2:X:307:LYS:HE2	2:X:435:GLY:HA2	2.01	0.42
2:X:456:GLN:NE2	2:X:465:ARG:NH1	2.68	0.42
1:A:71:PHE:HB3	1:A:120:VAL:HG11	2.02	0.42
2:E:306:LEU:HB2	2:E:313:VAL:HG13	2.01	0.42
2:E:349:ALA:N	3:E:69:HOH:O	2.52	0.42
2:G:441:SER:HB2	2:G:478:ASP:OD2	2.20	0.42
1:I:70:GLU:HB3	1:I:118:TYR:CD2	2.54	0.42
2:P:415:GLN:HE21	2:P:415:GLN:HB3	1.60	0.42
2:R:436:TYR:CD2	2:R:450:MET:HG2	2.55	0.42
1:B:28:LYS:HE2	1:B:46:PRO:HD3	2.02	0.41
2:C:301:THR:HG23	2:C:333:LYS:HD3	2.02	0.41
2:G:324:ASN:ND2	2:G:324:ASN:H	2.18	0.41
2:J:301:THR:HA	2:J:333:LYS:HZ2	1.85	0.41
2:N:334:VAL:HG22	3:N:120:HOH:O	2.20	0.41
2:T:505:VAL:HA	2:T:506:PRO:HD3	1.89	0.41
1:O:112:THR:CG2	1:U:115:ALA:HB3	2.49	0.41
1:W:123:CYS:HA	1:W:139:TYR:O	2.20	0.41
1:F:205:VAL:HG12	1:F:206:ALA:H	1.84	0.41
1:F:28:LYS:HE2	1:F:46:PRO:HD3	2.02	0.41
2:H:301:THR:HA	2:H:333:LYS:HZ3	1.84	0.41
1:A:89:TYR:HD1	2:P:382:ARG:HD3	1.84	0.41
1:S:217:ARG:HA	1:S:218:PRO:HD3	1.96	0.41
2:V:355:PHE:HD1	2:V:355:PHE:HA	1.76	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:LEU:HD12	1:B:222:PHE:HD1	1.86	0.41
1:D:182:ARG:HA	1:D:235:VAL:HB	2.02	0.41
1:D:43:ALA:HA	3:D:251:HOH:O	2.20	0.41
2:E:380:ILE:HD11	2:E:421:VAL:HG21	2.02	0.41
1:F:97:ARG:HH11	1:M:49:SER:HB2	1.86	0.41
1:K:30:VAL:HG23	1:K:65:ALA:HB2	2.03	0.41
1:M:85:ARG:NH1	1:M:85:ARG:CG	2.82	0.41
1:O:182:ARG:HA	1:O:235:VAL:HB	2.01	0.41
1:Q:56:LEU:HD13	1:Q:99:LEU:HD23	2.01	0.41
2:T:378:GLY:HA3	3:1:252:HOH:O	2.20	0.41
1:1:74:LEU:HD11	1:1:107:LEU:HD21	2.02	0.41
2:2:301:THR:N	2:2:441:SER:HG	2.17	0.41
1:B:205:VAL:HG12	1:B:206:ALA:H	1.84	0.41
2:C:441:SER:HB2	2:C:478:ASP:OD2	2.20	0.41
2:C:513:LEU:O	2:C:516:ALA:HB3	2.19	0.41
1:F:56:LEU:O	2:G:368:LYS:HD2	2.20	0.41
2:J:449:SER:HB2	2:Z:452:LYS:HZ3	1.85	0.41
1:K:39:VAL:N	3:K:249:HOH:O	2.53	0.41
2:N:456:GLN:HE22	2:N:465:ARG:NH1	2.18	0.41
1:S:57:TYR:O	1:S:58:ASP:C	2.59	0.41
2:Z:318:ARG:HD2	2:Z:492:PRO:HA	2.01	0.41
1:D:55:GLU:OE2	1:D:220:ARG:HD2	2.20	0.41
2:G:475:ALA:HA	2:G:481:THR:HB	2.03	0.41
2:J:437:GLN:OE1	2:J:447:LYS:HD3	2.21	0.41
2:J:496:ILE:HG13	2:J:505:VAL:CG2	2.50	0.41
1:F:97:ARG:NH1	1:M:49:SER:O	2.53	0.41
1:S:213:LEU:HD12	1:S:222:PHE:HD1	1.85	0.41
2:T:337:THR:HG21	2:T:359:TYR:CD2	2.55	0.41
2:V:514:ALA:O	2:V:518:ILE:HG13	2.19	0.41
1:W:182:ARG:HB2	1:W:182:ARG:NH1	2.35	0.41
2:X:496:ILE:O	2:X:502:ALA:HA	2.19	0.41
2:Z:313:VAL:HG23	2:Z:496:ILE:HG12	2.02	0.41
2:E:475:ALA:HB2	2:E:481:THR:HG22	2.01	0.41
1:I:217:ARG:HA	1:I:218:PRO:HD3	1.98	0.41
2:J:380:ILE:HD11	2:J:421:VAL:HG21	2.02	0.41
2:J:456:GLN:HE22	2:J:465:ARG:NH1	2.18	0.41
2:J:514:ALA:O	2:J:518:ILE:HG13	2.20	0.41
1:K:83:ASP:OD2	2:L:365:HIS:CD2	2.71	0.41
2:P:355:PHE:HA	2:P:355:PHE:HD1	1.78	0.41
2:T:412:SER:O	2:T:414:PRO:HD3	2.20	0.41
1:A:10:GLU:HA	1:O:19:LEU:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:205:VAL:C	1:D:207:SER:N	2.74	0.41
1:K:205:VAL:C	1:K:207:SER:N	2.74	0.41
1:K:40:LEU:HD12	1:K:212:VAL:CG1	2.50	0.41
2:X:485:ASP:OD2	2:X:488:ARG:CB	2.69	0.41
1:I:154:VAL:HG13	3:I:249:HOH:O	2.20	0.41
1:A:49:SER:HB2	1:B:97:ARG:HG3	2.03	0.41
1:B:135:ARG:HA	1:B:136:PRO:HD2	1.96	0.41
2:C:318:ARG:HD2	2:C:492:PRO:HA	2.03	0.41
2:C:514:ALA:O	2:C:518:ILE:HG13	2.21	0.41
2:E:321:THR:HG21	2:E:480:ALA:HB1	2.02	0.41
2:H:324:ASN:N	2:H:324:ASN:ND2	2.68	0.41
1:M:64:ALA:HB2	1:M:122:LEU:HG	2.02	0.41
1:O:30:VAL:HG23	1:O:65:ALA:HB2	2.02	0.41
1:Q:182:ARG:HA	1:Q:235:VAL:HB	2.02	0.41
1:Q:55:GLU:OE2	1:Q:220:ARG:CD	2.69	0.41
2:R:321:THR:HG21	2:R:480:ALA:HB1	2.03	0.41
1:W:205:VAL:C	1:W:207:SER:N	2.72	0.41
1:B:55:GLU:OE2	1:B:220:ARG:HD2	2.20	0.41
2:G:355:PHE:HD1	2:G:355:PHE:HA	1.77	0.41
1:I:55:GLU:OE2	1:I:220:ARG:CD	2.69	0.41
2:J:450:MET:HE3	2:J:470:ALA:CB	2.51	0.41
1:K:28:LYS:HB2	1:K:52:LYS:HZ2	1.83	0.41
1:K:63:ALA:O	1:K:156:MET:HE1	2.21	0.41
2:L:301:THR:HA	2:L:333:LYS:HZ3	1.86	0.41
1:S:182:ARG:HA	1:S:235:VAL:HB	2.01	0.41
2:X:320:SER:HB3	2:X:328:GLY:HA3	2.02	0.41
2:X:324:ASN:HD22	2:X:324:ASN:N	2.16	0.41
2:X:412:SER:O	2:X:414:PRO:HD3	2.21	0.41
1:Y:55:GLU:OE2	1:Y:220:ARG:CD	2.68	0.41
1:A:189:ARG:NH2	1:A:237:GLN:HB3	2.35	0.41
1:B:12:ALA:O	1:B:16:ARG:HG2	2.20	0.41
2:R:415:GLN:HB3	2:R:415:GLN:HE21	1.60	0.41
1:S:55:GLU:OE2	1:S:220:ARG:CD	2.69	0.41
2:Z:393:ALA:HB1	2:Z:398:LEU:HB2	2.03	0.41
1:U:93:ASP:HB3	2:2:366:TYR:OH	2.21	0.41
1:A:155:VAL:HG12	1:A:160:THR:HG22	2.03	0.41
1:F:182:ARG:HA	1:F:235:VAL:HB	2.03	0.41
1:K:55:GLU:OE2	1:K:220:ARG:HD2	2.21	0.41
1:O:43:ALA:HB1	3:O:252:HOH:O	2.21	0.41
2:R:318:ARG:HD2	2:R:492:PRO:HA	2.02	0.41
2:T:476:ASP:O	2:Z:329:ARG:NH2	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:VAL:C	1:A:207:SER:N	2.73	0.40
1:A:30:VAL:CG2	1:A:65:ALA:HB2	2.51	0.40
2:G:456:GLN:NE2	2:G:465:ARG:NH1	2.66	0.40
2:J:318:ARG:HD2	2:J:492:PRO:HA	2.03	0.40
1:K:205:VAL:HG12	1:K:206:ALA:H	1.85	0.40
1:O:163:ILE:HG23	1:O:188:LEU:HA	2.03	0.40
1:Q:12:ALA:O	1:Q:16:ARG:HG2	2.20	0.40
1:F:85:ARG:CG	1:F:85:ARG:NH1	2.80	0.40
2:G:397:GLY:O	2:G:399:LEU:N	2.54	0.40
1:I:134:LYS:HG3	1:I:135:ARG:N	2.36	0.40
1:K:48:ARG:HH22	1:M:135:ARG:HB3	1.86	0.40
1:Q:71:PHE:HB3	1:Q:120:VAL:HG11	2.04	0.40
2:V:393:ALA:HB1	2:V:398:LEU:HB2	2.03	0.40
1:W:163:ILE:HG23	1:W:188:LEU:HA	2.03	0.40
1:W:30:VAL:HG23	1:W:65:ALA:HB2	2.02	0.40
1:W:40:LEU:HD12	1:W:212:VAL:CG1	2.51	0.40
1:D:15:GLU:OE1	1:K:8:SER:HA	2.21	0.40
2:H:452:LYS:HZ3	2:E:449:SER:HB2	1.85	0.40
1:F:163:ILE:HG23	1:F:188:LEU:HA	2.04	0.40
2:H:393:ALA:HB1	2:H:398:LEU:HB2	2.04	0.40
2:J:321:THR:HG21	2:J:480:ALA:HB1	2.02	0.40
1:M:127:VAL:HG22	1:M:215:ALA:HB2	2.04	0.40
1:O:85:ARG:NH1	1:O:85:ARG:CG	2.79	0.40
2:X:301:THR:HG23	2:X:333:LYS:HD3	2.02	0.40
2:X:505:VAL:HA	2:X:506:PRO:HD3	1.91	0.40
2:2:496:ILE:HG13	2:2:505:VAL:CG2	2.52	0.40
2:C:321:THR:HG21	2:C:480:ALA:HB1	2.03	0.40
1:D:40:LEU:HD12	1:D:212:VAL:CG1	2.51	0.40
2:H:469:GLU:HG3	2:H:517:ILE:HG21	2.02	0.40
2:N:453:LEU:HB2	2:N:466:VAL:HG13	2.04	0.40
1:O:40:LEU:HD12	1:O:212:VAL:CG1	2.52	0.40
2:N:329:ARG:NH2	2:P:476:ASP:O	2.54	0.40
1:Q:134:LYS:HA	1:Q:134:LYS:HE2	2.03	0.40
1:U:55:GLU:OE2	1:U:220:ARG:HD2	2.22	0.40
1:U:40:LEU:HD12	1:U:212:VAL:CG1	2.51	0.40
2:Z:301:THR:N	2:Z:441:SER:HG	2.19	0.40
1:1:134:LYS:HA	1:1:134:LYS:HE2	2.02	0.40
1:A:56:LEU:HD13	1:A:99:LEU:HD23	2.04	0.40
1:K:182:ARG:HA	1:K:235:VAL:HB	2.02	0.40
1:M:134:LYS:HE2	1:M:134:LYS:HA	2.04	0.40
1:M:217:ARG:HA	1:M:218:PRO:HD3	1.97	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:496:ILE:HG13	2:N:505:VAL:CG2	2.51	0.40
1:Q:135:ARG:CB	1:Y:48:ARG:HH22	2.35	0.40
2:T:393:ALA:HB1	2:T:398:LEU:HB2	2.03	0.40

All (14) 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)
2:G:465:ARG:NE	2:X:458:THR:CG2[2_554]	1.40	0.80
1:A:236:ASP:O	1:D:133:THR:OG1[2_655]	1.59	0.61
2:N:456:GLN:NE2	2:Z:415:GLN:OE1[1_565]	1.83	0.37
1:W:228:SER:O	2:2:414:PRO:CB[2_544]	1.97	0.23
2:J:456:GLN:NE2	2:V:415:GLN:OE1[1_545]	2.00	0.20
1:A:170:SER:CB	1:D:216:ASN:OD1[2_655]	2.06	0.14
1:A:169:GLU:C	1:D:216:ASN:ND2[2_655]	2.07	0.13
1:I:190:ALA:O	1:U:14:ARG:NE[2_545]	2.08	0.12
1:I:192:SER:N	1:U:14:ARG:NH2[2_545]	2.08	0.12
2:E:519:GLU:OE1	2:P:412:SER:O[2_645]	2.09	0.11
2:G:465:ARG:CD	2:X:458:THR:OG1[2_554]	2.11	0.09
2:J:465:ARG:CD	2:V:415:GLN:NE2[1_545]	2.15	0.05
2:G:465:ARG:CD	2:X:458:THR:CG2[2_554]	2.16	0.04
1:A:169:GLU:O	1:D:216:ASN:ND2[2_655]	2.19	0.01

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	1	216/250 (86%)	188 (87%)	22 (10%)	6 (3%)	5	30
1	A	216/250 (86%)	192 (89%)	19 (9%)	5 (2%)	7	35
1	B	216/250 (86%)	189 (88%)	21 (10%)	6 (3%)	5	30
1	D	216/250 (86%)	193 (89%)	18 (8%)	5 (2%)	7	35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	216/250 (86%)	190 (88%)	20 (9%)	6 (3%)	5	30
1	I	216/250 (86%)	189 (88%)	22 (10%)	5 (2%)	7	35
1	K	216/250 (86%)	191 (88%)	20 (9%)	5 (2%)	7	35
1	M	216/250 (86%)	187 (87%)	24 (11%)	5 (2%)	7	35
1	O	216/250 (86%)	188 (87%)	23 (11%)	5 (2%)	7	35
1	Q	216/250 (86%)	188 (87%)	23 (11%)	5 (2%)	7	35
1	S	216/250 (86%)	189 (88%)	22 (10%)	5 (2%)	7	35
1	U	216/250 (86%)	189 (88%)	22 (10%)	5 (2%)	7	35
1	W	216/250 (86%)	192 (89%)	19 (9%)	5 (2%)	7	35
1	Y	216/250 (86%)	187 (87%)	23 (11%)	6 (3%)	5	30
2	2	220/240 (92%)	195 (89%)	22 (10%)	3 (1%)	12	47
2	C	220/240 (92%)	195 (89%)	22 (10%)	3 (1%)	12	47
2	E	220/240 (92%)	196 (89%)	19 (9%)	5 (2%)	7	35
2	G	220/240 (92%)	196 (89%)	18 (8%)	6 (3%)	5	31
2	H	220/240 (92%)	193 (88%)	22 (10%)	5 (2%)	7	35
2	J	220/240 (92%)	194 (88%)	22 (10%)	4 (2%)	9	42
2	L	220/240 (92%)	194 (88%)	21 (10%)	5 (2%)	7	35
2	N	220/240 (92%)	198 (90%)	16 (7%)	6 (3%)	5	31
2	P	220/240 (92%)	195 (89%)	19 (9%)	6 (3%)	5	31
2	R	220/240 (92%)	193 (88%)	22 (10%)	5 (2%)	7	35
2	T	220/240 (92%)	195 (89%)	19 (9%)	6 (3%)	5	31
2	V	220/240 (92%)	194 (88%)	21 (10%)	5 (2%)	7	35
2	X	220/240 (92%)	193 (88%)	23 (10%)	4 (2%)	9	42
2	Z	220/240 (92%)	192 (87%)	24 (11%)	4 (2%)	9	42
All	All	6104/6860 (89%)	5375 (88%)	588 (10%)	141 (2%)	7	35

All (141) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	128	ALA
1	B	128	ALA
1	D	128	ALA
1	F	128	ALA
1	I	128	ALA

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Mol	Chain	Res	Type
1	K	128	ALA
1	M	128	ALA
1	O	128	ALA
1	Q	128	ALA
1	S	128	ALA
1	U	128	ALA
1	W	128	ALA
1	Y	128	ALA
1	1	128	ALA
1	A	58	ASP
1	B	58	ASP
1	D	58	ASP
1	I	58	ASP
1	I	206	ALA
1	K	58	ASP
1	M	58	ASP
1	Q	58	ASP
1	S	58	ASP
1	S	206	ALA
2	T	317	ASP
1	U	58	ASP
2	V	317	ASP
1	W	58	ASP
1	Y	58	ASP
1	1	58	ASP
2	2	317	ASP
2	H	317	ASP
1	B	130	TYR
1	B	206	ALA
2	C	317	ASP
1	D	206	ALA
2	E	317	ASP
1	F	58	ASP
1	F	130	TYR
1	F	206	ALA
2	G	317	ASP
2	G	398	LEU
1	I	130	TYR
2	J	317	ASP
1	K	130	TYR
1	K	206	ALA
2	L	317	ASP

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Mol	Chain	Res	Type
1	M	130	TYR
1	M	206	ALA
2	N	398	LEU
1	O	58	ASP
1	O	130	TYR
1	O	206	ALA
2	P	317	ASP
1	Q	130	TYR
1	Q	206	ALA
2	R	317	ASP
1	S	130	TYR
2	T	398	LEU
1	U	130	TYR
1	U	206	ALA
1	W	206	ALA
2	X	317	ASP
1	Y	130	TYR
1	Y	206	ALA
2	Z	317	ASP
1	1	130	TYR
1	1	206	ALA
1	A	130	TYR
1	A	206	ALA
1	A	218	PRO
1	B	218	PRO
1	B	226	THR
2	C	434	GLU
1	D	130	TYR
1	F	218	PRO
1	I	218	PRO
1	K	218	PRO
1	M	218	PRO
1	O	218	PRO
1	Q	218	PRO
1	S	218	PRO
1	U	218	PRO
1	W	130	TYR
1	W	218	PRO
2	X	460	GLY
1	Y	218	PRO
2	Z	460	GLY
1	1	218	PRO

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Mol	Chain	Res	Type
2	2	460	GLY
2	H	460	GLY
1	D	218	PRO
1	F	226	THR
2	G	460	GLY
2	L	398	LEU
2	N	317	ASP
2	P	434	GLU
2	P	460	GLY
2	R	434	GLU
2	V	398	LEU
2	V	482	GLY
1	Y	226	THR
2	Z	434	GLU
1	1	226	THR
2	H	434	GLU
2	E	434	GLU
2	G	434	GLU
2	G	482	GLY
2	P	398	LEU
2	T	434	GLU
2	T	460	GLY
2	T	482	GLY
2	V	434	GLU
2	X	434	GLU
2	C	460	GLY
2	R	460	GLY
2	R	482	GLY
2	V	460	GLY
2	J	482	GLY
2	L	397	GLY
2	N	460	GLY
2	H	397	GLY
2	H	482	GLY
2	E	397	GLY
2	E	460	GLY
2	J	460	GLY
2	L	460	GLY
2	L	482	GLY
2	N	482	GLY
2	P	397	GLY
2	R	397	GLY

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Mol	Chain	Res	Type
2	X	482	GLY
2	E	482	GLY
2	G	397	GLY
2	J	397	GLY
2	P	482	GLY
2	T	397	GLY
2	Z	482	GLY
2	2	397	GLY
2	N	389	GLY
2	N	397	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	1	169/194 (87%)	156 (92%)	13 (8%)	14	45
1	A	169/194 (87%)	156 (92%)	13 (8%)	14	45
1	B	169/194 (87%)	156 (92%)	13 (8%)	14	45
1	D	169/194 (87%)	156 (92%)	13 (8%)	14	45
1	F	169/194 (87%)	155 (92%)	14 (8%)	12	42
1	I	169/194 (87%)	156 (92%)	13 (8%)	14	45
1	K	169/194 (87%)	156 (92%)	13 (8%)	14	45
1	M	169/194 (87%)	155 (92%)	14 (8%)	12	42
1	O	169/194 (87%)	156 (92%)	13 (8%)	14	45
1	Q	169/194 (87%)	155 (92%)	14 (8%)	12	42
1	S	169/194 (87%)	156 (92%)	13 (8%)	14	45
1	U	169/194 (87%)	156 (92%)	13 (8%)	14	45
1	W	169/194 (87%)	155 (92%)	14 (8%)	12	42
1	Y	169/194 (87%)	156 (92%)	13 (8%)	14	45
2	2	165/178 (93%)	150 (91%)	15 (9%)	10	35
2	C	165/178 (93%)	150 (91%)	15 (9%)	10	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	E	165/178 (93%)	150 (91%)	15 (9%)	10	35
2	G	165/178 (93%)	151 (92%)	14 (8%)	12	40
2	H	165/178 (93%)	150 (91%)	15 (9%)	10	35
2	J	165/178 (93%)	150 (91%)	15 (9%)	10	35
2	L	165/178 (93%)	150 (91%)	15 (9%)	10	35
2	N	165/178 (93%)	150 (91%)	15 (9%)	10	35
2	P	165/178 (93%)	151 (92%)	14 (8%)	12	40
2	R	165/178 (93%)	150 (91%)	15 (9%)	10	35
2	T	165/178 (93%)	150 (91%)	15 (9%)	10	35
2	V	165/178 (93%)	150 (91%)	15 (9%)	10	35
2	X	165/178 (93%)	150 (91%)	15 (9%)	10	35
2	Z	165/178 (93%)	149 (90%)	16 (10%)	9	33
All	All	4676/5208 (90%)	4281 (92%)	395 (8%)	12	40

All (395) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	LEU
1	A	85	ARG
1	A	92	ARG
1	A	93	ASP
1	A	113	GLU
1	A	134	LYS
1	A	135	ARG
1	A	140	ARG
1	A	147	ILE
1	A	150	GLU
1	A	173	GLU
1	A	182	ARG
1	A	203	LEU
2	H	318	ARG
2	H	319	ARG
2	H	324	ASN
2	H	329	ARG
2	H	332	ARG
2	H	345	ILE
2	H	355	PHE
2	H	391	LEU

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Mol	Chain	Res	Type
2	H	403	LEU
2	H	415	GLN
2	H	430	ASN
2	H	436	TYR
2	H	444	LEU
2	H	449	SER
2	H	508	SER
1	B	33	LEU
1	B	85	ARG
1	B	92	ARG
1	B	93	ASP
1	B	113	GLU
1	B	134	LYS
1	B	135	ARG
1	B	140	ARG
1	B	147	ILE
1	B	150	GLU
1	B	173	GLU
1	B	182	ARG
1	B	203	LEU
2	C	318	ARG
2	C	319	ARG
2	C	324	ASN
2	C	329	ARG
2	C	332	ARG
2	C	345	ILE
2	C	355	PHE
2	C	391	LEU
2	C	403	LEU
2	C	415	GLN
2	C	430	ASN
2	C	436	TYR
2	C	444	LEU
2	C	449	SER
2	C	508	SER
1	D	33	LEU
1	D	85	ARG
1	D	92	ARG
1	D	93	ASP
1	D	113	GLU
1	D	134	LYS
1	D	135	ARG

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Mol	Chain	Res	Type
1	D	140	ARG
1	D	147	ILE
1	D	150	GLU
1	D	173	GLU
1	D	182	ARG
1	D	203	LEU
2	E	318	ARG
2	E	319	ARG
2	E	324	ASN
2	E	329	ARG
2	E	332	ARG
2	E	345	ILE
2	E	355	PHE
2	E	391	LEU
2	E	403	LEU
2	E	415	GLN
2	E	430	ASN
2	E	436	TYR
2	E	444	LEU
2	E	449	SER
2	E	508	SER
1	F	33	LEU
1	F	85	ARG
1	F	92	ARG
1	F	93	ASP
1	F	113	GLU
1	F	134	LYS
1	F	135	ARG
1	F	140	ARG
1	F	144	ASP
1	F	147	ILE
1	F	150	GLU
1	F	173	GLU
1	F	182	ARG
1	F	203	LEU
2	G	318	ARG
2	G	319	ARG
2	G	324	ASN
2	G	329	ARG
2	G	345	ILE
2	G	355	PHE
2	G	391	LEU

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Mol	Chain	Res	Type
2	G	403	LEU
2	G	415	GLN
2	G	430	ASN
2	G	436	TYR
2	G	444	LEU
2	G	449	SER
2	G	508	SER
1	I	33	LEU
1	I	85	ARG
1	I	92	ARG
1	I	93	ASP
1	I	113	GLU
1	I	134	LYS
1	I	135	ARG
1	I	140	ARG
1	I	147	ILE
1	I	150	GLU
1	I	173	GLU
1	I	182	ARG
1	I	203	LEU
2	J	318	ARG
2	J	319	ARG
2	J	324	ASN
2	J	329	ARG
2	J	332	ARG
2	J	345	ILE
2	J	355	PHE
2	J	391	LEU
2	J	403	LEU
2	J	415	GLN
2	J	430	ASN
2	J	436	TYR
2	J	444	LEU
2	J	449	SER
2	J	508	SER
1	K	33	LEU
1	K	85	ARG
1	K	92	ARG
1	K	93	ASP
1	K	113	GLU
1	K	134	LYS
1	K	135	ARG

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Mol	Chain	Res	Type
1	K	140	ARG
1	K	147	ILE
1	K	150	GLU
1	K	173	GLU
1	K	182	ARG
1	K	203	LEU
2	L	318	ARG
2	L	319	ARG
2	L	324	ASN
2	L	329	ARG
2	L	332	ARG
2	L	345	ILE
2	L	355	PHE
2	L	391	LEU
2	L	403	LEU
2	L	415	GLN
2	L	430	ASN
2	L	436	TYR
2	L	444	LEU
2	L	449	SER
2	L	508	SER
1	M	33	LEU
1	M	85	ARG
1	M	92	ARG
1	M	93	ASP
1	M	113	GLU
1	M	134	LYS
1	M	135	ARG
1	M	140	ARG
1	M	144	ASP
1	M	147	ILE
1	M	150	GLU
1	M	173	GLU
1	M	182	ARG
1	M	203	LEU
2	N	318	ARG
2	N	319	ARG
2	N	324	ASN
2	N	329	ARG
2	N	332	ARG
2	N	345	ILE
2	N	355	PHE

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Mol	Chain	Res	Type
2	N	391	LEU
2	N	403	LEU
2	N	415	GLN
2	N	430	ASN
2	N	436	TYR
2	N	444	LEU
2	N	449	SER
2	N	508	SER
1	O	33	LEU
1	O	85	ARG
1	O	92	ARG
1	O	113	GLU
1	O	134	LYS
1	O	135	ARG
1	O	140	ARG
1	O	147	ILE
1	O	150	GLU
1	O	173	GLU
1	O	179	ASP
1	O	182	ARG
1	O	203	LEU
2	P	318	ARG
2	P	319	ARG
2	P	324	ASN
2	P	329	ARG
2	P	332	ARG
2	P	345	ILE
2	P	391	LEU
2	P	403	LEU
2	P	415	GLN
2	P	430	ASN
2	P	436	TYR
2	P	444	LEU
2	P	449	SER
2	P	508	SER
1	Q	33	LEU
1	Q	85	ARG
1	Q	92	ARG
1	Q	93	ASP
1	Q	113	GLU
1	Q	134	LYS
1	Q	135	ARG

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Mol	Chain	Res	Type
1	Q	140	ARG
1	Q	147	ILE
1	Q	150	GLU
1	Q	173	GLU
1	Q	179	ASP
1	Q	182	ARG
1	Q	203	LEU
2	R	318	ARG
2	R	319	ARG
2	R	324	ASN
2	R	329	ARG
2	R	332	ARG
2	R	345	ILE
2	R	355	PHE
2	R	391	LEU
2	R	403	LEU
2	R	415	GLN
2	R	430	ASN
2	R	436	TYR
2	R	444	LEU
2	R	449	SER
2	R	508	SER
1	S	33	LEU
1	S	85	ARG
1	S	92	ARG
1	S	93	ASP
1	S	113	GLU
1	S	134	LYS
1	S	135	ARG
1	S	140	ARG
1	S	147	ILE
1	S	150	GLU
1	S	173	GLU
1	S	182	ARG
1	S	203	LEU
2	T	318	ARG
2	T	319	ARG
2	T	324	ASN
2	T	329	ARG
2	T	332	ARG
2	T	345	ILE
2	T	355	PHE

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Mol	Chain	Res	Type
2	T	391	LEU
2	T	403	LEU
2	T	415	GLN
2	T	430	ASN
2	T	436	TYR
2	T	444	LEU
2	T	449	SER
2	T	508	SER
1	U	33	LEU
1	U	85	ARG
1	U	92	ARG
1	U	113	GLU
1	U	134	LYS
1	U	135	ARG
1	U	140	ARG
1	U	144	ASP
1	U	147	ILE
1	U	150	GLU
1	U	173	GLU
1	U	182	ARG
1	U	203	LEU
2	V	318	ARG
2	V	319	ARG
2	V	324	ASN
2	V	329	ARG
2	V	332	ARG
2	V	345	ILE
2	V	355	PHE
2	V	391	LEU
2	V	403	LEU
2	V	415	GLN
2	V	430	ASN
2	V	436	TYR
2	V	444	LEU
2	V	449	SER
2	V	508	SER
1	W	33	LEU
1	W	85	ARG
1	W	92	ARG
1	W	113	GLU
1	W	134	LYS
1	W	135	ARG

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Mol	Chain	Res	Type
1	W	140	ARG
1	W	144	ASP
1	W	147	ILE
1	W	150	GLU
1	W	173	GLU
1	W	179	ASP
1	W	182	ARG
1	W	203	LEU
2	X	318	ARG
2	X	319	ARG
2	X	324	ASN
2	X	329	ARG
2	X	345	ILE
2	X	355	PHE
2	X	391	LEU
2	X	403	LEU
2	X	415	GLN
2	X	430	ASN
2	X	436	TYR
2	X	444	LEU
2	X	449	SER
2	X	458	THR
2	X	508	SER
1	Y	33	LEU
1	Y	85	ARG
1	Y	92	ARG
1	Y	93	ASP
1	Y	113	GLU
1	Y	134	LYS
1	Y	135	ARG
1	Y	140	ARG
1	Y	147	ILE
1	Y	150	GLU
1	Y	173	GLU
1	Y	182	ARG
1	Y	203	LEU
2	Z	318	ARG
2	Z	319	ARG
2	Z	324	ASN
2	Z	329	ARG
2	Z	332	ARG
2	Z	341	THR

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Mol	Chain	Res	Type
2	Z	345	ILE
2	Z	355	PHE
2	Z	391	LEU
2	Z	403	LEU
2	Z	415	GLN
2	Z	430	ASN
2	Z	436	TYR
2	Z	444	LEU
2	Z	449	SER
2	Z	508	SER
1	1	33	LEU
1	1	85	ARG
1	1	92	ARG
1	1	93	ASP
1	1	113	GLU
1	1	134	LYS
1	1	135	ARG
1	1	140	ARG
1	1	147	ILE
1	1	150	GLU
1	1	173	GLU
1	1	182	ARG
1	1	203	LEU
2	2	318	ARG
2	2	319	ARG
2	2	324	ASN
2	2	329	ARG
2	2	332	ARG
2	2	345	ILE
2	2	355	PHE
2	2	391	LEU
2	2	403	LEU
2	2	415	GLN
2	2	430	ASN
2	2	436	TYR
2	2	444	LEU
2	2	449	SER
2	2	508	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (154) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	GLN
1	A	73	ASN
1	A	98	GLN
1	A	105	GLN
1	A	129	HIS
1	A	165	ASN
1	A	231	GLN
2	H	324	ASN
2	H	365	HIS
2	H	415	GLN
2	H	456	GLN
1	B	51	GLN
1	B	73	ASN
1	B	80	GLN
1	B	98	GLN
1	B	129	HIS
1	B	165	ASN
1	B	231	GLN
2	C	324	ASN
2	C	365	HIS
2	C	415	GLN
2	C	456	GLN
1	D	51	GLN
1	D	73	ASN
1	D	98	GLN
1	D	129	HIS
1	D	165	ASN
1	D	231	GLN
2	E	324	ASN
2	E	365	HIS
2	E	415	GLN
2	E	456	GLN
1	F	51	GLN
1	F	73	ASN
1	F	80	GLN
1	F	98	GLN
1	F	105	GLN
1	F	129	HIS
1	F	165	ASN
1	F	231	GLN
2	G	324	ASN
2	G	365	HIS
2	G	415	GLN

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Mol	Chain	Res	Type
2	G	456	GLN
1	I	51	GLN
1	I	73	ASN
1	I	80	GLN
1	I	98	GLN
1	I	105	GLN
1	I	129	HIS
1	I	165	ASN
1	I	231	GLN
2	J	324	ASN
2	J	365	HIS
2	J	415	GLN
2	J	456	GLN
1	K	51	GLN
1	K	73	ASN
1	K	80	GLN
1	K	98	GLN
1	K	129	HIS
1	K	165	ASN
1	K	231	GLN
2	L	324	ASN
2	L	365	HIS
2	L	415	GLN
2	L	456	GLN
1	M	51	GLN
1	M	80	GLN
1	M	98	GLN
1	M	129	HIS
1	M	165	ASN
1	M	231	GLN
2	N	324	ASN
2	N	365	HIS
2	N	415	GLN
2	N	456	GLN
1	O	51	GLN
1	O	73	ASN
1	O	98	GLN
1	O	105	GLN
1	O	129	HIS
1	O	165	ASN
1	O	231	GLN
2	P	324	ASN

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Mol	Chain	Res	Type
2	P	365	HIS
2	P	415	GLN
2	P	456	GLN
1	Q	51	GLN
1	Q	98	GLN
1	Q	105	GLN
1	Q	129	HIS
1	Q	165	ASN
1	Q	231	GLN
2	R	324	ASN
2	R	365	HIS
2	R	415	GLN
2	R	456	GLN
1	S	51	GLN
1	S	73	ASN
1	S	98	GLN
1	S	105	GLN
1	S	129	HIS
1	S	165	ASN
1	S	231	GLN
2	T	324	ASN
2	T	365	HIS
2	T	415	GLN
2	T	456	GLN
1	U	51	GLN
1	U	73	ASN
1	U	80	GLN
1	U	98	GLN
1	U	105	GLN
1	U	129	HIS
1	U	165	ASN
1	U	231	GLN
2	V	324	ASN
2	V	365	HIS
2	V	415	GLN
2	V	456	GLN
1	W	51	GLN
1	W	73	ASN
1	W	80	GLN
1	W	98	GLN
1	W	129	HIS
1	W	165	ASN

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Mol	Chain	Res	Type
1	W	231	GLN
2	X	324	ASN
2	X	365	HIS
2	X	415	GLN
2	X	456	GLN
1	Y	51	GLN
1	Y	73	ASN
1	Y	98	GLN
1	Y	129	HIS
1	Y	165	ASN
1	Y	231	GLN
2	Z	324	ASN
2	Z	365	HIS
2	Z	415	GLN
2	Z	456	GLN
1	1	51	GLN
1	1	73	ASN
1	1	80	GLN
1	1	98	GLN
1	1	105	GLN
1	1	129	HIS
1	1	165	ASN
1	1	231	GLN
2	2	324	ASN
2	2	365	HIS
2	2	415	GLN
2	2	456	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no 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, 95th 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	1	220/250 (88%)	0.63	20 (9%) 9 7	100, 100, 100, 100	0
1	A	220/250 (88%)	0.35	4 (1%) 68 58	100, 100, 100, 100	0
1	B	220/250 (88%)	0.35	6 (2%) 54 43	100, 100, 100, 100	0
1	D	220/250 (88%)	0.60	16 (7%) 15 10	100, 100, 100, 100	0
1	F	220/250 (88%)	0.42	11 (5%) 29 19	100, 100, 100, 100	0
1	I	220/250 (88%)	0.55	12 (5%) 25 16	100, 100, 100, 100	0
1	K	220/250 (88%)	0.98	38 (17%) 1 1	100, 100, 100, 100	0
1	M	220/250 (88%)	0.43	8 (3%) 42 31	100, 100, 100, 100	0
1	O	220/250 (88%)	0.68	20 (9%) 9 7	100, 100, 100, 100	0
1	Q	220/250 (88%)	0.77	25 (11%) 5 4	100, 100, 100, 100	0
1	S	220/250 (88%)	0.64	19 (8%) 10 8	100, 100, 100, 100	0
1	U	220/250 (88%)	0.66	17 (7%) 13 9	100, 100, 100, 100	0
1	W	220/250 (88%)	0.42	9 (4%) 37 27	100, 100, 100, 100	0
1	Y	220/250 (88%)	0.65	20 (9%) 9 7	100, 100, 100, 100	0
2	2	222/240 (92%)	0.40	6 (2%) 54 43	100, 100, 100, 100	0
2	C	222/240 (92%)	0.21	0 100 100	100, 100, 100, 100	0
2	E	222/240 (92%)	0.22	7 (3%) 47 35	100, 100, 100, 100	0
2	G	222/240 (92%)	0.22	0 100 100	100, 100, 100, 100	0
2	H	222/240 (92%)	0.20	0 100 100	100, 100, 100, 100	0
2	J	222/240 (92%)	0.21	0 100 100	100, 100, 100, 100	0
2	L	222/240 (92%)	0.20	2 (0%) 84 78	100, 100, 100, 100	0
2	N	222/240 (92%)	0.14	0 100 100	100, 100, 100, 100	0
2	P	222/240 (92%)	0.22	0 100 100	100, 100, 100, 100	0
2	R	222/240 (92%)	0.27	0 100 100	100, 100, 100, 100	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
2	T	222/240 (92%)	0.22	0 100 100	100, 100, 100, 100	0
2	V	222/240 (92%)	0.24	2 (0%) 84 78	100, 100, 100, 100	0
2	X	222/240 (92%)	0.13	0 100 100	100, 100, 100, 100	0
2	Z	222/240 (92%)	0.24	0 100 100	100, 100, 100, 100	0
All	All	6188/6860 (90%)	0.40	242 (3%) 39 29	100, 100, 100, 100	0

All (242) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	236	ASP	17.0
1	K	235	VAL	15.5
1	S	236	ASP	14.4
1	K	236	ASP	12.1
1	Q	236	ASP	11.5
1	S	235	VAL	11.3
1	O	236	ASP	11.1
1	U	236	ASP	10.8
1	A	235	VAL	10.5
1	M	235	VAL	10.5
1	F	236	ASP	10.4
1	O	237	GLN	10.3
1	B	236	ASP	9.6
1	I	235	VAL	9.6
1	D	235	VAL	9.5
1	Q	237	GLN	9.5
1	D	237	GLN	9.0
1	A	237	GLN	8.9
1	Q	235	VAL	8.8
1	W	235	VAL	8.7
1	U	235	VAL	8.5
1	O	235	VAL	8.4
1	I	236	ASP	8.4
1	1	236	ASP	7.6
1	K	237	GLN	7.5
1	Y	236	ASP	7.3
1	U	237	GLN	7.0
1	Y	237	GLN	6.7
1	B	235	VAL	6.2
1	W	236	ASP	6.1
1	1	235	VAL	6.1
1	A	236	ASP	6.0

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Mol	Chain	Res	Type	RSRZ
1	B	237	GLN	5.8
1	I	237	GLN	5.5
1	M	237	GLN	5.4
1	Y	235	VAL	5.4
1	F	237	GLN	5.2
1	F	235	VAL	5.2
1	Q	204	GLY	5.1
1	K	171	TYR	5.1
1	S	234	LEU	5.0
1	K	41	PHE	4.8
1	M	236	ASP	4.6
1	S	237	GLN	4.5
2	2	414	PRO	4.5
1	I	234	LEU	4.5
1	D	234	LEU	4.4
1	K	184	ALA	4.4
1	1	237	GLN	4.4
1	K	61	GLY	4.3
1	M	172	ALA	4.2
1	I	203	LEU	4.2
1	K	119	GLU	4.1
1	F	191	GLY	4.1
1	O	225	ILE	4.0
1	W	228	SER	4.0
1	Q	171	TYR	4.0
1	K	124	VAL	4.0
1	K	40	LEU	3.9
1	K	186	ALA	3.8
1	B	192	SER	3.8
1	I	204	GLY	3.8
1	1	10	GLU	3.7
1	O	167	LEU	3.7
1	1	192	SER	3.7
1	O	233	LEU	3.7
1	K	192	SER	3.6
1	K	127	VAL	3.6
1	K	143	TYR	3.6
1	Q	234	LEU	3.6
1	Y	204	GLY	3.6
1	K	204	GLY	3.6
1	F	171	TYR	3.5
1	O	171	TYR	3.4

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Mol	Chain	Res	Type	RSRZ
1	O	191	GLY	3.4
1	Q	137	GLU	3.4
2	E	363	LEU	3.3
1	U	132	GLU	3.3
1	K	64	ALA	3.3
1	B	41	PHE	3.2
1	W	237	GLN	3.2
1	K	125	ALA	3.2
1	U	177	LEU	3.2
1	1	188	LEU	3.2
1	S	171	TYR	3.2
1	Q	205	VAL	3.2
1	Y	41	PHE	3.1
1	1	167	LEU	3.1
1	Q	41	PHE	3.1
2	2	407	TYR	3.1
1	Y	205	VAL	3.1
1	Y	13	MET	3.0
1	M	234	LEU	3.0
1	U	234	LEU	3.0
1	O	41	PHE	3.0
1	K	167	LEU	3.0
1	K	153	PHE	3.0
1	K	34	ALA	3.0
1	O	143	TYR	3.0
1	1	171	TYR	3.0
1	D	41	PHE	3.0
1	I	172	ALA	2.9
1	O	172	ALA	2.9
1	U	225	ILE	2.9
1	1	41	PHE	2.9
1	Q	191	GLY	2.9
1	S	165	ASN	2.9
1	K	234	LEU	2.9
2	E	355	PHE	2.9
1	S	225	ILE	2.8
1	I	231	GLN	2.8
2	L	420	ILE	2.8
1	Q	233	LEU	2.8
1	S	167	LEU	2.8
1	1	191	GLY	2.8
1	W	188	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	O	234	LEU	2.8
1	D	163	ILE	2.8
1	K	33	LEU	2.8
2	E	350	ALA	2.8
1	W	163	ILE	2.8
1	Q	188	LEU	2.8
1	1	234	LEU	2.7
1	Y	154	VAL	2.7
1	S	111	PHE	2.7
1	Y	213	LEU	2.7
1	O	111	PHE	2.7
1	M	155	VAL	2.7
1	U	41	PHE	2.7
1	K	191	GLY	2.7
1	O	188	LEU	2.6
1	F	167	LEU	2.6
1	D	177	LEU	2.6
1	K	138	LEU	2.6
1	K	172	ALA	2.6
2	2	420	ILE	2.6
1	1	40	LEU	2.6
2	E	356	ALA	2.6
1	S	191	GLY	2.6
1	K	42	VAL	2.6
1	F	172	ALA	2.6
1	O	138	LEU	2.5
1	Q	155	VAL	2.5
1	Q	213	LEU	2.5
1	I	167	LEU	2.5
1	Y	171	TYR	2.5
1	D	188	LEU	2.5
2	E	337	THR	2.5
1	D	184	ALA	2.5
1	F	177	LEU	2.5
1	W	41	PHE	2.5
2	E	351	VAL	2.4
1	F	173	GLU	2.4
1	K	139	TYR	2.4
1	O	140	ARG	2.4
1	Q	225	ILE	2.4
2	E	343	THR	2.4
1	W	213	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	K	96	GLY	2.3
1	1	153	PHE	2.3
1	D	209	GLU	2.3
1	D	179	ASP	2.3
1	U	11	GLN	2.3
1	I	44	GLU	2.3
1	K	135	ARG	2.3
1	Q	21	ARG	2.3
1	I	159	THR	2.3
1	S	41	PHE	2.3
1	Q	230	LEU	2.3
1	1	124	VAL	2.3
1	W	229	ALA	2.3
1	U	203	LEU	2.3
1	K	65	ALA	2.3
1	I	227	GLY	2.3
1	U	33	LEU	2.2
1	Y	131	GLY	2.2
1	S	213	LEU	2.2
1	U	213	LEU	2.2
1	Y	138	LEU	2.2
1	K	60	VAL	2.2
1	Q	172	ALA	2.2
1	1	215	ALA	2.2
1	U	40	LEU	2.2
1	Y	210	VAL	2.2
1	Q	232	ALA	2.2
1	K	177	LEU	2.2
1	D	62	PHE	2.2
1	S	172	ALA	2.2
2	2	408	ASP	2.2
1	S	44	GLU	2.2
1	U	111	PHE	2.2
1	Q	183	ILE	2.2
1	1	163	ILE	2.2
1	A	177	LEU	2.2
1	D	141	ILE	2.2
1	S	135	ARG	2.2
1	D	178	THR	2.2
1	U	205	VAL	2.2
1	O	192	SER	2.2
1	Q	206	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	Q	203	LEU	2.1
1	U	138	LEU	2.1
1	1	147	ILE	2.1
1	M	177	LEU	2.1
1	K	111	PHE	2.1
1	1	33	LEU	2.1
1	D	185	VAL	2.1
1	Q	163	ILE	2.1
1	Y	233	LEU	2.1
1	Q	36	ALA	2.1
1	O	137	GLU	2.1
1	O	147	ILE	2.1
1	O	219	ARG	2.1
2	V	468	VAL	2.1
2	2	497	ILE	2.1
2	V	316	GLY	2.1
1	K	213	LEU	2.1
1	M	13	MET	2.1
1	Y	114	GLN	2.1
1	U	233	LEU	2.1
1	Y	177	LEU	2.1
1	1	13	MET	2.1
1	D	137	GLU	2.1
1	F	233	LEU	2.1
1	S	122	LEU	2.1
1	S	147	ILE	2.1
1	1	62	PHE	2.0
2	L	376	PHE	2.0
1	K	209	GLU	2.0
1	Y	10	GLU	2.0
1	S	13	MET	2.0
1	K	123	CYS	2.0
1	Y	155	VAL	2.0
1	K	122	LEU	2.0
1	B	171	TYR	2.0
1	Q	31	VAL	2.0
1	S	224	ARG	2.0
1	Y	40	LEU	2.0
1	Y	143	TYR	2.0
1	F	156	MET	2.0
2	2	325	MET	2.0
1	K	188	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 carbohydrates 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.