



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 04:23 AM UTC

PDB ID : 1PMA / pdb_00001pma
Title : PROTEASOME FROM THERMOPLASMA ACIDOPHILUM
Authors : Loewe, J.; Stock, D.; Jap, B.; Zwickl, P.; Baumeister, W.; Huber, R.
Deposited on : 1994-12-19
Resolution : 3.40 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

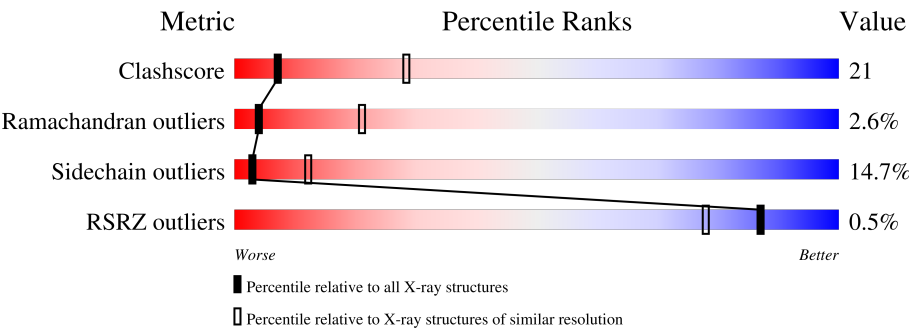
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	A	233	% 45%43%7%5%
1	C	233	% 49%36%9%5%
1	D	233	% 46%39%9%5%
1	E	233	% 46%38%10%5%
1	F	233	42%45%7%5%
1	G	233	% 41%47%6%5%
1	H	233	47%41%7%5%

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Mol	Chain	Length	Quality of chain
1	I	233	
1	J	233	
1	K	233	
1	L	233	
1	M	233	
1	N	233	
1	O	233	
2	1	211	
2	2	211	
2	B	211	
2	P	211	
2	Q	211	
2	R	211	
2	S	211	
2	T	211	
2	U	211	
2	V	211	
2	W	211	
2	X	211	
2	Y	211	
2	Z	211	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 56294 atoms, of which 10402 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 PROTEASOME.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	221	Total	C	H	N	O	S	0	0	0
			2113	1092	393	290	335	3			
1	C	221	Total	C	H	N	O	S	0	0	0
			2113	1092	393	290	335	3			
1	D	221	Total	C	H	N	O	S	0	0	0
			2113	1092	393	290	335	3			
1	E	221	Total	C	H	N	O	S	0	0	0
			2113	1092	393	290	335	3			
1	F	221	Total	C	H	N	O	S	0	0	0
			2113	1092	393	290	335	3			
1	G	221	Total	C	H	N	O	S	0	0	0
			2113	1092	393	290	335	3			
1	H	221	Total	C	H	N	O	S	0	0	0
			2113	1092	393	290	335	3			
1	I	221	Total	C	H	N	O	S	0	0	0
			2113	1092	393	290	335	3			
1	J	221	Total	C	H	N	O	S	0	0	0
			2113	1092	393	290	335	3			
1	K	221	Total	C	H	N	O	S	0	0	0
			2113	1092	393	290	335	3			
1	L	221	Total	C	H	N	O	S	0	0	0
			2113	1092	393	290	335	3			
1	M	221	Total	C	H	N	O	S	0	0	0
			2113	1092	393	290	335	3			
1	N	221	Total	C	H	N	O	S	0	0	0
			2113	1092	393	290	335	3			
1	O	221	Total	C	H	N	O	S	0	0	0
			2113	1092	393	290	335	3			

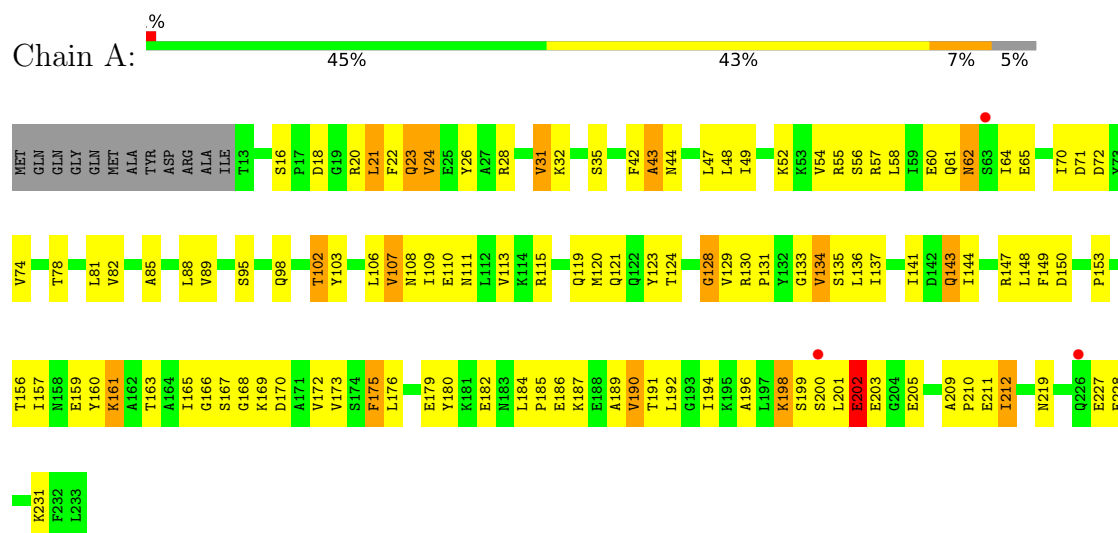
- Molecule 2 is a protein called PROTEASOME.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	203	Total 1908	C 985	H 350	N 264	O 298	S 11	0	0	0
2	P	203	Total 1908	C 985	H 350	N 264	O 298	S 11	0	0	0
2	Q	203	Total 1908	C 985	H 350	N 264	O 298	S 11	0	0	0
2	R	203	Total 1908	C 985	H 350	N 264	O 298	S 11	0	0	0
2	S	203	Total 1908	C 985	H 350	N 264	O 298	S 11	0	0	0
2	T	203	Total 1908	C 985	H 350	N 264	O 298	S 11	0	0	0
2	U	203	Total 1908	C 985	H 350	N 264	O 298	S 11	0	0	0
2	V	203	Total 1908	C 985	H 350	N 264	O 298	S 11	0	0	0
2	W	203	Total 1908	C 985	H 350	N 264	O 298	S 11	0	0	0
2	X	203	Total 1908	C 985	H 350	N 264	O 298	S 11	0	0	0
2	Y	203	Total 1908	C 985	H 350	N 264	O 298	S 11	0	0	0
2	Z	203	Total 1908	C 985	H 350	N 264	O 298	S 11	0	0	0
2	1	203	Total 1908	C 985	H 350	N 264	O 298	S 11	0	0	0
2	2	203	Total 1908	C 985	H 350	N 264	O 298	S 11	0	0	0

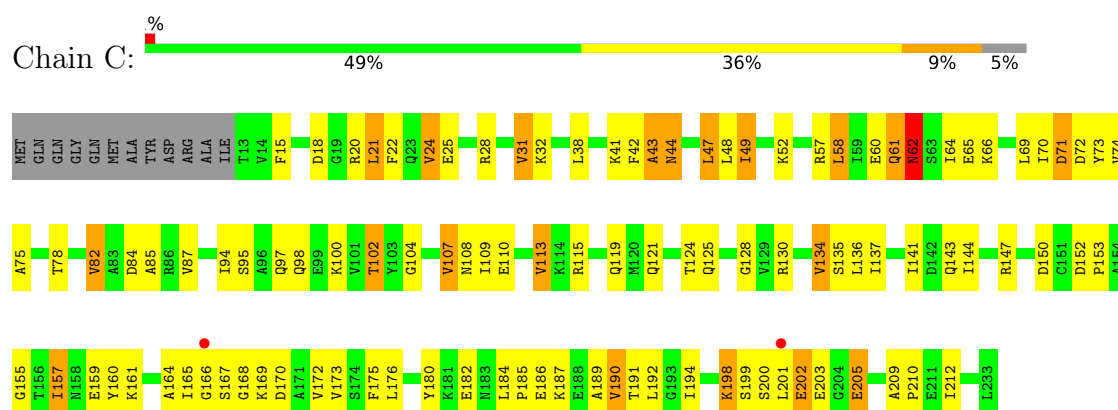
3 Residue-property plots

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

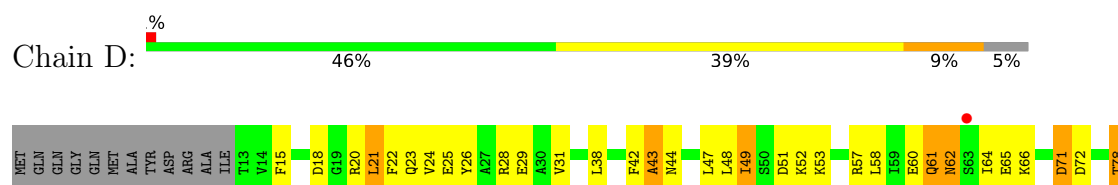
• Molecule 1: PROTEASOME

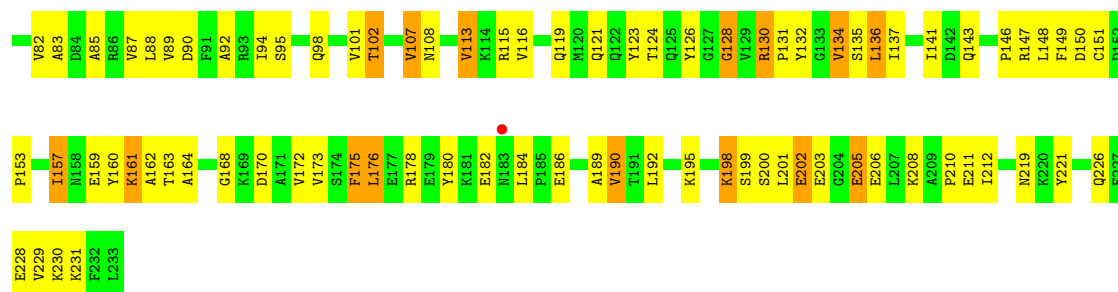


• Molecule 1: PROTEASOME

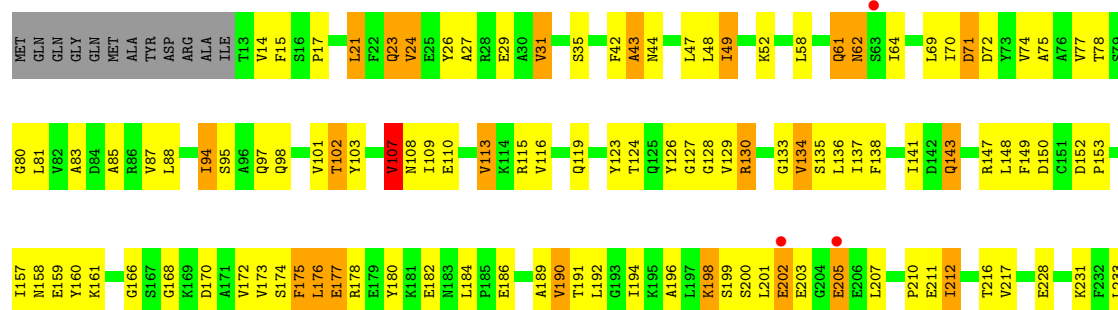


• Molecule 1: PROTEASOME

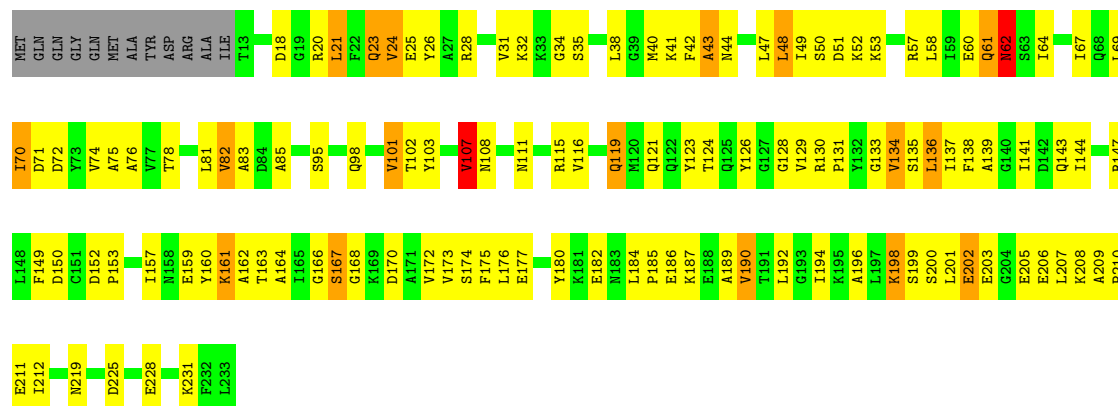




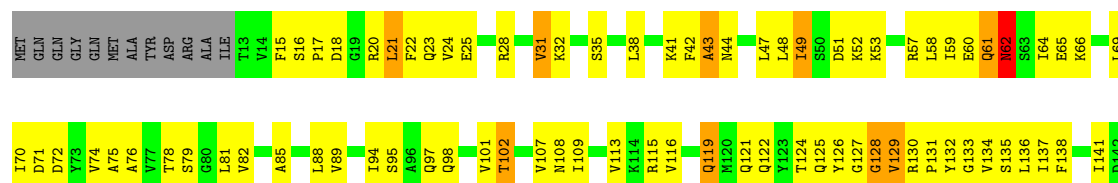
• Molecule 1: PROTEASOME

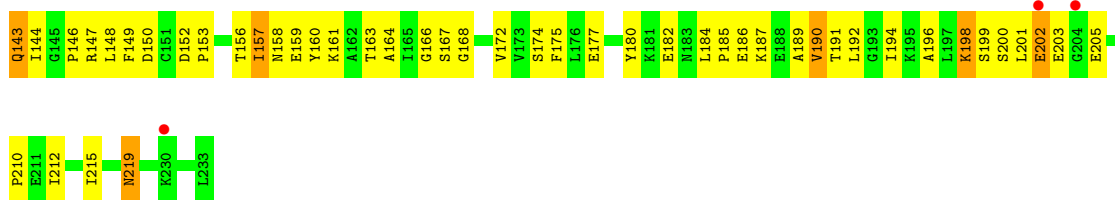


• Molecule 1: PROTEASOME



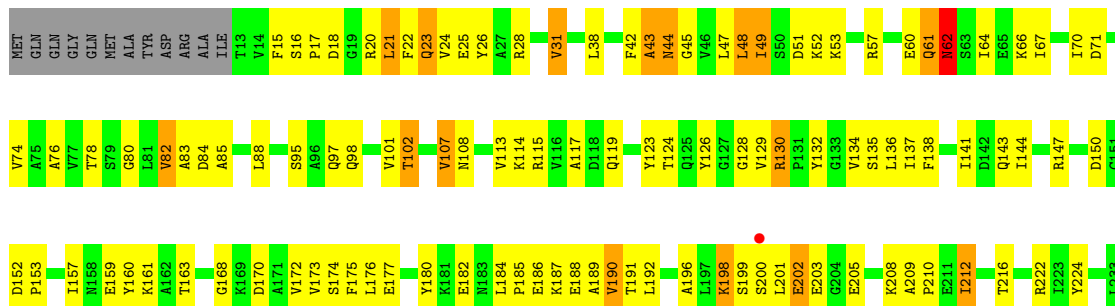
• Molecule 1: PROTEASOME





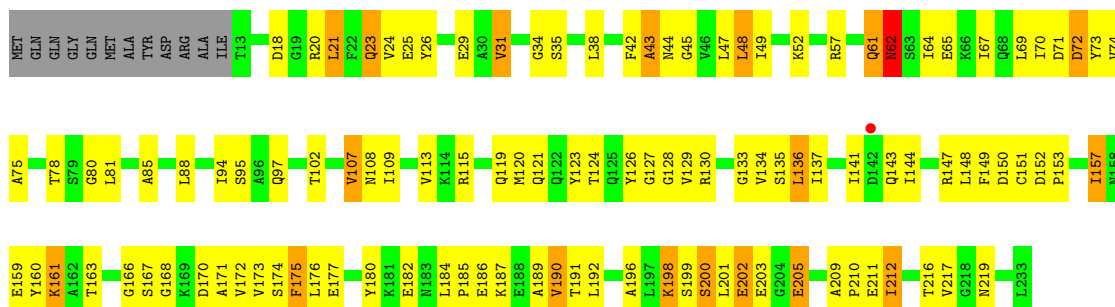
• Molecule 1: PROTEASOME

Chain H: 47% 41% 7% 5%



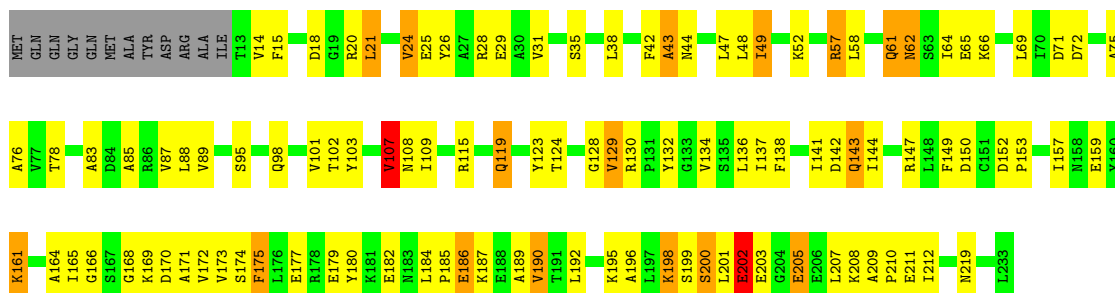
• Molecule 1: PROTEASOME

Chain I: 46% 40% 8% 5%



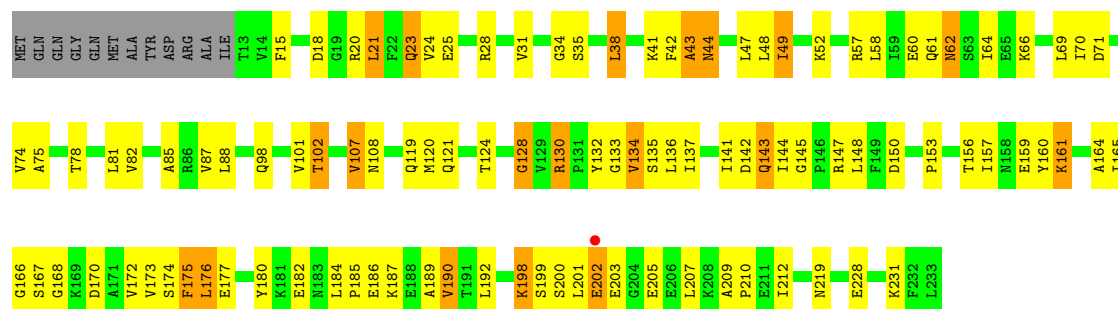
• Molecule 1: PROTEASOME

Chain J: 48% 38% 7% 5%

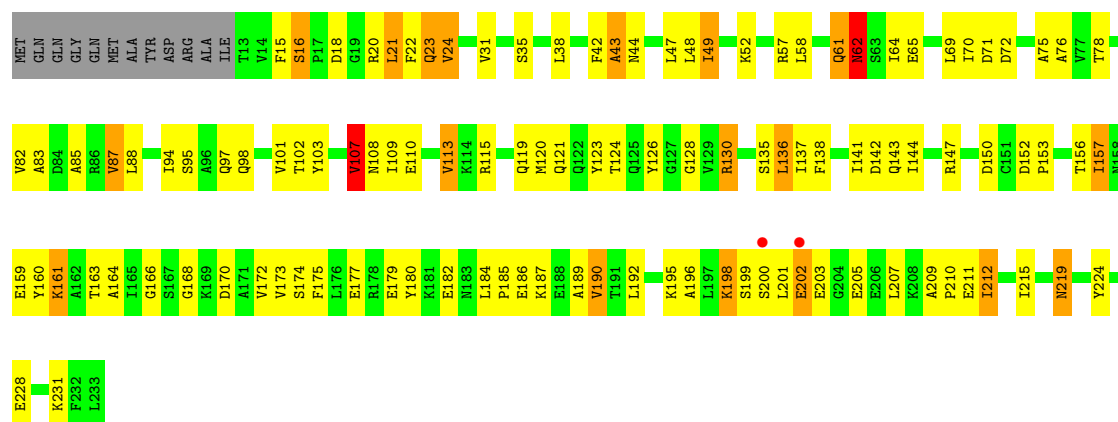


• Molecule 1: PROTEASOME

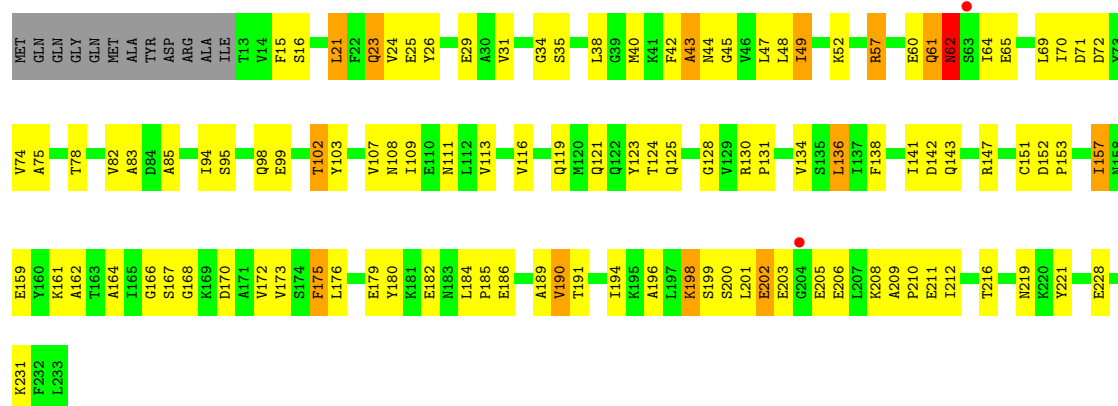
Chain K: 50% 36% 8% 5%



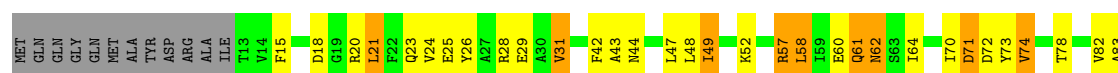
• Molecule 1: PROTEASOME

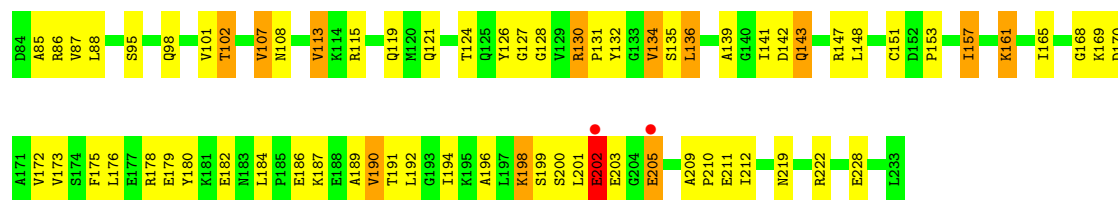


• Molecule 1: PROTEASOME

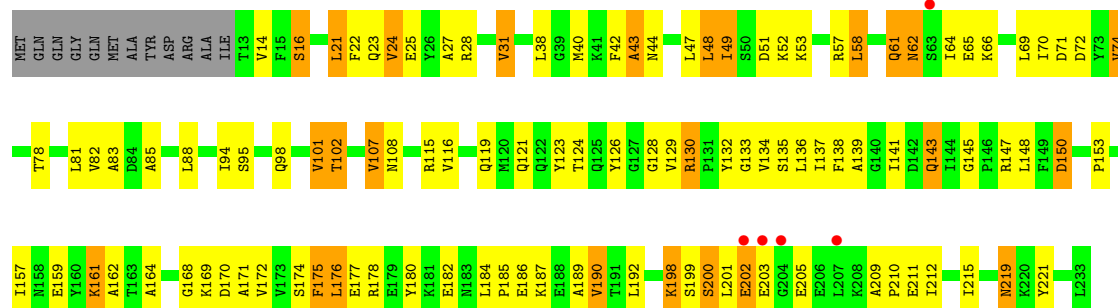


• Molecule 1: PROTEASOME

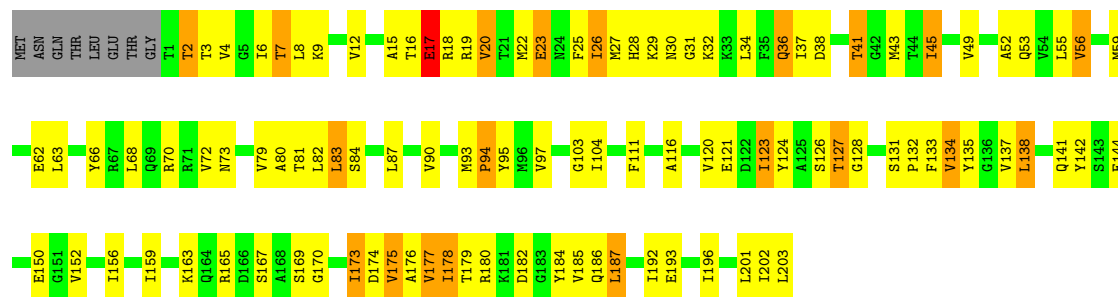




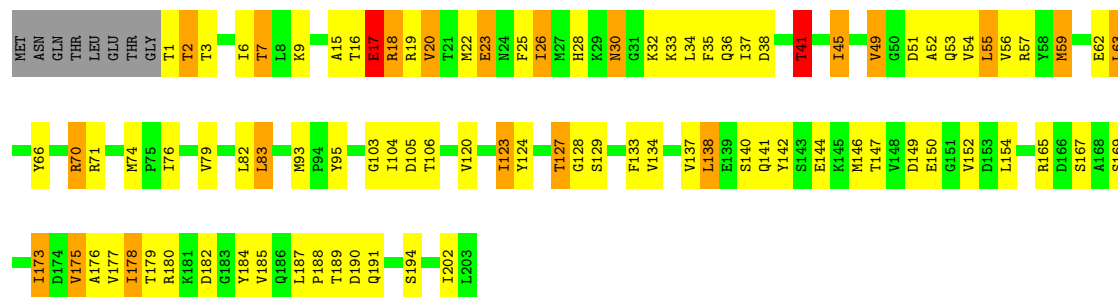
• Molecule 1: PROTEASOME



• Molecule 2: PROTEASOME

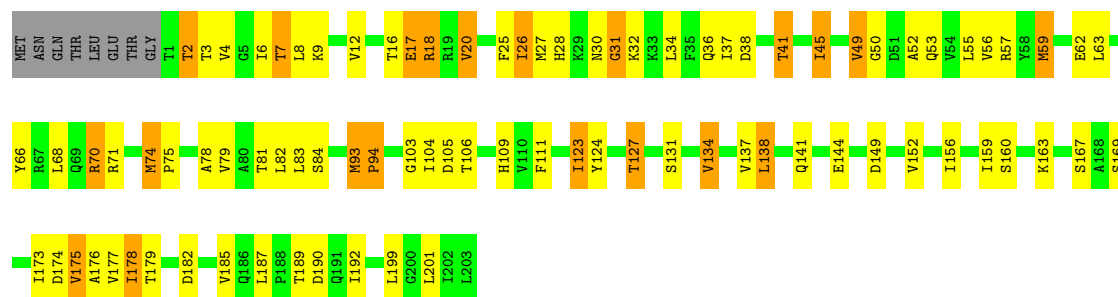


• Molecule 2: PROTEASOME



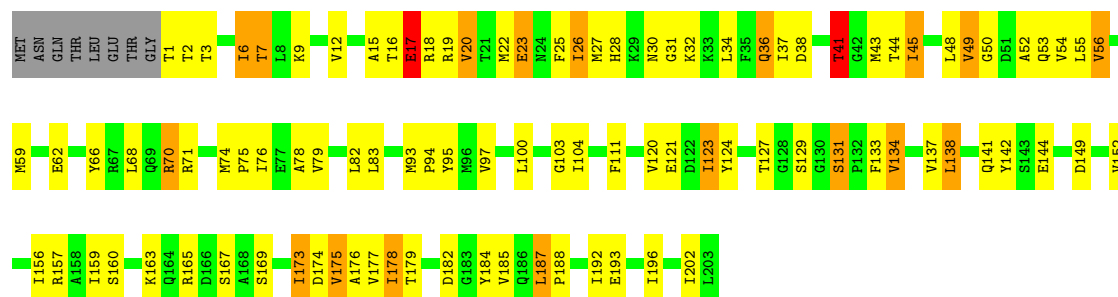
• Molecule 2: PROTEASOME





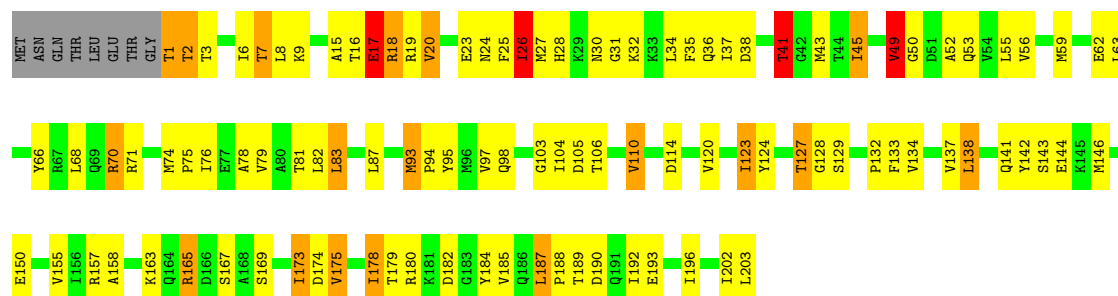
- Molecule 2: PROTEASOME

Chain R: 49% 37% 9% . .



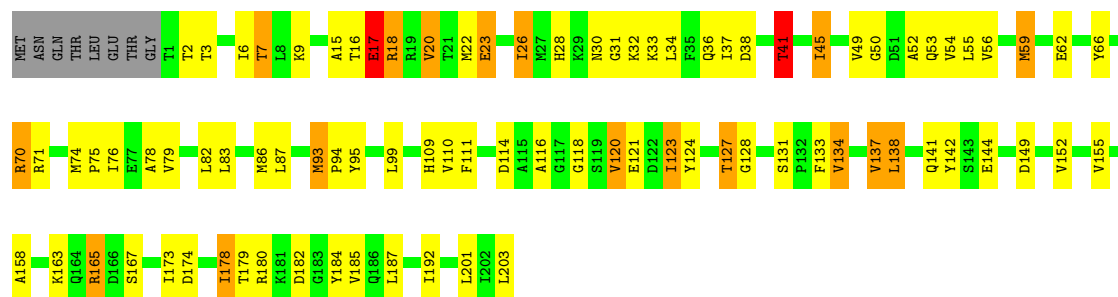
- Molecule 2: PROTEASOME

Chain S: 46% 39% 9% . .



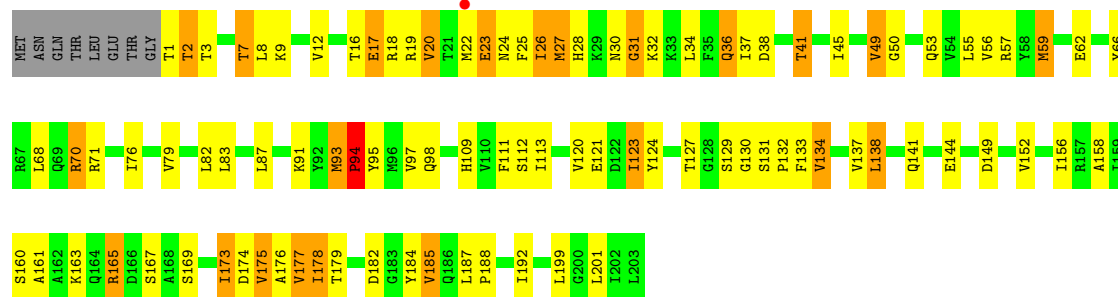
- Molecule 2: PROTEASOME

Chain T: 55% 33% 8% . .



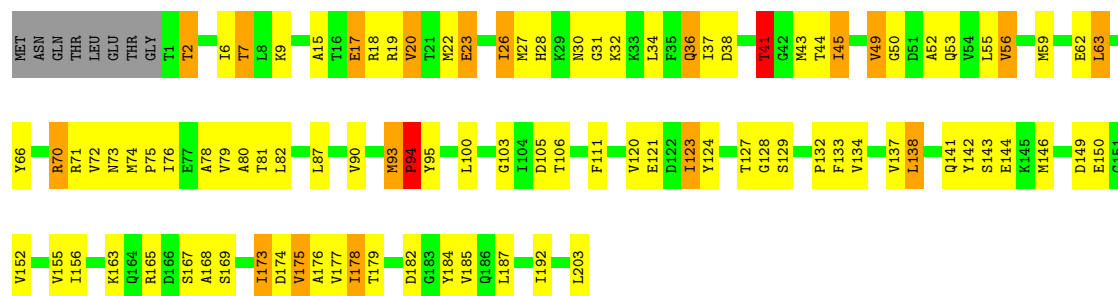
- Molecule 2: PROTEASOME

Chain U:  51% 34% 11% .



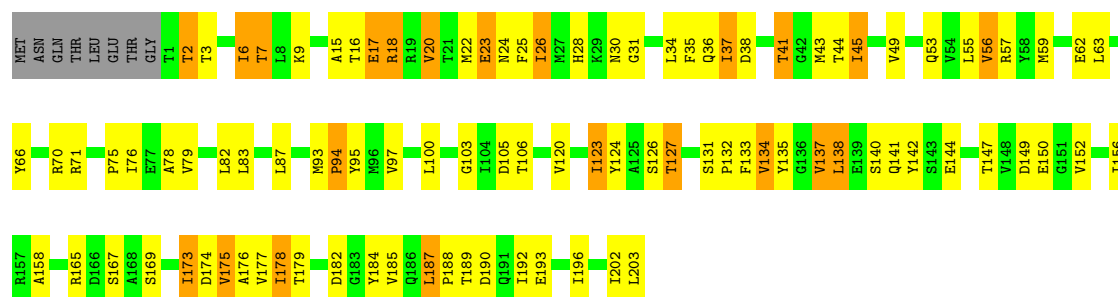
• Molecule 2: PROTEASOME

Chain V:  50% 36% 9% . .



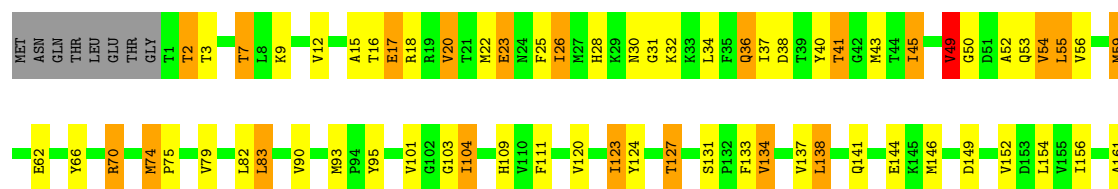
• Molecule 2: PROTEASOME

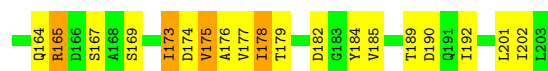
Chain W:  50% 36% 10% .



• Molecule 2: PROTEASOME

Chain X:  55% 29% 11% .

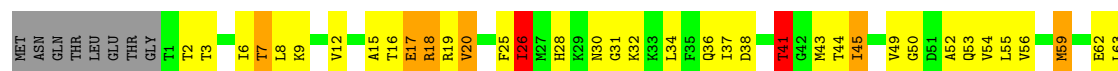




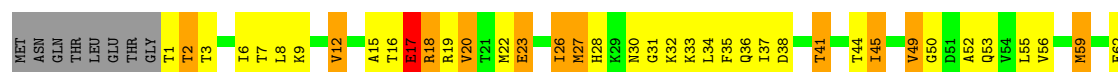
• Molecule 2: PROTEASOME



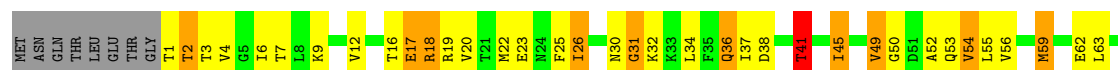
• Molecule 2: PROTEASOME

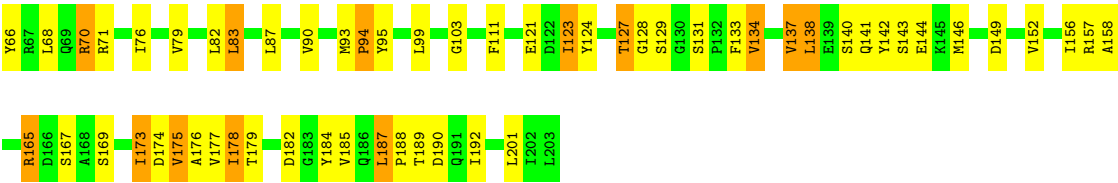


• Molecule 2: PROTEASOME



• Molecule 2: PROTEASOME





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	311.90Å 209.70Å 117.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 3.40 10.00 – 3.40	Depositor EDS
% Data completeness (in resolution range)	85.7 (10.00-3.40) 81.7 (10.00-3.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.72 (at 3.37Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.221 , (Not available) 0.208 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	80.4	Xtriage
Anisotropy	0.268	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 110.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	56294	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.52% 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 ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.61	0/1743	0.98	6/2348 (0.3%)
1	C	0.64	0/1743	1.03	5/2348 (0.2%)
1	D	0.64	0/1743	1.03	11/2348 (0.5%)
1	E	0.66	0/1743	1.00	6/2348 (0.3%)
1	F	0.64	0/1743	1.02	8/2348 (0.3%)
1	G	0.63	0/1743	1.04	7/2348 (0.3%)
1	H	0.63	0/1743	1.02	7/2348 (0.3%)
1	I	0.62	0/1743	1.00	5/2348 (0.2%)
1	J	0.60	0/1743	1.01	8/2348 (0.3%)
1	K	0.60	0/1743	1.04	9/2348 (0.4%)
1	L	0.65	0/1743	1.04	12/2348 (0.5%)
1	M	0.63	0/1743	1.01	6/2348 (0.3%)
1	N	0.65	0/1743	1.02	11/2348 (0.5%)
1	O	0.64	0/1743	1.02	8/2348 (0.3%)
2	1	0.73	0/1577	1.14	10/2129 (0.5%)
2	2	0.69	0/1577	1.13	14/2129 (0.7%)
2	B	0.75	0/1577	1.12	12/2129 (0.6%)
2	P	0.71	1/1577 (0.1%)	1.14	12/2129 (0.6%)
2	Q	0.71	0/1577	1.14	13/2129 (0.6%)
2	R	0.74	0/1577	1.13	11/2129 (0.5%)
2	S	0.75	1/1577 (0.1%)	1.14	15/2129 (0.7%)
2	T	0.73	0/1577	1.11	12/2129 (0.6%)
2	U	0.72	0/1577	1.11	10/2129 (0.5%)
2	V	0.74	0/1577	1.14	10/2129 (0.5%)
2	W	0.74	0/1577	1.16	12/2129 (0.6%)
2	X	0.73	0/1577	1.10	10/2129 (0.5%)
2	Y	0.71	0/1577	1.10	9/2129 (0.4%)
2	Z	0.73	2/1577 (0.1%)	1.13	13/2129 (0.6%)
All	All	0.68	4/46480 (0.0%)	1.07	272/62678 (0.4%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	S	26	ILE	CA-CB	6.70	1.60	1.53
2	Z	59	MET	SD-CE	-5.80	1.65	1.79
2	P	93	MET	SD-CE	5.15	1.92	1.79
2	Z	93	MET	SD-CE	5.00	1.92	1.79

All (272) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1	93	MET	CA-C-N	11.71	131.84	119.78
2	1	93	MET	C-N-CA	11.71	131.84	119.78
1	G	161	LYS	N-CA-C	-11.21	98.21	112.90
2	Z	93	MET	CA-C-N	11.02	131.71	119.92
2	Z	93	MET	C-N-CA	11.02	131.71	119.92
1	I	203	GLU	N-CA-C	-10.57	98.92	112.23
1	D	203	GLU	N-CA-C	-10.53	98.96	112.23
2	2	18	ARG	N-CA-C	10.39	122.67	110.41
1	K	203	GLU	N-CA-C	-10.31	99.24	112.23
1	L	161	LYS	N-CA-C	-10.27	100.88	113.41
1	F	203	GLU	N-CA-C	-10.21	99.36	112.23
2	W	93	MET	CA-C-N	10.19	130.12	120.03
2	W	93	MET	C-N-CA	10.19	130.12	120.03
1	G	203	GLU	N-CA-C	-10.10	99.51	112.23
1	C	203	GLU	N-CA-C	-10.09	99.52	112.23
1	K	161	LYS	N-CA-C	-10.02	101.19	113.41
1	C	161	LYS	N-CA-C	-10.01	101.19	113.41
1	H	203	GLU	N-CA-C	-9.96	100.26	111.82
1	J	203	GLU	N-CA-C	-9.93	99.72	112.23
1	A	203	GLU	N-CA-C	-9.88	100.35	111.82
2	Q	93	MET	CA-C-N	9.88	130.49	119.92
2	Q	93	MET	C-N-CA	9.88	130.49	119.92
1	L	203	GLU	N-CA-C	-9.87	99.79	112.23
1	O	203	GLU	N-CA-C	-9.67	100.05	112.23
2	P	93	MET	CA-C-N	9.65	130.24	119.92
2	P	93	MET	C-N-CA	9.65	130.24	119.92
1	I	161	LYS	N-CA-C	-9.64	100.27	112.90
1	E	203	GLU	N-CA-C	-9.64	100.09	112.23
2	T	18	ARG	N-CA-C	9.54	121.67	110.41
2	S	18	ARG	N-CA-C	9.52	121.64	110.41
1	H	161	LYS	N-CA-C	-9.42	101.92	113.41
1	N	203	GLU	N-CA-C	-9.37	100.95	111.82
1	J	161	LYS	N-CA-C	-9.07	102.35	113.41
1	E	161	LYS	N-CA-C	-9.04	102.38	113.41
1	M	203	GLU	N-CA-C	-8.97	100.93	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	161	LYS	N-CA-C	-8.79	102.68	113.41
2	V	36	GLN	N-CA-C	-8.77	97.51	110.48
2	W	187	LEU	CA-C-N	8.69	129.03	119.90
2	W	187	LEU	C-N-CA	8.69	129.03	119.90
1	D	161	LYS	N-CA-C	-8.69	102.81	113.50
1	F	70	ILE	N-CA-C	-8.66	104.30	112.96
2	Z	18	ARG	N-CA-C	8.61	120.57	110.41
2	Q	18	ARG	N-CA-C	8.52	120.46	110.41
2	W	18	ARG	N-CA-C	8.45	120.38	110.41
1	A	161	LYS	N-CA-C	-8.42	103.14	113.41
2	R	95	TYR	N-CA-C	-8.29	95.06	108.41
2	V	93	MET	CA-C-N	8.29	128.80	119.92
2	V	93	MET	C-N-CA	8.29	128.80	119.92
2	X	93	MET	CA-C-N	8.16	130.04	119.84
2	X	93	MET	C-N-CA	8.16	130.04	119.84
1	N	161	LYS	N-CA-C	-8.14	103.48	113.41
2	U	93	MET	CA-C-N	8.07	128.56	119.92
2	U	93	MET	C-N-CA	8.07	128.56	119.92
2	P	18	ARG	N-CA-C	8.03	119.88	110.41
2	B	93	MET	CA-C-N	8.01	128.49	119.92
2	B	93	MET	C-N-CA	8.01	128.49	119.92
2	T	31	GLY	N-CA-C	-7.86	101.80	112.57
2	2	93	MET	CA-C-N	7.86	127.81	120.03
2	2	93	MET	C-N-CA	7.86	127.81	120.03
2	1	18	ARG	N-CA-C	7.75	119.55	110.41
1	O	161	LYS	N-CA-C	-7.63	102.91	112.90
2	Q	31	GLY	N-CA-C	-7.53	100.69	112.58
1	L	70	ILE	N-CA-C	-7.41	105.55	112.96
2	T	93	MET	CA-C-N	7.38	129.06	119.84
2	T	93	MET	C-N-CA	7.38	129.06	119.84
1	F	161	LYS	N-CA-C	-7.27	103.37	112.90
2	Q	36	GLN	N-CA-C	-7.27	99.71	110.48
2	W	17	GLU	N-CA-C	-7.26	98.81	109.63
2	V	128	GLY	N-CA-C	7.23	119.41	112.04
2	R	36	GLN	N-CA-C	-7.17	98.87	110.20
2	1	17	GLU	N-CA-C	-7.15	98.98	109.63
1	O	219	ASN	N-CA-C	7.08	117.37	108.45
1	H	126	TYR	N-CA-C	7.07	121.67	110.70
2	Q	17	GLU	N-CA-C	-7.03	99.33	109.31
2	S	17	GLU	N-CA-C	-7.02	98.92	109.94
1	M	57	ARG	N-CA-C	-6.99	103.43	112.23
2	U	17	GLU	N-CA-C	-6.97	99.41	109.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	93	MET	CA-C-N	6.93	128.50	119.84
2	S	93	MET	C-N-CA	6.93	128.50	119.84
2	R	17	GLU	N-CA-C	-6.89	99.53	109.31
2	X	49	VAL	N-CA-C	6.88	117.39	110.23
2	2	95	TYR	N-CA-C	-6.86	97.37	108.41
2	B	36	GLN	N-CA-C	-6.83	99.40	110.20
2	T	95	TYR	N-CA-C	-6.83	97.41	108.41
2	U	36	GLN	N-CA-C	-6.83	99.41	110.20
2	Y	95	TYR	N-CA-C	-6.76	97.53	108.41
2	2	17	GLU	N-CA-C	-6.76	99.56	109.63
2	V	95	TYR	N-CA-C	-6.74	97.56	108.41
2	T	17	GLU	N-CA-C	-6.70	99.43	109.94
1	O	130	ARG	CA-C-N	6.69	126.71	119.89
1	O	130	ARG	C-N-CA	6.69	126.71	119.89
2	Q	94	PRO	N-CA-C	6.66	121.67	111.34
1	D	219	ASN	N-CA-C	6.58	116.97	108.34
2	1	36	GLN	N-CA-C	-6.57	100.75	110.48
1	A	57	ARG	N-CA-C	-6.55	104.76	112.89
2	2	140	SER	N-CA-C	6.55	118.22	111.14
2	R	93	MET	CA-C-N	6.53	128.00	119.84
2	R	93	MET	C-N-CA	6.53	128.00	119.84
1	D	126	TYR	N-CA-C	6.53	120.82	110.70
2	B	80	ALA	N-CA-C	-6.52	103.87	110.97
1	N	57	ARG	N-CA-C	-6.51	104.82	112.89
2	S	187	LEU	CA-C-N	6.51	126.86	119.83
2	S	187	LEU	C-N-CA	6.51	126.86	119.83
2	Z	95	TYR	N-CA-C	-6.45	98.02	108.41
2	W	95	TYR	N-CA-C	-6.44	98.04	108.41
2	Z	128	GLY	N-CA-C	6.44	118.61	112.04
2	W	94	PRO	N-CA-C	6.44	121.06	111.41
2	T	36	GLN	N-CA-C	-6.42	100.98	110.48
1	J	57	ARG	N-CA-C	-6.42	104.14	112.23
1	D	57	ARG	N-CA-C	-6.40	104.96	112.89
2	2	36	GLN	N-CA-C	-6.39	100.11	110.20
1	H	57	ARG	N-CA-C	-6.38	104.42	111.82
2	P	128	GLY	N-CA-C	6.37	118.54	112.04
1	C	57	ARG	N-CA-C	-6.36	104.44	111.82
2	B	128	GLY	N-CA-C	6.34	118.51	112.04
2	Y	17	GLU	N-CA-C	-6.34	100.18	109.63
2	P	95	TYR	N-CA-C	-6.31	98.89	108.67
1	N	107	VAL	N-CA-C	6.27	116.43	110.53
2	1	49	VAL	N-CA-C	6.27	116.75	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	107	VAL	N-CA-C	6.26	116.41	110.53
2	X	17	GLU	N-CA-C	-6.25	100.33	109.63
1	L	126	TYR	N-CA-C	6.21	120.33	110.70
2	Z	31	GLY	N-CA-C	-6.17	103.15	112.60
1	J	107	VAL	N-CA-C	6.16	116.32	110.53
1	D	82	VAL	N-CA-C	6.13	117.61	110.62
1	I	219	ASN	N-CA-C	6.12	116.35	108.34
2	S	128	GLY	N-CA-C	6.09	119.50	111.70
2	W	36	GLN	N-CA-C	-6.08	100.59	110.20
2	V	41	THR	N-CA-C	6.05	118.33	108.76
2	1	27	MET	N-CA-C	6.05	119.86	112.23
1	G	57	ARG	N-CA-C	-6.03	104.64	112.23
2	Y	93	MET	CA-C-N	6.02	126.36	119.92
2	Y	93	MET	C-N-CA	6.02	126.36	119.92
1	J	119	GLN	N-CA-C	-6.01	103.89	111.11
2	P	30	ASN	N-CA-C	6.01	117.02	108.54
1	L	57	ARG	N-CA-C	-6.00	105.45	112.89
2	U	94	PRO	N-CA-C	5.98	120.61	111.34
1	L	107	VAL	N-CA-C	5.97	116.75	110.72
2	X	31	GLY	N-CA-C	-5.96	103.48	112.60
2	W	24	ASN	N-CA-C	-5.94	106.36	113.97
1	I	57	ARG	N-CA-C	-5.93	105.31	112.54
1	K	130	ARG	CA-C-N	5.91	125.82	119.85
1	K	130	ARG	C-N-CA	5.91	125.82	119.85
1	G	219	ASN	N-CA-C	5.89	116.86	108.74
2	Y	36	GLN	N-CA-C	-5.88	100.92	110.20
2	T	118	GLY	N-CA-C	-5.86	100.84	111.15
1	L	219	ASN	N-CA-C	5.86	116.28	108.38
2	Z	36	GLN	N-CA-C	-5.85	100.95	110.20
2	S	95	TYR	N-CA-C	-5.85	98.19	108.20
1	O	57	ARG	N-CA-C	-5.84	105.64	112.89
2	B	95	TYR	N-CA-C	-5.83	97.73	107.99
2	T	187	LEU	CA-C-N	5.82	126.73	119.98
2	T	187	LEU	C-N-CA	5.82	126.73	119.98
2	2	94	PRO	N-CA-C	5.82	120.14	111.41
1	J	219	ASN	N-CA-C	5.82	116.77	108.74
1	D	78	THR	N-CA-C	5.81	118.24	109.41
2	Q	187	LEU	CA-C-N	5.80	125.99	119.90
2	Q	187	LEU	C-N-CA	5.80	125.99	119.90
2	B	150	GLU	N-CA-C	-5.79	104.97	111.28
2	P	17	GLU	N-CA-C	-5.78	101.02	109.63
2	W	140	SER	N-CA-C	5.77	118.79	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	U	27	MET	N-CA-C	5.77	120.46	112.90
2	V	94	PRO	N-CA-C	5.77	120.28	111.34
2	R	131	SER	N-CA-C	5.76	120.74	113.25
2	Q	4	VAL	N-CA-C	5.76	116.17	108.27
2	X	74	MET	CA-C-N	5.76	125.72	119.78
2	X	74	MET	C-N-CA	5.76	125.72	119.78
2	Q	74	MET	CA-C-N	5.76	125.71	119.78
2	Q	74	MET	C-N-CA	5.76	125.71	119.78
2	R	187	LEU	CA-C-N	5.76	125.94	119.90
2	R	187	LEU	C-N-CA	5.76	125.94	119.90
2	X	36	GLN	N-CA-C	-5.75	101.11	110.20
2	Z	94	PRO	N-CA-C	5.75	120.25	111.34
2	Y	41	THR	N-CA-C	5.74	117.85	108.55
2	1	94	PRO	N-CA-C	5.73	120.31	111.21
1	F	119	GLN	N-CA-C	-5.72	104.95	111.07
1	F	57	ARG	N-CA-C	-5.71	105.81	112.89
1	E	107	VAL	N-CA-C	5.70	115.89	110.42
2	V	27	MET	N-CA-C	5.68	120.34	112.90
2	U	31	GLY	N-CA-C	-5.67	103.61	112.58
1	E	126	TYR	N-CA-C	5.67	122.88	110.80
2	Y	202	ILE	N-CA-C	5.66	116.51	108.42
1	K	70	ILE	N-CA-C	-5.64	106.82	113.42
2	2	41	THR	N-CA-C	5.62	117.66	108.55
1	D	128	GLY	N-CA-C	5.62	126.49	113.18
1	M	219	ASN	N-CA-C	5.59	116.45	108.74
1	A	219	ASN	N-CA-C	5.59	116.45	108.74
2	P	202	ILE	N-CA-C	5.58	116.39	108.42
1	J	195	LYS	N-CA-C	-5.57	105.12	111.14
1	K	128	GLY	N-CA-C	5.57	126.39	113.18
2	2	31	GLY	N-CA-C	-5.57	104.09	112.89
2	P	36	GLN	N-CA-C	-5.53	101.46	110.20
1	A	179	GLU	N-CA-C	5.52	119.12	112.93
2	Z	26	ILE	CB-CA-C	5.50	117.64	111.80
2	Y	94	PRO	N-CA-C	5.49	119.85	111.34
2	R	41	THR	N-CA-C	5.49	117.43	108.76
1	G	126	TYR	N-CA-C	5.49	122.49	110.80
2	S	202	ILE	N-CA-C	5.48	117.69	108.81
2	X	95	TYR	N-CA-C	-5.46	98.37	107.99
2	S	26	ILE	CB-CA-C	5.46	117.59	111.80
2	R	31	GLY	N-CA-C	-5.46	104.25	112.60
1	O	16	SER	N-CA-C	-5.46	102.11	110.07
2	U	95	TYR	N-CA-C	-5.45	100.22	108.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	219	ASN	N-CA-C	5.44	116.25	108.74
1	E	130	ARG	CA-C-N	5.44	126.64	119.84
1	E	130	ARG	C-N-CA	5.44	126.64	119.84
1	L	179	GLU	N-CA-C	5.42	118.90	112.72
1	N	130	ARG	CA-C-N	5.40	125.35	119.78
1	N	130	ARG	C-N-CA	5.40	125.35	119.78
1	L	16	SER	N-CA-C	-5.40	102.29	110.39
2	S	27	MET	N-CA-C	5.39	118.31	111.69
2	P	41	THR	N-CA-C	5.38	117.26	108.76
2	B	187	LEU	CA-C-N	5.38	125.14	119.76
2	B	187	LEU	C-N-CA	5.38	125.14	119.76
2	U	49	VAL	N-CA-C	5.37	115.82	110.23
1	K	219	ASN	N-CA-C	5.36	116.14	108.74
2	B	94	PRO	N-CA-C	5.36	119.64	111.34
1	D	195	LYS	N-CA-C	-5.35	105.36	111.14
1	D	130	ARG	CA-C-N	5.35	125.64	119.92
1	D	130	ARG	C-N-CA	5.35	125.64	119.92
1	G	127	GLY	N-CA-C	5.33	120.93	111.02
1	A	128	GLY	N-CA-C	5.32	125.78	113.18
1	M	16	SER	N-CA-C	-5.31	102.43	110.39
1	C	155	GLY	N-CA-C	-5.30	107.91	115.64
2	B	17	GLU	N-CA-C	-5.29	99.53	110.80
2	Y	31	GLY	N-CA-C	-5.29	103.46	112.51
2	T	128	GLY	N-CA-C	5.29	118.47	111.70
1	N	127	GLY	N-CA-C	5.28	120.94	111.34
2	S	41	THR	N-CA-C	5.28	117.27	108.99
1	N	179	GLU	N-CA-C	5.26	118.72	112.72
2	Z	187	LEU	CA-C-N	5.25	125.50	119.83
2	Z	187	LEU	C-N-CA	5.25	125.50	119.83
2	Q	27	MET	N-CA-C	5.24	118.84	112.23
1	H	70	ILE	N-CA-C	-5.24	105.69	113.39
2	U	24	ASN	N-CA-C	-5.23	107.06	113.50
2	Z	41	THR	N-CA-C	5.23	117.02	108.55
1	M	179	GLU	N-CA-C	5.22	119.33	112.92
2	R	202	ILE	N-CA-C	5.22	117.26	108.81
2	1	202	ILE	N-CA-C	5.22	115.88	108.42
1	O	126	TYR	N-CA-C	5.20	121.89	110.80
2	Z	17	GLU	N-CA-C	-5.20	101.88	109.63
1	K	57	ARG	N-CA-C	-5.19	106.45	112.89
1	N	126	TYR	N-CA-C	5.17	121.80	110.80
2	S	24	ASN	N-CA-C	-5.16	107.36	113.97
1	I	126	TYR	N-CA-C	5.16	121.79	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	126	TYR	N-CA-C	5.15	121.77	110.80
1	F	219	ASN	N-CA-C	5.14	116.11	108.86
2	2	129	SER	N-CA-C	5.13	117.54	111.33
1	L	130	ARG	CA-C-N	5.13	125.07	119.78
1	L	130	ARG	C-N-CA	5.13	125.07	119.78
2	S	36	GLN	N-CA-C	-5.13	102.10	110.20
2	2	128	GLY	N-CA-C	5.12	118.25	111.70
2	V	31	GLY	N-CA-C	-5.12	104.49	112.58
2	T	41	THR	N-CA-C	5.08	116.78	108.55
1	H	130	ARG	N-CA-C	5.07	116.04	109.65
2	S	150	GLU	N-CA-C	-5.07	105.75	111.28
2	2	187	LEU	CA-C-N	5.07	125.22	119.90
2	2	187	LEU	C-N-CA	5.07	125.22	119.90
1	H	82	VAL	N-CA-C	5.06	115.68	110.36
1	L	195	LYS	N-CA-C	-5.05	105.69	111.14
2	P	49	VAL	N-CA-C	5.05	115.66	110.36
1	N	205	GLU	N-CA-C	5.04	121.53	110.80
1	C	82	VAL	N-CA-C	5.03	115.64	110.36
2	B	31	GLY	N-CA-C	-5.02	104.64	112.58
1	K	82	VAL	N-CA-C	5.02	115.63	110.36
2	W	31	GLY	N-CA-C	-5.02	104.33	112.31
2	1	87	LEU	N-CA-C	5.02	116.75	111.28
2	P	140	SER	N-CA-C	5.02	117.86	111.69
1	J	179	GLU	N-CA-C	5.01	118.54	112.93
2	X	202	ILE	N-CA-C	5.01	116.93	108.81
2	V	150	GLU	N-CA-C	-5.00	105.72	111.07
1	G	82	VAL	N-CA-C	5.00	115.61	110.36

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	A	1720	393	1753	80	0
1	C	1720	393	1753	76	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1720	393	1753	79	1
1	E	1720	393	1753	83	0
1	F	1720	393	1753	89	0
1	G	1720	393	1753	96	0
1	H	1720	393	1753	82	0
1	I	1720	393	1753	83	0
1	J	1720	393	1753	77	0
1	K	1720	393	1753	73	0
1	L	1720	393	1753	81	0
1	M	1720	393	1753	76	0
1	N	1720	393	1753	67	1
1	O	1720	393	1753	79	0
2	1	1558	350	1609	79	0
2	2	1558	350	1609	63	0
2	B	1558	350	1609	84	0
2	P	1558	350	1609	72	0
2	Q	1558	350	1609	59	0
2	R	1558	350	1609	70	0
2	S	1558	350	1609	82	0
2	T	1558	350	1609	66	0
2	U	1558	350	1609	73	0
2	V	1558	350	1609	79	0
2	W	1558	350	1609	70	0
2	X	1558	350	1609	68	0
2	Y	1558	350	1609	67	0
2	Z	1558	350	1609	72	0
All	All	45892	10402	47068	1933	1

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 21.

All (1933) 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:B:38:ASP:HB3	2:B:41:THR:HG23	1.38	1.03
2:T:38:ASP:HB3	2:T:41:THR:HG23	1.44	1.00
2:Q:45:ILE:HG12	2:Q:52:ALA:HB1	1.44	0.99
2:Q:38:ASP:HB3	2:Q:41:THR:HG23	1.46	0.98
2:R:38:ASP:HB3	2:R:41:THR:HG23	1.45	0.98
2:B:66:TYR:OH	1:H:107:VAL:HG11	1.62	0.97
2:T:45:ILE:HG12	2:T:52:ALA:HB1	1.46	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:107:VAL:HG11	2:1:66:TYR:OH	1.65	0.96
2:U:38:ASP:HB3	2:U:41:THR:HG23	1.47	0.95
2:Y:38:ASP:HB3	2:Y:41:THR:HG23	1.48	0.95
2:2:38:ASP:HB3	2:2:41:THR:HG23	1.47	0.95
2:W:38:ASP:HB3	2:W:41:THR:HG23	1.45	0.95
2:P:38:ASP:HB3	2:P:41:THR:HG23	1.49	0.94
1:K:107:VAL:HG11	2:Y:66:TYR:OH	1.68	0.94
1:I:107:VAL:HG11	2:W:66:TYR:OH	1.68	0.93
2:W:59:MET:HE1	2:W:82:LEU:HD23	1.48	0.93
2:1:38:ASP:HB3	2:1:41:THR:HG23	1.50	0.93
2:Z:38:ASP:HB3	2:Z:41:THR:HG23	1.50	0.93
1:A:107:VAL:HG11	2:P:66:TYR:OH	1.69	0.93
1:L:107:VAL:HG11	2:Z:66:TYR:OH	1.69	0.92
1:D:107:VAL:HG11	2:R:66:TYR:OH	1.70	0.91
1:N:107:VAL:HG11	2:2:66:TYR:OH	1.69	0.91
2:X:45:ILE:HG12	2:X:52:ALA:HB1	1.53	0.91
1:F:107:VAL:HG11	2:T:66:TYR:OH	1.71	0.90
2:1:37:ILE:HD11	2:1:59:MET:HB3	1.54	0.90
2:X:38:ASP:HB3	2:X:41:THR:HG23	1.54	0.89
1:E:107:VAL:HG11	2:S:66:TYR:OH	1.73	0.89
2:X:53:GLN:O	2:X:56:VAL:HG12	1.73	0.88
2:T:37:ILE:HD11	2:T:59:MET:HB3	1.56	0.87
1:J:107:VAL:HG11	2:X:66:TYR:OH	1.75	0.85
1:D:108:ASN:HB3	2:R:70:ARG:HG2	1.57	0.85
1:L:124:THR:HG22	1:M:130:ARG:HH21	1.42	0.85
2:S:38:ASP:HB3	2:S:41:THR:HG23	1.59	0.85
1:I:130:ARG:HH21	1:O:124:THR:HG22	1.41	0.84
1:K:124:THR:HG22	1:L:130:ARG:HH21	1.43	0.84
2:V:38:ASP:HB3	2:V:41:THR:HG23	1.57	0.84
1:O:107:VAL:HG11	2:V:66:TYR:OH	1.78	0.84
2:Z:59:MET:HE1	2:Z:82:LEU:HD23	1.60	0.83
1:M:168:GLY:O	1:M:172:VAL:HG12	1.77	0.83
2:U:53:GLN:O	2:U:56:VAL:HG12	1.78	0.83
2:P:123:ILE:HG12	2:P:124:TYR:HD1	1.44	0.83
2:Q:37:ILE:HD11	2:Q:59:MET:HB3	1.61	0.82
1:C:107:VAL:HG11	2:Q:66:TYR:OH	1.79	0.81
1:G:124:THR:HG22	1:H:130:ARG:HH21	1.44	0.81
2:Z:123:ILE:HG12	2:Z:124:TYR:HD1	1.44	0.81
2:T:20:VAL:HG13	2:T:28:HIS:HB2	1.62	0.81
1:A:52:LYS:NZ	1:A:62:ASN:HA	1.96	0.81
2:W:123:ILE:HG12	2:W:124:TYR:HD1	1.46	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:108:ASN:HB3	2:W:70:ARG:HG2	1.62	0.80
1:F:124:THR:HG22	1:G:130:ARG:HH21	1.45	0.80
2:X:59:MET:HE1	2:X:82:LEU:HD23	1.65	0.79
1:G:107:VAL:HG11	2:U:66:TYR:OH	1.83	0.79
2:R:123:ILE:HG12	2:R:124:TYR:HD1	1.48	0.78
2:B:123:ILE:HG12	2:B:124:TYR:HD1	1.48	0.78
2:1:123:ILE:HD13	2:1:123:ILE:H	1.47	0.78
2:R:59:MET:HE1	2:R:82:LEU:HD23	1.63	0.78
2:B:70:ARG:HG2	1:H:108:ASN:HB3	1.65	0.78
2:P:53:GLN:O	2:P:56:VAL:HG12	1.83	0.78
2:R:59:MET:HE2	2:R:79:VAL:HG23	1.64	0.78
1:A:186:GLU:O	1:A:190:VAL:HG12	1.84	0.78
2:Q:123:ILE:HD13	2:Q:123:ILE:H	1.49	0.78
2:Z:59:MET:HE2	2:Z:79:VAL:HG23	1.66	0.78
1:K:52:LYS:NZ	1:K:62:ASN:HA	2.00	0.77
2:W:53:GLN:O	2:W:56:VAL:HG12	1.86	0.76
2:2:59:MET:HE1	2:2:82:LEU:HD23	1.66	0.76
2:Y:59:MET:HE1	2:Y:82:LEU:HD23	1.68	0.76
2:B:43:MET:HE2	2:B:56:VAL:HG23	1.66	0.76
1:C:18:ASP:OD2	1:C:20:ARG:HD3	1.85	0.76
1:H:168:GLY:O	1:H:172:VAL:HG12	1.85	0.76
1:K:108:ASN:HB3	2:Y:70:ARG:HG2	1.66	0.76
2:2:53:GLN:O	2:2:56:VAL:HG12	1.86	0.76
1:A:124:THR:HG22	1:C:130:ARG:HH21	1.50	0.76
1:I:198:LYS:O	1:I:202:GLU:HB2	1.85	0.76
2:V:123:ILE:HG12	2:V:124:TYR:HD1	1.49	0.76
2:U:32:LYS:HE2	2:U:34:LEU:O	1.85	0.75
1:K:78:THR:HG21	1:K:85:ALA:HB1	1.67	0.75
1:F:21:LEU:HD11	1:G:130:ARG:HD2	1.68	0.75
2:S:53:GLN:O	2:S:56:VAL:HG12	1.87	0.75
2:1:3:THR:OG1	2:1:127:THR:HG22	1.86	0.75
2:1:53:GLN:O	2:1:56:VAL:HG12	1.86	0.74
2:Y:53:GLN:O	2:Y:56:VAL:HG12	1.87	0.74
1:G:21:LEU:O	1:G:24:VAL:HG12	1.87	0.73
2:S:2:THR:HG22	2:S:169:SER:OG	1.89	0.73
1:E:135:SER:OG	1:E:153:PRO:HD3	1.88	0.73
1:M:78:THR:HG21	1:M:85:ALA:HB1	1.71	0.73
2:W:43:MET:HE2	2:W:56:VAL:HG23	1.68	0.73
2:T:18:ARG:HE	2:T:30:ASN:HD22	1.37	0.73
1:A:78:THR:HG21	1:A:85:ALA:HB1	1.70	0.73
2:2:37:ILE:HD11	2:2:59:MET:HB3	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:130:ARG:HD2	1:O:21:LEU:HD11	1.69	0.73
2:V:123:ILE:HD13	2:V:123:ILE:H	1.53	0.73
2:P:38:ASP:HB3	2:P:41:THR:CG2	2.19	0.73
2:P:103:GLY:HA2	2:P:178:ILE:HD11	1.71	0.73
2:U:62:GLU:HG2	2:U:82:LEU:HD21	1.70	0.72
2:U:123:ILE:H	2:U:123:ILE:HD13	1.52	0.72
1:L:198:LYS:O	1:L:202:GLU:HB2	1.90	0.72
1:M:198:LYS:O	1:M:202:GLU:HB2	1.89	0.72
1:I:78:THR:HG21	1:I:85:ALA:HB1	1.71	0.72
1:D:52:LYS:NZ	1:D:62:ASN:HA	2.04	0.72
2:X:123:ILE:HG12	2:X:124:TYR:HD1	1.54	0.72
1:A:168:GLY:O	1:A:172:VAL:HG12	1.89	0.72
2:B:53:GLN:O	2:B:56:VAL:HG12	1.89	0.72
1:J:78:THR:HG21	1:J:85:ALA:HB1	1.70	0.72
1:J:184:LEU:HD23	1:J:189:ALA:HA	1.71	0.72
2:T:123:ILE:HG12	2:T:124:TYR:HD1	1.53	0.72
2:B:32:LYS:HE2	2:B:34:LEU:O	1.89	0.71
1:J:198:LYS:O	1:J:202:GLU:HB2	1.89	0.71
1:K:168:GLY:O	1:K:172:VAL:HG12	1.89	0.71
2:S:7:THR:HB	2:S:123:ILE:O	1.90	0.71
2:2:18:ARG:HB2	2:2:31:GLY:O	1.91	0.71
2:R:167:SER:HB2	2:V:167:SER:HB2	1.73	0.71
2:S:20:VAL:HG13	2:S:28:HIS:HB2	1.71	0.71
1:K:184:LEU:HD23	1:K:189:ALA:HA	1.73	0.71
1:F:52:LYS:NZ	1:F:62:ASN:HA	2.06	0.71
1:K:21:LEU:O	1:K:24:VAL:HG12	1.90	0.70
1:M:186:GLU:O	1:M:190:VAL:HG12	1.90	0.70
1:D:98:GLN:O	1:D:102:THR:HG22	1.91	0.70
2:V:149:ASP:O	2:V:152:VAL:HG12	1.91	0.70
2:U:37:ILE:HD11	2:U:59:MET:HB3	1.73	0.70
2:P:103:GLY:HA2	2:P:178:ILE:CD1	2.22	0.70
2:X:3:THR:OG1	2:X:127:THR:HG22	1.92	0.70
2:2:55:LEU:HD23	2:2:99:LEU:HD11	1.74	0.70
2:B:59:MET:HE1	2:B:82:LEU:HD23	1.73	0.69
1:H:21:LEU:O	1:H:24:VAL:HG12	1.92	0.69
2:Z:53:GLN:O	2:Z:56:VAL:HG12	1.92	0.69
2:1:62:GLU:HG2	2:1:82:LEU:HD21	1.73	0.69
2:B:45:ILE:HG12	2:B:52:ALA:HB1	1.74	0.69
1:J:42:PHE:HB2	1:J:184:LEU:O	1.91	0.69
2:Q:45:ILE:CG1	2:Q:52:ALA:HB1	2.22	0.69
1:G:198:LYS:O	1:G:202:GLU:HB2	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:38:ASP:HB3	2:W:41:THR:CG2	2.19	0.69
1:G:52:LYS:NZ	1:G:62:ASN:HA	2.06	0.69
2:P:62:GLU:HG2	2:P:82:LEU:HD21	1.74	0.69
2:V:124:TYR:CD2	2:V:138:LEU:HD23	2.28	0.69
2:W:18:ARG:HE	2:W:30:ASN:HD22	1.37	0.69
2:X:43:MET:HE2	2:X:56:VAL:HG23	1.73	0.69
1:G:52:LYS:HZ1	1:G:62:ASN:HA	1.56	0.69
2:Y:45:ILE:HG12	2:Y:52:ALA:HB1	1.74	0.69
2:S:193:GLU:HA	2:S:196:ILE:HD12	1.74	0.69
1:A:184:LEU:HD23	1:A:189:ALA:HA	1.75	0.69
2:B:167:SER:HB2	2:Y:167:SER:HB2	1.75	0.69
2:X:32:LYS:HE2	2:X:34:LEU:O	1.92	0.69
1:C:42:PHE:HB2	1:C:184:LEU:O	1.92	0.69
2:R:12:VAL:HG13	2:R:178:ILE:HG23	1.74	0.69
2:V:43:MET:HE2	2:V:56:VAL:HG23	1.73	0.69
1:D:135:SER:OG	1:D:153:PRO:HD3	1.92	0.69
2:Q:53:GLN:O	2:Q:56:VAL:HG12	1.91	0.69
2:Z:15:ALA:HB2	2:Z:175:VAL:HB	1.74	0.68
2:Z:18:ARG:HE	2:Z:30:ASN:HD22	1.39	0.68
2:T:53:GLN:O	2:T:56:VAL:HG12	1.93	0.68
2:Y:32:LYS:HE2	2:Y:34:LEU:O	1.93	0.68
2:1:32:LYS:HE2	2:1:34:LEU:O	1.93	0.68
2:T:3:THR:OG1	2:T:127:THR:HG22	1.93	0.68
2:X:37:ILE:HD11	2:X:59:MET:HB3	1.75	0.68
1:D:198:LYS:O	1:D:202:GLU:HB2	1.94	0.68
1:G:52:LYS:HE3	1:G:64:ILE:HG23	1.75	0.68
1:K:52:LYS:HZ1	1:K:62:ASN:HA	1.57	0.68
1:O:198:LYS:O	1:O:202:GLU:HB2	1.93	0.68
2:Q:149:ASP:O	2:Q:152:VAL:HG12	1.94	0.68
1:C:78:THR:HG21	1:C:85:ALA:HB1	1.74	0.68
1:O:52:LYS:NZ	1:O:62:ASN:HA	2.09	0.68
1:E:124:THR:HG22	1:F:130:ARG:HH21	1.58	0.68
1:J:186:GLU:O	1:J:190:VAL:HG12	1.94	0.68
1:M:109:ILE:CG2	1:M:147:ARG:HD3	2.24	0.68
1:M:184:LEU:HD23	1:M:189:ALA:HA	1.76	0.68
2:1:59:MET:HE1	2:1:82:LEU:HD23	1.76	0.68
1:I:52:LYS:NZ	1:I:62:ASN:HA	2.08	0.68
2:U:38:ASP:HB3	2:U:41:THR:CG2	2.21	0.67
1:L:168:GLY:O	1:L:172:VAL:HG12	1.94	0.67
1:N:78:THR:HG21	1:N:85:ALA:HB1	1.75	0.67
2:R:7:THR:HB	2:R:123:ILE:O	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:95:SER:OG	1:H:115:ARG:HD3	1.94	0.67
2:T:123:ILE:HD13	2:T:123:ILE:H	1.60	0.67
2:V:53:GLN:O	2:V:56:VAL:HG12	1.95	0.67
1:E:198:LYS:O	1:E:202:GLU:HB2	1.95	0.67
1:N:52:LYS:HZ1	1:N:62:ASN:HA	1.59	0.67
2:P:133:PHE:CZ	2:P:165:ARG:HB3	2.30	0.67
1:H:198:LYS:O	1:H:202:GLU:HB2	1.95	0.67
2:B:59:MET:SD	2:B:83:LEU:HD13	2.35	0.67
1:E:78:THR:HG21	1:E:85:ALA:HB1	1.75	0.67
1:C:168:GLY:O	1:C:172:VAL:HG12	1.95	0.67
1:I:23:GLN:OE1	1:O:14:VAL:HB	1.95	0.67
1:K:198:LYS:O	1:K:202:GLU:HB2	1.95	0.67
1:M:69:LEU:HD23	1:M:75:ALA:HB2	1.75	0.67
1:G:21:LEU:HD11	1:H:130:ARG:HD2	1.76	0.66
1:G:184:LEU:HD23	1:G:189:ALA:HA	1.77	0.66
1:G:186:GLU:O	1:G:190:VAL:HG12	1.95	0.66
2:V:6:ILE:HD11	2:V:142:TYR:CD1	2.31	0.66
2:Z:111:PHE:CE2	2:Z:121:GLU:HB2	2.29	0.66
2:R:28:HIS:CD2	2:S:120:VAL:HG11	2.31	0.66
2:W:124:TYR:CD2	2:W:138:LEU:HD23	2.31	0.66
1:C:108:ASN:HB3	2:Q:70:ARG:HG2	1.78	0.66
1:D:21:LEU:O	1:D:25:GLU:HG2	1.95	0.66
2:P:7:THR:HB	2:P:123:ILE:O	1.96	0.66
2:Q:2:THR:HG22	2:Q:169:SER:OG	1.96	0.66
1:D:108:ASN:CB	2:R:70:ARG:HG2	2.25	0.66
1:G:78:THR:HG21	1:G:85:ALA:HB1	1.76	0.66
2:Q:75:PRO:O	2:Q:78:ALA:HB3	1.96	0.66
2:R:123:ILE:HG12	2:R:124:TYR:CD1	2.31	0.66
1:F:168:GLY:O	1:F:172:VAL:HG12	1.96	0.66
2:2:45:ILE:HG12	2:2:52:ALA:HB1	1.77	0.66
1:A:198:LYS:O	1:A:202:GLU:HB2	1.96	0.66
2:V:7:THR:HB	2:V:123:ILE:O	1.96	0.65
1:F:69:LEU:HD23	1:F:75:ALA:HB2	1.79	0.65
1:L:49:ILE:HD11	1:L:210:PRO:HB3	1.78	0.65
2:V:45:ILE:HG12	2:V:52:ALA:HB1	1.78	0.65
1:D:15:PHE:HD2	1:E:23:GLN:HE22	1.45	0.65
1:F:186:GLU:O	1:F:190:VAL:HG12	1.96	0.65
1:I:43:ALA:HB2	1:I:185:PRO:HA	1.79	0.65
1:O:98:GLN:O	1:O:102:THR:HG22	1.96	0.65
2:Q:18:ARG:HE	2:Q:30:ASN:HD22	1.41	0.65
2:S:37:ILE:HD11	2:S:59:MET:HB3	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:52:LYS:HZ3	1:D:62:ASN:HA	1.60	0.65
1:I:21:LEU:HD11	1:J:130:ARG:HD2	1.79	0.65
2:S:59:MET:SD	2:S:83:LEU:HD13	2.36	0.65
1:A:159:GLU:HG2	1:C:60:GLU:HG3	1.79	0.65
1:E:52:LYS:NZ	1:E:62:ASN:HA	2.10	0.65
1:L:52:LYS:NZ	1:L:62:ASN:HA	2.11	0.65
2:2:32:LYS:HE2	2:2:34:LEU:O	1.97	0.65
2:B:38:ASP:HB3	2:B:41:THR:CG2	2.20	0.65
1:L:170:ASP:O	1:L:173:VAL:HG12	1.96	0.65
1:N:98:GLN:O	1:N:102:THR:HG22	1.97	0.65
2:T:45:ILE:CG1	2:T:52:ALA:HB1	2.26	0.65
1:F:198:LYS:O	1:F:202:GLU:HB2	1.97	0.65
2:P:123:ILE:H	2:P:123:ILE:HD13	1.62	0.65
2:S:123:ILE:HG12	2:S:124:TYR:HD1	1.61	0.65
1:M:21:LEU:O	1:M:24:VAL:HG12	1.97	0.65
1:N:198:LYS:O	1:N:202:GLU:HB2	1.96	0.65
1:F:21:LEU:O	1:F:24:VAL:HG12	1.98	0.64
1:H:61:GLN:O	1:H:64:ILE:HG22	1.96	0.64
1:J:124:THR:HG22	1:K:130:ARG:HH21	1.62	0.64
2:P:45:ILE:HG12	2:P:52:ALA:HB1	1.79	0.64
2:X:18:ARG:HE	2:X:30:ASN:HD22	1.42	0.64
1:A:21:LEU:HD11	1:C:130:ARG:HD2	1.79	0.64
1:A:52:LYS:HZ1	1:A:62:ASN:HA	1.59	0.64
1:A:61:GLN:O	1:A:64:ILE:HG22	1.95	0.64
2:T:124:TYR:CD2	2:T:138:LEU:HD23	2.31	0.64
2:1:59:MET:SD	2:1:83:LEU:HD13	2.37	0.64
1:N:21:LEU:O	1:N:24:VAL:HG12	1.97	0.64
2:P:20:VAL:HG13	2:P:28:HIS:HB2	1.79	0.64
2:Y:37:ILE:HD11	2:Y:59:MET:HB3	1.79	0.64
2:U:123:ILE:HG12	2:U:124:TYR:HD2	1.61	0.64
2:X:20:VAL:HG13	2:X:28:HIS:HB2	1.80	0.64
2:B:123:ILE:H	2:B:123:ILE:HD13	1.62	0.64
1:G:121:GLN:O	1:G:124:THR:HB	1.96	0.64
2:Y:124:TYR:CD1	2:Y:138:LEU:HD23	2.32	0.64
2:Z:149:ASP:O	2:Z:152:VAL:HG12	1.97	0.64
1:L:108:ASN:HB3	2:Z:70:ARG:HG2	1.80	0.64
1:N:52:LYS:NZ	1:N:62:ASN:HA	2.13	0.64
2:P:124:TYR:CD2	2:P:138:LEU:HD23	2.32	0.64
1:L:144:ILE:HD12	1:L:147:ARG:NH1	2.13	0.64
2:W:3:THR:OG1	2:W:127:THR:HG22	1.97	0.64
1:G:137:ILE:HG22	1:G:150:ASP:HB2	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:109:ILE:HG22	1:M:142:ASP:OD1	1.98	0.64
2:S:43:MET:HE2	2:S:56:VAL:HG23	1.78	0.64
2:V:103:GLY:HA2	2:V:178:ILE:CD1	2.28	0.64
1:G:135:SER:OG	1:G:153:PRO:HD3	1.98	0.63
2:S:18:ARG:HB2	2:S:31:GLY:O	1.98	0.63
2:S:124:TYR:CD2	2:S:138:LEU:HD23	2.33	0.63
2:Z:123:ILE:H	2:Z:123:ILE:HD13	1.64	0.63
1:J:21:LEU:O	1:J:24:VAL:HG12	1.98	0.63
2:R:123:ILE:H	2:R:123:ILE:HD13	1.63	0.63
2:T:49:VAL:HG23	2:T:50:GLY:H	1.62	0.63
2:V:76:ILE:O	2:V:79:VAL:HG12	1.98	0.63
2:Y:7:THR:HB	2:Y:123:ILE:O	1.98	0.63
1:H:52:LYS:NZ	1:H:62:ASN:HA	2.14	0.63
1:J:108:ASN:HB3	2:X:70:ARG:HG2	1.79	0.63
1:M:52:LYS:NZ	1:M:62:ASN:HA	2.12	0.63
2:U:179:THR:HG23	2:U:182:ASP:H	1.63	0.63
2:V:32:LYS:HE2	2:V:34:LEU:O	1.98	0.63
2:1:123:ILE:HG12	2:1:124:TYR:HD1	1.63	0.63
2:1:123:ILE:HG12	2:1:124:TYR:CD1	2.34	0.63
2:2:2:THR:HG22	2:2:169:SER:OG	1.98	0.63
1:F:180:TYR:HA	1:F:192:LEU:HD21	1.80	0.63
2:P:59:MET:HE1	2:P:82:LEU:HD23	1.79	0.63
1:F:108:ASN:HB3	2:T:70:ARG:HG2	1.78	0.63
1:J:52:LYS:NZ	1:J:62:ASN:HA	2.14	0.63
2:W:3:THR:HB	2:W:16:THR:HG22	1.80	0.63
1:C:52:LYS:HE3	1:C:64:ILE:HG23	1.81	0.63
1:G:168:GLY:O	1:G:172:VAL:HG12	1.99	0.63
1:I:137:ILE:HG22	1:I:150:ASP:HB2	1.81	0.63
1:J:168:GLY:O	1:J:172:VAL:HG12	1.99	0.63
1:N:168:GLY:O	1:N:172:VAL:HG12	1.97	0.63
2:Q:103:GLY:HA2	2:Q:178:ILE:HD13	1.81	0.63
2:B:124:TYR:CD2	2:B:138:LEU:HD23	2.33	0.63
2:B:123:ILE:HG12	2:B:124:TYR:CD1	2.33	0.63
1:D:49:ILE:HD11	1:D:210:PRO:HB3	1.80	0.63
2:R:193:GLU:HA	2:R:196:ILE:HD12	1.81	0.63
1:D:61:GLN:O	1:D:64:ILE:HG22	1.98	0.62
2:P:167:SER:HB2	2:X:167:SER:HB2	1.81	0.62
2:U:167:SER:HB2	2:Z:167:SER:HB2	1.81	0.62
1:C:94:ILE:HG13	1:C:95:SER:N	2.14	0.62
1:E:108:ASN:HB3	2:S:70:ARG:HG2	1.81	0.62
1:N:184:LEU:HD23	1:N:189:ALA:HA	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:15:ALA:HB2	2:S:175:VAL:HB	1.81	0.62
2:R:3:THR:HB	2:R:16:THR:HG22	1.80	0.62
2:B:55:LEU:HD21	2:B:87:LEU:HD11	1.80	0.62
2:U:133:PHE:CZ	2:U:165:ARG:HB3	2.34	0.62
2:V:124:TYR:HD2	2:V:138:LEU:HD23	1.61	0.62
1:D:21:LEU:O	1:D:24:VAL:HG12	2.00	0.62
1:O:108:ASN:HB3	2:V:70:ARG:HG2	1.81	0.62
2:P:1:THR:H3	2:P:129:SER:HB3	1.65	0.62
2:P:76:ILE:O	2:P:79:VAL:HG12	2.00	0.62
2:Z:38:ASP:HB3	2:Z:41:THR:CG2	2.27	0.62
2:2:123:ILE:H	2:2:123:ILE:HD13	1.63	0.62
2:Q:103:GLY:HA2	2:Q:178:ILE:CD1	2.29	0.62
2:Z:19:ARG:NE	2:Z:26:ILE:HG13	2.15	0.62
2:1:18:ARG:HB2	2:1:31:GLY:O	2.00	0.62
1:H:78:THR:HG21	1:H:85:ALA:HB1	1.82	0.62
1:I:168:GLY:O	1:I:172:VAL:HG12	1.99	0.62
1:K:88:LEU:HD21	1:K:120:MET:HE3	1.80	0.62
1:O:61:GLN:O	1:O:64:ILE:HG22	2.00	0.62
2:P:37:ILE:HD11	2:P:59:MET:HB3	1.82	0.62
2:R:141:GLN:NE2	2:W:141:GLN:HE21	1.98	0.62
1:F:52:LYS:HE3	1:F:64:ILE:HG23	1.82	0.62
1:G:18:ASP:OD2	1:G:20:ARG:HD3	2.00	0.62
1:M:21:LEU:O	1:M:25:GLU:HG2	1.99	0.62
1:N:70:ILE:HD12	1:N:74:VAL:HG22	1.81	0.62
2:X:124:TYR:CD2	2:X:138:LEU:HD23	2.35	0.62
2:Y:62:GLU:HG2	2:Y:82:LEU:HD21	1.82	0.62
1:C:186:GLU:O	1:C:190:VAL:HG12	1.99	0.61
1:F:70:ILE:HD12	1:F:74:VAL:HG22	1.82	0.61
2:T:123:ILE:HG12	2:T:124:TYR:CD1	2.33	0.61
2:T:149:ASP:O	2:T:152:VAL:HG12	1.99	0.61
1:F:78:THR:HG21	1:F:85:ALA:HB1	1.81	0.61
1:F:170:ASP:O	1:F:173:VAL:HG12	1.99	0.61
2:B:2:THR:HG22	2:B:169:SER:OG	2.00	0.61
1:M:175:PHE:CD2	1:M:196:ALA:HA	2.36	0.61
2:R:141:GLN:NE2	2:W:141:GLN:NE2	2.48	0.61
2:Y:174:ASP:HA	2:Y:192:ILE:HD13	1.83	0.61
1:J:170:ASP:O	1:J:173:VAL:HG12	2.01	0.61
2:B:43:MET:CE	2:B:56:VAL:HG23	2.29	0.61
1:N:124:THR:HG22	1:O:130:ARG:HH21	1.65	0.61
2:B:37:ILE:HD11	2:B:59:MET:HB3	1.82	0.61
2:U:76:ILE:O	2:U:79:VAL:HG12	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:44:THR:OG1	2:Z:100:LEU:HB3	2.00	0.61
1:L:124:THR:HG22	1:M:130:ARG:NH2	2.13	0.61
1:L:184:LEU:HD23	1:L:189:ALA:HA	1.82	0.61
2:Y:18:ARG:HE	2:Y:30:ASN:HD22	1.47	0.61
1:A:61:GLN:OE1	1:A:62:ASN:HB3	2.01	0.61
1:K:21:LEU:O	1:K:25:GLU:HG2	2.01	0.61
1:O:137:ILE:HG22	1:O:150:ASP:HB2	1.83	0.61
2:X:26:ILE:C	2:X:26:ILE:HD13	2.26	0.61
2:Y:123:ILE:HG12	2:Y:124:TYR:HD2	1.66	0.61
1:A:88:LEU:HD21	1:A:120:MET:SD	2.41	0.60
1:A:121:GLN:O	1:A:124:THR:HB	2.00	0.60
1:D:186:GLU:O	1:D:190:VAL:HG12	2.01	0.60
1:E:61:GLN:O	1:E:64:ILE:HG22	2.00	0.60
1:K:18:ASP:OD2	1:K:20:ARG:HD3	2.01	0.60
2:B:59:MET:HE2	2:B:79:VAL:HG23	1.83	0.60
1:K:52:LYS:HE3	1:K:64:ILE:HG23	1.83	0.60
1:L:21:LEU:O	1:L:24:VAL:HG12	2.02	0.60
1:L:43:ALA:HB2	1:L:185:PRO:HA	1.84	0.60
1:L:156:THR:HG23	1:M:82:VAL:HG11	1.82	0.60
1:H:170:ASP:O	1:H:173:VAL:HG12	2.01	0.60
2:S:38:ASP:HB3	2:S:41:THR:CG2	2.32	0.60
2:X:62:GLU:HG2	2:X:82:LEU:HD21	1.82	0.60
1:C:43:ALA:HB2	1:C:185:PRO:HA	1.82	0.60
1:D:168:GLY:O	1:D:172:VAL:HG12	2.02	0.60
1:I:135:SER:OG	1:I:153:PRO:HD3	2.01	0.60
1:J:18:ASP:OD2	1:J:20:ARG:HD3	2.00	0.60
1:K:21:LEU:HD11	1:L:130:ARG:HD2	1.83	0.60
2:W:178:ILE:HB	2:W:184:TYR:HA	1.83	0.60
1:E:24:VAL:O	1:E:27:ALA:HB3	2.02	0.60
2:1:38:ASP:HB3	2:1:41:THR:CG2	2.29	0.60
1:A:49:ILE:HD12	1:A:211:GLU:O	2.01	0.60
1:C:198:LYS:O	1:C:202:GLU:HB2	2.01	0.60
1:F:52:LYS:HZ3	1:F:62:ASN:HA	1.64	0.60
1:H:98:GLN:O	1:H:102:THR:HG22	2.01	0.60
1:N:135:SER:OG	1:N:153:PRO:HD3	2.01	0.60
2:U:26:ILE:C	2:U:26:ILE:HD13	2.27	0.60
2:V:111:PHE:CE2	2:V:121:GLU:HB2	2.37	0.60
1:G:61:GLN:O	1:G:64:ILE:HG22	2.01	0.60
1:A:28:ARG:O	1:A:31:VAL:HG22	2.02	0.60
1:A:42:PHE:HD1	1:A:43:ALA:N	2.00	0.60
1:C:198:LYS:HG2	1:C:202:GLU:HG2	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:49:ILE:HD12	1:I:211:GLU:O	2.01	0.60
1:K:88:LEU:HD13	1:K:132:TYR:CD2	2.36	0.60
2:Q:38:ASP:HB2	2:Q:63:LEU:HD23	1.84	0.60
2:S:3:THR:HB	2:S:16:THR:HG22	1.83	0.60
1:C:84:ASP:O	1:C:87:VAL:HG12	2.02	0.60
1:N:52:LYS:HB3	1:N:209:ALA:O	2.01	0.60
1:N:61:GLN:O	1:N:64:ILE:HG22	2.02	0.60
1:O:98:GLN:O	1:O:101:VAL:HG12	2.02	0.60
2:S:32:LYS:HE2	2:S:34:LEU:O	2.01	0.60
1:D:52:LYS:HA	1:D:66:LYS:NZ	2.17	0.60
1:O:52:LYS:HE3	1:O:64:ILE:HG23	1.83	0.60
2:X:2:THR:HG22	2:X:169:SER:OG	2.02	0.60
1:K:186:GLU:O	1:K:190:VAL:HG12	2.01	0.59
1:N:170:ASP:O	1:N:173:VAL:HG12	2.02	0.59
2:V:62:GLU:HG2	2:V:82:LEU:HD21	1.82	0.59
2:Y:133:PHE:CZ	2:Y:165:ARG:HB3	2.37	0.59
2:1:20:VAL:HG13	2:1:28:HIS:HB2	1.83	0.59
1:I:186:GLU:O	1:I:190:VAL:HG12	2.03	0.59
2:T:133:PHE:CZ	2:T:165:ARG:HB3	2.36	0.59
2:U:178:ILE:HB	2:U:184:TYR:HA	1.84	0.59
2:2:179:THR:HG23	2:2:182:ASP:H	1.68	0.59
2:R:152:VAL:O	2:R:156:ILE:HG13	2.03	0.59
2:Y:111:PHE:CE2	2:Y:121:GLU:HB2	2.37	0.59
2:Z:12:VAL:HG13	2:Z:178:ILE:HG23	1.82	0.59
1:J:61:GLN:O	1:J:64:ILE:HG22	2.00	0.59
1:K:98:GLN:O	1:K:102:THR:HG22	2.03	0.59
1:M:52:LYS:HB3	1:M:209:ALA:O	2.01	0.59
1:O:49:ILE:HD12	1:O:211:GLU:O	2.01	0.59
2:W:124:TYR:HD2	2:W:138:LEU:HD23	1.67	0.59
2:X:179:THR:HG23	2:X:182:ASP:H	1.66	0.59
2:Y:2:THR:HG22	2:Y:169:SER:OG	2.02	0.59
2:Z:37:ILE:HD11	2:Z:59:MET:HB3	1.84	0.59
1:M:94:ILE:HG13	1:M:95:SER:N	2.17	0.59
1:O:49:ILE:HD11	1:O:210:PRO:HB3	1.83	0.59
2:T:38:ASP:HB3	2:T:41:THR:CG2	2.27	0.59
2:1:66:TYR:CZ	2:1:70:ARG:HD2	2.37	0.59
1:A:49:ILE:HD11	1:A:210:PRO:HB3	1.85	0.59
2:R:32:LYS:HE2	2:R:34:LEU:O	2.02	0.59
2:R:38:ASP:HB3	2:R:41:THR:CG2	2.26	0.59
2:R:159:ILE:O	2:R:163:LYS:HG3	2.02	0.59
2:U:3:THR:HB	2:U:16:THR:HG22	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:121:GLN:O	1:F:124:THR:HB	2.03	0.59
2:R:124:TYR:CD2	2:R:138:LEU:HD23	2.37	0.59
2:2:26:ILE:C	2:2:26:ILE:HD13	2.27	0.59
2:B:8:LEU:HD12	2:B:8:LEU:O	2.03	0.59
1:G:95:SER:OG	1:G:115:ARG:HD3	2.03	0.59
1:G:148:LEU:O	1:G:159:GLU:HG3	2.03	0.59
2:2:36:GLN:HB2	2:2:184:TYR:CE1	2.37	0.59
1:F:95:SER:OG	1:F:115:ARG:HD3	2.03	0.59
1:M:136:LEU:HD13	1:M:138:PHE:CE2	2.37	0.59
1:A:103:TYR:HE1	2:P:74:MET:HE2	1.68	0.58
2:Q:7:THR:HB	2:Q:123:ILE:O	2.03	0.58
2:S:123:ILE:HD13	2:S:123:ILE:H	1.67	0.58
1:E:176:LEU:HB3	1:F:58:LEU:HD21	1.85	0.58
1:I:34:GLY:O	1:I:167:SER:HB2	2.03	0.58
1:I:42:PHE:HB2	1:I:184:LEU:O	2.03	0.58
1:E:21:LEU:HD11	1:F:130:ARG:HD2	1.85	0.58
1:L:18:ASP:OD2	1:L:20:ARG:HD3	2.03	0.58
2:2:3:THR:OG1	2:2:127:THR:HG22	2.02	0.58
2:B:26:ILE:C	2:B:26:ILE:HD13	2.28	0.58
1:I:184:LEU:HD23	1:I:189:ALA:HA	1.86	0.58
1:L:61:GLN:O	1:L:64:ILE:HG22	2.04	0.58
2:P:123:ILE:HG12	2:P:124:TYR:CD1	2.32	0.58
2:S:1:THR:H3	2:S:129:SER:HB3	1.69	0.58
1:K:121:GLN:O	1:K:124:THR:HB	2.04	0.58
1:O:81:LEU:HD23	1:O:133:GLY:HA3	1.84	0.58
2:R:1:THR:H3	2:R:129:SER:HB3	1.69	0.58
2:P:149:ASP:O	2:P:152:VAL:HG12	2.03	0.58
1:A:52:LYS:HZ3	1:A:62:ASN:HA	1.66	0.58
1:G:42:PHE:HB2	1:G:184:LEU:O	2.03	0.58
1:G:49:ILE:HD11	1:G:210:PRO:HB3	1.86	0.58
1:O:51:ASP:HB3	1:O:53:LYS:HZ3	1.68	0.58
2:W:133:PHE:CZ	2:W:165:ARG:HB3	2.39	0.58
2:1:59:MET:HE2	2:1:79:VAL:HG23	1.85	0.58
2:2:76:ILE:HG22	2:2:111:PHE:CE2	2.38	0.58
1:D:78:THR:HG21	1:D:85:ALA:HB1	1.85	0.58
2:R:131:SER:O	2:R:134:VAL:HG13	2.04	0.58
1:G:108:ASN:HB3	2:U:70:ARG:HG2	1.86	0.58
2:S:28:HIS:CD2	2:T:120:VAL:HG11	2.39	0.58
1:F:124:THR:HG22	1:G:130:ARG:NH2	2.18	0.58
1:N:21:LEU:O	1:N:25:GLU:HG2	2.03	0.58
2:Q:59:MET:HE1	2:Q:82:LEU:HD23	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:28:HIS:CD2	2:W:120:VAL:HG11	2.39	0.58
2:Z:133:PHE:CZ	2:Z:165:ARG:HB3	2.39	0.58
2:B:152:VAL:O	2:B:156:ILE:HG13	2.04	0.57
1:D:101:VAL:HG23	2:Q:57:ARG:HB3	1.85	0.57
1:M:42:PHE:HB2	1:M:184:LEU:O	2.03	0.57
2:Y:26:ILE:HD13	2:Y:26:ILE:C	2.29	0.57
2:2:149:ASP:O	2:2:152:VAL:HG12	2.04	0.57
1:I:95:SER:OG	1:I:115:ARG:HD3	2.04	0.57
1:L:121:GLN:O	1:L:124:THR:HB	2.04	0.57
1:L:186:GLU:O	1:L:190:VAL:HG12	2.05	0.57
2:R:20:VAL:HG22	2:R:28:HIS:HB2	1.86	0.57
2:2:18:ARG:HE	2:2:30:ASN:HD22	1.51	0.57
1:G:98:GLN:O	1:G:102:THR:HG22	2.04	0.57
1:O:70:ILE:HD12	1:O:74:VAL:HG22	1.86	0.57
2:Q:26:ILE:HD13	2:Q:26:ILE:C	2.29	0.57
2:Y:12:VAL:HG13	2:Y:178:ILE:HG23	1.85	0.57
1:A:135:SER:OG	1:A:153:PRO:HD3	2.04	0.57
1:F:61:GLN:O	1:F:64:ILE:HG22	2.05	0.57
2:P:51:ASP:O	2:P:55:LEU:HB2	2.04	0.57
2:S:179:THR:HG23	2:S:182:ASP:H	1.70	0.57
1:H:180:TYR:HA	1:H:192:LEU:HD21	1.85	0.57
1:I:49:ILE:HD11	1:I:210:PRO:HB3	1.86	0.57
1:J:42:PHE:HD1	1:J:43:ALA:N	2.02	0.57
1:J:49:ILE:HD11	1:J:210:PRO:HB3	1.85	0.57
1:L:78:THR:HG21	1:L:85:ALA:HB1	1.86	0.57
1:O:135:SER:OG	1:O:153:PRO:HD3	2.04	0.57
2:R:26:ILE:C	2:R:26:ILE:HD13	2.29	0.57
2:T:75:PRO:O	2:T:78:ALA:HB3	2.04	0.57
1:C:159:GLU:HG2	1:D:60:GLU:HG3	1.85	0.57
1:F:144:ILE:HD12	1:F:147:ARG:NH1	2.19	0.57
1:G:124:THR:HG22	1:H:130:ARG:NH2	2.16	0.57
2:V:20:VAL:HG13	2:V:28:HIS:HB2	1.85	0.57
2:W:55:LEU:HD21	2:W:87:LEU:HD11	1.87	0.57
1:K:81:LEU:HD23	1:K:133:GLY:HA3	1.85	0.57
2:Q:199:LEU:HB3	2:Q:201:LEU:HD13	1.85	0.57
2:R:173:ILE:C	2:R:173:ILE:HD13	2.30	0.57
2:W:20:VAL:HG13	2:W:28:HIS:HB2	1.87	0.57
1:E:49:ILE:HD13	1:E:212:ILE:HB	1.87	0.57
1:L:35:SER:O	1:L:166:GLY:HA3	2.05	0.57
2:Q:160:SER:O	2:Q:163:LYS:HB2	2.04	0.57
2:T:28:HIS:CD2	2:U:120:VAL:HG11	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:SER:O	1:A:166:GLY:HA3	2.03	0.57
1:H:76:ALA:HB2	1:H:138:PHE:CD1	2.40	0.57
2:R:45:ILE:HG12	2:R:52:ALA:HB1	1.87	0.57
2:W:173:ILE:C	2:W:173:ILE:HD13	2.30	0.57
2:2:7:THR:HB	2:2:123:ILE:O	2.05	0.57
1:E:94:ILE:HG13	1:E:95:SER:N	2.20	0.57
1:G:42:PHE:HD1	1:G:43:ALA:N	2.03	0.57
1:I:69:LEU:HD23	1:I:75:ALA:HB2	1.87	0.57
1:A:143:GLN:HA	1:A:143:GLN:HE21	1.70	0.56
2:B:37:ILE:HD11	2:B:59:MET:CG	2.35	0.56
2:B:66:TYR:HH	1:H:107:VAL:HG11	1.68	0.56
1:C:165:ILE:HG13	1:C:166:GLY:H	1.70	0.56
2:Q:3:THR:OG1	2:Q:127:THR:HG22	2.05	0.56
2:S:43:MET:CE	2:S:56:VAL:HG23	2.35	0.56
2:U:174:ASP:HA	2:U:192:ILE:HD13	1.87	0.56
2:Z:178:ILE:HB	2:Z:184:TYR:HA	1.86	0.56
1:I:21:LEU:O	1:I:24:VAL:HG12	2.05	0.56
2:R:141:GLN:HE21	2:W:141:GLN:NE2	2.03	0.56
2:Z:152:VAL:O	2:Z:156:ILE:HG13	2.05	0.56
1:E:175:PHE:C	1:E:175:PHE:HD1	2.14	0.56
1:J:88:LEU:HD13	1:J:132:TYR:CD2	2.39	0.56
2:U:124:TYR:CD1	2:U:138:LEU:HD23	2.39	0.56
2:U:152:VAL:O	2:U:156:ILE:HG13	2.05	0.56
2:V:6:ILE:HD11	2:V:142:TYR:HD1	1.68	0.56
2:X:133:PHE:CZ	2:X:165:ARG:HB3	2.40	0.56
2:Z:19:ARG:HE	2:Z:26:ILE:HG13	1.71	0.56
1:F:175:PHE:CD2	1:F:196:ALA:HA	2.39	0.56
1:O:184:LEU:HD23	1:O:189:ALA:HA	1.87	0.56
2:T:178:ILE:HB	2:T:184:TYR:HA	1.87	0.56
2:1:75:PRO:O	2:1:78:ALA:HB3	2.06	0.56
1:A:43:ALA:HB2	1:A:185:PRO:HA	1.88	0.56
1:E:81:LEU:HD23	1:E:133:GLY:HA3	1.85	0.56
1:L:76:ALA:HB2	1:L:138:PHE:CD2	2.41	0.56
2:R:18:ARG:HE	2:R:30:ASN:HD22	1.51	0.56
2:2:62:GLU:HG2	2:2:82:LEU:HD21	1.86	0.56
1:A:23:GLN:HE22	1:H:15:PHE:HB2	1.71	0.56
1:H:52:LYS:HB3	1:H:209:ALA:O	2.05	0.56
1:I:108:ASN:CB	2:W:70:ARG:HG2	2.33	0.56
2:B:120:VAL:HG11	2:U:28:HIS:CD2	2.41	0.56
2:B:174:ASP:HA	2:B:192:ILE:HD13	1.88	0.56
1:I:38:LEU:HG	1:I:49:ILE:HG23	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:175:PHE:CD1	1:I:175:PHE:C	2.83	0.56
2:Q:123:ILE:HG12	2:Q:124:TYR:HD1	1.69	0.56
2:T:32:LYS:HE2	2:T:34:LEU:O	2.06	0.56
2:Z:59:MET:CE	2:Z:82:LEU:HD23	2.34	0.56
2:B:70:ARG:HG2	1:H:108:ASN:CB	2.36	0.56
1:E:49:ILE:HD12	1:E:211:GLU:O	2.05	0.56
1:I:124:THR:HG22	1:J:130:ARG:HH21	1.71	0.56
1:I:198:LYS:HG2	1:I:202:GLU:HG2	1.88	0.56
2:Q:167:SER:HB2	2:W:167:SER:HB2	1.88	0.56
2:1:174:ASP:HA	2:1:192:ILE:HD13	1.87	0.56
1:H:137:ILE:HG22	1:H:150:ASP:HB2	1.86	0.56
1:K:61:GLN:O	1:K:64:ILE:HG22	2.06	0.56
2:R:25:PHE:CD1	2:R:25:PHE:C	2.80	0.56
2:X:149:ASP:O	2:X:152:VAL:HG12	2.06	0.56
1:I:61:GLN:O	1:I:64:ILE:HG22	2.06	0.55
1:J:21:LEU:HD11	1:K:130:ARG:HD2	1.88	0.55
1:L:49:ILE:HD12	1:L:211:GLU:O	2.06	0.55
2:V:152:VAL:O	2:V:156:ILE:HG13	2.06	0.55
2:W:43:MET:CE	2:W:56:VAL:HG23	2.33	0.55
1:L:38:LEU:HA	1:L:164:ALA:HA	1.87	0.55
1:N:108:ASN:HB3	2:2:70:ARG:HG2	1.88	0.55
2:B:173:ILE:C	2:B:173:ILE:HD13	2.31	0.55
1:E:175:PHE:C	1:E:175:PHE:CD1	2.83	0.55
1:G:70:ILE:HD12	1:G:74:VAL:HG22	1.88	0.55
1:G:85:ALA:O	1:G:89:VAL:HG23	2.06	0.55
1:H:42:PHE:HD1	1:H:43:ALA:N	2.04	0.55
1:H:186:GLU:O	1:H:190:VAL:HG12	2.06	0.55
2:R:43:MET:HE2	2:R:56:VAL:HG23	1.88	0.55
2:Z:6:ILE:HD11	2:Z:142:TYR:CD1	2.41	0.55
1:L:175:PHE:CD2	1:L:196:ALA:HA	2.41	0.55
1:O:186:GLU:O	1:O:190:VAL:HG12	2.06	0.55
2:X:37:ILE:HD11	2:X:59:MET:CG	2.36	0.55
1:I:175:PHE:C	1:I:175:PHE:HD1	2.15	0.55
2:T:76:ILE:HG21	2:T:109:HIS:HB2	1.87	0.55
2:B:179:THR:HG23	2:B:182:ASP:H	1.71	0.55
2:P:17:GLU:O	2:P:33:LYS:HD2	2.07	0.55
1:K:108:ASN:CB	2:Y:70:ARG:HG2	2.37	0.55
2:T:37:ILE:HD11	2:T:59:MET:CB	2.35	0.55
2:X:28:HIS:CD2	2:Y:120:VAL:HG11	2.42	0.55
2:Z:124:TYR:CD2	2:Z:138:LEU:HD23	2.41	0.55
1:E:170:ASP:O	1:E:173:VAL:HG12	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:156:THR:HG23	1:H:82:VAL:HG11	1.88	0.55
1:H:42:PHE:HB2	1:H:184:LEU:O	2.06	0.55
1:I:130:ARG:NH2	1:O:124:THR:HG22	2.15	0.55
1:C:121:GLN:O	1:C:124:THR:HB	2.06	0.55
1:F:38:LEU:HG	1:F:49:ILE:HG23	1.89	0.55
1:G:175:PHE:CD2	1:G:196:ALA:HA	2.41	0.55
1:L:137:ILE:HG22	1:L:150:ASP:HB2	1.89	0.55
1:O:48:LEU:HD13	1:O:139:ALA:HB3	1.89	0.55
2:U:66:TYR:CZ	2:U:70:ARG:HD2	2.41	0.55
2:X:123:ILE:H	2:X:123:ILE:HD13	1.71	0.55
2:Y:123:ILE:HD13	2:Y:123:ILE:H	1.71	0.55
2:1:131:SER:O	2:1:134:VAL:HG13	2.07	0.55
1:A:70:ILE:HD12	1:A:74:VAL:HG22	1.88	0.55
1:A:95:SER:OG	1:A:115:ARG:HD3	2.07	0.55
1:D:26:TYR:O	1:D:29:GLU:HB2	2.06	0.55
1:E:52:LYS:HZ1	1:E:62:ASN:HA	1.71	0.55
2:S:173:ILE:HD13	2:S:173:ILE:C	2.32	0.55
2:W:123:ILE:HD13	2:W:123:ILE:H	1.72	0.55
1:E:184:LEU:HD23	1:E:189:ALA:HA	1.87	0.54
1:D:175:PHE:CD1	1:D:175:PHE:C	2.85	0.54
1:M:49:ILE:HD11	1:M:210:PRO:HB3	1.88	0.54
1:H:21:LEU:O	1:H:25:GLU:HG2	2.08	0.54
1:I:42:PHE:HD1	1:I:43:ALA:N	2.05	0.54
1:L:52:LYS:HZ1	1:L:62:ASN:HA	1.73	0.54
2:B:62:GLU:HG2	2:B:82:LEU:HD21	1.87	0.54
1:C:38:LEU:HA	1:C:164:ALA:HA	1.89	0.54
1:K:52:LYS:HA	1:K:66:LYS:NZ	2.23	0.54
1:O:78:THR:HG21	1:O:85:ALA:HB1	1.88	0.54
1:A:175:PHE:CD1	1:A:175:PHE:C	2.84	0.54
1:A:175:PHE:C	1:A:175:PHE:HD1	2.15	0.54
2:B:159:ILE:O	2:B:163:LYS:HG3	2.08	0.54
1:K:198:LYS:HG2	1:K:202:GLU:HG2	1.89	0.54
2:S:132:PRO:HA	2:V:133:PHE:HE1	1.72	0.54
2:Z:124:TYR:HD2	2:Z:138:LEU:HD23	1.73	0.54
2:1:7:THR:HB	2:1:123:ILE:O	2.08	0.54
1:A:124:THR:HG22	1:C:130:ARG:NH2	2.23	0.54
1:C:61:GLN:O	1:C:64:ILE:HG22	2.08	0.54
1:C:109:ILE:CG2	1:C:147:ARG:HD3	2.37	0.54
1:D:38:LEU:HA	1:D:164:ALA:HA	1.89	0.54
1:D:52:LYS:HA	1:D:66:LYS:HZ2	1.71	0.54
1:H:174:SER:O	1:H:177:GLU:HB3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:109:ILE:CG2	1:I:147:ARG:HD3	2.37	0.54
2:Z:45:ILE:HG12	2:Z:52:ALA:HB1	1.90	0.54
1:J:69:LEU:HD23	1:J:75:ALA:HB2	1.89	0.54
1:L:94:ILE:HG13	1:L:95:SER:N	2.23	0.54
1:M:61:GLN:OE1	1:M:62:ASN:HB3	2.07	0.54
2:R:62:GLU:HG2	2:R:82:LEU:HD21	1.90	0.54
2:W:193:GLU:O	2:W:196:ILE:HB	2.08	0.54
1:F:187:LYS:O	1:F:190:VAL:HG13	2.08	0.54
2:Q:131:SER:O	2:Q:134:VAL:HG13	2.08	0.54
2:Z:62:GLU:HG2	2:Z:82:LEU:HD21	1.89	0.54
1:A:130:ARG:HH21	1:H:124:THR:HG22	1.73	0.54
1:K:137:ILE:HG22	1:K:150:ASP:HB2	1.89	0.54
1:K:143:GLN:HE21	1:K:143:GLN:HA	1.73	0.54
2:V:15:ALA:HB2	2:V:175:VAL:HB	1.89	0.54
2:W:59:MET:SD	2:W:83:LEU:HD13	2.48	0.54
1:A:42:PHE:HB2	1:A:184:LEU:O	2.08	0.54
1:A:198:LYS:HG2	1:A:202:GLU:HG2	1.88	0.54
2:B:6:ILE:HD11	2:B:142:TYR:CD1	2.42	0.54
1:I:31:VAL:HA	1:I:80:GLY:HA2	1.90	0.54
1:I:174:SER:O	1:I:177:GLU:HB3	2.08	0.54
1:O:51:ASP:HB3	1:O:53:LYS:NZ	2.23	0.54
2:X:59:MET:HE1	2:X:82:LEU:CD2	2.36	0.54
2:X:131:SER:O	2:X:134:VAL:HG13	2.08	0.54
1:C:95:SER:OG	1:C:115:ARG:HD3	2.08	0.53
1:I:144:ILE:HD12	1:I:147:ARG:NH1	2.22	0.53
1:O:168:GLY:O	1:O:172:VAL:HG12	2.09	0.53
2:S:45:ILE:HG12	2:S:52:ALA:HB1	1.90	0.53
2:U:199:LEU:HB3	2:U:201:LEU:HD13	1.90	0.53
2:V:59:MET:HE2	2:V:79:VAL:HG23	1.90	0.53
2:W:25:PHE:CD1	2:W:25:PHE:C	2.84	0.53
1:E:71:ASP:OD2	1:E:74:VAL:HG12	2.08	0.53
1:K:174:SER:O	1:K:177:GLU:HB3	2.08	0.53
2:Y:179:THR:HG23	2:Y:182:ASP:H	1.72	0.53
1:H:97:GLN:OE1	1:H:97:GLN:HA	2.07	0.53
1:M:52:LYS:HZ3	1:M:62:ASN:HA	1.72	0.53
1:N:88:LEU:HD13	1:N:132:TYR:CD2	2.42	0.53
2:V:55:LEU:HD21	2:V:87:LEU:HD11	1.90	0.53
1:D:88:LEU:HD13	1:D:132:TYR:CD2	2.44	0.53
1:E:180:TYR:HA	1:E:192:LEU:HD21	1.90	0.53
1:L:52:LYS:HE3	1:L:64:ILE:HG23	1.89	0.53
2:S:62:GLU:HG2	2:S:82:LEU:HD21	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:61:GLN:OE1	1:G:62:ASN:HB3	2.09	0.53
2:U:149:ASP:O	2:U:152:VAL:HG12	2.08	0.53
2:Z:173:ILE:C	2:Z:173:ILE:HD13	2.34	0.53
1:A:49:ILE:HD13	1:A:212:ILE:HB	1.89	0.53
1:N:15:PHE:HB2	1:O:23:GLN:HE22	1.74	0.53
1:O:52:LYS:HZ1	1:O:62:ASN:HA	1.74	0.53
2:Q:3:THR:HB	2:Q:16:THR:HG22	1.90	0.53
2:T:26:ILE:HD13	2:T:26:ILE:C	2.34	0.53
2:W:26:ILE:O	2:W:26:ILE:HD13	2.08	0.53
1:G:175:PHE:CD1	1:G:175:PHE:C	2.87	0.53
1:K:124:THR:HG22	1:L:130:ARG:NH2	2.20	0.53
1:N:113:VAL:HG22	1:N:157:ILE:HD12	1.91	0.53
1:O:175:PHE:CD1	1:O:175:PHE:C	2.87	0.53
2:P:3:THR:HB	2:P:16:THR:HG22	1.90	0.53
2:S:59:MET:HE1	2:S:82:LEU:HD23	1.91	0.53
2:W:35:PHE:CE2	2:W:45:ILE:HD12	2.43	0.53
2:W:37:ILE:HD11	2:W:59:MET:CG	2.39	0.53
2:1:1:THR:H3	2:1:129:SER:HB3	1.73	0.53
2:1:49:VAL:HG23	2:1:50:GLY:H	1.74	0.53
2:B:133:PHE:CZ	2:B:165:ARG:HB3	2.43	0.53
1:E:109:ILE:CG2	1:E:147:ARG:HD3	2.38	0.53
1:H:51:ASP:HB3	1:H:53:LYS:HZ3	1.72	0.53
1:J:202:GLU:HG3	1:J:205:GLU:O	2.08	0.53
2:Q:32:LYS:HE2	2:Q:34:LEU:O	2.08	0.53
2:Z:174:ASP:HA	2:Z:192:ILE:HD13	1.91	0.53
2:1:124:TYR:CD2	2:1:138:LEU:HD23	2.44	0.53
2:2:103:GLY:HA2	2:2:178:ILE:HD13	1.90	0.53
1:C:144:ILE:HD12	1:C:147:ARG:NH1	2.24	0.53
1:J:43:ALA:HB2	1:J:185:PRO:HA	1.91	0.53
2:S:26:ILE:O	2:S:26:ILE:HD13	2.09	0.53
2:U:18:ARG:HE	2:U:30:ASN:HD22	1.57	0.53
2:W:59:MET:HE2	2:W:79:VAL:HG23	1.91	0.53
2:Y:25:PHE:C	2:Y:25:PHE:CD1	2.83	0.53
2:1:111:PHE:CE2	2:1:121:GLU:HB2	2.44	0.53
1:C:165:ILE:HG13	1:C:166:GLY:N	2.24	0.53
1:E:175:PHE:CD2	1:E:196:ALA:HA	2.44	0.53
1:F:41:LYS:HE3	1:F:160:TYR:O	2.09	0.53
1:J:42:PHE:CD1	1:J:43:ALA:N	2.76	0.53
1:J:95:SER:OG	1:J:115:ARG:HD3	2.09	0.53
1:J:198:LYS:HG3	1:J:207:LEU:HD22	1.91	0.53
1:O:61:GLN:CD	1:O:62:ASN:H	2.16	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:35:PHE:CE2	2:S:45:ILE:HD12	2.43	0.53
2:X:50:GLY:O	2:X:54:VAL:HG12	2.08	0.53
1:F:159:GLU:HG2	1:G:60:GLU:HG3	1.91	0.52
1:H:184:LEU:HD23	1:H:189:ALA:HA	1.92	0.52
1:K:170:ASP:O	1:K:173:VAL:HG12	2.09	0.52
2:S:133:PHE:HE1	2:V:132:PRO:HA	1.74	0.52
2:T:6:ILE:HD11	2:T:142:TYR:CD1	2.44	0.52
2:V:133:PHE:CZ	2:V:165:ARG:HB3	2.43	0.52
1:C:175:PHE:C	1:C:175:PHE:CD1	2.88	0.52
1:J:52:LYS:HB3	1:J:209:ALA:O	2.10	0.52
1:M:35:SER:O	1:M:166:GLY:HA3	2.10	0.52
2:T:55:LEU:HD23	2:T:99:LEU:HD11	1.91	0.52
2:U:131:SER:O	2:U:134:VAL:HG13	2.09	0.52
2:Y:49:VAL:HG23	2:Y:50:GLY:H	1.74	0.52
1:A:144:ILE:HD12	1:A:147:ARG:NH1	2.24	0.52
1:C:180:TYR:HA	1:C:192:LEU:HD21	1.91	0.52
1:F:198:LYS:HG3	1:F:207:LEU:HD22	1.90	0.52
1:J:24:VAL:O	1:J:28:ARG:HG3	2.09	0.52
2:Q:28:HIS:CD2	2:R:120:VAL:HG11	2.44	0.52
2:Q:37:ILE:HD11	2:Q:59:MET:CB	2.38	0.52
2:R:37:ILE:HD11	2:R:59:MET:HB3	1.90	0.52
2:2:76:ILE:HG22	2:2:111:PHE:HE2	1.74	0.52
1:A:42:PHE:CD1	1:A:43:ALA:N	2.78	0.52
2:B:3:THR:HB	2:B:16:THR:HG22	1.90	0.52
1:E:143:GLN:HE21	1:E:143:GLN:HA	1.75	0.52
1:L:21:LEU:HD11	1:M:130:ARG:HD2	1.91	0.52
1:L:95:SER:OG	1:L:115:ARG:HD3	2.09	0.52
1:M:42:PHE:HD1	1:M:43:ALA:N	2.08	0.52
1:D:24:VAL:O	1:D:28:ARG:HG3	2.09	0.52
1:F:21:LEU:O	1:F:25:GLU:HG2	2.09	0.52
1:G:43:ALA:HB2	1:G:185:PRO:HA	1.91	0.52
1:G:51:ASP:HB3	1:G:53:LYS:HZ3	1.74	0.52
1:G:94:ILE:HG13	1:G:95:SER:N	2.24	0.52
1:G:144:ILE:HD12	1:G:147:ARG:NH1	2.24	0.52
2:P:45:ILE:CG1	2:P:52:ALA:HB1	2.39	0.52
2:R:103:GLY:HA2	2:R:178:ILE:HD13	1.91	0.52
1:D:175:PHE:C	1:D:175:PHE:HD1	2.18	0.52
1:J:61:GLN:OE1	1:J:62:ASN:HB3	2.07	0.52
1:L:42:PHE:HB2	1:L:184:LEU:O	2.09	0.52
1:L:109:ILE:CG2	1:L:147:ARG:HD3	2.39	0.52
2:R:15:ALA:HB2	2:R:175:VAL:HB	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:55:LEU:HD21	2:S:87:LEU:HD11	1.92	0.52
2:1:3:THR:HB	2:1:16:THR:HG22	1.91	0.52
1:A:70:ILE:HB	1:A:74:VAL:HG13	1.92	0.52
1:A:160:TYR:CD2	1:A:163:THR:HB	2.45	0.52
1:H:61:GLN:OE1	1:H:62:ASN:HB3	2.09	0.52
1:H:160:TYR:CD2	1:H:163:THR:HB	2.44	0.52
1:L:175:PHE:CD1	1:L:175:PHE:C	2.88	0.52
1:M:108:ASN:HB3	2:1:70:ARG:HG2	1.91	0.52
2:P:18:ARG:HE	2:P:30:ASN:HD22	1.57	0.52
2:P:26:ILE:C	2:P:26:ILE:HD13	2.35	0.52
1:G:21:LEU:O	1:G:25:GLU:HG2	2.09	0.52
1:G:160:TYR:CD2	1:G:163:THR:HB	2.45	0.52
1:H:135:SER:OG	1:H:153:PRO:HD3	2.10	0.52
2:P:63:LEU:HD11	2:P:74:MET:SD	2.48	0.52
2:R:165:ARG:HA	2:V:26:ILE:HG23	1.92	0.52
2:S:141:GLN:NE2	2:V:141:GLN:HE21	2.07	0.52
2:U:25:PHE:CD1	2:U:25:PHE:C	2.84	0.52
2:W:137:VAL:HG21	2:W:158:ALA:HA	1.90	0.52
2:R:36:GLN:HB2	2:R:184:TYR:CE1	2.43	0.52
1:H:49:ILE:HD11	1:H:210:PRO:HB3	1.92	0.52
2:P:179:THR:HG23	2:P:182:ASP:H	1.75	0.52
2:Q:124:TYR:CD2	2:Q:138:LEU:HD23	2.45	0.52
2:Q:189:THR:HG23	2:Q:190:ASP:N	2.25	0.52
2:R:53:GLN:O	2:R:56:VAL:HG12	2.10	0.52
2:S:103:GLY:HA2	2:S:178:ILE:CD1	2.39	0.52
2:V:103:GLY:HA2	2:V:178:ILE:HD11	1.91	0.52
1:F:108:ASN:CB	2:T:70:ARG:HG2	2.41	0.51
1:I:52:LYS:HZ3	1:I:62:ASN:HA	1.73	0.51
1:J:137:ILE:HG22	1:J:150:ASP:HA	1.91	0.51
1:M:109:ILE:HG22	1:M:147:ARG:HD3	1.92	0.51
1:M:113:VAL:HG22	1:M:157:ILE:HD12	1.91	0.51
2:U:2:THR:HG22	2:U:169:SER:OG	2.10	0.51
2:W:131:SER:O	2:W:134:VAL:HG13	2.10	0.51
2:X:146:MET:HE1	2:X:154:LEU:HB2	1.92	0.51
2:1:19:ARG:NE	2:1:26:ILE:HG13	2.25	0.51
1:D:15:PHE:HD2	1:E:23:GLN:NE2	2.09	0.51
1:J:21:LEU:O	1:J:25:GLU:HG2	2.10	0.51
1:J:26:TYR:O	1:J:29:GLU:HB2	2.09	0.51
2:T:20:VAL:CG1	2:T:28:HIS:HB2	2.36	0.51
2:Y:152:VAL:O	2:Y:156:ILE:HG13	2.10	0.51
2:2:111:PHE:CE1	2:2:121:GLU:HB2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:ALA:O	1:A:89:VAL:HG23	2.11	0.51
1:J:38:LEU:HA	1:J:164:ALA:HA	1.92	0.51
2:Y:28:HIS:CD2	2:Z:120:VAL:HG11	2.45	0.51
2:1:37:ILE:HD11	2:1:59:MET:CB	2.35	0.51
1:A:21:LEU:O	1:A:24:VAL:HG12	2.10	0.51
1:I:70:ILE:HB	1:I:74:VAL:HG13	1.91	0.51
1:K:15:PHE:HB2	1:L:23:GLN:HE22	1.75	0.51
1:L:69:LEU:HD23	1:L:75:ALA:HB2	1.93	0.51
1:L:135:SER:OG	1:L:153:PRO:HD3	2.11	0.51
2:X:174:ASP:HA	2:X:192:ILE:HD13	1.91	0.51
2:B:116:ALA:O	2:U:50:GLY:HA3	2.11	0.51
1:E:14:VAL:HB	1:F:23:GLN:OE1	2.10	0.51
1:H:18:ASP:OD2	1:H:20:ARG:HD3	2.11	0.51
1:I:107:VAL:HG11	2:W:66:TYR:HH	1.73	0.51
1:K:165:ILE:HG13	1:K:166:GLY:N	2.25	0.51
1:F:34:GLY:O	1:F:167:SER:HB2	2.11	0.51
1:G:198:LYS:HG2	1:G:202:GLU:HG2	1.91	0.51
1:H:175:PHE:CD1	1:H:175:PHE:C	2.88	0.51
1:J:109:ILE:CG2	1:J:147:ARG:HD3	2.40	0.51
1:J:174:SER:O	1:J:177:GLU:HB3	2.10	0.51
1:J:187:LYS:O	1:J:190:VAL:HG13	2.10	0.51
2:S:124:TYR:HD2	2:S:138:LEU:HD23	1.76	0.51
2:V:123:ILE:HG12	2:V:124:TYR:CD1	2.37	0.51
2:1:18:ARG:HE	2:1:30:ASN:HD22	1.57	0.51
2:B:45:ILE:CG1	2:B:52:ALA:HB1	2.39	0.51
1:C:113:VAL:HG22	1:C:157:ILE:HD12	1.92	0.51
1:G:35:SER:O	1:G:166:GLY:HA3	2.11	0.51
1:H:24:VAL:O	1:H:28:ARG:HG3	2.09	0.51
1:I:52:LYS:HB3	1:I:209:ALA:O	2.11	0.51
1:M:175:PHE:CD1	1:M:175:PHE:C	2.89	0.51
2:P:141:GLN:HE21	2:Y:141:GLN:NE2	2.09	0.51
2:R:174:ASP:HA	2:R:192:ILE:HD13	1.92	0.51
2:S:167:SER:HB2	2:2:167:SER:HB2	1.92	0.51
1:A:156:THR:HG23	1:C:82:VAL:HG11	1.92	0.51
1:D:198:LYS:O	1:D:199:SER:C	2.54	0.51
1:D:198:LYS:HG2	1:D:202:GLU:HG2	1.93	0.51
1:F:184:LEU:HD23	1:F:189:ALA:HA	1.92	0.51
1:K:49:ILE:HD11	1:K:210:PRO:HB3	1.92	0.51
1:M:159:GLU:HG2	1:N:60:GLU:HG3	1.92	0.51
1:N:175:PHE:C	1:N:175:PHE:CD1	2.86	0.51
2:V:174:ASP:HA	2:V:192:ILE:HD13	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:123:ILE:HG12	2:X:124:TYR:CD1	2.39	0.51
1:A:191:THR:O	1:A:194:ILE:HG22	2.11	0.51
1:C:52:LYS:NZ	1:C:62:ASN:HA	2.26	0.51
1:E:110:GLU:O	1:E:113:VAL:HG13	2.10	0.51
1:G:137:ILE:HG22	1:G:150:ASP:CB	2.40	0.51
2:T:49:VAL:HG23	2:T:50:GLY:N	2.25	0.51
2:U:141:GLN:HE21	2:1:141:GLN:NE2	2.08	0.51
2:1:6:ILE:HD11	2:1:142:TYR:CD1	2.45	0.51
2:2:124:TYR:CD1	2:2:138:LEU:HD23	2.46	0.51
1:F:40:MET:HA	1:F:162:ALA:HA	1.93	0.51
1:K:107:VAL:HG11	2:Y:66:TYR:HH	1.75	0.51
1:N:49:ILE:HD11	1:N:210:PRO:HB3	1.93	0.51
1:O:52:LYS:HZ3	1:O:62:ASN:HA	1.76	0.51
2:Q:160:SER:HA	2:Q:163:LYS:HD3	1.93	0.51
2:Z:123:ILE:HG12	2:Z:124:TYR:CD1	2.35	0.51
1:F:24:VAL:O	1:F:28:ARG:HG3	2.11	0.50
1:F:123:TYR:CD1	1:F:123:TYR:N	2.78	0.50
1:H:212:ILE:HG23	1:H:224:TYR:HB2	1.93	0.50
1:J:52:LYS:HE3	1:J:64:ILE:HG23	1.93	0.50
1:J:52:LYS:HZ1	1:J:62:ASN:HA	1.75	0.50
1:M:49:ILE:HD12	1:M:211:GLU:O	2.11	0.50
2:V:26:ILE:HD13	2:V:26:ILE:C	2.36	0.50
2:Y:3:THR:OG1	2:Y:127:THR:HG22	2.11	0.50
2:Y:19:ARG:HE	2:Y:26:ILE:HG13	1.75	0.50
2:Z:28:HIS:CD2	2:1:120:VAL:HG11	2.46	0.50
2:B:141:GLN:NE2	2:Z:141:GLN:HE21	2.08	0.50
1:F:43:ALA:HB2	1:F:185:PRO:HA	1.92	0.50
1:K:38:LEU:HG	1:K:49:ILE:HG23	1.92	0.50
1:K:69:LEU:HD23	1:K:75:ALA:HB2	1.92	0.50
1:O:52:LYS:HB3	1:O:209:ALA:O	2.11	0.50
1:O:180:TYR:HA	1:O:192:LEU:HD21	1.91	0.50
2:P:66:TYR:CZ	2:P:70:ARG:HD2	2.46	0.50
2:U:1:THR:H3	2:U:129:SER:HB3	1.76	0.50
2:X:59:MET:HE2	2:X:79:VAL:HG23	1.94	0.50
2:1:3:THR:CB	2:1:16:THR:HG22	2.42	0.50
2:2:50:GLY:O	2:2:54:VAL:HG12	2.10	0.50
2:B:178:ILE:HB	2:B:184:TYR:HA	1.93	0.50
1:D:95:SER:OG	1:D:115:ARG:HD3	2.10	0.50
1:H:43:ALA:HB2	1:H:185:PRO:HA	1.94	0.50
1:K:175:PHE:C	1:K:175:PHE:CD1	2.89	0.50
1:M:21:LEU:HD11	1:N:130:ARG:HD2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:98:GLN:O	1:M:102:THR:HG22	2.12	0.50
1:M:180:TYR:HB3	1:N:57:ARG:NH2	2.24	0.50
2:R:165:ARG:C	2:V:26:ILE:HG22	2.36	0.50
2:T:131:SER:O	2:T:134:VAL:HG13	2.10	0.50
1:A:180:TYR:HA	1:A:192:LEU:HD21	1.93	0.50
2:B:176:ALA:HA	2:B:186:GLN:HA	1.92	0.50
1:E:95:SER:OG	1:E:115:ARG:HD3	2.11	0.50
1:E:198:LYS:O	1:E:199:SER:C	2.54	0.50
1:I:62:ASN:O	1:I:65:GLU:HG2	2.11	0.50
1:J:175:PHE:HD2	1:J:199:SER:HG	1.60	0.50
2:U:36:GLN:HB2	2:U:184:TYR:CE1	2.46	0.50
2:X:12:VAL:HG13	2:X:178:ILE:HG23	1.93	0.50
2:X:37:ILE:HD11	2:X:59:MET:CB	2.39	0.50
1:E:98:GLN:O	1:E:102:THR:HG22	2.11	0.50
1:F:137:ILE:HG22	1:F:150:ASP:HB2	1.92	0.50
1:O:172:VAL:O	1:O:176:LEU:HD22	2.11	0.50
2:Q:62:GLU:HG2	2:Q:82:LEU:HD21	1.94	0.50
2:S:133:PHE:CZ	2:S:165:ARG:HB3	2.47	0.50
2:T:26:ILE:HD13	2:T:26:ILE:O	2.11	0.50
2:T:62:GLU:HG2	2:T:82:LEU:HD21	1.93	0.50
2:W:152:VAL:O	2:W:156:ILE:HG13	2.11	0.50
2:2:59:MET:HE1	2:2:82:LEU:CD2	2.37	0.50
1:A:149:PHE:CE1	1:A:159:GLU:HB2	2.46	0.50
2:U:20:VAL:HG13	2:U:28:HIS:HB2	1.93	0.50
2:X:15:ALA:HB2	2:X:175:VAL:HB	1.94	0.50
2:Z:3:THR:HB	2:Z:16:THR:HG22	1.94	0.50
1:D:137:ILE:HG22	1:D:150:ASP:HB2	1.93	0.50
1:G:17:PRO:HA	1:H:26:TYR:CD1	2.46	0.50
1:M:43:ALA:HB2	1:M:185:PRO:HA	1.94	0.50
1:M:103:TYR:CE1	2:1:74:MET:HE2	2.47	0.50
2:P:59:MET:CE	2:P:82:LEU:HD23	2.41	0.50
2:Q:123:ILE:H	2:Q:123:ILE:CD1	2.22	0.50
2:Y:189:THR:HG23	2:Y:190:ASP:H	1.76	0.50
2:1:123:ILE:H	2:1:123:ILE:CD1	2.22	0.50
2:2:133:PHE:CZ	2:2:165:ARG:HB3	2.47	0.50
1:C:70:ILE:HD12	1:C:74:VAL:HG22	1.92	0.50
1:E:61:GLN:OE1	1:E:62:ASN:HB3	2.12	0.50
2:V:43:MET:CE	2:V:56:VAL:HG23	2.41	0.50
1:A:26:TYR:CD1	1:H:17:PRO:HA	2.45	0.50
1:C:198:LYS:CG	1:C:202:GLU:HG2	2.42	0.50
1:E:49:ILE:HD11	1:E:210:PRO:HB3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:175:PHE:CD1	1:J:175:PHE:C	2.90	0.50
1:M:62:ASN:O	1:M:65:GLU:HG2	2.12	0.50
1:N:121:GLN:O	1:N:124:THR:HB	2.11	0.50
2:U:112:SER:O	2:U:113:ILE:HD13	2.12	0.50
2:W:26:ILE:HD13	2:W:26:ILE:C	2.35	0.50
2:W:28:HIS:CD2	2:X:120:VAL:HG11	2.47	0.50
2:1:152:VAL:O	2:1:156:ILE:HG13	2.11	0.50
1:C:170:ASP:O	1:C:173:VAL:HG12	2.10	0.49
1:C:198:LYS:O	1:C:199:SER:C	2.55	0.49
1:D:113:VAL:HG22	1:D:157:ILE:HD12	1.94	0.49
1:F:52:LYS:HB3	1:F:209:ALA:O	2.12	0.49
1:K:38:LEU:HA	1:K:164:ALA:HA	1.93	0.49
1:O:174:SER:O	1:O:177:GLU:HB3	2.11	0.49
1:O:198:LYS:O	1:O:199:SER:C	2.55	0.49
2:R:179:THR:HG23	2:R:182:ASP:H	1.77	0.49
2:U:123:ILE:HG12	2:U:124:TYR:CD2	2.44	0.49
2:X:161:ALA:O	2:X:164:GLN:HB2	2.12	0.49
1:H:52:LYS:HZ3	1:H:62:ASN:HA	1.76	0.49
1:O:28:ARG:O	1:O:31:VAL:HG22	2.12	0.49
2:P:173:ILE:HD13	2:P:173:ILE:C	2.37	0.49
2:2:3:THR:HB	2:2:16:THR:HG22	1.93	0.49
1:D:22:PHE:O	1:D:25:GLU:HB2	2.12	0.49
1:D:62:ASN:O	1:D:65:GLU:HG2	2.11	0.49
1:I:52:LYS:HZ1	1:I:62:ASN:HA	1.74	0.49
1:I:198:LYS:O	1:I:199:SER:C	2.55	0.49
1:O:21:LEU:O	1:O:24:VAL:HG12	2.12	0.49
1:O:38:LEU:HA	1:O:164:ALA:HA	1.94	0.49
2:V:75:PRO:O	2:V:78:ALA:HB3	2.12	0.49
2:X:38:ASP:HB3	2:X:41:THR:CG2	2.36	0.49
2:Y:189:THR:HG23	2:Y:190:ASP:N	2.27	0.49
2:2:174:ASP:HA	2:2:192:ILE:HD13	1.93	0.49
1:A:137:ILE:HG22	1:A:150:ASP:HB2	1.95	0.49
1:A:170:ASP:O	1:A:173:VAL:HG12	2.13	0.49
1:G:116:VAL:HG11	1:G:138:PHE:CZ	2.46	0.49
1:H:84:ASP:O	1:H:88:LEU:HB2	2.13	0.49
1:I:94:ILE:HG13	1:I:95:SER:N	2.27	0.49
1:O:95:SER:OG	1:O:115:ARG:HD3	2.12	0.49
2:W:149:ASP:O	2:W:152:VAL:HG12	2.11	0.49
2:X:173:ILE:HD13	2:X:173:ILE:C	2.37	0.49
2:Y:76:ILE:O	2:Y:79:VAL:HG12	2.13	0.49
2:1:19:ARG:HE	2:1:26:ILE:HG13	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:61:GLN:CD	1:H:62:ASN:H	2.20	0.49
1:N:61:GLN:CD	1:N:62:ASN:H	2.20	0.49
2:S:189:THR:HG23	2:S:190:ASP:N	2.28	0.49
2:T:124:TYR:HD2	2:T:138:LEU:HD23	1.76	0.49
2:W:123:ILE:HG12	2:W:124:TYR:CD1	2.36	0.49
1:A:110:GLU:O	1:A:113:VAL:HG12	2.13	0.49
1:E:42:PHE:HB2	1:E:184:LEU:O	2.13	0.49
1:L:198:LYS:O	1:L:199:SER:C	2.56	0.49
2:P:3:THR:OG1	2:P:127:THR:HG22	2.12	0.49
2:1:12:VAL:HG13	2:1:178:ILE:HG23	1.95	0.49
1:E:17:PRO:HA	1:F:26:TYR:CD1	2.48	0.49
1:F:134:VAL:CG2	1:F:135:SER:N	2.76	0.49
1:G:128:GLY:O	1:G:129:VAL:HB	2.13	0.49
1:I:49:ILE:HD13	1:I:212:ILE:HB	1.95	0.49
1:M:198:LYS:O	1:M:199:SER:C	2.56	0.49
2:Y:59:MET:HE2	2:Y:79:VAL:HG23	1.94	0.49
1:A:137:ILE:HG22	1:A:150:ASP:CB	2.43	0.49
1:E:135:SER:OG	1:E:152:ASP:HA	2.12	0.49
1:G:174:SER:O	1:G:177:GLU:HB3	2.12	0.49
1:K:52:LYS:HZ3	1:K:62:ASN:HA	1.75	0.49
2:R:175:VAL:CG2	2:R:176:ALA:N	2.75	0.49
2:V:15:ALA:HB3	2:V:155:VAL:HG11	1.95	0.49
2:2:157:ARG:HA	2:2:201:LEU:HD21	1.95	0.49
1:C:184:LEU:HD23	1:C:189:ALA:HA	1.95	0.49
1:H:88:LEU:HD13	1:H:132:TYR:CD2	2.47	0.49
1:L:110:GLU:O	1:L:113:VAL:HG13	2.13	0.49
2:Q:174:ASP:HA	2:Q:192:ILE:HD13	1.94	0.49
2:S:18:ARG:HE	2:S:30:ASN:HD22	1.61	0.49
2:1:149:ASP:O	2:1:152:VAL:HG12	2.12	0.49
2:B:25:PHE:CD1	2:B:25:PHE:C	2.90	0.49
1:C:175:PHE:C	1:C:175:PHE:HD1	2.20	0.49
1:D:38:LEU:HB3	1:D:164:ALA:HB2	1.94	0.49
1:L:42:PHE:HD1	1:L:43:ALA:N	2.11	0.49
2:Z:26:ILE:C	2:Z:26:ILE:HD13	2.38	0.49
1:H:42:PHE:CD1	1:H:43:ALA:N	2.81	0.48
1:L:187:LYS:O	1:L:190:VAL:HG13	2.14	0.48
2:R:133:PHE:CZ	2:R:165:ARG:HB3	2.48	0.48
2:V:38:ASP:HB3	2:V:41:THR:CG2	2.38	0.48
1:E:69:LEU:HD23	1:E:75:ALA:HB2	1.96	0.48
1:F:32:LYS:O	1:F:167:SER:HA	2.14	0.48
1:I:97:GLN:OE1	1:I:97:GLN:HA	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:21:LEU:HD11	1:O:130:ARG:HD2	1.94	0.48
1:N:186:GLU:O	1:N:190:VAL:HG12	2.13	0.48
1:O:187:LYS:O	1:O:190:VAL:HG13	2.13	0.48
2:P:25:PHE:CD1	2:P:25:PHE:C	2.91	0.48
2:Q:18:ARG:HB2	2:Q:31:GLY:O	2.13	0.48
2:X:152:VAL:O	2:X:156:ILE:HG13	2.13	0.48
1:C:187:LYS:O	1:C:190:VAL:HG13	2.14	0.48
1:D:148:LEU:O	1:D:159:GLU:HG3	2.13	0.48
1:G:70:ILE:HB	1:G:74:VAL:HG13	1.95	0.48
1:K:124:THR:CG2	1:L:130:ARG:HH21	2.22	0.48
1:M:136:LEU:HD12	1:M:151:CYS:HB3	1.94	0.48
2:P:15:ALA:HB2	2:P:175:VAL:HB	1.93	0.48
2:T:76:ILE:O	2:T:79:VAL:HG12	2.14	0.48
2:1:189:THR:HG23	2:1:190:ASP:N	2.29	0.48
1:A:228:GLU:O	1:A:231:LYS:HB3	2.13	0.48
2:B:12:VAL:HG13	2:B:178:ILE:HG23	1.96	0.48
1:C:124:THR:HG22	1:D:130:ARG:HH21	1.79	0.48
1:D:180:TYR:HA	1:D:192:LEU:HD21	1.95	0.48
1:E:35:SER:O	1:E:166:GLY:HA3	2.13	0.48
1:E:107:VAL:HG11	2:S:66:TYR:HH	1.77	0.48
1:H:175:PHE:C	1:H:175:PHE:HD1	2.22	0.48
1:K:34:GLY:O	1:K:167:SER:HB2	2.13	0.48
1:L:198:LYS:HG2	1:L:202:GLU:HG2	1.95	0.48
1:N:98:GLN:O	1:N:101:VAL:HG12	2.13	0.48
2:V:45:ILE:CG1	2:V:52:ALA:HB1	2.42	0.48
2:Y:38:ASP:HB3	2:Y:41:THR:CG2	2.32	0.48
2:2:131:SER:O	2:2:134:VAL:HG13	2.13	0.48
2:B:36:GLN:HB2	2:B:184:TYR:CE1	2.48	0.48
2:B:124:TYR:HD2	2:B:138:LEU:HD23	1.76	0.48
1:C:28:ARG:O	1:C:31:VAL:HG22	2.13	0.48
1:G:69:LEU:HD23	1:G:75:ALA:HB2	1.94	0.48
1:G:152:ASP:HB2	1:G:153:PRO:CD	2.43	0.48
1:J:123:TYR:CE2	1:J:129:VAL:HG21	2.48	0.48
1:O:215:ILE:HD11	1:O:219:ASN:O	2.13	0.48
2:X:104:ILE:HG22	2:X:178:ILE:HD11	1.94	0.48
1:A:62:ASN:O	1:A:65:GLU:HG2	2.13	0.48
1:F:49:ILE:HD11	1:F:210:PRO:HB3	1.94	0.48
1:J:144:ILE:HD12	1:J:147:ARG:NH1	2.28	0.48
1:M:175:PHE:C	1:M:175:PHE:HD1	2.20	0.48
2:Q:109:HIS:HB3	2:Q:111:PHE:HE1	1.79	0.48
1:A:148:LEU:O	1:A:159:GLU:HG3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:168:GLY:O	1:E:172:VAL:HG12	2.12	0.48
1:O:175:PHE:C	1:O:175:PHE:HD1	2.21	0.48
2:T:179:THR:HG23	2:T:182:ASP:H	1.79	0.48
2:B:17:GLU:HB2	2:B:170:GLY:O	2.14	0.48
2:B:141:GLN:NE2	2:Z:141:GLN:NE2	2.61	0.48
1:D:85:ALA:O	1:D:89:VAL:HG23	2.14	0.48
1:D:121:GLN:O	1:D:124:THR:HB	2.13	0.48
1:E:15:PHE:HD2	1:F:23:GLN:HE22	1.61	0.48
1:E:127:GLY:O	1:E:129:VAL:N	2.47	0.48
1:F:76:ALA:HB2	1:F:138:PHE:CD1	2.48	0.48
1:K:98:GLN:O	1:K:101:VAL:HG12	2.14	0.48
1:N:24:VAL:O	1:N:28:ARG:HG3	2.14	0.48
2:V:111:PHE:CD2	2:V:121:GLU:HB2	2.49	0.48
2:X:36:GLN:HB2	2:X:184:TYR:CE1	2.48	0.48
2:1:137:VAL:HG21	2:1:158:ALA:HA	1.95	0.48
1:C:61:GLN:CD	1:C:62:ASN:H	2.21	0.48
1:C:125:GLN:HB3	1:D:130:ARG:NH2	2.28	0.48
1:D:147:ARG:HB3	1:D:149:PHE:HE1	1.79	0.48
1:H:52:LYS:HA	1:H:66:LYS:NZ	2.29	0.48
1:M:42:PHE:CD1	1:M:43:ALA:N	2.81	0.48
2:T:167:SER:HB2	2:1:167:SER:HB2	1.95	0.48
2:U:141:GLN:NE2	2:1:141:GLN:HE21	2.12	0.48
2:Z:3:THR:OG1	2:Z:127:THR:HG22	2.14	0.48
2:2:55:LEU:HD21	2:2:87:LEU:HD11	1.96	0.48
1:G:175:PHE:C	1:G:175:PHE:HD1	2.21	0.48
1:J:49:ILE:HD12	1:J:211:GLU:O	2.13	0.48
1:M:61:GLN:O	1:M:64:ILE:HG22	2.12	0.48
2:Q:66:TYR:CD2	2:Q:74:MET:HE2	2.48	0.48
2:W:202:ILE:HG12	2:W:203:LEU:N	2.28	0.48
2:X:37:ILE:HD11	2:X:59:MET:HG3	1.96	0.48
2:Y:34:LEU:HD21	2:Y:176:ALA:HB3	1.95	0.48
2:Y:55:LEU:HD21	2:Y:87:LEU:HD11	1.94	0.48
1:C:24:VAL:O	1:C:28:ARG:HG3	2.14	0.47
1:F:42:PHE:HB2	1:F:184:LEU:O	2.14	0.47
1:H:48:LEU:HB3	1:H:67:ILE:HD13	1.96	0.47
1:I:113:VAL:HG22	1:I:157:ILE:HD12	1.96	0.47
1:O:94:ILE:HG13	1:O:95:SER:N	2.29	0.47
2:P:22:MET:O	2:P:23:GLU:HB2	2.14	0.47
2:V:26:ILE:HD13	2:V:26:ILE:O	2.13	0.47
1:A:108:ASN:HB3	2:P:70:ARG:HG2	1.95	0.47
2:B:66:TYR:CZ	2:B:70:ARG:HD2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:126:SER:HB3	2:B:135:TYR:CE2	2.49	0.47
1:D:90:ASP:O	1:D:94:ILE:HG23	2.14	0.47
1:E:191:THR:O	1:E:194:ILE:HG22	2.13	0.47
1:G:42:PHE:CD1	1:G:43:ALA:N	2.81	0.47
2:P:59:MET:HE1	2:P:82:LEU:CD2	2.42	0.47
2:Q:159:ILE:O	2:Q:163:LYS:HG3	2.14	0.47
2:R:44:THR:OG1	2:R:100:LEU:HB3	2.14	0.47
2:V:44:THR:OG1	2:V:100:LEU:HB3	2.14	0.47
2:1:15:ALA:HB2	2:1:175:VAL:HB	1.95	0.47
2:1:133:PHE:CZ	2:1:165:ARG:HB3	2.49	0.47
2:2:6:ILE:HD11	2:2:142:TYR:CD1	2.49	0.47
1:C:137:ILE:HG22	1:C:150:ASP:HB2	1.96	0.47
1:E:134:VAL:CG2	1:E:135:SER:N	2.76	0.47
1:F:38:LEU:CD2	1:F:49:ILE:HG23	2.44	0.47
1:G:198:LYS:CG	1:G:202:GLU:HG2	2.44	0.47
1:N:187:LYS:O	1:N:190:VAL:HG13	2.14	0.47
2:P:32:LYS:HE2	2:P:34:LEU:O	2.14	0.47
2:P:189:THR:HG23	2:P:190:ASP:N	2.28	0.47
2:P:189:THR:HG23	2:P:190:ASP:H	1.79	0.47
2:T:74:MET:HG2	2:T:78:ALA:HB3	1.95	0.47
2:2:123:ILE:HG12	2:2:124:TYR:CD2	2.49	0.47
1:E:202:GLU:HG3	1:E:205:GLU:O	2.14	0.47
1:F:49:ILE:HD12	1:F:211:GLU:O	2.14	0.47
1:I:81:LEU:HD23	1:I:133:GLY:HA3	1.97	0.47
1:K:165:ILE:HG13	1:K:166:GLY:H	1.79	0.47
1:L:113:VAL:HG22	1:L:157:ILE:HD12	1.96	0.47
1:N:26:TYR:O	1:N:29:GLU:HB2	2.15	0.47
1:N:95:SER:OG	1:N:115:ARG:HD3	2.14	0.47
2:R:103:GLY:HA2	2:R:178:ILE:CD1	2.44	0.47
2:U:175:VAL:CG2	2:U:176:ALA:N	2.78	0.47
2:V:103:GLY:HA2	2:V:178:ILE:HD13	1.95	0.47
2:W:62:GLU:HG2	2:W:82:LEU:HD21	1.96	0.47
2:1:66:TYR:CD1	2:1:66:TYR:C	2.92	0.47
2:2:173:ILE:HD13	2:2:173:ILE:C	2.39	0.47
1:E:130:ARG:HG2	1:E:130:ARG:HH11	1.80	0.47
1:H:198:LYS:O	1:H:199:SER:C	2.56	0.47
1:I:130:ARG:HH21	1:O:124:THR:CG2	2.20	0.47
1:I:160:TYR:CD2	1:I:163:THR:HB	2.49	0.47
1:M:94:ILE:CG1	1:M:95:SER:N	2.77	0.47
1:N:61:GLN:OE1	1:N:62:ASN:HB3	2.13	0.47
2:S:132:PRO:HA	2:V:133:PHE:CE1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:18:ARG:HB2	2:U:31:GLY:O	2.14	0.47
2:U:91:LYS:O	2:U:94:PRO:HD3	2.15	0.47
2:V:17:GLU:HA	2:V:173:ILE:HA	1.96	0.47
2:V:143:SER:O	2:V:146:MET:HG3	2.14	0.47
2:Y:22:MET:O	2:Y:23:GLU:HB2	2.14	0.47
2:Y:123:ILE:HG12	2:Y:124:TYR:CD2	2.49	0.47
1:C:94:ILE:CG1	1:C:95:SER:N	2.78	0.47
1:C:98:GLN:O	1:C:102:THR:HG23	2.15	0.47
1:J:62:ASN:O	1:J:65:GLU:HG2	2.14	0.47
1:L:174:SER:O	1:L:175:PHE:C	2.57	0.47
1:M:34:GLY:O	1:M:167:SER:HB2	2.14	0.47
1:N:82:VAL:HG13	1:N:83:ALA:N	2.29	0.47
2:T:7:THR:HB	2:T:123:ILE:O	2.14	0.47
2:Z:15:ALA:HB3	2:Z:155:VAL:CG1	2.44	0.47
2:1:2:THR:HG22	2:1:169:SER:OG	2.14	0.47
2:1:45:ILE:HG12	2:1:52:ALA:HB1	1.95	0.47
2:1:103:GLY:HA2	2:1:178:ILE:HD13	1.97	0.47
1:A:61:GLN:CD	1:A:62:ASN:H	2.22	0.47
1:A:134:VAL:O	1:A:153:PRO:HG3	2.14	0.47
2:B:83:LEU:HD12	2:B:83:LEU:HA	1.69	0.47
2:B:103:GLY:HA2	2:B:178:ILE:CD1	2.44	0.47
1:D:229:VAL:HG13	1:D:230:LYS:N	2.30	0.47
1:E:52:LYS:HE3	1:E:64:ILE:HG23	1.96	0.47
1:G:143:GLN:HA	1:G:143:GLN:HE21	1.80	0.47
1:G:198:LYS:O	1:G:199:SER:C	2.57	0.47
1:H:45:GLY:HA3	1:H:216:THR:HA	1.96	0.47
1:J:159:GLU:HG2	1:K:60:GLU:HG3	1.96	0.47
1:K:42:PHE:HB2	1:K:184:LEU:O	2.15	0.47
1:K:198:LYS:O	1:K:199:SER:C	2.57	0.47
1:L:175:PHE:C	1:L:175:PHE:HD1	2.21	0.47
2:P:35:PHE:CE2	2:P:45:ILE:HD12	2.50	0.47
2:Q:45:ILE:HD11	2:Q:52:ALA:O	2.14	0.47
2:Q:152:VAL:O	2:Q:156:ILE:HG13	2.14	0.47
2:S:174:ASP:HA	2:S:192:ILE:HD13	1.96	0.47
2:T:22:MET:O	2:T:23:GLU:HB2	2.15	0.47
2:U:27:MET:O	2:U:27:MET:HG2	2.15	0.47
2:1:104:ILE:HG22	2:1:178:ILE:HD11	1.96	0.47
2:B:6:ILE:HD11	2:B:142:TYR:HD1	1.80	0.47
2:B:20:VAL:HG22	2:B:28:HIS:HB2	1.96	0.47
1:C:21:LEU:HD11	1:D:130:ARG:HD2	1.97	0.47
1:G:38:LEU:HA	1:G:164:ALA:HA	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:16:SER:HB3	1:H:22:PHE:CE2	2.50	0.47
1:I:180:TYR:HB3	1:J:57:ARG:NH2	2.30	0.47
1:L:109:ILE:HG22	1:L:147:ARG:HD3	1.97	0.47
1:N:18:ASP:OD2	1:N:20:ARG:HD3	2.15	0.47
1:O:116:VAL:HG11	1:O:138:PHE:CZ	2.50	0.47
2:Q:175:VAL:CG2	2:Q:176:ALA:N	2.78	0.47
2:T:141:GLN:HE21	2:2:141:GLN:NE2	2.12	0.47
2:2:25:PHE:CD1	2:2:25:PHE:C	2.89	0.47
1:A:103:TYR:CE1	2:P:74:MET:HE2	2.48	0.47
2:B:37:ILE:HD11	2:B:59:MET:CB	2.45	0.47
2:B:165:ARG:C	2:Y:26:ILE:HG22	2.40	0.47
1:C:58:LEU:N	1:C:58:LEU:CD1	2.78	0.47
1:E:159:GLU:HG2	1:F:60:GLU:HG3	1.96	0.47
1:H:114:LYS:O	1:H:117:ALA:HB3	2.15	0.47
1:I:35:SER:O	1:I:166:GLY:HA3	2.15	0.47
1:L:108:ASN:HA	1:L:142:ASP:OD1	2.15	0.47
1:N:52:LYS:HE3	1:N:64:ILE:HG23	1.97	0.47
1:O:130:ARG:HG2	1:O:130:ARG:NH1	2.30	0.47
2:T:184:TYR:CD1	2:T:184:TYR:C	2.93	0.47
2:W:37:ILE:HD11	2:W:59:MET:HG3	1.97	0.47
2:2:189:THR:HG23	2:2:190:ASP:N	2.30	0.47
1:C:110:GLU:O	1:C:113:VAL:HG13	2.15	0.47
1:D:52:LYS:HZ1	1:D:62:ASN:HA	1.80	0.47
1:F:38:LEU:HA	1:F:164:ALA:HA	1.97	0.47
1:G:152:ASP:HB2	1:G:153:PRO:HD2	1.96	0.47
1:I:135:SER:OG	1:I:152:ASP:HA	2.15	0.47
1:I:187:LYS:O	1:I:190:VAL:HG13	2.14	0.47
1:K:130:ARG:HG2	1:K:130:ARG:HH11	1.80	0.47
1:N:142:ASP:OD2	1:N:147:ARG:HD2	2.16	0.47
2:Q:81:THR:O	2:Q:84:SER:HB3	2.15	0.47
2:S:165:ARG:C	2:2:26:ILE:HG22	2.40	0.47
2:V:175:VAL:CG2	2:V:176:ALA:N	2.78	0.47
2:V:177:VAL:HG12	2:V:187:LEU:HD11	1.96	0.47
1:E:134:VAL:O	1:E:153:PRO:HG3	2.15	0.46
1:F:135:SER:OG	1:F:153:PRO:HD3	2.15	0.46
2:R:74:MET:HG2	2:R:78:ALA:HB3	1.97	0.46
2:X:22:MET:O	2:X:23:GLU:HB2	2.16	0.46
2:X:124:TYR:HD2	2:X:138:LEU:HD23	1.80	0.46
2:Y:175:VAL:CG2	2:Y:176:ALA:N	2.78	0.46
2:2:66:TYR:CD1	2:2:66:TYR:C	2.93	0.46
2:2:123:ILE:HG12	2:2:124:TYR:HD2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:GLN:O	1:A:102:THR:HG23	2.15	0.46
1:F:98:GLN:O	1:F:101:VAL:HG12	2.16	0.46
1:L:152:ASP:HB2	1:L:153:PRO:HD2	1.97	0.46
1:O:108:ASN:CB	2:V:70:ARG:HG2	2.44	0.46
2:U:123:ILE:HD13	2:U:123:ILE:N	2.26	0.46
2:W:131:SER:HB2	2:W:132:PRO:HD3	1.97	0.46
2:Z:177:VAL:HG12	2:Z:187:LEU:HD11	1.97	0.46
2:B:177:VAL:HG12	2:B:187:LEU:CD1	2.46	0.46
1:D:42:PHE:O	1:D:43:ALA:C	2.59	0.46
1:E:103:TYR:CE1	2:S:74:MET:HE2	2.50	0.46
1:I:48:LEU:HB3	1:I:67:ILE:HD13	1.97	0.46
1:I:72:ASP:HB2	1:I:73:TYR:CD1	2.51	0.46
1:I:121:GLN:O	1:I:124:THR:HB	2.14	0.46
2:W:76:ILE:HA	2:W:79:VAL:HG12	1.96	0.46
2:W:138:LEU:HD12	2:W:138:LEU:HA	1.73	0.46
2:Y:36:GLN:HB2	2:Y:184:TYR:CE1	2.50	0.46
1:A:60:GLU:HG3	1:H:159:GLU:HG2	1.96	0.46
2:B:165:ARG:HA	2:Y:26:ILE:HG23	1.98	0.46
1:D:21:LEU:HD11	1:E:130:ARG:HD2	1.97	0.46
1:D:172:VAL:O	1:D:176:LEU:HD22	2.16	0.46
1:I:18:ASP:OD2	1:I:20:ARG:HD3	2.16	0.46
1:J:88:LEU:HD13	1:J:132:TYR:CE2	2.51	0.46
1:K:172:VAL:O	1:K:176:LEU:HD22	2.16	0.46
1:L:180:TYR:HA	1:L:192:LEU:HD21	1.97	0.46
2:P:20:VAL:CG1	2:P:28:HIS:HB2	2.44	0.46
2:R:50:GLY:O	2:R:54:VAL:HG12	2.14	0.46
2:S:25:PHE:CD1	2:S:25:PHE:C	2.91	0.46
2:V:19:ARG:HE	2:V:26:ILE:HG13	1.80	0.46
2:X:3:THR:HG1	2:X:127:THR:HG22	1.80	0.46
2:Y:34:LEU:HD21	2:Y:176:ALA:CB	2.46	0.46
2:Y:178:ILE:HB	2:Y:184:TYR:HA	1.96	0.46
2:1:15:ALA:HB3	2:1:155:VAL:HG11	1.98	0.46
1:A:175:PHE:CD2	1:A:196:ALA:HA	2.50	0.46
1:J:165:ILE:HD12	1:J:169:LYS:HD2	1.97	0.46
1:M:124:THR:HG22	1:N:130:ARG:HH21	1.81	0.46
2:U:132:PRO:HA	2:1:133:PHE:HE1	1.81	0.46
2:Z:8:LEU:HD12	2:Z:8:LEU:O	2.16	0.46
2:Z:43:MET:HE2	2:Z:56:VAL:HG23	1.97	0.46
2:Z:50:GLY:O	2:Z:54:VAL:HG12	2.16	0.46
1:F:81:LEU:HD23	1:F:133:GLY:HA3	1.97	0.46
1:F:160:TYR:C	1:G:60:GLU:HG2	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:228:GLU:O	1:F:231:LYS:HB3	2.15	0.46
1:H:31:VAL:HA	1:H:80:GLY:HA2	1.98	0.46
1:L:161:LYS:HD2	1:M:60:GLU:OE2	2.16	0.46
1:L:174:SER:O	1:L:177:GLU:HB3	2.15	0.46
2:R:48:LEU:HD12	2:R:49:VAL:N	2.31	0.46
2:W:15:ALA:HB2	2:W:175:VAL:HB	1.96	0.46
1:C:42:PHE:HD1	1:C:43:ALA:N	2.14	0.46
1:E:70:ILE:HB	1:E:74:VAL:HG13	1.98	0.46
1:F:152:ASP:HB2	1:F:153:PRO:CD	2.46	0.46
1:H:135:SER:OG	1:H:152:ASP:HA	2.16	0.46
1:O:61:GLN:OE1	1:O:62:ASN:HB3	2.16	0.46
1:O:88:LEU:HD13	1:O:132:TYR:CD2	2.51	0.46
2:R:160:SER:HA	2:R:163:LYS:HD3	1.98	0.46
2:S:75:PRO:O	2:S:78:ALA:HB3	2.16	0.46
2:U:55:LEU:HD21	2:U:87:LEU:HD11	1.97	0.46
2:U:76:ILE:HG21	2:U:109:HIS:HB2	1.96	0.46
2:V:37:ILE:HD11	2:V:59:MET:HB3	1.97	0.46
2:X:40:TYR:O	2:X:178:ILE:HD11	2.15	0.46
2:1:22:MET:O	2:1:23:GLU:HB2	2.15	0.46
1:A:198:LYS:O	1:A:199:SER:C	2.59	0.46
2:B:72:VAL:HG22	2:B:73:ASN:N	2.31	0.46
1:E:108:ASN:CB	2:S:70:ARG:HG2	2.43	0.46
1:H:52:LYS:HZ1	1:H:62:ASN:HA	1.81	0.46
1:J:198:LYS:HG2	1:J:202:GLU:HG2	1.96	0.46
1:K:228:GLU:O	1:K:231:LYS:HB3	2.16	0.46
2:S:103:GLY:HA2	2:S:178:ILE:HD11	1.98	0.46
2:1:15:ALA:HB3	2:1:155:VAL:CG1	2.46	0.46
1:E:42:PHE:CD1	1:E:43:ALA:N	2.84	0.46
1:G:130:ARG:HA	1:G:131:PRO:HD3	1.82	0.46
1:I:198:LYS:C	1:I:202:GLU:HB2	2.41	0.46
1:L:38:LEU:HG	1:L:49:ILE:HG23	1.98	0.46
2:P:175:VAL:CG2	2:P:176:ALA:N	2.78	0.46
2:X:59:MET:CE	2:X:82:LEU:HD23	2.42	0.46
2:Z:59:MET:CE	2:Z:79:VAL:HG23	2.38	0.46
2:B:193:GLU:HA	2:B:196:ILE:HD12	1.98	0.46
1:D:94:ILE:HG13	1:D:95:SER:N	2.29	0.46
1:E:77:VAL:CG1	1:E:137:ILE:HG12	2.46	0.46
1:G:109:ILE:CG2	1:G:147:ARG:HD3	2.46	0.46
1:H:187:LYS:O	1:H:190:VAL:HG13	2.16	0.46
1:I:137:ILE:HG22	1:I:150:ASP:CB	2.45	0.46
1:K:43:ALA:HB2	1:K:185:PRO:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:88:LEU:HD13	1:N:132:TYR:CE2	2.51	0.46
2:R:17:GLU:HA	2:R:173:ILE:HA	1.98	0.46
2:T:174:ASP:HA	2:T:192:ILE:HD13	1.98	0.46
2:U:109:HIS:HB3	2:U:111:PHE:HE1	1.81	0.46
2:1:26:ILE:HD13	2:1:26:ILE:O	2.16	0.46
1:G:81:LEU:HD23	1:G:133:GLY:HA3	1.97	0.45
1:H:38:LEU:HG	1:H:49:ILE:HG23	1.98	0.45
2:R:27:MET:O	2:R:27:MET:HG2	2.16	0.45
2:R:111:PHE:CE2	2:R:121:GLU:HB2	2.51	0.45
2:R:124:TYR:HD2	2:R:138:LEU:HD23	1.80	0.45
2:U:187:LEU:HA	2:U:188:PRO:HD3	1.81	0.45
2:Y:18:ARG:HB2	2:Y:31:GLY:O	2.16	0.45
2:Z:32:LYS:HE2	2:Z:34:LEU:O	2.16	0.45
2:1:26:ILE:HD13	2:1:26:ILE:C	2.41	0.45
2:1:189:THR:HG23	2:1:190:ASP:H	1.81	0.45
1:C:15:PHE:HD2	1:D:23:GLN:HE22	1.64	0.45
1:F:51:ASP:HB3	1:F:53:LYS:HZ3	1.81	0.45
1:F:194:ILE:O	1:F:198:LYS:HB2	2.16	0.45
1:F:198:LYS:O	1:F:199:SER:C	2.58	0.45
1:I:148:LEU:O	1:I:159:GLU:HG3	2.16	0.45
1:K:198:LYS:HG3	1:K:207:LEU:HD22	1.98	0.45
1:L:52:LYS:HZ3	1:L:62:ASN:HA	1.79	0.45
2:S:178:ILE:O	2:S:178:ILE:HG12	2.14	0.45
2:T:15:ALA:HB3	2:T:155:VAL:HG11	1.98	0.45
2:W:103:GLY:HA2	2:W:178:ILE:CD1	2.46	0.45
2:W:189:THR:HG23	2:W:190:ASP:N	2.31	0.45
2:B:55:LEU:HD12	2:B:55:LEU:HA	1.50	0.45
2:B:132:PRO:HA	2:Z:133:PHE:HE1	1.81	0.45
1:H:52:LYS:HE3	1:H:64:ILE:HG23	1.99	0.45
1:J:76:ALA:HB2	1:J:138:PHE:CD1	2.52	0.45
1:J:143:GLN:HA	1:J:143:GLN:HE21	1.82	0.45
1:N:58:LEU:N	1:N:58:LEU:CD1	2.79	0.45
2:Q:179:THR:HG23	2:Q:182:ASP:H	1.80	0.45
2:R:75:PRO:O	2:R:78:ALA:HB3	2.16	0.45
2:S:19:ARG:HE	2:S:26:ILE:HG13	1.82	0.45
2:T:110:VAL:O	2:T:110:VAL:HG13	2.16	0.45
2:U:124:TYR:HD1	2:U:138:LEU:HD23	1.81	0.45
2:V:18:ARG:HE	2:V:30:ASN:HD22	1.65	0.45
2:X:59:MET:SD	2:X:83:LEU:HD13	2.56	0.45
1:A:52:LYS:HE3	1:A:64:ILE:HG23	1.99	0.45
2:B:7:THR:HB	2:B:123:ILE:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:111:PHE:CE2	2:B:121:GLU:HB2	2.51	0.45
1:C:49:ILE:HD11	1:C:210:PRO:HB3	1.98	0.45
1:D:52:LYS:HE3	1:D:64:ILE:HG23	1.98	0.45
1:F:61:GLN:OE1	1:F:62:ASN:HB3	2.16	0.45
1:F:103:TYR:CE1	2:T:74:MET:HE2	2.52	0.45
1:N:175:PHE:C	1:N:175:PHE:HD1	2.23	0.45
2:P:105:ASP:OD1	2:P:106:THR:N	2.49	0.45
2:1:175:VAL:CG2	2:1:176:ALA:N	2.78	0.45
1:I:42:PHE:CD1	1:I:43:ALA:N	2.83	0.45
1:K:175:PHE:C	1:K:175:PHE:HD1	2.24	0.45
1:L:152:ASP:HB2	1:L:153:PRO:CD	2.46	0.45
1:N:198:LYS:O	1:N:199:SER:C	2.59	0.45
2:R:149:ASP:O	2:R:152:VAL:HG12	2.17	0.45
2:W:147:THR:OG1	2:W:150:GLU:HG3	2.16	0.45
2:X:189:THR:HG23	2:X:190:ASP:N	2.31	0.45
2:Z:15:ALA:HB3	2:Z:155:VAL:HG11	1.97	0.45
2:1:93:MET:N	2:1:94:PRO:CD	2.79	0.45
2:B:27:MET:O	2:B:27:MET:HG2	2.17	0.45
1:D:18:ASP:OD2	1:D:20:ARG:HD3	2.15	0.45
1:M:180:TYR:HB3	1:N:57:ARG:HH22	1.80	0.45
1:M:198:LYS:HG2	1:M:202:GLU:HG2	1.98	0.45
2:Q:20:VAL:HG13	2:Q:28:HIS:HB2	1.97	0.45
2:Q:141:GLN:HE21	2:X:141:GLN:NE2	2.14	0.45
2:U:130:GLY:O	2:U:134:VAL:HG12	2.17	0.45
2:2:76:ILE:O	2:2:79:VAL:HG12	2.17	0.45
1:C:69:LEU:HD23	1:C:75:ALA:HB2	1.98	0.45
1:E:148:LEU:O	1:E:159:GLU:HG3	2.17	0.45
1:G:16:SER:C	1:G:18:ASP:H	2.24	0.45
1:I:171:ALA:HB3	1:I:200:SER:OG	2.17	0.45
1:K:52:LYS:CE	1:K:64:ILE:HG23	2.46	0.45
1:M:228:GLU:O	1:M:231:LYS:HB3	2.17	0.45
2:Q:189:THR:HG23	2:Q:190:ASP:H	1.81	0.45
2:R:43:MET:CE	2:R:56:VAL:HG23	2.45	0.45
2:T:6:ILE:O	2:T:6:ILE:HG23	2.17	0.45
2:T:141:GLN:NE2	2:2:141:GLN:HE21	2.14	0.45
2:U:37:ILE:HD11	2:U:59:MET:CG	2.46	0.45
2:U:97:VAL:HG22	2:U:98:GLN:H	1.81	0.45
2:X:25:PHE:CD1	2:X:25:PHE:C	2.92	0.45
2:X:103:GLY:HA2	2:X:178:ILE:HD13	1.99	0.45
2:Y:190:ASP:HA	2:Y:193:GLU:HG2	1.99	0.45
2:Z:59:MET:SD	2:Z:83:LEU:HD13	2.57	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:66:TYR:CZ	2:2:70:ARG:HD2	2.52	0.45
1:A:24:VAL:O	1:A:28:ARG:HG3	2.17	0.45
1:E:21:LEU:O	1:E:24:VAL:HG12	2.16	0.45
1:H:123:TYR:N	1:H:123:TYR:CD1	2.85	0.45
1:M:42:PHE:O	1:M:43:ALA:C	2.60	0.45
1:M:99:GLU:HG3	1:M:103:TYR:HD2	1.81	0.45
1:N:136:LEU:HD12	1:N:151:CYS:HB3	1.97	0.45
2:U:93:MET:N	2:U:94:PRO:CD	2.78	0.45
2:1:97:VAL:HG22	2:1:98:GLN:H	1.81	0.45
1:A:49:ILE:HD11	1:A:210:PRO:CB	2.47	0.45
1:D:123:TYR:N	1:D:123:TYR:CD1	2.85	0.45
1:D:228:GLU:O	1:D:231:LYS:HB3	2.17	0.45
1:F:149:PHE:CE2	1:F:159:GLU:HB2	2.52	0.45
1:J:198:LYS:O	1:J:199:SER:C	2.59	0.45
2:S:19:ARG:NE	2:S:26:ILE:HG13	2.32	0.45
2:X:45:ILE:CG1	2:X:52:ALA:HB1	2.34	0.45
2:1:55:LEU:HD12	2:1:55:LEU:HA	1.85	0.45
2:2:143:SER:O	2:2:146:MET:HG3	2.17	0.45
2:B:180:ARG:HA	2:B:180:ARG:HD2	1.79	0.45
1:E:176:LEU:O	1:E:178:ARG:N	2.49	0.45
1:E:186:GLU:O	1:E:190:VAL:HG12	2.17	0.45
1:H:22:PHE:O	1:H:25:GLU:HB2	2.17	0.45
1:O:121:GLN:O	1:O:124:THR:HB	2.17	0.45
2:P:146:MET:HA	2:P:150:GLU:OE1	2.17	0.45
2:Q:105:ASP:OD1	2:Q:106:THR:N	2.50	0.45
2:Z:2:THR:HG22	2:Z:169:SER:OG	2.16	0.45
2:2:22:MET:O	2:2:23:GLU:HB2	2.16	0.45
1:G:51:ASP:HB3	1:G:53:LYS:NZ	2.31	0.44
1:I:161:LYS:HG2	1:I:180:TYR:HE2	1.82	0.44
1:I:175:PHE:CD2	1:I:196:ALA:HA	2.52	0.44
1:N:180:TYR:HA	1:N:192:LEU:HD21	1.99	0.44
2:P:6:ILE:HD11	2:P:142:TYR:CD1	2.52	0.44
2:S:6:ILE:HD11	2:S:142:TYR:CD1	2.52	0.44
2:Z:111:PHE:CD2	2:Z:121:GLU:HB2	2.53	0.44
2:2:103:GLY:HA2	2:2:178:ILE:CD1	2.47	0.44
1:C:42:PHE:HD2	1:C:47:LEU:HD23	1.83	0.44
1:E:15:PHE:HD2	1:F:23:GLN:NE2	2.15	0.44
1:I:170:ASP:O	1:I:173:VAL:HG12	2.16	0.44
1:J:175:PHE:C	1:J:175:PHE:HD1	2.25	0.44
1:K:24:VAL:O	1:K:28:ARG:HG3	2.17	0.44
1:L:82:VAL:HG13	1:L:83:ALA:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:52:LYS:HZ1	1:M:62:ASN:HA	1.81	0.44
1:M:82:VAL:HG13	1:M:83:ALA:N	2.32	0.44
1:N:49:ILE:HD12	1:N:211:GLU:O	2.17	0.44
2:P:138:LEU:HD12	2:P:154:LEU:HD11	1.98	0.44
2:Q:49:VAL:HG23	2:Q:50:GLY:H	1.82	0.44
2:S:110:VAL:HG13	2:S:110:VAL:O	2.16	0.44
2:U:97:VAL:HG22	2:U:98:GLN:N	2.32	0.44
2:U:160:SER:HA	2:U:163:LYS:HD3	2.00	0.44
2:Z:93:MET:N	2:Z:94:PRO:CD	2.79	0.44
2:B:22:MET:O	2:B:23:GLU:HB2	2.17	0.44
2:B:66:TYR:CD1	2:B:66:TYR:C	2.95	0.44
1:C:44:ASN:HD22	1:C:44:ASN:HA	1.56	0.44
1:J:58:LEU:N	1:J:58:LEU:CD1	2.81	0.44
1:L:212:ILE:HG23	1:L:224:TYR:HB2	1.99	0.44
1:M:159:GLU:O	1:N:60:GLU:HB2	2.17	0.44
1:N:42:PHE:HB2	1:N:184:LEU:O	2.17	0.44
1:N:143:GLN:HA	1:N:143:GLN:HE21	1.82	0.44
2:S:74:MET:HG2	2:S:78:ALA:HB3	2.00	0.44
2:U:173:ILE:HD13	2:U:173:ILE:C	2.43	0.44
2:W:75:PRO:O	2:W:78:ALA:HB3	2.18	0.44
2:2:90:VAL:O	2:2:90:VAL:HG22	2.17	0.44
1:A:18:ASP:OD2	1:A:20:ARG:HD3	2.17	0.44
1:D:49:ILE:HD12	1:D:211:GLU:O	2.17	0.44
1:G:149:PHE:CE2	1:G:159:GLU:HB2	2.53	0.44
1:G:187:LYS:O	1:G:190:VAL:HG13	2.17	0.44
1:I:70:ILE:HD12	1:I:74:VAL:HG22	1.99	0.44
1:K:148:LEU:O	1:K:159:GLU:HG3	2.17	0.44
1:M:125:GLN:HB3	1:N:130:ARG:NH2	2.32	0.44
1:M:170:ASP:O	1:M:173:VAL:HG12	2.17	0.44
2:P:2:THR:HG22	2:P:169:SER:OG	2.17	0.44
2:S:17:GLU:HA	2:S:173:ILE:HA	1.99	0.44
2:S:93:MET:N	2:S:94:PRO:CD	2.80	0.44
2:U:37:ILE:HD11	2:U:59:MET:CB	2.43	0.44
2:Y:59:MET:CE	2:Y:79:VAL:HG23	2.48	0.44
2:Z:20:VAL:HG22	2:Z:28:HIS:HB2	1.99	0.44
2:B:29:LYS:NZ	2:Y:164:GLN:NE2	2.64	0.44
1:E:174:SER:O	1:E:177:GLU:HB3	2.18	0.44
1:H:44:ASN:HD22	1:H:44:ASN:HA	1.60	0.44
1:J:180:TYR:HA	1:J:192:LEU:HD21	1.99	0.44
2:Y:133:PHE:CE2	2:Y:165:ARG:HB3	2.52	0.44
1:A:81:LEU:HD23	1:A:133:GLY:HA3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:123:TYR:N	1:E:123:TYR:CD1	2.84	0.44
1:G:28:ARG:O	1:G:31:VAL:HG13	2.18	0.44
1:G:180:TYR:HA	1:G:192:LEU:HD21	2.00	0.44
1:K:135:SER:OG	1:K:153:PRO:HD3	2.17	0.44
1:K:180:TYR:HA	1:K:192:LEU:HD21	2.00	0.44
1:L:62:ASN:O	1:L:65:GLU:HG2	2.18	0.44
1:L:83:ALA:O	1:L:87:VAL:HG12	2.18	0.44
1:L:107:VAL:HG11	2:Z:66:TYR:HH	1.79	0.44
1:N:165:ILE:HD12	1:N:169:LYS:HD2	2.00	0.44
1:O:123:TYR:CE2	1:O:129:VAL:HG21	2.53	0.44
1:A:32:LYS:O	1:A:167:SER:HA	2.18	0.44
1:A:78:THR:CG2	1:A:85:ALA:HB1	2.45	0.44
2:B:141:GLN:HE21	2:Z:141:GLN:NE2	2.15	0.44
1:G:15:PHE:HD2	1:H:23:GLN:HE22	1.65	0.44
1:G:52:LYS:HA	1:G:66:LYS:NZ	2.32	0.44
2:R:55:LEU:HD12	2:R:55:LEU:HA	1.79	0.44
2:U:7:THR:HB	2:U:123:ILE:O	2.18	0.44
2:U:19:ARG:HD2	2:U:169:SER:C	2.43	0.44
2:W:43:MET:HE1	2:W:56:VAL:HA	2.00	0.44
2:Y:161:ALA:O	2:Y:164:GLN:HB2	2.17	0.44
2:Z:55:LEU:HD21	2:Z:87:LEU:HD11	1.99	0.44
2:Z:74:MET:HG2	2:Z:78:ALA:HB3	2.00	0.44
2:B:165:ARG:CZ	2:Y:29:LYS:HE3	2.48	0.44
1:C:20:ARG:CZ	1:C:22:PHE:CE1	3.01	0.44
1:I:202:GLU:HG3	1:I:205:GLU:O	2.18	0.44
1:L:228:GLU:O	1:L:231:LYS:HB3	2.17	0.44
1:N:191:THR:O	1:N:194:ILE:HG22	2.18	0.44
1:O:38:LEU:HB3	1:O:164:ALA:HB2	1.99	0.44
2:U:8:LEU:HD12	2:U:8:LEU:O	2.17	0.44
2:B:133:PHE:HE1	2:Z:132:PRO:HA	1.83	0.44
1:C:134:VAL:CG2	1:C:135:SER:N	2.79	0.44
1:D:136:LEU:HD12	1:D:151:CYS:HB3	1.99	0.44
1:D:184:LEU:HD23	1:D:189:ALA:HA	1.99	0.44
1:J:52:LYS:HA	1:J:66:LYS:NZ	2.33	0.44
1:J:83:ALA:O	1:J:87:VAL:HG12	2.18	0.44
1:M:107:VAL:HG13	1:M:108:ASN:N	2.32	0.44
2:Q:123:ILE:HG12	2:Q:124:TYR:CD1	2.51	0.44
2:R:76:ILE:O	2:R:79:VAL:HG12	2.17	0.44
2:S:189:THR:HG23	2:S:190:ASP:H	1.83	0.44
2:X:101:VAL:O	2:X:101:VAL:HG13	2.18	0.44
2:Z:184:TYR:CD1	2:Z:184:TYR:C	2.96	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:225:ASP:OD1	1:F:228:GLU:HB2	2.18	0.43
1:O:145:GLY:O	1:O:147:ARG:HG3	2.18	0.43
2:S:8:LEU:HD12	2:S:8:LEU:O	2.17	0.43
2:S:180:ARG:HD2	2:S:180:ARG:HA	1.71	0.43
2:U:49:VAL:O	2:U:50:GLY:C	2.61	0.43
1:A:16:SER:HB3	1:A:22:PHE:CE2	2.53	0.43
1:D:130:ARG:HA	1:D:131:PRO:HD3	1.86	0.43
1:E:137:ILE:HG22	1:E:150:ASP:HB2	2.00	0.43
1:F:52:LYS:HZ1	1:F:62:ASN:HA	1.83	0.43
1:J:61:GLN:CD	1:J:62:ASN:H	2.26	0.43
1:L:16:SER:HB3	1:L:22:PHE:CE2	2.52	0.43
1:O:98:GLN:O	1:O:102:THR:CG2	2.66	0.43
2:Q:105:ASP:CG	2:Q:106:THR:H	2.26	0.43
2:T:49:VAL:O	2:T:50:GLY:C	2.61	0.43
2:T:86:MET:HE2	2:T:86:MET:HB3	1.92	0.43
2:T:141:GLN:NE2	2:2:141:GLN:NE2	2.67	0.43
2:U:25:PHE:C	2:U:25:PHE:HD1	2.26	0.43
2:W:6:ILE:HD11	2:W:142:TYR:CD1	2.53	0.43
2:Z:7:THR:HB	2:Z:123:ILE:O	2.19	0.43
1:C:32:LYS:O	1:C:167:SER:HA	2.18	0.43
1:C:52:LYS:HB3	1:C:209:ALA:O	2.18	0.43
1:C:202:GLU:HG3	1:C:205:GLU:O	2.19	0.43
1:F:107:VAL:HG13	1:F:108:ASN:H	1.82	0.43
1:F:107:VAL:HG13	1:F:108:ASN:N	2.33	0.43
1:F:175:PHE:C	1:F:175:PHE:CD1	2.96	0.43
1:G:97:GLN:OE1	1:G:97:GLN:HA	2.18	0.43
1:H:52:LYS:CE	1:H:64:ILE:HG23	2.48	0.43
1:J:147:ARG:HB3	1:J:149:PHE:HE1	1.83	0.43
1:K:145:GLY:O	1:K:147:ARG:HG3	2.19	0.43
1:L:52:LYS:HB3	1:L:209:ALA:O	2.18	0.43
1:M:38:LEU:HA	1:M:164:ALA:HA	1.98	0.43
1:O:198:LYS:C	1:O:202:GLU:HB2	2.44	0.43
2:R:19:ARG:HD2	2:R:169:SER:C	2.43	0.43
2:S:20:VAL:CG1	2:S:28:HIS:HB2	2.45	0.43
2:U:123:ILE:H	2:U:123:ILE:CD1	2.24	0.43
2:W:7:THR:HB	2:W:123:ILE:O	2.18	0.43
2:Z:179:THR:HG23	2:Z:182:ASP:H	1.83	0.43
1:A:109:ILE:CG2	1:A:147:ARG:HD3	2.48	0.43
1:D:205:GLU:HG3	1:D:206:GLU:N	2.34	0.43
1:E:158:ASN:HB2	1:E:160:TYR:CE1	2.53	0.43
1:I:136:LEU:HD12	1:I:151:CYS:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:159:GLU:HG2	1:M:60:GLU:HG3	2.00	0.43
2:S:76:ILE:HA	2:S:79:VAL:HG12	2.00	0.43
2:T:93:MET:N	2:T:94:PRO:CD	2.81	0.43
2:B:90:VAL:O	2:B:90:VAL:HG22	2.18	0.43
1:F:170:ASP:C	1:F:173:VAL:HG12	2.43	0.43
1:G:107:VAL:HG13	1:G:108:ASN:N	2.34	0.43
1:G:113:VAL:HA	1:G:116:VAL:HG12	2.01	0.43
1:J:14:VAL:O	1:J:21:LEU:HD12	2.18	0.43
2:P:141:GLN:NE2	2:Y:141:GLN:NE2	2.66	0.43
2:P:184:TYR:CD1	2:P:184:TYR:C	2.97	0.43
2:R:34:LEU:HD21	2:R:176:ALA:HB3	2.00	0.43
2:S:178:ILE:HB	2:S:184:TYR:HA	2.01	0.43
2:W:2:THR:HG22	2:W:169:SER:OG	2.18	0.43
2:W:187:LEU:HA	2:W:188:PRO:HD3	1.67	0.43
2:Y:180:ARG:HA	2:Y:180:ARG:HD2	1.75	0.43
1:A:52:LYS:HB3	1:A:209:ALA:O	2.19	0.43
1:A:130:ARG:NH1	1:A:131:PRO:O	2.51	0.43
2:B:17:GLU:HA	2:B:173:ILE:HA	2.01	0.43
2:P:124:TYR:HD2	2:P:138:LEU:HD23	1.78	0.43
2:Q:25:PHE:C	2:Q:25:PHE:CD1	2.96	0.43
2:Q:141:GLN:NE2	2:X:141:GLN:HE21	2.16	0.43
2:S:3:THR:OG1	2:S:127:THR:HG22	2.19	0.43
2:W:179:THR:HG23	2:W:182:ASP:H	1.84	0.43
2:X:3:THR:HB	2:X:16:THR:HG22	2.01	0.43
2:X:43:MET:HE1	2:X:56:VAL:HA	2.01	0.43
2:X:90:VAL:O	2:X:90:VAL:HG22	2.19	0.43
2:Z:25:PHE:CD1	2:Z:25:PHE:C	2.93	0.43
2:Z:131:SER:O	2:Z:134:VAL:HG13	2.19	0.43
2:1:97:VAL:HG22	2:1:98:GLN:N	2.34	0.43
2:2:2:THR:HG22	2:2:169:SER:CB	2.49	0.43
2:B:15:ALA:HB2	2:B:175:VAL:HB	1.99	0.43
1:F:107:VAL:HG11	2:T:66:TYR:HH	1.75	0.43
1:F:160:TYR:CD2	1:F:163:THR:HB	2.53	0.43
1:G:146:PRO:O	1:G:147:ARG:HG2	2.17	0.43
1:J:208:LYS:HD2	1:J:208:LYS:HA	1.82	0.43
1:M:26:TYR:O	1:M:29:GLU:HB2	2.18	0.43
1:N:25:GLU:O	1:N:28:ARG:HB2	2.18	0.43
1:O:24:VAL:O	1:O:28:ARG:HG3	2.18	0.43
2:R:6:ILE:HD11	2:R:142:TYR:CD1	2.53	0.43
2:S:49:VAL:O	2:S:50:GLY:C	2.62	0.43
2:T:87:LEU:HD23	2:T:114:ASP:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:138:LEU:HD12	2:T:138:LEU:HA	1.86	0.43
2:V:59:MET:HE1	2:V:82:LEU:HD23	2.01	0.43
2:Y:149:ASP:O	2:Y:152:VAL:HG12	2.18	0.43
2:2:59:MET:SD	2:2:83:LEU:HD13	2.58	0.43
2:B:28:HIS:CD2	2:P:120:VAL:HG11	2.54	0.43
2:B:131:SER:O	2:B:134:VAL:HG13	2.19	0.43
2:B:202:ILE:HG12	2:B:203:LEU:N	2.34	0.43
1:C:71:ASP:O	1:C:73:TYR:N	2.51	0.43
1:D:124:THR:HG22	1:E:130:ARG:HH21	1.84	0.43
1:J:109:ILE:HG22	1:J:147:ARG:HD3	2.01	0.43
1:K:142:ASP:OD2	1:K:147:ARG:HD2	2.18	0.43
1:O:148:LEU:O	1:O:159:GLU:HG3	2.19	0.43
2:U:111:PHE:CE2	2:U:121:GLU:HB2	2.53	0.43
2:V:19:ARG:NE	2:V:26:ILE:HG13	2.34	0.43
2:2:187:LEU:HA	2:2:188:PRO:HD3	1.81	0.43
1:E:83:ALA:O	1:E:87:VAL:HG12	2.19	0.43
2:V:76:ILE:HA	2:V:79:VAL:HG12	2.01	0.43
2:V:93:MET:N	2:V:94:PRO:CD	2.82	0.43
2:W:34:LEU:HD21	2:W:176:ALA:HB3	1.99	0.43
2:Y:15:ALA:HB2	2:Y:175:VAL:HB	2.01	0.43
1:C:21:LEU:O	1:C:25:GLU:HG2	2.19	0.43
1:F:82:VAL:HG13	1:F:83:ALA:H	1.84	0.43
1:F:198:LYS:HG2	1:F:202:GLU:HG2	2.01	0.43
1:G:125:GLN:HB3	1:H:130:ARG:NH2	2.34	0.43
2:S:26:ILE:HD13	2:S:26:ILE:C	2.44	0.43
2:U:59:MET:HE1	2:U:82:LEU:HD23	2.01	0.43
2:V:36:GLN:HB2	2:V:184:TYR:CE1	2.53	0.43
2:B:19:ARG:HE	2:B:26:ILE:HG13	1.84	0.42
1:C:62:ASN:O	1:C:65:GLU:HG2	2.18	0.42
1:C:165:ILE:HD12	1:C:169:LYS:HD2	2.01	0.42
1:D:42:PHE:HB2	1:D:184:LEU:O	2.20	0.42
1:D:198:LYS:C	1:D:202:GLU:HB2	2.44	0.42
1:F:35:SER:O	1:F:166:GLY:HA3	2.19	0.42
1:F:130:ARG:HA	1:F:131:PRO:HD3	1.91	0.42
1:L:198:LYS:HG3	1:L:207:LEU:HD22	2.01	0.42
1:N:107:VAL:HG11	2:2:66:TYR:HH	1.80	0.42
2:S:59:MET:HE1	2:S:82:LEU:CD2	2.48	0.42
2:U:141:GLN:HE21	2:1:141:GLN:HE21	1.66	0.42
2:V:22:MET:O	2:V:23:GLU:HB2	2.18	0.42
2:Y:59:MET:CE	2:Y:82:LEU:HD23	2.45	0.42
2:Z:176:ALA:HB2	2:Z:186:GLN:HG3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:152:VAL:O	2:2:156:ILE:HG13	2.19	0.42
1:A:58:LEU:N	1:A:58:LEU:CD1	2.83	0.42
1:D:51:ASP:HB3	1:D:53:LYS:HZ3	1.84	0.42
1:I:123:TYR:N	1:I:123:TYR:CD1	2.88	0.42
1:O:24:VAL:O	1:O:27:ALA:HB3	2.19	0.42
2:P:187:LEU:HA	2:P:188:PRO:HD3	1.83	0.42
2:S:157:ARG:O	2:S:158:ALA:C	2.63	0.42
2:U:141:GLN:NE2	2:1:141:GLN:NE2	2.66	0.42
2:1:49:VAL:O	2:1:50:GLY:C	2.62	0.42
2:B:103:GLY:HA2	2:B:178:ILE:HD13	2.01	0.42
1:F:159:GLU:O	1:G:60:GLU:HB2	2.19	0.42
1:I:149:PHE:CE2	1:I:159:GLU:HB2	2.54	0.42
1:J:15:PHE:HD2	1:K:23:GLN:HE22	1.67	0.42
1:M:40:MET:HA	1:M:162:ALA:HA	2.01	0.42
2:S:163:LYS:CE	2:S:203:LEU:HD23	2.50	0.42
2:T:109:HIS:HB3	2:T:111:PHE:HE1	1.84	0.42
2:W:174:ASP:HA	2:W:192:ILE:HD13	2.00	0.42
2:X:49:VAL:O	2:X:50:GLY:C	2.62	0.42
2:Z:20:VAL:HG13	2:Z:28:HIS:HB2	2.00	0.42
1:A:56:SER:OG	1:A:58:LEU:HB2	2.20	0.42
1:A:187:LYS:O	1:A:190:VAL:HG13	2.19	0.42
1:C:41:LYS:HE3	1:C:160:TYR:O	2.19	0.42
1:C:100:LYS:O	1:C:104:GLY:CA	2.68	0.42
1:D:146:PRO:O	1:D:147:ARG:HG2	2.19	0.42
1:E:176:LEU:C	1:E:178:ARG:N	2.75	0.42
1:F:49:ILE:HD12	1:F:50:SER:N	2.34	0.42
1:I:21:LEU:O	1:I:25:GLU:HG2	2.18	0.42
1:L:136:LEU:HD13	1:L:138:PHE:CE1	2.54	0.42
1:L:160:TYR:CD2	1:L:163:THR:HB	2.55	0.42
1:M:152:ASP:HB2	1:M:153:PRO:CD	2.49	0.42
1:O:88:LEU:HD12	1:O:88:LEU:HA	1.91	0.42
2:P:45:ILE:CD1	2:P:52:ALA:HB1	2.49	0.42
2:R:157:ARG:O	2:R:160:SER:HB2	2.19	0.42
2:R:187:LEU:HA	2:R:188:PRO:HD3	1.76	0.42
2:S:15:ALA:HB3	2:S:155:VAL:CG1	2.49	0.42
2:S:105:ASP:OD1	2:S:106:THR:N	2.52	0.42
2:S:165:ARG:HA	2:2:26:ILE:HG23	2.00	0.42
2:T:59:MET:HE1	2:T:82:LEU:HD23	2.01	0.42
2:T:114:ASP:OD1	2:T:116:ALA:HB3	2.20	0.42
2:V:2:THR:HG22	2:V:169:SER:OG	2.19	0.42
2:V:72:VAL:HG22	2:V:73:ASN:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:105:ASP:OD1	2:V:106:THR:N	2.53	0.42
2:Y:124:TYR:HD1	2:Y:138:LEU:HD23	1.83	0.42
2:1:34:LEU:HD21	2:1:176:ALA:HB3	2.00	0.42
2:2:137:VAL:HG21	2:2:158:ALA:HA	2.01	0.42
2:B:59:MET:HE2	2:B:79:VAL:CG2	2.47	0.42
1:C:97:GLN:OE1	1:C:97:GLN:HA	2.19	0.42
1:D:160:TYR:CD2	1:D:163:THR:HB	2.54	0.42
1:M:70:ILE:HB	1:M:74:VAL:HG13	2.01	0.42
1:M:109:ILE:HG22	1:M:142:ASP:CG	2.45	0.42
1:N:139:ALA:HB2	1:N:148:LEU:HD13	2.01	0.42
1:O:43:ALA:HB2	1:O:185:PRO:HA	2.00	0.42
1:O:143:GLN:HA	1:O:143:GLN:HE21	1.84	0.42
2:T:137:VAL:HG21	2:T:158:ALA:HA	2.01	0.42
2:U:22:MET:O	2:U:23:GLU:HB2	2.20	0.42
2:V:123:ILE:H	2:V:123:ILE:CD1	2.29	0.42
2:Z:87:LEU:HD23	2:Z:114:ASP:O	2.20	0.42
1:C:52:LYS:HA	1:C:66:LYS:NZ	2.34	0.42
1:C:108:ASN:CB	2:Q:70:ARG:HG2	2.48	0.42
1:C:191:THR:O	1:C:194:ILE:HG22	2.19	0.42
1:D:162:ALA:O	1:D:163:THR:HB	2.19	0.42
1:H:82:VAL:HG13	1:H:83:ALA:N	2.34	0.42
1:I:161:LYS:HG2	1:I:180:TYR:CE2	2.55	0.42
1:J:52:LYS:HZ3	1:J:62:ASN:HA	1.83	0.42
1:L:180:TYR:HB3	1:M:57:ARG:NH2	2.35	0.42
1:N:71:ASP:O	1:N:73:TYR:N	2.53	0.42
1:N:134:VAL:CG2	1:N:135:SER:N	2.83	0.42
1:O:40:MET:HA	1:O:162:ALA:HA	2.02	0.42
1:O:42:PHE:HB2	1:O:184:LEU:O	2.19	0.42
1:O:176:LEU:C	1:O:178:ARG:N	2.76	0.42
2:R:26:ILE:HG22	2:V:165:ARG:C	2.44	0.42
2:V:129:SER:OG	2:V:168:ALA:HB3	2.18	0.42
2:Y:19:ARG:NE	2:Y:26:ILE:HG13	2.35	0.42
2:1:44:THR:OG1	2:1:100:LEU:HB3	2.19	0.42
2:1:66:TYR:CE1	2:1:70:ARG:HD2	2.54	0.42
1:D:61:GLN:OE1	1:D:62:ASN:HB3	2.20	0.42
1:E:31:VAL:HA	1:E:80:GLY:HA2	2.01	0.42
1:E:147:ARG:HB3	1:E:149:PHE:HE1	1.83	0.42
1:G:79:SER:OG	1:G:166:GLY:HA2	2.20	0.42
1:G:125:GLN:O	1:H:129:VAL:HG23	2.20	0.42
1:I:26:TYR:N	1:I:26:TYR:CD1	2.88	0.42
1:L:15:PHE:HB2	1:M:23:GLN:HE22	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:215:ILE:HD11	1:L:219:ASN:O	2.19	0.42
1:M:123:TYR:N	1:M:123:TYR:CD1	2.87	0.42
1:M:206:GLU:HG2	1:M:208:LYS:H	1.84	0.42
2:S:15:ALA:HB3	2:S:155:VAL:HG11	2.00	0.42
2:S:190:ASP:HA	2:S:193:GLU:HG2	2.02	0.42
2:V:90:VAL:O	2:V:90:VAL:HG22	2.20	0.42
2:V:163:LYS:CE	2:V:203:LEU:HD23	2.49	0.42
2:X:74:MET:HA	2:X:75:PRO:HD3	1.88	0.42
2:1:173:ILE:O	2:1:192:ILE:HG21	2.20	0.42
2:1:176:ALA:HA	2:1:186:GLN:HA	2.02	0.42
1:E:130:ARG:HG2	1:E:130:ARG:NH1	2.34	0.42
1:G:191:THR:HA	1:G:194:ILE:HG22	2.02	0.42
1:G:215:ILE:HD11	1:G:219:ASN:O	2.19	0.42
1:H:88:LEU:HD13	1:H:132:TYR:CE2	2.55	0.42
1:I:107:VAL:HG13	1:I:108:ASN:H	1.84	0.42
1:K:44:ASN:HD22	1:K:44:ASN:HA	1.58	0.42
1:N:82:VAL:HG13	1:N:83:ALA:H	1.84	0.42
2:S:55:LEU:HD12	2:S:55:LEU:HA	1.67	0.42
2:X:175:VAL:CG2	2:X:176:ALA:N	2.83	0.42
2:Y:20:VAL:HG22	2:Y:28:HIS:HB2	2.02	0.42
2:1:34:LEU:HD21	2:1:176:ALA:CB	2.50	0.42
2:1:35:PHE:CE2	2:1:45:ILE:HD12	2.55	0.42
1:I:88:LEU:HD21	1:I:120:MET:SD	2.59	0.42
1:I:191:THR:O	1:I:192:LEU:C	2.62	0.42
1:J:98:GLN:O	1:J:101:VAL:HG12	2.20	0.42
1:K:144:ILE:HD12	1:K:147:ARG:NH1	2.35	0.42
1:K:174:SER:O	1:K:175:PHE:C	2.63	0.42
1:O:186:GLU:O	1:O:187:LYS:C	2.62	0.42
2:P:83:LEU:HD12	2:P:83:LEU:HA	1.88	0.42
2:T:180:ARG:HD2	2:T:180:ARG:HA	1.77	0.42
2:W:83:LEU:HD12	2:W:83:LEU:HA	1.79	0.42
2:1:27:MET:O	2:1:27:MET:HG2	2.20	0.42
1:A:54:VAL:HG22	1:A:55:ARG:N	2.34	0.42
1:D:64:ILE:HG23	1:D:64:ILE:O	2.20	0.42
1:D:176:LEU:C	1:D:178:ARG:N	2.74	0.42
1:F:58:LEU:N	1:F:58:LEU:CD1	2.83	0.42
1:G:22:PHE:O	1:G:25:GLU:HB2	2.20	0.42
1:G:59:ILE:HD13	1:G:59:ILE:HA	1.92	0.42
1:G:70:ILE:HD11	1:G:76:ALA:HB2	2.01	0.42
1:H:208:LYS:HD2	1:H:208:LYS:HA	1.90	0.42
1:J:85:ALA:O	1:J:89:VAL:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:134:VAL:CG2	1:K:135:SER:N	2.82	0.42
1:O:48:LEU:CD1	1:O:139:ALA:HB3	2.49	0.42
1:O:58:LEU:N	1:O:58:LEU:CD1	2.82	0.42
2:Q:109:HIS:HB3	2:Q:111:PHE:CE1	2.54	0.42
2:1:17:GLU:O	2:1:33:LYS:HD2	2.20	0.42
2:2:19:ARG:HE	2:2:26:ILE:HG13	1.85	0.42
2:B:3:THR:OG1	2:B:127:THR:HG22	2.19	0.41
1:C:121:GLN:HG3	1:D:83:ALA:HB1	2.02	0.41
1:D:170:ASP:O	1:D:173:VAL:HG12	2.20	0.41
1:G:41:LYS:HE3	1:G:160:TYR:O	2.20	0.41
1:G:62:ASN:O	1:G:65:GLU:HG2	2.20	0.41
1:J:58:LEU:N	1:J:58:LEU:HD12	2.35	0.41
1:M:107:VAL:HG13	1:M:108:ASN:H	1.85	0.41
2:Q:34:LEU:HD21	2:Q:176:ALA:CB	2.50	0.41
2:T:66:TYR:CZ	2:T:70:ARG:HD2	2.54	0.41
2:1:163:LYS:CE	2:1:203:LEU:HD23	2.50	0.41
1:E:102:THR:O	2:S:81:THR:HG22	2.20	0.41
1:F:174:SER:O	1:F:177:GLU:HB3	2.20	0.41
1:H:175:PHE:CD2	1:H:196:ALA:HA	2.56	0.41
1:K:156:THR:HG23	1:L:82:VAL:HG11	2.02	0.41
1:L:103:TYR:CE1	2:Z:74:MET:HE2	2.55	0.41
2:Q:141:GLN:HE21	2:X:141:GLN:HE21	1.68	0.41
2:U:138:LEU:HA	2:U:138:LEU:HD12	1.71	0.41
2:W:126:SER:HB3	2:W:135:TYR:CE2	2.55	0.41
2:Y:81:THR:O	2:Y:82:LEU:C	2.61	0.41
1:E:52:LYS:HZ3	1:E:62:ASN:HA	1.81	0.41
1:E:97:GLN:OE1	1:E:97:GLN:HA	2.19	0.41
1:G:88:LEU:HD13	1:G:132:TYR:CD2	2.54	0.41
1:O:130:ARG:HG2	1:O:130:ARG:HH11	1.84	0.41
2:P:188:PRO:O	2:P:189:THR:C	2.63	0.41
2:T:163:LYS:CE	2:T:203:LEU:HD23	2.50	0.41
2:V:124:TYR:CE2	2:V:138:LEU:HB3	2.54	0.41
2:W:44:THR:OG1	2:W:100:LEU:HB3	2.19	0.41
2:X:109:HIS:HB3	2:X:111:PHE:HE1	1.84	0.41
1:D:71:ASP:OD1	1:D:72:ASP:N	2.53	0.41
1:E:26:TYR:O	1:E:29:GLU:HB2	2.20	0.41
1:G:52:LYS:CE	1:G:64:ILE:HG23	2.46	0.41
1:G:94:ILE:CG1	1:G:95:SER:N	2.82	0.41
1:G:156:THR:CG2	1:H:82:VAL:HG11	2.50	0.41
1:I:124:THR:HG22	1:J:130:ARG:NH2	2.35	0.41
1:L:123:TYR:N	1:L:123:TYR:CD1	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:28:ARG:O	1:N:31:VAL:HG22	2.20	0.41
1:O:25:GLU:O	1:O:28:ARG:HB2	2.21	0.41
2:P:180:ARG:HD2	2:P:180:ARG:HA	1.81	0.41
2:P:191:GLN:O	2:P:194:SER:HB3	2.20	0.41
2:S:143:SER:O	2:S:146:MET:HG3	2.20	0.41
2:U:59:MET:SD	2:U:83:LEU:HD13	2.60	0.41
2:V:179:THR:HG23	2:V:182:ASP:H	1.86	0.41
2:W:105:ASP:CG	2:W:106:THR:H	2.28	0.41
2:W:193:GLU:HA	2:W:196:ILE:HD12	2.02	0.41
2:X:7:THR:HB	2:X:123:ILE:O	2.21	0.41
2:Z:189:THR:HG23	2:Z:190:ASP:N	2.35	0.41
2:1:184:TYR:CD1	2:1:184:TYR:C	2.98	0.41
2:B:18:ARG:HE	2:B:30:ASN:HD22	1.67	0.41
1:E:228:GLU:O	1:E:231:LYS:HB3	2.20	0.41
1:G:157:ILE:HG12	1:G:158:ASN:N	2.34	0.41
1:H:101:VAL:HG23	2:U:57:ARG:HB3	2.03	0.41
1:K:35:SER:O	1:K:166:GLY:HA3	2.20	0.41
1:L:42:PHE:CD1	1:L:43:ALA:N	2.89	0.41
1:L:88:LEU:HD21	1:L:120:MET:HE3	2.02	0.41
1:M:15:PHE:HD2	1:N:23:GLN:HE22	1.66	0.41
1:M:191:THR:O	1:M:194:ILE:HG22	2.21	0.41
1:N:222:ARG:HH21	1:N:228:GLU:CD	2.29	0.41
1:O:16:SER:HB3	1:O:22:PHE:CE2	2.56	0.41
2:P:147:THR:OG1	2:P:150:GLU:HG3	2.21	0.41
2:P:175:VAL:HG22	2:P:176:ALA:N	2.35	0.41
2:T:111:PHE:CE2	2:T:121:GLU:HB2	2.55	0.41
1:E:176:LEU:O	1:E:177:GLU:C	2.63	0.41
1:H:51:ASP:HB3	1:H:53:LYS:NZ	2.35	0.41
1:H:144:ILE:HD12	1:H:147:ARG:NH1	2.36	0.41
1:I:45:GLY:HA3	1:I:216:THR:HA	2.02	0.41
1:I:216:THR:O	1:I:217:VAL:C	2.64	0.41
1:L:16:SER:HB3	1:L:22:PHE:CD2	2.56	0.41
1:O:171:ALA:HB3	1:O:200:SER:OG	2.20	0.41
2:P:55:LEU:HD12	2:P:55:LEU:HA	1.90	0.41
2:S:87:LEU:HD23	2:S:114:ASP:O	2.20	0.41
2:T:17:GLU:O	2:T:33:LYS:HD2	2.20	0.41
2:V:37:ILE:HD11	2:V:59:MET:CG	2.50	0.41
2:W:56:VAL:CG1	2:W:57:ARG:N	2.83	0.41
2:1:138:LEU:HD12	2:1:138:LEU:HA	1.83	0.41
2:B:26:ILE:HG23	2:Y:165:ARG:HA	2.01	0.41
1:C:38:LEU:HG	1:C:49:ILE:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:38:LEU:HB3	1:D:164:ALA:CB	2.51	0.41
1:F:18:ASP:OD2	1:F:20:ARG:HD3	2.21	0.41
1:H:113:VAL:HG23	1:H:138:PHE:CE2	2.56	0.41
1:J:152:ASP:HB2	1:J:153:PRO:CD	2.50	0.41
1:K:41:LYS:HE3	1:K:160:TYR:O	2.20	0.41
1:L:97:GLN:O	1:L:98:GLN:C	2.63	0.41
1:M:45:GLY:HA3	1:M:216:THR:HA	2.01	0.41
1:N:130:ARG:HA	1:N:131:PRO:HD3	1.93	0.41
1:O:174:SER:O	1:O:175:PHE:C	2.63	0.41
2:P:105:ASP:CG	2:P:106:THR:H	2.28	0.41
2:S:97:VAL:HG22	2:S:98:GLN:N	2.36	0.41
2:U:158:ALA:O	2:U:161:ALA:HB3	2.21	0.41
2:V:59:MET:HE3	2:V:63:LEU:HD13	2.03	0.41
2:2:45:ILE:CG1	2:2:52:ALA:HB1	2.45	0.41
2:2:49:VAL:O	2:2:50:GLY:C	2.63	0.41
1:G:159:GLU:HG2	1:H:60:GLU:HG3	2.03	0.41
1:J:175:PHE:CD2	1:J:196:ALA:HA	2.56	0.41
2:R:49:VAL:O	2:R:50:GLY:C	2.64	0.41
2:W:22:MET:O	2:W:23:GLU:HB2	2.21	0.41
2:W:105:ASP:OD1	2:W:106:THR:N	2.54	0.41
2:1:180:ARG:HA	2:1:180:ARG:HD2	1.85	0.41
2:2:175:VAL:CG2	2:2:176:ALA:N	2.83	0.41
1:C:170:ASP:C	1:C:173:VAL:HG12	2.46	0.41
1:D:89:VAL:O	1:D:92:ALA:HB3	2.20	0.41
1:D:134:VAL:CG2	1:D:135:SER:N	2.83	0.41
1:F:48:LEU:HD13	1:F:139:ALA:HB3	2.02	0.41
1:F:136:LEU:HD13	1:F:138:PHE:CE2	2.56	0.41
1:H:107:VAL:H	1:H:107:VAL:HG12	1.60	0.41
1:I:26:TYR:O	1:I:29:GLU:HB2	2.21	0.41
1:J:103:TYR:CE1	2:X:74:MET:HE2	2.56	0.41
1:K:130:ARG:HG2	1:K:130:ARG:NH1	2.36	0.41
1:L:38:LEU:HB3	1:L:164:ALA:HB2	2.02	0.41
1:L:137:ILE:HG22	1:L:150:ASP:CB	2.50	0.41
1:O:82:VAL:HG13	1:O:83:ALA:H	1.86	0.41
1:O:169:LYS:O	1:O:170:ASP:C	2.64	0.41
2:P:59:MET:SD	2:P:83:LEU:HD13	2.61	0.41
2:R:22:MET:O	2:R:23:GLU:HB2	2.21	0.41
2:U:177:VAL:HG13	2:U:185:VAL:HG13	2.03	0.41
2:V:74:MET:HG2	2:V:78:ALA:HB3	2.02	0.41
2:X:20:VAL:O	2:X:20:VAL:HG22	2.20	0.41
2:X:55:LEU:HD12	2:X:55:LEU:HA	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:49:VAL:O	2:Y:50:GLY:C	2.64	0.41
1:A:227:GLU:CD	1:A:227:GLU:N	2.79	0.41
1:E:88:LEU:HD12	1:E:88:LEU:HA	1.84	0.41
1:E:98:GLN:O	1:E:102:THR:CG2	2.69	0.41
1:E:207:LEU:HD23	1:E:233:LEU:HD12	2.02	0.41
1:G:191:THR:O	1:G:194:ILE:HG22	2.20	0.41
1:H:188:GLU:O	1:H:191:THR:HB	2.20	0.41
1:I:127:GLY:O	1:I:129:VAL:N	2.53	0.41
1:J:123:TYR:N	1:J:123:TYR:CD1	2.88	0.41
1:J:165:ILE:HG13	1:J:166:GLY:H	1.84	0.41
1:K:98:GLN:O	1:K:102:THR:CG2	2.69	0.41
1:M:198:LYS:C	1:M:202:GLU:HB2	2.46	0.41
1:O:69:LEU:HD23	1:O:69:LEU:HA	1.90	0.41
2:P:56:VAL:CG1	2:P:57:ARG:N	2.84	0.41
2:V:6:ILE:HD11	2:V:142:TYR:CE1	2.56	0.41
2:V:138:LEU:HD12	2:V:138:LEU:HA	1.88	0.41
2:Y:3:THR:HB	2:Y:16:THR:HG22	2.03	0.41
2:Z:37:ILE:HD11	2:Z:59:MET:CG	2.51	0.41
2:2:55:LEU:HA	2:2:55:LEU:HD12	1.74	0.41
1:D:61:GLN:CD	1:D:62:ASN:H	2.29	0.40
1:D:226:GLN:O	1:D:229:VAL:HG12	2.20	0.40
1:E:42:PHE:HD1	1:E:43:ALA:N	2.19	0.40
1:E:116:VAL:HG11	1:E:138:PHE:CZ	2.56	0.40
1:F:61:GLN:CD	1:F:62:ASN:H	2.29	0.40
1:K:52:LYS:HB3	1:K:209:ALA:O	2.21	0.40
1:M:121:GLN:CG	1:N:83:ALA:HB1	2.51	0.40
2:S:66:TYR:CZ	2:S:70:ARG:HD2	2.56	0.40
2:U:55:LEU:HD12	2:U:55:LEU:HA	1.96	0.40
2:W:103:GLY:HA2	2:W:178:ILE:HD13	2.03	0.40
2:Z:163:LYS:HE2	2:Z:203:LEU:HD23	2.01	0.40
2:B:81:THR:O	2:B:84:SER:HB3	2.21	0.40
1:C:108:ASN:OD1	1:C:147:ARG:NH1	2.54	0.40
1:D:208:LYS:HD2	1:D:208:LYS:HA	1.93	0.40
1:G:38:LEU:HG	1:G:49:ILE:HG23	2.03	0.40
1:H:76:ALA:HA	1:H:137:ILE:O	2.21	0.40
1:J:107:VAL:H	1:J:107:VAL:HG12	1.67	0.40
1:J:142:ASP:OD2	1:J:147:ARG:HD2	2.21	0.40
1:K:187:LYS:O	1:K:190:VAL:HG13	2.21	0.40
1:M:130:ARG:HA	1:M:131:PRO:HD3	1.95	0.40
1:N:86:ARG:HH11	1:N:86:ARG:HD3	1.76	0.40
2:Q:93:MET:N	2:Q:94:PRO:CD	2.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:177:VAL:HG13	2:Y:185:VAL:HG13	2.02	0.40
2:Z:175:VAL:CG2	2:Z:176:ALA:N	2.84	0.40
1:A:123:TYR:CD1	1:A:123:TYR:N	2.88	0.40
1:A:165:ILE:HD12	1:A:169:LYS:HD2	2.03	0.40
1:C:152:ASP:HB2	1:C:153:PRO:CD	2.50	0.40
1:F:206:GLU:HG2	1:F:208:LYS:H	1.85	0.40
1:G:32:LYS:O	1:G:167:SER:HA	2.22	0.40
1:G:58:LEU:N	1:G:58:LEU:CD1	2.84	0.40
1:J:171:ALA:HB3	1:J:200:SER:OG	2.22	0.40
1:O:52:LYS:HA	1:O:66:LYS:NZ	2.36	0.40
2:S:20:VAL:HG13	2:S:28:HIS:CB	2.47	0.40
2:V:80:ALA:O	2:V:81:THR:C	2.64	0.40
2:W:134:VAL:HG23	2:W:158:ALA:HB1	2.04	0.40
2:X:20:VAL:CG1	2:X:28:HIS:HB2	2.50	0.40
1:A:107:VAL:HG11	2:P:66:TYR:HH	1.82	0.40
2:B:202:ILE:CG1	2:B:203:LEU:N	2.85	0.40
1:I:130:ARG:HH11	1:I:130:ARG:HG2	1.87	0.40
1:J:35:SER:O	1:J:166:GLY:HA3	2.21	0.40
2:P:19:ARG:NE	2:P:26:ILE:HG13	2.36	0.40
2:P:26:ILE:HD13	2:P:26:ILE:O	2.22	0.40
2:S:187:LEU:HA	2:S:188:PRO:HD3	1.76	0.40
2:T:3:THR:HB	2:T:16:THR:HG22	2.02	0.40
2:V:15:ALA:HB3	2:V:155:VAL:CG1	2.51	0.40
2:Z:187:LEU:HA	2:Z:188:PRO:HD3	1.87	0.40
1:C:107:VAL:HG11	2:Q:66:TYR:HH	1.80	0.40
1:E:216:THR:O	1:E:217:VAL:C	2.64	0.40
1:F:48:LEU:HB3	1:F:67:ILE:CD1	2.51	0.40
1:F:123:TYR:N	1:F:123:TYR:HD1	2.19	0.40
1:F:123:TYR:H	1:F:123:TYR:HD1	1.70	0.40
1:G:119:GLN:O	1:G:122:GLN:HB2	2.22	0.40
1:H:222:ARG:NH2	1:H:224:TYR:CZ	2.89	0.40
1:I:180:TYR:HA	1:I:192:LEU:HD21	2.02	0.40
1:K:52:LYS:HA	1:K:66:LYS:HZ1	1.86	0.40
1:N:175:PHE:CD2	1:N:196:ALA:HA	2.57	0.40
1:O:62:ASN:O	1:O:65:GLU:HG2	2.21	0.40
2:P:178:ILE:HB	2:P:184:TYR:HA	2.03	0.40
2:R:26:ILE:HG23	2:V:165:ARG:HA	2.03	0.40
2:R:49:VAL:HG23	2:R:50:GLY:H	1.86	0.40
2:V:49:VAL:O	2:V:50:GLY:C	2.65	0.40
2:Z:66:TYR:CZ	2:Z:70:ARG:HD2	2.57	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:178:ARG:HH22	1:N:178:ARG:HH22[4_457]	1.29	0.31

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	A	219/233 (94%)	184 (84%)	26 (12%)	9 (4%)	2	15
1	C	219/233 (94%)	185 (84%)	25 (11%)	9 (4%)	2	15
1	D	219/233 (94%)	184 (84%)	28 (13%)	7 (3%)	3	17
1	E	219/233 (94%)	188 (86%)	22 (10%)	9 (4%)	2	15
1	F	219/233 (94%)	183 (84%)	25 (11%)	11 (5%)	1	10
1	G	219/233 (94%)	186 (85%)	23 (10%)	10 (5%)	2	12
1	H	219/233 (94%)	186 (85%)	25 (11%)	8 (4%)	2	16
1	I	219/233 (94%)	188 (86%)	22 (10%)	9 (4%)	2	15
1	J	219/233 (94%)	182 (83%)	26 (12%)	11 (5%)	1	10
1	K	219/233 (94%)	187 (85%)	26 (12%)	6 (3%)	4	20
1	L	219/233 (94%)	186 (85%)	24 (11%)	9 (4%)	2	15
1	M	219/233 (94%)	184 (84%)	26 (12%)	9 (4%)	2	15
1	N	219/233 (94%)	187 (85%)	23 (10%)	9 (4%)	2	15
1	O	219/233 (94%)	188 (86%)	23 (10%)	8 (4%)	2	16
2	1	201/211 (95%)	184 (92%)	15 (8%)	2 (1%)	12	40
2	2	201/211 (95%)	181 (90%)	19 (10%)	1 (0%)	24	54
2	B	201/211 (95%)	185 (92%)	14 (7%)	2 (1%)	12	40
2	P	201/211 (95%)	183 (91%)	16 (8%)	2 (1%)	12	40
2	Q	201/211 (95%)	180 (90%)	20 (10%)	1 (0%)	24	54
2	R	201/211 (95%)	184 (92%)	15 (8%)	2 (1%)	12	40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	S	201/211 (95%)	181 (90%)	16 (8%)	4 (2%)	6	25
2	T	201/211 (95%)	176 (88%)	23 (11%)	2 (1%)	12	40
2	U	201/211 (95%)	184 (92%)	15 (8%)	2 (1%)	12	40
2	V	201/211 (95%)	179 (89%)	20 (10%)	2 (1%)	12	40
2	W	201/211 (95%)	186 (92%)	13 (6%)	2 (1%)	12	40
2	X	201/211 (95%)	181 (90%)	18 (9%)	2 (1%)	12	40
2	Y	201/211 (95%)	183 (91%)	16 (8%)	2 (1%)	12	40
2	Z	201/211 (95%)	185 (92%)	14 (7%)	2 (1%)	12	40
All	All	5880/6216 (95%)	5150 (88%)	578 (10%)	152 (3%)	4	21

All (152) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	128	GLY
1	A	182	GLU
1	A	200	SER
1	C	128	GLY
1	C	200	SER
1	D	128	GLY
1	D	182	GLU
1	D	200	SER
1	E	128	GLY
1	E	182	GLU
1	E	200	SER
1	F	128	GLY
1	F	182	GLU
1	F	200	SER
1	G	128	GLY
1	G	200	SER
1	H	128	GLY
1	H	182	GLU
1	H	200	SER
1	I	128	GLY
1	I	182	GLU
1	I	200	SER
1	I	205	GLU
1	J	128	GLY
1	J	182	GLU
1	J	200	SER

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Mol	Chain	Res	Type
1	K	128	GLY
1	K	182	GLU
1	K	200	SER
1	L	128	GLY
1	L	182	GLU
1	L	200	SER
1	M	43	ALA
1	M	128	GLY
1	M	182	GLU
1	M	200	SER
1	N	128	GLY
1	N	182	GLU
1	N	200	SER
1	O	182	GLU
1	O	200	SER
2	P	9	LYS
2	S	9	LYS
2	T	9	LYS
2	V	9	LYS
2	Y	9	LYS
1	A	43	ALA
1	A	72	ASP
1	A	205	GLU
2	B	9	LYS
1	C	43	ALA
1	C	72	ASP
1	C	182	GLU
1	C	205	GLU
1	D	43	ALA
1	D	205	GLU
1	E	43	ALA
1	E	205	GLU
1	F	72	ASP
1	G	43	ALA
1	G	129	VAL
1	G	182	GLU
1	G	205	GLU
1	H	43	ALA
1	J	43	ALA
1	J	72	ASP
1	J	205	GLU
1	K	43	ALA

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Mol	Chain	Res	Type
1	K	205	GLU
1	L	43	ALA
1	L	205	GLU
1	M	62	ASN
1	M	72	ASP
1	M	205	GLU
1	N	72	ASP
1	N	205	GLU
1	O	43	ALA
1	O	128	GLY
1	O	205	GLU
2	Q	9	LYS
2	R	9	LYS
2	U	9	LYS
2	W	9	LYS
2	X	9	LYS
2	Z	9	LYS
2	1	9	LYS
2	2	9	LYS
2	B	23	GLU
1	E	72	ASP
1	E	177	GLU
1	F	43	ALA
1	F	61	GLN
1	F	198	LYS
1	F	205	GLU
1	G	61	GLN
1	G	62	ASN
1	H	61	GLN
1	H	62	ASN
1	H	198	LYS
1	H	205	GLU
1	I	43	ALA
1	J	186	GLU
1	L	72	ASP
1	M	61	GLN
1	M	198	LYS
1	N	43	ALA
1	N	202	GLU
1	O	61	GLN
1	O	72	ASP
1	O	198	LYS

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Mol	Chain	Res	Type
2	R	23	GLU
2	Y	23	GLU
1	C	61	GLN
1	D	198	LYS
1	E	61	GLN
1	F	62	ASN
1	I	61	GLN
1	I	62	ASN
1	I	72	ASP
1	I	198	LYS
1	K	198	LYS
1	L	62	ASN
1	N	198	LYS
2	T	23	GLU
2	V	23	GLU
2	X	23	GLU
1	A	198	LYS
1	A	202	GLU
1	C	198	LYS
1	G	72	ASP
1	J	61	GLN
1	J	198	LYS
1	J	202	GLU
1	L	198	LYS
1	N	61	GLN
2	S	23	GLU
2	U	23	GLU
2	W	23	GLU
2	1	23	GLU
1	C	62	ASN
1	D	61	GLN
1	E	198	LYS
1	F	129	VAL
1	F	167	SER
1	G	198	LYS
1	L	61	GLN
2	P	23	GLU
2	S	49	VAL
2	Z	110	VAL
1	J	129	VAL
2	S	110	VAL
1	A	129	VAL

5.3.2 Protein sidechains ⓘ

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	A	184/193 (95%)	157 (85%)	27 (15%)	3	12
1	C	184/193 (95%)	160 (87%)	24 (13%)	4	16
1	D	184/193 (95%)	156 (85%)	28 (15%)	3	10
1	E	184/193 (95%)	156 (85%)	28 (15%)	3	10
1	F	184/193 (95%)	157 (85%)	27 (15%)	3	12
1	G	184/193 (95%)	163 (89%)	21 (11%)	5	21
1	H	184/193 (95%)	161 (88%)	23 (12%)	4	18
1	I	184/193 (95%)	162 (88%)	22 (12%)	5	19
1	J	184/193 (95%)	161 (88%)	23 (12%)	4	18
1	K	184/193 (95%)	156 (85%)	28 (15%)	3	10
1	L	184/193 (95%)	159 (86%)	25 (14%)	3	15
1	M	184/193 (95%)	159 (86%)	25 (14%)	3	15
1	N	184/193 (95%)	159 (86%)	25 (14%)	3	15
1	O	184/193 (95%)	155 (84%)	29 (16%)	2	10
2	1	170/177 (96%)	145 (85%)	25 (15%)	3	12
2	2	170/177 (96%)	140 (82%)	30 (18%)	2	8
2	B	170/177 (96%)	142 (84%)	28 (16%)	2	10
2	P	170/177 (96%)	143 (84%)	27 (16%)	2	10
2	Q	170/177 (96%)	140 (82%)	30 (18%)	2	8
2	R	170/177 (96%)	142 (84%)	28 (16%)	2	10
2	S	170/177 (96%)	144 (85%)	26 (15%)	3	10
2	T	170/177 (96%)	146 (86%)	24 (14%)	3	13
2	U	170/177 (96%)	145 (85%)	25 (15%)	3	12
2	V	170/177 (96%)	146 (86%)	24 (14%)	3	13
2	W	170/177 (96%)	144 (85%)	26 (15%)	3	10
2	X	170/177 (96%)	143 (84%)	27 (16%)	2	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	Y	170/177 (96%)	140 (82%)	30 (18%)	2	8
2	Z	170/177 (96%)	147 (86%)	23 (14%)	4	15
All	All	4956/5180 (96%)	4228 (85%)	728 (15%)	3	12

All (728) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	LEU
1	A	23	GLN
1	A	24	VAL
1	A	31	VAL
1	A	44	ASN
1	A	47	LEU
1	A	48	LEU
1	A	62	ASN
1	A	71	ASP
1	A	82	VAL
1	A	102	THR
1	A	106	LEU
1	A	107	VAL
1	A	111	ASN
1	A	119	GLN
1	A	134	VAL
1	A	136	LEU
1	A	141	ILE
1	A	143	GLN
1	A	157	ILE
1	A	161	LYS
1	A	175	PHE
1	A	176	LEU
1	A	190	VAL
1	A	201	LEU
1	A	202	GLU
1	A	212	ILE
2	B	2	THR
2	B	4	VAL
2	B	7	THR
2	B	17	GLU
2	B	20	VAL
2	B	26	ILE
2	B	41	THR

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Mol	Chain	Res	Type
2	B	45	ILE
2	B	49	VAL
2	B	56	VAL
2	B	63	LEU
2	B	68	LEU
2	B	83	LEU
2	B	94	PRO
2	B	97	VAL
2	B	104	ILE
2	B	123	ILE
2	B	127	THR
2	B	134	VAL
2	B	137	VAL
2	B	138	LEU
2	B	144	GLU
2	B	173	ILE
2	B	175	VAL
2	B	177	VAL
2	B	178	ILE
2	B	185	VAL
2	B	201	LEU
1	C	21	LEU
1	C	24	VAL
1	C	31	VAL
1	C	44	ASN
1	C	47	LEU
1	C	48	LEU
1	C	49	ILE
1	C	58	LEU
1	C	62	ASN
1	C	71	ASP
1	C	102	THR
1	C	107	VAL
1	C	113	VAL
1	C	119	GLN
1	C	134	VAL
1	C	136	LEU
1	C	141	ILE
1	C	143	GLN
1	C	157	ILE
1	C	176	LEU
1	C	190	VAL

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Mol	Chain	Res	Type
1	C	201	LEU
1	C	202	GLU
1	C	212	ILE
1	D	21	LEU
1	D	31	VAL
1	D	44	ASN
1	D	47	LEU
1	D	48	LEU
1	D	49	ILE
1	D	58	LEU
1	D	62	ASN
1	D	71	ASP
1	D	87	VAL
1	D	102	THR
1	D	107	VAL
1	D	113	VAL
1	D	116	VAL
1	D	119	GLN
1	D	134	VAL
1	D	136	LEU
1	D	141	ILE
1	D	143	GLN
1	D	157	ILE
1	D	161	LYS
1	D	175	PHE
1	D	176	LEU
1	D	190	VAL
1	D	201	LEU
1	D	202	GLU
1	D	212	ILE
1	D	221	TYR
1	E	21	LEU
1	E	23	GLN
1	E	24	VAL
1	E	31	VAL
1	E	44	ASN
1	E	47	LEU
1	E	48	LEU
1	E	49	ILE
1	E	58	LEU
1	E	62	ASN
1	E	71	ASP

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Mol	Chain	Res	Type
1	E	94	ILE
1	E	101	VAL
1	E	102	THR
1	E	107	VAL
1	E	113	VAL
1	E	119	GLN
1	E	134	VAL
1	E	136	LEU
1	E	141	ILE
1	E	143	GLN
1	E	157	ILE
1	E	175	PHE
1	E	176	LEU
1	E	190	VAL
1	E	201	LEU
1	E	202	GLU
1	E	212	ILE
1	F	21	LEU
1	F	23	GLN
1	F	24	VAL
1	F	31	VAL
1	F	44	ASN
1	F	47	LEU
1	F	48	LEU
1	F	62	ASN
1	F	71	ASP
1	F	82	VAL
1	F	101	VAL
1	F	102	THR
1	F	107	VAL
1	F	111	ASN
1	F	116	VAL
1	F	119	GLN
1	F	134	VAL
1	F	136	LEU
1	F	141	ILE
1	F	143	GLN
1	F	157	ILE
1	F	161	LYS
1	F	176	LEU
1	F	190	VAL
1	F	201	LEU

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Mol	Chain	Res	Type
1	F	202	GLU
1	F	212	ILE
1	G	21	LEU
1	G	23	GLN
1	G	31	VAL
1	G	44	ASN
1	G	47	LEU
1	G	48	LEU
1	G	49	ILE
1	G	62	ASN
1	G	71	ASP
1	G	101	VAL
1	G	102	THR
1	G	119	GLN
1	G	134	VAL
1	G	136	LEU
1	G	141	ILE
1	G	143	GLN
1	G	157	ILE
1	G	190	VAL
1	G	201	LEU
1	G	202	GLU
1	G	212	ILE
1	H	21	LEU
1	H	23	GLN
1	H	31	VAL
1	H	44	ASN
1	H	47	LEU
1	H	48	LEU
1	H	49	ILE
1	H	62	ASN
1	H	71	ASP
1	H	74	VAL
1	H	102	THR
1	H	107	VAL
1	H	119	GLN
1	H	134	VAL
1	H	136	LEU
1	H	141	ILE
1	H	143	GLN
1	H	157	ILE
1	H	176	LEU

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Mol	Chain	Res	Type
1	H	190	VAL
1	H	201	LEU
1	H	202	GLU
1	H	212	ILE
1	I	21	LEU
1	I	23	GLN
1	I	31	VAL
1	I	44	ASN
1	I	47	LEU
1	I	48	LEU
1	I	62	ASN
1	I	71	ASP
1	I	102	THR
1	I	107	VAL
1	I	119	GLN
1	I	134	VAL
1	I	136	LEU
1	I	141	ILE
1	I	143	GLN
1	I	157	ILE
1	I	175	PHE
1	I	176	LEU
1	I	190	VAL
1	I	201	LEU
1	I	202	GLU
1	I	212	ILE
1	J	21	LEU
1	J	24	VAL
1	J	31	VAL
1	J	44	ASN
1	J	47	LEU
1	J	48	LEU
1	J	49	ILE
1	J	62	ASN
1	J	71	ASP
1	J	102	THR
1	J	107	VAL
1	J	119	GLN
1	J	134	VAL
1	J	136	LEU
1	J	141	ILE
1	J	143	GLN

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Mol	Chain	Res	Type
1	J	157	ILE
1	J	161	LYS
1	J	175	PHE
1	J	190	VAL
1	J	201	LEU
1	J	202	GLU
1	J	212	ILE
1	K	21	LEU
1	K	23	GLN
1	K	31	VAL
1	K	38	LEU
1	K	44	ASN
1	K	47	LEU
1	K	48	LEU
1	K	49	ILE
1	K	58	LEU
1	K	62	ASN
1	K	71	ASP
1	K	74	VAL
1	K	87	VAL
1	K	102	THR
1	K	107	VAL
1	K	119	GLN
1	K	134	VAL
1	K	136	LEU
1	K	141	ILE
1	K	143	GLN
1	K	157	ILE
1	K	161	LYS
1	K	175	PHE
1	K	176	LEU
1	K	190	VAL
1	K	201	LEU
1	K	202	GLU
1	K	212	ILE
1	L	21	LEU
1	L	23	GLN
1	L	24	VAL
1	L	31	VAL
1	L	44	ASN
1	L	47	LEU
1	L	48	LEU

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Mol	Chain	Res	Type
1	L	49	ILE
1	L	58	LEU
1	L	62	ASN
1	L	71	ASP
1	L	87	VAL
1	L	101	VAL
1	L	102	THR
1	L	107	VAL
1	L	113	VAL
1	L	119	GLN
1	L	136	LEU
1	L	141	ILE
1	L	143	GLN
1	L	157	ILE
1	L	190	VAL
1	L	201	LEU
1	L	202	GLU
1	L	212	ILE
1	M	21	LEU
1	M	23	GLN
1	M	31	VAL
1	M	44	ASN
1	M	47	LEU
1	M	48	LEU
1	M	49	ILE
1	M	62	ASN
1	M	71	ASP
1	M	102	THR
1	M	111	ASN
1	M	116	VAL
1	M	119	GLN
1	M	134	VAL
1	M	136	LEU
1	M	141	ILE
1	M	143	GLN
1	M	157	ILE
1	M	175	PHE
1	M	176	LEU
1	M	190	VAL
1	M	201	LEU
1	M	202	GLU
1	M	212	ILE

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Mol	Chain	Res	Type
1	M	221	TYR
1	N	21	LEU
1	N	31	VAL
1	N	44	ASN
1	N	47	LEU
1	N	48	LEU
1	N	49	ILE
1	N	58	LEU
1	N	62	ASN
1	N	71	ASP
1	N	74	VAL
1	N	87	VAL
1	N	102	THR
1	N	113	VAL
1	N	119	GLN
1	N	134	VAL
1	N	136	LEU
1	N	141	ILE
1	N	143	GLN
1	N	157	ILE
1	N	161	LYS
1	N	176	LEU
1	N	190	VAL
1	N	201	LEU
1	N	202	GLU
1	N	212	ILE
1	O	21	LEU
1	O	24	VAL
1	O	31	VAL
1	O	44	ASN
1	O	47	LEU
1	O	48	LEU
1	O	49	ILE
1	O	58	LEU
1	O	62	ASN
1	O	71	ASP
1	O	74	VAL
1	O	101	VAL
1	O	102	THR
1	O	107	VAL
1	O	119	GLN
1	O	134	VAL

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Mol	Chain	Res	Type
1	O	136	LEU
1	O	141	ILE
1	O	143	GLN
1	O	150	ASP
1	O	157	ILE
1	O	161	LYS
1	O	175	PHE
1	O	176	LEU
1	O	190	VAL
1	O	201	LEU
1	O	202	GLU
1	O	212	ILE
1	O	221	TYR
2	P	2	THR
2	P	7	THR
2	P	17	GLU
2	P	20	VAL
2	P	26	ILE
2	P	41	THR
2	P	45	ILE
2	P	49	VAL
2	P	54	VAL
2	P	55	LEU
2	P	59	MET
2	P	63	LEU
2	P	70	ARG
2	P	71	ARG
2	P	83	LEU
2	P	104	ILE
2	P	123	ILE
2	P	127	THR
2	P	134	VAL
2	P	137	VAL
2	P	138	LEU
2	P	144	GLU
2	P	173	ILE
2	P	175	VAL
2	P	177	VAL
2	P	178	ILE
2	P	185	VAL
2	Q	2	THR
2	Q	6	ILE

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Mol	Chain	Res	Type
2	Q	7	THR
2	Q	8	LEU
2	Q	12	VAL
2	Q	17	GLU
2	Q	20	VAL
2	Q	26	ILE
2	Q	41	THR
2	Q	45	ILE
2	Q	49	VAL
2	Q	55	LEU
2	Q	59	MET
2	Q	68	LEU
2	Q	70	ARG
2	Q	71	ARG
2	Q	79	VAL
2	Q	83	LEU
2	Q	104	ILE
2	Q	123	ILE
2	Q	127	THR
2	Q	134	VAL
2	Q	137	VAL
2	Q	138	LEU
2	Q	144	GLU
2	Q	173	ILE
2	Q	175	VAL
2	Q	177	VAL
2	Q	178	ILE
2	Q	185	VAL
2	R	2	THR
2	R	6	ILE
2	R	7	THR
2	R	17	GLU
2	R	20	VAL
2	R	26	ILE
2	R	41	THR
2	R	45	ILE
2	R	49	VAL
2	R	56	VAL
2	R	68	LEU
2	R	70	ARG
2	R	71	ARG
2	R	83	LEU

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Mol	Chain	Res	Type
2	R	94	PRO
2	R	97	VAL
2	R	104	ILE
2	R	123	ILE
2	R	127	THR
2	R	134	VAL
2	R	137	VAL
2	R	138	LEU
2	R	144	GLU
2	R	173	ILE
2	R	175	VAL
2	R	177	VAL
2	R	178	ILE
2	R	185	VAL
2	S	1	THR
2	S	2	THR
2	S	7	THR
2	S	17	GLU
2	S	20	VAL
2	S	26	ILE
2	S	41	THR
2	S	45	ILE
2	S	49	VAL
2	S	63	LEU
2	S	68	LEU
2	S	70	ARG
2	S	71	ARG
2	S	83	LEU
2	S	104	ILE
2	S	123	ILE
2	S	127	THR
2	S	134	VAL
2	S	137	VAL
2	S	138	LEU
2	S	144	GLU
2	S	165	ARG
2	S	173	ILE
2	S	175	VAL
2	S	178	ILE
2	S	185	VAL
2	T	2	THR
2	T	7	THR

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Mol	Chain	Res	Type
2	T	17	GLU
2	T	20	VAL
2	T	26	ILE
2	T	41	THR
2	T	45	ILE
2	T	54	VAL
2	T	59	MET
2	T	70	ARG
2	T	71	ARG
2	T	83	LEU
2	T	120	VAL
2	T	123	ILE
2	T	127	THR
2	T	134	VAL
2	T	137	VAL
2	T	138	LEU
2	T	144	GLU
2	T	165	ARG
2	T	173	ILE
2	T	178	ILE
2	T	185	VAL
2	T	201	LEU
2	U	2	THR
2	U	7	THR
2	U	12	VAL
2	U	17	GLU
2	U	20	VAL
2	U	26	ILE
2	U	41	THR
2	U	45	ILE
2	U	59	MET
2	U	68	LEU
2	U	70	ARG
2	U	71	ARG
2	U	94	PRO
2	U	123	ILE
2	U	127	THR
2	U	134	VAL
2	U	137	VAL
2	U	138	LEU
2	U	144	GLU
2	U	165	ARG

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Mol	Chain	Res	Type
2	U	173	ILE
2	U	175	VAL
2	U	177	VAL
2	U	178	ILE
2	U	185	VAL
2	V	2	THR
2	V	7	THR
2	V	17	GLU
2	V	20	VAL
2	V	26	ILE
2	V	41	THR
2	V	45	ILE
2	V	49	VAL
2	V	56	VAL
2	V	63	LEU
2	V	70	ARG
2	V	71	ARG
2	V	94	PRO
2	V	120	VAL
2	V	123	ILE
2	V	127	THR
2	V	134	VAL
2	V	137	VAL
2	V	138	LEU
2	V	144	GLU
2	V	173	ILE
2	V	175	VAL
2	V	178	ILE
2	V	185	VAL
2	W	2	THR
2	W	6	ILE
2	W	7	THR
2	W	17	GLU
2	W	20	VAL
2	W	26	ILE
2	W	37	ILE
2	W	41	THR
2	W	45	ILE
2	W	49	VAL
2	W	56	VAL
2	W	63	LEU
2	W	71	ARG

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Mol	Chain	Res	Type
2	W	94	PRO
2	W	97	VAL
2	W	123	ILE
2	W	127	THR
2	W	134	VAL
2	W	137	VAL
2	W	138	LEU
2	W	144	GLU
2	W	173	ILE
2	W	175	VAL
2	W	177	VAL
2	W	178	ILE
2	W	185	VAL
2	X	2	THR
2	X	7	THR
2	X	17	GLU
2	X	20	VAL
2	X	26	ILE
2	X	41	THR
2	X	45	ILE
2	X	49	VAL
2	X	54	VAL
2	X	55	LEU
2	X	59	MET
2	X	70	ARG
2	X	83	LEU
2	X	104	ILE
2	X	123	ILE
2	X	127	THR
2	X	134	VAL
2	X	137	VAL
2	X	138	LEU
2	X	144	GLU
2	X	165	ARG
2	X	173	ILE
2	X	175	VAL
2	X	177	VAL
2	X	178	ILE
2	X	185	VAL
2	X	201	LEU
2	Y	2	THR
2	Y	4	VAL

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Mol	Chain	Res	Type
2	Y	7	THR
2	Y	12	VAL
2	Y	17	GLU
2	Y	20	VAL
2	Y	26	ILE
2	Y	41	THR
2	Y	45	ILE
2	Y	49	VAL
2	Y	59	MET
2	Y	63	LEU
2	Y	70	ARG
2	Y	71	ARG
2	Y	83	LEU
2	Y	87	LEU
2	Y	94	PRO
2	Y	123	ILE
2	Y	127	THR
2	Y	134	VAL
2	Y	137	VAL
2	Y	138	LEU
2	Y	144	GLU
2	Y	165	ARG
2	Y	173	ILE
2	Y	175	VAL
2	Y	177	VAL
2	Y	178	ILE
2	Y	185	VAL
2	Y	201	LEU
2	Z	7	THR
2	Z	17	GLU
2	Z	20	VAL
2	Z	26	ILE
2	Z	41	THR
2	Z	45	ILE
2	Z	49	VAL
2	Z	63	LEU
2	Z	70	ARG
2	Z	79	VAL
2	Z	83	LEU
2	Z	104	ILE
2	Z	123	ILE
2	Z	127	THR

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Mol	Chain	Res	Type
2	Z	134	VAL
2	Z	137	VAL
2	Z	138	LEU
2	Z	144	GLU
2	Z	165	ARG
2	Z	173	ILE
2	Z	175	VAL
2	Z	178	ILE
2	Z	185	VAL
2	1	2	THR
2	1	8	LEU
2	1	12	VAL
2	1	17	GLU
2	1	20	VAL
2	1	26	ILE
2	1	41	THR
2	1	45	ILE
2	1	59	MET
2	1	70	ARG
2	1	71	ARG
2	1	83	LEU
2	1	123	ILE
2	1	127	THR
2	1	134	VAL
2	1	137	VAL
2	1	138	LEU
2	1	144	GLU
2	1	165	ARG
2	1	173	ILE
2	1	175	VAL
2	1	177	VAL
2	1	178	ILE
2	1	185	VAL
2	1	201	LEU
2	2	1	THR
2	2	2	THR
2	2	4	VAL
2	2	12	VAL
2	2	17	GLU
2	2	20	VAL
2	2	26	ILE
2	2	41	THR

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Mol	Chain	Res	Type
2	2	45	ILE
2	2	49	VAL
2	2	54	VAL
2	2	59	MET
2	2	63	LEU
2	2	68	LEU
2	2	70	ARG
2	2	71	ARG
2	2	83	LEU
2	2	94	PRO
2	2	123	ILE
2	2	127	THR
2	2	134	VAL
2	2	137	VAL
2	2	138	LEU
2	2	144	GLU
2	2	165	ARG
2	2	173	ILE
2	2	175	VAL
2	2	177	VAL
2	2	178	ILE
2	2	185	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (163) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	44	ASN
1	A	98	GLN
1	A	119	GLN
1	A	121	GLN
1	A	125	GLN
1	A	143	GLN
2	B	28	HIS
2	B	30	ASN
2	B	36	GLN
2	B	85	ASN
1	C	44	ASN
1	C	98	GLN
1	C	119	GLN
1	C	121	GLN
1	C	125	GLN

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Mol	Chain	Res	Type
1	C	143	GLN
1	C	183	ASN
1	D	23	GLN
1	D	44	ASN
1	D	98	GLN
1	D	121	GLN
1	D	125	GLN
1	D	143	GLN
1	E	44	ASN
1	E	98	GLN
1	E	119	GLN
1	E	121	GLN
1	E	125	GLN
1	E	143	GLN
1	F	44	ASN
1	F	119	GLN
1	F	121	GLN
1	F	125	GLN
1	F	143	GLN
1	F	158	ASN
1	G	23	GLN
1	G	44	ASN
1	G	119	GLN
1	G	143	GLN
1	H	44	ASN
1	H	98	GLN
1	H	121	GLN
1	H	125	GLN
1	H	143	GLN
1	H	158	ASN
1	H	183	ASN
1	I	44	ASN
1	I	121	GLN
1	I	125	GLN
1	I	143	GLN
1	I	158	ASN
1	J	44	ASN
1	J	98	GLN
1	J	119	GLN
1	J	121	GLN
1	J	125	GLN
1	J	143	GLN

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Mol	Chain	Res	Type
1	J	158	ASN
1	K	44	ASN
1	K	98	GLN
1	K	119	GLN
1	K	122	GLN
1	K	143	GLN
1	K	158	ASN
1	L	23	GLN
1	L	44	ASN
1	L	121	GLN
1	L	125	GLN
1	L	143	GLN
1	L	158	ASN
1	L	183	ASN
1	L	226	GLN
1	M	44	ASN
1	M	119	GLN
1	M	121	GLN
1	M	125	GLN
1	M	143	GLN
1	M	183	ASN
1	N	23	GLN
1	N	44	ASN
1	N	121	GLN
1	N	125	GLN
1	N	143	GLN
1	N	183	ASN
1	O	23	GLN
1	O	44	ASN
1	O	98	GLN
1	O	121	GLN
1	O	125	GLN
1	O	143	GLN
1	O	158	ASN
2	P	28	HIS
2	P	30	ASN
2	P	36	GLN
2	P	73	ASN
2	P	85	ASN
2	P	164	GLN
2	Q	30	ASN
2	Q	36	GLN

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Mol	Chain	Res	Type
2	Q	141	GLN
2	Q	164	GLN
2	R	28	HIS
2	R	30	ASN
2	R	85	ASN
2	R	141	GLN
2	R	164	GLN
2	S	28	HIS
2	S	30	ASN
2	S	36	GLN
2	S	85	ASN
2	S	141	GLN
2	S	164	GLN
2	T	28	HIS
2	T	30	ASN
2	T	85	ASN
2	T	141	GLN
2	T	164	GLN
2	U	28	HIS
2	U	30	ASN
2	U	36	GLN
2	U	85	ASN
2	U	141	GLN
2	U	164	GLN
2	V	28	HIS
2	V	30	ASN
2	V	36	GLN
2	V	85	ASN
2	V	164	GLN
2	W	28	HIS
2	W	30	ASN
2	W	36	GLN
2	W	73	ASN
2	W	85	ASN
2	W	164	GLN
2	X	28	HIS
2	X	30	ASN
2	X	36	GLN
2	X	85	ASN
2	X	98	GLN
2	X	164	GLN
2	Y	30	ASN

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Mol	Chain	Res	Type
2	Y	85	ASN
2	Y	98	GLN
2	Y	141	GLN
2	Y	164	GLN
2	Z	28	HIS
2	Z	30	ASN
2	Z	36	GLN
2	Z	85	ASN
2	Z	141	GLN
2	Z	164	GLN
2	1	28	HIS
2	1	30	ASN
2	1	36	GLN
2	1	85	ASN
2	1	164	GLN
2	2	28	HIS
2	2	30	ASN
2	2	36	GLN
2	2	98	GLN
2	2	141	GLN
2	2	164	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	A	221/233 (94%)	-0.17	3 (1%) 73 59	21, 51, 101, 142	0
1	C	221/233 (94%)	-0.14	2 (0%) 81 68	15, 50, 100, 142	0
1	D	221/233 (94%)	-0.21	2 (0%) 81 68	22, 48, 97, 141	0
1	E	221/233 (94%)	-0.13	3 (1%) 73 59	19, 49, 98, 142	0
1	F	221/233 (94%)	-0.14	0 100 100	18, 52, 99, 141	0
1	G	221/233 (94%)	-0.05	3 (1%) 73 59	22, 52, 98, 143	0
1	H	221/233 (94%)	-0.15	1 (0%) 87 78	23, 52, 102, 141	0
1	I	221/233 (94%)	-0.20	1 (0%) 87 78	19, 51, 97, 142	0
1	J	221/233 (94%)	-0.22	0 100 100	22, 51, 100, 144	0
1	K	221/233 (94%)	-0.26	1 (0%) 87 78	22, 51, 99, 141	0
1	L	221/233 (94%)	-0.25	2 (0%) 81 68	16, 49, 98, 141	0
1	M	221/233 (94%)	-0.24	2 (0%) 81 68	19, 49, 97, 141	0
1	N	221/233 (94%)	-0.22	2 (0%) 81 68	21, 49, 97, 144	0
1	O	221/233 (94%)	-0.17	5 (2%) 61 46	19, 48, 97, 140	0
2	1	203/211 (96%)	-0.53	0 100 100	12, 33, 65, 74	0
2	2	203/211 (96%)	-0.49	0 100 100	11, 33, 64, 75	0
2	B	203/211 (96%)	-0.49	0 100 100	13, 34, 65, 77	0
2	P	203/211 (96%)	-0.51	0 100 100	10, 35, 63, 72	0
2	Q	203/211 (96%)	-0.56	0 100 100	11, 33, 63, 73	0
2	R	203/211 (96%)	-0.56	0 100 100	11, 32, 63, 73	0
2	S	203/211 (96%)	-0.48	0 100 100	10, 33, 64, 74	0
2	T	203/211 (96%)	-0.41	0 100 100	13, 35, 65, 77	0
2	U	203/211 (96%)	-0.50	1 (0%) 87 78	16, 34, 65, 76	0
2	V	203/211 (96%)	-0.55	0 100 100	14, 32, 64, 74	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
2	W	203/211 (96%)	-0.56	0	100	100	13, 34, 64, 76	0
2	X	203/211 (96%)	-0.60	0	100	100	11, 33, 63, 78	0
2	Y	203/211 (96%)	-0.58	0	100	100	12, 33, 62, 73	0
2	Z	203/211 (96%)	-0.60	0	100	100	12, 32, 64, 75	0
All	All	5936/6216 (95%)	-0.35	28 (0%)	87	78	10, 41, 92, 144	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	202	GLU	4.0
1	D	63	SER	3.6
1	K	202	GLU	3.5
1	C	166	GLY	3.2
1	N	205	GLU	3.1
1	G	202	GLU	3.0
1	A	200	SER	3.0
1	M	63	SER	3.0
1	L	202	GLU	2.9
1	E	63	SER	2.8
1	L	200	SER	2.7
1	O	204	GLY	2.7
1	A	63	SER	2.7
1	G	204	GLY	2.6
1	H	200	SER	2.6
1	O	63	SER	2.5
1	N	202	GLU	2.5
1	O	207	LEU	2.4
1	O	203	GLU	2.3
1	E	205	GLU	2.2
2	U	22	MET	2.2
1	E	202	GLU	2.2
1	G	230	LYS	2.2
1	M	204	GLY	2.2
1	D	183	ASN	2.1
1	C	201	LEU	2.1
1	A	226	GLN	2.0
1	I	142	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.