



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:41 PM UTC

PDB ID : 1W4C / pdb_00001w4c
Title : P4 protein from Bacteriophage PHI12 apo state
Authors : Mancini, E.J.; Kainov, D.E.; Grimes, J.M.; Tuma, R.; Bamford, D.H.; Stuart, D.I.
Deposited on : 2004-07-22
Resolution : 2.50 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:

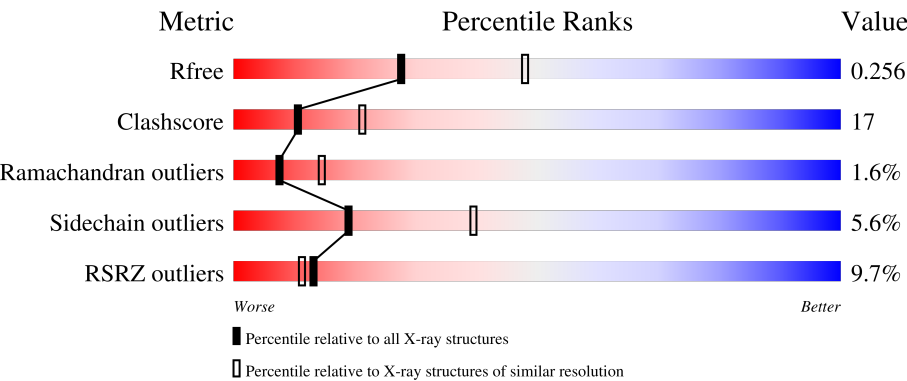
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	331	5% 63% 21% • • 13%
1	B	331	8% 63% 24% 5% 8%
1	C	331	8% 65% 22% 5% 8%
1	D	331	8% 62% 21% • • 13%
1	E	331	10% 64% 23% • 8%

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Mol	Chain	Length	Quality of chain
1	F	331	
1	G	331	
1	H	331	
1	I	331	
1	J	331	
1	K	331	
1	L	331	
1	M	331	
1	N	331	
1	O	331	
1	P	331	
1	Q	331	
1	R	331	
1	S	331	
1	T	331	
1	U	331	
1	V	331	
1	W	331	
1	X	331	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 57270 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called NTPASE P4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	289	Total	C	N	O	S	0	0	1
			2171	1361	379	424	7			
1	B	304	Total	C	N	O	S	0	0	0
			2288	1434	399	448	7			
1	C	304	Total	C	N	O	S	0	0	0
			2288	1433	399	449	7			
1	D	289	Total	C	N	O	S	0	0	1
			2171	1361	379	424	7			
1	E	304	Total	C	N	O	S	0	0	0
			2289	1434	399	449	7			
1	F	304	Total	C	N	O	S	0	0	0
			2289	1434	399	449	7			
1	G	304	Total	C	N	O	S	0	0	0
			2289	1434	399	449	7			
1	H	289	Total	C	N	O	S	0	0	1
			2171	1361	379	424	7			
1	I	289	Total	C	N	O	S	0	0	1
			2171	1361	379	424	7			
1	J	304	Total	C	N	O	S	0	0	0
			2289	1434	399	449	7			
1	K	304	Total	C	N	O	S	0	0	0
			2289	1434	399	449	7			
1	L	289	Total	C	N	O	S	0	0	1
			2171	1361	379	424	7			
1	M	304	Total	C	N	O	S	0	0	0
			2289	1434	399	449	7			
1	N	304	Total	C	N	O	S	0	0	0
			2289	1434	399	449	7			
1	O	304	Total	C	N	O	S	0	0	0
			2289	1434	399	449	7			
1	P	304	Total	C	N	O	S	0	0	0
			2289	1434	399	449	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	304	Total	C	N	O	S	0	0	0
			2289	1434	399	449	7			
1	R	304	Total	C	N	O	S	0	0	0
			2289	1434	399	449	7			
1	S	304	Total	C	N	O	S	0	0	0
			2289	1434	399	449	7			
1	T	304	Total	C	N	O	S	0	0	0
			2289	1434	399	449	7			
1	U	289	Total	C	N	O	S	0	0	1
			2171	1361	379	424	7			
1	V	304	Total	C	N	O	S	0	0	0
			2289	1434	399	449	7			
1	W	304	Total	C	N	O	S	0	0	0
			2289	1434	399	449	7			
1	X	289	Total	C	N	O	S	0	0	1
			2171	1361	379	424	7			

- Molecule 2 is water.

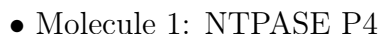
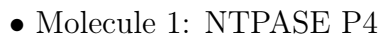
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	110	Total	O	0	0
			110	110		
2	B	119	Total	O	0	0
			119	119		
2	C	129	Total	O	0	0
			129	129		
2	D	145	Total	O	0	0
			145	145		
2	E	143	Total	O	0	0
			143	143		
2	F	151	Total	O	0	0
			151	151		
2	G	101	Total	O	0	0
			101	101		
2	H	178	Total	O	0	0
			178	178		
2	I	193	Total	O	0	0
			193	193		
2	J	159	Total	O	0	0
			159	159		
2	K	122	Total	O	0	0
			122	122		

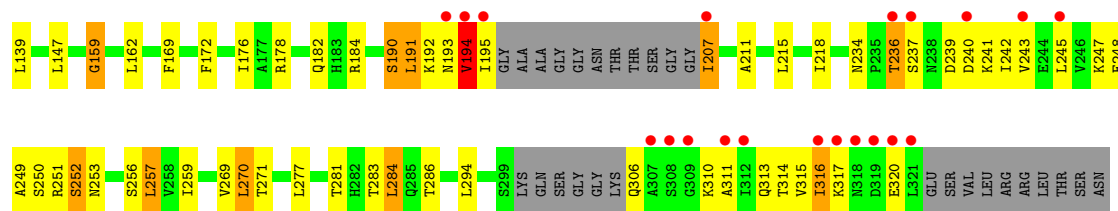
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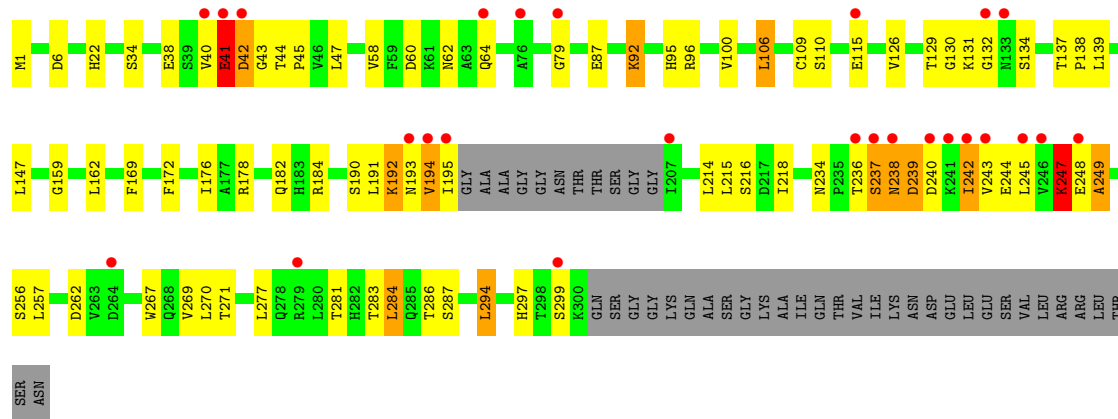
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	L	93	Total 93	O 93	0	0
2	M	169	Total 169	O 169	0	0
2	N	202	Total 202	O 202	0	0
2	O	144	Total 144	O 144	0	0
2	P	103	Total 103	O 103	0	0
2	Q	93	Total 93	O 93	0	0
2	R	110	Total 110	O 110	0	0
2	S	146	Total 146	O 146	0	0
2	T	88	Total 88	O 88	0	0
2	U	73	Total 73	O 73	0	0
2	V	118	Total 118	O 118	0	0
2	W	120	Total 120	O 120	0	0
2	X	153	Total 153	O 153	0	0

- Molecule 1: NTPASE P4

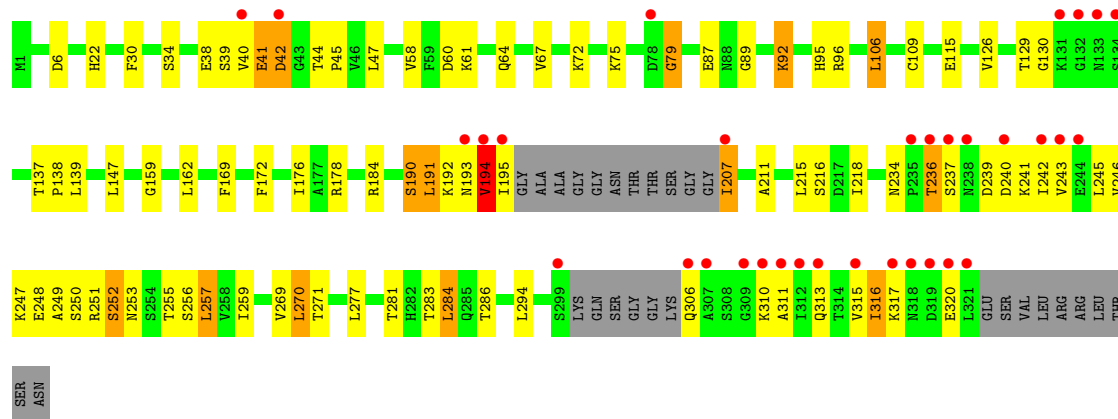




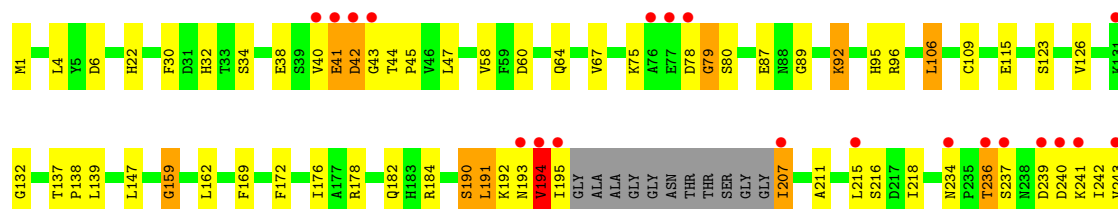
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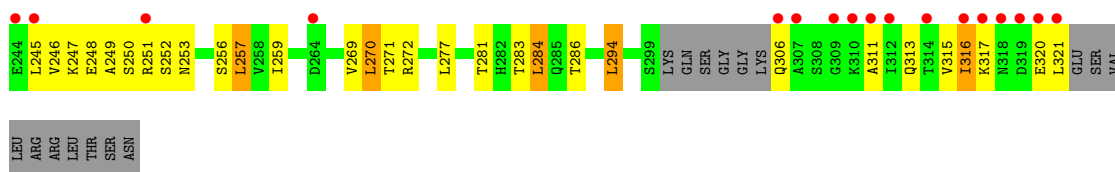


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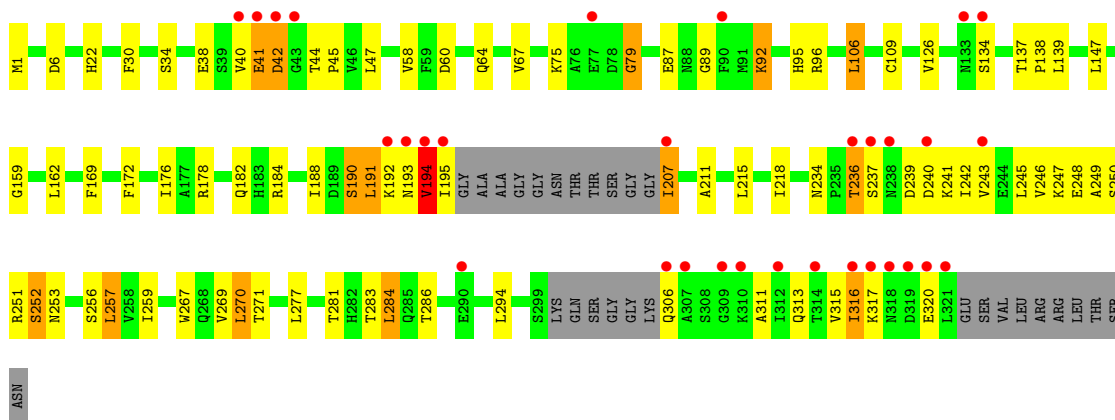


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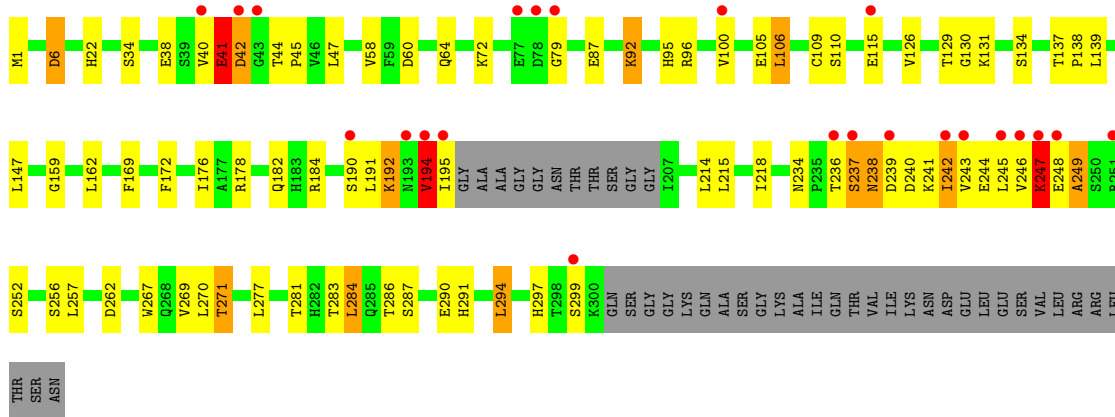




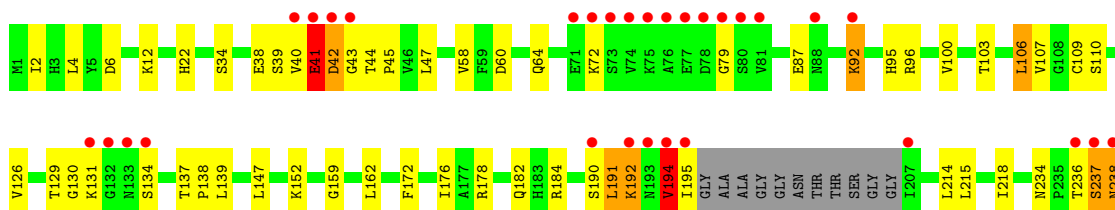
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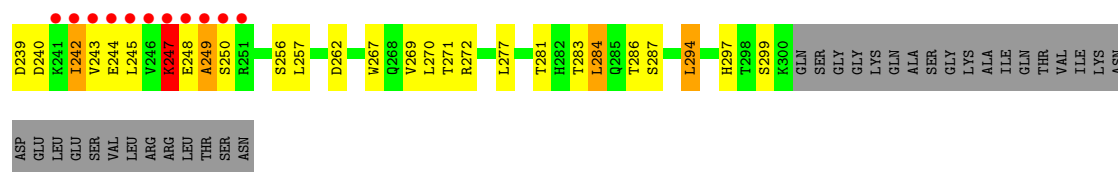


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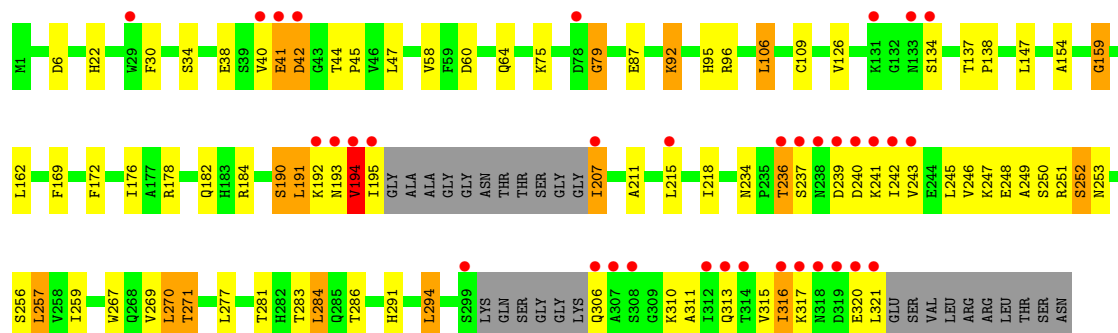


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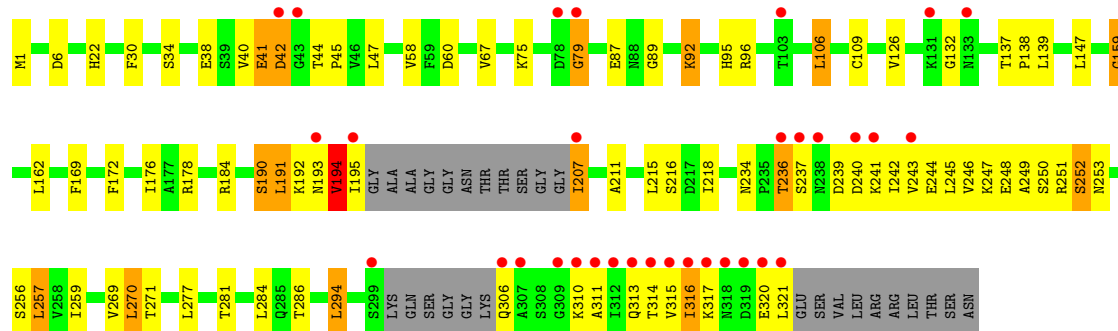




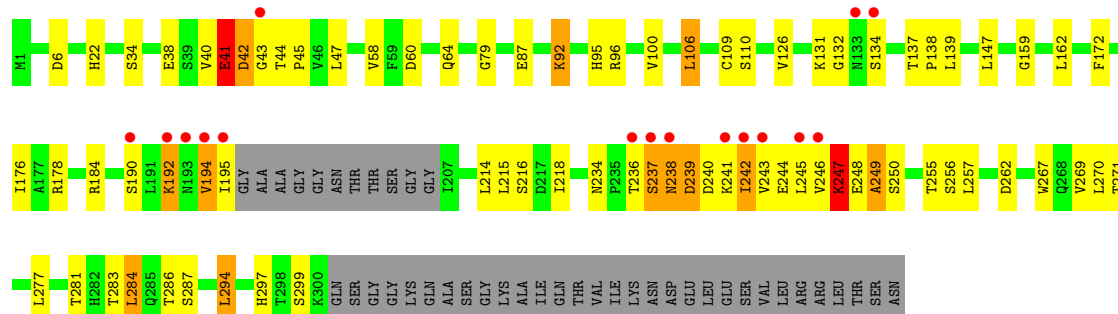
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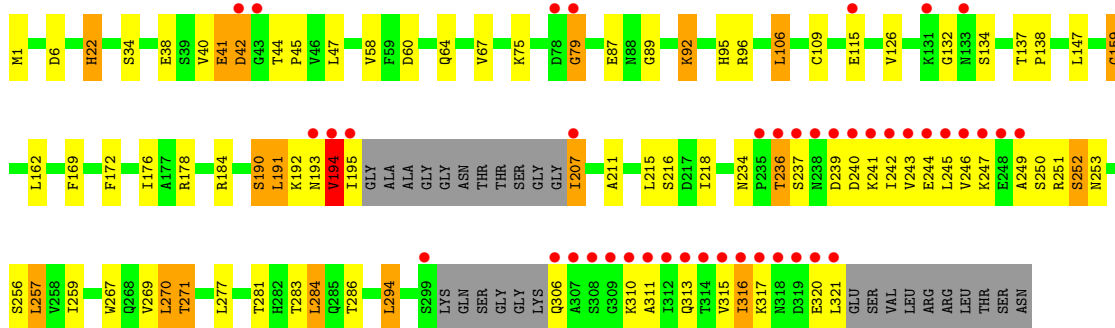
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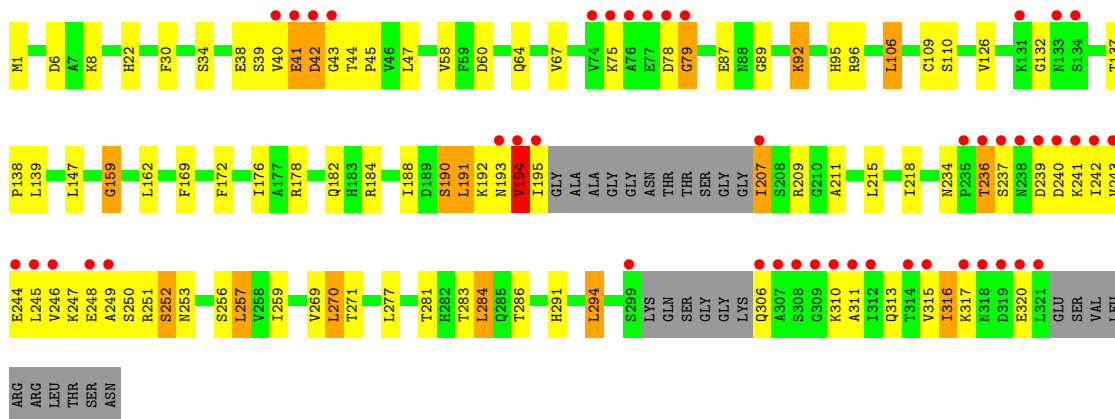
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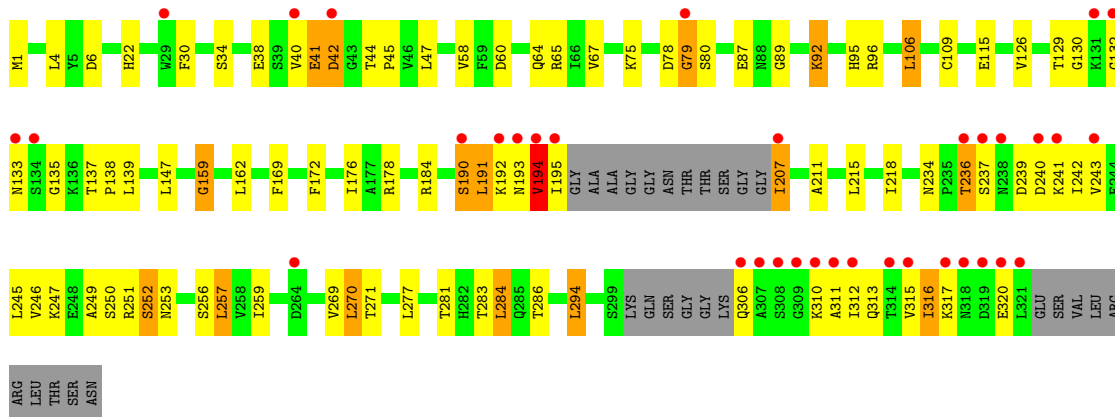
• Molecule 1: NTPASE P4



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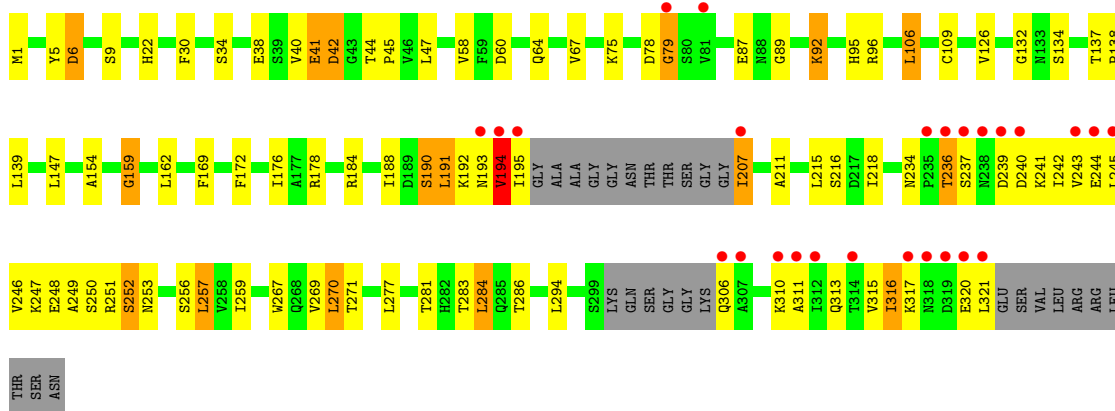


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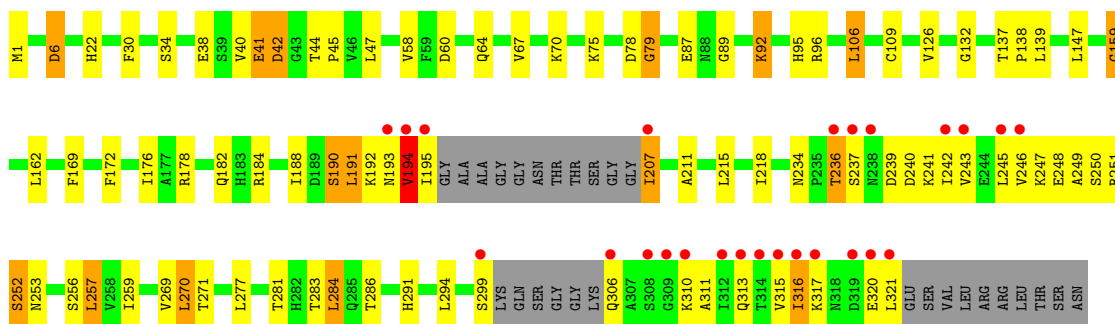


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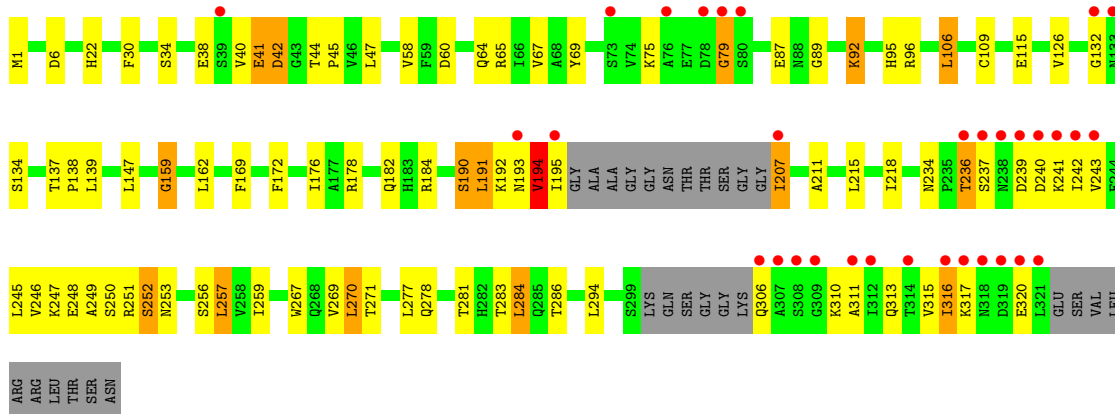




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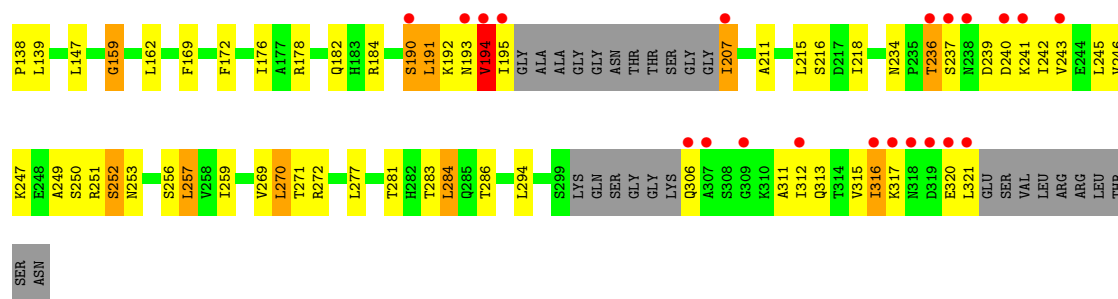


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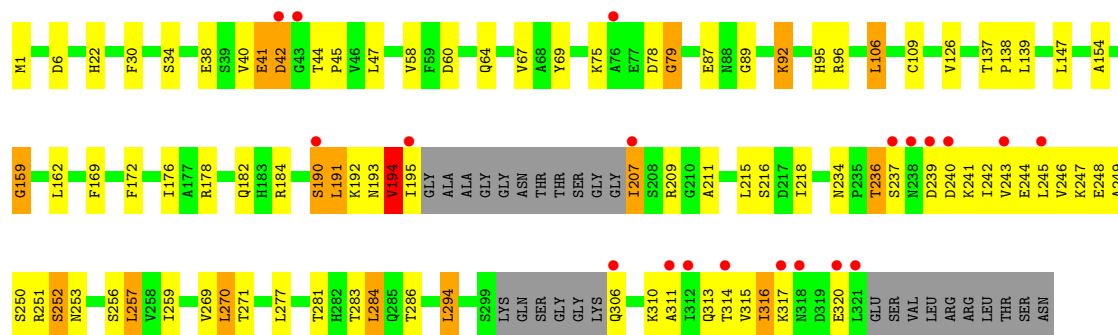


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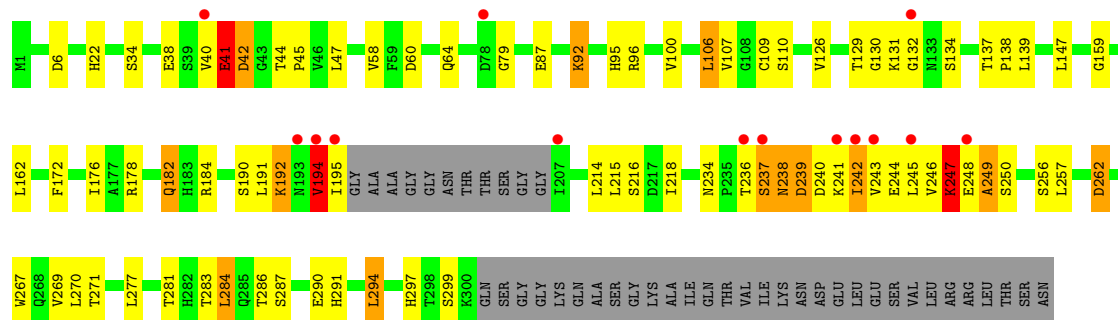




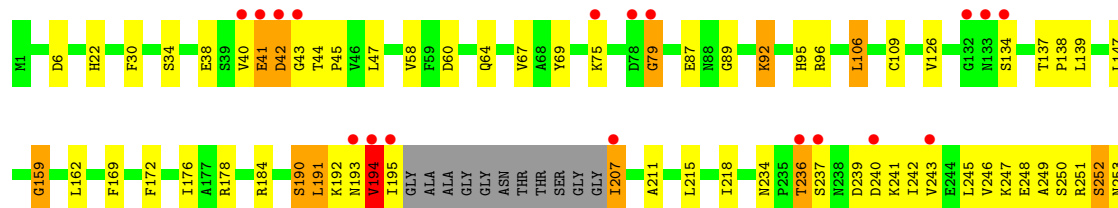
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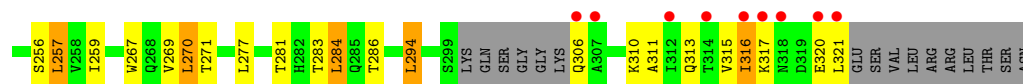


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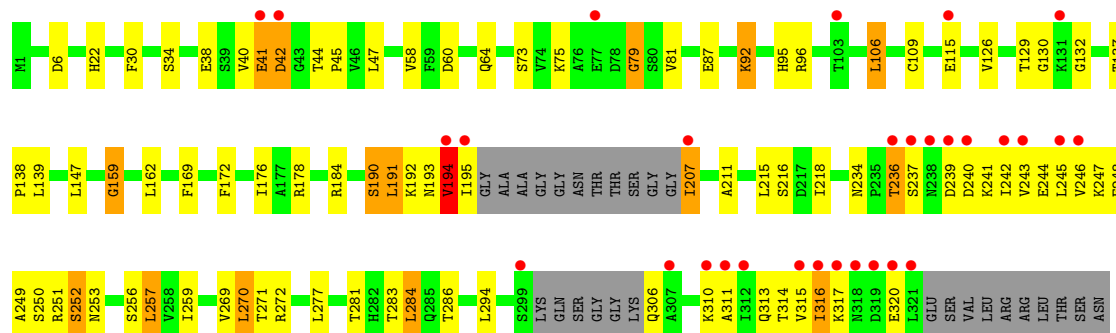


• Molecule 1: NTPASE P4

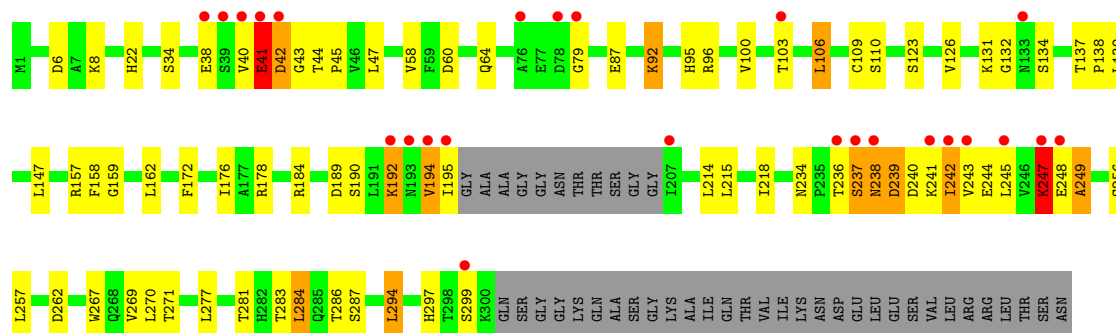




● Molecule 1: NTPASE P4



● Molecule 1: NTPASE P4



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	115.40Å 126.30Å 155.60Å 90.00° 91.60° 90.50°	Depositor
Resolution (Å)	20.00 – 2.50 20.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	96.0 (20.00-2.50) 96.0 (20.00-2.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.35 (at 2.50Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.251 , 0.224 (Not available) , 0.256	Depositor DCC
R_{free} test set	14484 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	41.2	Xtriage
Anisotropy	0.307	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 57.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.004 for h,-k,-l 0.006 for -h,k,-l 0.001 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	57270	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.17% 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	0.41	1/2208 (0.0%)	0.98	14/2991 (0.5%)
1	B	0.40	0/2324	0.95	11/3145 (0.3%)
1	C	0.40	0/2323	0.95	9/3142 (0.3%)
1	D	0.45	1/2208 (0.0%)	0.97	14/2991 (0.5%)
1	E	0.42	0/2325	0.95	8/3146 (0.3%)
1	F	0.43	0/2325	0.95	9/3146 (0.3%)
1	G	0.41	0/2325	0.95	10/3146 (0.3%)
1	H	0.46	1/2208 (0.0%)	0.98	13/2991 (0.4%)
1	I	0.48	1/2208 (0.0%)	0.98	16/2991 (0.5%)
1	J	0.45	0/2325	0.96	9/3146 (0.3%)
1	K	0.41	0/2325	0.96	8/3146 (0.3%)
1	L	0.42	1/2208 (0.0%)	0.98	14/2991 (0.5%)
1	M	0.45	0/2325	0.96	8/3146 (0.3%)
1	N	0.45	0/2325	0.96	12/3146 (0.4%)
1	O	0.43	0/2325	0.95	8/3146 (0.3%)
1	P	0.39	0/2325	0.96	10/3146 (0.3%)
1	Q	0.39	0/2325	0.95	11/3146 (0.3%)
1	R	0.42	0/2325	0.96	9/3146 (0.3%)
1	S	0.43	0/2325	0.96	9/3146 (0.3%)
1	T	0.38	0/2325	0.95	9/3146 (0.3%)
1	U	0.40	1/2208 (0.0%)	0.98	14/2991 (0.5%)
1	V	0.40	0/2325	0.95	8/3146 (0.3%)
1	W	0.40	0/2325	0.96	8/3146 (0.3%)
1	X	0.45	1/2208 (0.0%)	0.97	14/2991 (0.5%)
All	All	0.42	7/54978 (0.0%)	0.96	255/74414 (0.3%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	299	SER	C-N	-5.61	1.25	1.33
1	X	299	SER	C-N	-5.54	1.25	1.33
1	U	299	SER	C-N	-5.52	1.25	1.33
1	D	299	SER	C-N	-5.52	1.25	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	299	SER	C-N	-5.51	1.25	1.33
1	L	299	SER	C-N	-5.50	1.25	1.33
1	H	299	SER	C-N	-5.47	1.25	1.33

All (255) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	194	VAL	N-CA-C	-8.21	100.94	110.21
1	V	191	LEU	N-CA-C	-8.16	103.23	113.02
1	M	191	LEU	N-CA-C	-8.13	103.26	113.02
1	E	194	VAL	N-CA-C	-8.07	101.09	110.21
1	W	194	VAL	N-CA-C	-8.05	101.12	110.21
1	R	194	VAL	N-CA-C	-8.04	101.13	110.21
1	O	194	VAL	N-CA-C	-8.02	101.14	110.21
1	S	194	VAL	N-CA-C	-8.01	101.16	110.21
1	V	194	VAL	N-CA-C	-7.98	101.19	110.21
1	G	194	VAL	N-CA-C	-7.95	101.22	110.21
1	M	194	VAL	N-CA-C	-7.95	101.23	110.21
1	Q	194	VAL	N-CA-C	-7.95	101.23	110.21
1	P	194	VAL	N-CA-C	-7.93	101.24	110.21
1	K	194	VAL	N-CA-C	-7.92	101.26	110.21
1	E	191	LEU	N-CA-C	-7.89	103.55	113.02
1	B	194	VAL	N-CA-C	-7.88	101.30	110.21
1	N	194	VAL	N-CA-C	-7.88	101.30	110.21
1	T	191	LEU	N-CA-C	-7.86	103.59	113.02
1	W	191	LEU	N-CA-C	-7.85	103.60	113.02
1	J	194	VAL	N-CA-C	-7.84	101.35	110.21
1	G	191	LEU	N-CA-C	-7.82	103.64	113.02
1	F	194	VAL	N-CA-C	-7.81	101.38	110.21
1	B	191	LEU	N-CA-C	-7.81	103.65	113.02
1	X	242	ILE	N-CA-C	-7.80	103.83	112.80
1	C	194	VAL	N-CA-C	-7.80	101.39	110.21
1	N	191	LEU	N-CA-C	-7.75	103.72	113.02
1	P	191	LEU	N-CA-C	-7.72	103.76	113.02
1	L	242	ILE	N-CA-C	-7.71	103.93	112.80
1	S	191	LEU	N-CA-C	-7.71	103.77	113.02
1	U	242	ILE	N-CA-C	-7.69	103.96	112.80
1	I	242	ILE	N-CA-C	-7.68	103.97	112.80
1	D	242	ILE	N-CA-C	-7.68	103.97	112.80
1	Q	191	LEU	N-CA-C	-7.65	103.84	113.02
1	H	242	ILE	N-CA-C	-7.61	104.06	112.80
1	F	191	LEU	N-CA-C	-7.57	103.94	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	191	LEU	N-CA-C	-7.56	103.95	113.02
1	K	191	LEU	N-CA-C	-7.55	103.96	113.02
1	C	191	LEU	N-CA-C	-7.53	103.98	113.02
1	A	159	GLY	N-CA-C	7.49	125.41	114.10
1	A	242	ILE	N-CA-C	-7.46	104.23	112.80
1	H	159	GLY	N-CA-C	7.45	125.35	114.10
1	J	191	LEU	N-CA-C	-7.43	104.11	113.02
1	D	22	HIS	N-CA-C	7.39	120.78	111.69
1	U	159	GLY	N-CA-C	7.34	125.19	114.10
1	I	159	GLY	N-CA-C	7.32	125.15	114.10
1	W	159	GLY	N-CA-C	7.31	124.16	113.48
1	D	159	GLY	N-CA-C	7.29	125.10	114.10
1	R	191	LEU	N-CA-C	-7.27	104.29	113.02
1	L	159	GLY	N-CA-C	7.25	125.05	114.10
1	L	22	HIS	N-CA-C	7.23	120.59	111.69
1	X	159	GLY	N-CA-C	7.21	124.99	114.10
1	I	247	LYS	N-CA-C	-7.21	101.54	110.41
1	C	159	GLY	N-CA-C	7.15	123.92	113.48
1	K	159	GLY	N-CA-C	7.14	123.91	113.48
1	P	159	GLY	N-CA-C	7.14	123.90	113.48
1	M	22	HIS	N-CA-C	7.12	120.45	111.69
1	N	218	ILE	N-CA-C	7.12	118.74	110.62
1	O	22	HIS	N-CA-C	7.10	120.42	111.69
1	R	159	GLY	N-CA-C	7.09	123.84	113.48
1	I	22	HIS	N-CA-C	7.09	120.41	111.69
1	H	22	HIS	N-CA-C	7.09	120.41	111.69
1	J	22	HIS	N-CA-C	7.07	120.38	111.69
1	O	159	GLY	N-CA-C	7.06	123.79	113.48
1	W	218	ILE	N-CA-C	7.06	118.67	110.62
1	Q	22	HIS	N-CA-C	7.05	120.36	111.69
1	D	247	LYS	N-CA-C	-7.04	101.75	110.41
1	U	22	HIS	N-CA-C	6.99	120.29	111.69
1	U	247	LYS	N-CA-C	-6.99	101.81	110.41
1	H	247	LYS	N-CA-C	-6.97	101.83	110.41
1	S	159	GLY	N-CA-C	6.96	123.64	113.48
1	A	22	HIS	N-CA-C	6.96	120.25	111.69
1	L	247	LYS	N-CA-C	-6.96	101.85	110.41
1	S	22	HIS	N-CA-C	6.95	120.24	111.69
1	M	218	ILE	N-CA-C	6.95	118.55	110.62
1	A	247	LYS	N-CA-C	-6.93	101.89	110.41
1	G	218	ILE	N-CA-C	6.93	118.52	110.62
1	C	218	ILE	N-CA-C	6.92	118.50	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	218	ILE	N-CA-C	6.91	118.50	110.62
1	Q	218	ILE	N-CA-C	6.90	118.48	110.62
1	T	22	HIS	N-CA-C	6.89	120.17	111.69
1	F	218	ILE	N-CA-C	6.88	118.46	110.62
1	P	218	ILE	N-CA-C	6.88	118.46	110.62
1	R	218	ILE	N-CA-C	6.87	118.45	110.62
1	X	247	LYS	N-CA-C	-6.87	101.96	110.41
1	C	22	HIS	N-CA-C	6.87	120.14	111.69
1	K	22	HIS	N-CA-C	6.85	120.11	111.69
1	K	218	ILE	N-CA-C	6.83	118.41	110.62
1	L	218	ILE	N-CA-C	6.82	118.40	110.62
1	P	22	HIS	N-CA-C	6.80	120.06	111.69
1	S	218	ILE	N-CA-C	6.78	118.35	110.62
1	A	218	ILE	N-CA-C	6.78	118.35	110.62
1	V	218	ILE	N-CA-C	6.78	118.35	110.62
1	F	22	HIS	N-CA-C	6.78	120.03	111.69
1	G	22	HIS	N-CA-C	6.78	120.02	111.69
1	B	218	ILE	N-CA-C	6.76	118.33	110.62
1	H	218	ILE	N-CA-C	6.74	118.31	110.62
1	N	22	HIS	N-CA-C	6.73	119.97	111.69
1	X	22	HIS	N-CA-C	6.71	119.95	111.69
1	U	218	ILE	N-CA-C	6.66	118.21	110.62
1	E	218	ILE	N-CA-C	6.62	118.17	110.62
1	V	22	HIS	N-CA-C	6.62	119.83	111.69
1	O	218	ILE	N-CA-C	6.61	118.16	110.62
1	J	218	ILE	N-CA-C	6.61	118.16	110.62
1	R	22	HIS	N-CA-C	6.60	119.81	111.69
1	X	218	ILE	N-CA-C	6.59	118.13	110.62
1	T	218	ILE	N-CA-C	6.58	118.12	110.62
1	B	22	HIS	N-CA-C	6.51	119.70	111.69
1	W	22	HIS	N-CA-C	6.51	119.69	111.69
1	E	22	HIS	N-CA-C	6.49	119.68	111.69
1	D	218	ILE	N-CA-C	6.39	117.91	110.62
1	E	6	ASP	N-CA-C	-6.39	99.85	108.86
1	K	6	ASP	N-CA-C	-6.31	99.74	109.14
1	N	6	ASP	N-CA-C	-6.27	100.02	108.86
1	C	6	ASP	N-CA-C	-6.22	99.87	109.14
1	X	6	ASP	N-CA-C	-6.21	99.97	109.41
1	T	6	ASP	N-CA-C	-6.16	99.96	109.14
1	E	252	SER	N-CA-C	6.15	121.06	113.50
1	J	6	ASP	N-CA-C	-6.11	100.03	109.14
1	P	252	SER	N-CA-C	6.10	121.01	113.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	6	ASP	N-CA-C	-6.09	100.07	109.14
1	A	6	ASP	N-CA-C	-6.09	100.07	109.14
1	P	6	ASP	N-CA-C	-6.08	100.08	109.14
1	R	252	SER	N-CA-C	6.07	120.97	113.50
1	B	6	ASP	N-CA-C	-6.07	100.09	109.14
1	C	252	SER	N-CA-C	6.07	120.97	113.50
1	R	6	ASP	N-CA-C	-6.07	100.31	108.86
1	J	252	SER	N-CA-C	6.04	120.93	113.50
1	K	252	SER	N-CA-C	6.04	120.92	113.50
1	X	249	ALA	N-CA-C	-6.03	104.83	111.82
1	I	249	ALA	N-CA-C	-6.02	104.84	111.82
1	D	249	ALA	N-CA-C	-6.01	104.85	111.82
1	I	6	ASP	N-CA-C	-6.00	100.19	109.14
1	M	6	ASP	N-CA-C	-6.00	100.40	108.86
1	N	252	SER	N-CA-C	5.99	120.87	113.50
1	V	6	ASP	N-CA-C	-5.99	100.21	109.14
1	U	249	ALA	N-CA-C	-5.97	104.89	111.82
1	F	79	GLY	N-CA-C	-5.95	108.00	115.08
1	L	6	ASP	N-CA-C	-5.95	100.37	109.41
1	A	249	ALA	N-CA-C	-5.94	104.93	111.82
1	O	6	ASP	N-CA-C	-5.93	100.30	109.14
1	L	249	ALA	N-CA-C	-5.92	104.96	111.82
1	G	6	ASP	N-CA-C	-5.91	100.33	109.14
1	T	79	GLY	N-CA-C	-5.91	108.04	115.08
1	S	6	ASP	N-CA-C	-5.91	100.33	109.14
1	A	79	GLY	N-CA-C	-5.90	108.06	115.08
1	B	252	SER	N-CA-C	5.90	120.75	113.50
1	U	79	GLY	N-CA-C	-5.89	108.07	115.08
1	G	252	SER	N-CA-C	5.87	120.72	113.50
1	F	6	ASP	N-CA-C	-5.85	100.42	109.14
1	H	79	GLY	N-CA-C	-5.85	108.12	115.08
1	D	79	GLY	N-CA-C	-5.85	108.12	115.08
1	W	6	ASP	N-CA-C	-5.84	100.43	109.14
1	R	79	GLY	N-CA-C	-5.84	108.13	115.08
1	S	79	GLY	N-CA-C	-5.84	108.13	115.08
1	H	249	ALA	N-CA-C	-5.83	105.06	111.82
1	U	6	ASP	N-CA-C	-5.83	100.55	109.41
1	V	79	GLY	N-CA-C	-5.81	108.17	115.08
1	M	79	GLY	N-CA-C	-5.80	108.18	115.08
1	K	79	GLY	N-CA-C	-5.80	108.18	115.08
1	W	252	SER	N-CA-C	5.78	120.61	113.50
1	I	79	GLY	N-CA-C	-5.77	108.21	115.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	79	GLY	N-CA-C	-5.76	108.23	115.08
1	G	79	GLY	N-CA-C	-5.75	108.24	115.08
1	Q	79	GLY	N-CA-C	-5.75	108.24	115.08
1	M	252	SER	N-CA-C	5.74	120.56	113.50
1	D	6	ASP	N-CA-C	-5.73	100.70	109.41
1	B	79	GLY	N-CA-C	-5.72	108.27	115.08
1	L	79	GLY	N-CA-C	-5.71	108.29	115.08
1	T	252	SER	N-CA-C	5.71	120.52	113.50
1	P	79	GLY	N-CA-C	-5.71	108.29	115.08
1	W	79	GLY	N-CA-C	-5.70	108.30	115.08
1	N	79	GLY	N-CA-C	-5.69	108.31	115.08
1	X	79	GLY	N-CA-C	-5.67	108.33	115.08
1	H	41	GLU	N-CA-C	5.65	122.84	110.80
1	C	79	GLY	N-CA-C	-5.65	108.36	115.08
1	V	159	GLY	N-CA-C	5.64	123.92	113.76
1	Q	252	SER	N-CA-C	5.63	120.43	113.50
1	H	6	ASP	N-CA-C	-5.61	100.89	109.41
1	M	159	GLY	N-CA-C	5.58	123.81	113.76
1	E	79	GLY	N-CA-C	-5.54	108.49	115.08
1	T	159	GLY	N-CA-C	5.51	123.69	113.76
1	O	79	GLY	N-CA-C	-5.51	108.52	115.08
1	N	159	GLY	N-CA-C	5.50	123.66	113.76
1	J	159	GLY	N-CA-C	5.49	123.64	113.76
1	A	41	GLU	N-CA-C	5.48	122.47	110.80
1	U	41	GLU	N-CA-C	5.46	122.44	110.80
1	D	41	GLU	N-CA-C	5.45	122.40	110.80
1	U	182	GLN	N-CA-C	5.44	120.80	113.72
1	L	41	GLU	N-CA-C	5.42	122.35	110.80
1	Q	159	GLY	N-CA-C	5.41	123.49	113.76
1	H	194	VAL	N-CA-C	-5.40	102.61	109.58
1	C	182	GLN	N-CA-C	5.39	121.61	114.12
1	F	159	GLY	N-CA-C	5.36	123.41	113.76
1	X	41	GLU	N-CA-C	5.35	122.19	110.80
1	D	182	GLN	N-CA-C	5.34	120.66	113.72
1	B	159	GLY	N-CA-C	5.34	123.37	113.76
1	U	194	VAL	N-CA-C	-5.34	102.69	109.58
1	D	239	ASP	N-CA-C	-5.33	105.62	113.61
1	A	194	VAL	N-CA-C	-5.32	102.72	109.58
1	N	182	GLN	N-CA-C	5.31	121.50	114.12
1	J	182	GLN	N-CA-C	5.30	121.48	114.12
1	L	255	THR	N-CA-C	-5.29	105.57	112.23
1	R	182	GLN	N-CA-C	5.28	121.45	114.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	239	ASP	N-CA-C	-5.27	105.71	113.61
1	I	41	GLU	N-CA-C	5.26	122.01	110.80
1	T	182	GLN	N-CA-C	5.26	121.44	114.12
1	L	43	GLY	N-CA-C	-5.26	108.45	115.40
1	L	239	ASP	N-CA-C	-5.26	105.72	113.61
1	H	182	GLN	N-CA-C	5.26	120.56	113.72
1	G	182	GLN	N-CA-C	5.26	121.43	114.12
1	A	191	LEU	N-CA-C	-5.25	104.25	111.81
1	D	110	SER	N-CA-C	-5.25	99.70	108.94
1	L	110	SER	N-CA-C	-5.25	99.70	108.94
1	H	110	SER	N-CA-C	-5.25	99.71	108.94
1	I	194	VAL	N-CA-C	-5.24	102.82	109.58
1	A	239	ASP	N-CA-C	-5.23	105.76	113.61
1	U	239	ASP	N-CA-C	-5.23	105.77	113.61
1	I	182	GLN	N-CA-C	5.21	120.49	113.72
1	X	239	ASP	N-CA-C	-5.21	105.80	113.61
1	I	110	SER	N-CA-C	-5.20	99.78	108.94
1	Q	188	ILE	CA-C-N	-5.20	116.08	122.84
1	Q	188	ILE	C-N-CA	-5.20	116.08	122.84
1	A	182	GLN	N-CA-C	5.19	120.47	113.72
1	X	110	SER	N-CA-C	-5.18	99.83	108.94
1	F	123	SER	N-CA-C	-5.17	103.21	110.35
1	F	182	GLN	N-CA-C	5.17	121.31	114.12
1	A	43	GLY	N-CA-C	-5.16	108.58	115.40
1	H	239	ASP	N-CA-C	-5.16	105.87	113.61
1	X	123	SER	N-CA-C	-5.14	103.25	110.35
1	G	188	ILE	CA-C-N	-5.14	116.16	122.84
1	G	188	ILE	C-N-CA	-5.14	116.16	122.84
1	N	188	ILE	CA-C-N	-5.13	116.17	122.84
1	N	188	ILE	C-N-CA	-5.13	116.17	122.84
1	O	252	SER	N-CA-C	5.13	120.54	113.97
1	Q	182	GLN	N-CA-C	5.13	121.25	114.12
1	D	43	GLY	N-CA-C	-5.12	108.64	115.40
1	D	191	LEU	N-CA-C	-5.11	104.45	111.81
1	B	188	ILE	CA-C-N	-5.11	116.20	122.84
1	B	188	ILE	C-N-CA	-5.11	116.20	122.84
1	U	110	SER	N-CA-C	-5.10	99.97	108.94
1	S	252	SER	N-CA-C	5.06	120.30	113.72
1	V	252	SER	N-CA-C	5.06	120.44	113.97
1	I	43	GLY	N-CA-C	-5.05	108.74	115.40
1	S	182	GLN	N-CA-C	5.03	121.11	114.12
1	B	182	GLN	N-CA-C	5.03	121.11	114.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	U	250	SER	N-CA-C	-5.03	105.27	111.40
1	I	250	SER	N-CA-C	-5.03	105.27	111.40
1	N	110	SER	N-CA-C	-5.03	100.09	108.94
1	L	250	SER	N-CA-C	-5.02	105.27	111.40
1	I	191	LEU	N-CA-C	-5.02	104.58	111.81
1	E	255	THR	N-CA-C	-5.02	105.52	111.69
1	X	43	GLY	N-CA-C	-5.01	108.78	115.40
1	P	188	ILE	CA-C-N	-5.00	116.34	122.84
1	P	188	ILE	C-N-CA	-5.00	116.34	122.84
1	X	158	PHE	N-CA-C	5.00	116.65	108.55

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	2171	0	2147	76	0
1	B	2288	0	2271	77	0
1	C	2288	0	2266	82	0
1	D	2171	0	2147	77	1
1	E	2289	0	2271	81	1
1	F	2289	0	2271	85	0
1	G	2289	0	2271	68	0
1	H	2171	0	2147	81	1
1	I	2171	0	2147	87	0
1	J	2289	0	2271	67	0
1	K	2289	0	2271	82	0
1	L	2171	0	2147	73	0
1	M	2289	0	2271	100	0
1	N	2289	0	2271	92	1
1	O	2289	0	2271	93	0
1	P	2289	0	2271	94	0
1	Q	2289	0	2271	91	0
1	R	2289	0	2271	88	0
1	S	2289	0	2271	81	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	T	2289	0	2271	84	0
1	U	2171	0	2147	84	0
1	V	2289	0	2271	79	0
1	W	2289	0	2271	91	1
1	X	2171	0	2147	81	1
2	A	110	0	0	6	0
2	B	119	0	0	5	0
2	C	129	0	0	3	0
2	D	145	0	0	4	0
2	E	143	0	0	11	0
2	F	151	0	0	9	0
2	G	101	0	0	1	0
2	H	178	0	0	9	0
2	I	193	0	0	11	0
2	J	159	0	0	2	0
2	K	122	0	0	2	0
2	L	93	0	0	4	0
2	M	169	0	0	12	0
2	N	202	0	0	5	0
2	O	144	0	0	6	0
2	P	103	0	0	8	0
2	Q	93	0	0	6	0
2	R	110	0	0	3	0
2	S	146	0	0	8	0
2	T	88	0	0	4	0
2	U	73	0	0	7	0
2	V	118	0	0	5	0
2	W	120	0	0	7	0
2	X	153	0	0	7	0
All	All	57270	0	53631	1805	3

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 17.

All (1805) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:39:SER:HA	1:M:115:GLU:CD	1.56	1.31
1:I:39:SER:HA	1:M:115:GLU:OE2	1.15	1.28
1:S:251:ARG:HD2	1:T:236:THR:HG23	1.27	1.15
1:K:251:ARG:HD2	1:L:236:THR:HG23	1.14	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:251:ARG:HD2	1:U:236:THR:HG23	1.15	1.13
1:G:251:ARG:HD2	1:H:236:THR:HG23	1.30	1.10
1:M:237:SER:HB3	1:M:242:ILE:HD11	1.34	1.09
1:O:237:SER:HB3	1:O:242:ILE:HD11	1.34	1.09
1:B:251:ARG:HD2	1:C:236:THR:HG23	1.26	1.09
1:M:236:THR:HG23	1:R:251:ARG:HD2	1.18	1.09
1:S:237:SER:HB3	1:S:242:ILE:HD11	1.33	1.09
1:K:237:SER:HB3	1:K:242:ILE:HD11	1.34	1.08
1:C:237:SER:HB3	1:C:242:ILE:HD11	1.35	1.08
1:J:251:ARG:HD2	1:K:236:THR:HG23	1.35	1.08
1:Q:237:SER:HB3	1:Q:242:ILE:HD11	1.34	1.08
1:W:237:SER:HB3	1:W:242:ILE:HD11	1.34	1.08
1:E:237:SER:HB3	1:E:242:ILE:HD11	1.35	1.08
1:V:251:ARG:HD2	1:W:236:THR:HG23	1.23	1.08
1:G:237:SER:HB3	1:G:242:ILE:HD11	1.35	1.07
1:B:237:SER:HB3	1:B:242:ILE:HD11	1.36	1.07
1:O:251:ARG:HD2	1:P:236:THR:HG23	1.30	1.07
1:C:251:ARG:HD2	1:D:236:THR:HG23	1.36	1.06
1:J:237:SER:HB3	1:J:242:ILE:HD11	1.34	1.06
1:M:251:ARG:HD2	1:N:236:THR:CG2	1.84	1.06
1:F:237:SER:HB3	1:F:242:ILE:HD11	1.33	1.06
1:W:251:ARG:HD2	1:X:236:THR:HG23	1.09	1.06
1:E:251:ARG:HD2	1:F:236:THR:HG23	1.10	1.05
1:M:251:ARG:CD	1:N:236:THR:HG23	1.85	1.05
1:V:237:SER:HB3	1:V:242:ILE:HD11	1.34	1.05
1:Q:251:ARG:HD2	1:R:236:THR:HG23	1.09	1.04
1:N:237:SER:HB3	1:N:242:ILE:HD11	1.34	1.04
1:T:237:SER:HB3	1:T:242:ILE:HD11	1.34	1.04
1:P:237:SER:HB3	1:P:242:ILE:HD11	1.34	1.04
1:M:115:GLU:HG2	2:M:2068:HOH:O	1.57	1.03
1:R:237:SER:HB3	1:R:242:ILE:HD11	1.34	1.03
1:I:39:SER:CA	1:M:115:GLU:OE2	2.09	1.00
1:A:236:THR:HG23	1:F:251:ARG:HD2	1.43	1.00
1:N:251:ARG:HD2	1:O:236:THR:HG23	1.02	0.99
1:P:247:LYS:HA	2:P:2103:HOH:O	1.62	0.99
1:P:251:ARG:HD2	1:Q:236:THR:CG2	1.92	0.99
1:P:251:ARG:HD2	1:Q:236:THR:HG23	1.00	0.99
1:P:251:ARG:CD	1:Q:236:THR:HG23	1.93	0.98
1:M:251:ARG:HD2	1:N:236:THR:HG23	0.96	0.95
1:N:251:ARG:HD2	1:O:236:THR:CG2	1.96	0.95
1:E:251:ARG:HD2	1:F:236:THR:CG2	1.98	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:39:SER:CA	1:M:115:GLU:CD	2.41	0.94
1:E:251:ARG:CD	1:F:236:THR:HG23	1.98	0.93
1:N:251:ARG:CD	1:O:236:THR:HG23	1.97	0.92
1:W:251:ARG:HD2	1:X:236:THR:CG2	2.01	0.89
1:W:251:ARG:CD	1:X:236:THR:HG23	2.01	0.89
1:P:250:SER:HB2	2:P:2103:HOH:O	1.73	0.88
1:O:195:ILE:HD11	1:O:215:LEU:HD13	1.57	0.87
1:Q:195:ILE:HD11	1:Q:215:LEU:HD13	1.57	0.86
1:I:39:SER:CA	1:M:115:GLU:OE1	2.23	0.86
1:J:195:ILE:HD11	1:J:215:LEU:HD13	1.58	0.86
1:I:41:GLU:HG2	2:M:2024:HOH:O	1.75	0.86
1:B:195:ILE:HD11	1:B:215:LEU:HD13	1.58	0.85
1:F:195:ILE:HD11	1:F:215:LEU:HD13	1.57	0.85
1:P:195:ILE:HD11	1:P:215:LEU:HD13	1.59	0.85
1:V:195:ILE:HD11	1:V:215:LEU:HD13	1.58	0.85
1:W:81:VAL:HB	2:W:2032:HOH:O	1.76	0.85
1:Q:251:ARG:HD2	1:R:236:THR:CG2	2.02	0.85
1:R:195:ILE:HD11	1:R:215:LEU:HD13	1.58	0.85
1:C:1:MET:CG	1:C:1:MET:CA	2.55	0.84
1:N:310:LYS:HE3	2:O:2066:HOH:O	1.77	0.84
1:I:131:LYS:HB2	1:I:243:VAL:HG11	1.60	0.84
1:E:195:ILE:HD11	1:E:215:LEU:HD13	1.57	0.84
1:N:195:ILE:HD11	1:N:215:LEU:HD13	1.60	0.84
1:W:195:ILE:HD11	1:W:215:LEU:HD13	1.59	0.84
1:S:251:ARG:HD2	1:T:236:THR:CG2	2.07	0.83
1:K:251:ARG:HD2	1:L:236:THR:CG2	2.04	0.83
1:D:131:LYS:HB2	1:D:243:VAL:HG11	1.60	0.83
1:G:195:ILE:HD11	1:G:215:LEU:HD13	1.58	0.83
1:H:131:LYS:HB2	1:H:243:VAL:HG11	1.60	0.83
1:K:251:ARG:CD	1:L:236:THR:HG23	2.04	0.83
1:X:131:LYS:HB2	1:X:243:VAL:HG11	1.60	0.83
1:S:195:ILE:HD11	1:S:215:LEU:HD13	1.59	0.83
1:T:195:ILE:HD11	1:T:215:LEU:HD13	1.60	0.83
1:K:195:ILE:HD11	1:K:215:LEU:HD13	1.59	0.83
1:M:236:THR:CG2	1:R:251:ARG:HD2	2.07	0.83
1:I:39:SER:CB	1:M:115:GLU:OE1	2.28	0.82
1:L:131:LYS:HB2	1:L:243:VAL:HG11	1.60	0.82
1:A:194:VAL:HG22	1:A:195:ILE:HG13	1.61	0.82
1:C:195:ILE:HD11	1:C:215:LEU:HD13	1.58	0.82
1:M:195:ILE:HD11	1:M:215:LEU:HD13	1.60	0.82
1:D:194:VAL:HG22	1:D:195:ILE:HG13	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:251:ARG:CD	1:T:236:THR:HG23	2.08	0.81
1:X:194:VAL:HG22	1:X:195:ILE:HG13	1.62	0.81
1:A:131:LYS:HB2	1:A:243:VAL:HG11	1.60	0.81
1:H:194:VAL:HG22	1:H:195:ILE:HG13	1.62	0.80
1:T:251:ARG:CD	1:U:236:THR:HG23	2.05	0.80
1:U:131:LYS:HB2	1:U:243:VAL:HG11	1.60	0.80
1:I:194:VAL:HG22	1:I:195:ILE:HG13	1.63	0.80
1:C:194:VAL:HG22	1:C:195:ILE:HG13	1.64	0.80
1:J:92:LYS:HE3	1:J:92:LYS:HA	1.64	0.80
1:S:92:LYS:HA	1:S:92:LYS:HE3	1.64	0.80
1:I:39:SER:HA	1:M:115:GLU:OE1	1.82	0.80
1:U:194:VAL:HG22	1:U:195:ILE:HG13	1.62	0.79
1:N:92:LYS:HA	1:N:92:LYS:HE3	1.65	0.79
1:T:251:ARG:HD2	1:U:236:THR:CG2	2.05	0.79
1:F:194:VAL:HG22	1:F:195:ILE:HG13	1.65	0.79
1:M:194:VAL:HG22	1:M:195:ILE:HG13	1.64	0.79
1:N:194:VAL:HG22	1:N:195:ILE:HG13	1.65	0.79
1:T:92:LYS:HA	1:T:92:LYS:HE3	1.65	0.79
1:E:92:LYS:HA	1:E:92:LYS:HE3	1.65	0.79
1:W:92:LYS:HA	1:W:92:LYS:HE3	1.65	0.79
1:F:92:LYS:HA	1:F:92:LYS:HE3	1.65	0.78
1:O:92:LYS:HA	1:O:92:LYS:HE3	1.65	0.78
1:P:92:LYS:HA	1:P:92:LYS:HE3	1.65	0.78
1:P:194:VAL:HG22	1:P:195:ILE:HG13	1.65	0.78
1:M:92:LYS:HA	1:M:92:LYS:HE3	1.65	0.78
1:K:194:VAL:HG22	1:K:195:ILE:HG13	1.65	0.78
1:L:194:VAL:HG22	1:L:195:ILE:HG13	1.62	0.78
1:T:194:VAL:HG22	1:T:195:ILE:HG13	1.65	0.78
1:J:194:VAL:HG22	1:J:195:ILE:HG13	1.66	0.78
1:N:251:ARG:HH11	1:O:236:THR:HG22	1.48	0.78
1:V:194:VAL:HG22	1:V:195:ILE:HG13	1.66	0.78
1:G:92:LYS:HA	1:G:92:LYS:HE3	1.65	0.78
1:Q:251:ARG:CD	1:R:236:THR:HG23	2.02	0.78
1:W:194:VAL:HG22	1:W:195:ILE:HG13	1.65	0.78
1:Q:92:LYS:HA	1:Q:92:LYS:HE3	1.66	0.78
1:V:92:LYS:HA	1:V:92:LYS:HE3	1.66	0.78
1:B:194:VAL:HG22	1:B:195:ILE:HG13	1.66	0.78
1:C:92:LYS:HA	1:C:92:LYS:HE3	1.65	0.78
1:G:194:VAL:HG22	1:G:195:ILE:HG13	1.66	0.78
1:R:92:LYS:HE3	1:R:92:LYS:HA	1.66	0.77
1:R:194:VAL:HG22	1:R:195:ILE:HG13	1.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:194:VAL:HG22	1:O:195:ILE:HG13	1.65	0.77
1:Q:194:VAL:HG22	1:Q:195:ILE:HG13	1.65	0.77
1:X:157:ARG:HA	2:X:2102:HOH:O	1.82	0.77
1:B:92:LYS:HE3	1:B:92:LYS:HA	1.65	0.77
1:E:194:VAL:HG22	1:E:195:ILE:HG13	1.66	0.77
1:S:194:VAL:HG22	1:S:195:ILE:HG13	1.65	0.77
1:O:135:GLY:HA2	2:O:2066:HOH:O	1.85	0.77
1:N:251:ARG:HH11	1:O:236:THR:CG2	1.99	0.76
1:K:92:LYS:HA	1:K:92:LYS:HE3	1.66	0.76
1:M:236:THR:HG23	1:R:251:ARG:CD	2.08	0.75
1:R:191:LEU:O	1:R:194:VAL:HG13	1.85	0.75
1:I:39:SER:HB3	1:M:115:GLU:OE1	1.86	0.75
1:F:259:ILE:HD13	1:F:316:ILE:HG23	1.69	0.75
1:W:248:GLU:OE1	1:X:236:THR:HG22	1.88	0.74
1:P:251:ARG:HH11	1:Q:236:THR:HG22	1.53	0.74
1:K:259:ILE:HD13	1:K:316:ILE:HG23	1.70	0.74
1:B:259:ILE:HD13	1:B:316:ILE:HG23	1.70	0.74
1:E:259:ILE:HD13	1:E:316:ILE:HG23	1.69	0.74
1:P:191:LEU:O	1:P:194:VAL:HG13	1.88	0.74
1:G:259:ILE:HD13	1:G:316:ILE:HG23	1.69	0.74
1:N:310:LYS:HD2	1:O:132:GLY:O	1.86	0.74
1:S:259:ILE:HD13	1:S:316:ILE:HG23	1.69	0.74
1:F:191:LEU:O	1:F:194:VAL:HG13	1.88	0.73
1:N:259:ILE:HD13	1:N:316:ILE:HG23	1.70	0.73
1:C:259:ILE:HD13	1:C:316:ILE:HG23	1.70	0.73
1:G:191:LEU:O	1:G:194:VAL:HG13	1.89	0.73
1:R:259:ILE:HD13	1:R:316:ILE:HG23	1.70	0.73
1:M:251:ARG:HH11	1:N:236:THR:HG22	1.54	0.73
1:O:191:LEU:O	1:O:194:VAL:HG13	1.89	0.73
1:Q:259:ILE:HD13	1:Q:316:ILE:HG23	1.70	0.72
1:W:314:THR:HG21	1:X:239:ASP:CG	2.14	0.72
1:P:259:ILE:HD13	1:P:316:ILE:HG23	1.70	0.72
1:C:191:LEU:O	1:C:194:VAL:HG13	1.89	0.72
1:H:195:ILE:HA	2:H:2132:HOH:O	1.87	0.72
1:N:191:LEU:O	1:N:194:VAL:HG13	1.89	0.72
1:E:61:LYS:HE2	2:E:2030:HOH:O	1.89	0.72
1:J:259:ILE:HD13	1:J:316:ILE:HG23	1.69	0.72
1:Q:251:ARG:HH11	1:R:236:THR:CG2	2.03	0.72
1:V:191:LEU:O	1:V:194:VAL:HG13	1.90	0.72
1:V:259:ILE:HD13	1:V:316:ILE:HG23	1.71	0.72
1:W:259:ILE:HD13	1:W:316:ILE:HG23	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:314:THR:HG21	1:L:239:ASP:CG	2.13	0.72
1:R:34:SER:O	1:R:38:GLU:HG3	1.90	0.72
1:M:259:ILE:HD13	1:M:316:ILE:HG23	1.70	0.72
1:Q:191:LEU:O	1:Q:194:VAL:HG13	1.89	0.72
1:J:191:LEU:O	1:J:194:VAL:HG13	1.90	0.72
1:O:259:ILE:HD13	1:O:316:ILE:HG23	1.69	0.72
1:V:251:ARG:HD2	1:W:236:THR:CG2	2.11	0.72
1:X:189:ASP:HB3	2:X:2102:HOH:O	1.90	0.71
1:E:191:LEU:O	1:E:194:VAL:HG13	1.88	0.71
1:T:248:GLU:OE1	1:U:236:THR:HG22	1.89	0.71
1:T:259:ILE:HD13	1:T:316:ILE:HG23	1.71	0.71
1:W:191:LEU:O	1:W:194:VAL:HG13	1.90	0.71
1:G:251:ARG:CD	1:H:236:THR:HG23	2.15	0.71
1:Q:34:SER:O	1:Q:38:GLU:HG3	1.91	0.71
1:K:252:SER:OG	1:L:236:THR:HG21	1.89	0.70
1:U:34:SER:O	1:U:38:GLU:HG3	1.91	0.70
1:G:251:ARG:HD2	1:H:236:THR:CG2	2.15	0.70
1:N:8:LYS:HD2	2:N:2007:HOH:O	1.91	0.70
1:V:251:ARG:CD	1:W:236:THR:HG23	2.12	0.70
1:T:191:LEU:O	1:T:194:VAL:HG13	1.91	0.70
1:K:191:LEU:O	1:K:194:VAL:HG13	1.90	0.70
1:Q:251:ARG:HH11	1:R:236:THR:HG22	1.57	0.70
1:D:240:ASP:C	1:D:242:ILE:H	2.00	0.70
1:J:195:ILE:HG12	1:J:215:LEU:HD22	1.74	0.70
1:M:191:LEU:O	1:M:194:VAL:HG13	1.91	0.70
1:C:248:GLU:OE1	1:D:236:THR:HG22	1.92	0.69
1:I:192:LYS:NZ	1:I:192:LYS:HB3	2.07	0.69
1:G:34:SER:O	1:G:38:GLU:HG3	1.93	0.69
1:S:191:LEU:O	1:S:194:VAL:HG13	1.91	0.69
1:U:240:ASP:C	1:U:242:ILE:H	2.00	0.69
1:B:191:LEU:O	1:B:194:VAL:HG13	1.91	0.69
1:A:195:ILE:HA	2:A:2079:HOH:O	1.93	0.69
1:E:195:ILE:HG12	1:E:215:LEU:HD22	1.75	0.69
1:F:195:ILE:HG12	1:F:215:LEU:HD22	1.73	0.69
1:P:195:ILE:HG12	1:P:215:LEU:HD22	1.74	0.69
1:Q:195:ILE:HG12	1:Q:215:LEU:HD22	1.74	0.69
1:X:240:ASP:C	1:X:242:ILE:H	2.00	0.69
1:H:192:LYS:HB2	2:H:2127:HOH:O	1.90	0.69
1:I:72:LYS:HE2	2:M:2021:HOH:O	1.92	0.69
1:I:192:LYS:HB2	2:I:2130:HOH:O	1.93	0.69
1:K:248:GLU:OE1	1:L:236:THR:HG22	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:314:THR:HG21	1:U:239:ASP:CG	2.18	0.69
1:U:192:LYS:NZ	1:U:192:LYS:HB3	2.08	0.69
1:H:192:LYS:NZ	1:H:192:LYS:HB3	2.08	0.69
1:L:34:SER:O	1:L:38:GLU:HG3	1.92	0.69
1:P:251:ARG:HH11	1:Q:236:THR:CG2	2.06	0.69
1:X:34:SER:O	1:X:38:GLU:HG3	1.92	0.69
1:K:249:ALA:HA	1:K:253:ASN:HD22	1.58	0.69
1:O:195:ILE:HG12	1:O:215:LEU:HD22	1.74	0.69
1:T:34:SER:O	1:T:38:GLU:HG3	1.93	0.69
1:A:240:ASP:C	1:A:242:ILE:H	2.01	0.68
1:X:192:LYS:NZ	1:X:192:LYS:HB3	2.08	0.68
1:B:207:ILE:HD13	2:B:2079:HOH:O	1.91	0.68
1:E:34:SER:O	1:E:38:GLU:HG3	1.94	0.68
1:L:192:LYS:NZ	1:L:192:LYS:HB3	2.09	0.68
1:M:249:ALA:HA	1:M:253:ASN:HD22	1.59	0.68
1:P:184:ARG:HD3	2:P:2051:HOH:O	1.91	0.68
1:O:251:ARG:HD2	1:P:236:THR:CG2	2.14	0.68
1:D:192:LYS:HB3	1:D:192:LYS:NZ	2.08	0.68
1:H:240:ASP:C	1:H:242:ILE:H	2.00	0.68
1:J:251:ARG:HD2	1:K:236:THR:CG2	2.20	0.68
1:K:314:THR:HG21	1:L:239:ASP:CB	2.24	0.68
1:L:240:ASP:C	1:L:242:ILE:H	2.00	0.68
1:U:107:VAL:HA	2:U:2027:HOH:O	1.93	0.68
1:J:239:ASP:OD2	1:J:241:LYS:HG2	1.93	0.68
1:P:34:SER:O	1:P:38:GLU:HG3	1.93	0.68
1:C:249:ALA:HA	1:C:253:ASN:HD22	1.59	0.68
1:I:240:ASP:C	1:I:242:ILE:H	2.01	0.68
1:M:195:ILE:HG12	1:M:215:LEU:HD22	1.75	0.68
1:O:34:SER:O	1:O:38:GLU:HG3	1.94	0.68
1:B:195:ILE:HG12	1:B:215:LEU:HD22	1.76	0.68
1:E:251:ARG:HH11	1:F:236:THR:CG2	2.05	0.68
1:F:239:ASP:OD2	1:F:241:LYS:HG2	1.94	0.68
1:N:239:ASP:OD2	1:N:241:LYS:HG2	1.94	0.68
1:B:34:SER:O	1:B:38:GLU:HG3	1.93	0.68
1:I:195:ILE:HD11	1:I:215:LEU:HD13	1.75	0.68
1:K:195:ILE:HG12	1:K:215:LEU:HD22	1.75	0.68
1:O:251:ARG:CD	1:P:236:THR:HG23	2.15	0.68
1:V:239:ASP:OD2	1:V:241:LYS:HG2	1.94	0.68
1:W:239:ASP:OD2	1:W:241:LYS:HG2	1.94	0.68
1:B:239:ASP:OD2	1:B:241:LYS:HG2	1.94	0.68
1:F:249:ALA:HA	1:F:253:ASN:HD22	1.59	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:249:ALA:HA	1:R:253:ASN:HD22	1.59	0.68
1:S:239:ASP:OD2	1:S:241:LYS:HG2	1.93	0.67
1:F:34:SER:O	1:F:38:GLU:HG3	1.94	0.67
1:M:239:ASP:OD2	1:M:241:LYS:HG2	1.95	0.67
1:T:252:SER:OG	1:U:236:THR:HG21	1.95	0.67
1:W:195:ILE:HG12	1:W:215:LEU:HD22	1.75	0.67
1:C:34:SER:O	1:C:38:GLU:HG3	1.94	0.67
1:N:195:ILE:HG12	1:N:215:LEU:HD22	1.76	0.67
1:S:195:ILE:HG12	1:S:215:LEU:HD22	1.75	0.67
1:W:314:THR:HG21	1:X:239:ASP:CB	2.25	0.67
1:C:239:ASP:OD2	1:C:241:LYS:HG2	1.95	0.67
1:E:61:LYS:CE	2:E:2030:HOH:O	2.41	0.67
1:J:251:ARG:CD	1:K:236:THR:HG23	2.21	0.67
1:K:34:SER:O	1:K:38:GLU:HG3	1.94	0.67
1:Q:239:ASP:OD2	1:Q:241:LYS:HG2	1.94	0.67
1:S:249:ALA:HA	1:S:253:ASN:HD22	1.60	0.67
1:V:34:SER:O	1:V:38:GLU:HG3	1.93	0.67
1:W:252:SER:OG	1:X:236:THR:HG21	1.94	0.67
1:E:239:ASP:OD2	1:E:241:LYS:HG2	1.94	0.67
1:I:41:GLU:CD	1:M:22:HIS:HB3	2.20	0.67
1:Q:249:ALA:HA	1:Q:253:ASN:HD22	1.60	0.67
1:T:239:ASP:OD2	1:T:241:LYS:HG2	1.94	0.67
1:I:34:SER:O	1:I:38:GLU:HG3	1.95	0.67
1:N:34:SER:O	1:N:38:GLU:HG3	1.94	0.67
1:R:239:ASP:OD2	1:R:241:LYS:HG2	1.94	0.67
1:G:195:ILE:HG12	1:G:215:LEU:HD22	1.75	0.67
1:R:195:ILE:HG12	1:R:215:LEU:HD22	1.74	0.67
1:C:195:ILE:HG12	1:C:215:LEU:HD22	1.76	0.67
1:K:239:ASP:OD2	1:K:241:LYS:HG2	1.95	0.66
1:M:34:SER:O	1:M:38:GLU:HG3	1.95	0.66
1:O:239:ASP:OD2	1:O:241:LYS:HG2	1.94	0.66
1:G:239:ASP:OD2	1:G:241:LYS:HG2	1.94	0.66
1:P:239:ASP:OD2	1:P:241:LYS:HG2	1.95	0.66
1:U:192:LYS:HB2	2:U:2045:HOH:O	1.94	0.66
1:W:34:SER:O	1:W:38:GLU:HG3	1.95	0.66
1:W:73:SER:HB3	2:W:2032:HOH:O	1.93	0.66
1:A:192:LYS:NZ	1:A:192:LYS:HB3	2.10	0.66
1:E:249:ALA:HA	1:E:253:ASN:HD22	1.59	0.66
1:P:249:ALA:HA	1:P:253:ASN:HD22	1.59	0.66
1:B:251:ARG:HD2	1:C:236:THR:CG2	2.15	0.66
1:L:195:ILE:HD11	1:L:215:LEU:HD13	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:195:ILE:HG12	1:V:215:LEU:HD22	1.75	0.66
1:A:195:ILE:HD11	1:A:215:LEU:HD13	1.77	0.66
1:D:195:ILE:HD11	1:D:215:LEU:HD13	1.76	0.66
1:H:34:SER:O	1:H:38:GLU:HG3	1.96	0.66
1:Q:310:LYS:HD2	1:R:132:GLY:O	1.96	0.66
1:T:195:ILE:HG12	1:T:215:LEU:HD22	1.76	0.66
1:A:34:SER:O	1:A:38:GLU:HG3	1.95	0.66
1:D:195:ILE:HB	2:D:2102:HOH:O	1.96	0.66
1:U:195:ILE:HD11	1:U:215:LEU:HD13	1.77	0.66
1:Q:40:VAL:CG1	1:Q:44:THR:HB	2.26	0.66
1:V:249:ALA:HA	1:V:253:ASN:HD22	1.61	0.66
1:W:40:VAL:CG1	1:W:44:THR:HB	2.26	0.66
1:E:115:GLU:HG2	2:E:2055:HOH:O	1.97	0.65
1:J:34:SER:O	1:J:38:GLU:HG3	1.96	0.65
1:J:40:VAL:CG1	1:J:44:THR:HB	2.26	0.65
1:J:249:ALA:HA	1:J:253:ASN:HD22	1.60	0.65
1:L:172:PHE:CZ	1:L:176:ILE:HD11	2.31	0.65
1:H:195:ILE:HD11	1:H:215:LEU:HD13	1.77	0.65
1:I:41:GLU:HG3	2:M:2023:HOH:O	1.95	0.65
1:D:172:PHE:CZ	1:D:176:ILE:HD11	2.31	0.65
1:D:34:SER:O	1:D:38:GLU:HG3	1.96	0.65
1:D:247:LYS:HB2	1:D:247:LYS:NZ	2.12	0.65
1:O:249:ALA:HA	1:O:253:ASN:HD22	1.61	0.65
1:T:40:VAL:CG1	1:T:44:THR:HB	2.26	0.65
1:X:195:ILE:HD11	1:X:215:LEU:HD13	1.78	0.65
1:A:92:LYS:HA	1:A:92:LYS:HE3	1.79	0.65
1:D:92:LYS:HA	1:D:92:LYS:HE3	1.78	0.65
1:M:251:ARG:HH11	1:N:236:THR:CG2	2.09	0.65
1:N:249:ALA:HA	1:N:253:ASN:HD22	1.60	0.65
1:O:40:VAL:CG1	1:O:44:THR:HB	2.27	0.65
1:U:172:PHE:CZ	1:U:176:ILE:HD11	2.31	0.65
1:K:40:VAL:CG1	1:K:44:THR:HB	2.26	0.65
1:B:40:VAL:CG1	1:B:44:THR:HB	2.27	0.64
1:U:192:LYS:HA	2:U:2054:HOH:O	1.96	0.64
1:B:249:ALA:HA	1:B:253:ASN:HD22	1.62	0.64
1:E:40:VAL:CG1	1:E:44:THR:HB	2.27	0.64
1:E:251:ARG:HH11	1:F:236:THR:HG22	1.61	0.64
1:E:252:SER:HB3	1:F:192:LYS:HE3	1.79	0.64
1:N:251:ARG:HB2	1:N:317:LYS:HE2	1.79	0.64
1:P:40:VAL:CG1	1:P:44:THR:HB	2.27	0.64
1:C:252:SER:OG	1:D:236:THR:HG21	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:246:VAL:HA	2:L:2071:HOH:O	1.96	0.64
1:R:40:VAL:CG1	1:R:44:THR:HB	2.28	0.64
1:L:92:LYS:HA	1:L:92:LYS:HE3	1.79	0.64
1:O:251:ARG:HB2	1:O:317:LYS:HE2	1.79	0.64
1:V:251:ARG:HB2	1:V:317:LYS:HE2	1.80	0.64
1:W:249:ALA:HA	1:W:253:ASN:HD22	1.63	0.64
1:X:172:PHE:CZ	1:X:176:ILE:HD11	2.32	0.64
1:S:34:SER:O	1:S:38:GLU:HG3	1.98	0.64
1:T:67:VAL:HG12	2:T:2020:HOH:O	1.97	0.64
1:A:172:PHE:CZ	1:A:176:ILE:HD11	2.33	0.64
1:C:195:ILE:HG22	1:C:195:ILE:O	1.98	0.64
1:F:195:ILE:HG22	1:F:195:ILE:O	1.97	0.64
1:M:40:VAL:CG1	1:M:44:THR:HB	2.27	0.64
1:T:251:ARG:HB2	1:T:317:LYS:HE2	1.80	0.64
1:A:247:LYS:HB2	1:A:247:LYS:NZ	2.13	0.64
1:H:247:LYS:HB2	1:H:247:LYS:NZ	2.13	0.64
1:I:247:LYS:NZ	1:I:247:LYS:HB2	2.13	0.64
1:K:251:ARG:HB2	1:K:317:LYS:HE2	1.80	0.64
1:P:216:SER:HB2	2:P:2070:HOH:O	1.98	0.64
1:S:195:ILE:HG22	1:S:195:ILE:O	1.98	0.64
1:C:40:VAL:CG1	1:C:44:THR:HB	2.27	0.64
1:H:172:PHE:CZ	1:H:176:ILE:HD11	2.32	0.64
1:N:248:GLU:OE1	1:O:236:THR:HG22	1.98	0.64
1:U:92:LYS:HA	1:U:92:LYS:HE3	1.79	0.64
1:E:252:SER:HB3	1:F:192:LYS:CE	2.28	0.64
1:G:172:PHE:CZ	1:G:176:ILE:HD11	2.33	0.64
1:H:92:LYS:HA	1:H:92:LYS:HE3	1.80	0.64
1:K:195:ILE:HG22	1:K:195:ILE:O	1.98	0.64
1:L:41:GLU:O	1:L:42:ASP:HB2	1.98	0.64
1:O:195:ILE:O	1:O:195:ILE:HG22	1.97	0.64
1:E:195:ILE:O	1:E:195:ILE:HG22	1.98	0.63
1:H:192:LYS:HB3	1:H:192:LYS:HZ3	1.63	0.63
1:I:92:LYS:HA	1:I:92:LYS:HE3	1.79	0.63
1:M:195:ILE:O	1:M:195:ILE:HG22	1.98	0.63
1:W:195:ILE:O	1:W:195:ILE:HG22	1.98	0.63
1:A:41:GLU:O	1:A:42:ASP:HB2	1.98	0.63
1:P:310:LYS:HD2	1:Q:132:GLY:O	1.98	0.63
1:G:249:ALA:HA	1:G:253:ASN:HD22	1.62	0.63
1:I:192:LYS:O	1:I:194:VAL:N	2.30	0.63
1:L:192:LYS:HB3	1:L:192:LYS:HZ2	1.63	0.63
1:Q:195:ILE:HG22	1:Q:195:ILE:O	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:92:LYS:HA	1:X:92:LYS:HE3	1.79	0.63
1:B:251:ARG:CD	1:C:236:THR:HG23	2.16	0.63
1:G:40:VAL:CG1	1:G:44:THR:HB	2.28	0.63
1:P:172:PHE:CZ	1:P:176:ILE:HD11	2.33	0.63
1:N:195:ILE:HG22	1:N:195:ILE:O	1.98	0.63
1:V:195:ILE:HG22	1:V:195:ILE:O	1.98	0.63
1:F:43:GLY:HA2	2:F:2041:HOH:O	1.98	0.63
1:L:247:LYS:HB2	1:L:247:LYS:NZ	2.13	0.63
1:Q:251:ARG:HB2	1:Q:317:LYS:HE2	1.81	0.63
1:V:172:PHE:CZ	1:V:176:ILE:HD11	2.33	0.63
1:H:41:GLU:O	1:H:42:ASP:HB2	1.98	0.63
1:T:195:ILE:O	1:T:195:ILE:HG22	1.99	0.63
1:T:244:GLU:HG2	1:U:238:ASN:HD21	1.64	0.63
1:U:247:LYS:HB2	1:U:247:LYS:NZ	2.13	0.63
1:B:195:ILE:O	1:B:195:ILE:HG22	1.98	0.63
1:D:41:GLU:O	1:D:42:ASP:HB2	1.97	0.63
1:G:195:ILE:O	1:G:195:ILE:HG22	1.98	0.63
1:U:41:GLU:O	1:U:42:ASP:HB2	1.98	0.63
1:R:195:ILE:O	1:R:195:ILE:HG22	1.98	0.63
1:T:249:ALA:HA	1:T:253:ASN:HD22	1.62	0.63
1:G:251:ARG:HB2	1:G:317:LYS:HE2	1.80	0.62
1:U:192:LYS:O	1:U:194:VAL:N	2.32	0.62
1:W:251:ARG:HB2	1:W:317:LYS:HE2	1.80	0.62
1:E:251:ARG:HB2	1:E:317:LYS:HE2	1.81	0.62
1:M:251:ARG:HB2	1:M:317:LYS:HE2	1.81	0.62
1:P:195:ILE:HG22	1:P:195:ILE:O	1.99	0.62
1:R:172:PHE:CZ	1:R:176:ILE:HD11	2.34	0.62
1:V:40:VAL:CG1	1:V:44:THR:HB	2.29	0.62
1:X:192:LYS:O	1:X:194:VAL:N	2.31	0.62
1:C:251:ARG:HB2	1:C:317:LYS:HE2	1.81	0.62
1:R:251:ARG:HB2	1:R:317:LYS:HE2	1.81	0.62
1:S:40:VAL:CG1	1:S:44:THR:HB	2.29	0.62
1:X:41:GLU:O	1:X:42:ASP:HB2	1.99	0.62
1:J:195:ILE:O	1:J:195:ILE:HG22	1.98	0.62
1:V:41:GLU:HB3	2:V:2022:HOH:O	1.99	0.62
1:P:251:ARG:HB2	1:P:317:LYS:HE2	1.80	0.62
1:Q:172:PHE:CZ	1:Q:176:ILE:HD11	2.33	0.62
1:F:251:ARG:HB2	1:F:317:LYS:HE2	1.80	0.62
1:H:192:LYS:O	1:H:194:VAL:N	2.32	0.62
1:K:172:PHE:CZ	1:K:176:ILE:HD11	2.35	0.62
1:L:178:ARG:NH1	1:L:178:ARG:HB2	2.15	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:271:THR:HG21	2:M:2073:HOH:O	2.00	0.62
1:T:286:THR:HB	1:T:294:LEU:HD11	1.81	0.62
1:X:247:LYS:HB2	1:X:247:LYS:NZ	2.13	0.62
1:C:172:PHE:CZ	1:C:176:ILE:HD11	2.33	0.62
1:J:251:ARG:HB2	1:J:317:LYS:HE2	1.80	0.62
1:S:1:MET:HA	2:T:2052:HOH:O	1.98	0.62
1:F:40:VAL:CG1	1:F:44:THR:HB	2.29	0.62
1:B:251:ARG:HB2	1:B:317:LYS:HE2	1.81	0.62
1:N:40:VAL:CG1	1:N:44:THR:HB	2.29	0.62
1:P:317:LYS:HE3	2:P:2103:HOH:O	1.99	0.62
1:S:251:ARG:HB2	1:S:317:LYS:HE2	1.80	0.62
1:I:41:GLU:O	1:I:42:ASP:HB2	1.99	0.61
1:I:240:ASP:HB3	1:I:242:ILE:HG12	1.82	0.61
1:H:192:LYS:HA	2:H:2129:HOH:O	1.99	0.61
1:D:192:LYS:O	1:D:194:VAL:N	2.33	0.61
1:T:172:PHE:CZ	1:T:176:ILE:HD11	2.36	0.61
1:A:240:ASP:HB3	1:A:242:ILE:HG12	1.82	0.61
1:U:240:ASP:HB3	1:U:242:ILE:HG12	1.82	0.61
1:B:172:PHE:CZ	1:B:176:ILE:HD11	2.35	0.61
1:D:41:GLU:HG3	2:D:2031:HOH:O	1.99	0.61
1:D:178:ARG:NH1	1:D:178:ARG:HB2	2.16	0.61
1:H:178:ARG:NH1	1:H:178:ARG:HB2	2.15	0.61
1:L:192:LYS:O	1:L:194:VAL:N	2.32	0.61
1:L:240:ASP:HB3	1:L:242:ILE:HG12	1.82	0.61
1:Q:286:THR:HB	1:Q:294:LEU:HD11	1.83	0.61
1:V:286:THR:HB	1:V:294:LEU:HD11	1.83	0.61
1:W:172:PHE:CZ	1:W:176:ILE:HD11	2.35	0.61
1:I:172:PHE:CZ	1:I:176:ILE:HD11	2.36	0.61
1:O:172:PHE:CZ	1:O:176:ILE:HD11	2.36	0.61
1:U:178:ARG:NH1	1:U:178:ARG:HB2	2.16	0.61
1:B:308:SER:HB2	2:B:2114:HOH:O	2.00	0.60
1:T:314:THR:HG21	1:U:239:ASP:CB	2.31	0.60
1:M:172:PHE:CZ	1:M:176:ILE:HD11	2.36	0.60
1:F:286:THR:HB	1:F:294:LEU:HD11	1.83	0.60
1:S:216:SER:HB2	2:S:2109:HOH:O	2.01	0.60
1:W:244:GLU:HG2	1:X:238:ASN:HD21	1.65	0.60
1:X:189:ASP:O	2:X:2102:HOH:O	2.16	0.60
1:X:178:ARG:NH1	1:X:178:ARG:HB2	2.16	0.60
1:N:43:GLY:HA2	2:N:2052:HOH:O	2.00	0.60
1:W:286:THR:HB	1:W:294:LEU:HD11	1.83	0.60
1:F:172:PHE:CZ	1:F:176:ILE:HD11	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:172:PHE:CZ	1:J:176:ILE:HD11	2.37	0.60
1:X:240:ASP:HB3	1:X:242:ILE:HG12	1.83	0.60
1:H:240:ASP:HB3	1:H:242:ILE:HG12	1.82	0.60
1:S:286:THR:HB	1:S:294:LEU:HD11	1.83	0.60
1:X:247:LYS:O	1:X:249:ALA:N	2.34	0.60
1:D:240:ASP:HB3	1:D:242:ILE:HG12	1.83	0.60
1:F:257:LEU:HD22	1:F:259:ILE:HG23	1.84	0.60
1:I:41:GLU:OE2	1:M:22:HIS:HB3	2.00	0.60
1:K:257:LEU:HD22	1:K:259:ILE:HG23	1.84	0.60
1:D:87:GLU:HB3	1:D:92:LYS:HD2	1.84	0.59
1:V:257:LEU:HD22	1:V:259:ILE:HG23	1.84	0.59
1:G:286:THR:HB	1:G:294:LEU:HD11	1.83	0.59
1:S:172:PHE:CZ	1:S:176:ILE:HD11	2.36	0.59
1:A:192:LYS:O	1:A:194:VAL:N	2.32	0.59
1:B:286:THR:HB	1:B:294:LEU:HD11	1.84	0.59
1:M:252:SER:HB3	1:N:192:LYS:CE	2.31	0.59
1:H:87:GLU:HB3	1:H:92:LYS:HD2	1.84	0.59
1:E:172:PHE:CZ	1:E:176:ILE:HD11	2.37	0.59
1:I:41:GLU:OE2	1:M:22:HIS:ND1	2.35	0.59
1:A:178:ARG:NH1	1:A:178:ARG:HB2	2.17	0.59
1:C:257:LEU:HD22	1:C:259:ILE:HG23	1.85	0.59
1:G:257:LEU:HD22	1:G:259:ILE:HG23	1.84	0.59
1:L:87:GLU:HB3	1:L:92:LYS:HD2	1.84	0.59
1:I:87:GLU:HB3	1:I:92:LYS:HD2	1.84	0.59
1:P:106:LEU:HD22	1:P:109:CYS:SG	2.42	0.59
1:Q:257:LEU:HD22	1:Q:259:ILE:HG23	1.85	0.59
1:X:87:GLU:HB3	1:X:92:LYS:HD2	1.85	0.59
1:H:195:ILE:HB	2:H:2131:HOH:O	2.02	0.59
1:J:286:THR:HB	1:J:294:LEU:HD11	1.85	0.59
1:M:257:LEU:HD22	1:M:259:ILE:HG23	1.85	0.59
1:R:286:THR:HB	1:R:294:LEU:HD11	1.85	0.59
1:C:251:ARG:HD2	1:D:236:THR:CG2	2.23	0.59
1:C:286:THR:HB	1:C:294:LEU:HD11	1.83	0.59
1:I:192:LYS:O	1:I:194:VAL:HG12	2.03	0.59
1:W:257:LEU:HD22	1:W:259:ILE:HG23	1.85	0.59
1:O:286:THR:HB	1:O:294:LEU:HD11	1.83	0.59
1:P:257:LEU:HD22	1:P:259:ILE:HG23	1.84	0.59
1:X:192:LYS:O	1:X:194:VAL:HG12	2.03	0.58
1:F:106:LEU:HD22	1:F:109:CYS:SG	2.43	0.58
1:M:236:THR:CG2	1:R:251:ARG:HH11	2.16	0.58
1:N:248:GLU:OE1	1:O:236:THR:CG2	2.52	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:87:GLU:HB3	1:U:92:LYS:HD2	1.84	0.58
1:A:247:LYS:O	1:A:248:GLU:HB3	2.03	0.58
1:J:271:THR:HG21	2:J:2067:HOH:O	2.04	0.58
1:J:257:LEU:HD22	1:J:259:ILE:HG23	1.86	0.58
1:K:244:GLU:HG2	1:L:238:ASN:HD21	1.69	0.58
1:O:106:LEU:HD22	1:O:109:CYS:SG	2.44	0.58
1:U:192:LYS:HB3	1:U:192:LYS:HZ3	1.66	0.58
1:U:216:SER:HB3	2:U:2055:HOH:O	2.04	0.58
1:D:247:LYS:O	1:D:248:GLU:HB3	2.04	0.58
1:I:178:ARG:NH1	1:I:178:ARG:HB2	2.18	0.58
1:K:286:THR:HB	1:K:294:LEU:HD11	1.85	0.58
1:N:286:THR:HB	1:N:294:LEU:HD11	1.85	0.58
1:Q:248:GLU:OE1	1:R:236:THR:HG22	2.03	0.58
1:A:87:GLU:HB3	1:A:92:LYS:HD2	1.84	0.58
1:M:236:THR:HG22	1:R:251:ARG:HH11	1.69	0.58
1:I:2:ILE:HD11	2:J:2108:HOH:O	2.02	0.58
1:N:172:PHE:CZ	1:N:176:ILE:HD11	2.39	0.58
1:V:310:LYS:HD2	1:W:132:GLY:O	2.04	0.58
1:R:115:GLU:HG2	2:R:2051:HOH:O	2.04	0.57
1:U:192:LYS:O	1:U:194:VAL:HG12	2.04	0.57
1:L:60:ASP:OD2	1:L:64:GLN:HB3	2.05	0.57
1:P:286:THR:HB	1:P:294:LEU:HD11	1.86	0.57
1:U:247:LYS:O	1:U:248:GLU:HB3	2.04	0.57
1:L:247:LYS:O	1:L:248:GLU:HB3	2.03	0.57
1:M:286:THR:HB	1:M:294:LEU:HD11	1.84	0.57
1:B:257:LEU:HD22	1:B:259:ILE:HG23	1.85	0.57
1:L:287:SER:OG	1:L:297:HIS:HE1	1.88	0.57
1:L:234:ASN:C	1:L:236:THR:H	2.13	0.57
1:N:251:ARG:NH1	1:O:236:THR:HG22	2.18	0.57
1:R:106:LEU:HD22	1:R:109:CYS:SG	2.45	0.57
1:U:60:ASP:OD2	1:U:64:GLN:HB3	2.05	0.57
1:B:310:LYS:HD2	1:C:132:GLY:O	2.04	0.57
1:D:192:LYS:O	1:D:194:VAL:HG12	2.04	0.57
1:E:286:THR:HB	1:E:294:LEU:HD11	1.87	0.57
1:F:178:ARG:NH1	1:F:178:ARG:HB2	2.20	0.57
1:H:287:SER:OG	1:H:297:HIS:HE1	1.88	0.57
1:M:247:LYS:HZ3	1:M:321:LEU:HB2	1.70	0.57
1:X:247:LYS:O	1:X:248:GLU:HB3	2.04	0.57
1:A:192:LYS:O	1:A:194:VAL:HG12	2.04	0.57
1:Q:178:ARG:NH1	1:Q:178:ARG:HB2	2.20	0.57
2:Q:2075:HOH:O	1:U:262:ASP:HB2	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:238:ASN:HD22	1:U:238:ASN:N	2.02	0.57
1:A:236:THR:HG21	1:F:252:SER:OG	2.05	0.56
1:B:251:ARG:HH11	1:C:236:THR:CG2	2.18	0.56
1:A:236:THR:HG22	1:F:248:GLU:OE1	2.04	0.56
1:L:192:LYS:O	1:L:194:VAL:HG12	2.04	0.56
1:S:257:LEU:HD22	1:S:259:ILE:HG23	1.85	0.56
1:V:106:LEU:HD22	1:V:109:CYS:SG	2.45	0.56
1:H:192:LYS:O	1:H:194:VAL:HG12	2.04	0.56
1:H:238:ASN:HD22	1:H:238:ASN:N	2.04	0.56
1:H:247:LYS:O	1:H:248:GLU:HB3	2.05	0.56
1:I:245:LEU:O	1:I:247:LYS:O	2.24	0.56
1:L:238:ASN:HD22	1:L:238:ASN:N	2.03	0.56
1:V:178:ARG:NH1	1:V:178:ARG:HB2	2.20	0.56
1:Q:247:LYS:HZ2	1:Q:321:LEU:HB2	1.70	0.56
1:T:234:ASN:C	1:T:236:THR:H	2.14	0.56
1:T:257:LEU:HD22	1:T:259:ILE:HG23	1.86	0.56
1:M:132:GLY:O	1:R:310:LYS:HD2	2.05	0.56
1:O:257:LEU:HD22	1:O:259:ILE:HG23	1.87	0.56
1:T:106:LEU:HD22	1:T:109:CYS:SG	2.46	0.56
1:U:234:ASN:C	1:U:236:THR:H	2.14	0.56
1:W:310:LYS:HD2	1:X:132:GLY:O	2.05	0.56
1:E:216:SER:HB2	2:F:2113:HOH:O	2.06	0.56
1:E:257:LEU:HD22	1:E:259:ILE:HG23	1.88	0.56
1:H:234:ASN:C	1:H:236:THR:H	2.13	0.56
1:I:247:LYS:O	1:I:248:GLU:HB3	2.05	0.56
1:Q:248:GLU:OE1	1:R:236:THR:CG2	2.53	0.56
1:A:236:THR:CG2	1:F:251:ARG:HD2	2.27	0.56
1:C:234:ASN:C	1:C:236:THR:H	2.13	0.56
1:E:251:ARG:NH1	1:F:236:THR:HG22	2.21	0.56
1:G:42:ASP:HB3	2:G:2025:HOH:O	2.04	0.56
1:G:234:ASN:C	1:G:236:THR:H	2.14	0.56
1:L:245:LEU:O	1:L:247:LYS:O	2.24	0.56
1:B:234:ASN:C	1:B:236:THR:H	2.14	0.56
1:C:251:ARG:CD	1:D:236:THR:HG23	2.23	0.56
1:E:234:ASN:C	1:E:236:THR:H	2.14	0.56
1:I:41:GLU:OE2	1:M:22:HIS:CG	2.58	0.56
1:O:234:ASN:C	1:O:236:THR:H	2.14	0.56
1:S:106:LEU:HD22	1:S:109:CYS:SG	2.46	0.56
1:W:106:LEU:HD22	1:W:109:CYS:SG	2.46	0.56
1:X:238:ASN:HD22	1:X:238:ASN:N	2.03	0.56
1:D:238:ASN:HD22	1:D:238:ASN:N	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:245:LEU:O	1:H:247:LYS:O	2.24	0.56
1:H:247:LYS:O	1:H:249:ALA:N	2.36	0.56
1:I:234:ASN:C	1:I:236:THR:H	2.13	0.56
1:D:192:LYS:HB3	1:D:192:LYS:HZ3	1.69	0.56
1:N:92:LYS:HE3	1:N:92:LYS:CA	2.36	0.56
1:R:234:ASN:C	1:R:236:THR:H	2.14	0.56
1:X:234:ASN:C	1:X:236:THR:H	2.14	0.56
1:N:234:ASN:C	1:N:236:THR:H	2.14	0.55
1:Q:234:ASN:C	1:Q:236:THR:H	2.14	0.55
1:V:234:ASN:C	1:V:236:THR:H	2.14	0.55
1:X:192:LYS:HB3	1:X:192:LYS:HZ3	1.69	0.55
1:C:106:LEU:HD22	1:C:109:CYS:SG	2.46	0.55
1:D:60:ASP:OD2	1:D:64:GLN:HB3	2.06	0.55
1:K:234:ASN:C	1:K:236:THR:H	2.14	0.55
1:N:178:ARG:NH1	1:N:178:ARG:HB2	2.21	0.55
1:S:207:ILE:HD13	2:S:2104:HOH:O	2.06	0.55
1:W:234:ASN:C	1:W:236:THR:H	2.13	0.55
1:I:72:LYS:HE3	2:I:2031:HOH:O	2.05	0.55
1:N:92:LYS:HA	1:N:92:LYS:CE	2.36	0.55
1:S:178:ARG:NH1	1:S:178:ARG:HB2	2.21	0.55
1:A:60:ASP:OD2	1:A:64:GLN:HB3	2.06	0.55
1:A:247:LYS:O	1:A:249:ALA:N	2.36	0.55
1:I:247:LYS:O	1:I:249:ALA:N	2.36	0.55
1:J:92:LYS:HE3	1:J:92:LYS:CA	2.36	0.55
1:P:234:ASN:C	1:P:236:THR:H	2.13	0.55
1:U:247:LYS:O	1:U:249:ALA:N	2.37	0.55
1:D:247:LYS:O	1:D:249:ALA:N	2.37	0.55
1:F:234:ASN:C	1:F:236:THR:H	2.14	0.55
1:I:238:ASN:HD22	1:I:238:ASN:N	2.04	0.55
1:J:234:ASN:C	1:J:236:THR:H	2.15	0.55
1:R:257:LEU:HD22	1:R:259:ILE:HG23	1.87	0.55
1:U:184:ARG:HD3	2:U:2040:HOH:O	2.05	0.55
1:U:287:SER:OG	1:U:297:HIS:HE1	1.90	0.55
1:A:234:ASN:C	1:A:236:THR:H	2.14	0.55
1:B:106:LEU:HD22	1:B:109:CYS:SG	2.46	0.55
1:D:234:ASN:C	1:D:236:THR:H	2.14	0.55
1:D:245:LEU:O	1:D:247:LYS:O	2.25	0.55
1:E:72:LYS:HE3	2:E:2039:HOH:O	2.06	0.55
1:G:1:MET:HA	2:H:2118:HOH:O	2.07	0.55
1:M:234:ASN:C	1:M:236:THR:H	2.14	0.55
1:S:234:ASN:C	1:S:236:THR:H	2.15	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:60:ASP:OD2	1:X:64:GLN:HB3	2.06	0.55
1:A:238:ASN:HD22	1:A:238:ASN:N	2.04	0.55
1:U:106:LEU:HD22	1:U:109:CYS:SG	2.47	0.55
1:B:95:HIS:HD2	1:B:96:ARG:O	1.89	0.55
1:H:72:LYS:HE3	2:H:2018:HOH:O	2.06	0.55
1:M:106:LEU:HD22	1:M:109:CYS:SG	2.47	0.55
1:A:245:LEU:O	1:A:247:LYS:O	2.25	0.54
1:K:310:LYS:HD2	1:L:132:GLY:O	2.06	0.54
1:N:257:LEU:HD22	1:N:259:ILE:HG23	1.87	0.54
1:U:95:HIS:HD2	1:U:96:ARG:O	1.89	0.54
1:L:247:LYS:O	1:L:249:ALA:N	2.37	0.54
1:M:252:SER:HB3	1:N:192:LYS:HE3	1.89	0.54
1:U:245:LEU:O	1:U:247:LYS:O	2.23	0.54
1:X:245:LEU:O	1:X:247:LYS:O	2.25	0.54
1:D:247:LYS:HB2	1:D:247:LYS:HZ2	1.72	0.54
1:E:106:LEU:HD22	1:E:109:CYS:SG	2.47	0.54
1:M:244:GLU:HG2	1:N:239:ASP:HB2	1.90	0.54
1:P:251:ARG:NH1	1:Q:236:THR:HG22	2.22	0.54
1:F:92:LYS:HE3	1:F:92:LYS:CA	2.36	0.54
1:M:178:ARG:NH1	1:M:178:ARG:HB2	2.23	0.54
1:B:178:ARG:NH1	1:B:178:ARG:HB2	2.23	0.54
1:D:287:SER:OG	1:D:297:HIS:HE1	1.90	0.54
1:K:259:ILE:CD1	1:K:316:ILE:HG23	2.37	0.54
1:Q:92:LYS:HA	1:Q:92:LYS:CE	2.38	0.54
1:Q:251:ARG:NH1	1:R:236:THR:HG22	2.21	0.54
1:U:40:VAL:CG1	1:U:44:THR:HB	2.38	0.54
1:A:236:THR:HG23	1:F:251:ARG:CD	2.27	0.54
1:G:92:LYS:HE3	1:G:92:LYS:CA	2.36	0.54
1:S:92:LYS:HE3	1:S:92:LYS:CA	2.36	0.54
1:W:132:GLY:HA3	2:W:2049:HOH:O	2.07	0.54
1:C:92:LYS:HA	1:C:92:LYS:CE	2.37	0.54
1:E:40:VAL:O	2:E:2030:HOH:O	2.18	0.54
1:Q:106:LEU:HD22	1:Q:109:CYS:SG	2.48	0.54
1:R:178:ARG:HB2	1:R:178:ARG:NH1	2.23	0.54
1:F:92:LYS:HA	1:F:92:LYS:CE	2.37	0.54
1:H:60:ASP:OD2	1:H:64:GLN:HB3	2.07	0.54
1:K:106:LEU:HD22	1:K:109:CYS:SG	2.48	0.54
1:O:178:ARG:HB2	1:O:178:ARG:NH1	2.23	0.54
1:P:178:ARG:NH1	1:P:178:ARG:HB2	2.23	0.54
1:P:259:ILE:CD1	1:P:316:ILE:HG23	2.38	0.54
1:T:259:ILE:CD1	1:T:316:ILE:HG23	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:134:SER:HB3	1:U:267:TRP:CZ2	2.43	0.54
1:C:178:ARG:NH1	1:C:178:ARG:HB2	2.23	0.53
1:D:195:ILE:HG12	1:D:215:LEU:HD22	1.90	0.53
1:L:40:VAL:CG1	1:L:44:THR:HB	2.38	0.53
1:W:259:ILE:CD1	1:W:316:ILE:HG23	2.38	0.53
1:H:95:HIS:HD2	1:H:96:ARG:O	1.91	0.53
1:I:134:SER:HB3	1:I:267:TRP:CZ2	2.43	0.53
1:K:92:LYS:HE3	1:K:92:LYS:CA	2.37	0.53
1:N:209:ARG:HD3	2:N:2158:HOH:O	2.07	0.53
1:N:311:ALA:O	1:N:315:VAL:HG23	2.09	0.53
1:T:178:ARG:NH1	1:T:178:ARG:HB2	2.22	0.53
1:W:92:LYS:HA	1:W:92:LYS:CE	2.37	0.53
1:A:40:VAL:CG1	1:A:44:THR:HB	2.39	0.53
1:L:134:SER:HB3	1:L:267:TRP:CZ2	2.43	0.53
1:W:192:LYS:O	1:W:193:ASN:HB2	2.09	0.53
1:A:95:HIS:HD2	1:A:96:ARG:O	1.92	0.53
1:A:106:LEU:HD22	1:A:109:CYS:SG	2.49	0.53
1:B:259:ILE:CD1	1:B:316:ILE:HG23	2.38	0.53
1:G:95:HIS:HD2	1:G:96:ARG:O	1.91	0.53
1:K:178:ARG:NH1	1:K:178:ARG:HB2	2.24	0.53
1:N:259:ILE:CD1	1:N:316:ILE:HG23	2.38	0.53
1:G:178:ARG:HB2	1:G:178:ARG:NH1	2.24	0.53
1:G:192:LYS:O	1:G:193:ASN:HB2	2.09	0.53
1:I:106:LEU:HD22	1:I:109:CYS:SG	2.48	0.53
1:M:92:LYS:HE3	1:M:92:LYS:CA	2.37	0.53
1:O:192:LYS:O	1:O:193:ASN:HB2	2.09	0.53
1:W:178:ARG:HB2	1:W:178:ARG:NH1	2.23	0.53
1:D:134:SER:HB3	1:D:267:TRP:CZ2	2.44	0.53
1:E:92:LYS:HE3	1:E:92:LYS:CA	2.37	0.53
1:I:287:SER:OG	1:I:297:HIS:HE1	1.92	0.53
1:T:310:LYS:HD2	1:U:132:GLY:O	2.09	0.53
1:U:131:LYS:HA	2:U:2032:HOH:O	2.07	0.53
1:W:92:LYS:HE3	1:W:92:LYS:CA	2.37	0.53
1:D:286:THR:HB	1:D:294:LEU:HD11	1.90	0.53
1:E:178:ARG:NH1	1:E:178:ARG:HB2	2.24	0.53
1:I:107:VAL:HA	2:I:2090:HOH:O	2.09	0.53
2:M:2109:HOH:O	1:R:1:MET:HA	2.08	0.53
1:P:311:ALA:O	1:P:315:VAL:HG23	2.09	0.53
1:S:92:LYS:HA	1:S:92:LYS:CE	2.36	0.53
1:S:247:LYS:HZ2	1:S:321:LEU:HB2	1.73	0.53
1:C:195:ILE:HG23	1:C:245:LEU:HG	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:40:VAL:CG1	1:H:44:THR:HB	2.38	0.53
1:P:92:LYS:HE3	1:P:92:LYS:CA	2.37	0.53
1:Q:259:ILE:CD1	1:Q:316:ILE:HG23	2.38	0.53
1:S:137:THR:HB	1:S:138:PRO:HD3	1.91	0.53
1:T:311:ALA:O	1:T:315:VAL:HG23	2.09	0.53
1:A:134:SER:HB3	1:A:267:TRP:CZ2	2.44	0.53
1:B:248:GLU:OE1	1:C:236:THR:HG22	2.08	0.53
1:G:106:LEU:HD22	1:G:109:CYS:SG	2.49	0.53
1:G:259:ILE:CD1	1:G:316:ILE:HG23	2.36	0.53
1:M:95:HIS:HD2	1:M:96:ARG:O	1.92	0.53
1:M:137:THR:HB	1:M:138:PRO:HD3	1.91	0.53
1:N:310:LYS:HB3	1:O:133:ASN:HA	1.91	0.53
1:Q:311:ALA:O	1:Q:315:VAL:HG23	2.08	0.53
1:X:95:HIS:HD2	1:X:96:ARG:O	1.92	0.53
1:T:92:LYS:HE3	1:T:92:LYS:CA	2.37	0.53
1:B:311:ALA:O	1:B:315:VAL:HG23	2.09	0.52
1:Q:237:SER:HB3	1:Q:242:ILE:CD1	2.25	0.52
1:T:92:LYS:HA	1:T:92:LYS:CE	2.37	0.52
1:U:247:LYS:HB2	1:U:247:LYS:HZ2	1.74	0.52
1:X:134:SER:HB3	1:X:267:TRP:CZ2	2.44	0.52
1:C:192:LYS:O	1:C:193:ASN:HB2	2.09	0.52
1:F:192:LYS:O	1:F:193:ASN:HB2	2.09	0.52
1:F:259:ILE:CD1	1:F:316:ILE:HG23	2.37	0.52
1:K:311:ALA:O	1:K:315:VAL:HG23	2.09	0.52
1:L:95:HIS:HD2	1:L:96:ARG:O	1.92	0.52
1:M:251:ARG:NH1	1:N:236:THR:HG22	2.21	0.52
1:P:195:ILE:HG23	1:P:245:LEU:HG	1.90	0.52
1:R:195:ILE:HG23	1:R:245:LEU:HG	1.91	0.52
1:J:178:ARG:NH1	1:J:178:ARG:HB2	2.25	0.52
1:M:195:ILE:HG23	1:M:245:LEU:HG	1.91	0.52
1:V:195:ILE:HG23	1:V:245:LEU:HG	1.91	0.52
1:C:311:ALA:O	1:C:315:VAL:HG23	2.10	0.52
1:H:195:ILE:HG12	1:H:215:LEU:HD22	1.92	0.52
1:I:95:HIS:HD2	1:I:96:ARG:O	1.93	0.52
1:M:192:LYS:O	1:M:193:ASN:HB2	2.09	0.52
1:O:259:ILE:CD1	1:O:316:ILE:HG23	2.37	0.52
1:V:92:LYS:HA	1:V:92:LYS:CE	2.38	0.52
1:V:311:ALA:O	1:V:315:VAL:HG23	2.09	0.52
1:D:40:VAL:CG1	1:D:44:THR:HB	2.39	0.52
1:F:95:HIS:HD2	1:F:96:ARG:O	1.92	0.52
1:H:252:SER:HB2	1:I:236:THR:HG21	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:195:ILE:HG12	1:L:215:LEU:HD22	1.92	0.52
1:M:259:ILE:CD1	1:M:316:ILE:HG23	2.38	0.52
1:N:106:LEU:HD22	1:N:109:CYS:SG	2.49	0.52
1:P:244:GLU:HG2	1:Q:239:ASP:HB2	1.91	0.52
1:Q:195:ILE:HG23	1:Q:245:LEU:HG	1.91	0.52
1:T:195:ILE:HG23	1:T:245:LEU:HG	1.91	0.52
1:X:242:ILE:O	1:X:242:ILE:HG22	2.10	0.52
1:B:248:GLU:OE1	1:C:236:THR:CG2	2.58	0.52
1:D:106:LEU:HD22	1:D:109:CYS:SG	2.49	0.52
1:G:311:ALA:O	1:G:315:VAL:HG23	2.10	0.52
1:I:242:ILE:HG22	1:I:242:ILE:O	2.09	0.52
1:M:311:ALA:O	1:M:315:VAL:HG23	2.10	0.52
1:O:92:LYS:HE3	1:O:92:LYS:CA	2.37	0.52
1:R:237:SER:HB3	1:R:242:ILE:CD1	2.24	0.52
1:B:195:ILE:HG23	1:B:245:LEU:HG	1.92	0.52
1:C:313:GLN:HE22	1:C:317:LYS:HZ3	1.58	0.52
1:E:42:ASP:N	2:E:2030:HOH:O	2.42	0.52
1:E:192:LYS:O	1:E:193:ASN:HB2	2.10	0.52
1:E:195:ILE:HG23	1:E:245:LEU:HG	1.91	0.52
1:H:106:LEU:HD22	1:H:109:CYS:SG	2.50	0.52
1:I:240:ASP:C	1:I:242:ILE:N	2.68	0.52
1:R:259:ILE:CD1	1:R:316:ILE:HG23	2.39	0.52
1:S:88:ASN:HB2	2:S:2049:HOH:O	2.10	0.52
1:V:92:LYS:HE3	1:V:92:LYS:CA	2.37	0.52
1:V:259:ILE:CD1	1:V:316:ILE:HG23	2.39	0.52
1:W:311:ALA:O	1:W:315:VAL:HG23	2.09	0.52
1:B:92:LYS:HA	1:B:92:LYS:CE	2.37	0.52
1:L:286:THR:HB	1:L:294:LEU:HD11	1.91	0.52
1:M:92:LYS:HA	1:M:92:LYS:CE	2.37	0.52
1:N:195:ILE:HG23	1:N:245:LEU:HG	1.92	0.52
1:O:92:LYS:HA	1:O:92:LYS:CE	2.37	0.52
1:R:311:ALA:O	1:R:315:VAL:HG23	2.10	0.52
1:S:259:ILE:CD1	1:S:316:ILE:HG23	2.38	0.52
1:X:40:VAL:CG1	1:X:44:THR:HB	2.40	0.52
1:F:195:ILE:HG23	1:F:245:LEU:HG	1.91	0.52
1:R:95:HIS:HD2	1:R:96:ARG:O	1.93	0.52
1:T:244:GLU:HG2	1:U:238:ASN:ND2	2.25	0.52
1:W:251:ARG:HH11	1:X:236:THR:HG22	1.75	0.52
2:I:2015:HOH:O	1:J:291:HIS:HD2	1.93	0.52
1:J:92:LYS:HA	1:J:92:LYS:CE	2.37	0.52
1:K:195:ILE:HG23	1:K:245:LEU:HG	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:311:ALA:O	1:O:315:VAL:HG23	2.10	0.52
1:Q:95:HIS:HD2	1:Q:96:ARG:O	1.92	0.52
1:R:92:LYS:HE3	1:R:92:LYS:CA	2.38	0.52
1:S:252:SER:HB3	1:T:192:LYS:CE	2.40	0.52
1:V:313:GLN:HE22	1:V:317:LYS:HZ3	1.58	0.52
1:X:195:ILE:HG12	1:X:215:LEU:HD22	1.92	0.52
1:A:240:ASP:C	1:A:242:ILE:N	2.68	0.51
1:D:95:HIS:HD2	1:D:96:ARG:O	1.93	0.51
1:G:195:ILE:HG23	1:G:245:LEU:HG	1.91	0.51
1:H:41:GLU:OE2	1:X:8:LYS:NZ	2.40	0.51
1:J:259:ILE:CD1	1:J:316:ILE:HG23	2.37	0.51
1:O:195:ILE:HG23	1:O:245:LEU:HG	1.92	0.51
1:S:252:SER:HB3	1:T:192:LYS:HE3	1.91	0.51
1:T:192:LYS:O	1:T:193:ASN:HB2	2.11	0.51
1:W:195:ILE:HG23	1:W:245:LEU:HG	1.91	0.51
1:X:192:LYS:HA	2:X:2108:HOH:O	2.10	0.51
1:K:92:LYS:HA	1:K:92:LYS:CE	2.38	0.51
1:P:248:GLU:OE1	1:Q:236:THR:HG22	2.10	0.51
1:A:147:LEU:O	1:A:184:ARG:NH2	2.44	0.51
1:D:1:MET:HA	2:E:2089:HOH:O	2.10	0.51
1:D:242:ILE:HG22	1:D:242:ILE:O	2.09	0.51
1:H:286:THR:HB	1:H:294:LEU:HD11	1.91	0.51
1:M:236:THR:HG22	1:R:248:GLU:OE1	2.09	0.51
1:Q:137:THR:HB	1:Q:138:PRO:HD3	1.92	0.51
1:S:311:ALA:O	1:S:315:VAL:HG23	2.09	0.51
1:T:209:ARG:HD3	2:T:2059:HOH:O	2.10	0.51
1:E:259:ILE:CD1	1:E:316:ILE:HG23	2.38	0.51
1:F:311:ALA:O	1:F:315:VAL:HG23	2.10	0.51
1:I:195:ILE:HG12	1:I:215:LEU:HD22	1.92	0.51
1:S:195:ILE:HG23	1:S:245:LEU:HG	1.92	0.51
1:A:287:SER:OG	1:A:297:HIS:HE1	1.94	0.51
1:B:92:LYS:HE3	1:B:92:LYS:CA	2.37	0.51
1:G:92:LYS:HA	1:G:92:LYS:CE	2.36	0.51
1:J:106:LEU:HD22	1:J:109:CYS:SG	2.50	0.51
1:O:259:ILE:HD13	1:O:316:ILE:CG2	2.41	0.51
1:P:192:LYS:O	1:P:193:ASN:HB2	2.11	0.51
1:Q:92:LYS:HE3	1:Q:92:LYS:CA	2.38	0.51
1:R:92:LYS:HA	1:R:92:LYS:CE	2.38	0.51
1:S:192:LYS:O	1:S:193:ASN:HB2	2.10	0.51
1:X:147:LEU:O	1:X:184:ARG:NH2	2.44	0.51
1:E:92:LYS:HA	1:E:92:LYS:CE	2.37	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:147:LEU:O	1:F:184:ARG:NH2	2.44	0.51
1:H:105:GLU:HB3	2:H:2062:HOH:O	2.10	0.51
1:L:147:LEU:O	1:L:184:ARG:NH2	2.44	0.51
1:P:190:SER:OG	1:P:192:LYS:HB3	2.10	0.51
1:U:195:ILE:HG12	1:U:215:LEU:HD22	1.93	0.51
1:X:286:THR:HB	1:X:294:LEU:HD11	1.93	0.51
1:C:92:LYS:HE3	1:C:92:LYS:CA	2.37	0.51
1:F:115:GLU:HG2	2:F:2070:HOH:O	2.11	0.51
1:H:242:ILE:O	1:H:242:ILE:HG22	2.10	0.51
1:I:192:LYS:HA	2:I:2153:HOH:O	2.11	0.51
1:A:154:ALA:HA	1:F:4:LEU:HD23	1.93	0.51
1:B:251:ARG:HH11	1:C:236:THR:HG22	1.75	0.51
1:G:313:GLN:HE22	1:G:317:LYS:NZ	2.09	0.51
1:I:272:ARG:NH1	2:I:2169:HOH:O	2.42	0.51
1:M:190:SER:OG	1:M:192:LYS:HB3	2.10	0.51
1:V:95:HIS:HD2	1:V:96:ARG:O	1.94	0.51
1:W:250:SER:HB2	1:W:317:LYS:HE3	1.93	0.51
1:F:313:GLN:HE22	1:F:317:LYS:NZ	2.08	0.51
1:G:137:THR:HB	1:G:138:PRO:HD3	1.93	0.51
1:S:250:SER:HB2	1:S:317:LYS:HE3	1.92	0.51
1:U:242:ILE:O	1:U:242:ILE:HG22	2.10	0.51
1:G:248:GLU:OE1	1:H:236:THR:HG22	2.11	0.51
1:I:60:ASP:OD2	1:I:64:GLN:HB3	2.11	0.51
1:J:207:ILE:HG23	1:J:211:ALA:HB3	1.93	0.51
1:J:311:ALA:O	1:J:315:VAL:HG23	2.10	0.51
1:N:313:GLN:HE22	1:N:317:LYS:HZ3	1.57	0.51
1:E:313:GLN:HE22	1:E:317:LYS:HZ3	1.58	0.50
2:M:2130:HOH:O	1:S:312:ILE:HD13	2.11	0.50
1:P:92:LYS:HA	1:P:92:LYS:CE	2.37	0.50
1:Q:70:LYS:HG2	2:Q:2022:HOH:O	2.11	0.50
1:R:190:SER:OG	1:R:192:LYS:HB3	2.12	0.50
1:X:287:SER:OG	1:X:297:HIS:HE1	1.93	0.50
1:E:313:GLN:HE22	1:E:317:LYS:NZ	2.09	0.50
1:H:1:MET:HA	2:I:2142:HOH:O	2.11	0.50
1:H:247:LYS:HB2	1:H:247:LYS:HZ2	1.76	0.50
1:K:95:HIS:HD2	1:K:96:ARG:O	1.94	0.50
1:P:313:GLN:HE22	1:P:317:LYS:HZ3	1.58	0.50
1:Q:192:LYS:O	1:Q:193:ASN:HB2	2.10	0.50
1:T:313:GLN:HE22	1:T:317:LYS:HZ3	1.58	0.50
1:A:195:ILE:HG12	1:A:215:LEU:HD22	1.91	0.50
1:C:137:THR:HB	1:C:138:PRO:HD3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:134:SER:HB3	1:H:267:TRP:CZ2	2.47	0.50
1:I:40:VAL:CG1	1:I:44:THR:HB	2.40	0.50
1:J:192:LYS:O	1:J:193:ASN:HB2	2.11	0.50
1:V:251:ARG:HH11	1:W:236:THR:CG2	2.24	0.50
1:D:216:SER:HB2	2:E:2096:HOH:O	2.11	0.50
1:J:195:ILE:HG23	1:J:245:LEU:HG	1.93	0.50
1:J:313:GLN:HE22	1:J:317:LYS:NZ	2.10	0.50
1:K:192:LYS:O	1:K:193:ASN:HB2	2.11	0.50
1:O:252:SER:HB3	1:P:192:LYS:HE3	1.92	0.50
1:W:244:GLU:HG2	1:X:238:ASN:ND2	2.26	0.50
1:B:192:LYS:O	1:B:193:ASN:HB2	2.10	0.50
1:K:216:SER:HB2	2:L:2059:HOH:O	2.11	0.50
1:L:242:ILE:HG22	1:L:242:ILE:O	2.11	0.50
1:R:65:ARG:HD2	2:R:2032:HOH:O	2.11	0.50
1:G:250:SER:HB2	1:G:317:LYS:HE3	1.93	0.50
1:N:95:HIS:HD2	1:N:96:ARG:O	1.94	0.50
2:P:2005:HOH:O	1:Q:291:HIS:HD2	1.94	0.50
1:W:137:THR:HB	1:W:138:PRO:HD3	1.93	0.50
1:A:286:THR:HB	1:A:294:LEU:HD11	1.93	0.50
1:C:313:GLN:HE22	1:C:317:LYS:NZ	2.09	0.50
1:S:159:GLY:HA3	1:S:193:ASN:ND2	2.26	0.50
1:S:313:GLN:HE22	1:S:317:LYS:NZ	2.10	0.50
1:U:182:GLN:NE2	2:U:2051:HOH:O	2.45	0.50
1:B:159:GLY:HA3	1:B:193:ASN:ND2	2.27	0.50
1:D:147:LEU:O	1:D:184:ARG:NH2	2.44	0.50
1:E:95:HIS:HD2	1:E:96:ARG:O	1.95	0.50
1:N:244:GLU:HG2	1:O:239:ASP:HB2	1.93	0.50
1:S:115:GLU:HG2	2:S:2062:HOH:O	2.10	0.50
1:A:192:LYS:HB3	1:A:192:LYS:HZ3	1.77	0.50
1:E:252:SER:HA	2:F:2093:HOH:O	2.12	0.50
1:I:286:THR:HB	1:I:294:LEU:HD11	1.92	0.50
1:J:159:GLY:HA3	1:J:193:ASN:ND2	2.27	0.50
1:K:313:GLN:HE22	1:K:317:LYS:NZ	2.09	0.50
1:L:106:LEU:HD22	1:L:109:CYS:SG	2.51	0.50
1:M:310:LYS:HD2	1:N:132:GLY:O	2.12	0.50
1:M:313:GLN:HE22	1:M:317:LYS:NZ	2.10	0.50
1:R:313:GLN:HE22	1:R:317:LYS:NZ	2.10	0.50
1:V:134:SER:HA	2:V:2104:HOH:O	2.11	0.50
1:B:313:GLN:HE22	1:B:317:LYS:NZ	2.09	0.49
1:F:250:SER:HB2	1:F:317:LYS:HE3	1.93	0.49
1:O:313:GLN:HE22	1:O:317:LYS:NZ	2.10	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:252:SER:HB3	1:R:192:LYS:HE3	1.94	0.49
1:R:192:LYS:O	1:R:193:ASN:HB2	2.12	0.49
1:V:190:SER:OG	1:V:192:LYS:HB3	2.12	0.49
1:V:313:GLN:HE22	1:V:317:LYS:NZ	2.10	0.49
1:W:313:GLN:HE22	1:W:317:LYS:NZ	2.10	0.49
1:B:259:ILE:HD13	1:B:316:ILE:CG2	2.41	0.49
1:C:147:LEU:O	1:C:184:ARG:NH2	2.45	0.49
1:C:259:ILE:CD1	1:C:316:ILE:HG23	2.38	0.49
1:E:159:GLY:HA3	1:E:193:ASN:ND2	2.27	0.49
1:G:147:LEU:O	1:G:184:ARG:NH2	2.45	0.49
1:N:237:SER:HB3	1:N:242:ILE:CD1	2.25	0.49
1:N:313:GLN:HE22	1:N:317:LYS:NZ	2.10	0.49
1:O:250:SER:HB2	1:O:317:LYS:HE3	1.94	0.49
1:P:247:LYS:HZ2	1:P:321:LEU:HB2	1.77	0.49
1:P:259:ILE:HD13	1:P:316:ILE:CG2	2.41	0.49
1:T:313:GLN:HE22	1:T:317:LYS:NZ	2.10	0.49
1:G:259:ILE:HD13	1:G:316:ILE:CG2	2.39	0.49
1:L:126:VAL:HG22	1:L:256:SER:HB2	1.94	0.49
1:M:259:ILE:HD13	1:M:316:ILE:CG2	2.41	0.49
1:N:193:ASN:N	2:N:2154:HOH:O	2.45	0.49
1:O:95:HIS:HD2	1:O:96:ARG:O	1.95	0.49
1:V:42:ASP:HB3	2:V:2024:HOH:O	2.12	0.49
1:X:126:VAL:HG22	1:X:256:SER:HB2	1.93	0.49
1:B:250:SER:HB2	1:B:317:LYS:HE3	1.95	0.49
1:B:313:GLN:HE22	1:B:317:LYS:HZ3	1.60	0.49
1:C:250:SER:HB2	1:C:317:LYS:HE3	1.93	0.49
1:G:159:GLY:HA3	1:G:193:ASN:ND2	2.27	0.49
1:H:147:LEU:O	1:H:184:ARG:NH2	2.46	0.49
1:O:159:GLY:HA3	1:O:193:ASN:ND2	2.28	0.49
1:B:257:LEU:HD22	1:B:259:ILE:CG2	2.43	0.49
1:C:184:ARG:HD3	2:C:2067:HOH:O	2.12	0.49
1:E:311:ALA:O	1:E:315:VAL:HG23	2.10	0.49
1:H:271:THR:HG21	2:H:2085:HOH:O	2.11	0.49
1:J:137:THR:HB	1:J:138:PRO:HD3	1.93	0.49
1:K:137:THR:HB	1:K:138:PRO:HD3	1.95	0.49
1:M:60:ASP:HB2	2:M:2045:HOH:O	2.11	0.49
1:P:313:GLN:HE22	1:P:317:LYS:NZ	2.10	0.49
1:R:137:THR:HB	1:R:138:PRO:HD3	1.93	0.49
1:R:259:ILE:HD13	1:R:316:ILE:CG2	2.41	0.49
1:S:45:PRO:HB3	1:S:58:VAL:HG11	1.94	0.49
1:V:159:GLY:HA3	1:V:193:ASN:ND2	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:ILE:HG22	1:A:242:ILE:O	2.11	0.49
1:C:95:HIS:HD2	1:C:96:ARG:O	1.95	0.49
1:N:207:ILE:HG23	1:N:211:ALA:HB3	1.94	0.49
1:O:147:LEU:O	1:O:184:ARG:NH2	2.46	0.49
1:P:159:GLY:HA3	1:P:193:ASN:ND2	2.28	0.49
1:Q:313:GLN:HE22	1:Q:317:LYS:NZ	2.10	0.49
1:R:313:GLN:HE22	1:R:317:LYS:HZ3	1.59	0.49
1:S:147:LEU:O	1:S:184:ARG:NH2	2.46	0.49
1:S:190:SER:OG	1:S:192:LYS:HB3	2.13	0.49
1:V:250:SER:HB2	1:V:317:LYS:HE3	1.94	0.49
1:A:236:THR:HB	2:A:2086:HOH:O	2.12	0.49
1:D:126:VAL:HG22	1:D:256:SER:HB2	1.94	0.49
1:E:207:ILE:HG23	1:E:211:ALA:HB3	1.94	0.49
1:J:250:SER:HB2	1:J:317:LYS:HE3	1.94	0.49
1:J:310:LYS:HD2	1:K:132:GLY:O	2.12	0.49
1:M:216:SER:HB2	2:M:2119:HOH:O	2.11	0.49
1:M:250:SER:HB2	1:M:317:LYS:HE3	1.94	0.49
1:P:95:HIS:HD2	1:P:96:ARG:O	1.95	0.49
1:U:147:LEU:O	1:U:184:ARG:NH2	2.45	0.49
1:U:286:THR:HB	1:U:294:LEU:HD11	1.93	0.49
1:C:190:SER:OG	1:C:192:LYS:HB3	2.13	0.49
1:J:313:GLN:HE22	1:J:317:LYS:HZ3	1.59	0.49
1:K:147:LEU:O	1:K:184:ARG:NH2	2.46	0.49
1:N:192:LYS:O	1:N:193:ASN:HB2	2.12	0.49
1:O:193:ASN:HA	2:O:2106:HOH:O	2.12	0.49
1:T:95:HIS:HD2	1:T:96:ARG:O	1.95	0.49
1:V:192:LYS:O	1:V:193:ASN:HB2	2.12	0.49
1:W:313:GLN:HE22	1:W:317:LYS:HZ3	1.61	0.49
1:B:137:THR:HB	1:B:138:PRO:HD3	1.95	0.49
1:F:32:HIS:HD2	2:F:2030:HOH:O	1.95	0.49
1:N:41:GLU:O	1:N:42:ASP:HB2	2.13	0.49
1:O:41:GLU:O	1:O:42:ASP:HB2	2.13	0.49
1:Q:252:SER:HB3	1:R:192:LYS:CE	2.43	0.49
1:R:45:PRO:HB3	1:R:58:VAL:HG11	1.94	0.49
1:W:190:SER:OG	1:W:192:LYS:HB3	2.12	0.49
1:E:147:LEU:O	1:E:184:ARG:NH2	2.46	0.49
1:K:159:GLY:HA3	1:K:193:ASN:ND2	2.28	0.49
1:M:64:GLN:HG3	2:M:2048:HOH:O	2.13	0.49
1:P:137:THR:HB	1:P:138:PRO:HD3	1.93	0.49
1:R:147:LEU:O	1:R:184:ARG:NH2	2.46	0.49
1:V:137:THR:HB	1:V:138:PRO:HD3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:147:LEU:O	1:V:184:ARG:NH2	2.46	0.49
1:W:95:HIS:HD2	1:W:96:ARG:O	1.95	0.49
1:B:75:LYS:HE3	1:B:79:GLY:O	2.13	0.48
1:E:259:ILE:HD13	1:E:316:ILE:CG2	2.41	0.48
1:J:190:SER:OG	1:J:192:LYS:HB3	2.13	0.48
1:O:207:ILE:HG23	1:O:211:ALA:HB3	1.95	0.48
1:P:252:SER:HB3	1:Q:192:LYS:CE	2.42	0.48
1:Q:147:LEU:O	1:Q:184:ARG:NH2	2.45	0.48
1:Q:159:GLY:HA3	1:Q:193:ASN:ND2	2.28	0.48
1:T:137:THR:HB	1:T:138:PRO:HD3	1.94	0.48
1:T:207:ILE:HG23	1:T:211:ALA:HB3	1.95	0.48
1:W:192:LYS:HA	2:W:2080:HOH:O	2.12	0.48
1:G:207:ILE:HG23	1:G:211:ALA:HB3	1.94	0.48
1:Q:45:PRO:HB3	1:Q:58:VAL:HG11	1.94	0.48
1:T:216:SER:HB2	2:T:2060:HOH:O	2.13	0.48
1:T:250:SER:HB2	1:T:317:LYS:HE3	1.94	0.48
1:V:257:LEU:HD22	1:V:259:ILE:CG2	2.43	0.48
1:K:313:GLN:HE22	1:K:317:LYS:HZ3	1.61	0.48
2:M:2130:HOH:O	1:S:312:ILE:HG21	2.13	0.48
1:X:195:ILE:HA	2:X:2110:HOH:O	2.12	0.48
1:E:137:THR:HB	1:E:138:PRO:HD3	1.94	0.48
1:F:247:LYS:HZ2	1:F:321:LEU:HB2	1.77	0.48
1:F:259:ILE:HD13	1:F:316:ILE:CG2	2.41	0.48
1:J:41:GLU:O	1:J:42:ASP:HB2	2.12	0.48
1:N:190:SER:OG	1:N:192:LYS:HB3	2.13	0.48
1:S:193:ASN:HA	2:S:2105:HOH:O	2.13	0.48
1:F:137:THR:HB	1:F:138:PRO:HD3	1.94	0.48
1:J:147:LEU:O	1:J:184:ARG:NH2	2.47	0.48
1:K:75:LYS:HE3	1:K:79:GLY:O	2.14	0.48
1:K:259:ILE:HD13	1:K:316:ILE:CG2	2.40	0.48
1:O:190:SER:OG	1:O:192:LYS:HB3	2.13	0.48
1:Q:207:ILE:HG23	1:Q:211:ALA:HB3	1.95	0.48
1:U:238:ASN:N	1:U:238:ASN:ND2	2.61	0.48
1:V:251:ARG:HH11	1:W:236:THR:HG22	1.78	0.48
1:B:192:LYS:O	1:B:194:VAL:N	2.47	0.48
1:C:159:GLY:HA3	1:C:193:ASN:ND2	2.29	0.48
1:F:159:GLY:HA3	1:F:193:ASN:ND2	2.29	0.48
1:N:250:SER:HB2	1:N:317:LYS:HE3	1.96	0.48
1:T:190:SER:OG	1:T:192:LYS:HB3	2.13	0.48
1:W:159:GLY:HA3	1:W:193:ASN:ND2	2.29	0.48
1:D:92:LYS:HE3	1:D:92:LYS:CA	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:75:LYS:HE3	1:E:79:GLY:O	2.14	0.48
1:L:139:LEU:C	1:L:139:LEU:HD13	2.39	0.48
1:M:41:GLU:O	1:M:42:ASP:HB2	2.14	0.48
1:N:236:THR:HG22	1:N:237:SER:N	2.28	0.48
1:N:270:LEU:HD22	1:N:270:LEU:N	2.29	0.48
1:V:75:LYS:HE3	1:V:79:GLY:O	2.14	0.48
1:X:106:LEU:HD22	1:X:109:CYS:SG	2.54	0.48
1:A:38:GLU:HB3	2:A:2020:HOH:O	2.14	0.48
1:G:190:SER:OG	1:G:192:LYS:HB3	2.14	0.48
1:P:250:SER:HB2	1:P:317:LYS:HE3	1.95	0.48
1:V:248:GLU:OE1	1:W:236:THR:HG22	2.13	0.48
1:D:137:THR:HB	1:D:138:PRO:HD3	1.96	0.48
1:E:190:SER:OG	1:E:192:LYS:HB3	2.13	0.48
1:E:250:SER:HB2	1:E:317:LYS:HE3	1.94	0.48
1:K:250:SER:HB2	1:K:317:LYS:HE3	1.95	0.48
1:V:169:PHE:O	1:V:172:PHE:HB3	2.13	0.48
1:E:41:GLU:O	1:E:42:ASP:HB2	2.14	0.48
1:I:147:LEU:O	1:I:184:ARG:NH2	2.47	0.48
1:J:259:ILE:HD13	1:J:316:ILE:CG2	2.40	0.48
1:K:190:SER:OG	1:K:192:LYS:HB3	2.14	0.48
1:S:95:HIS:HD2	1:S:96:ARG:O	1.95	0.48
1:U:240:ASP:C	1:U:242:ILE:N	2.67	0.48
1:A:283:THR:HG22	1:A:284:LEU:N	2.29	0.47
1:F:257:LEU:HD22	1:F:259:ILE:CG2	2.44	0.47
1:J:95:HIS:HD2	1:J:96:ARG:O	1.97	0.47
1:Q:190:SER:OG	1:Q:192:LYS:HB3	2.14	0.47
1:Q:250:SER:HB2	1:Q:317:LYS:HE3	1.96	0.47
1:C:310:LYS:HD2	1:D:132:GLY:O	2.14	0.47
1:F:192:LYS:O	1:F:194:VAL:N	2.47	0.47
1:O:75:LYS:HE3	1:O:79:GLY:O	2.14	0.47
1:P:147:LEU:O	1:P:184:ARG:NH2	2.47	0.47
1:T:159:GLY:HA3	1:T:193:ASN:ND2	2.28	0.47
1:T:169:PHE:O	1:T:172:PHE:HB3	2.14	0.47
1:U:139:LEU:C	1:U:139:LEU:HD13	2.39	0.47
1:B:41:GLU:O	1:B:42:ASP:HB2	2.14	0.47
1:B:147:LEU:O	1:B:184:ARG:NH2	2.48	0.47
1:F:41:GLU:O	1:F:42:ASP:HB2	2.14	0.47
1:F:45:PRO:HB3	1:F:58:VAL:HG11	1.96	0.47
1:F:190:SER:OG	1:F:192:LYS:HB3	2.14	0.47
1:H:6:ASP:HB3	1:I:152:LYS:HG2	1.96	0.47
1:K:1:MET:HA	2:L:2055:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:45:PRO:HB3	1:K:58:VAL:HG11	1.96	0.47
1:M:236:THR:CG2	1:R:248:GLU:OE1	2.62	0.47
1:O:137:THR:HB	1:O:138:PRO:HD3	1.96	0.47
1:R:250:SER:HB2	1:R:317:LYS:HE3	1.96	0.47
1:U:92:LYS:HE3	1:U:92:LYS:CA	2.45	0.47
1:X:238:ASN:N	1:X:238:ASN:ND2	2.62	0.47
1:E:169:PHE:O	1:E:172:PHE:HB3	2.14	0.47
1:F:207:ILE:HG23	1:F:211:ALA:HB3	1.95	0.47
1:G:257:LEU:HD22	1:G:259:ILE:CG2	2.44	0.47
1:H:234:ASN:HB3	2:H:2139:HOH:O	2.13	0.47
1:K:257:LEU:HD22	1:K:259:ILE:CG2	2.44	0.47
1:L:270:LEU:N	1:L:270:LEU:HD22	2.29	0.47
1:M:159:GLY:HA3	1:M:193:ASN:ND2	2.28	0.47
1:N:147:LEU:O	1:N:184:ARG:NH2	2.47	0.47
1:R:159:GLY:HA3	1:R:193:ASN:ND2	2.29	0.47
1:S:207:ILE:HG23	1:S:211:ALA:HB3	1.95	0.47
1:U:283:THR:HG22	1:U:284:LEU:N	2.29	0.47
1:V:207:ILE:HG23	1:V:211:ALA:HB3	1.96	0.47
1:V:259:ILE:HD13	1:V:316:ILE:CG2	2.43	0.47
1:C:45:PRO:HB3	1:C:58:VAL:HG11	1.96	0.47
1:C:257:LEU:HD22	1:C:259:ILE:CG2	2.43	0.47
1:H:92:LYS:HE3	1:H:92:LYS:CA	2.45	0.47
1:I:247:LYS:HB2	1:I:247:LYS:HZ2	1.78	0.47
1:M:75:LYS:HE3	1:M:79:GLY:O	2.14	0.47
1:N:75:LYS:HE3	1:N:79:GLY:O	2.13	0.47
1:P:257:LEU:HD22	1:P:259:ILE:CG2	2.45	0.47
1:T:45:PRO:HB3	1:T:58:VAL:HG11	1.96	0.47
1:E:45:PRO:HB3	1:E:58:VAL:HG11	1.96	0.47
1:I:192:LYS:HB3	1:I:192:LYS:HZ3	1.76	0.47
1:J:257:LEU:HD22	1:J:259:ILE:CG2	2.45	0.47
1:Q:75:LYS:HE3	1:Q:79:GLY:O	2.15	0.47
1:S:257:LEU:HD22	1:S:259:ILE:CG2	2.45	0.47
1:W:45:PRO:HB3	1:W:58:VAL:HG11	1.95	0.47
1:W:257:LEU:HD22	1:W:259:ILE:CG2	2.45	0.47
1:G:45:PRO:HB3	1:G:58:VAL:HG11	1.95	0.47
1:G:75:LYS:HE3	1:G:79:GLY:O	2.14	0.47
1:I:126:VAL:HG22	1:I:256:SER:HB2	1.97	0.47
1:N:259:ILE:HD13	1:N:316:ILE:CG2	2.42	0.47
1:P:169:PHE:O	1:P:172:PHE:HB3	2.15	0.47
1:Q:313:GLN:HE22	1:Q:317:LYS:HZ3	1.63	0.47
1:S:41:GLU:O	1:S:42:ASP:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:147:LEU:O	1:T:184:ARG:NH2	2.48	0.47
1:W:207:ILE:HG23	1:W:211:ALA:HB3	1.96	0.47
1:W:243:VAL:O	1:W:247:LYS:HG3	2.15	0.47
1:B:252:SER:HB3	1:C:192:LYS:HE3	1.97	0.47
1:G:237:SER:HB3	1:G:242:ILE:CD1	2.26	0.47
1:I:139:LEU:HD13	1:I:139:LEU:C	2.40	0.47
1:L:137:THR:HB	1:L:138:PRO:HD3	1.97	0.47
1:M:45:PRO:HB3	1:M:58:VAL:HG11	1.96	0.47
1:R:169:PHE:O	1:R:172:PHE:HB3	2.14	0.47
1:A:126:VAL:HG22	1:A:256:SER:HB2	1.97	0.47
1:E:310:LYS:HD2	1:F:132:GLY:O	2.14	0.47
1:G:41:GLU:O	1:G:42:ASP:HB2	2.15	0.47
1:H:238:ASN:N	1:H:238:ASN:ND2	2.62	0.47
1:I:192:LYS:HB3	1:I:192:LYS:HZ2	1.80	0.47
1:R:281:THR:HG22	1:R:306:GLN:O	2.15	0.47
1:V:45:PRO:HB3	1:V:58:VAL:HG11	1.96	0.47
1:N:137:THR:HB	1:N:138:PRO:HD3	1.96	0.47
1:Q:243:VAL:O	1:Q:247:LYS:HG3	2.15	0.47
1:R:41:GLU:O	1:R:42:ASP:HB2	2.14	0.47
1:R:207:ILE:HG23	1:R:211:ALA:HB3	1.97	0.47
1:T:41:GLU:O	1:T:42:ASP:HB2	2.15	0.47
1:B:45:PRO:HB3	1:B:58:VAL:HG11	1.96	0.46
1:B:247:LYS:HZ2	1:B:321:LEU:HB2	1.79	0.46
1:F:75:LYS:HE3	1:F:79:GLY:O	2.15	0.46
1:G:169:PHE:O	1:G:172:PHE:HB3	2.14	0.46
1:G:313:GLN:HE22	1:G:317:LYS:HZ3	1.61	0.46
1:O:252:SER:HB3	1:P:192:LYS:CE	2.45	0.46
1:O:257:LEU:HD22	1:O:259:ILE:CG2	2.45	0.46
1:P:45:PRO:HB3	1:P:58:VAL:HG11	1.97	0.46
1:Q:236:THR:HG22	1:Q:237:SER:N	2.30	0.46
1:Q:257:LEU:HD22	1:Q:259:ILE:CG2	2.44	0.46
1:T:75:LYS:HE3	1:T:79:GLY:O	2.15	0.46
1:C:259:ILE:HD13	1:C:316:ILE:CG2	2.41	0.46
1:F:272:ARG:HA	2:F:2131:HOH:O	2.15	0.46
1:G:236:THR:HG22	1:G:237:SER:N	2.31	0.46
1:J:45:PRO:HB3	1:J:58:VAL:HG11	1.97	0.46
1:J:75:LYS:HE3	1:J:79:GLY:O	2.16	0.46
1:K:192:LYS:O	1:K:194:VAL:N	2.47	0.46
1:N:192:LYS:O	1:N:194:VAL:N	2.48	0.46
1:N:243:VAL:O	1:N:247:LYS:HG3	2.15	0.46
1:O:310:LYS:HD2	1:P:132:GLY:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:259:ILE:HD13	1:S:316:ILE:CG2	2.41	0.46
1:V:281:THR:HG22	1:V:306:GLN:O	2.16	0.46
1:C:126:VAL:HG22	1:C:256:SER:HB2	1.97	0.46
1:F:236:THR:HG22	1:F:237:SER:N	2.30	0.46
1:N:252:SER:HB3	1:O:192:LYS:CE	2.45	0.46
1:R:278:GLN:HB2	2:R:2095:HOH:O	2.14	0.46
1:T:236:THR:HG22	1:T:237:SER:N	2.29	0.46
1:T:251:ARG:HH11	1:U:236:THR:HG22	1.80	0.46
1:A:92:LYS:HE3	1:A:92:LYS:CA	2.45	0.46
1:B:190:SER:OG	1:B:192:LYS:HB3	2.15	0.46
1:M:147:LEU:O	1:M:184:ARG:NH2	2.48	0.46
1:M:192:LYS:HE3	1:R:252:SER:HB3	1.98	0.46
1:M:236:THR:HB	2:M:2125:HOH:O	2.15	0.46
1:O:192:LYS:O	1:O:194:VAL:N	2.47	0.46
1:T:243:VAL:O	1:T:247:LYS:HG3	2.16	0.46
1:T:257:LEU:HD22	1:T:259:ILE:CG2	2.46	0.46
1:U:126:VAL:HG22	1:U:256:SER:HB2	1.96	0.46
1:V:192:LYS:O	1:V:194:VAL:N	2.48	0.46
1:A:247:LYS:HB2	1:A:247:LYS:HZ2	1.79	0.46
1:C:41:GLU:O	1:C:42:ASP:HB2	2.15	0.46
1:D:92:LYS:HA	1:D:92:LYS:CE	2.45	0.46
2:I:2073:HOH:O	1:N:291:HIS:HE1	1.99	0.46
1:O:237:SER:HB3	1:O:242:ILE:CD1	2.25	0.46
1:P:207:ILE:HG23	1:P:211:ALA:HB3	1.96	0.46
1:W:75:LYS:HE3	1:W:79:GLY:O	2.15	0.46
1:B:236:THR:HG22	1:B:237:SER:N	2.31	0.46
1:C:169:PHE:O	1:C:172:PHE:HB3	2.15	0.46
1:C:281:THR:HG22	1:C:306:GLN:O	2.16	0.46
1:E:126:VAL:HG22	1:E:256:SER:HB2	1.98	0.46
1:H:45:PRO:HB3	1:H:58:VAL:HG11	1.98	0.46
1:I:12:LYS:HG3	2:I:2013:HOH:O	2.16	0.46
1:I:283:THR:HG22	1:I:284:LEU:N	2.31	0.46
1:K:87:GLU:HB3	1:K:92:LYS:HD2	1.98	0.46
1:L:236:THR:O	1:L:237:SER:C	2.59	0.46
1:L:283:THR:HG22	1:L:284:LEU:N	2.31	0.46
1:W:169:PHE:O	1:W:172:PHE:HB3	2.15	0.46
1:H:126:VAL:HG22	1:H:256:SER:HB2	1.97	0.46
1:K:41:GLU:O	1:K:42:ASP:HB2	2.15	0.46
1:Q:281:THR:HG22	1:Q:306:GLN:O	2.16	0.46
1:S:75:LYS:HE3	1:S:79:GLY:O	2.14	0.46
1:U:92:LYS:HA	1:U:92:LYS:CE	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:236:THR:O	1:D:237:SER:C	2.59	0.46
1:M:192:LYS:O	1:M:194:VAL:N	2.48	0.46
1:O:45:PRO:HB3	1:O:58:VAL:HG11	1.97	0.46
1:P:41:GLU:O	1:P:42:ASP:HB2	2.16	0.46
1:P:191:LEU:HD23	1:P:191:LEU:HA	1.81	0.46
1:S:30:PHE:CG	1:S:184:ARG:HG3	2.51	0.46
1:S:281:THR:HG22	1:S:306:GLN:O	2.16	0.46
1:X:92:LYS:HE3	1:X:92:LYS:CA	2.45	0.46
1:A:139:LEU:HD13	1:A:139:LEU:C	2.40	0.46
1:B:87:GLU:HB3	1:B:92:LYS:HD2	1.97	0.46
1:D:193:ASN:HA	2:D:2101:HOH:O	2.15	0.46
1:E:87:GLU:HB3	1:E:92:LYS:HD2	1.98	0.46
1:K:40:VAL:HA	2:K:2016:HOH:O	2.15	0.46
1:P:236:THR:HG22	1:P:237:SER:N	2.31	0.46
1:R:192:LYS:O	1:R:194:VAL:N	2.49	0.46
1:V:126:VAL:HG22	1:V:256:SER:HB2	1.97	0.46
1:X:137:THR:HB	1:X:138:PRO:HD3	1.98	0.46
1:X:236:THR:O	1:X:237:SER:C	2.59	0.46
1:A:238:ASN:N	1:A:238:ASN:ND2	2.63	0.46
1:D:240:ASP:C	1:D:242:ILE:N	2.68	0.46
1:E:192:LYS:O	1:E:194:VAL:N	2.49	0.46
1:J:236:THR:HG22	1:J:237:SER:N	2.31	0.46
1:K:244:GLU:HG2	1:L:238:ASN:ND2	2.30	0.46
1:K:247:LYS:HZ3	1:K:321:LEU:HB2	1.81	0.46
1:L:216:SER:HB3	2:L:2062:HOH:O	2.15	0.46
1:L:287:SER:OG	1:L:297:HIS:CE1	2.67	0.46
1:M:281:THR:HG22	1:M:306:GLN:O	2.16	0.46
1:O:126:VAL:HG22	1:O:256:SER:HB2	1.97	0.46
1:Q:270:LEU:HD22	1:Q:270:LEU:N	2.31	0.46
1:R:243:VAL:O	1:R:247:LYS:HG3	2.16	0.46
1:V:286:THR:HB	1:V:294:LEU:CD1	2.46	0.46
1:W:236:THR:HG22	1:W:237:SER:N	2.31	0.46
1:C:243:VAL:O	1:C:247:LYS:HG3	2.16	0.45
1:H:240:ASP:O	1:H:242:ILE:N	2.48	0.45
1:K:169:PHE:O	1:K:172:PHE:HB3	2.16	0.45
1:K:243:VAL:O	1:K:247:LYS:HG3	2.16	0.45
1:K:251:ARG:HH11	1:L:236:THR:HG22	1.81	0.45
1:N:159:GLY:HA3	1:N:193:ASN:ND2	2.31	0.45
1:U:236:THR:O	1:U:237:SER:C	2.59	0.45
1:W:270:LEU:N	1:W:270:LEU:HD22	2.31	0.45
1:X:139:LEU:HD13	1:X:139:LEU:C	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:THR:O	1:A:237:SER:C	2.59	0.45
1:L:238:ASN:N	1:L:238:ASN:ND2	2.62	0.45
1:M:87:GLU:HB3	1:M:92:LYS:HD2	1.99	0.45
1:N:126:VAL:HG22	1:N:256:SER:HB2	1.98	0.45
1:N:281:THR:HG22	1:N:306:GLN:O	2.17	0.45
1:P:126:VAL:HG22	1:P:256:SER:HB2	1.97	0.45
1:T:192:LYS:O	1:T:194:VAL:N	2.48	0.45
1:V:270:LEU:HD22	1:V:270:LEU:N	2.31	0.45
1:W:41:GLU:O	1:W:42:ASP:HB2	2.15	0.45
1:C:60:ASP:OD2	1:C:64:GLN:HB3	2.17	0.45
1:C:207:ILE:HG23	1:C:211:ALA:HB3	1.98	0.45
1:C:248:GLU:OE2	1:D:236:THR:HG21	2.17	0.45
1:D:139:LEU:C	1:D:139:LEU:HD13	2.42	0.45
1:E:283:THR:HG22	1:E:284:LEU:N	2.31	0.45
1:L:178:ARG:HB2	1:L:178:ARG:HH11	1.81	0.45
1:P:243:VAL:O	1:P:247:LYS:HG3	2.15	0.45
1:S:192:LYS:O	1:S:194:VAL:N	2.49	0.45
1:S:286:THR:HB	1:S:294:LEU:CD1	2.46	0.45
1:U:240:ASP:O	1:U:242:ILE:N	2.48	0.45
1:A:178:ARG:NH2	1:F:80:SER:HA	2.32	0.45
1:B:281:THR:HG22	1:B:306:GLN:O	2.17	0.45
1:E:243:VAL:O	1:E:247:LYS:HG3	2.15	0.45
1:H:139:LEU:HD13	1:H:139:LEU:C	2.42	0.45
1:J:243:VAL:O	1:J:247:LYS:HG3	2.17	0.45
1:M:207:ILE:HG23	1:M:211:ALA:HB3	1.98	0.45
1:M:243:VAL:O	1:M:247:LYS:HG3	2.16	0.45
1:O:236:THR:HG22	1:O:237:SER:N	2.32	0.45
1:Q:41:GLU:O	1:Q:42:ASP:HB2	2.15	0.45
1:C:191:LEU:HA	1:C:191:LEU:HD23	1.80	0.45
1:E:236:THR:HG22	1:E:237:SER:N	2.30	0.45
1:G:281:THR:HG22	1:G:306:GLN:O	2.17	0.45
1:I:238:ASN:N	1:I:238:ASN:ND2	2.63	0.45
1:K:126:VAL:HG22	1:K:256:SER:HB2	1.99	0.45
1:M:236:THR:HG22	1:M:237:SER:N	2.31	0.45
1:O:243:VAL:O	1:O:247:LYS:HG3	2.16	0.45
1:O:313:GLN:HE22	1:O:317:LYS:HZ3	1.64	0.45
1:P:192:LYS:O	1:P:194:VAL:N	2.49	0.45
1:S:87:GLU:HB3	1:S:92:LYS:HD2	1.98	0.45
1:U:270:LEU:HD22	1:U:270:LEU:N	2.31	0.45
1:V:87:GLU:HB3	1:V:92:LYS:HD2	1.98	0.45
1:V:207:ILE:HD13	2:V:2083:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:236:THR:HG22	1:V:237:SER:N	2.31	0.45
1:B:169:PHE:O	1:B:172:PHE:HB3	2.17	0.45
1:C:87:GLU:HB3	1:C:92:LYS:HD2	1.98	0.45
1:C:286:THR:HB	1:C:294:LEU:CD1	2.47	0.45
1:C:314:THR:HG21	1:D:239:ASP:CG	2.42	0.45
1:F:126:VAL:HG22	1:F:256:SER:HB2	1.99	0.45
1:H:270:LEU:HD22	1:H:270:LEU:N	2.31	0.45
1:Q:87:GLU:HB3	1:Q:92:LYS:HD2	1.99	0.45
1:W:87:GLU:HB3	1:W:92:LYS:HD2	1.99	0.45
1:X:45:PRO:HB3	1:X:58:VAL:HG11	1.98	0.45
1:A:137:THR:HB	1:A:138:PRO:HD3	1.99	0.45
1:A:240:ASP:O	1:A:242:ILE:N	2.49	0.45
1:D:283:THR:HG22	1:D:284:LEU:N	2.32	0.45
1:H:92:LYS:HA	1:H:92:LYS:CE	2.47	0.45
1:J:192:LYS:O	1:J:194:VAL:N	2.49	0.45
1:K:184:ARG:HD3	2:K:2063:HOH:O	2.15	0.45
1:L:234:ASN:C	1:L:236:THR:N	2.75	0.45
1:N:169:PHE:O	1:N:172:PHE:HB3	2.17	0.45
1:G:243:VAL:O	1:G:247:LYS:HG3	2.17	0.45
1:K:236:THR:HG22	1:K:237:SER:N	2.31	0.45
1:O:169:PHE:O	1:O:172:PHE:HB3	2.16	0.45
1:P:87:GLU:HB3	1:P:92:LYS:HD2	1.99	0.45
1:P:269:VAL:O	1:P:281:THR:HA	2.17	0.45
1:Q:259:ILE:HD13	1:Q:316:ILE:CG2	2.41	0.45
1:T:270:LEU:HD22	1:T:270:LEU:N	2.32	0.45
1:V:41:GLU:O	1:V:42:ASP:HB2	2.16	0.45
1:W:259:ILE:HD13	1:W:316:ILE:CG2	2.41	0.45
1:W:281:THR:HG22	1:W:306:GLN:O	2.17	0.45
1:C:75:LYS:HE3	1:C:79:GLY:O	2.16	0.45
1:F:30:PHE:CG	1:F:184:ARG:HG3	2.51	0.45
1:G:270:LEU:HD22	1:G:270:LEU:N	2.31	0.45
1:J:126:VAL:HG22	1:J:256:SER:HB2	1.99	0.45
1:P:30:PHE:CG	1:P:184:ARG:HG3	2.52	0.45
1:R:236:THR:HG22	1:R:237:SER:N	2.32	0.45
1:B:207:ILE:HG23	1:B:211:ALA:HB3	1.98	0.45
1:B:283:THR:HG22	1:B:284:LEU:N	2.32	0.45
1:B:286:THR:HB	1:B:294:LEU:CD1	2.47	0.45
1:F:87:GLU:HB3	1:F:92:LYS:HD2	1.98	0.45
1:H:287:SER:OG	1:H:297:HIS:CE1	2.68	0.45
1:Q:169:PHE:O	1:Q:172:PHE:HB3	2.16	0.45
1:T:126:VAL:HG22	1:T:256:SER:HB2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:259:ILE:HD13	1:T:316:ILE:CG2	2.42	0.45
1:U:195:ILE:O	1:U:195:ILE:HG22	2.17	0.45
1:C:192:LYS:O	1:C:194:VAL:N	2.48	0.44
1:D:234:ASN:C	1:D:236:THR:N	2.75	0.44
1:D:287:SER:OG	1:D:297:HIS:CE1	2.70	0.44
1:G:87:GLU:HB3	1:G:92:LYS:HD2	1.99	0.44
1:H:137:THR:HB	1:H:138:PRO:HD3	1.98	0.44
1:H:234:ASN:C	1:H:236:THR:N	2.75	0.44
1:H:283:THR:HG22	1:H:284:LEU:N	2.32	0.44
1:J:270:LEU:HD22	1:J:270:LEU:N	2.32	0.44
1:N:191:LEU:HD23	1:N:191:LEU:HA	1.83	0.44
1:O:30:PHE:CG	1:O:184:ARG:HG3	2.52	0.44
1:R:283:THR:HG22	1:R:284:LEU:N	2.32	0.44
1:V:243:VAL:O	1:V:247:LYS:HG3	2.17	0.44
1:X:195:ILE:O	1:X:195:ILE:HG22	2.17	0.44
1:D:270:LEU:N	1:D:270:LEU:HD22	2.32	0.44
1:P:248:GLU:OE1	1:Q:236:THR:CG2	2.65	0.44
1:U:269:VAL:O	1:U:281:THR:HA	2.18	0.44
1:V:191:LEU:HD23	1:V:191:LEU:HA	1.82	0.44
1:V:283:THR:HG22	1:V:284:LEU:N	2.32	0.44
1:E:270:LEU:HD22	1:E:270:LEU:N	2.32	0.44
1:I:92:LYS:HE3	1:I:92:LYS:CA	2.44	0.44
1:I:236:THR:O	1:I:237:SER:C	2.59	0.44
1:L:92:LYS:HA	1:L:92:LYS:CE	2.47	0.44
1:O:87:GLU:HB3	1:O:92:LYS:HD2	1.99	0.44
1:O:191:LEU:HD23	1:O:191:LEU:HA	1.83	0.44
1:Q:283:THR:HG22	1:Q:284:LEU:N	2.32	0.44
1:Q:286:THR:HB	1:Q:294:LEU:CD1	2.47	0.44
1:R:257:LEU:HD22	1:R:259:ILE:CG2	2.47	0.44
1:R:317:LYS:HD3	1:R:320:GLU:OE2	2.18	0.44
1:S:169:PHE:O	1:S:172:PHE:HB3	2.17	0.44
1:W:147:LEU:O	1:W:184:ARG:NH2	2.50	0.44
1:A:270:LEU:HD22	1:A:270:LEU:N	2.32	0.44
1:B:131:LYS:HD3	2:B:2089:HOH:O	2.18	0.44
1:C:30:PHE:CG	1:C:184:ARG:HG3	2.52	0.44
1:D:195:ILE:O	1:D:195:ILE:HG22	2.18	0.44
1:F:169:PHE:O	1:F:172:PHE:HB3	2.17	0.44
1:F:283:THR:HG22	1:F:284:LEU:N	2.32	0.44
1:G:192:LYS:O	1:G:194:VAL:N	2.48	0.44
1:I:270:LEU:HD22	1:I:270:LEU:N	2.33	0.44
1:J:87:GLU:HB3	1:J:92:LYS:HD2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:30:PHE:CG	1:K:184:ARG:HG3	2.52	0.44
1:K:207:ILE:HG23	1:K:211:ALA:HB3	1.98	0.44
1:P:216:SER:HB3	2:Q:2054:HOH:O	2.17	0.44
1:Q:191:LEU:HD23	1:Q:191:LEU:HA	1.85	0.44
1:T:87:GLU:HB3	1:T:92:LYS:HD2	1.99	0.44
1:X:270:LEU:HD22	1:X:270:LEU:N	2.33	0.44
1:B:126:VAL:HG22	1:B:256:SER:HB2	2.00	0.44
1:C:236:THR:HG22	1:C:237:SER:N	2.32	0.44
1:C:237:SER:HB3	1:C:242:ILE:CD1	2.26	0.44
1:D:216:SER:HB3	2:E:2097:HOH:O	2.17	0.44
1:E:257:LEU:HD22	1:E:259:ILE:CG2	2.47	0.44
1:E:281:THR:HG22	1:E:306:GLN:O	2.17	0.44
1:I:195:ILE:O	1:I:195:ILE:HG22	2.18	0.44
1:J:169:PHE:O	1:J:172:PHE:HB3	2.18	0.44
1:Q:30:PHE:CG	1:Q:184:ARG:HG3	2.52	0.44
1:Q:299:SER:HA	2:Q:2091:HOH:O	2.18	0.44
1:Q:317:LYS:HD3	1:Q:320:GLU:OE2	2.18	0.44
1:V:247:LYS:HZ2	1:V:321:LEU:HB2	1.82	0.44
1:W:126:VAL:HG22	1:W:256:SER:HB2	2.00	0.44
1:W:216:SER:HB2	2:X:2105:HOH:O	2.15	0.44
1:X:269:VAL:O	1:X:281:THR:HA	2.18	0.44
1:A:92:LYS:HA	1:A:92:LYS:CE	2.46	0.44
1:C:270:LEU:HD22	1:C:270:LEU:N	2.32	0.44
1:G:60:ASP:OD2	1:G:64:GLN:HB3	2.18	0.44
1:L:240:ASP:O	1:L:242:ILE:N	2.48	0.44
1:M:1:MET:HA	2:N:2145:HOH:O	2.17	0.44
1:M:192:LYS:CE	1:R:252:SER:HB3	2.47	0.44
1:M:257:LEU:HD22	1:M:259:ILE:CG2	2.46	0.44
1:U:137:THR:HB	1:U:138:PRO:HD3	1.99	0.44
1:B:191:LEU:HD23	1:B:191:LEU:HA	1.80	0.44
1:F:281:THR:HG22	1:F:306:GLN:O	2.17	0.44
1:I:234:ASN:C	1:I:236:THR:N	2.76	0.44
1:M:169:PHE:O	1:M:172:PHE:HB3	2.18	0.44
1:N:45:PRO:HB3	1:N:58:VAL:HG11	1.98	0.44
1:O:60:ASP:OD2	1:O:64:GLN:HB3	2.18	0.44
1:S:236:THR:HG22	1:S:237:SER:N	2.32	0.44
1:T:30:PHE:CG	1:T:184:ARG:HG3	2.53	0.44
1:T:281:THR:HG22	1:T:306:GLN:O	2.18	0.44
1:A:45:PRO:HB3	1:A:58:VAL:HG11	1.99	0.44
1:A:119:HIS:HA	2:A:2049:HOH:O	2.17	0.44
1:B:30:PHE:CG	1:B:184:ARG:HG3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:242:ILE:O	1:D:245:LEU:HB3	2.18	0.44
1:F:313:GLN:HE22	1:F:317:LYS:HZ3	1.66	0.44
1:I:137:THR:HB	1:I:138:PRO:HD3	2.00	0.44
1:I:242:ILE:O	1:I:245:LEU:HB3	2.18	0.44
1:L:92:LYS:HE3	1:L:92:LYS:CA	2.45	0.44
1:M:270:LEU:HD22	1:M:270:LEU:N	2.33	0.44
1:N:87:GLU:HB3	1:N:92:LYS:HD2	1.99	0.44
1:N:192:LYS:HG2	1:N:193:ASN:N	2.33	0.44
1:O:139:LEU:C	1:O:139:LEU:HD13	2.43	0.44
1:P:75:LYS:HE3	1:P:79:GLY:O	2.17	0.44
1:P:281:THR:HG22	1:P:306:GLN:O	2.17	0.44
1:Q:192:LYS:HG2	1:Q:193:ASN:N	2.33	0.44
1:U:129:THR:OG1	1:U:130:GLY:N	2.50	0.44
1:V:192:LYS:HG2	1:V:193:ASN:N	2.33	0.44
1:A:240:ASP:OD2	1:A:241:LYS:N	2.51	0.44
1:K:242:ILE:O	1:K:246:VAL:HG23	2.18	0.44
1:N:317:LYS:HD3	1:N:320:GLU:OE2	2.18	0.44
1:O:192:LYS:HG2	1:O:193:ASN:N	2.33	0.44
1:S:270:LEU:HD22	1:S:270:LEU:N	2.33	0.44
1:S:272:ARG:NH1	2:S:2122:HOH:O	2.41	0.44
1:V:248:GLU:OE1	1:W:236:THR:CG2	2.66	0.44
1:V:269:VAL:O	1:V:281:THR:HA	2.18	0.44
1:W:251:ARG:HH11	1:X:236:THR:CG2	2.30	0.44
1:W:286:THR:HB	1:W:294:LEU:CD1	2.47	0.44
1:A:234:ASN:C	1:A:236:THR:N	2.76	0.43
1:A:269:VAL:O	1:A:281:THR:HA	2.18	0.43
1:L:269:VAL:O	1:L:281:THR:HA	2.17	0.43
1:M:236:THR:HG22	1:R:251:ARG:NH1	2.33	0.43
1:O:286:THR:HB	1:O:294:LEU:CD1	2.47	0.43
1:R:75:LYS:HE3	1:R:79:GLY:O	2.18	0.43
1:R:270:LEU:HD22	1:R:270:LEU:N	2.33	0.43
1:S:126:VAL:HG22	1:S:256:SER:HB2	1.98	0.43
1:V:139:LEU:HD13	1:V:139:LEU:C	2.42	0.43
1:W:314:THR:HG21	1:X:239:ASP:HB2	2.00	0.43
1:B:317:LYS:HD3	1:B:320:GLU:OE2	2.18	0.43
1:D:242:ILE:C	1:D:244:GLU:H	2.26	0.43
1:D:269:VAL:O	1:D:281:THR:HA	2.18	0.43
1:G:283:THR:HG22	1:G:284:LEU:N	2.33	0.43
1:H:178:ARG:HB2	1:H:178:ARG:HH11	1.83	0.43
1:H:195:ILE:HG22	1:H:195:ILE:O	2.18	0.43
1:I:4:LEU:HD23	1:J:154:ALA:HA	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:103:THR:HG21	2:I:2090:HOH:O	2.18	0.43
1:I:247:LYS:C	1:I:249:ALA:N	2.76	0.43
1:I:269:VAL:O	1:I:281:THR:HA	2.18	0.43
1:M:126:VAL:HG22	1:M:256:SER:HB2	2.00	0.43
1:N:257:LEU:HD22	1:N:259:ILE:CG2	2.48	0.43
1:S:178:ARG:HD2	2:S:2096:HOH:O	2.18	0.43
1:S:313:GLN:HE22	1:S:317:LYS:HZ3	1.66	0.43
1:W:192:LYS:O	1:W:194:VAL:N	2.49	0.43
1:W:237:SER:HB3	1:W:242:ILE:CD1	2.25	0.43
1:A:209:ARG:HD3	2:A:2080:HOH:O	2.18	0.43
1:D:238:ASN:N	1:D:238:ASN:ND2	2.63	0.43
1:E:30:PHE:CG	1:E:184:ARG:HG3	2.54	0.43
1:E:317:LYS:HD3	1:E:320:GLU:OE2	2.18	0.43
1:H:236:THR:O	1:H:237:SER:C	2.59	0.43
1:J:281:THR:HG22	1:J:306:GLN:O	2.18	0.43
1:K:269:VAL:O	1:K:281:THR:HA	2.19	0.43
1:K:270:LEU:HD22	1:K:270:LEU:N	2.33	0.43
1:L:240:ASP:C	1:L:242:ILE:N	2.67	0.43
1:P:270:LEU:HD22	1:P:270:LEU:N	2.32	0.43
1:S:243:VAL:O	1:S:247:LYS:HG3	2.19	0.43
1:U:45:PRO:HB3	1:U:58:VAL:HG11	2.00	0.43
1:X:283:THR:HG22	1:X:284:LEU:N	2.33	0.43
1:A:115:GLU:HG2	2:A:2048:HOH:O	2.18	0.43
1:F:139:LEU:HD13	1:F:139:LEU:C	2.43	0.43
1:F:243:VAL:O	1:F:247:LYS:HG3	2.18	0.43
1:I:40:VAL:HG12	1:I:44:THR:HB	2.00	0.43
1:I:92:LYS:HA	1:I:92:LYS:CE	2.46	0.43
1:L:247:LYS:HB2	1:L:247:LYS:HZ2	1.79	0.43
1:S:237:SER:HB3	1:S:242:ILE:CD1	2.24	0.43
1:T:139:LEU:C	1:T:139:LEU:HD13	2.43	0.43
1:U:242:ILE:C	1:U:244:GLU:H	2.27	0.43
1:V:30:PHE:CG	1:V:184:ARG:HG3	2.54	0.43
1:X:247:LYS:C	1:X:249:ALA:N	2.77	0.43
1:A:242:ILE:C	1:A:244:GLU:H	2.26	0.43
1:C:269:VAL:O	1:C:281:THR:HA	2.18	0.43
1:F:216:SER:HB3	2:F:2120:HOH:O	2.18	0.43
1:G:192:LYS:HG2	1:G:193:ASN:N	2.34	0.43
1:J:247:LYS:HZ2	1:J:321:LEU:HB2	1.84	0.43
1:L:40:VAL:HG12	1:L:44:THR:HB	2.01	0.43
1:M:317:LYS:HD3	1:M:320:GLU:OE2	2.18	0.43
1:Q:70:LYS:HA	2:Q:2022:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:139:LEU:HD13	1:Q:139:LEU:C	2.43	0.43
1:Q:269:VAL:O	1:Q:281:THR:HA	2.19	0.43
1:W:242:ILE:O	1:W:246:VAL:HG23	2.18	0.43
1:B:192:LYS:HG2	1:B:193:ASN:N	2.34	0.43
1:C:192:LYS:HG2	1:C:193:ASN:N	2.33	0.43
1:D:242:ILE:C	1:D:244:GLU:N	2.77	0.43
1:G:252:SER:OG	1:H:236:THR:HG21	2.18	0.43
1:H:242:ILE:O	1:H:245:LEU:HB3	2.19	0.43
1:J:248:GLU:OE1	1:K:236:THR:HG22	2.19	0.43
1:K:281:THR:HG22	1:K:306:GLN:O	2.18	0.43
1:L:195:ILE:O	1:L:195:ILE:HG22	2.17	0.43
1:O:207:ILE:HD13	1:O:207:ILE:HA	1.92	0.43
1:S:192:LYS:HG2	1:S:193:ASN:N	2.34	0.43
1:B:243:VAL:O	1:B:247:LYS:HG3	2.19	0.43
1:F:237:SER:HB3	1:F:242:ILE:CD1	2.24	0.43
1:F:270:LEU:HD22	1:F:270:LEU:N	2.34	0.43
1:G:317:LYS:HD3	1:G:320:GLU:OE2	2.19	0.43
1:L:41:GLU:HB2	1:L:44:THR:OG1	2.19	0.43
1:L:42:ASP:C	1:L:44:THR:H	2.27	0.43
1:M:60:ASP:OD2	1:M:64:GLN:HB3	2.18	0.43
1:M:286:THR:HB	1:M:294:LEU:CD1	2.48	0.43
1:T:286:THR:HB	1:T:294:LEU:CD1	2.47	0.43
1:V:252:SER:HB3	1:W:192:LYS:HE3	1.99	0.43
1:A:195:ILE:O	1:A:195:ILE:HG22	2.18	0.43
1:B:60:ASP:OD2	1:B:64:GLN:HB3	2.18	0.43
1:G:30:PHE:CG	1:G:184:ARG:HG3	2.54	0.43
1:G:126:VAL:HG22	1:G:256:SER:HB2	2.01	0.43
1:H:242:ILE:C	1:H:244:GLU:H	2.26	0.43
1:H:247:LYS:C	1:H:249:ALA:N	2.77	0.43
1:P:192:LYS:HG2	1:P:193:ASN:N	2.33	0.43
1:R:139:LEU:C	1:R:139:LEU:HD13	2.43	0.43
1:R:192:LYS:HG2	1:R:193:ASN:N	2.34	0.43
1:R:269:VAL:O	1:R:281:THR:HA	2.18	0.43
1:T:269:VAL:O	1:T:281:THR:HA	2.18	0.43
1:V:317:LYS:HD3	1:V:320:GLU:OE2	2.19	0.43
1:X:242:ILE:C	1:X:244:GLU:H	2.26	0.43
1:X:247:LYS:HB2	1:X:247:LYS:HZ3	1.81	0.43
1:C:138:PRO:HD3	2:C:2060:HOH:O	2.19	0.43
1:C:283:THR:HG22	1:C:284:LEU:N	2.34	0.43
1:E:139:LEU:C	1:E:139:LEU:HD13	2.44	0.43
1:E:192:LYS:HG2	1:E:193:ASN:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:216:SER:HB2	2:F:2116:HOH:O	2.19	0.43
1:J:192:LYS:HG2	1:J:193:ASN:N	2.34	0.43
1:O:317:LYS:HD3	1:O:320:GLU:OE2	2.18	0.43
1:Q:242:ILE:O	1:Q:246:VAL:HG23	2.19	0.43
1:B:269:VAL:O	1:B:281:THR:HA	2.18	0.43
1:J:30:PHE:CG	1:J:184:ARG:HG3	2.54	0.43
1:K:286:THR:HB	1:K:294:LEU:CD1	2.48	0.43
1:M:237:SER:HB3	1:M:242:ILE:CD1	2.25	0.43
1:R:191:LEU:HD23	1:R:191:LEU:HA	1.81	0.43
1:T:283:THR:HG22	1:T:284:LEU:N	2.33	0.43
1:U:234:ASN:C	1:U:236:THR:N	2.76	0.43
1:A:242:ILE:O	1:A:245:LEU:HB3	2.18	0.42
1:B:67:VAL:HA	1:B:89:GLY:HA2	2.01	0.42
1:E:61:LYS:NZ	2:E:2030:HOH:O	2.52	0.42
1:E:269:VAL:O	1:E:281:THR:HA	2.19	0.42
1:I:240:ASP:O	1:I:242:ILE:N	2.50	0.42
1:I:242:ILE:C	1:I:244:GLU:N	2.77	0.42
1:J:60:ASP:OD2	1:J:64:GLN:HB3	2.19	0.42
1:J:237:SER:HB3	1:J:242:ILE:CD1	2.25	0.42
1:Q:192:LYS:O	1:Q:194:VAL:N	2.50	0.42
1:R:87:GLU:HB3	1:R:92:LYS:HD2	1.99	0.42
1:X:242:ILE:C	1:X:244:GLU:N	2.77	0.42
1:A:40:VAL:HG12	1:A:44:THR:HB	2.00	0.42
1:B:270:LEU:HD22	1:B:270:LEU:N	2.34	0.42
1:C:139:LEU:HD13	1:C:139:LEU:C	2.45	0.42
1:C:317:LYS:HD3	1:C:320:GLU:OE2	2.19	0.42
1:E:60:ASP:OD2	1:E:64:GLN:HB3	2.19	0.42
1:F:317:LYS:HD3	1:F:320:GLU:OE2	2.19	0.42
1:H:41:GLU:HB2	1:H:44:THR:OG1	2.18	0.42
1:Q:234:ASN:C	1:Q:236:THR:N	2.77	0.42
1:R:60:ASP:OD2	1:R:64:GLN:HB3	2.19	0.42
1:A:41:GLU:HB2	1:A:44:THR:OG1	2.19	0.42
1:F:192:LYS:HG2	1:F:193:ASN:N	2.34	0.42
1:J:242:ILE:O	1:J:246:VAL:HG23	2.19	0.42
1:K:192:LYS:HG2	1:K:193:ASN:N	2.34	0.42
1:L:247:LYS:C	1:L:249:ALA:N	2.77	0.42
1:R:67:VAL:HA	1:R:89:GLY:HA2	2.02	0.42
1:S:67:VAL:HA	1:S:89:GLY:HA2	2.02	0.42
1:S:286:THR:CB	1:S:294:LEU:HD11	2.49	0.42
1:T:192:LYS:HG2	1:T:193:ASN:N	2.34	0.42
1:U:242:ILE:O	1:U:245:LEU:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:242:ILE:C	1:U:244:GLU:N	2.77	0.42
1:W:192:LYS:HG2	1:W:193:ASN:N	2.34	0.42
1:X:40:VAL:HG12	1:X:44:THR:HB	2.01	0.42
1:X:92:LYS:HA	1:X:92:LYS:CE	2.46	0.42
1:A:41:GLU:O	1:A:42:ASP:CB	2.68	0.42
1:C:67:VAL:HA	1:C:89:GLY:HA2	2.02	0.42
1:D:247:LYS:C	1:D:249:ALA:N	2.77	0.42
1:E:237:SER:HB3	1:E:242:ILE:CD1	2.25	0.42
1:F:286:THR:HB	1:F:294:LEU:CD1	2.47	0.42
1:H:240:ASP:OD2	1:H:241:LYS:N	2.51	0.42
1:I:242:ILE:C	1:I:244:GLU:H	2.26	0.42
1:J:283:THR:HG22	1:J:284:LEU:N	2.34	0.42
1:L:242:ILE:O	1:L:245:LEU:HB3	2.20	0.42
1:M:242:ILE:O	1:M:246:VAL:HG23	2.18	0.42
1:N:139:LEU:HD13	1:N:139:LEU:C	2.44	0.42
1:U:41:GLU:HB2	1:U:44:THR:OG1	2.20	0.42
1:W:269:VAL:O	1:W:281:THR:HA	2.19	0.42
1:W:317:LYS:HD3	1:W:320:GLU:OE2	2.19	0.42
1:D:40:VAL:HG12	1:D:44:THR:HB	2.01	0.42
1:K:317:LYS:HD3	1:K:320:GLU:OE2	2.19	0.42
1:P:75:LYS:HD3	2:P:2027:HOH:O	2.19	0.42
1:P:283:THR:HG22	1:P:284:LEU:N	2.33	0.42
1:S:283:THR:HG22	1:S:284:LEU:N	2.34	0.42
1:T:244:GLU:CG	1:U:238:ASN:ND2	2.82	0.42
1:U:40:VAL:HG12	1:U:44:THR:HB	2.00	0.42
1:U:287:SER:OG	1:U:297:HIS:CE1	2.69	0.42
1:V:242:ILE:O	1:V:246:VAL:HG23	2.20	0.42
1:G:286:THR:HB	1:G:294:LEU:CD1	2.48	0.42
1:H:290:GLU:HG2	1:H:291:HIS:CD2	2.55	0.42
1:L:45:PRO:HB3	1:L:58:VAL:HG11	2.00	0.42
1:M:234:ASN:C	1:M:236:THR:N	2.78	0.42
1:M:313:GLN:HE22	1:M:317:LYS:HZ3	1.67	0.42
1:N:242:ILE:O	1:N:246:VAL:HG23	2.20	0.42
1:O:65:ARG:HD2	2:O:2095:HOH:O	2.19	0.42
1:O:129:THR:OG1	1:O:130:GLY:N	2.52	0.42
1:O:251:ARG:HH11	1:P:236:THR:CG2	2.32	0.42
1:O:312:ILE:HG21	2:W:2092:HOH:O	2.20	0.42
1:Q:6:ASP:HB2	2:Q:2004:HOH:O	2.20	0.42
1:R:234:ASN:C	1:R:236:THR:N	2.78	0.42
1:A:236:THR:O	1:A:238:ASN:N	2.53	0.42
1:B:134:SER:HB3	1:B:267:TRP:CZ2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:129:THR:OG1	1:E:130:GLY:N	2.51	0.42
1:N:207:ILE:HD13	1:N:207:ILE:HA	1.91	0.42
1:O:115:GLU:HG2	2:O:2061:HOH:O	2.18	0.42
1:T:317:LYS:HD3	1:T:320:GLU:OE2	2.20	0.42
1:V:60:ASP:OD2	1:V:64:GLN:HB3	2.20	0.42
2:W:2085:HOH:O	1:X:238:ASN:HA	2.19	0.42
1:B:49:ILE:HG13	2:B:2029:HOH:O	2.19	0.42
1:D:42:ASP:C	1:D:44:THR:H	2.27	0.42
1:H:40:VAL:HG12	1:H:44:THR:HB	2.01	0.42
1:J:317:LYS:HD3	1:J:320:GLU:OE2	2.19	0.42
1:K:234:ASN:C	1:K:236:THR:N	2.78	0.42
1:M:192:LYS:HG2	1:M:193:ASN:N	2.34	0.42
1:O:251:ARG:HH11	1:P:236:THR:HG22	1.85	0.42
1:P:234:ASN:C	1:P:236:THR:N	2.77	0.42
1:P:317:LYS:HD3	1:P:320:GLU:OE2	2.20	0.42
1:Q:126:VAL:HG22	1:Q:256:SER:HB2	2.01	0.42
1:R:30:PHE:CG	1:R:184:ARG:HG3	2.54	0.42
1:A:247:LYS:C	1:A:249:ALA:N	2.77	0.42
1:B:216:SER:HB2	2:B:2084:HOH:O	2.19	0.42
1:D:41:GLU:HB2	1:D:44:THR:OG1	2.20	0.42
1:D:45:PRO:HB3	1:D:58:VAL:HG11	2.01	0.42
1:E:242:ILE:O	1:E:246:VAL:HG23	2.19	0.42
1:G:67:VAL:HA	1:G:89:GLY:HA2	2.01	0.42
1:G:242:ILE:O	1:G:246:VAL:HG23	2.20	0.42
1:H:242:ILE:C	1:H:244:GLU:N	2.77	0.42
1:N:286:THR:HB	1:N:294:LEU:CD1	2.50	0.42
1:O:270:LEU:N	1:O:270:LEU:HD22	2.34	0.42
1:P:6:ASP:H	1:P:9:SER:HG	1.68	0.42
1:P:252:SER:HB3	1:Q:192:LYS:HE3	2.01	0.42
1:U:247:LYS:C	1:U:249:ALA:N	2.78	0.42
1:W:30:PHE:CG	1:W:184:ARG:HG3	2.55	0.42
1:A:129:THR:OG1	1:A:130:GLY:N	2.50	0.42
1:A:178:ARG:HB2	1:A:178:ARG:HH11	1.85	0.42
1:F:207:ILE:HD13	1:F:207:ILE:HA	1.92	0.42
1:H:169:PHE:O	1:H:172:PHE:HB3	2.20	0.42
1:L:242:ILE:C	1:L:244:GLU:H	2.27	0.42
1:L:242:ILE:C	1:L:244:GLU:N	2.77	0.42
1:N:283:THR:HG22	1:N:284:LEU:N	2.34	0.42
1:O:286:THR:CB	1:O:294:LEU:HD11	2.50	0.42
1:Q:60:ASP:OD2	1:Q:64:GLN:HB3	2.20	0.42
1:R:126:VAL:HG22	1:R:256:SER:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:234:ASN:C	1:T:236:THR:N	2.78	0.42
1:W:244:GLU:OE1	1:X:238:ASN:ND2	2.53	0.42
1:X:240:ASP:C	1:X:242:ILE:N	2.68	0.42
1:C:65:ARG:HD2	2:C:2032:HOH:O	2.19	0.41
1:F:1:MET:HB2	1:F:78:ASP:OD1	2.20	0.41
1:M:67:VAL:HA	1:M:89:GLY:HA2	2.02	0.41
1:N:234:ASN:C	1:N:236:THR:N	2.78	0.41
1:P:286:THR:HB	1:P:294:LEU:CD1	2.48	0.41
1:S:60:ASP:OD2	1:S:64:GLN:HB3	2.20	0.41
1:T:248:GLU:OE2	1:U:236:THR:HG21	2.20	0.41
1:U:42:ASP:C	1:U:44:THR:H	2.28	0.41
1:V:237:SER:HB3	1:V:242:ILE:CD1	2.25	0.41
1:X:236:THR:O	1:X:238:ASN:N	2.53	0.41
1:H:269:VAL:O	1:H:281:THR:HA	2.19	0.41
1:I:41:GLU:O	1:I:42:ASP:CB	2.68	0.41
1:I:191:LEU:O	1:I:194:VAL:HG13	2.20	0.41
1:K:139:LEU:HD13	1:K:139:LEU:C	2.46	0.41
1:O:4:LEU:HD23	1:P:154:ALA:HA	2.01	0.41
1:O:67:VAL:HA	1:O:89:GLY:HA2	2.01	0.41
1:O:269:VAL:O	1:O:281:THR:HA	2.19	0.41
1:P:134:SER:HB3	1:P:267:TRP:CZ2	2.55	0.41
1:R:286:THR:HB	1:R:294:LEU:CD1	2.48	0.41
1:S:242:ILE:O	1:S:246:VAL:HG23	2.20	0.41
1:S:269:VAL:O	1:S:281:THR:HA	2.20	0.41
1:T:60:ASP:OD2	1:T:64:GLN:HB3	2.20	0.41
1:T:242:ILE:O	1:T:246:VAL:HG23	2.20	0.41
1:W:234:ASN:C	1:W:236:THR:N	2.77	0.41
1:X:242:ILE:O	1:X:245:LEU:HB3	2.19	0.41
1:D:286:THR:HB	1:D:294:LEU:CD1	2.49	0.41
1:E:248:GLU:OE1	1:F:236:THR:CG2	2.68	0.41
1:G:269:VAL:O	1:G:281:THR:HA	2.20	0.41
1:H:191:LEU:O	1:H:194:VAL:HG13	2.21	0.41
1:I:45:PRO:HB3	1:I:58:VAL:HG11	2.03	0.41
2:I:2073:HOH:O	1:N:291:HIS:CE1	2.73	0.41
1:L:240:ASP:OD2	1:L:241:LYS:N	2.51	0.41
1:P:5:TYR:HA	2:P:2003:HOH:O	2.19	0.41
1:P:60:ASP:OD2	1:P:64:GLN:HB3	2.20	0.41
1:S:234:ASN:C	1:S:236:THR:N	2.78	0.41
1:X:103:THR:C	2:X:2054:HOH:O	2.63	0.41
1:X:178:ARG:HB2	1:X:178:ARG:HH11	1.84	0.41
1:A:192:LYS:HB3	1:A:192:LYS:HZ2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:ILE:C	1:A:244:GLU:N	2.76	0.41
1:D:129:THR:OG1	1:D:130:GLY:N	2.50	0.41
1:Q:67:VAL:HA	1:Q:89:GLY:HA2	2.01	0.41
1:T:286:THR:CB	1:T:294:LEU:HD11	2.50	0.41
1:U:240:ASP:OD2	1:U:241:LYS:N	2.52	0.41
1:W:139:LEU:C	1:W:139:LEU:HD13	2.46	0.41
1:W:283:THR:HG22	1:W:284:LEU:N	2.35	0.41
1:D:62:ASN:ND2	2:D:2039:HOH:O	2.52	0.41
1:D:169:PHE:O	1:D:172:PHE:HB3	2.21	0.41
1:J:252:SER:HB3	1:K:192:LYS:HE3	2.02	0.41
1:J:269:VAL:O	1:J:281:THR:HA	2.20	0.41
1:M:134:SER:HB3	1:M:267:TRP:CZ2	2.55	0.41
1:O:234:ASN:C	1:O:236:THR:N	2.78	0.41
1:S:1:MET:HB2	1:S:78:ASP:OD1	2.21	0.41
1:U:191:LEU:O	1:U:194:VAL:HG13	2.20	0.41
1:V:67:VAL:HA	1:V:89:GLY:HA2	2.03	0.41
1:V:207:ILE:HD13	1:V:207:ILE:HA	1.92	0.41
1:W:244:GLU:CG	1:X:238:ASN:ND2	2.83	0.41
1:X:41:GLU:HB2	1:X:44:THR:OG1	2.20	0.41
1:A:42:ASP:C	1:A:44:THR:H	2.28	0.41
1:A:237:SER:O	1:A:238:ASN:HB2	2.20	0.41
1:G:134:SER:HB3	1:G:267:TRP:CZ2	2.56	0.41
1:K:237:SER:HB3	1:K:242:ILE:CD1	2.25	0.41
1:O:242:ILE:O	1:O:246:VAL:HG23	2.21	0.41
1:Q:1:MET:HB2	1:Q:78:ASP:OD1	2.21	0.41
1:T:1:MET:HB2	1:T:78:ASP:OD1	2.20	0.41
1:T:67:VAL:HA	1:T:89:GLY:HA2	2.02	0.41
1:V:43:GLY:N	2:V:2024:HOH:O	2.52	0.41
1:B:242:ILE:O	1:B:246:VAL:HG23	2.19	0.41
1:F:242:ILE:O	1:F:246:VAL:HG23	2.21	0.41
1:J:286:THR:HB	1:J:294:LEU:CD1	2.48	0.41
1:M:283:THR:HG22	1:M:284:LEU:N	2.35	0.41
1:N:67:VAL:HA	1:N:89:GLY:HA2	2.03	0.41
1:O:281:THR:HG22	1:O:306:GLN:O	2.20	0.41
1:P:67:VAL:HA	1:P:89:GLY:HA2	2.02	0.41
1:R:242:ILE:O	1:R:246:VAL:HG23	2.19	0.41
1:V:252:SER:HB3	1:W:192:LYS:CE	2.51	0.41
1:B:139:LEU:C	1:B:139:LEU:HD13	2.45	0.41
1:D:178:ARG:HB2	1:D:178:ARG:HH11	1.83	0.41
1:H:236:THR:O	1:H:238:ASN:N	2.53	0.41
1:I:41:GLU:OE2	1:M:22:HIS:CB	2.66	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:236:THR:O	1:L:238:ASN:N	2.54	0.41
1:N:60:ASP:OD2	1:N:64:GLN:HB3	2.20	0.41
1:N:269:VAL:O	1:N:281:THR:HA	2.20	0.41
1:O:80:SER:HA	1:P:178:ARG:NH2	2.36	0.41
1:U:236:THR:O	1:U:238:ASN:N	2.54	0.41
1:B:129:THR:OG1	1:B:130:GLY:N	2.52	0.41
1:F:60:ASP:OD2	1:F:64:GLN:HB3	2.21	0.41
1:F:269:VAL:O	1:F:281:THR:HA	2.20	0.41
1:I:129:THR:OG1	1:I:130:GLY:N	2.51	0.41
1:J:134:SER:HB3	1:J:267:TRP:CZ2	2.56	0.41
1:K:60:ASP:OD1	1:K:60:ASP:C	2.64	0.41
1:O:87:GLU:HB2	2:O:2043:HOH:O	2.21	0.41
1:O:283:THR:HG22	1:O:284:LEU:N	2.35	0.41
1:R:134:SER:HB3	1:R:267:TRP:CZ2	2.56	0.41
1:S:139:LEU:HD13	1:S:139:LEU:C	2.46	0.41
1:S:317:LYS:HD3	1:S:320:GLU:OE2	2.20	0.41
1:U:237:SER:O	1:U:238:ASN:HB2	2.21	0.41
1:V:234:ASN:C	1:V:236:THR:N	2.78	0.41
1:W:129:THR:OG1	1:W:130:GLY:N	2.51	0.41
1:D:236:THR:O	1:D:238:ASN:N	2.53	0.41
1:D:248:GLU:OE1	1:E:236:THR:HG23	2.20	0.41
1:F:64:GLN:HG3	2:F:2043:HOH:O	2.20	0.41
1:I:131:LYS:HD3	1:I:243:VAL:HG11	2.03	0.41
1:I:236:THR:O	1:I:238:ASN:N	2.53	0.41
1:M:269:VAL:O	1:M:281:THR:HA	2.21	0.41
1:Q:286:THR:CB	1:Q:294:LEU:HD11	2.50	0.41
1:S:60:ASP:HB2	2:S:2037:HOH:O	2.21	0.41
1:W:248:GLU:OE2	1:X:236:THR:HG21	2.21	0.41
1:W:272:ARG:NH1	2:W:2097:HOH:O	2.44	0.41
1:X:240:ASP:O	1:X:242:ILE:N	2.48	0.41
1:B:286:THR:CB	1:B:294:LEU:HD11	2.51	0.40
1:D:237:SER:O	1:D:238:ASN:HB2	2.21	0.40
1:E:207:ILE:HD13	1:E:207:ILE:HA	1.92	0.40
1:E:236:THR:HB	2:E:2107:HOH:O	2.21	0.40
1:F:67:VAL:HA	1:F:89:GLY:HA2	2.03	0.40
1:H:246:VAL:HG23	1:H:247:LYS:N	2.37	0.40
1:K:191:LEU:HD23	1:K:191:LEU:HA	1.79	0.40
1:L:41:GLU:O	1:L:42:ASP:CB	2.67	0.40
1:N:30:PHE:CG	1:N:184:ARG:HG3	2.56	0.40
1:R:45:PRO:HD3	1:R:69:TYR:CE2	2.57	0.40
1:S:191:LEU:HD23	1:S:191:LEU:HA	1.82	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:178:ARG:HB2	1:U:178:ARG:HH11	1.85	0.40
1:U:290:GLU:HG2	1:U:291:HIS:CD2	2.56	0.40
1:W:60:ASP:OD2	1:W:64:GLN:HB3	2.20	0.40
1:A:287:SER:OG	1:A:297:HIS:CE1	2.75	0.40
1:D:240:ASP:O	1:D:242:ILE:N	2.48	0.40
1:G:286:THR:CB	1:G:294:LEU:HD11	2.51	0.40
1:H:42:ASP:C	1:H:44:THR:H	2.27	0.40
1:H:129:THR:OG1	1:H:130:GLY:N	2.53	0.40
1:H:286:THR:HB	1:H:294:LEU:CD1	2.51	0.40
1:K:248:GLU:OE2	1:L:236:THR:HG21	2.21	0.40
1:V:134:SER:HB3	1:V:267:TRP:CZ2	2.56	0.40
1:A:1:MET:HB2	1:A:78:ASP:OD1	2.22	0.40
1:B:252:SER:HB3	1:C:192:LYS:CE	2.51	0.40
1:C:286:THR:CB	1:C:294:LEU:HD11	2.50	0.40
1:E:67:VAL:HA	1:E:89:GLY:HA2	2.02	0.40
1:E:286:THR:HB	1:E:294:LEU:CD1	2.50	0.40
1:G:234:ASN:C	1:G:236:THR:N	2.78	0.40
1:H:237:SER:O	1:H:238:ASN:HB2	2.21	0.40
1:I:237:SER:O	1:I:238:ASN:HB2	2.22	0.40
1:K:67:VAL:HA	1:K:89:GLY:HA2	2.02	0.40
1:N:1:MET:HB2	1:N:78:ASP:OD1	2.21	0.40
1:N:310:LYS:HB3	1:O:132:GLY:O	2.22	0.40
1:O:1:MET:HB2	1:O:78:ASP:OD1	2.21	0.40
1:P:1:MET:HB2	1:P:78:ASP:OD1	2.21	0.40
1:P:207:ILE:HD13	1:P:207:ILE:HA	1.91	0.40
1:P:242:ILE:O	1:P:246:VAL:HG23	2.20	0.40
1:S:80:SER:HA	1:T:178:ARG:NH2	2.37	0.40
1:U:246:VAL:HG23	1:U:247:LYS:N	2.37	0.40
1:V:45:PRO:HD3	1:V:69:TYR:CE2	2.56	0.40
1:I:287:SER:OG	1:I:297:HIS:CE1	2.72	0.40
1:T:45:PRO:HD3	1:T:69:TYR:CE2	2.57	0.40
1:X:42:ASP:C	1:X:44:THR:H	2.29	0.40
1:X:240:ASP:OD2	1:X:241:LYS:N	2.52	0.40
1:C:129:THR:OG1	1:C:130:GLY:N	2.53	0.40
1:G:139:LEU:HD13	1:G:139:LEU:C	2.47	0.40
1:P:139:LEU:C	1:P:139:LEU:HD13	2.46	0.40
1:S:4:LEU:HD23	1:T:154:ALA:HA	2.03	0.40
1:X:241:LYS:N	1:X:241:LYS:HD2	2.37	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:115:GLU:OE2	1:N:39:SER:OG[1_655]	1.92	0.28
1:E:39:SER:CB	1:W:115:GLU:OE1[1_645]	2.04	0.16
1:D:115:GLU:OE2	1:X:38:GLU:O[1_545]	2.17	0.03

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	285/331 (86%)	265 (93%)	16 (6%)	4 (1%)	9	17
1	B	298/331 (90%)	286 (96%)	7 (2%)	5 (2%)	7	13
1	C	298/331 (90%)	286 (96%)	7 (2%)	5 (2%)	7	13
1	D	285/331 (86%)	266 (93%)	15 (5%)	4 (1%)	9	17
1	E	298/331 (90%)	288 (97%)	5 (2%)	5 (2%)	7	13
1	F	298/331 (90%)	285 (96%)	8 (3%)	5 (2%)	7	13
1	G	298/331 (90%)	287 (96%)	6 (2%)	5 (2%)	7	13
1	H	285/331 (86%)	266 (93%)	15 (5%)	4 (1%)	9	17
1	I	285/331 (86%)	266 (93%)	15 (5%)	4 (1%)	9	17
1	J	298/331 (90%)	285 (96%)	8 (3%)	5 (2%)	7	13
1	K	298/331 (90%)	284 (95%)	9 (3%)	5 (2%)	7	13
1	L	285/331 (86%)	265 (93%)	16 (6%)	4 (1%)	9	17
1	M	298/331 (90%)	287 (96%)	6 (2%)	5 (2%)	7	13
1	N	298/331 (90%)	286 (96%)	7 (2%)	5 (2%)	7	13
1	O	298/331 (90%)	285 (96%)	8 (3%)	5 (2%)	7	13
1	P	298/331 (90%)	287 (96%)	6 (2%)	5 (2%)	7	13
1	Q	298/331 (90%)	287 (96%)	6 (2%)	5 (2%)	7	13
1	R	298/331 (90%)	286 (96%)	7 (2%)	5 (2%)	7	13
1	S	298/331 (90%)	288 (97%)	5 (2%)	5 (2%)	7	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	T	298/331 (90%)	286 (96%)	7 (2%)	5 (2%)	7	13
1	U	285/331 (86%)	266 (93%)	15 (5%)	4 (1%)	9	17
1	V	298/331 (90%)	285 (96%)	8 (3%)	5 (2%)	7	13
1	W	298/331 (90%)	286 (96%)	7 (2%)	5 (2%)	7	13
1	X	285/331 (86%)	265 (93%)	16 (6%)	4 (1%)	9	17
All	All	7061/7944 (89%)	6723 (95%)	225 (3%)	113 (2%)	7	14

All (113) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	236	THR
1	C	236	THR
1	E	236	THR
1	F	236	THR
1	G	236	THR
1	J	236	THR
1	K	236	THR
1	M	236	THR
1	N	236	THR
1	O	236	THR
1	P	236	THR
1	Q	236	THR
1	R	236	THR
1	S	236	THR
1	T	236	THR
1	V	236	THR
1	W	236	THR
1	B	41	GLU
1	B	240	ASP
1	C	41	GLU
1	C	240	ASP
1	E	41	GLU
1	E	240	ASP
1	F	41	GLU
1	F	240	ASP
1	G	41	GLU
1	G	240	ASP
1	J	41	GLU
1	J	240	ASP
1	K	41	GLU

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Mol	Chain	Res	Type
1	K	240	ASP
1	M	41	GLU
1	M	240	ASP
1	N	41	GLU
1	N	240	ASP
1	O	41	GLU
1	O	240	ASP
1	P	41	GLU
1	P	240	ASP
1	Q	41	GLU
1	Q	240	ASP
1	R	41	GLU
1	R	240	ASP
1	S	41	GLU
1	S	240	ASP
1	T	41	GLU
1	T	240	ASP
1	V	41	GLU
1	V	240	ASP
1	W	41	GLU
1	W	240	ASP
1	B	42	ASP
1	B	190	SER
1	C	42	ASP
1	C	190	SER
1	E	42	ASP
1	E	190	SER
1	F	42	ASP
1	F	190	SER
1	G	42	ASP
1	G	190	SER
1	J	42	ASP
1	J	190	SER
1	K	42	ASP
1	K	190	SER
1	M	42	ASP
1	M	190	SER
1	N	42	ASP
1	N	190	SER
1	O	42	ASP
1	O	190	SER
1	P	42	ASP

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Mol	Chain	Res	Type
1	P	190	SER
1	Q	42	ASP
1	Q	190	SER
1	R	42	ASP
1	R	190	SER
1	S	42	ASP
1	S	190	SER
1	T	42	ASP
1	T	190	SER
1	V	42	ASP
1	V	190	SER
1	W	42	ASP
1	W	190	SER
1	A	237	SER
1	D	237	SER
1	H	237	SER
1	I	41	GLU
1	I	237	SER
1	L	237	SER
1	U	41	GLU
1	U	237	SER
1	X	41	GLU
1	X	237	SER
1	A	190	SER
1	D	41	GLU
1	D	42	ASP
1	D	190	SER
1	H	190	SER
1	I	42	ASP
1	L	42	ASP
1	L	190	SER
1	X	42	ASP
1	X	190	SER
1	A	41	GLU
1	A	42	ASP
1	H	41	GLU
1	H	42	ASP
1	I	190	SER
1	L	41	GLU
1	U	42	ASP
1	U	190	SER

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	234/265 (88%)	218 (93%)	16 (7%)	14	31
1	B	247/265 (93%)	235 (95%)	12 (5%)	22	45
1	C	246/265 (93%)	234 (95%)	12 (5%)	22	45
1	D	234/265 (88%)	218 (93%)	16 (7%)	14	31
1	E	247/265 (93%)	235 (95%)	12 (5%)	22	45
1	F	247/265 (93%)	234 (95%)	13 (5%)	20	42
1	G	247/265 (93%)	235 (95%)	12 (5%)	22	45
1	H	234/265 (88%)	218 (93%)	16 (7%)	14	31
1	I	234/265 (88%)	218 (93%)	16 (7%)	14	31
1	J	247/265 (93%)	234 (95%)	13 (5%)	20	42
1	K	247/265 (93%)	234 (95%)	13 (5%)	20	42
1	L	234/265 (88%)	218 (93%)	16 (7%)	14	31
1	M	247/265 (93%)	234 (95%)	13 (5%)	20	42
1	N	247/265 (93%)	234 (95%)	13 (5%)	20	42
1	O	247/265 (93%)	234 (95%)	13 (5%)	20	42
1	P	247/265 (93%)	235 (95%)	12 (5%)	22	45
1	Q	247/265 (93%)	235 (95%)	12 (5%)	22	45
1	R	247/265 (93%)	235 (95%)	12 (5%)	22	45
1	S	247/265 (93%)	235 (95%)	12 (5%)	22	45
1	T	247/265 (93%)	234 (95%)	13 (5%)	20	42
1	U	234/265 (88%)	218 (93%)	16 (7%)	14	31
1	V	247/265 (93%)	234 (95%)	13 (5%)	20	42
1	W	247/265 (93%)	235 (95%)	12 (5%)	22	45
1	X	234/265 (88%)	218 (93%)	16 (7%)	14	31
All	All	5836/6360 (92%)	5512 (94%)	324 (6%)	19	39

All (324) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	LEU
1	A	92	LYS
1	A	100	VAL
1	A	106	LEU
1	A	162	LEU
1	A	192	LYS
1	A	194	VAL
1	A	214	LEU
1	A	238	ASN
1	A	247	LYS
1	A	257	LEU
1	A	262	ASP
1	A	271	THR
1	A	277	LEU
1	A	284	LEU
1	A	294	LEU
1	B	47	LEU
1	B	92	LYS
1	B	106	LEU
1	B	162	LEU
1	B	194	VAL
1	B	207	ILE
1	B	257	LEU
1	B	270	LEU
1	B	271	THR
1	B	277	LEU
1	B	284	LEU
1	B	316	ILE
1	C	47	LEU
1	C	92	LYS
1	C	106	LEU
1	C	162	LEU
1	C	194	VAL
1	C	207	ILE
1	C	257	LEU
1	C	270	LEU
1	C	271	THR
1	C	277	LEU
1	C	284	LEU
1	C	316	ILE
1	D	47	LEU
1	D	92	LYS
1	D	100	VAL

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Mol	Chain	Res	Type
1	D	106	LEU
1	D	162	LEU
1	D	192	LYS
1	D	194	VAL
1	D	214	LEU
1	D	238	ASN
1	D	247	LYS
1	D	257	LEU
1	D	262	ASP
1	D	271	THR
1	D	277	LEU
1	D	284	LEU
1	D	294	LEU
1	E	47	LEU
1	E	92	LYS
1	E	106	LEU
1	E	162	LEU
1	E	194	VAL
1	E	207	ILE
1	E	257	LEU
1	E	270	LEU
1	E	271	THR
1	E	277	LEU
1	E	284	LEU
1	E	316	ILE
1	F	47	LEU
1	F	92	LYS
1	F	106	LEU
1	F	162	LEU
1	F	194	VAL
1	F	207	ILE
1	F	257	LEU
1	F	270	LEU
1	F	271	THR
1	F	277	LEU
1	F	284	LEU
1	F	294	LEU
1	F	316	ILE
1	G	47	LEU
1	G	92	LYS
1	G	106	LEU
1	G	162	LEU

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Mol	Chain	Res	Type
1	G	194	VAL
1	G	207	ILE
1	G	257	LEU
1	G	270	LEU
1	G	271	THR
1	G	277	LEU
1	G	284	LEU
1	G	316	ILE
1	H	47	LEU
1	H	92	LYS
1	H	100	VAL
1	H	106	LEU
1	H	162	LEU
1	H	192	LYS
1	H	194	VAL
1	H	214	LEU
1	H	238	ASN
1	H	247	LYS
1	H	257	LEU
1	H	262	ASP
1	H	271	THR
1	H	277	LEU
1	H	284	LEU
1	H	294	LEU
1	I	47	LEU
1	I	92	LYS
1	I	100	VAL
1	I	106	LEU
1	I	162	LEU
1	I	192	LYS
1	I	194	VAL
1	I	214	LEU
1	I	238	ASN
1	I	247	LYS
1	I	257	LEU
1	I	262	ASP
1	I	271	THR
1	I	277	LEU
1	I	284	LEU
1	I	294	LEU
1	J	47	LEU
1	J	92	LYS

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Mol	Chain	Res	Type
1	J	106	LEU
1	J	162	LEU
1	J	194	VAL
1	J	207	ILE
1	J	257	LEU
1	J	270	LEU
1	J	271	THR
1	J	277	LEU
1	J	284	LEU
1	J	294	LEU
1	J	316	ILE
1	K	47	LEU
1	K	92	LYS
1	K	106	LEU
1	K	162	LEU
1	K	194	VAL
1	K	207	ILE
1	K	257	LEU
1	K	270	LEU
1	K	271	THR
1	K	277	LEU
1	K	284	LEU
1	K	294	LEU
1	K	316	ILE
1	L	47	LEU
1	L	92	LYS
1	L	100	VAL
1	L	106	LEU
1	L	162	LEU
1	L	192	LYS
1	L	194	VAL
1	L	214	LEU
1	L	238	ASN
1	L	247	LYS
1	L	257	LEU
1	L	262	ASP
1	L	271	THR
1	L	277	LEU
1	L	284	LEU
1	L	294	LEU
1	M	47	LEU
1	M	92	LYS

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Mol	Chain	Res	Type
1	M	106	LEU
1	M	162	LEU
1	M	194	VAL
1	M	207	ILE
1	M	257	LEU
1	M	270	LEU
1	M	271	THR
1	M	277	LEU
1	M	284	LEU
1	M	294	LEU
1	M	316	ILE
1	N	47	LEU
1	N	92	LYS
1	N	106	LEU
1	N	162	LEU
1	N	194	VAL
1	N	207	ILE
1	N	257	LEU
1	N	270	LEU
1	N	271	THR
1	N	277	LEU
1	N	284	LEU
1	N	294	LEU
1	N	316	ILE
1	O	47	LEU
1	O	92	LYS
1	O	106	LEU
1	O	162	LEU
1	O	194	VAL
1	O	207	ILE
1	O	257	LEU
1	O	270	LEU
1	O	271	THR
1	O	277	LEU
1	O	284	LEU
1	O	294	LEU
1	O	316	ILE
1	P	47	LEU
1	P	92	LYS
1	P	106	LEU
1	P	162	LEU
1	P	194	VAL

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Mol	Chain	Res	Type
1	P	207	ILE
1	P	257	LEU
1	P	270	LEU
1	P	271	THR
1	P	277	LEU
1	P	284	LEU
1	P	316	ILE
1	Q	47	LEU
1	Q	92	LYS
1	Q	106	LEU
1	Q	162	LEU
1	Q	194	VAL
1	Q	207	ILE
1	Q	257	LEU
1	Q	270	LEU
1	Q	271	THR
1	Q	277	LEU
1	Q	284	LEU
1	Q	316	ILE
1	R	47	LEU
1	R	92	LYS
1	R	106	LEU
1	R	162	LEU
1	R	194	VAL
1	R	207	ILE
1	R	257	LEU
1	R	270	LEU
1	R	271	THR
1	R	277	LEU
1	R	284	LEU
1	R	316	ILE
1	S	47	LEU
1	S	92	LYS
1	S	106	LEU
1	S	162	LEU
1	S	194	VAL
1	S	207	ILE
1	S	257	LEU
1	S	270	LEU
1	S	271	THR
1	S	277	LEU
1	S	284	LEU

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Mol	Chain	Res	Type
1	S	316	ILE
1	T	47	LEU
1	T	92	LYS
1	T	106	LEU
1	T	162	LEU
1	T	194	VAL
1	T	207	ILE
1	T	257	LEU
1	T	270	LEU
1	T	271	THR
1	T	277	LEU
1	T	284	LEU
1	T	294	LEU
1	T	316	ILE
1	U	47	LEU
1	U	92	LYS
1	U	100	VAL
1	U	106	LEU
1	U	162	LEU
1	U	192	LYS
1	U	194	VAL
1	U	214	LEU
1	U	238	ASN
1	U	247	LYS
1	U	257	LEU
1	U	262	ASP
1	U	271	THR
1	U	277	LEU
1	U	284	LEU
1	U	294	LEU
1	V	47	LEU
1	V	92	LYS
1	V	106	LEU
1	V	162	LEU
1	V	194	VAL
1	V	207	ILE
1	V	257	LEU
1	V	270	LEU
1	V	271	THR
1	V	277	LEU
1	V	284	LEU
1	V	294	LEU

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Mol	Chain	Res	Type
1	V	316	ILE
1	W	47	LEU
1	W	92	LYS
1	W	106	LEU
1	W	162	LEU
1	W	194	VAL
1	W	207	ILE
1	W	257	LEU
1	W	270	LEU
1	W	271	THR
1	W	277	LEU
1	W	284	LEU
1	W	316	ILE
1	X	47	LEU
1	X	92	LYS
1	X	100	VAL
1	X	106	LEU
1	X	162	LEU
1	X	192	LYS
1	X	194	VAL
1	X	214	LEU
1	X	238	ASN
1	X	247	LYS
1	X	257	LEU
1	X	262	ASP
1	X	271	THR
1	X	277	LEU
1	X	284	LEU
1	X	294	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (291) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	HIS
1	A	22	HIS
1	A	95	HIS
1	A	182	GLN
1	A	193	ASN
1	A	238	ASN
1	A	268	GLN
1	A	278	GLN
1	A	291	HIS

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Mol	Chain	Res	Type
1	A	297	HIS
1	B	22	HIS
1	B	62	ASN
1	B	95	HIS
1	B	182	GLN
1	B	234	ASN
1	B	238	ASN
1	B	253	ASN
1	B	268	GLN
1	B	278	GLN
1	B	291	HIS
1	B	297	HIS
1	B	306	GLN
1	B	313	GLN
1	C	22	HIS
1	C	62	ASN
1	C	95	HIS
1	C	182	GLN
1	C	234	ASN
1	C	238	ASN
1	C	253	ASN
1	C	268	GLN
1	C	278	GLN
1	C	291	HIS
1	C	297	HIS
1	C	306	GLN
1	C	313	GLN
1	D	95	HIS
1	D	182	GLN
1	D	193	ASN
1	D	238	ASN
1	D	268	GLN
1	D	278	GLN
1	D	291	HIS
1	D	297	HIS
1	E	22	HIS
1	E	62	ASN
1	E	95	HIS
1	E	182	GLN
1	E	234	ASN
1	E	238	ASN
1	E	253	ASN

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Mol	Chain	Res	Type
1	E	268	GLN
1	E	278	GLN
1	E	291	HIS
1	E	297	HIS
1	E	306	GLN
1	E	313	GLN
1	F	22	HIS
1	F	32	HIS
1	F	62	ASN
1	F	95	HIS
1	F	182	GLN
1	F	234	ASN
1	F	238	ASN
1	F	253	ASN
1	F	268	GLN
1	F	278	GLN
1	F	291	HIS
1	F	297	HIS
1	F	306	GLN
1	F	313	GLN
1	G	22	HIS
1	G	62	ASN
1	G	95	HIS
1	G	182	GLN
1	G	234	ASN
1	G	238	ASN
1	G	253	ASN
1	G	268	GLN
1	G	278	GLN
1	G	291	HIS
1	G	297	HIS
1	G	306	GLN
1	G	313	GLN
1	H	62	ASN
1	H	95	HIS
1	H	133	ASN
1	H	182	GLN
1	H	193	ASN
1	H	238	ASN
1	H	268	GLN
1	H	278	GLN
1	H	291	HIS

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Mol	Chain	Res	Type
1	H	297	HIS
1	I	3	HIS
1	I	22	HIS
1	I	95	HIS
1	I	182	GLN
1	I	193	ASN
1	I	238	ASN
1	I	268	GLN
1	I	278	GLN
1	I	291	HIS
1	I	297	HIS
1	J	32	HIS
1	J	62	ASN
1	J	95	HIS
1	J	182	GLN
1	J	234	ASN
1	J	238	ASN
1	J	253	ASN
1	J	268	GLN
1	J	278	GLN
1	J	291	HIS
1	J	297	HIS
1	J	306	GLN
1	J	313	GLN
1	K	22	HIS
1	K	62	ASN
1	K	95	HIS
1	K	182	GLN
1	K	234	ASN
1	K	238	ASN
1	K	253	ASN
1	K	268	GLN
1	K	278	GLN
1	K	291	HIS
1	K	297	HIS
1	K	306	GLN
1	K	313	GLN
1	L	22	HIS
1	L	95	HIS
1	L	182	GLN
1	L	193	ASN
1	L	238	ASN

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Mol	Chain	Res	Type
1	L	268	GLN
1	L	278	GLN
1	L	291	HIS
1	L	297	HIS
1	M	62	ASN
1	M	95	HIS
1	M	182	GLN
1	M	234	ASN
1	M	238	ASN
1	M	253	ASN
1	M	268	GLN
1	M	278	GLN
1	M	291	HIS
1	M	297	HIS
1	M	306	GLN
1	M	313	GLN
1	N	22	HIS
1	N	62	ASN
1	N	95	HIS
1	N	182	GLN
1	N	234	ASN
1	N	238	ASN
1	N	253	ASN
1	N	268	GLN
1	N	278	GLN
1	N	291	HIS
1	N	297	HIS
1	N	306	GLN
1	N	313	GLN
1	O	22	HIS
1	O	32	HIS
1	O	62	ASN
1	O	95	HIS
1	O	182	GLN
1	O	234	ASN
1	O	238	ASN
1	O	253	ASN
1	O	268	GLN
1	O	278	GLN
1	O	291	HIS
1	O	297	HIS
1	O	306	GLN

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Mol	Chain	Res	Type
1	O	313	GLN
1	P	22	HIS
1	P	62	ASN
1	P	95	HIS
1	P	182	GLN
1	P	234	ASN
1	P	238	ASN
1	P	253	ASN
1	P	268	GLN
1	P	278	GLN
1	P	291	HIS
1	P	297	HIS
1	P	306	GLN
1	P	313	GLN
1	Q	22	HIS
1	Q	62	ASN
1	Q	95	HIS
1	Q	182	GLN
1	Q	234	ASN
1	Q	238	ASN
1	Q	253	ASN
1	Q	268	GLN
1	Q	278	GLN
1	Q	291	HIS
1	Q	297	HIS
1	Q	306	GLN
1	Q	313	GLN
1	R	22	HIS
1	R	62	ASN
1	R	95	HIS
1	R	182	GLN
1	R	234	ASN
1	R	238	ASN
1	R	253	ASN
1	R	268	GLN
1	R	278	GLN
1	R	291	HIS
1	R	297	HIS
1	R	306	GLN
1	R	313	GLN
1	S	22	HIS
1	S	32	HIS

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Mol	Chain	Res	Type
1	S	62	ASN
1	S	95	HIS
1	S	182	GLN
1	S	234	ASN
1	S	238	ASN
1	S	253	ASN
1	S	268	GLN
1	S	278	GLN
1	S	291	HIS
1	S	297	HIS
1	S	306	GLN
1	S	313	GLN
1	T	22	HIS
1	T	62	ASN
1	T	95	HIS
1	T	182	GLN
1	T	234	ASN
1	T	238	ASN
1	T	253	ASN
1	T	268	GLN
1	T	278	GLN
1	T	291	HIS
1	T	297	HIS
1	T	306	GLN
1	T	313	GLN
1	U	3	HIS
1	U	22	HIS
1	U	62	ASN
1	U	95	HIS
1	U	182	GLN
1	U	193	ASN
1	U	238	ASN
1	U	268	GLN
1	U	278	GLN
1	U	291	HIS
1	U	297	HIS
1	V	22	HIS
1	V	62	ASN
1	V	95	HIS
1	V	182	GLN
1	V	234	ASN
1	V	238	ASN

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Mol	Chain	Res	Type
1	V	253	ASN
1	V	268	GLN
1	V	278	GLN
1	V	291	HIS
1	V	297	HIS
1	V	306	GLN
1	V	313	GLN
1	W	22	HIS
1	W	62	ASN
1	W	95	HIS
1	W	182	GLN
1	W	234	ASN
1	W	238	ASN
1	W	253	ASN
1	W	268	GLN
1	W	278	GLN
1	W	291	HIS
1	W	297	HIS
1	W	306	GLN
1	W	313	GLN
1	X	22	HIS
1	X	95	HIS
1	X	182	GLN
1	X	193	ASN
1	X	238	ASN
1	X	253	ASN
1	X	268	GLN
1	X	278	GLN
1	X	291	HIS
1	X	297	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [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	289/331 (87%)	0.38	18 (6%) 26 23	25, 38, 90, 114	0
1	B	304/331 (91%)	0.55	28 (9%) 14 13	26, 39, 89, 118	0
1	C	304/331 (91%)	0.45	26 (8%) 16 14	24, 37, 89, 119	0
1	D	289/331 (87%)	0.19	26 (8%) 15 13	22, 36, 90, 113	0
1	E	304/331 (91%)	0.37	33 (10%) 10 9	23, 37, 90, 119	0
1	F	304/331 (91%)	0.45	37 (12%) 8 7	23, 37, 89, 118	0
1	G	304/331 (91%)	0.47	31 (10%) 12 10	25, 38, 88, 119	0
1	H	289/331 (87%)	0.29	23 (7%) 18 16	20, 34, 90, 113	0
1	I	289/331 (87%)	0.49	41 (14%) 6 5	19, 33, 90, 113	0
1	J	304/331 (91%)	0.41	35 (11%) 9 8	20, 34, 88, 118	0
1	K	304/331 (91%)	0.46	32 (10%) 11 10	24, 38, 89, 119	0
1	L	289/331 (87%)	0.45	16 (5%) 30 27	25, 39, 90, 114	0
1	M	304/331 (91%)	0.53	43 (14%) 6 5	18, 34, 89, 119	0
1	N	304/331 (91%)	0.54	46 (15%) 5 4	19, 34, 90, 119	0
1	O	304/331 (91%)	0.39	35 (11%) 9 8	23, 36, 89, 119	0
1	P	304/331 (91%)	0.46	26 (8%) 16 14	26, 39, 90, 119	0
1	Q	304/331 (91%)	0.56	25 (8%) 17 15	27, 40, 90, 119	0
1	R	304/331 (91%)	0.51	32 (10%) 11 10	23, 37, 89, 119	0
1	S	304/331 (91%)	0.42	28 (9%) 14 13	22, 37, 89, 118	0
1	T	304/331 (91%)	0.43	20 (6%) 24 21	24, 40, 89, 118	0
1	U	289/331 (87%)	0.43	14 (4%) 35 31	27, 40, 91, 114	0
1	V	304/331 (91%)	0.42	27 (8%) 15 13	26, 39, 89, 119	0
1	W	304/331 (91%)	0.32	30 (9%) 13 11	25, 38, 90, 118	0
1	X	289/331 (87%)	0.22	25 (8%) 16 14	21, 36, 91, 114	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	7191/7944 (90%)	0.43	697 (9%) 13 11	18, 37, 91, 119	0

All (697) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	321	LEU	8.8
1	F	195	ILE	8.4
1	I	195	ILE	8.1
1	J	195	ILE	8.0
1	N	309	GLY	7.7
1	S	195	ILE	7.6
1	P	321	LEU	7.4
1	O	195	ILE	7.4
1	G	195	ILE	7.4
1	A	195	ILE	7.3
1	M	321	LEU	7.2
1	N	195	ILE	7.2
1	T	321	LEU	6.9
1	O	321	LEU	6.9
1	R	195	ILE	6.8
1	T	195	ILE	6.8
1	E	195	ILE	6.7
1	R	321	LEU	6.6
1	E	321	LEU	6.5
1	N	321	LEU	6.4
1	M	317	LYS	6.3
1	B	195	ILE	6.3
1	Q	321	LEU	6.3
1	G	321	LEU	6.2
1	V	321	LEU	6.2
1	I	41	GLU	6.2
1	M	320	GLU	6.1
1	W	321	LEU	6.0
1	K	321	LEU	5.9
1	C	321	LEU	5.9
1	I	193	ASN	5.8
1	I	236	THR	5.8
1	I	132	GLY	5.8
1	C	195	ILE	5.7
1	M	318	ASN	5.7
1	P	243	VAL	5.6
1	E	320	GLU	5.6

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Mol	Chain	Res	Type	RSRZ
1	P	195	ILE	5.6
1	J	207	ILE	5.5
1	I	80	SER	5.5
1	N	236	THR	5.5
1	J	321	LEU	5.5
1	K	195	ILE	5.4
1	N	237	SER	5.4
1	F	207	ILE	5.4
1	I	245	LEU	5.4
1	O	320	GLU	5.3
1	I	76	ALA	5.3
1	I	74	VAL	5.3
1	X	195	ILE	5.3
1	X	236	THR	5.3
1	S	321	LEU	5.3
1	V	195	ILE	5.2
1	F	321	LEU	5.2
1	G	42	ASP	5.2
1	I	79	GLY	5.2
1	M	195	ILE	5.2
1	W	195	ILE	5.2
1	J	320	GLU	5.2
1	L	193	ASN	5.2
1	V	42	ASP	5.1
1	Q	195	ILE	5.1
1	I	243	VAL	5.0
1	Q	320	GLU	5.0
1	X	242	ILE	5.0
1	D	195	ILE	5.0
1	M	243	VAL	5.0
1	N	243	VAL	5.0
1	X	245	LEU	4.9
1	I	194	VAL	4.9
1	N	307	ALA	4.9
1	J	317	LYS	4.9
1	N	245	LEU	4.9
1	G	207	ILE	4.9
1	G	320	GLU	4.9
1	I	81	VAL	4.9
1	H	195	ILE	4.8
1	A	237	SER	4.8
1	K	318	ASN	4.8

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Mol	Chain	Res	Type	RSRZ
1	J	306	GLN	4.8
1	U	245	LEU	4.8
1	K	320	GLU	4.8
1	U	195	ILE	4.8
1	O	307	ALA	4.8
1	H	42	ASP	4.7
1	N	318	ASN	4.7
1	A	236	THR	4.7
1	C	207	ILE	4.6
1	N	238	ASN	4.6
1	J	237	SER	4.6
1	N	320	GLU	4.6
1	S	320	GLU	4.6
1	I	237	SER	4.5
1	I	72	LYS	4.5
1	I	42	ASP	4.5
1	H	236	THR	4.5
1	J	193	ASN	4.5
1	H	115	GLU	4.5
1	C	320	GLU	4.5
1	W	320	GLU	4.5
1	N	315	VAL	4.4
1	E	237	SER	4.4
1	H	245	LEU	4.4
1	N	319	ASP	4.4
1	O	237	SER	4.4
1	N	240	ASP	4.4
1	V	207	ILE	4.3
1	O	132	GLY	4.3
1	D	237	SER	4.3
1	L	195	ILE	4.3
1	R	243	VAL	4.3
1	T	243	VAL	4.3
1	M	115	GLU	4.3
1	J	319	ASP	4.2
1	X	42	ASP	4.2
1	R	309	GLY	4.2
1	I	75	LYS	4.2
1	L	245	LEU	4.2
1	U	242	ILE	4.2
1	V	43	GLY	4.2
1	N	314	THR	4.2

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Mol	Chain	Res	Type	RSRZ
1	N	40	VAL	4.2
1	F	306	GLN	4.1
1	N	42	ASP	4.1
1	I	73	SER	4.1
1	N	207	ILE	4.1
1	S	207	ILE	4.1
1	J	236	THR	4.1
1	N	248	GLU	4.1
1	G	43	GLY	4.1
1	D	245	LEU	4.1
1	G	317	LYS	4.0
1	G	237	SER	4.0
1	N	242	ILE	4.0
1	V	237	SER	4.0
1	R	319	ASP	4.0
1	A	242	ILE	3.9
1	E	312	ILE	3.9
1	K	207	ILE	3.9
1	P	207	ILE	3.9
1	M	237	SER	3.9
1	F	243	VAL	3.9
1	N	77	GLU	3.9
1	X	243	VAL	3.9
1	I	133	ASN	3.9
1	O	133	ASN	3.9
1	C	309	GLY	3.9
1	B	134	SER	3.9
1	F	320	GLU	3.9
1	A	193	ASN	3.9
1	N	312	ILE	3.9
1	B	320	GLU	3.9
1	O	306	GLN	3.9
1	V	320	GLU	3.9
1	E	236	THR	3.9
1	G	134	SER	3.8
1	E	243	VAL	3.8
1	O	29	TRP	3.8
1	I	78	ASP	3.8
1	I	242	ILE	3.8
1	J	240	ASP	3.8
1	E	317	LYS	3.8
1	O	317	LYS	3.8

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Mol	Chain	Res	Type	RSRZ
1	P	320	GLU	3.8
1	B	207	ILE	3.8
1	N	244	GLU	3.8
1	W	237	SER	3.7
1	F	307	ALA	3.7
1	G	307	ALA	3.7
1	O	193	ASN	3.7
1	T	42	ASP	3.7
1	J	194	VAL	3.7
1	H	243	VAL	3.7
1	X	207	ILE	3.7
1	M	308	SER	3.7
1	X	41	GLU	3.7
1	S	306	GLN	3.7
1	J	238	ASN	3.7
1	N	317	LYS	3.7
1	H	194	VAL	3.6
1	W	317	LYS	3.6
1	A	245	LEU	3.6
1	Q	238	ASN	3.6
1	M	236	THR	3.6
1	R	320	GLU	3.6
1	K	317	LYS	3.6
1	P	317	LYS	3.6
1	N	308	SER	3.6
1	O	207	ILE	3.6
1	H	193	ASN	3.6
1	N	193	ASN	3.6
1	R	308	SER	3.5
1	M	309	GLY	3.5
1	N	79	GLY	3.5
1	M	238	ASN	3.5
1	M	319	ASP	3.5
1	N	78	ASP	3.5
1	R	236	THR	3.5
1	V	236	THR	3.5
1	H	237	SER	3.5
1	M	249	ALA	3.5
1	D	193	ASN	3.5
1	H	248	GLU	3.5
1	K	243	VAL	3.5
1	T	207	ILE	3.5

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Mol	Chain	Res	Type	RSRZ
1	I	247	LYS	3.5
1	M	193	ASN	3.5
1	X	78	ASP	3.5
1	G	306	GLN	3.5
1	S	243	VAL	3.5
1	U	194	VAL	3.5
1	W	243	VAL	3.5
1	D	242	ILE	3.5
1	J	316	ILE	3.5
1	P	238	ASN	3.4
1	R	133	ASN	3.4
1	U	193	ASN	3.4
1	M	314	THR	3.4
1	N	134	SER	3.4
1	C	319	ASP	3.4
1	S	133	ASN	3.4
1	F	314	THR	3.4
1	B	242	ILE	3.4
1	C	312	ILE	3.4
1	M	239	ASP	3.4
1	D	238	ASN	3.4
1	F	193	ASN	3.4
1	F	318	ASN	3.4
1	W	238	ASN	3.4
1	N	311	ALA	3.4
1	Q	207	ILE	3.4
1	N	43	GLY	3.4
1	V	132	GLY	3.4
1	R	207	ILE	3.4
1	H	77	GLU	3.4
1	W	319	ASP	3.3
1	J	131	LYS	3.3
1	M	316	ILE	3.3
1	X	193	ASN	3.3
1	A	299	SER	3.3
1	B	318	ASN	3.3
1	B	243	VAL	3.3
1	E	307	ALA	3.3
1	K	78	ASP	3.3
1	I	40	VAL	3.3
1	S	132	GLY	3.3
1	J	29	TRP	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	237	SER	3.2
1	C	237	SER	3.2
1	J	243	VAL	3.2
1	B	132	GLY	3.2
1	P	314	THR	3.2
1	W	312	ILE	3.2
1	F	237	SER	3.2
1	S	237	SER	3.2
1	I	251	ARG	3.2
1	D	115	GLU	3.2
1	O	309	GLY	3.2
1	Q	309	GLY	3.2
1	K	311	ALA	3.2
1	C	193	ASN	3.2
1	B	317	LYS	3.2
1	G	40	VAL	3.2
1	L	243	VAL	3.2
1	K	236	THR	3.2
1	L	236	THR	3.2
1	J	41	GLU	3.2
1	M	245	LEU	3.2
1	T	318	ASN	3.2
1	C	243	VAL	3.2
1	F	194	VAL	3.2
1	U	243	VAL	3.2
1	N	41	GLU	3.1
1	Q	317	LYS	3.1
1	B	193	ASN	3.1
1	G	193	ASN	3.1
1	E	207	ILE	3.1
1	H	242	ILE	3.1
1	W	236	THR	3.1
1	C	311	ALA	3.1
1	I	131	LYS	3.1
1	E	240	ASP	3.1
1	O	318	ASN	3.1
1	D	194	VAL	3.1
1	L	242	ILE	3.1
1	T	317	LYS	3.1
1	J	312	ILE	3.1
1	V	314	THR	3.1
1	N	249	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	J	134	SER	3.1
1	R	193	ASN	3.1
1	V	318	ASN	3.1
1	N	246	VAL	3.1
1	C	317	LYS	3.0
1	D	236	THR	3.0
1	U	236	THR	3.0
1	V	307	ALA	3.0
1	G	41	GLU	3.0
1	G	319	ASP	3.0
1	B	133	ASN	3.0
1	V	193	ASN	3.0
1	S	317	LYS	3.0
1	L	194	VAL	3.0
1	M	306	GLN	3.0
1	F	236	THR	3.0
1	M	235	PRO	3.0
1	P	319	ASP	3.0
1	A	238	ASN	3.0
1	V	312	ILE	3.0
1	Q	314	THR	3.0
1	F	78	ASP	3.0
1	C	131	LYS	3.0
1	F	234	ASN	3.0
1	J	318	ASN	3.0
1	S	193	ASN	3.0
1	I	43	GLY	3.0
1	M	315	VAL	3.0
1	E	244	GLU	3.0
1	N	131	LYS	3.0
1	L	237	SER	3.0
1	I	207	ILE	2.9
1	I	248	GLU	2.9
1	O	236	THR	2.9
1	E	319	ASP	2.9
1	O	319	ASP	2.9
1	M	299	SER	2.9
1	N	133	ASN	2.9
1	D	248	GLU	2.9
1	U	207	ILE	2.9
1	W	207	ILE	2.9
1	E	40	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	H	246	VAL	2.9
1	W	315	VAL	2.9
1	Q	310	LYS	2.9
1	J	78	ASP	2.9
1	R	240	ASP	2.9
1	X	237	SER	2.9
1	S	238	ASN	2.9
1	V	40	VAL	2.9
1	W	311	ALA	2.9
1	F	245	LEU	2.9
1	E	78	ASP	2.9
1	F	319	ASP	2.9
1	K	319	ASP	2.9
1	M	78	ASP	2.9
1	Q	319	ASP	2.9
1	B	309	GLY	2.9
1	E	134	SER	2.9
1	E	193	ASN	2.9
1	G	77	GLU	2.9
1	G	316	ILE	2.9
1	L	192	LYS	2.9
1	V	317	LYS	2.9
1	O	311	ALA	2.9
1	K	240	ASP	2.9
1	H	299	SER	2.8
1	B	312	ILE	2.8
1	M	241	LYS	2.8
1	W	242	ILE	2.8
1	K	315	VAL	2.8
1	Q	243	VAL	2.8
1	E	306	GLN	2.8
1	N	306	GLN	2.8
1	I	192	LYS	2.8
1	C	308	SER	2.8
1	E	238	ASN	2.8
1	I	238	ASN	2.8
1	L	238	ASN	2.8
1	M	207	ILE	2.8
1	R	237	SER	2.8
1	R	317	LYS	2.8
1	Q	242	ILE	2.8
1	I	134	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	K	313	GLN	2.8
1	M	313	GLN	2.8
1	O	241	LYS	2.8
1	O	42	ASP	2.8
1	S	78	ASP	2.8
1	S	240	ASP	2.8
1	W	42	ASP	2.8
1	F	43	GLY	2.8
1	T	312	ILE	2.8
1	C	73	SER	2.8
1	D	299	SER	2.8
1	S	134	SER	2.8
1	T	190	SER	2.8
1	T	237	SER	2.8
1	W	318	ASN	2.8
1	M	246	VAL	2.8
1	S	40	VAL	2.8
1	X	40	VAL	2.8
1	N	76	ALA	2.8
1	M	131	LYS	2.8
1	O	192	LYS	2.8
1	J	42	ASP	2.8
1	H	79	GLY	2.7
1	R	132	GLY	2.7
1	K	238	ASN	2.7
1	E	194	VAL	2.7
1	O	40	VAL	2.7
1	X	194	VAL	2.7
1	A	76	ALA	2.7
1	X	76	ALA	2.7
1	N	241	LYS	2.7
1	A	239	ASP	2.7
1	M	242	ILE	2.7
1	B	194	VAL	2.7
1	E	299	SER	2.7
1	J	40	VAL	2.7
1	O	134	SER	2.7
1	B	236	THR	2.7
1	R	306	GLN	2.7
1	R	316	ILE	2.7
1	T	238	ASN	2.7
1	A	194	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	I	190	SER	2.7
1	M	194	VAL	2.7
1	X	241	LYS	2.7
1	X	103	THR	2.7
1	V	306	GLN	2.7
1	W	239	ASP	2.7
1	K	312	ILE	2.7
1	A	246	VAL	2.7
1	F	40	VAL	2.7
1	K	237	SER	2.7
1	L	190	SER	2.7
1	N	299	SER	2.7
1	P	245	LEU	2.7
1	V	194	VAL	2.7
1	B	307	ALA	2.7
1	I	77	GLU	2.7
1	P	306	GLN	2.7
1	H	78	ASP	2.6
1	F	312	ILE	2.6
1	Q	312	ILE	2.6
1	V	316	ILE	2.6
1	G	238	ASN	2.6
1	K	193	ASN	2.6
1	R	238	ASN	2.6
1	S	318	ASN	2.6
1	W	194	VAL	2.6
1	U	248	GLU	2.6
1	S	319	ASP	2.6
1	F	241	LYS	2.6
1	Q	194	VAL	2.6
1	V	243	VAL	2.6
1	K	307	ALA	2.6
1	R	314	THR	2.6
1	F	42	ASP	2.6
1	P	79	GLY	2.6
1	E	242	ILE	2.6
1	S	316	ILE	2.6
1	F	215	LEU	2.6
1	C	194	VAL	2.6
1	Q	193	ASN	2.6
1	S	194	VAL	2.6
1	F	311	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	R	311	ALA	2.6
1	M	240	ASP	2.6
1	O	79	GLY	2.6
1	W	316	ILE	2.6
1	P	237	SER	2.6
1	P	307	ALA	2.6
1	C	240	ASP	2.5
1	E	132	GLY	2.5
1	K	79	GLY	2.5
1	N	235	PRO	2.5
1	W	240	ASP	2.5
1	X	79	GLY	2.5
1	R	312	ILE	2.5
1	S	312	ILE	2.5
1	Q	245	LEU	2.5
1	T	245	LEU	2.5
1	A	190	SER	2.5
1	F	131	LYS	2.5
1	J	313	GLN	2.5
1	A	81	VAL	2.5
1	N	194	VAL	2.5
1	T	311	ALA	2.5
1	J	308	SER	2.5
1	P	236	THR	2.5
1	S	236	THR	2.5
1	B	79	GLY	2.5
1	C	132	GLY	2.5
1	B	319	ASP	2.5
1	D	240	ASP	2.5
1	F	240	ASP	2.5
1	B	310	LYS	2.5
1	F	317	LYS	2.5
1	H	40	VAL	2.5
1	M	311	ALA	2.5
1	W	299	SER	2.5
1	G	290	GLU	2.5
1	P	244	GLU	2.5
1	T	320	GLU	2.5
1	B	240	ASP	2.5
1	D	241	LYS	2.5
1	Q	306	GLN	2.5
1	L	246	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	M	133	ASN	2.5
1	P	193	ASN	2.5
1	K	103	THR	2.5
1	D	132	GLY	2.4
1	S	79	GLY	2.4
1	S	309	GLY	2.4
1	V	79	GLY	2.4
1	J	239	ASP	2.4
1	J	242	ILE	2.4
1	K	316	ILE	2.4
1	R	242	ILE	2.4
1	Q	315	VAL	2.4
1	J	314	THR	2.4
1	T	314	THR	2.4
1	U	237	SER	2.4
1	M	244	GLU	2.4
1	K	43	GLY	2.4
1	F	239	ASP	2.4
1	M	312	ILE	2.4
1	N	239	ASP	2.4
1	T	240	ASP	2.4
1	Q	313	GLN	2.4
1	R	76	ALA	2.4
1	K	314	THR	2.4
1	O	190	SER	2.4
1	A	300	LYS	2.4
1	D	79	GLY	2.4
1	L	43	GLY	2.4
1	E	313	GLN	2.4
1	O	243	VAL	2.4
1	X	133	ASN	2.4
1	X	238	ASN	2.4
1	J	307	ALA	2.4
1	E	310	LYS	2.4
1	I	71	GLU	2.4
1	P	310	LYS	2.4
1	V	75	LYS	2.4
1	H	190	SER	2.4
1	R	73	SER	2.4
1	X	39	SER	2.4
1	H	43	GLY	2.4
1	M	79	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	207	ILE	2.4
1	K	306	GLN	2.4
1	D	40	VAL	2.4
1	P	194	VAL	2.4
1	E	133	ASN	2.4
1	E	318	ASN	2.4
1	F	76	ALA	2.4
1	M	248	GLU	2.4
1	X	248	GLU	2.4
1	B	306	GLN	2.3
1	C	64	GLN	2.3
1	J	215	LEU	2.3
1	T	306	GLN	2.3
1	P	240	ASP	2.3
1	R	78	ASP	2.3
1	W	245	LEU	2.3
1	A	241	LYS	2.3
1	E	315	VAL	2.3
1	J	241	LYS	2.3
1	J	133	ASN	2.3
1	M	307	ALA	2.3
1	X	38	GLU	2.3
1	K	131	LYS	2.3
1	O	131	LYS	2.3
1	B	315	VAL	2.3
1	G	194	VAL	2.3
1	L	133	ASN	2.3
1	E	311	ALA	2.3
1	O	314	THR	2.3
1	E	309	GLY	2.3
1	K	299	SER	2.3
1	Q	299	SER	2.3
1	V	134	SER	2.3
1	C	78	ASP	2.3
1	V	240	ASP	2.3
1	K	310	LYS	2.3
1	U	241	LYS	2.3
1	F	77	GLU	2.3
1	E	235	PRO	2.3
1	S	76	ALA	2.3
1	T	43	GLY	2.3
1	I	250	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	245	LEU	2.3
1	P	312	ILE	2.3
1	Q	316	ILE	2.3
1	G	243	VAL	2.3
1	B	76	ALA	2.2
1	C	76	ALA	2.2
1	G	318	ASN	2.2
1	Q	236	THR	2.2
1	B	43	GLY	2.2
1	K	309	GLY	2.2
1	C	316	ILE	2.2
1	F	316	ILE	2.2
1	J	192	LYS	2.2
1	R	241	LYS	2.2
1	R	307	ALA	2.2
1	S	307	ALA	2.2
1	Q	237	SER	2.2
1	A	262	ASP	2.2
1	W	77	GLU	2.2
1	O	315	VAL	2.2
1	T	76	ALA	2.2
1	F	310	LYS	2.2
1	O	310	LYS	2.2
1	Q	308	SER	2.2
1	S	190	SER	2.2
1	D	42	ASP	2.2
1	I	246	VAL	2.2
1	E	131	LYS	2.2
1	I	92	LYS	2.2
1	M	247	LYS	2.2
1	W	310	LYS	2.2
1	C	318	ASN	2.2
1	G	309	GLY	2.2
1	H	239	ASP	2.2
1	P	239	ASP	2.2
1	T	239	ASP	2.2
1	H	251	ARG	2.2
1	P	235	PRO	2.2
1	M	310	LYS	2.2
1	D	243	VAL	2.1
1	I	88	ASN	2.1
1	I	249	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	R	318	ASN	2.1
1	B	316	ILE	2.1
1	F	244	GLU	2.1
1	V	78	ASP	2.1
1	H	247	LYS	2.1
1	U	40	VAL	2.1
1	D	76	ALA	2.1
1	G	133	ASN	2.1
1	O	238	ASN	2.1
1	F	309	GLY	2.1
1	M	42	ASP	2.1
1	O	308	SER	2.1
1	R	39	SER	2.1
1	R	80	SER	2.1
1	R	239	ASP	2.1
1	G	192	LYS	2.1
1	I	241	LYS	2.1
1	X	247	LYS	2.1
1	G	90	PHE	2.1
1	D	246	VAL	2.1
1	H	100	VAL	2.1
1	N	74	VAL	2.1
1	O	194	VAL	2.1
1	C	236	THR	2.1
1	D	207	ILE	2.1
1	W	115	GLU	2.1
1	L	241	LYS	2.1
1	O	264	ASP	2.1
1	U	78	ASP	2.1
1	W	131	LYS	2.1
1	L	134	SER	2.1
1	D	64	GLN	2.1
1	B	311	ALA	2.1
1	W	307	ALA	2.1
1	D	133	ASN	2.1
1	K	133	ASN	2.1
1	I	244	GLU	2.1
1	G	312	ILE	2.1
1	O	312	ILE	2.1
1	K	241	LYS	2.1
1	D	264	ASP	2.1
1	G	240	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	K	42	ASP	2.1
1	O	240	ASP	2.1
1	X	299	SER	2.1
1	W	246	VAL	2.0
1	C	307	ALA	2.0
1	P	311	ALA	2.0
1	P	318	ASN	2.0
1	D	41	GLU	2.0
1	F	41	GLU	2.0
1	M	43	GLY	2.0
1	W	41	GLU	2.0
1	G	310	LYS	2.0
1	G	314	THR	2.0
1	N	75	LYS	2.0
1	N	310	LYS	2.0
1	S	241	LYS	2.0
1	W	103	THR	2.0
1	X	192	LYS	2.0
1	E	42	ASP	2.0
1	J	299	SER	2.0
1	D	279	ARG	2.0
1	F	251	ARG	2.0
1	P	81	VAL	2.0
1	Q	246	VAL	2.0
1	V	41	GLU	2.0
1	R	79	GLY	2.0
1	U	132	GLY	2.0
1	V	133	ASN	2.0
1	G	236	THR	2.0
1	F	264	ASP	2.0

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

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

6.3 Carbohydrates ⓘ

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.