



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 07:42 PM UTC

PDB ID : 4HOK / pdb_00004hok
Title : crystal structure of apo ck1e
Authors : Huang, X.; Long, A.M.; Zhao, H.
Deposited on : 2012-10-22
Resolution : 2.77 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:

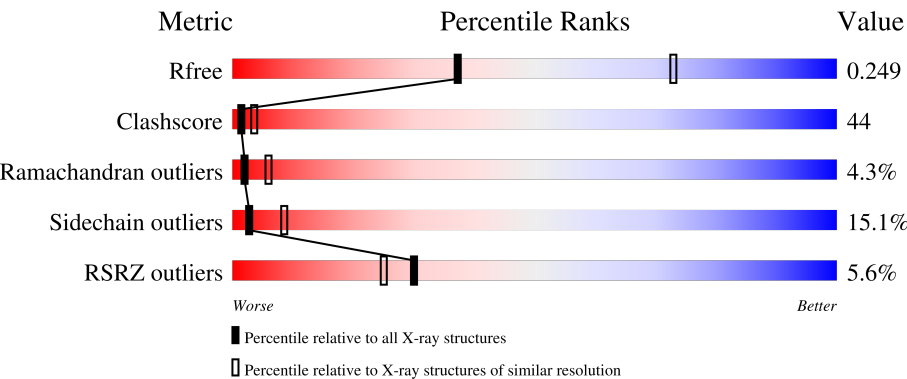
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 2.77 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	5248 (2.80-2.76)
Clashscore	190562	5693 (2.80-2.76)
Ramachandran outliers	187476	5590 (2.80-2.76)
Sidechain outliers	187428	5592 (2.80-2.76)
RSRZ outliers	180081	5251 (2.80-2.76)

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	296	58%32%7%..
1	C	296	50%40%7%..
1	E	296	43%44%11%..
1	G	296	2%44%42%12%..
1	I	296	2%44%43%8%..

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Mol	Chain	Length	Quality of chain
1	K	296	
1	M	296	
1	O	296	
1	Q	296	
1	S	296	
1	U	296	
1	W	296	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	U	301	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 28954 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 Casein kinase I isoform epsilon.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	290	Total	C	N	O	S	0	0	0
			2368	1520	410	423	15			
1	C	289	Total	C	N	O	S	0	0	0
			2370	1521	413	422	14			
1	E	291	Total	C	N	O	S	0	0	0
			2371	1521	414	422	14			
1	G	290	Total	C	N	O	S	0	0	0
			2358	1515	408	420	15			
1	I	291	Total	C	N	O	S	0	0	0
			2373	1522	413	423	15			
1	K	290	Total	C	N	O	S	0	0	0
			2354	1511	406	422	15			
1	M	291	Total	C	N	O	S	0	0	0
			2349	1507	409	419	14			
1	O	290	Total	C	N	O	S	0	0	0
			2364	1518	410	421	15			
1	Q	290	Total	C	N	O	S	0	0	0
			2365	1518	412	420	15			
1	S	286	Total	C	N	O	S	0	0	0
			2327	1495	403	415	14			
1	U	289	Total	C	N	O	S	0	0	0
			2349	1508	405	421	15			
1	W	289	Total	C	N	O	S	0	0	0
			2355	1512	407	422	14			

There are 24 discrepancies between the modelled and reference sequences:

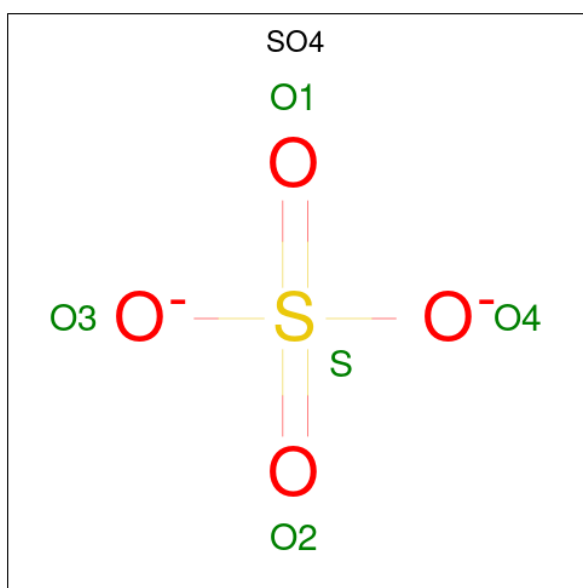
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P49674
A	0	SER	-	expression tag	UNP P49674
C	-1	GLY	-	expression tag	UNP P49674
C	0	SER	-	expression tag	UNP P49674
E	-1	GLY	-	expression tag	UNP P49674

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Chain	Residue	Modelled	Actual	Comment	Reference
E	0	SER	-	expression tag	UNP P49674
G	-1	GLY	-	expression tag	UNP P49674
G	0	SER	-	expression tag	UNP P49674
I	-1	GLY	-	expression tag	UNP P49674
I	0	SER	-	expression tag	UNP P49674
K	-1	GLY	-	expression tag	UNP P49674
K	0	SER	-	expression tag	UNP P49674
M	-1	GLY	-	expression tag	UNP P49674
M	0	SER	-	expression tag	UNP P49674
O	-1	GLY	-	expression tag	UNP P49674
O	0	SER	-	expression tag	UNP P49674
Q	-1	GLY	-	expression tag	UNP P49674
Q	0	SER	-	expression tag	UNP P49674
S	-1	GLY	-	expression tag	UNP P49674
S	0	SER	-	expression tag	UNP P49674
U	-1	GLY	-	expression tag	UNP P49674
U	0	SER	-	expression tag	UNP P49674
W	-1	GLY	-	expression tag	UNP P49674
W	0	SER	-	expression tag	UNP P49674

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	E	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	I	1	Total	O	S	0	0
			5	4	1		
2	K	1	Total	O	S	0	0
			5	4	1		
2	M	1	Total	O	S	0	0
			5	4	1		
2	O	1	Total	O	S	0	0
			5	4	1		
2	Q	1	Total	O	S	0	0
			5	4	1		
2	S	1	Total	O	S	0	0
			5	4	1		
2	U	1	Total	O	S	0	0
			5	4	1		
2	W	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	79	Total	O	0	0
			79	79		
3	C	70	Total	O	0	0
			70	70		
3	E	61	Total	O	0	0
			61	61		
3	G	62	Total	O	0	0
			62	62		
3	I	57	Total	O	0	0
			57	57		
3	K	40	Total	O	0	0
			40	40		
3	M	40	Total	O	0	0
			40	40		
3	O	42	Total	O	0	0
			42	42		
3	Q	45	Total	O	0	0
			45	45		

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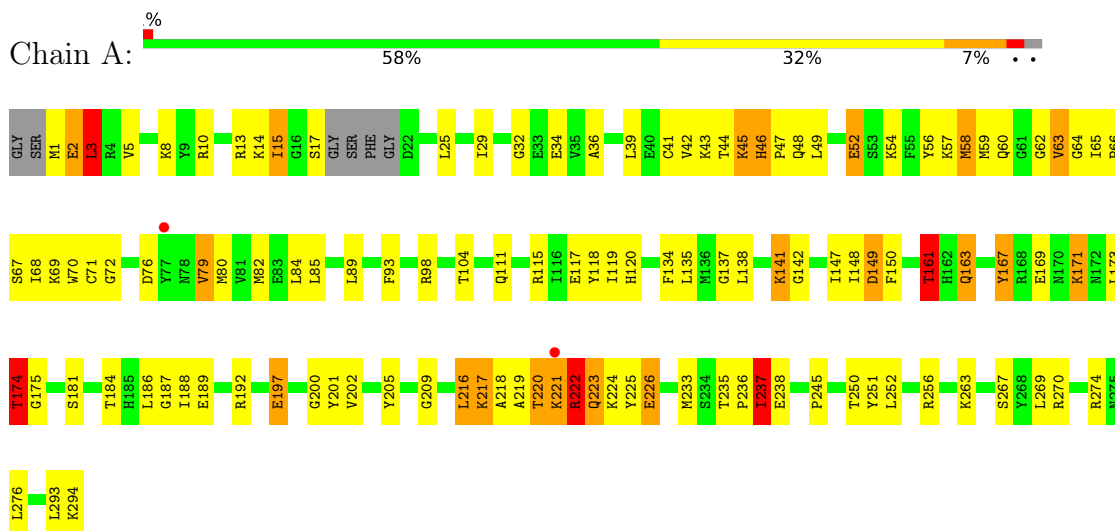
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	S	33	Total 33	O 33	0	0
3	U	29	Total 29	O 29	0	0
3	W	33	Total 33	O 33	0	0

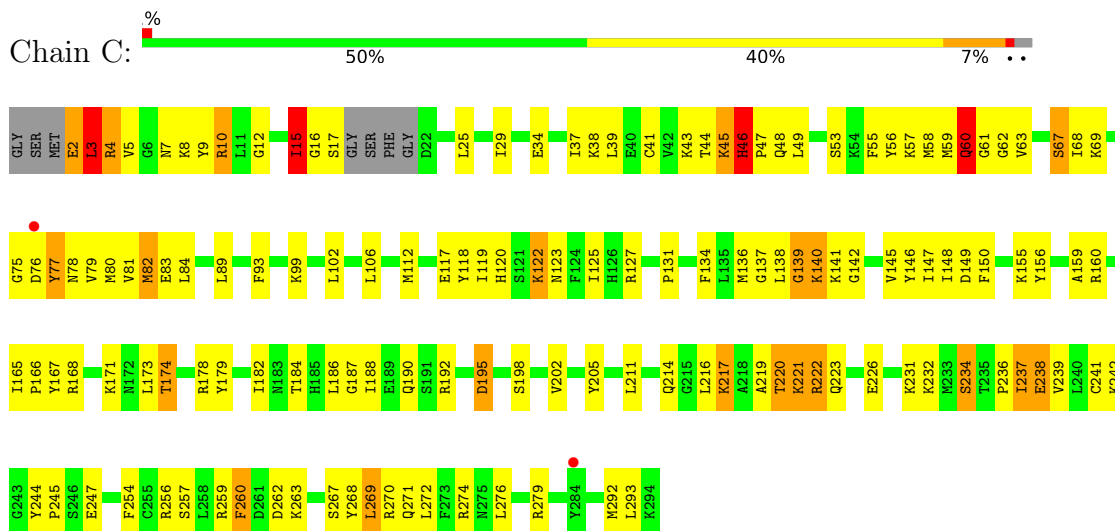
3 Residue-property plots [i](#)

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

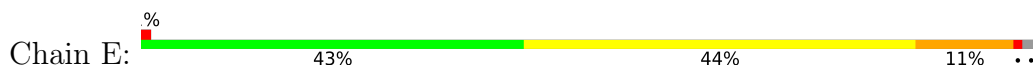
• Molecule 1: Casein kinase I isoform epsilon

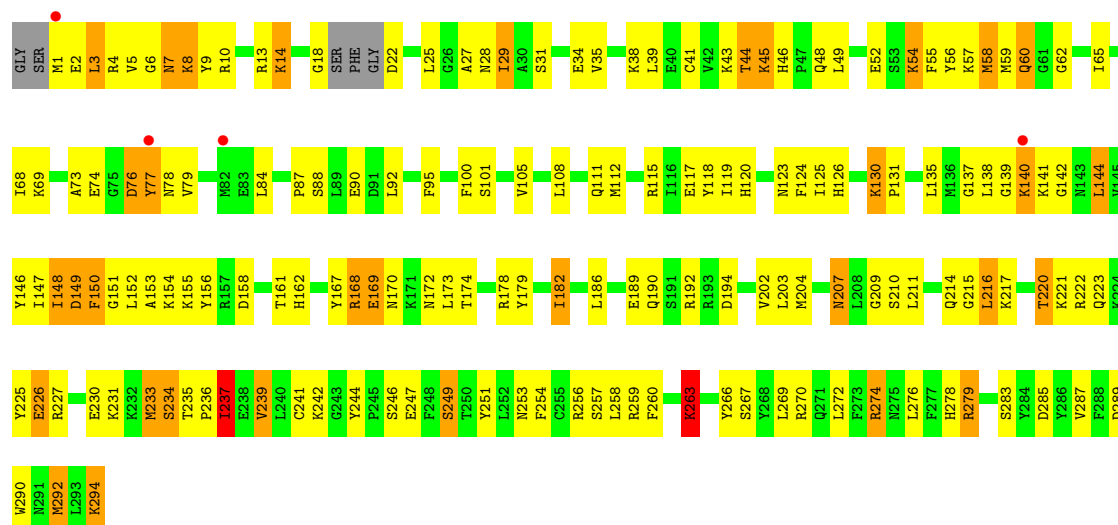


• Molecule 1: Casein kinase I isoform epsilon

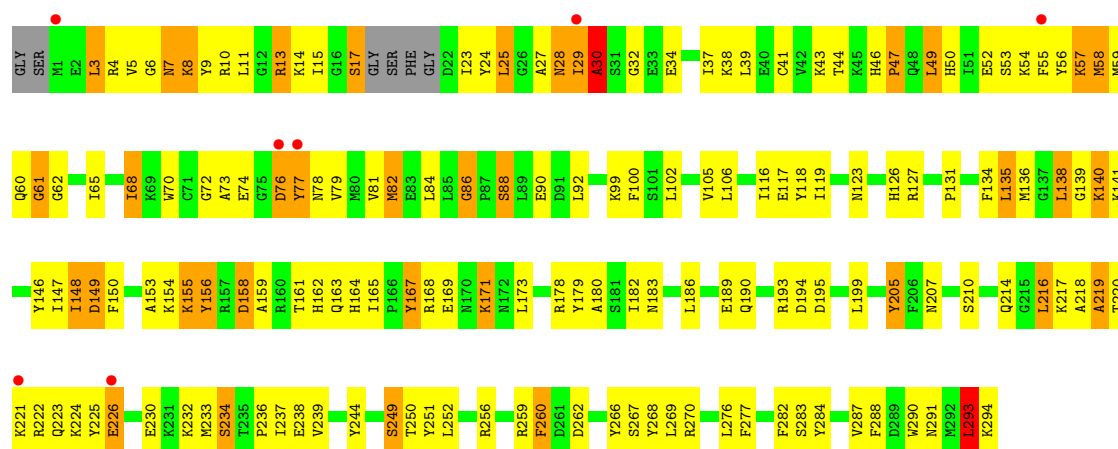
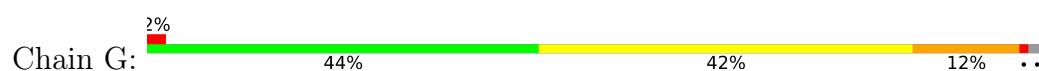


• Molecule 1: Casein kinase I isoform epsilon

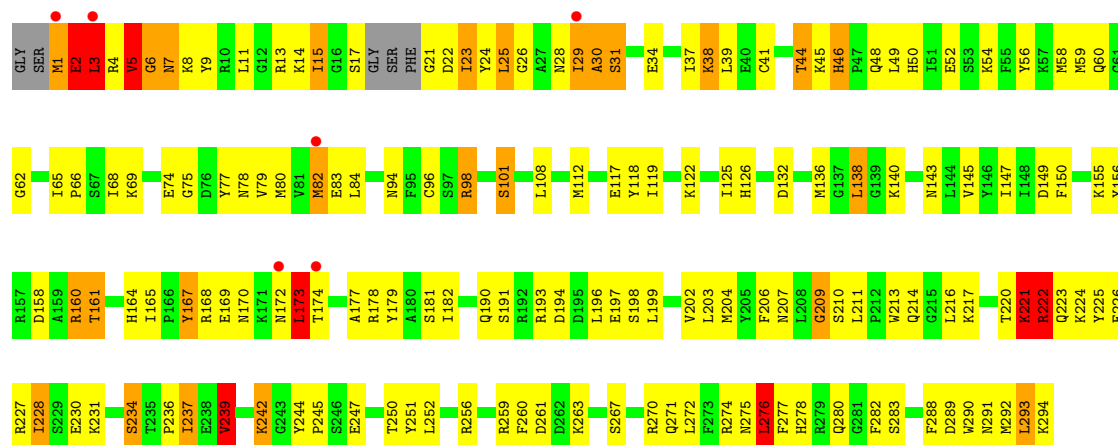




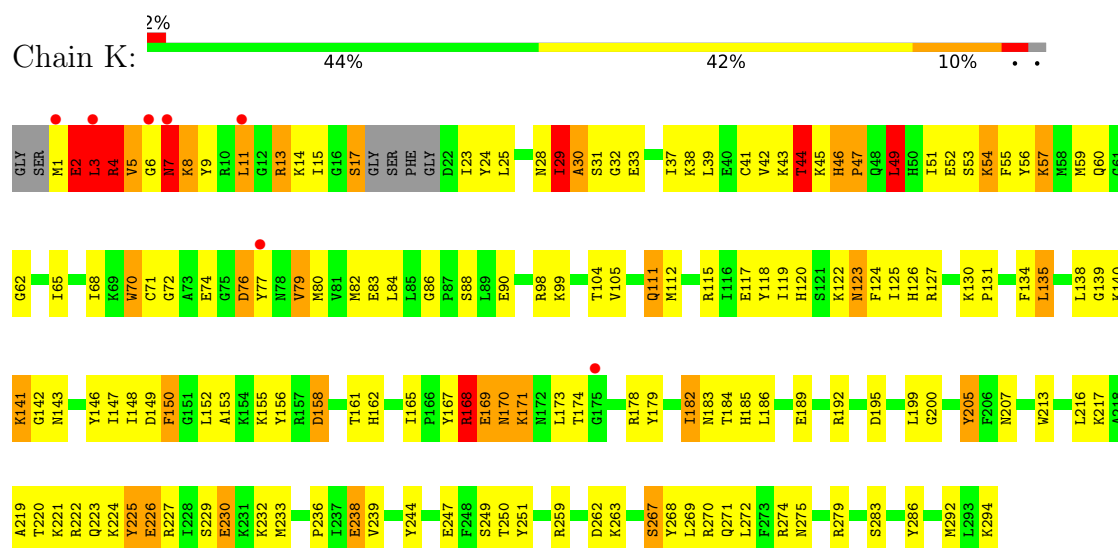
• Molecule 1: Casein kinase I isoform epsilon



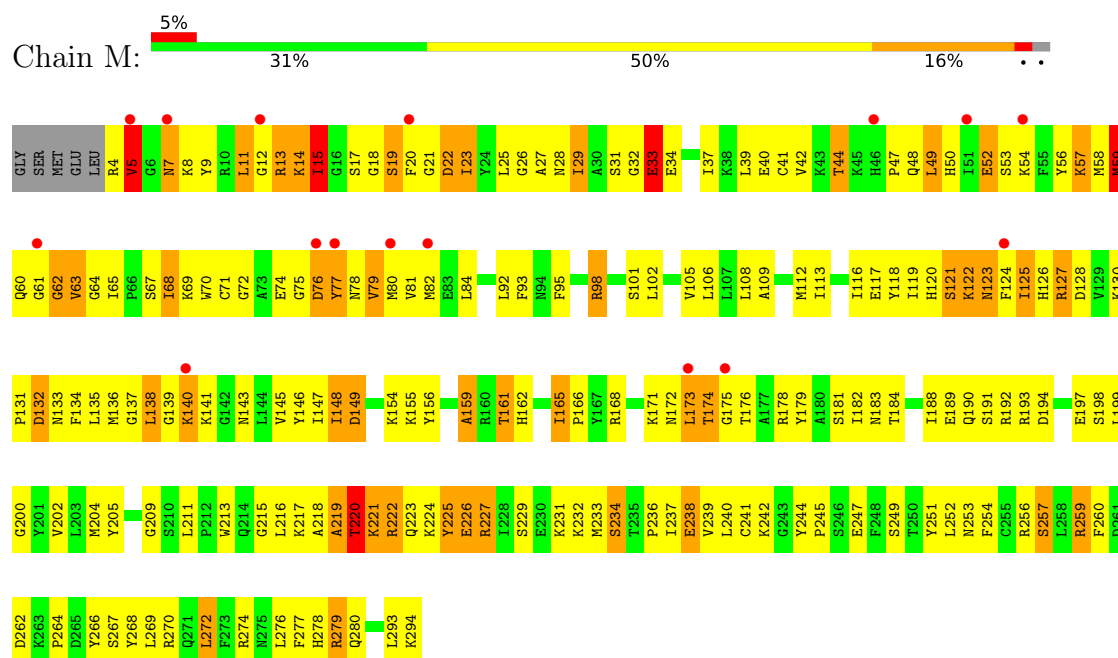
• Molecule 1: Casein kinase I isoform epsilon



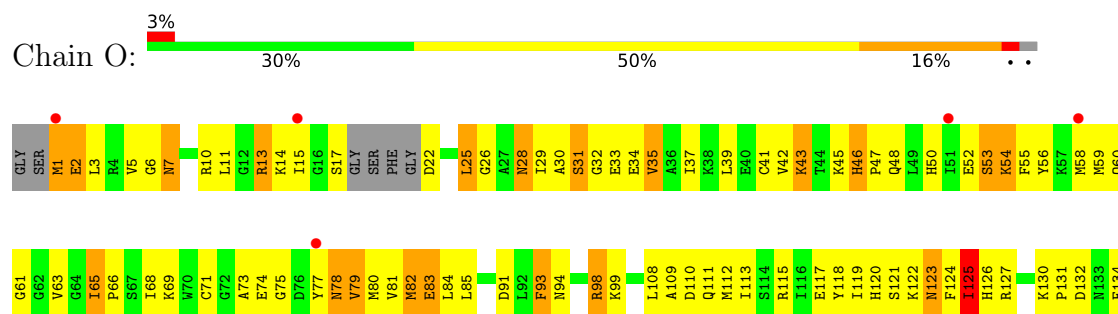
- Molecule 1: Casein kinase I isoform epsilon

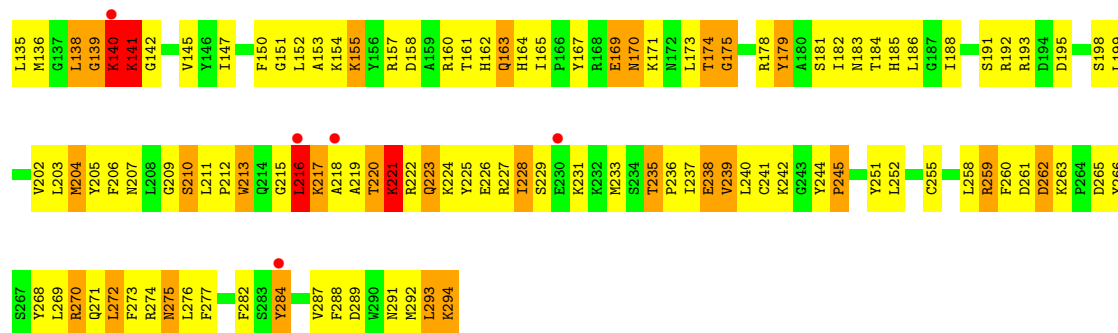


- Molecule 1: Casein kinase I isoform epsilon

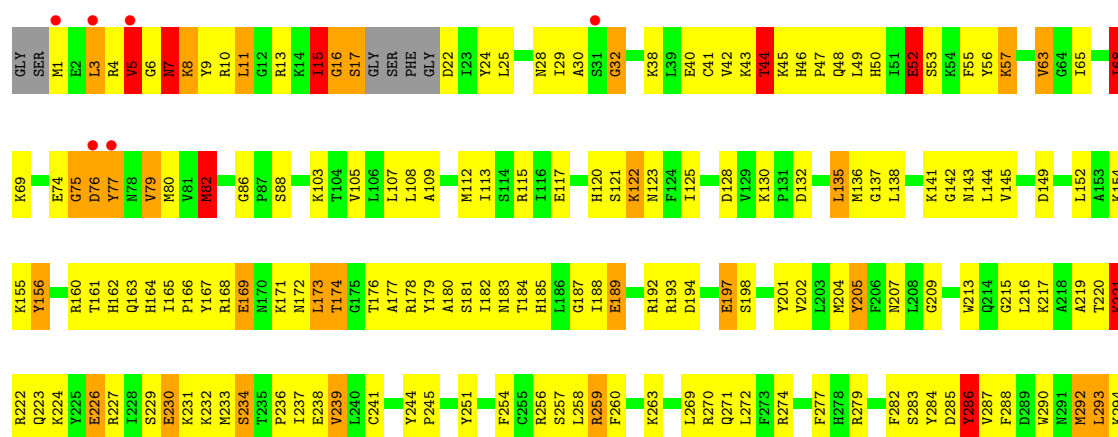
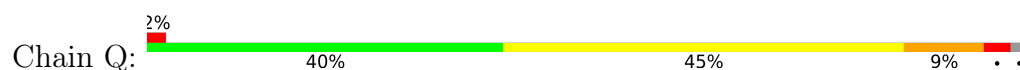


- Molecule 1: Casein kinase I isoform epsilon

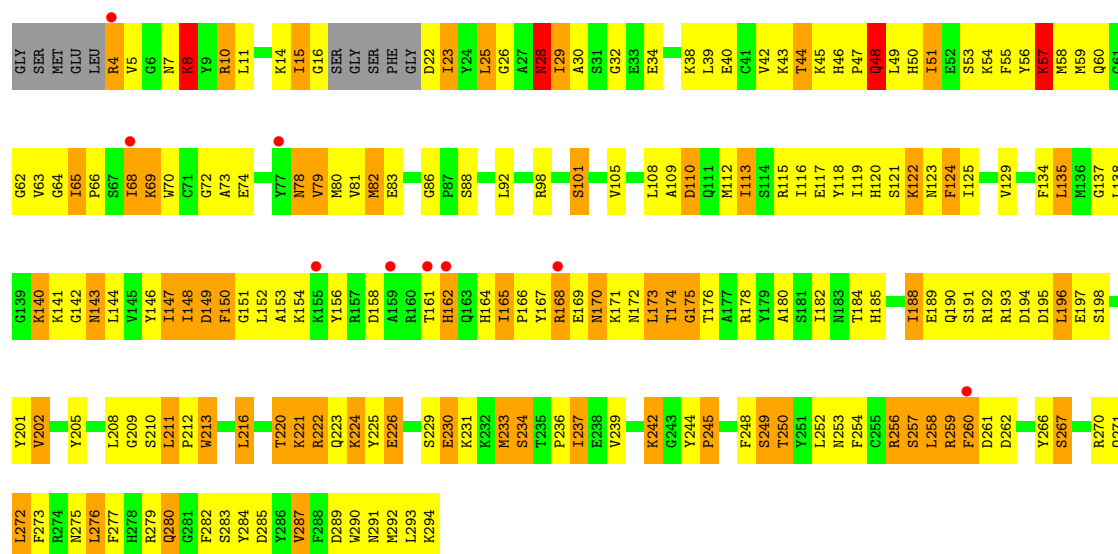




• Molecule 1: Casein kinase I isoform epsilon



• Molecule 1: Casein kinase I isoform epsilon



• Molecule 1: Casein kinase I isoform epsilon

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	180.36Å 142.50Å 232.46Å 90.00° 108.57° 90.00°	Depositor
Resolution (Å)	50.00 – 2.77 50.00 – 2.77	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.77) 99.8 (50.00-2.77)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 2.77Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.241 , 0.262 0.233 , 0.249	Depositor DCC
R_{free} test set	7082 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	56.2	Xtriage
Anisotropy	0.177	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 61.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	28954	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0.69	1/2422 (0.0%)	1.15	17/3251 (0.5%)
1	C	0.65	1/2424 (0.0%)	1.13	13/3252 (0.4%)
1	E	0.62	1/2425 (0.0%)	1.19	22/3255 (0.7%)
1	G	0.64	0/2411	1.20	26/3237 (0.8%)
1	I	0.66	1/2427 (0.0%)	1.18	25/3258 (0.8%)
1	K	0.64	0/2407	1.22	27/3234 (0.8%)
1	M	0.65	1/2404 (0.0%)	1.28	25/3232 (0.8%)
1	O	0.63	0/2418	1.18	22/3246 (0.7%)
1	Q	0.68	3/2419 (0.1%)	1.23	29/3248 (0.9%)
1	S	0.64	0/2380	1.24	26/3197 (0.8%)
1	U	0.69	0/2402	1.36	38/3228 (1.2%)
1	W	0.80	2/2408 (0.1%)	1.37	41/3233 (1.3%)
All	All	0.67	10/28947 (0.0%)	1.23	311/38871 (0.8%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	W	0	1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	2	GLU	CA-C	7.62	1.62	1.52
1	Q	5	VAL	CA-CB	7.22	1.61	1.54
1	Q	1	MET	SD-CE	7.08	1.97	1.79
1	W	59	MET	SD-CE	6.88	1.96	1.79
1	W	124	PHE	CG-CD1	6.67	1.52	1.38
1	Q	82	MET	SD-CE	-5.79	1.65	1.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	222	ARG	CD-NE	5.51	1.53	1.46
1	E	58	MET	SD-CE	5.42	1.93	1.79
1	C	67	SER	C-O	-5.40	1.17	1.24
1	M	5	VAL	N-CA	5.01	1.52	1.46

All (311) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	20	PHE	N-CA-C	-15.84	87.33	111.56
1	M	14	LYS	N-CA-C	-12.65	94.84	110.41
1	W	123	ASN	N-CA-C	10.30	128.54	113.40
1	Q	77	TYR	N-CA-C	10.29	126.01	109.24
1	M	23	ILE	N-CA-C	-10.23	93.39	108.12
1	W	224	LYS	N-CA-C	-9.93	99.28	111.40
1	U	239	VAL	N-CA-C	-9.90	101.11	110.42
1	O	65	ILE	N-CA-C	-9.76	98.49	108.15
1	Q	63	VAL	N-CA-C	-9.74	96.84	109.80
1	I	209	GLY	N-CA-C	-9.63	101.84	114.85
1	Q	68	ILE	N-CA-C	-9.60	99.59	110.05
1	K	5	VAL	N-CA-C	9.57	121.92	108.23
1	M	17	SER	N-CA-C	-9.57	98.18	110.53
1	U	224	LYS	N-CA-C	-9.26	101.24	112.54
1	K	31	SER	N-CA-C	9.17	124.53	113.16
1	K	3	LEU	N-CA-C	9.06	130.09	110.80
1	S	250	THR	N-CA-C	-8.99	100.32	111.11
1	S	78	ASN	N-CA-C	-8.98	97.19	110.48
1	I	3	LEU	N-CA-C	8.94	129.84	110.80
1	E	209	GLY	N-CA-C	-8.91	103.88	114.48
1	C	45	LYS	N-CA-C	-8.87	99.48	110.65
1	O	25	LEU	N-CA-C	-8.85	99.12	110.53
1	M	77	TYR	N-CA-C	8.83	123.80	109.59
1	U	86	GLY	CA-C-N	8.78	128.84	119.89
1	U	86	GLY	C-N-CA	8.78	128.84	119.89
1	G	159	ALA	N-CA-C	8.77	122.98	111.75
1	U	140	LYS	N-CA-C	-8.70	101.11	112.68
1	U	281	GLY	N-CA-C	8.64	126.15	114.92
1	M	125	ILE	N-CA-C	-8.51	96.19	108.53
1	A	235	THR	CA-C-N	-8.51	111.12	120.14
1	A	235	THR	C-N-CA	-8.51	111.12	120.14
1	I	2	GLU	N-CA-C	8.46	128.83	110.80
1	O	83	GLU	N-CA-C	-8.41	99.42	110.53
1	U	155	LYS	N-CA-C	-8.39	96.42	109.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	31	SER	N-CA-C	8.38	122.06	111.24
1	G	239	VAL	N-CA-C	-8.27	103.76	111.45
1	M	78	ASN	N-CA-C	-8.25	98.27	110.48
1	K	4	ARG	N-CA-C	8.19	128.25	110.80
1	Q	160	ARG	N-CA-C	8.07	122.41	112.23
1	U	211	LEU	CA-C-N	8.05	129.91	119.84
1	U	211	LEU	C-N-CA	8.05	129.91	119.84
1	Q	141	LYS	N-CA-C	-8.01	103.06	112.92
1	C	3	LEU	N-CA-C	7.96	127.76	110.80
1	W	114	SER	N-CA-C	7.95	120.03	111.36
1	U	68	ILE	N-CA-C	-7.91	97.05	108.36
1	W	276	LEU	N-CA-C	-7.84	102.81	111.36
1	O	125	ILE	N-CA-C	-7.84	97.16	108.53
1	E	239	VAL	N-CA-C	-7.76	103.68	110.74
1	O	46	HIS	CA-C-N	7.72	127.71	119.76
1	O	46	HIS	C-N-CA	7.72	127.71	119.76
1	U	5	VAL	N-CA-C	7.71	119.95	108.46
1	M	174	THR	N-CA-C	7.71	120.24	110.61
1	W	86	GLY	CA-C-N	7.66	129.41	119.84
1	W	86	GLY	C-N-CA	7.66	129.41	119.84
1	I	221	LYS	N-CA-C	-7.61	101.73	111.02
1	O	73	ALA	N-CA-C	7.59	120.80	110.55
1	G	163	GLN	N-CA-C	-7.57	99.25	110.23
1	A	175	GLY	N-CA-C	-7.52	98.90	111.08
1	E	4	ARG	CA-C-N	-7.46	113.47	123.10
1	E	4	ARG	C-N-CA	-7.46	113.47	123.10
1	A	167	TYR	N-CA-C	-7.41	99.32	110.28
1	A	3	LEU	N-CA-C	7.37	126.50	110.80
1	G	78	ASN	N-CA-C	-7.33	98.66	110.32
1	K	174	THR	N-CA-C	7.29	121.43	112.54
1	G	148	ILE	N-CA-C	7.29	117.71	108.82
1	W	272	LEU	N-CA-C	-7.26	103.68	112.54
1	U	183	ASN	N-CA-C	7.25	119.26	111.36
1	U	144	LEU	N-CA-C	7.23	120.05	108.41
1	K	13	ARG	N-CA-C	7.22	119.62	110.24
1	K	148	ILE	N-CA-C	7.19	118.52	108.23
1	U	53	SER	N-CA-C	-7.18	103.39	111.14
1	W	45	LYS	N-CA-C	-7.17	102.34	113.02
1	M	149	ASP	N-CA-C	7.09	119.21	110.91
1	K	49	LEU	N-CA-C	7.09	119.62	111.11
1	W	31	SER	N-CA-C	7.08	125.88	110.80
1	A	174	THR	N-CA-C	7.07	120.17	110.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	125	ILE	N-CA-C	-7.07	98.30	108.48
1	U	250	THR	N-CA-C	-7.06	103.19	111.03
1	I	14	LYS	N-CA-C	-7.04	101.21	110.43
1	Q	75	GLY	N-CA-C	-7.01	99.60	111.73
1	W	3	LEU	N-CA-C	7.00	125.71	110.80
1	U	38	LYS	N-CA-C	-6.98	101.52	110.53
1	G	49	LEU	N-CA-C	6.98	119.73	111.71
1	W	49	LEU	N-CA-C	-6.98	103.60	111.07
1	K	263	LYS	CA-C-N	6.96	127.00	119.90
1	K	263	LYS	C-N-CA	6.96	127.00	119.90
1	U	276	LEU	N-CA-C	-6.96	103.39	110.97
1	I	6	GLY	N-CA-C	-6.95	104.26	114.61
1	O	93	PHE	N-CA-C	-6.94	103.40	110.97
1	U	167	TYR	N-CA-C	-6.94	101.58	110.53
1	E	31	SER	N-CA-C	6.89	121.44	112.89
1	Q	53	SER	N-CA-C	-6.88	103.71	111.07
1	K	2	GLU	N-CA-C	6.88	125.44	110.80
1	M	21	GLY	N-CA-C	6.88	124.96	115.27
1	S	65	ILE	CA-C-N	6.88	128.69	120.23
1	S	65	ILE	C-N-CA	6.88	128.69	120.23
1	S	57	LYS	N-CA-C	-6.84	103.51	110.97
1	C	148	ILE	N-CA-C	6.84	116.87	108.53
1	U	226	GLU	N-CA-C	-6.83	103.76	111.14
1	O	79	VAL	N-CA-C	6.83	118.13	108.17
1	A	63	VAL	N-CA-C	-6.81	102.51	110.21
1	E	169	GLU	N-CA-C	6.72	117.35	108.07
1	Q	16	GLY	N-CA-C	6.72	120.93	111.19
1	K	79	VAL	N-CA-C	6.68	117.75	108.12
1	S	276	LEU	N-CA-C	-6.68	103.92	111.07
1	E	246	SER	N-CA-C	6.67	120.28	111.75
1	S	32	GLY	N-CA-C	-6.65	105.33	114.64
1	W	227	ARG	N-CA-C	-6.64	103.97	111.07
1	M	127	ARG	N-CA-C	6.63	121.14	113.38
1	U	125	ILE	N-CA-C	-6.61	99.00	109.17
1	A	250	THR	N-CA-C	-6.58	104.11	111.28
1	Q	79	VAL	N-CA-C	6.58	118.98	108.85
1	C	237	ILE	N-CA-C	6.58	117.07	110.23
1	K	170	ASN	N-CA-C	6.55	120.85	112.86
1	O	78	ASN	N-CA-C	-6.55	100.79	110.48
1	E	28	ASN	N-CA-C	-6.53	99.75	109.15
1	O	239	VAL	N-CA-C	-6.51	104.41	110.53
1	W	173	LEU	N-CA-C	-6.51	100.91	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	W	76	ASP	N-CA-C	-6.51	96.94	110.80
1	E	14	LYS	N-CA-C	-6.50	101.33	110.50
1	E	259	ARG	N-CA-C	-6.49	100.88	110.48
1	U	235	THR	N-CA-C	6.49	124.14	109.81
1	G	72	GLY	N-CA-C	6.45	118.55	110.29
1	C	63	VAL	N-CA-C	-6.44	101.24	109.80
1	G	68	ILE	N-CA-C	-6.44	100.39	108.89
1	G	293	LEU	N-CA-C	-6.43	101.60	110.35
1	S	197	GLU	N-CA-C	-6.43	104.19	111.07
1	G	205	TYR	N-CA-C	-6.42	104.20	111.07
1	S	124	PHE	N-CA-C	6.41	118.92	109.24
1	M	33	GLU	N-CA-C	6.41	120.12	110.64
1	E	237	ILE	N-CA-C	6.40	117.92	110.62
1	I	25	LEU	N-CA-C	-6.40	101.48	110.50
1	E	73	ALA	N-CA-C	6.32	118.92	108.99
1	I	31	SER	N-CA-C	6.32	120.71	113.19
1	U	145	VAL	N-CA-C	-6.30	101.46	109.58
1	E	292	MET	N-CA-C	6.27	118.97	109.95
1	S	213	TRP	N-CA-C	6.26	120.53	113.02
1	G	73	ALA	N-CA-C	6.22	119.68	109.85
1	U	98	ARG	N-CA-C	6.21	120.12	111.74
1	E	77	TYR	N-CA-C	6.14	119.41	109.40
1	W	152	LEU	N-CA-C	-6.14	104.40	113.61
1	U	249	SER	N-CA-C	-6.13	105.96	113.50
1	Q	169	GLU	N-CA-C	6.11	116.35	108.34
1	A	197	GLU	N-CA-C	-6.11	104.54	111.14
1	U	184	THR	N-CA-C	-6.09	104.56	111.07
1	W	218	ALA	N-CA-C	6.05	118.90	109.52
1	W	257	SER	N-CA-C	6.03	119.89	112.54
1	W	98	ARG	N-CA-C	6.03	119.56	111.24
1	I	78	ASN	N-CA-C	-6.01	99.49	109.46
1	I	46	HIS	CA-C-N	6.00	126.20	119.90
1	I	46	HIS	C-N-CA	6.00	126.20	119.90
1	K	268	TYR	N-CA-C	-6.00	104.65	111.07
1	W	105	VAL	N-CA-C	-6.00	104.48	110.30
1	U	287	VAL	N-CA-C	-5.99	96.88	109.34
1	I	167	TYR	N-CA-C	-5.97	102.23	110.35
1	U	213	TRP	N-CA-C	-5.97	104.66	113.61
1	S	188	ILE	N-CA-C	5.95	117.26	109.58
1	W	13	ARG	N-CA-C	5.95	123.47	110.80
1	I	5	VAL	N-CA-C	5.94	118.43	108.81
1	S	28	ASN	N-CA-C	-5.93	98.16	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	209	GLY	N-CA-C	-5.92	106.35	114.64
1	M	227	ARG	N-CA-C	-5.92	104.74	111.07
1	U	33	GLU	N-CA-C	5.92	118.40	110.35
1	M	123	ASN	N-CA-C	5.91	123.39	110.80
1	C	48	GLN	N-CA-C	-5.91	107.89	114.62
1	Q	68	ILE	CB-CA-C	-5.89	105.11	111.59
1	G	90	GLU	N-CA-C	-5.88	104.95	111.36
1	O	235	THR	CA-C-N	-5.88	113.10	120.51
1	O	235	THR	C-N-CA	-5.88	113.10	120.51
1	M	173	LEU	N-CA-C	-5.88	101.60	110.24
1	Q	163	GLN	N-CA-C	-5.86	101.73	110.23
1	A	45	LYS	N-CA-C	-5.85	102.80	111.81
1	Q	11	LEU	N-CA-C	5.85	117.74	108.67
1	U	146	TYR	N-CA-C	-5.81	100.58	109.41
1	W	28	ASN	N-CA-C	-5.80	98.28	108.20
1	S	249	SER	N-CA-C	-5.80	105.87	113.12
1	K	56	TYR	N-CA-C	-5.80	105.05	111.71
1	W	127	ARG	N-CA-C	5.80	121.62	113.56
1	G	216	LEU	N-CA-C	-5.78	99.10	108.52
1	W	5	VAL	N-CA-C	5.78	116.69	108.42
1	K	44	THR	N-CA-C	5.78	118.63	109.50
1	S	86	GLY	CA-C-N	5.78	125.75	120.03
1	S	86	GLY	C-N-CA	5.78	125.75	120.03
1	W	211	LEU	CA-C-N	5.76	125.47	119.82
1	W	211	LEU	C-N-CA	5.76	125.47	119.82
1	I	169	GLU	N-CA-C	5.75	118.62	109.65
1	W	135	LEU	N-CA-C	-5.73	100.55	109.72
1	S	79	VAL	N-CA-C	5.73	116.32	107.78
1	G	30	ALA	N-CA-C	-5.73	98.60	110.80
1	U	244	TYR	CA-C-N	5.72	126.98	119.84
1	U	244	TYR	C-N-CA	5.72	126.98	119.84
1	E	130	LYS	CA-C-N	5.71	126.98	119.84
1	E	130	LYS	C-N-CA	5.71	126.98	119.84
1	C	99	LYS	N-CA-C	-5.69	99.03	108.75
1	A	269	LEU	N-CA-C	5.67	117.46	111.28
1	S	172	ASN	N-CA-C	5.67	117.86	110.43
1	O	98	ARG	N-CA-C	5.67	119.21	111.39
1	Q	230	GLU	N-CA-C	-5.67	104.31	111.11
1	E	25	LEU	N-CA-C	-5.66	102.91	110.55
1	U	127	ARG	N-CA-C	5.64	122.81	110.80
1	W	240	LEU	N-CA-C	-5.64	105.50	112.38
1	C	78	ASN	N-CA-C	-5.63	100.50	109.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	179	TYR	N-CA-C	5.63	120.26	113.17
1	K	65	ILE	CA-C-N	-5.62	113.99	119.78
1	K	65	ILE	C-N-CA	-5.62	113.99	119.78
1	M	98	ARG	N-CA-C	5.61	119.17	111.54
1	M	22	ASP	N-CA-C	-5.60	98.87	110.80
1	I	276	LEU	N-CA-C	-5.58	105.27	111.36
1	K	83	GLU	N-CA-C	-5.58	102.22	110.48
1	K	111	GLN	N-CA-C	5.57	117.03	111.07
1	Q	65	ILE	CB-CA-C	-5.51	104.44	110.78
1	Q	221	LYS	N-CA-C	-5.50	104.30	111.02
1	G	25	LEU	N-CA-C	-5.50	102.75	110.50
1	I	37	ILE	N-CA-C	5.50	116.65	108.46
1	I	54	LYS	N-CA-C	-5.50	105.20	111.14
1	G	276	LEU	N-CA-C	-5.47	105.22	111.07
1	K	275	ASN	N-CA-C	-5.46	104.36	111.02
1	M	161	THR	N-CA-C	-5.46	105.25	111.14
1	S	25	LEU	N-CA-C	-5.45	101.97	110.42
1	E	148	ILE	N-CA-C	5.44	115.17	108.53
1	E	150	PHE	N-CA-C	-5.43	105.09	112.26
1	G	156	TYR	N-CA-C	-5.43	106.66	113.72
1	I	237	ILE	N-CA-C	5.43	116.16	110.62
1	W	68	ILE	CB-CA-C	-5.42	102.49	111.32
1	W	136	MET	N-CA-C	-5.41	100.87	109.96
1	Q	32	GLY	N-CA-C	-5.41	100.37	113.18
1	G	86	GLY	CA-C-N	5.40	126.58	119.84
1	G	86	GLY	C-N-CA	5.40	126.58	119.84
1	Q	15	ILE	N-CA-C	5.39	118.92	113.47
1	W	111	GLN	N-CA-C	-5.39	105.09	110.97
1	K	205	TYR	N-CA-C	-5.39	105.49	111.36
1	W	81	VAL	N-CA-C	-5.39	99.75	107.78
1	A	161	THR	N-CA-C	5.38	119.57	112.89
1	O	123	ASN	N-CA-C	5.37	124.27	113.31
1	E	144	LEU	N-CA-C	5.36	117.26	108.52
1	I	173	LEU	N-CA-C	-5.35	102.70	110.24
1	W	171	LYS	N-CA-C	-5.34	102.98	110.35
1	O	275	ASN	N-CA-C	-5.33	105.37	111.07
1	U	44	THR	N-CA-C	5.32	117.39	109.25
1	M	168	ARG	CG-CD-NE	-5.31	100.31	112.00
1	K	53	SER	CA-C-N	-5.31	113.17	120.28
1	K	53	SER	C-N-CA	-5.31	113.17	120.28
1	G	77	TYR	N-CA-C	5.30	118.21	109.72
1	M	27	ALA	N-CA-C	-5.30	101.92	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	64	GLY	CA-C-N	-5.30	117.60	123.43
1	S	64	GLY	C-N-CA	-5.30	117.60	123.43
1	G	88	SER	N-CA-C	-5.30	102.21	110.42
1	C	232	LYS	N-CA-C	-5.29	105.41	111.07
1	Q	156	TYR	N-CA-C	-5.28	106.85	113.72
1	A	237	ILE	N-CA-C	5.28	115.90	110.36
1	A	79	VAL	N-CA-C	5.28	115.72	108.12
1	M	34	GLU	N-CA-C	-5.26	101.88	110.20
1	M	168	ARG	CB-CG-CD	5.26	123.41	111.30
1	C	15	ILE	CB-CA-C	-5.26	106.25	111.30
1	Q	205	TYR	N-CA-C	-5.25	104.81	111.11
1	S	98	ARG	N-CA-C	5.25	118.63	111.39
1	I	4	ARG	N-CA-CB	-5.24	102.43	111.55
1	U	246	SER	N-CA-C	-5.24	105.68	111.71
1	Q	7	ASN	N-CA-C	-5.22	99.68	110.80
1	O	291	ASN	N-CA-C	-5.22	106.86	113.18
1	C	77	TYR	N-CA-C	5.22	117.40	108.90
1	A	148	ILE	N-CA-C	5.21	114.89	108.53
1	G	99	LYS	N-CA-C	-5.21	99.77	108.32
1	Q	9	TYR	N-CA-C	5.21	117.39	108.90
1	A	63	VAL	CB-CA-C	-5.20	105.62	111.45
1	M	168	ARG	CA-CB-CG	-5.20	103.69	114.10
1	M	79	VAL	N-CA-C	5.19	115.75	108.17
1	W	159	ALA	N-CA-C	5.19	117.61	111.33
1	W	178	ARG	N-CA-C	5.19	117.61	111.33
1	I	259	ARG	N-CA-C	-5.18	103.69	110.53
1	W	37	ILE	N-CA-C	5.18	115.50	107.78
1	Q	263	LYS	CA-C-N	5.18	125.10	119.76
1	Q	263	LYS	C-N-CA	5.18	125.10	119.76
1	S	287	VAL	CB-CA-C	-5.18	106.31	111.80
1	U	105	VAL	N-CA-C	-5.18	105.49	110.72
1	C	269	LEU	N-CA-C	5.18	116.61	110.97
1	W	148	ILE	N-CA-C	5.18	120.11	109.34
1	W	166	PRO	N-CA-C	5.17	120.17	111.32
1	K	150	PHE	N-CA-C	-5.16	107.15	112.93
1	C	195	ASP	N-CA-C	-5.15	105.56	111.07
1	W	7	ASN	N-CA-C	5.14	119.14	112.86
1	Q	125	ILE	N-CA-C	-5.14	100.80	108.46
1	S	196	LEU	N-CA-C	5.14	116.96	111.36
1	A	32	GLY	N-CA-C	-5.14	108.62	115.40
1	W	54	LYS	N-CA-C	-5.14	105.17	111.75
1	W	145	VAL	N-CA-C	5.14	115.71	108.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	W	43	LYS	N-CA-C	5.13	120.18	113.20
1	G	268	TYR	N-CA-C	-5.11	105.60	111.07
1	I	228	ILE	CB-CA-C	-5.11	105.34	111.88
1	U	153	ALA	N-CA-C	5.10	116.69	110.41
1	I	98	ARG	N-CA-C	5.09	118.34	111.17
1	K	168	ARG	N-CA-C	5.09	116.14	108.46
1	G	61	GLY	N-CA-C	5.08	122.30	115.59
1	U	257	SER	N-CA-C	5.08	117.94	111.69
1	S	113	ILE	N-CA-C	-5.08	105.64	110.42
1	O	231	LYS	N-CA-C	-5.08	105.44	110.97
1	Q	120	HIS	N-CA-C	-5.07	105.76	111.28
1	M	159	ALA	N-CA-C	5.06	117.18	111.11
1	Q	145	VAL	CB-CA-C	-5.06	105.16	111.08
1	O	181	SER	N-CA-C	-5.05	103.82	110.33
1	G	250	THR	N-CA-C	-5.03	105.79	111.28
1	O	213	TRP	N-CA-C	5.03	118.91	112.87
1	S	273	PHE	N-CA-C	5.02	116.75	111.28
1	G	167	TYR	N-CA-C	-5.02	103.85	110.33
1	S	68	ILE	N-CA-C	-5.02	102.62	109.55
1	E	263	LYS	N-CA-C	-5.01	99.49	108.47
1	U	212	PRO	N-CA-C	5.01	122.80	112.47
1	I	239	VAL	N-CA-C	-5.01	106.18	110.74
1	Q	52	GLU	N-CA-C	5.01	117.63	111.82
1	K	195	ASP	N-CA-C	-5.01	105.71	111.07
1	E	78	ASN	N-CA-C	-5.00	101.16	109.46

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	W	284	TYR	Sidechain

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	2368	0	2366	126	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2370	0	2376	119	1
1	E	2371	0	2369	164	0
1	G	2358	0	2354	159	0
1	I	2373	0	2366	150	0
1	K	2354	0	2336	162	0
1	M	2349	0	2321	203	0
1	O	2364	0	2362	265	0
1	Q	2365	0	2359	187	1
1	S	2327	0	2313	272	1
1	U	2349	0	2337	389	0
1	W	2355	0	2346	395	0
2	A	5	0	0	0	0
2	C	5	0	0	0	0
2	E	5	0	0	0	0
2	G	5	0	0	1	0
2	I	5	0	0	0	0
2	K	5	0	0	0	0
2	M	5	0	0	1	0
2	O	5	0	0	0	0
2	Q	5	0	0	1	0
2	S	5	0	0	1	0
2	U	5	0	0	3	0
2	W	5	0	0	0	0
3	A	79	0	0	12	0
3	C	70	0	0	7	0
3	E	61	0	0	7	0
3	G	62	0	0	12	0
3	I	57	0	0	8	0
3	K	40	0	0	6	0
3	M	40	0	0	6	0
3	O	42	0	0	9	0
3	Q	45	0	0	6	0
3	S	33	0	0	7	0
3	U	29	0	0	6	0
3	W	33	0	0	13	0
All	All	28954	0	28205	2476	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 44.

All (2476) 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:W:120:HIS:ND1	1:W:192:ARG:HG2	1.41	1.35
1:E:52:GLU:OE2	1:E:149:ASP:HA	1.31	1.24
1:K:3:LEU:CD2	1:K:11:LEU:HB3	1.71	1.20
1:W:53:SER:HB3	1:W:71:CYS:SG	1.79	1.20
1:M:13:ARG:H	1:M:13:ARG:CD	1.54	1.19
1:O:56:TYR:HB2	1:O:68:ILE:HD11	1.23	1.18
1:W:69:LYS:HB2	1:W:81:VAL:O	1.40	1.17
1:W:192:ARG:NH1	1:W:264:PRO:HD2	1.62	1.15
1:M:13:ARG:HD3	1:M:13:ARG:N	1.35	1.14
1:A:220:THR:HG22	1:A:223:GLN:H	1.10	1.13
1:S:191:SER:HB3	1:S:260:PHE:HE1	0.98	1.12
1:W:192:ARG:NH1	1:W:263:LYS:HA	1.65	1.11
1:W:158:ASP:HB3	1:W:163:GLN:HB2	1.26	1.11
1:W:29:ILE:HA	3:W:420:HOH:O	1.48	1.10
1:C:3:LEU:HD21	1:K:238:GLU:HG3	1.21	1.10
1:S:280:GLN:HA	1:S:280:GLN:HE21	1.01	1.10
1:M:222:ARG:HB2	1:M:222:ARG:HH11	1.16	1.09
1:W:192:ARG:HH12	1:W:263:LYS:HA	1.18	1.09
1:O:13:ARG:HH11	1:O:13:ARG:HG3	1.13	1.09
1:O:58:MET:HE2	1:O:59:MET:HE2	1.29	1.09
1:W:285:ASP:OD1	1:W:287:VAL:HG23	1.49	1.09
1:S:174:THR:CG2	1:S:175:GLY:H	1.65	1.08
1:O:28:ASN:ND2	1:O:31:SER:H	1.51	1.08
1:W:219:ALA:O	1:W:220:THR:HG22	1.51	1.08
1:S:191:SER:HB3	1:S:260:PHE:CE1	1.88	1.07
1:W:68:ILE:HD13	1:W:80:MET:HE3	1.34	1.07
1:K:3:LEU:HD22	1:K:11:LEU:HB3	1.34	1.07
1:U:47:PRO:O	1:U:48:GLN:HG3	1.56	1.06
1:I:160:ARG:HG2	1:I:160:ARG:HH11	1.20	1.05
1:S:174:THR:HG23	1:S:175:GLY:H	0.97	1.05
1:U:237:ILE:HG13	1:U:256:ARG:NH1	1.68	1.05
1:E:249:SER:HB2	1:O:1:MET:HE3	1.36	1.05
1:Q:17:SER:H	1:S:294:LYS:HD3	1.13	1.05
1:S:173:LEU:HD23	1:S:225:TYR:HD2	1.19	1.04
1:Q:4:ARG:HH21	1:Q:7:ASN:HA	1.20	1.04
1:O:56:TYR:CB	1:O:68:ILE:HD11	1.87	1.04
1:I:220:THR:HG23	1:I:223:GLN:H	1.21	1.03
1:U:56:TYR:CE1	1:U:66:PRO:HG2	1.92	1.03
1:W:192:ARG:HH11	1:W:264:PRO:HD2	0.89	1.03
1:S:140:LYS:H	1:S:140:LYS:HD3	1.21	1.03
1:U:205:TYR:HB2	1:U:211:LEU:CD1	1.86	1.03
1:U:4:ARG:HH21	1:U:7:ASN:HA	1.22	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:220:THR:HG22	1:E:223:GLN:HG3	1.34	1.02
1:U:169:GLU:H	1:U:169:GLU:CD	1.67	1.02
1:S:170:ASN:HD22	1:S:170:ASN:N	1.58	1.01
1:S:173:LEU:HD23	1:S:225:TYR:CD2	1.94	1.01
1:U:4:ARG:NH2	1:U:7:ASN:HA	1.75	1.01
1:A:34:GLU:HG3	3:C:414:HOH:O	1.59	1.00
1:Q:259:ARG:HD2	1:Q:260:PHE:H	1.26	1.00
1:U:7:ASN:HD22	1:U:7:ASN:C	1.67	0.99
1:S:174:THR:HG23	1:S:175:GLY:N	1.70	0.99
1:W:2:GLU:HG3	1:W:3:LEU:H	1.27	0.99
1:I:278:HIS:HB3	3:I:411:HOH:O	1.64	0.98
1:U:156:TYR:HA	1:U:165:ILE:HD13	1.45	0.97
1:G:178:ARG:CZ	1:G:214:GLN:HE21	1.77	0.97
1:S:280:GLN:HE21	1:S:280:GLN:CA	1.77	0.97
1:U:264:PRO:HG2	1:U:266:TYR:CZ	1.99	0.97
1:M:274:ARG:HH11	1:M:274:ARG:HG2	1.29	0.97
1:O:140:LYS:HG3	1:O:141:LYS:HD3	1.43	0.97
1:G:186:LEU:HD21	1:G:233:MET:HE1	1.46	0.96
1:W:41:CYS:HA	1:W:77:TYR:HD1	1.31	0.96
1:S:156:TYR:O	1:S:165:ILE:HG23	1.65	0.96
1:W:10:ARG:HG2	1:W:10:ARG:HH11	1.30	0.96
1:M:84:LEU:HD21	1:O:292:MET:HE2	1.45	0.96
1:S:10:ARG:HG3	1:S:10:ARG:HH11	1.30	0.96
1:S:271:GLN:HA	1:S:271:GLN:NE2	1.80	0.96
1:U:66:PRO:HA	1:U:83:GLU:OE2	1.66	0.96
1:Q:220:THR:HG23	1:Q:223:GLN:H	1.31	0.96
1:O:255:CYS:HA	1:O:258:LEU:HD12	1.47	0.95
1:M:40:GLU:OE2	1:M:47:PRO:HA	1.67	0.95
1:C:3:LEU:CD2	1:K:238:GLU:HG3	1.97	0.95
1:G:15:ILE:HG21	1:G:25:LEU:HB2	1.49	0.95
1:A:186:LEU:HD21	1:A:233:MET:HE1	1.48	0.95
1:W:4:ARG:HD3	1:W:29:ILE:HD12	1.49	0.95
1:M:15:ILE:HD12	1:M:25:LEU:HB2	1.45	0.94
1:O:28:ASN:C	1:O:28:ASN:HD22	1.73	0.94
1:S:280:GLN:HA	1:S:280:GLN:NE2	1.72	0.94
1:O:13:ARG:HH11	1:O:13:ARG:CG	1.80	0.94
1:W:120:HIS:CE1	1:W:192:ARG:HG2	2.03	0.94
1:O:204:MET:HA	1:O:204:MET:HE3	1.49	0.94
1:U:208:LEU:O	1:U:210:SER:N	2.00	0.94
1:U:211:LEU:HD22	1:U:213:TRP:CZ2	2.03	0.94
1:W:278:HIS:O	1:W:281:GLY:N	2.01	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:68:ILE:HD11	1:K:71:CYS:HB2	1.50	0.93
1:W:293:LEU:O	1:W:294:LYS:HD3	1.68	0.93
1:U:14:LYS:HG3	1:U:15:ILE:N	1.84	0.93
1:Q:4:ARG:NH2	1:Q:7:ASN:HA	1.82	0.93
1:Q:171:LYS:HB2	1:Q:187:GLY:O	1.69	0.93
1:K:259:ARG:HB2	1:K:262:ASP:OD1	1.69	0.92
1:W:173:LEU:HD12	1:W:184:THR:HG22	1.49	0.92
1:Q:17:SER:N	1:S:294:LYS:HD3	1.84	0.92
1:S:140:LYS:HD3	1:S:140:LYS:N	1.83	0.92
1:I:15:ILE:HD12	1:I:25:LEU:HB2	1.51	0.92
1:S:182:ILE:HD11	1:S:256:ARG:NH2	1.84	0.92
1:S:188:ILE:HG22	1:S:189:GLU:O	1.70	0.92
1:E:249:SER:CB	1:O:1:MET:HE3	1.99	0.92
1:Q:15:ILE:HD13	1:Q:25:LEU:HB2	1.52	0.92
1:U:116:ILE:HG22	1:U:120:HIS:CE1	2.06	0.91
1:W:56:TYR:HB2	1:W:68:ILE:CD1	1.99	0.91
1:E:44:THR:HG22	1:E:45:LYS:H	1.33	0.91
1:W:148:ILE:HA	1:W:150:PHE:HE1	1.35	0.91
1:W:56:TYR:HB2	1:W:68:ILE:HG12	1.53	0.90
1:W:173:LEU:HD12	1:W:184:THR:CG2	2.02	0.90
1:M:5:VAL:HA	1:M:74:GLU:OE2	1.71	0.90
1:O:39:LEU:HD23	1:O:79:VAL:HG22	1.51	0.90
1:O:140:LYS:CG	1:O:141:LYS:H	1.83	0.90
1:I:293:LEU:HD21	1:K:15:ILE:HG13	1.52	0.89
1:U:5:VAL:HG23	1:U:9:TYR:HB2	1.54	0.89
1:U:237:ILE:CD1	1:U:252:LEU:HB3	2.02	0.89
1:M:237:ILE:HD12	1:M:253:ASN:OD1	1.72	0.89
1:E:58:MET:HG2	1:E:59:MET:HE2	1.53	0.89
1:G:171:LYS:HD2	1:G:189:GLU:OE1	1.71	0.89
1:U:28:ASN:CG	1:U:31:SER:HB2	1.97	0.89
1:U:205:TYR:HB2	1:U:211:LEU:HD12	1.53	0.89
1:G:39:LEU:HD23	1:G:79:VAL:HG22	1.54	0.89
1:E:52:GLU:OE2	1:E:149:ASP:CA	2.20	0.89
1:I:217:LYS:O	1:I:227:ARG:NH1	2.06	0.89
1:K:39:LEU:CD2	1:K:79:VAL:HG22	2.02	0.89
1:O:284:TYR:CD1	1:O:284:TYR:N	2.40	0.88
1:U:235:THR:O	1:U:235:THR:HG22	1.74	0.88
1:W:41:CYS:HA	1:W:77:TYR:CD1	2.08	0.88
1:U:235:THR:HG22	1:U:240:LEU:HB2	1.55	0.88
1:W:158:ASP:HB3	1:W:163:GLN:CB	2.02	0.88
1:A:1:MET:CE	1:G:249:SER:HB3	2.03	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:55:PHE:CD2	1:G:150:PHE:HB2	2.07	0.88
1:U:56:TYR:HB3	1:U:68:ILE:HD11	1.54	0.87
1:A:293:LEU:HD11	1:C:15:ILE:CG2	2.05	0.87
1:K:46:HIS:H	1:K:47:PRO:CD	1.87	0.87
1:S:4:ARG:HG3	1:S:4:ARG:HH11	1.39	0.87
1:S:101:SER:O	1:S:105:VAL:HG23	1.74	0.87
1:U:28:ASN:HD22	1:U:28:ASN:C	1.82	0.87
1:W:56:TYR:HB2	1:W:68:ILE:CG1	2.03	0.87
1:K:52:GLU:OE1	1:K:149:ASP:HA	1.75	0.87
1:O:293:LEU:O	1:O:294:LYS:HE3	1.73	0.87
1:U:56:TYR:CB	1:U:68:ILE:HD11	2.05	0.87
1:W:17:SER:HB3	3:W:426:HOH:O	1.73	0.86
1:A:117:GLU:OE1	1:A:270:ARG:NH2	2.07	0.86
1:G:178:ARG:CZ	1:G:214:GLN:NE2	2.37	0.86
1:U:112:MET:HE2	1:U:199:LEU:HD11	1.54	0.86
1:I:45:LYS:C	1:I:46:HIS:HD1	1.83	0.86
1:G:117:GLU:OE1	1:G:270:ARG:NH2	2.07	0.86
1:M:76:ASP:OD2	1:M:76:ASP:N	2.07	0.86
1:Q:136:MET:HE2	1:Q:290:TRP:HZ2	1.41	0.86
1:U:112:MET:HE2	1:U:199:LEU:CD1	2.06	0.86
1:W:9:TYR:HB3	1:W:27:ALA:O	1.75	0.86
1:U:91:ASP:OD2	1:W:294:LYS:HB2	1.75	0.85
1:W:70:TRP:O	1:W:70:TRP:CE3	2.29	0.85
1:E:126:HIS:CD2	1:E:147:ILE:HD11	2.11	0.85
1:O:284:TYR:H	1:O:284:TYR:HD1	1.20	0.85
1:U:242:LYS:HG3	1:U:243:GLY:N	1.89	0.85
1:M:13:ARG:CD	1:M:13:ARG:N	2.23	0.85
1:S:108:LEU:O	1:S:112:MET:HG3	1.77	0.85
1:A:68:ILE:HD12	1:A:80:MET:HE3	1.59	0.85
1:A:270:ARG:NH1	3:A:401:HOH:O	2.08	0.85
1:K:17:SER:HB2	3:K:405:HOH:O	1.75	0.85
1:M:59:MET:HB2	1:M:65:ILE:HG21	1.58	0.85
1:U:237:ILE:CD1	1:U:256:ARG:HD2	2.05	0.85
1:U:52:GLU:OE2	1:U:149:ASP:HA	1.75	0.85
1:I:160:ARG:HH11	1:I:160:ARG:CG	1.89	0.84
1:Q:236:PRO:HG2	1:Q:239:VAL:HB	1.56	0.84
1:A:217:LYS:H	1:A:217:LYS:HD2	1.42	0.84
1:S:140:LYS:H	1:S:140:LYS:CD	1.83	0.84
1:W:192:ARG:HH12	1:W:263:LYS:CA	1.89	0.84
1:C:117:GLU:OE1	1:C:270:ARG:NH2	2.10	0.84
1:S:191:SER:CB	1:S:260:PHE:HE1	1.86	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:140:LYS:HG3	1:O:141:LYS:H	1.38	0.84
1:U:117:GLU:HG3	1:U:266:TYR:CG	2.12	0.84
1:W:117:GLU:HB2	1:W:266:TYR:CE1	2.13	0.84
1:W:120:HIS:ND1	1:W:192:ARG:CG	2.35	0.84
1:S:154:LYS:HD2	3:S:410:HOH:O	1.77	0.84
1:O:174:THR:HG22	1:O:175:GLY:N	1.92	0.83
1:W:49:LEU:HD11	1:W:80:MET:HB2	1.60	0.83
1:W:259:ARG:HB2	1:W:262:ASP:OD2	1.78	0.83
1:W:148:ILE:HA	1:W:150:PHE:CE1	2.13	0.83
1:I:271:GLN:NE2	1:I:271:GLN:HA	1.93	0.83
1:S:248:PHE:O	1:S:252:LEU:HD12	1.78	0.83
1:A:115:ARG:HB3	3:A:419:HOH:O	1.78	0.83
1:G:43:LYS:HB2	1:M:233:MET:HE1	1.60	0.83
1:S:10:ARG:HG3	1:S:10:ARG:NH1	1.88	0.83
1:W:10:ARG:HG2	1:W:10:ARG:NH1	1.91	0.83
1:I:237:ILE:HD13	1:I:252:LEU:HB3	1.58	0.82
1:W:117:GLU:HB2	1:W:266:TYR:CD1	2.13	0.82
1:U:237:ILE:HD12	1:U:256:ARG:HD2	1.60	0.82
1:S:10:ARG:HH11	1:S:10:ARG:CG	1.92	0.82
1:U:118:TYR:CZ	1:U:122:LYS:HE3	2.14	0.82
1:W:14:LYS:HD2	1:W:22:ASP:OD2	1.79	0.82
1:W:57:LYS:HE3	1:W:68:ILE:HB	1.60	0.82
1:C:5:VAL:HG23	1:C:9:TYR:HB2	1.59	0.82
1:G:173:LEU:HD23	1:G:225:TYR:CE2	2.14	0.82
1:K:259:ARG:HH11	1:K:259:ARG:HG3	1.42	0.82
1:O:45:LYS:O	1:O:46:HIS:HD2	1.63	0.82
1:I:221:LYS:HE2	1:I:221:LYS:H	1.45	0.82
1:U:237:ILE:HD13	1:U:252:LEU:HB3	1.61	0.82
1:W:13:ARG:H	1:W:13:ARG:HD3	1.45	0.82
1:W:64:GLY:HA3	1:W:115:ARG:NE	1.94	0.82
1:A:15:ILE:HD12	1:C:292:MET:HE3	1.62	0.82
1:C:15:ILE:HD11	1:C:25:LEU:HD13	1.61	0.82
1:I:58:MET:O	1:I:58:MET:HG2	1.80	0.81
1:W:39:LEU:N	1:W:39:LEU:HD23	1.94	0.81
1:W:84:LEU:HD12	1:W:85:LEU:N	1.96	0.81
1:A:220:THR:HG22	1:A:223:GLN:N	1.93	0.81
1:A:222:ARG:HG3	1:A:222:ARG:HH11	1.45	0.81
1:O:117:GLU:OE1	1:O:270:ARG:NH2	2.12	0.81
1:A:68:ILE:CD1	1:A:80:MET:HE3	2.10	0.81
1:I:80:MET:HE3	1:I:82:MET:HE3	1.62	0.81
1:G:55:PHE:HA	1:G:58:MET:HE3	1.63	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:124:PHE:HA	1:U:154:LYS:O	1.81	0.81
1:W:191:SER:HB3	1:W:260:PHE:CE1	2.16	0.81
1:E:126:HIS:HD2	1:E:147:ILE:HD11	1.45	0.81
1:M:217:LYS:O	1:M:227:ARG:NH1	2.12	0.81
1:U:7:ASN:C	1:U:7:ASN:ND2	2.35	0.81
1:W:269:LEU:O	1:W:271:GLN:N	2.13	0.81
1:A:221:LYS:HE2	1:A:221:LYS:H	1.45	0.81
1:M:138:LEU:HD13	1:M:139:GLY:N	1.96	0.80
1:Q:88:SER:HA	1:Q:135:LEU:HD12	1.63	0.80
1:Q:117:GLU:OE1	1:Q:270:ARG:NH2	2.14	0.80
1:S:237:ILE:HG13	1:S:256:ARG:NH1	1.96	0.80
1:S:271:GLN:HA	1:S:271:GLN:HE21	1.47	0.80
1:I:181:SER:HB2	1:I:197:GLU:OE2	1.81	0.80
1:U:178:ARG:HH21	1:U:214:GLN:HG3	1.46	0.80
1:W:60:GLN:HA	3:W:401:HOH:O	1.81	0.80
1:I:293:LEU:CD2	1:K:15:ILE:HG13	2.12	0.80
1:W:269:LEU:O	1:W:272:LEU:N	2.11	0.80
1:W:56:TYR:CB	1:W:68:ILE:HG12	2.12	0.80
1:U:178:ARG:NH2	1:U:214:GLN:HG3	1.96	0.80
1:S:4:ARG:NH1	1:S:29:ILE:HD11	1.95	0.80
1:E:39:LEU:HD22	1:E:79:VAL:HG22	1.64	0.80
1:K:43:LYS:O	1:O:233:MET:HE1	1.80	0.80
1:M:161:THR:O	1:M:162:HIS:HB2	1.82	0.80
1:M:220:THR:OG1	1:M:221:LYS:N	2.09	0.80
1:U:137:GLY:O	1:U:142:GLY:HA2	1.83	0.79
1:O:222:ARG:HB3	3:O:417:HOH:O	1.82	0.79
1:Q:220:THR:HG22	1:Q:223:GLN:HE21	1.47	0.79
1:U:140:LYS:C	1:U:142:GLY:H	1.87	0.79
1:I:25:LEU:HD23	1:I:26:GLY:N	1.97	0.79
1:M:120:HIS:ND1	1:M:192:ARG:HG2	1.98	0.79
1:U:151:GLY:O	1:U:152:LEU:HD23	1.83	0.79
1:U:283:SER:C	1:U:285:ASP:H	1.91	0.79
1:W:283:SER:HB2	1:W:285:ASP:OD2	1.83	0.79
1:C:5:VAL:CG2	1:C:9:TYR:HB2	2.12	0.79
1:I:17:SER:HA	1:I:21:GLY:O	1.83	0.79
1:K:6:GLY:O	1:K:8:LYS:N	2.15	0.79
1:Q:219:ALA:HB3	1:Q:223:GLN:HE22	1.45	0.79
1:Q:230:GLU:HG2	3:Q:406:HOH:O	1.83	0.79
1:U:100:PHE:HE2	1:U:206:PHE:CE1	2.01	0.79
1:O:219:ALA:HB3	1:O:223:GLN:OE1	1.83	0.78
1:O:222:ARG:HG3	1:O:223:GLN:N	1.98	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:174:THR:HG21	1:S:190:GLN:OE1	1.83	0.78
1:W:37:ILE:HG23	1:W:81:VAL:HG13	1.64	0.78
1:E:220:THR:CG2	1:E:223:GLN:HG3	2.12	0.78
1:K:84:LEU:O	1:K:138:LEU:HD22	1.83	0.78
1:U:204:MET:O	1:U:207:ASN:N	2.15	0.78
1:W:56:TYR:HB2	1:W:68:ILE:HD11	1.63	0.78
1:W:264:PRO:HG2	1:W:266:TYR:CE2	2.17	0.78
1:I:204:MET:HA	1:I:207:ASN:HD22	1.48	0.78
1:S:213:TRP:O	1:S:216:LEU:HD22	1.84	0.78
1:K:158:ASP:OD1	1:K:161:THR:N	2.17	0.78
1:K:49:LEU:HD12	1:K:49:LEU:O	1.84	0.78
1:W:4:ARG:CD	1:W:29:ILE:HD12	2.12	0.78
1:U:276:LEU:HD13	1:U:280:GLN:HG3	1.65	0.78
1:O:66:PRO:HA	1:O:83:GLU:OE2	1.84	0.78
1:G:5:VAL:C	1:G:7:ASN:H	1.91	0.78
1:M:31:SER:O	1:M:33:GLU:N	2.17	0.77
1:K:3:LEU:HD11	1:O:242:LYS:HE3	1.66	0.77
1:K:46:HIS:H	1:K:47:PRO:HD2	1.48	0.77
1:U:205:TYR:HB2	1:U:211:LEU:HD11	1.64	0.77
1:C:259:ARG:HB2	1:C:262:ASP:OD2	1.84	0.77
1:W:173:LEU:CD1	1:W:184:THR:HG22	2.14	0.77
1:Q:221:LYS:H	1:Q:221:LYS:HD2	1.49	0.77
1:E:274:ARG:NH1	1:Q:274:ARG:NH1	2.33	0.77
1:O:56:TYR:CE1	1:O:66:PRO:HG2	2.20	0.77
1:U:14:LYS:O	1:U:15:ILE:HG12	1.85	0.77
1:U:22:ASP:N	3:U:419:HOH:O	2.17	0.77
1:W:269:LEU:O	1:W:270:ARG:C	2.25	0.77
1:S:150:PHE:O	1:S:152:LEU:N	2.17	0.77
1:U:87:PRO:HD3	1:W:291:ASN:O	1.83	0.77
1:Q:259:ARG:HD2	1:Q:260:PHE:N	1.99	0.77
1:S:220:THR:HG22	1:S:223:GLN:NE2	2.00	0.77
1:S:69:LYS:HB2	1:S:81:VAL:O	1.85	0.77
1:G:207:ASN:HB3	1:G:244:TYR:CE1	2.20	0.76
1:M:8:LYS:HD3	1:M:9:TYR:CE2	2.20	0.76
1:M:222:ARG:HB2	1:M:222:ARG:NH1	1.96	0.76
1:U:202:VAL:O	1:U:206:PHE:CD2	2.38	0.76
1:S:109:ALA:O	1:S:113:ILE:HG13	1.84	0.76
1:S:161:THR:O	1:S:162:HIS:HB2	1.84	0.76
1:U:169:GLU:CD	1:U:169:GLU:N	2.43	0.76
1:U:249:SER:O	1:U:253:ASN:ND2	2.17	0.76
1:A:171:LYS:HB2	1:A:187:GLY:O	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:219:ALA:O	1:W:220:THR:CG2	2.32	0.76
1:W:167:TYR:HE1	1:W:169:GLU:OE2	1.68	0.76
1:G:219:ALA:O	1:G:220:THR:HB	1.85	0.76
1:C:46:HIS:H	1:C:47:PRO:HD3	1.50	0.76
1:Q:80:MET:CE	1:Q:82:MET:HE3	2.16	0.76
1:U:56:TYR:HE1	1:U:66:PRO:HG2	1.48	0.76
1:M:236:PRO:HG2	1:M:239:VAL:HG23	1.67	0.76
1:K:217:LYS:O	1:K:227:ARG:NH1	2.19	0.76
1:M:293:LEU:O	1:M:294:LYS:HD2	1.86	0.76
1:W:15:ILE:HG22	1:W:16:GLY:N	2.01	0.76
1:Q:221:LYS:H	1:Q:221:LYS:CD	1.99	0.76
1:C:43:LYS:HB2	1:K:233:MET:HE2	1.67	0.75
1:A:80:MET:HE2	1:A:82:MET:SD	2.26	0.75
1:S:221:LYS:O	1:S:225:TYR:HD1	1.69	0.75
1:U:293:LEU:HB3	1:W:15:ILE:CG2	2.17	0.75
1:E:217:LYS:O	1:E:227:ARG:NH1	2.18	0.75
1:K:247:GLU:OE2	1:K:279:ARG:NH1	2.19	0.75
1:U:250:THR:HG21	1:U:272:LEU:HD11	1.67	0.75
1:W:64:GLY:HA3	1:W:115:ARG:CD	2.17	0.75
1:A:15:ILE:HG21	1:A:25:LEU:HB2	1.68	0.75
1:G:9:TYR:HA	1:G:27:ALA:O	1.86	0.75
1:U:292:MET:HG3	1:U:293:LEU:H	1.51	0.75
1:Q:293:LEU:C	1:Q:293:LEU:HD12	2.11	0.75
1:U:137:GLY:C	1:U:142:GLY:HA2	2.11	0.75
1:W:69:LYS:CB	1:W:81:VAL:O	2.30	0.75
1:G:220:THR:HG22	1:G:223:GLN:OE1	1.86	0.75
1:U:4:ARG:HH21	1:U:7:ASN:CA	1.98	0.74
1:M:42:VAL:HG23	1:M:76:ASP:O	1.86	0.74
1:M:118:TYR:O	1:M:121:SER:HB3	1.86	0.74
1:U:155:LYS:HE2	3:U:414:HOH:O	1.87	0.74
1:U:254:PHE:CD2	1:U:269:LEU:HD21	2.21	0.74
1:W:280:GLN:HB3	1:W:282:PHE:CE2	2.23	0.74
1:K:270:ARG:NH1	3:K:408:HOH:O	2.19	0.74
1:S:234:SER:O	1:S:236:PRO:HD3	1.88	0.74
1:U:237:ILE:HD13	1:U:252:LEU:CB	2.16	0.74
1:W:56:TYR:CE2	1:W:82:MET:CE	2.71	0.74
1:Q:221:LYS:HD2	1:Q:221:LYS:N	2.02	0.74
1:U:4:ARG:CZ	1:U:7:ASN:HA	2.17	0.74
1:K:3:LEU:HD23	1:K:11:LEU:HB3	1.67	0.74
1:W:181:SER:HB2	1:W:197:GLU:OE1	1.87	0.74
1:G:41:CYS:O	1:G:44:THR:HG22	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:158:ASP:O	1:S:162:HIS:HD2	1.71	0.74
1:S:169:GLU:CB	1:S:170:ASN:HD22	2.01	0.74
1:W:52:GLU:HG2	1:W:56:TYR:CE2	2.23	0.74
1:M:259:ARG:HB2	1:M:262:ASP:OD2	1.88	0.74
1:U:123:ASN:O	1:U:155:LYS:HA	1.87	0.74
1:U:183:ASN:HA	1:U:186:LEU:HG	1.68	0.74
1:W:164:HIS:NE2	1:W:261:ASP:HA	2.03	0.74
1:U:208:LEU:C	1:U:210:SER:H	1.96	0.73
1:W:53:SER:HA	1:W:68:ILE:CD1	2.18	0.73
1:A:174:THR:O	1:A:174:THR:CG2	2.35	0.73
1:W:103:LYS:HG3	1:W:282:PHE:CD1	2.23	0.73
1:O:28:ASN:HD21	1:O:31:SER:H	1.36	0.73
1:U:241:CYS:O	1:U:244:TYR:HB2	1.88	0.73
1:O:13:ARG:CG	1:O:13:ARG:NH1	2.48	0.73
1:S:39:LEU:HD23	1:S:79:VAL:HG22	1.70	0.73
1:S:143:ASN:C	1:S:143:ASN:HD22	1.97	0.73
1:W:53:SER:CB	1:W:71:CYS:SG	2.70	0.73
1:U:112:MET:O	1:U:116:ILE:HD12	1.88	0.73
1:U:224:LYS:NZ	2:U:301:SO4:O3	2.19	0.73
1:W:138:LEU:O	1:W:139:GLY:C	2.32	0.73
1:K:1:MET:O	1:K:2:GLU:HB2	1.87	0.73
1:Q:10:ARG:HB2	1:Q:29:ILE:HD11	1.70	0.73
1:W:56:TYR:HE1	1:W:150:PHE:CE1	2.06	0.73
1:Q:226:GLU:O	1:Q:230:GLU:HG3	1.89	0.72
1:E:220:THR:HG22	1:E:223:GLN:CG	2.18	0.72
1:S:10:ARG:HG2	1:S:10:ARG:O	1.89	0.72
1:O:58:MET:HE2	1:O:59:MET:CE	2.15	0.72
1:Q:221:LYS:HG2	1:Q:222:ARG:H	1.54	0.72
1:U:109:ALA:O	1:U:113:ILE:HG13	1.89	0.72
1:W:111:GLN:CD	1:W:145:VAL:HG23	2.14	0.72
1:U:60:GLN:HG3	1:U:61:GLY:N	2.03	0.72
1:W:271:GLN:OE1	1:W:275:ASN:OD1	2.07	0.72
1:M:124:PHE:CE2	1:M:155:LYS:HG3	2.24	0.72
1:O:52:GLU:O	1:O:54:LYS:N	2.23	0.72
1:O:140:LYS:HG3	1:O:141:LYS:CD	2.19	0.72
1:W:63:VAL:HA	3:W:425:HOH:O	1.89	0.72
1:W:191:SER:HB3	1:W:260:PHE:CD1	2.25	0.72
1:E:117:GLU:OE1	1:E:270:ARG:NH2	2.21	0.72
1:S:137:GLY:HA3	1:S:141:LYS:HB2	1.71	0.72
1:U:100:PHE:HE2	1:U:206:PHE:HE1	1.35	0.72
1:U:234:SER:O	1:U:236:PRO:HD3	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:28:ASN:OD1	1:U:31:SER:HB2	1.88	0.72
1:G:5:VAL:C	1:G:7:ASN:N	2.42	0.71
1:K:3:LEU:CD1	1:O:242:LYS:HE3	2.20	0.71
1:U:46:HIS:H	1:U:47:PRO:HD3	1.55	0.71
1:G:220:THR:HG22	1:G:223:GLN:CD	2.15	0.71
1:U:117:GLU:HG3	1:U:266:TYR:CD1	2.25	0.71
1:W:111:GLN:OE1	1:W:145:VAL:HG23	1.90	0.71
1:O:13:ARG:HG3	1:O:13:ARG:NH1	1.94	0.71
1:U:135:LEU:HD13	1:U:148:ILE:HD13	1.70	0.71
1:O:204:MET:HE3	1:O:207:ASN:HB2	1.73	0.71
1:O:222:ARG:CG	1:O:223:GLN:N	2.54	0.71
1:K:140:LYS:HG3	1:K:141:LYS:HG2	1.73	0.71
1:G:28:ASN:O	1:G:32:GLY:N	2.24	0.71
1:S:25:LEU:HD23	1:S:26:GLY:N	2.06	0.71
1:U:140:LYS:O	1:U:142:GLY:N	2.23	0.71
1:K:39:LEU:HD21	1:K:79:VAL:HG22	1.71	0.71
1:M:200:GLY:HA3	1:M:252:LEU:HD21	1.73	0.71
1:Q:204:MET:HE2	1:Q:241:CYS:HA	1.73	0.71
1:S:221:LYS:H	1:S:221:LYS:HZ3	1.37	0.71
1:W:66:PRO:HB3	1:W:85:LEU:HD11	1.71	0.71
1:S:4:ARG:N	3:S:402:HOH:O	2.23	0.71
1:A:47:PRO:O	1:A:48:GLN:HG2	1.90	0.71
1:A:111:GLN:O	1:A:115:ARG:HG2	1.90	0.71
1:C:140:LYS:HA	1:C:140:LYS:HE3	1.71	0.71
1:O:17:SER:C	3:O:402:HOH:O	2.33	0.71
1:W:168:ARG:HG3	1:W:169:GLU:H	1.55	0.71
1:G:82:MET:HE1	3:G:427:HOH:O	1.91	0.71
1:O:140:LYS:HG3	1:O:141:LYS:N	2.06	0.71
1:O:220:THR:HG23	1:O:222:ARG:HG2	1.71	0.71
1:U:237:ILE:HG13	1:U:256:ARG:CZ	2.21	0.71
1:W:59:MET:HE1	1:W:122:LYS:HB2	1.72	0.71
1:W:247:GLU:HB2	1:W:276:LEU:CD2	2.21	0.71
1:W:278:HIS:O	1:W:280:GLN:N	2.24	0.71
1:O:174:THR:HG22	1:O:175:GLY:H	1.53	0.70
1:U:185:HIS:NE2	1:U:232:LYS:HE3	2.06	0.70
1:S:56:TYR:CE1	1:S:66:PRO:HG2	2.26	0.70
1:S:254:PHE:C	1:S:254:PHE:CD2	2.69	0.70
1:W:128:ASP:O	1:W:133:ASN:ND2	2.23	0.70
1:E:38:LYS:O	1:E:39:LEU:HD23	1.91	0.70
1:S:169:GLU:HB2	1:S:170:ASN:ND2	2.06	0.70
1:U:41:CYS:O	1:U:44:THR:HG22	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:59:MET:CE	1:W:122:LYS:HB2	2.21	0.70
1:C:10:ARG:HB2	1:C:29:ILE:CD1	2.20	0.70
1:Q:213:TRP:HB3	1:Q:231:LYS:HG3	1.73	0.70
1:E:101:SER:O	1:E:105:VAL:HG23	1.90	0.70
1:A:56:TYR:HD2	1:A:68:ILE:HD11	1.55	0.70
1:K:161:THR:O	1:K:162:HIS:HB2	1.90	0.70
1:S:140:LYS:C	1:S:142:GLY:H	1.99	0.70
1:S:45:LYS:O	1:S:47:PRO:HD3	1.92	0.70
1:W:192:ARG:HH11	1:W:264:PRO:CD	1.85	0.70
1:C:39:LEU:CD2	1:C:79:VAL:HG22	2.21	0.70
1:E:10:ARG:HB2	1:E:29:ILE:HD11	1.73	0.70
1:K:39:LEU:HD22	1:K:79:VAL:HG22	1.72	0.70
1:O:123:ASN:O	1:O:155:LYS:HA	1.92	0.70
1:U:140:LYS:C	1:U:142:GLY:N	2.47	0.70
1:W:251:TYR:CD1	1:W:251:TYR:C	2.69	0.70
1:I:41:CYS:O	1:I:44:THR:HG22	1.92	0.69
1:S:167:TYR:O	1:S:167:TYR:HD1	1.73	0.69
1:W:182:ILE:HD12	1:W:256:ARG:NE	2.06	0.69
1:Q:220:THR:HG22	1:Q:223:GLN:NE2	2.07	0.69
1:S:182:ILE:HG23	1:S:233:MET:HE3	1.74	0.69
1:S:259:ARG:HD3	1:S:260:PHE:H	1.56	0.69
1:O:259:ARG:HB2	1:O:262:ASP:HB2	1.74	0.69
1:S:120:HIS:HA	1:S:124:PHE:O	1.93	0.69
1:A:222:ARG:HG3	1:A:222:ARG:NH1	2.08	0.69
1:C:219:ALA:O	1:C:220:THR:HG22	1.92	0.69
1:M:84:LEU:CD2	1:O:292:MET:HE2	2.22	0.69
1:S:169:GLU:CB	1:S:170:ASN:ND2	2.56	0.69
1:G:88:SER:HA	1:G:135:LEU:HD12	1.74	0.69
1:K:11:LEU:HD12	1:K:37:ILE:CD1	2.23	0.69
1:S:208:LEU:HD23	1:S:244:TYR:CE2	2.28	0.69
1:W:220:THR:OG1	1:W:221:LYS:HE2	1.92	0.69
1:A:120:HIS:CG	1:A:192:ARG:HG2	2.27	0.69
1:E:44:THR:HG22	1:E:45:LYS:N	2.07	0.69
1:M:191:SER:HB3	1:M:260:PHE:CE1	2.27	0.69
1:M:293:LEU:HD21	1:O:135:LEU:HD23	1.74	0.69
1:U:5:VAL:CG2	1:U:9:TYR:HB2	2.23	0.69
1:G:222:ARG:O	1:G:226:GLU:OE1	2.11	0.69
1:O:140:LYS:C	1:O:142:GLY:H	2.01	0.69
1:Q:17:SER:H	1:S:294:LYS:CD	1.97	0.69
1:S:120:HIS:CG	1:S:192:ARG:HG2	2.28	0.69
1:C:3:LEU:HD21	1:K:238:GLU:CG	2.12	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:54:LYS:HG3	1:O:55:PHE:N	2.08	0.68
1:A:1:MET:O	1:A:2:GLU:HB2	1.93	0.68
1:G:28:ASN:HD21	1:G:30:ALA:HB3	1.58	0.68
1:K:5:VAL:HG12	1:K:74:GLU:HG2	1.76	0.68
1:U:127:ARG:HB3	1:U:190:GLN:NE2	2.07	0.68
1:C:10:ARG:HB2	1:C:29:ILE:HD11	1.74	0.68
1:M:41:CYS:O	1:M:44:THR:HG22	1.92	0.68
1:U:191:SER:HB3	1:U:260:PHE:CE1	2.28	0.68
1:W:127:ARG:HG2	1:W:190:GLN:NE2	2.08	0.68
1:I:13:ARG:HG2	3:I:416:HOH:O	1.93	0.68
1:O:56:TYR:CB	1:O:68:ILE:CD1	2.70	0.68
1:G:105:VAL:HG21	1:G:207:ASN:OD1	1.93	0.68
1:S:82:MET:HE2	3:S:409:HOH:O	1.92	0.68
1:U:254:PHE:CG	1:U:269:LEU:HD21	2.29	0.68
1:I:222:ARG:HG3	1:I:222:ARG:HH11	1.59	0.68
1:U:23:ILE:HD13	1:U:23:ILE:N	2.08	0.68
1:M:123:ASN:HD21	1:M:159:ALA:HA	1.59	0.68
1:U:28:ASN:ND2	1:U:30:ALA:H	1.92	0.68
1:U:217:LYS:O	1:U:218:ALA:HB2	1.94	0.68
1:W:12:GLY:HA2	3:W:432:HOH:O	1.93	0.68
1:W:73:ALA:O	1:W:74:GLU:HB3	1.93	0.68
1:E:111:GLN:O	1:E:115:ARG:HG2	1.93	0.68
1:M:134:PHE:C	1:M:135:LEU:HD12	2.18	0.68
1:W:13:ARG:HD3	1:W:13:ARG:N	2.06	0.68
1:E:39:LEU:CD2	1:E:79:VAL:HG13	2.24	0.68
1:E:92:LEU:HD22	1:E:290:TRP:CG	2.28	0.68
1:S:170:ASN:N	1:S:170:ASN:ND2	2.32	0.68
1:U:120:HIS:CG	1:U:192:ARG:HG2	2.28	0.68
1:M:31:SER:C	1:M:33:GLU:H	2.01	0.67
1:W:190:GLN:HA	1:W:194:ASP:OD2	1.94	0.67
1:E:182:ILE:HD11	1:E:256:ARG:NH2	2.08	0.67
1:W:143:ASN:ND2	1:W:286:TYR:CD2	2.62	0.67
1:A:1:MET:CE	1:G:249:SER:CB	2.73	0.67
1:O:118:TYR:CZ	1:O:122:LYS:HE3	2.29	0.67
1:W:41:CYS:HB2	1:W:77:TYR:CE1	2.29	0.67
1:A:186:LEU:HD21	1:A:233:MET:CE	2.22	0.67
1:E:210:SER:HB2	1:E:214:GLN:OE1	1.94	0.67
1:U:259:ARG:CB	1:U:262:ASP:OD2	2.42	0.67
1:W:14:LYS:NZ	1:W:16:GLY:O	2.24	0.67
1:Q:229:SER:O	1:Q:233:MET:HG3	1.93	0.67
1:U:218:ALA:O	1:U:219:ALA:O	2.12	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:261:ASP:O	1:U:262:ASP:O	2.12	0.67
1:O:130:LYS:HE3	1:O:132:ASP:HB2	1.76	0.67
1:U:202:VAL:O	1:U:206:PHE:HD2	1.77	0.67
1:U:276:LEU:CD1	1:U:280:GLN:HG3	2.24	0.67
1:I:56:TYR:CE2	1:I:82:MET:HE2	2.30	0.67
1:M:156:TYR:C	1:M:165:ILE:HG23	2.20	0.67
1:W:92:LEU:HD13	1:W:290:TRP:CD2	2.30	0.67
1:C:4:ARG:HD3	3:C:428:HOH:O	1.93	0.67
1:C:219:ALA:C	1:C:220:THR:HG22	2.20	0.67
1:M:293:LEU:HD21	1:O:135:LEU:CD2	2.24	0.67
1:O:41:CYS:SG	1:O:43:LYS:CE	2.82	0.67
1:O:155:LYS:HD2	1:O:157:ARG:O	1.95	0.67
1:O:220:THR:HG23	1:O:223:GLN:HG3	1.77	0.67
1:I:56:TYR:HE1	1:I:150:PHE:HE1	1.42	0.67
1:W:31:SER:HB2	1:W:33:GLU:HB3	1.76	0.67
1:A:119:ILE:HD13	1:A:150:PHE:HE2	1.58	0.67
1:M:274:ARG:HG2	1:M:274:ARG:NH1	2.00	0.67
1:O:58:MET:HE1	1:O:124:PHE:CD1	2.29	0.67
1:Q:271:GLN:HE22	1:Q:274:ARG:NH1	1.93	0.67
1:S:115:ARG:O	1:S:119:ILE:HG13	1.96	0.67
1:E:43:LYS:O	1:E:44:THR:O	2.12	0.66
1:S:167:TYR:HE2	1:S:259:ARG:NH1	1.93	0.66
1:S:173:LEU:HD12	1:S:174:THR:N	2.09	0.66
1:S:167:TYR:CE2	1:S:259:ARG:NH1	2.64	0.66
1:O:22:ASP:HA	3:O:405:HOH:O	1.94	0.66
1:O:30:ALA:HB2	1:S:284:TYR:CZ	2.30	0.66
1:U:4:ARG:NH2	1:U:7:ASN:CA	2.56	0.66
1:E:44:THR:HG22	1:E:46:HIS:H	1.60	0.66
1:I:132:ASP:HB2	3:I:424:HOH:O	1.94	0.66
1:Q:215:GLY:N	2:Q:301:SO4:O3	2.29	0.66
1:W:200:GLY:HA3	1:W:252:LEU:HD21	1.76	0.66
1:S:236:PRO:HD2	1:S:239:VAL:HG21	1.78	0.66
1:A:10:ARG:HB2	1:A:29:ILE:CD1	2.25	0.66
1:C:140:LYS:HA	1:C:140:LYS:CE	2.26	0.66
1:U:237:ILE:HD11	1:U:252:LEU:HB3	1.77	0.66
1:K:62:GLY:HA3	1:K:118:TYR:CZ	2.30	0.66
1:S:4:ARG:HH12	1:S:29:ILE:HD11	1.61	0.66
1:U:164:HIS:HE1	1:U:260:PHE:CZ	2.13	0.66
1:W:130:LYS:O	1:W:131:PRO:C	2.39	0.66
1:W:192:ARG:NH1	1:W:264:PRO:CD	2.52	0.66
1:C:39:LEU:HD23	1:C:79:VAL:HG22	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:183:ASN:O	1:K:184:THR:C	2.38	0.66
1:M:102:LEU:HG	1:M:106:LEU:CD1	2.25	0.66
1:O:140:LYS:CG	1:O:141:LYS:N	2.51	0.66
1:Q:220:THR:HG23	1:Q:223:GLN:N	2.09	0.66
1:S:193:ARG:HG3	1:S:194:ASP:N	2.10	0.66
1:W:56:TYR:CE2	1:W:82:MET:HE1	2.31	0.66
1:W:266:TYR:CB	1:W:270:ARG:HH12	2.09	0.66
1:K:5:VAL:HG12	1:K:74:GLU:CG	2.26	0.66
1:K:247:GLU:OE1	1:K:247:GLU:N	2.29	0.66
1:K:267:SER:OG	3:K:433:HOH:O	2.13	0.66
1:U:56:TYR:HB3	1:U:68:ILE:CD1	2.26	0.66
1:O:120:HIS:CE1	1:O:192:ARG:HG2	2.32	0.65
1:G:168:ARG:NH1	1:G:171:LYS:HG2	2.11	0.65
1:I:28:ASN:ND2	1:I:31:SER:H	1.94	0.65
1:I:56:TYR:CE2	1:I:82:MET:CE	2.79	0.65
1:O:229:SER:O	1:O:233:MET:HG3	1.96	0.65
1:S:221:LYS:O	1:S:225:TYR:CD1	2.48	0.65
1:E:56:TYR:HB2	1:E:68:ILE:HD11	1.77	0.65
1:E:58:MET:CG	1:E:59:MET:HE2	2.26	0.65
1:G:161:THR:O	1:G:162:HIS:HB2	1.96	0.65
1:K:183:ASN:O	1:K:186:LEU:N	2.28	0.65
1:U:150:PHE:O	1:U:152:LEU:N	2.29	0.65
1:U:293:LEU:HB3	1:W:15:ILE:HG22	1.78	0.65
1:W:111:GLN:OE1	1:W:144:LEU:HA	1.96	0.65
1:A:147:ILE:CG2	3:A:419:HOH:O	2.44	0.65
1:M:220:THR:OG1	1:M:221:LYS:HE2	1.96	0.65
1:U:1:MET:SD	3:U:407:HOH:O	2.54	0.65
1:U:56:TYR:CG	1:U:68:ILE:HD11	2.31	0.65
1:U:267:SER:HA	1:U:270:ARG:NH1	2.10	0.65
1:I:222:ARG:HG3	1:I:222:ARG:NH1	2.11	0.65
1:M:15:ILE:HD11	1:O:292:MET:SD	2.37	0.65
1:S:117:GLU:OE1	1:S:270:ARG:NH2	2.30	0.65
1:S:167:TYR:O	1:S:167:TYR:CD1	2.50	0.65
1:W:111:GLN:OE1	1:W:145:VAL:N	2.28	0.65
1:I:23:ILE:HD11	1:I:38:LYS:HE2	1.79	0.65
1:K:143:ASN:OD1	1:K:286:TYR:HB3	1.96	0.65
1:S:22:ASP:N	3:S:418:HOH:O	2.28	0.65
1:S:23:ILE:HD11	1:S:38:LYS:HE3	1.78	0.65
1:U:204:MET:HE3	1:U:207:ASN:HB2	1.78	0.65
1:U:235:THR:O	1:U:235:THR:CG2	2.43	0.65
1:U:237:ILE:HG22	1:U:249:SER:OG	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:117:GLU:OE1	1:W:270:ARG:NH2	2.30	0.65
1:I:221:LYS:H	1:I:221:LYS:CE	2.10	0.65
1:U:4:ARG:NE	1:U:7:ASN:HA	2.12	0.65
1:U:14:LYS:HG3	1:U:15:ILE:H	1.61	0.65
1:U:94:ASN:OD1	1:U:98:ARG:NH1	2.28	0.65
1:U:259:ARG:HB2	1:U:262:ASP:OD2	1.96	0.65
1:W:48:GLN:HA	1:W:51:ILE:HG13	1.76	0.65
1:A:82:MET:HE2	3:A:404:HOH:O	1.96	0.65
1:O:276:LEU:HD12	1:O:276:LEU:O	1.96	0.65
1:O:58:MET:HE1	1:O:124:PHE:CE1	2.32	0.65
1:U:62:GLY:HA3	1:U:118:TYR:CE2	2.32	0.65
1:W:41:CYS:CA	1:W:77:TYR:HD1	2.07	0.65
1:C:15:ILE:CD1	1:C:25:LEU:HD13	2.27	0.65
1:U:15:ILE:O	1:U:15:ILE:HG22	1.96	0.65
1:U:289:ASP:O	1:U:292:MET:HG2	1.97	0.65
1:W:161:THR:O	1:W:162:HIS:HB2	1.97	0.65
1:M:236:PRO:HG2	1:M:239:VAL:CG2	2.27	0.64
1:U:28:ASN:HB3	1:U:31:SER:HB3	1.78	0.64
1:U:216:LEU:HB3	1:U:227:ARG:NH1	2.13	0.64
1:U:292:MET:O	1:W:87:PRO:HD3	1.97	0.64
1:A:226:GLU:HA	1:A:226:GLU:OE1	1.96	0.64
1:O:199:LEU:O	1:O:203:LEU:HG	1.98	0.64
1:W:2:GLU:CG	1:W:3:LEU:H	2.05	0.64
1:W:41:CYS:HB2	1:W:77:TYR:HE1	1.62	0.64
1:I:220:THR:HG23	1:I:223:GLN:N	2.05	0.64
1:S:169:GLU:C	1:S:170:ASN:HD22	2.06	0.64
1:M:173:LEU:HD12	1:M:184:THR:HG22	1.79	0.64
1:Q:41:CYS:O	1:Q:44:THR:HG23	1.97	0.64
1:K:186:LEU:HD21	1:K:233:MET:CE	2.27	0.64
1:O:174:THR:CG2	1:O:175:GLY:N	2.57	0.64
1:S:150:PHE:C	1:S:152:LEU:H	2.06	0.64
1:W:69:LYS:HB2	1:W:81:VAL:C	2.20	0.64
1:G:5:VAL:HG23	1:G:9:TYR:HB2	1.79	0.64
1:S:229:SER:O	1:S:233:MET:HG2	1.97	0.64
1:W:57:LYS:NZ	1:W:68:ILE:HG21	2.13	0.64
1:A:293:LEU:CD1	1:C:15:ILE:CG2	2.76	0.64
1:M:69:LYS:HB2	1:M:81:VAL:O	1.98	0.64
1:U:23:ILE:N	1:U:23:ILE:CD1	2.60	0.64
1:K:259:ARG:HG3	1:K:259:ARG:NH1	2.12	0.64
1:E:74:GLU:OE1	3:E:445:HOH:O	2.15	0.64
1:I:197:GLU:OE1	1:I:256:ARG:HG2	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:220:THR:O	1:O:223:GLN:N	2.30	0.64
1:O:222:ARG:CG	1:O:223:GLN:H	2.10	0.64
1:W:164:HIS:CD2	1:W:261:ASP:HB2	2.32	0.64
1:O:7:ASN:HD21	1:S:283:SER:CA	2.11	0.63
1:S:68:ILE:HG22	1:S:69:LYS:N	2.13	0.63
1:U:6:GLY:HA3	1:U:70:TRP:CZ2	2.34	0.63
1:K:186:LEU:HD21	1:K:233:MET:HE1	1.79	0.63
1:S:150:PHE:N	1:S:150:PHE:CD1	2.65	0.63
1:W:123:ASN:HA	1:W:156:TYR:CE2	2.33	0.63
1:I:56:TYR:HE2	1:I:82:MET:CE	2.11	0.63
1:K:46:HIS:N	1:K:47:PRO:HD2	2.13	0.63
1:U:100:PHE:CE2	1:U:206:PHE:CE1	2.84	0.63
1:W:33:GLU:HG3	1:W:33:GLU:O	1.97	0.63
1:G:74:GLU:OE1	1:G:74:GLU:HA	1.98	0.63
1:I:84:LEU:HD21	1:K:292:MET:HG3	1.79	0.63
1:I:173:LEU:HD23	1:I:225:TYR:CE2	2.33	0.63
1:O:120:HIS:ND1	1:O:192:ARG:HG2	2.13	0.63
1:W:134:PHE:C	1:W:135:LEU:HD12	2.23	0.63
1:S:15:ILE:HG21	1:S:25:LEU:HB2	1.79	0.63
1:S:223:GLN:O	1:S:224:LYS:C	2.42	0.63
1:U:283:SER:O	1:U:285:ASP:N	2.31	0.63
1:W:7:ASN:HA	3:W:405:HOH:O	1.99	0.63
1:U:213:TRP:CE3	1:U:232:LYS:HG3	2.33	0.63
1:A:42:VAL:HG23	1:A:76:ASP:O	1.99	0.63
1:G:5:VAL:HG21	1:G:37:ILE:HD13	1.81	0.63
1:O:28:ASN:ND2	1:O:31:SER:N	2.36	0.63
1:S:59:MET:HE3	1:S:150:PHE:CE2	2.34	0.63
1:W:73:ALA:O	1:W:74:GLU:CB	2.46	0.63
1:O:28:ASN:ND2	1:O:28:ASN:C	2.46	0.63
1:Q:8:LYS:CB	1:Q:8:LYS:NZ	2.62	0.63
1:S:293:LEU:C	1:S:293:LEU:HD12	2.23	0.63
1:W:88:SER:HA	1:W:134:PHE:O	1.99	0.63
1:U:15:ILE:HD13	1:W:292:MET:CE	2.29	0.62
1:W:84:LEU:HD12	1:W:85:LEU:H	1.64	0.62
1:W:131:PRO:O	1:W:133:ASN:N	2.32	0.62
1:M:14:LYS:HE3	3:M:429:HOH:O	1.99	0.62
1:G:135:LEU:HD22	1:G:148:ILE:HD13	1.81	0.62
1:S:56:TYR:CE1	1:S:66:PRO:CG	2.83	0.62
1:S:56:TYR:CD1	1:S:66:PRO:HG2	2.34	0.62
1:S:239:VAL:O	1:S:242:LYS:HB2	1.99	0.62
1:U:178:ARG:NH2	2:U:301:SO4:O1	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:167:TYR:CE1	1:W:169:GLU:OE2	2.51	0.62
1:S:222:ARG:HG2	1:S:222:ARG:NH1	2.14	0.62
1:C:247:GLU:HG3	1:C:272:LEU:HD11	1.82	0.62
1:M:198:SER:O	1:M:202:VAL:HG23	1.99	0.62
1:S:120:HIS:CE1	1:S:192:ARG:HG2	2.34	0.62
1:S:236:PRO:HB2	1:S:239:VAL:HG23	1.80	0.62
1:U:235:THR:CG2	1:U:240:LEU:HB2	2.28	0.62
1:W:150:PHE:CD1	1:W:150:PHE:N	2.68	0.62
1:Q:173:LEU:HD12	1:Q:184:THR:HG22	1.81	0.62
1:S:70:TRP:HZ3	1:S:72:GLY:O	1.81	0.62
1:U:193:ARG:HG3	1:U:194:ASP:H	1.65	0.62
1:W:123:ASN:C	1:W:156:TYR:CD2	2.78	0.62
1:W:280:GLN:HB3	1:W:282:PHE:CD2	2.35	0.62
1:A:220:THR:HG23	1:A:222:ARG:H	1.65	0.62
1:U:283:SER:C	1:U:285:ASP:N	2.57	0.62
1:A:238:GLU:HG2	1:I:3:LEU:HB2	1.81	0.62
1:G:210:SER:HB2	1:G:214:GLN:OE1	2.00	0.62
1:S:39:LEU:CD2	1:S:79:VAL:HG22	2.30	0.62
1:C:222:ARG:HH11	1:C:222:ARG:CG	2.12	0.62
1:Q:76:ASP:OD1	1:Q:76:ASP:N	2.20	0.62
1:U:191:SER:O	1:U:193:ARG:N	2.32	0.62
1:C:37:ILE:HG12	1:C:81:VAL:HG22	1.82	0.62
1:G:127:ARG:HD2	1:G:190:GLN:NE2	2.15	0.62
1:I:222:ARG:O	1:I:226:GLU:OE1	2.17	0.62
1:K:221:LYS:O	1:K:224:LYS:N	2.33	0.62
1:M:140:LYS:O	1:M:141:LYS:HD3	1.99	0.62
1:M:174:THR:HG23	1:M:190:GLN:OE1	1.99	0.62
1:Q:220:THR:OG1	1:Q:221:LYS:HD2	1.99	0.62
1:U:251:TYR:CD1	1:U:251:TYR:C	2.78	0.62
1:G:23:ILE:CD1	1:G:38:LYS:HG3	2.30	0.61
1:K:98:ARG:NH2	1:K:205:TYR:OH	2.33	0.61
1:S:112:MET:O	1:S:116:ILE:HD12	2.00	0.61
1:S:222:ARG:HG2	1:S:222:ARG:HH11	1.65	0.61
1:U:84:LEU:HD21	1:W:292:MET:HG2	1.82	0.61
1:U:184:THR:HG23	1:U:190:GLN:OE1	2.00	0.61
1:W:47:PRO:C	1:W:48:GLN:HG3	2.25	0.61
1:A:66:PRO:HB3	1:A:85:LEU:HD11	1.82	0.61
1:W:192:ARG:HH12	1:W:263:LYS:CB	2.12	0.61
1:K:6:GLY:C	1:K:8:LYS:H	2.07	0.61
1:M:254:PHE:CD2	1:M:269:LEU:HD21	2.35	0.61
1:S:4:ARG:HG3	1:S:4:ARG:NH1	2.03	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:247:GLU:OE1	1:W:247:GLU:N	2.33	0.61
1:E:174:THR:HG23	1:E:174:THR:O	2.01	0.61
1:M:93:PHE:CE1	1:M:98:ARG:C	2.79	0.61
1:S:182:ILE:CD1	1:S:256:ARG:NH2	2.62	0.61
1:S:221:LYS:H	1:S:221:LYS:NZ	1.98	0.61
1:U:250:THR:CG2	1:U:272:LEU:HD21	2.30	0.61
1:A:293:LEU:HD11	1:C:15:ILE:HG21	1.82	0.61
1:M:220:THR:CG2	1:M:223:GLN:CD	2.73	0.61
1:Q:285:ASP:O	1:Q:285:ASP:OD1	2.19	0.61
1:K:120:HIS:ND1	1:K:192:ARG:HG2	2.15	0.61
1:K:173:LEU:HD23	1:K:225:TYR:CE2	2.35	0.61
1:W:222:ARG:HG3	1:W:222:ARG:HH11	1.65	0.61
1:K:158:ASP:O	1:K:162:HIS:HA	2.00	0.61
1:O:41:CYS:SG	1:O:43:LYS:HE3	2.39	0.61
1:O:220:THR:O	1:O:221:LYS:C	2.42	0.61
1:Q:40:GLU:HG2	1:Q:44:THR:HG21	1.82	0.61
1:Q:136:MET:HE2	1:Q:290:TRP:CZ2	2.29	0.61
1:U:164:HIS:HE1	1:U:260:PHE:CE2	2.18	0.61
1:W:55:PHE:CE1	1:W:58:MET:HE1	2.36	0.61
1:W:57:LYS:HD3	1:W:68:ILE:CG1	2.30	0.61
1:A:137:GLY:HA3	1:A:141:LYS:O	2.01	0.61
1:C:56:TYR:HB2	1:C:68:ILE:HD11	1.83	0.61
1:M:18:GLY:O	1:M:19:SER:CB	2.48	0.61
1:M:174:THR:CG2	1:M:190:GLN:OE1	2.48	0.61
1:S:117:GLU:HG3	1:S:266:TYR:CD2	2.35	0.61
1:S:201:TYR:O	1:S:202:VAL:C	2.43	0.61
1:W:14:LYS:HZ3	1:W:16:GLY:C	2.07	0.61
1:W:191:SER:OG	1:W:193:ARG:HG2	1.99	0.61
1:A:56:TYR:CD2	1:A:68:ILE:HD11	2.36	0.61
1:S:254:PHE:C	1:S:254:PHE:HD2	2.08	0.61
1:U:15:ILE:CD1	1:W:292:MET:HE3	2.31	0.61
1:A:42:VAL:HG12	1:A:42:VAL:O	2.01	0.60
1:C:270:ARG:NH1	3:C:467:HOH:O	2.33	0.60
1:I:29:ILE:HG22	1:I:30:ALA:N	2.16	0.60
1:K:182:ILE:HD13	1:K:233:MET:HG3	1.82	0.60
1:I:80:MET:HE3	1:I:82:MET:CE	2.31	0.60
1:M:109:ALA:O	1:M:113:ILE:HG13	2.00	0.60
1:M:124:PHE:HD2	1:M:154:LYS:C	2.09	0.60
1:O:141:LYS:HD3	1:O:141:LYS:N	2.15	0.60
1:O:204:MET:HA	1:O:204:MET:CE	2.25	0.60
1:S:80:MET:HE3	1:S:82:MET:SD	2.40	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:253:ASN:O	1:U:257:SER:OG	2.20	0.60
1:W:68:ILE:HD13	1:W:80:MET:CE	2.21	0.60
1:M:204:MET:HA	1:M:204:MET:HE3	1.83	0.60
1:O:169:GLU:O	1:O:170:ASN:HB2	2.00	0.60
1:C:15:ILE:HG22	1:C:16:GLY:N	2.16	0.60
1:I:15:ILE:CD1	1:I:25:LEU:HB2	2.29	0.60
1:O:118:TYR:CE1	1:O:122:LYS:HE3	2.36	0.60
1:Q:6:GLY:O	1:Q:7:ASN:CB	2.49	0.60
1:S:108:LEU:O	1:S:112:MET:CG	2.48	0.60
1:U:28:ASN:ND2	1:U:30:ALA:N	2.49	0.60
1:W:177:ALA:HB1	1:W:228:ILE:HD12	1.82	0.60
1:E:247:GLU:CD	1:E:276:LEU:HD22	2.27	0.60
1:I:1:MET:O	1:I:2:GLU:HB2	2.01	0.60
1:O:11:LEU:HD12	1:O:37:ILE:HD12	1.81	0.60
1:W:266:TYR:HB3	1:W:270:ARG:HH12	1.66	0.60
1:O:1:MET:O	1:O:2:GLU:CB	2.49	0.60
1:O:33:GLU:OE2	1:O:69:LYS:HE2	2.01	0.60
1:U:118:TYR:CZ	1:U:122:LYS:CE	2.84	0.60
1:U:191:SER:HB3	1:U:260:PHE:HE1	1.66	0.60
1:S:173:LEU:HD12	1:S:174:THR:H	1.67	0.60
1:U:213:TRP:CD2	1:U:232:LYS:HG3	2.36	0.60
1:G:84:LEU:HG	1:G:138:LEU:HD11	1.83	0.60
1:I:158:ASP:OD1	1:I:161:THR:HG23	2.02	0.60
1:O:117:GLU:HG3	1:O:266:TYR:CD2	2.37	0.60
1:A:58:MET:SD	1:A:59:MET:HE2	2.42	0.60
1:A:147:ILE:HG22	3:A:419:HOH:O	2.01	0.60
1:G:168:ARG:NH1	1:G:169:GLU:O	2.35	0.60
1:G:171:LYS:HE2	3:G:402:HOH:O	2.02	0.60
1:M:253:ASN:O	1:M:257:SER:OG	2.19	0.60
1:W:242:LYS:NZ	3:W:423:HOH:O	2.34	0.60
1:A:1:MET:HE3	1:G:249:SER:HB3	1.83	0.59
1:A:181:SER:HB2	1:A:197:GLU:CD	2.26	0.59
1:E:34:GLU:O	1:E:35:VAL:HG13	2.02	0.59
1:G:46:HIS:N	1:G:47:PRO:HD3	2.17	0.59
1:K:11:LEU:HD12	1:K:37:ILE:HD12	1.82	0.59
1:Q:11:LEU:HD11	1:Q:24:TYR:CB	2.32	0.59
1:W:31:SER:C	1:W:33:GLU:H	2.07	0.59
1:Q:63:VAL:HG22	1:Q:144:LEU:HD21	1.84	0.59
1:W:84:LEU:HG	1:W:138:LEU:HD12	1.85	0.59
1:M:57:LYS:HD2	1:M:68:ILE:HD12	1.83	0.59
1:O:7:ASN:HD21	1:S:283:SER:HA	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:213:TRP:HB2	1:O:228:ILE:HG23	1.84	0.59
1:Q:7:ASN:C	1:Q:7:ASN:HD22	2.09	0.59
1:S:174:THR:CG2	1:S:175:GLY:N	2.37	0.59
1:U:13:ARG:HG2	3:U:401:HOH:O	2.02	0.59
1:O:58:MET:CE	1:O:59:MET:HE2	2.20	0.59
1:Q:221:LYS:HG2	1:Q:222:ARG:N	2.17	0.59
1:S:191:SER:CB	1:S:260:PHE:CE1	2.72	0.59
1:U:124:PHE:HD1	1:U:154:LYS:C	2.09	0.59
1:U:215:GLY:N	2:U:301:SO4:O4	2.23	0.59
1:W:39:LEU:HD23	1:W:39:LEU:H	1.66	0.59
1:W:47:PRO:O	1:W:48:GLN:HG3	2.02	0.59
1:A:219:ALA:HB3	1:A:223:GLN:OE1	2.02	0.59
1:I:221:LYS:O	1:I:222:ARG:C	2.44	0.59
1:O:7:ASN:ND2	1:S:283:SER:HA	2.17	0.59
1:O:220:THR:HG23	1:O:223:GLN:CG	2.32	0.59
1:S:169:GLU:HB3	1:S:170:ASN:HD22	1.67	0.59
1:U:4:ARG:HE	1:U:7:ASN:HA	1.67	0.59
1:W:56:TYR:HD2	1:W:80:MET:HE2	1.67	0.59
1:G:186:LEU:CD2	1:G:233:MET:HE1	2.28	0.59
1:I:80:MET:CE	1:I:82:MET:HE3	2.32	0.59
1:K:32:GLY:O	1:K:33:GLU:C	2.43	0.59
1:O:84:LEU:HG	1:O:138:LEU:CD1	2.33	0.59
1:U:242:LYS:HG3	1:U:243:GLY:H	1.66	0.59
1:E:9:TYR:HA	1:E:27:ALA:O	2.02	0.59
1:G:3:LEU:HD23	1:G:4:ARG:N	2.18	0.59
1:G:41:CYS:SG	1:M:233:MET:HE2	2.43	0.59
1:K:167:TYR:CD1	1:K:168:ARG:N	2.70	0.59
1:M:141:LYS:C	1:M:143:ASN:H	2.10	0.59
1:O:134:PHE:C	1:O:135:LEU:HD12	2.27	0.59
1:U:185:HIS:HB3	1:U:229:SER:OG	2.02	0.59
1:S:257:SER:O	1:S:258:LEU:O	2.20	0.59
1:S:271:GLN:HE21	1:S:271:GLN:CA	2.08	0.59
1:U:167:TYR:CD1	1:U:168:ARG:N	2.71	0.59
1:W:293:LEU:C	1:W:294:LYS:HD3	2.27	0.59
1:W:57:LYS:HD3	1:W:68:ILE:HD12	1.85	0.59
1:W:204:MET:HE3	1:W:208:LEU:HD11	1.83	0.59
1:A:70:TRP:CH2	1:A:72:GLY:HA3	2.37	0.59
1:M:102:LEU:HG	1:M:106:LEU:HD11	1.84	0.59
1:U:109:ALA:O	1:U:113:ILE:CG1	2.51	0.59
1:E:151:GLY:O	1:E:152:LEU:HD23	2.03	0.58
1:U:28:ASN:HD22	1:U:30:ALA:N	2.01	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:114:SER:HB2	1:U:115:ARG:NH1	2.17	0.58
1:W:9:TYR:CE1	1:W:69:LYS:HD3	2.38	0.58
1:W:57:LYS:HE3	1:W:68:ILE:CB	2.32	0.58
1:W:106:LEU:O	1:W:109:ALA:HB3	2.03	0.58
1:W:222:ARG:HG3	1:W:222:ARG:NH1	2.18	0.58
1:C:102:LEU:O	1:C:106:LEU:HG	2.02	0.58
1:I:178:ARG:HD2	1:I:179:TYR:CZ	2.38	0.58
1:K:4:ARG:NH2	1:K:7:ASN:ND2	2.51	0.58
1:K:15:ILE:HG21	1:K:25:LEU:HB2	1.85	0.58
1:M:28:ASN:C	1:M:28:ASN:OD1	2.45	0.58
1:O:52:GLU:O	1:O:55:PHE:N	2.36	0.58
1:S:55:PHE:CZ	1:S:153:ALA:HB3	2.37	0.58
1:S:164:HIS:CD2	1:S:261:ASP:HA	2.39	0.58
1:U:86:GLY:HA2	1:W:291:ASN:O	2.02	0.58
1:A:174:THR:O	1:A:174:THR:HG22	2.01	0.58
1:A:293:LEU:CD1	1:C:15:ILE:HG23	2.33	0.58
1:O:39:LEU:HD23	1:O:79:VAL:CG2	2.30	0.58
1:U:228:ILE:O	1:U:232:LYS:HB2	2.03	0.58
1:W:10:ARG:HB2	1:W:29:ILE:HD13	1.85	0.58
1:C:165:ILE:HB	1:C:166:PRO:HD2	1.84	0.58
1:E:140:LYS:CG	1:E:141:LYS:HG2	2.34	0.58
1:O:182:ILE:O	1:O:185:HIS:HB2	2.02	0.58
1:Q:43:LYS:O	1:Q:44:THR:O	2.22	0.58
1:U:277:PHE:CZ	1:U:282:PHE:HB2	2.39	0.58
1:A:3:LEU:CD1	1:G:238:GLU:OE1	2.51	0.58
1:A:52:GLU:OE1	1:A:56:TYR:CZ	2.56	0.58
1:A:115:ARG:HD2	3:A:419:HOH:O	2.02	0.58
1:C:237:ILE:HD11	1:C:256:ARG:HD2	1.85	0.58
1:S:117:GLU:O	1:S:120:HIS:HB2	2.03	0.58
1:K:5:VAL:HG12	1:K:74:GLU:CD	2.29	0.58
1:K:41:CYS:O	1:K:44:THR:HG23	2.03	0.58
1:Q:221:LYS:CG	1:Q:222:ARG:H	2.16	0.58
1:U:14:LYS:CG	1:U:15:ILE:N	2.64	0.58
1:U:100:PHE:HA	1:U:289:ASP:OD2	2.03	0.58
1:W:4:ARG:CD	1:W:29:ILE:CD1	2.82	0.58
1:C:80:MET:HE3	1:C:82:MET:HE3	1.86	0.58
1:U:28:ASN:CG	1:U:31:SER:CB	2.75	0.58
1:U:49:LEU:CD1	1:U:80:MET:HE3	2.33	0.58
1:U:201:TYR:O	1:U:202:VAL:C	2.47	0.58
1:W:79:VAL:HG12	1:W:80:MET:N	2.17	0.58
1:W:156:TYR:HA	1:W:165:ILE:HD13	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:45:LYS:O	1:O:46:HIS:CD2	2.51	0.58
1:Q:17:SER:OG	1:S:294:LYS:HE2	2.04	0.58
1:U:237:ILE:HG13	1:U:256:ARG:HH11	1.65	0.58
1:W:56:TYR:HD2	1:W:80:MET:CE	2.16	0.58
1:G:23:ILE:HD12	1:G:38:LYS:HG3	1.84	0.58
1:M:74:GLU:O	1:M:75:GLY:C	2.46	0.58
1:S:165:ILE:HB	1:S:166:PRO:HD2	1.86	0.58
1:A:56:TYR:CD2	1:A:80:MET:HE1	2.38	0.58
1:E:74:GLU:OE1	1:E:74:GLU:HA	2.03	0.58
1:K:156:TYR:HA	1:K:165:ILE:HD13	1.85	0.58
1:K:171:LYS:HD3	1:K:189:GLU:OE1	2.03	0.58
1:S:143:ASN:HB3	3:S:411:HOH:O	2.02	0.58
1:S:260:PHE:CD1	1:S:260:PHE:C	2.80	0.58
1:W:37:ILE:CG2	1:W:81:VAL:HG13	2.34	0.58
1:C:165:ILE:HB	1:C:166:PRO:CD	2.33	0.57
1:M:267:SER:HA	1:M:270:ARG:NH1	2.19	0.57
1:W:15:ILE:HG22	1:W:16:GLY:H	1.69	0.57
1:W:124:PHE:CG	1:W:155:LYS:HA	2.39	0.57
1:W:285:ASP:O	1:W:286:TYR:HB2	2.04	0.57
1:Q:4:ARG:NH2	1:Q:7:ASN:CA	2.62	0.57
1:S:23:ILE:HD12	1:S:38:LYS:HG3	1.86	0.57
1:U:122:LYS:O	1:U:123:ASN:HB2	2.02	0.57
1:W:57:LYS:HD3	1:W:68:ILE:HG13	1.86	0.57
1:G:82:MET:CE	3:G:427:HOH:O	2.49	0.57
1:U:234:SER:O	1:U:236:PRO:CD	2.52	0.57
1:I:28:ASN:ND2	1:I:31:SER:N	2.51	0.57
1:I:158:ASP:OD1	1:I:161:THR:N	2.35	0.57
1:O:7:ASN:HD21	1:S:283:SER:HB2	1.69	0.57
1:Q:32:GLY:O	1:S:283:SER:HB3	2.04	0.57
1:Q:154:LYS:NZ	1:Q:189:GLU:OE2	2.31	0.57
1:Q:293:LEU:HD12	1:Q:294:LYS:N	2.19	0.57
1:U:129:VAL:HG13	1:U:134:PHE:CZ	2.39	0.57
1:W:56:TYR:HE2	1:W:82:MET:CE	2.16	0.57
1:W:57:LYS:CD	1:W:68:ILE:HG13	2.34	0.57
1:E:182:ILE:CD1	1:E:256:ARG:CZ	2.83	0.57
1:G:178:ARG:HD2	1:G:179:TYR:CZ	2.39	0.57
1:E:220:THR:CG2	1:E:223:GLN:H	2.17	0.57
1:O:251:TYR:CD1	1:O:251:TYR:C	2.82	0.57
1:Q:88:SER:CA	1:Q:135:LEU:HD12	2.34	0.57
1:S:202:VAL:O	1:S:205:TYR:HB3	2.04	0.57
1:W:247:GLU:CD	1:W:276:LEU:HD22	2.30	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:VAL:O	1:A:205:TYR:HB3	2.05	0.57
1:C:60:GLN:HG3	1:C:61:GLY:N	2.20	0.57
1:G:168:ARG:HG2	1:G:169:GLU:H	1.68	0.57
1:Q:52:GLU:OE2	1:Q:149:ASP:HA	2.04	0.57
1:S:176:THR:HG23	3:S:407:HOH:O	2.05	0.57
1:E:44:THR:CG2	1:E:45:LYS:H	2.06	0.57
1:M:200:GLY:HA3	1:M:252:LEU:CD2	2.34	0.57
1:O:58:MET:HE3	1:O:122:LYS:HB3	1.85	0.57
1:O:222:ARG:O	1:O:226:GLU:OE1	2.23	0.57
1:S:80:MET:CE	1:S:82:MET:SD	2.93	0.57
1:W:44:THR:HG23	1:W:46:HIS:H	1.69	0.57
1:M:11:LEU:HG	1:M:12:GLY:H	1.69	0.57
1:S:260:PHE:C	1:S:260:PHE:HD1	2.12	0.57
1:U:47:PRO:O	1:U:48:GLN:CG	2.44	0.57
1:U:193:ARG:HG3	1:U:194:ASP:N	2.20	0.57
1:E:289:ASP:O	1:E:294:LYS:NZ	2.38	0.57
1:Q:122:LYS:O	1:Q:123:ASN:HB2	2.05	0.57
1:I:8:LYS:HE3	1:I:9:TYR:CZ	2.40	0.56
1:K:3:LEU:CD2	1:K:11:LEU:CB	2.66	0.56
1:K:167:TYR:CD1	1:K:167:TYR:C	2.83	0.56
1:O:178:ARG:HD2	1:O:179:TYR:CZ	2.40	0.56
1:W:12:GLY:O	1:W:25:LEU:HB3	2.05	0.56
1:W:39:LEU:N	1:W:39:LEU:CD2	2.67	0.56
1:A:1:MET:HE2	1:G:249:SER:CB	2.34	0.56
1:A:59:MET:HB2	1:A:65:ILE:HG21	1.86	0.56
1:G:17:SER:C	3:G:425:HOH:O	2.47	0.56
1:W:193:ARG:HB3	1:W:258:LEU:HD12	1.87	0.56
1:A:236:PRO:HB3	1:I:77:TYR:CE2	2.40	0.56
1:C:220:THR:HG23	1:C:223:GLN:CD	2.30	0.56
1:G:37:ILE:HG12	1:G:81:VAL:HG22	1.86	0.56
1:G:76:ASP:OD1	1:G:76:ASP:N	2.32	0.56
1:I:23:ILE:HD13	1:I:23:ILE:N	2.20	0.56
1:I:117:GLU:OE1	1:I:270:ARG:NH2	2.39	0.56
1:O:28:ASN:HD21	1:O:30:ALA:HB3	1.69	0.56
1:Q:41:CYS:SG	3:Q:416:HOH:O	2.57	0.56
1:Q:173:LEU:CD1	1:Q:184:THR:HG22	2.36	0.56
1:Q:251:TYR:C	1:Q:251:TYR:CD1	2.83	0.56
1:U:42:VAL:HG12	1:U:43:LYS:N	2.20	0.56
1:U:186:LEU:HD21	1:U:233:MET:CE	2.36	0.56
1:W:12:GLY:O	1:W:13:ARG:O	2.24	0.56
1:W:56:TYR:CD2	1:W:80:MET:HE2	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:254:PHE:O	1:W:257:SER:HB2	2.06	0.56
1:K:207:ASN:HB3	1:K:244:TYR:CE1	2.41	0.56
1:Q:76:ASP:HA	3:Q:429:HOH:O	2.04	0.56
1:S:140:LYS:C	1:S:142:GLY:N	2.61	0.56
1:S:164:HIS:NE2	1:S:261:ASP:HA	2.20	0.56
1:W:83:GLU:HG3	1:W:83:GLU:O	2.04	0.56
1:A:84:LEU:HD21	1:C:292:MET:HG2	1.88	0.56
1:G:38:LYS:HE2	1:G:49:LEU:HD13	1.86	0.56
1:W:92:LEU:HD13	1:W:290:TRP:CE2	2.41	0.56
1:W:244:TYR:O	1:W:245:PRO:C	2.48	0.56
1:E:249:SER:OG	1:O:1:MET:HE3	2.06	0.56
1:G:28:ASN:ND2	1:G:28:ASN:C	2.63	0.56
1:I:136:MET:SD	1:I:145:VAL:HG22	2.45	0.56
1:K:70:TRP:CZ3	1:K:72:GLY:HA3	2.40	0.56
1:M:229:SER:O	1:M:233:MET:HG3	2.06	0.56
1:M:245:PRO:HG2	1:M:276:LEU:HD21	1.88	0.56
1:O:7:ASN:ND2	1:S:283:SER:HB2	2.20	0.56
1:O:219:ALA:HB3	1:O:223:GLN:CD	2.31	0.56
1:U:129:VAL:HG13	1:U:134:PHE:CE2	2.41	0.56
1:W:116:ILE:O	1:W:119:ILE:HB	2.05	0.56
1:G:28:ASN:C	1:G:28:ASN:HD22	2.13	0.56
1:S:121:SER:C	1:S:123:ASN:H	2.13	0.56
1:W:250:THR:O	1:W:251:TYR:C	2.47	0.56
1:E:56:TYR:CB	1:E:68:ILE:HD11	2.36	0.56
1:E:84:LEU:HG	1:E:138:LEU:HD11	1.88	0.56
1:O:193:ARG:NH1	1:O:260:PHE:HA	2.20	0.56
1:S:49:LEU:HD11	1:S:80:MET:HB2	1.87	0.56
1:U:60:GLN:HA	3:U:412:HOH:O	2.05	0.56
1:U:62:GLY:CA	1:U:118:TYR:CZ	2.89	0.56
1:M:156:TYR:O	1:M:165:ILE:HG23	2.06	0.56
1:O:204:MET:HE3	1:O:204:MET:CA	2.31	0.56
1:O:268:TYR:CE1	1:O:272:LEU:HD22	2.41	0.56
1:Q:143:ASN:OD1	1:Q:288:PHE:HE2	1.88	0.56
1:Q:269:LEU:O	1:Q:272:LEU:HB3	2.06	0.56
1:W:264:PRO:O	1:W:266:TYR:CD2	2.59	0.56
1:A:56:TYR:HE1	1:A:150:PHE:HE1	1.54	0.56
1:G:150:PHE:HB3	1:G:153:ALA:CB	2.36	0.56
1:I:56:TYR:HE1	1:I:150:PHE:CE1	2.21	0.56
1:K:3:LEU:HD22	1:K:11:LEU:CB	2.22	0.56
1:M:251:TYR:CD2	1:M:269:LEU:HD22	2.40	0.56
1:U:28:ASN:C	1:U:28:ASN:ND2	2.55	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:219:ALA:C	1:C:220:THR:CG2	2.78	0.55
1:E:6:GLY:O	1:E:8:LYS:N	2.39	0.55
1:O:52:GLU:O	1:O:53:SER:C	2.49	0.55
1:Q:279:ARG:HG3	1:Q:279:ARG:HH11	1.71	0.55
1:S:120:HIS:ND1	1:S:192:ARG:HG2	2.21	0.55
1:W:196:LEU:O	1:W:199:LEU:N	2.39	0.55
1:A:161:THR:OG1	1:A:163:GLN:HB2	2.07	0.55
1:I:271:GLN:HA	1:I:271:GLN:HE21	1.66	0.55
1:M:116:ILE:HD12	1:M:199:LEU:HD22	1.87	0.55
1:U:13:ARG:NH2	1:W:292:MET:HE1	2.22	0.55
1:U:211:LEU:O	1:U:214:GLN:HB3	2.06	0.55
1:W:56:TYR:CE1	1:W:150:PHE:CE1	2.92	0.55
1:W:109:ALA:O	1:W:113:ILE:HG13	2.05	0.55
1:W:280:GLN:CB	1:W:282:PHE:CD2	2.89	0.55
1:C:174:THR:HG22	1:C:190:GLN:OE1	2.05	0.55
1:E:140:LYS:HG3	1:E:141:LYS:HG2	1.89	0.55
1:M:13:ARG:H	1:M:13:ARG:HD3	0.59	0.55
1:M:171:LYS:NZ	3:M:408:HOH:O	2.38	0.55
1:M:182:ILE:HD12	1:M:256:ARG:CZ	2.36	0.55
1:O:117:GLU:O	1:O:120:HIS:HB2	2.07	0.55
1:Q:41:CYS:HB3	1:Q:44:THR:HG22	1.87	0.55
1:Q:220:THR:HG22	1:Q:223:GLN:CG	2.35	0.55
1:W:56:TYR:CD2	1:W:80:MET:CE	2.89	0.55
1:W:79:VAL:CG1	1:W:80:MET:N	2.68	0.55
1:W:124:PHE:HB3	1:W:154:LYS:C	2.32	0.55
1:G:15:ILE:HG21	1:G:25:LEU:CB	2.31	0.55
1:S:174:THR:CG2	1:S:190:GLN:OE1	2.53	0.55
1:E:178:ARG:HD2	1:E:179:TYR:CZ	2.41	0.55
1:U:138:LEU:CD1	1:U:138:LEU:C	2.80	0.55
1:U:292:MET:O	1:W:87:PRO:CD	2.54	0.55
1:W:59:MET:HE1	1:W:119:ILE:O	2.06	0.55
1:C:46:HIS:N	1:C:47:PRO:HD3	2.20	0.55
1:O:124:PHE:CD2	1:O:155:LYS:N	2.75	0.55
1:O:287:VAL:O	1:O:287:VAL:HG12	2.05	0.55
1:S:194:ASP:O	1:S:195:ASP:C	2.50	0.55
1:U:127:ARG:HD2	1:U:190:GLN:NE2	2.21	0.55
1:U:204:MET:O	1:U:207:ASN:HB2	2.07	0.55
1:K:123:ASN:OD1	1:K:123:ASN:N	2.40	0.55
1:M:59:MET:HB3	1:M:118:TYR:HE2	1.70	0.55
1:M:222:ARG:HH11	1:M:222:ARG:CB	2.05	0.55
1:Q:8:LYS:NZ	1:Q:8:LYS:HB2	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:271:GLN:NE2	1:S:271:GLN:CA	2.54	0.55
1:W:117:GLU:O	1:W:118:TYR:C	2.48	0.55
1:A:52:GLU:OE1	1:A:56:TYR:CE2	2.59	0.55
1:A:69:LYS:HE3	3:A:447:HOH:O	2.06	0.55
1:E:274:ARG:HH11	1:Q:274:ARG:NH1	2.04	0.55
1:G:178:ARG:NH1	1:G:214:GLN:NE2	2.55	0.55
1:Q:7:ASN:C	1:Q:7:ASN:ND2	2.64	0.55
1:W:213:TRP:HB3	1:W:231:LYS:HG3	1.89	0.55
1:C:25:LEU:HD21	1:C:34:GLU:OE2	2.06	0.55
1:K:251:TYR:CD2	1:K:269:LEU:HD22	2.42	0.55
1:O:215:GLY:O	1:O:216:LEU:C	2.49	0.55
1:Q:254:PHE:C	1:Q:254:PHE:CD2	2.84	0.55
1:U:204:MET:O	1:U:205:TYR:C	2.50	0.55
1:M:173:LEU:HD23	1:M:225:TYR:CD2	2.42	0.55
1:O:56:TYR:HB2	1:O:68:ILE:CD1	2.15	0.55
1:O:124:PHE:CD2	1:O:154:LYS:C	2.85	0.55
1:Q:8:LYS:HB3	1:Q:8:LYS:HZ3	1.72	0.55
1:U:182:ILE:O	1:U:185:HIS:HB2	2.07	0.55
1:W:13:ARG:H	1:W:13:ARG:CD	2.17	0.55
1:W:59:MET:CE	1:W:122:LYS:CB	2.85	0.55
1:A:59:MET:O	1:A:60:GLN:C	2.49	0.54
1:C:17:SER:C	3:C:431:HOH:O	2.50	0.54
1:E:140:LYS:HG2	1:E:141:LYS:CG	2.37	0.54
1:I:5:VAL:C	1:I:7:ASN:N	2.64	0.54
1:I:156:TYR:O	1:I:165:ILE:HG23	2.07	0.54
1:M:80:MET:CE	1:M:82:MET:HB3	2.37	0.54
1:W:86:GLY:O	1:W:135:LEU:HB3	2.06	0.54
1:W:272:LEU:HD12	1:W:272:LEU:O	2.07	0.54
1:A:56:TYR:CE2	1:A:80:MET:HE1	2.43	0.54
1:G:62:GLY:HA3	1:G:118:TYR:CZ	2.42	0.54
1:I:221:LYS:HE2	1:I:221:LYS:N	2.20	0.54
1:I:247:GLU:OE1	1:I:247:GLU:N	2.36	0.54
1:U:192:ARG:HD2	1:U:266:TYR:OH	2.06	0.54
1:W:209:GLY:O	1:W:210:SER:HB3	2.07	0.54
1:W:267:SER:O	1:W:271:GLN:HB3	2.07	0.54
1:E:220:THR:HG22	1:E:223:GLN:H	1.72	0.54
1:G:41:CYS:SG	1:M:233:MET:HB3	2.47	0.54
1:M:82:MET:HE1	3:M:405:HOH:O	2.06	0.54
1:O:167:TYR:HB2	1:O:260:PHE:CD2	2.43	0.54
1:S:7:ASN:O	1:S:7:ASN:CG	2.50	0.54
1:S:208:LEU:CD2	1:S:244:TYR:CE2	2.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:15:ILE:CD1	1:W:292:MET:CE	2.84	0.54
1:U:237:ILE:CD1	1:U:256:ARG:CD	2.83	0.54
1:E:172:ASN:O	1:E:173:LEU:C	2.49	0.54
1:Q:178:ARG:HD2	1:Q:179:TYR:CZ	2.42	0.54
1:Q:213:TRP:HB3	1:Q:231:LYS:CG	2.38	0.54
1:S:120:HIS:CD2	1:S:192:ARG:HG2	2.42	0.54
1:U:89:LEU:HD13	1:U:206:PHE:HZ	1.72	0.54
1:I:11:LEU:HD11	1:I:24:TYR:CG	2.43	0.54
1:I:160:ARG:HG2	1:I:160:ARG:NH1	2.01	0.54
1:M:193:ARG:CZ	1:M:260:PHE:HA	2.37	0.54
1:S:59:MET:HB2	1:S:65:ILE:HG21	1.89	0.54
1:U:169:GLU:N	1:U:169:GLU:OE1	2.39	0.54
1:W:17:SER:C	3:W:413:HOH:O	2.51	0.54
1:W:57:LYS:HD3	1:W:68:ILE:CD1	2.38	0.54
1:A:89:LEU:O	1:A:93:PHE:HB2	2.08	0.54
1:A:217:LYS:H	1:A:217:LYS:CD	2.09	0.54
1:I:230:GLU:O	1:I:234:SER:OG	2.24	0.54
1:M:52:GLU:OE2	1:M:149:ASP:HA	2.07	0.54
1:Q:74:GLU:N	1:Q:77:TYR:O	2.35	0.54
1:S:56:TYR:HB3	1:S:68:ILE:HG12	1.89	0.54
1:U:30:ALA:O	1:U:31:SER:C	2.49	0.54
1:W:15:ILE:CG2	1:W:16:GLY:N	2.70	0.54
1:W:27:ALA:CB	3:W:418:HOH:O	2.54	0.54
1:W:247:GLU:HG3	1:W:272:LEU:HD11	1.88	0.54
1:W:277:PHE:CZ	1:W:282:PHE:HB3	2.43	0.54
1:C:123:ASN:ND2	1:C:159:ALA:HA	2.23	0.54
1:K:11:LEU:HD12	1:K:37:ILE:HD13	1.89	0.54
1:M:101:SER:O	1:M:105:VAL:HG23	2.08	0.54
1:S:8:LYS:HG3	1:S:8:LYS:O	2.08	0.54
1:U:118:TYR:OH	1:U:122:LYS:HE3	2.08	0.54
1:U:271:GLN:O	1:U:272:LEU:C	2.50	0.54
1:W:88:SER:OG	1:W:91:ASP:OD2	2.25	0.54
1:G:7:ASN:CG	1:G:7:ASN:O	2.50	0.54
1:G:49:LEU:HG	1:G:49:LEU:O	2.06	0.54
1:G:150:PHE:N	1:G:150:PHE:CD1	2.75	0.54
1:I:94:ASN:OD1	1:I:98:ARG:NH1	2.39	0.54
1:M:128:ASP:OD2	1:M:130:LYS:HE2	2.07	0.54
1:O:124:PHE:HD2	1:O:154:LYS:C	2.16	0.54
1:U:56:TYR:HE1	1:U:66:PRO:CG	2.18	0.54
1:W:13:ARG:N	1:W:13:ARG:CD	2.71	0.54
1:W:44:THR:HG21	1:W:47:PRO:N	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:65:ILE:HD13	1:W:118:TYR:CD2	2.42	0.54
1:W:289:ASP:O	1:W:294:LYS:NZ	2.32	0.54
1:E:95:PHE:CE2	1:E:294:LYS:HE2	2.43	0.54
1:G:134:PHE:O	1:G:135:LEU:HD12	2.08	0.54
1:O:225:TYR:N	1:O:225:TYR:CD1	2.76	0.54
1:Q:292:MET:O	1:Q:294:LYS:NZ	2.30	0.54
1:U:235:THR:O	1:U:236:PRO:C	2.51	0.54
1:W:229:SER:O	1:W:233:MET:HG3	2.08	0.54
1:G:43:LYS:HB2	1:M:233:MET:CE	2.35	0.54
1:O:50:HIS:C	1:O:52:GLU:N	2.65	0.54
1:Q:56:TYR:HE2	1:Q:82:MET:CE	2.21	0.54
1:W:173:LEU:HD11	1:W:180:ALA:CB	2.38	0.54
1:W:200:GLY:HA3	1:W:252:LEU:CD2	2.38	0.54
1:E:52:GLU:OE1	1:E:56:TYR:CZ	2.60	0.53
1:O:7:ASN:HD21	1:S:283:SER:CB	2.21	0.53
1:Q:143:ASN:OD1	1:Q:288:PHE:CE2	2.60	0.53
1:S:55:PHE:O	1:S:59:MET:HG2	2.07	0.53
1:S:62:GLY:O	1:S:65:ILE:HG12	2.08	0.53
1:S:168:ARG:HG3	1:S:169:GLU:H	1.72	0.53
1:W:32:GLY:HA2	3:W:419:HOH:O	2.08	0.53
1:W:122:LYS:C	1:W:123:ASN:ND2	2.65	0.53
1:W:192:ARG:NH1	1:W:263:LYS:HG3	2.23	0.53
1:K:274:ARG:NH2	3:K:418:HOH:O	2.35	0.53
1:O:108:LEU:O	1:O:112:MET:HG3	2.07	0.53
1:O:198:SER:O	1:O:202:VAL:HG23	2.08	0.53
1:U:60:GLN:CG	1:U:61:GLY:N	2.72	0.53
1:U:191:SER:OG	1:U:193:ARG:HG2	2.07	0.53
1:A:223:GLN:O	1:A:226:GLU:HB2	2.08	0.53
1:I:160:ARG:CG	1:I:160:ARG:NH1	2.56	0.53
1:Q:10:ARG:HG2	1:Q:10:ARG:NH1	2.23	0.53
1:Q:156:TYR:CZ	1:Q:192:ARG:HD3	2.44	0.53
1:S:173:LEU:HD23	1:S:225:TYR:CE2	2.42	0.53
1:U:116:ILE:CG2	1:U:120:HIS:CE1	2.88	0.53
1:U:127:ARG:HB3	1:U:190:GLN:HE22	1.72	0.53
1:A:1:MET:O	1:A:2:GLU:CB	2.57	0.53
1:I:23:ILE:CD1	1:I:38:LYS:HE2	2.37	0.53
1:I:28:ASN:HD21	1:I:31:SER:H	1.56	0.53
1:S:14:LYS:HE3	1:S:22:ASP:OD2	2.07	0.53
1:I:173:LEU:HD21	1:I:177:ALA:HB2	1.91	0.53
1:M:135:LEU:HD12	1:M:135:LEU:N	2.23	0.53
1:M:241:CYS:O	1:M:242:LYS:C	2.51	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:74:GLU:O	1:O:75:GLY:C	2.51	0.53
1:Q:5:VAL:HG21	1:Q:79:VAL:HG11	1.90	0.53
1:S:141:LYS:O	1:S:142:GLY:C	2.50	0.53
1:U:103:LYS:HG3	1:U:282:PHE:HB3	1.89	0.53
1:E:62:GLY:HA3	1:E:118:TYR:CZ	2.44	0.53
1:Q:68:ILE:HG22	1:Q:69:LYS:N	2.23	0.53
1:U:17:SER:C	3:U:403:HOH:O	2.50	0.53
1:W:93:PHE:CZ	1:W:206:PHE:HA	2.43	0.53
1:M:40:GLU:OE1	1:M:49:LEU:HB2	2.08	0.53
1:M:156:TYR:HA	1:M:165:ILE:CG2	2.38	0.53
1:O:25:LEU:HG	1:O:26:GLY:N	2.24	0.53
1:O:126:HIS:N	1:O:195:ASP:OD2	2.41	0.53
1:Q:181:SER:HB2	1:Q:197:GLU:CD	2.34	0.53
1:S:22:ASP:C	1:S:23:ILE:HD13	2.33	0.53
1:S:70:TRP:CZ3	1:S:72:GLY:O	2.62	0.53
1:S:120:HIS:HD2	1:S:124:PHE:O	1.90	0.53
1:S:250:THR:CG2	1:S:272:LEU:HD21	2.39	0.53
1:W:247:GLU:HG3	1:W:272:LEU:CD1	2.39	0.53
1:A:39:LEU:CD2	1:A:79:VAL:HG22	2.39	0.53
1:C:259:ARG:CB	1:C:262:ASP:OD2	2.57	0.53
1:E:39:LEU:HD21	1:E:79:VAL:HG13	1.91	0.53
1:I:167:TYR:HA	1:I:260:PHE:CE2	2.43	0.53
1:K:5:VAL:HG12	1:K:74:GLU:OE1	2.08	0.53
1:W:70:TRP:O	1:W:70:TRP:HE3	1.86	0.53
1:Q:220:THR:CG2	1:Q:223:GLN:H	2.14	0.53
1:S:189:GLU:HB3	1:S:260:PHE:HE2	1.74	0.53
1:U:248:PHE:O	1:U:252:LEU:HD12	2.08	0.53
1:W:119:ILE:HD11	1:W:150:PHE:CE2	2.44	0.53
1:W:124:PHE:N	1:W:124:PHE:CD1	2.77	0.53
1:A:200:GLY:HA3	1:A:252:LEU:HD21	1.91	0.53
1:K:125:ILE:O	1:K:153:ALA:HA	2.09	0.53
1:K:274:ARG:NH1	3:K:418:HOH:O	2.41	0.53
1:Q:217:LYS:O	1:Q:227:ARG:NH1	2.37	0.53
1:S:92:LEU:HD13	1:S:290:TRP:CD2	2.44	0.53
1:U:186:LEU:HD21	1:U:233:MET:HE3	1.91	0.53
1:W:41:CYS:CA	1:W:77:TYR:CD1	2.85	0.53
1:E:138:LEU:CD2	1:G:287:VAL:HG13	2.39	0.52
1:G:178:ARG:NH2	2:G:301:SO4:O1	2.39	0.52
1:K:54:LYS:O	1:K:57:LYS:CB	2.57	0.52
1:O:140:LYS:O	1:O:142:GLY:N	2.40	0.52
1:Q:222:ARG:HG3	1:Q:222:ARG:HH11	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:182:ILE:HG23	1:S:233:MET:CE	2.40	0.52
1:S:191:SER:O	1:S:192:ARG:C	2.52	0.52
1:U:38:LYS:O	1:U:39:LEU:HD23	2.09	0.52
1:U:156:TYR:HA	1:U:165:ILE:CD1	2.31	0.52
1:U:246:SER:O	1:U:250:THR:N	2.37	0.52
1:A:221:LYS:HE2	1:A:221:LYS:N	2.18	0.52
1:C:41:CYS:SG	3:C:411:HOH:O	2.59	0.52
1:E:57:LYS:N	1:E:68:ILE:HD11	2.24	0.52
1:O:161:THR:OG1	1:O:163:GLN:HB2	2.09	0.52
1:U:247:GLU:CD	1:U:276:LEU:HD23	2.33	0.52
1:U:249:SER:O	1:U:253:ASN:HB2	2.10	0.52
1:U:292:MET:CG	1:U:293:LEU:H	2.18	0.52
1:G:183:ASN:ND2	3:G:434:HOH:O	2.41	0.52
1:M:102:LEU:HG	1:M:106:LEU:HD12	1.89	0.52
1:M:274:ARG:O	1:M:277:PHE:HB3	2.10	0.52
1:S:254:PHE:CD2	1:S:254:PHE:O	2.62	0.52
1:A:13:ARG:O	1:A:15:ILE:HG22	2.10	0.52
1:E:190:GLN:HA	1:E:194:ASP:OD2	2.10	0.52
1:E:279:ARG:HH11	1:E:279:ARG:HG3	1.74	0.52
1:O:112:MET:HE3	1:O:134:PHE:CD2	2.44	0.52
1:U:178:ARG:CG	1:U:178:ARG:O	2.57	0.52
1:W:157:ARG:HA	1:W:163:GLN:O	2.09	0.52
1:K:43:LYS:CB	1:O:233:MET:HE1	2.40	0.52
1:M:172:ASN:O	1:M:173:LEU:C	2.52	0.52
1:M:173:LEU:CD1	1:M:184:THR:HG22	2.38	0.52
1:O:220:THR:O	1:O:222:ARG:N	2.43	0.52
1:Q:44:THR:OG1	1:Q:45:LYS:N	2.42	0.52
1:Q:293:LEU:HD11	1:S:16:GLY:HA3	1.92	0.52
1:S:66:PRO:HA	1:S:83:GLU:OE2	2.09	0.52
1:U:259:ARG:O	1:U:262:ASP:HB2	2.09	0.52
1:U:264:PRO:HG2	1:U:266:TYR:CE1	2.45	0.52
1:C:60:GLN:CG	1:C:61:GLY:N	2.71	0.52
1:C:222:ARG:NH1	1:C:222:ARG:HG2	2.24	0.52
1:E:237:ILE:HD11	1:E:256:ARG:CZ	2.40	0.52
1:G:54:LYS:HE2	3:G:444:HOH:O	2.08	0.52
1:K:41:CYS:O	1:K:44:THR:CG2	2.58	0.52
1:O:119:ILE:CD1	1:O:147:ILE:HD13	2.40	0.52
1:U:127:ARG:NE	1:U:152:LEU:O	2.34	0.52
1:U:216:LEU:HB3	1:U:227:ARG:CZ	2.38	0.52
1:G:259:ARG:HD2	3:G:403:HOH:O	2.09	0.52
1:M:215:GLY:N	2:M:301:SO4:O3	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:52:GLU:OE2	1:O:56:TYR:HE2	1.91	0.52
1:O:183:ASN:O	1:O:186:LEU:N	2.42	0.52
1:U:285:ASP:O	1:U:286:TYR:HB2	2.10	0.52
1:G:131:PRO:HG2	1:G:205:TYR:CE2	2.44	0.52
1:G:251:TYR:CD1	1:G:251:TYR:C	2.88	0.52
1:O:54:LYS:HG3	1:O:55:PHE:H	1.74	0.52
1:S:229:SER:O	1:S:233:MET:CG	2.58	0.52
1:U:138:LEU:C	1:U:138:LEU:HD13	2.34	0.52
1:W:105:VAL:HG21	1:W:207:ASN:OD1	2.10	0.52
1:W:250:THR:HA	1:W:253:ASN:HB2	1.91	0.52
1:W:280:GLN:CB	1:W:282:PHE:CE2	2.92	0.52
1:G:164:HIS:O	1:G:165:ILE:C	2.52	0.52
1:I:22:ASP:C	1:I:23:ILE:HD13	2.35	0.52
1:M:122:LYS:O	1:M:123:ASN:HB2	2.09	0.52
1:Q:138:LEU:HD11	1:S:287:VAL:HG13	1.91	0.52
1:W:269:LEU:C	1:W:271:GLN:N	2.68	0.52
1:A:263:LYS:HD2	3:A:448:HOH:O	2.10	0.52
1:E:58:MET:SD	1:E:124:PHE:CE1	3.03	0.52
1:I:108:LEU:O	1:I:112:MET:HG3	2.10	0.52
1:Q:11:LEU:HD11	1:Q:24:TYR:HB3	1.90	0.52
1:W:124:PHE:CB	1:W:155:LYS:HA	2.40	0.52
1:W:271:GLN:O	1:W:275:ASN:ND2	2.32	0.52
1:K:139:GLY:O	1:K:140:LYS:C	2.51	0.51
1:Q:41:CYS:O	1:Q:44:THR:CG2	2.57	0.51
1:Q:105:VAL:HG21	1:Q:207:ASN:OD1	2.10	0.51
1:U:276:LEU:O	1:U:277:PHE:C	2.52	0.51
1:W:163:GLN:HA	1:W:163:GLN:OE1	2.11	0.51
1:A:237:ILE:HD11	1:A:256:ARG:CZ	2.40	0.51
1:E:90:GLU:HA	1:E:90:GLU:OE1	2.09	0.51
1:U:152:LEU:HD13	1:U:174:THR:HG22	1.92	0.51
1:U:167:TYR:HD2	1:U:260:PHE:CD2	2.28	0.51
1:U:242:LYS:C	1:U:244:TYR:N	2.68	0.51
1:U:264:PRO:CG	1:U:266:TYR:CZ	2.83	0.51
1:W:185:HIS:NE2	1:W:232:LYS:NZ	2.56	0.51
1:I:292:MET:O	1:I:294:LYS:NZ	2.42	0.51
1:M:141:LYS:C	1:M:143:ASN:N	2.65	0.51
1:U:207:ASN:C	1:U:209:GLY:H	2.18	0.51
1:W:116:ILE:HD11	1:W:129:VAL:CG2	2.40	0.51
1:W:247:GLU:HB2	1:W:276:LEU:HD23	1.91	0.51
1:E:1:MET:O	3:E:432:HOH:O	2.19	0.51
1:M:57:LYS:HD3	3:M:434:HOH:O	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:125:ILE:HG21	1:O:191:SER:C	2.35	0.51
1:S:149:ASP:C	1:S:149:ASP:OD1	2.53	0.51
1:C:137:GLY:O	1:C:142:GLY:HA2	2.10	0.51
1:E:222:ARG:HG3	1:E:222:ARG:NH1	2.24	0.51
1:G:150:PHE:HB3	1:G:153:ALA:HB3	1.91	0.51
1:M:237:ILE:O	1:M:240:LEU:HB3	2.10	0.51
1:O:28:ASN:CG	1:O:31:SER:HB3	2.36	0.51
1:Q:182:ILE:CD1	1:Q:256:ARG:CZ	2.88	0.51
1:Q:285:ASP:O	1:Q:287:VAL:N	2.42	0.51
1:U:49:LEU:HD11	1:U:80:MET:HE3	1.91	0.51
1:W:22:ASP:N	3:W:413:HOH:O	2.43	0.51
1:M:8:LYS:HD3	1:M:9:TYR:CZ	2.46	0.51
1:U:103:LYS:HB2	1:U:282:PHE:CD1	2.45	0.51
1:W:194:ASP:O	1:W:195:ASP:C	2.54	0.51
1:W:270:ARG:HG3	1:W:270:ARG:NH1	2.26	0.51
1:E:34:GLU:O	1:E:35:VAL:CG1	2.58	0.51
1:I:23:ILE:HD12	1:I:38:LYS:HG3	1.93	0.51
1:O:56:TYR:HE1	1:O:66:PRO:HG2	1.72	0.51
1:O:66:PRO:HB3	1:O:85:LEU:HD11	1.91	0.51
1:O:84:LEU:HG	1:O:138:LEU:HD11	1.93	0.51
1:O:161:THR:C	1:O:163:GLN:H	2.19	0.51
1:O:289:ASP:O	1:O:292:MET:HB3	2.10	0.51
1:S:43:LYS:C	1:S:44:THR:O	2.49	0.51
1:S:237:ILE:CG1	1:S:256:ARG:NH1	2.72	0.51
1:E:88:SER:HA	1:E:135:LEU:HD23	1.91	0.51
1:E:222:ARG:HG3	1:E:222:ARG:HH11	1.74	0.51
1:G:156:TYR:C	1:G:165:ILE:HG23	2.36	0.51
1:M:274:ARG:NH1	1:M:274:ARG:CG	2.72	0.51
1:O:183:ASN:O	1:O:184:THR:C	2.54	0.51
1:U:165:ILE:HB	1:U:166:PRO:HD2	1.93	0.51
1:U:213:TRP:O	1:U:216:LEU:HD22	2.11	0.51
1:U:284:TYR:O	1:U:286:TYR:CE2	2.64	0.51
1:W:36:ALA:O	1:W:81:VAL:HA	2.10	0.51
1:W:54:LYS:O	1:W:58:MET:HB2	2.11	0.51
1:W:134:PHE:HA	1:W:146:TYR:O	2.11	0.51
1:C:259:ARG:N	1:C:262:ASP:OD2	2.38	0.51
1:E:137:GLY:O	1:E:142:GLY:HA2	2.11	0.51
1:E:138:LEU:HD22	1:G:287:VAL:HG13	1.93	0.51
1:Q:16:GLY:CA	1:S:294:LYS:HD3	2.41	0.51
1:Q:221:LYS:H	1:Q:221:LYS:HE3	1.76	0.51
1:U:45:LYS:O	1:U:46:HIS:CB	2.59	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:127:ARG:CB	1:U:190:GLN:NE2	2.74	0.51
1:U:277:PHE:CE2	1:U:282:PHE:O	2.63	0.51
1:W:2:GLU:HG3	1:W:3:LEU:N	2.08	0.51
1:C:76:ASP:OD1	1:C:77:TYR:CD2	2.64	0.51
1:I:69:LYS:HE2	3:I:417:HOH:O	2.11	0.51
1:U:167:TYR:O	1:U:168:ARG:HB2	2.11	0.51
1:W:57:LYS:CE	1:W:68:ILE:HB	2.36	0.51
1:W:150:PHE:O	1:W:153:ALA:HB3	2.11	0.51
1:A:47:PRO:C	1:A:48:GLN:CG	2.85	0.50
1:C:3:LEU:CG	1:K:238:GLU:HG3	2.39	0.50
1:E:84:LEU:HG	1:E:138:LEU:CD1	2.41	0.50
1:G:84:LEU:O	1:G:138:LEU:HD12	2.11	0.50
1:G:222:ARG:O	1:G:226:GLU:HG2	2.10	0.50
1:I:45:LYS:C	1:I:46:HIS:ND1	2.64	0.50
1:M:68:ILE:HG22	1:M:69:LYS:N	2.26	0.50
1:O:80:MET:HE3	1:O:82:MET:HE2	1.93	0.50
1:Q:165:ILE:HB	1:Q:166:PRO:HD2	1.92	0.50
1:Q:185:HIS:CG	1:Q:229:SER:HB2	2.46	0.50
1:U:103:LYS:HB2	1:U:282:PHE:CG	2.45	0.50
1:W:94:ASN:OD1	1:W:98:ARG:HD2	2.11	0.50
1:W:211:LEU:HB3	1:W:212:PRO:HD2	1.93	0.50
1:W:223:GLN:O	1:W:227:ARG:HG3	2.11	0.50
1:C:186:LEU:O	1:C:188:ILE:N	2.44	0.50
1:I:220:THR:CG2	1:I:223:GLN:H	2.08	0.50
1:K:38:LYS:O	1:K:39:LEU:HD23	2.11	0.50
1:O:28:ASN:ND2	1:O:30:ALA:N	2.59	0.50
1:S:4:ARG:HH11	1:S:4:ARG:CG	2.13	0.50
1:U:28:ASN:HD22	1:U:30:ALA:H	1.56	0.50
1:M:23:ILE:HG21	1:O:293:LEU:HD23	1.94	0.50
1:O:202:VAL:O	1:O:205:TYR:HB3	2.11	0.50
1:S:237:ILE:HG13	1:S:256:ARG:HH12	1.75	0.50
1:U:157:ARG:HA	1:U:164:HIS:HA	1.94	0.50
1:W:84:LEU:HG	1:W:138:LEU:CD1	2.42	0.50
1:W:124:PHE:HB3	1:W:154:LYS:O	2.12	0.50
1:E:220:THR:HG23	1:E:222:ARG:HB3	1.93	0.50
1:G:178:ARG:NH2	1:G:214:GLN:HE21	2.06	0.50
1:K:250:THR:HG21	1:K:272:LEU:HD11	1.92	0.50
1:Q:4:ARG:NH2	1:Q:7:ASN:HD22	2.08	0.50
1:Q:43:LYS:C	1:Q:44:THR:O	2.55	0.50
1:Q:221:LYS:H	1:Q:221:LYS:CE	2.23	0.50
1:S:169:GLU:HB3	1:S:170:ASN:ND2	2.24	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:42:VAL:HG22	1:W:76:ASP:C	2.36	0.50
1:W:102:LEU:HD13	1:W:245:PRO:HG2	1.92	0.50
1:C:62:GLY:HA3	1:C:118:TYR:CE2	2.47	0.50
1:C:67:SER:HB3	1:C:83:GLU:OE2	2.12	0.50
1:E:131:PRO:HD3	1:E:202:VAL:HG22	1.93	0.50
1:E:236:PRO:HB3	1:O:77:TYR:CE2	2.47	0.50
1:G:141:LYS:HD3	1:G:146:TYR:OH	2.12	0.50
1:G:168:ARG:HG2	1:G:169:GLU:N	2.27	0.50
1:M:71:CYS:SG	3:M:404:HOH:O	2.60	0.50
1:Q:108:LEU:O	1:Q:112:MET:HG3	2.12	0.50
1:S:25:LEU:HD23	1:S:25:LEU:C	2.37	0.50
1:W:44:THR:HG23	1:W:46:HIS:N	2.27	0.50
1:E:241:CYS:O	1:E:242:LYS:C	2.53	0.50
1:I:276:LEU:HD12	1:I:280:GLN:HG2	1.94	0.50
1:K:120:HIS:CG	1:K:192:ARG:HG2	2.46	0.50
1:K:220:THR:CG2	1:K:223:GLN:HG3	2.42	0.50
1:M:120:HIS:CG	1:M:192:ARG:HG2	2.47	0.50
1:M:219:ALA:HB3	1:M:223:GLN:OE1	2.11	0.50
1:O:52:GLU:OE2	1:O:56:TYR:CE2	2.64	0.50
1:Q:76:ASP:HB3	3:Q:429:HOH:O	2.10	0.50
1:U:6:GLY:C	1:U:8:LYS:H	2.20	0.50
1:U:242:LYS:O	1:U:244:TYR:N	2.45	0.50
1:W:123:ASN:C	1:W:156:TYR:HD2	2.19	0.50
1:W:172:ASN:O	1:W:173:LEU:C	2.54	0.50
1:E:203:LEU:O	1:E:207:ASN:ND2	2.44	0.50
1:G:259:ARG:HG2	1:G:259:ARG:HH11	1.76	0.50
1:O:58:MET:HE1	1:O:122:LYS:O	2.11	0.50
1:U:52:GLU:OE2	1:U:150:PHE:N	2.44	0.50
1:U:126:HIS:CD2	1:U:147:ILE:HD11	2.46	0.50
1:E:7:ASN:CG	1:E:7:ASN:O	2.53	0.50
1:K:49:LEU:HD12	1:K:49:LEU:C	2.36	0.50
1:K:62:GLY:CA	1:K:118:TYR:CZ	2.95	0.50
1:K:213:TRP:CE2	1:K:232:LYS:HE2	2.47	0.50
1:M:293:LEU:CD2	1:O:135:LEU:HD23	2.40	0.50
1:O:140:LYS:C	1:O:142:GLY:N	2.69	0.50
1:O:169:GLU:HA	1:O:188:ILE:HA	1.94	0.50
1:Q:167:TYR:CD1	1:Q:168:ARG:N	2.80	0.50
1:Q:220:THR:N	1:Q:223:GLN:HE21	2.10	0.50
1:U:130:LYS:HB2	1:U:131:PRO:HD2	1.94	0.50
1:U:167:TYR:HA	1:U:260:PHE:CE2	2.46	0.50
1:U:234:SER:C	1:U:236:PRO:HD3	2.36	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:57:LYS:HZ2	1:W:68:ILE:HG21	1.77	0.50
1:W:70:TRP:O	1:W:70:TRP:CD2	2.65	0.50
1:W:254:PHE:CD2	1:W:258:LEU:HD21	2.46	0.50
1:A:120:HIS:ND1	1:A:192:ARG:HG2	2.26	0.50
1:A:293:LEU:HD12	1:C:15:ILE:HG23	1.94	0.50
1:I:17:SER:C	3:I:409:HOH:O	2.55	0.50
1:I:251:TYR:C	1:I:251:TYR:CD1	2.90	0.50
1:I:271:GLN:HG3	1:I:275:ASN:ND2	2.26	0.50
1:K:55:PHE:O	1:K:59:MET:HG2	2.12	0.50
1:O:219:ALA:CB	1:O:223:GLN:OE1	2.57	0.50
1:U:3:LEU:C	1:U:3:LEU:HD12	2.37	0.50
1:U:207:ASN:O	1:U:209:GLY:N	2.38	0.50
1:W:258:LEU:HD23	1:W:258:LEU:N	2.26	0.50
1:E:269:LEU:O	1:E:272:LEU:HB3	2.12	0.49
1:I:25:LEU:HD23	1:I:25:LEU:C	2.37	0.49
1:I:59:MET:O	1:I:60:GLN:C	2.54	0.49
1:K:90:GLU:OE2	1:K:98:ARG:NH2	2.45	0.49
1:K:140:LYS:HG3	1:K:141:LYS:H	1.77	0.49
1:M:156:TYR:HA	1:M:165:ILE:HG23	1.94	0.49
1:M:220:THR:HG22	1:M:223:GLN:CD	2.35	0.49
1:Q:8:LYS:O	1:Q:29:ILE:HG12	2.12	0.49
1:S:118:TYR:C	1:S:118:TYR:CD2	2.90	0.49
1:S:137:GLY:HA3	1:S:141:LYS:CB	2.41	0.49
1:S:167:TYR:CD2	1:S:260:PHE:HD2	2.29	0.49
1:S:180:ALA:HB3	1:S:185:HIS:NE2	2.26	0.49
1:U:28:ASN:ND2	1:U:31:SER:N	2.59	0.49
1:C:12:GLY:N	1:C:25:LEU:O	2.45	0.49
1:K:29:ILE:HG22	1:K:30:ALA:N	2.26	0.49
1:M:125:ILE:HG13	1:M:127:ARG:HG3	1.95	0.49
1:Q:8:LYS:HB2	1:Q:8:LYS:HZ2	1.76	0.49
1:S:68:ILE:CG2	1:S:69:LYS:N	2.75	0.49
1:U:5:VAL:N	1:U:9:TYR:O	2.39	0.49
1:W:164:HIS:CE1	1:W:261:ASP:HA	2.46	0.49
1:C:58:MET:HG2	1:C:59:MET:HE2	1.94	0.49
1:E:182:ILE:HD11	1:E:256:ARG:CZ	2.41	0.49
1:G:131:PRO:HG2	1:G:205:TYR:HE2	1.76	0.49
1:I:6:GLY:O	1:I:7:ASN:C	2.55	0.49
1:M:80:MET:HE3	1:M:82:MET:HB3	1.93	0.49
1:M:218:ALA:HB2	1:M:227:ARG:HD3	1.93	0.49
1:O:14:LYS:HD2	1:O:22:ASP:OD2	2.12	0.49
1:W:90:GLU:HB2	1:W:131:PRO:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:128:ASP:OD2	1:W:130:LYS:HD3	2.13	0.49
1:W:270:ARG:HG3	1:W:270:ARG:HH11	1.77	0.49
1:E:211:LEU:O	1:E:214:GLN:HB2	2.12	0.49
1:E:231:LYS:HA	1:E:234:SER:OG	2.12	0.49
1:G:5:VAL:O	1:G:7:ASN:N	2.45	0.49
1:G:92:LEU:HD13	1:G:290:TRP:CE2	2.47	0.49
1:M:135:LEU:HD13	1:M:148:ILE:HD13	1.93	0.49
1:M:251:TYR:O	1:M:254:PHE:HB3	2.13	0.49
1:Q:220:THR:H	1:Q:223:GLN:HE21	1.58	0.49
1:S:40:GLU:OE1	1:S:49:LEU:HB3	2.12	0.49
1:S:208:LEU:CD2	1:S:244:TYR:HE2	2.24	0.49
1:U:28:ASN:HD21	1:U:30:ALA:HB3	1.77	0.49
1:U:52:GLU:OE1	1:U:56:TYR:HE2	1.94	0.49
1:I:234:SER:O	1:I:236:PRO:CD	2.61	0.49
1:K:4:ARG:NH2	1:K:7:ASN:HD22	2.11	0.49
1:K:117:GLU:OE1	1:K:270:ARG:NH2	2.46	0.49
1:M:41:CYS:HB2	1:M:77:TYR:CE1	2.48	0.49
1:M:58:MET:O	1:M:60:GLN:N	2.45	0.49
1:O:221:LYS:O	1:O:222:ARG:C	2.55	0.49
1:S:193:ARG:CG	1:S:194:ASP:N	2.76	0.49
1:W:213:TRP:HB3	1:W:231:LYS:CG	2.43	0.49
1:C:173:LEU:HD12	1:C:184:THR:HG22	1.94	0.49
1:E:237:ILE:HD11	1:E:256:ARG:NE	2.28	0.49
1:O:60:GLN:CG	1:O:61:GLY:N	2.75	0.49
1:O:124:PHE:HD2	1:O:154:LYS:CA	2.26	0.49
1:U:277:PHE:CE1	1:U:282:PHE:HB2	2.48	0.49
1:W:10:ARG:HB2	1:W:29:ILE:CD1	2.42	0.49
1:W:135:LEU:N	1:W:135:LEU:CD1	2.76	0.49
1:A:174:THR:O	1:A:174:THR:HG23	2.13	0.49
1:A:238:GLU:CG	1:I:3:LEU:HB2	2.43	0.49
3:A:476:HOH:O	1:I:1:MET:HE3	2.13	0.49
1:G:224:LYS:O	1:G:225:TYR:C	2.56	0.49
1:I:174:THR:O	1:I:174:THR:HG23	2.13	0.49
1:K:226:GLU:O	1:K:230:GLU:HB2	2.12	0.49
1:O:150:PHE:C	1:O:152:LEU:H	2.20	0.49
1:O:158:ASP:OD1	1:O:160:ARG:N	2.44	0.49
1:S:134:PHE:CZ	1:S:147:ILE:HD12	2.48	0.49
1:S:222:ARG:HH11	1:S:222:ARG:CG	2.23	0.49
1:E:57:LYS:HG3	1:E:68:ILE:HD12	1.95	0.49
1:K:42:VAL:HG23	1:K:76:ASP:C	2.38	0.49
1:K:111:GLN:OE1	1:K:115:ARG:NH2	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:119:ILE:CD1	1:K:147:ILE:HD13	2.43	0.49
1:O:120:HIS:CG	1:O:192:ARG:HG2	2.48	0.49
1:S:28:ASN:HD22	1:S:28:ASN:C	2.20	0.49
1:W:86:GLY:N	1:W:136:MET:O	2.44	0.49
1:A:222:ARG:HH11	1:A:222:ARG:CG	2.20	0.49
1:E:207:ASN:HB3	1:E:244:TYR:CE1	2.48	0.49
1:G:226:GLU:CD	1:G:226:GLU:N	2.70	0.49
1:K:41:CYS:HB3	1:K:44:THR:HG22	1.94	0.49
1:M:279:ARG:HG2	1:S:63:VAL:HG22	1.95	0.49
1:Q:28:ASN:OD1	1:Q:30:ALA:N	2.45	0.49
1:S:147:ILE:HG13	1:S:148:ILE:N	2.27	0.49
1:A:47:PRO:C	1:A:48:GLN:HG2	2.38	0.49
1:A:221:LYS:H	1:A:221:LYS:CE	2.21	0.49
1:C:231:LYS:HA	1:C:234:SER:OG	2.13	0.49
1:C:236:PRO:HB3	1:E:77:TYR:CE2	2.48	0.49
1:M:278:HIS:O	1:M:280:GLN:N	2.46	0.49
1:O:217:LYS:O	1:O:227:ARG:NH1	2.40	0.49
1:Q:172:ASN:O	1:Q:173:LEU:C	2.55	0.49
1:Q:181:SER:O	1:Q:184:THR:HB	2.13	0.49
1:Q:222:ARG:HG3	1:Q:222:ARG:NH1	2.26	0.49
1:S:150:PHE:C	1:S:152:LEU:N	2.67	0.49
1:U:138:LEU:HD13	1:U:139:GLY:N	2.28	0.49
1:U:208:LEU:C	1:U:210:SER:N	2.62	0.49
1:U:254:PHE:O	1:U:257:SER:N	2.44	0.49
1:U:276:LEU:HD13	1:U:276:LEU:C	2.37	0.49
1:W:4:ARG:HD2	1:W:29:ILE:CD1	2.43	0.49
1:W:140:LYS:CE	1:W:140:LYS:HA	2.43	0.49
1:W:147:ILE:O	1:W:147:ILE:HG23	2.12	0.49
1:W:150:PHE:N	1:W:150:PHE:HD1	2.08	0.49
1:W:164:HIS:NE2	1:W:261:ASP:CA	2.76	0.49
1:W:259:ARG:O	1:W:262:ASP:HB2	2.12	0.49
1:A:245:PRO:CB	1:A:276:LEU:HD21	2.43	0.48
1:C:46:HIS:H	1:C:47:PRO:CD	2.22	0.48
1:C:186:LEU:O	1:C:188:ILE:HG13	2.12	0.48
1:E:54:LYS:HD3	1:E:54:LYS:HA	1.59	0.48
1:G:28:ASN:HD21	1:G:30:ALA:CB	2.24	0.48
1:G:116:ILE:HD12	1:G:199:LEU:HD22	1.95	0.48
1:G:158:ASP:C	1:G:158:ASP:OD1	2.56	0.48
1:G:158:ASP:CG	1:G:161:THR:OG1	2.56	0.48
1:G:178:ARG:HD2	1:G:179:TYR:CE1	2.48	0.48
1:I:15:ILE:HD11	1:I:25:LEU:HD12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:230:GLU:O	1:U:231:LYS:C	2.56	0.48
1:W:14:LYS:NZ	1:W:16:GLY:C	2.70	0.48
1:E:230:GLU:HA	1:E:233:MET:HE3	1.94	0.48
1:K:15:ILE:CG2	1:K:25:LEU:HB2	2.43	0.48
1:C:222:ARG:CG	1:C:222:ARG:NH1	2.72	0.48
1:M:138:LEU:HD21	1:O:287:VAL:HG13	1.94	0.48
1:O:50:HIS:O	1:O:52:GLU:N	2.46	0.48
1:O:221:LYS:CG	1:O:222:ARG:N	2.74	0.48
1:W:71:CYS:HA	1:W:79:VAL:O	2.14	0.48
1:W:196:LEU:O	1:W:197:GLU:C	2.56	0.48
1:C:219:ALA:HB3	1:C:223:GLN:OE1	2.14	0.48
1:E:5:VAL:N	1:E:9:TYR:O	2.43	0.48
1:E:285:ASP:C	1:E:285:ASP:OD1	2.56	0.48
1:G:6:GLY:HA2	1:G:70:TRP:CZ2	2.48	0.48
1:I:17:SER:HB3	3:I:409:HOH:O	2.13	0.48
1:K:221:LYS:O	1:K:222:ARG:C	2.55	0.48
1:O:52:GLU:C	1:O:54:LYS:N	2.71	0.48
1:O:94:ASN:OD1	1:O:98:ARG:NH1	2.44	0.48
1:O:237:ILE:O	1:O:240:LEU:HB3	2.13	0.48
1:Q:13:ARG:N	3:Q:418:HOH:O	2.32	0.48
1:Q:161:THR:O	1:Q:162:HIS:HB2	2.11	0.48
1:S:4:ARG:NH1	1:S:29:ILE:CD1	2.71	0.48
1:U:9:TYR:CE2	1:U:81:VAL:HG11	2.48	0.48
1:U:44:THR:O	1:U:46:HIS:N	2.47	0.48
1:U:127:ARG:CB	1:U:190:GLN:HE21	2.26	0.48
1:U:184:THR:CG2	1:U:190:GLN:OE1	2.61	0.48
1:U:237:ILE:HG21	1:U:253:ASN:ND2	2.28	0.48
1:U:293:LEU:HD13	1:U:293:LEU:C	2.38	0.48
1:E:287:VAL:HG13	1:G:138:LEU:HD21	1.95	0.48
1:I:211:LEU:O	1:I:214:GLN:HB2	2.13	0.48
1:M:63:VAL:O	1:M:65:ILE:HG12	2.14	0.48
1:Q:16:GLY:HA2	1:S:294:LYS:HG2	1.95	0.48
1:U:193:ARG:HG3	1:U:194:ASP:OD2	2.12	0.48
1:A:45:LYS:O	1:A:46:HIS:CD2	2.67	0.48
1:E:119:ILE:HD11	1:E:147:ILE:HG21	1.94	0.48
1:K:156:TYR:O	1:K:165:ILE:HG23	2.13	0.48
1:M:56:TYR:HB2	1:M:68:ILE:HD11	1.96	0.48
1:Q:17:SER:N	1:S:294:LYS:CD	2.67	0.48
1:Q:257:SER:O	1:Q:258:LEU:C	2.57	0.48
1:C:269:LEU:O	1:C:272:LEU:HB3	2.14	0.48
1:E:56:TYR:HB2	1:E:68:ILE:CD1	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:147:ILE:HG12	1:M:148:ILE:N	2.29	0.48
1:M:237:ILE:HD13	1:M:252:LEU:HB3	1.94	0.48
1:O:58:MET:HE1	1:O:124:PHE:HD1	1.78	0.48
1:Q:277:PHE:CE1	1:Q:282:PHE:HD2	2.31	0.48
1:W:57:LYS:O	1:W:58:MET:C	2.54	0.48
1:W:89:LEU:HG	1:W:134:PHE:HB2	1.96	0.48
1:A:63:VAL:HG12	1:A:64:GLY:N	2.28	0.48
1:E:236:PRO:HG2	1:E:239:VAL:CG2	2.44	0.48
1:G:182:ILE:HD12	1:G:256:ARG:CZ	2.43	0.48
1:K:171:LYS:HE2	1:K:171:LYS:HB3	1.77	0.48
1:Q:80:MET:HE1	1:Q:82:MET:HE3	1.92	0.48
1:C:38:LYS:HG2	1:C:49:LEU:HD13	1.95	0.48
1:C:46:HIS:N	1:C:47:PRO:CD	2.77	0.48
1:E:55:PHE:O	1:E:59:MET:HG2	2.14	0.48
1:G:76:ASP:HB2	3:G:438:HOH:O	2.14	0.48
1:K:14:LYS:HB2	1:K:24:TYR:CE2	2.49	0.48
1:K:59:MET:O	1:K:60:GLN:C	2.57	0.48
1:O:222:ARG:HG2	1:O:223:GLN:H	1.79	0.48
1:S:43:LYS:O	1:S:44:THR:C	2.57	0.48
1:S:57:LYS:O	1:S:58:MET:C	2.55	0.48
1:W:70:TRP:CH2	1:W:72:GLY:HA3	2.49	0.48
1:W:192:ARG:HD2	1:W:264:PRO:CD	2.44	0.48
1:U:4:ARG:CZ	1:U:7:ASN:O	2.61	0.48
1:U:14:LYS:C	1:U:15:ILE:CG1	2.86	0.48
1:U:39:LEU:CD2	1:U:79:VAL:HG13	2.44	0.48
1:U:111:GLN:O	1:U:115:ARG:HG2	2.14	0.48
1:C:270:ARG:O	1:C:274:ARG:HG3	2.14	0.47
1:K:150:PHE:N	1:K:150:PHE:CD1	2.81	0.47
1:M:31:SER:C	1:M:33:GLU:N	2.71	0.47
1:Q:128:ASP:HB2	1:Q:152:LEU:HD12	1.96	0.47
1:Q:182:ILE:HD12	1:Q:256:ARG:CZ	2.44	0.47
1:U:211:LEU:O	1:U:214:GLN:CB	2.62	0.47
1:W:37:ILE:HG23	1:W:80:MET:O	2.12	0.47
1:W:201:TYR:O	1:W:202:VAL:C	2.57	0.47
1:C:119:ILE:CD1	1:C:147:ILE:HD13	2.44	0.47
1:E:22:ASP:N	3:E:433:HOH:O	2.47	0.47
1:M:61:GLY:O	1:M:62:GLY:C	2.57	0.47
1:M:64:GLY:HA2	1:M:146:TYR:CD2	2.48	0.47
1:Q:4:ARG:NH2	1:Q:7:ASN:ND2	2.62	0.47
1:Q:181:SER:HA	1:Q:197:GLU:OE2	2.14	0.47
1:Q:193:ARG:HG3	1:Q:194:ASP:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:189:GLU:HB3	1:S:260:PHE:CE2	2.48	0.47
1:W:165:ILE:HB	1:W:166:PRO:CD	2.44	0.47
1:C:59:MET:O	1:C:60:GLN:C	2.56	0.47
1:K:118:TYR:OH	1:K:122:LYS:HE3	2.13	0.47
1:K:221:LYS:NZ	1:K:225:TYR:OH	2.47	0.47
1:M:181:SER:OG	1:M:194:ASP:OD1	2.28	0.47
1:U:130:LYS:HB2	1:U:131:PRO:CD	2.44	0.47
1:U:224:LYS:O	1:U:228:ILE:HG13	2.14	0.47
1:C:120:HIS:CG	1:C:192:ARG:HG2	2.49	0.47
1:C:138:LEU:HA	1:C:138:LEU:HD23	1.75	0.47
1:E:8:LYS:HD3	1:E:9:TYR:CE2	2.49	0.47
1:E:274:ARG:HH12	1:Q:274:ARG:NH1	2.11	0.47
1:G:28:ASN:ND2	1:G:30:ALA:H	2.12	0.47
1:G:55:PHE:CE2	1:G:150:PHE:O	2.68	0.47
1:K:44:THR:O	1:K:47:PRO:HD3	2.14	0.47
1:M:178:ARG:HD2	1:M:179:TYR:CZ	2.49	0.47
1:O:150:PHE:N	1:O:150:PHE:CD1	2.82	0.47
1:U:201:TYR:C	1:U:203:LEU:N	2.70	0.47
1:W:53:SER:HA	1:W:68:ILE:HD12	1.96	0.47
1:W:87:PRO:O	1:W:135:LEU:HA	2.13	0.47
1:A:98:ARG:NH2	1:A:205:TYR:OH	2.48	0.47
1:A:137:GLY:C	1:A:142:GLY:HA2	2.39	0.47
1:C:127:ARG:NH1	1:C:174:THR:HG21	2.29	0.47
1:I:291:ASN:O	1:K:86:GLY:HA2	2.14	0.47
1:K:185:HIS:HB3	1:K:229:SER:OG	2.13	0.47
1:O:150:PHE:O	1:O:152:LEU:N	2.47	0.47
1:O:167:TYR:HB2	1:O:260:PHE:CE2	2.49	0.47
1:S:120:HIS:CD2	1:S:125:ILE:HG22	2.49	0.47
1:S:276:LEU:O	1:S:277:PHE:C	2.58	0.47
1:U:120:HIS:C	1:U:122:LYS:N	2.72	0.47
1:W:6:GLY:HA2	1:W:70:TRP:CH2	2.50	0.47
1:E:140:LYS:HG2	1:E:141:LYS:HG3	1.97	0.47
1:E:168:ARG:HG2	1:E:169:GLU:N	2.29	0.47
1:G:41:CYS:SG	3:G:438:HOH:O	2.60	0.47
1:I:222:ARG:HH11	1:I:222:ARG:CG	2.26	0.47
1:I:271:GLN:HE21	1:I:271:GLN:CA	2.21	0.47
1:M:294:LYS:HB2	1:O:91:ASP:OD2	2.14	0.47
1:W:6:GLY:HA2	1:W:70:TRP:CZ2	2.50	0.47
1:E:251:TYR:CD1	1:E:251:TYR:C	2.93	0.47
1:G:10:ARG:NH2	3:G:450:HOH:O	2.47	0.47
1:G:50:HIS:O	1:G:53:SER:OG	2.31	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:57:LYS:HA	1:G:57:LYS:HD2	1.59	0.47
1:G:259:ARG:O	1:G:260:PHE:C	2.58	0.47
1:I:270:ARG:NH1	3:I:452:HOH:O	2.47	0.47
1:K:140:LYS:C	1:K:142:GLY:H	2.22	0.47
1:M:108:LEU:O	1:M:109:ALA:C	2.57	0.47
1:O:11:LEU:CD1	1:O:37:ILE:HD12	2.45	0.47
1:O:33:GLU:OE2	1:O:69:LYS:CE	2.62	0.47
1:O:35:VAL:HG21	1:O:81:VAL:CG1	2.43	0.47
1:O:119:ILE:HD11	1:O:147:ILE:HG21	1.96	0.47
1:O:259:ARG:HB2	1:O:262:ASP:CB	2.43	0.47
1:S:134:PHE:CE1	1:S:147:ILE:HD12	2.49	0.47
1:U:62:GLY:HA3	1:U:118:TYR:CZ	2.49	0.47
1:W:117:GLU:CB	1:W:266:TYR:CE1	2.94	0.47
1:A:17:SER:HA	3:A:413:HOH:O	2.13	0.47
1:A:41:CYS:C	1:A:43:LYS:N	2.71	0.47
1:E:57:LYS:HG3	1:E:68:ILE:CD1	2.45	0.47
1:G:29:ILE:O	1:G:30:ALA:O	2.33	0.47
1:U:29:ILE:HD13	1:U:29:ILE:HA	1.77	0.47
1:W:250:THR:HB	1:W:272:LEU:HD21	1.97	0.47
1:E:41:CYS:O	1:E:44:THR:OG1	2.21	0.47
1:E:57:LYS:O	1:E:60:GLN:HB3	2.15	0.47
1:E:76:ASP:OD1	1:E:76:ASP:N	2.28	0.47
1:K:45:LYS:O	1:K:46:HIS:CB	2.63	0.47
1:O:268:TYR:CZ	1:O:272:LEU:CD2	2.98	0.47
1:Q:182:ILE:O	1:Q:183:ASN:C	2.57	0.47
1:U:208:LEU:HD23	1:U:244:TYR:CE2	2.50	0.47
1:U:257:SER:O	1:U:258:LEU:C	2.58	0.47
1:C:59:MET:HE1	1:C:122:LYS:HB3	1.97	0.47
1:G:126:HIS:O	1:G:127:ARG:HB2	2.15	0.47
1:K:8:LYS:HB2	1:K:8:LYS:HE2	1.62	0.47
1:M:93:PHE:HZ	1:M:209:GLY:HA2	1.80	0.47
1:S:154:LYS:NZ	3:S:401:HOH:O	2.29	0.47
1:U:66:PRO:CA	1:U:83:GLU:OE2	2.52	0.47
1:U:197:GLU:O	1:U:200:GLY:N	2.45	0.47
1:W:56:TYR:CE2	1:W:82:MET:HE2	2.50	0.47
1:W:123:ASN:HA	1:W:156:TYR:HE2	1.76	0.47
1:C:2:GLU:HB3	1:C:3:LEU:H	1.58	0.46
1:C:244:TYR:O	1:C:245:PRO:C	2.56	0.46
1:G:56:TYR:HB3	1:G:68:ILE:HG12	1.96	0.46
1:I:84:LEU:HD23	1:I:138:LEU:HD11	1.97	0.46
1:I:174:THR:CG2	1:I:190:GLN:OE1	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:54:LYS:O	1:K:57:LYS:HB2	2.15	0.46
1:K:134:PHE:HA	1:K:146:TYR:O	2.15	0.46
1:M:102:LEU:CG	1:M:106:LEU:HD11	2.45	0.46
1:S:293:LEU:HD12	1:S:294:LYS:HB2	1.96	0.46
1:U:156:TYR:O	1:U:165:ILE:HG12	2.15	0.46
1:U:293:LEU:HB3	1:W:15:ILE:HG23	1.94	0.46
1:A:98:ARG:NH1	1:A:209:GLY:O	2.48	0.46
1:A:119:ILE:CD1	1:A:150:PHE:HE2	2.26	0.46
1:A:217:LYS:HD2	1:A:217:LYS:N	2.21	0.46
1:E:6:GLY:N	3:E:445:HOH:O	2.21	0.46
1:E:167:TYR:HA	1:E:260:PHE:CE2	2.50	0.46
1:G:119:ILE:HD11	1:G:147:ILE:HD13	1.98	0.46
1:K:49:LEU:HD11	1:K:80:MET:HE2	1.96	0.46
1:M:244:TYR:O	1:M:245:PRO:C	2.57	0.46
1:U:35:VAL:HG23	1:U:36:ALA:O	2.16	0.46
1:W:164:HIS:CD2	1:W:261:ASP:O	2.67	0.46
1:A:120:HIS:CE1	1:A:192:ARG:HG2	2.51	0.46
1:I:56:TYR:CE1	1:I:150:PHE:CE1	3.03	0.46
1:S:43:LYS:O	1:S:44:THR:O	2.34	0.46
1:S:150:PHE:N	1:S:150:PHE:HD1	2.10	0.46
1:U:226:GLU:O	1:U:227:ARG:C	2.58	0.46
1:U:292:MET:HE2	1:U:292:MET:HB3	1.78	0.46
1:A:10:ARG:HB2	1:A:29:ILE:HD11	1.96	0.46
1:A:167:TYR:OH	1:A:169:GLU:OE2	2.22	0.46
1:C:263:LYS:NZ	3:C:464:HOH:O	2.49	0.46
1:G:25:LEU:HD11	1:G:34:GLU:HB3	1.97	0.46
1:Q:57:LYS:HD2	1:Q:57:LYS:HA	1.42	0.46
1:Q:220:THR:HG22	1:Q:223:GLN:HG3	1.96	0.46
1:Q:223:GLN:O	1:Q:227:ARG:HG3	2.15	0.46
1:S:209:GLY:O	1:S:210:SER:HB3	2.13	0.46
1:A:36:ALA:HB3	1:A:82:MET:HG3	1.97	0.46
1:C:119:ILE:HD11	1:C:147:ILE:HD13	1.97	0.46
1:E:3:LEU:HD23	1:E:3:LEU:HA	1.64	0.46
1:E:6:GLY:O	1:E:7:ASN:C	2.59	0.46
1:E:123:ASN:HA	1:E:156:TYR:CE2	2.51	0.46
1:G:136:MET:HA	1:G:136:MET:HE3	1.98	0.46
1:M:13:ARG:C	1:M:14:LYS:O	2.53	0.46
1:M:117:GLU:O	1:M:118:TYR:C	2.57	0.46
1:M:135:LEU:HD23	1:O:293:LEU:HD13	1.98	0.46
1:M:191:SER:HB3	1:M:260:PHE:HE1	1.80	0.46
1:O:58:MET:CE	1:O:122:LYS:O	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:111:GLN:O	1:O:115:ARG:HG2	2.15	0.46
1:S:23:ILE:HD11	1:S:38:LYS:CE	2.45	0.46
1:W:134:PHE:C	1:W:135:LEU:CD1	2.88	0.46
1:E:130:LYS:HA	1:E:202:VAL:HG21	1.98	0.46
1:G:234:SER:O	1:G:236:PRO:HD3	2.16	0.46
1:M:231:LYS:HA	1:M:234:SER:OG	2.15	0.46
1:O:289:ASP:O	1:O:294:LYS:NZ	2.47	0.46
1:Q:10:ARG:HG2	1:Q:10:ARG:HH11	1.80	0.46
1:U:6:GLY:HA3	1:U:70:TRP:CE2	2.50	0.46
1:U:6:GLY:CA	1:U:70:TRP:CZ2	2.99	0.46
1:U:237:ILE:HD11	1:U:256:ARG:CD	2.45	0.46
1:W:266:TYR:HB3	1:W:270:ARG:NH1	2.30	0.46
1:C:136:MET:SD	1:C:145:VAL:HG22	2.56	0.46
1:E:215:GLY:O	1:E:216:LEU:C	2.59	0.46
1:G:14:LYS:HA	1:G:24:TYR:CD1	2.51	0.46
1:I:28:ASN:HD22	1:I:31:SER:N	2.12	0.46
1:I:196:LEU:O	1:I:199:LEU:HB3	2.15	0.46
1:M:204:MET:HE3	1:M:204:MET:CA	2.45	0.46
1:O:41:CYS:SG	1:O:43:LYS:HE2	2.56	0.46
1:O:164:HIS:HE1	1:O:260:PHE:CZ	2.34	0.46
1:O:293:LEU:HD12	1:O:294:LYS:H	1.80	0.46
1:S:59:MET:HE3	1:S:150:PHE:HE2	1.81	0.46
1:S:198:SER:O	1:S:202:VAL:HG23	2.15	0.46
1:U:49:LEU:HD11	1:U:80:MET:HB3	1.97	0.46
1:U:150:PHE:C	1:U:152:LEU:N	2.74	0.46
1:U:161:THR:O	1:U:163:GLN:N	2.49	0.46
1:U:267:SER:HA	1:U:270:ARG:HH11	1.80	0.46
1:W:44:THR:CG2	1:W:46:HIS:H	2.28	0.46
1:W:85:LEU:HD22	1:W:146:TYR:CD1	2.51	0.46
1:C:238:GLU:H	1:C:238:GLU:CD	2.24	0.46
1:E:92:LEU:HD22	1:E:290:TRP:CD2	2.51	0.46
1:G:84:LEU:HG	1:G:138:LEU:CD1	2.45	0.46
1:G:123:ASN:O	1:G:155:LYS:HA	2.15	0.46
1:K:8:LYS:NZ	1:K:28:ASN:HD21	2.13	0.46
1:M:70:TRP:CZ3	1:M:72:GLY:N	2.83	0.46
1:O:59:MET:O	1:O:60:GLN:C	2.59	0.46
1:S:57:LYS:HD3	1:S:57:LYS:HA	1.79	0.46
1:S:117:GLU:O	1:S:120:HIS:N	2.46	0.46
1:U:185:HIS:NE2	1:U:232:LYS:CE	2.78	0.46
1:W:57:LYS:HA	1:W:57:LYS:HD2	1.66	0.46
1:W:93:PHE:CE1	1:W:206:PHE:HD1	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:124:PHE:CE2	1:W:155:LYS:HG3	2.50	0.46
1:A:1:MET:O	1:A:2:GLU:OE1	2.34	0.46
1:E:241:CYS:HB2	1:O:1:MET:HE2	1.98	0.46
1:I:6:GLY:C	1:I:8:LYS:N	2.72	0.46
1:K:118:TYR:CZ	1:K:122:LYS:HE3	2.51	0.46
1:O:56:TYR:HE1	1:O:66:PRO:CG	2.29	0.46
1:O:169:GLU:O	1:O:170:ASN:CB	2.62	0.46
1:O:238:GLU:H	1:O:238:GLU:HG2	1.29	0.46
1:S:51:ILE:O	1:S:54:LYS:HB2	2.15	0.46
1:S:237:ILE:HD13	1:S:252:LEU:HB3	1.97	0.46
1:S:277:PHE:CE2	1:S:282:PHE:HB2	2.51	0.46
1:U:120:HIS:C	1:U:122:LYS:H	2.22	0.46
1:U:120:HIS:HB3	1:U:192:ARG:HD3	1.98	0.46
1:U:173:LEU:CD1	1:U:174:THR:N	2.79	0.46
1:U:222:ARG:O	1:U:225:TYR:HB2	2.15	0.46
1:W:112:MET:O	1:W:113:ILE:C	2.55	0.46
1:A:216:LEU:HD12	1:A:216:LEU:HA	1.77	0.46
1:I:126:HIS:CD2	1:I:147:ILE:HD11	2.51	0.46
1:K:182:ILE:CD1	1:K:233:MET:HG3	2.46	0.46
1:O:22:ASP:N	3:O:405:HOH:O	2.48	0.46
1:O:209:GLY:O	1:O:210:SER:HB3	2.16	0.46
1:O:224:LYS:O	1:O:228:ILE:HG13	2.16	0.46
1:O:225:TYR:N	1:O:225:TYR:HD1	2.12	0.46
1:O:271:GLN:O	1:O:272:LEU:C	2.58	0.46
1:Q:107:LEU:HD22	1:Q:286:TYR:CE1	2.50	0.46
1:S:250:THR:HG22	1:S:272:LEU:HD21	1.98	0.46
1:U:89:LEU:HD13	1:U:206:PHE:CZ	2.51	0.46
1:W:88:SER:HA	1:W:135:LEU:HA	1.98	0.46
1:W:211:LEU:HD13	1:W:213:TRP:CZ2	2.51	0.46
1:C:75:GLY:C	1:C:77:TYR:H	2.24	0.45
1:K:156:TYR:C	1:K:165:ILE:HG23	2.41	0.45
1:O:22:ASP:CA	3:O:405:HOH:O	2.61	0.45
1:O:43:LYS:HE3	1:O:43:LYS:HB2	1.58	0.45
1:O:58:MET:SD	1:O:124:PHE:HE1	2.39	0.45
1:Q:8:LYS:CB	1:Q:8:LYS:HZ3	2.27	0.45
1:U:181:SER:HB2	1:U:197:GLU:CD	2.41	0.45
1:C:56:TYR:HE1	1:C:150:PHE:HE1	1.64	0.45
1:E:186:LEU:HD23	1:E:186:LEU:HA	1.72	0.45
1:I:17:SER:CB	3:I:409:HOH:O	2.63	0.45
1:K:3:LEU:HD22	1:K:11:LEU:C	2.42	0.45
1:K:88:SER:HA	1:K:135:LEU:HD12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:62:GLY:HA3	1:M:118:TYR:CZ	2.50	0.45
1:M:156:TYR:CA	1:M:165:ILE:HG23	2.47	0.45
1:M:171:LYS:HD2	1:M:189:GLU:OE1	2.16	0.45
1:O:50:HIS:C	1:O:52:GLU:H	2.25	0.45
1:O:261:ASP:C	1:O:261:ASP:OD1	2.58	0.45
1:Q:56:TYR:CE2	1:Q:82:MET:CE	2.99	0.45
1:Q:74:GLU:O	1:Q:75:GLY:C	2.58	0.45
1:Q:176:THR:O	1:Q:177:ALA:C	2.59	0.45
1:S:50:HIS:HA	1:S:53:SER:OG	2.16	0.45
1:S:260:PHE:HD1	1:S:260:PHE:O	1.99	0.45
1:U:116:ILE:HG22	1:U:120:HIS:NE2	2.27	0.45
1:A:220:THR:CG2	1:A:222:ARG:HB3	2.46	0.45
1:C:259:ARG:O	1:C:260:PHE:C	2.58	0.45
1:E:173:LEU:HD23	1:E:225:TYR:CE2	2.51	0.45
1:K:3:LEU:HD23	1:K:11:LEU:CB	2.43	0.45
1:O:60:GLN:HG3	1:O:61:GLY:H	1.81	0.45
1:S:150:PHE:HD1	1:S:150:PHE:H	1.65	0.45
1:U:70:TRP:CH2	1:U:72:GLY:HA3	2.51	0.45
1:W:116:ILE:HG22	1:W:117:GLU:N	2.31	0.45
1:W:164:HIS:O	1:W:165:ILE:O	2.35	0.45
1:W:219:ALA:O	1:W:220:THR:CB	2.65	0.45
1:A:134:PHE:O	1:A:135:LEU:HD23	2.16	0.45
1:E:192:ARG:CZ	1:E:263:LYS:HA	2.47	0.45
1:G:167:TYR:CD1	1:G:168:ARG:N	2.84	0.45
1:M:26:GLY:HA3	1:M:37:ILE:HD11	1.98	0.45
1:M:223:GLN:O	1:M:227:ARG:HG3	2.16	0.45
1:O:269:LEU:O	1:O:270:ARG:C	2.59	0.45
1:Q:174:THR:O	1:Q:174:THR:CG2	2.63	0.45
1:U:94:ASN:O	1:U:97:SER:N	2.49	0.45
1:K:43:LYS:C	1:O:233:MET:HE1	2.41	0.45
1:M:58:MET:C	1:M:60:GLN:H	2.25	0.45
1:S:158:ASP:O	1:S:162:HIS:HA	2.17	0.45
1:U:85:LEU:HB2	1:U:135:LEU:HD23	1.97	0.45
1:U:220:THR:O	1:U:221:LYS:C	2.58	0.45
1:W:259:ARG:N	1:W:262:ASP:OD2	2.43	0.45
1:C:76:ASP:OD1	1:C:76:ASP:N	2.49	0.45
1:C:182:ILE:HD12	1:C:256:ARG:CZ	2.46	0.45
1:E:43:LYS:C	1:E:44:THR:O	2.60	0.45
1:E:292:MET:HA	1:G:86:GLY:HA2	1.97	0.45
1:I:62:GLY:HA3	1:I:118:TYR:CZ	2.52	0.45
1:I:164:HIS:CD2	1:I:261:ASP:HB2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:173:LEU:HD12	1:M:173:LEU:HA	1.69	0.45
1:O:45:LYS:C	1:O:46:HIS:CD2	2.95	0.45
1:Q:15:ILE:HD13	1:Q:25:LEU:CB	2.34	0.45
1:Q:115:ARG:HA	1:Q:115:ARG:HD3	1.76	0.45
1:U:161:THR:O	1:U:162:HIS:C	2.60	0.45
1:W:56:TYR:OH	1:W:148:ILE:HB	2.16	0.45
1:G:88:SER:HB2	1:G:135:LEU:CD1	2.46	0.45
1:K:158:ASP:OD1	1:K:161:THR:OG1	2.28	0.45
1:S:116:ILE:HG21	1:S:196:LEU:CD2	2.47	0.45
1:S:220:THR:CG2	1:S:223:GLN:NE2	2.75	0.45
1:S:237:ILE:HD13	1:S:252:LEU:CB	2.47	0.45
1:U:182:ILE:HD11	1:U:256:ARG:NH2	2.30	0.45
1:W:156:TYR:C	1:W:165:ILE:HG23	2.42	0.45
1:W:236:PRO:HG2	1:W:239:VAL:HB	1.98	0.45
1:A:39:LEU:HD22	1:A:79:VAL:HG22	1.98	0.45
1:C:217:LYS:HE2	1:C:217:LYS:HB3	1.51	0.45
1:E:18:GLY:O	3:E:448:HOH:O	2.21	0.45
1:I:56:TYR:HB3	1:I:68:ILE:HG12	1.99	0.45
1:I:74:GLU:O	1:I:75:GLY:C	2.59	0.45
1:M:213:TRP:CE2	1:M:232:LYS:HE2	2.52	0.45
1:O:60:GLN:HG3	1:O:61:GLY:N	2.30	0.45
1:O:259:ARG:NH1	3:O:408:HOH:O	2.27	0.45
1:U:5:VAL:HG11	1:U:79:VAL:HG11	1.99	0.45
1:W:59:MET:HE3	1:W:119:ILE:HG23	1.98	0.45
1:G:220:THR:O	1:G:221:LYS:C	2.60	0.45
1:O:10:ARG:CZ	1:O:29:ILE:CD1	2.95	0.45
1:W:69:LYS:N	1:W:81:VAL:O	2.50	0.45
1:W:123:ASN:O	1:W:156:TYR:CD2	2.70	0.45
1:E:120:HIS:ND1	1:E:266:TYR:OH	2.36	0.45
1:G:218:ALA:C	1:G:220:THR:H	2.25	0.45
1:M:139:GLY:C	1:M:141:LYS:H	2.25	0.45
1:Q:6:GLY:O	1:Q:7:ASN:HB2	2.17	0.45
1:S:267:SER:O	1:S:271:GLN:HB2	2.17	0.45
1:U:120:HIS:CD2	1:U:192:ARG:HG2	2.51	0.45
1:W:167:TYR:C	1:W:167:TYR:CD1	2.95	0.45
1:A:41:CYS:C	1:A:43:LYS:H	2.25	0.44
1:E:38:LYS:HE3	3:E:457:HOH:O	2.17	0.44
1:I:223:GLN:O	1:I:227:ARG:HG3	2.17	0.44
1:K:178:ARG:HD2	1:K:179:TYR:CZ	2.51	0.44
1:K:269:LEU:HD23	1:K:269:LEU:HA	1.69	0.44
1:M:122:LYS:O	1:M:123:ASN:CB	2.64	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:181:SER:HB2	1:M:197:GLU:CD	2.41	0.44
1:Q:181:SER:HB2	1:Q:197:GLU:OE2	2.17	0.44
1:S:80:MET:HE3	1:S:82:MET:CG	2.47	0.44
1:U:6:GLY:O	1:U:8:LYS:N	2.50	0.44
1:U:23:ILE:HD13	1:U:23:ILE:H	1.82	0.44
1:U:252:LEU:O	1:U:256:ARG:HG3	2.17	0.44
1:W:112:MET:HB3	1:W:199:LEU:HD11	1.99	0.44
1:I:277:PHE:CZ	1:I:282:PHE:HB2	2.52	0.44
1:M:92:LEU:O	1:M:95:PHE:HB3	2.18	0.44
1:O:47:PRO:C	1:O:48:GLN:CG	2.90	0.44
1:Q:86:GLY:C	1:S:293:LEU:HA	2.42	0.44
1:Q:109:ALA:O	1:Q:113:ILE:HG13	2.17	0.44
1:Q:236:PRO:HG2	1:Q:239:VAL:CB	2.39	0.44
1:S:161:THR:O	1:S:162:HIS:CB	2.57	0.44
1:U:161:THR:C	1:U:163:GLN:N	2.75	0.44
1:C:220:THR:HG21	1:C:223:GLN:NE2	2.32	0.44
1:G:220:THR:OG1	1:G:221:LYS:NZ	2.48	0.44
1:I:271:GLN:HE22	1:I:274:ARG:HD2	1.81	0.44
1:I:293:LEU:HD21	1:K:15:ILE:CG1	2.36	0.44
1:K:222:ARG:HG3	1:K:223:GLN:N	2.32	0.44
1:O:56:TYR:HB3	1:O:68:ILE:CD1	2.48	0.44
1:Q:28:ASN:OD1	1:Q:29:ILE:N	2.49	0.44
1:Q:122:LYS:O	1:Q:123:ASN:CB	2.64	0.44
1:U:56:TYR:HB3	1:U:68:ILE:CG1	2.47	0.44
1:U:223:GLN:O	1:U:227:ARG:HG3	2.17	0.44
1:W:9:TYR:CE2	1:W:81:VAL:HG21	2.52	0.44
1:W:87:PRO:HB2	1:W:92:LEU:HD21	1.99	0.44
1:W:133:ASN:C	1:W:134:PHE:CD2	2.95	0.44
1:W:216:LEU:HD12	1:W:216:LEU:HA	1.75	0.44
1:C:84:LEU:HD12	1:C:84:LEU:HA	1.79	0.44
1:M:127:ARG:HG2	1:M:190:GLN:NE2	2.32	0.44
1:M:266:TYR:O	1:M:270:ARG:HB2	2.18	0.44
1:U:273:PHE:O	1:U:276:LEU:N	2.51	0.44
1:W:186:LEU:HA	1:W:186:LEU:HD23	1.63	0.44
1:A:120:HIS:CD2	1:A:192:ARG:HG2	2.52	0.44
1:E:56:TYR:C	1:E:68:ILE:HD11	2.42	0.44
1:E:130:LYS:HB2	1:E:131:PRO:HD2	2.00	0.44
1:G:154:LYS:NZ	1:G:189:GLU:OE2	2.42	0.44
1:I:236:PRO:HB3	1:M:77:TYR:CE2	2.53	0.44
1:M:93:PHE:CD1	1:M:98:ARG:HA	2.52	0.44
1:Q:171:LYS:HE2	3:Q:405:HOH:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:182:ILE:HD11	1:S:256:ARG:HH21	1.76	0.44
1:U:92:LEU:HA	1:U:92:LEU:HD23	1.79	0.44
1:W:56:TYR:CB	1:W:68:ILE:CG1	2.79	0.44
1:W:129:VAL:HG11	1:W:198:SER:HB2	2.00	0.44
1:W:278:HIS:O	1:W:279:ARG:C	2.60	0.44
1:E:59:MET:HB2	1:E:65:ILE:HG21	1.99	0.44
1:E:125:ILE:O	1:E:153:ALA:HA	2.18	0.44
1:E:140:LYS:HG2	1:E:141:LYS:HG2	1.97	0.44
1:E:144:LEU:HD23	1:E:146:TYR:CE1	2.53	0.44
1:G:58:MET:SD	1:G:59:MET:HE2	2.58	0.44
1:G:59:MET:O	1:G:60:GLN:C	2.60	0.44
1:S:134:PHE:HA	1:S:146:TYR:O	2.18	0.44
1:S:280:GLN:CA	1:S:280:GLN:NE2	2.49	0.44
1:U:204:MET:CE	1:U:207:ASN:HB2	2.48	0.44
1:U:276:LEU:HD13	1:U:276:LEU:O	2.17	0.44
1:W:117:GLU:OE1	1:W:266:TYR:CG	2.71	0.44
1:W:129:VAL:O	1:W:130:LYS:HB3	2.17	0.44
1:W:211:LEU:HD13	1:W:213:TRP:CE2	2.53	0.44
1:W:278:HIS:C	1:W:280:GLN:N	2.74	0.44
1:E:45:LYS:HB3	1:E:45:LYS:HE2	1.62	0.44
1:G:60:GLN:HG2	1:G:61:GLY:N	2.31	0.44
1:I:172:ASN:O	1:I:173:LEU:C	2.60	0.44
1:K:236:PRO:HD2	1:K:239:VAL:HB	2.00	0.44
1:O:58:MET:SD	1:O:124:PHE:CE1	3.10	0.44
1:Q:4:ARG:CZ	1:Q:7:ASN:O	2.66	0.44
1:S:14:LYS:CE	1:S:22:ASP:OD2	2.66	0.44
1:U:150:PHE:C	1:U:152:LEU:H	2.25	0.44
1:C:49:LEU:HD12	1:C:49:LEU:HA	1.76	0.44
1:I:66:PRO:HA	1:I:83:GLU:OE2	2.18	0.44
1:M:136:MET:SD	1:M:145:VAL:HG22	2.58	0.44
1:O:263:LYS:HD2	3:O:416:HOH:O	2.17	0.44
1:Q:52:GLU:OE1	1:Q:56:TYR:CZ	2.70	0.44
1:Q:103:LYS:NZ	1:Q:285:ASP:OD1	2.51	0.44
1:Q:221:LYS:O	1:Q:224:LYS:N	2.51	0.44
1:Q:259:ARG:HA	1:Q:259:ARG:HD3	1.35	0.44
1:U:14:LYS:C	1:U:15:ILE:HG12	2.43	0.44
1:U:291:ASN:O	1:W:87:PRO:HD3	2.18	0.44
1:W:86:GLY:O	1:W:87:PRO:O	2.34	0.44
1:W:125:ILE:HD13	1:W:190:GLN:O	2.17	0.44
1:A:49:LEU:HA	1:A:49:LEU:HD12	1.53	0.44
1:A:188:ILE:O	1:A:189:GLU:C	2.61	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:178:ARG:HD2	1:C:179:TYR:CZ	2.53	0.44
1:E:253:ASN:O	1:E:254:PHE:C	2.60	0.44
1:G:88:SER:CB	1:G:135:LEU:CD1	2.96	0.44
1:I:207:ASN:HB3	1:I:244:TYR:CE1	2.53	0.44
1:I:250:THR:O	1:I:251:TYR:C	2.59	0.44
1:M:128:ASP:O	1:M:133:ASN:ND2	2.45	0.44
1:M:188:ILE:HG22	1:M:189:GLU:N	2.32	0.44
1:M:220:THR:CG2	1:M:223:GLN:NE2	2.81	0.44
1:O:275:ASN:O	1:O:276:LEU:C	2.60	0.44
1:O:277:PHE:CE1	1:O:282:PHE:CB	3.00	0.44
1:U:4:ARG:HH21	1:U:7:ASN:CB	2.31	0.44
1:U:82:MET:HG3	1:U:83:GLU:O	2.18	0.44
1:W:78:ASN:O	1:W:79:VAL:HG23	2.18	0.44
1:W:86:GLY:CA	1:W:136:MET:O	2.65	0.44
1:W:90:GLU:HB2	1:W:131:PRO:CB	2.48	0.44
1:C:156:TYR:CZ	1:C:192:ARG:HD3	2.52	0.43
1:G:82:MET:HB2	1:G:82:MET:HE2	1.42	0.43
1:M:220:THR:HG23	1:M:223:GLN:CG	2.47	0.43
1:O:211:LEU:O	1:O:212:PRO:C	2.59	0.43
1:S:14:LYS:NZ	1:S:22:ASP:OD2	2.47	0.43
1:S:56:TYR:CE1	1:S:66:PRO:HG3	2.53	0.43
1:S:120:HIS:ND1	1:S:266:TYR:OH	2.43	0.43
1:U:199:LEU:HD12	1:U:199:LEU:O	2.17	0.43
1:U:279:ARG:HG2	1:U:280:GLN:HG2	1.99	0.43
1:W:4:ARG:HD3	1:W:29:ILE:CD1	2.33	0.43
1:W:56:TYR:HB3	1:W:68:ILE:HG12	1.94	0.43
1:W:167:TYR:C	1:W:167:TYR:HD1	2.26	0.43
1:A:173:LEU:HD23	1:A:225:TYR:CE2	2.53	0.43
1:E:29:ILE:HD13	1:E:29:ILE:HA	1.78	0.43
1:G:149:ASP:OD1	1:G:149:ASP:C	2.60	0.43
1:G:252:LEU:HA	1:G:252:LEU:HD23	1.84	0.43
1:I:49:LEU:HA	1:I:49:LEU:HD12	1.79	0.43
1:I:191:SER:HB3	1:I:260:PHE:CE1	2.54	0.43
1:I:213:TRP:HB2	1:I:228:ILE:HG23	2.00	0.43
1:M:40:GLU:OE1	1:M:49:LEU:CB	2.66	0.43
1:M:48:GLN:O	1:M:50:HIS:N	2.51	0.43
1:U:58:MET:O	1:U:60:GLN:N	2.51	0.43
1:U:107:LEU:HD21	1:U:277:PHE:CE1	2.53	0.43
1:U:176:THR:HG22	1:U:178:ARG:H	1.83	0.43
1:U:226:GLU:OE1	1:U:226:GLU:N	2.51	0.43
1:U:252:LEU:O	1:U:253:ASN:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:27:ALA:HB2	3:W:418:HOH:O	2.18	0.43
1:W:83:GLU:O	1:W:83:GLU:CG	2.66	0.43
1:C:43:LYS:HB2	1:K:233:MET:CE	2.44	0.43
1:E:150:PHE:N	1:E:150:PHE:CD1	2.86	0.43
1:E:236:PRO:HG2	1:E:239:VAL:HG23	2.00	0.43
1:E:257:SER:O	1:E:258:LEU:C	2.60	0.43
1:G:102:LEU:O	1:G:106:LEU:HG	2.18	0.43
1:K:134:PHE:O	1:K:135:LEU:HD12	2.18	0.43
1:M:41:CYS:HA	1:M:77:TYR:CD1	2.53	0.43
1:M:74:GLU:OE1	1:M:74:GLU:HA	2.18	0.43
1:S:223:GLN:O	1:S:226:GLU:N	2.52	0.43
1:U:9:TYR:HD2	1:U:81:VAL:HG21	1.83	0.43
1:U:191:SER:O	1:U:192:ARG:C	2.61	0.43
1:U:242:LYS:C	1:U:244:TYR:H	2.25	0.43
1:W:57:LYS:HE3	1:W:68:ILE:CG2	2.47	0.43
1:W:207:ASN:HB3	1:W:244:TYR:CE1	2.53	0.43
1:W:238:GLU:CD	1:W:238:GLU:N	2.76	0.43
1:C:131:PRO:HG3	1:C:202:VAL:HG13	2.01	0.43
1:E:241:CYS:HB2	1:O:1:MET:CE	2.49	0.43
1:O:251:TYR:HD2	1:O:273:PHE:CE2	2.36	0.43
1:Q:202:VAL:O	1:Q:205:TYR:HB3	2.18	0.43
1:Q:234:SER:O	1:Q:236:PRO:HD3	2.18	0.43
1:S:88:SER:HA	1:S:135:LEU:HD12	1.99	0.43
1:S:259:ARG:O	1:S:262:ASP:HB2	2.19	0.43
1:U:46:HIS:N	1:U:47:PRO:HD3	2.28	0.43
1:U:263:LYS:HA	1:U:264:PRO:HD2	1.86	0.43
1:W:22:ASP:CA	3:W:413:HOH:O	2.66	0.43
1:A:44:THR:OG1	1:G:230:GLU:OE2	2.16	0.43
1:A:56:TYR:HE1	1:A:150:PHE:CE1	2.36	0.43
1:C:167:TYR:CD1	1:C:167:TYR:C	2.96	0.43
1:G:259:ARG:HB2	1:G:262:ASP:CG	2.43	0.43
1:I:5:VAL:C	1:I:7:ASN:H	2.24	0.43
1:I:239:VAL:O	1:I:242:LYS:N	2.45	0.43
1:K:46:HIS:N	1:K:47:PRO:CD	2.62	0.43
1:M:93:PHE:CE1	1:M:98:ARG:HA	2.53	0.43
1:M:112:MET:HE2	1:M:199:LEU:CD1	2.49	0.43
1:O:54:LYS:CG	1:O:55:PHE:N	2.79	0.43
1:O:127:ARG:NH1	3:O:419:HOH:O	2.48	0.43
1:O:136:MET:SD	1:O:145:VAL:HG22	2.57	0.43
1:S:69:LYS:HZ2	1:S:69:LYS:HG2	1.48	0.43
1:U:126:HIS:ND1	1:U:126:HIS:O	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:173:LEU:HD13	1:U:174:THR:H	1.84	0.43
1:W:57:LYS:O	1:W:60:GLN:HB3	2.19	0.43
1:C:236:PRO:HG2	1:C:239:VAL:CG2	2.48	0.43
1:E:5:VAL:O	1:E:6:GLY:C	2.60	0.43
1:M:268:TYR:CE1	1:M:272:LEU:HD13	2.53	0.43
1:O:150:PHE:C	1:O:152:LEU:N	2.76	0.43
1:Q:221:LYS:O	1:Q:222:ARG:C	2.61	0.43
1:S:237:ILE:HD11	1:S:256:ARG:CD	2.48	0.43
1:U:102:LEU:HD12	1:U:102:LEU:HA	1.73	0.43
1:W:128:ASP:HB2	1:W:152:LEU:HD12	1.99	0.43
1:W:251:TYR:CD1	1:W:252:LEU:N	2.87	0.43
1:C:89:LEU:O	1:C:93:PHE:HB2	2.19	0.43
1:C:220:THR:CG2	1:C:223:GLN:NE2	2.82	0.43
1:C:267:SER:O	1:C:268:TYR:C	2.62	0.43
1:G:134:PHE:C	1:G:135:LEU:HD12	2.43	0.43
1:I:119:ILE:CD1	1:I:147:ILE:HD13	2.49	0.43
1:K:5:VAL:CG1	1:K:74:GLU:HG2	2.45	0.43
1:M:224:LYS:O	1:M:226:GLU:N	2.52	0.43
1:O:233:MET:HE2	1:O:233:MET:HB3	1.70	0.43
1:O:251:TYR:CE1	1:O:255:CYS:SG	3.06	0.43
1:Q:15:ILE:O	1:S:294:LYS:HB3	2.18	0.43
1:Q:49:LEU:HD12	1:Q:49:LEU:HA	1.85	0.43
1:S:257:SER:O	1:S:258:LEU:C	2.60	0.43
1:U:117:GLU:CG	1:U:266:TYR:CG	2.93	0.43
1:W:280:GLN:HB2	1:W:282:PHE:CD2	2.54	0.43
1:A:62:GLY:HA3	1:A:118:TYR:CZ	2.54	0.43
1:G:277:PHE:CE2	1:G:282:PHE:HB2	2.54	0.43
1:K:23:ILE:HD13	1:K:38:LYS:HG3	2.00	0.43
1:K:70:TRP:CZ3	1:K:72:GLY:CA	3.01	0.43
1:K:105:VAL:HG21	1:K:207:ASN:OD1	2.19	0.43
1:M:119:ILE:CD1	1:M:147:ILE:HD13	2.49	0.43
1:M:137:GLY:HA3	1:M:141:LYS:HB2	2.01	0.43
1:O:292:MET:HB2	1:O:292:MET:HE3	1.71	0.43
1:S:121:SER:C	1:S:123:ASN:N	2.77	0.43
1:S:143:ASN:C	1:S:143:ASN:ND2	2.66	0.43
1:U:124:PHE:CA	1:U:154:LYS:O	2.60	0.43
1:U:183:ASN:O	1:U:186:LEU:HB2	2.18	0.43
1:W:56:TYR:HE2	1:W:82:MET:HE1	1.75	0.43
1:K:9:TYR:HE1	1:K:28:ASN:HD22	1.66	0.43
1:M:126:HIS:CD2	1:M:147:ILE:HD11	2.53	0.43
1:O:259:ARG:CB	1:O:262:ASP:HB2	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:32:GLY:O	1:S:283:SER:CB	2.67	0.43
1:S:244:TYR:O	1:S:245:PRO:C	2.60	0.43
1:U:128:ASP:OD1	1:U:176:THR:N	2.42	0.43
1:U:152:LEU:HD13	1:U:174:THR:CG2	2.49	0.43
1:U:223:GLN:C	1:U:225:TYR:N	2.76	0.43
1:M:53:SER:O	1:M:57:LYS:HB2	2.19	0.43
1:M:267:SER:HA	1:M:270:ARG:HH12	1.84	0.43
1:O:244:TYR:O	1:O:245:PRO:C	2.62	0.43
1:Q:3:LEU:HD23	1:Q:4:ARG:H	1.84	0.43
1:Q:16:GLY:HA2	1:S:294:LYS:CG	2.49	0.43
1:Q:103:LYS:HG3	1:Q:277:PHE:HE1	1.84	0.43
1:S:285:ASP:CG	1:S:287:VAL:HG23	2.44	0.43
1:U:49:LEU:HD12	1:U:80:MET:CE	2.49	0.43
1:U:49:LEU:HD12	1:U:80:MET:HE3	1.99	0.43
1:U:101:SER:O	1:U:105:VAL:HG23	2.19	0.43
1:U:124:PHE:CD1	1:U:154:LYS:C	2.95	0.43
1:U:210:SER:OG	1:U:211:LEU:N	2.51	0.43
1:W:22:ASP:O	1:W:23:ILE:HD13	2.19	0.43
1:W:185:HIS:ND1	1:W:229:SER:HB2	2.34	0.43
1:W:264:PRO:HG2	1:W:266:TYR:CZ	2.53	0.43
1:C:182:ILE:CD1	1:C:256:ARG:CZ	2.97	0.42
1:I:101:SER:OG	1:I:289:ASP:OD1	2.36	0.42
1:M:224:LYS:C	1:M:226:GLU:N	2.75	0.42
1:M:278:HIS:C	1:M:280:GLN:N	2.76	0.42
1:O:140:LYS:HG2	1:O:141:LYS:H	1.75	0.42
1:O:152:LEU:HD22	1:O:174:THR:HG23	2.01	0.42
1:O:228:ILE:O	1:O:229:SER:C	2.61	0.42
1:Q:180:ALA:O	1:Q:232:LYS:NZ	2.49	0.42
1:W:251:TYR:HD1	1:W:252:LEU:N	2.16	0.42
1:W:288:PHE:O	1:W:291:ASN:HB2	2.19	0.42
1:I:193:ARG:HG3	1:I:194:ASP:N	2.34	0.42
1:I:276:LEU:HD12	1:I:276:LEU:O	2.19	0.42
1:K:112:MET:HE2	1:K:134:PHE:CE2	2.54	0.42
1:O:42:VAL:HG22	1:O:78:ASN:ND2	2.33	0.42
1:O:93:PHE:CZ	1:O:206:PHE:HA	2.53	0.42
1:O:204:MET:SD	1:O:241:CYS:SG	3.11	0.42
1:Q:28:ASN:OD1	1:Q:28:ASN:C	2.62	0.42
1:U:35:VAL:HG21	1:U:81:VAL:HG13	2.01	0.42
1:W:43:LYS:C	1:W:44:THR:O	2.58	0.42
1:A:15:ILE:HG21	1:A:15:ILE:HD13	1.73	0.42
1:A:98:ARG:NH1	3:A:435:HOH:O	2.46	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:254:PHE:CD2	1:C:254:PHE:C	2.97	0.42
1:E:49:LEU:HD12	1:E:49:LEU:HA	1.83	0.42
1:I:277:PHE:CE2	1:I:282:PHE:HB2	2.54	0.42
1:M:39:LEU:HD22	1:M:79:VAL:HG22	2.01	0.42
1:M:41:CYS:HB2	1:M:77:TYR:HE1	1.84	0.42
1:O:223:GLN:O	1:O:224:LYS:C	2.61	0.42
1:Q:229:SER:O	1:Q:230:GLU:C	2.62	0.42
1:S:173:LEU:HD13	1:S:184:THR:HG22	2.01	0.42
1:W:111:GLN:CB	1:W:145:VAL:HG23	2.49	0.42
1:C:41:CYS:O	1:C:44:THR:HG22	2.19	0.42
1:E:154:LYS:HE2	1:E:189:GLU:OE2	2.19	0.42
1:E:247:GLU:OE1	1:E:247:GLU:N	2.42	0.42
1:G:59:MET:HB2	1:G:65:ILE:HG21	2.00	0.42
1:K:54:LYS:HD3	1:K:54:LYS:HA	1.74	0.42
1:Q:55:PHE:O	1:Q:56:TYR:C	2.61	0.42
1:Q:237:ILE:C	1:Q:239:VAL:N	2.76	0.42
1:Q:293:LEU:C	1:Q:293:LEU:CD1	2.83	0.42
1:U:112:MET:HE2	1:U:199:LEU:HD13	1.94	0.42
1:U:196:LEU:O	1:U:199:LEU:HB3	2.19	0.42
1:U:207:ASN:C	1:U:209:GLY:N	2.78	0.42
1:U:261:ASP:OD1	1:U:261:ASP:N	2.36	0.42
1:U:288:PHE:O	1:U:289:ASP:C	2.62	0.42
1:W:70:TRP:HB3	1:W:81:VAL:CG2	2.49	0.42
1:W:192:ARG:NH1	1:W:263:LYS:CA	2.53	0.42
1:A:220:THR:CG2	1:A:222:ARG:H	2.32	0.42
1:I:15:ILE:HD11	1:K:292:MET:SD	2.58	0.42
1:M:5:VAL:C	1:M:7:ASN:H	2.25	0.42
1:O:118:TYR:OH	1:O:122:LYS:HE3	2.18	0.42
1:O:217:LYS:HA	1:O:217:LYS:HD3	1.48	0.42
1:Q:41:CYS:C	1:Q:43:LYS:N	2.75	0.42
1:Q:164:HIS:ND1	1:Q:165:ILE:N	2.67	0.42
1:Q:244:TYR:O	1:Q:245:PRO:C	2.62	0.42
1:S:192:ARG:O	1:S:193:ARG:C	2.61	0.42
1:U:62:GLY:O	1:U:63:VAL:C	2.61	0.42
1:U:202:VAL:HG12	1:U:206:PHE:CE2	2.55	0.42
1:U:276:LEU:HD22	1:U:276:LEU:HA	1.85	0.42
1:W:149:ASP:C	1:W:149:ASP:OD1	2.62	0.42
1:C:138:LEU:O	1:C:139:GLY:C	2.63	0.42
1:E:221:LYS:H	1:E:221:LYS:HG3	1.63	0.42
1:E:274:ARG:NH1	1:Q:274:ARG:CZ	2.81	0.42
1:E:274:ARG:NH1	1:Q:274:ARG:HH12	2.16	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:56:TYR:HE2	1:I:82:MET:HE1	1.82	0.42
1:M:205:TYR:HB2	1:M:211:LEU:HD11	2.01	0.42
1:O:182:ILE:HG22	1:O:183:ASN:N	2.35	0.42
1:U:117:GLU:HG3	1:U:266:TYR:CD2	2.52	0.42
1:U:118:TYR:O	1:U:122:LYS:HD2	2.19	0.42
1:U:178:ARG:HG2	1:U:179:TYR:CD2	2.54	0.42
1:U:203:LEU:HD23	1:U:203:LEU:HA	1.70	0.42
1:U:264:PRO:CG	1:U:266:TYR:CE1	3.02	0.42
1:W:115:ARG:O	1:W:116:ILE:C	2.62	0.42
1:W:293:LEU:H	1:W:293:LEU:HD23	1.85	0.42
1:C:8:LYS:O	1:C:29:ILE:HG12	2.19	0.42
1:C:234:SER:O	1:C:236:PRO:HD3	2.20	0.42
1:C:245:PRO:HG2	1:C:276:LEU:HD21	2.01	0.42
1:I:94:ASN:C	1:I:96:CYS:N	2.77	0.42
1:I:239:VAL:O	1:I:242:LYS:HB2	2.19	0.42
1:K:119:ILE:HG22	1:K:124:PHE:O	2.19	0.42
1:O:265:ASP:OD1	1:O:268:TYR:CB	2.68	0.42
1:O:268:TYR:CZ	1:O:272:LEU:HD21	2.55	0.42
1:S:65:ILE:CG2	1:S:66:PRO:HD2	2.50	0.42
1:U:9:TYR:CD2	1:U:81:VAL:HG21	2.54	0.42
1:G:29:ILE:O	1:G:30:ALA:C	2.63	0.42
1:K:199:LEU:O	1:K:200:GLY:C	2.60	0.42
1:M:125:ILE:HG23	1:M:156:TYR:CD2	2.55	0.42
1:M:220:THR:HG22	1:M:223:GLN:NE2	2.34	0.42
1:W:57:LYS:CE	1:W:68:ILE:HG21	2.50	0.42
1:A:115:ARG:CD	3:A:419:HOH:O	2.65	0.42
1:C:125:ILE:HG23	1:C:156:TYR:CD2	2.55	0.42
1:E:100:PHE:HA	1:E:289:ASP:OD2	2.20	0.42
1:E:278:HIS:HB3	1:Q:284:TYR:CG	2.55	0.42
1:G:46:HIS:N	1:G:47:PRO:CD	2.82	0.42
1:G:134:PHE:C	1:G:135:LEU:CD1	2.92	0.42
1:K:28:ASN:O	1:K:29:ILE:C	2.63	0.42
1:O:13:ARG:NH1	3:O:407:HOH:O	2.53	0.42
1:O:130:LYS:HB2	1:O:131:PRO:HD2	2.01	0.42
1:O:220:THR:H	1:O:223:GLN:HG3	1.85	0.42
1:Q:57:LYS:HD3	1:Q:68:ILE:HG12	2.00	0.42
1:S:125:ILE:O	1:S:125:ILE:HG13	2.19	0.42
1:S:289:ASP:O	1:S:292:MET:HB2	2.20	0.42
1:U:42:VAL:HB	1:U:76:ASP:OD1	2.20	0.42
1:U:54:LYS:O	1:U:57:LYS:HB2	2.20	0.42
1:U:178:ARG:HG2	1:U:179:TYR:CE2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:193:ARG:CB	1:W:258:LEU:HD12	2.49	0.42
1:A:39:LEU:HD23	1:A:79:VAL:HG22	2.01	0.42
1:A:42:VAL:O	1:A:42:VAL:CG1	2.68	0.42
1:A:171:LYS:HA	1:A:171:LYS:HD2	1.73	0.42
1:E:14:LYS:HD2	1:E:22:ASP:OD2	2.20	0.42
1:E:156:TYR:CZ	1:E:192:ARG:HD3	2.55	0.42
1:E:274:ARG:HH12	1:Q:274:ARG:HH12	1.68	0.42
1:I:237:ILE:HD11	1:I:256:ARG:CZ	2.50	0.42
1:I:288:PHE:CG	1:I:290:TRP:CZ2	3.08	0.42
1:M:48:GLN:O	1:M:49:LEU:C	2.62	0.42
1:Q:49:LEU:O	1:Q:50:HIS:C	2.63	0.42
1:S:23:ILE:HD13	1:S:23:ILE:N	2.35	0.42
1:S:167:TYR:CD1	1:S:167:TYR:C	2.97	0.42
1:S:182:ILE:CD1	1:S:256:ARG:CZ	2.98	0.42
1:S:189:GLU:HG3	1:S:260:PHE:HZ	1.85	0.42
1:S:193:ARG:NH1	1:S:260:PHE:N	2.67	0.42
1:U:100:PHE:CD2	1:U:206:PHE:CD1	3.08	0.42
1:W:53:SER:C	1:W:55:PHE:N	2.77	0.42
1:W:122:LYS:HA	1:W:122:LYS:HD2	1.80	0.42
1:C:195:ASP:O	1:C:198:SER:HB2	2.19	0.41
1:E:216:LEU:HD12	1:E:216:LEU:HA	1.81	0.41
1:I:220:THR:O	1:I:221:LYS:C	2.63	0.41
1:K:130:LYS:HB2	1:K:131:PRO:HD2	2.01	0.41
1:M:8:LYS:O	1:M:29:ILE:HG12	2.20	0.41
1:M:126:HIS:ND1	1:M:126:HIS:C	2.77	0.41
1:M:183:ASN:HB3	1:M:188:ILE:HB	2.02	0.41
1:M:245:PRO:C	1:M:247:GLU:N	2.77	0.41
1:M:254:PHE:CD2	1:M:269:LEU:HD11	2.55	0.41
1:W:6:GLY:CA	1:W:70:TRP:CH2	3.03	0.41
1:A:251:TYR:CD1	1:A:251:TYR:C	2.98	0.41
1:G:38:LYS:NZ	1:G:52:GLU:OE1	2.38	0.41
1:G:59:MET:CB	1:G:65:ILE:HG21	2.50	0.41
1:G:218:ALA:C	1:G:220:THR:N	2.78	0.41
1:I:25:LEU:HD12	1:K:292:MET:SD	2.59	0.41
1:I:203:LEU:HD23	1:I:203:LEU:HA	1.71	0.41
1:M:124:PHE:CZ	1:M:155:LYS:HG3	2.54	0.41
1:O:34:GLU:C	1:O:35:VAL:CG1	2.93	0.41
1:O:218:ALA:HB1	1:O:223:GLN:HB2	2.02	0.41
1:Q:188:ILE:HG22	1:Q:189:GLU:N	2.35	0.41
1:Q:220:THR:CG2	1:Q:223:GLN:HG3	2.50	0.41
1:S:80:MET:HE2	1:S:82:MET:SD	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:231:LYS:HA	1:S:234:SER:OG	2.21	0.41
1:U:89:LEU:HB2	1:U:131:PRO:O	2.20	0.41
1:U:221:LYS:H	1:U:221:LYS:HG3	1.46	0.41
1:W:121:SER:C	1:W:123:ASN:H	2.28	0.41
1:W:158:ASP:OD1	1:W:161:THR:N	2.54	0.41
1:W:271:GLN:NE2	1:W:274:ARG:HD2	2.35	0.41
1:A:220:THR:O	1:A:221:LYS:C	2.63	0.41
1:C:222:ARG:HH11	1:C:222:ARG:HG2	1.81	0.41
1:G:183:ASN:O	1:G:186:LEU:N	2.54	0.41
1:K:152:LEU:O	1:K:153:ALA:C	2.63	0.41
1:K:169:GLU:HB2	1:K:170:ASN:H	1.66	0.41
1:M:293:LEU:CD2	1:O:135:LEU:CD2	2.94	0.41
1:Q:52:GLU:OE2	1:Q:149:ASP:CA	2.67	0.41
1:Q:165:ILE:HB	1:Q:166:PRO:CD	2.50	0.41
1:Q:167:TYR:CD1	1:Q:167:TYR:C	2.98	0.41
1:S:178:ARG:NE	2:S:301:SO4:O2	2.44	0.41
1:U:55:PHE:O	1:U:56:TYR:C	2.63	0.41
1:U:58:MET:C	1:U:60:GLN:H	2.29	0.41
1:U:285:ASP:CG	1:U:287:VAL:HG23	2.45	0.41
1:W:4:ARG:HD2	1:W:29:ILE:HD12	1.98	0.41
1:C:211:LEU:O	1:C:214:GLN:HB2	2.20	0.41
1:C:271:GLN:NE2	1:C:274:ARG:HD2	2.35	0.41
1:E:38:LYS:C	1:E:39:LEU:HD23	2.45	0.41
1:E:233:MET:HE3	1:E:233:MET:HB2	1.70	0.41
1:G:194:ASP:O	1:G:195:ASP:C	2.63	0.41
1:I:15:ILE:CD1	1:K:292:MET:SD	3.09	0.41
1:I:49:LEU:O	1:I:50:HIS:C	2.62	0.41
1:M:101:SER:CB	1:O:13:ARG:NH2	2.83	0.41
1:M:219:ALA:O	1:M:220:THR:O	2.39	0.41
1:M:238:GLU:H	1:M:238:GLU:HG2	1.09	0.41
1:O:85:LEU:C	1:O:138:LEU:HD12	2.46	0.41
1:O:223:GLN:HA	1:O:226:GLU:OE1	2.20	0.41
1:Q:4:ARG:CZ	1:Q:7:ASN:HA	2.48	0.41
1:S:92:LEU:HD13	1:S:290:TRP:CE2	2.55	0.41
1:U:199:LEU:HD12	1:U:199:LEU:HA	1.73	0.41
1:U:242:LYS:O	1:U:244:TYR:CD2	2.73	0.41
1:U:285:ASP:OD1	1:U:286:TYR:N	2.53	0.41
1:A:14:LYS:C	1:A:15:ILE:HG22	2.46	0.41
1:A:70:TRP:CZ3	1:A:72:GLY:HA3	2.55	0.41
1:E:168:ARG:HG2	1:E:169:GLU:H	1.86	0.41
1:G:180:ALA:O	1:G:232:LYS:NZ	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:101:SER:HB3	1:K:13:ARG:CZ	2.50	0.41
1:I:203:LEU:O	1:I:206:PHE:HB2	2.20	0.41
1:O:109:ALA:O	1:O:113:ILE:HG13	2.21	0.41
1:O:164:HIS:ND1	1:O:165:ILE:O	2.45	0.41
1:O:274:ARG:O	1:O:277:PHE:HB3	2.21	0.41
1:Q:40:GLU:HB2	1:Q:49:LEU:HD22	2.03	0.41
1:Q:182:ILE:O	1:Q:185:HIS:N	2.51	0.41
1:S:109:ALA:O	1:S:110:ASP:C	2.63	0.41
1:S:205:TYR:HB2	1:S:211:LEU:HD11	2.02	0.41
1:U:15:ILE:HD13	1:W:292:MET:HE1	2.02	0.41
1:U:15:ILE:HD12	1:W:292:MET:HE3	1.99	0.41
1:U:93:PHE:HA	1:U:100:PHE:CZ	2.55	0.41
1:U:128:ASP:O	1:U:133:ASN:ND2	2.46	0.41
1:U:135:LEU:CD1	1:U:148:ILE:HD13	2.46	0.41
1:W:246:SER:O	1:W:249:SER:HB2	2.21	0.41
1:C:112:MET:HE3	1:C:134:PHE:CG	2.56	0.41
1:C:221:LYS:H	1:C:221:LYS:HE2	1.86	0.41
1:G:14:LYS:HB2	1:G:24:TYR:CE1	2.55	0.41
1:G:251:TYR:CD2	1:G:269:LEU:HD22	2.55	0.41
1:I:164:HIS:O	1:I:165:ILE:C	2.64	0.41
1:I:198:SER:O	1:I:202:VAL:HG23	2.20	0.41
1:I:276:LEU:O	1:I:280:GLN:HG2	2.19	0.41
1:K:222:ARG:HG3	1:K:223:GLN:H	1.85	0.41
1:K:251:TYR:C	1:K:251:TYR:CD1	2.98	0.41
1:M:8:LYS:CD	1:M:9:TYR:CE2	2.98	0.41
1:M:130:LYS:HD2	1:M:132:ASP:OD2	2.21	0.41
1:M:138:LEU:HD21	1:O:287:VAL:CG1	2.50	0.41
1:M:220:THR:HG23	1:M:223:GLN:HB2	2.02	0.41
1:M:262:ASP:O	1:M:264:PRO:HD3	2.21	0.41
1:O:5:VAL:O	1:O:6:GLY:C	2.64	0.41
1:O:126:HIS:ND1	1:O:126:HIS:C	2.79	0.41
1:O:161:THR:O	1:O:163:GLN:N	2.54	0.41
1:S:275:ASN:O	1:S:279:ARG:HG3	2.21	0.41
1:U:150:PHE:N	1:U:150:PHE:CD1	2.88	0.41
1:U:198:SER:C	1:U:200:GLY:N	2.77	0.41
1:W:104:THR:O	1:W:108:LEU:HG	2.20	0.41
1:W:116:ILE:HD11	1:W:129:VAL:HG22	2.02	0.41
1:C:138:LEU:O	1:C:141:LYS:N	2.51	0.41
1:G:3:LEU:HD23	1:G:3:LEU:C	2.46	0.41
1:K:17:SER:CB	3:K:405:HOH:O	2.52	0.41
1:Q:137:GLY:O	1:Q:142:GLY:HA2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:70:TRP:HZ3	1:U:79:VAL:HB	1.86	0.41
1:U:110:ASP:OD1	1:U:270:ARG:HG3	2.20	0.41
1:U:241:CYS:O	1:U:242:LYS:O	2.38	0.41
1:U:247:GLU:OE1	1:U:276:LEU:HD23	2.21	0.41
1:U:251:TYR:CE1	1:U:255:CYS:SG	3.13	0.41
1:W:3:LEU:O	1:W:4:ARG:C	2.63	0.41
1:C:134:PHE:HA	1:C:146:TYR:O	2.20	0.41
1:E:88:SER:CA	1:E:135:LEU:HD23	2.50	0.41
1:E:220:THR:O	1:E:221:LYS:C	2.63	0.41
1:G:15:ILE:HG23	1:G:25:LEU:H	1.84	0.41
1:I:221:LYS:O	1:I:224:LYS:N	2.54	0.41
1:I:226:GLU:N	1:I:226:GLU:CD	2.79	0.41
1:K:1:MET:O	1:K:2:GLU:CB	2.66	0.41
1:O:122:LYS:O	1:O:123:ASN:HB2	2.20	0.41
1:O:252:LEU:HD23	1:O:252:LEU:HA	1.94	0.41
1:Q:138:LEU:HD12	1:S:291:ASN:HB3	2.03	0.41
1:U:250:THR:HG22	1:U:272:LEU:HD21	2.03	0.41
1:W:119:ILE:HD11	1:W:150:PHE:HE2	1.86	0.41
1:W:213:TRP:CZ3	1:W:232:LYS:HG2	2.56	0.41
1:E:34:GLU:C	1:E:35:VAL:HG13	2.46	0.41
1:E:55:PHE:HE2	1:E:124:PHE:CD2	2.39	0.41
1:E:108:LEU:O	1:E:112:MET:HG3	2.21	0.41
1:E:140:LYS:CG	1:E:141:LYS:N	2.84	0.41
1:E:158:ASP:O	1:E:162:HIS:HA	2.21	0.41
1:E:204:MET:HA	1:E:207:ASN:HD22	1.86	0.41
1:E:226:GLU:O	1:E:230:GLU:HB2	2.21	0.41
1:E:249:SER:HB2	1:O:1:MET:CE	2.26	0.41
1:G:13:ARG:HD3	3:M:423:HOH:O	2.20	0.41
1:G:77:TYR:OH	1:M:236:PRO:HA	2.21	0.41
1:G:88:SER:HB2	1:G:135:LEU:HD12	2.03	0.41
1:I:231:LYS:HD2	1:I:231:LYS:O	2.21	0.41
1:I:234:SER:O	1:I:236:PRO:HD3	2.21	0.41
1:I:244:TYR:O	1:I:245:PRO:C	2.64	0.41
1:K:77:TYR:CZ	1:O:236:PRO:HB3	2.56	0.41
1:K:259:ARG:HB2	1:K:262:ASP:CG	2.43	0.41
1:M:278:HIS:O	1:M:279:ARG:C	2.64	0.41
1:O:32:GLY:O	1:O:33:GLU:C	2.64	0.41
1:O:204:MET:CE	1:O:204:MET:CA	2.93	0.41
1:O:211:LEU:HD22	1:O:213:TRP:CZ2	2.55	0.41
1:Q:46:HIS:O	1:Q:48:GLN:HG3	2.21	0.41
1:Q:47:PRO:C	1:Q:48:GLN:HG3	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:198:SER:O	1:Q:201:TYR:N	2.53	0.41
1:S:11:LEU:CD1	1:S:39:LEU:HD11	2.51	0.41
1:S:46:HIS:O	1:S:48:GLN:NE2	2.54	0.41
1:S:78:ASN:C	1:S:79:VAL:HG23	2.46	0.41
1:S:185:HIS:HB3	1:S:229:SER:OG	2.21	0.41
1:U:4:ARG:CG	1:U:5:VAL:N	2.82	0.41
1:U:27:ALA:HA	1:U:33:GLU:O	2.21	0.41
1:U:185:HIS:CE1	1:U:228:ILE:HG22	2.56	0.41
1:U:254:PHE:HB3	1:U:255:CYS:H	1.71	0.41
1:W:125:ILE:CD1	1:W:127:ARG:HD3	2.51	0.41
1:W:156:TYR:HE1	1:W:192:ARG:HE	1.62	0.41
1:W:259:ARG:O	1:W:260:PHE:C	2.64	0.41
1:A:218:ALA:HB2	1:A:224:LYS:HA	2.03	0.41
1:E:169:GLU:HB2	1:E:170:ASN:H	1.64	0.41
1:G:193:ARG:CZ	1:G:260:PHE:HA	2.51	0.41
1:M:254:PHE:CE2	1:M:269:LEU:HD11	2.56	0.41
1:O:236:PRO:HG2	1:O:239:VAL:HG23	2.02	0.41
1:U:41:CYS:O	1:U:42:VAL:C	2.64	0.41
1:U:103:LYS:CG	1:U:282:PHE:HB3	2.50	0.41
1:U:173:LEU:HD12	1:U:174:THR:N	2.36	0.41
1:U:182:ILE:O	1:U:186:LEU:HG	2.20	0.41
1:U:244:TYR:HA	1:U:245:PRO:HD3	1.88	0.41
1:W:57:LYS:CD	1:W:68:ILE:CG1	2.94	0.41
1:W:225:TYR:N	1:W:225:TYR:CD1	2.89	0.41
1:W:274:ARG:O	1:W:277:PHE:HB3	2.21	0.41
1:W:285:ASP:OD1	1:W:287:VAL:CG2	2.42	0.41
1:A:52:GLU:OE2	1:A:149:ASP:HA	2.21	0.40
1:G:8:LYS:HB2	1:G:8:LYS:HE2	1.63	0.40
1:G:117:GLU:HG3	1:G:266:TYR:CE2	2.57	0.40
1:I:118:TYR:OH	1:I:122:LYS:HE2	2.21	0.40
1:I:196:LEU:HD23	1:I:196:LEU:HA	1.86	0.40
1:K:6:GLY:C	1:K:8:LYS:N	2.69	0.40
1:K:158:ASP:CG	1:K:161:THR:HG1	2.26	0.40
1:K:292:MET:HE3	1:K:292:MET:HB2	1.90	0.40
1:O:139:GLY:O	1:O:140:LYS:C	2.64	0.40
1:O:259:ARG:O	1:O:260:PHE:C	2.62	0.40
1:O:292:MET:O	1:O:293:LEU:O	2.40	0.40
1:S:28:ASN:HD21	1:S:30:ALA:HB3	1.85	0.40
1:S:220:THR:OG1	1:S:221:LYS:N	2.54	0.40
1:S:230:GLU:O	1:S:233:MET:N	2.55	0.40
1:S:290:TRP:CD1	1:S:291:ASN:ND2	2.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:192:ARG:HD2	1:W:264:PRO:HD2	2.03	0.40
1:E:87:PRO:HA	1:G:293:LEU:HA	2.03	0.40
1:E:140:LYS:HG2	1:E:141:LYS:N	2.37	0.40
1:G:139:GLY:O	1:G:140:LYS:C	2.64	0.40
1:K:126:HIS:O	1:K:127:ARG:HB2	2.21	0.40
1:K:156:TYR:CZ	1:K:192:ARG:HD3	2.55	0.40
1:M:130:LYS:O	1:M:131:PRO:C	2.63	0.40
1:O:150:PHE:O	1:O:153:ALA:N	2.47	0.40
1:O:161:THR:C	1:O:163:GLN:N	2.77	0.40
1:S:49:LEU:HD11	1:S:80:MET:CB	2.49	0.40
1:S:49:LEU:HD12	1:S:49:LEU:O	2.21	0.40
1:S:237:ILE:CD1	1:S:256:ARG:NH1	2.84	0.40
1:U:211:LEU:CD2	1:U:213:TRP:CZ2	2.92	0.40
1:U:276:LEU:CD1	1:U:276:LEU:C	2.93	0.40
1:W:90:GLU:O	1:W:93:PHE:N	2.54	0.40
1:A:171:LYS:CB	1:A:187:GLY:O	2.64	0.40
1:C:202:VAL:O	1:C:205:TYR:HB3	2.22	0.40
1:E:52:GLU:OE2	1:E:149:ASP:N	2.54	0.40
1:E:270:ARG:NH1	3:E:401:HOH:O	2.55	0.40
1:G:3:LEU:HD13	1:G:11:LEU:HD22	2.03	0.40
1:G:284:TYR:HB2	3:G:445:HOH:O	2.22	0.40
1:K:39:LEU:HD23	1:K:39:LEU:HA	1.70	0.40
1:M:70:TRP:CZ3	1:M:72:GLY:CA	3.04	0.40
1:O:277:PHE:CE1	1:O:282:PHE:HB2	2.56	0.40
1:S:65:ILE:HA	1:S:66:PRO:HD2	1.82	0.40
1:U:250:THR:HG21	1:U:272:LEU:HD21	2.02	0.40
1:W:24:TYR:CD2	1:W:39:LEU:HD21	2.56	0.40
1:W:150:PHE:O	1:W:153:ALA:CB	2.69	0.40
1:W:183:ASN:HA	1:W:186:LEU:HB2	2.04	0.40
1:A:173:LEU:HD12	1:A:184:THR:HG22	2.03	0.40
1:A:201:TYR:O	1:A:202:VAL:C	2.64	0.40
1:C:171:LYS:HD3	3:C:429:HOH:O	2.21	0.40
1:G:50:HIS:HE1	3:G:444:HOH:O	2.04	0.40
1:I:39:LEU:CD2	1:I:79:VAL:HG22	2.51	0.40
1:I:181:SER:CB	1:I:197:GLU:OE2	2.59	0.40
1:M:175:GLY:O	1:M:176:THR:C	2.64	0.40
1:Q:68:ILE:CG2	1:Q:69:LYS:N	2.83	0.40
1:S:193:ARG:HG3	1:S:194:ASP:H	1.83	0.40
1:U:52:GLU:OE1	1:U:56:TYR:CE2	2.74	0.40
1:U:265:ASP:O	1:U:268:TYR:HB3	2.22	0.40
1:W:62:GLY:HA3	1:W:118:TYR:CZ	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:65:ILE:HG22	1:W:66:PRO:O	2.22	0.40
1:W:108:LEU:O	1:W:109:ALA:C	2.64	0.40
1:W:173:LEU:CD1	1:W:184:THR:CG2	2.83	0.40
1:A:56:TYR:HD2	1:A:80:MET:HE1	1.84	0.40
1:C:241:CYS:O	1:C:242:LYS:C	2.64	0.40
1:E:156:TYR:CE1	1:E:192:ARG:HD3	2.56	0.40
1:G:288:PHE:O	1:G:291:ASN:HB2	2.21	0.40
1:I:45:LYS:O	1:I:46:HIS:ND1	2.38	0.40
1:I:165:ILE:O	1:I:165:ILE:HG13	2.21	0.40
1:I:209:GLY:O	1:I:210:SER:HB3	2.21	0.40
1:K:182:ILE:HD11	1:K:233:MET:HA	2.04	0.40
1:S:182:ILE:CG2	1:S:233:MET:CE	2.99	0.40
1:S:253:ASN:O	1:S:254:PHE:C	2.64	0.40
1:W:115:ARG:HH11	1:W:115:ARG:HA	1.87	0.40
1:W:124:PHE:CD2	1:W:155:LYS:CA	3.05	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:160:ARG:NH2	1:C:160:ARG:NH2[2_454]	1.82	0.38
1:Q:77:TYR:OH	1:S:233:MET:O[2_453]	2.14	0.06

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	286/296 (97%)	257 (90%)	26 (9%)	3 (1%)	12	35
1	C	285/296 (96%)	255 (90%)	23 (8%)	7 (2%)	4	14
1	E	287/296 (97%)	257 (90%)	25 (9%)	5 (2%)	7	22
1	G	286/296 (97%)	244 (85%)	37 (13%)	5 (2%)	7	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	287/296 (97%)	245 (85%)	37 (13%)	5 (2%)	7	22
1	K	286/296 (97%)	240 (84%)	33 (12%)	13 (4%)	2	5
1	M	289/296 (98%)	227 (78%)	46 (16%)	16 (6%)	1	4
1	O	286/296 (97%)	233 (82%)	38 (13%)	15 (5%)	1	4
1	Q	286/296 (97%)	251 (88%)	31 (11%)	4 (1%)	9	26
1	S	282/296 (95%)	217 (77%)	48 (17%)	17 (6%)	1	3
1	U	285/296 (96%)	211 (74%)	43 (15%)	31 (11%)	0	0
1	W	285/296 (96%)	195 (68%)	65 (23%)	25 (9%)	0	1
All	All	3430/3552 (97%)	2832 (83%)	452 (13%)	146 (4%)	2	6

All (146) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	C	46	HIS
1	C	187	GLY
1	E	7	ASN
1	E	44	THR
1	G	260	PHE
1	I	2	GLU
1	I	3	LEU
1	K	2	GLU
1	K	4	ARG
1	K	46	HIS
1	K	219	ALA
1	M	219	ALA
1	M	220	THR
1	O	2	GLU
1	O	53	SER
1	O	141	LYS
1	O	288	PHE
1	O	293	LEU
1	Q	44	THR
1	S	162	HIS
1	S	257	SER
1	S	258	LEU
1	U	31	SER
1	U	46	HIS
1	U	151	GLY

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Mol	Chain	Res	Type
1	U	192	ARG
1	U	209	GLY
1	U	219	ALA
1	U	235	THR
1	U	236	PRO
1	U	242	LYS
1	U	262	ASP
1	W	3	LEU
1	W	13	ARG
1	W	31	SER
1	W	74	GLU
1	W	87	PRO
1	W	132	ASP
1	W	165	ILE
1	W	220	THR
1	W	270	ARG
1	W	279	ARG
1	C	139	GLY
1	E	139	GLY
1	E	149	ASP
1	I	30	ALA
1	K	141	LYS
1	M	11	LEU
1	M	19	SER
1	M	32	GLY
1	M	49	LEU
1	M	59	MET
1	M	279	ARG
1	O	139	GLY
1	O	151	GLY
1	O	221	LYS
1	Q	7	ASN
1	Q	286	TYR
1	S	74	GLU
1	S	110	ASP
1	S	151	GLY
1	S	175	GLY
1	U	48	GLN
1	U	59	MET
1	U	141	LYS
1	U	162	HIS
1	U	208	LEU

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Mol	Chain	Res	Type
1	U	218	ALA
1	U	254	PHE
1	U	284	TYR
1	U	290	TRP
1	W	15	ILE
1	W	70	TRP
1	W	139	GLY
1	W	140	LYS
1	W	164	HIS
1	W	210	SER
1	W	269	LEU
1	W	278	HIS
1	C	3	LEU
1	C	149	ASP
1	C	260	PHE
1	G	30	ALA
1	I	149	ASP
1	K	7	ASN
1	K	29	ILE
1	K	30	ALA
1	K	70	TRP
1	M	140	LYS
1	M	225	TYR
1	O	216	LEU
1	Q	173	LEU
1	S	8	LYS
1	S	44	THR
1	S	48	GLN
1	S	149	ASP
1	S	202	VAL
1	U	127	ARG
1	U	212	PRO
1	U	237	ILE
1	U	260	PHE
1	U	286	TYR
1	W	4	ARG
1	W	30	ALA
1	W	44	THR
1	G	219	ALA
1	K	3	LEU
1	K	225	TYR
1	M	22	ASP

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Mol	Chain	Res	Type
1	O	110	ASP
1	O	140	LYS
1	O	162	HIS
1	O	210	SER
1	S	60	GLN
1	S	260	PHE
1	U	170	ASN
1	U	258	LEU
1	W	131	PRO
1	W	217	LYS
1	A	149	ASP
1	E	2	GLU
1	G	47	PRO
1	G	149	ASP
1	I	222	ARG
1	K	51	ILE
1	O	7	ASN
1	O	175	GLY
1	S	224	LYS
1	U	15	ILE
1	U	245	PRO
1	W	221	LYS
1	C	60	GLN
1	M	15	ILE
1	M	148	ILE
1	S	73	ALA
1	S	122	LYS
1	U	142	GLY
1	W	149	ASP
1	A	46	HIS
1	K	47	PRO
1	M	62	GLY
1	U	243	GLY
1	M	166	PRO
1	M	29	ILE
1	U	42	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	255/260 (98%)	227 (89%)	28 (11%)	6	18
1	C	256/260 (98%)	227 (89%)	29 (11%)	5	17
1	E	254/260 (98%)	223 (88%)	31 (12%)	5	14
1	G	252/260 (97%)	224 (89%)	28 (11%)	6	18
1	I	254/260 (98%)	217 (85%)	37 (15%)	3	9
1	K	251/260 (96%)	219 (87%)	32 (13%)	4	13
1	M	248/260 (95%)	217 (88%)	31 (12%)	4	13
1	O	254/260 (98%)	213 (84%)	41 (16%)	2	7
1	Q	253/260 (97%)	217 (86%)	36 (14%)	3	10
1	S	248/260 (95%)	197 (79%)	51 (21%)	1	3
1	U	252/260 (97%)	202 (80%)	50 (20%)	1	4
1	W	253/260 (97%)	190 (75%)	63 (25%)	0	2
All	All	3030/3120 (97%)	2573 (85%)	457 (15%)	3	8

All (457) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	5	VAL
1	A	8	LYS
1	A	15	ILE
1	A	52	GLU
1	A	54	LYS
1	A	57	LYS
1	A	58	MET
1	A	67	SER
1	A	71	CYS
1	A	104	THR
1	A	138	LEU
1	A	141	LYS
1	A	161	THR
1	A	163	GLN
1	A	171	LYS
1	A	174	THR
1	A	216	LEU
1	A	217	LYS

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Mol	Chain	Res	Type
1	A	220	THR
1	A	221	LYS
1	A	222	ARG
1	A	223	GLN
1	A	226	GLU
1	A	237	ILE
1	A	267	SER
1	A	274	ARG
1	A	294	LYS
1	C	2	GLU
1	C	4	ARG
1	C	7	ASN
1	C	10	ARG
1	C	15	ILE
1	C	45	LYS
1	C	46	HIS
1	C	53	SER
1	C	55	PHE
1	C	57	LYS
1	C	60	GLN
1	C	69	LYS
1	C	82	MET
1	C	122	LYS
1	C	140	LYS
1	C	155	LYS
1	C	168	ARG
1	C	174	THR
1	C	216	LEU
1	C	217	LYS
1	C	220	THR
1	C	221	LYS
1	C	222	ARG
1	C	226	GLU
1	C	234	SER
1	C	238	GLU
1	C	257	SER
1	C	279	ARG
1	C	293	LEU
1	E	3	LEU
1	E	8	LYS
1	E	13	ARG
1	E	29	ILE

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Mol	Chain	Res	Type
1	E	45	LYS
1	E	48	GLN
1	E	54	LYS
1	E	60	GLN
1	E	69	LYS
1	E	76	ASP
1	E	140	LYS
1	E	148	ILE
1	E	155	LYS
1	E	161	THR
1	E	168	ARG
1	E	182	ILE
1	E	207	ASN
1	E	216	LEU
1	E	220	THR
1	E	226	GLU
1	E	233	MET
1	E	234	SER
1	E	235	THR
1	E	237	ILE
1	E	249	SER
1	E	263	LYS
1	E	267	SER
1	E	274	ARG
1	E	279	ARG
1	E	283	SER
1	E	294	LYS
1	G	3	LEU
1	G	7	ASN
1	G	8	LYS
1	G	13	ARG
1	G	17	SER
1	G	28	ASN
1	G	29	ILE
1	G	57	LYS
1	G	58	MET
1	G	76	ASP
1	G	82	MET
1	G	100	PHE
1	G	135	LEU
1	G	138	LEU
1	G	140	LYS

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Mol	Chain	Res	Type
1	G	155	LYS
1	G	158	ASP
1	G	171	LYS
1	G	216	LEU
1	G	217	LYS
1	G	226	GLU
1	G	234	SER
1	G	237	ILE
1	G	249	SER
1	G	267	SER
1	G	283	SER
1	G	293	LEU
1	G	294	LYS
1	I	1	MET
1	I	2	GLU
1	I	5	VAL
1	I	7	ASN
1	I	15	ILE
1	I	23	ILE
1	I	29	ILE
1	I	34	GLU
1	I	38	LYS
1	I	44	THR
1	I	48	GLN
1	I	52	GLU
1	I	65	ILE
1	I	82	MET
1	I	101	SER
1	I	138	LEU
1	I	140	LYS
1	I	143	ASN
1	I	155	LYS
1	I	160	ARG
1	I	161	THR
1	I	168	ARG
1	I	170	ASN
1	I	173	LEU
1	I	182	ILE
1	I	216	LEU
1	I	221	LYS
1	I	222	ARG
1	I	234	SER

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Mol	Chain	Res	Type
1	I	239	VAL
1	I	242	LYS
1	I	263	LYS
1	I	267	SER
1	I	272	LEU
1	I	276	LEU
1	I	283	SER
1	I	293	LEU
1	K	2	GLU
1	K	3	LEU
1	K	7	ASN
1	K	8	LYS
1	K	11	LEU
1	K	17	SER
1	K	29	ILE
1	K	44	THR
1	K	49	LEU
1	K	54	LYS
1	K	57	LYS
1	K	76	ASP
1	K	82	MET
1	K	99	LYS
1	K	104	THR
1	K	123	ASN
1	K	135	LEU
1	K	155	LYS
1	K	158	ASP
1	K	168	ARG
1	K	169	GLU
1	K	171	LYS
1	K	182	ILE
1	K	216	LEU
1	K	226	GLU
1	K	230	GLU
1	K	238	GLU
1	K	249	SER
1	K	267	SER
1	K	271	GLN
1	K	283	SER
1	K	294	LYS
1	M	4	ARG
1	M	5	VAL

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Mol	Chain	Res	Type
1	M	7	ASN
1	M	13	ARG
1	M	15	ILE
1	M	33	GLU
1	M	44	THR
1	M	52	GLU
1	M	54	LYS
1	M	57	LYS
1	M	59	MET
1	M	63	VAL
1	M	67	SER
1	M	68	ILE
1	M	76	ASP
1	M	121	SER
1	M	122	LYS
1	M	132	ASP
1	M	138	LEU
1	M	165	ILE
1	M	216	LEU
1	M	220	THR
1	M	221	LYS
1	M	222	ARG
1	M	226	GLU
1	M	234	SER
1	M	238	GLU
1	M	249	SER
1	M	257	SER
1	M	259	ARG
1	M	272	LEU
1	O	1	MET
1	O	3	LEU
1	O	13	ARG
1	O	15	ILE
1	O	28	ASN
1	O	35	VAL
1	O	43	LYS
1	O	54	LYS
1	O	63	VAL
1	O	65	ILE
1	O	71	CYS
1	O	82	MET
1	O	99	LYS

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Mol	Chain	Res	Type
1	O	121	SER
1	O	125	ILE
1	O	138	LEU
1	O	140	LYS
1	O	141	LYS
1	O	155	LYS
1	O	163	GLN
1	O	169	GLU
1	O	170	ASN
1	O	171	LYS
1	O	173	LEU
1	O	174	THR
1	O	204	MET
1	O	216	LEU
1	O	217	LYS
1	O	220	THR
1	O	221	LYS
1	O	223	GLN
1	O	228	ILE
1	O	235	THR
1	O	238	GLU
1	O	245	PRO
1	O	259	ARG
1	O	262	ASP
1	O	270	ARG
1	O	272	LEU
1	O	284	TYR
1	O	294	LYS
1	Q	3	LEU
1	Q	5	VAL
1	Q	7	ASN
1	Q	8	LYS
1	Q	15	ILE
1	Q	17	SER
1	Q	22	ASP
1	Q	38	LYS
1	Q	42	VAL
1	Q	44	THR
1	Q	52	GLU
1	Q	57	LYS
1	Q	68	ILE
1	Q	76	ASP

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Mol	Chain	Res	Type
1	Q	82	MET
1	Q	121	SER
1	Q	122	LYS
1	Q	130	LYS
1	Q	132	ASP
1	Q	135	LEU
1	Q	155	LYS
1	Q	169	GLU
1	Q	174	THR
1	Q	189	GLU
1	Q	197	GLU
1	Q	216	LEU
1	Q	221	LYS
1	Q	226	GLU
1	Q	234	SER
1	Q	238	GLU
1	Q	239	VAL
1	Q	259	ARG
1	Q	283	SER
1	Q	286	TYR
1	Q	292	MET
1	Q	293	LEU
1	S	4	ARG
1	S	5	VAL
1	S	8	LYS
1	S	10	ARG
1	S	15	ILE
1	S	23	ILE
1	S	28	ASN
1	S	29	ILE
1	S	34	GLU
1	S	42	VAL
1	S	48	GLN
1	S	51	ILE
1	S	57	LYS
1	S	69	LYS
1	S	82	MET
1	S	101	SER
1	S	122	LYS
1	S	129	VAL
1	S	135	LEU
1	S	138	LEU

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Mol	Chain	Res	Type
1	S	140	LYS
1	S	143	ASN
1	S	144	LEU
1	S	147	ILE
1	S	148	ILE
1	S	150	PHE
1	S	165	ILE
1	S	168	ARG
1	S	170	ASN
1	S	171	LYS
1	S	173	LEU
1	S	174	THR
1	S	211	LEU
1	S	212	PRO
1	S	216	LEU
1	S	220	THR
1	S	221	LYS
1	S	222	ARG
1	S	226	GLU
1	S	230	GLU
1	S	233	MET
1	S	234	SER
1	S	237	ILE
1	S	242	LYS
1	S	245	PRO
1	S	249	SER
1	S	256	ARG
1	S	259	ARG
1	S	267	SER
1	S	272	LEU
1	S	280	GLN
1	U	1	MET
1	U	7	ASN
1	U	8	LYS
1	U	13	ARG
1	U	17	SER
1	U	23	ILE
1	U	25	LEU
1	U	28	ASN
1	U	31	SER
1	U	35	VAL
1	U	42	VAL

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Mol	Chain	Res	Type
1	U	43	LYS
1	U	44	THR
1	U	52	GLU
1	U	69	LYS
1	U	71	CYS
1	U	83	GLU
1	U	88	SER
1	U	97	SER
1	U	104	THR
1	U	113	ILE
1	U	122	LYS
1	U	125	ILE
1	U	138	LEU
1	U	144	LEU
1	U	158	ASP
1	U	169	GLU
1	U	173	LEU
1	U	190	GLN
1	U	204	MET
1	U	205	TYR
1	U	208	LEU
1	U	210	SER
1	U	211	LEU
1	U	216	LEU
1	U	220	THR
1	U	221	LYS
1	U	226	GLU
1	U	229	SER
1	U	230	GLU
1	U	234	SER
1	U	236	PRO
1	U	237	ILE
1	U	238	GLU
1	U	246	SER
1	U	257	SER
1	U	267	SER
1	U	279	ARG
1	U	288	PHE
1	U	291	ASN
1	W	3	LEU
1	W	5	VAL
1	W	9	TYR

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Mol	Chain	Res	Type
1	W	10	ARG
1	W	29	ILE
1	W	33	GLU
1	W	37	ILE
1	W	39	LEU
1	W	42	VAL
1	W	48	GLN
1	W	52	GLU
1	W	53	SER
1	W	57	LYS
1	W	60	GLN
1	W	63	VAL
1	W	67	SER
1	W	68	ILE
1	W	69	LYS
1	W	71	CYS
1	W	74	GLU
1	W	76	ASP
1	W	78	ASN
1	W	81	VAL
1	W	82	MET
1	W	84	LEU
1	W	87	PRO
1	W	98	ARG
1	W	113	ILE
1	W	115	ARG
1	W	122	LYS
1	W	124	PHE
1	W	129	VAL
1	W	135	LEU
1	W	140	LYS
1	W	141	LYS
1	W	145	VAL
1	W	147	ILE
1	W	150	PHE
1	W	154	LYS
1	W	158	ASP
1	W	163	GLN
1	W	167	TYR
1	W	168	ARG
1	W	169	GLU
1	W	174	THR

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Mol	Chain	Res	Type
1	W	182	ILE
1	W	184	THR
1	W	188	ILE
1	W	216	LEU
1	W	221	LYS
1	W	226	GLU
1	W	234	SER
1	W	238	GLU
1	W	246	SER
1	W	249	SER
1	W	261	ASP
1	W	272	LEU
1	W	275	ASN
1	W	276	LEU
1	W	284	TYR
1	W	287	VAL
1	W	289	ASP
1	W	293	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (68) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	HIS
1	A	60	GLN
1	A	162	HIS
1	C	280	GLN
1	C	291	ASN
1	E	60	GLN
1	E	126	HIS
1	E	163	GLN
1	E	190	GLN
1	E	207	ASN
1	E	271	GLN
1	G	28	ASN
1	G	170	ASN
1	G	278	HIS
1	G	291	ASN
1	I	28	ASN
1	I	50	HIS
1	I	60	GLN
1	I	170	ASN
1	I	207	ASN

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Mol	Chain	Res	Type
1	I	271	GLN
1	I	278	HIS
1	K	7	ASN
1	K	28	ASN
1	K	60	GLN
1	K	162	HIS
1	M	7	ASN
1	M	60	GLN
1	M	271	GLN
1	M	280	GLN
1	O	7	ASN
1	O	28	ASN
1	O	46	HIS
1	O	60	GLN
1	O	78	ASN
1	O	163	GLN
1	O	271	GLN
1	O	278	HIS
1	O	280	GLN
1	Q	7	ASN
1	Q	60	GLN
1	Q	170	ASN
1	Q	223	GLN
1	Q	271	GLN
1	Q	291	ASN
1	S	7	ASN
1	S	28	ASN
1	S	48	GLN
1	S	60	GLN
1	S	143	ASN
1	S	162	HIS
1	S	170	ASN
1	S	271	GLN
1	S	280	GLN
1	S	291	ASN
1	U	7	ASN
1	U	28	ASN
1	U	163	GLN
1	U	164	HIS
1	U	190	GLN
1	U	271	GLN
1	U	278	HIS

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Mol	Chain	Res	Type
1	U	280	GLN
1	U	291	ASN
1	W	50	HIS
1	W	133	ASN
1	W	190	GLN
1	W	271	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	G	301	-	4,4,4	0.52	0	6,6,6	0.64	0
2	SO4	O	301	-	4,4,4	0.28	0	6,6,6	0.47	0
2	SO4	I	301	-	4,4,4	0.33	0	6,6,6	0.32	0
2	SO4	W	301	-	4,4,4	0.71	0	6,6,6	0.35	0
2	SO4	A	301	-	4,4,4	0.47	0	6,6,6	0.32	0
2	SO4	C	301	-	4,4,4	0.67	0	6,6,6	0.37	0
2	SO4	K	301	-	4,4,4	0.54	0	6,6,6	0.18	0
2	SO4	S	301	-	4,4,4	0.48	0	6,6,6	0.23	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	Q	301	-	4,4,4	0.49	0	6,6,6	0.33	0
2	SO4	M	301	-	4,4,4	0.41	0	6,6,6	0.28	0
2	SO4	U	301	-	4,4,4	0.61	0	6,6,6	0.41	0
2	SO4	E	301	-	4,4,4	0.53	0	6,6,6	0.42	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	301	SO4	1	0
2	S	301	SO4	1	0
2	Q	301	SO4	1	0
2	M	301	SO4	1	0
2	U	301	SO4	3	0

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	290/296 (97%)	-0.15	2 (0%) 84 79	11, 31, 56, 84	1 (0%)
1	C	289/296 (97%)	-0.09	2 (0%) 84 79	11, 34, 60, 82	1 (0%)
1	E	291/296 (98%)	-0.03	4 (1%) 73 67	18, 38, 60, 84	1 (0%)
1	G	290/296 (97%)	0.11	7 (2%) 59 52	17, 41, 70, 90	1 (0%)
1	I	291/296 (98%)	0.10	6 (2%) 63 56	23, 41, 63, 83	1 (0%)
1	K	290/296 (97%)	0.22	7 (2%) 59 52	24, 47, 76, 92	1 (0%)
1	M	291/296 (98%)	0.49	16 (5%) 30 25	24, 49, 74, 81	1 (0%)
1	O	290/296 (97%)	0.50	10 (3%) 48 41	33, 53, 75, 94	1 (0%)
1	Q	290/296 (97%)	0.20	6 (2%) 63 56	24, 47, 72, 91	1 (0%)
1	S	286/296 (96%)	0.50	9 (3%) 51 44	25, 55, 77, 89	1 (0%)
1	U	289/296 (97%)	1.28	54 (18%) 3 2	26, 68, 86, 93	1 (0%)
1	W	289/296 (97%)	1.37	72 (24%) 2 1	28, 82, 93, 97	1 (0%)
All	All	3476/3552 (97%)	0.37	195 (5%) 30 25	11, 47, 83, 97	12 (0%)

All (195) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	U	293	LEU	6.7
1	K	1	MET	5.3
1	W	284	TYR	5.1
1	W	3	LEU	5.0
1	W	11	LEU	5.0
1	E	1	MET	4.9
1	W	27	ALA	4.9
1	W	67	SER	4.8
1	W	77	TYR	4.7
1	K	3	LEU	4.6
1	W	15	ILE	4.5

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Mol	Chain	Res	Type	RSRZ
1	S	77	TYR	4.3
1	W	35	VAL	4.0
1	U	284	TYR	3.9
1	W	150	PHE	3.8
1	U	77	TYR	3.7
1	W	29	ILE	3.7
1	W	59	MET	3.7
1	W	51	ILE	3.6
1	K	7	ASN	3.6
1	W	66	PRO	3.6
1	K	175	GLY	3.5
1	W	56	TYR	3.5
1	W	39	LEU	3.5
1	W	69	LYS	3.5
1	U	6	GLY	3.5
1	U	82	MET	3.4
1	U	8	LYS	3.4
1	U	240	LEU	3.4
1	W	30	ALA	3.4
1	W	41	CYS	3.4
1	M	5	VAL	3.4
1	M	76	ASP	3.3
1	U	221	LYS	3.3
1	U	92	LEU	3.2
1	Q	77	TYR	3.2
1	W	5	VAL	3.2
1	U	213	TRP	3.2
1	S	260	PHE	3.1
1	O	58	MET	3.1
1	O	284	TYR	3.1
1	K	77	TYR	3.1
1	W	65	ILE	3.1
1	W	73	ALA	3.1
1	U	254	PHE	3.1
1	W	143	ASN	3.0
1	S	68	ILE	3.0
1	E	140	LYS	3.0
1	W	141	LYS	3.0
1	U	105	VAL	3.0
1	Q	1	MET	3.0
1	O	51	ILE	3.0
1	W	25	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	U	209	GLY	2.9
1	W	151	GLY	2.9
1	W	9	TYR	2.9
1	K	11	LEU	2.9
1	W	37	ILE	2.9
1	W	188	ILE	2.9
1	G	55	PHE	2.8
1	M	77	TYR	2.8
1	U	256	ARG	2.8
1	U	208	LEU	2.8
1	Q	5	VAL	2.8
1	U	247	GLU	2.8
1	W	58	MET	2.8
1	W	81	VAL	2.8
1	G	77	TYR	2.8
1	I	1	MET	2.7
1	U	287	VAL	2.7
1	W	55	PHE	2.7
1	W	42	VAL	2.7
1	W	153	ALA	2.7
1	W	24	TYR	2.7
1	W	23	ILE	2.7
1	U	188	ILE	2.6
1	W	147	ILE	2.6
1	M	46	HIS	2.6
1	U	278	HIS	2.6
1	W	52	GLU	2.6
1	U	159	ALA	2.6
1	W	182	ILE	2.6
1	O	230	GLU	2.6
1	W	83	GLU	2.6
1	W	129	VAL	2.6
1	M	54	LYS	2.6
1	W	79	VAL	2.6
1	U	54	LYS	2.6
1	M	20	PHE	2.6
1	S	159	ALA	2.6
1	U	68	ILE	2.5
1	U	255	CYS	2.5
1	M	124	PHE	2.5
1	W	260	PHE	2.5
1	O	140	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	S	4	ARG	2.5
1	U	272	LEU	2.5
1	U	251	TYR	2.5
1	U	252	LEU	2.5
1	C	76	ASP	2.5
1	U	203	LEU	2.4
1	W	84	LEU	2.4
1	G	76	ASP	2.4
1	W	82	MET	2.4
1	G	221	LYS	2.4
1	U	227	ARG	2.4
1	W	144	LEU	2.4
1	U	100	PHE	2.4
1	G	29	ILE	2.4
1	U	106	LEU	2.4
1	W	165	ILE	2.4
1	W	26	GLY	2.4
1	W	63	VAL	2.4
1	W	36	ALA	2.4
1	U	220	THR	2.4
1	M	7	ASN	2.4
1	O	1	MET	2.4
1	U	99	LYS	2.4
1	W	75	GLY	2.4
1	W	74	GLU	2.3
1	I	29	ILE	2.3
1	U	179	TYR	2.3
1	W	31	SER	2.3
1	W	216	LEU	2.3
1	U	237	ILE	2.3
1	S	161	THR	2.3
1	U	242	LYS	2.3
1	U	107	LEU	2.3
1	U	282	PHE	2.3
1	W	49	LEU	2.3
1	M	51	ILE	2.3
1	U	73	ALA	2.3
1	I	172	ASN	2.3
1	U	245	PRO	2.3
1	M	12	GLY	2.3
1	W	145	VAL	2.3
1	W	159	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	U	238	GLU	2.2
1	W	286	TYR	2.2
1	Q	76	ASP	2.2
1	M	61	GLY	2.2
1	W	269	LEU	2.2
1	U	51	ILE	2.2
1	S	168	ARG	2.2
1	U	7	ASN	2.2
1	I	3	LEU	2.2
1	Q	3	LEU	2.2
1	W	217	LYS	2.2
1	O	15	ILE	2.2
1	W	148	ILE	2.2
1	U	104	THR	2.2
1	E	77	TYR	2.2
1	W	152	LEU	2.2
1	G	226	GLU	2.2
1	W	268	TYR	2.2
1	M	140	LYS	2.2
1	W	38	LYS	2.2
1	W	139	GLY	2.2
1	M	80	MET	2.2
1	Q	31	SER	2.2
1	U	5	VAL	2.2
1	W	164	HIS	2.2
1	U	279	ARG	2.1
1	O	77	TYR	2.1
1	U	103	LYS	2.1
1	I	82	MET	2.1
1	M	175	GLY	2.1
1	W	127	ARG	2.1
1	W	43	LYS	2.1
1	W	54	LYS	2.1
1	W	140	LYS	2.1
1	M	173	LEU	2.1
1	U	175	GLY	2.1
1	W	273	PHE	2.1
1	O	218	ALA	2.1
1	O	216	LEU	2.1
1	U	145	VAL	2.1
1	W	222	ARG	2.1
1	S	155	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	1	MET	2.1
1	U	48	GLN	2.1
1	S	162	HIS	2.1
1	A	77	TYR	2.1
1	U	202	VAL	2.1
1	M	82	MET	2.0
1	U	216	LEU	2.0
1	W	85	LEU	2.0
1	K	6	GLY	2.0
1	U	9	TYR	2.0
1	U	195	ASP	2.0
1	A	221	LYS	2.0
1	E	82	MET	2.0
1	I	174	THR	2.0
1	U	64	GLY	2.0
1	C	284	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SO4	U	301	5/5	0.79	0.16	78,79,80,80	0
2	SO4	I	301	5/5	0.85	0.13	51,53,54,55	0
2	SO4	W	301	5/5	0.87	0.12	65,67,68,69	0
2	SO4	S	301	5/5	0.88	0.12	68,69,70,71	0
2	SO4	O	301	5/5	0.89	0.10	62,62,63,66	0
2	SO4	G	301	5/5	0.89	0.11	50,51,54,55	0
2	SO4	M	301	5/5	0.92	0.09	52,53,54,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	E	301	5/5	0.92	0.08	50,51,53,55	0
2	SO4	Q	301	5/5	0.92	0.11	55,55,55,56	0
2	SO4	K	301	5/5	0.94	0.09	55,55,57,59	0
2	SO4	C	301	5/5	0.95	0.07	43,46,47,48	0
2	SO4	A	301	5/5	0.97	0.07	30,33,34,40	0

6.5 Other polymers [i](#)

There are no such residues in this entry.