



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:40 PM UTC

PDB ID : 2EIV / pdb_00002eiv
Title : Crystal Structure of the arginase from *Thermus thermophilus*
Authors : Kumarevel, T.S.; Karthe, P.; Kuramitsu, S.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2007-03-13
Resolution : 2.91 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

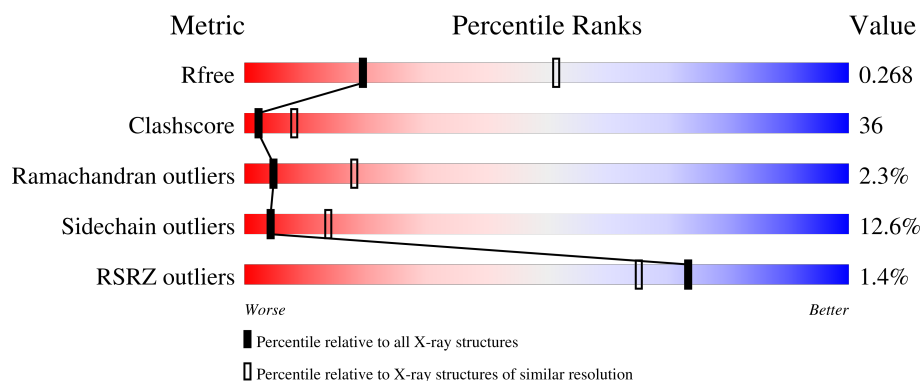
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.91 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	2995 (2.94-2.90)
Clashscore	190562	3213 (2.94-2.90)
Ramachandran outliers	187476	3128 (2.94-2.90)
Sidechain outliers	187428	3130 (2.94-2.90)
RSRZ outliers	180081	2995 (2.94-2.90)

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	291	
1	C	291	
1	D	291	
1	E	291	
1	F	291	

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Mol	Chain	Length	Quality of chain
1	G	291	%44%41%9%6%
1	H	291	%45%39%9%6%
1	I	291	%34%49%10%6%
1	J	291	%39%43%11%6%
1	K	291	%26%53%14%6%
1	L	291	%29%46%18%6%
1	M	291	7%23%51%18%6%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 24799 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 Arginase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	273	Total	C	N	O	S	0	0	0
			2052	1300	363	382	7			
1	C	273	Total	C	N	O	S	0	0	0
			2052	1300	363	382	7			
1	D	273	Total	C	N	O	S	0	0	0
			2052	1300	363	382	7			
1	E	273	Total	C	N	O	S	0	0	0
			2052	1300	363	382	7			
1	F	273	Total	C	N	O	S	0	0	0
			2052	1300	363	382	7			
1	G	273	Total	C	N	O	S	0	0	0
			2052	1300	363	382	7			
1	H	273	Total	C	N	O	S	0	0	0
			2052	1300	363	382	7			
1	I	273	Total	C	N	O	S	0	0	0
			2052	1300	363	382	7			
1	J	273	Total	C	N	O	S	0	0	0
			2052	1300	363	382	7			
1	K	273	Total	C	N	O	S	0	0	0
			2052	1300	363	382	7			
1	L	273	Total	C	N	O	S	0	0	0
			2052	1300	363	382	7			
1	M	273	Total	C	N	O	S	0	0	0
			2052	1300	363	382	7			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	26	Total	O	0	0
			26	26		
2	C	12	Total	O	0	0
			12	12		

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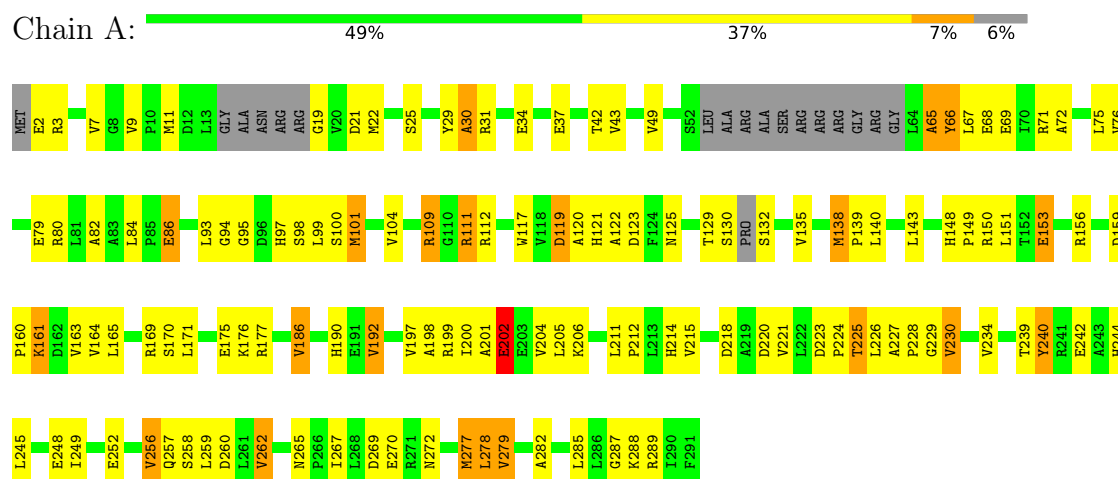
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	9	Total	O	0	0
			9	9		
2	E	18	Total	O	0	0
			18	18		
2	F	17	Total	O	0	0
			17	17		
2	G	10	Total	O	0	0
			10	10		
2	H	19	Total	O	0	0
			19	19		
2	I	14	Total	O	0	0
			14	14		
2	J	17	Total	O	0	0
			17	17		
2	K	5	Total	O	0	0
			5	5		
2	L	17	Total	O	0	0
			17	17		
2	M	11	Total	O	0	0
			11	11		

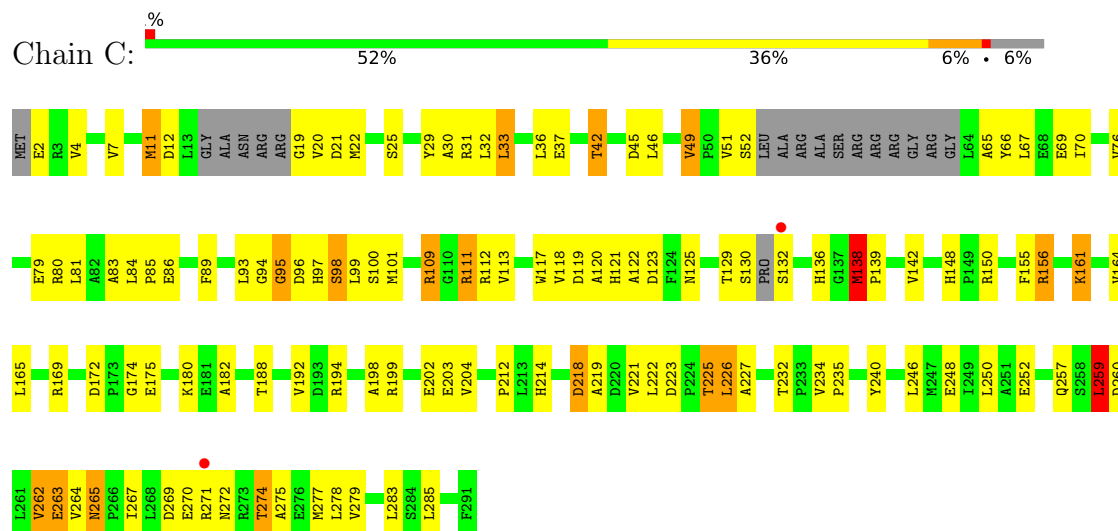
3 Residue-property plots

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

• Molecule 1: Arginase

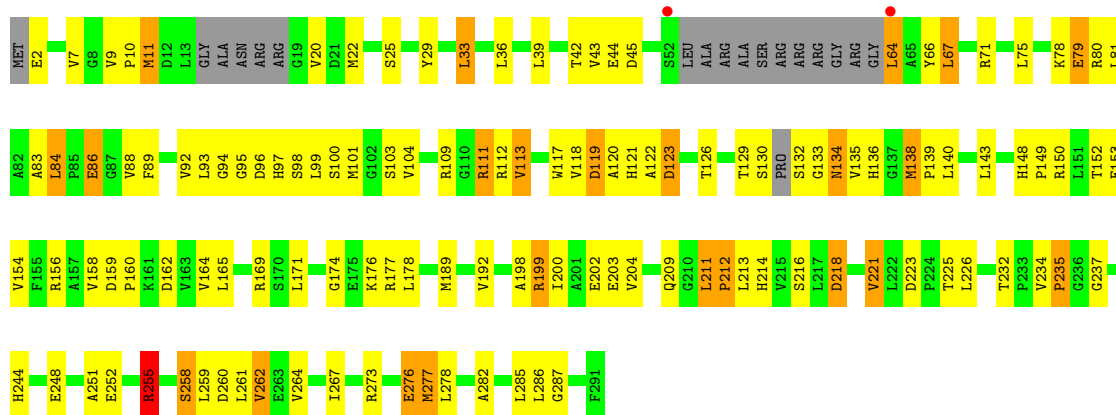


• Molecule 1: Arginase

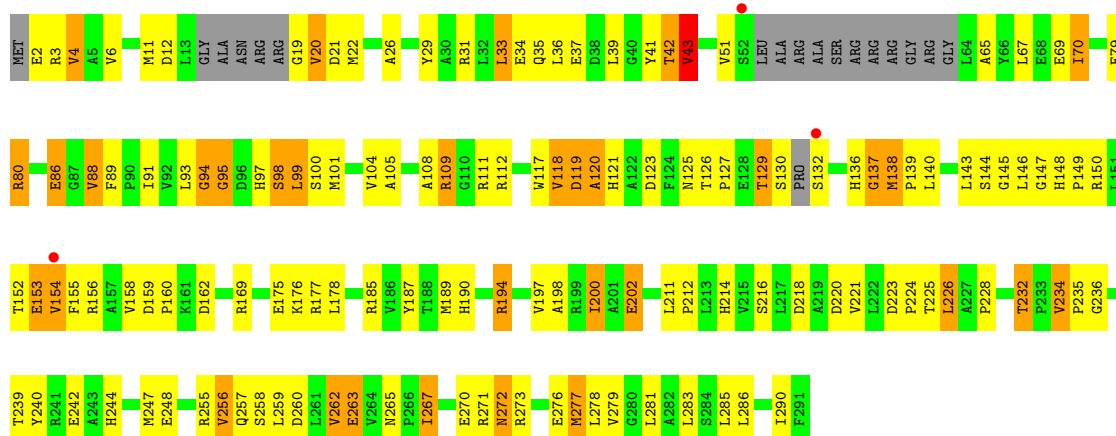


• Molecule 1: Arginase

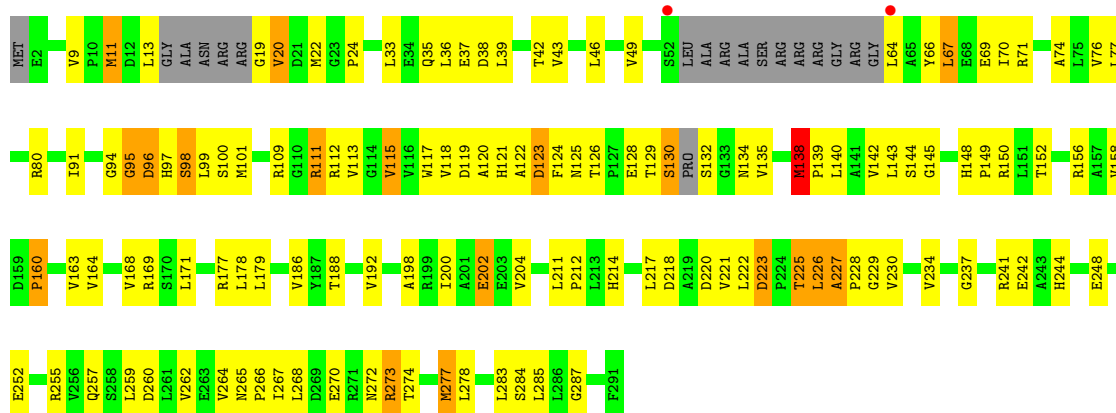




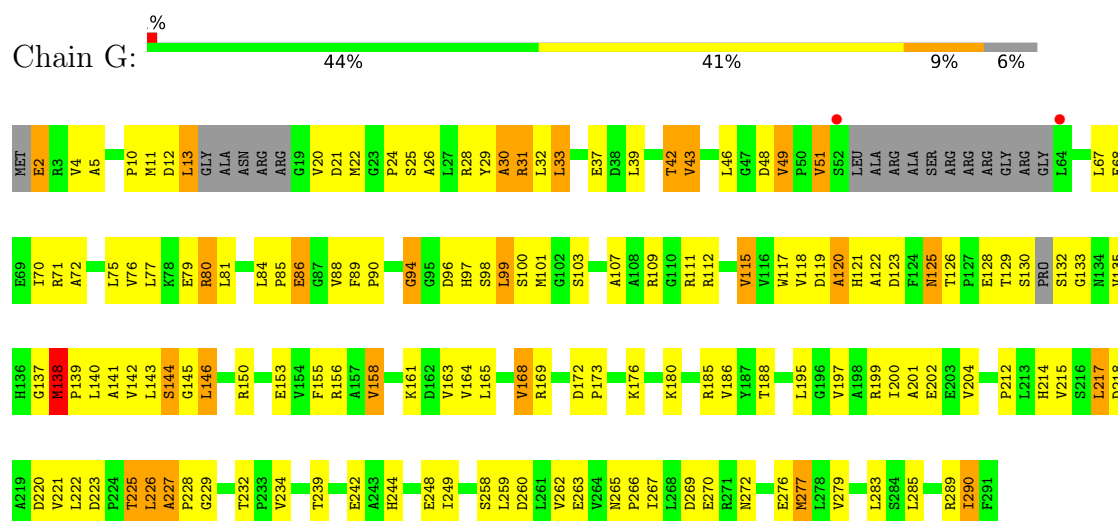
• Molecule 1: Arginase



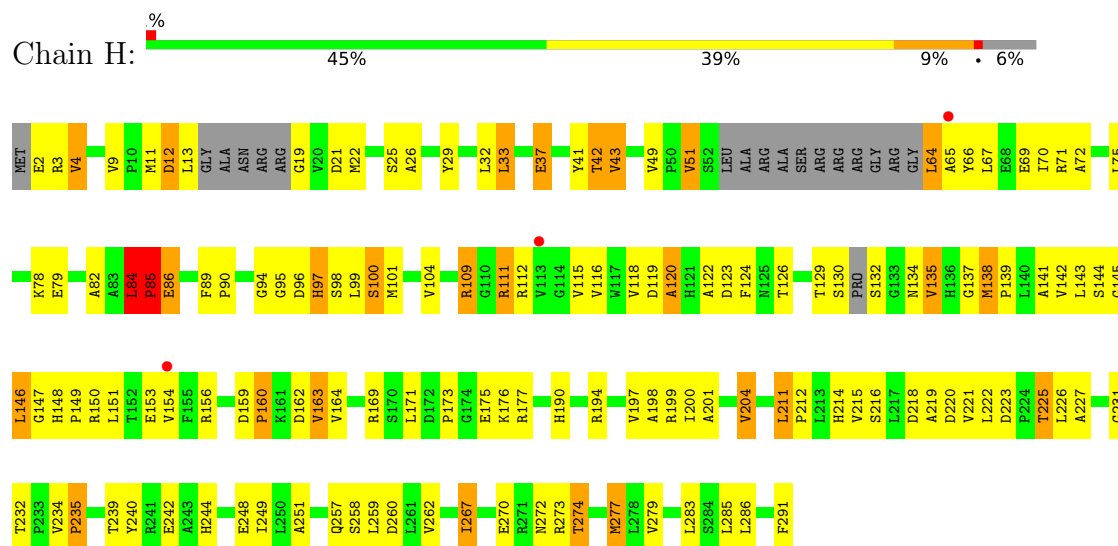
• Molecule 1: Arginase



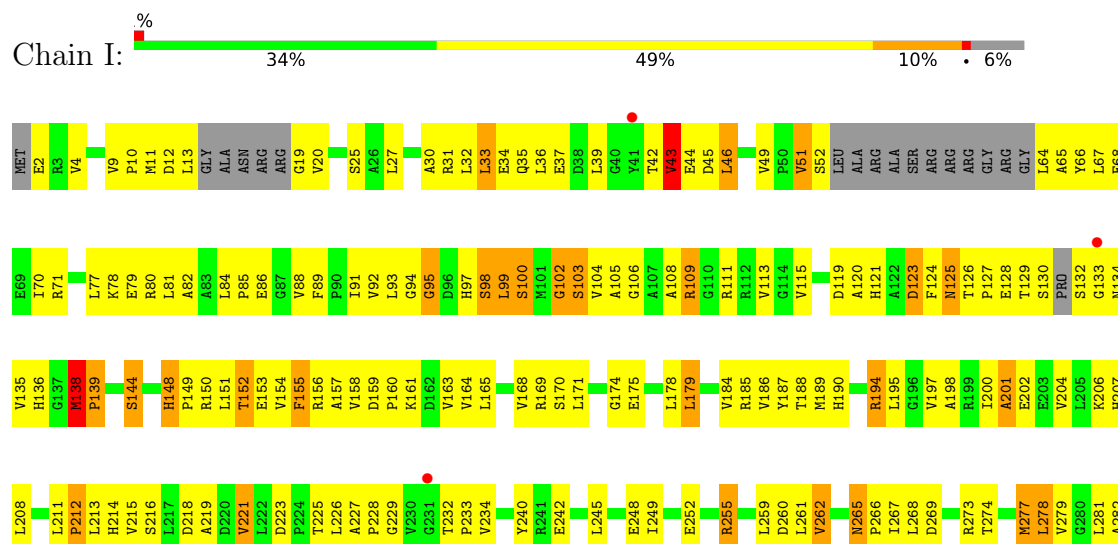
• Molecule 1: Arginase

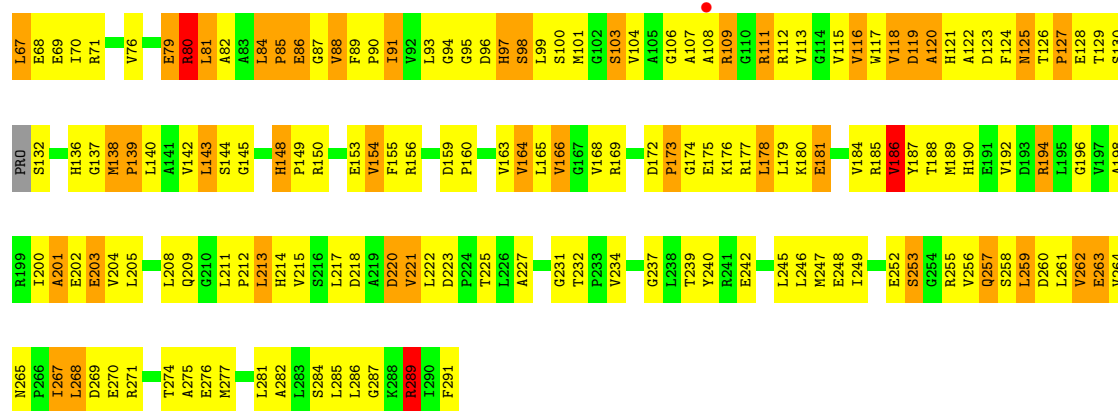


- Molecule 1: Arginase

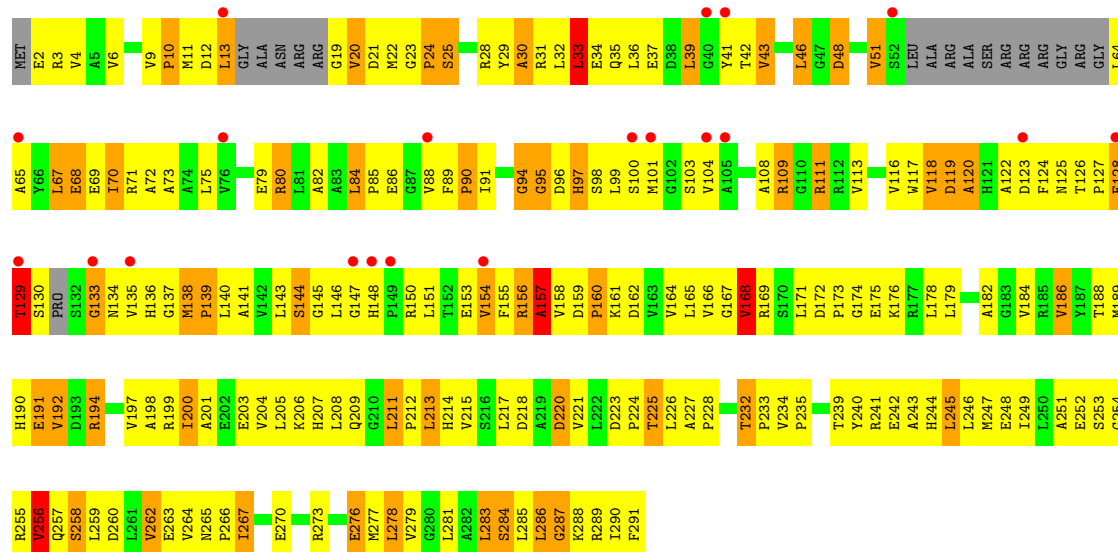


- Molecule 1: Arginase





• Molecule 1: Arginase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	159.98Å 139.89Å 84.37Å 90.00° 90.26° 90.00°	Depositor
Resolution (Å)	20.00 – 2.91 20.00 – 2.91	Depositor EDS
% Data completeness (in resolution range)	98.9 (20.00-2.91) 98.9 (20.00-2.91)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 2.90Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.232 , 0.269 0.231 , 0.268	Depositor DCC
R_{free} test set	4082 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	60.3	Xtriage
Anisotropy	0.511	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 59.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.019 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	24799	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.70	0/2083	1.19	22/2828 (0.8%)
1	C	0.67	0/2083	1.21	22/2828 (0.8%)
1	D	0.65	0/2083	1.20	17/2828 (0.6%)
1	E	0.65	0/2083	1.15	19/2828 (0.7%)
1	F	0.63	0/2083	1.19	17/2828 (0.6%)
1	G	0.63	0/2083	1.20	21/2828 (0.7%)
1	H	0.62	0/2083	1.23	19/2828 (0.7%)
1	I	0.62	0/2083	1.24	19/2828 (0.7%)
1	J	0.60	0/2083	1.16	18/2828 (0.6%)
1	K	0.55	0/2083	1.28	32/2828 (1.1%)
1	L	0.58	0/2083	1.29	30/2828 (1.1%)
1	M	0.59	0/2083	1.36	38/2828 (1.3%)
All	All	0.62	0/24996	1.23	274/33936 (0.8%)

There are no bond length outliers.

All (274) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	138	MET	CA-C-N	-11.91	104.95	119.84
1	K	138	MET	C-N-CA	-11.91	104.95	119.84
1	A	66	TYR	N-CA-C	10.67	126.24	113.23
1	G	67	LEU	N-CA-C	10.36	122.15	111.07
1	M	67	LEU	N-CA-C	10.36	122.65	111.36
1	L	49	VAL	N-CA-C	-10.18	97.86	108.96
1	D	120	ALA	N-CA-C	-9.89	99.94	112.90
1	I	133	GLY	N-CA-C	9.86	136.55	113.18
1	L	213	LEU	N-CA-C	9.85	124.39	110.50
1	H	262	VAL	N-CA-C	9.73	120.69	108.82
1	D	133	GLY	N-CA-C	9.55	127.63	115.21
1	J	95	GLY	N-CA-C	-9.48	90.71	113.18
1	F	76	VAL	N-CA-C	-9.27	101.82	110.53
1	J	43	VAL	N-CA-C	8.89	120.62	108.17
1	K	225	THR	N-CA-C	-8.83	101.11	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	158	VAL	N-CA-CB	-8.73	97.81	112.47
1	K	262	VAL	N-CA-C	8.72	121.53	108.80
1	K	94	GLY	N-CA-C	8.65	126.78	113.02
1	L	287	GLY	N-CA-C	8.65	123.91	113.79
1	C	42	THR	N-CA-C	-8.64	95.44	109.96
1	L	101	MET	N-CA-C	-8.62	101.88	111.28
1	M	158	VAL	N-CA-C	8.40	122.09	108.99
1	M	95	GLY	N-CA-C	-8.32	93.46	113.18
1	C	120	ALA	N-CA-C	-8.18	103.28	113.18
1	F	43	VAL	N-CA-C	8.09	119.78	108.12
1	K	120	ALA	N-CA-C	-8.09	103.19	113.23
1	G	172	ASP	N-CA-C	-8.09	100.83	110.13
1	I	95	GLY	N-CA-C	-8.02	94.17	113.18
1	C	94	GLY	N-CA-C	8.00	122.78	111.10
1	E	120	ALA	N-CA-C	-7.95	103.58	113.28
1	K	290	ILE	N-CA-C	-7.92	102.97	110.42
1	D	262	VAL	N-CA-C	7.91	120.34	108.80
1	M	227	ALA	CA-C-N	7.84	127.76	119.05
1	M	227	ALA	C-N-CA	7.84	127.76	119.05
1	F	120	ALA	N-CA-C	-7.83	103.87	113.50
1	G	212	PRO	N-CA-C	-7.72	99.11	111.38
1	M	133	GLY	N-CA-C	7.70	131.43	113.18
1	L	263	GLU	N-CA-C	7.69	122.61	113.23
1	K	30	ALA	N-CA-C	-7.69	104.32	112.93
1	M	94	GLY	N-CA-C	7.65	125.19	113.02
1	J	287	GLY	N-CA-C	7.65	124.87	114.92
1	K	137	GLY	N-CA-C	-7.64	102.32	115.61
1	H	49	VAL	N-CA-C	-7.62	101.48	108.95
1	G	120	ALA	N-CA-C	-7.60	103.81	113.23
1	M	48	ASP	N-CA-C	7.58	121.48	109.50
1	A	95	GLY	N-CA-C	-7.55	95.29	113.18
1	L	43	VAL	N-CA-C	7.54	118.72	108.17
1	F	134	ASN	N-CA-C	7.53	121.60	110.30
1	L	203	GLU	N-CA-C	7.49	119.53	111.36
1	C	182	ALA	N-CA-C	7.39	120.39	111.82
1	H	120	ALA	N-CA-C	-7.38	104.08	113.23
1	E	43	VAL	N-CA-C	7.35	118.40	108.11
1	L	84	LEU	N-CA-C	7.35	120.07	109.48
1	D	78	LYS	N-CA-C	-7.34	103.27	111.71
1	D	42	THR	N-CA-C	-7.30	95.07	107.99
1	L	119	ASP	N-CA-C	-7.29	99.42	110.14
1	L	97	HIS	N-CA-C	-7.24	103.92	112.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	70	ILE	N-CA-C	-7.15	102.79	110.23
1	G	227	ALA	CA-C-N	7.15	126.65	118.85
1	G	227	ALA	C-N-CA	7.15	126.65	118.85
1	M	262	VAL	N-CA-C	7.13	120.26	109.20
1	K	43	VAL	N-CA-C	7.11	118.82	108.58
1	I	120	ALA	N-CA-C	-7.09	104.37	113.16
1	I	212	PRO	N-CA-C	-7.05	100.86	111.57
1	L	262	VAL	N-CA-C	7.02	117.70	110.05
1	L	94	GLY	N-CA-C	7.01	123.98	110.66
1	M	69	GLU	N-CA-C	-6.96	104.92	113.41
1	G	155	PHE	N-CA-C	6.96	122.77	113.72
1	E	95	GLY	N-CA-C	-6.92	96.79	113.18
1	F	95	GLY	N-CA-C	-6.90	96.83	113.18
1	J	120	ALA	N-CA-C	-6.89	104.34	112.89
1	L	34	GLU	N-CA-C	-6.89	102.88	112.45
1	C	262	VAL	N-CA-C	6.87	118.72	108.96
1	H	212	PRO	N-CA-C	-6.87	100.46	111.38
1	H	95	GLY	N-CA-C	-6.76	97.15	113.18
1	E	256	VAL	N-CA-C	-6.76	100.02	109.21
1	L	180	LYS	N-CA-C	-6.76	103.91	111.28
1	A	120	ALA	N-CA-C	-6.72	105.08	113.28
1	M	70	ILE	N-CA-C	-6.69	104.25	110.53
1	L	120	ALA	N-CA-C	-6.65	105.17	113.28
1	C	265	ASN	CA-C-N	6.62	126.39	119.05
1	C	265	ASN	C-N-CA	6.62	126.39	119.05
1	J	225	THR	N-CA-C	-6.59	104.17	111.36
1	K	37	GLU	N-CA-C	-6.58	104.03	111.14
1	H	37	GLU	N-CA-C	-6.58	104.11	111.28
1	I	265	ASN	CA-C-N	6.57	126.26	119.56
1	I	265	ASN	C-N-CA	6.57	126.26	119.56
1	K	213	LEU	N-CA-C	6.55	120.08	109.40
1	L	42	THR	N-CA-C	-6.55	98.05	108.73
1	M	157	ALA	CB-CA-C	6.54	123.42	110.42
1	C	212	PRO	N-CA-C	-6.53	100.93	111.19
1	A	202	GLU	N-CA-C	-6.53	104.16	111.28
1	K	148	HIS	CA-C-N	6.53	128.00	119.84
1	K	148	HIS	C-N-CA	6.53	128.00	119.84
1	M	30	ALA	N-CA-C	-6.53	105.43	113.19
1	K	25	SER	N-CA-C	6.50	119.19	111.33
1	L	115	VAL	N-CA-C	6.49	116.98	107.37
1	F	227	ALA	CA-C-N	6.46	125.96	119.24
1	F	227	ALA	C-N-CA	6.46	125.96	119.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	11	MET	N-CA-C	6.45	119.04	108.52
1	M	156	ARG	N-CA-C	-6.41	102.07	110.53
1	A	262	VAL	N-CA-C	6.40	122.65	109.34
1	E	119	ASP	N-CA-C	-6.34	100.10	109.81
1	H	124	PHE	N-CA-C	6.34	121.89	112.94
1	A	93	LEU	CA-C-N	-6.34	116.53	122.17
1	A	93	LEU	C-N-CA	-6.34	116.53	122.17
1	L	181	GLU	N-CA-C	6.33	118.18	111.28
1	I	155	PHE	N-CA-C	6.30	122.44	114.31
1	G	94	GLY	N-CA-C	6.29	122.62	110.66
1	M	232	THR	CA-C-N	-6.29	113.81	120.03
1	M	232	THR	C-N-CA	-6.29	113.81	120.03
1	H	43	VAL	N-CA-C	6.24	116.87	107.75
1	C	65	ALA	N-CA-C	6.24	119.09	110.35
1	C	49	VAL	CA-C-N	-6.18	112.72	120.51
1	C	49	VAL	C-N-CA	-6.18	112.72	120.51
1	D	287	GLY	N-CA-C	6.18	122.95	114.92
1	I	148	HIS	CA-C-N	6.17	127.56	119.84
1	I	148	HIS	C-N-CA	6.17	127.56	119.84
1	M	42	THR	N-CA-C	-6.15	100.54	109.59
1	E	262	VAL	N-CA-C	6.14	118.01	109.29
1	M	119	ASP	N-CA-C	-6.14	100.00	109.52
1	C	259	LEU	N-CA-C	6.14	119.49	109.06
1	L	186	VAL	N-CA-C	6.13	117.54	107.24
1	D	11	MET	N-CA-C	6.10	118.68	108.73
1	L	155	PHE	N-CA-C	6.09	120.87	113.38
1	M	75	LEU	N-CA-C	-6.07	104.29	111.03
1	C	274	THR	N-CA-C	-6.05	104.25	111.69
1	A	43	VAL	N-CA-C	6.03	117.17	108.48
1	G	42	THR	N-CA-C	-6.02	99.38	108.96
1	M	205	LEU	N-CA-C	-5.99	104.87	111.82
1	G	49	VAL	CA-C-N	5.97	126.32	119.93
1	G	49	VAL	C-N-CA	5.97	126.32	119.93
1	K	287	GLY	N-CA-C	5.97	122.91	114.85
1	M	127	PRO	N-CA-C	-5.97	106.28	113.98
1	M	256	VAL	CB-CA-C	-5.97	105.47	111.80
1	D	212	PRO	N-CA-C	-5.96	101.90	111.38
1	C	95	GLY	N-CA-C	-5.96	99.05	113.18
1	I	42	THR	N-CA-C	-5.95	99.50	108.96
1	C	70	ILE	N-CA-C	-5.95	104.53	110.30
1	J	213	LEU	N-CA-C	5.93	119.72	110.17
1	H	190	HIS	N-CA-C	-5.93	104.16	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	97	HIS	N-CA-C	-5.92	105.91	113.01
1	F	115	VAL	N-CA-C	5.90	116.30	107.51
1	M	120	ALA	N-CA-C	-5.87	104.83	112.23
1	K	154	VAL	N-CA-C	5.87	118.83	113.20
1	M	101	MET	N-CA-C	-5.85	103.89	111.02
1	F	42	THR	N-CA-C	-5.83	100.98	110.20
1	G	43	VAL	N-CA-C	5.83	116.88	108.48
1	H	137	GLY	N-CA-C	-5.82	105.97	115.46
1	I	195	LEU	N-CA-C	5.82	121.04	113.88
1	M	65	ALA	N-CA-C	5.81	123.17	110.80
1	M	225	THR	N-CA-C	-5.80	104.96	111.28
1	L	282	ALA	N-CA-C	-5.78	104.58	111.69
1	G	126	THR	CA-C-N	-5.78	113.72	119.56
1	G	126	THR	C-N-CA	-5.78	113.72	119.56
1	A	282	ALA	N-CA-C	-5.75	104.93	111.14
1	H	84	LEU	N-CA-C	5.74	122.49	109.81
1	E	212	PRO	N-CA-C	-5.72	102.28	111.38
1	K	95	GLY	N-CA-C	-5.72	99.61	113.18
1	K	259	LEU	N-CA-C	5.71	118.51	108.75
1	J	205	LEU	N-CA-C	-5.69	104.94	112.34
1	G	217	LEU	N-CA-C	5.67	118.02	107.99
1	I	134	ASN	N-CA-C	5.66	118.40	109.96
1	A	42	THR	N-CA-C	-5.65	99.97	108.96
1	J	262	VAL	N-CA-C	5.63	121.05	109.34
1	M	73	ALA	N-CA-C	5.63	117.11	110.97
1	M	186	VAL	N-CA-C	5.63	115.96	107.80
1	A	101	MET	N-CA-C	-5.62	105.15	111.28
1	L	148	HIS	CA-C-N	5.61	124.80	118.97
1	L	148	HIS	C-N-CA	5.61	124.80	118.97
1	G	290	ILE	N-CA-C	-5.60	105.38	110.82
1	G	30	ALA	N-CA-C	-5.58	106.50	113.15
1	K	179	LEU	N-CA-C	-5.58	104.84	111.03
1	A	287	GLY	N-CA-C	5.57	121.39	114.37
1	E	93	LEU	CA-C-N	-5.57	116.55	122.67
1	E	93	LEU	C-N-CA	-5.57	116.55	122.67
1	G	31	ARG	N-CA-C	5.54	119.33	112.24
1	A	119	ASP	N-CA-C	-5.54	100.88	109.24
1	I	65	ALA	N-CA-C	5.53	118.82	110.64
1	H	134	ASN	N-CA-C	5.52	117.70	109.25
1	E	94	GLY	N-CA-C	5.52	121.22	112.06
1	M	228	PRO	N-CA-C	5.51	121.19	113.53
1	J	279	VAL	N-CA-C	-5.51	104.20	111.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	76	VAL	N-CA-C	-5.51	104.16	111.05
1	L	201	ALA	N-CA-C	-5.50	104.97	110.97
1	K	8	GLY	N-CA-C	5.49	119.11	110.71
1	A	256	VAL	N-CA-C	-5.49	101.73	109.63
1	L	103	SER	N-CA-C	5.48	118.44	111.69
1	M	213	LEU	N-CA-C	5.48	118.42	109.59
1	K	119	ASP	N-CA-C	-5.47	100.99	109.14
1	G	186	VAL	N-CA-C	5.46	115.85	107.77
1	J	42	THR	N-CA-C	-5.46	99.51	108.41
1	D	93	LEU	N-CA-C	-5.45	101.28	109.95
1	A	49	VAL	N-CA-C	-5.43	103.96	108.63
1	J	9	VAL	CA-C-N	5.43	126.62	119.84
1	J	9	VAL	C-N-CA	5.43	126.62	119.84
1	C	218	ASP	N-CA-C	-5.42	100.47	109.46
1	F	223	ASP	CA-C-N	5.41	125.12	119.82
1	F	223	ASP	C-N-CA	5.41	125.12	119.82
1	F	262	VAL	N-CA-C	5.38	120.54	109.34
1	D	36	LEU	N-CA-C	-5.37	105.51	111.36
1	A	279	VAL	N-CA-C	-5.35	104.53	110.62
1	C	93	LEU	N-CA-C	-5.34	102.57	110.48
1	K	212	PRO	N-CA-C	-5.34	101.17	111.69
1	H	42	THR	N-CA-C	-5.33	100.55	109.24
1	J	115	VAL	N-CA-C	5.33	115.53	107.80
1	D	218	ASP	N-CA-C	-5.33	101.78	110.20
1	E	263	GLU	N-CA-C	5.33	119.06	112.24
1	I	43	VAL	N-CA-C	5.33	115.63	108.17
1	J	212	PRO	N-CA-C	-5.31	102.82	111.68
1	K	218	ASP	N-CA-C	-5.28	101.36	109.76
1	I	287	GLY	N-CA-C	5.28	121.02	114.37
1	K	36	LEU	N-CA-C	-5.27	105.59	112.23
1	J	148	HIS	CA-C-N	5.27	125.58	119.47
1	J	148	HIS	C-N-CA	5.27	125.58	119.47
1	L	139	PRO	N-CA-C	5.26	121.59	113.75
1	G	115	VAL	N-CA-C	5.26	115.15	107.37
1	I	201	ALA	N-CA-C	-5.25	105.45	111.07
1	J	163	VAL	N-CA-C	5.24	116.13	108.53
1	H	163	VAL	N-CA-C	5.23	116.91	108.85
1	A	30	ALA	N-CA-C	-5.23	106.93	113.15
1	E	65	ALA	N-CA-C	5.22	118.14	110.30
1	M	290	ILE	N-CA-C	-5.22	105.62	110.53
1	F	217	LEU	N-CA-C	5.22	117.16	108.02
1	L	48	ASP	N-CA-C	5.22	117.96	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	20	VAL	N-CA-C	5.21	120.18	109.34
1	L	245	LEU	N-CA-C	-5.21	105.50	111.07
1	M	287	GLY	N-CA-C	5.21	122.29	115.36
1	D	134	ASN	CB-CA-C	5.21	117.65	109.84
1	K	232	THR	CA-C-N	5.21	126.35	119.84
1	K	232	THR	C-N-CA	5.21	126.35	119.84
1	M	97	HIS	N-CA-C	-5.21	106.99	113.19
1	M	251	ALA	N-CA-C	-5.20	105.53	111.14
1	G	77	LEU	N-CA-C	-5.18	105.33	110.97
1	F	272	ASN	N-CA-C	5.17	118.89	112.58
1	J	65	ALA	N-CA-C	5.17	121.81	110.80
1	H	135	VAL	N-CA-C	5.16	116.50	110.62
1	L	289	ARG	N-CA-C	5.16	116.68	108.79
1	M	235	PRO	N-CA-C	5.15	118.43	111.22
1	K	186	VAL	N-CA-C	5.14	115.67	108.17
1	C	172	ASP	CA-C-N	5.13	124.58	119.24
1	C	172	ASP	C-N-CA	5.13	124.58	119.24
1	E	129	THR	N-CA-C	5.13	119.41	113.20
1	E	137	GLY	N-CA-C	-5.12	106.89	115.80
1	A	186	VAL	N-CA-C	5.12	115.22	107.75
1	F	49	VAL	CA-C-N	-5.12	114.97	120.03
1	F	49	VAL	C-N-CA	-5.12	114.97	120.03
1	E	42	THR	N-CA-C	-5.11	100.91	109.24
1	A	212	PRO	N-CA-C	-5.11	103.25	111.38
1	E	105	ALA	N-CA-C	-5.11	105.60	111.07
1	D	159	ASP	N-CA-C	-5.11	103.64	110.07
1	F	287	GLY	N-CA-C	5.09	120.79	114.37
1	A	66	TYR	N-CA-CB	-5.09	104.43	112.63
1	A	272	ASN	N-CA-C	5.08	118.60	111.74
1	E	234	VAL	CA-C-N	5.07	126.18	119.84
1	E	234	VAL	C-N-CA	5.07	126.18	119.84
1	C	263	GLU	N-CA-C	5.07	118.73	112.24
1	H	4	VAL	N-CA-C	5.07	115.56	108.17
1	H	126	THR	N-CA-C	-5.06	100.05	109.06
1	C	37	GLU	N-CA-C	-5.06	105.67	111.14
1	M	51	VAL	N-CA-C	5.06	115.94	108.45
1	A	192	VAL	N-CA-C	-5.06	105.77	110.53
1	D	88	VAL	N-CA-C	5.05	114.56	106.88
1	K	7	VAL	N-CA-C	5.05	115.99	108.46
1	I	30	ALA	N-CA-C	-5.05	106.81	113.17
1	H	274	THR	N-CA-C	-5.04	105.78	111.28
1	M	245	LEU	N-CA-C	-5.03	105.26	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	262	VAL	CB-CA-C	-5.02	106.06	111.59
1	C	11	MET	N-CA-C	5.01	116.69	108.52
1	D	235	PRO	N-CA-C	5.01	119.08	111.11
1	I	123	ASP	N-CA-C	-5.01	104.73	111.54
1	D	255	ARG	N-CA-C	5.00	118.43	112.72
1	D	119	ASP	N-CA-C	-5.00	101.77	109.52
1	I	82	ALA	N-CA-C	-5.00	105.83	111.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2052	0	2101	132	0
1	C	2052	0	2101	132	0
1	D	2052	0	2101	140	0
1	E	2052	0	2101	129	0
1	F	2052	0	2101	112	0
1	G	2052	0	2101	117	0
1	H	2052	0	2101	146	0
1	I	2052	0	2101	153	0
1	J	2052	0	2101	166	0
1	K	2052	0	2101	198	0
1	L	2052	0	2101	195	0
1	M	2052	0	2101	242	0
2	A	26	0	0	1	0
2	C	12	0	0	2	0
2	D	9	0	0	2	0
2	E	18	0	0	4	0
2	F	17	0	0	2	0
2	G	10	0	0	2	0
2	H	19	0	0	2	0
2	I	14	0	0	1	0
2	J	17	0	0	3	0
2	K	5	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	L	17	0	0	6	0
2	M	11	0	0	6	0
All	All	24799	0	25212	1779	0

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 36.

All (1779) 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:A:111:ARG:NH2	1:D:79:GLU:HA	1.57	1.19
1:F:111:ARG:HD3	1:F:112:ARG:N	1.62	1.14
1:F:111:ARG:HD3	1:F:112:ARG:H	0.97	1.11
1:H:109:ARG:HH11	1:H:109:ARG:HG2	1.05	1.11
1:A:79:GLU:HB3	1:D:111:ARG:HH22	1.16	1.10
1:J:109:ARG:HB3	1:J:109:ARG:HH11	1.11	1.10
1:C:109:ARG:HG2	1:C:109:ARG:HH11	0.92	1.09
1:H:111:ARG:HD3	1:H:112:ARG:H	1.17	1.08
1:F:130:SER:HG	1:F:132:SER:N	1.52	1.08
1:L:111:ARG:HD3	1:L:112:ARG:H	1.14	1.06
1:M:138:MET:H	1:M:139:PRO:HD2	1.17	1.04
1:M:129:THR:HB	1:M:174:GLY:HA3	1.38	1.03
1:G:145:GLY:HA2	1:G:156:ARG:HD3	1.39	1.01
1:K:113:VAL:HG12	1:K:212:PRO:HG2	1.41	1.01
1:K:130:SER:HG	1:K:132:SER:N	1.59	0.98
1:L:109:ARG:HG2	1:L:109:ARG:HH11	1.26	0.98
1:J:130:SER:HG	1:J:132:SER:N	1.61	0.98
1:H:111:ARG:CD	1:H:112:ARG:H	1.77	0.97
1:C:109:ARG:HG2	1:C:109:ARG:NH1	1.72	0.96
1:I:25:SER:HB3	1:M:22:MET:HE3	1.48	0.94
1:J:72:ALA:O	1:J:76:VAL:HG23	1.66	0.94
1:L:138:MET:H	1:L:139:PRO:HD2	1.32	0.94
1:M:113:VAL:HA	2:M:296:HOH:O	1.68	0.93
1:A:111:ARG:HH21	1:D:79:GLU:HA	1.13	0.93
1:M:140:LEU:HA	1:M:143:LEU:HD12	1.50	0.93
1:M:145:GLY:HA3	1:M:156:ARG:HH11	1.32	0.93
1:C:83:ALA:C	1:H:111:ARG:HH12	1.77	0.93
1:M:199:ARG:O	1:M:203:GLU:HG3	1.69	0.92
1:C:86:GLU:HG2	1:C:109:ARG:HE	1.35	0.92
1:K:111:ARG:HD3	1:K:112:ARG:H	1.34	0.92
1:C:271:ARG:NH2	1:K:228:PRO:HB2	1.84	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:111:ARG:HA	1:H:111:ARG:HE	1.34	0.91
1:H:111:ARG:HD3	1:H:112:ARG:N	1.85	0.91
1:M:80:ARG:HG2	1:M:80:ARG:HH11	1.36	0.91
1:M:138:MET:N	1:M:139:PRO:HD2	1.85	0.91
1:E:138:MET:N	1:E:139:PRO:HD2	1.86	0.91
1:G:101:MET:HA	1:G:143:LEU:HD21	1.53	0.91
1:I:130:SER:HG	1:I:132:SER:N	1.68	0.90
1:A:22:MET:HE3	1:H:25:SER:HB2	1.52	0.90
1:K:123:ASP:HB3	1:K:139:PRO:HD2	1.52	0.90
1:K:227:ALA:HB1	1:K:274:THR:HG23	1.53	0.90
1:A:79:GLU:CB	1:D:111:ARG:HH22	1.85	0.90
1:H:109:ARG:HG2	1:H:109:ARG:NH1	1.85	0.90
1:H:223:ASP:OD2	1:H:225:THR:HB	1.72	0.90
1:J:216:SER:HA	1:J:260:ASP:HB2	1.51	0.90
1:G:117:TRP:HB3	1:G:165:LEU:HD23	1.52	0.89
1:K:259:LEU:HD22	1:K:285:LEU:HD23	1.55	0.89
1:H:4:VAL:HG22	1:H:89:PHE:HB3	1.53	0.89
1:A:111:ARG:NH2	1:D:79:GLU:CA	2.34	0.88
1:H:111:ARG:HA	1:H:111:ARG:NE	1.84	0.88
1:J:109:ARG:HB3	1:J:109:ARG:NH1	1.89	0.88
1:E:138:MET:H	1:E:139:PRO:HD2	1.38	0.88
1:M:153:GLU:HG3	1:M:154:VAL:H	1.39	0.88
1:C:79:GLU:HB2	1:H:86:GLU:OE1	1.73	0.87
1:I:197:VAL:HG21	1:I:242:GLU:HB3	1.57	0.87
1:H:197:VAL:HG21	1:H:242:GLU:HG2	1.55	0.87
1:L:33:LEU:HD23	1:L:43:VAL:HB	1.56	0.87
1:D:111:ARG:HE	1:D:112:ARG:H	1.23	0.87
1:I:227:ALA:HB1	1:I:274:THR:HG23	1.56	0.87
1:K:164:VAL:HG23	1:K:208:LEU:HD11	1.56	0.86
1:K:129:THR:O	1:K:130:SER:HB2	1.75	0.85
1:J:164:VAL:HG11	1:J:204:VAL:HG22	1.58	0.85
1:M:34:GLU:CD	1:M:34:GLU:H	1.85	0.85
1:M:111:ARG:HA	1:M:111:ARG:HE	1.41	0.85
1:L:111:ARG:HD3	1:L:112:ARG:N	1.92	0.85
1:C:148:HIS:HD2	1:C:150:ARG:H	1.25	0.85
1:A:111:ARG:HD3	1:A:112:ARG:H	1.42	0.85
1:J:125:ASN:ND2	1:J:175:GLU:HG3	1.92	0.85
1:L:223:ASP:HB3	1:L:225:THR:HG22	1.58	0.85
1:M:82:ALA:HA	1:M:109:ARG:HH12	1.42	0.85
1:C:83:ALA:HB1	1:H:111:ARG:CZ	2.07	0.84
1:I:36:LEU:HD21	1:I:286:LEU:HD23	1.59	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:125:ASN:O	1:G:138:MET:HB3	1.78	0.84
1:A:111:ARG:HH12	1:D:83:ALA:HB2	1.42	0.84
1:L:25:SER:O	1:L:29:TYR:HD2	1.60	0.84
1:E:197:VAL:HG21	1:E:242:GLU:HG2	1.58	0.84
1:I:67:LEU:C	1:I:67:LEU:HD23	2.02	0.84
1:F:111:ARG:CD	1:F:112:ARG:H	1.88	0.83
1:H:109:ARG:HH11	1:H:109:ARG:CG	1.91	0.83
1:H:239:THR:OG1	1:H:242:GLU:HB2	1.78	0.83
1:I:4:VAL:HG22	1:I:89:PHE:HB3	1.60	0.83
1:J:156:ARG:HG2	1:J:156:ARG:HH11	1.42	0.83
1:F:244:HIS:O	1:F:248:GLU:HG3	1.79	0.83
1:J:195:LEU:HD12	1:J:200:ILE:HD11	1.60	0.83
1:L:4:VAL:HG22	1:L:89:PHE:HB3	1.58	0.83
1:F:148:HIS:HD2	1:F:150:ARG:H	1.27	0.83
1:J:109:ARG:HH11	1:J:109:ARG:CB	1.89	0.83
1:J:66:TYR:O	1:J:70:ILE:HD13	1.79	0.82
1:M:226:LEU:HD21	1:M:240:TYR:HB2	1.59	0.82
1:H:82:ALA:HA	1:H:109:ARG:HH12	1.44	0.82
1:C:83:ALA:O	1:H:111:ARG:NH1	2.13	0.81
1:K:200:ILE:O	1:K:204:VAL:HG23	1.79	0.81
1:L:138:MET:N	1:L:139:PRO:HD2	1.95	0.81
1:L:215:VAL:HG21	1:L:285:LEU:HD21	1.61	0.81
1:I:138:MET:N	1:I:139:PRO:HD2	1.94	0.81
1:L:138:MET:H	1:L:139:PRO:CD	1.92	0.81
1:A:138:MET:N	1:A:139:PRO:HD2	1.96	0.81
1:L:138:MET:HA	2:L:301:HOH:O	1.80	0.81
1:L:190:HIS:HE1	1:L:194:ARG:HE	1.27	0.81
1:M:36:LEU:HD21	1:M:286:LEU:HD23	1.62	0.80
1:A:79:GLU:HB3	1:D:111:ARG:NH2	1.96	0.80
1:F:227:ALA:HB1	1:F:274:THR:HG23	1.63	0.80
1:J:138:MET:N	1:J:139:PRO:HD2	1.96	0.80
1:L:165:LEU:HD12	1:L:186:VAL:CG2	2.11	0.80
1:M:13:LEU:HD12	1:M:70:ILE:HG12	1.61	0.80
1:E:119:ASP:HA	1:E:218:ASP:HB3	1.64	0.80
1:D:11:MET:HE3	1:D:98:SER:HB2	1.63	0.80
1:F:119:ASP:OD2	1:F:123:ASP:OD2	2.00	0.80
1:M:113:VAL:HG12	1:M:212:PRO:HG2	1.61	0.80
1:C:25:SER:HB2	1:K:22:MET:HE3	1.65	0.79
1:E:37:GLU:HG2	1:E:43:VAL:HG23	1.64	0.79
1:E:130:SER:HG	1:E:132:SER:N	1.80	0.79
1:H:216:SER:HA	1:H:260:ASP:HB2	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:SER:HG	1:A:132:SER:N	1.80	0.79
1:C:109:ARG:HH11	1:C:109:ARG:CG	1.85	0.79
1:G:197:VAL:HG21	1:G:242:GLU:HB3	1.63	0.79
1:E:153:GLU:HG3	1:E:154:VAL:HG13	1.65	0.78
1:K:193:ASP:HB3	1:M:245:LEU:HD22	1.65	0.78
1:M:211:LEU:HB3	2:M:296:HOH:O	1.83	0.78
1:C:218:ASP:OD2	2:C:292:HOH:O	1.99	0.78
1:M:208:LEU:O	1:M:211:LEU:HG	1.83	0.78
1:K:144:SER:HB3	1:K:160:PRO:HG3	1.66	0.78
1:F:259:LEU:HD13	1:F:285:LEU:HD23	1.65	0.78
1:E:120:ALA:HB2	1:E:220:ASP:O	1.82	0.78
1:M:218:ASP:HA	1:M:262:VAL:HG23	1.65	0.78
1:A:111:ARG:HD3	1:A:112:ARG:N	1.98	0.78
1:H:259:LEU:HD13	1:H:285:LEU:HD23	1.66	0.78
1:I:164:VAL:HG22	1:I:185:ARG:HB3	1.66	0.78
1:M:12:ASP:HB2	1:M:21:ASP:HB3	1.66	0.78
1:E:145:GLY:O	1:E:146:LEU:HD23	1.84	0.77
1:G:138:MET:N	1:G:139:PRO:HD2	1.99	0.77
1:M:168:VAL:HG12	1:M:188:THR:HA	1.67	0.77
1:G:109:ARG:HG2	1:G:109:ARG:HH11	1.50	0.77
1:G:12:ASP:O	1:G:13:LEU:HD23	1.85	0.77
1:G:272:ASN:O	1:G:276:GLU:HG3	1.84	0.77
1:M:109:ARG:HG2	1:M:109:ARG:HH11	1.49	0.77
1:C:84:LEU:O	1:C:109:ARG:NH2	2.19	0.76
1:C:97:HIS:ND1	1:C:123:ASP:OD2	2.18	0.76
1:L:122:ALA:HB3	1:L:175:GLU:OE2	1.84	0.76
1:C:164:VAL:HG11	1:C:204:VAL:HG22	1.66	0.76
1:A:149:PRO:O	1:A:153:GLU:HB3	1.85	0.76
1:I:109:ARG:HG2	1:I:109:ARG:HH11	1.48	0.76
1:K:109:ARG:HB3	1:K:109:ARG:HH11	1.50	0.76
1:K:19:GLY:HA3	1:K:265:ASN:ND2	2.01	0.76
1:A:111:ARG:HH22	1:D:79:GLU:C	1.92	0.76
1:J:99:LEU:C	1:J:99:LEU:HD12	2.11	0.76
1:K:12:ASP:HB2	1:K:21:ASP:HB3	1.68	0.76
1:M:111:ARG:HA	1:M:111:ARG:NE	1.99	0.76
1:M:146:LEU:HD13	1:M:178:LEU:HD22	1.67	0.76
1:F:101:MET:HA	1:F:143:LEU:HD21	1.67	0.75
1:C:19:GLY:N	1:C:265:ASN:HD21	1.84	0.75
1:G:4:VAL:HG22	1:G:89:PHE:HB3	1.68	0.75
1:M:138:MET:H	1:M:139:PRO:CD	1.97	0.75
1:D:11:MET:CE	1:D:98:SER:HB2	2.15	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:100:SER:HA	1:J:103:SER:OG	1.86	0.75
1:J:168:VAL:HG11	1:J:171:LEU:HD21	1.69	0.75
1:K:165:LEU:HD12	1:K:186:VAL:HG22	1.69	0.75
1:H:11:MET:CE	1:H:98:SER:HB2	2.17	0.75
1:M:145:GLY:HA2	1:M:156:ARG:CG	2.17	0.75
1:G:115:VAL:HG23	1:G:158:VAL:HG21	1.69	0.75
1:M:168:VAL:HG21	1:M:171:LEU:HD21	1.69	0.75
1:J:272:ASN:O	1:J:276:GLU:HG3	1.87	0.74
1:M:97:HIS:ND1	1:M:123:ASP:OD2	2.20	0.74
1:F:130:SER:OG	1:F:132:SER:N	2.20	0.74
1:M:126:THR:HG22	1:M:147:GLY:HA2	1.69	0.74
1:L:109:ARG:HH11	1:L:109:ARG:CG	1.99	0.74
1:D:22:MET:HE3	1:J:25:SER:HB2	1.68	0.74
1:I:169:ARG:NH1	1:I:234:VAL:O	2.20	0.74
1:M:36:LEU:CD2	1:M:286:LEU:HD23	2.16	0.74
1:L:198:ALA:O	1:L:202:GLU:HG2	1.86	0.74
1:L:208:LEU:O	1:L:255:ARG:NH1	2.19	0.74
1:A:159:ASP:OD1	1:A:161:LYS:HD3	1.87	0.73
1:C:156:ARG:HG2	1:C:156:ARG:HH11	1.53	0.73
1:G:84:LEU:O	1:G:109:ARG:NH2	2.21	0.73
1:L:240:TYR:CE1	1:L:277:MET:HE1	2.23	0.73
1:H:25:SER:O	1:H:29:TYR:HD2	1.71	0.73
1:M:145:GLY:CA	1:M:156:ARG:HH11	2.00	0.73
1:F:145:GLY:HA3	1:F:156:ARG:HD3	1.70	0.73
1:L:33:LEU:O	1:L:37:GLU:HG3	1.88	0.73
1:D:244:HIS:O	1:D:248:GLU:HG3	1.89	0.73
1:H:97:HIS:ND1	1:H:123:ASP:OD2	2.21	0.73
1:K:70:ILE:HD13	1:K:135:VAL:HG11	1.70	0.73
1:C:227:ALA:HB1	1:C:274:THR:HG23	1.69	0.73
1:I:278:LEU:HD12	1:I:281:LEU:HD12	1.71	0.73
1:G:146:LEU:HD23	1:G:146:LEU:N	2.04	0.73
1:J:97:HIS:ND1	1:J:123:ASP:OD2	2.22	0.73
1:M:11:MET:HE3	1:M:98:SER:HB2	1.71	0.73
1:F:200:ILE:O	1:F:204:VAL:HG23	1.89	0.73
1:E:149:PRO:O	1:E:153:GLU:HG2	1.89	0.72
1:F:125:ASN:O	1:F:138:MET:HB3	1.88	0.72
1:M:117:TRP:CD1	1:M:165:LEU:HD21	2.24	0.72
1:C:83:ALA:CA	1:H:111:ARG:HH12	2.02	0.72
1:C:83:ALA:CA	1:H:111:ARG:NH1	2.52	0.72
1:D:273:ARG:HA	1:D:276:GLU:HG3	1.72	0.72
1:M:153:GLU:HG3	1:M:154:VAL:HG13	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:148:HIS:CD2	1:F:150:ARG:H	2.08	0.72
1:M:84:LEU:HD13	1:M:88:VAL:HG11	1.71	0.72
1:D:104:VAL:HG22	1:D:214:HIS:CE1	2.25	0.71
1:H:222:LEU:HD13	1:H:277:MET:HE2	1.71	0.71
1:I:184:VAL:O	1:I:186:VAL:HG23	1.91	0.71
1:M:80:ARG:HH11	1:M:80:ARG:CG	2.02	0.71
1:E:126:THR:C	1:E:138:MET:HE2	2.14	0.71
1:M:172:ASP:HB3	2:M:293:HOH:O	1.90	0.71
1:D:9:VAL:O	1:D:11:MET:N	2.23	0.71
1:D:119:ASP:HB3	1:D:121:HIS:O	1.90	0.71
1:H:66:TYR:O	1:H:70:ILE:HD13	1.91	0.71
1:J:201:ALA:HB1	1:J:249:ILE:HG21	1.73	0.71
1:M:36:LEU:HD21	1:M:286:LEU:CD2	2.20	0.71
1:G:115:VAL:HB	1:G:163:VAL:HG22	1.71	0.71
1:A:223:ASP:OD2	1:A:225:THR:HB	1.92	0.70
1:G:109:ARG:HG2	1:G:109:ARG:NH1	2.03	0.70
1:K:164:VAL:CG2	1:K:208:LEU:HD11	2.21	0.70
1:A:84:LEU:O	1:A:109:ARG:NH2	2.23	0.70
1:D:214:HIS:CD2	1:D:258:SER:HB2	2.26	0.70
1:H:101:MET:HA	1:H:143:LEU:HD21	1.73	0.70
1:M:29:TYR:C	1:M:31:ARG:H	1.98	0.70
1:D:99:LEU:HD21	1:D:262:VAL:HG12	1.74	0.70
1:G:130:SER:HG	1:G:132:SER:N	1.88	0.70
1:H:129:THR:O	1:H:130:SER:HB2	1.89	0.70
1:K:214:HIS:HE1	1:K:260:ASP:OD2	1.73	0.70
1:A:25:SER:HB2	1:H:22:MET:HE3	1.74	0.70
1:C:119:ASP:OD2	1:C:123:ASP:OD2	2.10	0.70
1:J:30:ALA:HB3	1:J:279:VAL:HG21	1.73	0.70
1:C:22:MET:HE3	1:K:25:SER:CB	2.22	0.70
1:H:130:SER:HG	1:H:132:SER:N	1.89	0.70
1:K:118:VAL:HG23	1:K:216:SER:O	1.92	0.70
1:G:111:ARG:HD3	1:G:112:ARG:H	1.56	0.70
1:I:119:ASP:OD2	1:I:123:ASP:OD2	2.10	0.70
1:L:97:HIS:ND1	1:L:123:ASP:OD2	2.25	0.70
1:I:11:MET:CE	1:I:98:SER:HB2	2.22	0.69
1:A:119:ASP:OD2	1:A:218:ASP:OD2	2.09	0.69
1:D:129:THR:O	1:D:130:SER:HB2	1.91	0.69
1:C:148:HIS:CD2	1:C:150:ARG:H	2.07	0.69
1:F:169:ARG:HG3	1:F:234:VAL:HG11	1.74	0.69
1:A:220:ASP:OD2	2:A:293:HOH:O	2.10	0.69
1:G:97:HIS:ND1	1:G:123:ASP:OD2	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:TRP:CE3	1:A:140:LEU:HD13	2.27	0.69
1:M:190:HIS:HE1	1:M:194:ARG:HG3	1.57	0.69
1:I:12:ASP:OD2	1:I:19:GLY:HA2	1.92	0.69
1:K:19:GLY:HA3	1:K:265:ASN:HD21	1.57	0.69
1:A:198:ALA:O	1:A:202:GLU:HG2	1.93	0.69
1:A:79:GLU:CB	1:D:111:ARG:NH2	2.56	0.69
1:J:6:VAL:HG13	1:J:93:LEU:HD21	1.74	0.69
1:M:80:ARG:HD2	1:M:80:ARG:O	1.93	0.69
1:J:119:ASP:OD2	1:J:123:ASP:OD2	2.11	0.69
1:L:149:PRO:O	1:L:153:GLU:HB3	1.93	0.68
1:M:125:ASN:HB2	1:M:137:GLY:O	1.92	0.68
1:A:109:ARG:HG2	1:A:109:ARG:HH11	1.56	0.68
1:L:156:ARG:HG2	1:L:156:ARG:HH11	1.57	0.68
1:E:239:THR:OG1	1:E:242:GLU:HB2	1.93	0.68
1:E:99:LEU:HD12	1:E:100:SER:N	2.08	0.68
1:J:66:TYR:HB3	1:J:70:ILE:CD1	2.23	0.68
1:L:108:ALA:C	1:L:109:ARG:HG3	2.19	0.68
1:G:195:LEU:HD22	1:G:199:ARG:NH1	2.09	0.68
1:I:67:LEU:C	1:I:67:LEU:CD2	2.66	0.68
1:M:11:MET:HG2	1:M:96:ASP:HB2	1.75	0.68
1:I:11:MET:HE3	1:I:70:ILE:HG12	1.74	0.68
1:J:66:TYR:HB3	1:J:70:ILE:HD11	1.74	0.68
1:J:211:LEU:O	1:J:255:ARG:NH1	2.25	0.68
1:K:78:LYS:HA	1:K:102:GLY:O	1.93	0.68
1:M:190:HIS:CE1	1:M:194:ARG:HG3	2.29	0.68
1:M:244:HIS:O	1:M:248:GLU:HG3	1.94	0.68
1:H:11:MET:HE1	1:H:98:SER:HB2	1.74	0.68
1:I:259:LEU:HD13	1:I:285:LEU:HD23	1.76	0.68
1:J:125:ASN:HD21	1:J:175:GLU:HG3	1.58	0.68
1:G:12:ASP:C	1:G:13:LEU:HD23	2.19	0.67
1:D:86:GLU:HG2	1:D:109:ARG:HH21	1.58	0.67
1:L:119:ASP:OD1	1:L:121:HIS:ND1	2.27	0.67
1:I:179:LEU:HD22	1:I:186:VAL:HG21	1.77	0.67
1:G:218:ASP:OD1	1:G:263:GLU:HG3	1.93	0.67
1:I:119:ASP:OD2	1:I:218:ASP:OD2	2.13	0.67
1:J:164:VAL:HG11	1:J:204:VAL:CG2	2.25	0.67
1:K:246:LEU:HG	1:K:247:MET:HE2	1.75	0.67
1:D:101:MET:HA	1:D:143:LEU:HD21	1.76	0.67
1:F:223:ASP:OD2	1:F:225:THR:HB	1.93	0.67
1:M:124:PHE:HE2	1:M:178:LEU:HB3	1.60	0.67
1:A:156:ARG:NH2	1:D:156:ARG:NH2	2.42	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:120:ALA:O	1:M:168:VAL:HA	1.95	0.67
1:E:240:TYR:HB3	2:E:306:HOH:O	1.95	0.67
1:H:84:LEU:O	1:H:85:PRO:O	2.12	0.67
1:H:111:ARG:NE	1:H:112:ARG:H	1.92	0.67
1:I:148:HIS:HD2	1:I:149:PRO:HD2	1.60	0.67
1:J:148:HIS:HD2	1:J:150:ARG:HB2	1.59	0.67
1:K:119:ASP:OD2	1:K:123:ASP:OD2	2.13	0.67
1:J:177:ARG:HB3	1:J:177:ARG:HH11	1.59	0.67
1:M:153:GLU:HG3	1:M:154:VAL:N	2.08	0.67
1:C:83:ALA:C	1:H:111:ARG:NH1	2.53	0.67
1:J:86:GLU:HG2	1:J:109:ARG:HE	1.60	0.67
1:L:130:SER:OG	1:L:132:SER:N	2.27	0.67
1:A:119:ASP:OD2	1:A:123:ASP:OD2	2.13	0.66
1:M:109:ARG:HG2	1:M:109:ARG:NH1	2.08	0.66
1:M:128:GLU:O	1:M:130:SER:N	2.27	0.66
1:D:43:VAL:HG12	1:D:44:GLU:N	2.10	0.66
1:K:41:TYR:OH	1:K:286:LEU:O	2.12	0.66
1:K:117:TRP:HB3	1:K:165:LEU:HD23	1.75	0.66
1:L:140:LEU:HD21	1:L:163:VAL:HG11	1.77	0.66
1:M:125:ASN:ND2	1:M:129:THR:OG1	2.28	0.66
1:C:117:TRP:HB3	1:C:165:LEU:HD23	1.78	0.66
1:K:9:VAL:HB	1:K:99:LEU:HD22	1.77	0.66
1:L:96:ASP:HB3	1:L:98:SER:OG	1.94	0.66
1:M:12:ASP:OD2	1:M:19:GLY:HA2	1.95	0.66
1:G:11:MET:CE	1:G:98:SER:HB2	2.24	0.66
1:H:111:ARG:NE	1:H:111:ARG:CA	2.58	0.66
1:K:211:LEU:O	1:K:255:ARG:HD2	1.96	0.66
1:K:214:HIS:CE1	1:K:260:ASP:OD2	2.49	0.66
1:M:117:TRP:HD1	1:M:165:LEU:HD21	1.61	0.66
1:D:138:MET:H	1:D:139:PRO:HD3	1.60	0.66
1:L:189:MET:HA	1:L:192:VAL:HG23	1.77	0.66
1:F:259:LEU:HD13	1:F:285:LEU:CD2	2.25	0.66
1:L:129:THR:O	1:L:130:SER:HB3	1.96	0.66
1:D:119:ASP:OD2	1:D:123:ASP:OD2	2.13	0.66
1:I:97:HIS:CD2	1:I:262:VAL:HG21	2.31	0.66
1:L:239:THR:OG1	1:L:242:GLU:HG3	1.96	0.66
1:M:165:LEU:HB2	1:M:186:VAL:HG22	1.77	0.66
1:C:25:SER:CB	1:K:22:MET:HE3	2.25	0.66
1:E:4:VAL:HG11	1:E:36:LEU:HD13	1.77	0.66
1:H:22:MET:SD	1:H:267:ILE:HD13	2.35	0.66
1:H:33:LEU:HG	1:H:43:VAL:HG11	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:81:LEU:HA	1:I:84:LEU:HD12	1.77	0.66
1:E:138:MET:H	1:E:139:PRO:CD	2.10	0.65
1:I:169:ARG:NH2	1:I:221:VAL:O	2.28	0.65
1:K:72:ALA:O	1:K:76:VAL:HG23	1.96	0.65
1:A:11:MET:CE	1:A:98:SER:HB2	2.26	0.65
1:L:169:ARG:HD2	1:L:234:VAL:HB	1.77	0.65
1:M:12:ASP:C	1:M:13:LEU:HD23	2.22	0.65
1:A:130:SER:OG	1:A:132:SER:N	2.29	0.65
1:F:99:LEU:C	1:F:99:LEU:HD12	2.22	0.65
1:A:169:ARG:HG3	1:A:234:VAL:HG11	1.79	0.65
1:C:86:GLU:HG2	1:C:109:ARG:NE	2.11	0.65
1:H:129:THR:O	1:H:130:SER:CB	2.44	0.65
1:J:129:THR:O	1:J:130:SER:HB2	1.96	0.65
1:L:3:ARG:NH2	1:L:88:VAL:N	2.44	0.65
1:L:97:HIS:CD2	1:L:262:VAL:HG21	2.32	0.65
1:L:201:ALA:HB1	1:L:249:ILE:HG21	1.78	0.65
1:F:149:PRO:HA	1:F:152:THR:OG1	1.97	0.65
1:I:11:MET:HE1	1:I:98:SER:HB2	1.78	0.65
1:G:244:HIS:O	1:G:248:GLU:HG3	1.97	0.65
1:I:109:ARG:HG2	1:I:109:ARG:NH1	2.12	0.65
1:K:239:THR:OG1	1:K:242:GLU:HG3	1.96	0.65
1:L:3:ARG:NH2	1:L:87:GLY:C	2.54	0.65
1:E:290:ILE:H	1:E:290:ILE:HD12	1.62	0.65
1:M:31:ARG:O	1:M:35:GLN:HG3	1.96	0.65
1:A:68:GLU:CD	1:A:150:ARG:HH21	2.05	0.65
1:J:122:ALA:O	1:J:123:ASP:C	2.39	0.65
1:M:35:GLN:HB3	1:M:283:LEU:HD11	1.79	0.65
1:K:71:ARG:NH2	1:K:153:GLU:OE2	2.30	0.64
1:A:256:VAL:HG21	1:A:285:LEU:HD11	1.79	0.64
1:J:138:MET:N	1:J:139:PRO:CD	2.60	0.64
1:A:111:ARG:HH22	1:D:79:GLU:CA	2.10	0.64
1:E:31:ARG:NH2	1:E:34:GLU:HG2	2.12	0.64
1:E:149:PRO:HA	1:E:152:THR:OG1	1.97	0.64
1:K:218:ASP:HA	1:K:262:VAL:HG23	1.78	0.64
1:L:218:ASP:OD1	1:L:220:ASP:OD2	2.15	0.64
1:L:277:MET:HA	1:L:277:MET:HE3	1.78	0.64
1:M:145:GLY:HA3	1:M:156:ARG:NH1	2.08	0.64
1:C:83:ALA:HA	1:H:111:ARG:NH1	2.12	0.64
1:C:248:GLU:OE1	1:I:190:HIS:HD2	1.81	0.64
1:I:164:VAL:HG11	1:I:204:VAL:HG22	1.79	0.64
1:K:94:GLY:HA2	1:K:99:LEU:HD21	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:99:LEU:C	1:C:99:LEU:HD12	2.23	0.64
1:H:130:SER:OG	1:H:132:SER:N	2.31	0.64
1:I:85:PRO:O	1:I:88:VAL:HG23	1.97	0.64
1:G:169:ARG:NH2	1:G:221:VAL:O	2.31	0.64
1:J:101:MET:HA	1:J:143:LEU:HD21	1.79	0.64
1:K:11:MET:HE2	1:K:96:ASP:HB2	1.78	0.64
1:K:67:LEU:HD23	1:K:67:LEU:C	2.23	0.64
1:D:214:HIS:HD2	1:D:258:SER:HB2	1.62	0.64
1:F:98:SER:HA	1:F:139:PRO:HG3	1.79	0.64
1:J:7:VAL:CG1	1:J:92:VAL:HG22	2.28	0.64
1:K:205:LEU:O	1:K:209:GLN:N	2.30	0.64
1:D:111:ARG:HE	1:D:112:ARG:N	1.96	0.64
1:E:101:MET:HA	1:E:143:LEU:HD21	1.80	0.64
1:E:197:VAL:HG21	1:E:242:GLU:CG	2.27	0.64
1:I:99:LEU:C	1:I:99:LEU:HD12	2.22	0.64
1:A:156:ARG:NH2	1:D:156:ARG:HH21	1.95	0.64
1:D:71:ARG:O	1:D:75:LEU:HB2	1.98	0.64
1:E:80:ARG:HD3	2:E:293:HOH:O	1.97	0.64
1:H:171:LEU:HB2	1:H:176:LYS:HE2	1.80	0.64
1:J:156:ARG:HH11	1:J:156:ARG:CG	2.10	0.64
1:E:6:VAL:HG22	1:E:91:ILE:HB	1.80	0.63
1:E:99:LEU:HD12	1:E:99:LEU:C	2.23	0.63
1:E:138:MET:N	1:E:139:PRO:CD	2.61	0.63
1:I:31:ARG:HD2	2:I:294:HOH:O	1.97	0.63
1:J:169:ARG:NH1	1:J:234:VAL:O	2.29	0.63
1:K:226:LEU:HD21	1:K:240:TYR:N	2.13	0.63
1:E:156:ARG:HG2	1:E:156:ARG:HH11	1.63	0.63
1:L:112:ARG:NH1	1:L:211:LEU:HD21	2.12	0.63
1:L:164:VAL:HG13	1:L:185:ARG:HB3	1.79	0.63
1:C:271:ARG:HH21	1:K:228:PRO:HB2	1.61	0.63
1:G:138:MET:N	1:G:139:PRO:CD	2.61	0.63
1:K:243:ALA:HB1	1:K:281:LEU:HD11	1.79	0.63
1:M:126:THR:OG1	1:M:129:THR:HG23	1.98	0.63
1:A:71:ARG:O	1:A:75:LEU:HB2	1.97	0.63
1:A:109:ARG:HG2	1:A:109:ARG:NH1	2.11	0.63
1:A:226:LEU:HD21	1:A:240:TYR:HB2	1.80	0.63
1:E:145:GLY:C	1:E:146:LEU:HD23	2.23	0.63
1:K:159:ASP:O	1:K:161:LYS:N	2.32	0.63
1:C:119:ASP:HB3	1:C:121:HIS:O	1.98	0.63
1:D:259:LEU:HD13	1:D:285:LEU:HD23	1.79	0.63
1:F:115:VAL:HG23	1:F:158:VAL:HG21	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:130:SER:HG	1:L:132:SER:N	1.96	0.63
1:M:20:VAL:HG12	1:M:264:VAL:O	1.99	0.63
1:L:27:LEU:HD21	1:L:264:VAL:HG21	1.81	0.63
1:L:93:LEU:CD2	1:L:261:LEU:HD12	2.29	0.63
1:K:192:VAL:HA	1:K:200:ILE:HD11	1.80	0.63
1:G:119:ASP:OD2	1:G:218:ASP:OD2	2.17	0.62
1:M:259:LEU:HD13	1:M:285:LEU:CD2	2.28	0.62
1:H:244:HIS:O	1:H:248:GLU:HG3	1.99	0.62
1:E:51:VAL:O	1:E:51:VAL:HG12	1.99	0.62
1:I:216:SER:HA	1:I:260:ASP:HB2	1.80	0.62
1:M:138:MET:N	1:M:139:PRO:CD	2.60	0.62
1:A:104:VAL:HG22	1:A:214:HIS:CE1	2.33	0.62
1:F:99:LEU:HD12	1:F:100:SER:N	2.14	0.62
1:L:247:MET:HG3	1:L:281:LEU:O	1.99	0.62
1:D:117:TRP:CE3	1:D:140:LEU:HD13	2.35	0.62
1:E:119:ASP:HB3	1:E:121:HIS:O	1.99	0.62
1:I:49:VAL:HG21	1:I:77:LEU:HD13	1.81	0.62
1:A:67:LEU:HD11	1:A:148:HIS:CD2	2.35	0.62
1:J:104:VAL:HB	1:J:143:LEU:HD22	1.81	0.62
1:A:69:GLU:OE1	1:A:69:GLU:N	2.31	0.62
1:A:119:ASP:HA	1:A:218:ASP:HB3	1.82	0.62
1:E:256:VAL:HG11	1:E:285:LEU:HD11	1.80	0.62
1:J:148:HIS:CD2	1:J:150:ARG:HB2	2.34	0.62
1:K:176:LYS:HB3	1:M:291:PHE:HE2	1.64	0.62
1:A:25:SER:O	1:A:29:TYR:HD2	1.81	0.62
1:A:164:VAL:HG11	1:A:204:VAL:HG22	1.81	0.62
1:H:145:GLY:C	1:H:146:LEU:HD23	2.25	0.62
1:K:159:ASP:C	1:K:161:LYS:H	2.06	0.62
1:K:165:LEU:HD12	1:K:186:VAL:CG2	2.29	0.62
1:I:126:THR:HG23	1:I:178:LEU:HD13	1.81	0.62
1:J:46:LEU:HD22	1:J:80:ARG:NH2	2.15	0.62
1:D:138:MET:N	1:D:139:PRO:CD	2.62	0.62
1:F:13:LEU:HB2	1:F:70:ILE:HD11	1.82	0.62
1:L:12:ASP:HA	1:L:96:ASP:OD1	1.99	0.62
1:G:11:MET:HE1	1:G:98:SER:HB2	1.80	0.61
1:I:198:ALA:O	1:I:202:GLU:HG2	1.99	0.61
1:K:100:SER:HA	1:K:103:SER:OG	2.00	0.61
1:M:164:VAL:HG11	1:M:204:VAL:CG2	2.30	0.61
1:D:223:ASP:OD2	1:D:225:THR:HG22	2.00	0.61
1:L:119:ASP:HA	1:L:218:ASP:HB3	1.81	0.61
1:L:169:ARG:HG3	1:L:234:VAL:HG11	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:240:TYR:HE1	1:L:277:MET:HE1	1.62	0.61
1:F:179:LEU:HD13	1:F:186:VAL:HG21	1.82	0.61
1:H:94:GLY:HA3	1:H:99:LEU:CD2	2.30	0.61
1:M:30:ALA:HB3	1:M:279:VAL:HG21	1.83	0.61
1:A:11:MET:HE3	1:A:98:SER:HB2	1.83	0.61
1:A:138:MET:N	1:A:139:PRO:CD	2.63	0.61
1:A:169:ARG:HA	1:E:290:ILE:HG21	1.82	0.61
1:J:130:SER:OG	1:J:132:SER:N	2.33	0.61
1:K:101:MET:HA	1:K:143:LEU:HD21	1.83	0.61
1:I:25:SER:HB3	1:M:22:MET:CE	2.26	0.61
1:M:4:VAL:HG23	1:M:41:TYR:HD1	1.65	0.61
1:D:94:GLY:HA3	1:D:99:LEU:CD2	2.30	0.61
1:E:129:THR:O	1:E:130:SER:CB	2.49	0.61
1:G:195:LEU:HD22	1:G:199:ARG:HH11	1.66	0.61
1:H:201:ALA:HB1	1:H:249:ILE:HG21	1.83	0.61
1:I:248:GLU:O	1:I:252:GLU:HG3	2.00	0.61
1:I:123:ASP:HB3	1:I:139:PRO:HG2	1.81	0.61
1:M:244:HIS:CE1	1:M:281:LEU:HD23	2.35	0.61
1:A:79:GLU:HG2	1:D:111:ARG:NH2	2.15	0.61
1:A:94:GLY:HA3	1:A:99:LEU:CD2	2.31	0.61
1:C:80:ARG:O	1:C:83:ALA:HB3	2.00	0.61
1:F:71:ARG:HD3	2:F:299:HOH:O	2.00	0.61
1:J:119:ASP:HA	1:J:218:ASP:HB3	1.83	0.61
1:K:253:SER:C	1:K:255:ARG:H	2.09	0.61
1:D:81:LEU:O	1:D:84:LEU:HD12	2.01	0.60
1:F:138:MET:H	1:F:139:PRO:HD3	1.64	0.60
1:G:2:GLU:HB2	2:G:294:HOH:O	2.00	0.60
1:K:113:VAL:CG1	1:K:212:PRO:HG2	2.25	0.60
1:M:31:ARG:HB2	1:M:31:ARG:HH11	1.66	0.60
1:M:84:LEU:CD1	1:M:88:VAL:HG11	2.29	0.60
1:E:11:MET:HE1	1:E:98:SER:HB2	1.83	0.60
1:E:130:SER:OG	1:E:132:SER:N	2.34	0.60
1:E:148:HIS:CD2	1:E:150:ARG:HB2	2.36	0.60
1:H:84:LEU:O	1:H:109:ARG:NH2	2.33	0.60
1:K:124:PHE:HD1	1:K:140:LEU:HB3	1.66	0.60
1:L:11:MET:HG3	1:L:12:ASP:N	2.16	0.60
1:D:129:THR:O	1:D:130:SER:CB	2.49	0.60
1:H:111:ARG:CD	1:H:112:ARG:N	2.51	0.60
1:L:112:ARG:HD3	1:L:211:LEU:CD2	2.31	0.60
1:A:97:HIS:CE1	1:A:117:TRP:CZ2	2.89	0.60
1:C:22:MET:HE3	1:K:25:SER:HB3	1.81	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:25:SER:O	1:C:29:TYR:HD2	1.84	0.60
1:G:122:ALA:O	1:G:123:ASP:C	2.44	0.60
1:K:169:ARG:NH1	1:K:234:VAL:O	2.34	0.60
1:G:119:ASP:HB3	1:G:121:HIS:O	2.02	0.60
1:G:138:MET:H	1:G:139:PRO:CD	2.14	0.60
1:H:138:MET:N	1:H:139:PRO:HD2	2.16	0.60
1:I:149:PRO:HA	1:I:152:THR:OG1	2.02	0.60
1:J:35:GLN:HA	1:J:38:ASP:OD2	2.01	0.60
1:L:119:ASP:OD2	1:L:123:ASP:OD2	2.19	0.60
1:C:22:MET:HE3	1:K:25:SER:HB2	1.83	0.60
1:K:124:PHE:HD2	1:K:179:LEU:HG	1.67	0.60
1:K:277:MET:HA	1:K:277:MET:HE3	1.83	0.60
1:L:209:GLN:HA	1:L:255:ARG:HH22	1.65	0.60
1:C:225:THR:CG2	1:C:226:LEU:N	2.63	0.60
1:J:269:ASP:OD1	1:J:270:GLU:N	2.30	0.60
1:I:37:GLU:HG2	1:I:43:VAL:HG23	1.83	0.60
1:M:117:TRP:CE3	1:M:140:LEU:HD13	2.37	0.60
1:G:262:VAL:O	1:G:263:GLU:HB2	2.01	0.60
1:H:169:ARG:NH2	1:H:221:VAL:O	2.35	0.60
1:L:4:VAL:HG13	1:L:91:ILE:HD11	1.84	0.60
1:C:32:LEU:O	1:C:36:LEU:HD12	2.02	0.60
1:C:125:ASN:ND2	1:C:175:GLU:HG3	2.16	0.60
1:C:169:ARG:HH22	1:C:221:VAL:C	2.09	0.60
1:C:218:ASP:O	1:C:221:VAL:HG12	2.02	0.60
1:H:111:ARG:HE	1:H:111:ARG:CA	2.10	0.60
1:K:111:ARG:HD3	1:K:112:ARG:N	2.12	0.60
1:L:165:LEU:HB2	1:L:186:VAL:HG22	1.83	0.60
1:A:153:GLU:HA	1:D:156:ARG:CZ	2.31	0.59
1:C:119:ASP:OD2	1:C:218:ASP:OD2	2.20	0.59
1:H:71:ARG:NH2	1:H:154:VAL:HG11	2.17	0.59
1:J:81:LEU:HD23	1:J:84:LEU:HD11	1.82	0.59
1:K:25:SER:O	1:K:29:TYR:HD2	1.85	0.59
1:D:92:VAL:HG11	1:D:99:LEU:HD13	1.84	0.59
1:E:33:LEU:HD23	1:E:43:VAL:HB	1.84	0.59
1:F:112:ARG:CZ	1:F:211:LEU:HD21	2.32	0.59
1:J:30:ALA:CB	1:J:279:VAL:HG21	2.33	0.59
1:J:261:LEU:HD11	1:J:282:ALA:HB2	1.84	0.59
1:L:33:LEU:CD2	1:L:43:VAL:HB	2.30	0.59
1:M:194:ARG:HG2	1:M:194:ARG:HH11	1.67	0.59
1:C:12:ASP:OD2	1:C:19:GLY:HA2	2.02	0.59
1:A:239:THR:OG1	1:A:242:GLU:HG3	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:223:ASP:OD2	1:C:225:THR:HB	2.02	0.59
1:C:225:THR:HG22	1:C:226:LEU:N	2.18	0.59
1:J:22:MET:SD	1:J:267:ILE:HD12	2.43	0.59
1:M:29:TYR:C	1:M:31:ARG:N	2.60	0.59
1:D:97:HIS:CE1	1:D:119:ASP:OD2	2.56	0.59
1:G:169:ARG:HH22	1:G:221:VAL:C	2.10	0.59
1:J:177:ARG:HB3	1:J:177:ARG:NH1	2.17	0.59
1:H:149:PRO:O	1:H:153:GLU:HG2	2.03	0.59
1:K:109:ARG:C	1:K:111:ARG:H	2.10	0.59
1:A:138:MET:H	1:A:139:PRO:HD2	1.66	0.59
1:L:37:GLU:HG2	1:L:43:VAL:CG2	2.32	0.59
1:L:156:ARG:HG2	1:L:156:ARG:NH1	2.16	0.59
1:M:11:MET:SD	1:M:70:ILE:HD13	2.42	0.59
1:E:119:ASP:OD2	1:E:218:ASP:OD2	2.21	0.59
1:K:49:VAL:O	1:K:51:VAL:HG23	2.02	0.59
1:D:153:GLU:HG3	1:D:154:VAL:HG13	1.84	0.59
1:L:91:ILE:HD13	1:L:91:ILE:N	2.18	0.59
1:M:82:ALA:C	1:M:84:LEU:H	2.09	0.59
1:A:99:LEU:C	1:A:99:LEU:HD12	2.28	0.58
1:C:96:ASP:HA	1:C:263:GLU:OE2	2.03	0.58
1:D:97:HIS:CD2	1:D:262:VAL:HG21	2.38	0.58
1:E:97:HIS:CD2	1:E:262:VAL:HG21	2.38	0.58
1:E:148:HIS:HD2	1:E:150:ARG:H	1.51	0.58
1:K:104:VAL:HG22	1:K:214:HIS:CE1	2.38	0.58
1:G:223:ASP:OD2	1:G:225:THR:HB	2.02	0.58
1:I:125:ASN:O	1:I:138:MET:HG2	2.03	0.58
1:L:138:MET:N	1:L:139:PRO:CD	2.60	0.58
1:M:31:ARG:HH11	1:M:31:ARG:CB	2.15	0.58
1:D:138:MET:N	1:D:139:PRO:HD3	2.17	0.58
1:I:94:GLY:HA3	1:I:99:LEU:HD21	1.86	0.58
1:I:259:LEU:HG	1:I:260:ASP:N	2.18	0.58
1:K:119:ASP:HB3	1:K:121:HIS:O	2.04	0.58
1:L:129:THR:O	1:L:130:SER:CB	2.51	0.58
1:L:129:THR:CG2	1:L:174:GLY:HA3	2.34	0.58
1:A:161:LYS:HD3	1:A:161:LYS:H	1.67	0.58
1:F:214:HIS:HE1	1:F:260:ASP:OD2	1.86	0.58
1:L:104:VAL:HB	1:L:143:LEU:HD21	1.84	0.58
1:E:119:ASP:OD2	1:E:123:ASP:OD2	2.20	0.58
1:G:129:THR:O	1:G:130:SER:HB3	2.03	0.58
1:L:165:LEU:HD12	1:L:186:VAL:HG22	1.85	0.58
1:M:31:ARG:CB	1:M:31:ARG:NH1	2.66	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:253:SER:O	1:M:255:ARG:HG3	2.02	0.58
1:J:34:GLU:N	1:J:34:GLU:OE1	2.36	0.58
1:F:13:LEU:HD22	1:F:66:TYR:CG	2.38	0.58
1:H:94:GLY:HA3	1:H:99:LEU:HD21	1.84	0.58
1:K:169:ARG:HG3	1:K:234:VAL:HG11	1.85	0.58
1:M:164:VAL:HG11	1:M:204:VAL:HG22	1.84	0.58
1:A:82:ALA:HA	1:A:109:ARG:NH1	2.19	0.58
1:H:270:GLU:O	1:H:273:ARG:HG2	2.03	0.58
1:I:130:SER:OG	1:I:132:SER:N	2.36	0.58
1:K:159:ASP:HB3	1:K:162:ASP:OD1	2.03	0.58
1:M:2:GLU:OE2	1:M:3:ARG:HG3	2.04	0.58
1:M:145:GLY:HA2	1:M:156:ARG:HG2	1.86	0.58
1:A:215:VAL:O	1:A:259:LEU:HD12	2.04	0.58
1:C:30:ALA:HB3	1:C:279:VAL:HG21	1.85	0.58
1:D:164:VAL:HG11	1:D:204:VAL:HG22	1.85	0.58
1:H:144:SER:HB3	1:H:160:PRO:HG3	1.86	0.58
1:I:232:THR:O	1:I:234:VAL:HG23	2.04	0.58
1:L:220:ASP:O	1:L:220:ASP:OD1	2.22	0.58
1:M:124:PHE:HA	1:M:141:ALA:HB2	1.86	0.58
1:C:161:LYS:HD3	2:C:296:HOH:O	2.04	0.58
1:C:214:HIS:HE1	1:C:260:ASP:OD2	1.87	0.58
1:E:69:GLU:N	1:E:69:GLU:OE1	2.37	0.58
1:K:169:ARG:NH2	1:K:237:GLY:HA3	2.19	0.57
1:L:118:VAL:HB	1:L:217:LEU:CD1	2.34	0.57
1:M:22:MET:HB2	1:M:266:PRO:HG3	1.84	0.57
1:D:169:ARG:NH1	1:D:234:VAL:O	2.37	0.57
1:H:12:ASP:OD1	1:H:12:ASP:O	2.21	0.57
1:M:247:MET:N	1:M:247:MET:HE2	2.18	0.57
1:G:10:PRO:HG3	1:G:48:ASP:OD2	2.04	0.57
1:I:36:LEU:CD2	1:I:286:LEU:HD23	2.32	0.57
1:L:153:GLU:HG2	1:L:154:VAL:CG1	2.34	0.57
1:F:24:PRO:HD3	1:F:94:GLY:O	2.04	0.57
1:C:130:SER:HG	1:C:132:SER:N	2.02	0.57
1:G:68:GLU:OE1	1:G:150:ARG:NH2	2.26	0.57
1:K:192:VAL:HA	1:K:200:ILE:CD1	2.35	0.57
1:L:148:HIS:HD2	1:L:150:ARG:HB2	1.69	0.57
1:C:156:ARG:HG2	1:C:156:ARG:NH1	2.18	0.57
1:E:273:ARG:O	1:E:277:MET:HG3	2.04	0.57
1:G:239:THR:OG1	1:G:242:GLU:HG3	2.04	0.57
1:L:153:GLU:HG2	1:L:154:VAL:HG13	1.85	0.57
1:C:81:LEU:C	1:C:83:ALA:H	2.12	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:198:ALA:O	1:C:202:GLU:HG2	2.05	0.57
1:I:31:ARG:O	1:I:35:GLN:HG3	2.04	0.57
1:D:118:VAL:HG12	1:D:221:VAL:HG11	1.87	0.57
1:D:134:ASN:O	1:D:138:MET:HE3	2.05	0.57
1:E:22:MET:CE	1:F:22:MET:HE2	2.35	0.57
1:F:111:ARG:HH22	1:G:249:ILE:HG23	1.70	0.57
1:L:89:PHE:HZ	1:L:256:VAL:HG12	1.69	0.57
1:M:108:ALA:HB2	1:M:113:VAL:HG21	1.86	0.57
1:E:190:HIS:O	1:E:194:ARG:HB2	2.05	0.57
1:E:244:HIS:O	1:E:248:GLU:HG3	2.05	0.57
1:H:156:ARG:HG2	1:H:156:ARG:HH11	1.69	0.57
1:M:71:ARG:HG3	1:M:155:PHE:HE2	1.68	0.57
1:M:80:ARG:HD2	1:M:80:ARG:C	2.29	0.57
1:E:2:GLU:O	1:E:42:THR:HG23	2.05	0.57
1:G:24:PRO:O	1:G:28:ARG:HG3	2.04	0.57
1:M:129:THR:O	1:M:130:SER:CB	2.53	0.57
1:M:270:GLU:O	1:M:273:ARG:HG2	2.04	0.57
1:G:25:SER:O	1:G:29:TYR:HD2	1.88	0.56
1:I:187:TYR:CD1	1:I:200:ILE:HD12	2.39	0.56
1:K:74:ALA:O	1:K:77:LEU:HB3	2.05	0.56
1:E:177:ARG:HB3	1:E:177:ARG:HH11	1.69	0.56
1:G:138:MET:H	1:G:139:PRO:HD2	1.68	0.56
1:I:104:VAL:HG22	1:I:214:HIS:ND1	2.20	0.56
1:I:190:HIS:CE1	1:I:194:ARG:HE	2.24	0.56
1:H:11:MET:HE3	1:H:98:SER:HB2	1.87	0.56
1:I:67:LEU:HD23	1:I:67:LEU:O	2.04	0.56
1:M:97:HIS:CE1	1:M:119:ASP:OD2	2.57	0.56
1:M:125:ASN:C	1:M:138:MET:HG2	2.30	0.56
1:M:156:ARG:O	1:M:157:ALA:HB2	2.04	0.56
1:G:81:LEU:HD13	1:G:107:ALA:HB2	1.86	0.56
1:G:109:ARG:HH11	1:G:109:ARG:CG	2.16	0.56
1:J:52:SER:O	1:J:69:GLU:HB3	2.06	0.56
1:A:94:GLY:HA3	1:A:99:LEU:HD21	1.88	0.56
1:E:177:ARG:HB3	1:E:177:ARG:NH1	2.21	0.56
1:H:119:ASP:OD2	1:H:218:ASP:OD2	2.24	0.56
1:M:211:LEU:CB	2:M:296:HOH:O	2.47	0.56
1:M:239:THR:OG1	1:M:242:GLU:HG3	2.05	0.56
1:D:122:ALA:O	1:D:123:ASP:C	2.48	0.56
1:M:128:GLU:C	1:M:130:SER:H	2.13	0.56
1:A:148:HIS:HD2	1:A:150:ARG:HB2	1.71	0.56
1:D:22:MET:HE2	1:J:22:MET:HE2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:126:THR:C	1:M:128:GLU:N	2.61	0.56
1:M:283:LEU:HD23	1:M:283:LEU:N	2.21	0.56
1:C:83:ALA:HA	1:H:111:ARG:HH12	1.69	0.56
1:J:169:ARG:HG3	1:J:234:VAL:HG11	1.87	0.56
1:K:245:LEU:O	1:K:249:ILE:HG12	2.05	0.56
1:L:112:ARG:HH11	1:L:211:LEU:HD21	1.69	0.56
1:A:214:HIS:HD2	1:A:258:SER:OG	1.88	0.56
1:C:125:ASN:O	1:C:138:MET:HB3	2.06	0.56
1:J:37:GLU:HB2	2:J:298:HOH:O	2.05	0.56
1:J:161:LYS:HG3	2:J:293:HOH:O	2.06	0.56
1:K:243:ALA:C	1:K:281:LEU:HD21	2.31	0.56
1:A:244:HIS:O	1:A:248:GLU:HG3	2.06	0.56
1:H:239:THR:HG1	1:H:242:GLU:HB2	1.69	0.56
1:K:124:PHE:CD2	1:K:179:LEU:HG	2.41	0.56
1:M:188:THR:O	1:M:191:GLU:HB2	2.05	0.56
1:M:244:HIS:O	1:M:248:GLU:CG	2.54	0.56
1:A:156:ARG:NH1	1:D:153:GLU:O	2.39	0.55
1:F:265:ASN:HD22	1:F:268:LEU:HD12	1.71	0.55
1:J:204:VAL:C	1:J:206:LYS:N	2.62	0.55
1:A:169:ARG:HA	1:E:290:ILE:CG2	2.36	0.55
1:C:129:THR:O	1:C:130:SER:CB	2.53	0.55
1:I:169:ARG:HD2	1:I:234:VAL:HG12	1.89	0.55
1:J:7:VAL:HG13	1:J:92:VAL:HG22	1.88	0.55
1:L:97:HIS:HE1	1:L:119:ASP:HB2	1.70	0.55
1:M:31:ARG:NH1	1:M:31:ARG:HB3	2.20	0.55
1:C:199:ARG:O	1:C:203:GLU:HG3	2.05	0.55
1:F:169:ARG:NH1	1:F:234:VAL:O	2.40	0.55
1:L:13:LEU:HB2	1:L:70:ILE:HD11	1.88	0.55
1:L:124:PHE:HD1	1:L:140:LEU:HD23	1.71	0.55
1:L:214:HIS:HD2	1:L:258:SER:OG	1.88	0.55
1:G:128:GLU:OE1	1:G:128:GLU:N	2.29	0.55
1:K:290:ILE:HD12	1:K:290:ILE:H	1.71	0.55
1:M:259:LEU:HD13	1:M:285:LEU:HD23	1.87	0.55
1:F:91:ILE:HG23	1:F:259:LEU:HD23	1.89	0.55
1:I:228:PRO:HD3	1:I:273:ARG:HH21	1.71	0.55
1:J:117:TRP:CD2	1:J:140:LEU:HD22	2.42	0.55
1:K:124:PHE:CD1	1:K:140:LEU:HG	2.42	0.55
1:K:244:HIS:O	1:K:248:GLU:HG3	2.07	0.55
1:D:169:ARG:NH2	1:D:221:VAL:O	2.40	0.55
1:D:169:ARG:NH2	1:D:237:GLY:HA3	2.22	0.55
1:F:122:ALA:O	1:F:123:ASP:C	2.49	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:119:ASP:HB3	1:I:121:HIS:O	2.05	0.55
1:M:125:ASN:O	1:M:138:MET:HG2	2.06	0.55
1:M:225:THR:HG23	1:M:226:LEU:N	2.21	0.55
1:C:169:ARG:HD2	1:C:234:VAL:O	2.06	0.55
1:G:145:GLY:HA2	1:G:156:ARG:CD	2.25	0.55
1:G:145:GLY:CA	1:G:156:ARG:HD3	2.24	0.55
1:L:248:GLU:HA	2:L:294:HOH:O	2.06	0.55
1:M:197:VAL:HG21	1:M:242:GLU:HB3	1.89	0.55
1:D:112:ARG:NH1	1:D:211:LEU:HD21	2.21	0.55
1:G:94:GLY:HA3	1:G:99:LEU:HD21	1.88	0.55
1:I:98:SER:OG	1:I:136:HIS:HB3	2.07	0.55
1:I:127:PRO:HD2	1:I:128:GLU:OE1	2.06	0.55
1:L:66:TYR:O	1:L:68:GLU:N	2.40	0.55
1:K:124:PHE:CD1	1:K:141:ALA:N	2.75	0.55
1:K:159:ASP:O	1:K:162:ASP:N	2.40	0.55
1:K:176:LYS:HB3	1:M:291:PHE:CE2	2.41	0.55
1:L:188:THR:O	1:L:192:VAL:HG23	2.07	0.55
1:M:13:LEU:N	1:M:96:ASP:OD2	2.36	0.55
1:C:81:LEU:C	1:C:83:ALA:N	2.61	0.55
1:G:201:ALA:HB1	1:G:249:ILE:HG21	1.89	0.55
1:I:144:SER:HA	1:I:158:VAL:O	2.07	0.55
1:M:109:ARG:HH11	1:M:109:ARG:CG	2.19	0.55
1:M:150:ARG:O	1:M:150:ARG:HD3	2.07	0.55
1:D:96:ASP:HB3	1:D:136:HIS:HB3	1.89	0.54
1:H:97:HIS:O	1:H:100:SER:HB2	2.07	0.54
1:J:129:THR:O	1:J:130:SER:CB	2.54	0.54
1:M:159:ASP:O	1:M:162:ASP:HB2	2.07	0.54
1:D:143:LEU:O	1:D:158:VAL:HG12	2.07	0.54
1:G:26:ALA:HB1	1:G:272:ASN:OD1	2.07	0.54
1:G:156:ARG:HG2	1:G:156:ARG:HH11	1.72	0.54
1:H:173:PRO:HA	1:H:176:LYS:HG3	1.89	0.54
1:D:192:VAL:HA	1:D:200:ILE:HD11	1.90	0.54
1:C:148:HIS:HD2	1:C:150:ARG:N	2.01	0.54
1:H:112:ARG:HD3	1:H:211:LEU:HD22	1.90	0.54
1:L:3:ARG:CZ	1:L:88:VAL:HG23	2.38	0.54
1:H:119:ASP:OD2	1:H:123:ASP:OD2	2.25	0.54
1:I:138:MET:N	1:I:139:PRO:CD	2.68	0.54
1:I:148:HIS:CD2	1:I:149:PRO:HD2	2.42	0.54
1:K:128:GLU:H	1:K:128:GLU:CD	2.15	0.54
1:M:4:VAL:CG2	1:M:41:TYR:HD1	2.20	0.54
1:C:30:ALA:CB	1:C:279:VAL:HG21	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:91:ILE:HD11	1:I:286:LEU:HD21	1.89	0.54
1:L:205:LEU:HD13	1:L:253:SER:HB3	1.89	0.54
1:J:187:TYR:CD1	1:J:200:ILE:HD12	2.43	0.54
1:M:247:MET:HB2	1:M:284:SER:HB3	1.90	0.54
1:J:125:ASN:ND2	1:J:175:GLU:CG	2.67	0.54
1:K:112:ARG:HD3	1:K:211:LEU:HD21	1.90	0.54
1:L:126:THR:HG23	1:L:178:LEU:HD13	1.90	0.54
1:A:79:GLU:CG	1:D:111:ARG:NH2	2.70	0.54
1:I:261:LEU:HD11	1:I:282:ALA:HB2	1.90	0.54
1:J:86:GLU:HG2	1:J:109:ARG:NE	2.21	0.54
1:L:12:ASP:HB2	1:L:20:VAL:HG23	1.90	0.54
1:M:22:MET:HB2	1:M:266:PRO:CG	2.38	0.54
1:A:125:ASN:ND2	1:A:175:GLU:HG3	2.23	0.54
1:D:113:VAL:HG12	1:D:212:PRO:HG2	1.90	0.54
1:D:117:TRP:HB3	1:D:165:LEU:HD23	1.91	0.54
1:F:123:ASP:HB3	1:F:139:PRO:HD2	1.88	0.54
1:H:169:ARG:HH22	1:H:221:VAL:C	2.16	0.54
1:M:22:MET:SD	1:M:267:ILE:HD13	2.48	0.54
1:A:153:GLU:HA	1:D:156:ARG:NH2	2.23	0.53
1:G:279:VAL:O	1:G:283:LEU:HG	2.08	0.53
1:L:265:ASN:ND2	1:L:268:LEU:HD13	2.23	0.53
1:M:124:PHE:CE2	1:M:178:LEU:HB3	2.41	0.53
1:M:129:THR:HB	1:M:174:GLY:CA	2.25	0.53
1:L:196:GLY:O	1:L:200:ILE:HG13	2.08	0.53
1:M:117:TRP:O	1:M:165:LEU:HD23	2.08	0.53
1:M:122:ALA:HB2	1:M:171:LEU:CD2	2.38	0.53
1:D:11:MET:HG2	1:D:96:ASP:OD2	2.08	0.53
1:E:67:LEU:HD23	1:E:67:LEU:C	2.33	0.53
1:K:159:ASP:C	1:K:161:LYS:N	2.63	0.53
1:K:215:VAL:HB	1:K:259:LEU:HD13	1.89	0.53
1:K:215:VAL:O	1:K:259:LEU:HD12	2.07	0.53
1:L:100:SER:HA	1:L:103:SER:OG	2.08	0.53
1:M:226:LEU:HD21	1:M:240:TYR:CB	2.33	0.53
1:D:189:MET:HA	1:D:189:MET:HE3	1.89	0.53
1:E:216:SER:HA	1:E:260:ASP:HB2	1.90	0.53
1:F:270:GLU:O	1:F:273:ARG:HG2	2.08	0.53
1:I:35:GLN:OE1	1:I:283:LEU:HD11	2.08	0.53
1:L:189:MET:HA	1:L:192:VAL:CG2	2.38	0.53
1:E:34:GLU:H	1:E:34:GLU:CD	2.16	0.53
1:F:177:ARG:HG2	1:F:177:ARG:HH11	1.74	0.53
1:J:4:VAL:HG22	1:J:89:PHE:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:122:ALA:O	1:J:124:PHE:HB2	2.09	0.53
1:K:97:HIS:ND1	1:K:119:ASP:OD2	2.42	0.53
1:K:175:GLU:O	1:K:176:LYS:C	2.52	0.53
1:L:145:GLY:HA3	1:L:156:ARG:CD	2.38	0.53
1:M:124:PHE:O	1:M:124:PHE:CD2	2.62	0.53
1:F:140:LEU:HD11	1:F:163:VAL:HG11	1.89	0.53
1:K:159:ASP:HB3	1:K:162:ASP:CG	2.33	0.53
1:L:33:LEU:HD23	1:L:43:VAL:CB	2.36	0.53
1:A:228:PRO:HG2	1:A:269:ASP:OD1	2.09	0.53
1:H:97:HIS:CE1	1:H:218:ASP:HB2	2.43	0.53
1:K:277:MET:HA	1:K:277:MET:CE	2.39	0.53
1:L:64:LEU:HD13	1:L:65:ALA:N	2.24	0.53
1:M:94:GLY:HA2	1:M:99:LEU:CD2	2.39	0.53
1:M:148:HIS:HD2	1:M:150:ARG:H	1.57	0.53
1:I:32:LEU:HD12	1:I:279:VAL:HG13	1.90	0.53
1:K:29:TYR:C	1:K:31:ARG:H	2.17	0.53
1:L:37:GLU:O	1:L:40:GLY:N	2.35	0.53
1:L:81:LEU:HD13	1:L:107:ALA:HB2	1.90	0.53
1:A:31:ARG:HA	1:A:34:GLU:OE1	2.09	0.53
1:D:169:ARG:HG3	1:D:234:VAL:HG11	1.90	0.53
1:H:51:VAL:O	1:H:51:VAL:HG12	2.09	0.53
1:I:165:LEU:HD12	1:I:186:VAL:HG22	1.90	0.53
1:J:111:ARG:HD3	1:J:112:ARG:H	1.74	0.53
1:J:117:TRP:HB3	1:J:165:LEU:HD23	1.90	0.53
1:K:270:GLU:HB2	1:K:273:ARG:HD3	1.89	0.53
1:K:272:ASN:O	1:K:276:GLU:HG3	2.09	0.53
1:L:97:HIS:ND1	1:L:218:ASP:OD2	2.42	0.53
1:M:41:TYR:O	1:M:43:VAL:HG23	2.09	0.53
1:M:167:GLY:O	1:M:168:VAL:C	2.51	0.53
1:A:138:MET:H	1:A:139:PRO:CD	2.21	0.53
1:D:169:ARG:HD3	1:D:235:PRO:O	2.09	0.53
1:H:156:ARG:HG2	1:H:156:ARG:NH1	2.23	0.53
1:M:144:SER:OG	1:M:160:PRO:HG3	2.09	0.53
1:M:287:GLY:O	1:M:289:ARG:HD3	2.08	0.53
1:C:138:MET:N	1:C:139:PRO:CD	2.72	0.52
1:F:198:ALA:O	1:F:202:GLU:HG2	2.08	0.52
1:G:75:LEU:O	1:G:79:GLU:HG3	2.09	0.52
1:I:20:VAL:HG12	1:I:265:ASN:HB2	1.91	0.52
1:J:149:PRO:HA	1:J:152:THR:OG1	2.08	0.52
1:K:91:ILE:HA	1:K:259:LEU:O	2.09	0.52
1:D:119:ASP:OD2	1:D:218:ASP:OD2	2.26	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:156:ARG:HG2	1:D:156:ARG:HH11	1.73	0.52
1:I:179:LEU:HD23	1:I:184:VAL:HB	1.91	0.52
1:K:97:HIS:ND1	1:K:123:ASP:OD2	2.42	0.52
1:D:169:ARG:HH22	1:D:221:VAL:C	2.18	0.52
1:K:243:ALA:O	1:K:247:MET:HG2	2.10	0.52
1:M:213:LEU:O	1:M:257:GLN:N	2.43	0.52
1:M:225:THR:CG2	1:M:226:LEU:N	2.72	0.52
1:D:22:MET:HE2	1:J:22:MET:HB3	1.92	0.52
1:G:12:ASP:HB2	1:G:21:ASP:HB3	1.92	0.52
1:G:99:LEU:C	1:G:99:LEU:HD12	2.34	0.52
1:J:169:ARG:NH2	1:J:237:GLY:HA3	2.25	0.52
1:K:8:GLY:O	1:K:48:ASP:HA	2.09	0.52
1:K:30:ALA:C	1:K:31:ARG:HG2	2.34	0.52
1:M:29:TYR:O	1:M:31:ARG:HG3	2.09	0.52
1:A:111:ARG:CD	1:A:112:ARG:H	2.18	0.52
1:E:19:GLY:N	1:E:265:ASN:HD21	2.08	0.52
1:E:221:VAL:O	1:E:221:VAL:HG22	2.08	0.52
1:I:13:LEU:HD22	1:I:66:TYR:CD1	2.45	0.52
1:J:66:TYR:C	1:J:70:ILE:HD13	2.34	0.52
1:K:237:GLY:O	1:M:241:ARG:NH1	2.42	0.52
1:F:11:MET:CE	1:F:98:SER:HB2	2.39	0.52
1:F:214:HIS:CE1	1:F:260:ASP:OD2	2.62	0.52
1:H:13:LEU:HB2	1:H:70:ILE:HD11	1.91	0.52
1:H:109:ARG:NH1	1:H:109:ARG:CG	2.61	0.52
1:M:153:GLU:CG	1:M:154:VAL:H	2.18	0.52
1:A:109:ARG:HH11	1:A:109:ARG:CG	2.21	0.52
1:C:83:ALA:HB1	1:H:111:ARG:NH1	2.23	0.52
1:E:22:MET:HE3	1:F:22:MET:HE2	1.90	0.52
1:K:181:GLU:C	1:K:183:GLY:H	2.18	0.52
1:L:124:PHE:CD1	1:L:140:LEU:HD23	2.44	0.52
1:E:259:LEU:HD22	1:E:285:LEU:HD23	1.91	0.52
1:F:94:GLY:HA3	1:F:99:LEU:HD21	1.92	0.52
1:I:13:LEU:HD13	1:I:70:ILE:HG13	1.92	0.52
1:K:265:ASN:C	1:K:265:ASN:OD1	2.53	0.52
1:M:118:VAL:HG13	1:M:166:VAL:HB	1.91	0.52
1:I:119:ASP:C	1:I:221:VAL:HG23	2.34	0.52
1:I:170:SER:O	1:I:171:LEU:HD23	2.10	0.52
1:F:222:LEU:O	1:F:223:ASP:C	2.53	0.52
1:L:190:HIS:HE1	1:L:194:ARG:NE	2.03	0.52
1:E:271:ARG:HH22	1:F:228:PRO:HB3	1.75	0.51
1:K:109:ARG:O	1:K:111:ARG:N	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:169:ARG:NH1	1:M:234:VAL:O	2.42	0.51
1:D:129:THR:HB	1:D:174:GLY:HA3	1.93	0.51
1:F:20:VAL:HB	1:F:95:GLY:HA2	1.92	0.51
1:M:22:MET:O	1:M:23:GLY:C	2.52	0.51
1:A:156:ARG:CZ	1:D:156:ARG:NH2	2.74	0.51
1:D:22:MET:CE	1:J:22:MET:HB3	2.40	0.51
1:G:120:ALA:HB2	1:G:220:ASP:O	2.11	0.51
1:M:20:VAL:O	1:M:95:GLY:HA2	2.11	0.51
1:C:97:HIS:CE1	1:C:119:ASP:OD2	2.64	0.51
1:D:216:SER:HA	1:D:260:ASP:HB2	1.92	0.51
1:G:218:ASP:CG	1:G:263:GLU:HG3	2.35	0.51
1:J:118:VAL:HG12	1:J:221:VAL:HG21	1.93	0.51
1:J:119:ASP:OD2	1:J:218:ASP:OD2	2.29	0.51
1:E:26:ALA:HB1	1:E:272:ASN:OD1	2.11	0.51
1:E:118:VAL:HG12	1:E:221:VAL:HG21	1.92	0.51
1:H:97:HIS:ND1	1:H:218:ASP:OD2	2.44	0.51
1:I:20:VAL:HB	1:I:95:GLY:HA2	1.92	0.51
1:I:44:GLU:HG2	1:I:46:LEU:HD23	1.92	0.51
1:M:126:THR:C	1:M:138:MET:HE2	2.36	0.51
1:G:117:TRP:HB3	1:G:165:LEU:CD2	2.35	0.51
1:H:119:ASP:HA	1:H:218:ASP:HB3	1.93	0.51
1:I:94:GLY:HA3	1:I:99:LEU:CD2	2.40	0.51
1:I:259:LEU:HD21	1:I:261:LEU:HD21	1.91	0.51
1:K:77:LEU:O	1:K:78:LYS:C	2.53	0.51
1:L:169:ARG:NH2	1:L:237:GLY:HA2	2.25	0.51
1:M:13:LEU:HD23	1:M:13:LEU:N	2.25	0.51
1:A:122:ALA:O	1:A:123:ASP:C	2.54	0.51
1:A:129:THR:O	1:A:130:SER:CB	2.59	0.51
1:E:98:SER:OG	1:E:136:HIS:HB3	2.11	0.51
1:M:223:ASP:OD2	1:M:225:THR:HG22	2.11	0.51
1:A:65:ALA:O	1:A:66:TYR:HB2	2.09	0.51
1:A:248:GLU:O	1:A:252:GLU:HG3	2.11	0.51
1:C:4:VAL:HG22	1:C:89:PHE:HB3	1.92	0.51
1:I:68:GLU:OE2	1:I:150:ARG:NE	2.44	0.51
1:A:148:HIS:CD2	1:A:150:ARG:HB2	2.46	0.51
1:G:226:LEU:HD11	1:G:277:MET:SD	2.50	0.51
1:I:126:THR:HG23	1:I:178:LEU:CD1	2.41	0.51
1:K:190:HIS:HD2	1:M:248:GLU:OE1	1.94	0.51
1:M:168:VAL:O	1:M:168:VAL:CG1	2.58	0.51
1:C:29:TYR:C	1:C:31:ARG:H	2.19	0.51
1:C:83:ALA:C	1:H:111:ARG:HH22	2.19	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:22:MET:SD	1:G:267:ILE:HD11	2.50	0.51
1:M:203:GLU:O	1:M:206:LYS:HB3	2.11	0.51
1:M:278:LEU:O	1:M:279:VAL:C	2.54	0.51
1:C:111:ARG:CD	1:C:112:ARG:H	2.23	0.50
1:C:169:ARG:NH2	1:C:221:VAL:O	2.44	0.50
1:E:4:VAL:HG12	1:E:43:VAL:HG13	1.91	0.50
1:I:109:ARG:HH11	1:I:109:ARG:CG	2.22	0.50
1:M:169:ARG:HB3	1:M:189:MET:HG2	1.93	0.50
1:A:72:ALA:O	1:A:76:VAL:HG23	2.11	0.50
1:C:83:ALA:HB1	1:H:111:ARG:NH2	2.25	0.50
1:D:43:VAL:CG1	1:D:44:GLU:N	2.73	0.50
1:K:97:HIS:CD2	1:K:262:VAL:HG21	2.45	0.50
1:M:169:ARG:HH22	1:M:221:VAL:C	2.19	0.50
1:A:97:HIS:ND1	1:A:123:ASP:OD2	2.44	0.50
1:E:104:VAL:O	1:E:108:ALA:HB2	2.12	0.50
1:G:33:LEU:HG	1:G:43:VAL:HG11	1.94	0.50
1:H:26:ALA:HB1	1:H:272:ASN:OD1	2.12	0.50
1:H:32:LEU:HA	1:H:279:VAL:HG13	1.93	0.50
1:M:33:LEU:O	1:M:34:GLU:C	2.55	0.50
1:M:129:THR:O	1:M:130:SER:HB2	2.12	0.50
1:C:11:MET:CE	1:C:98:SER:HB2	2.42	0.50
1:H:90:PRO:HD2	1:H:257:GLN:O	2.10	0.50
1:J:33:LEU:O	1:J:34:GLU:C	2.54	0.50
1:J:187:TYR:OH	1:J:203:GLU:HG2	2.11	0.50
1:K:122:ALA:C	1:K:124:PHE:N	2.67	0.50
1:L:118:VAL:HB	1:L:217:LEU:HD12	1.93	0.50
1:M:249:ILE:O	1:M:252:GLU:HB2	2.11	0.50
1:A:79:GLU:CG	1:D:111:ARG:HH22	2.24	0.50
1:E:97:HIS:ND1	1:E:119:ASP:OD2	2.44	0.50
1:F:142:VAL:O	1:F:145:GLY:N	2.42	0.50
1:F:169:ARG:NH2	1:F:221:VAL:O	2.44	0.50
1:H:99:LEU:HD12	1:H:100:SER:N	2.27	0.50
1:I:212:PRO:HA	1:I:255:ARG:O	2.12	0.50
1:K:115:VAL:HB	1:K:163:VAL:HG22	1.94	0.50
1:L:98:SER:OG	1:L:136:HIS:HB3	2.11	0.50
1:L:148:HIS:CD2	1:L:150:ARG:HB2	2.45	0.50
1:M:30:ALA:HB1	1:M:276:GLU:HA	1.92	0.50
1:M:122:ALA:HB2	1:M:171:LEU:HD21	1.93	0.50
1:C:118:VAL:HG12	1:C:221:VAL:HG21	1.94	0.50
1:M:126:THR:C	1:M:128:GLU:H	2.18	0.50
1:M:188:THR:O	1:M:192:VAL:HG23	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:169:ARG:NH1	1:E:234:VAL:O	2.45	0.50
1:H:111:ARG:NE	1:H:112:ARG:N	2.59	0.50
1:H:115:VAL:HB	1:H:163:VAL:HG22	1.94	0.50
1:H:153:GLU:HG3	1:H:154:VAL:HG13	1.92	0.50
1:L:177:ARG:O	1:L:179:LEU:N	2.44	0.50
1:L:189:MET:O	1:L:190:HIS:C	2.55	0.50
1:C:222:LEU:O	1:C:223:ASP:C	2.54	0.50
1:D:97:HIS:ND1	1:D:119:ASP:OD2	2.45	0.50
1:E:228:PRO:HG3	1:E:270:GLU:HG3	1.93	0.50
1:F:144:SER:HB3	1:F:160:PRO:HG3	1.94	0.50
1:H:82:ALA:HA	1:H:109:ARG:NH1	2.20	0.50
1:I:27:LEU:HD13	1:I:93:LEU:HD22	1.93	0.50
1:I:89:PHE:CE2	1:I:286:LEU:HD11	2.46	0.50
1:E:169:ARG:HH22	1:E:221:VAL:C	2.20	0.50
1:I:100:SER:HA	1:I:103:SER:OG	2.12	0.50
1:I:168:VAL:O	1:I:188:THR:HA	2.12	0.50
1:M:173:PRO:HG2	2:M:293:HOH:O	2.11	0.50
1:A:29:TYR:C	1:A:31:ARG:H	2.19	0.49
1:C:11:MET:HE1	1:C:98:SER:HB2	1.94	0.49
1:C:221:VAL:O	1:C:221:VAL:HG22	2.12	0.49
1:D:259:LEU:HD13	1:D:285:LEU:CD2	2.41	0.49
1:E:12:ASP:HB2	1:E:21:ASP:HB3	1.93	0.49
1:G:97:HIS:NE2	1:G:117:TRP:CZ2	2.80	0.49
1:I:138:MET:O	1:I:139:PRO:C	2.55	0.49
1:J:143:LEU:O	1:J:158:VAL:HG12	2.11	0.49
1:K:124:PHE:CE1	1:K:140:LEU:HG	2.47	0.49
1:M:97:HIS:ND1	1:M:119:ASP:OD2	2.45	0.49
1:D:33:LEU:HD11	1:D:45:ASP:HB2	1.94	0.49
1:F:138:MET:N	1:F:139:PRO:HD3	2.26	0.49
1:H:119:ASP:OD1	1:H:120:ALA:N	2.44	0.49
1:I:32:LEU:CD1	1:I:279:VAL:HG13	2.42	0.49
1:I:51:VAL:CG1	1:I:52:SER:N	2.75	0.49
1:I:213:LEU:HD11	1:I:255:ARG:NH1	2.26	0.49
1:J:89:PHE:HD2	1:J:91:ILE:HD12	1.78	0.49
1:L:67:LEU:C	1:L:67:LEU:HD23	2.38	0.49
1:L:109:ARG:CG	1:L:109:ARG:NH1	2.65	0.49
1:M:96:ASP:C	1:M:98:SER:H	2.20	0.49
1:C:122:ALA:O	1:C:123:ASP:C	2.55	0.49
1:E:169:ARG:HH11	1:E:234:VAL:HB	1.76	0.49
1:F:19:GLY:N	2:F:302:HOH:O	2.45	0.49
1:F:122:ALA:O	1:F:124:PHE:HB2	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:188:THR:HG21	1:H:291:PHE:HB2	1.94	0.49
1:G:99:LEU:HD12	1:G:100:SER:N	2.26	0.49
1:G:195:LEU:HB2	1:G:200:ILE:HD11	1.94	0.49
1:H:135:VAL:O	1:H:139:PRO:HD3	2.12	0.49
1:J:124:PHE:HD1	1:J:140:LEU:HB3	1.78	0.49
1:K:174:GLY:C	1:K:178:LEU:HD12	2.37	0.49
1:A:111:ARG:NH1	1:D:83:ALA:HB2	2.19	0.49
1:E:112:ARG:HD3	1:E:211:LEU:HD21	1.93	0.49
1:E:198:ALA:O	1:E:202:GLU:HG2	2.13	0.49
1:F:192:VAL:HA	1:F:200:ILE:HD12	1.95	0.49
1:G:119:ASP:HA	1:G:218:ASP:HB3	1.93	0.49
1:G:130:SER:OG	1:G:132:SER:N	2.46	0.49
1:I:169:ARG:HH22	1:I:221:VAL:C	2.20	0.49
1:K:128:GLU:CD	1:K:128:GLU:N	2.70	0.49
1:M:41:TYR:CD2	1:M:41:TYR:N	2.79	0.49
1:E:79:GLU:HB3	2:E:303:HOH:O	2.13	0.49
1:F:138:MET:N	1:F:139:PRO:CD	2.75	0.49
1:I:155:PHE:O	1:I:156:ARG:C	2.55	0.49
1:J:152:THR:O	1:J:156:ARG:HB2	2.11	0.49
1:J:207:HIS:CD2	1:J:207:HIS:O	2.66	0.49
1:L:112:ARG:HD3	1:L:211:LEU:HD22	1.94	0.49
1:L:186:VAL:O	1:L:186:VAL:HG12	2.11	0.49
1:C:83:ALA:CB	1:H:111:ARG:NH1	2.76	0.49
1:D:43:VAL:HG12	1:D:44:GLU:H	1.77	0.49
1:E:88:VAL:O	1:E:88:VAL:HG12	2.12	0.49
1:E:127:PRO:N	1:E:138:MET:HE2	2.27	0.49
1:G:100:SER:HA	1:G:103:SER:OG	2.13	0.49
1:J:169:ARG:NH2	1:J:221:VAL:O	2.46	0.49
1:C:11:MET:HG2	1:C:96:ASP:OD2	2.12	0.49
1:C:86:GLU:OE2	1:C:109:ARG:HD3	2.12	0.49
1:D:223:ASP:OD2	1:D:225:THR:CG2	2.61	0.49
1:I:77:LEU:C	1:I:79:GLU:N	2.68	0.49
1:J:99:LEU:HD12	1:J:100:SER:N	2.27	0.49
1:K:279:VAL:O	1:K:283:LEU:HG	2.12	0.49
1:E:156:ARG:HG2	1:E:156:ARG:NH1	2.28	0.49
1:E:158:VAL:HG22	1:E:159:ASP:N	2.27	0.49
1:G:173:PRO:HA	1:G:176:LYS:HG3	1.95	0.49
1:K:158:VAL:HG22	1:K:159:ASP:N	2.27	0.49
1:C:169:ARG:HD2	1:C:234:VAL:HB	1.93	0.49
1:F:66:TYR:HB3	1:F:69:GLU:HB2	1.95	0.49
1:F:66:TYR:O	1:F:67:LEU:C	2.56	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:115:VAL:CG2	1:F:158:VAL:HG21	2.42	0.49
1:H:84:LEU:C	1:H:85:PRO:O	2.56	0.49
1:H:122:ALA:O	1:H:123:ASP:C	2.56	0.49
1:J:226:LEU:HD21	1:J:240:TYR:HB2	1.94	0.49
1:K:75:LEU:O	1:K:79:GLU:HB2	2.13	0.49
1:K:137:GLY:HA3	2:K:293:HOH:O	2.13	0.49
1:K:270:GLU:O	1:K:273:ARG:HG2	2.13	0.49
1:L:200:ILE:HA	1:L:203:GLU:HB2	1.95	0.49
1:L:201:ALA:CB	1:L:249:ILE:HG21	2.42	0.49
1:D:199:ARG:O	1:D:203:GLU:HG3	2.13	0.48
1:H:84:LEU:O	1:H:85:PRO:C	2.55	0.48
1:K:4:VAL:HG12	1:K:43:VAL:HG13	1.95	0.48
1:K:124:PHE:CE1	1:K:141:ALA:HA	2.48	0.48
1:K:264:VAL:CG2	1:K:278:LEU:HD22	2.43	0.48
1:L:117:TRP:HB3	1:L:165:LEU:HD23	1.95	0.48
1:M:19:GLY:N	1:M:265:ASN:HD21	2.11	0.48
1:A:171:LEU:HB2	1:A:176:LYS:HE2	1.95	0.48
1:C:226:LEU:HD21	1:C:240:TYR:HB2	1.95	0.48
1:G:164:VAL:HG22	1:G:185:ARG:HB3	1.95	0.48
1:H:147:GLY:O	1:H:148:HIS:C	2.56	0.48
1:I:33:LEU:HD11	1:I:45:ASP:HB2	1.95	0.48
1:L:25:SER:O	1:L:29:TYR:CD2	2.52	0.48
1:M:135:VAL:O	1:M:139:PRO:HD3	2.14	0.48
1:A:30:ALA:HB3	1:A:279:VAL:HG21	1.95	0.48
1:C:169:ARG:HG3	1:C:234:VAL:HG11	1.94	0.48
1:D:97:HIS:ND1	1:D:123:ASP:OD2	2.46	0.48
1:D:198:ALA:O	1:D:202:GLU:HG2	2.13	0.48
1:H:214:HIS:CD2	1:H:258:SER:OG	2.66	0.48
1:J:260:ASP:O	1:J:261:LEU:HD23	2.13	0.48
1:K:169:ARG:NH2	1:K:221:VAL:O	2.46	0.48
1:A:214:HIS:HE1	1:A:260:ASP:OD2	1.96	0.48
1:C:33:LEU:HD21	1:C:45:ASP:HB2	1.95	0.48
1:D:100:SER:HA	1:D:103:SER:OG	2.12	0.48
1:F:112:ARG:NE	1:F:211:LEU:HD21	2.28	0.48
1:G:119:ASP:OD2	1:G:123:ASP:OD2	2.32	0.48
1:J:126:THR:O	1:J:127:PRO:C	2.56	0.48
1:K:119:ASP:OD2	1:K:218:ASP:OD2	2.30	0.48
1:K:148:HIS:CD2	1:K:150:ARG:HB2	2.48	0.48
1:K:185:ARG:CZ	1:K:207:HIS:ND1	2.76	0.48
1:L:213:LEU:O	1:L:257:GLN:HG3	2.13	0.48
1:A:86:GLU:OE1	1:D:86:GLU:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:HIS:NE2	1:A:117:TRP:CZ2	2.81	0.48
1:C:97:HIS:CD2	1:C:262:VAL:HG21	2.48	0.48
1:E:271:ARG:NH2	1:F:228:PRO:HB3	2.28	0.48
1:F:264:VAL:CG2	1:F:278:LEU:HD22	2.43	0.48
1:G:29:TYR:C	1:G:31:ARG:H	2.20	0.48
1:D:71:ARG:HD3	2:D:295:HOH:O	2.12	0.48
1:F:119:ASP:HB3	1:F:121:HIS:O	2.13	0.48
1:J:100:SER:O	1:J:101:MET:C	2.57	0.48
1:M:46:LEU:N	1:M:46:LEU:HD23	2.28	0.48
1:A:169:ARG:HG3	1:A:234:VAL:CG1	2.44	0.48
1:C:97:HIS:ND1	1:C:119:ASP:OD2	2.46	0.48
1:D:130:SER:HG	1:D:132:SER:N	2.11	0.48
1:E:214:HIS:CD2	1:E:258:SER:OG	2.66	0.48
1:E:279:VAL:O	1:E:283:LEU:HG	2.13	0.48
1:I:115:VAL:HB	1:I:163:VAL:HG22	1.95	0.48
1:J:81:LEU:O	1:J:84:LEU:HD12	2.13	0.48
1:L:222:LEU:HD13	1:L:277:MET:HG2	1.95	0.48
1:C:275:ALA:O	1:C:279:VAL:HG23	2.13	0.48
1:D:225:THR:O	1:D:273:ARG:NH2	2.46	0.48
1:E:117:TRP:CE3	1:E:140:LEU:HD13	2.48	0.48
1:F:221:VAL:O	1:F:221:VAL:HG22	2.14	0.48
1:G:128:GLU:H	1:G:128:GLU:CD	2.21	0.48
1:J:33:LEU:HD11	1:J:45:ASP:HB2	1.96	0.48
1:K:84:LEU:O	1:K:109:ARG:NH2	2.47	0.48
1:K:97:HIS:CE1	1:K:119:ASP:OD2	2.67	0.48
1:K:161:LYS:HA	2:K:294:HOH:O	2.14	0.48
1:L:116:VAL:CG1	1:L:204:VAL:HG11	2.44	0.48
1:H:177:ARG:NH1	2:H:304:HOH:O	2.44	0.48
1:I:78:LYS:O	1:I:78:LYS:HG2	2.13	0.48
1:J:32:LEU:HA	1:J:279:VAL:HG13	1.95	0.48
1:K:32:LEU:CD1	1:K:279:VAL:HG13	2.43	0.48
1:K:222:LEU:O	1:K:223:ASP:C	2.56	0.48
1:M:70:ILE:HG21	1:M:135:VAL:HG11	1.95	0.48
1:D:214:HIS:HD2	1:D:258:SER:CB	2.26	0.48
1:E:109:ARG:HH11	1:E:109:ARG:CG	2.27	0.48
1:J:138:MET:H	1:J:139:PRO:CD	2.26	0.48
1:M:100:SER:HA	1:M:103:SER:OG	2.14	0.48
1:A:156:ARG:CZ	1:D:153:GLU:HA	2.44	0.47
1:A:200:ILE:O	1:A:204:VAL:HG23	2.14	0.47
1:F:37:GLU:O	1:F:38:ASP:C	2.54	0.47
1:G:51:VAL:O	1:G:51:VAL:HG12	2.12	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:215:VAL:O	1:I:259:LEU:HD12	2.14	0.47
1:J:198:ALA:O	1:J:202:GLU:HG2	2.14	0.47
1:K:8:GLY:HA2	1:K:93:LEU:HB2	1.95	0.47
1:K:96:ASP:C	1:K:98:SER:H	2.21	0.47
1:L:153:GLU:HG2	1:L:154:VAL:N	2.29	0.47
1:M:151:LEU:HD22	1:M:155:PHE:CD2	2.49	0.47
1:D:214:HIS:HE1	1:D:260:ASP:OD2	1.97	0.47
1:I:97:HIS:ND1	1:I:123:ASP:OD2	2.47	0.47
1:J:247:MET:N	1:J:247:MET:HE2	2.29	0.47
1:K:221:VAL:HG22	1:K:238:LEU:HD12	1.96	0.47
1:K:253:SER:C	1:K:255:ARG:N	2.72	0.47
1:L:112:ARG:HD3	1:L:211:LEU:HD21	1.97	0.47
1:L:125:ASN:N	2:L:301:HOH:O	2.47	0.47
1:F:20:VAL:HB	1:F:95:GLY:CA	2.45	0.47
1:I:92:VAL:HG21	1:I:103:SER:HB3	1.97	0.47
1:I:214:HIS:CE1	1:I:260:ASP:OD2	2.67	0.47
1:J:149:PRO:O	1:J:153:GLU:HB3	2.13	0.47
1:K:152:THR:O	1:K:156:ARG:HB3	2.15	0.47
1:K:259:LEU:HD12	1:K:260:ASP:H	1.79	0.47
1:L:145:GLY:N	1:L:156:ARG:HG3	2.30	0.47
1:C:20:VAL:HB	1:C:95:GLY:HA2	1.96	0.47
1:G:146:LEU:N	1:G:146:LEU:CD2	2.70	0.47
1:I:92:VAL:HG11	1:I:99:LEU:HD13	1.95	0.47
1:L:13:LEU:HD23	1:L:66:TYR:CD1	2.49	0.47
1:L:149:PRO:O	1:L:153:GLU:CB	2.62	0.47
1:M:116:VAL:HB	1:M:215:VAL:HG22	1.96	0.47
1:D:95:GLY:O	1:D:96:ASP:C	2.58	0.47
1:D:225:THR:CG2	1:D:226:LEU:N	2.78	0.47
1:F:228:PRO:O	1:F:230:VAL:N	2.41	0.47
1:J:77:LEU:C	1:J:79:GLU:N	2.71	0.47
1:K:78:LYS:O	1:K:106:GLY:HA3	2.14	0.47
1:M:97:HIS:CD2	1:M:262:VAL:HG21	2.50	0.47
1:E:189:MET:HE2	1:E:236:GLY:O	2.14	0.47
1:G:86:GLU:OE2	1:G:109:ARG:HD3	2.14	0.47
1:I:9:VAL:HG21	1:I:77:LEU:HD22	1.97	0.47
1:I:67:LEU:HD21	1:I:151:LEU:HD21	1.96	0.47
1:I:229:GLY:O	1:I:274:THR:HG21	2.14	0.47
1:J:2:GLU:HG2	2:J:303:HOH:O	2.15	0.47
1:K:33:LEU:HD23	1:K:43:VAL:CG1	2.44	0.47
1:L:275:ALA:O	1:L:276:GLU:C	2.58	0.47
1:A:140:LEU:HD21	1:A:163:VAL:HG11	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:MET:HE2	1:A:277:MET:HB3	1.66	0.47
1:A:278:LEU:O	1:A:279:VAL:C	2.58	0.47
1:C:155:PHE:O	1:C:156:ARG:C	2.55	0.47
1:E:20:VAL:HG11	1:E:263:GLU:HA	1.97	0.47
1:E:36:LEU:HD22	1:E:286:LEU:HD23	1.97	0.47
1:G:70:ILE:O	1:G:71:ARG:C	2.56	0.47
1:H:11:MET:HE3	1:H:96:ASP:HB2	1.97	0.47
1:H:226:LEU:HD21	1:H:240:TYR:HB2	1.97	0.47
1:H:259:LEU:HD13	1:H:285:LEU:CD2	2.40	0.47
1:J:124:PHE:O	1:J:124:PHE:HD2	1.97	0.47
1:J:156:ARG:CG	1:J:156:ARG:NH1	2.73	0.47
1:J:214:HIS:HD2	1:J:258:SER:OG	1.98	0.47
1:K:201:ALA:O	1:K:204:VAL:HB	2.14	0.47
1:L:125:ASN:HD22	1:L:125:ASN:HA	1.53	0.47
1:L:177:ARG:C	1:L:179:LEU:H	2.21	0.47
1:L:214:HIS:CD2	1:L:258:SER:OG	2.68	0.47
1:L:227:ALA:HB1	1:L:274:THR:HG23	1.97	0.47
1:L:291:PHE:C	1:L:291:PHE:CD2	2.90	0.47
1:E:31:ARG:O	1:E:35:GLN:HG3	2.15	0.47
1:G:42:THR:HG23	2:G:294:HOH:O	2.13	0.47
1:G:214:HIS:HE1	1:G:260:ASP:OD2	1.97	0.47
1:J:145:GLY:C	1:J:146:LEU:HD23	2.39	0.47
1:J:204:VAL:C	1:J:206:LYS:H	2.22	0.47
1:M:32:LEU:HB2	1:M:279:VAL:HG22	1.97	0.47
1:A:170:SER:O	1:A:171:LEU:HD23	2.14	0.47
1:A:259:LEU:HD13	1:A:285:LEU:CD2	2.44	0.47
1:A:269:ASP:CG	1:A:270:GLU:H	2.23	0.47
1:D:2:GLU:HB2	2:D:293:HOH:O	2.14	0.47
1:J:100:SER:C	1:J:103:SER:HG	2.21	0.47
1:J:206:LYS:C	1:J:208:LEU:H	2.23	0.47
1:K:92:VAL:HG23	1:K:260:ASP:HA	1.97	0.47
1:K:219:ALA:C	1:K:221:VAL:H	2.22	0.47
1:K:290:ILE:HD12	1:K:290:ILE:N	2.30	0.47
1:C:76:VAL:HA	1:H:86:GLU:HG3	1.96	0.47
1:D:189:MET:HE3	1:D:189:MET:CA	2.45	0.47
1:H:149:PRO:C	1:H:151:LEU:N	2.73	0.47
1:M:169:ARG:HD2	1:M:234:VAL:HB	1.97	0.47
1:M:218:ASP:CG	1:M:263:GLU:HG3	2.40	0.47
1:A:214:HIS:CD2	1:A:258:SER:OG	2.67	0.46
1:E:4:VAL:HG22	1:E:89:PHE:HB3	1.96	0.46
1:I:34:GLU:H	1:I:34:GLU:CD	2.22	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:179:LEU:CD2	1:I:186:VAL:HG21	2.44	0.46
1:J:187:TYR:CE1	1:J:200:ILE:HD12	2.50	0.46
1:K:78:LYS:CA	1:K:102:GLY:O	2.63	0.46
1:K:257:GLN:HG3	1:K:258:SER:N	2.29	0.46
1:M:9:VAL:O	1:M:11:MET:N	2.47	0.46
1:M:145:GLY:HA2	1:M:156:ARG:CD	2.45	0.46
1:D:97:HIS:O	1:D:100:SER:HB2	2.15	0.46
1:D:209:GLN:HA	1:D:255:ARG:NH2	2.30	0.46
1:F:111:ARG:CD	1:F:112:ARG:N	2.54	0.46
1:I:138:MET:H	1:I:139:PRO:HD2	1.73	0.46
1:J:99:LEU:C	1:J:99:LEU:CD1	2.82	0.46
1:J:124:PHE:O	1:J:124:PHE:CD2	2.68	0.46
1:K:176:LYS:HD3	1:M:291:PHE:CD2	2.50	0.46
1:K:275:ALA:O	1:K:276:GLU:C	2.58	0.46
1:L:13:LEU:HD23	1:L:66:TYR:CE1	2.50	0.46
1:L:129:THR:HG21	1:L:174:GLY:HA3	1.97	0.46
1:M:79:GLU:HA	1:M:82:ALA:HB3	1.96	0.46
1:E:214:HIS:HD2	1:E:258:SER:OG	1.98	0.46
1:E:247:MET:HA	1:E:247:MET:HE2	1.97	0.46
1:H:75:LEU:HD12	1:H:75:LEU:HA	1.78	0.46
1:I:135:VAL:HA	1:I:138:MET:SD	2.55	0.46
1:J:4:VAL:HG13	1:J:91:ILE:HD13	1.96	0.46
1:L:201:ALA:HB1	1:L:249:ILE:CG2	2.44	0.46
1:M:12:ASP:OD1	1:M:20:VAL:HG23	2.15	0.46
1:M:145:GLY:HA2	1:M:156:ARG:HD2	1.97	0.46
1:M:220:ASP:C	1:M:220:ASP:OD1	2.58	0.46
1:D:277:MET:HE3	1:D:277:MET:HB3	1.72	0.46
1:F:69:GLU:OE1	1:F:69:GLU:N	2.41	0.46
1:G:46:LEU:HD13	1:G:80:ARG:CZ	2.45	0.46
1:G:115:VAL:CG2	1:G:158:VAL:HG21	2.44	0.46
1:I:279:VAL:O	1:I:283:LEU:HG	2.16	0.46
1:L:99:LEU:C	1:L:99:LEU:HD12	2.40	0.46
1:L:163:VAL:HG12	1:L:184:VAL:CG1	2.46	0.46
1:M:160:PRO:HB2	1:M:182:ALA:O	2.15	0.46
1:C:76:VAL:HG22	1:H:86:GLU:HG3	1.98	0.46
1:C:97:HIS:O	1:C:100:SER:HB2	2.15	0.46
1:D:213:LEU:N	1:D:255:ARG:O	2.36	0.46
1:E:129:THR:O	1:E:130:SER:HB2	2.15	0.46
1:H:11:MET:CE	1:H:96:ASP:HB2	2.45	0.46
1:H:64:LEU:HB3	1:H:65:ALA:H	1.51	0.46
1:J:160:PRO:C	1:J:162:ASP:H	2.24	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:144:SER:CB	1:K:160:PRO:HG3	2.41	0.46
1:L:20:VAL:C	1:L:22:MET:H	2.23	0.46
1:M:99:LEU:HD12	1:M:99:LEU:C	2.41	0.46
1:C:214:HIS:CE1	1:C:260:ASP:OD2	2.68	0.46
1:H:138:MET:N	1:H:139:PRO:CD	2.77	0.46
1:K:32:LEU:HD13	1:K:279:VAL:HG13	1.97	0.46
1:L:138:MET:C	2:L:301:HOH:O	2.58	0.46
1:C:84:LEU:O	1:C:85:PRO:C	2.58	0.46
1:H:145:GLY:HA3	1:H:156:ARG:HD2	1.97	0.46
1:H:199:ARG:O	1:H:200:ILE:C	2.57	0.46
1:K:92:VAL:CG2	1:K:260:ASP:OD1	2.64	0.46
1:C:46:LEU:HD22	1:C:80:ARG:NH2	2.30	0.46
1:C:109:ARG:NH1	1:C:109:ARG:CG	2.55	0.46
1:C:225:THR:HG22	1:C:226:LEU:H	1.81	0.46
1:C:272:ASN:HB2	1:K:267:ILE:HA	1.98	0.46
1:D:248:GLU:O	1:D:252:GLU:HG3	2.15	0.46
1:E:109:ARG:C	1:E:111:ARG:H	2.24	0.46
1:I:274:THR:O	1:I:277:MET:HB2	2.16	0.46
1:M:68:GLU:O	1:M:72:ALA:HB2	2.16	0.46
1:M:82:ALA:C	1:M:84:LEU:N	2.71	0.46
1:I:159:ASP:C	1:I:159:ASP:OD1	2.59	0.46
1:J:11:MET:HE3	1:J:98:SER:HB2	1.97	0.46
1:J:150:ARG:O	1:J:153:GLU:HG2	2.14	0.46
1:K:70:ILE:CD1	1:K:135:VAL:HG21	2.46	0.46
1:A:101:MET:HA	1:A:143:LEU:HD21	1.98	0.46
1:D:149:PRO:HA	1:D:152:THR:OG1	2.16	0.46
1:G:11:MET:O	1:G:96:ASP:CG	2.59	0.46
1:I:214:HIS:HE1	1:I:260:ASP:OD2	1.99	0.46
1:J:124:PHE:CD1	1:J:140:LEU:HB3	2.51	0.46
1:L:42:THR:HA	2:L:299:HOH:O	2.15	0.46
1:G:259:LEU:HD22	1:G:285:LEU:HD23	1.98	0.45
1:I:97:HIS:CG	1:I:262:VAL:HG21	2.51	0.45
1:K:94:GLY:HA3	1:K:262:VAL:HG12	1.97	0.45
1:K:157:ALA:O	1:K:158:VAL:HB	2.16	0.45
1:A:99:LEU:HD12	1:A:100:SER:N	2.30	0.45
1:A:190:HIS:HD2	1:E:248:GLU:OE1	1.99	0.45
1:C:279:VAL:O	1:C:283:LEU:HG	2.15	0.45
1:I:105:ALA:O	1:I:108:ALA:HB3	2.16	0.45
1:J:22:MET:SD	1:J:267:ILE:CD1	3.04	0.45
1:A:67:LEU:HD21	1:A:151:LEU:HG	1.98	0.45
1:A:135:VAL:HA	1:A:138:MET:SD	2.57	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:52:SER:O	1:C:69:GLU:HG2	2.17	0.45
1:D:126:THR:HG23	1:D:178:LEU:CD1	2.46	0.45
1:E:277:MET:HE2	1:E:277:MET:HB3	1.71	0.45
1:H:148:HIS:HD2	1:H:150:ARG:H	1.63	0.45
1:H:169:ARG:NH1	1:H:234:VAL:O	2.48	0.45
1:J:79:GLU:C	1:J:81:LEU:N	2.74	0.45
1:K:35:GLN:HB2	1:K:283:LEU:HD21	1.98	0.45
1:L:142:VAL:O	1:L:145:GLY:N	2.49	0.45
1:M:245:LEU:HD12	1:M:245:LEU:HA	1.78	0.45
1:A:119:ASP:HB3	1:A:121:HIS:O	2.16	0.45
1:C:150:ARG:HD2	1:C:150:ARG:HA	1.79	0.45
1:D:135:VAL:O	1:D:139:PRO:HD3	2.17	0.45
1:G:135:VAL:C	1:G:137:GLY:H	2.24	0.45
1:H:25:SER:O	1:H:29:TYR:CD2	2.61	0.45
1:I:232:THR:O	1:I:233:PRO:C	2.60	0.45
1:J:33:LEU:O	1:J:36:LEU:N	2.48	0.45
1:K:81:LEU:HD12	1:K:103:SER:HA	1.97	0.45
1:M:120:ALA:HB2	1:M:220:ASP:O	2.17	0.45
1:M:128:GLU:C	1:M:130:SER:N	2.74	0.45
1:C:138:MET:O	1:C:142:VAL:HG23	2.17	0.45
1:I:206:LYS:C	1:I:208:LEU:H	2.25	0.45
1:L:84:LEU:HA	1:L:85:PRO:HD2	1.87	0.45
1:A:97:HIS:CE1	1:A:117:TRP:CE2	3.04	0.45
1:E:86:GLU:HA	1:E:109:ARG:HH21	1.81	0.45
1:E:94:GLY:HA3	1:E:99:LEU:HD21	1.98	0.45
1:F:66:TYR:HA	1:F:69:GLU:OE1	2.17	0.45
1:F:97:HIS:ND1	1:F:123:ASP:OD2	2.50	0.45
1:H:120:ALA:HB2	1:H:220:ASP:O	2.17	0.45
1:H:277:MET:HE3	1:H:277:MET:HB3	1.75	0.45
1:I:201:ALA:HB1	1:I:249:ILE:HG21	1.98	0.45
1:M:179:LEU:HD13	1:M:186:VAL:HG21	1.98	0.45
1:J:9:VAL:C	1:J:11:MET:H	2.25	0.45
1:K:8:GLY:HA3	1:K:48:ASP:OD1	2.16	0.45
1:K:70:ILE:O	1:K:73:ALA:N	2.50	0.45
1:L:3:ARG:HH21	1:L:87:GLY:C	2.23	0.45
1:A:205:LEU:HD23	1:A:205:LEU:HA	1.75	0.45
1:F:80:ARG:HA	1:F:80:ARG:HD2	1.60	0.45
1:G:169:ARG:HG3	1:G:234:VAL:HG11	1.99	0.45
1:H:231:GLY:N	2:H:299:HOH:O	2.30	0.45
1:I:175:GLU:O	1:I:179:LEU:HB2	2.17	0.45
1:L:79:GLU:O	1:L:80:ARG:C	2.60	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:90:PRO:C	1:L:91:ILE:HD13	2.42	0.45
1:L:173:PRO:O	1:L:174:GLY:C	2.58	0.45
1:F:113:VAL:HG12	1:F:212:PRO:HG2	1.99	0.45
1:G:128:GLU:N	1:G:128:GLU:CD	2.74	0.45
1:G:215:VAL:O	1:G:259:LEU:HA	2.16	0.45
1:H:197:VAL:CG2	1:H:242:GLU:HG2	2.38	0.45
1:I:99:LEU:HD12	1:I:100:SER:N	2.32	0.45
1:I:125:ASN:ND2	1:I:129:THR:OG1	2.50	0.45
1:J:77:LEU:O	1:J:78:LYS:C	2.59	0.45
1:J:77:LEU:O	1:J:79:GLU:N	2.50	0.45
1:J:95:GLY:O	1:J:96:ASP:C	2.59	0.45
1:J:223:ASP:OD2	1:J:225:THR:HB	2.16	0.45
1:K:149:PRO:O	1:K:153:GLU:HG2	2.17	0.45
1:K:150:ARG:HA	1:K:153:GLU:HG2	1.99	0.45
1:K:240:TYR:CD1	1:K:277:MET:HE1	2.52	0.45
1:L:189:MET:O	1:L:192:VAL:N	2.49	0.45
1:M:223:ASP:OD2	1:M:225:THR:CG2	2.64	0.45
1:A:19:GLY:HA3	1:A:267:ILE:HD12	1.98	0.45
1:A:79:GLU:HG2	1:D:111:ARG:HH21	1.80	0.45
1:C:240:TYR:CD1	1:C:277:MET:HE3	2.52	0.45
1:F:119:ASP:HA	1:F:218:ASP:HB3	1.99	0.45
1:F:169:ARG:HD2	1:F:234:VAL:CG1	2.47	0.45
1:J:104:VAL:HB	1:J:143:LEU:CD2	2.46	0.45
1:M:160:PRO:C	1:M:162:ASP:H	2.26	0.45
1:C:29:TYR:C	1:C:31:ARG:N	2.74	0.44
1:I:265:ASN:HA	1:I:266:PRO:HD2	1.76	0.44
1:K:169:ARG:HB3	1:K:189:MET:HG2	1.99	0.44
1:L:82:ALA:HA	1:L:109:ARG:HH12	1.82	0.44
1:L:125:ASN:HB2	1:L:137:GLY:O	2.17	0.44
1:L:159:ASP:OD1	1:L:160:PRO:HD2	2.17	0.44
1:C:19:GLY:N	1:C:265:ASN:ND2	2.61	0.44
1:C:97:HIS:CE1	1:C:117:TRP:CZ2	3.06	0.44
1:E:20:VAL:O	1:E:95:GLY:HA2	2.17	0.44
1:E:29:TYR:C	1:E:31:ARG:H	2.24	0.44
1:I:9:VAL:O	1:I:11:MET:N	2.47	0.44
1:I:102:GLY:O	1:I:103:SER:C	2.60	0.44
1:I:169:ARG:HB3	1:I:189:MET:HG2	1.99	0.44
1:L:22:MET:SD	1:L:267:ILE:HD13	2.57	0.44
1:L:269:ASP:OD1	1:L:274:THR:OG1	2.29	0.44
1:D:66:TYR:O	1:D:67:LEU:C	2.60	0.44
1:E:178:LEU:HD23	1:E:178:LEU:HA	1.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:140:LEU:O	1:G:144:SER:OG	2.36	0.44
1:G:141:ALA:O	1:G:142:VAL:C	2.60	0.44
1:H:11:MET:HE3	1:H:96:ASP:CB	2.47	0.44
1:K:205:LEU:O	1:K:206:LYS:C	2.60	0.44
1:K:238:LEU:HA	1:M:241:ARG:HH12	1.83	0.44
1:L:69:GLU:OE1	1:L:69:GLU:N	2.47	0.44
1:L:82:ALA:HB2	1:L:106:GLY:O	2.17	0.44
1:L:122:ALA:O	1:L:123:ASP:C	2.60	0.44
1:L:122:ALA:C	1:L:124:PHE:N	2.73	0.44
1:M:24:PRO:HB2	2:M:294:HOH:O	2.17	0.44
1:D:225:THR:HG23	1:D:226:LEU:N	2.33	0.44
1:E:278:LEU:O	1:E:281:LEU:N	2.49	0.44
1:G:229:GLY:HA3	1:G:269:ASP:HB2	1.99	0.44
1:I:226:LEU:HD21	1:I:240:TYR:HB2	1.99	0.44
1:K:124:PHE:CD1	1:K:140:LEU:HB3	2.51	0.44
1:A:165:LEU:HD12	1:A:186:VAL:HG22	1.99	0.44
1:A:223:ASP:HA	1:A:224:PRO:HD3	1.92	0.44
1:D:192:VAL:HA	1:D:200:ILE:CD1	2.48	0.44
1:F:277:MET:HE2	1:F:277:MET:HB3	1.72	0.44
1:J:66:TYR:HB3	1:J:70:ILE:HD13	1.99	0.44
1:J:79:GLU:O	1:J:81:LEU:N	2.51	0.44
1:J:244:HIS:O	1:J:248:GLU:HG3	2.16	0.44
1:L:145:GLY:HA3	1:L:156:ARG:HD3	1.99	0.44
1:L:246:LEU:HG	1:L:247:MET:HE2	1.99	0.44
1:L:289:ARG:HB2	1:L:289:ARG:HH11	1.82	0.44
1:D:80:ARG:HD2	1:D:80:ARG:HA	1.63	0.44
1:D:214:HIS:CE1	1:D:260:ASP:OD2	2.71	0.44
1:E:2:GLU:HB2	2:E:300:HOH:O	2.17	0.44
1:F:119:ASP:OD2	1:F:218:ASP:OD2	2.35	0.44
1:I:129:THR:HB	1:I:174:GLY:HA3	1.99	0.44
1:I:223:ASP:OD2	1:I:225:THR:HG22	2.17	0.44
1:J:177:ARG:NH1	1:J:177:ARG:CB	2.80	0.44
1:J:197:VAL:HG21	1:J:242:GLU:HB3	1.99	0.44
1:K:11:MET:CE	1:K:96:ASP:HB2	2.47	0.44
1:K:251:ALA:O	1:K:254:GLY:N	2.40	0.44
1:M:10:PRO:CD	1:M:48:ASP:OD2	2.65	0.44
1:C:32:LEU:HD11	1:C:36:LEU:HD11	2.00	0.44
1:C:99:LEU:HD21	1:C:262:VAL:HG12	1.98	0.44
1:F:164:VAL:HG11	1:F:204:VAL:HG22	2.00	0.44
1:G:169:ARG:NH1	1:G:234:VAL:O	2.49	0.44
1:I:278:LEU:HD12	1:I:281:LEU:CD1	2.44	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:223:ASP:O	1:J:226:LEU:N	2.51	0.44
1:K:9:VAL:HB	1:K:99:LEU:CD2	2.48	0.44
1:L:9:VAL:O	1:L:11:MET:N	2.50	0.44
1:L:169:ARG:HG3	1:L:234:VAL:CG1	2.46	0.44
1:M:161:LYS:H	1:M:161:LYS:HG2	1.60	0.44
1:F:97:HIS:CE1	1:F:117:TRP:CZ2	3.05	0.44
1:F:111:ARG:HG2	1:F:111:ARG:HH11	1.81	0.44
1:G:290:ILE:HD12	1:G:290:ILE:N	2.32	0.44
1:I:213:LEU:HD11	1:I:255:ARG:HH12	1.82	0.44
1:L:126:THR:C	1:L:128:GLU:N	2.73	0.44
1:L:144:SER:HB3	1:L:160:PRO:HG3	1.99	0.44
1:M:4:VAL:HA	1:M:89:PHE:O	2.18	0.44
1:M:226:LEU:HD21	1:M:240:TYR:CA	2.48	0.44
1:C:234:VAL:HA	1:C:235:PRO:HD2	1.80	0.44
1:I:46:LEU:HD23	1:I:46:LEU:N	2.33	0.44
1:L:39:LEU:O	1:L:39:LEU:HG	2.17	0.44
1:L:71:ARG:NH2	1:L:154:VAL:HG11	2.33	0.44
1:L:124:PHE:C	2:L:301:HOH:O	2.61	0.44
1:M:104:VAL:HG22	1:M:214:HIS:CE1	2.52	0.44
1:C:188:THR:O	1:C:192:VAL:HG23	2.18	0.43
1:C:264:VAL:CG2	1:C:278:LEU:HD22	2.48	0.43
1:K:112:ARG:HD3	1:K:211:LEU:CD2	2.48	0.43
1:L:177:ARG:C	1:L:179:LEU:N	2.75	0.43
1:L:270:GLU:O	1:L:271:ARG:HB2	2.17	0.43
1:M:32:LEU:HA	1:M:279:VAL:HG13	2.00	0.43
1:M:119:ASP:OD2	1:M:123:ASP:OD2	2.36	0.43
1:M:224:PRO:CG	1:M:233:PRO:HB2	2.48	0.43
1:A:199:ARG:HA	1:A:202:GLU:HG3	1.99	0.43
1:D:169:ARG:NH2	1:D:237:GLY:CA	2.80	0.43
1:D:169:ARG:HB3	1:D:189:MET:HG2	1.99	0.43
1:G:97:HIS:ND1	1:G:119:ASP:OD2	2.51	0.43
1:H:13:LEU:CB	1:H:70:ILE:HD11	2.47	0.43
1:I:153:GLU:HG3	1:I:154:VAL:HG13	2.01	0.43
1:J:148:HIS:HA	1:J:149:PRO:HD3	1.82	0.43
1:K:124:PHE:O	1:K:175:GLU:HG2	2.18	0.43
1:L:240:TYR:CD1	1:L:277:MET:HE1	2.53	0.43
1:M:198:ALA:C	1:M:200:ILE:H	2.25	0.43
1:M:218:ASP:CG	1:M:220:ASP:OD2	2.62	0.43
1:D:104:VAL:CG2	1:D:214:HIS:CE1	2.99	0.43
1:F:109:ARG:NH1	1:F:109:ARG:HG2	2.32	0.43
1:G:32:LEU:HD12	1:G:279:VAL:HG13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:97:HIS:CE1	1:G:119:ASP:OD2	2.71	0.43
1:H:227:ALA:HB1	1:H:274:THR:HG23	2.00	0.43
1:H:279:VAL:O	1:H:283:LEU:HG	2.18	0.43
1:L:113:VAL:HB	1:L:212:PRO:O	2.18	0.43
1:L:172:ASP:O	1:L:175:GLU:HB2	2.18	0.43
1:L:277:MET:HE3	1:L:277:MET:CA	2.48	0.43
1:A:229:GLY:HA3	1:A:269:ASP:HB2	2.00	0.43
1:G:118:VAL:HB	1:G:217:LEU:HD12	1.99	0.43
1:G:129:THR:O	1:G:130:SER:CB	2.66	0.43
1:J:100:SER:HA	1:J:103:SER:HG	1.78	0.43
1:J:165:LEU:HD12	1:J:186:VAL:HG22	2.00	0.43
1:J:269:ASP:CG	1:J:270:GLU:H	2.20	0.43
1:L:247:MET:SD	1:L:285:LEU:HD22	2.58	0.43
1:M:3:ARG:HH12	1:M:85:PRO:HB2	1.84	0.43
1:M:80:ARG:CG	1:M:80:ARG:NH1	2.69	0.43
1:C:83:ALA:O	1:C:84:LEU:C	2.61	0.43
1:D:264:VAL:CG2	1:D:278:LEU:HD22	2.48	0.43
1:E:187:TYR:CD1	1:E:200:ILE:HG12	2.54	0.43
1:F:13:LEU:N	1:F:96:ASP:OD2	2.43	0.43
1:I:78:LYS:HE3	1:I:105:ALA:HB1	2.00	0.43
1:K:69:GLU:O	1:K:72:ALA:HB3	2.18	0.43
1:K:269:ASP:CG	1:K:270:GLU:H	2.26	0.43
1:A:123:ASP:HB3	1:A:139:PRO:HG2	2.01	0.43
1:C:98:SER:O	1:C:101:MET:HG3	2.18	0.43
1:D:43:VAL:CG1	1:D:44:GLU:H	2.32	0.43
1:D:98:SER:C	1:D:100:SER:N	2.76	0.43
1:E:169:ARG:NH2	1:E:221:VAL:O	2.51	0.43
1:E:290:ILE:HD12	1:E:290:ILE:N	2.33	0.43
1:F:169:ARG:CZ	1:F:237:GLY:HA2	2.48	0.43
1:J:50:PRO:C	1:J:51:VAL:CG2	2.92	0.43
1:J:225:THR:HG22	1:J:226:LEU:N	2.33	0.43
1:K:124:PHE:HD1	1:K:140:LEU:CB	2.30	0.43
1:L:262:VAL:O	1:L:263:GLU:HB2	2.18	0.43
1:A:244:HIS:O	1:A:245:LEU:C	2.62	0.43
1:C:269:ASP:OD1	1:C:270:GLU:N	2.46	0.43
1:E:19:GLY:C	1:E:21:ASP:H	2.25	0.43
1:F:122:ALA:O	1:F:124:PHE:N	2.52	0.43
1:J:70:ILE:HD12	1:J:70:ILE:N	2.34	0.43
1:J:145:GLY:HA2	1:J:156:ARG:HG3	2.00	0.43
1:J:214:HIS:CD2	1:J:258:SER:OG	2.72	0.43
1:K:70:ILE:O	1:K:71:ARG:C	2.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:173:PRO:O	1:L:176:LYS:HB2	2.19	0.43
1:C:246:LEU:O	1:C:250:LEU:HG	2.19	0.43
1:F:169:ARG:HD2	1:F:234:VAL:HG12	2.01	0.43
1:L:190:HIS:CE1	1:L:194:ARG:HE	2.19	0.43
1:A:256:VAL:HG21	1:A:285:LEU:CD1	2.48	0.43
1:E:11:MET:CE	1:E:98:SER:HB2	2.49	0.43
1:E:147:GLY:O	1:E:148:HIS:C	2.61	0.43
1:E:226:LEU:HD11	1:E:240:TYR:HB2	2.01	0.43
1:G:164:VAL:HG11	1:G:204:VAL:HG22	2.00	0.43
1:I:278:LEU:HA	1:I:281:LEU:HD12	2.00	0.43
1:K:12:ASP:O	1:K:13:LEU:HD23	2.19	0.43
1:K:243:ALA:HB1	1:K:281:LEU:CD1	2.47	0.43
1:M:135:VAL:C	1:M:137:GLY:H	2.26	0.43
1:M:172:ASP:O	1:M:176:LYS:HG3	2.19	0.43
1:A:177:ARG:HG2	1:A:177:ARG:HH11	1.83	0.43
1:A:201:ALA:HB1	1:A:249:ILE:HG21	2.01	0.43
1:C:129:THR:O	1:C:130:SER:HB3	2.18	0.43
1:E:119:ASP:OD1	1:E:220:ASP:OD2	2.36	0.43
1:F:169:ARG:HH22	1:F:221:VAL:C	2.27	0.43
1:J:24:PRO:O	1:J:28:ARG:HG3	2.19	0.43
1:J:251:ALA:HB2	1:J:285:LEU:HA	2.01	0.43
1:L:6:VAL:O	1:L:6:VAL:HG12	2.18	0.43
1:A:197:VAL:HG21	1:A:242:GLU:HB3	2.00	0.42
1:C:199:ARG:HA	1:C:202:GLU:HG3	2.01	0.42
1:E:3:ARG:HB3	1:E:88:VAL:HG22	2.01	0.42
1:E:185:ARG:NH1	1:E:185:ARG:HG2	2.34	0.42
1:F:128:GLU:H	1:F:128:GLU:CD	2.27	0.42
1:J:5:ALA:HA	1:J:44:GLU:O	2.19	0.42
1:L:247:MET:HA	1:L:285:LEU:HD13	2.00	0.42
1:M:80:ARG:HG2	1:M:80:ARG:NH1	2.17	0.42
1:M:124:PHE:CA	1:M:141:ALA:HB2	2.49	0.42
1:M:146:LEU:CD1	1:M:178:LEU:HD22	2.43	0.42
1:M:201:ALA:CB	1:M:249:ILE:HG21	2.50	0.42
1:M:208:LEU:O	1:M:209:GLN:C	2.60	0.42
1:G:218:ASP:O	1:G:221:VAL:HG12	2.18	0.42
1:I:106:GLY:C	1:I:108:ALA:N	2.77	0.42
1:I:207:HIS:CG	1:I:207:HIS:O	2.72	0.42
1:L:215:VAL:O	1:L:259:LEU:HA	2.19	0.42
1:L:291:PHE:HD2	1:L:291:PHE:OXT	2.02	0.42
1:M:3:ARG:NH1	1:M:85:PRO:HB2	2.35	0.42
1:M:84:LEU:O	1:M:109:ARG:NH2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:96:ASP:C	1:M:98:SER:N	2.76	0.42
1:H:148:HIS:CD2	1:H:150:ARG:HB2	2.55	0.42
1:H:214:HIS:ND1	1:H:214:HIS:C	2.77	0.42
1:I:12:ASP:OD1	1:I:12:ASP:C	2.62	0.42
1:I:245:LEU:O	1:I:245:LEU:HG	2.15	0.42
1:K:165:LEU:HB2	1:K:186:VAL:HG22	2.00	0.42
1:L:124:PHE:CD2	1:L:179:LEU:HG	2.54	0.42
1:M:25:SER:O	1:M:28:ARG:HB2	2.19	0.42
1:D:25:SER:O	1:D:29:TYR:HD2	2.03	0.42
1:H:251:ALA:HB2	1:H:285:LEU:HA	2.01	0.42
1:I:168:VAL:CG1	1:I:171:LEU:HD21	2.49	0.42
1:I:219:ALA:C	1:I:221:VAL:H	2.27	0.42
1:J:22:MET:HB2	1:J:266:PRO:HG2	2.01	0.42
1:J:89:PHE:HA	1:J:90:PRO:HD3	1.89	0.42
1:J:169:ARG:HG3	1:J:234:VAL:CG1	2.49	0.42
1:M:148:HIS:CD2	1:M:150:ARG:H	2.36	0.42
1:D:98:SER:O	1:D:99:LEU:C	2.61	0.42
1:E:108:ALA:O	1:E:109:ARG:HB2	2.19	0.42
1:F:143:LEU:C	1:F:145:GLY:H	2.26	0.42
1:H:164:VAL:HG11	1:H:204:VAL:HG22	2.01	0.42
1:I:20:VAL:CG1	1:I:265:ASN:HB2	2.48	0.42
1:L:90:PRO:HG2	1:L:258:SER:HB3	2.02	0.42
1:L:119:ASP:C	1:L:221:VAL:HG23	2.44	0.42
1:M:165:LEU:CB	1:M:186:VAL:HG22	2.49	0.42
1:M:240:TYR:HD1	1:M:277:MET:SD	2.42	0.42
1:A:169:ARG:HH22	1:A:221:VAL:C	2.27	0.42
1:E:22:MET:SD	1:E:267:ILE:CD1	3.08	0.42
1:F:74:ALA:O	1:F:77:LEU:HB3	2.19	0.42
1:G:39:LEU:HA	1:G:39:LEU:HD12	1.75	0.42
1:H:101:MET:HG3	1:H:139:PRO:HB3	2.02	0.42
1:H:111:ARG:HE	1:H:112:ARG:N	2.17	0.42
1:I:37:GLU:C	1:I:39:LEU:N	2.76	0.42
1:I:269:ASP:CG	1:I:274:THR:HG1	2.27	0.42
1:K:96:ASP:C	1:K:98:SER:N	2.77	0.42
1:K:221:VAL:O	1:K:221:VAL:HG22	2.20	0.42
1:M:11:MET:O	1:M:96:ASP:N	2.50	0.42
1:D:64:LEU:O	1:D:67:LEU:HB2	2.20	0.42
1:E:155:PHE:O	1:E:156:ARG:C	2.63	0.42
1:F:35:GLN:HB3	1:F:283:LEU:HD11	2.02	0.42
1:G:5:ALA:O	1:G:90:PRO:HA	2.19	0.42
1:J:179:LEU:HD23	1:J:184:VAL:HG21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:188:THR:C	1:K:190:HIS:N	2.76	0.42
1:L:36:LEU:HD22	1:L:286:LEU:HD23	2.02	0.42
1:L:118:VAL:HG13	1:L:166:VAL:HB	2.01	0.42
1:L:120:ALA:HB2	1:L:220:ASP:O	2.19	0.42
1:L:126:THR:CG2	1:L:178:LEU:HD13	2.49	0.42
1:A:9:VAL:O	1:A:11:MET:N	2.52	0.42
1:A:21:ASP:CG	1:H:29:TYR:HH	2.28	0.42
1:A:111:ARG:NE	1:A:111:ARG:HA	2.35	0.42
1:A:192:VAL:HA	1:A:200:ILE:CD1	2.49	0.42
1:D:160:PRO:C	1:D:162:ASP:H	2.27	0.42
1:E:202:GLU:HG2	1:E:202:GLU:H	1.66	0.42
1:F:95:GLY:O	1:F:96:ASP:O	2.38	0.42
1:F:169:ARG:HH11	1:F:234:VAL:HB	1.85	0.42
1:H:32:LEU:HA	1:H:279:VAL:CG1	2.49	0.42
1:H:104:VAL:HG22	1:H:214:HIS:CE1	2.55	0.42
1:J:249:ILE:HA	1:J:249:ILE:HD13	1.75	0.42
1:M:211:LEU:N	1:M:211:LEU:HD23	2.35	0.42
1:A:202:GLU:HG2	1:A:202:GLU:H	1.63	0.42
1:C:125:ASN:ND2	1:C:129:THR:OG1	2.52	0.42
1:D:149:PRO:HA	1:D:152:THR:HG1	1.85	0.42
1:E:159:ASP:C	1:E:159:ASP:OD1	2.63	0.42
1:F:99:LEU:C	1:F:99:LEU:CD1	2.90	0.42
1:F:126:THR:HG23	1:F:178:LEU:HD13	2.00	0.42
1:H:69:GLU:O	1:H:72:ALA:HB3	2.19	0.42
1:H:82:ALA:CA	1:H:109:ARG:HH12	2.24	0.42
1:I:278:LEU:HD12	1:I:278:LEU:HA	1.75	0.42
1:L:37:GLU:HG2	1:L:43:VAL:HG23	2.01	0.42
1:L:163:VAL:HB	1:L:184:VAL:HG13	2.01	0.42
1:L:177:ARG:O	1:L:181:GLU:HB2	2.20	0.42
1:M:256:VAL:HG11	1:M:285:LEU:HD21	2.01	0.42
1:C:129:THR:HB	1:C:174:GLY:HA3	2.02	0.42
1:D:22:MET:HE3	1:J:25:SER:CB	2.44	0.42
1:E:177:ARG:NH1	1:E:177:ARG:CB	2.81	0.42
1:F:36:LEU:O	1:F:39:LEU:N	2.53	0.42
1:H:163:VAL:CG1	1:H:164:VAL:N	2.83	0.42
1:J:89:PHE:HE1	1:J:256:VAL:O	2.03	0.42
1:M:99:LEU:HD12	1:M:100:SER:N	2.34	0.42
1:A:29:TYR:C	1:A:31:ARG:N	2.79	0.41
1:C:271:ARG:CZ	1:K:268:LEU:O	2.68	0.41
1:D:261:LEU:HD11	1:D:282:ALA:HB2	2.01	0.41
1:F:113:VAL:HG11	1:F:257:GLN:NE2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:71:ARG:NH2	1:G:153:GLU:OE2	2.51	0.41
1:G:201:ALA:CB	1:G:249:ILE:HG21	2.49	0.41
1:H:116:VAL:HB	1:H:215:VAL:HG22	2.01	0.41
1:H:234:VAL:HA	1:H:235:PRO:HD2	1.81	0.41
1:I:119:ASP:HA	1:I:218:ASP:HB3	2.02	0.41
1:J:50:PRO:C	1:J:51:VAL:HG23	2.45	0.41
1:J:115:VAL:CG2	1:J:158:VAL:HG21	2.50	0.41
1:K:94:GLY:N	1:K:261:LEU:O	2.44	0.41
1:K:226:LEU:HD21	1:K:240:TYR:CA	2.49	0.41
1:L:187:TYR:OH	1:L:203:GLU:OE1	2.35	0.41
1:M:140:LEU:HD23	1:M:165:LEU:HD11	2.01	0.41
1:M:214:HIS:CD2	1:M:258:SER:HB2	2.55	0.41
1:C:12:ASP:C	1:C:12:ASP:OD1	2.62	0.41
1:C:111:ARG:CD	1:C:112:ARG:N	2.82	0.41
1:D:39:LEU:HD12	1:D:39:LEU:HA	1.84	0.41
1:D:119:ASP:C	1:D:221:VAL:HG23	2.45	0.41
1:E:121:HIS:HE1	1:E:232:THR:HB	1.85	0.41
1:E:159:ASP:O	1:E:160:PRO:C	2.61	0.41
1:E:160:PRO:C	1:E:162:ASP:H	2.28	0.41
1:G:227:ALA:N	1:G:228:PRO:HD3	2.34	0.41
1:J:6:VAL:CG1	1:J:93:LEU:HD21	2.47	0.41
1:K:119:ASP:HA	1:K:218:ASP:HB3	2.01	0.41
1:K:122:ALA:O	1:K:123:ASP:C	2.63	0.41
1:M:91:ILE:HG23	1:M:259:LEU:HD23	2.01	0.41
1:C:252:GLU:OE2	1:I:194:ARG:NH2	2.53	0.41
1:D:99:LEU:C	1:D:99:LEU:HD12	2.45	0.41
1:D:148:HIS:CD2	1:D:150:ARG:H	2.38	0.41
1:E:138:MET:O	1:E:139:PRO:C	2.62	0.41
1:G:168:VAL:HG12	1:G:188:THR:HG22	2.02	0.41
1:G:222:LEU:CD1	1:G:277:MET:HE2	2.50	0.41
1:H:12:ASP:O	1:H:13:LEU:HD23	2.21	0.41
1:I:11:MET:HE2	1:I:98:SER:HB2	2.02	0.41
1:I:124:PHE:CD2	1:I:124:PHE:O	2.73	0.41
1:J:108:ALA:O	1:J:109:ARG:C	2.63	0.41
1:K:22:MET:SD	1:K:267:ILE:CD1	3.09	0.41
1:K:277:MET:CE	1:K:277:MET:CA	2.98	0.41
1:M:39:LEU:HD12	1:M:39:LEU:HA	1.75	0.41
1:M:119:ASP:OD2	1:M:218:ASP:OD2	2.38	0.41
1:M:277:MET:HB3	1:M:277:MET:HE3	1.78	0.41
1:E:119:ASP:CG	1:E:218:ASP:OD2	2.63	0.41
1:F:95:GLY:O	1:F:96:ASP:C	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:265:ASN:HA	1:F:266:PRO:HD2	1.93	0.41
1:G:84:LEU:O	1:G:85:PRO:C	2.63	0.41
1:H:3:ARG:HE	1:H:3:ARG:HB2	1.59	0.41
1:I:265:ASN:ND2	1:I:268:LEU:HG	2.36	0.41
1:J:119:ASP:HB3	1:J:121:HIS:O	2.19	0.41
1:J:139:PRO:O	1:J:143:LEU:HD12	2.20	0.41
1:J:247:MET:SD	1:J:285:LEU:HD13	2.61	0.41
1:K:35:GLN:OE1	1:K:283:LEU:HD11	2.19	0.41
1:K:251:ALA:O	1:K:252:GLU:C	2.63	0.41
1:L:89:PHE:CZ	1:L:256:VAL:HG12	2.52	0.41
1:A:97:HIS:CD2	1:A:262:VAL:HG21	2.56	0.41
1:D:234:VAL:HA	1:D:235:PRO:HD3	1.91	0.41
1:E:34:GLU:OE1	1:E:34:GLU:N	2.34	0.41
1:E:37:GLU:C	1:E:39:LEU:N	2.77	0.41
1:E:153:GLU:HG3	1:E:154:VAL:N	2.35	0.41
1:F:9:VAL:O	1:F:11:MET:N	2.53	0.41
1:F:168:VAL:HG11	1:F:171:LEU:HD21	2.02	0.41
1:G:32:LEU:CD1	1:G:279:VAL:HG13	2.50	0.41
1:G:139:PRO:O	1:G:143:LEU:HG	2.20	0.41
1:I:288:LYS:O	1:I:289:ARG:HG3	2.21	0.41
1:K:148:HIS:HA	1:K:149:PRO:HD3	1.85	0.41
1:K:193:ASP:HB2	1:M:245:LEU:HD13	2.01	0.41
1:L:93:LEU:HD22	1:L:261:LEU:HD12	2.03	0.41
1:M:71:ARG:O	1:M:72:ALA:C	2.62	0.41
1:C:19:GLY:C	1:C:21:ASP:N	2.77	0.41
1:C:67:LEU:HD21	1:C:150:ARG:HB2	2.02	0.41
1:C:148:HIS:CD2	1:C:150:ARG:HB2	2.56	0.41
1:C:248:GLU:OE1	1:I:190:HIS:CD2	2.68	0.41
1:D:171:LEU:HB2	1:D:176:LYS:HE2	2.03	0.41
1:E:37:GLU:HG2	1:E:43:VAL:CG2	2.42	0.41
1:E:175:GLU:O	1:E:176:LYS:C	2.64	0.41
1:G:11:MET:O	1:G:96:ASP:OD2	2.39	0.41
1:G:22:MET:CB	1:G:266:PRO:HG2	2.51	0.41
1:G:94:GLY:HA3	1:G:99:LEU:CD2	2.50	0.41
1:H:146:LEU:HD23	1:H:146:LEU:N	2.36	0.41
1:K:190:HIS:O	1:K:194:ARG:HB2	2.21	0.41
1:K:276:GLU:O	1:K:277:MET:C	2.62	0.41
1:M:13:LEU:HD12	1:M:70:ILE:CG1	2.42	0.41
1:M:243:ALA:HB1	1:M:281:LEU:CD1	2.50	0.41
1:A:117:TRP:HB3	1:A:165:LEU:HD23	2.03	0.41
1:D:251:ALA:O	1:D:252:GLU:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:46:LEU:HD13	1:F:80:ARG:NH2	2.35	0.41
1:G:265:ASN:OD1	1:G:267:ILE:HB	2.20	0.41
1:I:225:THR:O	1:I:273:ARG:NH2	2.54	0.41
1:J:277:MET:HE2	1:J:277:MET:HB3	1.88	0.41
1:L:64:LEU:HD13	1:L:65:ALA:H	1.84	0.41
1:M:150:ARG:O	1:M:150:ARG:CD	2.67	0.41
1:M:172:ASP:HB3	1:M:173:PRO:HD2	2.03	0.41
1:M:286:LEU:N	1:M:286:LEU:CD1	2.83	0.41
1:A:67:LEU:HD11	1:A:148:HIS:CG	2.55	0.41
1:C:259:LEU:HD13	1:C:285:LEU:HD22	2.03	0.41
1:J:34:GLU:H	1:J:34:GLU:CD	2.24	0.41
1:M:150:ARG:O	1:M:153:GLU:OE2	2.38	0.41
1:M:217:LEU:HD12	1:M:217:LEU:HA	1.85	0.41
1:M:243:ALA:O	1:M:247:MET:HG2	2.21	0.41
1:C:96:ASP:HB3	1:C:136:HIS:HB3	2.02	0.41
1:D:99:LEU:HD21	1:D:262:VAL:CG1	2.47	0.41
1:E:37:GLU:HA	1:E:41:TYR:O	2.20	0.41
1:F:67:LEU:O	1:F:71:ARG:HB2	2.21	0.41
1:F:241:ARG:O	1:F:242:GLU:C	2.60	0.41
1:G:72:ALA:O	1:G:76:VAL:HG23	2.20	0.41
1:H:12:ASP:HB3	1:H:21:ASP:HB3	2.03	0.41
1:H:141:ALA:O	1:H:142:VAL:C	2.64	0.41
1:H:159:ASP:O	1:H:160:PRO:C	2.64	0.41
1:H:159:ASP:O	1:H:162:ASP:N	2.47	0.41
1:I:153:GLU:CG	1:I:154:VAL:HG13	2.51	0.41
1:I:163:VAL:HG12	1:I:184:VAL:HG13	2.03	0.41
1:I:168:VAL:HG11	1:I:171:LEU:HD21	2.03	0.41
1:J:140:LEU:HD23	1:J:165:LEU:HD21	2.03	0.41
1:J:145:GLY:CA	1:J:156:ARG:HD2	2.51	0.41
1:J:168:VAL:CG1	1:J:171:LEU:HD21	2.45	0.41
1:J:208:LEU:HD23	1:J:208:LEU:HA	1.91	0.41
1:K:4:VAL:HG22	1:K:89:PHE:HB3	2.03	0.41
1:K:75:LEU:HG	1:K:79:GLU:HG3	2.03	0.41
1:K:176:LYS:HD3	1:M:291:PHE:HD2	1.85	0.41
1:K:185:ARG:NH1	1:K:207:HIS:ND1	2.69	0.41
1:K:242:GLU:O	1:K:243:ALA:C	2.64	0.41
1:L:10:PRO:O	1:L:51:VAL:HG21	2.20	0.41
1:L:95:GLY:O	1:L:96:ASP:C	2.64	0.41
1:L:97:HIS:ND1	1:L:119:ASP:OD2	2.53	0.41
1:M:99:LEU:HD21	1:M:262:VAL:HG12	2.03	0.41
1:M:218:ASP:OD1	1:M:263:GLU:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:19:GLY:C	1:C:21:ASP:H	2.29	0.41
1:D:160:PRO:C	1:D:162:ASP:N	2.79	0.41
1:H:135:VAL:O	1:H:138:MET:N	2.46	0.41
1:J:138:MET:H	1:J:139:PRO:HD2	1.76	0.41
1:J:191:GLU:H	1:J:191:GLU:CD	2.29	0.41
1:J:278:LEU:HD12	1:J:278:LEU:HA	1.84	0.41
1:K:68:GLU:CD	1:K:150:ARG:HH21	2.29	0.41
1:K:167:GLY:O	1:K:168:VAL:C	2.64	0.41
1:K:169:ARG:CZ	1:K:237:GLY:HA3	2.51	0.41
1:M:194:ARG:HH11	1:M:194:ARG:CG	2.33	0.41
1:C:84:LEU:H	1:C:84:LEU:HG	1.67	0.40
1:D:89:PHE:CZ	1:D:286:LEU:HD11	2.56	0.40
1:E:125:ASN:HB2	1:E:137:GLY:O	2.21	0.40
1:E:223:ASP:HA	1:E:224:PRO:HD3	1.96	0.40
1:F:67:LEU:HD21	1:F:150:ARG:HB2	2.03	0.40
1:F:111:ARG:NH2	1:G:249:ILE:O	2.54	0.40
1:F:145:GLY:CA	1:F:156:ARG:HD3	2.47	0.40
1:F:211:LEU:H	1:F:255:ARG:NH1	2.19	0.40
1:F:220:ASP:C	1:F:220:ASP:OD1	2.64	0.40
1:K:39:LEU:HA	1:K:39:LEU:HD12	1.60	0.40
1:L:81:LEU:HD12	1:L:103:SER:HA	2.02	0.40
1:L:202:GLU:HA	1:L:202:GLU:OE1	2.21	0.40
1:L:205:LEU:O	1:L:255:ARG:NH2	2.54	0.40
1:M:82:ALA:O	1:M:84:LEU:N	2.48	0.40
1:M:253:SER:O	1:M:254:GLY:C	2.64	0.40
1:A:19:GLY:N	1:A:265:ASN:HD21	2.20	0.40
1:A:29:TYR:CE1	1:H:19:GLY:HA2	2.57	0.40
1:A:288:LYS:O	1:A:289:ARG:HG3	2.20	0.40
1:C:219:ALA:C	1:C:221:VAL:H	2.30	0.40
1:H:12:ASP:CB	1:H:21:ASP:HB3	2.51	0.40
1:I:71:ARG:CZ	1:I:150:ARG:NH1	2.84	0.40
1:J:153:GLU:HG3	1:J:154:VAL:HG13	2.02	0.40
1:J:156:ARG:O	1:J:157:ALA:HB2	2.21	0.40
1:L:285:LEU:HD12	1:L:285:LEU:HA	1.84	0.40
1:A:86:GLU:HB2	1:D:86:GLU:HG3	2.02	0.40
1:A:220:ASP:OD1	1:A:220:ASP:C	2.64	0.40
1:A:227:ALA:O	1:A:230:VAL:HG13	2.21	0.40
1:C:272:ASN:CG	1:C:272:ASN:O	2.63	0.40
1:E:112:ARG:CZ	1:E:211:LEU:HD21	2.51	0.40
1:H:138:MET:H	1:H:139:PRO:HD2	1.86	0.40
1:H:197:VAL:O	1:H:198:ALA:C	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:219:ALA:C	1:H:221:VAL:H	2.30	0.40
1:I:277:MET:HB3	1:I:277:MET:HE2	1.84	0.40
1:J:145:GLY:HA2	1:J:156:ARG:CG	2.52	0.40
1:K:67:LEU:HA	1:K:70:ILE:HD12	2.03	0.40
1:M:214:HIS:CD2	1:M:258:SER:OG	2.74	0.40
1:D:112:ARG:HH11	1:D:211:LEU:HD21	1.84	0.40
1:D:204:VAL:O	1:D:204:VAL:HG12	2.20	0.40
1:G:30:ALA:HB3	1:G:279:VAL:HG21	2.04	0.40
1:H:37:GLU:HA	1:H:41:TYR:O	2.21	0.40
1:K:97:HIS:CE1	1:K:117:TRP:CZ2	3.10	0.40
1:L:79:GLU:O	1:L:81:LEU:N	2.54	0.40
1:M:174:GLY:O	1:M:175:GLU:C	2.65	0.40
1:A:111:ARG:NH2	1:D:79:GLU:O	2.28	0.40
1:D:98:SER:HA	1:D:139:PRO:HG3	2.04	0.40
1:E:69:GLU:O	1:E:70:ILE:C	2.64	0.40
1:F:129:THR:O	1:F:130:SER:CB	2.69	0.40
1:F:225:THR:HG22	1:F:226:LEU:N	2.35	0.40
1:G:22:MET:CE	1:L:22:MET:HE2	2.51	0.40
1:J:202:GLU:HG2	1:J:202:GLU:H	1.67	0.40
1:J:206:LYS:C	1:J:208:LEU:N	2.79	0.40
1:J:225:THR:CG2	1:J:226:LEU:N	2.82	0.40
1:K:252:GLU:C	1:K:254:GLY:N	2.75	0.40
1:L:104:VAL:HG21	1:L:143:LEU:CD1	2.52	0.40
1:L:126:THR:O	1:L:127:PRO:C	2.63	0.40
1:M:209:GLN:HA	1:M:255:ARG:NH2	2.37	0.40
1:M:283:LEU:O	1:M:288:LYS:CB	2.69	0.40

There are no symmetry-related clashes.

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	265/291 (91%)	246 (93%)	17 (6%)	2 (1%)	16	43
1	C	265/291 (91%)	245 (92%)	18 (7%)	2 (1%)	16	43
1	D	265/291 (91%)	248 (94%)	14 (5%)	3 (1%)	11	35
1	E	265/291 (91%)	236 (89%)	25 (9%)	4 (2%)	8	27
1	F	265/291 (91%)	242 (91%)	19 (7%)	4 (2%)	8	27
1	G	265/291 (91%)	231 (87%)	32 (12%)	2 (1%)	16	43
1	H	265/291 (91%)	240 (91%)	21 (8%)	4 (2%)	8	27
1	I	265/291 (91%)	225 (85%)	34 (13%)	6 (2%)	5	18
1	J	265/291 (91%)	217 (82%)	37 (14%)	11 (4%)	2	7
1	K	265/291 (91%)	206 (78%)	50 (19%)	9 (3%)	3	11
1	L	265/291 (91%)	220 (83%)	34 (13%)	11 (4%)	2	7
1	M	265/291 (91%)	217 (82%)	33 (12%)	15 (6%)	1	4
All	All	3180/3492 (91%)	2773 (87%)	334 (10%)	73 (2%)	5	18

All (73) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	K	67	LEU
1	L	67	LEU
1	L	138	MET
1	M	129	THR
1	M	133	GLY
1	C	66	TYR
1	F	96	ASP
1	F	229	GLY
1	H	85	PRO
1	J	33	LEU
1	J	111	ARG
1	J	157	ALA
1	K	168	VAL
1	L	66	TYR
1	L	80	ARG
1	L	253	SER
1	M	33	LEU
1	M	139	PRO
1	M	168	VAL
1	H	235	PRO
1	J	65	ALA
1	J	78	LYS

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Mol	Chain	Res	Type
1	J	207	HIS
1	K	157	ALA
1	K	160	PRO
1	K	182	ALA
1	L	178	LEU
1	L	231	GLY
1	M	157	ALA
1	M	184	VAL
1	M	246	LEU
1	D	10	PRO
1	D	123	ASP
1	E	153	GLU
1	E	235	PRO
1	F	123	ASP
1	G	138	MET
1	I	103	SER
1	J	96	ASP
1	K	177	ARG
1	L	12	ASP
1	L	79	GLU
1	L	86	GLU
1	M	90	PRO
1	M	128	GLU
1	M	136	HIS
1	M	207	HIS
1	M	220	ASP
1	A	65	ALA
1	E	272	ASN
1	F	138	MET
1	G	133	GLY
1	I	157	ALA
1	J	67	LEU
1	K	110	GLY
1	M	10	PRO
1	M	138	MET
1	E	138	MET
1	I	10	PRO
1	I	139	PRO
1	J	127	PRO
1	K	267	ILE
1	A	138	MET
1	K	90	PRO

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Mol	Chain	Res	Type
1	I	102	GLY
1	J	10	PRO
1	C	138	MET
1	J	138	MET
1	L	85	PRO
1	D	138	MET
1	H	84	LEU
1	H	138	MET
1	I	138	MET

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	218/232 (94%)	198 (91%)	20 (9%)	8	26
1	C	218/232 (94%)	197 (90%)	21 (10%)	8	25
1	D	218/232 (94%)	198 (91%)	20 (9%)	8	26
1	E	218/232 (94%)	194 (89%)	24 (11%)	6	19
1	F	218/232 (94%)	198 (91%)	20 (9%)	8	26
1	G	218/232 (94%)	191 (88%)	27 (12%)	4	14
1	H	218/232 (94%)	191 (88%)	27 (12%)	4	14
1	I	218/232 (94%)	188 (86%)	30 (14%)	3	11
1	J	218/232 (94%)	192 (88%)	26 (12%)	5	16
1	K	218/232 (94%)	187 (86%)	31 (14%)	3	10
1	L	218/232 (94%)	177 (81%)	41 (19%)	1	5
1	M	218/232 (94%)	176 (81%)	42 (19%)	1	4
All	All	2616/2784 (94%)	2287 (87%)	329 (13%)	4	14

All (329) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU

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Mol	Chain	Res	Type
1	A	3	ARG
1	A	7	VAL
1	A	37	GLU
1	A	80	ARG
1	A	86	GLU
1	A	109	ARG
1	A	111	ARG
1	A	153	GLU
1	A	160	PRO
1	A	161	LYS
1	A	202	GLU
1	A	206	LYS
1	A	211	LEU
1	A	225	THR
1	A	230	VAL
1	A	240	TYR
1	A	257	GLN
1	A	277	MET
1	A	278	LEU
1	C	2	GLU
1	C	7	VAL
1	C	33	LEU
1	C	42	THR
1	C	49	VAL
1	C	51	VAL
1	C	98	SER
1	C	109	ARG
1	C	111	ARG
1	C	113	VAL
1	C	138	MET
1	C	156	ARG
1	C	161	LYS
1	C	180	LYS
1	C	194	ARG
1	C	225	THR
1	C	226	LEU
1	C	232	THR
1	C	257	GLN
1	C	259	LEU
1	C	267	ILE
1	D	7	VAL
1	D	20	VAL

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Mol	Chain	Res	Type
1	D	33	LEU
1	D	64	LEU
1	D	67	LEU
1	D	79	GLU
1	D	84	LEU
1	D	86	GLU
1	D	111	ARG
1	D	113	VAL
1	D	177	ARG
1	D	199	ARG
1	D	211	LEU
1	D	221	VAL
1	D	232	THR
1	D	255	ARG
1	D	258	SER
1	D	267	ILE
1	D	276	GLU
1	D	277	MET
1	E	4	VAL
1	E	20	VAL
1	E	33	LEU
1	E	43	VAL
1	E	80	ARG
1	E	86	GLU
1	E	88	VAL
1	E	98	SER
1	E	99	LEU
1	E	109	ARG
1	E	118	VAL
1	E	144	SER
1	E	154	VAL
1	E	194	ARG
1	E	200	ILE
1	E	202	GLU
1	E	225	THR
1	E	226	LEU
1	E	232	THR
1	E	255	ARG
1	E	257	GLN
1	E	267	ILE
1	E	276	GLU
1	E	277	MET

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Mol	Chain	Res	Type
1	F	11	MET
1	F	20	VAL
1	F	33	LEU
1	F	64	LEU
1	F	67	LEU
1	F	98	SER
1	F	111	ARG
1	F	118	VAL
1	F	130	SER
1	F	135	VAL
1	F	138	MET
1	F	160	PRO
1	F	202	GLU
1	F	225	THR
1	F	226	LEU
1	F	252	GLU
1	F	267	ILE
1	F	273	ARG
1	F	277	MET
1	F	284	SER
1	G	2	GLU
1	G	13	LEU
1	G	20	VAL
1	G	33	LEU
1	G	37	GLU
1	G	49	VAL
1	G	51	VAL
1	G	80	ARG
1	G	86	GLU
1	G	88	VAL
1	G	99	LEU
1	G	125	ASN
1	G	138	MET
1	G	144	SER
1	G	146	LEU
1	G	158	VAL
1	G	161	LYS
1	G	168	VAL
1	G	180	LYS
1	G	202	GLU
1	G	225	THR
1	G	226	LEU

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Mol	Chain	Res	Type
1	G	232	THR
1	G	258	SER
1	G	270	GLU
1	G	277	MET
1	G	289	ARG
1	H	2	GLU
1	H	9	VAL
1	H	12	ASP
1	H	33	LEU
1	H	42	THR
1	H	51	VAL
1	H	64	LEU
1	H	67	LEU
1	H	78	LYS
1	H	79	GLU
1	H	85	PRO
1	H	86	GLU
1	H	100	SER
1	H	109	ARG
1	H	111	ARG
1	H	118	VAL
1	H	146	LEU
1	H	160	PRO
1	H	175	GLU
1	H	194	ARG
1	H	204	VAL
1	H	211	LEU
1	H	225	THR
1	H	232	THR
1	H	267	ILE
1	H	277	MET
1	H	286	LEU
1	I	2	GLU
1	I	33	LEU
1	I	43	VAL
1	I	46	LEU
1	I	51	VAL
1	I	64	LEU
1	I	80	ARG
1	I	86	GLU
1	I	98	SER
1	I	99	LEU

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Mol	Chain	Res	Type
1	I	100	SER
1	I	109	ARG
1	I	111	ARG
1	I	113	VAL
1	I	125	ASN
1	I	138	MET
1	I	144	SER
1	I	152	THR
1	I	160	PRO
1	I	161	LYS
1	I	179	LEU
1	I	194	ARG
1	I	211	LEU
1	I	221	VAL
1	I	255	ARG
1	I	262	VAL
1	I	267	ILE
1	I	277	MET
1	I	278	LEU
1	I	286	LEU
1	J	2	GLU
1	J	13	LEU
1	J	33	LEU
1	J	44	GLU
1	J	64	LEU
1	J	67	LEU
1	J	78	LYS
1	J	93	LEU
1	J	109	ARG
1	J	118	VAL
1	J	125	ASN
1	J	130	SER
1	J	140	LEU
1	J	156	ARG
1	J	158	VAL
1	J	166	VAL
1	J	184	VAL
1	J	194	ARG
1	J	206	LYS
1	J	225	THR
1	J	247	MET
1	J	249	ILE

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Mol	Chain	Res	Type
1	J	267	ILE
1	J	270	GLU
1	J	277	MET
1	J	278	LEU
1	K	2	GLU
1	K	4	VAL
1	K	28	ARG
1	K	31	ARG
1	K	33	LEU
1	K	37	GLU
1	K	44	GLU
1	K	46	LEU
1	K	64	LEU
1	K	68	GLU
1	K	90	PRO
1	K	92	VAL
1	K	98	SER
1	K	109	ARG
1	K	113	VAL
1	K	118	VAL
1	K	126	THR
1	K	130	SER
1	K	134	ASN
1	K	156	ARG
1	K	160	PRO
1	K	162	ASP
1	K	166	VAL
1	K	194	ARG
1	K	216	SER
1	K	225	THR
1	K	226	LEU
1	K	230	VAL
1	K	246	LEU
1	K	267	ILE
1	K	277	MET
1	L	2	GLU
1	L	4	VAL
1	L	6	VAL
1	L	11	MET
1	L	24	PRO
1	L	33	LEU
1	L	43	VAL

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Mol	Chain	Res	Type
1	L	51	VAL
1	L	64	LEU
1	L	76	VAL
1	L	80	ARG
1	L	81	LEU
1	L	86	GLU
1	L	88	VAL
1	L	91	ILE
1	L	98	SER
1	L	109	ARG
1	L	111	ARG
1	L	116	VAL
1	L	118	VAL
1	L	125	ASN
1	L	127	PRO
1	L	143	LEU
1	L	154	VAL
1	L	164	VAL
1	L	166	VAL
1	L	168	VAL
1	L	173	PRO
1	L	186	VAL
1	L	194	ARG
1	L	220	ASP
1	L	221	VAL
1	L	232	THR
1	L	252	GLU
1	L	257	GLN
1	L	259	LEU
1	L	260	ASP
1	L	267	ILE
1	L	268	LEU
1	L	284	SER
1	L	289	ARG
1	M	6	VAL
1	M	13	LEU
1	M	20	VAL
1	M	24	PRO
1	M	25	SER
1	M	33	LEU
1	M	37	GLU
1	M	39	LEU

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Mol	Chain	Res	Type
1	M	43	VAL
1	M	46	LEU
1	M	51	VAL
1	M	64	LEU
1	M	67	LEU
1	M	68	GLU
1	M	80	ARG
1	M	84	LEU
1	M	86	GLU
1	M	90	PRO
1	M	109	ARG
1	M	111	ARG
1	M	118	VAL
1	M	129	THR
1	M	134	ASN
1	M	144	SER
1	M	154	VAL
1	M	160	PRO
1	M	168	VAL
1	M	191	GLU
1	M	192	VAL
1	M	194	ARG
1	M	200	ILE
1	M	211	LEU
1	M	232	THR
1	M	256	VAL
1	M	258	SER
1	M	260	ASP
1	M	267	ILE
1	M	276	GLU
1	M	278	LEU
1	M	283	LEU
1	M	284	SER
1	M	286	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (67) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	125	ASN
1	A	148	HIS
1	A	190	HIS
1	A	214	HIS

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Mol	Chain	Res	Type
1	A	257	GLN
1	C	35	GLN
1	C	125	ASN
1	C	134	ASN
1	C	148	HIS
1	C	207	HIS
1	C	214	HIS
1	D	125	ASN
1	D	134	ASN
1	D	136	HIS
1	D	148	HIS
1	D	207	HIS
1	D	214	HIS
1	D	265	ASN
1	E	125	ASN
1	E	134	ASN
1	E	148	HIS
1	E	190	HIS
1	E	207	HIS
1	E	214	HIS
1	F	121	HIS
1	F	125	ASN
1	F	134	ASN
1	F	148	HIS
1	F	214	HIS
1	F	257	GLN
1	F	265	ASN
1	G	125	ASN
1	G	134	ASN
1	G	148	HIS
1	G	207	HIS
1	G	209	GLN
1	G	214	HIS
1	H	136	HIS
1	H	148	HIS
1	H	214	HIS
1	I	125	ASN
1	I	134	ASN
1	I	190	HIS
1	I	207	HIS
1	I	214	HIS
1	J	121	HIS

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Mol	Chain	Res	Type
1	J	125	ASN
1	J	134	ASN
1	J	148	HIS
1	J	207	HIS
1	J	214	HIS
1	K	134	ASN
1	K	148	HIS
1	K	190	HIS
1	K	214	HIS
1	L	35	GLN
1	L	125	ASN
1	L	134	ASN
1	L	148	HIS
1	L	190	HIS
1	L	214	HIS
1	L	265	ASN
1	M	125	ASN
1	M	148	HIS
1	M	190	HIS
1	M	207	HIS
1	M	214	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	273/291 (93%)	-0.39	0 100 100	26, 42, 57, 68	0
1	C	273/291 (93%)	-0.26	2 (0%) 84 79	28, 48, 60, 72	0
1	D	273/291 (93%)	-0.29	2 (0%) 84 79	31, 45, 60, 70	0
1	E	273/291 (93%)	-0.22	3 (1%) 78 71	28, 48, 62, 72	0
1	F	273/291 (93%)	-0.31	2 (0%) 84 79	34, 47, 61, 68	0
1	G	273/291 (93%)	-0.20	2 (0%) 84 79	27, 53, 70, 79	0
1	H	273/291 (93%)	-0.14	3 (1%) 78 71	35, 55, 68, 74	0
1	I	273/291 (93%)	-0.12	3 (1%) 78 71	37, 56, 69, 72	0
1	J	273/291 (93%)	-0.03	2 (0%) 84 79	42, 60, 74, 79	0
1	K	273/291 (93%)	0.18	4 (1%) 72 64	50, 68, 78, 81	0
1	L	273/291 (93%)	0.22	2 (0%) 84 79	52, 67, 76, 84	0
1	M	273/291 (93%)	0.63	20 (7%) 21 17	54, 73, 82, 88	0
All	All	3276/3492 (93%)	-0.08	45 (1%) 73 65	26, 55, 75, 88	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	65	ALA	4.5
1	G	52	SER	4.1
1	M	88	VAL	3.3
1	M	101	MET	3.3
1	M	40	GLY	3.3
1	E	132	SER	3.1
1	M	100	SER	3.0
1	D	64	LEU	3.0
1	M	41	TYR	3.0
1	M	52	SER	3.0
1	D	52	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	M	104	VAL	2.9
1	M	154	VAL	2.9
1	M	133	GLY	2.7
1	M	13	LEU	2.7
1	M	147	GLY	2.7
1	E	52	SER	2.6
1	I	41	TYR	2.6
1	K	231	GLY	2.6
1	M	135	VAL	2.6
1	M	129	THR	2.5
1	H	154	VAL	2.5
1	K	52	SER	2.4
1	M	128	GLU	2.4
1	L	64	LEU	2.4
1	M	123	ASP	2.3
1	L	108	ALA	2.3
1	E	154	VAL	2.3
1	G	64	LEU	2.3
1	C	132	SER	2.2
1	M	149	PRO	2.2
1	F	52	SER	2.2
1	J	87	GLY	2.2
1	I	231	GLY	2.2
1	H	113	VAL	2.1
1	M	76	VAL	2.1
1	F	64	LEU	2.1
1	K	291	PHE	2.1
1	K	19	GLY	2.1
1	C	271	ARG	2.1
1	J	52	SER	2.0
1	I	133	GLY	2.0
1	M	148	HIS	2.0
1	M	65	ALA	2.0
1	M	105	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.