



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:06 AM UTC

PDB ID : 2CB6 / pdb\_00002cb6  
Title : Crystal structure of the catalytic domain of the mosquitocidal toxin from *Bacillus sphaericus*, mutant E195Q  
Authors : Reinert, D.J.; Carpusca, I.; Aktories, K.; Schulz, G.E.  
Deposited on : 2005-12-29  
Resolution : 3.00 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](mailto: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>.

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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

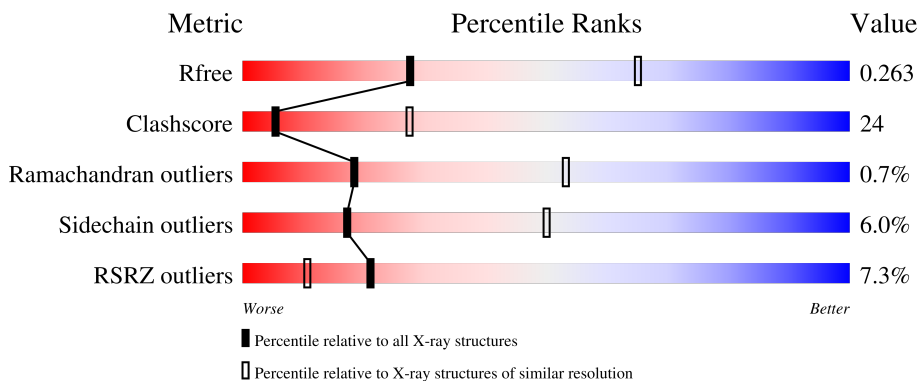
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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.



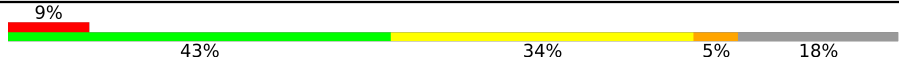
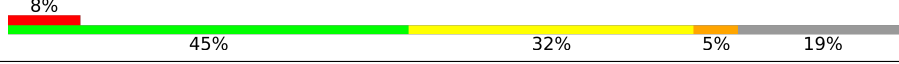
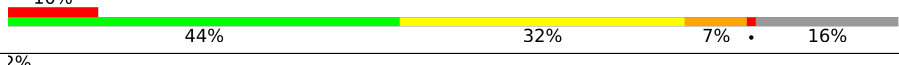
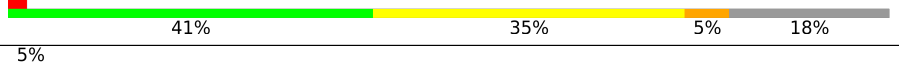
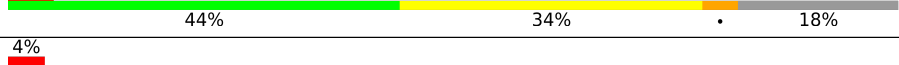

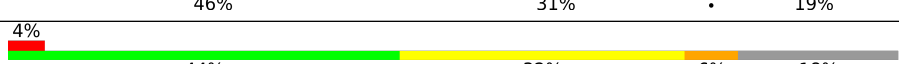
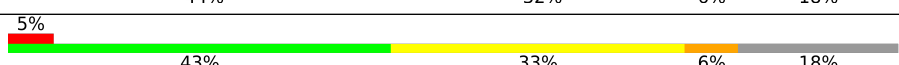



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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  $\geq 3$ , 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	B	291	
1	C	291	
1	D	291	
1	E	291	

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Mol	Chain	Length	Quality of chain
1	F	291	
1	G	291	
1	H	291	
1	I	291	
1	J	291	
1	K	291	
1	L	291	
1	M	291	
1	N	291	
1	O	291	
1	P	291	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 31202 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 MOSQUITOCIDAL TOXIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	238	Total 1939	C 1223	N 346	O 367	S 3	0	0	0
1	B	238	Total 1939	C 1223	N 346	O 367	S 3	0	0	0
1	C	244	Total 1986	C 1252	N 353	O 378	S 3	0	0	0
1	D	244	Total 1986	C 1252	N 353	O 378	S 3	0	0	0
1	E	238	Total 1939	C 1223	N 346	O 367	S 3	0	0	0
1	F	238	Total 1939	C 1223	N 346	O 367	S 3	0	0	0
1	G	236	Total 1918	C 1210	N 338	O 367	S 3	0	0	0
1	H	245	Total 1992	C 1255	N 354	O 380	S 3	0	0	0
1	I	238	Total 1939	C 1223	N 346	O 367	S 3	0	0	0
1	J	238	Total 1939	C 1223	N 346	O 367	S 3	0	0	0
1	K	244	Total 1986	C 1252	N 353	O 378	S 3	0	0	0
1	L	236	Total 1918	C 1210	N 338	O 367	S 3	0	0	0
1	M	238	Total 1939	C 1223	N 346	O 367	S 3	0	0	0
1	N	238	Total 1939	C 1223	N 346	O 367	S 3	0	0	0
1	O	236	Total 1918	C 1210	N 338	O 367	S 3	0	0	0
1	P	244	Total 1986	C 1252	N 353	O 378	S 3	0	0	0

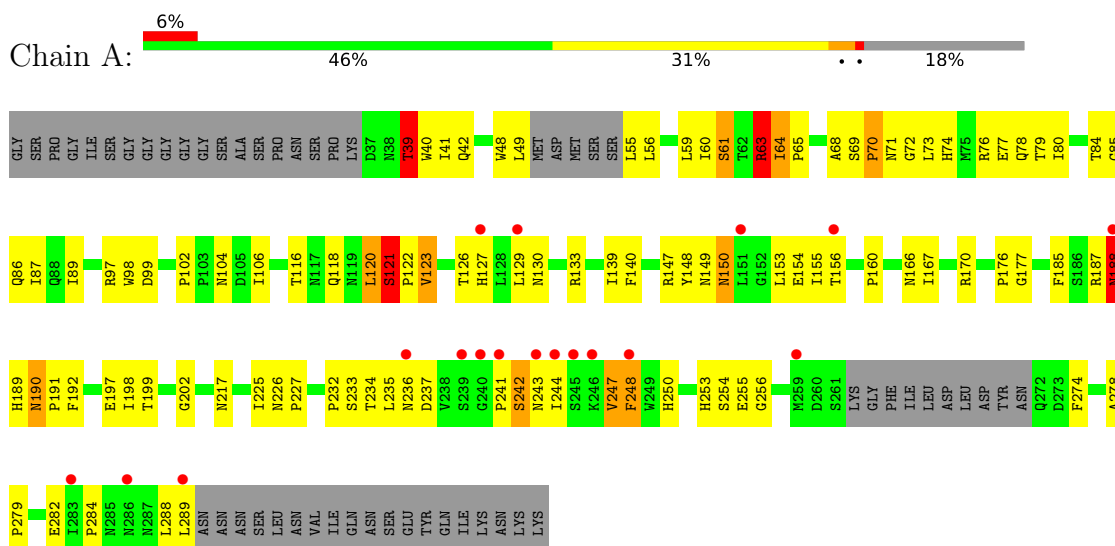
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	195	GLN	GLU	engineered mutation	UNP Q03988
B	195	GLN	GLU	engineered mutation	UNP Q03988
C	195	GLN	GLU	engineered mutation	UNP Q03988
D	195	GLN	GLU	engineered mutation	UNP Q03988
E	195	GLN	GLU	engineered mutation	UNP Q03988
F	195	GLN	GLU	engineered mutation	UNP Q03988
G	195	GLN	GLU	engineered mutation	UNP Q03988
H	195	GLN	GLU	engineered mutation	UNP Q03988
I	195	GLN	GLU	engineered mutation	UNP Q03988
J	195	GLN	GLU	engineered mutation	UNP Q03988
K	195	GLN	GLU	engineered mutation	UNP Q03988
L	195	GLN	GLU	engineered mutation	UNP Q03988
M	195	GLN	GLU	engineered mutation	UNP Q03988
N	195	GLN	GLU	engineered mutation	UNP Q03988
O	195	GLN	GLU	engineered mutation	UNP Q03988
P	195	GLN	GLU	engineered mutation	UNP Q03988

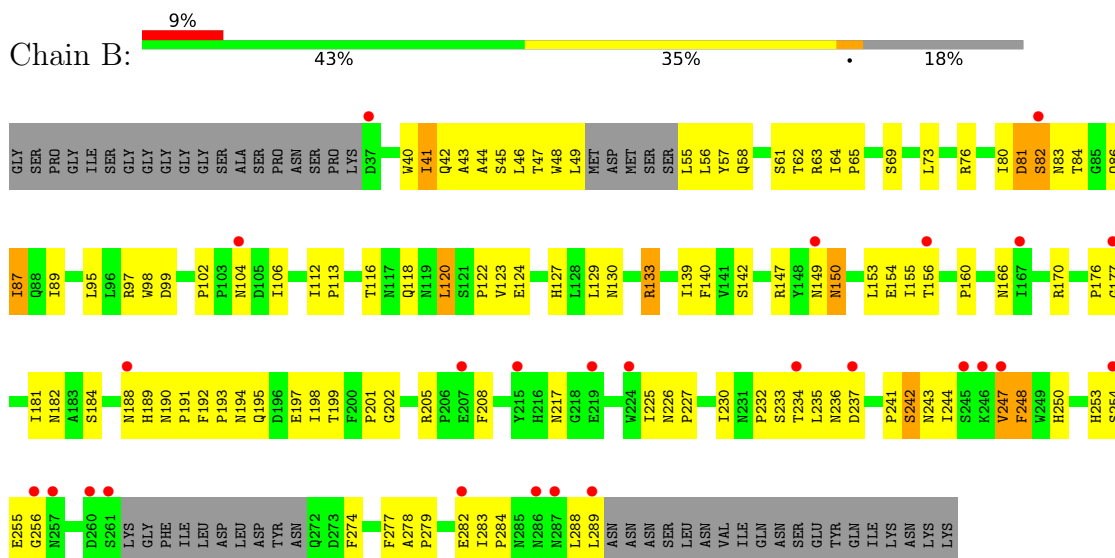
### 3 Residue-property plots i

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

#### • Molecule 1: MOSQUITOCIDAL TOXIN

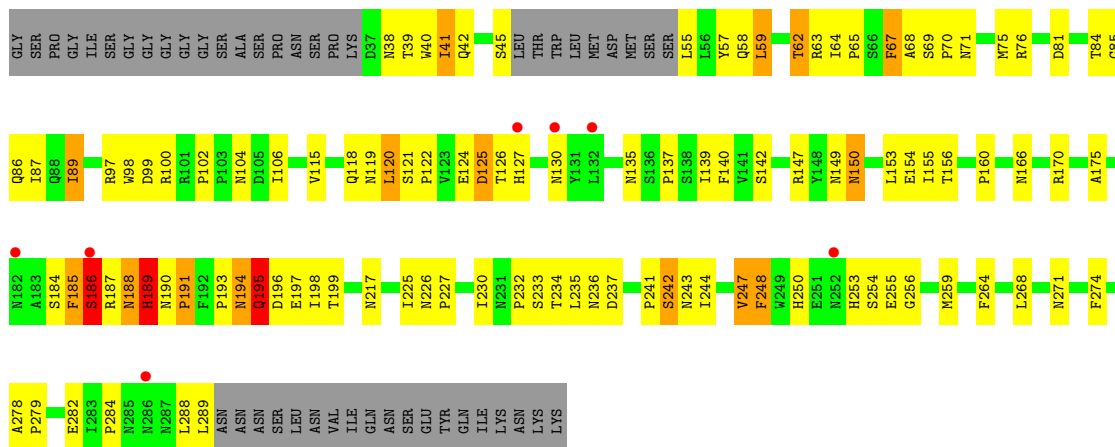


#### • Molecule 1: MOSQUITOCIDAL TOXIN

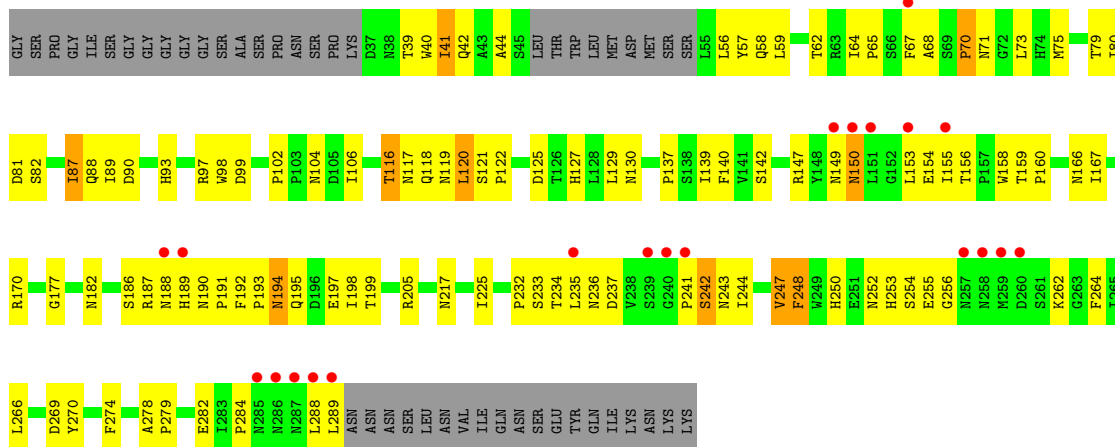


#### • Molecule 1: MOSQUITOCIDAL TOXIN

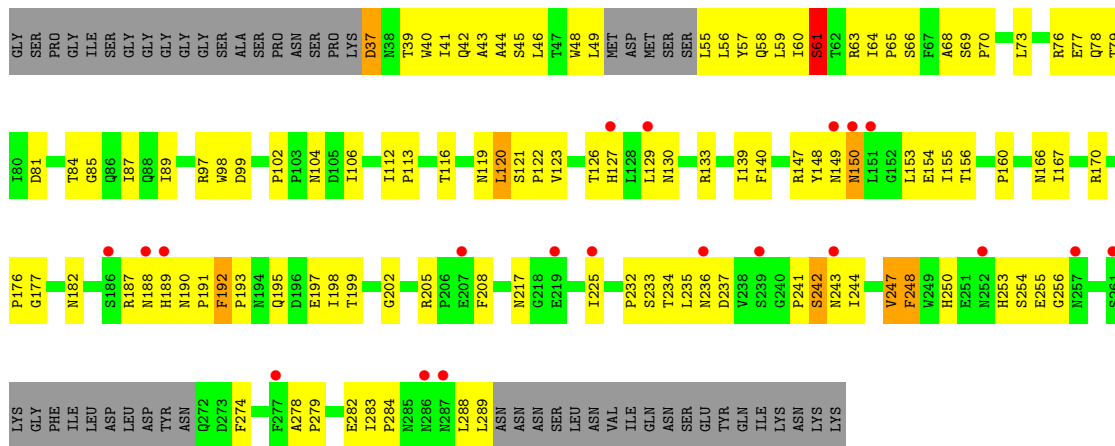
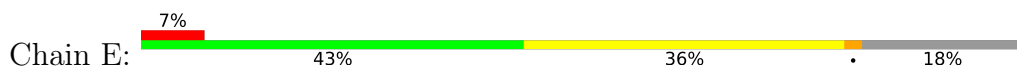




• Molecule 1: MOSQUITOCIDAL TOXIN



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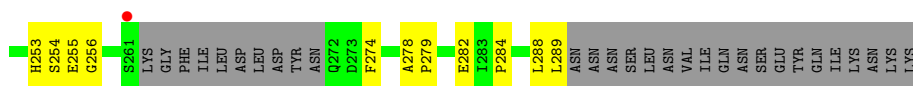
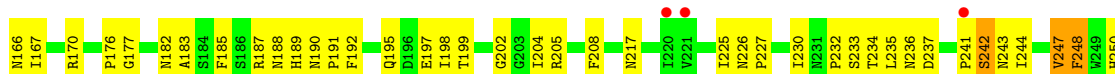
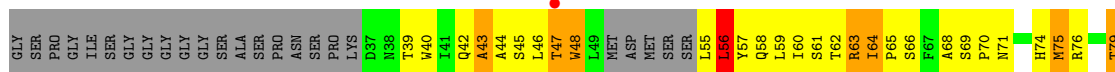


• Molecule 1: MOSQUITOCIDAL TOXIN

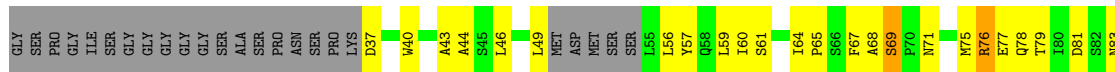
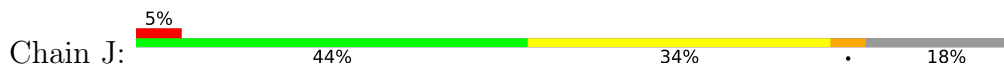




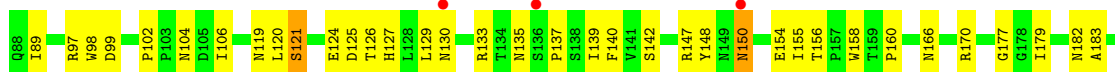
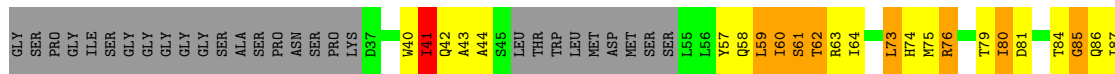
- Molecule 1: MOSQUITOCIDAL TOXIN

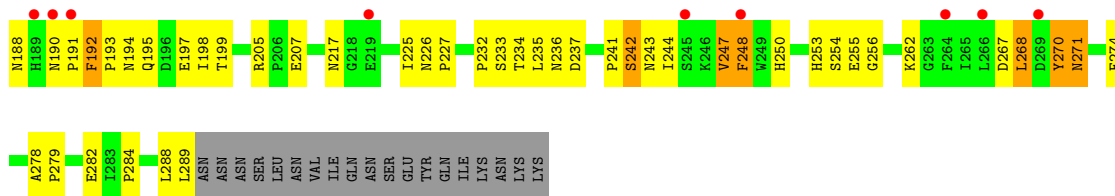


- Molecule 1: MOSQUITOCIDAL TOXIN

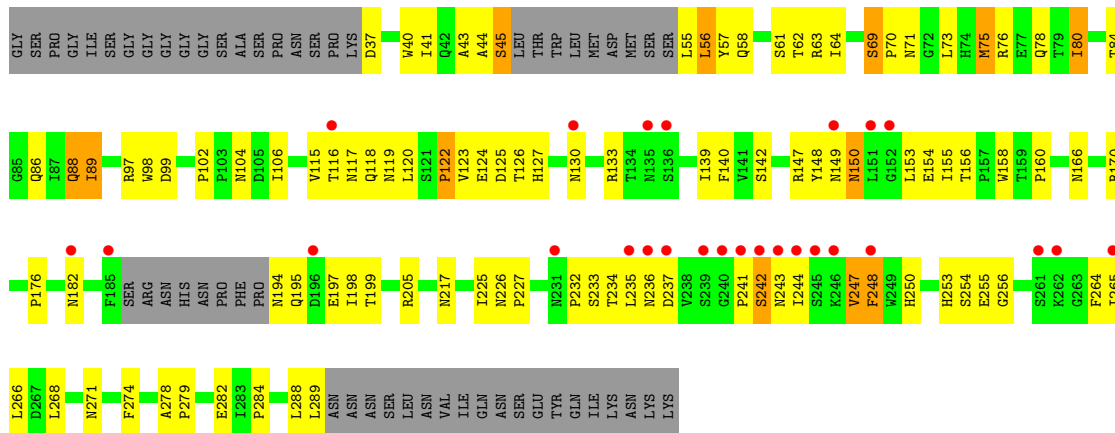


- Molecule 1: MOSQUITOCIDAL TOXIN

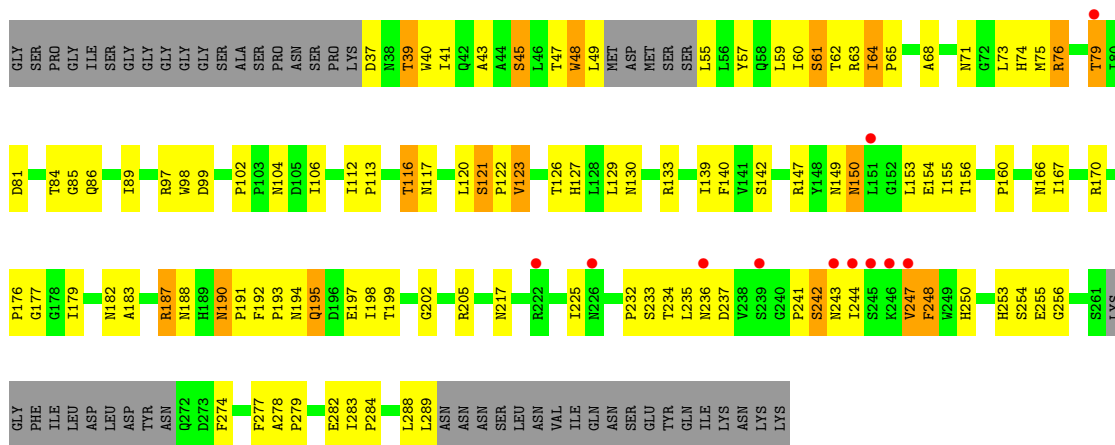




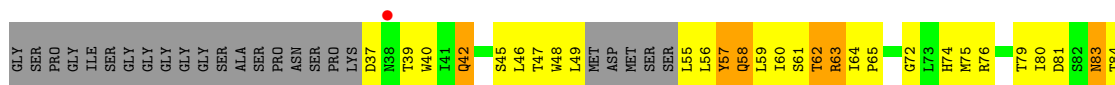
● Molecule 1: MOSQUITOCIDAL TOXIN

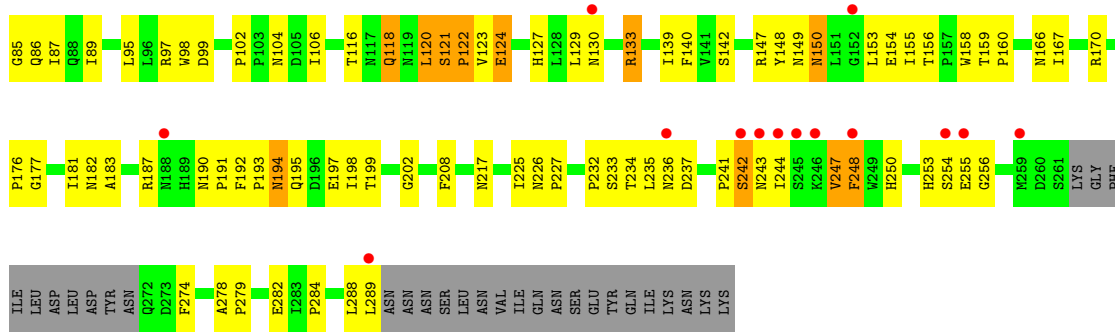


● Molecule 1: MOSQUITOCIDAL TOXIN

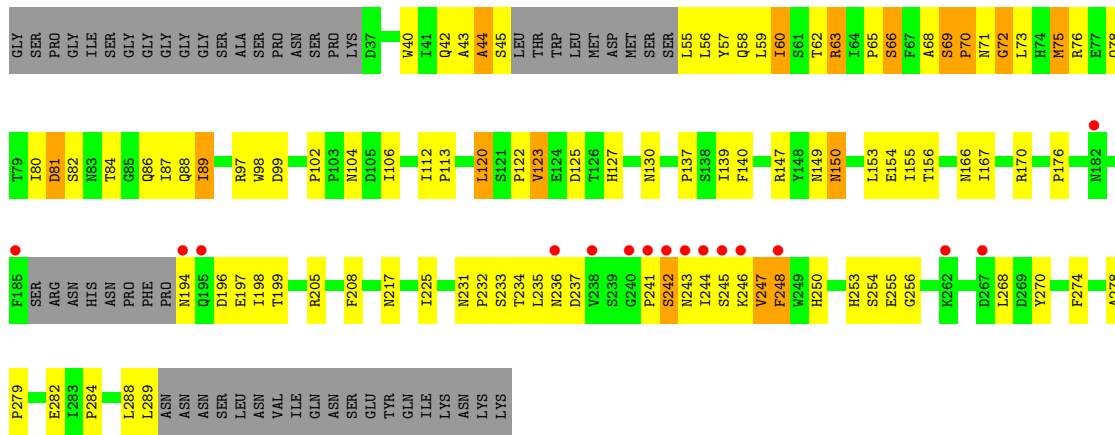


● Molecule 1: MOSQUITOCIDAL TOXIN

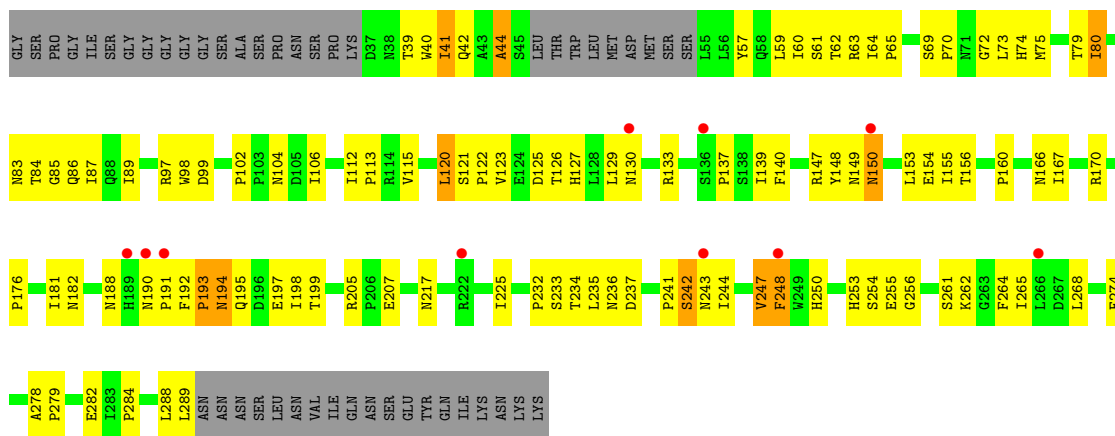




● Molecule 1: MOSQUITOCIDAL TOXIN



● Molecule 1: MOSQUITOCIDAL TOXIN



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	106.30Å 175.80Å 335.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.00 50.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.00) 99.6 (50.00-3.00)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.22 (at 3.01Å)	Xtrriage
Refinement program	TNT 5.6.1	Depositor
R, $R_{free}$	0.227 , 0.246 (Not available) , 0.263	Depositor DCC
$R_{free}$ test set	6301 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	49.0	Xtrriage
Anisotropy	0.207	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 48.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.23$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.85	EDS
Total number of atoms	31202	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 24.83 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.5553e-03.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality i

### 5.1 Standard geometry i

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.61	0/1995	1.14	16/2726 (0.6%)
1	B	0.57	0/1995	1.05	9/2726 (0.3%)
1	C	0.62	0/2043	1.13	19/2790 (0.7%)
1	D	0.62	0/2043	1.12	14/2790 (0.5%)
1	E	0.62	1/1995 (0.1%)	1.10	12/2726 (0.4%)
1	F	0.55	0/1995	1.05	9/2726 (0.3%)
1	G	0.58	0/1970	1.08	11/2688 (0.4%)
1	H	0.63	1/2049 (0.0%)	1.19	21/2798 (0.8%)
1	I	0.58	1/1995 (0.1%)	1.09	13/2726 (0.5%)
1	J	0.58	0/1995	1.12	13/2726 (0.5%)
1	K	0.57	0/2043	1.08	12/2790 (0.4%)
1	L	0.61	1/1970 (0.1%)	1.15	13/2688 (0.5%)
1	M	0.54	0/1995	1.12	15/2726 (0.6%)
1	N	0.59	1/1995 (0.1%)	1.10	15/2726 (0.6%)
1	O	0.62	0/1970	1.18	17/2688 (0.6%)
1	P	0.60	0/2043	1.08	10/2790 (0.4%)
All	All	0.59	5/32091 (0.0%)	1.11	219/43830 (0.5%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	75	MET	SD-CE	6.70	1.96	1.79
1	H	195	GLN	CA-C	-5.76	1.45	1.52
1	I	115	VAL	CA-CB	5.33	1.60	1.53
1	N	123	VAL	CA-CB	-5.09	1.48	1.54
1	E	60	ILE	CA-C	-5.06	1.46	1.52

All (219) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	187	ARG	N-CA-C	13.29	125.76	111.28
1	H	187	ARG	N-CA-C	-11.90	95.09	111.87
1	H	60	ILE	N-CA-C	10.96	120.94	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	83	ASN	N-CA-C	-10.95	98.52	114.39
1	M	85	GLY	N-CA-C	-10.54	98.73	116.01
1	A	187	ARG	N-CA-C	10.51	126.00	112.34
1	O	69	SER	N-CA-C	-10.50	96.06	108.14
1	L	88	GLN	CA-C-N	-10.30	111.96	121.65
1	L	88	GLN	C-N-CA	-10.30	111.96	121.65
1	H	117	ASN	N-CA-C	-10.06	100.54	113.12
1	A	123	VAL	N-CA-C	10.05	119.87	110.42
1	L	61	SER	N-CA-C	9.71	121.86	111.28
1	O	69	SER	C-N-CD	-9.61	85.62	125.00
1	E	61	SER	N-CA-C	9.34	121.54	111.36
1	K	61	SER	N-CA-C	9.26	120.98	111.07
1	O	72	GLY	N-CA-C	9.17	128.03	111.34
1	A	64	ILE	N-CA-C	9.15	118.85	108.05
1	G	195	GLN	N-CA-C	-9.09	102.19	113.28
1	P	194	ASN	N-CA-C	-8.97	92.86	108.20
1	C	85	GLY	N-CA-C	-8.89	101.38	115.08
1	N	85	GLY	N-CA-C	-8.87	102.22	115.00
1	H	195	GLN	CB-CA-C	-8.82	92.87	110.42
1	N	187	ARG	N-CA-C	8.74	120.73	111.03
1	O	73	LEU	N-CA-C	-8.73	96.40	110.20
1	M	187	ARG	N-CA-C	8.68	121.61	111.02
1	I	187	ARG	N-CA-C	8.47	120.13	111.07
1	O	71	ASN	CA-C-N	8.47	133.70	120.07
1	O	71	ASN	C-N-CA	8.47	133.70	120.07
1	J	44	ALA	N-CA-C	8.21	122.80	110.64
1	C	185	PHE	CA-C-N	-8.13	106.02	121.54
1	C	185	PHE	C-N-CA	-8.13	106.02	121.54
1	D	190	ASN	C-N-CD	-8.13	102.72	120.60
1	J	84	THR	N-CA-C	8.11	123.52	112.90
1	H	59	LEU	N-CA-C	-7.93	101.59	111.11
1	E	44	ALA	N-CA-C	7.88	121.92	110.42
1	C	185	PHE	O-C-N	-7.79	112.27	122.94
1	F	61	SER	N-CA-C	7.73	120.78	111.82
1	D	188	ASN	N-CA-C	-7.71	101.76	112.25
1	P	60	ILE	N-CA-C	7.65	117.72	110.53
1	A	39	THR	N-CA-C	-7.64	102.95	111.82
1	A	85	GLY	N-CA-C	-7.59	101.86	114.76
1	B	82	SER	N-CA-C	-7.58	103.91	113.01
1	B	47	THR	N-CA-C	7.58	120.27	111.02
1	M	79	THR	N-CA-C	-7.52	103.91	113.23
1	H	185	PHE	CA-C-N	-7.46	107.30	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	185	PHE	C-N-CA	-7.46	107.30	121.54
1	I	87	ILE	N-CA-C	7.39	124.72	109.34
1	K	188	ASN	N-CA-C	7.34	119.17	111.03
1	L	271	ASN	N-CA-C	-7.28	97.38	108.67
1	E	42	GLN	N-CA-C	7.28	119.21	111.28
1	N	61	SER	N-CA-C	7.21	118.83	110.97
1	J	79	THR	N-CA-C	-7.21	104.45	113.18
1	B	61	SER	N-CA-C	7.21	119.76	111.11
1	I	64	ILE	N-CA-C	7.15	116.48	108.05
1	P	106	ILE	N-CA-C	7.10	117.23	110.42
1	N	106	ILE	N-CA-C	7.08	117.22	110.42
1	H	106	ILE	N-CA-C	7.07	117.21	110.42
1	C	106	ILE	N-CA-C	7.07	117.20	110.42
1	E	106	ILE	N-CA-C	7.07	117.20	110.42
1	L	106	ILE	N-CA-C	7.06	117.20	110.42
1	A	106	ILE	N-CA-C	7.06	117.20	110.42
1	J	106	ILE	N-CA-C	7.06	117.19	110.42
1	F	106	ILE	N-CA-C	7.06	117.19	110.42
1	O	106	ILE	N-CA-C	7.05	117.19	110.42
1	D	106	ILE	N-CA-C	7.05	117.19	110.42
1	G	106	ILE	N-CA-C	7.05	117.19	110.42
1	B	106	ILE	N-CA-C	7.05	117.19	110.42
1	I	106	ILE	N-CA-C	7.03	117.17	110.42
1	K	106	ILE	N-CA-C	7.03	117.17	110.42
1	F	59	LEU	N-CA-C	-7.03	103.70	112.90
1	C	195	GLN	CB-CA-C	-7.02	97.02	110.57
1	M	106	ILE	N-CA-C	7.02	117.16	110.42
1	M	61	SER	N-CA-C	6.99	118.69	111.14
1	D	269	ASP	N-CA-C	6.98	120.61	110.28
1	H	185	PHE	O-C-N	-6.97	113.39	122.94
1	F	56	LEU	N-CA-C	-6.89	103.70	111.07
1	C	189	HIS	N-CA-C	-6.85	105.08	113.50
1	I	56	LEU	N-CA-C	-6.77	103.90	111.28
1	L	265	ILE	N-CA-C	-6.77	99.05	108.12
1	K	270	TYR	N-CA-C	6.75	119.74	108.73
1	B	44	ALA	N-CA-C	6.75	120.63	110.64
1	I	66	SER	N-CA-C	-6.63	104.05	111.28
1	H	186	SER	N-CA-CB	6.59	121.63	110.49
1	H	262	LYS	N-CA-C	6.58	119.00	111.11
1	H	55	LEU	N-CA-C	-6.57	103.23	111.11
1	A	121	SER	N-CA-C	-6.55	95.34	109.81
1	K	41	ILE	CB-CA-C	-6.51	104.70	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	61	SER	N-CA-C	6.43	119.10	111.71
1	E	192	PHE	CB-CA-C	-6.37	106.68	111.20
1	P	44	ALA	N-CA-C	6.33	118.05	110.19
1	G	62	THR	N-CA-C	6.30	118.67	111.11
1	G	117	ASN	N-CA-C	-6.22	104.60	111.82
1	M	48	TRP	N-CA-C	6.21	120.47	113.01
1	D	79	THR	N-CA-C	-6.20	104.63	111.82
1	D	194	ASN	N-CA-C	-6.17	100.91	110.10
1	A	40	TRP	N-CA-C	6.17	120.36	112.34
1	G	85	GLY	N-CA-C	-6.13	106.57	114.85
1	L	89	ILE	N-CA-C	6.08	112.72	106.21
1	C	89	ILE	N-CA-C	6.08	112.72	106.21
1	H	89	ILE	N-CA-C	6.08	112.72	106.21
1	O	89	ILE	N-CA-C	6.05	112.69	106.21
1	J	71	ASN	N-CA-C	6.03	119.60	112.72
1	G	44	ALA	N-CA-C	5.92	117.93	110.24
1	O	70	PRO	N-CA-C	-5.92	100.29	112.47
1	C	194	ASN	N-CA-C	-5.91	95.81	107.69
1	I	79	THR	N-CA-C	-5.91	104.97	111.82
1	J	116	THR	CB-CA-C	-5.91	101.95	111.28
1	A	63	ARG	N-CA-C	-5.89	105.75	113.17
1	C	64	ILE	N-CA-C	5.88	113.97	108.15
1	E	45	SER	N-CA-C	-5.86	105.96	113.23
1	O	270	TYR	N-CA-C	5.85	118.26	108.73
1	N	83	ASN	N-CA-C	-5.83	104.88	112.23
1	D	262	LYS	N-CA-C	5.82	119.19	111.75
1	G	120	LEU	N-CA-C	5.82	119.11	109.46
1	P	120	LEU	N-CA-C	5.80	119.37	110.20
1	A	61	SER	N-CA-C	5.80	123.15	110.80
1	C	67	PHE	N-CA-C	-5.76	106.29	113.38
1	K	271	ASN	N-CA-CB	5.76	118.87	110.58
1	P	41	ILE	CB-CA-C	-5.74	104.50	112.36
1	E	85	GLY	N-CA-C	-5.73	106.08	114.90
1	H	66	SER	N-CA-C	5.73	117.20	111.07
1	H	188	ASN	N-CA-C	5.65	120.30	112.90
1	O	81	ASP	N-CA-C	-5.64	102.68	110.35
1	C	188	ASN	N-CA-C	5.63	119.96	112.30
1	D	270	TYR	N-CA-C	5.63	117.91	108.96
1	N	57	TYR	N-CA-C	-5.61	105.17	111.28
1	D	120	LEU	N-CA-C	5.59	118.74	109.46
1	F	83	ASN	N-CA-C	-5.58	103.03	111.34
1	O	71	ASN	CA-C-O	5.56	126.68	119.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	194	ASN	N-CA-C	-5.55	100.14	108.96
1	N	72	GLY	N-CA-C	-5.54	104.61	111.70
1	J	189	HIS	N-CA-C	-5.53	102.33	110.52
1	E	274	PHE	N-CA-C	5.53	117.74	111.11
1	N	274	PHE	N-CA-C	5.52	117.74	111.11
1	L	274	PHE	N-CA-C	5.52	117.73	111.11
1	D	274	PHE	N-CA-C	5.52	117.73	111.11
1	G	274	PHE	N-CA-C	5.52	117.73	111.11
1	P	274	PHE	N-CA-C	5.51	117.73	111.11
1	F	274	PHE	N-CA-C	5.51	117.72	111.11
1	N	62	THR	N-CA-C	5.51	122.54	110.80
1	J	124	GLU	CA-C-N	-5.51	113.95	122.49
1	J	124	GLU	C-N-CA	-5.51	113.95	122.49
1	H	86	GLN	N-CA-C	5.51	118.26	110.50
1	H	274	PHE	N-CA-C	5.51	117.72	111.11
1	O	274	PHE	N-CA-C	5.50	117.71	111.11
1	M	274	PHE	N-CA-C	5.50	117.70	111.11
1	K	274	PHE	N-CA-C	5.50	117.70	111.11
1	C	191	PRO	N-CA-C	-5.49	106.04	113.40
1	J	274	PHE	N-CA-C	5.49	117.70	111.11
1	C	274	PHE	N-CA-C	5.48	117.69	111.11
1	A	274	PHE	N-CA-C	5.48	117.69	111.11
1	I	274	PHE	N-CA-C	5.47	117.68	111.11
1	B	274	PHE	N-CA-C	5.47	117.67	111.11
1	G	262	LYS	N-CA-C	5.46	120.37	111.37
1	N	118	GLN	N-CA-C	-5.42	106.17	112.89
1	K	43	ALA	N-CA-C	-5.38	106.73	113.72
1	K	85	GLY	N-CA-C	-5.37	107.69	115.27
1	D	41	ILE	CB-CA-C	-5.35	102.51	111.29
1	C	120	LEU	N-CA-C	5.32	118.60	110.20
1	M	121	SER	CA-C-N	5.31	126.48	119.84
1	M	121	SER	C-N-CA	5.31	126.48	119.84
1	J	247	VAL	N-CA-C	5.31	116.86	109.80
1	O	247	VAL	N-CA-C	5.30	116.86	109.80
1	P	247	VAL	N-CA-C	5.30	116.85	109.80
1	D	247	VAL	N-CA-C	5.29	116.84	109.80
1	I	247	VAL	N-CA-C	5.29	116.84	109.80
1	M	39	THR	N-CA-C	5.29	117.46	111.11
1	M	247	VAL	N-CA-C	5.29	116.83	109.80
1	F	247	VAL	N-CA-C	5.29	116.83	109.80
1	E	247	VAL	N-CA-C	5.28	116.83	109.80
1	N	247	VAL	N-CA-C	5.28	116.83	109.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	247	VAL	N-CA-C	5.28	116.83	109.80
1	A	247	VAL	N-CA-C	5.27	116.81	109.80
1	C	247	VAL	N-CA-C	5.27	116.81	109.80
1	K	247	VAL	N-CA-C	5.27	116.81	109.80
1	H	247	VAL	N-CA-C	5.26	116.80	109.80
1	L	247	VAL	N-CA-C	5.26	116.80	109.80
1	B	247	VAL	N-CA-C	5.25	116.78	109.80
1	L	69	SER	CA-C-N	5.25	126.40	119.84
1	L	69	SER	C-N-CA	5.25	126.40	119.84
1	K	121	SER	N-CA-C	-5.21	97.19	108.81
1	O	60	ILE	CB-CA-C	-5.20	105.31	111.97
1	M	188	ASN	N-CA-C	5.20	119.61	113.16
1	A	116	THR	N-CA-C	5.19	120.46	113.72
1	G	139	ILE	N-CA-C	-5.14	107.74	112.83
1	A	188	ASN	N-CA-C	-5.12	107.07	113.72
1	N	139	ILE	N-CA-C	-5.09	107.79	112.83
1	M	139	ILE	N-CA-C	-5.09	107.80	112.83
1	L	139	ILE	N-CA-C	-5.08	107.80	112.83
1	C	186	SER	N-CA-C	-5.08	99.98	110.80
1	E	139	ILE	N-CA-C	-5.07	107.81	112.83
1	D	139	ILE	N-CA-C	-5.07	107.81	112.83
1	J	139	ILE	N-CA-C	-5.07	107.81	112.83
1	F	139	ILE	N-CA-C	-5.07	107.82	112.83
1	I	139	ILE	N-CA-C	-5.07	107.81	112.83
1	P	139	ILE	N-CA-C	-5.07	107.82	112.83
1	B	139	ILE	N-CA-C	-5.06	107.82	112.83
1	K	139	ILE	N-CA-C	-5.06	107.82	112.83
1	O	139	ILE	N-CA-C	-5.06	107.82	112.83
1	C	139	ILE	N-CA-C	-5.06	107.82	112.83
1	E	119	ASN	N-CA-C	5.06	118.54	110.70
1	C	62	THR	N-CA-C	5.04	118.59	112.23
1	A	139	ILE	N-CA-C	-5.04	107.84	112.83
1	B	124	GLU	N-CA-C	-5.04	107.18	113.38
1	I	167	ILE	N-CA-C	5.04	115.94	108.23
1	N	120	LEU	N-CA-C	5.04	117.18	110.53
1	D	167	ILE	N-CA-C	5.03	115.93	108.23
1	H	139	ILE	N-CA-C	-5.03	107.85	112.83
1	O	167	ILE	N-CA-C	5.03	115.92	108.23
1	F	167	ILE	N-CA-C	5.03	115.92	108.23
1	P	167	ILE	N-CA-C	5.02	115.91	108.23
1	M	64	ILE	N-CA-C	5.02	119.72	108.88
1	H	122	PRO	N-CA-C	5.01	122.80	112.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	167	ILE	N-CA-C	5.01	115.89	108.23
1	L	119	ASN	N-CA-C	5.01	118.43	112.72
1	E	167	ILE	N-CA-C	5.00	115.89	108.23
1	M	167	ILE	N-CA-C	5.00	115.89	108.23
1	A	167	ILE	N-CA-C	5.00	115.89	108.23
1	N	167	ILE	N-CA-C	5.00	115.88	108.23

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1939	0	1829	103	0
1	B	1939	0	1829	110	0
1	C	1986	0	1872	99	0
1	D	1986	0	1872	93	1
1	E	1939	0	1829	120	0
1	F	1939	0	1829	110	0
1	G	1918	0	1811	95	0
1	H	1992	0	1877	104	1
1	I	1939	0	1829	110	0
1	J	1939	0	1829	90	0
1	K	1986	0	1872	104	0
1	L	1918	0	1811	87	0
1	M	1939	0	1829	88	0
1	N	1939	0	1829	94	0
1	O	1918	0	1811	86	0
1	P	1986	0	1872	89	0
All	All	31202	0	29430	1450	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 24.

All (1450) 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:J:87:ILE:HD12	1:J:230:ILE:HG21	1.22	1.15
1:I:64:ILE:HG23	1:I:129:LEU:HD11	1.25	1.11
1:A:84:THR:HB	1:A:86:GLN:HG2	1.11	1.10
1:A:64:ILE:HG23	1:A:129:LEU:HD11	1.17	1.08
1:D:254:SER:HB3	1:O:244:ILE:O	1.53	1.07
1:G:116:THR:HG22	1:G:118:GLN:H	1.18	1.07
1:D:254:SER:CB	1:O:244:ILE:O	2.03	1.06
1:E:133:ARG:HD3	1:E:190:ASN:HD21	1.20	1.06
1:K:133:ARG:HG3	1:K:191:PRO:HB3	1.37	1.06
1:I:63:ARG:HD2	1:L:123:VAL:HG21	1.28	1.06
1:A:63:ARG:HG2	1:A:63:ARG:HH11	1.17	1.05
1:E:46:LEU:HD12	1:E:202:GLY:HA2	1.37	1.04
1:D:116:THR:HG22	1:D:118:GLN:H	1.23	1.03
1:E:133:ARG:HH11	1:E:190:ASN:ND2	1.54	1.03
1:C:185:PHE:HB2	1:C:189:HIS:HD2	1.24	1.01
1:C:87:ILE:HD12	1:C:230:ILE:HG21	1.44	0.99
1:K:190:ASN:HA	1:K:192:PHE:HD2	1.27	0.99
1:C:40:TRP:CE2	1:C:41:ILE:HD13	2.00	0.97
1:E:129:LEU:HD23	1:E:191:PRO:HD3	1.48	0.96
1:M:84:THR:HG21	1:M:86:GLN:HB2	1.47	0.96
1:M:123:VAL:HG22	1:P:123:VAL:HG22	1.48	0.96
1:P:190:ASN:HB2	1:P:191:PRO:HA	1.45	0.96
1:G:80:ILE:HG22	1:G:87:ILE:HD13	1.46	0.95
1:I:43:ALA:HB2	1:I:176:PRO:HD2	1.45	0.95
1:F:64:ILE:HG23	1:F:129:LEU:HD11	1.46	0.95
1:F:87:ILE:HD12	1:F:230:ILE:HG12	1.48	0.94
1:I:46:LEU:HD12	1:I:202:GLY:HA2	1.48	0.93
1:G:254:SER:OG	1:L:243:ASN:N	2.01	0.93
1:P:133:ARG:HG3	1:P:191:PRO:HB3	1.50	0.93
1:G:254:SER:CB	1:L:243:ASN:H	1.83	0.92
1:H:120:LEU:HG	1:H:122:PRO:HD3	1.52	0.91
1:C:87:ILE:CD1	1:C:230:ILE:HG21	2.01	0.91
1:B:129:LEU:HD23	1:B:191:PRO:CG	2.00	0.91
1:I:87:ILE:HD12	1:I:230:ILE:HG21	1.53	0.91
1:J:190:ASN:HB2	1:J:191:PRO:HA	1.54	0.90
1:E:283:ILE:CG2	1:H:268:LEU:HD21	2.02	0.90
1:K:190:ASN:HB2	1:K:191:PRO:HA	1.54	0.89
1:J:129:LEU:HD23	1:J:191:PRO:HD3	1.54	0.89
1:G:254:SER:CB	1:L:243:ASN:N	2.36	0.89
1:O:69:SER:HB2	1:O:72:GLY:HA2	1.52	0.89
1:L:127:HIS:ND1	1:L:130:ASN:HB2	1.88	0.88
1:J:127:HIS:ND1	1:J:130:ASN:HB2	1.89	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:127:HIS:ND1	1:K:130:ASN:HB2	1.89	0.88
1:O:127:HIS:ND1	1:O:130:ASN:HB2	1.88	0.88
1:I:64:ILE:HG23	1:I:129:LEU:CD1	2.03	0.88
1:N:127:HIS:ND1	1:N:130:ASN:HB2	1.88	0.88
1:I:127:HIS:ND1	1:I:130:ASN:HB2	1.89	0.88
1:A:127:HIS:ND1	1:A:130:ASN:HB2	1.89	0.88
1:P:127:HIS:ND1	1:P:130:ASN:HB2	1.88	0.88
1:B:127:HIS:ND1	1:B:130:ASN:HB2	1.89	0.88
1:A:133:ARG:HD3	1:A:190:ASN:HD22	1.38	0.88
1:E:127:HIS:ND1	1:E:130:ASN:HB2	1.89	0.88
1:M:127:HIS:ND1	1:M:130:ASN:HB2	1.89	0.87
1:H:127:HIS:ND1	1:H:130:ASN:HB2	1.88	0.87
1:C:127:HIS:ND1	1:C:130:ASN:HB2	1.88	0.87
1:E:64:ILE:HG23	1:E:129:LEU:HD11	1.55	0.87
1:F:127:HIS:ND1	1:F:130:ASN:HB2	1.89	0.87
1:N:133:ARG:HE	1:N:190:ASN:HD21	1.23	0.87
1:G:127:HIS:ND1	1:G:130:ASN:HB2	1.88	0.87
1:K:133:ARG:CG	1:K:191:PRO:HB3	2.03	0.87
1:K:190:ASN:HA	1:K:192:PHE:CD2	2.08	0.86
1:A:190:ASN:HA	1:A:192:PHE:H	1.38	0.86
1:D:127:HIS:ND1	1:D:130:ASN:HB2	1.88	0.86
1:I:63:ARG:HD2	1:L:123:VAL:CG2	2.06	0.86
1:A:84:THR:CB	1:A:86:GLN:HG2	2.02	0.86
1:A:129:LEU:HD23	1:A:191:PRO:HD3	1.58	0.86
1:I:133:ARG:HH11	1:I:190:ASN:ND2	1.73	0.85
1:O:241:PRO:HB2	1:O:244:ILE:HD12	1.59	0.85
1:L:241:PRO:HB2	1:L:244:ILE:HD12	1.59	0.85
1:M:241:PRO:HB2	1:M:244:ILE:HD12	1.59	0.85
1:M:283:ILE:HB	1:O:268:LEU:HD22	1.57	0.85
1:D:241:PRO:HB2	1:D:244:ILE:HD12	1.59	0.84
1:G:254:SER:HB3	1:L:244:ILE:H	1.42	0.84
1:E:241:PRO:HB2	1:E:244:ILE:HD12	1.59	0.84
1:P:64:ILE:HD13	1:P:73:LEU:HD13	1.59	0.84
1:H:241:PRO:HB2	1:H:244:ILE:HD12	1.59	0.84
1:B:133:ARG:HG2	1:B:191:PRO:HB3	1.57	0.84
1:F:241:PRO:HB2	1:F:244:ILE:HD12	1.59	0.84
1:A:241:PRO:HB2	1:A:244:ILE:HD12	1.59	0.84
1:A:64:ILE:HG23	1:A:129:LEU:CD1	2.06	0.83
1:C:135:ASN:HD22	1:C:271:ASN:HD21	1.26	0.83
1:N:87:ILE:HD11	1:N:208:PHE:CE1	2.13	0.83
1:G:241:PRO:HB2	1:G:244:ILE:HD12	1.59	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:241:PRO:HB2	1:C:244:ILE:CD1	2.09	0.83
1:I:241:PRO:HB2	1:I:244:ILE:CD1	2.09	0.83
1:J:241:PRO:HB2	1:J:244:ILE:HD12	1.59	0.83
1:N:241:PRO:HB2	1:N:244:ILE:HD12	1.59	0.83
1:D:254:SER:HB3	1:O:244:ILE:C	2.03	0.83
1:I:79:THR:HG21	1:I:177:GLY:H	1.43	0.83
1:E:241:PRO:HB2	1:E:244:ILE:CD1	2.09	0.83
1:G:241:PRO:HB2	1:G:244:ILE:CD1	2.09	0.83
1:F:241:PRO:HB2	1:F:244:ILE:CD1	2.09	0.83
1:A:241:PRO:HB2	1:A:244:ILE:CD1	2.09	0.83
1:F:87:ILE:HD12	1:F:230:ILE:HG21	1.61	0.83
1:L:78:GLN:O	1:L:88:GLN:HG3	1.78	0.82
1:N:241:PRO:HB2	1:N:244:ILE:CD1	2.09	0.82
1:P:241:PRO:HB2	1:P:244:ILE:CD1	2.09	0.82
1:C:185:PHE:HB2	1:C:189:HIS:CD2	2.13	0.82
1:O:241:PRO:HB2	1:O:244:ILE:CD1	2.09	0.82
1:N:48:TRP:CH2	1:N:120:LEU:HD23	2.13	0.82
1:B:241:PRO:HB2	1:B:244:ILE:CD1	2.09	0.82
1:K:194:ASN:HB3	1:K:197:GLU:HB2	1.61	0.82
1:K:241:PRO:HB2	1:K:244:ILE:CD1	2.09	0.82
1:P:241:PRO:HB2	1:P:244:ILE:HD12	1.59	0.82
1:C:40:TRP:CD2	1:C:41:ILE:HG23	2.15	0.82
1:H:241:PRO:HB2	1:H:244:ILE:CD1	2.09	0.82
1:K:241:PRO:HB2	1:K:244:ILE:HD12	1.59	0.82
1:B:241:PRO:HB2	1:B:244:ILE:HD12	1.59	0.82
1:D:241:PRO:HB2	1:D:244:ILE:CD1	2.09	0.81
1:C:241:PRO:HB2	1:C:244:ILE:HD12	1.59	0.81
1:I:241:PRO:HB2	1:I:244:ILE:HD12	1.59	0.81
1:G:254:SER:HB3	1:L:244:ILE:N	1.95	0.81
1:M:133:ARG:HH11	1:M:190:ASN:HB2	1.46	0.81
1:M:241:PRO:HB2	1:M:244:ILE:CD1	2.09	0.81
1:C:154:GLU:HG2	1:C:289:LEU:HD22	1.63	0.81
1:J:241:PRO:HB2	1:J:244:ILE:CD1	2.09	0.81
1:I:154:GLU:HG2	1:I:289:LEU:HD22	1.63	0.81
1:L:154:GLU:HG2	1:L:289:LEU:HD22	1.63	0.81
1:L:241:PRO:HB2	1:L:244:ILE:CD1	2.09	0.80
1:B:129:LEU:HD23	1:B:191:PRO:HG3	1.60	0.80
1:H:63:ARG:HG3	1:H:63:ARG:HH11	1.46	0.80
1:P:133:ARG:CG	1:P:191:PRO:HB3	2.10	0.80
1:D:186:SER:HB2	1:D:189:HIS:HB2	1.62	0.80
1:O:154:GLU:HG2	1:O:289:LEU:HD22	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:154:GLU:HG2	1:K:289:LEU:HD22	1.63	0.80
1:E:129:LEU:CD2	1:E:191:PRO:HD3	2.12	0.80
1:D:154:GLU:HG2	1:D:289:LEU:HD22	1.63	0.80
1:E:133:ARG:HH11	1:E:190:ASN:HD21	1.30	0.80
1:G:154:GLU:HG2	1:G:289:LEU:HD22	1.63	0.80
1:P:57:TYR:HE1	1:P:73:LEU:HD23	1.45	0.80
1:A:154:GLU:HG2	1:A:289:LEU:HD22	1.63	0.79
1:F:87:ILE:CD1	1:F:230:ILE:HG21	2.12	0.79
1:E:129:LEU:HD23	1:E:191:PRO:CD	2.13	0.79
1:N:154:GLU:HG2	1:N:289:LEU:HD22	1.63	0.79
1:D:255:GLU:OE2	1:O:242:SER:HB3	1.83	0.79
1:J:154:GLU:HG2	1:J:289:LEU:HD22	1.63	0.79
1:P:154:GLU:HG2	1:P:289:LEU:HD22	1.63	0.79
1:H:154:GLU:HG2	1:H:289:LEU:HD22	1.63	0.79
1:G:254:SER:HG	1:L:243:ASN:H	1.28	0.79
1:B:154:GLU:HG2	1:B:289:LEU:HD22	1.63	0.78
1:F:79:THR:HG21	1:F:177:GLY:H	1.48	0.78
1:M:84:THR:CG2	1:M:86:GLN:HB2	2.12	0.78
1:E:154:GLU:HG2	1:E:289:LEU:HD22	1.63	0.78
1:M:154:GLU:HG2	1:M:289:LEU:HD22	1.63	0.78
1:F:154:GLU:HG2	1:F:289:LEU:HD22	1.63	0.78
1:B:133:ARG:HE	1:B:190:ASN:HD22	1.29	0.78
1:B:43:ALA:HB2	1:B:176:PRO:HD2	1.66	0.78
1:H:185:PHE:HB2	1:H:189:HIS:HD2	1.47	0.78
1:I:46:LEU:HD11	1:I:113:PRO:HG2	1.66	0.78
1:E:87:ILE:CD1	1:E:176:PRO:HD3	2.14	0.78
1:J:84:THR:HB	1:J:86:GLN:HG3	1.66	0.77
1:E:133:ARG:HD3	1:E:190:ASN:ND2	1.98	0.77
1:D:40:TRP:CD2	1:D:41:ILE:HG23	2.19	0.77
1:J:40:TRP:CE3	1:J:75:MET:HE2	2.19	0.77
1:J:46:LEU:HD12	1:J:202:GLY:HA2	1.66	0.77
1:C:84:THR:OG1	1:C:86:GLN:HB2	1.85	0.77
1:H:115:VAL:HG11	1:H:125:ASP:HB3	1.66	0.77
1:J:87:ILE:CD1	1:J:230:ILE:HG21	2.12	0.77
1:A:49:LEU:HD21	1:A:56:LEU:HD21	1.65	0.76
1:F:87:ILE:CD1	1:F:230:ILE:HG12	2.15	0.76
1:G:39:THR:HA	1:G:42:GLN:HG3	1.67	0.76
1:B:122:PRO:HD3	1:D:62:THR:HG21	1.65	0.76
1:M:283:ILE:HB	1:O:268:LEU:CD2	2.14	0.76
1:D:252:ASN:O	1:O:245:SER:HA	1.85	0.76
1:N:182:ASN:HB2	1:N:195:GLN:O	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:87:ILE:HD11	1:G:176:PRO:HB3	1.67	0.76
1:A:63:ARG:HG2	1:A:63:ARG:NH1	1.97	0.76
1:G:254:SER:HB3	1:L:243:ASN:N	1.99	0.76
1:I:129:LEU:HD23	1:I:191:PRO:HD3	1.67	0.76
1:J:87:ILE:HD11	1:J:208:PHE:CE1	2.20	0.76
1:E:150:ASN:ND2	1:P:207:GLU:OE1	2.18	0.76
1:P:129:LEU:HD23	1:P:191:PRO:HD3	1.65	0.76
1:N:59:LEU:HA	1:O:122:PRO:HG2	1.67	0.76
1:C:40:TRP:NE1	1:C:41:ILE:HD13	2.01	0.75
1:D:254:SER:O	1:O:246:LYS:HE3	1.86	0.75
1:A:129:LEU:HD23	1:A:191:PRO:CD	2.17	0.75
1:D:58:GLN:O	1:D:62:THR:HG23	1.87	0.75
1:E:288:LEU:HD13	1:P:86:GLN:NE2	2.02	0.75
1:L:84:THR:OG1	1:L:86:GLN:HG2	1.85	0.74
1:F:76:ARG:HD2	1:F:198:ILE:HG21	1.69	0.74
1:L:56:LEU:HD12	1:L:56:LEU:O	1.85	0.74
1:N:133:ARG:HE	1:N:190:ASN:ND2	1.84	0.74
1:L:57:TYR:HE1	1:L:75:MET:HE3	1.53	0.74
1:C:58:GLN:O	1:C:62:THR:HB	1.87	0.74
1:A:122:PRO:HG2	1:C:59:LEU:HA	1.70	0.74
1:E:133:ARG:NH1	1:E:190:ASN:ND2	2.33	0.74
1:G:254:SER:CB	1:L:244:ILE:H	2.01	0.74
1:O:80:ILE:HG22	1:O:81:ASP:O	1.87	0.74
1:B:129:LEU:HD23	1:B:191:PRO:CD	2.17	0.74
1:C:185:PHE:CB	1:C:189:HIS:HD2	2.00	0.74
1:N:59:LEU:HD13	1:O:122:PRO:HB2	1.68	0.73
1:M:64:ILE:HG12	1:M:129:LEU:HD12	1.70	0.73
1:I:40:TRP:CH2	1:I:57:TYR:HB2	2.24	0.73
1:L:57:TYR:CE1	1:L:75:MET:HE3	2.23	0.73
1:N:76:ARG:NH1	1:N:95:LEU:HD11	2.04	0.73
1:B:129:LEU:HD23	1:B:191:PRO:HD3	1.70	0.73
1:P:40:TRP:CE3	1:P:75:MET:HE3	2.23	0.73
1:M:187:ARG:NH1	1:M:195:GLN:HG3	2.03	0.73
1:J:129:LEU:CD2	1:J:191:PRO:HD3	2.18	0.73
1:E:87:ILE:O	1:E:89:ILE:HG13	1.89	0.73
1:F:79:THR:HB	1:F:176:PRO:HA	1.69	0.73
1:K:262:LYS:HG2	1:K:270:TYR:HE1	1.53	0.72
1:K:58:GLN:O	1:K:62:THR:HG23	1.89	0.72
1:K:133:ARG:CB	1:K:191:PRO:HB3	2.20	0.72
1:L:120:LEU:HG	1:L:122:PRO:HD3	1.71	0.72
1:P:79:THR:OG1	1:P:176:PRO:HA	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:84:THR:HB	1:N:86:GLN:HG2	1.72	0.72
1:E:65:PRO:HB3	1:F:62:THR:O	1.90	0.71
1:K:80:ILE:HG22	1:K:87:ILE:HD13	1.72	0.71
1:E:156:THR:HG21	1:E:284:PRO:HG2	1.73	0.71
1:O:76:ARG:HD3	1:O:198:ILE:HG13	1.71	0.71
1:G:156:THR:HG21	1:G:284:PRO:HG2	1.72	0.71
1:H:156:THR:HG21	1:H:284:PRO:HG2	1.73	0.71
1:J:156:THR:HG21	1:J:284:PRO:HG2	1.73	0.71
1:O:156:THR:HG21	1:O:284:PRO:HG2	1.72	0.71
1:H:115:VAL:HG12	1:H:115:VAL:O	1.89	0.71
1:P:65:PRO:HD3	1:P:129:LEU:CD1	2.21	0.71
1:A:129:LEU:CD2	1:A:191:PRO:HD3	2.20	0.71
1:A:156:THR:HG21	1:A:284:PRO:HG2	1.73	0.71
1:F:129:LEU:HD23	1:F:191:PRO:HD3	1.73	0.71
1:L:156:THR:HG21	1:L:284:PRO:HG2	1.72	0.71
1:D:156:THR:HG21	1:D:284:PRO:HG2	1.73	0.71
1:H:186:SER:N	1:H:188:ASN:OD1	2.24	0.71
1:I:156:THR:HG21	1:I:284:PRO:HG2	1.73	0.70
1:A:190:ASN:HA	1:A:192:PHE:N	2.06	0.70
1:K:268:LEU:HD23	1:K:268:LEU:N	2.05	0.70
1:B:156:THR:HG21	1:B:284:PRO:HG2	1.73	0.70
1:E:87:ILE:HD11	1:E:176:PRO:HD3	1.73	0.70
1:J:76:ARG:HD3	1:J:177:GLY:O	1.91	0.70
1:N:156:THR:HG21	1:N:284:PRO:HG2	1.73	0.70
1:K:156:THR:HG21	1:K:284:PRO:HG2	1.73	0.70
1:C:156:THR:HG21	1:C:284:PRO:HG2	1.73	0.70
1:I:64:ILE:CG2	1:I:129:LEU:HD11	2.14	0.70
1:K:135:ASN:ND2	1:K:271:ASN:HD21	1.90	0.70
1:G:182:ASN:HB2	1:G:195:GLN:O	1.92	0.70
1:B:40:TRP:HA	1:B:177:GLY:HA3	1.74	0.70
1:D:40:TRP:CE3	1:D:41:ILE:HG23	2.27	0.70
1:F:156:THR:HG21	1:F:284:PRO:HG2	1.73	0.70
1:P:133:ARG:CB	1:P:191:PRO:HB3	2.22	0.70
1:A:129:LEU:HD23	1:A:191:PRO:HG3	1.74	0.70
1:G:182:ASN:HA	1:G:195:GLN:OE1	1.92	0.70
1:J:194:ASN:HB3	1:J:197:GLU:HB2	1.72	0.69
1:M:156:THR:HG21	1:M:284:PRO:HG2	1.73	0.69
1:N:87:ILE:HD11	1:N:208:PHE:HE1	1.55	0.69
1:H:264:PHE:HB3	1:P:248:PHE:CD2	2.27	0.69
1:F:76:ARG:HD2	1:F:198:ILE:CG2	2.21	0.69
1:N:120:LEU:HD12	1:N:120:LEU:O	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:GLN:HE21	1:B:176:PRO:HG3	1.57	0.69
1:G:194:ASN:HD21	1:G:197:GLU:HB2	1.58	0.69
1:J:190:ASN:CB	1:J:191:PRO:HA	2.18	0.69
1:P:156:THR:HG21	1:P:284:PRO:HG2	1.73	0.69
1:N:76:ARG:HD2	1:N:198:ILE:HG23	1.74	0.69
1:A:76:ARG:NH1	1:A:177:GLY:O	2.26	0.69
1:K:44:ALA:O	1:K:205:ARG:NH1	2.26	0.69
1:A:87:ILE:CD1	1:A:176:PRO:HD3	2.23	0.68
1:I:63:ARG:NH2	1:I:123:VAL:O	2.26	0.68
1:M:64:ILE:HG23	1:M:129:LEU:HD11	1.74	0.68
1:G:254:SER:HB3	1:L:243:ASN:CA	2.24	0.68
1:L:45:SER:HA	1:L:205:ARG:HG2	1.75	0.68
1:P:57:TYR:CE1	1:P:73:LEU:HD23	2.29	0.68
1:J:84:THR:CB	1:J:86:GLN:HG3	2.24	0.68
1:J:43:ALA:O	1:J:205:ARG:HG3	1.94	0.67
1:J:87:ILE:HD12	1:J:230:ILE:CG2	2.14	0.67
1:L:116:THR:HG22	1:L:117:ASN:H	1.58	0.67
1:I:129:LEU:CD2	1:I:191:PRO:HD3	2.24	0.67
1:H:185:PHE:HB2	1:H:189:HIS:CD2	2.30	0.67
1:K:158:TRP:CG	1:K:194:ASN:HD21	2.13	0.67
1:L:116:THR:CG2	1:L:117:ASN:H	2.07	0.67
1:F:79:THR:HG21	1:F:177:GLY:N	2.09	0.67
1:B:129:LEU:CD2	1:B:191:PRO:HD3	2.25	0.67
1:E:49:LEU:HD21	1:E:56:LEU:HD22	1.76	0.67
1:A:70:PRO:HG2	1:A:71:ASN:H	1.58	0.67
1:F:64:ILE:CG2	1:F:69:SER:HB3	2.24	0.67
1:L:264:PHE:O	1:L:266:LEU:HG	1.95	0.67
1:E:283:ILE:HG22	1:H:268:LEU:HD21	1.76	0.66
1:P:194:ASN:HB3	1:P:197:GLU:HB2	1.77	0.66
1:G:116:THR:HG22	1:G:118:GLN:N	2.01	0.66
1:N:48:TRP:HH2	1:N:120:LEU:HD23	1.57	0.66
1:O:59:LEU:O	1:O:63:ARG:NH1	2.28	0.66
1:D:254:SER:HB2	1:O:244:ILE:O	1.93	0.66
1:I:188:ASN:OD1	1:K:119:ASN:ND2	2.28	0.66
1:N:76:ARG:HD2	1:N:198:ILE:CG2	2.25	0.66
1:D:40:TRP:H	1:D:40:TRP:CD1	2.13	0.66
1:I:48:TRP:HB2	1:I:118:GLN:HG3	1.79	0.65
1:B:150:ASN:ND2	1:K:207:GLU:OE1	2.30	0.65
1:H:59:LEU:O	1:H:63:ARG:NH1	2.29	0.65
1:I:133:ARG:NH2	1:K:137:PRO:O	2.29	0.65
1:L:44:ALA:O	1:L:205:ARG:NH1	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:182:ASN:HB2	1:K:195:GLN:O	1.96	0.65
1:L:116:THR:HG22	1:L:117:ASN:N	2.12	0.65
1:N:87:ILE:HD11	1:N:208:PHE:CD1	2.32	0.65
1:H:120:LEU:HD12	1:H:125:ASP:HB2	1.77	0.65
1:A:129:LEU:HD23	1:A:191:PRO:CG	2.27	0.65
1:O:63:ARG:HH11	1:O:63:ARG:CG	2.09	0.65
1:O:69:SER:CB	1:O:72:GLY:HA2	2.25	0.65
1:A:49:LEU:HD21	1:A:56:LEU:CD2	2.27	0.65
1:I:87:ILE:HD11	1:I:208:PHE:HE1	1.62	0.65
1:F:192:PHE:CG	1:G:137:PRO:HG2	2.32	0.64
1:K:40:TRP:CE3	1:K:75:MET:HE3	2.32	0.64
1:N:46:LEU:HD21	1:N:116:THR:HA	1.77	0.64
1:A:48:TRP:CG	1:A:118:GLN:HG2	2.32	0.64
1:M:190:ASN:CB	1:M:191:PRO:HA	2.26	0.64
1:M:182:ASN:HB2	1:M:195:GLN:O	1.96	0.64
1:M:190:ASN:HB2	1:M:191:PRO:HA	1.77	0.64
1:F:63:ARG:O	1:F:65:PRO:HD3	1.96	0.64
1:G:40:TRP:CE3	1:G:75:MET:HE3	2.32	0.64
1:H:65:PRO:O	1:H:68:ALA:HB3	1.97	0.64
1:B:194:ASN:O	1:B:197:GLU:N	2.28	0.64
1:K:129:LEU:HD23	1:K:191:PRO:HD3	1.80	0.64
1:E:46:LEU:HD11	1:E:113:PRO:HG2	1.79	0.64
1:J:123:VAL:CB	1:K:63:ARG:HH21	2.10	0.64
1:E:187:ARG:O	1:E:189:HIS:ND1	2.30	0.64
1:H:84:THR:OG1	1:H:86:GLN:HB2	1.98	0.64
1:I:87:ILE:HD11	1:I:208:PHE:CE1	2.33	0.64
1:B:84:THR:CB	1:B:86:GLN:HG3	2.28	0.64
1:E:68:ALA:HB1	1:E:129:LEU:HD21	1.78	0.64
1:M:76:ARG:HB3	1:M:79:THR:CG2	2.28	0.64
1:C:81:ASP:HB3	1:C:84:THR:OG1	1.98	0.64
1:E:55:LEU:HD23	1:G:55:LEU:HD23	1.80	0.64
1:M:133:ARG:NH1	1:M:190:ASN:HB2	2.13	0.64
1:F:87:ILE:HD12	1:F:230:ILE:CG1	2.25	0.63
1:I:43:ALA:HB2	1:I:176:PRO:CD	2.24	0.63
1:I:123:VAL:HG21	1:L:63:ARG:HH11	1.62	0.63
1:N:133:ARG:NH2	1:P:125:ASP:OD1	2.30	0.63
1:J:123:VAL:HB	1:K:63:ARG:HH21	1.64	0.63
1:G:194:ASN:ND2	1:G:197:GLU:HB2	2.13	0.63
1:I:48:TRP:CB	1:I:118:GLN:HG3	2.28	0.63
1:N:40:TRP:CZ2	1:N:57:TYR:HB2	2.33	0.63
1:N:64:ILE:HG23	1:N:129:LEU:HD11	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:123:VAL:CG1	1:K:63:ARG:HH21	2.11	0.63
1:E:283:ILE:HB	1:H:268:LEU:CD2	2.27	0.63
1:K:74:HIS:HD2	1:K:183:ALA:O	1.81	0.63
1:N:84:THR:CB	1:N:86:GLN:HG2	2.28	0.63
1:B:76:ARG:NH1	1:B:95:LEU:HD11	2.12	0.63
1:F:76:ARG:HD3	1:F:177:GLY:O	1.99	0.63
1:O:57:TYR:CE1	1:O:75:MET:HE3	2.34	0.63
1:B:64:ILE:HG23	1:B:129:LEU:HD11	1.79	0.63
1:J:75:MET:HE1	1:J:179:ILE:CG1	2.28	0.63
1:B:64:ILE:HG21	1:B:69:SER:HB3	1.81	0.62
1:F:49:LEU:HD22	1:F:202:GLY:HA3	1.79	0.62
1:M:194:ASN:O	1:M:197:GLU:N	2.28	0.62
1:A:55:LEU:HD12	1:A:55:LEU:O	1.98	0.62
1:A:120:LEU:O	1:A:122:PRO:HD3	1.99	0.62
1:N:59:LEU:CA	1:O:122:PRO:HG2	2.28	0.62
1:A:68:ALA:HB1	1:A:129:LEU:HD21	1.82	0.62
1:C:120:LEU:HD21	1:C:122:PRO:HG3	1.80	0.62
1:D:155:ILE:HG22	1:D:288:LEU:HD23	1.82	0.62
1:E:155:ILE:HG22	1:E:288:LEU:HD23	1.82	0.62
1:H:190:ASN:CG	1:H:191:PRO:HD2	2.23	0.62
1:I:75:MET:HA	1:I:75:MET:HE2	1.81	0.62
1:H:38:ASN:OD1	1:H:42:GLN:NE2	2.32	0.62
1:H:155:ILE:HG22	1:H:288:LEU:HD23	1.82	0.62
1:B:42:GLN:NE2	1:B:176:PRO:HG3	2.15	0.62
1:N:155:ILE:HG22	1:N:288:LEU:HD23	1.82	0.62
1:K:135:ASN:HD22	1:K:271:ASN:HD21	1.45	0.62
1:A:155:ILE:HG22	1:A:288:LEU:HD23	1.82	0.62
1:E:133:ARG:CD	1:E:190:ASN:HD21	2.05	0.62
1:J:75:MET:HE1	1:J:179:ILE:HG12	1.82	0.62
1:J:182:ASN:HB2	1:J:195:GLN:O	1.99	0.62
1:M:155:ILE:HG22	1:M:288:LEU:HD23	1.82	0.62
1:G:155:ILE:HG22	1:G:288:LEU:HD23	1.82	0.62
1:G:264:PHE:HE2	1:L:236:ASN:HA	1.64	0.62
1:O:63:ARG:HH11	1:O:63:ARG:HG3	1.64	0.62
1:A:63:ARG:HH11	1:A:63:ARG:CG	2.03	0.61
1:B:155:ILE:HG22	1:B:288:LEU:HD23	1.82	0.61
1:C:135:ASN:ND2	1:C:271:ASN:HD21	1.96	0.61
1:I:133:ARG:NH1	1:I:190:ASN:ND2	2.47	0.61
1:K:262:LYS:HG2	1:K:270:TYR:CE1	2.35	0.61
1:I:40:TRP:CZ2	1:I:57:TYR:HB2	2.35	0.61
1:B:133:ARG:HE	1:B:190:ASN:ND2	1.98	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:129:LEU:CD2	1:F:191:PRO:HD3	2.30	0.61
1:B:76:ARG:HD3	1:B:177:GLY:O	2.00	0.61
1:F:155:ILE:HG22	1:F:288:LEU:HD23	1.82	0.61
1:J:155:ILE:HG22	1:J:288:LEU:HD23	1.82	0.61
1:D:39:THR:HA	1:D:42:GLN:HG3	1.83	0.61
1:E:43:ALA:O	1:E:205:ARG:HG3	2.00	0.61
1:M:64:ILE:HG12	1:M:129:LEU:CD1	2.31	0.61
1:O:56:LEU:O	1:O:60:ILE:HD12	2.00	0.61
1:E:39:THR:HG23	1:E:40:TRP:N	2.16	0.61
1:H:87:ILE:HD13	1:H:87:ILE:N	2.16	0.61
1:I:155:ILE:HG22	1:I:288:LEU:HD23	1.82	0.61
1:L:76:ARG:HD3	1:L:198:ILE:HG13	1.81	0.61
1:L:155:ILE:HG22	1:L:288:LEU:HD23	1.82	0.61
1:P:155:ILE:HG22	1:P:288:LEU:HD23	1.82	0.61
1:F:87:ILE:HD12	1:F:230:ILE:CG2	2.31	0.61
1:C:155:ILE:HG22	1:C:288:LEU:HD23	1.82	0.61
1:K:155:ILE:HG22	1:K:288:LEU:HD23	1.82	0.61
1:C:62:THR:HG23	1:C:63:ARG:HG3	1.81	0.60
1:A:133:ARG:NH1	1:A:190:ASN:HB2	2.17	0.60
1:C:39:THR:HA	1:C:42:GLN:HG2	1.83	0.60
1:E:40:TRP:CE3	1:E:41:ILE:HG23	2.36	0.60
1:O:155:ILE:HG22	1:O:288:LEU:HD23	1.82	0.60
1:G:116:THR:N	1:G:119:ASN:OD1	2.33	0.60
1:O:78:GLN:O	1:O:88:GLN:HG3	2.00	0.60
1:B:65:PRO:HD2	1:B:129:LEU:CD1	2.31	0.60
1:F:64:ILE:HG21	1:F:69:SER:HB3	1.82	0.60
1:J:64:ILE:HG21	1:J:69:SER:HB3	1.82	0.60
1:B:65:PRO:HD2	1:B:129:LEU:HD13	1.82	0.60
1:G:261:SER:O	1:G:264:PHE:HB2	2.02	0.60
1:M:55:LEU:HD12	1:M:55:LEU:O	2.02	0.60
1:E:283:ILE:CB	1:H:268:LEU:HD21	2.31	0.60
1:I:190:ASN:ND2	1:I:191:PRO:HA	2.17	0.60
1:N:133:ARG:NE	1:N:190:ASN:ND2	2.48	0.60
1:B:87:ILE:HG13	1:B:230:ILE:HG21	1.84	0.59
1:C:194:ASN:C	1:C:196:ASP:H	2.10	0.59
1:P:84:THR:OG1	1:P:85:GLY:N	2.35	0.59
1:J:87:ILE:HD11	1:J:208:PHE:HE1	1.65	0.59
1:J:64:ILE:HG23	1:J:129:LEU:HD11	1.85	0.59
1:P:65:PRO:HD3	1:P:129:LEU:HD11	1.83	0.59
1:I:129:LEU:HD23	1:I:191:PRO:CD	2.33	0.59
1:N:121:SER:HA	1:O:62:THR:HG21	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:186:SER:C	1:C:188:ASN:H	2.10	0.59
1:E:61:SER:HA	1:E:64:ILE:CD1	2.33	0.59
1:O:63:ARG:NH1	1:O:63:ARG:HG3	2.17	0.59
1:A:133:ARG:HD3	1:A:190:ASN:ND2	2.15	0.59
1:J:123:VAL:HG11	1:K:63:ARG:HH21	1.68	0.59
1:A:133:ARG:HH11	1:A:190:ASN:HB2	1.68	0.58
1:H:63:ARG:HG3	1:H:63:ARG:NH1	2.13	0.58
1:H:135:ASN:HD22	1:H:271:ASN:HD21	1.50	0.58
1:N:55:LEU:HD23	1:O:55:LEU:HD23	1.85	0.58
1:E:283:ILE:HB	1:H:268:LEU:HD21	1.83	0.58
1:J:129:LEU:HD23	1:J:191:PRO:CD	2.30	0.58
1:E:40:TRP:CD2	1:E:41:ILE:HG23	2.38	0.58
1:D:252:ASN:O	1:O:245:SER:CA	2.51	0.58
1:E:190:ASN:CG	1:E:191:PRO:HA	2.28	0.58
1:F:70:PRO:HG2	1:F:71:ASN:H	1.68	0.58
1:E:77:GLU:O	1:E:78:GLN:HB2	2.02	0.58
1:F:42:GLN:O	1:F:205:ARG:NH1	2.37	0.58
1:I:65:PRO:HA	1:J:65:PRO:HA	1.84	0.58
1:B:63:ARG:NH1	1:B:123:VAL:O	2.35	0.58
1:H:115:VAL:HB	1:H:138:SER:C	2.28	0.58
1:E:49:LEU:C	1:E:49:LEU:HD23	2.29	0.58
1:F:70:PRO:CG	1:F:71:ASN:H	2.15	0.58
1:O:58:GLN:O	1:O:62:THR:HG23	2.03	0.58
1:B:55:LEU:HD12	1:B:55:LEU:O	2.03	0.58
1:B:64:ILE:CD1	1:B:73:LEU:HD11	2.34	0.58
1:F:123:VAL:HG21	1:H:63:ARG:HD3	1.85	0.58
1:M:43:ALA:HB2	1:M:176:PRO:HD2	1.86	0.58
1:B:43:ALA:O	1:B:205:ARG:HG3	2.04	0.58
1:G:254:SER:OG	1:G:255:GLU:HG3	2.04	0.58
1:A:254:SER:OG	1:A:255:GLU:HG3	2.04	0.57
1:B:42:GLN:O	1:B:205:ARG:NH1	2.35	0.57
1:B:288:LEU:HD13	1:K:86:GLN:NE2	2.19	0.57
1:H:194:ASN:OD1	1:H:196:ASP:HB2	2.04	0.57
1:G:80:ILE:HG22	1:G:87:ILE:CD1	2.28	0.57
1:H:254:SER:OG	1:H:255:GLU:HG3	2.04	0.57
1:H:264:PHE:HB3	1:P:248:PHE:HD2	1.70	0.57
1:I:254:SER:OG	1:I:255:GLU:HG3	2.04	0.57
1:B:87:ILE:CD1	1:B:208:PHE:HE1	2.16	0.57
1:C:62:THR:CG2	1:C:63:ARG:HG3	2.34	0.57
1:D:254:SER:OG	1:D:255:GLU:HG3	2.04	0.57
1:M:68:ALA:HB1	1:M:129:LEU:HD21	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:PRO:HD2	1:B:123:VAL:H	1.70	0.57
1:B:254:SER:OG	1:B:255:GLU:HG3	2.04	0.57
1:O:194:ASN:HD21	1:O:196:ASP:HB2	1.68	0.57
1:E:254:SER:OG	1:E:255:GLU:HG3	2.04	0.57
1:I:84:THR:HB	1:I:86:GLN:HG2	1.87	0.57
1:K:254:SER:OG	1:K:255:GLU:HG3	2.04	0.57
1:P:254:SER:OG	1:P:255:GLU:HG3	2.05	0.57
1:B:49:LEU:CD1	1:B:202:GLY:HA3	2.35	0.57
1:J:56:LEU:O	1:J:60:ILE:HG13	2.05	0.57
1:A:79:THR:HG21	1:A:177:GLY:H	1.70	0.57
1:J:254:SER:OG	1:J:255:GLU:HG3	2.04	0.57
1:M:254:SER:OG	1:M:255:GLU:HG3	2.04	0.57
1:N:42:GLN:HG2	1:N:176:PRO:HG3	1.87	0.57
1:C:120:LEU:CD2	1:C:122:PRO:HG3	2.35	0.56
1:F:63:ARG:HE	1:F:127:HIS:CD2	2.22	0.56
1:L:116:THR:CG2	1:L:117:ASN:N	2.68	0.56
1:B:84:THR:HB	1:B:86:GLN:HG3	1.87	0.56
1:A:61:SER:HB2	1:A:73:LEU:HD12	1.87	0.56
1:B:192:PHE:CE2	1:C:137:PRO:HB2	2.40	0.56
1:C:40:TRP:CE2	1:C:41:ILE:HG23	2.39	0.56
1:C:65:PRO:HG2	1:C:68:ALA:HB2	1.86	0.56
1:C:254:SER:OG	1:C:255:GLU:HG3	2.05	0.56
1:F:254:SER:OG	1:F:255:GLU:HG3	2.04	0.56
1:K:61:SER:HA	1:K:64:ILE:HD12	1.86	0.56
1:N:254:SER:OG	1:N:255:GLU:HG3	2.04	0.56
1:F:81:ASP:OD1	1:F:83:ASN:HB2	2.05	0.56
1:O:254:SER:OG	1:O:255:GLU:HG3	2.04	0.56
1:K:42:GLN:O	1:K:42:GLN:HG2	2.04	0.56
1:L:73:LEU:HD23	1:L:75:MET:HE2	1.87	0.56
1:L:254:SER:OG	1:L:255:GLU:HG3	2.04	0.56
1:M:65:PRO:HA	1:N:64:ILE:O	2.06	0.56
1:H:118:GLN:O	1:H:118:GLN:HG3	2.04	0.56
1:L:56:LEU:HD12	1:L:56:LEU:C	2.28	0.56
1:B:133:ARG:HG3	1:B:190:ASN:HD21	1.71	0.56
1:B:63:ARG:O	1:B:65:PRO:HD3	2.06	0.56
1:K:129:LEU:HD23	1:K:191:PRO:CD	2.36	0.56
1:C:76:ARG:HD3	1:C:198:ILE:HG13	1.88	0.56
1:C:264:PHE:HB3	1:K:248:PHE:CD2	2.41	0.56
1:D:116:THR:CG2	1:D:117:ASN:N	2.69	0.56
1:F:129:LEU:HD23	1:F:191:PRO:HG3	1.88	0.56
1:B:49:LEU:O	1:B:49:LEU:HD23	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:123:VAL:HG21	1:L:63:ARG:NH1	2.20	0.56
1:F:87:ILE:HD11	1:F:208:PHE:CE1	2.42	0.55
1:G:116:THR:HG22	1:G:117:ASN:N	2.21	0.55
1:A:65:PRO:HB3	1:B:62:THR:O	2.07	0.55
1:B:84:THR:OG1	1:B:86:GLN:HG3	2.05	0.55
1:C:264:PHE:HB3	1:K:248:PHE:HD2	1.70	0.55
1:P:190:ASN:HA	1:P:192:PHE:H	1.72	0.55
1:B:188:ASN:HD21	1:C:119:ASN:ND2	2.03	0.55
1:I:59:LEU:HA	1:L:122:PRO:HG2	1.88	0.55
1:O:87:ILE:HD11	1:O:208:PHE:HE1	1.70	0.55
1:E:43:ALA:HB2	1:E:176:PRO:HD2	1.88	0.55
1:F:43:ALA:O	1:F:205:ARG:HG3	2.07	0.55
1:F:45:SER:OG	1:F:112:ILE:HG12	2.06	0.55
1:F:55:LEU:HG	1:H:55:LEU:HD23	1.87	0.55
1:H:194:ASN:C	1:H:196:ASP:H	2.12	0.55
1:A:87:ILE:HD12	1:A:176:PRO:HD3	1.88	0.55
1:H:197:GLU:O	1:H:198:ILE:HD13	2.07	0.55
1:N:197:GLU:O	1:N:198:ILE:HD13	2.07	0.55
1:D:197:GLU:O	1:D:198:ILE:HD13	2.07	0.55
1:I:133:ARG:NH1	1:I:190:ASN:HD22	2.05	0.55
1:I:197:GLU:O	1:I:198:ILE:HD13	2.07	0.55
1:J:197:GLU:O	1:J:198:ILE:HD13	2.07	0.55
1:K:158:TRP:CG	1:K:194:ASN:ND2	2.75	0.55
1:L:197:GLU:O	1:L:198:ILE:HD13	2.07	0.55
1:D:116:THR:HG22	1:D:118:GLN:N	2.06	0.55
1:E:87:ILE:HD11	1:E:208:PHE:HE1	1.72	0.55
1:D:67:PHE:CD1	1:D:68:ALA:N	2.75	0.55
1:F:64:ILE:HG21	1:F:69:SER:CB	2.37	0.55
1:F:197:GLU:O	1:F:198:ILE:HD13	2.07	0.55
1:K:192:PHE:N	1:K:193:PRO:HD3	2.21	0.55
1:N:158:TRP:CD1	1:N:194:ASN:ND2	2.75	0.55
1:E:197:GLU:O	1:E:198:ILE:HD13	2.07	0.55
1:F:40:TRP:H	1:F:40:TRP:CD1	2.25	0.55
1:P:197:GLU:O	1:P:198:ILE:HD13	2.07	0.55
1:B:80:ILE:O	1:B:80:ILE:HG13	2.06	0.54
1:F:81:ASP:HB3	1:F:84:THR:HB	1.90	0.54
1:K:197:GLU:O	1:K:198:ILE:HD13	2.07	0.54
1:A:64:ILE:HG12	1:A:129:LEU:HD12	1.89	0.54
1:B:49:LEU:HD23	1:B:49:LEU:C	2.33	0.54
1:C:278:ALA:HB3	1:C:279:PRO:HD3	1.90	0.54
1:M:197:GLU:O	1:M:198:ILE:HD13	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:120:LEU:O	1:N:122:PRO:HD3	2.06	0.54
1:P:61:SER:HA	1:P:64:ILE:HD12	1.89	0.54
1:B:197:GLU:O	1:B:198:ILE:HD13	2.07	0.54
1:P:64:ILE:CD1	1:P:73:LEU:HD13	2.34	0.54
1:A:48:TRP:CD2	1:A:118:GLN:HG2	2.43	0.54
1:I:247:VAL:HG12	1:I:248:PHE:N	2.23	0.54
1:K:247:VAL:HG12	1:K:248:PHE:N	2.23	0.54
1:O:278:ALA:HB3	1:O:279:PRO:HD3	1.90	0.54
1:I:182:ASN:HB2	1:I:195:GLN:O	2.07	0.54
1:I:278:ALA:HB3	1:I:279:PRO:HD3	1.90	0.54
1:O:197:GLU:O	1:O:198:ILE:HD13	2.07	0.54
1:A:247:VAL:HG12	1:A:248:PHE:N	2.23	0.54
1:B:192:PHE:CG	1:C:137:PRO:HG2	2.42	0.54
1:D:278:ALA:HB3	1:D:279:PRO:HD3	1.90	0.54
1:G:197:GLU:O	1:G:198:ILE:HD13	2.07	0.54
1:J:68:ALA:HB1	1:J:129:LEU:HD21	1.88	0.54
1:J:283:ILE:O	1:L:268:LEU:HD13	2.07	0.54
1:K:81:ASP:HB3	1:K:84:THR:OG1	2.07	0.54
1:L:278:ALA:HB3	1:L:279:PRO:HD3	1.90	0.54
1:P:65:PRO:CD	1:P:129:LEU:HD11	2.38	0.54
1:A:79:THR:HG21	1:A:177:GLY:N	2.22	0.54
1:E:116:THR:HG23	1:E:116:THR:O	2.08	0.54
1:F:57:TYR:HE1	1:F:75:MET:HE3	1.72	0.54
1:H:262:LYS:C	1:H:264:PHE:H	2.14	0.54
1:K:278:ALA:HB3	1:K:279:PRO:HD3	1.90	0.54
1:L:247:VAL:HG12	1:L:248:PHE:N	2.23	0.54
1:M:247:VAL:HG12	1:M:248:PHE:N	2.23	0.54
1:E:188:ASN:O	1:H:119:ASN:HB2	2.08	0.54
1:F:192:PHE:CD1	1:G:137:PRO:HG2	2.43	0.54
1:G:278:ALA:HB3	1:G:279:PRO:HD3	1.90	0.54
1:M:57:TYR:C	1:M:57:TYR:CD2	2.86	0.54
1:A:49:LEU:HD13	1:A:202:GLY:HA3	1.89	0.54
1:B:247:VAL:HG12	1:B:248:PHE:N	2.23	0.54
1:C:197:GLU:O	1:C:198:ILE:HD13	2.07	0.54
1:E:40:TRP:HA	1:E:177:GLY:HA3	1.90	0.54
1:N:74:HIS:HD2	1:N:183:ALA:O	1.91	0.54
1:A:197:GLU:O	1:A:198:ILE:HD13	2.07	0.53
1:A:278:ALA:HB3	1:A:279:PRO:HD3	1.90	0.53
1:E:56:LEU:O	1:E:59:LEU:HB3	2.09	0.53
1:F:278:ALA:HB3	1:F:279:PRO:HD3	1.90	0.53
1:I:122:PRO:O	1:I:126:THR:HG23	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:40:TRP:CZ2	1:K:57:TYR:HB2	2.42	0.53
1:C:118:GLN:O	1:C:118:GLN:HG3	2.08	0.53
1:E:79:THR:HG21	1:E:177:GLY:H	1.72	0.53
1:E:97:ARG:NH1	1:E:99:ASP:OD2	2.41	0.53
1:H:97:ARG:NH1	1:H:99:ASP:OD2	2.41	0.53
1:J:112:ILE:HG22	1:J:116:THR:HG22	1.90	0.53
1:B:278:ALA:HB3	1:B:279:PRO:HD3	1.90	0.53
1:H:115:VAL:HB	1:H:138:SER:O	2.08	0.53
1:H:278:ALA:HB3	1:H:279:PRO:HD3	1.90	0.53
1:C:87:ILE:HD11	1:C:230:ILE:HG21	1.87	0.53
1:D:97:ARG:NH1	1:D:99:ASP:OD2	2.42	0.53
1:F:79:THR:CG2	1:F:177:GLY:H	2.20	0.53
1:M:60:ILE:HG12	1:M:126:THR:HB	1.90	0.53
1:N:247:VAL:HG12	1:N:248:PHE:N	2.23	0.53
1:P:278:ALA:HB3	1:P:279:PRO:HD3	1.90	0.53
1:C:247:VAL:HG12	1:C:248:PHE:N	2.23	0.53
1:E:278:ALA:HB3	1:E:279:PRO:HD3	1.90	0.53
1:F:97:ARG:NH1	1:F:99:ASP:OD2	2.42	0.53
1:F:129:LEU:HD23	1:F:191:PRO:CD	2.38	0.53
1:H:247:VAL:HG12	1:H:248:PHE:N	2.23	0.53
1:K:73:LEU:HD21	1:K:179:ILE:HG23	1.91	0.53
1:K:120:LEU:HD12	1:K:125:ASP:HB2	1.91	0.53
1:L:97:ARG:NH1	1:L:99:ASP:OD2	2.41	0.53
1:O:97:ARG:NH1	1:O:99:ASP:OD2	2.42	0.53
1:P:40:TRP:H	1:P:40:TRP:CD1	2.27	0.53
1:P:87:ILE:HD13	1:P:87:ILE:N	2.22	0.53
1:F:87:ILE:HD13	1:F:230:ILE:HG21	1.90	0.53
1:H:265:ILE:C	1:H:267:ASP:H	2.16	0.53
1:J:247:VAL:HG12	1:J:248:PHE:N	2.23	0.53
1:J:278:ALA:HB3	1:J:279:PRO:HD3	1.90	0.53
1:N:97:ARG:NH1	1:N:99:ASP:OD2	2.42	0.53
1:O:44:ALA:O	1:O:205:ARG:NH1	2.37	0.53
1:O:63:ARG:HH11	1:O:63:ARG:HB2	1.73	0.53
1:C:97:ARG:NH1	1:C:99:ASP:OD2	2.41	0.53
1:G:247:VAL:HG12	1:G:248:PHE:N	2.23	0.53
1:P:97:ARG:NH1	1:P:99:ASP:OD2	2.42	0.53
1:I:64:ILE:O	1:J:65:PRO:HA	2.09	0.53
1:I:97:ARG:NH1	1:I:99:ASP:OD2	2.41	0.53
1:K:97:ARG:NH1	1:K:99:ASP:OD2	2.42	0.53
1:O:247:VAL:HG12	1:O:248:PHE:N	2.23	0.53
1:P:247:VAL:HG12	1:P:248:PHE:N	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:ARG:NH1	1:B:99:ASP:OD2	2.42	0.53
1:D:254:SER:HB3	1:O:244:ILE:H	1.74	0.53
1:F:46:LEU:HD11	1:F:115:VAL:O	2.09	0.53
1:G:97:ARG:NH1	1:G:99:ASP:OD2	2.42	0.53
1:G:116:THR:CG2	1:G:117:ASN:N	2.72	0.53
1:I:63:ARG:CD	1:L:123:VAL:HG21	2.19	0.53
1:M:278:ALA:HB3	1:M:279:PRO:HD3	1.90	0.53
1:A:80:ILE:HD11	1:A:176:PRO:HB3	1.91	0.52
1:D:247:VAL:HG12	1:D:248:PHE:N	2.23	0.52
1:J:97:ARG:NH1	1:J:99:ASP:OD2	2.42	0.52
1:N:80:ILE:HD13	1:N:87:ILE:HA	1.91	0.52
1:C:76:ARG:NH2	1:C:175:ALA:O	2.42	0.52
1:E:247:VAL:HG12	1:E:248:PHE:N	2.23	0.52
1:K:76:ARG:NH2	1:K:79:THR:HG22	2.24	0.52
1:M:59:LEU:HD13	1:P:122:PRO:HB2	1.91	0.52
1:A:97:ARG:NH1	1:A:99:ASP:OD2	2.41	0.52
1:E:63:ARG:NH1	1:E:123:VAL:O	2.28	0.52
1:I:55:LEU:HD23	1:L:55:LEU:HD23	1.90	0.52
1:M:97:ARG:NH1	1:M:99:ASP:OD2	2.41	0.52
1:C:70:PRO:HG2	1:C:71:ASN:H	1.74	0.52
1:L:40:TRP:CE3	1:L:41:ILE:HG23	2.43	0.52
1:M:45:SER:HA	1:M:205:ARG:HG2	1.90	0.52
1:P:115:VAL:HG11	1:P:120:LEU:HD12	1.90	0.52
1:I:79:THR:OG1	1:I:176:PRO:HA	2.09	0.52
1:K:192:PHE:CD2	1:K:192:PHE:N	2.77	0.52
1:N:278:ALA:HB3	1:N:279:PRO:HD3	1.90	0.52
1:C:40:TRP:CZ2	1:C:41:ILE:HD13	2.44	0.52
1:E:120:LEU:O	1:E:122:PRO:HD3	2.10	0.52
1:A:189:HIS:CD2	1:D:119:ASN:HB2	2.45	0.52
1:D:70:PRO:CG	1:D:71:ASN:H	2.22	0.52
1:O:78:GLN:OE1	1:O:78:GLN:HA	2.09	0.52
1:G:40:TRP:HB3	1:G:75:MET:HG3	1.91	0.52
1:I:46:LEU:CD1	1:I:202:GLY:HA2	2.31	0.52
1:I:188:ASN:C	1:I:189:HIS:HD2	2.18	0.52
1:D:44:ALA:O	1:D:205:ARG:NH1	2.41	0.52
1:F:64:ILE:HG22	1:F:69:SER:HB3	1.91	0.52
1:M:79:THR:HG21	1:M:177:GLY:H	1.75	0.52
1:B:58:GLN:NE2	1:D:120:LEU:O	2.43	0.51
1:F:247:VAL:HG12	1:F:248:PHE:N	2.23	0.51
1:L:40:TRP:CD2	1:L:41:ILE:HG23	2.45	0.51
1:M:48:TRP:HH2	1:M:120:LEU:HD23	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:55:LEU:HD12	1:M:55:LEU:C	2.35	0.51
1:H:265:ILE:HG22	1:H:267:ASP:HB2	1.92	0.51
1:I:75:MET:HE2	1:I:75:MET:CA	2.40	0.51
1:N:42:GLN:HG2	1:N:176:PRO:CG	2.40	0.51
1:A:79:THR:HB	1:A:176:PRO:HA	1.91	0.51
1:E:65:PRO:HA	1:F:65:PRO:HA	1.92	0.51
1:F:46:LEU:HG	1:F:113:PRO:HD2	1.93	0.51
1:F:122:PRO:HG2	1:H:59:LEU:HA	1.93	0.51
1:G:87:ILE:HD11	1:G:176:PRO:CB	2.38	0.51
1:I:48:TRP:CG	1:I:118:GLN:HG3	2.46	0.51
1:I:76:ARG:HD2	1:I:198:ILE:HG13	1.93	0.51
1:N:56:LEU:HD11	1:N:60:ILE:HD11	1.93	0.51
1:O:66:SER:O	1:O:69:SER:O	2.28	0.51
1:A:122:PRO:HG2	1:C:59:LEU:CA	2.39	0.51
1:B:45:SER:HA	1:B:205:ARG:HG2	1.92	0.51
1:H:133:ARG:HG3	1:H:133:ARG:O	2.09	0.51
1:I:150:ASN:OD1	1:I:150:ASN:N	2.44	0.51
1:J:122:PRO:HB2	1:K:59:LEU:HD13	1.93	0.51
1:K:133:ARG:HG3	1:K:191:PRO:CB	2.25	0.51
1:N:181:ILE:HG21	1:N:193:PRO:HB2	1.92	0.51
1:P:181:ILE:HG21	1:P:193:PRO:HB2	1.92	0.51
1:A:150:ASN:OD1	1:A:150:ASN:N	2.44	0.51
1:K:150:ASN:OD1	1:K:150:ASN:N	2.44	0.51
1:J:69:SER:HB2	1:J:184:SER:O	2.11	0.51
1:I:46:LEU:HD12	1:I:202:GLY:CA	2.33	0.51
1:J:67:PHE:CZ	1:J:189:HIS:CD2	2.99	0.51
1:N:150:ASN:OD1	1:N:150:ASN:N	2.44	0.51
1:B:87:ILE:HD12	1:B:208:PHE:HE1	1.76	0.50
1:B:181:ILE:HG21	1:B:193:PRO:HB2	1.93	0.50
1:F:250:HIS:O	1:F:253:HIS:HB2	2.12	0.50
1:D:254:SER:HA	1:O:246:LYS:HB2	1.93	0.50
1:E:250:HIS:O	1:E:253:HIS:HB2	2.12	0.50
1:H:264:PHE:CB	1:P:248:PHE:CD2	2.93	0.50
1:M:129:LEU:HD23	1:M:191:PRO:HD3	1.94	0.50
1:A:48:TRP:CG	1:A:118:GLN:CG	2.94	0.50
1:G:69:SER:OG	1:G:184:SER:O	2.28	0.50
1:P:61:SER:C	1:P:63:ARG:H	2.20	0.50
1:C:120:LEU:HD12	1:C:125:ASP:HB2	1.93	0.50
1:E:288:LEU:HD13	1:P:86:GLN:HE21	1.77	0.50
1:J:40:TRP:HA	1:J:177:GLY:HA3	1.94	0.50
1:M:63:ARG:C	1:M:64:ILE:HG13	2.37	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:73:LEU:HD21	1:K:179:ILE:CG2	2.41	0.50
1:K:250:HIS:O	1:K:253:HIS:HB2	2.12	0.50
1:N:250:HIS:O	1:N:253:HIS:HB2	2.12	0.50
1:F:87:ILE:O	1:F:89:ILE:HG13	2.12	0.50
1:G:264:PHE:CE2	1:L:236:ASN:HA	2.45	0.50
1:I:250:HIS:O	1:I:253:HIS:HB2	2.12	0.50
1:M:250:HIS:O	1:M:253:HIS:HB2	2.12	0.50
1:O:45:SER:HA	1:O:205:ARG:HG2	1.94	0.50
1:P:63:ARG:NH2	1:P:126:THR:OG1	2.44	0.50
1:B:57:TYR:C	1:B:57:TYR:CD2	2.88	0.50
1:C:150:ASN:OD1	1:C:150:ASN:N	2.44	0.50
1:G:250:HIS:O	1:G:253:HIS:HB2	2.12	0.50
1:L:182:ASN:HB2	1:L:195:GLN:O	2.11	0.50
1:N:49:LEU:HD13	1:N:202:GLY:HA3	1.93	0.50
1:C:39:THR:HA	1:C:42:GLN:CG	2.41	0.49
1:E:49:LEU:HD21	1:E:56:LEU:CD2	2.40	0.49
1:E:129:LEU:HD23	1:E:191:PRO:CG	2.42	0.49
1:E:192:PHE:CD1	1:H:137:PRO:HG2	2.47	0.49
1:F:181:ILE:HG21	1:F:193:PRO:HB2	1.93	0.49
1:H:185:PHE:CB	1:H:189:HIS:HD2	2.18	0.49
1:D:40:TRP:HA	1:D:177:GLY:HA3	1.94	0.49
1:J:250:HIS:O	1:J:253:HIS:HB2	2.12	0.49
1:L:250:HIS:O	1:L:253:HIS:HB2	2.12	0.49
1:M:79:THR:HB	1:M:176:PRO:HA	1.94	0.49
1:F:61:SER:HB3	1:F:73:LEU:HD23	1.95	0.49
1:P:250:HIS:O	1:P:253:HIS:HB2	2.12	0.49
1:D:250:HIS:O	1:D:253:HIS:HB2	2.12	0.49
1:I:63:ARG:NH1	1:I:63:ARG:HG2	2.28	0.49
1:I:123:VAL:CG2	1:L:63:ARG:NH1	2.75	0.49
1:K:158:TRP:CD1	1:K:194:ASN:ND2	2.80	0.49
1:O:250:HIS:O	1:O:253:HIS:HB2	2.12	0.49
1:P:39:THR:HA	1:P:42:GLN:HB2	1.93	0.49
1:M:74:HIS:HD2	1:M:183:ALA:O	1.95	0.49
1:B:48:TRP:H	1:B:48:TRP:CD1	2.30	0.49
1:B:232:PRO:HA	1:B:235:LEU:HG	1.95	0.49
1:E:192:PHE:N	1:E:193:PRO:HD3	2.28	0.49
1:F:87:ILE:HD11	1:F:208:PHE:HE1	1.78	0.49
1:N:120:LEU:HD12	1:N:120:LEU:C	2.37	0.49
1:I:76:ARG:HH21	1:I:93:HIS:HB3	1.76	0.49
1:J:64:ILE:HG12	1:J:129:LEU:CD1	2.43	0.49
1:K:232:PRO:HA	1:K:235:LEU:HG	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:HIS:O	1:A:253:HIS:HB2	2.12	0.49
1:B:250:HIS:O	1:B:253:HIS:HB2	2.12	0.49
1:D:57:TYR:CE1	1:D:75:MET:HE3	2.47	0.49
1:F:232:PRO:HA	1:F:235:LEU:HG	1.95	0.49
1:H:104:ASN:HB2	1:H:256:GLY:O	2.13	0.49
1:H:250:HIS:O	1:H:253:HIS:HB2	2.12	0.49
1:H:265:ILE:HG22	1:H:267:ASP:CB	2.42	0.49
1:L:57:TYR:CE1	1:L:75:MET:CE	2.93	0.49
1:L:150:ASN:OD1	1:L:150:ASN:N	2.44	0.49
1:L:232:PRO:HA	1:L:235:LEU:HG	1.95	0.49
1:A:70:PRO:HG2	1:A:71:ASN:ND2	2.28	0.49
1:A:77:GLU:O	1:A:78:GLN:HB2	2.13	0.49
1:B:104:ASN:HB2	1:B:256:GLY:O	2.13	0.49
1:C:250:HIS:O	1:C:253:HIS:HB2	2.12	0.49
1:G:254:SER:OG	1:L:242:SER:HA	2.12	0.49
1:I:59:LEU:HD21	1:I:126:THR:HG21	1.93	0.49
1:J:69:SER:O	1:J:69:SER:OG	2.27	0.49
1:J:115:VAL:HG23	1:J:138:SER:O	2.13	0.49
1:K:104:ASN:HB2	1:K:256:GLY:O	2.13	0.49
1:N:55:LEU:CD2	1:O:55:LEU:HD23	2.43	0.49
1:O:232:PRO:HA	1:O:235:LEU:HG	1.95	0.49
1:A:192:PHE:CG	1:D:137:PRO:HG2	2.48	0.48
1:B:48:TRP:HB2	1:B:118:GLN:HG3	1.95	0.48
1:E:79:THR:HG21	1:E:177:GLY:N	2.28	0.48
1:I:232:PRO:HA	1:I:235:LEU:HG	1.95	0.48
1:J:112:ILE:HG22	1:J:116:THR:CG2	2.42	0.48
1:O:84:THR:OG1	1:O:86:GLN:HG2	2.13	0.48
1:P:59:LEU:HD12	1:P:63:ARG:HH12	1.77	0.48
1:P:232:PRO:HA	1:P:235:LEU:HG	1.95	0.48
1:C:190:ASN:CG	1:C:191:PRO:HD2	2.37	0.48
1:E:79:THR:OG1	1:E:176:PRO:HA	2.13	0.48
1:E:104:ASN:HB2	1:E:256:GLY:O	2.13	0.48
1:G:76:ARG:HD3	1:G:198:ILE:HG13	1.94	0.48
1:K:81:ASP:HB3	1:K:84:THR:HG1	1.78	0.48
1:M:63:ARG:NH1	1:M:123:VAL:O	2.34	0.48
1:P:190:ASN:HB2	1:P:191:PRO:CA	2.32	0.48
1:E:232:PRO:HA	1:E:235:LEU:HG	1.95	0.48
1:J:60:ILE:HG12	1:J:126:THR:HB	1.95	0.48
1:F:63:ARG:HH11	1:H:123:VAL:HG21	1.79	0.48
1:O:63:ARG:HH11	1:O:63:ARG:CB	2.25	0.48
1:C:104:ASN:HB2	1:C:256:GLY:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:40:TRP:CE3	1:D:41:ILE:CG2	2.96	0.48
1:G:158:TRP:CD1	1:G:194:ASN:HB3	2.48	0.48
1:J:123:VAL:HG11	1:K:63:ARG:NH2	2.29	0.48
1:K:81:ASP:OD1	1:K:84:THR:HG23	2.14	0.48
1:M:49:LEU:HD22	1:M:202:GLY:HA3	1.95	0.48
1:M:104:ASN:HB2	1:M:256:GLY:O	2.13	0.48
1:P:182:ASN:HB2	1:P:195:GLN:O	2.11	0.48
1:D:129:LEU:HD23	1:D:191:PRO:CD	2.44	0.48
1:H:40:TRP:CH2	1:H:57:TYR:HA	2.48	0.48
1:H:242:SER:O	1:H:243:ASN:HB2	2.14	0.48
1:I:45:SER:CB	1:I:205:ARG:HG2	2.43	0.48
1:B:46:LEU:HD23	1:B:46:LEU:HA	1.53	0.48
1:D:40:TRP:CZ3	1:D:41:ILE:CG2	2.97	0.48
1:H:259:MET:CG	1:H:264:PHE:CE2	2.96	0.48
1:I:242:SER:O	1:I:243:ASN:HB2	2.14	0.48
1:M:242:SER:O	1:M:243:ASN:HB2	2.14	0.48
1:P:104:ASN:HB2	1:P:256:GLY:O	2.13	0.48
1:C:65:PRO:HB3	1:C:67:PHE:CE2	2.48	0.48
1:G:39:THR:CA	1:G:42:GLN:HG3	2.42	0.48
1:N:104:ASN:HB2	1:N:256:GLY:O	2.13	0.48
1:K:192:PHE:HD2	1:K:192:PHE:N	2.12	0.48
1:P:242:SER:O	1:P:243:ASN:HB2	2.14	0.48
1:C:186:SER:C	1:C:188:ASN:N	2.72	0.48
1:D:232:PRO:HA	1:D:235:LEU:HG	1.95	0.48
1:F:104:ASN:HB2	1:F:256:GLY:O	2.13	0.48
1:G:232:PRO:HA	1:G:235:LEU:HG	1.95	0.48
1:H:232:PRO:HA	1:H:235:LEU:HG	1.95	0.48
1:I:45:SER:HB3	1:I:204:ILE:C	2.39	0.48
1:I:104:ASN:HB2	1:I:256:GLY:O	2.13	0.48
1:J:104:ASN:HB2	1:J:256:GLY:O	2.13	0.48
1:J:242:SER:O	1:J:243:ASN:HB2	2.14	0.48
1:L:104:ASN:HB2	1:L:256:GLY:O	2.13	0.48
1:L:142:SER:OG	1:L:197:GLU:OE2	2.27	0.48
1:M:133:ARG:NH1	1:M:190:ASN:CB	2.75	0.48
1:M:142:SER:OG	1:M:197:GLU:OE2	2.27	0.48
1:N:80:ILE:CG2	1:N:81:ASP:N	2.76	0.48
1:O:104:ASN:HB2	1:O:256:GLY:O	2.13	0.48
1:P:64:ILE:HA	1:P:129:LEU:HD11	1.96	0.48
1:C:264:PHE:CB	1:K:248:PHE:CD2	2.97	0.47
1:J:232:PRO:HA	1:J:235:LEU:HG	1.95	0.47
1:A:48:TRP:HB2	1:A:118:GLN:HE21	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:242:SER:O	1:C:243:ASN:HB2	2.14	0.47
1:F:120:LEU:HD13	1:F:120:LEU:O	2.13	0.47
1:F:242:SER:O	1:F:243:ASN:HB2	2.14	0.47
1:G:262:LYS:C	1:G:264:PHE:H	2.20	0.47
1:K:40:TRP:CE3	1:K:75:MET:CE	2.97	0.47
1:P:40:TRP:CE3	1:P:41:ILE:HG23	2.50	0.47
1:P:150:ASN:OD1	1:P:150:ASN:N	2.44	0.47
1:B:87:ILE:HD12	1:B:208:PHE:CE1	2.49	0.47
1:N:80:ILE:HG22	1:N:81:ASP:N	2.28	0.47
1:P:65:PRO:HD3	1:P:129:LEU:HD13	1.95	0.47
1:C:232:PRO:HA	1:C:235:LEU:HG	1.95	0.47
1:D:39:THR:HA	1:D:42:GLN:CG	2.44	0.47
1:G:104:ASN:HB2	1:G:256:GLY:O	2.13	0.47
1:G:120:LEU:CD1	1:G:125:ASP:HB2	2.44	0.47
1:I:63:ARG:HG2	1:I:63:ARG:HH11	1.78	0.47
1:N:242:SER:O	1:N:243:ASN:HB2	2.14	0.47
1:A:60:ILE:HG22	1:A:73:LEU:HD11	1.95	0.47
1:A:242:SER:O	1:A:243:ASN:HB2	2.14	0.47
1:B:41:ILE:HG22	1:B:201:PRO:O	2.15	0.47
1:C:70:PRO:CG	1:C:71:ASN:H	2.26	0.47
1:D:242:SER:O	1:D:243:ASN:HB2	2.14	0.47
1:E:133:ARG:NH1	1:E:190:ASN:HD22	2.10	0.47
1:I:43:ALA:H	1:I:176:PRO:HG2	1.79	0.47
1:I:189:HIS:CD2	1:K:119:ASN:HB2	2.50	0.47
1:K:89:ILE:HG22	1:K:89:ILE:O	2.15	0.47
1:O:65:PRO:HG2	1:O:68:ALA:HB3	1.96	0.47
1:O:89:ILE:HG22	1:O:89:ILE:O	2.15	0.47
1:A:104:ASN:HB2	1:A:256:GLY:O	2.13	0.47
1:A:188:ASN:O	1:D:119:ASN:ND2	2.43	0.47
1:A:190:ASN:ND2	1:A:191:PRO:HA	2.30	0.47
1:B:288:LEU:CD1	1:K:86:GLN:NE2	2.78	0.47
1:D:104:ASN:HB2	1:D:256:GLY:O	2.13	0.47
1:F:41:ILE:HG22	1:F:201:PRO:HB2	1.97	0.47
1:F:89:ILE:HG22	1:F:89:ILE:O	2.15	0.47
1:G:70:PRO:HD2	1:G:71:ASN:H	1.80	0.47
1:I:89:ILE:O	1:I:89:ILE:HG22	2.15	0.47
1:K:60:ILE:HG22	1:K:61:SER:N	2.29	0.47
1:M:232:PRO:HA	1:M:235:LEU:HG	1.95	0.47
1:N:124:GLU:H	1:N:124:GLU:HG2	1.57	0.47
1:A:232:PRO:HA	1:A:235:LEU:HG	1.95	0.47
1:C:120:LEU:HG	1:C:121:SER:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:56:LEU:HD23	1:D:56:LEU:C	2.38	0.47
1:D:142:SER:OG	1:D:197:GLU:OE2	2.27	0.47
1:E:89:ILE:HG22	1:E:89:ILE:O	2.15	0.47
1:H:89:ILE:O	1:H:89:ILE:HG22	2.15	0.47
1:L:89:ILE:O	1:L:89:ILE:HG22	2.15	0.47
1:L:242:SER:O	1:L:243:ASN:HB2	2.14	0.47
1:N:40:TRP:HA	1:N:177:GLY:HA3	1.97	0.47
1:N:48:TRP:CZ3	1:N:120:LEU:HD23	2.49	0.47
1:N:57:TYR:CD2	1:N:57:TYR:C	2.92	0.47
1:N:89:ILE:O	1:N:89:ILE:HG22	2.15	0.47
1:N:190:ASN:CG	1:N:191:PRO:HA	2.40	0.47
1:N:232:PRO:HA	1:N:235:LEU:HG	1.95	0.47
1:P:115:VAL:CG1	1:P:120:LEU:HD12	2.44	0.47
1:C:190:ASN:OD1	1:C:191:PRO:HD2	2.15	0.47
1:G:254:SER:HB3	1:L:243:ASN:C	2.39	0.47
1:H:84:THR:C	1:H:86:GLN:H	2.23	0.47
1:J:89:ILE:HG22	1:J:89:ILE:O	2.15	0.47
1:J:133:ARG:NH1	1:J:192:PHE:HE2	2.12	0.47
1:O:242:SER:O	1:O:243:ASN:HB2	2.14	0.47
1:E:64:ILE:HD12	1:E:64:ILE:H	1.79	0.47
1:E:242:SER:O	1:E:243:ASN:HB2	2.14	0.47
1:F:129:LEU:HD23	1:F:191:PRO:CG	2.44	0.47
1:H:150:ASN:OD1	1:H:150:ASN:N	2.44	0.47
1:C:67:PHE:CD1	1:C:67:PHE:C	2.93	0.47
1:D:89:ILE:O	1:D:89:ILE:HG22	2.15	0.47
1:G:242:SER:O	1:G:243:ASN:HB2	2.14	0.47
1:L:43:ALA:O	1:L:205:ARG:HG3	2.15	0.47
1:M:40:TRP:CZ2	1:M:57:TYR:HB2	2.49	0.47
1:O:150:ASN:OD1	1:O:150:ASN:N	2.44	0.47
1:P:133:ARG:HB2	1:P:191:PRO:HB3	1.97	0.47
1:C:98:TRP:CH2	1:C:170:ARG:HD2	2.50	0.46
1:D:70:PRO:HG2	1:D:71:ASN:H	1.80	0.46
1:G:147:ARG:HD3	1:G:156:THR:O	2.16	0.46
1:H:98:TRP:CH2	1:H:170:ARG:HD2	2.51	0.46
1:I:68:ALA:O	1:I:185:PHE:HA	2.15	0.46
1:I:142:SER:OG	1:I:197:GLU:OE2	2.27	0.46
1:K:147:ARG:HD3	1:K:156:THR:O	2.16	0.46
1:O:81:ASP:OD1	1:O:82:SER:N	2.47	0.46
1:P:64:ILE:HA	1:P:129:LEU:CD1	2.46	0.46
1:A:122:PRO:HB2	1:C:59:LEU:HD13	1.97	0.46
1:C:89:ILE:HG22	1:C:89:ILE:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:40:TRP:HB2	1:D:75:MET:SD	2.55	0.46
1:E:133:ARG:CD	1:E:190:ASN:ND2	2.73	0.46
1:E:147:ARG:HD3	1:E:156:THR:O	2.16	0.46
1:H:59:LEU:HD21	1:H:122:PRO:HB3	1.96	0.46
1:I:188:ASN:O	1:I:189:HIS:HD2	1.99	0.46
1:J:59:LEU:HD13	1:K:59:LEU:HD21	1.97	0.46
1:K:98:TRP:CH2	1:K:170:ARG:HD2	2.50	0.46
1:K:190:ASN:CB	1:K:191:PRO:HA	2.29	0.46
1:L:45:SER:HA	1:L:205:ARG:CG	2.44	0.46
1:L:147:ARG:HD3	1:L:156:THR:O	2.16	0.46
1:O:81:ASP:HB3	1:O:84:THR:OG1	2.15	0.46
1:O:98:TRP:CH2	1:O:170:ARG:HD2	2.51	0.46
1:O:120:LEU:HD12	1:O:125:ASP:HB2	1.97	0.46
1:A:55:LEU:HG	1:C:55:LEU:HD23	1.97	0.46
1:D:98:TRP:CH2	1:D:170:ARG:HD2	2.51	0.46
1:E:153:LEU:HD13	1:P:86:GLN:HG2	1.97	0.46
1:F:98:TRP:CH2	1:F:170:ARG:HD2	2.51	0.46
1:H:147:ARG:HD3	1:H:156:THR:O	2.16	0.46
1:J:98:TRP:CH2	1:J:170:ARG:HD2	2.50	0.46
1:N:87:ILE:CD1	1:N:208:PHE:CD1	2.99	0.46
1:N:98:TRP:CH2	1:N:170:ARG:HD2	2.51	0.46
1:B:192:PHE:CZ	1:C:137:PRO:HB2	2.51	0.46
1:D:150:ASN:OD1	1:D:150:ASN:N	2.44	0.46
1:E:123:VAL:HG21	1:G:63:ARG:HD2	1.98	0.46
1:F:150:ASN:OD1	1:F:150:ASN:N	2.44	0.46
1:G:98:TRP:CH2	1:G:170:ARG:HD2	2.51	0.46
1:I:147:ARG:HD3	1:I:156:THR:O	2.16	0.46
1:K:142:SER:OG	1:K:197:GLU:OE2	2.27	0.46
1:M:98:TRP:CH2	1:M:170:ARG:HD2	2.51	0.46
1:N:46:LEU:HD22	1:N:48:TRP:CE2	2.51	0.46
1:A:147:ARG:HD3	1:A:156:THR:O	2.16	0.46
1:B:98:TRP:CH2	1:B:170:ARG:HD2	2.51	0.46
1:B:153:LEU:HD21	1:K:84:THR:O	2.16	0.46
1:D:147:ARG:HD3	1:D:156:THR:O	2.16	0.46
1:I:98:TRP:CH2	1:I:170:ARG:HD2	2.51	0.46
1:I:121:SER:HA	1:I:122:PRO:HD3	1.68	0.46
1:L:158:TRP:CD1	1:L:194:ASN:ND2	2.84	0.46
1:M:68:ALA:CB	1:M:129:LEU:HD21	2.46	0.46
1:N:40:TRP:HB3	1:N:75:MET:HG3	1.98	0.46
1:N:46:LEU:HD22	1:N:48:TRP:NE1	2.30	0.46
1:N:147:ARG:HD3	1:N:156:THR:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:147:ARG:HD3	1:C:156:THR:O	2.16	0.46
1:D:254:SER:HB3	1:O:244:ILE:N	2.29	0.46
1:E:49:LEU:HD23	1:E:49:LEU:O	2.15	0.46
1:F:147:ARG:HD3	1:F:156:THR:O	2.16	0.46
1:H:135:ASN:ND2	1:H:271:ASN:HD21	2.13	0.46
1:H:259:MET:HG2	1:H:264:PHE:CZ	2.50	0.46
1:I:58:GLN:O	1:I:62:THR:HG22	2.16	0.46
1:K:133:ARG:HB2	1:K:191:PRO:CG	2.46	0.46
1:K:242:SER:O	1:K:243:ASN:HB2	2.14	0.46
1:A:98:TRP:CH2	1:A:170:ARG:HD2	2.51	0.46
1:B:133:ARG:O	1:B:277:PHE:HZ	1.98	0.46
1:B:192:PHE:HZ	1:C:115:VAL:HG22	1.80	0.46
1:C:65:PRO:CB	1:C:67:PHE:CE2	2.99	0.46
1:G:37:ASP:HB2	1:G:38:ASN:H	1.56	0.46
1:G:40:TRP:CB	1:G:75:MET:HG3	2.45	0.46
1:G:73:LEU:HD22	1:G:179:ILE:CG2	2.46	0.46
1:J:147:ARG:HD3	1:J:156:THR:O	2.16	0.46
1:A:89:ILE:HG22	1:A:89:ILE:O	2.15	0.46
1:A:122:PRO:O	1:A:126:THR:HG23	2.16	0.46
1:C:186:SER:O	1:C:188:ASN:N	2.45	0.46
1:E:81:ASP:HB3	1:E:84:THR:OG1	2.15	0.46
1:H:189:HIS:CE1	1:H:193:PRO:HB3	2.51	0.46
1:H:247:VAL:CG1	1:H:248:PHE:N	2.79	0.46
1:I:48:TRP:CD1	1:I:118:GLN:HB2	2.50	0.46
1:I:247:VAL:CG1	1:I:248:PHE:N	2.79	0.46
1:N:64:ILE:HA	1:N:65:PRO:HD3	1.80	0.46
1:O:147:ARG:HD3	1:O:156:THR:O	2.16	0.46
1:P:247:VAL:CG1	1:P:248:PHE:N	2.79	0.46
1:A:133:ARG:HH11	1:A:190:ASN:HD22	1.64	0.46
1:C:187:ARG:HB3	1:C:193:PRO:HG3	1.97	0.46
1:E:150:ASN:OD1	1:E:150:ASN:N	2.44	0.46
1:L:124:GLU:C	1:L:126:THR:H	2.24	0.46
1:O:40:TRP:HB2	1:O:75:MET:SD	2.56	0.46
1:P:89:ILE:HG22	1:P:89:ILE:O	2.15	0.46
1:P:147:ARG:HD3	1:P:156:THR:O	2.16	0.46
1:B:147:ARG:HD3	1:B:156:THR:O	2.16	0.46
1:C:142:SER:OG	1:C:197:GLU:OE2	2.27	0.46
1:D:192:PHE:N	1:D:193:PRO:HD3	2.31	0.46
1:G:74:HIS:O	1:G:180:ASP:HB3	2.16	0.46
1:K:84:THR:OG1	1:K:85:GLY:N	2.48	0.46
1:M:283:ILE:O	1:O:268:LEU:HD13	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:VAL:HG21	1:C:63:ARG:HD2	1.97	0.45
1:B:89:ILE:O	1:B:89:ILE:HG22	2.15	0.45
1:D:80:ILE:HG12	1:D:87:ILE:HD13	1.97	0.45
1:M:89:ILE:HG22	1:M:89:ILE:O	2.15	0.45
1:M:133:ARG:HH11	1:M:190:ASN:CB	2.21	0.45
1:M:147:ARG:HD3	1:M:156:THR:O	2.16	0.45
1:N:247:VAL:CG1	1:N:248:PHE:N	2.79	0.45
1:A:226:ASN:HA	1:A:227:PRO:HD2	1.82	0.45
1:B:142:SER:OG	1:B:197:GLU:OE2	2.27	0.45
1:B:242:SER:O	1:B:243:ASN:HB2	2.14	0.45
1:C:124:GLU:C	1:C:126:THR:H	2.24	0.45
1:C:247:VAL:CG1	1:C:248:PHE:N	2.79	0.45
1:E:57:TYR:CD2	1:E:58:GLN:N	2.84	0.45
1:F:61:SER:HB3	1:F:73:LEU:CD2	2.47	0.45
1:F:65:PRO:HD2	1:F:129:LEU:HD13	1.96	0.45
1:F:87:ILE:CD1	1:F:208:PHE:CE1	3.00	0.45
1:J:40:TRP:HE3	1:J:75:MET:HE2	1.77	0.45
1:K:64:ILE:HA	1:K:129:LEU:HD11	1.98	0.45
1:K:190:ASN:CA	1:K:192:PHE:CD2	2.93	0.45
1:N:48:TRP:CZ3	1:N:120:LEU:CD2	2.99	0.45
1:E:40:TRP:CZ2	1:E:57:TYR:HB2	2.51	0.45
1:F:70:PRO:CG	1:F:71:ASN:N	2.78	0.45
1:G:247:VAL:CG1	1:G:248:PHE:N	2.79	0.45
1:N:192:PHE:CG	1:P:137:PRO:HG2	2.51	0.45
1:I:56:LEU:CD2	1:I:60:ILE:HD11	2.46	0.45
1:L:247:VAL:CG1	1:L:248:PHE:N	2.79	0.45
1:M:121:SER:HA	1:M:122:PRO:HD3	1.63	0.45
1:O:247:VAL:CG1	1:O:248:PHE:N	2.79	0.45
1:D:182:ASN:HB2	1:D:195:GLN:O	2.15	0.45
1:E:98:TRP:CH2	1:E:170:ARG:HD2	2.51	0.45
1:F:120:LEU:HD13	1:F:120:LEU:C	2.42	0.45
1:G:89:ILE:O	1:G:89:ILE:HG22	2.15	0.45
1:I:129:LEU:HD23	1:I:191:PRO:CG	2.47	0.45
1:L:98:TRP:CH2	1:L:170:ARG:HD2	2.51	0.45
1:M:234:THR:C	1:M:236:ASN:N	2.75	0.45
1:P:40:TRP:CE3	1:P:75:MET:CE	2.96	0.45
1:B:64:ILE:HD13	1:B:73:LEU:HD11	1.98	0.45
1:B:247:VAL:CG1	1:B:248:PHE:N	2.79	0.45
1:D:264:PHE:O	1:D:266:LEU:HD13	2.17	0.45
1:F:247:VAL:CG1	1:F:248:PHE:N	2.79	0.45
1:H:262:LYS:C	1:H:264:PHE:N	2.74	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:268:LEU:N	1:K:268:LEU:CD2	2.76	0.45
1:M:113:PRO:O	1:M:116:THR:HG22	2.17	0.45
1:M:192:PHE:CG	1:O:137:PRO:HG2	2.51	0.45
1:P:98:TRP:CH2	1:P:170:ARG:HD2	2.50	0.45
1:B:234:THR:C	1:B:236:ASN:N	2.75	0.45
1:G:67:PHE:CD1	1:G:68:ALA:N	2.85	0.45
1:H:56:LEU:HD12	1:H:56:LEU:HA	1.60	0.45
1:J:247:VAL:CG1	1:J:248:PHE:N	2.79	0.45
1:M:150:ASN:OD1	1:M:150:ASN:N	2.44	0.45
1:C:57:TYR:HE1	1:C:75:MET:HE3	1.82	0.45
1:C:65:PRO:O	1:C:68:ALA:HB3	2.17	0.45
1:G:41:ILE:HG12	1:G:41:ILE:O	2.17	0.45
1:G:55:LEU:O	1:G:58:GLN:N	2.50	0.45
1:H:42:GLN:HB3	1:H:176:PRO:CG	2.47	0.45
1:H:115:VAL:HG12	1:H:139:ILE:HG22	1.97	0.45
1:I:117:ASN:OD1	1:I:117:ASN:N	2.43	0.45
1:I:226:ASN:HA	1:I:227:PRO:HD2	1.82	0.45
1:A:48:TRP:HB2	1:A:118:GLN:NE2	2.32	0.45
1:A:156:THR:HG21	1:A:284:PRO:CG	2.46	0.45
1:A:247:VAL:CG1	1:A:248:PHE:N	2.79	0.45
1:D:282:GLU:O	1:D:284:PRO:HD3	2.17	0.45
1:E:234:THR:C	1:E:236:ASN:N	2.75	0.45
1:F:282:GLU:O	1:F:284:PRO:HD3	2.17	0.45
1:J:75:MET:HE1	1:J:179:ILE:HG13	1.98	0.45
1:K:73:LEU:CD2	1:K:179:ILE:HG23	2.47	0.45
1:N:49:LEU:HD13	1:N:202:GLY:CA	2.47	0.45
1:P:72:GLY:O	1:P:74:HIS:HD2	1.99	0.45
1:A:87:ILE:HD11	1:A:176:PRO:HD3	1.98	0.45
1:B:156:THR:HG21	1:B:284:PRO:CG	2.46	0.45
1:D:247:VAL:CG1	1:D:248:PHE:N	2.79	0.45
1:E:40:TRP:CD1	1:E:40:TRP:H	2.35	0.45
1:E:46:LEU:HD12	1:E:202:GLY:CA	2.28	0.45
1:K:156:THR:HG21	1:K:284:PRO:CG	2.46	0.45
1:E:182:ASN:HB2	1:E:195:GLN:O	2.17	0.44
1:E:247:VAL:CG1	1:E:248:PHE:N	2.79	0.44
1:E:282:GLU:O	1:E:284:PRO:HD3	2.17	0.44
1:F:133:ARG:HH11	1:F:190:ASN:HD22	1.64	0.44
1:A:69:SER:HB2	1:A:185:PHE:CE1	2.52	0.44
1:A:72:GLY:O	1:A:74:HIS:HD2	2.01	0.44
1:A:282:GLU:O	1:A:284:PRO:HD3	2.17	0.44
1:G:150:ASN:OD1	1:G:150:ASN:N	2.44	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:156:THR:HG21	1:G:284:PRO:CG	2.46	0.44
1:G:262:LYS:C	1:G:264:PHE:N	2.75	0.44
1:H:282:GLU:O	1:H:284:PRO:HD3	2.17	0.44
1:I:64:ILE:HA	1:I:65:PRO:HD3	1.92	0.44
1:I:188:ASN:C	1:I:189:HIS:CD2	2.95	0.44
1:L:226:ASN:HA	1:L:227:PRO:HD2	1.82	0.44
1:E:41:ILE:HD12	1:E:49:LEU:HD22	1.97	0.44
1:K:226:ASN:HA	1:K:227:PRO:HD2	1.82	0.44
1:K:247:VAL:CG1	1:K:248:PHE:N	2.79	0.44
1:L:234:THR:C	1:L:236:ASN:N	2.75	0.44
1:L:282:GLU:O	1:L:284:PRO:HD3	2.17	0.44
1:M:37:ASP:OD2	1:M:39:THR:OG1	2.35	0.44
1:P:282:GLU:O	1:P:284:PRO:HD3	2.17	0.44
1:F:57:TYR:CE1	1:F:75:MET:HE3	2.50	0.44
1:H:142:SER:OG	1:H:197:GLU:OE2	2.27	0.44
1:M:84:THR:HB	1:M:86:GLN:H	1.82	0.44
1:M:122:PRO:HG2	1:P:59:LEU:HA	1.99	0.44
1:O:282:GLU:O	1:O:284:PRO:HD3	2.17	0.44
1:B:182:ASN:HB2	1:B:195:GLN:O	2.18	0.44
1:C:195:GLN:HE21	1:C:195:GLN:HB2	1.48	0.44
1:C:259:MET:HG2	1:C:264:PHE:CZ	2.52	0.44
1:H:70:PRO:CD	1:H:71:ASN:H	2.31	0.44
1:J:81:ASP:HB3	1:J:84:THR:OG1	2.18	0.44
1:M:247:VAL:CG1	1:M:248:PHE:N	2.79	0.44
1:N:282:GLU:O	1:N:284:PRO:HD3	2.17	0.44
1:P:261:SER:O	1:P:264:PHE:HB2	2.18	0.44
1:B:122:PRO:HG2	1:D:59:LEU:HA	1.99	0.44
1:E:87:ILE:HD11	1:E:208:PHE:CE1	2.53	0.44
1:G:87:ILE:O	1:G:87:ILE:HG22	2.17	0.44
1:G:282:GLU:O	1:G:284:PRO:HD3	2.17	0.44
1:H:59:LEU:HD23	1:H:126:THR:HG21	2.00	0.44
1:K:129:LEU:CD2	1:K:191:PRO:HD3	2.45	0.44
1:K:190:ASN:HA	1:K:192:PHE:N	2.32	0.44
1:L:140:PHE:HB3	1:L:199:THR:CG2	2.48	0.44
1:N:58:GLN:NE2	1:O:120:LEU:O	2.50	0.44
1:B:81:ASP:OD1	1:B:83:ASN:HB2	2.17	0.44
1:D:116:THR:HG22	1:D:117:ASN:N	2.32	0.44
1:E:140:PHE:HB3	1:E:199:THR:CG2	2.48	0.44
1:F:140:PHE:HB3	1:F:199:THR:CG2	2.48	0.44
1:H:140:PHE:HB3	1:H:199:THR:CG2	2.48	0.44
1:K:282:GLU:O	1:K:284:PRO:HD3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:61:SER:OG	1:M:62:THR:N	2.50	0.44
1:B:140:PHE:HB3	1:B:199:THR:CG2	2.48	0.44
1:B:282:GLU:O	1:B:284:PRO:HD3	2.17	0.44
1:C:69:SER:HB2	1:C:184:SER:O	2.17	0.44
1:O:81:ASP:OD2	1:O:84:THR:HG23	2.18	0.44
1:B:283:ILE:CG2	1:C:268:LEU:HD21	2.48	0.44
1:D:57:TYR:HE1	1:D:75:MET:HE3	1.83	0.44
1:E:64:ILE:HG21	1:E:69:SER:HB2	1.99	0.44
1:F:186:SER:OG	1:F:189:HIS:HB2	2.18	0.44
1:I:140:PHE:HB3	1:I:199:THR:CG2	2.48	0.44
1:K:102:PRO:HB2	1:K:256:GLY:O	2.18	0.44
1:M:76:ARG:NH1	1:M:177:GLY:O	2.51	0.44
1:M:140:PHE:HB3	1:M:199:THR:CG2	2.48	0.44
1:M:282:GLU:O	1:M:284:PRO:HD3	2.17	0.44
1:N:84:THR:HB	1:N:86:GLN:H	1.83	0.44
1:N:234:THR:C	1:N:236:ASN:N	2.75	0.44
1:A:140:PHE:HB3	1:A:199:THR:CG2	2.48	0.43
1:B:46:LEU:HD13	1:B:48:TRP:CZ2	2.53	0.43
1:B:64:ILE:HD12	1:B:73:LEU:CD1	2.48	0.43
1:B:112:ILE:HA	1:B:113:PRO:HD3	1.91	0.43
1:D:102:PRO:HB2	1:D:256:GLY:O	2.18	0.43
1:F:64:ILE:HA	1:F:65:PRO:HD2	1.94	0.43
1:F:120:LEU:O	1:F:122:PRO:HD3	2.18	0.43
1:I:56:LEU:HD23	1:I:56:LEU:O	2.18	0.43
1:I:102:PRO:HB2	1:I:256:GLY:O	2.18	0.43
1:J:102:PRO:HB2	1:J:256:GLY:O	2.18	0.43
1:P:188:ASN:O	1:P:192:PHE:HE1	2.00	0.43
1:D:234:THR:C	1:D:236:ASN:N	2.75	0.43
1:H:192:PHE:N	1:H:193:PRO:CD	2.81	0.43
1:J:140:PHE:HB3	1:J:199:THR:CG2	2.48	0.43
1:K:234:THR:C	1:K:236:ASN:N	2.75	0.43
1:L:102:PRO:HB2	1:L:256:GLY:O	2.18	0.43
1:M:40:TRP:CD2	1:M:75:MET:HE3	2.53	0.43
1:N:45:SER:N	1:N:202:GLY:O	2.51	0.43
1:N:76:ARG:HH12	1:N:95:LEU:HD11	1.81	0.43
1:O:154:GLU:CG	1:O:289:LEU:HD22	2.43	0.43
1:B:122:PRO:HG2	1:D:59:LEU:HD23	2.00	0.43
1:C:282:GLU:O	1:C:284:PRO:HD3	2.17	0.43
1:E:102:PRO:HB2	1:E:256:GLY:O	2.18	0.43
1:E:122:PRO:O	1:E:126:THR:HG23	2.18	0.43
1:G:102:PRO:HB2	1:G:256:GLY:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:56:LEU:HG	1:H:60:ILE:HD12	1.99	0.43
1:I:234:THR:C	1:I:236:ASN:N	2.75	0.43
1:J:133:ARG:O	1:J:133:ARG:HG3	2.16	0.43
1:N:102:PRO:HB2	1:N:256:GLY:O	2.18	0.43
1:N:156:THR:HG21	1:N:284:PRO:CG	2.46	0.43
1:A:69:SER:HA	1:A:70:PRO:HD2	1.83	0.43
1:C:84:THR:HB	1:C:86:GLN:HG3	2.00	0.43
1:C:234:THR:C	1:C:236:ASN:N	2.75	0.43
1:E:68:ALA:CB	1:E:129:LEU:HD21	2.46	0.43
1:F:76:ARG:NH1	1:F:177:GLY:O	2.48	0.43
1:G:194:ASN:HD21	1:G:197:GLU:CB	2.30	0.43
1:H:76:ARG:HD3	1:H:198:ILE:HG13	2.00	0.43
1:I:133:ARG:HD2	1:I:190:ASN:HD21	1.84	0.43
1:M:102:PRO:HB2	1:M:256:GLY:O	2.18	0.43
1:M:129:LEU:HD23	1:M:191:PRO:HG3	2.00	0.43
1:O:102:PRO:HB2	1:O:256:GLY:O	2.18	0.43
1:A:55:LEU:HD12	1:A:55:LEU:C	2.43	0.43
1:A:154:GLU:CG	1:A:289:LEU:HD22	2.43	0.43
1:D:65:PRO:HB2	1:D:67:PHE:CD2	2.53	0.43
1:D:120:LEU:HG	1:D:121:SER:N	2.27	0.43
1:H:156:THR:HG21	1:H:284:PRO:CG	2.46	0.43
1:I:63:ARG:HH11	1:I:63:ARG:CG	2.31	0.43
1:J:282:GLU:O	1:J:284:PRO:HD3	2.17	0.43
1:M:112:ILE:HA	1:M:113:PRO:HD3	1.91	0.43
1:O:140:PHE:HB3	1:O:199:THR:CG2	2.48	0.43
1:A:102:PRO:HB2	1:A:256:GLY:O	2.18	0.43
1:D:140:PHE:HB3	1:D:199:THR:CG2	2.48	0.43
1:E:283:ILE:O	1:H:268:LEU:HD23	2.19	0.43
1:F:234:THR:C	1:F:236:ASN:N	2.75	0.43
1:G:44:ALA:O	1:G:205:ARG:NH1	2.50	0.43
1:H:124:GLU:N	1:H:124:GLU:OE1	2.52	0.43
1:H:234:THR:C	1:H:236:ASN:N	2.75	0.43
1:I:43:ALA:CB	1:I:176:PRO:HD2	2.33	0.43
1:I:282:GLU:O	1:I:284:PRO:HD3	2.17	0.43
1:K:76:ARG:NH2	1:K:79:THR:CG2	2.82	0.43
1:G:234:THR:C	1:G:236:ASN:N	2.75	0.43
1:K:40:TRP:HA	1:K:177:GLY:HA3	1.99	0.43
1:K:140:PHE:HB3	1:K:199:THR:CG2	2.48	0.43
1:M:283:ILE:HB	1:O:268:LEU:HD21	1.97	0.43
1:P:40:TRP:HB3	1:P:75:MET:HG3	2.01	0.43
1:P:140:PHE:HB3	1:P:199:THR:CG2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:190:ASN:HA	1:P:192:PHE:N	2.33	0.43
1:B:64:ILE:CG2	1:B:69:SER:HB3	2.48	0.43
1:B:69:SER:HA	1:B:184:SER:O	2.18	0.43
1:C:102:PRO:HB2	1:C:256:GLY:O	2.18	0.43
1:D:154:GLU:CG	1:D:289:LEU:HD22	2.43	0.43
1:E:39:THR:CG2	1:E:40:TRP:N	2.81	0.43
1:E:46:LEU:CD1	1:E:113:PRO:HG2	2.48	0.43
1:J:37:ASP:OD1	1:J:37:ASP:N	2.51	0.43
1:K:267:ASP:HB2	1:K:268:LEU:HD23	2.00	0.43
1:M:79:THR:HG21	1:M:177:GLY:N	2.33	0.43
1:N:284:PRO:O	1:P:262:LYS:HD3	2.18	0.43
1:O:156:THR:HG21	1:O:284:PRO:CG	2.46	0.43
1:B:102:PRO:HB2	1:B:256:GLY:O	2.18	0.43
1:C:140:PHE:HB3	1:C:199:THR:CG2	2.48	0.43
1:E:59:LEU:HA	1:G:122:PRO:HG2	2.01	0.43
1:E:190:ASN:ND2	1:E:191:PRO:HA	2.34	0.43
1:F:120:LEU:H	1:F:120:LEU:HD12	1.84	0.43
1:F:189:HIS:HD2	1:G:119:ASN:HB2	1.84	0.43
1:F:192:PHE:CZ	1:G:137:PRO:HB2	2.54	0.43
1:G:80:ILE:CG2	1:G:87:ILE:HD13	2.33	0.43
1:D:88:GLN:NE2	1:D:90:ASP:OD2	2.51	0.43
1:D:255:GLU:CD	1:O:242:SER:HB3	2.44	0.43
1:E:288:LEU:CD1	1:P:86:GLN:NE2	2.76	0.43
1:F:64:ILE:HA	1:F:129:LEU:CD1	2.48	0.43
1:G:140:PHE:HB3	1:G:199:THR:CG2	2.48	0.43
1:J:87:ILE:CD1	1:J:208:PHE:CD1	3.01	0.43
1:K:120:LEU:HG	1:K:121:SER:N	2.33	0.43
1:A:234:THR:C	1:A:236:ASN:N	2.75	0.42
1:D:80:ILE:HG22	1:D:81:ASP:N	2.34	0.42
1:D:120:LEU:HD12	1:D:125:ASP:HB2	2.01	0.42
1:L:76:ARG:HD3	1:L:198:ILE:CG1	2.46	0.42
1:L:84:THR:HG1	1:L:86:GLN:HG2	1.84	0.42
1:N:140:PHE:HB3	1:N:199:THR:CG2	2.48	0.42
1:N:226:ASN:HA	1:N:227:PRO:HD2	1.82	0.42
1:P:102:PRO:HB2	1:P:256:GLY:O	2.18	0.42
1:A:133:ARG:O	1:A:133:ARG:HG3	2.19	0.42
1:A:192:PHE:CD1	1:D:137:PRO:HG2	2.54	0.42
1:B:49:LEU:HD21	1:B:56:LEU:HD22	2.01	0.42
1:J:226:ASN:HA	1:J:227:PRO:HD2	1.82	0.42
1:L:73:LEU:CD2	1:L:75:MET:HE2	2.48	0.42
1:P:234:THR:C	1:P:236:ASN:N	2.75	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:THR:O	1:A:42:GLN:HB3	2.19	0.42
1:A:65:PRO:HA	1:B:65:PRO:HA	2.01	0.42
1:B:192:PHE:CD1	1:C:137:PRO:HG2	2.55	0.42
1:D:65:PRO:HB2	1:D:67:PHE:CE2	2.55	0.42
1:D:159:THR:HA	1:D:160:PRO:HD3	1.93	0.42
1:E:79:THR:CB	1:E:176:PRO:HA	2.49	0.42
1:F:59:LEU:HD23	1:F:126:THR:HG21	2.01	0.42
1:G:55:LEU:O	1:G:59:LEU:N	2.41	0.42
1:H:102:PRO:HB2	1:H:256:GLY:O	2.18	0.42
1:J:64:ILE:HA	1:J:65:PRO:HD3	1.67	0.42
1:J:87:ILE:CD1	1:J:208:PHE:CE1	2.97	0.42
1:K:80:ILE:HG22	1:K:87:ILE:CD1	2.47	0.42
1:N:37:ASP:OD1	1:N:39:THR:N	2.40	0.42
1:N:81:ASP:OD1	1:N:83:ASN:HB2	2.19	0.42
1:O:234:THR:C	1:O:236:ASN:N	2.75	0.42
1:B:288:LEU:HD13	1:K:86:GLN:HE21	1.85	0.42
1:E:48:TRP:C	1:E:48:TRP:CE3	2.97	0.42
1:E:57:TYR:CD2	1:E:57:TYR:C	2.97	0.42
1:E:156:THR:HG21	1:E:284:PRO:CG	2.46	0.42
1:E:283:ILE:HG21	1:H:268:LEU:HD21	1.94	0.42
1:F:81:ASP:C	1:F:83:ASN:H	2.26	0.42
1:G:194:ASN:ND2	1:G:197:GLU:N	2.67	0.42
1:J:77:GLU:HB3	1:J:78:GLN:NE2	2.34	0.42
1:N:48:TRP:HB3	1:N:118:GLN:OE1	2.19	0.42
1:D:40:TRP:CD1	1:D:40:TRP:N	2.81	0.42
1:D:158:TRP:CD1	1:D:194:ASN:HB3	2.55	0.42
1:I:47:THR:HG23	1:I:48:TRP:H	1.84	0.42
1:L:115:VAL:HG12	1:L:116:THR:O	2.19	0.42
1:A:121:SER:C	1:A:123:VAL:N	2.76	0.42
1:D:186:SER:HB2	1:D:189:HIS:CB	2.43	0.42
1:H:123:VAL:H	1:H:123:VAL:HG23	1.62	0.42
1:H:194:ASN:C	1:H:196:ASP:N	2.78	0.42
1:P:188:ASN:O	1:P:192:PHE:CE1	2.72	0.42
1:F:84:THR:HG21	1:F:86:GLN:HB2	2.02	0.42
1:F:226:ASN:HA	1:F:227:PRO:HD2	1.82	0.42
1:H:112:ILE:HA	1:H:113:PRO:HD3	1.91	0.42
1:I:56:LEU:HD21	1:I:60:ILE:HD11	2.02	0.42
1:M:156:THR:HG21	1:M:284:PRO:CG	2.46	0.42
1:E:61:SER:HA	1:E:64:ILE:HD12	2.00	0.42
1:F:159:THR:HA	1:F:160:PRO:HD3	1.93	0.42
1:O:42:GLN:HE21	1:O:42:GLN:HB3	1.69	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:65:PRO:HG2	1:O:68:ALA:CB	2.50	0.42
1:A:68:ALA:CB	1:A:129:LEU:HD21	2.47	0.42
1:F:55:LEU:CD2	1:H:55:LEU:HD23	2.49	0.42
1:F:102:PRO:HB2	1:F:256:GLY:O	2.18	0.42
1:I:70:PRO:HD2	1:I:71:ASN:H	1.84	0.42
1:L:78:GLN:OE1	1:L:78:GLN:HA	2.19	0.42
1:N:142:SER:OG	1:N:197:GLU:OE2	2.27	0.42
1:B:64:ILE:CD1	1:B:73:LEU:CD1	2.97	0.42
1:B:226:ASN:HA	1:B:227:PRO:HD2	1.82	0.42
1:D:149:ASN:HD21	1:D:153:LEU:HD12	1.85	0.42
1:M:73:LEU:HA	1:M:73:LEU:HD23	1.83	0.42
1:H:60:ILE:HG22	1:H:73:LEU:HD11	2.01	0.41
1:I:74:HIS:HD2	1:I:183:ALA:O	2.03	0.41
1:J:40:TRP:CE3	1:J:75:MET:CE	2.97	0.41
1:J:87:ILE:HD11	1:J:208:PHE:CD1	2.54	0.41
1:J:166:ASN:H	1:J:217:ASN:ND2	2.18	0.41
1:L:116:THR:HG22	1:L:118:GLN:H	1.85	0.41
1:L:156:THR:HG21	1:L:284:PRO:CG	2.46	0.41
1:M:133:ARG:O	1:M:277:PHE:HZ	2.03	0.41
1:M:192:PHE:N	1:M:193:PRO:HD3	2.35	0.41
1:O:166:ASN:H	1:O:217:ASN:ND2	2.18	0.41
1:B:87:ILE:HD11	1:B:208:PHE:HE1	1.84	0.41
1:B:98:TRP:CD1	1:B:160:PRO:HD3	2.56	0.41
1:F:81:ASP:HB3	1:F:85:GLY:H	1.85	0.41
1:F:166:ASN:H	1:F:217:ASN:ND2	2.18	0.41
1:H:166:ASN:H	1:H:217:ASN:ND2	2.18	0.41
1:I:159:THR:HA	1:I:160:PRO:HD3	1.93	0.41
1:I:166:ASN:H	1:I:217:ASN:ND2	2.18	0.41
1:J:98:TRP:CD1	1:J:160:PRO:HD3	2.56	0.41
1:J:234:THR:C	1:J:236:ASN:N	2.75	0.41
1:L:80:ILE:HD11	1:L:176:PRO:HB3	2.02	0.41
1:M:129:LEU:HD23	1:M:191:PRO:CG	2.51	0.41
1:M:149:ASN:HD21	1:M:153:LEU:HD12	1.85	0.41
1:A:98:TRP:CD1	1:A:160:PRO:HD3	2.56	0.41
1:B:120:LEU:C	1:B:120:LEU:HD13	2.45	0.41
1:C:156:THR:HG21	1:C:284:PRO:CG	2.46	0.41
1:D:156:THR:HG21	1:D:284:PRO:CG	2.46	0.41
1:H:55:LEU:O	1:H:58:GLN:HB2	2.20	0.41
1:A:48:TRP:HE3	1:A:48:TRP:O	2.03	0.41
1:D:98:TRP:CD1	1:D:160:PRO:HD3	2.56	0.41
1:E:59:LEU:CA	1:G:122:PRO:HG2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:98:TRP:CD1	1:G:160:PRO:HD3	2.56	0.41
1:H:149:ASN:HD21	1:H:153:LEU:HD12	1.85	0.41
1:N:98:TRP:CD1	1:N:160:PRO:HD3	2.56	0.41
1:O:76:ARG:HD3	1:O:198:ILE:CG1	2.45	0.41
1:O:112:ILE:HA	1:O:113:PRO:HD3	1.91	0.41
1:P:166:ASN:H	1:P:217:ASN:ND2	2.18	0.41
1:B:166:ASN:H	1:B:217:ASN:ND2	2.18	0.41
1:E:37:ASP:OD1	1:E:37:ASP:N	2.54	0.41
1:E:64:ILE:HG21	1:E:69:SER:CB	2.51	0.41
1:F:190:ASN:HA	1:F:191:PRO:HA	1.83	0.41
1:H:241:PRO:HB2	1:H:244:ILE:HD11	2.00	0.41
1:I:149:ASN:HD21	1:I:153:LEU:HD12	1.86	0.41
1:L:58:GLN:O	1:L:62:THR:OG1	2.28	0.41
1:M:73:LEU:HD22	1:M:179:ILE:HG23	2.01	0.41
1:P:69:SER:HA	1:P:70:PRO:HD2	1.77	0.41
1:P:98:TRP:CD1	1:P:160:PRO:HD3	2.56	0.41
1:A:60:ILE:HG22	1:A:61:SER:N	2.36	0.41
1:B:149:ASN:HD21	1:B:153:LEU:HD12	1.85	0.41
1:C:154:GLU:CG	1:C:289:LEU:HD22	2.43	0.41
1:D:80:ILE:CG2	1:D:81:ASP:N	2.83	0.41
1:E:187:ARG:HG2	1:E:195:GLN:NE2	2.35	0.41
1:E:241:PRO:HB2	1:E:244:ILE:HD11	2.00	0.41
1:H:98:TRP:CD1	1:H:160:PRO:HD3	2.56	0.41
1:I:42:GLN:C	1:I:44:ALA:H	2.29	0.41
1:I:98:TRP:CD1	1:I:160:PRO:HD3	2.56	0.41
1:L:98:TRP:CD1	1:L:160:PRO:HD3	2.56	0.41
1:L:166:ASN:H	1:L:217:ASN:ND2	2.18	0.41
1:M:129:LEU:CD2	1:M:191:PRO:HD3	2.51	0.41
1:B:48:TRP:CD2	1:B:118:GLN:HA	2.55	0.41
1:C:98:TRP:CD1	1:C:160:PRO:HD3	2.56	0.41
1:D:56:LEU:HD23	1:D:56:LEU:O	2.21	0.41
1:F:76:ARG:HD2	1:F:198:ILE:HG23	2.02	0.41
1:K:98:TRP:CD1	1:K:160:PRO:HD3	2.56	0.41
1:K:124:GLU:C	1:K:126:THR:H	2.29	0.41
1:L:69:SER:HA	1:L:70:PRO:HD2	1.49	0.41
1:N:159:THR:HA	1:N:160:PRO:HD3	1.93	0.41
1:A:123:VAL:HG11	1:C:63:ARG:NH1	2.36	0.41
1:B:64:ILE:HD12	1:B:73:LEU:HD13	2.01	0.41
1:B:188:ASN:HD21	1:C:119:ASN:CG	2.29	0.41
1:D:166:ASN:H	1:D:217:ASN:ND2	2.18	0.41
1:E:40:TRP:N	1:E:40:TRP:CD1	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:59:LEU:N	1:G:122:PRO:HG2	2.36	0.41
1:F:98:TRP:CD1	1:F:160:PRO:HD3	2.56	0.41
1:F:156:THR:HG21	1:F:284:PRO:CG	2.46	0.41
1:G:61:SER:HA	1:G:64:ILE:HD12	2.02	0.41
1:G:120:LEU:HD11	1:G:125:ASP:HB2	2.01	0.41
1:H:59:LEU:HA	1:H:59:LEU:HD12	1.90	0.41
1:H:159:THR:HA	1:H:160:PRO:HD3	1.93	0.41
1:J:151:LEU:HD23	1:J:151:LEU:HA	1.90	0.41
1:P:112:ILE:HA	1:P:113:PRO:HD3	1.91	0.41
1:A:42:GLN:O	1:A:42:GLN:HG3	2.21	0.41
1:A:149:ASN:HD21	1:A:153:LEU:HD12	1.85	0.41
1:C:100:ARG:HH11	1:C:100:ARG:HD3	1.75	0.41
1:E:98:TRP:CD1	1:E:160:PRO:HD3	2.56	0.41
1:E:133:ARG:HB2	1:E:191:PRO:HB2	2.03	0.41
1:E:192:PHE:CG	1:H:137:PRO:HG2	2.56	0.41
1:F:40:TRP:CZ2	1:F:57:TYR:HB2	2.56	0.41
1:F:148:TYR:CE1	1:F:154:GLU:HB2	2.56	0.41
1:F:149:ASN:HD21	1:F:153:LEU:HD12	1.85	0.41
1:F:154:GLU:CG	1:F:289:LEU:HD22	2.43	0.41
1:H:148:TYR:CE1	1:H:154:GLU:HB2	2.56	0.41
1:H:262:LYS:O	1:H:264:PHE:N	2.53	0.41
1:I:43:ALA:N	1:I:176:PRO:HG2	2.35	0.41
1:I:79:THR:HG23	1:I:80:ILE:N	2.36	0.41
1:I:148:TYR:CE1	1:I:154:GLU:HB2	2.56	0.41
1:K:148:TYR:CE1	1:K:154:GLU:HB2	2.56	0.41
1:K:166:ASN:H	1:K:217:ASN:ND2	2.18	0.41
1:L:148:TYR:CE1	1:L:154:GLU:HB2	2.56	0.41
1:L:149:ASN:HD21	1:L:153:LEU:HD12	1.85	0.41
1:O:43:ALA:HB2	1:O:176:PRO:O	2.21	0.41
1:A:166:ASN:H	1:A:217:ASN:ND2	2.18	0.41
1:C:41:ILE:HD13	1:C:41:ILE:HG23	1.89	0.41
1:D:88:GLN:HG2	1:D:93:HIS:ND1	2.36	0.41
1:D:129:LEU:HD23	1:D:191:PRO:HD3	2.02	0.41
1:D:194:ASN:OD1	1:D:194:ASN:N	2.53	0.41
1:E:149:ASN:HD21	1:E:153:LEU:HD12	1.85	0.41
1:G:142:SER:OG	1:G:197:GLU:OE2	2.27	0.41
1:I:42:GLN:HE21	1:I:176:PRO:HG3	1.84	0.41
1:J:112:ILE:HA	1:J:113:PRO:HD3	1.91	0.41
1:J:148:TYR:CE1	1:J:154:GLU:HB2	2.56	0.41
1:J:149:ASN:HD21	1:J:153:LEU:HD12	1.85	0.41
1:J:156:THR:HG21	1:J:284:PRO:CG	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:98:TRP:CD1	1:M:160:PRO:HD3	2.56	0.41
1:M:129:LEU:HD23	1:M:191:PRO:CD	2.50	0.41
1:N:120:LEU:C	1:N:120:LEU:CD1	2.93	0.41
1:N:148:TYR:CE1	1:N:154:GLU:HB2	2.56	0.41
1:P:44:ALA:O	1:P:205:ARG:NH1	2.42	0.41
1:P:149:ASN:HD21	1:P:153:LEU:HD12	1.85	0.41
1:P:156:THR:HG21	1:P:284:PRO:CG	2.46	0.41
1:B:122:PRO:CD	1:B:123:VAL:H	2.34	0.40
1:D:64:ILE:HD12	1:D:73:LEU:HG	2.03	0.40
1:F:76:ARG:CD	1:F:198:ILE:HG21	2.45	0.40
1:G:73:LEU:HD23	1:G:184:SER:HB3	2.01	0.40
1:G:231:ASN:HA	1:G:232:PRO:HD3	1.85	0.40
1:N:127:HIS:CE1	1:N:130:ASN:HB2	2.55	0.40
1:N:166:ASN:H	1:N:217:ASN:ND2	2.18	0.40
1:O:63:ARG:HH21	1:O:123:VAL:HA	1.85	0.40
1:P:148:TYR:CE1	1:P:154:GLU:HB2	2.56	0.40
1:C:226:ASN:HA	1:C:227:PRO:HD2	1.82	0.40
1:E:148:TYR:CE1	1:E:154:GLU:HB2	2.56	0.40
1:E:166:ASN:H	1:E:217:ASN:ND2	2.18	0.40
1:I:120:LEU:CD1	1:I:120:LEU:C	2.94	0.40
1:J:68:ALA:CB	1:J:129:LEU:HD21	2.51	0.40
1:M:166:ASN:H	1:M:217:ASN:ND2	2.18	0.40
1:P:79:THR:HG23	1:P:80:ILE:HG23	2.02	0.40
1:P:262:LYS:NZ	1:P:268:LEU:HB3	2.37	0.40
1:B:190:ASN:ND2	1:B:191:PRO:HA	2.36	0.40
1:C:40:TRP:CD2	1:C:41:ILE:CG2	2.98	0.40
1:H:259:MET:HG2	1:H:264:PHE:CE2	2.56	0.40
1:K:40:TRP:CD2	1:K:41:ILE:HG23	2.56	0.40
1:O:149:ASN:HD21	1:O:153:LEU:HD12	1.85	0.40
1:A:120:LEU:O	1:A:120:LEU:HD12	2.21	0.40
1:A:148:TYR:CE1	1:A:154:GLU:HB2	2.56	0.40
1:C:149:ASN:HD21	1:C:153:LEU:HD12	1.85	0.40
1:C:166:ASN:H	1:C:217:ASN:ND2	2.18	0.40
1:C:185:PHE:CB	1:C:189:HIS:CD2	2.89	0.40
1:G:226:ASN:HA	1:G:227:PRO:HD2	1.82	0.40
1:H:43:ALA:O	1:H:204:ILE:HA	2.22	0.40
1:I:56:LEU:HD23	1:I:56:LEU:C	2.47	0.40
1:J:117:ASN:C	1:J:119:ASN:N	2.79	0.40
1:J:150:ASN:OD1	1:J:150:ASN:N	2.44	0.40
1:O:231:ASN:HA	1:O:232:PRO:HD3	1.85	0.40
1:A:48:TRP:O	1:A:48:TRP:CE3	2.74	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:ARG:HB2	1:A:191:PRO:HB3	2.02	0.40
1:E:112:ILE:HA	1:E:113:PRO:HD3	1.91	0.40
1:E:127:HIS:CE1	1:E:130:ASN:HB2	2.55	0.40
1:F:44:ALA:HA	1:F:202:GLY:O	2.22	0.40
1:G:79:THR:O	1:G:88:GLN:HB3	2.21	0.40
1:G:149:ASN:HD21	1:G:153:LEU:HD12	1.85	0.40
1:G:159:THR:HA	1:G:160:PRO:HD3	1.93	0.40
1:H:154:GLU:CG	1:H:289:LEU:HD22	2.43	0.40
1:I:192:PHE:CG	1:K:137:PRO:HG2	2.56	0.40
1:J:40:TRP:CZ2	1:J:57:TYR:HB2	2.57	0.40
1:L:73:LEU:HD23	1:L:75:MET:CE	2.50	0.40
1:M:235:LEU:HD23	1:M:235:LEU:HA	1.91	0.40
1:N:63:ARG:HE	1:N:63:ARG:HB2	1.37	0.40
1:N:149:ASN:HD21	1:N:153:LEU:HD12	1.85	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:150:ASN:O	1:H:148:TYR:N[2_664]	1.96	0.24

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	232/291 (80%)	202 (87%)	29 (12%)	1 (0%)	30 65
1	B	232/291 (80%)	205 (88%)	27 (12%)	0	100 100
1	C	240/291 (82%)	211 (88%)	28 (12%)	1 (0%)	30 65
1	D	240/291 (82%)	216 (90%)	21 (9%)	3 (1%)	9 38
1	E	232/291 (80%)	200 (86%)	30 (13%)	2 (1%)	14 48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	232/291 (80%)	205 (88%)	25 (11%)	2 (1%)	14	48
1	G	230/291 (79%)	208 (90%)	22 (10%)	0	100	100
1	H	241/291 (83%)	211 (88%)	27 (11%)	3 (1%)	10	40
1	I	232/291 (80%)	208 (90%)	21 (9%)	3 (1%)	9	38
1	J	232/291 (80%)	208 (90%)	23 (10%)	1 (0%)	30	65
1	K	240/291 (82%)	211 (88%)	28 (12%)	1 (0%)	30	65
1	L	230/291 (79%)	202 (88%)	26 (11%)	2 (1%)	14	48
1	M	232/291 (80%)	206 (89%)	25 (11%)	1 (0%)	30	65
1	N	232/291 (80%)	206 (89%)	23 (10%)	3 (1%)	9	38
1	O	230/291 (79%)	201 (87%)	27 (12%)	2 (1%)	14	48
1	P	240/291 (82%)	212 (88%)	25 (10%)	3 (1%)	9	38
All	All	3747/4656 (80%)	3312 (88%)	407 (11%)	28 (1%)	18	53

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	70	PRO
1	O	70	PRO
1	A	70	PRO
1	N	62	THR
1	P	83	ASN
1	C	125	ASP
1	H	39	THR
1	K	62	THR
1	L	125	ASP
1	D	122	PRO
1	E	70	PRO
1	E	121	SER
1	I	43	ALA
1	I	47	THR
1	M	195	GLN
1	N	122	PRO
1	O	44	ALA
1	P	62	THR
1	D	82	SER
1	H	195	GLN
1	P	193	PRO
1	D	70	PRO

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Mol	Chain	Res	Type
1	F	44	ALA
1	H	263	GLY
1	I	48	TRP
1	J	122	PRO
1	N	121	SER
1	L	122	PRO

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	218/262 (83%)	204 (94%)	14 (6%)	16 48
1	B	218/262 (83%)	204 (94%)	14 (6%)	16 48
1	C	223/262 (85%)	210 (94%)	13 (6%)	18 51
1	D	223/262 (85%)	214 (96%)	9 (4%)	28 62
1	E	218/262 (83%)	206 (94%)	12 (6%)	19 53
1	F	218/262 (83%)	203 (93%)	15 (7%)	14 45
1	G	215/262 (82%)	199 (93%)	16 (7%)	13 42
1	H	224/262 (86%)	208 (93%)	16 (7%)	13 43
1	I	218/262 (83%)	204 (94%)	14 (6%)	16 48
1	J	218/262 (83%)	205 (94%)	13 (6%)	17 50
1	K	223/262 (85%)	209 (94%)	14 (6%)	16 48
1	L	215/262 (82%)	202 (94%)	13 (6%)	17 50
1	M	218/262 (83%)	202 (93%)	16 (7%)	13 42
1	N	218/262 (83%)	205 (94%)	13 (6%)	17 50
1	O	215/262 (82%)	204 (95%)	11 (5%)	21 55
1	P	223/262 (85%)	214 (96%)	9 (4%)	28 62
All	All	3505/4192 (84%)	3293 (94%)	212 (6%)	17 50

All (212) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	THR
1	A	41	ILE
1	A	59	LEU
1	A	63	ARG
1	A	120	LEU
1	A	121	SER
1	A	150	ASN
1	A	188	ASN
1	A	190	ASN
1	A	225	ILE
1	A	233	SER
1	A	237	ASP
1	A	242	SER
1	A	248	PHE
1	B	41	ILE
1	B	81	ASP
1	B	82	SER
1	B	87	ILE
1	B	116	THR
1	B	120	LEU
1	B	133	ARG
1	B	150	ASN
1	B	189	HIS
1	B	225	ILE
1	B	233	SER
1	B	237	ASP
1	B	242	SER
1	B	248	PHE
1	C	38	ASN
1	C	41	ILE
1	C	45	SER
1	C	59	LEU
1	C	150	ASN
1	C	186	SER
1	C	189	HIS
1	C	195	GLN
1	C	225	ILE
1	C	233	SER
1	C	237	ASP
1	C	242	SER
1	C	248	PHE
1	D	87	ILE
1	D	116	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	D	150	ASN
1	D	187	ARG
1	D	225	ILE
1	D	233	SER
1	D	237	ASP
1	D	242	SER
1	D	248	PHE
1	E	37	ASP
1	E	61	SER
1	E	66	SER
1	E	73	LEU
1	E	76	ARG
1	E	120	LEU
1	E	150	ASN
1	E	225	ILE
1	E	233	SER
1	E	237	ASP
1	E	242	SER
1	E	248	PHE
1	F	39	THR
1	F	49	LEU
1	F	75	MET
1	F	120	LEU
1	F	124	GLU
1	F	150	ASN
1	F	186	SER
1	F	188	ASN
1	F	190	ASN
1	F	194	ASN
1	F	225	ILE
1	F	233	SER
1	F	237	ASP
1	F	242	SER
1	F	248	PHE
1	G	37	ASP
1	G	59	LEU
1	G	66	SER
1	G	71	ASN
1	G	74	HIS
1	G	83	ASN
1	G	84	THR
1	G	87	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	G	133	ARG
1	G	150	ASN
1	G	225	ILE
1	G	233	SER
1	G	237	ASP
1	G	242	SER
1	G	248	PHE
1	G	269	ASP
1	H	42	GLN
1	H	64	ILE
1	H	84	THR
1	H	87	ILE
1	H	115	VAL
1	H	116	THR
1	H	119	ASN
1	H	133	ARG
1	H	150	ASN
1	H	186	SER
1	H	195	GLN
1	H	225	ILE
1	H	233	SER
1	H	237	ASP
1	H	242	SER
1	H	248	PHE
1	I	39	THR
1	I	56	LEU
1	I	63	ARG
1	I	69	SER
1	I	75	MET
1	I	117	ASN
1	I	120	LEU
1	I	133	ARG
1	I	150	ASN
1	I	225	ILE
1	I	233	SER
1	I	237	ASP
1	I	242	SER
1	I	248	PHE
1	J	49	LEU
1	J	61	SER
1	J	69	SER
1	J	76	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	J	83	ASN
1	J	120	LEU
1	J	150	ASN
1	J	190	ASN
1	J	225	ILE
1	J	233	SER
1	J	237	ASP
1	J	242	SER
1	J	248	PHE
1	K	41	ILE
1	K	59	LEU
1	K	60	ILE
1	K	73	LEU
1	K	76	ARG
1	K	80	ILE
1	K	150	ASN
1	K	192	PHE
1	K	225	ILE
1	K	233	SER
1	K	237	ASP
1	K	242	SER
1	K	248	PHE
1	K	268	LEU
1	L	37	ASP
1	L	45	SER
1	L	56	LEU
1	L	64	ILE
1	L	71	ASN
1	L	80	ILE
1	L	133	ARG
1	L	150	ASN
1	L	225	ILE
1	L	233	SER
1	L	237	ASP
1	L	242	SER
1	L	248	PHE
1	M	41	ILE
1	M	45	SER
1	M	47	THR
1	M	71	ASN
1	M	76	ARG
1	M	81	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	M	116	THR
1	M	117	ASN
1	M	123	VAL
1	M	150	ASN
1	M	190	ASN
1	M	225	ILE
1	M	233	SER
1	M	237	ASP
1	M	242	SER
1	M	248	PHE
1	N	42	GLN
1	N	47	THR
1	N	58	GLN
1	N	63	ARG
1	N	79	THR
1	N	124	GLU
1	N	133	ARG
1	N	150	ASN
1	N	225	ILE
1	N	233	SER
1	N	237	ASP
1	N	242	SER
1	N	248	PHE
1	O	63	ARG
1	O	66	SER
1	O	75	MET
1	O	120	LEU
1	O	123	VAL
1	O	150	ASN
1	O	225	ILE
1	O	233	SER
1	O	237	ASP
1	O	242	SER
1	O	248	PHE
1	P	80	ILE
1	P	121	SER
1	P	150	ASN
1	P	225	ILE
1	P	233	SER
1	P	237	ASP
1	P	242	SER
1	P	248	PHE

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Mol	Chain	Res	Type
1	P	265	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (104) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	GLN
1	A	71	ASN
1	A	74	HIS
1	A	118	GLN
1	A	189	HIS
1	A	190	ASN
1	A	217	ASN
1	A	252	ASN
1	B	42	GLN
1	B	58	GLN
1	B	109	ASN
1	B	182	ASN
1	B	188	ASN
1	B	190	ASN
1	B	217	ASN
1	C	119	ASN
1	C	135	ASN
1	C	189	HIS
1	C	195	GLN
1	C	217	ASN
1	C	252	ASN
1	C	271	ASN
1	D	58	GLN
1	D	189	HIS
1	D	217	ASN
1	D	252	ASN
1	E	86	GLN
1	E	190	ASN
1	E	217	ASN
1	E	252	ASN
1	F	58	GLN
1	F	86	GLN
1	F	109	ASN
1	F	182	ASN
1	F	189	HIS
1	F	190	ASN
1	F	217	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	F	252	ASN
1	G	58	GLN
1	G	135	ASN
1	G	182	ASN
1	G	194	ASN
1	G	217	ASN
1	H	109	ASN
1	H	135	ASN
1	H	189	HIS
1	H	195	GLN
1	H	217	ASN
1	H	252	ASN
1	H	271	ASN
1	I	42	GLN
1	I	58	GLN
1	I	71	ASN
1	I	74	HIS
1	I	109	ASN
1	I	182	ASN
1	I	189	HIS
1	I	190	ASN
1	I	217	ASN
1	J	78	GLN
1	J	83	ASN
1	J	109	ASN
1	J	182	ASN
1	J	189	HIS
1	J	190	ASN
1	J	195	GLN
1	J	217	ASN
1	J	252	ASN
1	K	42	GLN
1	K	58	GLN
1	K	74	HIS
1	K	86	GLN
1	K	109	ASN
1	K	135	ASN
1	K	182	ASN
1	K	188	ASN
1	K	217	ASN
1	K	272	GLN
1	L	42	GLN

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Mol	Chain	Res	Type
1	L	88	GLN
1	L	194	ASN
1	L	217	ASN
1	M	58	GLN
1	M	74	HIS
1	M	78	GLN
1	M	119	ASN
1	M	217	ASN
1	N	182	ASN
1	N	189	HIS
1	N	190	ASN
1	N	194	ASN
1	N	195	GLN
1	N	217	ASN
1	N	252	ASN
1	O	42	GLN
1	O	88	GLN
1	O	109	ASN
1	O	217	ASN
1	P	74	HIS
1	P	117	ASN
1	P	135	ASN
1	P	182	ASN
1	P	189	HIS
1	P	217	ASN

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	238/291 (81%)	0.61	18 (7%) 20 10	15, 35, 66, 84	0
1	B	238/291 (81%)	0.79	26 (10%) 10 6	17, 41, 71, 84	0
1	C	244/291 (83%)	0.34	7 (2%) 53 31	13, 32, 58, 78	0
1	D	244/291 (83%)	0.59	21 (8%) 16 8	14, 36, 65, 92	0
1	E	238/291 (81%)	0.73	20 (8%) 17 9	15, 40, 71, 83	0
1	F	238/291 (81%)	0.85	26 (10%) 10 6	14, 36, 67, 86	0
1	G	236/291 (81%)	0.71	22 (9%) 14 7	18, 37, 66, 77	0
1	H	245/291 (84%)	0.75	29 (11%) 9 5	13, 30, 57, 71	0
1	I	238/291 (81%)	0.63	6 (2%) 58 35	23, 42, 72, 85	0
1	J	238/291 (81%)	0.59	14 (5%) 28 14	16, 39, 68, 81	0
1	K	244/291 (83%)	0.34	12 (4%) 35 18	10, 35, 68, 85	0
1	L	236/291 (81%)	0.78	26 (11%) 10 6	18, 34, 64, 76	0
1	M	238/291 (81%)	0.75	11 (4%) 37 20	17, 40, 71, 87	0
1	N	238/291 (81%)	0.48	15 (6%) 26 13	14, 40, 69, 83	0
1	O	236/291 (81%)	0.50	16 (6%) 23 12	9, 34, 64, 79	0
1	P	244/291 (83%)	0.41	10 (4%) 41 23	12, 35, 67, 87	0
All	All	3833/4656 (82%)	0.61	279 (7%) 21 11	9, 37, 67, 92	0

All (279) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	150	ASN	8.5
1	J	245	SER	7.4
1	G	150	ASN	6.5
1	L	243	ASN	6.1
1	N	243	ASN	5.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	H	242	SER	4.5
1	L	241	PRO	4.4
1	O	244	ILE	4.4
1	L	236	ASN	4.3
1	L	242	SER	4.3
1	M	239	SER	4.3
1	O	185	PHE	4.2
1	P	150	ASN	4.1
1	L	245	SER	4.0
1	F	261	SER	3.9
1	H	245	SER	3.9
1	F	239	SER	3.9
1	L	261	SER	3.9
1	O	242	SER	3.9
1	H	259	MET	3.9
1	O	248	PHE	3.9
1	J	243	ASN	3.8
1	D	149	ASN	3.8
1	L	248	PHE	3.7
1	D	188	ASN	3.7
1	H	251	GLU	3.7
1	B	261	SER	3.6
1	M	247	VAL	3.6
1	C	130	ASN	3.6
1	G	288	LEU	3.6
1	L	262	LYS	3.6
1	O	236	ASN	3.6
1	G	194	ASN	3.5
1	A	245	SER	3.5
1	K	191	PRO	3.5
1	D	287	ASN	3.5
1	K	190	ASN	3.4
1	P	190	ASN	3.4
1	F	104	ASN	3.4
1	D	286	ASN	3.3
1	J	236	ASN	3.3
1	M	244	ILE	3.3
1	C	186	SER	3.2
1	D	288	LEU	3.2
1	A	246	LYS	3.2
1	D	189	HIS	3.2
1	A	129	LEU	3.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	O	262	LYS	3.2
1	H	254	SER	3.2
1	N	246	LYS	3.2
1	O	243	ASN	3.2
1	A	240	GLY	3.1
1	E	149	ASN	3.1
1	L	185	PHE	3.1
1	B	149	ASN	3.1
1	E	257	ASN	3.1
1	L	244	ILE	3.1
1	J	246	LYS	3.1
1	L	130	ASN	3.1
1	F	177	GLY	3.1
1	L	237	ASP	3.1
1	H	257	ASN	3.0
1	H	279	PRO	3.0
1	A	127	HIS	3.0
1	A	236	ASN	3.0
1	D	257	ASN	3.0
1	O	240	GLY	3.0
1	J	244	ILE	3.0
1	P	191	PRO	3.0
1	E	150	ASN	3.0
1	F	188	ASN	3.0
1	F	240	GLY	3.0
1	L	149	ASN	3.0
1	J	240	GLY	3.0
1	H	130	ASN	3.0
1	K	130	ASN	2.9
1	M	226	ASN	2.9
1	P	136	SER	2.9
1	F	241	PRO	2.9
1	O	245	SER	2.9
1	G	153	LEU	2.9
1	G	222	ARG	2.9
1	B	207	GLU	2.9
1	O	241	PRO	2.9
1	D	153	LEU	2.9
1	B	286	ASN	2.9
1	H	222	ARG	2.9
1	H	252	ASN	2.8
1	D	289	LEU	2.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	F	286	ASN	2.8
1	H	248	PHE	2.8
1	L	136	SER	2.8
1	A	241	PRO	2.8
1	A	156	THR	2.8
1	N	255	GLU	2.8
1	H	185	PHE	2.7
1	G	285	ASN	2.7
1	A	239	SER	2.7
1	N	242	SER	2.7
1	B	246	LYS	2.7
1	J	248	PHE	2.7
1	F	207	GLU	2.7
1	G	245	SER	2.7
1	G	254	SER	2.7
1	O	246	LYS	2.7
1	P	130	ASN	2.7
1	O	195	GLN	2.7
1	N	152	GLY	2.7
1	I	47	THR	2.7
1	B	247	VAL	2.7
1	B	287	ASN	2.7
1	F	252	ASN	2.7
1	B	245	SER	2.6
1	H	132	LEU	2.6
1	I	83	ASN	2.6
1	K	219	GLU	2.6
1	J	130	ASN	2.6
1	N	236	ASN	2.6
1	B	256	GLY	2.6
1	G	218	GLY	2.6
1	G	156	THR	2.6
1	P	248	PHE	2.6
1	A	243	ASN	2.6
1	G	259	MET	2.6
1	D	241	PRO	2.6
1	N	245	SER	2.6
1	N	254	SER	2.6
1	D	285	ASN	2.6
1	N	244	ILE	2.5
1	G	241	PRO	2.5
1	I	261	SER	2.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	E	286	ASN	2.5
1	H	150	ASN	2.5
1	H	258	ASN	2.5
1	F	156	THR	2.5
1	D	239	SER	2.5
1	C	252	ASN	2.5
1	E	127	HIS	2.5
1	M	151	LEU	2.5
1	P	266	LEU	2.5
1	E	261	SER	2.5
1	A	188	ASN	2.5
1	B	237	ASP	2.5
1	N	188	ASN	2.5
1	O	194	ASN	2.5
1	N	248	PHE	2.5
1	E	239	SER	2.5
1	H	280	ASN	2.5
1	K	150	ASN	2.5
1	F	108	LEU	2.5
1	F	151	LEU	2.5
1	F	127	HIS	2.5
1	F	256	GLY	2.5
1	G	243	ASN	2.4
1	E	277	PHE	2.4
1	G	248	PHE	2.4
1	B	188	ASN	2.4
1	E	236	ASN	2.4
1	J	241	PRO	2.4
1	L	246	LYS	2.4
1	M	246	LYS	2.4
1	A	248	PHE	2.4
1	H	186	SER	2.4
1	H	243	ASN	2.4
1	B	37	ASP	2.4
1	F	102	PRO	2.4
1	F	259	MET	2.4
1	K	266	LEU	2.4
1	D	240	GLY	2.3
1	L	135	ASN	2.3
1	B	82	SER	2.3
1	G	130	ASN	2.3
1	B	289	LEU	2.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	F	284	PRO	2.3
1	K	245	SER	2.3
1	L	235	LEU	2.3
1	P	243	ASN	2.3
1	B	282	GLU	2.3
1	I	241	PRO	2.3
1	E	189	HIS	2.3
1	K	136	SER	2.3
1	M	236	ASN	2.3
1	J	207	GLU	2.3
1	B	177	GLY	2.3
1	B	104	ASN	2.3
1	C	286	ASN	2.3
1	F	246	LYS	2.3
1	J	119	ASN	2.3
1	N	130	ASN	2.3
1	G	255	GLU	2.2
1	B	167	ILE	2.2
1	L	265	ILE	2.2
1	D	235	LEU	2.2
1	H	246	LYS	2.2
1	E	188	ASN	2.2
1	E	243	ASN	2.2
1	F	285	ASN	2.2
1	D	151	LEU	2.2
1	E	129	LEU	2.2
1	M	222	ARG	2.2
1	E	287	ASN	2.2
1	H	83	ASN	2.2
1	E	207	GLU	2.2
1	I	220	ILE	2.2
1	K	269	ASP	2.2
1	H	241	PRO	2.2
1	L	152	GLY	2.2
1	F	248	PHE	2.2
1	L	116	THR	2.2
1	M	79	THR	2.2
1	B	215	TYR	2.2
1	B	254	SER	2.2
1	J	242	SER	2.2
1	M	243	ASN	2.2
1	L	240	GLY	2.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	L	196	ASP	2.2
1	O	267	ASP	2.2
1	H	127	HIS	2.2
1	H	268	LEU	2.2
1	D	260	ASP	2.2
1	H	260	ASP	2.2
1	K	248	PHE	2.2
1	B	224	TRP	2.2
1	A	244	ILE	2.1
1	A	289	LEU	2.1
1	E	151	LEU	2.1
1	F	288	LEU	2.1
1	A	259	MET	2.1
1	D	259	MET	2.1
1	J	259	MET	2.1
1	P	222	ARG	2.1
1	F	236	ASN	2.1
1	F	258	ASN	2.1
1	G	236	ASN	2.1
1	H	135	ASN	2.1
1	B	260	ASP	2.1
1	N	259	MET	2.1
1	A	286	ASN	2.1
1	P	189	HIS	2.1
1	A	151	LEU	2.1
1	G	220	ILE	2.1
1	M	245	SER	2.1
1	D	258	ASN	2.1
1	E	252	ASN	2.1
1	L	182	ASN	2.1
1	N	38	ASN	2.1
1	I	221	VAL	2.1
1	H	244	ILE	2.1
1	H	131	TYR	2.1
1	L	239	SER	2.1
1	F	260	ASP	2.1
1	B	234	THR	2.1
1	D	67	PHE	2.1
1	B	257	ASN	2.0
1	C	132	LEU	2.0
1	C	182	ASN	2.0
1	D	155	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	225	ILE	2.0
1	H	109	ASN	2.0
1	C	127	HIS	2.0
1	B	156	THR	2.0
1	H	227	PRO	2.0
1	K	264	PHE	2.0
1	B	219	GLU	2.0
1	E	219	GLU	2.0
1	G	246	LYS	2.0
1	N	289	LEU	2.0
1	A	283	ILE	2.0
1	E	186	SER	2.0
1	G	242	SER	2.0
1	F	83	ASN	2.0
1	G	287	ASN	2.0
1	L	231	ASN	2.0
1	O	182	ASN	2.0
1	K	189	HIS	2.0
1	G	247	VAL	2.0
1	O	238	VAL	2.0
1	J	289	LEU	2.0
1	L	151	LEU	2.0

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

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

## 6.3 Carbohydrates [\(i\)](#)

There are no 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.