Full wwPDB EM Validation Report (i)

Nov 20, 2022 – 02:56 pm GMT

PDB ID	:	5LDF
EMDB ID	:	EMD-4039
Title	:	Maltose binding protein genetically fused to dodecameric glutamine synthetase
Authors	:	Coscia, F.; Petosa, C.; Schoehn, G.
Deposited on	:	2016-06-25
Resolution	:	6.20 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

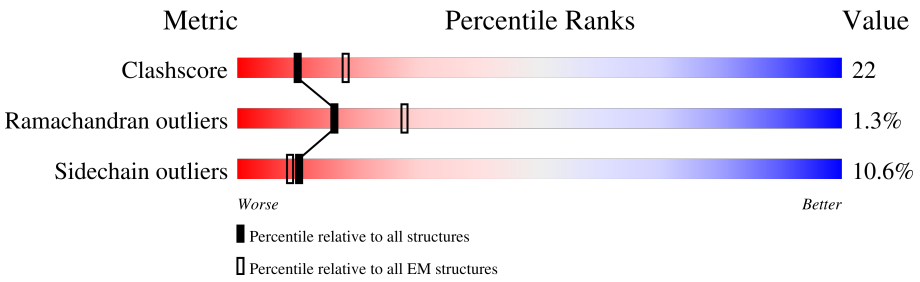
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 6.20 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)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	466	66% 27% 6% •
1	B	466	67% 26% 6% •
1	C	466	67% 26% 6% •
1	D	466	66% 27% 6% •
1	E	466	67% 26% 6% •
1	F	466	65% 27% 6% •
1	G	466	67% 25% 6% •
1	H	466	67% 26% 6% •

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Mol	Chain	Length	Quality of chain
1	I	466	67% 26% 6%
1	J	466	67% 26% 6%
1	K	466	67% 26% 6%
1	L	466	67% 26% 6%
2	M	370	5% 54% 30% 12%
2	N	370	5% 53% 31% 12%
2	O	370	54% 31% 12%
2	P	370	5% 52% 33% 11%
2	Q	370	5% 54% 31% 11%
2	R	370	54% 31% 11%
2	S	370	5% 54% 31% 11%
2	T	370	5% 54% 31% 11%
2	U	370	5% 53% 32% 11%
2	V	370	5% 53% 32% 11%
2	W	370	5% 54% 31% 12%
2	X	370	5% 54% 31% 12%
3	Y	2	100%
3	Z	2	100%
3	a	2	100%
3	b	2	100%
3	c	2	100%
3	d	2	100%
3	e	2	100%
3	f	2	100%
3	g	2	100%

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Mol	Chain	Length	Quality of chain
3	h	2	100%
3	i	2	100%
3	j	2	100%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 78120 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Glutamine synthetase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	466	3626	2295	622	689	20	0	0
1	B	466	3626	2295	622	689	20	0	0
1	C	466	3626	2295	622	689	20	0	0
1	D	466	3626	2295	622	689	20	0	0
1	E	466	3626	2295	622	689	20	0	0
1	F	466	3626	2295	622	689	20	0	0
1	G	466	3626	2295	622	689	20	0	0
1	H	466	3626	2295	622	689	20	0	0
1	I	466	3626	2295	622	689	20	0	0
1	J	466	3626	2295	622	689	20	0	0
1	K	466	3626	2295	622	689	20	0	0
1	L	466	3626	2295	622	689	20	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	391	PRO	ALA	conflict	UNP P0A1P7
B	391	PRO	ALA	conflict	UNP P0A1P7
C	391	PRO	ALA	conflict	UNP P0A1P7
D	391	PRO	ALA	conflict	UNP P0A1P7
E	391	PRO	ALA	conflict	UNP P0A1P7
F	391	PRO	ALA	conflict	UNP P0A1P7

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Chain	Residue	Modelled	Actual	Comment	Reference
G	391	PRO	ALA	conflict	UNP P0A1P7
H	391	PRO	ALA	conflict	UNP P0A1P7
I	391	PRO	ALA	conflict	UNP P0A1P7
J	391	PRO	ALA	conflict	UNP P0A1P7
K	391	PRO	ALA	conflict	UNP P0A1P7
L	391	PRO	ALA	conflict	UNP P0A1P7

- Molecule 2 is a protein called Maltose-binding periplasmic protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	M	370	2861	1843	468	544	6	0	0
2	N	370	2861	1843	468	544	6	0	0
2	O	370	2861	1843	468	544	6	0	0
2	P	370	2861	1843	468	544	6	0	0
2	Q	370	2861	1843	468	544	6	0	0
2	R	370	2861	1843	468	544	6	0	0
2	S	370	2861	1843	468	544	6	0	0
2	T	370	2861	1843	468	544	6	0	0
2	U	370	2861	1843	468	544	6	0	0
2	V	370	2861	1843	468	544	6	0	0
2	W	370	2861	1843	468	544	6	0	0
2	X	370	2861	1843	468	544	6	0	0

- Molecule 3 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.

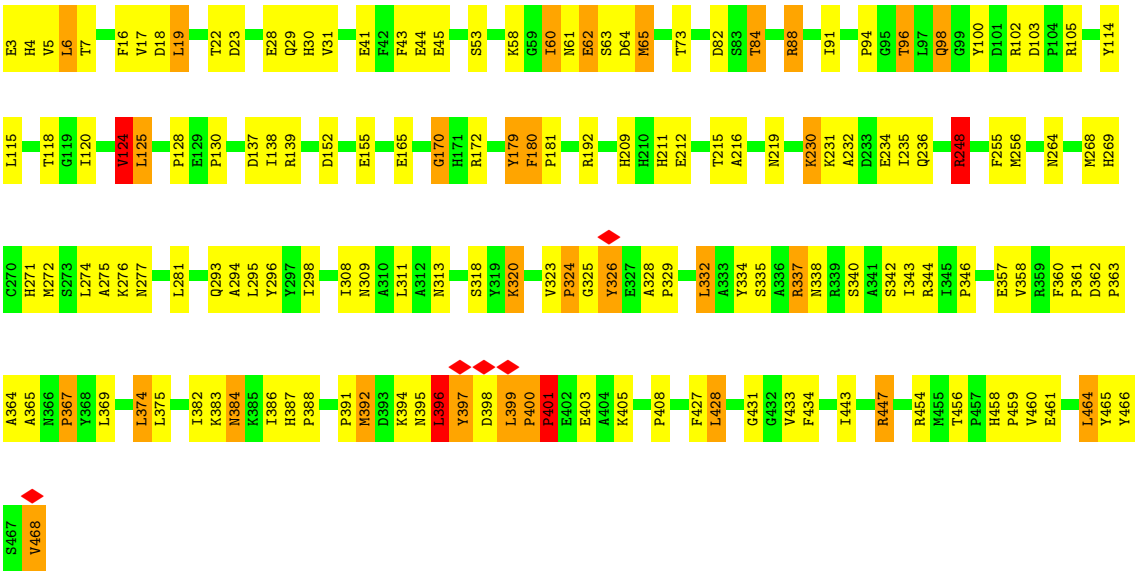
Mol	Chain	Residues	Atoms			AltConf	Trace
			Total	C	O		
3	Y	2	23	12	11	0	0
			Total	C	O		
3	Z	2	23	12	11	0	0
			Total	C	O		
3	a	2	23	12	11	0	0
			Total	C	O		
3	b	2	23	12	11	0	0
			Total	C	O		
3	c	2	23	12	11	0	0
			Total	C	O		
3	d	2	23	12	11	0	0
			Total	C	O		
3	e	2	23	12	11	0	0
			Total	C	O		
3	f	2	23	12	11	0	0
			Total	C	O		
3	g	2	23	12	11	0	0
			Total	C	O		
3	h	2	23	12	11	0	0
			Total	C	O		
3	i	2	23	12	11	0	0
			Total	C	O		
3	j	2	23	12	11	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

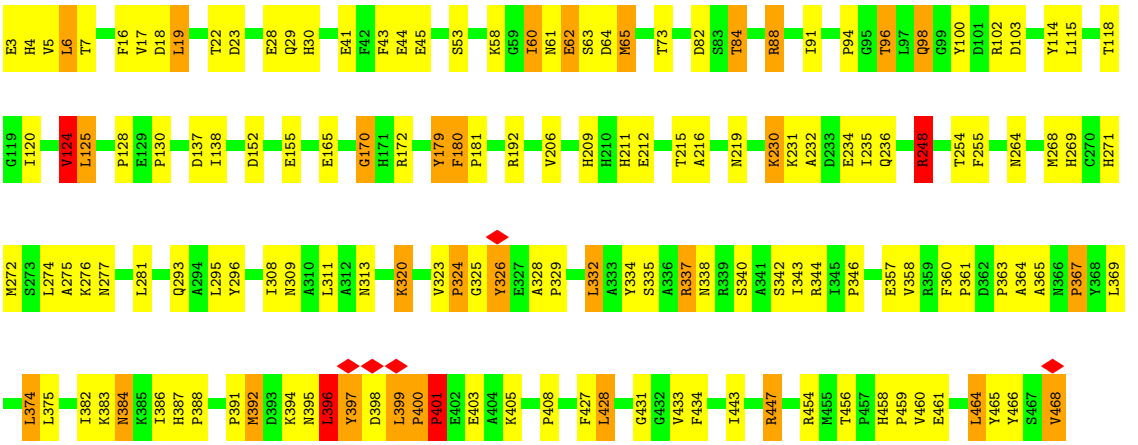
- Molecule 1: Glutamine synthetase

Chain A:



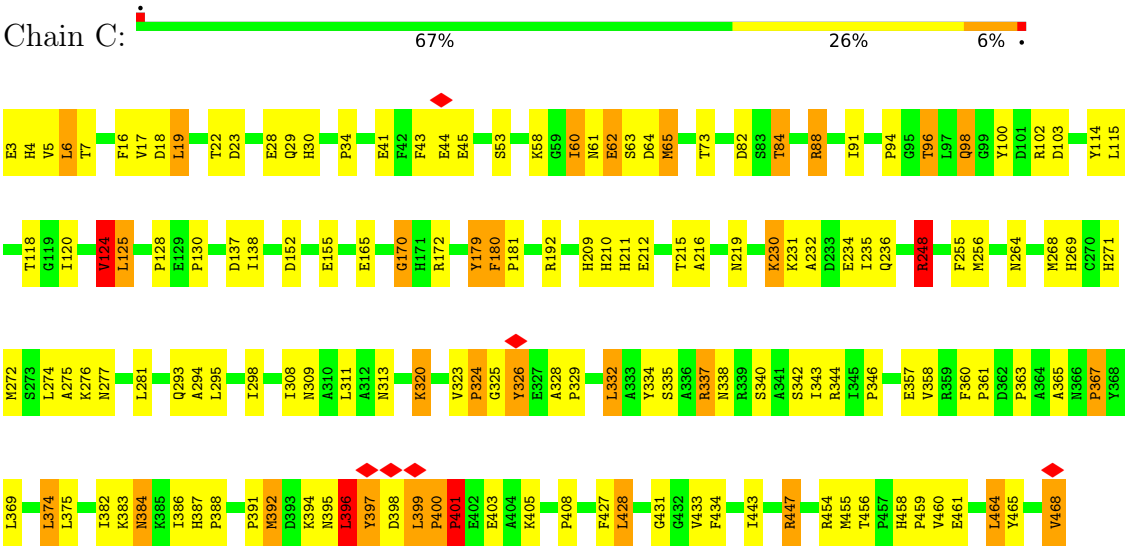
- Molecule 1: Glutamine synthetase

Chain B:



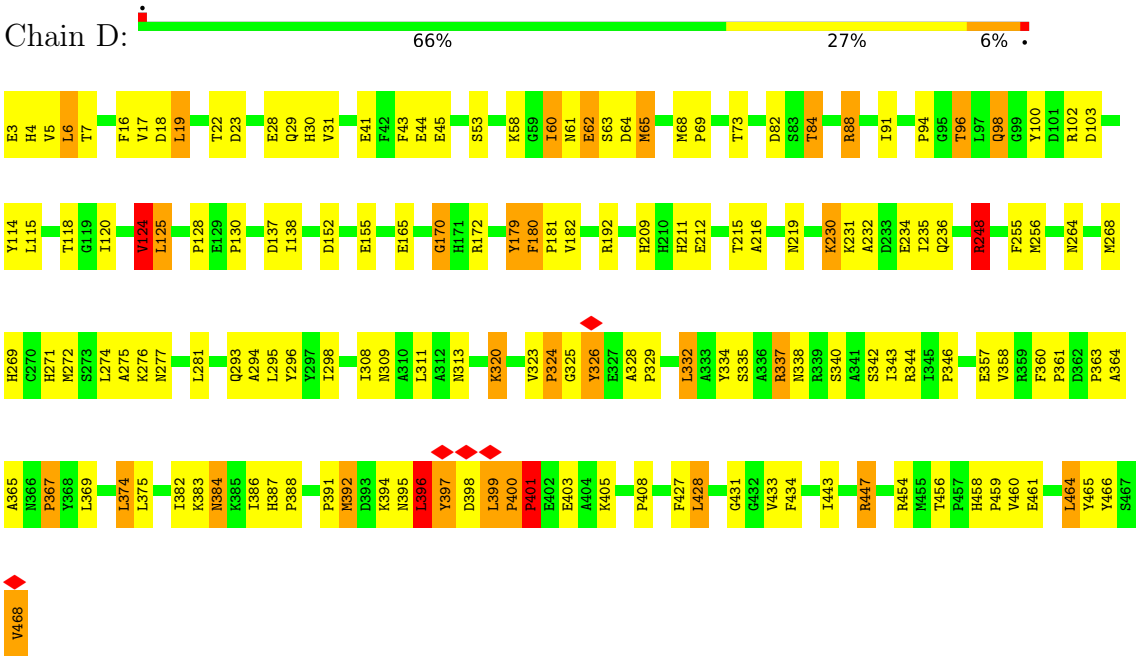
- Molecule 1: Glutamine synthetase

Chain C:



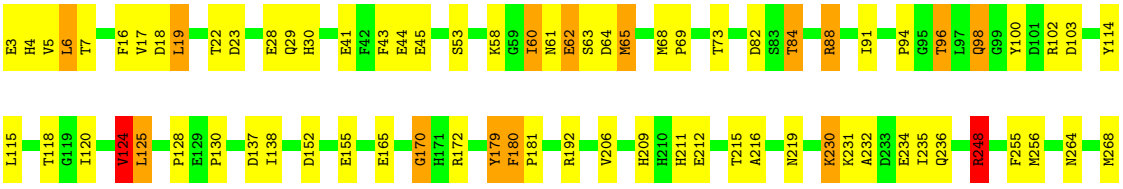
- Molecule 1: Glutamine synthetase

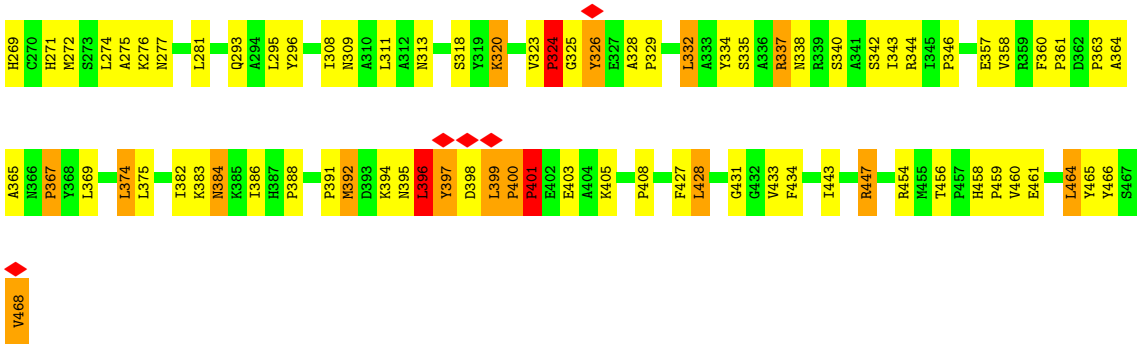
Chain D:



- Molecule 1: Glutamine synthetase

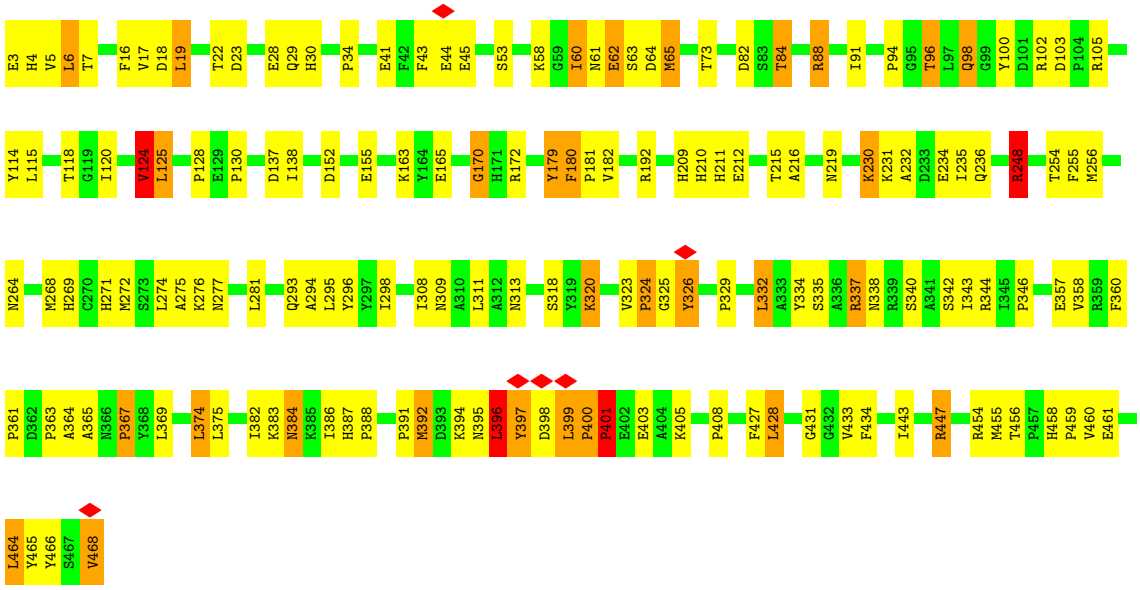
Chain E:





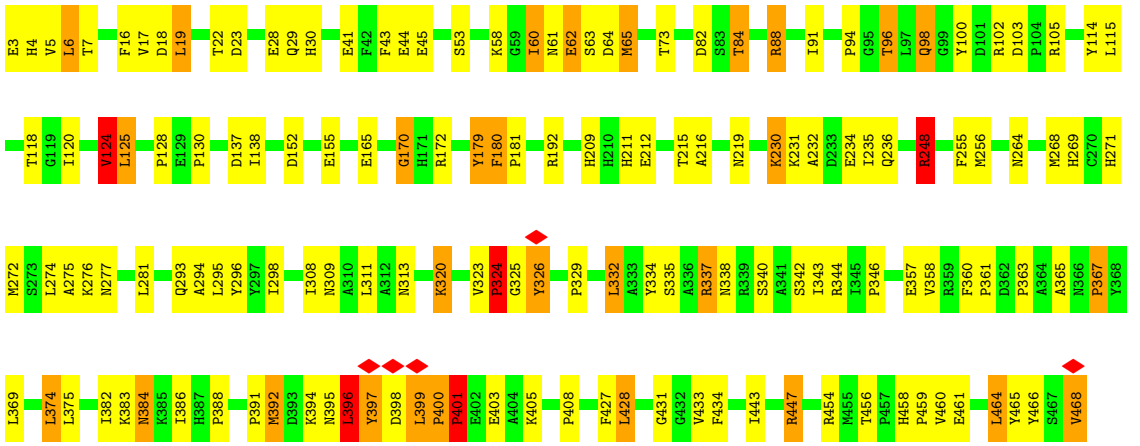
• Molecule 1: Glutamine synthetase

Chain F:



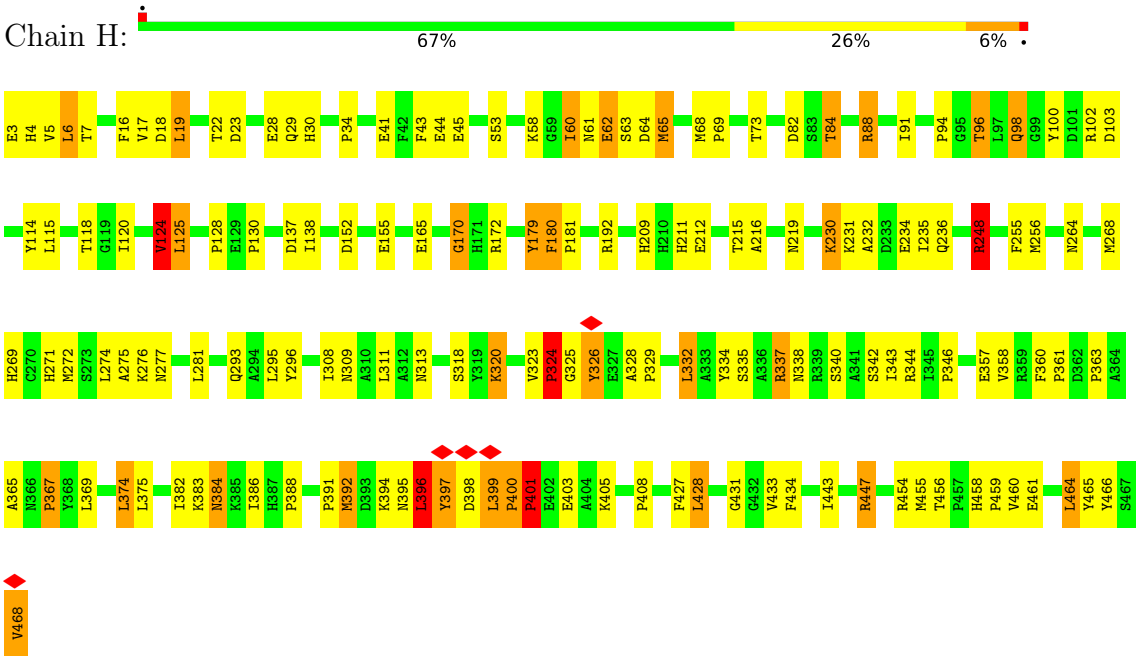
• Molecule 1: Glutamine synthetase

Chain G:



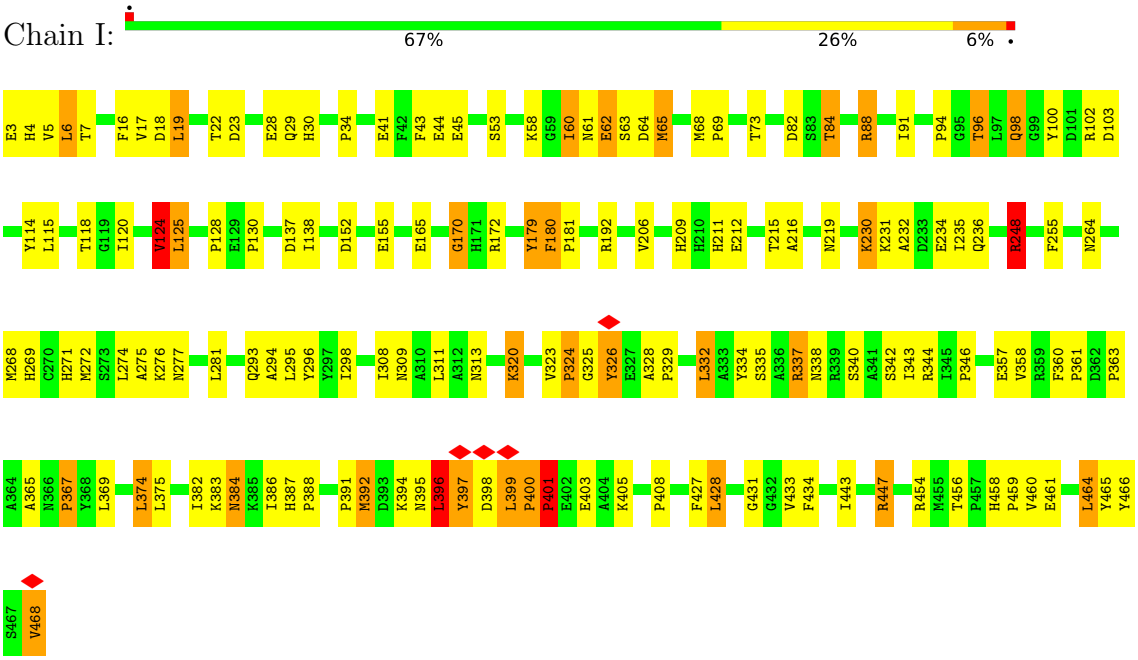
- Molecule 1: Glutamine synthetase

Chain H:



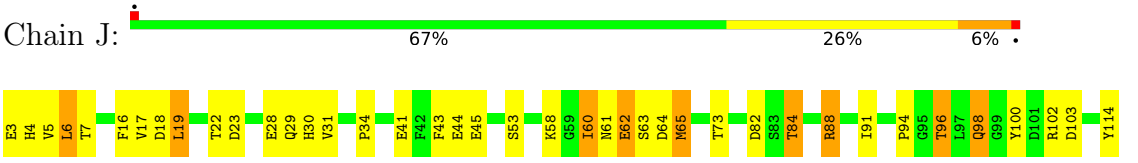
- Molecule 1: Glutamine synthetase

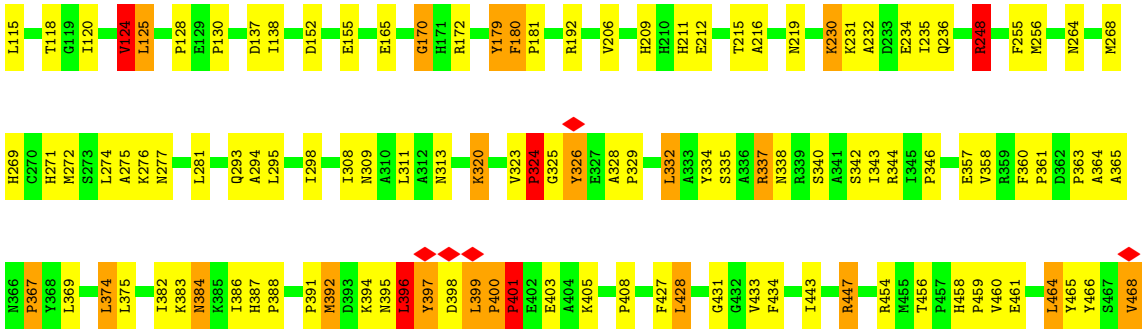
Chain I:



- Molecule 1: Glutamine synthetase

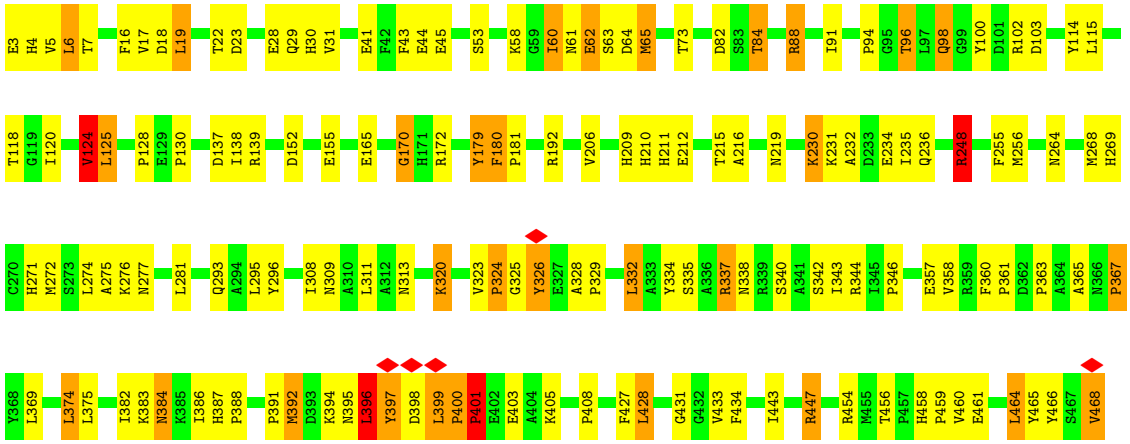
Chain J:





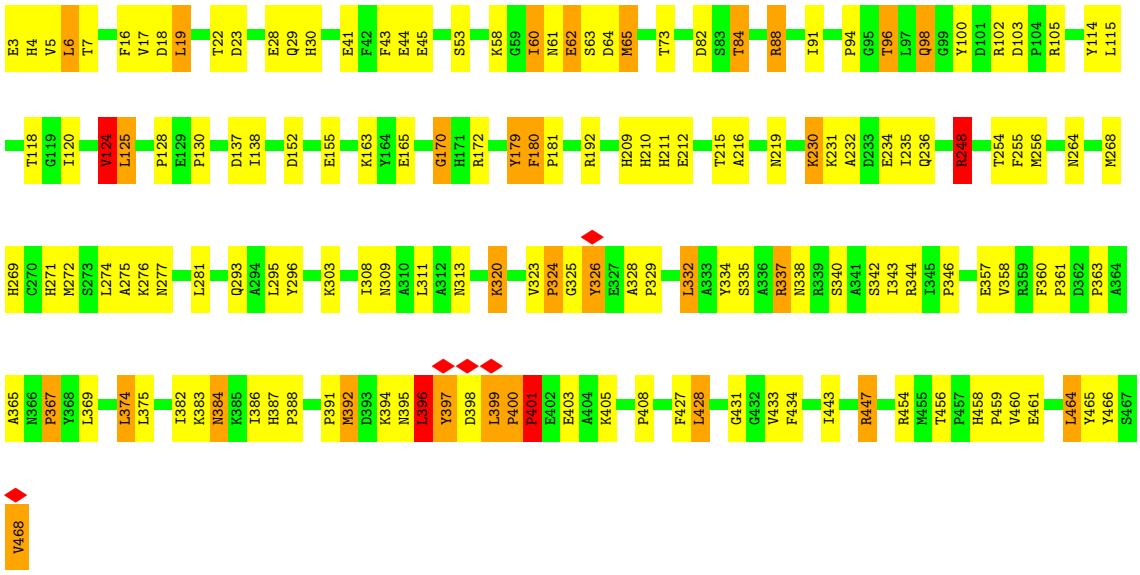
• Molecule 1: Glutamine synthetase

Chain K:



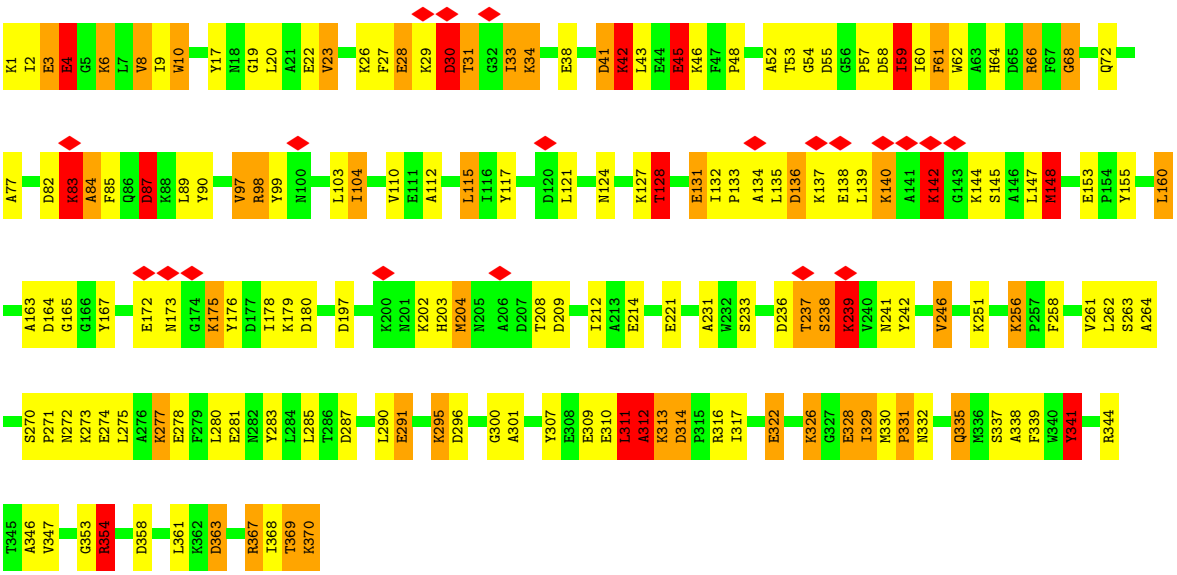
• Molecule 1: Glutamine synthetase

Chain L:



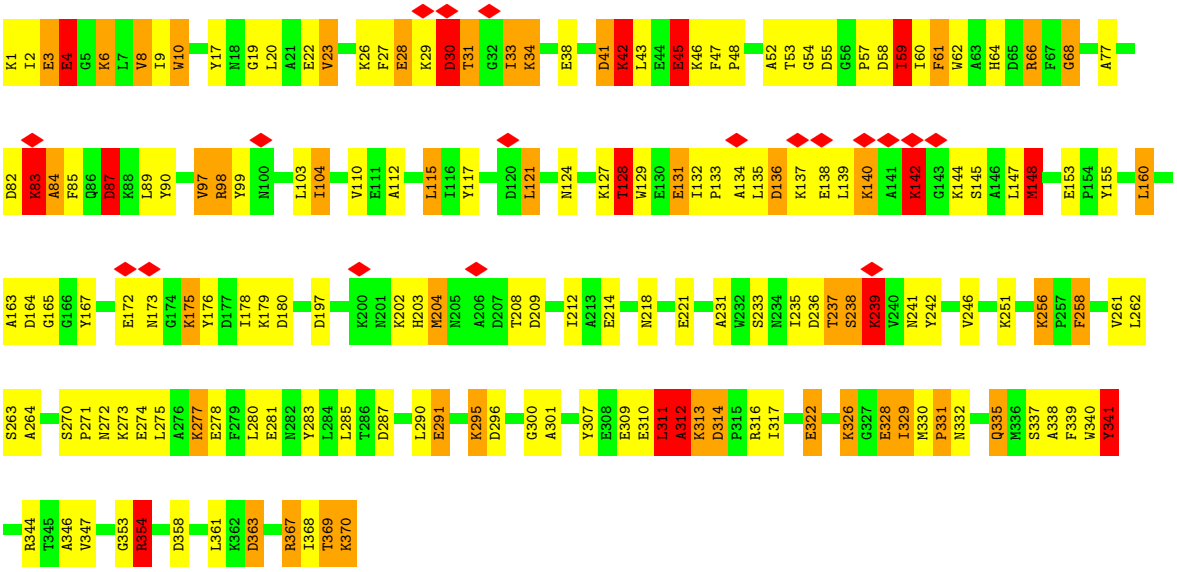
• Molecule 2: Maltose-binding periplasmic protein

Chain M:



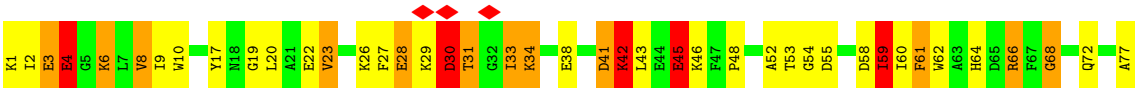
- Molecule 2: Maltose-binding periplasmic protein

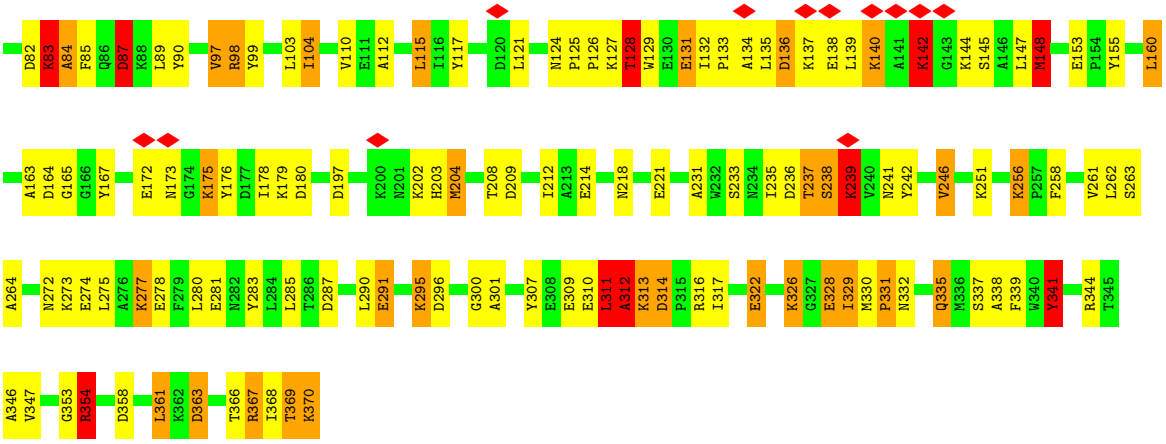
Chain N:



- Molecule 2: Maltose-binding periplasmic protein

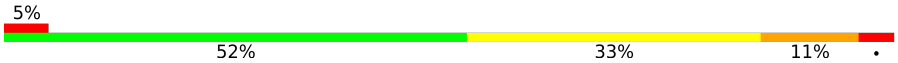
Chain O:

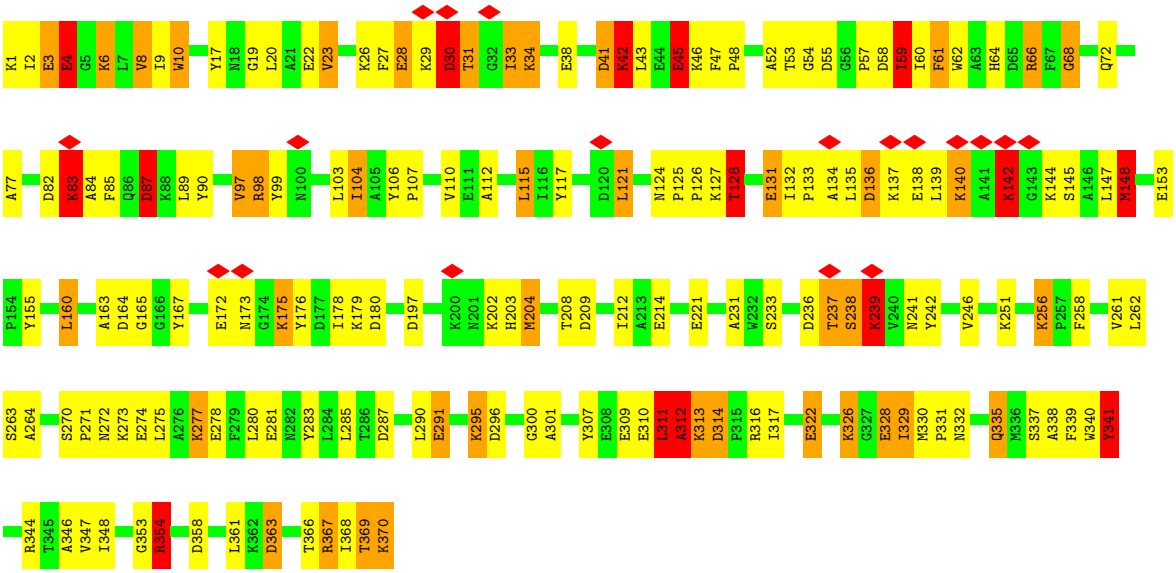




• Molecule 2: Maltose-binding periplasmic protein

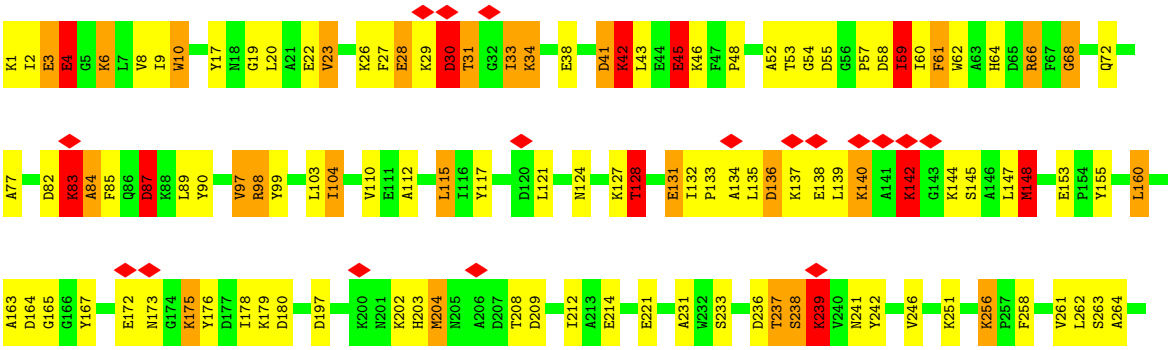
Chain P:

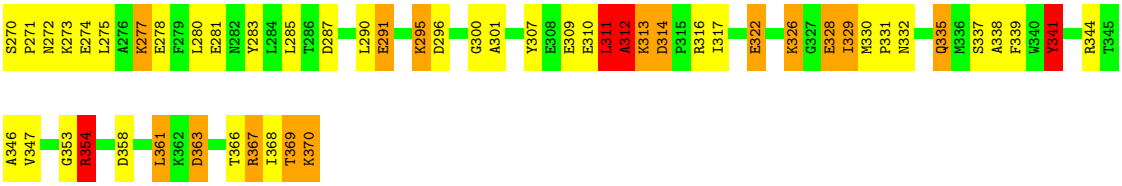




• Molecule 2: Maltose-binding periplasmic protein

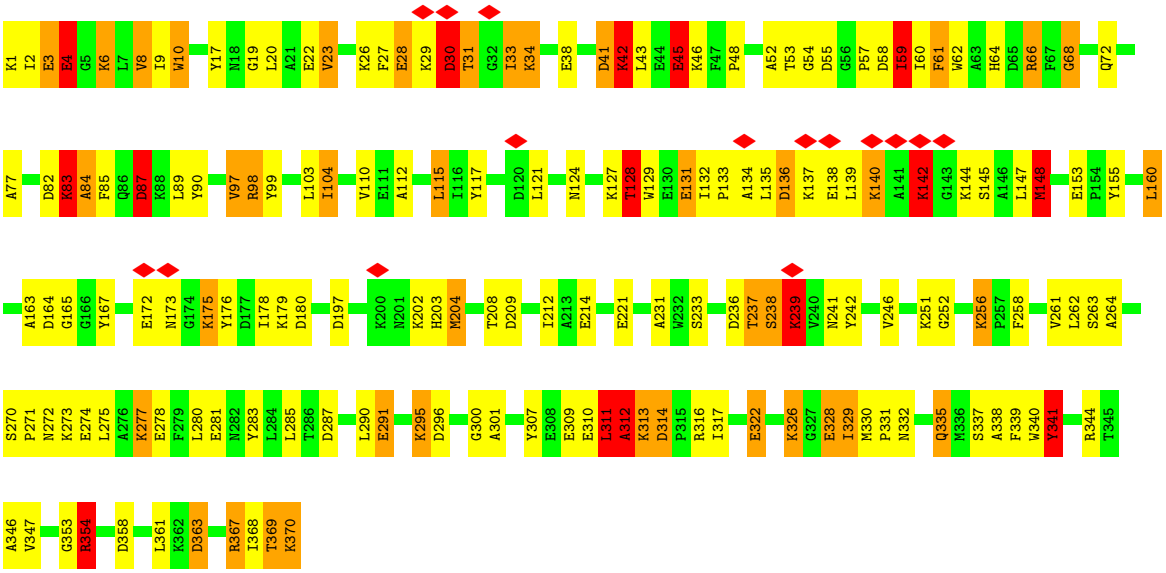
Chain Q:





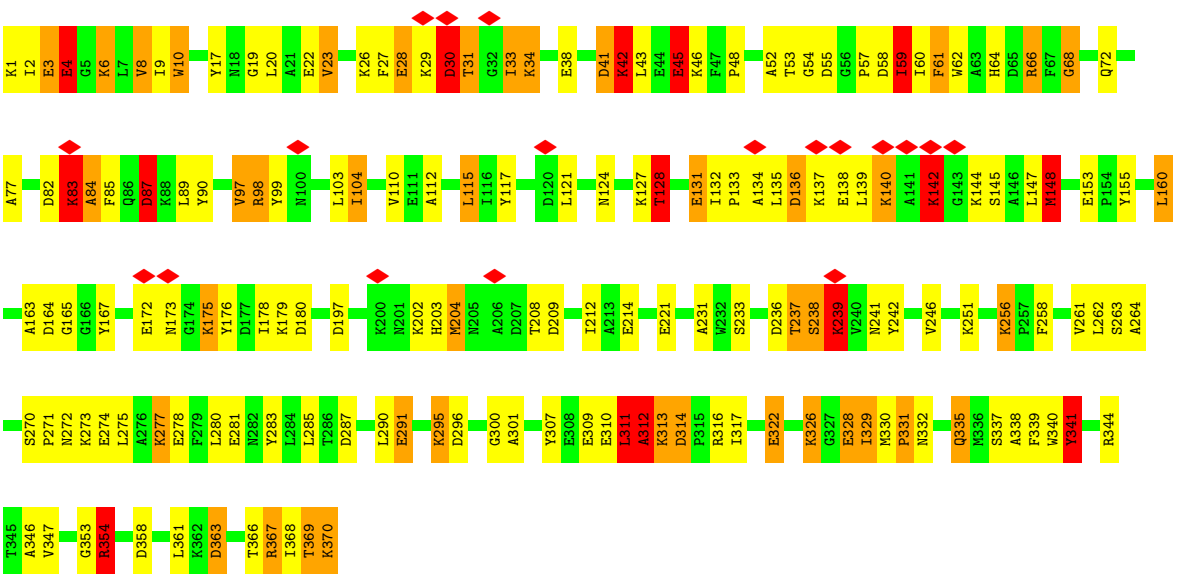
• Molecule 2: Maltose-binding periplasmic protein

Chain R:



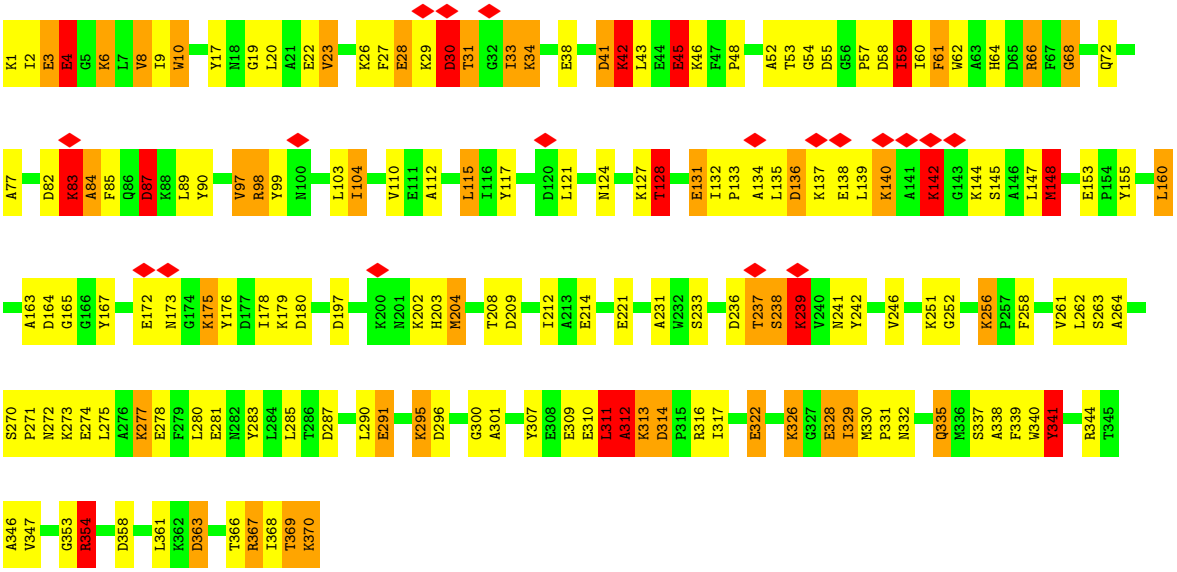
• Molecule 2: Maltose-binding periplasmic protein

Chain S:



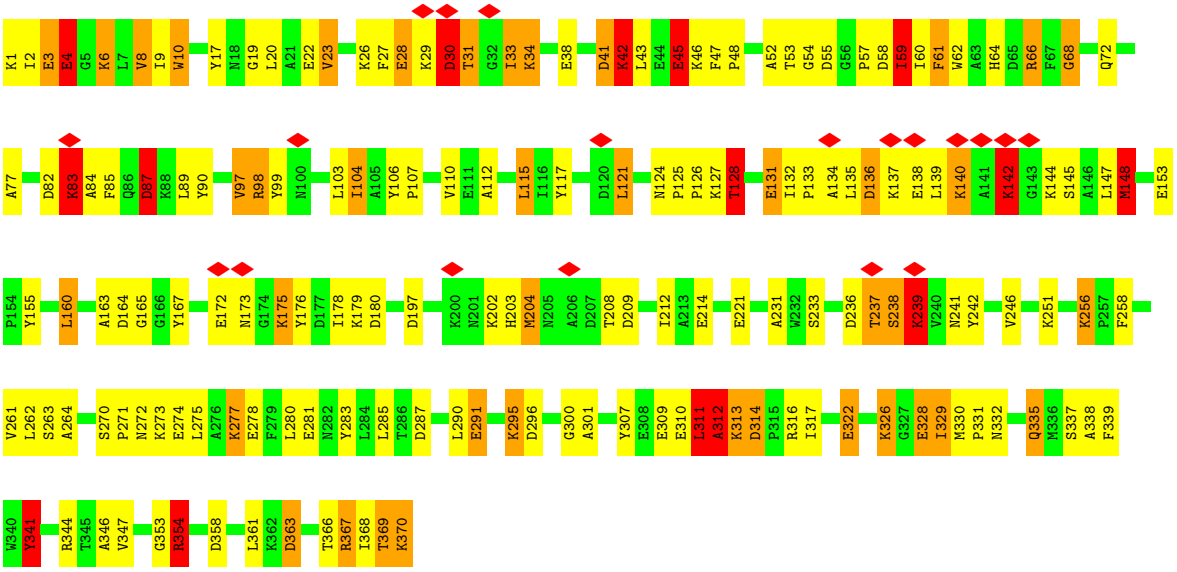
• Molecule 2: Maltose-binding periplasmic protein

Chain T:



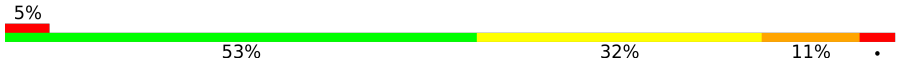
- Molecule 2: Maltose-binding periplasmic protein

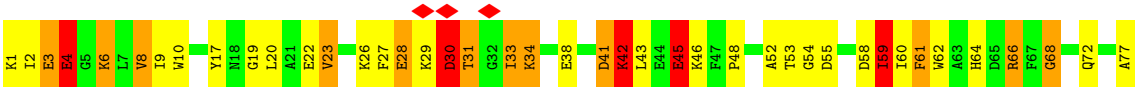
Chain U:

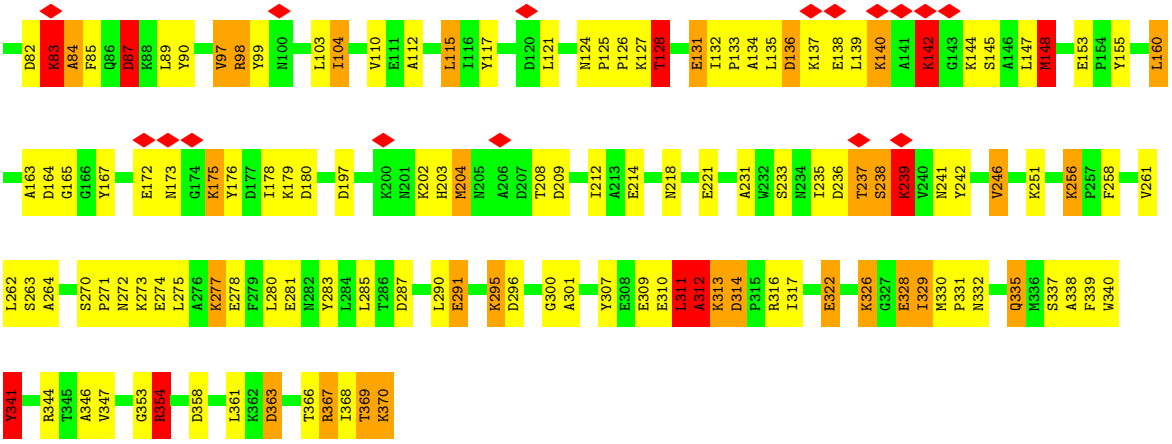


- Molecule 2: Maltose-binding periplasmic protein

Chain V:

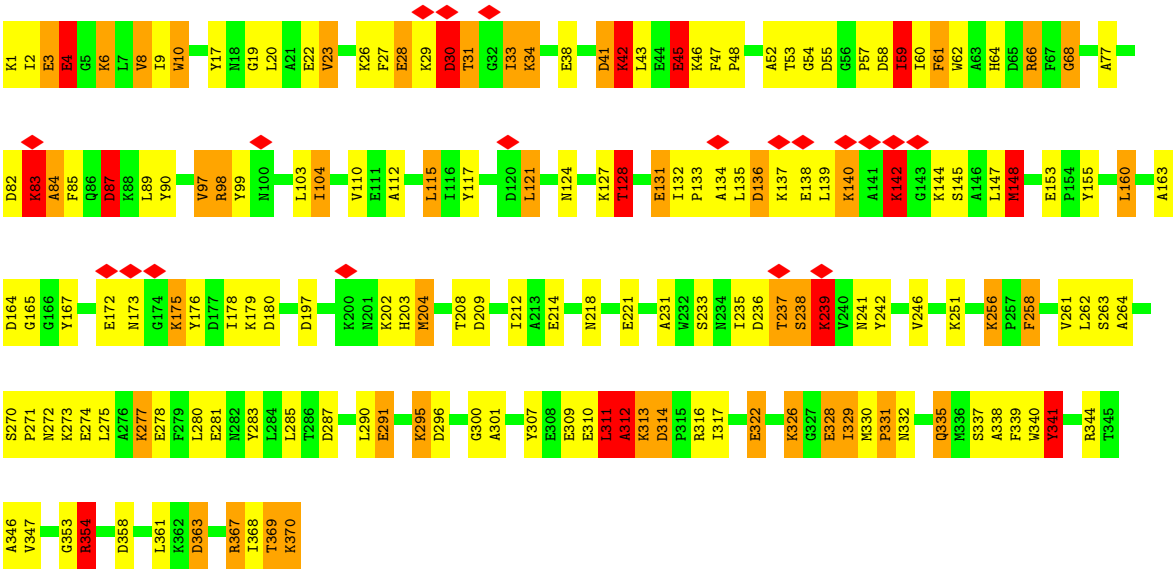






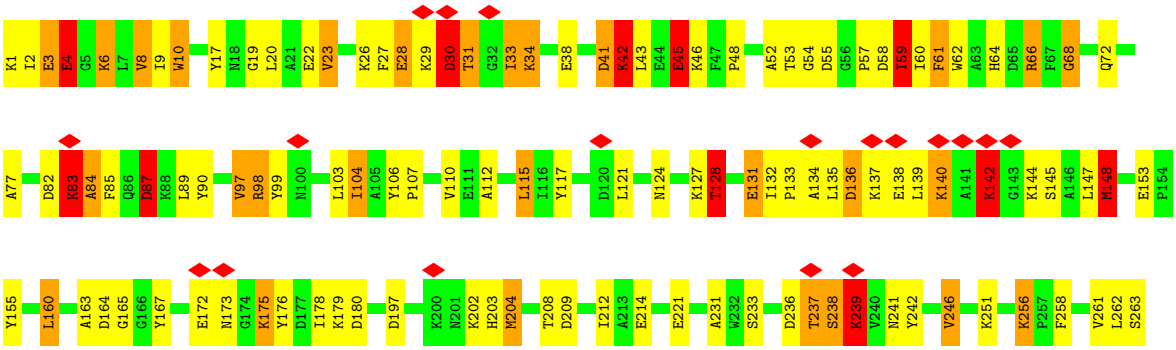
- Molecule 2: Maltose-binding periplasmic protein

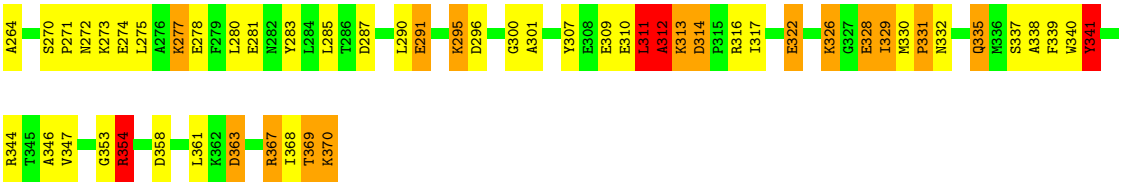
Chain W:



- Molecule 2: Maltose-binding periplasmic protein

Chain X:





- Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain Y: 100%

- Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain Z: 100%

- Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain a: 100%

- Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain b: 100%

- Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain c: 100%

- Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain d: 100%

- Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain e: 100%

GLC1
GLC2

• Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain f: 100%

GLC1
GLC2

• Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain g: 100%

GLC1
GLC2

• Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain h: 100%

GLC1
GLC2

• Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain i: 100%

GLC1
GLC2

• Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain j: 100%

GLC1
GLC2

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D6	Depositor
Number of particles used	13847	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	25	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.009	Depositor
Minimum map value	-0.003	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0015	Depositor
Map size (Å)	326.2, 326.2, 326.2	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8155, 0.8155, 0.8155	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.53	0/3713	0.85	4/5028 (0.1%)
1	B	0.53	0/3713	0.85	4/5028 (0.1%)
1	C	0.53	0/3713	0.85	4/5028 (0.1%)
1	D	0.53	0/3713	0.85	4/5028 (0.1%)
1	E	0.53	0/3713	0.85	4/5028 (0.1%)
1	F	0.53	0/3713	0.85	4/5028 (0.1%)
1	G	0.53	0/3713	0.85	4/5028 (0.1%)
1	H	0.53	0/3713	0.85	4/5028 (0.1%)
1	I	0.53	0/3713	0.85	4/5028 (0.1%)
1	J	0.53	0/3713	0.85	4/5028 (0.1%)
1	K	0.53	0/3713	0.85	4/5028 (0.1%)
1	L	0.53	0/3713	0.85	4/5028 (0.1%)
2	M	1.51	12/2930 (0.4%)	2.43	146/3979 (3.7%)
2	N	1.51	11/2930 (0.4%)	2.43	146/3979 (3.7%)
2	O	1.51	11/2930 (0.4%)	2.43	147/3979 (3.7%)
2	P	1.51	11/2930 (0.4%)	2.43	145/3979 (3.6%)
2	Q	1.51	11/2930 (0.4%)	2.43	144/3979 (3.6%)
2	R	1.51	13/2930 (0.4%)	2.43	148/3979 (3.7%)
2	S	1.51	11/2930 (0.4%)	2.43	146/3979 (3.7%)
2	T	1.51	12/2930 (0.4%)	2.43	147/3979 (3.7%)
2	U	1.51	11/2930 (0.4%)	2.43	145/3979 (3.6%)
2	V	1.51	11/2930 (0.4%)	2.43	146/3979 (3.7%)
2	W	1.51	11/2930 (0.4%)	2.43	146/3979 (3.7%)
2	X	1.51	12/2930 (0.4%)	2.43	145/3979 (3.6%)
All	All	1.08	137/79716 (0.2%)	1.74	1799/108084 (1.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	M	0	2
2	N	0	2
2	O	0	2
2	P	0	2
2	Q	0	2
2	R	0	2
2	S	0	2
2	T	0	2
2	U	0	2
2	V	0	2
2	W	0	2
2	X	0	2
All	All	0	24

All (137) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	369	THR	C-N	15.02	1.68	1.34
2	O	369	THR	C-N	14.75	1.68	1.34
2	T	369	THR	C-N	14.75	1.68	1.34
2	P	369	THR	C-N	14.75	1.68	1.34
2	Q	369	THR	C-N	14.74	1.68	1.34
2	U	369	THR	C-N	14.73	1.68	1.34
2	V	369	THR	C-N	14.72	1.68	1.34
2	R	369	THR	C-N	14.71	1.67	1.34
2	S	369	THR	C-N	14.71	1.67	1.34
2	W	369	THR	C-N	14.70	1.67	1.34
2	N	369	THR	C-N	14.69	1.67	1.34
2	X	369	THR	C-N	14.69	1.67	1.34
2	U	370	LYS	C-O	13.43	1.48	1.23
2	V	370	LYS	C-O	13.43	1.48	1.23
2	R	370	LYS	C-O	13.41	1.48	1.23
2	N	370	LYS	C-O	13.40	1.48	1.23
2	W	370	LYS	C-O	13.40	1.48	1.23
2	M	370	LYS	C-O	13.38	1.48	1.23
2	X	370	LYS	C-O	13.38	1.48	1.23
2	T	370	LYS	C-O	13.37	1.48	1.23
2	S	370	LYS	C-O	13.37	1.48	1.23
2	Q	370	LYS	C-O	13.36	1.48	1.23
2	P	370	LYS	C-O	13.35	1.48	1.23
2	O	370	LYS	C-O	13.35	1.48	1.23
2	R	238	SER	CB-OG	7.21	1.51	1.42
2	P	238	SER	CB-OG	7.19	1.51	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	238	SER	CB-OG	7.18	1.51	1.42
2	W	238	SER	CB-OG	7.18	1.51	1.42
2	M	238	SER	CB-OG	7.18	1.51	1.42
2	S	238	SER	CB-OG	7.15	1.51	1.42
2	O	238	SER	CB-OG	7.15	1.51	1.42
2	V	238	SER	CB-OG	7.14	1.51	1.42
2	X	238	SER	CB-OG	7.14	1.51	1.42
2	Q	238	SER	CB-OG	7.14	1.51	1.42
2	U	238	SER	CB-OG	7.13	1.51	1.42
2	T	238	SER	CB-OG	7.08	1.51	1.42
2	X	28	GLU	CD-OE2	-6.08	1.19	1.25
2	M	28	GLU	CD-OE2	-6.03	1.19	1.25
2	U	28	GLU	CD-OE2	-6.02	1.19	1.25
2	T	28	GLU	CD-OE2	-6.01	1.19	1.25
2	P	28	GLU	CD-OE2	-6.01	1.19	1.25
2	W	28	GLU	CD-OE2	-6.01	1.19	1.25
2	V	28	GLU	CD-OE2	-6.01	1.19	1.25
2	N	28	GLU	CD-OE2	-5.98	1.19	1.25
2	Q	28	GLU	CD-OE2	-5.98	1.19	1.25
2	R	28	GLU	CD-OE2	-5.96	1.19	1.25
2	O	28	GLU	CD-OE2	-5.94	1.19	1.25
2	S	28	GLU	CD-OE2	-5.93	1.19	1.25
2	W	214	GLU	CD-OE1	-5.74	1.19	1.25
2	O	214	GLU	CD-OE1	-5.71	1.19	1.25
2	M	214	GLU	CD-OE1	-5.70	1.19	1.25
2	Q	214	GLU	CD-OE1	-5.69	1.19	1.25
2	V	214	GLU	CD-OE1	-5.69	1.19	1.25
2	P	214	GLU	CD-OE1	-5.68	1.19	1.25
2	S	214	GLU	CD-OE1	-5.67	1.19	1.25
2	T	214	GLU	CD-OE1	-5.67	1.19	1.25
2	X	214	GLU	CD-OE1	-5.67	1.19	1.25
2	U	214	GLU	CD-OE1	-5.67	1.19	1.25
2	N	214	GLU	CD-OE1	-5.66	1.19	1.25
2	R	214	GLU	CD-OE1	-5.64	1.19	1.25
2	U	117	TYR	CG-CD2	5.56	1.46	1.39
2	N	117	TYR	CG-CD2	5.56	1.46	1.39
2	M	117	TYR	CG-CD2	5.55	1.46	1.39
2	P	117	TYR	CG-CD2	5.53	1.46	1.39
2	O	117	TYR	CG-CD2	5.52	1.46	1.39
2	T	117	TYR	CG-CD2	5.52	1.46	1.39
2	V	117	TYR	CG-CD2	5.52	1.46	1.39
2	T	138	GLU	C-O	5.51	1.33	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	X	138	GLU	C-O	5.51	1.33	1.23
2	P	138	GLU	C-O	5.51	1.33	1.23
2	R	117	TYR	CG-CD2	5.50	1.46	1.39
2	X	117	TYR	CG-CD2	5.50	1.46	1.39
2	Q	138	GLU	C-O	5.50	1.33	1.23
2	S	117	TYR	CG-CD2	5.50	1.46	1.39
2	V	138	GLU	C-O	5.50	1.33	1.23
2	N	138	GLU	C-O	5.49	1.33	1.23
2	S	138	GLU	C-O	5.49	1.33	1.23
2	U	138	GLU	C-O	5.49	1.33	1.23
2	O	138	GLU	C-O	5.48	1.33	1.23
2	W	117	TYR	CG-CD2	5.48	1.46	1.39
2	R	138	GLU	C-O	5.46	1.33	1.23
2	Q	117	TYR	CG-CD2	5.46	1.46	1.39
2	M	138	GLU	C-O	5.46	1.33	1.23
2	U	22	GLU	CD-OE2	5.45	1.31	1.25
2	W	138	GLU	C-O	5.45	1.33	1.23
2	T	22	GLU	CD-OE2	5.43	1.31	1.25
2	N	22	GLU	CD-OE2	5.42	1.31	1.25
2	P	22	GLU	CD-OE2	5.42	1.31	1.25
2	X	22	GLU	CD-OE2	5.40	1.31	1.25
2	V	22	GLU	CD-OE2	5.39	1.31	1.25
2	Q	22	GLU	CD-OE2	5.38	1.31	1.25
2	M	22	GLU	CD-OE2	5.37	1.31	1.25
2	R	22	GLU	CD-OE2	5.37	1.31	1.25
2	O	22	GLU	CD-OE2	5.37	1.31	1.25
2	W	22	GLU	CD-OE2	5.35	1.31	1.25
2	S	22	GLU	CD-OE2	5.35	1.31	1.25
2	R	300	GLY	CA-C	5.20	1.60	1.51
2	N	300	GLY	CA-C	5.20	1.60	1.51
2	M	300	GLY	CA-C	5.20	1.60	1.51
2	T	300	GLY	CA-C	5.19	1.60	1.51
2	V	300	GLY	CA-C	5.19	1.60	1.51
2	P	300	GLY	CA-C	5.19	1.60	1.51
2	O	300	GLY	CA-C	5.18	1.60	1.51
2	Q	300	GLY	CA-C	5.18	1.60	1.51
2	U	300	GLY	CA-C	5.16	1.60	1.51
2	W	300	GLY	CA-C	5.16	1.60	1.51
2	X	300	GLY	CA-C	5.15	1.60	1.51
2	S	300	GLY	CA-C	5.15	1.60	1.51
2	M	155	TYR	CE2-CZ	5.12	1.45	1.38
2	Q	155	TYR	CE2-CZ	5.12	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	U	66	ARG	CZ-NH1	5.11	1.39	1.33
2	Q	66	ARG	CZ-NH1	5.10	1.39	1.33
2	S	155	TYR	CE2-CZ	5.09	1.45	1.38
2	T	155	TYR	CE2-CZ	5.09	1.45	1.38
2	O	66	ARG	CZ-NH1	5.07	1.39	1.33
2	N	155	TYR	CE2-CZ	5.07	1.45	1.38
2	S	66	ARG	CZ-NH1	5.07	1.39	1.33
2	R	66	ARG	CZ-NH1	5.06	1.39	1.33
2	X	155	TYR	CE2-CZ	5.06	1.45	1.38
2	W	66	ARG	CZ-NH1	5.06	1.39	1.33
2	P	66	ARG	CZ-NH1	5.06	1.39	1.33
2	V	155	TYR	CE2-CZ	5.06	1.45	1.38
2	T	66	ARG	CZ-NH1	5.05	1.39	1.33
2	V	66	ARG	CZ-NH1	5.04	1.39	1.33
2	R	155	TYR	CE2-CZ	5.03	1.45	1.38
2	X	66	ARG	CZ-NH1	5.03	1.39	1.33
2	P	155	TYR	CE2-CZ	5.03	1.45	1.38
2	U	155	TYR	CE2-CZ	5.03	1.45	1.38
2	M	66	ARG	CZ-NH1	5.03	1.39	1.33
2	N	66	ARG	CZ-NH1	5.02	1.39	1.33
2	R	316	ARG	CZ-NH1	5.02	1.39	1.33
2	X	316	ARG	CZ-NH1	5.02	1.39	1.33
2	M	316	ARG	CZ-NH1	5.01	1.39	1.33
2	T	252	GLY	C-O	5.01	1.31	1.23
2	W	155	TYR	CE2-CZ	5.01	1.45	1.38
2	O	155	TYR	CE2-CZ	5.01	1.45	1.38
2	R	252	GLY	C-O	5.00	1.31	1.23

All (1799) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	P	354	ARG	NE-CZ-NH1	40.58	140.59	120.30
2	N	354	ARG	NE-CZ-NH1	40.56	140.58	120.30
2	S	354	ARG	NE-CZ-NH1	40.55	140.57	120.30
2	R	354	ARG	NE-CZ-NH1	40.53	140.56	120.30
2	T	354	ARG	NE-CZ-NH1	40.52	140.56	120.30
2	X	354	ARG	NE-CZ-NH1	40.52	140.56	120.30
2	M	354	ARG	NE-CZ-NH1	40.51	140.56	120.30
2	Q	354	ARG	NE-CZ-NH1	40.51	140.55	120.30
2	V	354	ARG	NE-CZ-NH1	40.50	140.55	120.30
2	W	354	ARG	NE-CZ-NH1	40.48	140.54	120.30
2	U	354	ARG	NE-CZ-NH1	40.45	140.52	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	O	354	ARG	NE-CZ-NH1	40.43	140.51	120.30
2	X	312	ALA	C-N-CA	19.80	171.19	121.70
2	W	312	ALA	C-N-CA	19.78	171.16	121.70
2	O	312	ALA	C-N-CA	19.78	171.15	121.70
2	M	312	ALA	C-N-CA	19.78	171.15	121.70
2	P	312	ALA	C-N-CA	19.77	171.13	121.70
2	Q	312	ALA	C-N-CA	19.77	171.13	121.70
2	R	312	ALA	C-N-CA	19.77	171.13	121.70
2	S	312	ALA	C-N-CA	19.77	171.12	121.70
2	V	312	ALA	C-N-CA	19.77	171.12	121.70
2	N	312	ALA	C-N-CA	19.77	171.12	121.70
2	U	312	ALA	C-N-CA	19.76	171.10	121.70
2	T	312	ALA	C-N-CA	19.76	171.09	121.70
2	U	341	TYR	CB-CG-CD2	-15.30	111.82	121.00
2	W	341	TYR	CB-CG-CD2	-15.30	111.82	121.00
2	M	341	TYR	CB-CG-CD2	-15.29	111.83	121.00
2	Q	341	TYR	CB-CG-CD2	-15.26	111.84	121.00
2	V	341	TYR	CB-CG-CD2	-15.26	111.84	121.00
2	R	341	TYR	CB-CG-CD2	-15.26	111.84	121.00
2	P	341	TYR	CB-CG-CD2	-15.26	111.85	121.00
2	T	341	TYR	CB-CG-CD2	-15.25	111.85	121.00
2	O	341	TYR	CB-CG-CD2	-15.25	111.85	121.00
2	N	341	TYR	CB-CG-CD2	-15.24	111.86	121.00
2	S	341	TYR	CB-CG-CD2	-15.22	111.87	121.00
2	X	341	TYR	CB-CG-CD2	-15.21	111.87	121.00
2	Q	341	TYR	CB-CG-CD1	15.14	130.09	121.00
2	P	341	TYR	CB-CG-CD1	15.14	130.08	121.00
2	S	341	TYR	CB-CG-CD1	15.13	130.08	121.00
2	W	341	TYR	CB-CG-CD1	15.12	130.07	121.00
2	T	341	TYR	CB-CG-CD1	15.11	130.07	121.00
2	O	341	TYR	CB-CG-CD1	15.11	130.06	121.00
2	N	341	TYR	CB-CG-CD1	15.10	130.06	121.00
2	V	341	TYR	CB-CG-CD1	15.10	130.06	121.00
2	M	341	TYR	CB-CG-CD1	15.08	130.05	121.00
2	U	341	TYR	CB-CG-CD1	15.07	130.04	121.00
2	R	341	TYR	CB-CG-CD1	15.05	130.03	121.00
2	X	341	TYR	CB-CG-CD1	15.03	130.02	121.00
2	N	45	GLU	OE1-CD-OE2	15.00	141.30	123.30
2	Q	45	GLU	OE1-CD-OE2	14.99	141.29	123.30
2	R	45	GLU	OE1-CD-OE2	14.98	141.28	123.30
2	W	45	GLU	OE1-CD-OE2	14.98	141.28	123.30
2	T	45	GLU	OE1-CD-OE2	14.97	141.26	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	U	45	GLU	OE1-CD-OE2	14.97	141.26	123.30
2	X	45	GLU	OE1-CD-OE2	14.97	141.26	123.30
2	P	45	GLU	OE1-CD-OE2	14.96	141.26	123.30
2	S	45	GLU	OE1-CD-OE2	14.96	141.26	123.30
2	V	45	GLU	OE1-CD-OE2	14.97	141.26	123.30
2	O	45	GLU	OE1-CD-OE2	14.94	141.23	123.30
2	M	45	GLU	OE1-CD-OE2	14.92	141.20	123.30
2	P	354	ARG	NE-CZ-NH2	-14.35	113.12	120.30
2	R	354	ARG	NE-CZ-NH2	-14.33	113.13	120.30
2	X	354	ARG	NE-CZ-NH2	-14.33	113.14	120.30
2	M	354	ARG	NE-CZ-NH2	-14.32	113.14	120.30
2	N	354	ARG	NE-CZ-NH2	-14.29	113.16	120.30
2	S	354	ARG	NE-CZ-NH2	-14.28	113.16	120.30
2	W	354	ARG	NE-CZ-NH2	-14.27	113.17	120.30
2	T	354	ARG	NE-CZ-NH2	-14.26	113.17	120.30
2	V	354	ARG	NE-CZ-NH2	-14.26	113.17	120.30
2	Q	354	ARG	NE-CZ-NH2	-14.25	113.18	120.30
2	U	354	ARG	NE-CZ-NH2	-14.25	113.18	120.30
2	O	354	ARG	NE-CZ-NH2	-14.24	113.18	120.30
2	S	316	ARG	NE-CZ-NH1	13.98	127.29	120.30
2	P	316	ARG	NE-CZ-NH1	13.94	127.27	120.30
2	Q	316	ARG	NE-CZ-NH1	13.94	127.27	120.30
2	T	316	ARG	NE-CZ-NH1	13.92	127.26	120.30
2	W	316	ARG	NE-CZ-NH1	13.91	127.25	120.30
2	V	316	ARG	NE-CZ-NH1	13.88	127.24	120.30
2	N	316	ARG	NE-CZ-NH1	13.87	127.23	120.30
2	R	316	ARG	NE-CZ-NH1	13.84	127.22	120.30
2	U	316	ARG	NE-CZ-NH1	13.84	127.22	120.30
2	X	316	ARG	NE-CZ-NH1	13.82	127.21	120.30
2	M	316	ARG	NE-CZ-NH1	13.79	127.20	120.30
2	O	316	ARG	NE-CZ-NH1	13.76	127.18	120.30
2	R	291	GLU	OE1-CD-OE2	13.45	139.44	123.30
2	X	291	GLU	OE1-CD-OE2	13.44	139.43	123.30
2	P	291	GLU	OE1-CD-OE2	13.43	139.41	123.30
2	N	291	GLU	OE1-CD-OE2	13.41	139.40	123.30
2	W	291	GLU	OE1-CD-OE2	13.41	139.39	123.30
2	S	291	GLU	OE1-CD-OE2	13.41	139.39	123.30
2	T	291	GLU	OE1-CD-OE2	13.40	139.38	123.30
2	M	291	GLU	OE1-CD-OE2	13.40	139.38	123.30
2	V	291	GLU	OE1-CD-OE2	13.40	139.38	123.30
2	Q	291	GLU	OE1-CD-OE2	13.38	139.36	123.30
2	U	291	GLU	OE1-CD-OE2	13.38	139.36	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	O	291	GLU	OE1-CD-OE2	13.35	139.32	123.30
2	S	354	ARG	NH1-CZ-NH2	-12.68	105.45	119.40
2	Q	354	ARG	NH1-CZ-NH2	-12.67	105.47	119.40
2	N	354	ARG	NH1-CZ-NH2	-12.66	105.47	119.40
2	T	354	ARG	NH1-CZ-NH2	-12.66	105.48	119.40
2	V	354	ARG	NH1-CZ-NH2	-12.66	105.48	119.40
2	P	354	ARG	NH1-CZ-NH2	-12.65	105.48	119.40
2	W	354	ARG	NH1-CZ-NH2	-12.65	105.48	119.40
2	U	354	ARG	NH1-CZ-NH2	-12.65	105.49	119.40
2	X	354	ARG	NH1-CZ-NH2	-12.64	105.50	119.40
2	O	354	ARG	NH1-CZ-NH2	-12.63	105.50	119.40
2	M	354	ARG	NH1-CZ-NH2	-12.63	105.51	119.40
2	R	354	ARG	NH1-CZ-NH2	-12.63	105.51	119.40
2	N	137	LYS	CA-CB-CG	12.47	140.84	113.40
2	X	137	LYS	CA-CB-CG	12.47	140.84	113.40
2	P	137	LYS	CA-CB-CG	12.46	140.82	113.40
2	Q	137	LYS	CA-CB-CG	12.46	140.81	113.40
2	O	137	LYS	CA-CB-CG	12.45	140.79	113.40
2	R	137	LYS	CA-CB-CG	12.45	140.79	113.40
2	T	137	LYS	CA-CB-CG	12.45	140.79	113.40
2	U	137	LYS	CA-CB-CG	12.45	140.79	113.40
2	V	137	LYS	CA-CB-CG	12.45	140.79	113.40
2	W	137	LYS	CA-CB-CG	12.45	140.79	113.40
2	M	137	LYS	CA-CB-CG	12.45	140.78	113.40
2	S	137	LYS	CA-CB-CG	12.44	140.77	113.40
2	O	287	ASP	CB-CG-OD1	12.01	129.11	118.30
2	N	287	ASP	CB-CG-OD1	11.99	129.10	118.30
2	Q	287	ASP	CB-CG-OD1	11.95	129.06	118.30
2	W	287	ASP	CB-CG-OD1	11.94	129.05	118.30
2	R	287	ASP	CB-CG-OD1	11.94	129.05	118.30
2	U	287	ASP	CB-CG-OD1	11.94	129.05	118.30
2	V	287	ASP	CB-CG-OD1	11.94	129.05	118.30
2	S	287	ASP	CB-CG-OD1	11.94	129.04	118.30
2	P	287	ASP	CB-CG-OD1	11.92	129.03	118.30
2	M	287	ASP	CB-CG-OD1	11.91	129.02	118.30
2	T	287	ASP	CB-CG-OD1	11.91	129.02	118.30
2	X	287	ASP	CB-CG-OD1	11.91	129.02	118.30
2	Q	30	ASP	CB-CG-OD2	11.08	128.27	118.30
2	N	30	ASP	CB-CG-OD2	11.07	128.26	118.30
2	X	30	ASP	CB-CG-OD2	11.07	128.26	118.30
2	U	30	ASP	CB-CG-OD2	11.06	128.26	118.30
2	P	30	ASP	CB-CG-OD2	11.05	128.25	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	S	30	ASP	CB-CG-OD2	11.05	128.25	118.30
2	V	30	ASP	CB-CG-OD2	11.04	128.24	118.30
2	W	30	ASP	CB-CG-OD2	11.04	128.24	118.30
2	O	30	ASP	CB-CG-OD2	11.03	128.22	118.30
2	T	30	ASP	CB-CG-OD2	11.02	128.22	118.30
2	M	30	ASP	CB-CG-OD2	10.99	128.19	118.30
2	R	30	ASP	CB-CG-OD2	10.99	128.19	118.30
2	M	341	TYR	CA-CB-CG	10.75	133.82	113.40
2	R	341	TYR	CA-CB-CG	10.75	133.82	113.40
2	T	341	TYR	CA-CB-CG	10.74	133.81	113.40
2	O	341	TYR	CA-CB-CG	10.74	133.81	113.40
2	R	311	LEU	C-N-CA	-10.74	94.85	121.70
2	N	341	TYR	CA-CB-CG	10.74	133.80	113.40
2	O	311	LEU	C-N-CA	-10.73	94.86	121.70
2	Q	341	TYR	CA-CB-CG	10.73	133.79	113.40
2	U	341	TYR	CA-CB-CG	10.73	133.80	113.40
2	S	341	TYR	CA-CB-CG	10.73	133.79	113.40
2	W	311	LEU	C-N-CA	-10.73	94.88	121.70
2	X	341	TYR	CA-CB-CG	10.73	133.79	113.40
2	P	311	LEU	C-N-CA	-10.73	94.88	121.70
2	V	341	TYR	CA-CB-CG	10.73	133.79	113.40
2	M	311	LEU	C-N-CA	-10.73	94.89	121.70
2	W	341	TYR	CA-CB-CG	10.73	133.78	113.40
2	Q	311	LEU	C-N-CA	-10.72	94.89	121.70
2	S	311	LEU	C-N-CA	-10.72	94.89	121.70
2	V	311	LEU	C-N-CA	-10.72	94.89	121.70
2	N	311	LEU	C-N-CA	-10.72	94.90	121.70
2	U	311	LEU	C-N-CA	-10.72	94.90	121.70
2	P	341	TYR	CA-CB-CG	10.72	133.77	113.40
2	T	311	LEU	C-N-CA	-10.71	94.91	121.70
2	X	311	LEU	C-N-CA	-10.71	94.92	121.70
2	R	312	ALA	O-C-N	10.27	139.13	122.70
2	Q	312	ALA	O-C-N	10.27	139.13	122.70
2	N	312	ALA	O-C-N	10.26	139.12	122.70
2	T	312	ALA	O-C-N	10.25	139.10	122.70
2	V	312	ALA	O-C-N	10.25	139.10	122.70
2	X	312	ALA	O-C-N	10.25	139.10	122.70
2	O	312	ALA	O-C-N	10.25	139.09	122.70
2	W	312	ALA	O-C-N	10.25	139.09	122.70
2	P	312	ALA	O-C-N	10.24	139.09	122.70
2	S	312	ALA	O-C-N	10.24	139.08	122.70
2	U	312	ALA	O-C-N	10.24	139.08	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	M	312	ALA	O-C-N	10.23	139.07	122.70
2	R	4	GLU	C-N-CA	9.92	143.13	122.30
2	U	4	GLU	C-N-CA	9.91	143.12	122.30
2	S	4	GLU	C-N-CA	9.91	143.11	122.30
2	P	4	GLU	C-N-CA	9.90	143.10	122.30
2	Q	4	GLU	C-N-CA	9.90	143.09	122.30
2	V	4	GLU	C-N-CA	9.90	143.09	122.30
2	W	4	GLU	C-N-CA	9.89	143.08	122.30
2	X	4	GLU	C-N-CA	9.89	143.07	122.30
2	O	316	ARG	CD-NE-CZ	9.89	137.45	123.60
2	T	4	GLU	C-N-CA	9.89	143.06	122.30
2	O	4	GLU	C-N-CA	9.88	143.06	122.30
2	M	316	ARG	CD-NE-CZ	9.88	137.43	123.60
2	N	4	GLU	C-N-CA	9.88	143.05	122.30
2	R	316	ARG	CD-NE-CZ	9.87	137.42	123.60
2	X	316	ARG	CD-NE-CZ	9.87	137.42	123.60
2	M	4	GLU	C-N-CA	9.87	143.03	122.30
2	Q	30	ASP	CA-CB-CG	9.87	135.10	113.40
2	U	316	ARG	CD-NE-CZ	9.86	137.40	123.60
2	V	316	ARG	CD-NE-CZ	9.86	137.40	123.60
2	P	30	ASP	CA-CB-CG	9.85	135.08	113.40
2	W	316	ARG	CD-NE-CZ	9.85	137.39	123.60
2	N	316	ARG	CD-NE-CZ	9.85	137.39	123.60
2	S	316	ARG	CD-NE-CZ	9.85	137.39	123.60
2	U	30	ASP	CA-CB-CG	9.84	135.06	113.40
2	T	30	ASP	CA-CB-CG	9.84	135.05	113.40
2	O	30	ASP	CA-CB-CG	9.84	135.05	113.40
2	T	316	ARG	CD-NE-CZ	9.84	137.38	123.60
2	V	30	ASP	CA-CB-CG	9.84	135.05	113.40
2	N	30	ASP	CA-CB-CG	9.84	135.04	113.40
2	Q	316	ARG	CD-NE-CZ	9.84	137.37	123.60
2	R	30	ASP	CA-CB-CG	9.84	135.04	113.40
2	M	30	ASP	CA-CB-CG	9.83	135.03	113.40
2	W	30	ASP	CA-CB-CG	9.83	135.03	113.40
2	X	30	ASP	CA-CB-CG	9.83	135.03	113.40
2	S	30	ASP	CA-CB-CG	9.83	135.02	113.40
2	P	316	ARG	CD-NE-CZ	9.82	137.34	123.60
2	O	236	ASP	CB-CG-OD2	-9.75	109.52	118.30
2	U	236	ASP	CB-CG-OD2	-9.73	109.54	118.30
2	S	236	ASP	CB-CG-OD2	-9.73	109.54	118.30
2	P	236	ASP	CB-CG-OD2	-9.71	109.56	118.30
2	N	236	ASP	CB-CG-OD2	-9.70	109.57	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	T	84	ALA	N-CA-CB	9.70	123.68	110.10
2	U	84	ALA	N-CA-CB	9.70	123.68	110.10
2	V	236	ASP	CB-CG-OD2	-9.70	109.57	118.30
2	W	84	ALA	N-CA-CB	9.69	123.66	110.10
2	W	236	ASP	CB-CG-OD2	-9.69	109.58	118.30
2	M	84	ALA	N-CA-CB	9.69	123.66	110.10
2	O	84	ALA	N-CA-CB	9.69	123.66	110.10
2	U	367	ARG	NE-CZ-NH2	9.68	125.14	120.30
2	Q	367	ARG	NE-CZ-NH2	9.68	125.14	120.30
2	R	367	ARG	NE-CZ-NH2	9.68	125.14	120.30
2	P	84	ALA	N-CA-CB	9.68	123.65	110.10
2	N	367	ARG	NE-CZ-NH2	9.68	125.14	120.30
2	S	84	ALA	N-CA-CB	9.67	123.64	110.10
2	R	84	ALA	N-CA-CB	9.67	123.64	110.10
2	Q	84	ALA	N-CA-CB	9.67	123.63	110.10
2	V	84	ALA	N-CA-CB	9.67	123.63	110.10
2	Q	236	ASP	CB-CG-OD2	-9.66	109.60	118.30
2	X	84	ALA	N-CA-CB	9.66	123.63	110.10
2	T	236	ASP	CB-CG-OD2	-9.66	109.61	118.30
2	T	367	ARG	NE-CZ-NH2	9.66	125.13	120.30
2	M	236	ASP	CB-CG-OD2	-9.66	109.61	118.30
2	O	367	ARG	NE-CZ-NH2	9.66	125.13	120.30
2	R	236	ASP	CB-CG-OD2	-9.66	109.61	118.30
2	X	236	ASP	CB-CG-OD2	-9.65	109.61	118.30
2	N	84	ALA	N-CA-CB	9.65	123.61	110.10
2	V	367	ARG	NE-CZ-NH2	9.63	125.12	120.30
2	W	367	ARG	NE-CZ-NH2	9.63	125.11	120.30
2	P	367	ARG	NE-CZ-NH2	9.61	125.11	120.30
2	X	367	ARG	NE-CZ-NH2	9.61	125.11	120.30
2	M	367	ARG	NE-CZ-NH2	9.57	125.08	120.30
2	S	367	ARG	NE-CZ-NH2	9.54	125.07	120.30
2	N	117	TYR	CB-CG-CD1	9.51	126.70	121.00
2	T	117	TYR	CB-CG-CD1	9.48	126.69	121.00
2	U	117	TYR	CB-CG-CD1	9.48	126.69	121.00
2	M	117	TYR	CB-CG-CD1	9.45	126.67	121.00
2	V	117	TYR	CB-CG-CD1	9.44	126.66	121.00
2	P	117	TYR	CB-CG-CD1	9.44	126.66	121.00
2	O	117	TYR	CB-CG-CD1	9.42	126.65	121.00
2	Q	117	TYR	CB-CG-CD1	9.41	126.65	121.00
2	S	117	TYR	CB-CG-CD1	9.41	126.65	121.00
2	R	117	TYR	CB-CG-CD1	9.39	126.64	121.00
2	W	117	TYR	CB-CG-CD1	9.38	126.62	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	X	117	TYR	CB-CG-CD1	9.36	126.62	121.00
2	U	41	ASP	CB-CG-OD1	9.29	126.66	118.30
2	S	41	ASP	CB-CG-OD1	9.29	126.66	118.30
2	W	41	ASP	CB-CG-OD1	9.28	126.66	118.30
2	O	41	ASP	CB-CG-OD1	9.28	126.65	118.30
2	P	41	ASP	CB-CG-OD1	9.28	126.65	118.30
2	S	369	THR	O-C-N	9.26	137.51	122.70
2	V	41	ASP	CB-CG-OD1	9.25	126.63	118.30
2	T	41	ASP	CB-CG-OD1	9.25	126.62	118.30
2	X	41	ASP	CB-CG-OD1	9.24	126.62	118.30
2	N	369	THR	O-C-N	9.23	137.47	122.70
2	X	369	THR	O-C-N	9.23	137.47	122.70
2	Q	41	ASP	CB-CG-OD1	9.23	126.61	118.30
2	R	41	ASP	CB-CG-OD1	9.23	126.61	118.30
2	O	369	THR	O-C-N	9.22	137.45	122.70
2	V	369	THR	O-C-N	9.22	137.45	122.70
2	Q	369	THR	O-C-N	9.21	137.44	122.70
2	T	369	THR	O-C-N	9.21	137.44	122.70
2	M	41	ASP	CB-CG-OD1	9.21	126.59	118.30
2	R	369	THR	O-C-N	9.21	137.43	122.70
2	N	41	ASP	CB-CG-OD1	9.21	126.59	118.30
2	P	369	THR	O-C-N	9.20	137.42	122.70
2	U	369	THR	O-C-N	9.20	137.42	122.70
2	W	369	THR	O-C-N	9.20	137.42	122.70
2	M	369	THR	O-C-N	9.18	137.39	122.70
2	X	41	ASP	CB-CG-OD2	-9.18	110.04	118.30
2	W	41	ASP	CB-CG-OD2	-9.17	110.04	118.30
2	S	41	ASP	CB-CG-OD2	-9.17	110.05	118.30
2	P	41	ASP	CB-CG-OD2	-9.15	110.06	118.30
2	Q	41	ASP	CB-CG-OD2	-9.15	110.06	118.30
2	W	197	ASP	CB-CG-OD2	-9.15	110.07	118.30
2	N	41	ASP	CB-CG-OD2	-9.14	110.07	118.30
2	U	41	ASP	CB-CG-OD2	-9.14	110.08	118.30
2	R	197	ASP	CB-CG-OD2	-9.13	110.08	118.30
2	V	41	ASP	CB-CG-OD2	-9.14	110.08	118.30
2	S	197	ASP	CB-CG-OD2	-9.13	110.08	118.30
2	N	197	ASP	CB-CG-OD2	-9.12	110.09	118.30
2	T	41	ASP	CB-CG-OD2	-9.12	110.09	118.30
2	Q	59	ILE	CA-CB-CG2	9.12	129.14	110.90
2	M	41	ASP	CB-CG-OD2	-9.11	110.10	118.30
2	O	41	ASP	CB-CG-OD2	-9.11	110.10	118.30
2	R	59	ILE	CA-CB-CG2	9.11	129.12	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	N	59	ILE	CA-CB-CG2	9.11	129.12	110.90
2	R	41	ASP	CB-CG-OD2	-9.11	110.10	118.30
2	W	59	ILE	CA-CB-CG2	9.11	129.12	110.90
2	V	59	ILE	CA-CB-CG2	9.10	129.10	110.90
2	V	197	ASP	CB-CG-OD2	-9.10	110.11	118.30
2	M	59	ILE	CA-CB-CG2	9.10	129.10	110.90
2	P	59	ILE	CA-CB-CG2	9.10	129.10	110.90
2	Q	197	ASP	CB-CG-OD2	-9.10	110.11	118.30
2	S	59	ILE	CA-CB-CG2	9.10	129.09	110.90
2	O	59	ILE	CA-CB-CG2	9.09	129.09	110.90
2	X	59	ILE	CA-CB-CG2	9.09	129.09	110.90
2	T	59	ILE	CA-CB-CG2	9.09	129.08	110.90
2	O	197	ASP	CB-CG-OD2	-9.09	110.12	118.30
2	U	59	ILE	CA-CB-CG2	9.09	129.07	110.90
2	X	197	ASP	CB-CG-OD2	-9.08	110.12	118.30
2	M	197	ASP	CB-CG-OD2	-9.08	110.13	118.30
2	T	197	ASP	CB-CG-OD2	-9.08	110.13	118.30
2	U	197	ASP	CB-CG-OD2	-9.08	110.13	118.30
2	P	197	ASP	CB-CG-OD2	-9.07	110.13	118.30
2	U	103	LEU	CB-CG-CD1	-8.89	95.89	111.00
2	W	197	ASP	CB-CG-OD1	8.88	126.29	118.30
2	M	197	ASP	CB-CG-OD1	8.88	126.29	118.30
2	W	103	LEU	CB-CG-CD1	-8.88	95.91	111.00
2	N	103	LEU	CB-CG-CD1	-8.87	95.91	111.00
2	Q	197	ASP	CB-CG-OD1	8.87	126.29	118.30
2	S	103	LEU	CB-CG-CD1	-8.87	95.92	111.00
2	Q	103	LEU	CB-CG-CD1	-8.87	95.93	111.00
2	T	103	LEU	CB-CG-CD1	-8.87	95.93	111.00
2	P	103	LEU	CB-CG-CD1	-8.86	95.94	111.00
2	R	103	LEU	CB-CG-CD1	-8.86	95.94	111.00
2	V	103	LEU	CB-CG-CD1	-8.86	95.93	111.00
2	N	197	ASP	CB-CG-OD1	8.86	126.27	118.30
2	P	197	ASP	CB-CG-OD1	8.85	126.26	118.30
2	S	197	ASP	CB-CG-OD1	8.85	126.26	118.30
2	M	103	LEU	CB-CG-CD1	-8.84	95.97	111.00
2	X	103	LEU	CB-CG-CD1	-8.84	95.97	111.00
2	V	197	ASP	CB-CG-OD1	8.84	126.26	118.30
2	O	103	LEU	CB-CG-CD1	-8.84	95.98	111.00
2	R	197	ASP	CB-CG-OD1	8.81	126.23	118.30
2	U	197	ASP	CB-CG-OD1	8.80	126.22	118.30
2	T	197	ASP	CB-CG-OD1	8.80	126.22	118.30
2	O	197	ASP	CB-CG-OD1	8.79	126.21	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	X	197	ASP	CB-CG-OD1	8.79	126.21	118.30
2	X	17	TYR	CB-CG-CD2	8.45	126.07	121.00
2	N	17	TYR	CB-CG-CD2	8.44	126.06	121.00
2	S	17	TYR	CB-CG-CD2	8.44	126.06	121.00
2	V	17	TYR	CB-CG-CD2	8.43	126.06	121.00
2	W	17	TYR	CB-CG-CD2	8.41	126.05	121.00
2	P	17	TYR	CB-CG-CD2	8.41	126.05	121.00
2	M	322	GLU	OE1-CD-OE2	8.41	133.39	123.30
2	O	17	TYR	CB-CG-CD2	8.40	126.04	121.00
2	R	17	TYR	CB-CG-CD2	8.40	126.04	121.00
2	Q	17	TYR	CB-CG-CD2	8.39	126.04	121.00
2	U	17	TYR	CB-CG-CD2	8.39	126.03	121.00
2	T	17	TYR	CB-CG-CD2	8.39	126.03	121.00
2	M	17	TYR	CB-CG-CD2	8.39	126.03	121.00
2	W	322	GLU	OE1-CD-OE2	8.37	133.35	123.30
2	S	322	GLU	OE1-CD-OE2	8.37	133.34	123.30
2	X	322	GLU	OE1-CD-OE2	8.37	133.34	123.30
2	N	322	GLU	OE1-CD-OE2	8.36	133.34	123.30
2	T	322	GLU	OE1-CD-OE2	8.36	133.34	123.30
2	T	314	ASP	CB-CG-OD1	8.36	125.82	118.30
2	V	322	GLU	OE1-CD-OE2	8.36	133.33	123.30
2	Q	322	GLU	OE1-CD-OE2	8.35	133.32	123.30
2	P	322	GLU	OE1-CD-OE2	8.35	133.32	123.30
2	N	314	ASP	CB-CG-OD1	8.35	125.81	118.30
2	M	314	ASP	CB-CG-OD1	8.34	125.80	118.30
2	U	314	ASP	CB-CG-OD1	8.34	125.80	118.30
2	S	314	ASP	CB-CG-OD1	8.33	125.80	118.30
2	R	322	GLU	OE1-CD-OE2	8.33	133.29	123.30
2	W	314	ASP	CB-CG-OD1	8.32	125.79	118.30
2	O	322	GLU	OE1-CD-OE2	8.32	133.28	123.30
2	X	314	ASP	CB-CG-OD1	8.32	125.79	118.30
2	V	314	ASP	CB-CG-OD1	8.30	125.77	118.30
2	O	314	ASP	CB-CG-OD1	8.30	125.77	118.30
2	U	322	GLU	OE1-CD-OE2	8.30	133.26	123.30
2	P	314	ASP	CB-CG-OD1	8.29	125.76	118.30
2	R	314	ASP	CB-CG-OD1	8.29	125.76	118.30
2	Q	314	ASP	CB-CG-OD1	8.26	125.73	118.30
2	R	99	TYR	CB-CG-CD2	-8.20	116.08	121.00
2	M	99	TYR	CB-CG-CD2	-8.20	116.08	121.00
2	O	87	ASP	CB-CG-OD2	-8.19	110.93	118.30
2	P	87	ASP	CB-CG-OD2	-8.19	110.93	118.30
2	Q	99	TYR	CB-CG-CD2	-8.19	116.08	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	T	99	TYR	CB-CG-CD2	-8.19	116.08	121.00
2	N	17	TYR	CB-CG-CD1	-8.19	116.09	121.00
2	T	87	ASP	CB-CG-OD2	-8.19	110.93	118.30
2	X	99	TYR	CB-CG-CD2	-8.19	116.09	121.00
2	N	87	ASP	CB-CG-OD2	-8.19	110.93	118.30
2	R	87	ASP	CB-CG-OD2	-8.18	110.94	118.30
2	N	99	TYR	CB-CG-CD2	-8.18	116.09	121.00
2	V	87	ASP	CB-CG-OD2	-8.18	110.94	118.30
2	V	99	TYR	CB-CG-CD2	-8.18	116.09	121.00
2	U	99	TYR	CB-CG-CD2	-8.17	116.10	121.00
2	M	87	ASP	CB-CG-OD2	-8.17	110.95	118.30
2	P	99	TYR	CB-CG-CD2	-8.16	116.10	121.00
2	U	87	ASP	CB-CG-OD2	-8.16	110.95	118.30
2	O	99	TYR	CB-CG-CD2	-8.16	116.10	121.00
2	S	99	TYR	CB-CG-CD2	-8.16	116.11	121.00
2	O	17	TYR	CB-CG-CD1	-8.15	116.11	121.00
2	X	87	ASP	CB-CG-OD2	-8.15	110.96	118.30
2	R	17	TYR	CB-CG-CD1	-8.15	116.11	121.00
2	P	17	TYR	CB-CG-CD1	-8.15	116.11	121.00
2	W	87	ASP	CB-CG-OD2	-8.15	110.97	118.30
2	S	17	TYR	CB-CG-CD1	-8.14	116.11	121.00
2	X	17	TYR	CB-CG-CD1	-8.14	116.11	121.00
2	W	99	TYR	CB-CG-CD2	-8.13	116.12	121.00
2	V	17	TYR	CB-CG-CD1	-8.12	116.13	121.00
2	S	87	ASP	CB-CG-OD2	-8.12	111.00	118.30
2	Q	87	ASP	CB-CG-OD2	-8.10	111.01	118.30
2	O	239	LYS	CB-CG-CD	8.09	132.64	111.60
2	S	239	LYS	CB-CG-CD	8.09	132.64	111.60
2	M	17	TYR	CB-CG-CD1	-8.09	116.14	121.00
2	P	239	LYS	CB-CG-CD	8.09	132.64	111.60
2	R	239	LYS	CB-CG-CD	8.09	132.63	111.60
2	X	239	LYS	CB-CG-CD	8.09	132.63	111.60
2	N	239	LYS	CB-CG-CD	8.08	132.61	111.60
2	Q	239	LYS	CB-CG-CD	8.08	132.62	111.60
2	T	239	LYS	CB-CG-CD	8.08	132.61	111.60
2	V	239	LYS	CB-CG-CD	8.08	132.62	111.60
2	T	17	TYR	CB-CG-CD1	-8.08	116.15	121.00
2	M	239	LYS	CB-CG-CD	8.08	132.60	111.60
2	U	239	LYS	CB-CG-CD	8.08	132.60	111.60
2	W	17	TYR	CB-CG-CD1	-8.08	116.16	121.00
2	U	17	TYR	CB-CG-CD1	-8.07	116.16	121.00
2	W	239	LYS	CB-CG-CD	8.07	132.57	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	Q	17	TYR	CB-CG-CD1	-8.06	116.16	121.00
2	T	61	PHE	CB-CG-CD2	-8.05	115.17	120.80
2	O	58	ASP	CB-CG-OD2	-8.04	111.07	118.30
2	P	61	PHE	CB-CG-CD2	-8.04	115.17	120.80
2	M	61	PHE	CB-CG-CD2	-8.03	115.18	120.80
2	M	58	ASP	CB-CG-OD2	-8.02	111.08	118.30
2	R	58	ASP	CB-CG-OD2	-8.02	111.08	118.30
2	N	58	ASP	CB-CG-OD2	-8.02	111.08	118.30
2	S	61	PHE	CB-CG-CD2	-8.02	115.19	120.80
2	V	61	PHE	CB-CG-CD2	-8.01	115.19	120.80
2	N	61	PHE	CB-CG-CD2	-8.01	115.19	120.80
2	O	61	PHE	CB-CG-CD2	-8.01	115.19	120.80
2	Q	58	ASP	CB-CG-OD2	-8.01	111.09	118.30
2	U	61	PHE	CB-CG-CD2	-8.01	115.19	120.80
2	N	98	ARG	NE-CZ-NH1	8.01	124.30	120.30
2	Q	61	PHE	CB-CG-CD2	-8.00	115.20	120.80
2	P	58	ASP	CB-CG-OD2	-8.00	111.10	118.30
2	X	58	ASP	CB-CG-OD2	-8.00	111.10	118.30
2	R	61	PHE	CB-CG-CD2	-7.99	115.21	120.80
2	V	58	ASP	CB-CG-OD2	-7.99	111.11	118.30
2	W	58	ASP	CB-CG-OD2	-7.99	111.11	118.30
2	Q	98	ARG	NE-CZ-NH1	7.99	124.29	120.30
2	T	98	ARG	NE-CZ-NH1	7.97	124.29	120.30
2	X	61	PHE	CB-CG-CD2	-7.96	115.23	120.80
2	W	61	PHE	CB-CG-CD2	-7.96	115.23	120.80
2	U	153	GLU	OE1-CD-OE2	-7.96	113.75	123.30
2	S	58	ASP	CB-CG-OD2	-7.95	111.14	118.30
2	W	98	ARG	NE-CZ-NH1	7.95	124.28	120.30
2	T	58	ASP	CB-CG-OD2	-7.95	111.14	118.30
2	U	58	ASP	CB-CG-OD2	-7.95	111.15	118.30
2	S	98	ARG	NE-CZ-NH1	7.94	124.27	120.30
2	R	98	ARG	NE-CZ-NH1	7.94	124.27	120.30
2	N	153	GLU	OE1-CD-OE2	-7.93	113.78	123.30
2	S	153	GLU	OE1-CD-OE2	-7.93	113.78	123.30
2	V	153	GLU	OE1-CD-OE2	-7.93	113.78	123.30
2	X	153	GLU	OE1-CD-OE2	-7.93	113.78	123.30
2	M	153	GLU	OE1-CD-OE2	-7.93	113.79	123.30
2	V	98	ARG	NE-CZ-NH1	7.92	124.26	120.30
2	T	153	GLU	OE1-CD-OE2	-7.92	113.80	123.30
2	P	153	GLU	OE1-CD-OE2	-7.92	113.80	123.30
2	P	98	ARG	NE-CZ-NH1	7.91	124.26	120.30
2	Q	153	GLU	OE1-CD-OE2	-7.91	113.81	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	O	153	GLU	OE1-CD-OE2	-7.91	113.81	123.30
2	R	153	GLU	OE1-CD-OE2	-7.89	113.83	123.30
2	W	153	GLU	OE1-CD-OE2	-7.89	113.83	123.30
2	X	98	ARG	NE-CZ-NH1	7.89	124.25	120.30
2	M	98	ARG	NE-CZ-NH1	7.88	124.24	120.30
2	O	98	ARG	NE-CZ-NH1	7.88	124.24	120.30
2	U	98	ARG	NE-CZ-NH1	7.88	124.24	120.30
2	O	278	GLU	CA-CB-CG	7.69	130.32	113.40
2	P	278	GLU	CA-CB-CG	7.68	130.30	113.40
2	W	278	GLU	CA-CB-CG	7.68	130.30	113.40
2	T	278	GLU	CA-CB-CG	7.67	130.28	113.40
2	M	278	GLU	CA-CB-CG	7.67	130.27	113.40
2	U	278	GLU	CA-CB-CG	7.67	130.27	113.40
2	V	278	GLU	CA-CB-CG	7.67	130.27	113.40
2	X	278	GLU	CA-CB-CG	7.67	130.26	113.40
2	N	278	GLU	CA-CB-CG	7.66	130.26	113.40
2	Q	278	GLU	CA-CB-CG	7.66	130.26	113.40
2	S	278	GLU	CA-CB-CG	7.66	130.25	113.40
2	R	278	GLU	CA-CB-CG	7.66	130.25	113.40
2	R	328	GLU	CA-CB-CG	7.65	130.24	113.40
2	W	328	GLU	CA-CB-CG	7.65	130.23	113.40
2	P	328	GLU	CA-CB-CG	7.65	130.23	113.40
2	Q	328	GLU	CA-CB-CG	7.65	130.22	113.40
2	U	328	GLU	CA-CB-CG	7.64	130.20	113.40
2	V	328	GLU	CA-CB-CG	7.63	130.19	113.40
2	N	328	GLU	CA-CB-CG	7.63	130.18	113.40
2	S	328	GLU	CA-CB-CG	7.63	130.18	113.40
2	T	328	GLU	CA-CB-CG	7.63	130.18	113.40
2	X	328	GLU	CA-CB-CG	7.62	130.17	113.40
2	M	328	GLU	CA-CB-CG	7.62	130.16	113.40
2	O	328	GLU	CA-CB-CG	7.61	130.15	113.40
2	M	164	ASP	CB-CG-OD2	-7.33	111.71	118.30
2	P	121	LEU	CB-CG-CD2	-7.32	98.56	111.00
2	W	121	LEU	CB-CG-CD2	-7.32	98.56	111.00
2	Q	121	LEU	CB-CG-CD2	-7.31	98.57	111.00
2	R	121	LEU	CB-CG-CD2	-7.31	98.57	111.00
2	X	164	ASP	CB-CG-OD2	-7.31	111.72	118.30
2	V	121	LEU	CB-CG-CD2	-7.31	98.57	111.00
2	X	121	LEU	CB-CG-CD2	-7.31	98.57	111.00
2	U	121	LEU	CB-CG-CD2	-7.31	98.58	111.00
2	N	121	LEU	CB-CG-CD2	-7.30	98.58	111.00
2	S	121	LEU	CB-CG-CD2	-7.30	98.58	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	W	164	ASP	CB-CG-OD2	-7.30	111.73	118.30
2	M	121	LEU	CB-CG-CD2	-7.30	98.59	111.00
2	S	164	ASP	CB-CG-OD2	-7.30	111.73	118.30
2	T	121	LEU	CB-CG-CD2	-7.30	98.59	111.00
2	T	164	ASP	CB-CG-OD2	-7.30	111.73	118.30
2	O	121	LEU	CB-CG-CD2	-7.30	98.60	111.00
2	N	164	ASP	CB-CG-OD2	-7.29	111.73	118.30
2	U	164	ASP	CB-CG-OD2	-7.29	111.74	118.30
2	Q	164	ASP	CB-CG-OD2	-7.29	111.74	118.30
2	O	164	ASP	CB-CG-OD2	-7.28	111.75	118.30
2	V	164	ASP	CB-CG-OD2	-7.28	111.75	118.30
2	R	164	ASP	CB-CG-OD2	-7.27	111.75	118.30
2	P	164	ASP	CB-CG-OD2	-7.24	111.78	118.30
2	S	358	ASP	CB-CG-OD2	7.18	124.76	118.30
2	N	358	ASP	CB-CG-OD2	7.16	124.74	118.30
2	M	176	TYR	CB-CG-CD2	-7.16	116.71	121.00
2	P	358	ASP	CB-CG-OD2	7.15	124.73	118.30
2	O	358	ASP	CB-CG-OD2	7.15	124.73	118.30
2	U	358	ASP	CB-CG-OD2	7.14	124.73	118.30
2	W	176	TYR	CB-CG-CD2	-7.13	116.72	121.00
2	X	99	TYR	CB-CG-CD1	7.13	125.28	121.00
2	M	358	ASP	CB-CG-OD2	7.13	124.71	118.30
2	N	239	LYS	CD-CE-NZ	7.12	128.06	111.70
2	V	358	ASP	CB-CG-OD2	7.12	124.70	118.30
2	Q	358	ASP	CB-CG-OD2	7.11	124.70	118.30
2	N	176	TYR	CB-CG-CD2	-7.11	116.73	121.00
2	Q	99	TYR	CB-CG-CD1	7.11	125.26	121.00
2	X	358	ASP	CB-CG-OD2	7.11	124.70	118.30
2	T	176	TYR	CB-CG-CD2	-7.10	116.74	121.00
2	V	176	TYR	CB-CG-CD2	-7.10	116.74	121.00
2	U	176	TYR	CB-CG-CD2	-7.10	116.74	121.00
2	O	99	TYR	CB-CG-CD1	7.09	125.26	121.00
2	T	358	ASP	CB-CG-OD2	7.09	124.68	118.30
2	U	239	LYS	CD-CE-NZ	7.09	128.02	111.70
2	R	99	TYR	CB-CG-CD1	7.09	125.25	121.00
2	R	239	LYS	CD-CE-NZ	7.09	128.00	111.70
2	T	99	TYR	CB-CG-CD1	7.09	125.25	121.00
2	O	239	LYS	CD-CE-NZ	7.09	128.00	111.70
2	X	239	LYS	CD-CE-NZ	7.09	128.00	111.70
2	P	239	LYS	CD-CE-NZ	7.08	128.00	111.70
2	Q	176	TYR	CB-CG-CD2	-7.08	116.75	121.00
2	V	239	LYS	CD-CE-NZ	7.08	128.00	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	W	358	ASP	CB-CG-OD2	7.08	124.68	118.30
2	T	239	LYS	CD-CE-NZ	7.08	127.99	111.70
2	P	99	TYR	CB-CG-CD1	7.08	125.25	121.00
2	S	239	LYS	CD-CE-NZ	7.08	127.99	111.70
2	M	239	LYS	CD-CE-NZ	7.08	127.98	111.70
2	Q	239	LYS	CD-CE-NZ	7.08	127.98	111.70
2	M	99	TYR	CB-CG-CD1	7.08	125.25	121.00
2	O	176	TYR	CB-CG-CD2	-7.08	116.75	121.00
2	S	99	TYR	CB-CG-CD1	7.07	125.24	121.00
2	R	358	ASP	CB-CG-OD2	7.07	124.66	118.30
2	U	99	TYR	CB-CG-CD1	7.07	125.24	121.00
2	R	176	TYR	CB-CG-CD2	-7.07	116.76	121.00
2	W	239	LYS	CD-CE-NZ	7.07	127.95	111.70
2	Q	136	ASP	O-C-N	7.07	134.00	122.70
2	V	99	TYR	CB-CG-CD1	7.07	125.24	121.00
2	P	176	TYR	CB-CG-CD2	-7.06	116.76	121.00
2	T	136	ASP	O-C-N	7.06	134.00	122.70
2	X	176	TYR	CB-CG-CD2	-7.05	116.77	121.00
2	O	136	ASP	O-C-N	7.05	133.99	122.70
2	M	236	ASP	O-C-N	7.05	133.98	122.70
2	N	236	ASP	O-C-N	7.05	133.98	122.70
2	R	136	ASP	O-C-N	7.04	133.97	122.70
2	X	136	ASP	O-C-N	7.04	133.96	122.70
2	S	236	ASP	O-C-N	7.04	133.96	122.70
2	M	136	ASP	O-C-N	7.04	133.96	122.70
2	N	136	ASP	O-C-N	7.04	133.96	122.70
2	W	136	ASP	O-C-N	7.04	133.96	122.70
2	W	236	ASP	O-C-N	7.04	133.96	122.70
2	U	236	ASP	O-C-N	7.03	133.95	122.70
2	X	236	ASP	O-C-N	7.03	133.95	122.70
2	V	136	ASP	O-C-N	7.03	133.95	122.70
2	S	136	ASP	O-C-N	7.03	133.95	122.70
2	W	328	GLU	OE1-CD-OE2	7.03	131.73	123.30
2	R	236	ASP	O-C-N	7.03	133.94	122.70
2	U	136	ASP	O-C-N	7.03	133.94	122.70
2	O	236	ASP	O-C-N	7.02	133.94	122.70
2	T	236	ASP	O-C-N	7.02	133.93	122.70
2	V	236	ASP	O-C-N	7.02	133.93	122.70
2	N	328	GLU	OE1-CD-OE2	7.01	131.72	123.30
2	P	236	ASP	O-C-N	7.01	133.92	122.70
2	Q	236	ASP	O-C-N	7.01	133.91	122.70
2	P	136	ASP	O-C-N	7.00	133.90	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	V	328	GLU	OE1-CD-OE2	7.00	131.71	123.30
2	Q	328	GLU	OE1-CD-OE2	7.00	131.70	123.30
2	S	328	GLU	OE1-CD-OE2	7.00	131.70	123.30
2	S	176	TYR	CB-CG-CD2	-7.00	116.80	121.00
2	M	328	GLU	OE1-CD-OE2	7.00	131.70	123.30
2	O	328	GLU	OE1-CD-OE2	7.00	131.69	123.30
2	U	328	GLU	OE1-CD-OE2	6.99	131.69	123.30
2	N	99	TYR	CB-CG-CD1	6.99	125.19	121.00
2	T	328	GLU	OE1-CD-OE2	6.99	131.69	123.30
2	N	272	ASN	CA-C-N	6.99	132.57	117.20
2	P	328	GLU	OE1-CD-OE2	6.99	131.68	123.30
2	R	328	GLU	OE1-CD-OE2	6.99	131.68	123.30
2	W	99	TYR	CB-CG-CD1	6.98	125.19	121.00
2	O	272	ASN	CA-C-N	6.97	132.53	117.20
2	X	328	GLU	OE1-CD-OE2	6.97	131.66	123.30
2	P	272	ASN	CA-C-N	6.96	132.51	117.20
2	S	272	ASN	CA-C-N	6.96	132.50	117.20
2	R	272	ASN	CA-C-N	6.95	132.50	117.20
2	V	272	ASN	CA-C-N	6.95	132.50	117.20
2	W	272	ASN	CA-C-N	6.95	132.49	117.20
2	M	272	ASN	CA-C-N	6.94	132.48	117.20
2	T	272	ASN	CA-C-N	6.94	132.48	117.20
2	Q	272	ASN	CA-C-N	6.94	132.47	117.20
2	Q	142	LYS	CA-CB-CG	6.94	128.67	113.40
2	U	142	LYS	CA-CB-CG	6.94	128.67	113.40
2	X	131	GLU	CG-CD-OE1	6.94	132.18	118.30
2	O	131	GLU	CG-CD-OE1	6.93	132.17	118.30
2	U	131	GLU	CG-CD-OE1	6.93	132.17	118.30
2	M	344	ARG	NE-CZ-NH2	6.93	123.77	120.30
2	P	142	LYS	CA-CB-CG	6.93	128.65	113.40
2	W	131	GLU	CG-CD-OE1	6.93	132.16	118.30
2	M	142	LYS	CA-CB-CG	6.93	128.65	113.40
2	Q	131	GLU	CG-CD-OE1	6.93	132.16	118.30
2	M	131	GLU	CG-CD-OE1	6.93	132.16	118.30
2	U	272	ASN	CA-C-N	6.93	132.44	117.20
2	T	131	GLU	CG-CD-OE1	6.93	132.15	118.30
2	X	272	ASN	CA-C-N	6.93	132.44	117.20
2	V	142	LYS	CA-CB-CG	6.92	128.63	113.40
2	X	142	LYS	CA-CB-CG	6.92	128.63	113.40
2	P	131	GLU	CG-CD-OE1	6.92	132.15	118.30
2	W	142	LYS	CA-CB-CG	6.92	128.63	113.40
2	S	142	LYS	CA-CB-CG	6.92	128.62	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	V	131	GLU	CG-CD-OE1	6.92	132.14	118.30
2	R	142	LYS	CA-CB-CG	6.92	128.62	113.40
2	R	131	GLU	CG-CD-OE1	6.92	132.13	118.30
2	T	142	LYS	CA-CB-CG	6.92	128.61	113.40
2	N	131	GLU	CG-CD-OE1	6.91	132.13	118.30
2	N	142	LYS	CA-CB-CG	6.91	128.60	113.40
1	H	401	PRO	CA-N-CD	-6.91	101.83	111.50
2	O	142	LYS	CA-CB-CG	6.91	128.59	113.40
1	C	401	PRO	CA-N-CD	-6.90	101.84	111.50
1	D	401	PRO	CA-N-CD	-6.90	101.84	111.50
2	S	131	GLU	CG-CD-OE1	6.90	132.09	118.30
1	A	401	PRO	CA-N-CD	-6.89	101.86	111.50
1	B	401	PRO	CA-N-CD	-6.89	101.85	111.50
1	J	401	PRO	CA-N-CD	-6.89	101.86	111.50
1	I	401	PRO	CA-N-CD	-6.88	101.86	111.50
1	G	401	PRO	CA-N-CD	-6.88	101.87	111.50
1	K	401	PRO	CA-N-CD	-6.88	101.87	111.50
1	L	401	PRO	CA-N-CD	-6.88	101.87	111.50
2	M	209	ASP	CB-CG-OD2	6.87	124.48	118.30
1	E	401	PRO	CA-N-CD	-6.87	101.88	111.50
2	N	209	ASP	CB-CG-OD2	6.86	124.47	118.30
2	Q	209	ASP	CB-CG-OD2	6.84	124.45	118.30
1	F	401	PRO	CA-N-CD	-6.84	101.93	111.50
2	M	148	MET	CG-SD-CE	-6.83	89.27	100.20
2	T	148	MET	CG-SD-CE	-6.83	89.27	100.20
2	T	209	ASP	CB-CG-OD2	6.83	124.44	118.30
2	O	344	ARG	NE-CZ-NH2	6.83	123.71	120.30
2	P	344	ARG	NE-CZ-NH2	6.83	123.71	120.30
2	P	55	ASP	CB-CA-C	6.83	124.05	110.40
2	R	148	MET	CG-SD-CE	-6.83	89.28	100.20
2	P	148	MET	CG-SD-CE	-6.82	89.28	100.20
2	V	148	MET	CG-SD-CE	-6.82	89.28	100.20
2	X	148	MET	CG-SD-CE	-6.82	89.28	100.20
2	N	148	MET	CG-SD-CE	-6.82	89.29	100.20
2	T	344	ARG	NE-CZ-NH2	6.82	123.71	120.30
2	T	55	ASP	CB-CA-C	6.82	124.03	110.40
2	W	148	MET	CG-SD-CE	-6.82	89.29	100.20
2	S	148	MET	CG-SD-CE	-6.81	89.30	100.20
2	U	209	ASP	CB-CG-OD2	6.81	124.43	118.30
2	W	55	ASP	CB-CA-C	6.81	124.02	110.40
2	O	148	MET	CG-SD-CE	-6.81	89.31	100.20
2	Q	55	ASP	CB-CA-C	6.81	124.02	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	Q	148	MET	CG-SD-CE	-6.81	89.31	100.20
2	R	55	ASP	CB-CA-C	6.81	124.02	110.40
2	X	344	ARG	NE-CZ-NH2	6.81	123.70	120.30
2	M	55	ASP	CB-CA-C	6.81	124.01	110.40
2	V	344	ARG	NE-CZ-NH2	6.81	123.70	120.30
2	W	344	ARG	NE-CZ-NH2	6.81	123.70	120.30
2	U	55	ASP	CB-CA-C	6.80	124.01	110.40
2	U	344	ARG	NE-CZ-NH2	6.80	123.70	120.30
2	N	291	GLU	CG-CD-OE2	-6.80	104.69	118.30
2	V	209	ASP	CB-CG-OD2	6.80	124.42	118.30
2	N	55	ASP	CB-CA-C	6.80	124.00	110.40
2	S	291	GLU	CG-CD-OE2	-6.80	104.69	118.30
2	V	55	ASP	CB-CA-C	6.80	124.00	110.40
2	W	209	ASP	CB-CG-OD2	6.80	124.42	118.30
2	T	291	GLU	CG-CD-OE2	-6.80	104.70	118.30
2	R	291	GLU	CG-CD-OE2	-6.80	104.70	118.30
2	U	148	MET	CG-SD-CE	-6.80	89.33	100.20
2	X	291	GLU	CG-CD-OE2	-6.80	104.71	118.30
2	P	209	ASP	CB-CG-OD2	6.79	124.41	118.30
2	P	291	GLU	CG-CD-OE2	-6.79	104.72	118.30
2	V	291	GLU	CG-CD-OE2	-6.79	104.72	118.30
2	U	291	GLU	CG-CD-OE2	-6.79	104.72	118.30
2	W	291	GLU	CG-CD-OE2	-6.79	104.72	118.30
2	O	55	ASP	CB-CA-C	6.79	123.97	110.40
2	S	55	ASP	CB-CA-C	6.79	123.97	110.40
2	S	209	ASP	CB-CG-OD2	6.78	124.41	118.30
2	X	180	ASP	CB-CG-OD2	6.78	124.40	118.30
2	O	291	GLU	CG-CD-OE2	-6.78	104.75	118.30
2	X	55	ASP	CB-CA-C	6.78	123.95	110.40
2	M	291	GLU	CG-CD-OE2	-6.77	104.75	118.30
2	Q	291	GLU	CG-CD-OE2	-6.76	104.77	118.30
2	X	209	ASP	CB-CG-OD2	6.76	124.39	118.30
2	R	209	ASP	CB-CG-OD2	6.76	124.38	118.30
2	Q	344	ARG	NE-CZ-NH2	6.76	123.68	120.30
2	N	344	ARG	NE-CZ-NH2	6.75	123.68	120.30
2	O	209	ASP	CB-CG-OD2	6.75	124.37	118.30
2	R	344	ARG	NE-CZ-NH2	6.75	123.67	120.30
2	U	180	ASP	CB-CG-OD2	6.73	124.36	118.30
2	N	180	ASP	CB-CG-OD2	6.72	124.35	118.30
2	V	180	ASP	CB-CG-OD2	6.72	124.35	118.30
2	Q	180	ASP	CB-CG-OD2	6.71	124.34	118.30
2	R	180	ASP	CB-CG-OD2	6.71	124.34	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	S	344	ARG	NE-CZ-NH2	6.71	123.65	120.30
2	S	180	ASP	CB-CG-OD2	6.71	124.34	118.30
2	M	180	ASP	CB-CG-OD2	6.70	124.33	118.30
2	P	180	ASP	CB-CG-OD2	6.68	124.31	118.30
2	T	180	ASP	CB-CG-OD2	6.68	124.31	118.30
2	O	180	ASP	CB-CG-OD2	6.67	124.30	118.30
2	W	180	ASP	CB-CG-OD2	6.67	124.30	118.30
2	T	358	ASP	CB-CG-OD1	6.56	124.20	118.30
2	U	45	GLU	N-CA-CB	-6.54	98.84	110.60
2	T	45	GLU	N-CA-CB	-6.53	98.84	110.60
2	W	45	GLU	N-CA-CB	-6.53	98.85	110.60
2	O	45	GLU	N-CA-CB	-6.52	98.86	110.60
2	X	358	ASP	CB-CG-OD1	6.52	124.17	118.30
2	M	45	GLU	N-CA-CB	-6.52	98.86	110.60
2	Q	45	GLU	N-CA-CB	-6.52	98.86	110.60
2	Q	358	ASP	CB-CG-OD1	6.52	124.17	118.30
2	P	45	GLU	N-CA-CB	-6.52	98.87	110.60
2	R	45	GLU	N-CA-CB	-6.51	98.87	110.60
2	S	45	GLU	N-CA-CB	-6.51	98.87	110.60
2	V	45	GLU	N-CA-CB	-6.51	98.87	110.60
2	N	45	GLU	N-CA-CB	-6.51	98.88	110.60
2	T	358	ASP	OD1-CG-OD2	-6.51	110.93	123.30
2	N	358	ASP	OD1-CG-OD2	-6.51	110.94	123.30
2	S	358	ASP	OD1-CG-OD2	-6.51	110.94	123.30
2	R	358	ASP	CB-CG-OD1	6.50	124.16	118.30
2	X	45	GLU	N-CA-CB	-6.50	98.89	110.60
2	P	358	ASP	OD1-CG-OD2	-6.50	110.95	123.30
2	M	326	LYS	CD-CE-NZ	-6.50	96.75	111.70
2	N	326	LYS	CD-CE-NZ	-6.50	96.75	111.70
2	Q	358	ASP	OD1-CG-OD2	-6.50	110.95	123.30
2	X	358	ASP	OD1-CG-OD2	-6.50	110.96	123.30
2	O	358	ASP	OD1-CG-OD2	-6.50	110.96	123.30
2	X	326	LYS	CD-CE-NZ	-6.49	96.77	111.70
2	M	358	ASP	OD1-CG-OD2	-6.49	110.97	123.30
2	T	326	LYS	CD-CE-NZ	-6.49	96.77	111.70
2	N	233	SER	CA-CB-OG	-6.49	93.68	111.20
2	O	233	SER	CA-CB-OG	-6.49	93.68	111.20
2	Q	326	LYS	CD-CE-NZ	-6.49	96.78	111.70
2	U	358	ASP	OD1-CG-OD2	-6.49	110.97	123.30
2	M	358	ASP	CB-CG-OD1	6.49	124.14	118.30
2	N	358	ASP	CB-CG-OD1	6.49	124.14	118.30
2	O	326	LYS	CD-CE-NZ	-6.49	96.78	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	P	326	LYS	CD-CE-NZ	-6.49	96.78	111.70
2	R	10	TRP	CB-CG-CD2	-6.49	118.17	126.60
2	V	326	LYS	CD-CE-NZ	-6.49	96.78	111.70
2	V	358	ASP	CB-CG-OD1	6.49	124.14	118.30
2	V	358	ASP	OD1-CG-OD2	-6.49	110.98	123.30
2	U	326	LYS	CD-CE-NZ	-6.48	96.79	111.70
2	N	124	ASN	CA-CB-CG	6.48	127.66	113.40
2	R	124	ASN	CA-CB-CG	6.48	127.65	113.40
2	R	233	SER	CA-CB-OG	-6.48	93.71	111.20
2	W	10	TRP	CB-CG-CD2	-6.48	118.18	126.60
2	P	358	ASP	CB-CG-OD1	6.48	124.13	118.30
2	W	358	ASP	CB-CG-OD1	6.48	124.13	118.30
2	X	233	SER	CA-CB-OG	-6.48	93.71	111.20
2	O	124	ASN	CA-CB-CG	6.48	127.65	113.40
2	M	10	TRP	CB-CG-CD2	-6.47	118.18	126.60
2	R	358	ASP	OD1-CG-OD2	-6.47	111.00	123.30
2	T	233	SER	CA-CB-OG	-6.47	93.72	111.20
2	W	124	ASN	CA-CB-CG	6.47	127.64	113.40
2	O	358	ASP	CB-CG-OD1	6.47	124.12	118.30
2	T	10	TRP	CB-CG-CD2	-6.47	118.19	126.60
2	T	38	GLU	O-C-N	6.47	133.06	122.70
2	T	124	ASN	CA-CB-CG	6.47	127.64	113.40
2	U	233	SER	CA-CB-OG	-6.47	93.72	111.20
2	V	124	ASN	CA-CB-CG	6.47	127.64	113.40
2	V	233	SER	CA-CB-OG	-6.47	93.72	111.20
2	S	326	LYS	CD-CE-NZ	-6.47	96.82	111.70
2	U	358	ASP	CB-CG-OD1	6.47	124.12	118.30
2	M	233	SER	CA-CB-OG	-6.47	93.73	111.20
2	O	10	TRP	CB-CG-CD2	-6.47	118.19	126.60
2	Q	233	SER	CA-CB-OG	-6.47	93.73	111.20
2	U	10	TRP	CB-CG-CD2	-6.47	118.19	126.60
2	W	358	ASP	OD1-CG-OD2	-6.47	111.01	123.30
2	S	358	ASP	CB-CG-OD1	6.47	124.12	118.30
2	P	124	ASN	CA-CB-CG	6.46	127.62	113.40
2	R	326	LYS	CD-CE-NZ	-6.46	96.83	111.70
2	S	233	SER	CA-CB-OG	-6.46	93.74	111.20
2	V	10	TRP	CB-CG-CD2	-6.46	118.20	126.60
2	W	326	LYS	CD-CE-NZ	-6.46	96.84	111.70
2	X	124	ASN	CA-CB-CG	6.46	127.61	113.40
2	S	124	ASN	CA-CB-CG	6.46	127.61	113.40
2	P	10	TRP	CB-CG-CD2	-6.46	118.20	126.60
2	S	38	GLU	O-C-N	6.46	133.03	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	W	38	GLU	O-C-N	6.46	133.03	122.70
2	Q	124	ASN	CA-CB-CG	6.46	127.60	113.40
2	U	124	ASN	CA-CB-CG	6.46	127.60	113.40
2	W	233	SER	CA-CB-OG	-6.46	93.77	111.20
2	P	38	GLU	O-C-N	6.45	133.03	122.70
2	P	233	SER	CA-CB-OG	-6.45	93.78	111.20
2	S	10	TRP	CB-CG-CD2	-6.45	118.21	126.60
2	O	38	GLU	O-C-N	6.45	133.02	122.70
2	Q	10	TRP	CB-CG-CD2	-6.45	118.22	126.60
2	X	38	GLU	O-C-N	6.45	133.02	122.70
2	N	10	TRP	CB-CG-CD2	-6.45	118.22	126.60
2	X	10	TRP	CB-CG-CD2	-6.45	118.22	126.60
2	M	124	ASN	CA-CB-CG	6.44	127.58	113.40
2	R	38	GLU	O-C-N	6.44	133.01	122.70
2	V	38	GLU	O-C-N	6.44	133.01	122.70
2	U	38	GLU	O-C-N	6.44	133.00	122.70
2	N	38	GLU	O-C-N	6.43	132.99	122.70
2	Q	38	GLU	O-C-N	6.43	132.98	122.70
2	M	38	GLU	O-C-N	6.41	132.95	122.70
2	S	316	ARG	NH1-CZ-NH2	-6.39	112.37	119.40
2	R	316	ARG	NH1-CZ-NH2	-6.39	112.38	119.40
2	X	316	ARG	NH1-CZ-NH2	-6.38	112.38	119.40
2	V	316	ARG	NH1-CZ-NH2	-6.38	112.38	119.40
2	P	316	ARG	NH1-CZ-NH2	-6.38	112.39	119.40
2	M	316	ARG	NH1-CZ-NH2	-6.37	112.39	119.40
2	Q	316	ARG	NH1-CZ-NH2	-6.37	112.39	119.40
2	S	363	ASP	CB-CG-OD2	-6.37	112.57	118.30
2	U	316	ARG	NH1-CZ-NH2	-6.37	112.40	119.40
2	N	316	ARG	NH1-CZ-NH2	-6.36	112.40	119.40
2	T	316	ARG	NH1-CZ-NH2	-6.36	112.40	119.40
2	R	363	ASP	CB-CG-OD2	-6.35	112.58	118.30
2	M	363	ASP	CB-CG-OD2	-6.34	112.59	118.30
2	W	316	ARG	NH1-CZ-NH2	-6.34	112.42	119.40
2	U	363	ASP	CB-CG-OD2	-6.33	112.60	118.30
2	T	363	ASP	CB-CG-OD2	-6.33	112.60	118.30
2	M	167	TYR	CB-CG-CD1	-6.33	117.20	121.00
2	S	98	ARG	NE-CZ-NH2	-6.33	117.14	120.30
2	T	167	TYR	CB-CG-CD1	-6.32	117.21	121.00
2	U	167	TYR	CB-CG-CD1	-6.32	117.21	121.00
2	O	316	ARG	NH1-CZ-NH2	-6.31	112.46	119.40
2	V	363	ASP	CB-CG-OD2	-6.31	112.62	118.30
2	T	98	ARG	NE-CZ-NH2	-6.30	117.15	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	S	167	TYR	CB-CG-CD1	-6.30	117.22	121.00
2	X	363	ASP	CB-CG-OD2	-6.30	112.63	118.30
2	P	98	ARG	NE-CZ-NH2	-6.30	117.15	120.30
2	Q	128	THR	N-CA-CB	-6.29	98.34	110.30
2	Q	363	ASP	CB-CG-OD2	-6.29	112.64	118.30
2	S	128	THR	N-CA-CB	-6.29	98.35	110.30
2	O	363	ASP	CB-CG-OD2	-6.29	112.64	118.30
2	R	128	THR	N-CA-CB	-6.28	98.36	110.30
2	M	128	THR	N-CA-CB	-6.28	98.37	110.30
2	O	128	THR	N-CA-CB	-6.28	98.37	110.30
2	N	128	THR	N-CA-CB	-6.27	98.38	110.30
2	T	128	THR	N-CA-CB	-6.27	98.38	110.30
2	V	128	THR	N-CA-CB	-6.27	98.38	110.30
2	W	363	ASP	CB-CG-OD2	-6.27	112.66	118.30
2	P	363	ASP	CB-CG-OD2	-6.27	112.66	118.30
2	W	128	THR	N-CA-CB	-6.27	98.39	110.30
2	O	167	TYR	CB-CG-CD1	-6.27	117.24	121.00
2	X	128	THR	N-CA-CB	-6.26	98.41	110.30
2	N	363	ASP	CB-CG-OD2	-6.25	112.67	118.30
2	W	167	TYR	CB-CG-CD1	-6.25	117.25	121.00
2	P	128	THR	N-CA-CB	-6.25	98.42	110.30
2	V	167	TYR	CB-CG-CD1	-6.25	117.25	121.00
2	U	128	THR	N-CA-CB	-6.25	98.43	110.30
2	R	167	TYR	CB-CG-CD1	-6.25	117.25	121.00
2	X	167	TYR	CB-CG-CD1	-6.24	117.25	121.00
2	U	98	ARG	NE-CZ-NH2	-6.24	117.18	120.30
2	N	167	TYR	CB-CG-CD1	-6.22	117.27	121.00
2	W	98	ARG	NE-CZ-NH2	-6.22	117.19	120.30
2	O	236	ASP	CB-CG-OD1	6.21	123.89	118.30
2	Q	167	TYR	CB-CG-CD1	-6.21	117.27	121.00
2	Q	236	ASP	CB-CG-OD1	6.21	123.89	118.30
2	V	98	ARG	NE-CZ-NH2	-6.21	117.20	120.30
2	Q	98	ARG	NE-CZ-NH2	-6.20	117.20	120.30
2	N	98	ARG	NE-CZ-NH2	-6.20	117.20	120.30
2	R	98	ARG	NE-CZ-NH2	-6.20	117.20	120.30
2	X	165	GLY	CA-C-O	-6.19	109.46	120.60
2	S	30	ASP	CB-CA-C	6.19	122.78	110.40
2	T	175	LYS	CB-CA-C	6.18	122.77	110.40
2	P	175	LYS	CB-CA-C	6.18	122.76	110.40
2	U	236	ASP	CB-CG-OD1	6.18	123.86	118.30
2	V	236	ASP	CB-CG-OD1	6.18	123.86	118.30
2	M	165	GLY	CA-C-O	-6.18	109.48	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	Q	175	LYS	CB-CA-C	6.18	122.76	110.40
2	U	165	GLY	CA-C-O	-6.18	109.47	120.60
2	X	30	ASP	CB-CA-C	6.18	122.76	110.40
2	O	3	GLU	CB-CA-C	6.18	122.75	110.40
2	S	175	LYS	CB-CA-C	6.18	122.75	110.40
2	V	175	LYS	CB-CA-C	6.18	122.75	110.40
2	W	3	GLU	CB-CA-C	6.18	122.75	110.40
2	R	165	GLY	CA-C-O	-6.17	109.49	120.60
2	V	3	GLU	CB-CA-C	6.17	122.75	110.40
2	X	175	LYS	CB-CA-C	6.17	122.75	110.40
2	P	165	GLY	CA-C-O	-6.17	109.49	120.60
2	M	3	GLU	CB-CA-C	6.17	122.74	110.40
2	M	175	LYS	CB-CA-C	6.17	122.74	110.40
2	P	236	ASP	CB-CG-OD1	6.17	123.85	118.30
2	R	175	LYS	CB-CA-C	6.17	122.74	110.40
2	P	3	GLU	CB-CA-C	6.17	122.74	110.40
2	U	175	LYS	CB-CA-C	6.17	122.74	110.40
2	W	236	ASP	CB-CG-OD1	6.17	123.85	118.30
2	N	3	GLU	CB-CA-C	6.17	122.74	110.40
2	N	30	ASP	CB-CA-C	6.17	122.74	110.40
2	N	175	LYS	CB-CA-C	6.17	122.74	110.40
2	Q	3	GLU	CB-CA-C	6.17	122.73	110.40
2	R	3	GLU	CB-CA-C	6.17	122.74	110.40
2	S	3	GLU	CB-CA-C	6.17	122.74	110.40
2	X	98	ARG	NE-CZ-NH2	-6.17	117.22	120.30
2	M	236	ASP	CB-CG-OD1	6.17	123.85	118.30
2	U	30	ASP	CB-CA-C	6.17	122.73	110.40
2	O	30	ASP	CB-CA-C	6.17	122.73	110.40
2	P	167	TYR	CB-CG-CD1	-6.16	117.30	121.00
2	S	165	GLY	CA-C-O	-6.16	109.51	120.60
2	V	30	ASP	CB-CA-C	6.16	122.73	110.40
2	V	165	GLY	CA-C-O	-6.16	109.51	120.60
2	O	175	LYS	CB-CA-C	6.16	122.72	110.40
2	S	236	ASP	CB-CG-OD1	6.16	123.85	118.30
2	T	3	GLU	CB-CA-C	6.16	122.72	110.40
2	O	165	GLY	CA-C-O	-6.16	109.51	120.60
2	W	30	ASP	CB-CA-C	6.16	122.72	110.40
2	M	98	ARG	NE-CZ-NH2	-6.16	117.22	120.30
2	N	236	ASP	CB-CG-OD1	6.16	123.84	118.30
2	T	30	ASP	CB-CA-C	6.16	122.72	110.40
2	U	3	GLU	CB-CA-C	6.16	122.72	110.40
2	T	165	GLY	CA-C-O	-6.16	109.52	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	M	30	ASP	CB-CA-C	6.16	122.71	110.40
2	W	165	GLY	CA-C-O	-6.16	109.52	120.60
2	X	3	GLU	CB-CA-C	6.16	122.71	110.40
2	T	236	ASP	CB-CG-OD1	6.15	123.84	118.30
2	X	236	ASP	CB-CG-OD1	6.15	123.84	118.30
2	N	165	GLY	CA-C-O	-6.15	109.53	120.60
2	Q	354	ARG	N-CA-CB	6.15	121.67	110.60
2	R	30	ASP	CB-CA-C	6.15	122.70	110.40
2	P	30	ASP	CB-CA-C	6.15	122.70	110.40
2	Q	165	GLY	CA-C-O	-6.15	109.53	120.60
2	W	175	LYS	CB-CA-C	6.15	122.70	110.40
2	Q	30	ASP	CB-CA-C	6.14	122.69	110.40
2	O	98	ARG	NE-CZ-NH2	-6.14	117.23	120.30
2	R	354	ARG	N-CA-CB	6.14	121.65	110.60
2	W	354	ARG	N-CA-CB	6.14	121.65	110.60
2	R	236	ASP	CB-CG-OD1	6.14	123.82	118.30
2	S	354	ARG	N-CA-CB	6.13	121.63	110.60
2	O	354	ARG	N-CA-CB	6.13	121.63	110.60
2	T	354	ARG	N-CA-CB	6.13	121.63	110.60
2	X	354	ARG	N-CA-CB	6.13	121.63	110.60
2	V	354	ARG	N-CA-CB	6.12	121.62	110.60
2	M	354	ARG	N-CA-CB	6.12	121.61	110.60
2	P	354	ARG	N-CA-CB	6.12	121.61	110.60
2	N	354	ARG	N-CA-CB	6.12	121.61	110.60
2	U	354	ARG	N-CA-CB	6.11	121.59	110.60
2	X	231	ALA	N-CA-CB	-6.10	101.56	110.10
2	S	231	ALA	N-CA-CB	-6.10	101.56	110.10
2	W	231	ALA	N-CA-CB	-6.08	101.59	110.10
2	N	231	ALA	N-CA-CB	-6.08	101.59	110.10
2	O	231	ALA	N-CA-CB	-6.08	101.59	110.10
2	P	231	ALA	N-CA-CB	-6.08	101.59	110.10
2	T	231	ALA	N-CA-CB	-6.08	101.59	110.10
2	U	231	ALA	N-CA-CB	-6.07	101.60	110.10
2	V	231	ALA	N-CA-CB	-6.07	101.60	110.10
2	Q	231	ALA	N-CA-CB	-6.07	101.60	110.10
2	O	29	LYS	CA-CB-CG	6.07	126.75	113.40
2	M	231	ALA	N-CA-CB	-6.07	101.61	110.10
2	Q	29	LYS	CA-CB-CG	6.07	126.74	113.40
2	T	29	LYS	CA-CB-CG	6.06	126.74	113.40
2	R	29	LYS	CA-CB-CG	6.06	126.73	113.40
2	V	29	LYS	CA-CB-CG	6.06	126.73	113.40
2	X	28	GLU	CG-CD-OE1	-6.06	106.19	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	S	29	LYS	CA-CB-CG	6.06	126.72	113.40
2	W	29	LYS	CA-CB-CG	6.06	126.72	113.40
2	R	28	GLU	CG-CD-OE1	-6.05	106.19	118.30
2	R	231	ALA	N-CA-CB	-6.05	101.62	110.10
2	U	29	LYS	CA-CB-CG	6.05	126.72	113.40
2	N	28	GLU	CG-CD-OE1	-6.05	106.20	118.30
2	N	29	LYS	CA-CB-CG	6.05	126.72	113.40
2	P	29	LYS	CA-CB-CG	6.05	126.71	113.40
2	V	28	GLU	CG-CD-OE1	-6.05	106.21	118.30
2	N	172	GLU	CG-CD-OE2	-6.04	106.21	118.30
2	T	28	GLU	CG-CD-OE1	-6.04	106.21	118.30
2	U	28	GLU	CG-CD-OE1	-6.04	106.21	118.30
2	U	172	GLU	CG-CD-OE2	-6.04	106.21	118.30
2	X	28	GLU	CG-CD-OE2	6.04	130.39	118.30
2	X	29	LYS	CA-CB-CG	6.04	126.69	113.40
2	N	28	GLU	CG-CD-OE2	6.04	130.38	118.30
2	S	28	GLU	CG-CD-OE1	-6.04	106.22	118.30
2	M	29	LYS	CA-CB-CG	6.04	126.68	113.40
2	O	172	GLU	CG-CD-OE2	-6.03	106.23	118.30
2	P	172	GLU	CG-CD-OE2	-6.03	106.23	118.30
2	Q	28	GLU	CG-CD-OE2	6.03	130.36	118.30
2	Q	172	GLU	CG-CD-OE2	-6.03	106.24	118.30
2	R	172	GLU	CG-CD-OE2	-6.03	106.24	118.30
2	P	28	GLU	CG-CD-OE1	-6.03	106.24	118.30
2	M	28	GLU	CG-CD-OE1	-6.03	106.24	118.30
2	M	172	GLU	CG-CD-OE2	-6.03	106.25	118.30
2	O	28	GLU	CG-CD-OE1	-6.03	106.25	118.30
2	R	28	GLU	CG-CD-OE2	6.03	130.36	118.30
2	V	172	GLU	CG-CD-OE2	-6.03	106.24	118.30
2	W	28	GLU	CG-CD-OE1	-6.03	106.24	118.30
2	P	28	GLU	CG-CD-OE2	6.02	130.34	118.30
2	T	28	GLU	CG-CD-OE2	6.02	130.35	118.30
2	Q	28	GLU	CG-CD-OE1	-6.02	106.26	118.30
2	T	172	GLU	CG-CD-OE2	-6.02	106.26	118.30
2	V	28	GLU	CG-CD-OE2	6.02	130.34	118.30
2	S	172	GLU	CG-CD-OE2	-6.02	106.27	118.30
2	W	28	GLU	CG-CD-OE2	6.02	130.34	118.30
2	M	28	GLU	CG-CD-OE2	6.01	130.33	118.30
2	O	239	LYS	CG-CD-CE	6.01	129.94	111.90
2	U	28	GLU	CG-CD-OE2	6.01	130.32	118.30
2	W	172	GLU	CG-CD-OE2	-6.01	106.28	118.30
2	X	172	GLU	CG-CD-OE2	-6.01	106.28	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	O	28	GLU	CG-CD-OE2	6.01	130.32	118.30
2	N	239	LYS	CG-CD-CE	6.01	129.92	111.90
2	M	239	LYS	CG-CD-CE	6.00	129.91	111.90
2	Q	239	LYS	CG-CD-CE	6.00	129.91	111.90
2	S	239	LYS	CG-CD-CE	6.00	129.90	111.90
2	U	239	LYS	CG-CD-CE	6.00	129.90	111.90
2	R	239	LYS	CG-CD-CE	6.00	129.90	111.90
2	X	239	LYS	CG-CD-CE	6.00	129.89	111.90
2	P	239	LYS	CG-CD-CE	6.00	129.89	111.90
2	T	239	LYS	CG-CD-CE	6.00	129.88	111.90
2	V	239	LYS	CG-CD-CE	6.00	129.89	111.90
2	S	28	GLU	CG-CD-OE2	5.99	130.28	118.30
2	W	239	LYS	CG-CD-CE	5.99	129.86	111.90
2	X	136	ASP	CB-CG-OD2	5.96	123.66	118.30
2	Q	331	PRO	O-C-N	-5.95	113.18	122.70
2	O	331	PRO	O-C-N	-5.94	113.19	122.70
2	M	136	ASP	CB-CG-OD2	5.94	123.65	118.30
2	T	331	PRO	O-C-N	-5.94	113.20	122.70
2	S	331	PRO	O-C-N	-5.93	113.21	122.70
2	U	136	ASP	CB-CG-OD2	5.93	123.64	118.30
2	W	136	ASP	CB-CG-OD2	5.93	123.64	118.30
2	P	331	PRO	O-C-N	-5.93	113.21	122.70
2	T	136	ASP	CB-CG-OD2	5.93	123.64	118.30
2	X	331	PRO	O-C-N	-5.92	113.22	122.70
2	O	136	ASP	CB-CG-OD2	5.92	123.63	118.30
2	P	136	ASP	CB-CG-OD2	5.92	123.63	118.30
2	W	331	PRO	O-C-N	-5.92	113.23	122.70
2	S	136	ASP	CB-CG-OD2	5.92	123.63	118.30
2	U	354	ARG	CA-CB-CG	5.92	126.42	113.40
2	N	331	PRO	O-C-N	-5.91	113.24	122.70
2	R	136	ASP	CB-CG-OD2	5.91	123.62	118.30
2	V	331	PRO	O-C-N	-5.91	113.24	122.70
2	V	136	ASP	CB-CG-OD2	5.91	123.62	118.30
2	M	331	PRO	O-C-N	-5.90	113.25	122.70
2	S	354	ARG	CA-CB-CG	5.90	126.39	113.40
2	Q	136	ASP	CB-CG-OD2	5.90	123.61	118.30
2	P	354	ARG	CA-CB-CG	5.90	126.38	113.40
2	R	331	PRO	O-C-N	-5.90	113.26	122.70
2	M	354	ARG	CA-CB-CG	5.89	126.36	113.40
2	V	354	ARG	CA-CB-CG	5.89	126.36	113.40
2	W	354	ARG	CA-CB-CG	5.88	126.34	113.40
2	O	354	ARG	CA-CB-CG	5.88	126.34	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	U	331	PRO	O-C-N	-5.88	113.29	122.70
2	X	354	ARG	CA-CB-CG	5.88	126.34	113.40
2	R	354	ARG	CA-CB-CG	5.88	126.33	113.40
2	N	136	ASP	CB-CG-OD2	5.88	123.59	118.30
2	N	354	ARG	CA-CB-CG	5.88	126.33	113.40
2	T	354	ARG	CA-CB-CG	5.88	126.33	113.40
2	Q	354	ARG	CA-CB-CG	5.87	126.31	113.40
2	P	341	TYR	CB-CA-C	5.86	122.12	110.40
2	T	341	TYR	CB-CA-C	5.85	122.11	110.40
2	W	341	TYR	CB-CA-C	5.85	122.10	110.40
2	U	341	TYR	CB-CA-C	5.85	122.10	110.40
2	V	341	TYR	CB-CA-C	5.85	122.09	110.40
2	Q	341	TYR	CB-CA-C	5.84	122.08	110.40
2	X	341	TYR	CB-CA-C	5.84	122.08	110.40
2	M	341	TYR	CB-CA-C	5.84	122.08	110.40
2	N	341	TYR	CB-CA-C	5.83	122.07	110.40
2	S	341	TYR	CB-CA-C	5.83	122.06	110.40
2	O	341	TYR	CB-CA-C	5.83	122.06	110.40
2	R	341	TYR	CB-CA-C	5.82	122.04	110.40
2	W	23	VAL	CG1-CB-CG2	5.80	120.18	110.90
2	P	23	VAL	CG1-CB-CG2	5.80	120.17	110.90
2	R	23	VAL	CG1-CB-CG2	5.79	120.17	110.90
2	X	264	ALA	N-CA-CB	5.79	118.21	110.10
2	T	347	VAL	O-C-N	5.79	131.97	122.70
2	U	23	VAL	CG1-CB-CG2	5.79	120.16	110.90
2	O	23	VAL	CG1-CB-CG2	5.79	120.16	110.90
2	S	23	VAL	CG1-CB-CG2	5.79	120.16	110.90
2	S	264	ALA	N-CA-CB	5.78	118.20	110.10
2	T	264	ALA	N-CA-CB	5.78	118.19	110.10
2	W	347	VAL	O-C-N	5.78	131.95	122.70
2	M	23	VAL	CG1-CB-CG2	5.78	120.15	110.90
2	N	23	VAL	CG1-CB-CG2	5.78	120.15	110.90
2	V	23	VAL	CG1-CB-CG2	5.78	120.14	110.90
2	Q	264	ALA	N-CA-CB	5.78	118.19	110.10
2	O	347	VAL	O-C-N	5.77	131.94	122.70
2	R	264	ALA	N-CA-CB	5.77	118.18	110.10
2	O	264	ALA	N-CA-CB	5.77	118.18	110.10
2	M	347	VAL	O-C-N	5.77	131.93	122.70
2	Q	23	VAL	CG1-CB-CG2	5.77	120.13	110.90
2	V	264	ALA	N-CA-CB	5.76	118.17	110.10
2	X	23	VAL	CG1-CB-CG2	5.76	120.12	110.90
2	P	347	VAL	O-C-N	5.76	131.92	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	S	347	VAL	O-C-N	5.76	131.92	122.70
2	U	347	VAL	O-C-N	5.76	131.92	122.70
2	V	347	VAL	O-C-N	5.76	131.91	122.70
2	U	264	ALA	N-CA-CB	5.76	118.16	110.10
2	W	264	ALA	N-CA-CB	5.75	118.16	110.10
2	T	23	VAL	CG1-CB-CG2	5.75	120.10	110.90
2	M	264	ALA	N-CA-CB	5.75	118.15	110.10
2	N	347	VAL	O-C-N	5.75	131.89	122.70
2	Q	347	VAL	O-C-N	5.74	131.89	122.70
2	X	347	VAL	O-C-N	5.74	131.89	122.70
2	U	251	LYS	CG-CD-CE	5.74	129.12	111.90
2	T	251	LYS	CG-CD-CE	5.74	129.12	111.90
2	W	251	LYS	CG-CD-CE	5.74	129.12	111.90
2	O	251	LYS	CG-CD-CE	5.74	129.11	111.90
2	Q	251	LYS	CG-CD-CE	5.74	129.11	111.90
2	R	347	VAL	O-C-N	5.74	131.88	122.70
2	N	251	LYS	CG-CD-CE	5.73	129.09	111.90
2	N	264	ALA	N-CA-CB	5.73	118.12	110.10
2	P	251	LYS	CG-CD-CE	5.73	129.10	111.90
2	R	251	LYS	CG-CD-CE	5.73	129.10	111.90
2	V	251	LYS	CG-CD-CE	5.73	129.10	111.90
2	P	264	ALA	N-CA-CB	5.73	118.12	110.10
2	S	251	LYS	CG-CD-CE	5.73	129.09	111.90
2	M	251	LYS	CG-CD-CE	5.72	129.07	111.90
2	X	251	LYS	CG-CD-CE	5.72	129.06	111.90
2	P	272	ASN	CB-CG-ND2	5.69	130.35	116.70
2	X	256	LYS	CA-CB-CG	5.69	125.91	113.40
2	R	256	LYS	CA-CB-CG	5.68	125.91	113.40
2	U	272	ASN	CB-CG-ND2	5.68	130.34	116.70
2	Q	272	ASN	CB-CG-ND2	5.68	130.34	116.70
2	O	256	LYS	CA-CB-CG	5.67	125.88	113.40
2	S	256	LYS	CA-CB-CG	5.67	125.88	113.40
2	S	272	ASN	CB-CG-ND2	5.67	130.32	116.70
2	N	97	VAL	O-C-N	5.67	131.78	122.70
2	U	256	LYS	CA-CB-CG	5.67	125.88	113.40
2	M	272	ASN	CB-CG-ND2	5.67	130.31	116.70
2	W	272	ASN	CB-CG-ND2	5.67	130.31	116.70
2	M	97	VAL	O-C-N	5.67	131.77	122.70
2	V	256	LYS	CA-CB-CG	5.67	125.87	113.40
2	V	272	ASN	CB-CG-ND2	5.67	130.30	116.70
2	P	256	LYS	CA-CB-CG	5.67	125.87	113.40
2	R	272	ASN	CB-CG-ND2	5.67	130.30	116.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	T	272	ASN	CB-CG-ND2	5.67	130.30	116.70
2	X	272	ASN	CB-CG-ND2	5.67	130.30	116.70
2	N	272	ASN	CB-CG-ND2	5.66	130.29	116.70
2	T	256	LYS	CA-CB-CG	5.66	125.86	113.40
2	U	97	VAL	O-C-N	5.66	131.76	122.70
2	M	256	LYS	CA-CB-CG	5.66	125.86	113.40
2	W	256	LYS	CA-CB-CG	5.66	125.85	113.40
2	O	272	ASN	CB-CG-ND2	5.66	130.28	116.70
2	Q	256	LYS	CA-CB-CG	5.66	125.85	113.40
2	N	256	LYS	CA-CB-CG	5.65	125.83	113.40
2	P	97	VAL	O-C-N	5.65	131.74	122.70
2	Q	97	VAL	O-C-N	5.65	131.75	122.70
2	R	97	VAL	O-C-N	5.65	131.74	122.70
2	V	97	VAL	O-C-N	5.65	131.74	122.70
2	W	53	THR	CA-CB-CG2	5.65	120.31	112.40
2	X	53	THR	CA-CB-CG2	5.65	120.31	112.40
2	T	97	VAL	O-C-N	5.65	131.73	122.70
2	T	61	PHE	CB-CG-CD1	5.64	124.75	120.80
2	M	53	THR	CA-CB-CG2	5.64	120.30	112.40
2	S	97	VAL	O-C-N	5.64	131.72	122.70
2	N	53	THR	CA-CB-CG2	5.64	120.29	112.40
2	P	53	THR	CA-CB-CG2	5.63	120.28	112.40
2	Q	262	LEU	O-C-N	5.63	131.71	122.70
2	R	53	THR	CA-CB-CG2	5.63	120.28	112.40
2	T	53	THR	CA-CB-CG2	5.63	120.28	112.40
2	V	53	THR	CA-CB-CG2	5.63	120.28	112.40
2	W	97	VAL	O-C-N	5.63	131.70	122.70
2	Q	53	THR	CA-CB-CG2	5.62	120.28	112.40
2	T	262	LEU	O-C-N	5.62	131.70	122.70
2	O	97	VAL	O-C-N	5.62	131.69	122.70
2	X	97	VAL	O-C-N	5.62	131.69	122.70
2	S	53	THR	CA-CB-CG2	5.62	120.26	112.40
2	U	53	THR	CA-CB-CG2	5.62	120.26	112.40
2	O	262	LEU	O-C-N	5.61	131.68	122.70
2	P	61	PHE	CB-CG-CD1	5.61	124.73	120.80
2	R	134	ALA	CA-C-O	5.61	131.89	120.10
2	O	53	THR	CA-CB-CG2	5.61	120.25	112.40
2	S	262	LEU	O-C-N	5.61	131.67	122.70
2	R	262	LEU	O-C-N	5.60	131.66	122.70
2	S	134	ALA	CA-C-O	5.60	131.87	120.10
2	M	61	PHE	CB-CG-CD1	5.60	124.72	120.80
2	O	134	ALA	CA-C-O	5.60	131.86	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	V	134	ALA	CA-C-O	5.60	131.85	120.10
2	W	134	ALA	CA-C-O	5.59	131.85	120.10
2	P	134	ALA	CA-C-O	5.59	131.84	120.10
2	V	262	LEU	O-C-N	5.59	131.64	122.70
2	M	310	GLU	CG-CD-OE1	5.59	129.47	118.30
2	Q	134	ALA	CA-C-O	5.59	131.83	120.10
2	U	310	GLU	CG-CD-OE1	5.59	129.47	118.30
2	W	262	LEU	O-C-N	5.59	131.64	122.70
2	Q	310	GLU	CG-CD-OE1	5.58	129.47	118.30
2	W	310	GLU	CG-CD-OE1	5.58	129.47	118.30
2	T	134	ALA	CA-C-O	5.58	131.82	120.10
1	F	248	ARG	NE-CZ-NH2	5.58	123.09	120.30
2	M	262	LEU	O-C-N	5.58	131.62	122.70
2	U	134	ALA	CA-C-O	5.58	131.82	120.10
2	U	262	LEU	O-C-N	5.58	131.62	122.70
2	X	165	GLY	CA-C-N	5.58	127.36	116.20
2	M	134	ALA	CA-C-O	5.58	131.81	120.10
2	Q	61	PHE	CB-CG-CD1	5.58	124.70	120.80
2	V	310	GLU	CG-CD-OE1	5.58	129.45	118.30
2	X	134	ALA	CA-C-O	5.58	131.81	120.10
2	X	310	GLU	CG-CD-OE1	5.58	129.45	118.30
2	X	262	LEU	O-C-N	5.57	131.62	122.70
2	N	134	ALA	CA-C-O	5.57	131.80	120.10
2	O	165	GLY	CA-C-N	5.57	127.34	116.20
2	P	262	LEU	O-C-N	5.57	131.61	122.70
2	V	61	PHE	CB-CG-CD1	5.57	124.70	120.80
2	M	165	GLY	CA-C-N	5.57	127.33	116.20
2	S	310	GLU	CG-CD-OE1	5.57	129.44	118.30
2	N	61	PHE	CB-CG-CD1	5.57	124.70	120.80
2	O	310	GLU	CG-CD-OE1	5.57	129.43	118.30
2	M	115	LEU	CA-CB-CG	5.56	128.10	115.30
2	O	61	PHE	CB-CG-CD1	5.56	124.69	120.80
2	T	310	GLU	CG-CD-OE1	5.56	129.42	118.30
2	U	165	GLY	CA-C-N	5.56	127.32	116.20
2	T	115	LEU	CA-CB-CG	5.56	128.09	115.30
2	R	310	GLU	CG-CD-OE1	5.56	129.41	118.30
2	N	310	GLU	CG-CD-OE1	5.56	129.41	118.30
2	M	301	ALA	CA-C-N	5.55	129.42	117.20
2	N	165	GLY	CA-C-N	5.55	127.31	116.20
2	R	165	GLY	CA-C-N	5.55	127.31	116.20
2	S	165	GLY	CA-C-N	5.55	127.31	116.20
2	U	61	PHE	CB-CG-CD1	5.55	124.69	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	R	61	PHE	CB-CG-CD1	5.55	124.69	120.80
2	U	301	ALA	CA-C-N	5.55	129.42	117.20
2	P	310	GLU	CG-CD-OE1	5.55	129.40	118.30
2	U	115	LEU	CA-CB-CG	5.55	128.07	115.30
2	V	165	GLY	CA-C-N	5.55	127.30	116.20
1	B	248	ARG	NE-CZ-NH2	5.55	123.08	120.30
2	N	301	ALA	CA-C-N	5.55	129.41	117.20
2	R	115	LEU	CA-CB-CG	5.55	128.07	115.30
2	N	262	LEU	O-C-N	5.55	131.58	122.70
2	P	115	LEU	CA-CB-CG	5.55	128.06	115.30
2	O	115	LEU	CA-CB-CG	5.55	128.06	115.30
2	W	115	LEU	CA-CB-CG	5.55	128.06	115.30
2	O	301	ALA	CA-C-N	5.54	129.40	117.20
2	P	301	ALA	CA-C-N	5.54	129.40	117.20
2	S	301	ALA	CA-C-N	5.54	129.40	117.20
2	T	165	GLY	CA-C-N	5.54	127.29	116.20
2	V	115	LEU	CA-CB-CG	5.54	128.05	115.30
1	E	248	ARG	NE-CZ-NH2	5.54	123.07	120.30
2	S	277	LYS	CB-CG-CD	5.54	126.01	111.60
2	W	165	GLY	CA-C-N	5.54	127.28	116.20
2	X	115	LEU	CA-CB-CG	5.54	128.05	115.30
2	X	301	ALA	CA-C-N	5.54	129.39	117.20
2	V	301	ALA	CA-C-N	5.54	129.39	117.20
2	S	61	PHE	CB-CG-CD1	5.54	124.68	120.80
2	U	277	LYS	CB-CG-CD	5.54	126.00	111.60
2	N	115	LEU	CA-CB-CG	5.54	128.04	115.30
2	P	165	GLY	CA-C-N	5.54	127.28	116.20
2	T	301	ALA	CA-C-N	5.54	129.38	117.20
2	N	42	LYS	CB-CA-C	-5.54	99.33	110.40
2	Q	115	LEU	CA-CB-CG	5.54	128.03	115.30
2	Q	165	GLY	CA-C-N	5.54	127.27	116.20
2	Q	301	ALA	CA-C-N	5.54	129.38	117.20
2	Q	312	ALA	CB-CA-C	5.54	118.40	110.10
2	X	61	PHE	CB-CG-CD1	5.54	124.67	120.80
2	P	42	LYS	CB-CA-C	-5.53	99.33	110.40
2	S	115	LEU	CA-CB-CG	5.53	128.03	115.30
2	M	277	LYS	CB-CG-CD	5.53	125.98	111.60
2	W	301	ALA	CA-C-N	5.53	129.37	117.20
2	W	42	LYS	CB-CA-C	-5.53	99.34	110.40
2	X	128	THR	OG1-CB-CG2	5.53	122.72	110.00
2	S	312	ALA	CB-CA-C	5.53	118.39	110.10
2	W	61	PHE	CB-CG-CD1	5.53	124.67	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	X	312	ALA	CB-CA-C	5.53	118.39	110.10
2	P	277	LYS	CB-CG-CD	5.53	125.97	111.60
2	R	301	ALA	CA-C-N	5.53	129.36	117.20
2	R	312	ALA	CB-CA-C	5.53	118.39	110.10
1	I	248	ARG	NE-CZ-NH2	5.53	123.06	120.30
2	P	312	ALA	CB-CA-C	5.53	118.39	110.10
2	W	277	LYS	CB-CG-CD	5.52	125.96	111.60
2	V	277	LYS	CB-CG-CD	5.52	125.96	111.60
2	X	277	LYS	CB-CG-CD	5.52	125.96	111.60
2	O	42	LYS	CB-CA-C	-5.52	99.36	110.40
2	T	42	LYS	CB-CA-C	-5.52	99.36	110.40
2	T	312	ALA	CB-CA-C	5.52	118.38	110.10
2	X	42	LYS	CB-CA-C	-5.52	99.36	110.40
2	M	42	LYS	CB-CA-C	-5.52	99.37	110.40
2	M	312	ALA	CB-CA-C	5.52	118.38	110.10
2	Q	277	LYS	CB-CG-CD	5.52	125.94	111.60
2	S	353	GLY	CA-C-O	-5.52	110.67	120.60
2	T	277	LYS	CB-CG-CD	5.52	125.94	111.60
2	N	277	LYS	CB-CG-CD	5.51	125.94	111.60
2	R	353	GLY	CA-C-O	-5.51	110.67	120.60
2	R	277	LYS	CB-CG-CD	5.51	125.94	111.60
2	U	312	ALA	CB-CA-C	5.51	118.37	110.10
2	U	353	GLY	CA-C-O	-5.51	110.68	120.60
2	O	277	LYS	CB-CG-CD	5.51	125.93	111.60
2	V	42	LYS	CB-CA-C	-5.51	99.38	110.40
2	W	128	THR	OG1-CB-CG2	5.51	122.68	110.00
2	W	353	GLY	CA-C-O	-5.51	110.68	120.60
2	M	128	THR	OG1-CB-CG2	5.51	122.67	110.00
2	Q	128	THR	OG1-CB-CG2	5.51	122.67	110.00
2	U	128	THR	OG1-CB-CG2	5.51	122.66	110.00
2	W	312	ALA	CB-CA-C	5.51	118.36	110.10
2	P	128	THR	OG1-CB-CG2	5.50	122.66	110.00
2	T	128	THR	OG1-CB-CG2	5.50	122.66	110.00
2	V	128	THR	OG1-CB-CG2	5.50	122.66	110.00
2	V	312	ALA	CB-CA-C	5.50	118.36	110.10
2	V	353	GLY	CA-C-O	-5.50	110.69	120.60
2	U	42	LYS	CB-CA-C	-5.50	99.40	110.40
2	X	353	GLY	CA-C-O	-5.50	110.70	120.60
2	M	353	GLY	CA-C-O	-5.50	110.70	120.60
2	N	312	ALA	CB-CA-C	5.50	118.35	110.10
2	O	128	THR	OG1-CB-CG2	5.50	122.65	110.00
2	Q	353	GLY	CA-C-O	-5.50	110.70	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	R	42	LYS	CB-CA-C	-5.50	99.40	110.40
2	S	42	LYS	CB-CA-C	-5.50	99.40	110.40
2	Q	42	LYS	CB-CA-C	-5.50	99.41	110.40
2	N	128	THR	OG1-CB-CG2	5.50	122.64	110.00
2	O	353	GLY	CA-C-O	-5.50	110.71	120.60
2	P	353	GLY	CA-C-O	-5.50	110.71	120.60
2	S	128	THR	OG1-CB-CG2	5.49	122.64	110.00
2	X	204	MET	N-CA-CB	-5.49	100.72	110.60
1	C	248	ARG	NE-CZ-NH2	5.49	123.04	120.30
2	O	312	ALA	CB-CA-C	5.49	118.33	110.10
2	T	353	GLY	CA-C-O	-5.49	110.72	120.60
2	N	353	GLY	CA-C-O	-5.49	110.73	120.60
2	M	204	MET	N-CA-CB	-5.48	100.73	110.60
2	R	128	THR	OG1-CB-CG2	5.48	122.61	110.00
2	U	285	LEU	O-C-N	-5.48	113.93	122.70
2	W	145	SER	N-CA-CB	5.48	118.72	110.50
1	J	248	ARG	NE-CZ-NH2	5.48	123.04	120.30
2	P	204	MET	N-CA-CB	-5.48	100.74	110.60
2	W	204	MET	N-CA-CB	-5.48	100.74	110.60
2	Q	145	SER	N-CA-CB	5.47	118.71	110.50
1	G	248	ARG	NE-CZ-NH2	5.47	123.04	120.30
2	M	145	SER	N-CA-CB	5.47	118.71	110.50
2	N	145	SER	N-CA-CB	5.47	118.71	110.50
2	O	285	LEU	O-C-N	-5.47	113.95	122.70
2	P	285	LEU	O-C-N	-5.47	113.94	122.70
1	K	248	ARG	NE-CZ-NH2	5.47	123.04	120.30
2	S	145	SER	N-CA-CB	5.47	118.71	110.50
2	N	204	MET	N-CA-CB	-5.47	100.75	110.60
2	S	204	MET	N-CA-CB	-5.47	100.75	110.60
2	V	204	MET	N-CA-CB	-5.47	100.76	110.60
2	Q	204	MET	N-CA-CB	-5.47	100.76	110.60
2	X	145	SER	N-CA-CB	5.47	118.70	110.50
2	X	285	LEU	O-C-N	-5.47	113.95	122.70
2	R	145	SER	N-CA-CB	5.46	118.70	110.50
2	U	204	MET	N-CA-CB	-5.46	100.77	110.60
2	V	285	LEU	O-C-N	-5.46	113.96	122.70
2	U	145	SER	N-CA-CB	5.46	118.69	110.50
2	V	145	SER	N-CA-CB	5.46	118.69	110.50
2	M	285	LEU	O-C-N	-5.46	113.97	122.70
2	O	145	SER	N-CA-CB	5.46	118.68	110.50
2	P	145	SER	N-CA-CB	5.46	118.68	110.50
2	T	204	MET	N-CA-CB	-5.46	100.78	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	T	285	LEU	O-C-N	-5.46	113.97	122.70
2	S	285	LEU	O-C-N	-5.45	113.98	122.70
2	N	285	LEU	O-C-N	-5.45	113.98	122.70
2	O	204	MET	N-CA-CB	-5.45	100.79	110.60
2	R	204	MET	N-CA-CB	-5.45	100.79	110.60
2	R	285	LEU	O-C-N	-5.45	113.98	122.70
2	T	145	SER	N-CA-CB	5.45	118.68	110.50
2	M	242	TYR	CB-CG-CD2	5.45	124.27	121.00
2	U	307	TYR	CB-CG-CD1	-5.45	117.73	121.00
2	W	285	LEU	O-C-N	-5.44	113.99	122.70
1	D	248	ARG	NE-CZ-NH2	5.44	123.02	120.30
2	P	361	LEU	O-C-N	5.43	131.38	122.70
2	Q	285	LEU	O-C-N	-5.43	114.02	122.70
1	A	248	ARG	NE-CZ-NH2	5.42	123.01	120.30
2	O	361	LEU	O-C-N	5.42	131.38	122.70
2	S	361	LEU	O-C-N	5.42	131.38	122.70
2	U	361	LEU	O-C-N	5.42	131.37	122.70
2	W	361	LEU	O-C-N	5.42	131.37	122.70
2	X	361	LEU	O-C-N	5.42	131.37	122.70
2	V	361	LEU	O-C-N	5.41	131.36	122.70
2	M	361	LEU	O-C-N	5.41	131.35	122.70
2	T	361	LEU	O-C-N	5.41	131.35	122.70
2	X	307	TYR	CB-CG-CD1	-5.40	117.76	121.00
2	R	361	LEU	O-C-N	5.40	131.34	122.70
2	M	208	THR	O-C-N	5.39	131.33	122.70
2	N	361	LEU	O-C-N	5.39	131.33	122.70
2	X	84	ALA	O-C-N	5.39	131.33	122.70
2	N	84	ALA	O-C-N	5.39	131.33	122.70
1	C	367	PRO	O-C-N	5.39	131.32	122.70
2	S	84	ALA	O-C-N	5.39	131.32	122.70
2	Q	33	ILE	O-C-N	5.39	131.32	122.70
2	U	84	ALA	O-C-N	5.39	131.32	122.70
2	T	307	TYR	CB-CG-CD1	-5.39	117.77	121.00
2	O	242	TYR	CB-CG-CD2	5.38	124.23	121.00
2	Q	361	LEU	O-C-N	5.38	131.31	122.70
2	S	307	TYR	CB-CG-CD1	-5.38	117.77	121.00
2	Q	208	THR	O-C-N	5.38	131.31	122.70
2	P	84	ALA	O-C-N	5.38	131.30	122.70
2	T	84	ALA	O-C-N	5.38	131.30	122.70
2	O	208	THR	O-C-N	5.37	131.30	122.70
2	O	307	TYR	CB-CG-CD1	-5.37	117.78	121.00
2	V	84	ALA	O-C-N	5.37	131.29	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	U	208	THR	O-C-N	5.37	131.29	122.70
2	W	208	THR	O-C-N	5.37	131.29	122.70
2	T	33	ILE	O-C-N	5.37	131.29	122.70
2	X	242	TYR	CB-CG-CD2	5.37	124.22	121.00
2	R	242	TYR	CB-CG-CD2	5.37	124.22	121.00
2	X	135	LEU	CB-CA-C	5.37	120.40	110.20
2	O	84	ALA	O-C-N	5.37	131.29	122.70
2	T	110	VAL	CG1-CB-CG2	5.37	119.48	110.90
2	V	208	THR	O-C-N	5.37	131.28	122.70
1	J	367	PRO	O-C-N	5.36	131.28	122.70
2	T	242	TYR	CB-CG-CD2	5.36	124.22	121.00
2	W	84	ALA	O-C-N	5.36	131.28	122.70
1	H	248	ARG	NE-CZ-NH2	5.36	122.98	120.30
2	N	33	ILE	O-C-N	5.36	131.28	122.70
2	Q	84	ALA	O-C-N	5.36	131.28	122.70
2	W	33	ILE	O-C-N	5.36	131.28	122.70
2	X	208	THR	O-C-N	5.36	131.28	122.70
1	A	367	PRO	O-C-N	5.36	131.27	122.70
1	L	248	ARG	NE-CZ-NH2	5.36	122.98	120.30
2	M	84	ALA	O-C-N	5.36	131.28	122.70
2	M	110	VAL	CG1-CB-CG2	5.36	119.47	110.90
2	N	307	TYR	CB-CG-CD1	-5.36	117.78	121.00
2	O	110	VAL	CG1-CB-CG2	5.36	119.47	110.90
2	R	84	ALA	O-C-N	5.36	131.27	122.70
2	R	33	ILE	O-C-N	5.36	131.27	122.70
2	S	33	ILE	O-C-N	5.36	131.27	122.70
2	V	33	ILE	O-C-N	5.35	131.26	122.70
2	P	208	THR	O-C-N	5.35	131.26	122.70
1	H	367	PRO	O-C-N	5.35	131.26	122.70
2	U	110	VAL	CG1-CB-CG2	5.35	119.46	110.90
2	Q	135	LEU	CB-CA-C	5.35	120.36	110.20
2	S	208	THR	O-C-N	5.35	131.26	122.70
2	R	208	THR	O-C-N	5.34	131.25	122.70
2	T	208	THR	O-C-N	5.34	131.25	122.70
2	U	242	TYR	CB-CG-CD2	5.34	124.21	121.00
2	N	208	THR	O-C-N	5.34	131.25	122.70
2	P	33	ILE	O-C-N	5.34	131.25	122.70
2	R	135	LEU	CB-CA-C	5.34	120.35	110.20
2	V	110	VAL	CG1-CB-CG2	5.34	119.45	110.90
2	V	242	TYR	CB-CG-CD2	5.34	124.20	121.00
2	M	33	ILE	O-C-N	5.34	131.24	122.70
2	R	110	VAL	CG1-CB-CG2	5.34	119.44	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	U	135	LEU	CB-CA-C	5.34	120.34	110.20
2	W	307	TYR	CB-CG-CD1	-5.34	117.80	121.00
1	K	367	PRO	O-C-N	5.34	131.24	122.70
2	V	307	TYR	CB-CG-CD1	-5.34	117.80	121.00
2	S	110	VAL	CG1-CB-CG2	5.34	119.44	110.90
2	W	110	VAL	CG1-CB-CG2	5.34	119.44	110.90
1	F	367	PRO	O-C-N	5.33	131.24	122.70
2	N	110	VAL	CG1-CB-CG2	5.33	119.44	110.90
1	D	367	PRO	O-C-N	5.33	131.23	122.70
2	M	135	LEU	CB-CA-C	5.33	120.33	110.20
2	O	135	LEU	CB-CA-C	5.33	120.33	110.20
2	P	242	TYR	CB-CG-CD2	5.33	124.20	121.00
2	Q	110	VAL	CG1-CB-CG2	5.33	119.44	110.90
1	G	367	PRO	O-C-N	5.33	131.23	122.70
2	N	55	ASP	CB-CG-OD1	5.33	123.10	118.30
2	N	242	TYR	CB-CG-CD2	5.33	124.20	121.00
2	P	110	VAL	CG1-CB-CG2	5.33	119.43	110.90
2	V	135	LEU	CB-CA-C	5.33	120.33	110.20
2	X	110	VAL	CG1-CB-CG2	5.33	119.43	110.90
2	O	33	ILE	O-C-N	5.33	131.23	122.70
2	W	135	LEU	CB-CA-C	5.33	120.33	110.20
2	T	135	LEU	CB-CA-C	5.33	120.33	110.20
1	L	367	PRO	O-C-N	5.33	131.22	122.70
2	X	33	ILE	O-C-N	5.33	131.22	122.70
2	M	307	TYR	CB-CG-CD1	-5.32	117.81	121.00
2	S	135	LEU	CB-CA-C	5.32	120.31	110.20
1	I	367	PRO	O-C-N	5.32	131.21	122.70
2	P	135	LEU	CB-CA-C	5.32	120.31	110.20
2	R	307	TYR	CB-CG-CD1	-5.32	117.81	121.00
2	U	33	ILE	O-C-N	5.32	131.21	122.70
1	E	367	PRO	O-C-N	5.32	131.20	122.70
2	P	55	ASP	CB-CG-OD1	5.31	123.08	118.30
2	R	55	ASP	CB-CG-OD1	5.31	123.08	118.30
2	T	55	ASP	CB-CG-OD1	5.31	123.08	118.30
2	W	242	TYR	CB-CG-CD2	5.31	124.19	121.00
2	M	55	ASP	CB-CG-OD1	5.31	123.08	118.30
2	R	160	LEU	CA-CB-CG	5.31	127.51	115.30
2	P	307	TYR	CB-CG-CD1	-5.31	117.81	121.00
2	N	135	LEU	CB-CA-C	5.30	120.28	110.20
2	U	160	LEU	CA-CB-CG	5.30	127.50	115.30
2	Q	307	TYR	CB-CG-CD1	-5.30	117.82	121.00
2	Q	160	LEU	CA-CB-CG	5.30	127.49	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	S	242	TYR	CB-CG-CD2	5.30	124.18	121.00
2	V	160	LEU	CA-CB-CG	5.30	127.49	115.30
2	M	335	GLN	CG-CD-NE2	5.30	129.41	116.70
2	O	160	LEU	CA-CB-CG	5.30	127.48	115.30
2	P	160	LEU	CA-CB-CG	5.30	127.48	115.30
2	Q	55	ASP	CB-CG-OD1	5.30	123.07	118.30
2	O	55	ASP	CB-CG-OD1	5.29	123.07	118.30
2	N	160	LEU	CA-CB-CG	5.29	127.47	115.30
2	O	335	GLN	CG-CD-NE2	5.29	129.40	116.70
2	V	55	ASP	CB-CG-OD1	5.29	123.06	118.30
2	W	160	LEU	CA-CB-CG	5.29	127.47	115.30
2	W	335	GLN	CG-CD-NE2	5.29	129.40	116.70
2	X	160	LEU	CA-CB-CG	5.29	127.47	115.30
1	B	367	PRO	O-C-N	5.29	131.16	122.70
2	S	335	GLN	CG-CD-NE2	5.29	129.39	116.70
2	T	160	LEU	CA-CB-CG	5.29	127.47	115.30
2	W	55	ASP	CB-CG-OD1	5.29	123.06	118.30
1	L	124	VAL	CB-CA-C	-5.29	101.36	111.40
2	T	335	GLN	CG-CD-NE2	5.29	129.39	116.70
2	U	335	GLN	CG-CD-NE2	5.29	129.39	116.70
1	D	124	VAL	CB-CA-C	-5.28	101.36	111.40
2	M	237	THR	CA-CB-CG2	-5.28	105.00	112.40
2	Q	335	GLN	CG-CD-NE2	5.28	129.38	116.70
2	U	55	ASP	CB-CG-OD1	5.28	123.06	118.30
2	V	335	GLN	CG-CD-NE2	5.28	129.38	116.70
2	S	160	LEU	CA-CB-CG	5.28	127.45	115.30
2	M	160	LEU	CA-CB-CG	5.28	127.45	115.30
2	S	55	ASP	CB-CG-OD1	5.28	123.05	118.30
2	P	335	GLN	CG-CD-NE2	5.28	129.37	116.70
2	N	335	GLN	CG-CD-NE2	5.28	129.36	116.70
2	R	335	GLN	CG-CD-NE2	5.27	129.35	116.70
2	X	335	GLN	CG-CD-NE2	5.27	129.35	116.70
2	Q	237	THR	CA-CB-CG2	-5.27	105.03	112.40
2	N	237	THR	CA-CB-CG2	-5.26	105.03	112.40
1	F	124	VAL	CB-CA-C	-5.26	101.40	111.40
1	I	124	VAL	CB-CA-C	-5.26	101.40	111.40
1	K	124	VAL	CB-CA-C	-5.26	101.41	111.40
1	C	124	VAL	CB-CA-C	-5.26	101.41	111.40
1	H	124	VAL	CB-CA-C	-5.26	101.41	111.40
1	J	124	VAL	CB-CA-C	-5.26	101.41	111.40
2	T	237	THR	CA-CB-CG2	-5.26	105.04	112.40
1	G	124	VAL	CB-CA-C	-5.26	101.41	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	124	VAL	CB-CA-C	-5.26	101.41	111.40
2	S	237	THR	CA-CB-CG2	-5.25	105.04	112.40
2	V	237	THR	CA-CB-CG2	-5.25	105.04	112.40
1	A	124	VAL	CB-CA-C	-5.25	101.42	111.40
2	R	237	THR	CA-CB-CG2	-5.25	105.05	112.40
2	U	237	THR	CA-CB-CG2	-5.25	105.05	112.40
1	E	124	VAL	CB-CA-C	-5.25	101.43	111.40
2	Q	242	TYR	CB-CG-CD2	5.25	124.15	121.00
2	X	237	THR	CA-CB-CG2	-5.25	105.06	112.40
2	P	237	THR	CA-CB-CG2	-5.24	105.06	112.40
2	W	237	THR	CA-CB-CG2	-5.24	105.06	112.40
2	X	55	ASP	CB-CG-OD1	5.24	123.02	118.30
2	N	103	LEU	CB-CA-C	5.24	120.15	110.20
2	P	103	LEU	CB-CA-C	5.24	120.15	110.20
2	W	103	LEU	CB-CA-C	5.24	120.15	110.20
2	O	237	THR	CA-CB-CG2	-5.23	105.07	112.40
2	X	103	LEU	CB-CA-C	5.23	120.14	110.20
2	U	103	LEU	CB-CA-C	5.23	120.13	110.20
2	Q	103	LEU	CB-CA-C	5.23	120.13	110.20
2	S	103	LEU	CB-CA-C	5.22	120.13	110.20
2	V	103	LEU	CB-CA-C	5.22	120.13	110.20
2	M	103	LEU	CB-CA-C	5.22	120.12	110.20
2	T	103	LEU	CB-CA-C	5.22	120.11	110.20
2	R	103	LEU	CB-CA-C	5.21	120.11	110.20
2	O	103	LEU	CB-CA-C	5.21	120.10	110.20
2	R	353	GLY	O-C-N	5.21	131.03	122.70
2	U	353	GLY	O-C-N	5.21	131.03	122.70
2	W	339	PHE	CB-CG-CD2	-5.20	117.16	120.80
2	Q	311	LEU	CB-CG-CD2	-5.20	102.16	111.00
2	U	311	LEU	CB-CG-CD2	-5.20	102.16	111.00
2	W	155	TYR	CD1-CE1-CZ	5.20	124.48	119.80
2	M	353	GLY	O-C-N	5.20	131.01	122.70
2	N	312	ALA	CA-C-N	-5.19	105.78	117.20
2	S	307	TYR	CB-CG-CD2	5.19	124.12	121.00
2	S	322	GLU	CG-CD-OE1	-5.19	107.92	118.30
2	M	322	GLU	CG-CD-OE1	-5.19	107.92	118.30
2	N	311	LEU	CB-CG-CD2	-5.19	102.18	111.00
2	X	353	GLY	O-C-N	5.19	131.00	122.70
2	T	339	PHE	CB-CG-CD2	-5.19	117.17	120.80
2	O	10	TRP	CB-CG-CD1	5.19	133.74	127.00
2	W	322	GLU	CG-CD-OE1	-5.19	107.93	118.30
2	X	311	LEU	CB-CG-CD2	-5.19	102.18	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	R	312	ALA	CA-C-N	-5.19	105.79	117.20
2	T	307	TYR	CB-CG-CD2	5.18	124.11	121.00
2	U	90	TYR	CB-CG-CD1	-5.18	117.89	121.00
2	V	311	LEU	CB-CG-CD2	-5.18	102.19	111.00
2	V	353	GLY	O-C-N	5.18	131.00	122.70
2	O	311	LEU	CB-CG-CD2	-5.18	102.19	111.00
2	P	272	ASN	CA-C-O	-5.18	109.22	120.10
2	T	322	GLU	CG-CD-OE1	-5.18	107.94	118.30
2	W	312	ALA	CA-C-N	-5.18	105.80	117.20
2	N	272	ASN	CA-C-O	-5.18	109.22	120.10
2	O	322	GLU	CG-CD-OE1	-5.18	107.94	118.30
2	P	311	LEU	CB-CG-CD2	-5.18	102.19	111.00
2	V	322	GLU	CG-CD-OE1	-5.18	107.94	118.30
2	M	311	LEU	CB-CG-CD2	-5.18	102.20	111.00
2	O	272	ASN	CA-C-O	-5.18	109.22	120.10
2	S	353	GLY	O-C-N	5.18	130.98	122.70
2	N	10	TRP	CB-CG-CD1	5.18	133.73	127.00
2	N	322	GLU	CG-CD-OE1	-5.18	107.95	118.30
2	Q	322	GLU	CG-CD-OE1	-5.18	107.95	118.30
2	R	311	LEU	CB-CG-CD2	-5.18	102.20	111.00
2	S	311	LEU	CB-CG-CD2	-5.18	102.20	111.00
2	U	307	TYR	CB-CG-CD2	5.18	124.11	121.00
2	P	322	GLU	CG-CD-OE1	-5.17	107.95	118.30
2	Q	312	ALA	CA-C-N	-5.17	105.82	117.20
2	T	311	LEU	CB-CG-CD2	-5.17	102.20	111.00
2	U	322	GLU	CG-CD-OE1	-5.17	107.95	118.30
2	W	272	ASN	CA-C-O	-5.17	109.23	120.10
2	W	353	GLY	O-C-N	5.17	130.98	122.70
2	M	312	ALA	CA-C-N	-5.17	105.82	117.20
2	R	322	GLU	CG-CD-OE1	-5.17	107.95	118.30
2	V	90	TYR	CB-CG-CD1	-5.17	117.90	121.00
2	M	90	TYR	CB-CG-CD1	-5.17	117.90	121.00
2	N	353	GLY	O-C-N	5.17	130.98	122.70
2	Q	155	TYR	CD1-CE1-CZ	5.17	124.45	119.80
2	R	272	ASN	CA-C-O	-5.17	109.24	120.10
2	X	312	ALA	CA-C-N	-5.17	105.82	117.20
2	M	155	TYR	CD1-CE1-CZ	5.17	124.45	119.80
2	R	90	TYR	CB-CG-CD1	-5.17	117.90	121.00
2	S	90	TYR	CB-CG-CD1	-5.17	117.90	121.00
2	V	312	ALA	CA-C-N	-5.17	105.83	117.20
2	O	353	GLY	O-C-N	5.17	130.97	122.70
2	P	353	GLY	O-C-N	5.17	130.97	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	Q	68	GLY	O-C-N	-5.17	114.42	123.20
2	R	10	TRP	CB-CG-CD1	5.17	133.72	127.00
2	T	353	GLY	O-C-N	5.17	130.97	122.70
2	U	312	ALA	CA-C-N	-5.17	105.83	117.20
2	X	246	VAL	CA-CB-CG2	-5.17	103.15	110.90
2	X	339	PHE	CB-CG-CD2	-5.17	117.18	120.80
2	N	68	GLY	O-C-N	-5.17	114.42	123.20
2	P	246	VAL	CA-CB-CG2	-5.17	103.15	110.90
2	P	312	ALA	CA-C-N	-5.17	105.84	117.20
2	X	155	TYR	CD1-CE1-CZ	5.17	124.45	119.80
2	S	68	GLY	O-C-N	-5.17	114.42	123.20
2	M	272	ASN	CA-C-O	-5.16	109.26	120.10
2	O	312	ALA	CA-C-N	-5.16	105.84	117.20
2	T	246	VAL	CA-CB-CG2	-5.16	103.16	110.90
2	T	312	ALA	CA-C-N	-5.16	105.84	117.20
2	V	10	TRP	CB-CG-CD1	5.16	133.71	127.00
2	V	272	ASN	CA-C-O	-5.16	109.26	120.10
2	W	10	TRP	CB-CG-CD1	5.16	133.71	127.00
2	W	68	GLY	O-C-N	-5.16	114.42	123.20
2	P	90	TYR	CB-CG-CD1	-5.16	117.90	121.00
2	Q	90	TYR	CB-CG-CD1	-5.16	117.90	121.00
2	S	312	ALA	CA-C-N	-5.16	105.84	117.20
2	U	155	TYR	CD1-CE1-CZ	5.16	124.45	119.80
2	W	311	LEU	CB-CG-CD2	-5.16	102.22	111.00
2	X	10	TRP	CB-CG-CD1	5.16	133.71	127.00
2	M	246	VAL	CA-CB-CG2	-5.16	103.16	110.90
2	Q	353	GLY	O-C-N	5.16	130.96	122.70
2	R	155	TYR	CD1-CE1-CZ	5.16	124.44	119.80
2	R	246	VAL	CA-CB-CG2	-5.16	103.16	110.90
2	T	339	PHE	CG-CD2-CE2	-5.16	115.12	120.80
2	X	322	GLU	CG-CD-OE1	-5.16	107.98	118.30
2	M	10	TRP	CB-CG-CD1	5.16	133.70	127.00
2	Q	272	ASN	CA-C-O	-5.16	109.27	120.10
2	T	10	TRP	CB-CG-CD1	5.16	133.70	127.00
2	U	10	TRP	CB-CG-CD1	5.16	133.70	127.00
2	X	346	ALA	O-C-N	-5.16	114.45	122.70
2	Q	346	ALA	O-C-N	-5.16	114.45	122.70
2	W	90	TYR	CB-CG-CD1	-5.16	117.91	121.00
2	M	339	PHE	CB-CG-CD2	-5.15	117.19	120.80
2	R	68	GLY	O-C-N	-5.15	114.44	123.20
2	S	339	PHE	CB-CG-CD2	-5.15	117.19	120.80
2	X	272	ASN	CA-C-O	-5.15	109.28	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	O	246	VAL	CA-CB-CG2	-5.15	103.17	110.90
2	T	155	TYR	CD1-CE1-CZ	5.15	124.44	119.80
2	V	155	TYR	CD1-CE1-CZ	5.15	124.44	119.80
2	P	10	TRP	CB-CG-CD1	5.15	133.70	127.00
2	T	90	TYR	CB-CG-CD1	-5.15	117.91	121.00
2	U	272	ASN	CA-C-O	-5.15	109.28	120.10
2	X	90	TYR	CB-CG-CD1	-5.15	117.91	121.00
2	M	68	GLY	O-C-N	-5.15	114.45	123.20
2	M	339	PHE	CG-CD2-CE2	-5.15	115.14	120.80
2	Q	307	TYR	CB-CG-CD2	5.15	124.09	121.00
2	S	246	VAL	CA-CB-CG2	-5.15	103.18	110.90
2	T	68	GLY	O-C-N	-5.15	114.45	123.20
2	V	246	VAL	CA-CB-CG2	-5.15	103.18	110.90
2	M	346	ALA	O-C-N	-5.14	114.47	122.70
2	S	272	ASN	CA-C-O	-5.14	109.30	120.10
2	Q	246	VAL	CA-CB-CG2	-5.14	103.19	110.90
2	S	10	TRP	CB-CG-CD1	5.14	133.69	127.00
2	T	272	ASN	CA-C-O	-5.14	109.30	120.10
2	V	68	GLY	O-C-N	-5.14	114.46	123.20
2	S	339	PHE	CG-CD2-CE2	-5.14	115.14	120.80
2	U	68	GLY	O-C-N	-5.14	114.46	123.20
2	W	339	PHE	CG-CD2-CE2	-5.14	115.15	120.80
2	O	155	TYR	CD1-CE1-CZ	5.14	124.42	119.80
2	Q	339	PHE	CG-CD2-CE2	-5.13	115.15	120.80
2	O	339	PHE	CG-CD2-CE2	-5.13	115.15	120.80
2	P	155	TYR	CD1-CE1-CZ	5.13	124.42	119.80
2	U	246	VAL	CA-CB-CG2	-5.13	103.20	110.90
2	V	339	PHE	CB-CG-CD2	-5.13	117.21	120.80
2	N	246	VAL	CA-CB-CG2	-5.13	103.20	110.90
2	N	339	PHE	CB-CG-CD2	-5.13	117.21	120.80
2	O	68	GLY	O-C-N	-5.13	114.48	123.20
2	Q	10	TRP	CB-CG-CD1	5.13	133.67	127.00
2	R	339	PHE	CB-CG-CD2	-5.13	117.21	120.80
2	R	346	ALA	O-C-N	-5.13	114.49	122.70
2	W	246	VAL	CA-CB-CG2	-5.13	103.20	110.90
2	N	346	ALA	O-C-N	-5.13	114.49	122.70
2	M	307	TYR	CB-CG-CD2	5.13	124.08	121.00
2	V	346	ALA	O-C-N	-5.13	114.50	122.70
2	U	339	PHE	CB-CG-CD2	-5.12	117.21	120.80
2	V	339	PHE	CG-CD2-CE2	-5.12	115.16	120.80
2	P	346	ALA	O-C-N	-5.12	114.50	122.70
2	S	155	TYR	CD1-CE1-CZ	5.12	124.41	119.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	S	367	ARG	CD-NE-CZ	-5.12	116.43	123.60
2	X	307	TYR	CB-CG-CD2	5.12	124.07	121.00
2	N	155	TYR	CD1-CE1-CZ	5.12	124.41	119.80
2	Q	339	PHE	CB-CG-CD2	-5.12	117.22	120.80
2	T	346	ALA	O-C-N	-5.12	114.50	122.70
2	U	346	ALA	O-C-N	-5.12	114.50	122.70
2	X	339	PHE	CG-CD2-CE2	-5.12	115.17	120.80
2	P	339	PHE	CB-CG-CD2	-5.12	117.22	120.80
2	P	367	ARG	CD-NE-CZ	-5.12	116.43	123.60
2	P	68	GLY	O-C-N	-5.12	114.50	123.20
2	N	104	ILE	O-C-N	5.12	130.89	122.70
2	P	339	PHE	CG-CD2-CE2	-5.12	115.17	120.80
2	S	346	ALA	O-C-N	-5.12	114.51	122.70
2	S	104	ILE	O-C-N	5.11	130.88	122.70
2	N	339	PHE	CG-CD2-CE2	-5.11	115.18	120.80
2	O	339	PHE	CB-CG-CD2	-5.11	117.22	120.80
2	V	307	TYR	CB-CG-CD2	5.11	124.07	121.00
2	X	68	GLY	O-C-N	-5.11	114.52	123.20
2	N	307	TYR	CB-CG-CD2	5.11	124.06	121.00
2	P	307	TYR	CB-CG-CD2	5.11	124.06	121.00
2	R	339	PHE	CG-CD2-CE2	-5.11	115.18	120.80
2	W	346	ALA	O-C-N	-5.11	114.53	122.70
2	M	367	ARG	CD-NE-CZ	-5.10	116.45	123.60
2	N	90	TYR	CB-CG-CD1	-5.10	117.94	121.00
2	O	346	ALA	O-C-N	-5.10	114.53	122.70
2	O	307	TYR	CB-CG-CD2	5.10	124.06	121.00
2	O	90	TYR	CB-CG-CD1	-5.10	117.94	121.00
2	W	307	TYR	CB-CG-CD2	5.10	124.06	121.00
2	X	104	ILE	O-C-N	5.10	130.86	122.70
2	W	367	ARG	CD-NE-CZ	-5.09	116.47	123.60
2	O	367	ARG	CD-NE-CZ	-5.09	116.47	123.60
2	U	104	ILE	O-C-N	5.09	130.85	122.70
2	Q	104	ILE	O-C-N	5.09	130.84	122.70
2	U	339	PHE	CG-CD2-CE2	-5.09	115.20	120.80
2	R	367	ARG	CD-NE-CZ	-5.09	116.47	123.60
2	Q	117	TYR	O-C-N	5.09	130.84	122.70
2	V	104	ILE	O-C-N	5.09	130.84	122.70
2	V	367	ARG	CD-NE-CZ	-5.09	116.48	123.60
2	M	117	TYR	O-C-N	5.08	130.84	122.70
2	P	117	TYR	O-C-N	5.08	130.84	122.70
2	T	117	TYR	O-C-N	5.08	130.83	122.70
2	U	112	ALA	N-CA-CB	5.08	117.22	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	U	117	TYR	O-C-N	5.08	130.83	122.70
2	X	367	ARG	CD-NE-CZ	-5.08	116.48	123.60
2	Q	367	ARG	CD-NE-CZ	-5.08	116.49	123.60
2	W	104	ILE	O-C-N	5.08	130.83	122.70
2	O	117	TYR	O-C-N	5.08	130.82	122.70
2	T	367	ARG	CD-NE-CZ	-5.08	116.49	123.60
2	R	307	TYR	CB-CG-CD2	5.07	124.04	121.00
2	V	117	TYR	O-C-N	5.07	130.82	122.70
2	O	104	ILE	O-C-N	5.07	130.81	122.70
2	T	104	ILE	O-C-N	5.07	130.81	122.70
2	N	112	ALA	N-CA-CB	5.07	117.20	110.10
2	P	104	ILE	O-C-N	5.07	130.81	122.70
2	M	104	ILE	O-C-N	5.07	130.81	122.70
2	X	117	TYR	O-C-N	5.07	130.81	122.70
2	M	167	TYR	CG-CD1-CE1	-5.07	117.25	121.30
2	S	117	TYR	O-C-N	5.06	130.80	122.70
2	N	117	TYR	O-C-N	5.06	130.79	122.70
2	O	167	TYR	CG-CD1-CE1	-5.06	117.25	121.30
2	R	117	TYR	O-C-N	5.06	130.80	122.70
2	U	367	ARG	CD-NE-CZ	-5.06	116.52	123.60
2	M	112	ALA	N-CA-CB	5.06	117.18	110.10
2	R	104	ILE	O-C-N	5.06	130.79	122.70
2	X	112	ALA	N-CA-CB	5.06	117.18	110.10
2	V	112	ALA	N-CA-CB	5.05	117.17	110.10
2	W	117	TYR	O-C-N	5.05	130.78	122.70
2	O	112	ALA	N-CA-CB	5.04	117.16	110.10
2	N	340	TRP	CD1-NE1-CE2	5.04	113.54	109.00
2	N	367	ARG	CD-NE-CZ	-5.04	116.54	123.60
2	R	112	ALA	N-CA-CB	5.04	117.16	110.10
2	Q	167	TYR	CG-CD1-CE1	-5.04	117.27	121.30
2	S	167	TYR	CG-CD1-CE1	-5.04	117.27	121.30
2	U	8	VAL	CB-CA-C	5.04	120.97	111.40
2	T	112	ALA	N-CA-CB	5.04	117.15	110.10
2	T	167	TYR	CG-CD1-CE1	-5.04	117.27	121.30
2	X	340	TRP	CD1-NE1-CE2	5.03	113.53	109.00
2	N	8	VAL	CB-CA-C	5.03	120.96	111.40
2	S	112	ALA	N-CA-CB	5.03	117.14	110.10
2	U	167	TYR	CG-CD1-CE1	-5.03	117.28	121.30
2	T	340	TRP	CD1-NE1-CE2	5.03	113.53	109.00
2	P	112	ALA	N-CA-CB	5.03	117.14	110.10
2	Q	112	ALA	N-CA-CB	5.03	117.14	110.10
2	S	8	VAL	CB-CA-C	5.03	120.95	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	V	167	TYR	CG-CD1-CE1	-5.03	117.28	121.30
2	W	340	TRP	CD1-NE1-CE2	5.02	113.52	109.00
2	R	340	TRP	CD1-NE1-CE2	5.02	113.52	109.00
2	N	129	TRP	CH2-CZ2-CE2	-5.02	112.38	117.40
2	V	340	TRP	CD1-NE1-CE2	5.02	113.52	109.00
2	R	129	TRP	CH2-CZ2-CE2	-5.02	112.38	117.40
2	V	8	VAL	CB-CA-C	5.01	120.93	111.40
2	P	340	TRP	CD1-NE1-CE2	5.01	113.51	109.00
2	W	112	ALA	N-CA-CB	5.01	117.12	110.10
2	O	129	TRP	CH2-CZ2-CE2	-5.01	112.39	117.40
2	S	340	TRP	CD1-NE1-CE2	5.01	113.51	109.00
2	T	8	VAL	CB-CA-C	5.01	120.92	111.40
2	R	167	TYR	CG-CD1-CE1	-5.01	117.29	121.30
2	X	8	VAL	CB-CA-C	5.01	120.91	111.40
2	O	8	VAL	CB-CA-C	5.00	120.91	111.40
2	P	8	VAL	CB-CA-C	5.00	120.91	111.40
2	W	8	VAL	CB-CA-C	5.00	120.91	111.40
2	M	8	VAL	CB-CA-C	5.00	120.91	111.40
2	M	278	GLU	CB-CG-CD	5.00	127.70	114.20
2	O	335	GLN	CG-CD-OE1	-5.00	111.60	121.60
2	R	8	VAL	CB-CA-C	5.00	120.90	111.40
2	R	278	GLU	CB-CG-CD	5.00	127.70	114.20
2	T	110	VAL	O-C-N	5.00	130.70	122.70
2	W	167	TYR	CG-CD1-CE1	-5.00	117.30	121.30

There are no chirality outliers.

All (24) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	M	312	ALA	Peptide
2	M	354	ARG	Sidechain
2	N	312	ALA	Peptide
2	N	354	ARG	Sidechain
2	O	312	ALA	Peptide
2	O	354	ARG	Sidechain
2	P	312	ALA	Peptide
2	P	354	ARG	Sidechain
2	Q	312	ALA	Peptide
2	Q	354	ARG	Sidechain
2	R	312	ALA	Peptide
2	R	354	ARG	Sidechain
2	S	312	ALA	Peptide

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Mol	Chain	Res	Type	Group
2	S	354	ARG	Sidechain
2	T	312	ALA	Peptide
2	T	354	ARG	Sidechain
2	U	312	ALA	Peptide
2	U	354	ARG	Sidechain
2	V	312	ALA	Peptide
2	V	354	ARG	Sidechain
2	W	312	ALA	Peptide
2	W	354	ARG	Sidechain
2	X	312	ALA	Peptide
2	X	354	ARG	Sidechain

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	3626	0	3531	193	0
1	B	3626	0	3531	187	0
1	C	3626	0	3531	183	0
1	D	3626	0	3531	194	0
1	E	3626	0	3531	187	0
1	F	3626	0	3531	193	0
1	G	3626	0	3531	190	0
1	H	3626	0	3531	192	0
1	I	3626	0	3531	189	0
1	J	3626	0	3531	192	0
1	K	3626	0	3531	188	0
1	L	3626	0	3531	193	0
2	M	2861	0	2826	144	0
2	N	2861	0	2826	152	0
2	O	2861	0	2826	149	0
2	P	2861	0	2826	155	0
2	Q	2861	0	2826	149	0
2	R	2861	0	2826	147	0
2	S	2861	0	2826	152	0
2	T	2861	0	2826	146	0
2	U	2861	0	2826	153	0
2	V	2861	0	2826	151	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	W	2861	0	2826	152	0
2	X	2861	0	2826	144	0
3	Y	23	0	20	0	0
3	Z	23	0	20	0	0
3	a	23	0	20	0	0
3	b	23	0	20	0	0
3	c	23	0	20	0	0
3	d	23	0	20	0	0
3	e	23	0	20	0	0
3	f	23	0	20	0	0
3	g	23	0	20	0	0
3	h	23	0	20	0	0
3	i	23	0	20	0	0
3	j	23	0	20	0	0
All	All	78120	0	76524	3377	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 22.

All (3377) 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:K:43:PHE:HB3	2:W:370:LYS:CE	1.36	1.55
1:B:43:PHE:HB3	2:N:370:LYS:CE	1.36	1.55
1:L:43:PHE:HB3	2:X:370:LYS:CE	1.36	1.54
1:A:43:PHE:HB3	2:M:370:LYS:CE	1.36	1.54
1:E:43:PHE:HB3	2:Q:370:LYS:CE	1.36	1.51
1:J:43:PHE:HB3	2:V:370:LYS:CE	1.36	1.51
1:C:43:PHE:HB3	2:O:370:LYS:CE	1.36	1.51
1:H:43:PHE:HB3	2:T:370:LYS:CE	1.36	1.50
1:D:43:PHE:HB3	2:P:370:LYS:CE	1.36	1.50
1:I:43:PHE:HB3	2:U:370:LYS:CE	1.36	1.50
1:G:43:PHE:HB3	2:S:370:LYS:CE	1.36	1.49
1:F:43:PHE:HB3	2:R:370:LYS:CE	1.36	1.48
2:P:369:THR:C	2:P:370:LYS:N	1.68	1.47
2:U:369:THR:C	2:U:370:LYS:N	1.67	1.47
1:D:43:PHE:CB	2:P:370:LYS:HE2	1.44	1.47
2:Q:369:THR:C	2:Q:370:LYS:N	1.68	1.47
1:I:43:PHE:CB	2:U:370:LYS:HE2	1.45	1.47
2:T:369:THR:C	2:T:370:LYS:N	1.68	1.47
1:C:43:PHE:CB	2:O:370:LYS:HE2	1.45	1.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:43:PHE:CB	2:V:370:LYS:HE2	1.45	1.46
2:O:369:THR:C	2:O:370:LYS:N	1.68	1.46
2:V:369:THR:C	2:V:370:LYS:N	1.67	1.46
2:X:369:THR:C	2:X:370:LYS:N	1.67	1.45
1:E:43:PHE:CB	2:Q:370:LYS:HE2	1.44	1.45
1:H:43:PHE:CB	2:T:370:LYS:HE2	1.44	1.45
2:W:369:THR:C	2:W:370:LYS:N	1.67	1.44
1:B:43:PHE:CB	2:N:370:LYS:HE2	1.44	1.44
1:K:43:PHE:CB	2:W:370:LYS:HE2	1.44	1.44
2:M:369:THR:C	2:M:370:LYS:N	1.68	1.44
2:N:369:THR:C	2:N:370:LYS:N	1.67	1.44
1:A:43:PHE:CB	2:M:370:LYS:HE2	1.44	1.44
1:G:43:PHE:CB	2:S:370:LYS:HE2	1.45	1.44
2:S:369:THR:C	2:S:370:LYS:N	1.67	1.44
1:L:43:PHE:CB	2:X:370:LYS:HE2	1.45	1.43
1:F:43:PHE:CB	2:R:370:LYS:HE2	1.44	1.43
2:R:369:THR:C	2:R:370:LYS:N	1.67	1.42
1:C:4:HIS:C	2:O:179:LYS:HZ3	1.22	1.42
1:B:4:HIS:C	2:N:179:LYS:HZ3	1.21	1.42
1:J:4:HIS:C	2:V:179:LYS:HZ3	1.20	1.42
1:K:4:HIS:C	2:W:179:LYS:HZ3	1.21	1.42
1:L:4:HIS:C	2:X:179:LYS:HZ3	1.22	1.42
1:A:4:HIS:C	2:M:179:LYS:HZ3	1.23	1.42
1:H:4:HIS:C	2:T:179:LYS:HZ3	1.20	1.42
1:E:4:HIS:C	2:Q:179:LYS:HZ3	1.20	1.40
1:G:4:HIS:C	2:S:179:LYS:HZ3	1.21	1.40
1:F:4:HIS:C	2:R:179:LYS:HZ3	1.23	1.39
1:I:4:HIS:C	2:U:179:LYS:HZ3	1.20	1.38
1:D:4:HIS:C	2:P:179:LYS:HZ3	1.20	1.37
1:A:337:ARG:HB2	1:B:61:ASN:O	1.36	1.25
1:I:61:ASN:O	1:J:337:ARG:HB2	1.30	1.24
1:F:5:VAL:N	2:R:179:LYS:NZ	1.87	1.23
1:G:5:VAL:N	2:S:179:LYS:NZ	1.87	1.23
1:A:5:VAL:N	2:M:179:LYS:NZ	1.87	1.23
1:B:5:VAL:N	2:N:179:LYS:NZ	1.87	1.23
1:E:4:HIS:CD2	2:Q:178:ILE:HG13	1.74	1.23
1:F:4:HIS:CD2	2:R:178:ILE:HG13	1.74	1.23
1:G:4:HIS:CD2	2:S:178:ILE:HG13	1.74	1.23
1:H:4:HIS:CD2	2:T:178:ILE:HG13	1.74	1.23
1:H:5:VAL:N	2:T:179:LYS:NZ	1.87	1.23
1:L:5:VAL:N	2:X:179:LYS:NZ	1.87	1.23

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:239:LYS:O	2:R:239:LYS:HE3	1.39	1.23
1:K:5:VAL:N	2:W:179:LYS:NZ	1.87	1.22
2:M:239:LYS:O	2:M:239:LYS:HE3	1.39	1.22
2:S:239:LYS:O	2:S:239:LYS:HE3	1.39	1.22
1:E:5:VAL:N	2:Q:179:LYS:NZ	1.87	1.22
2:X:239:LYS:O	2:X:239:LYS:HE3	1.39	1.22
1:A:4:HIS:CD2	2:M:178:ILE:HG13	1.74	1.22
1:C:5:VAL:N	2:O:179:LYS:NZ	1.87	1.22
1:I:4:HIS:CD2	2:U:178:ILE:HG13	1.74	1.22
1:D:4:HIS:CD2	2:P:178:ILE:HG13	1.74	1.21
1:J:5:VAL:N	2:V:179:LYS:NZ	1.87	1.21
1:L:4:HIS:CD2	2:X:178:ILE:HG13	1.74	1.21
1:D:5:VAL:N	2:P:179:LYS:NZ	1.87	1.21
1:G:61:ASN:O	1:H:337:ARG:HB2	1.35	1.21
1:K:4:HIS:CD2	2:W:178:ILE:HG13	1.74	1.21
2:W:239:LYS:O	2:W:239:LYS:HE3	1.39	1.21
1:B:4:HIS:CD2	2:N:178:ILE:HG13	1.74	1.21
1:C:4:HIS:CD2	2:O:178:ILE:HG13	1.74	1.21
1:I:5:VAL:N	2:U:179:LYS:NZ	1.87	1.21
1:J:4:HIS:CD2	2:V:178:ILE:HG13	1.74	1.21
2:N:239:LYS:HE3	2:N:239:LYS:O	1.39	1.21
2:T:239:LYS:O	2:T:239:LYS:HE3	1.39	1.21
2:Q:239:LYS:HE3	2:Q:239:LYS:O	1.39	1.20
1:J:61:ASN:O	1:K:337:ARG:HB2	1.42	1.20
1:C:337:ARG:HB2	1:D:61:ASN:O	1.37	1.19
2:U:239:LYS:O	2:U:239:LYS:HE3	1.39	1.18
2:O:239:LYS:O	2:O:239:LYS:HE3	1.39	1.18
2:P:239:LYS:O	2:P:239:LYS:HE3	1.39	1.17
2:V:239:LYS:HE3	2:V:239:LYS:O	1.39	1.17
1:B:4:HIS:C	2:N:179:LYS:NZ	1.99	1.16
1:F:4:HIS:C	2:R:179:LYS:NZ	1.99	1.16
1:K:4:HIS:C	2:W:179:LYS:NZ	1.99	1.16
2:S:311:LEU:O	2:S:312:ALA:HB2	1.34	1.16
1:G:4:HIS:C	2:S:179:LYS:NZ	1.99	1.15
1:E:360:PHE:CD2	1:E:361:PRO:HD3	1.81	1.15
1:F:360:PHE:CD2	1:F:361:PRO:HD3	1.81	1.15
2:R:311:LEU:O	2:R:312:ALA:HB2	1.34	1.15
1:G:360:PHE:CD2	1:G:361:PRO:HD3	1.81	1.15
1:H:360:PHE:CD2	1:H:361:PRO:HD3	1.81	1.15
1:C:360:PHE:CD2	1:C:361:PRO:HD3	1.81	1.14
1:H:4:HIS:C	2:T:179:LYS:NZ	1.99	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:360:PHE:CD2	1:J:361:PRO:HD3	1.81	1.14
2:M:311:LEU:O	2:M:312:ALA:HB2	1.34	1.14
2:T:311:LEU:O	2:T:312:ALA:HB2	1.34	1.14
1:E:4:HIS:C	2:Q:179:LYS:NZ	1.99	1.14
1:J:4:HIS:C	2:V:179:LYS:NZ	1.99	1.14
1:G:337:ARG:HB2	1:L:61:ASN:O	1.46	1.14
1:A:360:PHE:CD2	1:A:361:PRO:HD3	1.81	1.14
1:C:4:HIS:C	2:O:179:LYS:NZ	1.99	1.14
1:D:360:PHE:CD2	1:D:361:PRO:HD3	1.81	1.14
1:I:4:HIS:C	2:U:179:LYS:NZ	1.99	1.14
1:D:4:HIS:C	2:P:179:LYS:NZ	1.99	1.14
1:I:360:PHE:CD2	1:I:361:PRO:HD3	1.81	1.14
1:K:360:PHE:CD2	1:K:361:PRO:HD3	1.81	1.14
1:L:360:PHE:CD2	1:L:361:PRO:HD3	1.81	1.14
1:B:360:PHE:CD2	1:B:361:PRO:HD3	1.81	1.13
2:Q:311:LEU:O	2:Q:312:ALA:HB2	1.34	1.13
2:X:311:LEU:O	2:X:312:ALA:HB2	1.34	1.13
1:A:399:LEU:N	1:A:401:PRO:HG2	1.64	1.13
1:G:399:LEU:N	1:G:401:PRO:HG2	1.64	1.13
1:L:399:LEU:N	1:L:401:PRO:HG2	1.64	1.13
1:B:4:HIS:HD2	2:N:178:ILE:HG13	1.00	1.12
1:F:399:LEU:N	1:F:401:PRO:HG2	1.64	1.12
1:K:4:HIS:HD2	2:W:178:ILE:HG13	1.00	1.12
2:N:311:LEU:O	2:N:312:ALA:HB2	1.34	1.12
2:W:31:THR:HG23	2:W:33:ILE:H	1.09	1.12
1:A:4:HIS:C	2:M:179:LYS:NZ	1.99	1.12
1:L:4:HIS:C	2:X:179:LYS:NZ	1.99	1.12
2:N:31:THR:HG23	2:N:33:ILE:H	1.09	1.12
2:P:311:LEU:O	2:P:312:ALA:HB2	1.34	1.12
2:U:311:LEU:O	2:U:312:ALA:HB2	1.34	1.11
2:O:311:LEU:O	2:O:312:ALA:HB2	1.34	1.11
2:W:311:LEU:O	2:W:312:ALA:HB2	1.34	1.11
1:D:399:LEU:N	1:D:401:PRO:HG2	1.64	1.11
1:E:399:LEU:N	1:E:401:PRO:HG2	1.64	1.11
1:H:399:LEU:N	1:H:401:PRO:HG2	1.64	1.11
1:I:399:LEU:N	1:I:401:PRO:HG2	1.64	1.11
1:B:399:LEU:N	1:B:401:PRO:HG2	1.64	1.10
1:J:399:LEU:N	1:J:401:PRO:HG2	1.64	1.10
2:V:31:THR:HG23	2:V:33:ILE:H	1.09	1.10
2:V:311:LEU:O	2:V:312:ALA:HB2	1.34	1.10
2:X:31:THR:HG23	2:X:33:ILE:H	1.09	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:ILE:HD13	1:A:60:ILE:H	1.08	1.10
1:C:399:LEU:N	1:C:401:PRO:HG2	1.64	1.10
1:J:4:HIS:HD2	2:V:178:ILE:HG13	1.00	1.10
1:K:399:LEU:N	1:K:401:PRO:HG2	1.64	1.10
2:M:31:THR:HG23	2:M:33:ILE:H	1.09	1.10
1:C:4:HIS:HD2	2:O:178:ILE:HG13	1.00	1.10
1:A:4:HIS:HD2	2:M:178:ILE:HG13	1.00	1.10
1:L:60:ILE:HD13	1:L:60:ILE:H	1.08	1.10
1:L:4:HIS:HD2	2:X:178:ILE:HG13	1.00	1.09
2:Q:31:THR:HG23	2:Q:33:ILE:H	1.09	1.09
2:O:31:THR:HG23	2:O:33:ILE:H	1.09	1.09
2:T:31:THR:HG23	2:T:33:ILE:H	1.08	1.09
1:F:399:LEU:H	1:F:401:PRO:HG2	0.95	1.09
1:K:60:ILE:HD13	1:K:60:ILE:H	1.08	1.09
2:S:31:THR:HG23	2:S:33:ILE:H	1.08	1.09
1:B:60:ILE:H	1:B:60:ILE:HD13	1.08	1.09
2:P:31:THR:HG23	2:P:33:ILE:H	1.09	1.09
1:B:400:PRO:HB3	1:B:405:LYS:HE3	1.35	1.08
1:K:400:PRO:HB3	1:K:405:LYS:HE3	1.35	1.08
2:R:31:THR:HG23	2:R:33:ILE:H	1.09	1.08
1:F:60:ILE:HD13	1:F:60:ILE:H	1.08	1.08
1:J:60:ILE:H	1:J:60:ILE:HD13	1.08	1.08
1:A:399:LEU:H	1:A:401:PRO:HG2	0.95	1.08
1:G:399:LEU:H	1:G:401:PRO:HG2	0.95	1.08
1:E:60:ILE:HD13	1:E:60:ILE:H	1.08	1.08
1:J:400:PRO:HB3	1:J:405:LYS:HE3	1.35	1.08
1:L:399:LEU:H	1:L:401:PRO:HG2	0.95	1.08
2:U:31:THR:HG23	2:U:33:ILE:H	1.09	1.08
1:L:400:PRO:HB3	1:L:405:LYS:HE3	1.35	1.07
1:C:60:ILE:HD13	1:C:60:ILE:H	1.08	1.07
1:C:400:PRO:HB3	1:C:405:LYS:HE3	1.35	1.07
1:D:4:HIS:HD2	2:P:178:ILE:HG13	1.00	1.07
1:A:400:PRO:HB3	1:A:405:LYS:HE3	1.35	1.07
1:H:60:ILE:HD13	1:H:60:ILE:H	1.08	1.07
1:I:4:HIS:HD2	2:U:178:ILE:HG13	1.00	1.07
1:G:60:ILE:H	1:G:60:ILE:HD13	1.08	1.07
1:E:399:LEU:H	1:E:401:PRO:HG2	0.95	1.07
1:H:399:LEU:H	1:H:401:PRO:HG2	0.95	1.07
1:D:60:ILE:H	1:D:60:ILE:HD13	1.08	1.06
1:D:400:PRO:HB3	1:D:405:LYS:HE3	1.35	1.06
1:I:400:PRO:HB3	1:I:405:LYS:HE3	1.35	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:60:ILE:HD13	1:I:60:ILE:H	1.08	1.06
1:F:4:HIS:HD2	2:R:178:ILE:HG13	1.00	1.06
1:A:61:ASN:O	1:F:337:ARG:HB2	1.54	1.05
1:B:399:LEU:H	1:B:401:PRO:HG2	0.95	1.05
1:G:4:HIS:HD2	2:S:178:ILE:HG13	1.00	1.05
1:K:399:LEU:H	1:K:401:PRO:HG2	0.95	1.05
1:H:4:HIS:HD2	2:T:178:ILE:HG13	1.00	1.04
1:C:4:HIS:HA	2:O:178:ILE:CD1	1.88	1.04
1:D:4:HIS:HA	2:P:178:ILE:CD1	1.88	1.04
1:D:399:LEU:H	1:D:401:PRO:HG2	0.95	1.04
1:I:4:HIS:HA	2:U:178:ILE:CD1	1.88	1.04
1:J:4:HIS:HA	2:V:178:ILE:CD1	1.88	1.04
1:B:4:HIS:HA	2:N:178:ILE:CD1	1.88	1.04
1:E:4:HIS:HD2	2:Q:178:ILE:HG13	1.00	1.04
1:E:4:HIS:HA	2:Q:178:ILE:CD1	1.88	1.04
1:H:4:HIS:HA	2:T:178:ILE:CD1	1.88	1.04
1:I:399:LEU:H	1:I:401:PRO:HG2	0.95	1.04
1:K:4:HIS:HA	2:W:178:ILE:CD1	1.88	1.04
1:C:399:LEU:H	1:C:401:PRO:HG2	0.95	1.03
1:E:400:PRO:HB3	1:E:405:LYS:HE3	1.35	1.03
1:H:400:PRO:HB3	1:H:405:LYS:HE3	1.34	1.03
1:J:399:LEU:H	1:J:401:PRO:HG2	0.95	1.03
1:F:400:PRO:HB3	1:F:405:LYS:HE3	1.35	1.03
1:G:400:PRO:HB3	1:G:405:LYS:HE3	1.34	1.03
1:I:4:HIS:CB	2:U:179:LYS:NZ	2.21	1.03
1:A:4:HIS:HA	2:M:178:ILE:CD1	1.88	1.03
1:D:4:HIS:CB	2:P:179:LYS:NZ	2.21	1.03
1:L:4:HIS:HA	2:X:178:ILE:CD1	1.88	1.03
2:P:239:LYS:O	2:P:239:LYS:CE	2.07	1.03
2:U:239:LYS:O	2:U:239:LYS:CE	2.07	1.03
1:D:4:HIS:HB3	2:P:179:LYS:HZ2	1.24	1.03
1:F:4:HIS:HD2	2:R:178:ILE:CG1	1.72	1.03
2:U:311:LEU:O	2:U:312:ALA:CB	1.98	1.03
1:E:4:HIS:HD2	2:Q:178:ILE:CG1	1.72	1.02
1:G:4:HIS:HD2	2:S:178:ILE:CG1	1.72	1.02
1:G:4:HIS:HA	2:S:178:ILE:CD1	1.88	1.02
1:H:4:HIS:HD2	2:T:178:ILE:CG1	1.72	1.02
2:P:311:LEU:O	2:P:312:ALA:CB	1.98	1.02
2:S:239:LYS:O	2:S:239:LYS:CE	2.07	1.02
2:O:311:LEU:O	2:O:312:ALA:CB	1.98	1.02
2:R:239:LYS:O	2:R:239:LYS:CE	2.07	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:311:LEU:O	2:V:312:ALA:CB	1.98	1.02
1:F:4:HIS:HA	2:R:178:ILE:CD1	1.88	1.02
1:A:4:HIS:HD2	2:M:178:ILE:CG1	1.72	1.02
1:K:4:HIS:HD2	2:W:178:ILE:CG1	1.72	1.02
2:O:239:LYS:O	2:O:239:LYS:CE	2.07	1.02
1:B:4:HIS:HD2	2:N:178:ILE:CG1	1.72	1.02
1:C:4:HIS:CB	2:O:179:LYS:NZ	2.21	1.02
1:J:4:HIS:HD2	2:V:178:ILE:CG1	1.72	1.02
1:L:4:HIS:HD2	2:X:178:ILE:CG1	1.72	1.02
2:T:239:LYS:O	2:T:239:LYS:CE	2.07	1.02
2:V:239:LYS:O	2:V:239:LYS:CE	2.07	1.02
1:C:4:HIS:HD2	2:O:178:ILE:CG1	1.72	1.01
1:E:4:HIS:HB3	2:Q:179:LYS:HZ2	1.24	1.01
1:G:4:HIS:CB	2:S:179:LYS:NZ	2.21	1.01
2:N:239:LYS:O	2:N:239:LYS:CE	2.07	1.01
2:Q:239:LYS:O	2:Q:239:LYS:CE	2.07	1.01
2:W:239:LYS:O	2:W:239:LYS:CE	2.07	1.01
1:D:4:HIS:HD2	2:P:178:ILE:CG1	1.72	1.01
1:J:4:HIS:CB	2:V:179:LYS:NZ	2.21	1.01
1:L:5:VAL:N	2:X:179:LYS:HZ1	1.56	1.01
1:F:4:HIS:CB	2:R:179:LYS:NZ	2.21	1.01
1:I:4:HIS:HD2	2:U:178:ILE:CG1	1.72	1.01
1:B:4:HIS:CB	2:N:179:LYS:NZ	2.21	1.01
1:K:4:HIS:CB	2:W:179:LYS:NZ	2.21	1.01
1:A:5:VAL:N	2:M:179:LYS:HZ1	1.56	1.01
1:E:4:HIS:CB	2:Q:179:LYS:NZ	2.21	1.01
1:F:5:VAL:N	2:R:179:LYS:HZ1	1.55	1.01
1:I:4:HIS:HB3	2:U:179:LYS:HZ2	1.26	1.01
2:X:239:LYS:O	2:X:239:LYS:CE	2.07	1.01
2:M:239:LYS:O	2:M:239:LYS:CE	2.07	1.00
1:E:337:ARG:HB2	1:F:61:ASN:O	1.61	1.00
1:H:4:HIS:CB	2:T:179:LYS:NZ	2.21	1.00
1:H:61:ASN:O	1:I:337:ARG:HB2	1.61	1.00
1:H:4:HIS:HB3	2:T:179:LYS:HZ2	1.25	1.00
1:C:4:HIS:CA	2:O:178:ILE:HD12	1.91	1.00
1:D:4:HIS:CA	2:P:178:ILE:HD12	1.91	1.00
1:F:4:HIS:CA	2:R:178:ILE:HD12	1.91	1.00
1:K:61:ASN:O	1:L:337:ARG:HB2	1.61	1.00
1:H:4:HIS:CA	2:T:178:ILE:HD12	1.91	1.00
1:J:4:HIS:CA	2:V:178:ILE:HD12	1.91	1.00
2:Q:312:ALA:HB3	2:Q:317:ILE:CG2	1.92	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:312:ALA:HB3	2:T:317:ILE:CG2	1.92	1.00
2:W:31:THR:CG2	2:W:33:ILE:H	1.75	1.00
1:E:4:HIS:CA	2:Q:178:ILE:HD12	1.91	0.99
2:N:31:THR:CG2	2:N:33:ILE:H	1.75	0.99
2:O:312:ALA:HB3	2:O:317:ILE:CG2	1.92	0.99
2:V:312:ALA:HB3	2:V:317:ILE:CG2	1.92	0.99
1:B:4:HIS:CA	2:N:178:ILE:HD12	1.91	0.99
1:G:4:HIS:CA	2:S:178:ILE:HD12	1.91	0.99
1:I:4:HIS:CA	2:U:178:ILE:HD12	1.91	0.99
1:K:4:HIS:CA	2:W:178:ILE:HD12	1.91	0.99
2:M:31:THR:CG2	2:M:33:ILE:H	1.75	0.99
2:N:311:LEU:O	2:N:312:ALA:CB	1.98	0.99
2:V:31:THR:CG2	2:V:33:ILE:H	1.75	0.99
2:O:31:THR:CG2	2:O:33:ILE:H	1.75	0.99
2:W:311:LEU:O	2:W:312:ALA:CB	1.98	0.99
2:X:31:THR:CG2	2:X:33:ILE:H	1.75	0.99
1:A:4:HIS:CA	2:M:178:ILE:HD12	1.91	0.99
1:L:4:HIS:CA	2:X:178:ILE:HD12	1.91	0.99
2:Q:311:LEU:O	2:Q:312:ALA:CB	1.98	0.99
2:R:31:THR:CG2	2:R:33:ILE:H	1.75	0.99
2:S:31:THR:CG2	2:S:33:ILE:H	1.75	0.99
2:T:311:LEU:O	2:T:312:ALA:CB	1.98	0.99
1:A:4:HIS:CB	2:M:179:LYS:NZ	2.21	0.99
2:Q:31:THR:CG2	2:Q:33:ILE:H	1.75	0.99
2:T:31:THR:CG2	2:T:33:ILE:H	1.75	0.99
1:D:337:ARG:HB2	1:E:61:ASN:O	1.60	0.99
2:U:31:THR:CG2	2:U:33:ILE:H	1.75	0.99
2:R:312:ALA:HB3	2:R:317:ILE:CG2	1.92	0.98
1:B:337:ARG:HB2	1:C:61:ASN:O	1.60	0.98
1:L:4:HIS:CB	2:X:179:LYS:NZ	2.21	0.98
2:P:31:THR:CG2	2:P:33:ILE:H	1.75	0.98
2:M:312:ALA:HB3	2:M:317:ILE:CG2	1.92	0.98
2:S:312:ALA:HB3	2:S:317:ILE:CG2	1.92	0.98
2:X:312:ALA:HB3	2:X:317:ILE:CG2	1.92	0.98
2:P:312:ALA:HB3	2:P:317:ILE:CG2	1.92	0.98
2:U:312:ALA:HB3	2:U:317:ILE:CG2	1.92	0.98
1:G:4:HIS:HB3	2:S:179:LYS:HZ2	1.29	0.98
2:N:312:ALA:HB3	2:N:317:ILE:CG2	1.92	0.98
2:W:312:ALA:HB3	2:W:317:ILE:CG2	1.92	0.98
1:J:4:HIS:HB3	2:V:179:LYS:HZ2	1.26	0.98
1:L:4:HIS:HA	2:X:178:ILE:HD12	0.98	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:HIS:HA	2:M:178:ILE:HD12	0.98	0.97
1:B:4:HIS:HB3	2:N:179:LYS:HZ2	1.28	0.97
1:G:4:HIS:HA	2:S:178:ILE:HD12	0.98	0.97
1:J:4:HIS:HA	2:V:178:ILE:HD12	0.98	0.97
1:B:5:VAL:N	2:N:179:LYS:HZ1	1.58	0.97
1:C:4:HIS:HA	2:O:178:ILE:HD12	0.98	0.97
1:F:4:HIS:HA	2:R:178:ILE:HD12	0.98	0.97
1:D:4:HIS:HA	2:P:178:ILE:HD12	0.98	0.97
1:I:4:HIS:HA	2:U:178:ILE:HD12	0.98	0.97
1:C:5:VAL:N	2:O:179:LYS:HZ1	1.57	0.97
1:H:5:VAL:N	2:T:179:LYS:HZ1	1.60	0.97
1:B:4:HIS:HA	2:N:178:ILE:HD12	0.98	0.96
1:C:4:HIS:HB3	2:O:179:LYS:HZ2	1.30	0.96
1:E:4:HIS:HA	2:Q:178:ILE:HD12	0.98	0.96
1:K:4:HIS:HA	2:W:178:ILE:HD12	0.98	0.96
1:K:5:VAL:N	2:W:179:LYS:HZ1	1.58	0.96
1:H:4:HIS:HA	2:T:178:ILE:HD12	0.98	0.96
1:K:4:HIS:HB3	2:W:179:LYS:HZ2	1.29	0.96
2:P:239:LYS:O	2:P:239:LYS:CD	2.14	0.96
2:T:239:LYS:O	2:T:239:LYS:CD	2.14	0.96
2:U:239:LYS:O	2:U:239:LYS:CD	2.14	0.96
2:Q:239:LYS:O	2:Q:239:LYS:CD	2.14	0.96
1:E:5:VAL:N	2:Q:179:LYS:HZ1	1.61	0.95
2:T:312:ALA:CB	2:T:317:ILE:CG2	2.45	0.95
2:Q:312:ALA:CB	2:Q:317:ILE:CG2	2.45	0.95
2:N:312:ALA:CB	2:N:317:ILE:CG2	2.45	0.95
2:O:239:LYS:O	2:O:239:LYS:CD	2.14	0.95
2:O:312:ALA:CB	2:O:317:ILE:CG2	2.45	0.95
2:V:312:ALA:CB	2:V:317:ILE:CG2	2.45	0.95
2:W:312:ALA:CB	2:W:317:ILE:CG2	2.45	0.95
2:R:312:ALA:CB	2:R:317:ILE:CG2	2.45	0.95
2:S:312:ALA:CB	2:S:317:ILE:CG2	2.45	0.95
2:V:239:LYS:O	2:V:239:LYS:CD	2.14	0.95
2:X:239:LYS:O	2:X:239:LYS:CD	2.14	0.95
2:M:312:ALA:CB	2:M:317:ILE:CG2	2.45	0.95
2:P:312:ALA:CB	2:P:317:ILE:CG2	2.45	0.95
2:M:239:LYS:O	2:M:239:LYS:CD	2.14	0.94
2:U:312:ALA:CB	2:U:317:ILE:CG2	2.45	0.94
2:X:312:ALA:CB	2:X:317:ILE:CG2	2.45	0.94
2:R:239:LYS:O	2:R:239:LYS:CD	2.14	0.94
2:N:239:LYS:O	2:N:239:LYS:CD	2.14	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:239:LYS:O	2:W:239:LYS:CD	2.14	0.94
2:S:239:LYS:O	2:S:239:LYS:CD	2.14	0.94
1:G:5:VAL:N	2:S:179:LYS:HZ1	1.58	0.94
1:C:235:ILE:HG21	1:C:367:PRO:HG3	1.49	0.94
1:J:235:ILE:HG21	1:J:367:PRO:HG3	1.49	0.94
1:L:4:HIS:HB3	2:X:179:LYS:HZ2	1.32	0.93
1:K:235:ILE:HG21	1:K:367:PRO:HG3	1.49	0.93
1:B:235:ILE:HG21	1:B:367:PRO:HG3	1.49	0.93
1:K:60:ILE:H	1:K:60:ILE:CD1	1.82	0.93
1:B:60:ILE:H	1:B:60:ILE:CD1	1.82	0.92
1:J:5:VAL:N	2:V:179:LYS:HZ1	1.59	0.92
1:D:235:ILE:HG21	1:D:367:PRO:HG3	1.49	0.92
1:A:4:HIS:HB3	2:M:179:LYS:HZ2	1.33	0.92
1:I:235:ILE:HG21	1:I:367:PRO:HG3	1.49	0.92
1:F:4:HIS:HB3	2:R:179:LYS:HZ2	1.34	0.92
1:G:235:ILE:HG21	1:G:367:PRO:HG3	1.49	0.92
1:A:235:ILE:HG21	1:A:367:PRO:HG3	1.49	0.92
1:L:235:ILE:HG21	1:L:367:PRO:HG3	1.49	0.92
1:F:235:ILE:HG21	1:F:367:PRO:HG3	1.49	0.91
1:D:60:ILE:H	1:D:60:ILE:CD1	1.82	0.91
1:I:60:ILE:H	1:I:60:ILE:CD1	1.82	0.91
1:D:5:VAL:N	2:P:179:LYS:HZ1	1.61	0.91
1:E:235:ILE:HG21	1:E:367:PRO:HG3	1.49	0.90
1:H:235:ILE:HG21	1:H:367:PRO:HG3	1.49	0.90
1:I:5:VAL:N	2:U:179:LYS:HZ1	1.59	0.90
1:F:4:HIS:CA	2:R:179:LYS:HZ3	1.83	0.90
2:W:1:LYS:HA	2:W:54:GLY:O	1.72	0.90
1:J:395:ASN:HB3	1:J:400:PRO:HD2	1.54	0.90
2:N:1:LYS:HA	2:N:54:GLY:O	1.72	0.90
1:C:395:ASN:HB3	1:C:400:PRO:HD2	1.54	0.90
2:V:1:LYS:HA	2:V:54:GLY:O	1.72	0.90
2:X:1:LYS:HA	2:X:54:GLY:O	1.72	0.90
1:E:4:HIS:CB	2:Q:179:LYS:HZ2	1.82	0.90
2:M:1:LYS:HA	2:M:54:GLY:O	1.72	0.90
2:O:1:LYS:HA	2:O:54:GLY:O	1.72	0.90
1:K:395:ASN:HB3	1:K:400:PRO:HD2	1.54	0.89
2:S:1:LYS:HA	2:S:54:GLY:O	1.72	0.89
1:E:60:ILE:H	1:E:60:ILE:CD1	1.82	0.89
1:G:60:ILE:HD13	1:G:60:ILE:N	1.87	0.89
1:C:60:ILE:H	1:C:60:ILE:CD1	1.82	0.89
2:R:1:LYS:HA	2:R:54:GLY:O	1.72	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:395:ASN:HB3	1:B:400:PRO:HD2	1.54	0.89
1:D:395:ASN:HB3	1:D:400:PRO:HD2	1.54	0.89
1:H:60:ILE:H	1:H:60:ILE:CD1	1.82	0.89
1:I:395:ASN:HB3	1:I:400:PRO:HD2	1.54	0.89
2:P:1:LYS:HA	2:P:54:GLY:O	1.72	0.89
1:A:4:HIS:CA	2:M:179:LYS:HZ3	1.84	0.89
1:C:4:HIS:CA	2:O:179:LYS:HZ3	1.86	0.89
1:F:60:ILE:HD13	1:F:60:ILE:N	1.87	0.89
2:U:1:LYS:HA	2:U:54:GLY:O	1.72	0.89
1:C:60:ILE:HD13	1:C:60:ILE:N	1.87	0.89
1:E:60:ILE:HD13	1:E:60:ILE:N	1.87	0.89
1:J:60:ILE:H	1:J:60:ILE:CD1	1.82	0.89
1:E:395:ASN:HB3	1:E:400:PRO:HD2	1.54	0.88
1:F:60:ILE:H	1:F:60:ILE:CD1	1.82	0.88
1:H:60:ILE:HD13	1:H:60:ILE:N	1.87	0.88
1:D:60:ILE:HD13	1:D:60:ILE:N	1.87	0.88
1:H:395:ASN:HB3	1:H:400:PRO:HD2	1.54	0.88
1:J:60:ILE:HD13	1:J:60:ILE:N	1.87	0.88
1:D:4:HIS:CB	2:P:179:LYS:HZ2	1.82	0.88
1:K:60:ILE:HD13	1:K:60:ILE:N	1.87	0.88
1:L:4:HIS:CA	2:X:179:LYS:HZ3	1.85	0.88
1:G:60:ILE:H	1:G:60:ILE:CD1	1.82	0.88
1:I:60:ILE:HD13	1:I:60:ILE:N	1.87	0.88
1:L:60:ILE:HD13	1:L:60:ILE:N	1.87	0.88
2:M:312:ALA:CB	2:M:317:ILE:HB	2.04	0.88
2:P:312:ALA:CB	2:P:317:ILE:HB	2.04	0.88
1:B:60:ILE:HD13	1:B:60:ILE:N	1.87	0.88
1:H:4:HIS:CB	2:T:179:LYS:HZ2	1.84	0.88
2:T:312:ALA:CB	2:T:317:ILE:HB	2.04	0.88
2:X:312:ALA:CB	2:X:317:ILE:HB	2.04	0.88
1:A:60:ILE:HD13	1:A:60:ILE:N	1.87	0.88
2:P:309:GLU:O	2:P:313:LYS:HE3	1.74	0.88
2:Q:309:GLU:O	2:Q:313:LYS:HE3	1.74	0.88
2:Q:312:ALA:CB	2:Q:317:ILE:HB	2.04	0.88
2:T:309:GLU:O	2:T:313:LYS:HE3	1.74	0.88
2:U:309:GLU:O	2:U:313:LYS:HE3	1.74	0.88
2:U:312:ALA:CB	2:U:317:ILE:HB	2.04	0.88
1:A:395:ASN:HB3	1:A:400:PRO:HD2	1.54	0.88
1:L:395:ASN:HB3	1:L:400:PRO:HD2	1.54	0.88
2:Q:1:LYS:HA	2:Q:54:GLY:O	1.72	0.87
1:E:5:VAL:N	2:Q:179:LYS:HZ3	1.62	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:312:ALA:CB	2:N:317:ILE:HB	2.04	0.87
2:O:312:ALA:CB	2:O:317:ILE:HB	2.04	0.87
2:V:312:ALA:CB	2:V:317:ILE:HB	2.04	0.87
2:W:312:ALA:CB	2:W:317:ILE:HB	2.04	0.87
2:R:312:ALA:CB	2:R:317:ILE:HB	2.04	0.87
2:T:1:LYS:HA	2:T:54:GLY:O	1.72	0.87
1:K:4:HIS:CA	2:W:179:LYS:HZ3	1.87	0.87
2:M:309:GLU:O	2:M:313:LYS:HE3	1.74	0.87
1:G:395:ASN:HB3	1:G:400:PRO:HD2	1.54	0.87
2:S:312:ALA:CB	2:S:317:ILE:HB	2.04	0.87
2:X:309:GLU:O	2:X:313:LYS:HE3	1.74	0.87
1:F:395:ASN:HB3	1:F:400:PRO:HD2	1.54	0.86
2:S:309:GLU:O	2:S:313:LYS:HE3	1.74	0.86
1:B:4:HIS:CA	2:N:179:LYS:HZ3	1.87	0.86
2:N:309:GLU:O	2:N:313:LYS:HE3	1.74	0.86
2:W:309:GLU:O	2:W:313:LYS:HE3	1.74	0.86
1:G:4:HIS:CA	2:S:179:LYS:HZ3	1.87	0.86
2:M:31:THR:HG23	2:M:33:ILE:N	1.91	0.86
2:X:31:THR:HG23	2:X:33:ILE:N	1.91	0.86
2:O:309:GLU:O	2:O:313:LYS:HE3	1.74	0.86
2:R:309:GLU:O	2:R:313:LYS:HE3	1.74	0.86
1:I:4:HIS:CB	2:U:179:LYS:HZ2	1.85	0.86
2:S:31:THR:HG23	2:S:33:ILE:N	1.91	0.86
2:V:309:GLU:O	2:V:313:LYS:HE3	1.74	0.85
2:R:31:THR:HG23	2:R:33:ILE:N	1.91	0.85
1:A:60:ILE:H	1:A:60:ILE:CD1	1.82	0.85
1:J:82:ASP:O	1:J:84:THR:HG22	1.76	0.85
2:V:31:THR:HG23	2:V:33:ILE:N	1.91	0.85
1:C:82:ASP:O	1:C:84:THR:HG22	1.76	0.85
1:E:458:HIS:HD2	1:E:460:VAL:H	1.25	0.85
2:O:31:THR:HG23	2:O:33:ILE:N	1.91	0.85
1:B:398:ASP:O	1:B:399:LEU:C	2.11	0.85
1:K:398:ASP:O	1:K:399:LEU:C	2.11	0.85
1:H:458:HIS:HD2	1:H:460:VAL:H	1.25	0.85
1:A:458:HIS:HD2	1:A:460:VAL:H	1.25	0.85
1:L:60:ILE:H	1:L:60:ILE:CD1	1.82	0.85
1:D:458:HIS:HD2	1:D:460:VAL:H	1.25	0.85
1:E:82:ASP:O	1:E:84:THR:HG22	1.76	0.85
1:H:82:ASP:O	1:H:84:THR:HG22	1.76	0.85
1:I:61:ASN:O	1:J:337:ARG:CB	2.21	0.85
1:I:458:HIS:HD2	1:I:460:VAL:H	1.25	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:4:HIS:CA	2:V:179:LYS:HZ3	1.90	0.85
1:K:82:ASP:O	1:K:84:THR:HG22	1.76	0.85
1:L:458:HIS:HD2	1:L:460:VAL:H	1.25	0.85
1:B:82:ASP:O	1:B:84:THR:HG22	1.76	0.85
2:P:31:THR:HG23	2:P:33:ILE:N	1.91	0.84
1:G:458:HIS:HD2	1:G:460:VAL:H	1.25	0.84
1:I:4:HIS:CA	2:U:179:LYS:HZ3	1.89	0.84
1:A:398:ASP:O	1:A:399:LEU:C	2.11	0.84
1:I:82:ASP:O	1:I:84:THR:HG22	1.76	0.84
2:R:311:LEU:O	2:R:312:ALA:CB	1.98	0.84
2:X:311:LEU:O	2:X:312:ALA:CB	1.98	0.84
1:L:398:ASP:O	1:L:399:LEU:C	2.11	0.84
2:N:31:THR:HG23	2:N:33:ILE:N	1.91	0.84
2:W:31:THR:HG23	2:W:33:ILE:N	1.91	0.84
1:D:82:ASP:O	1:D:84:THR:HG22	1.76	0.84
1:F:458:HIS:HD2	1:F:460:VAL:H	1.25	0.84
2:U:31:THR:HG23	2:U:33:ILE:N	1.91	0.84
1:F:82:ASP:O	1:F:84:THR:HG22	1.76	0.84
1:J:458:HIS:HD2	1:J:460:VAL:H	1.25	0.84
1:B:458:HIS:HD2	1:B:460:VAL:H	1.25	0.84
1:C:458:HIS:HD2	1:C:460:VAL:H	1.25	0.84
1:K:458:HIS:HD2	1:K:460:VAL:H	1.25	0.84
2:S:311:LEU:O	2:S:312:ALA:CB	1.98	0.84
1:H:4:HIS:CA	2:T:179:LYS:HZ3	1.90	0.83
2:M:311:LEU:O	2:M:312:ALA:CB	1.98	0.83
1:G:82:ASP:O	1:G:84:THR:HG22	1.76	0.83
1:J:398:ASP:O	1:J:399:LEU:C	2.11	0.83
1:F:398:ASP:O	1:F:399:LEU:C	2.11	0.83
2:P:312:ALA:HB3	2:P:317:ILE:HG21	1.61	0.83
2:T:31:THR:HG23	2:T:33:ILE:N	1.90	0.83
1:C:398:ASP:O	1:C:399:LEU:C	2.11	0.83
1:D:43:PHE:CB	2:P:370:LYS:CE	2.25	0.83
2:N:367:ARG:O	2:N:370:LYS:HB2	1.78	0.83
2:Q:31:THR:HG23	2:Q:33:ILE:N	1.91	0.83
2:U:312:ALA:HB3	2:U:317:ILE:HG21	1.61	0.83
2:V:367:ARG:O	2:V:370:LYS:HB2	1.78	0.83
2:W:367:ARG:O	2:W:370:LYS:HB2	1.78	0.83
1:A:43:PHE:CB	2:M:370:LYS:CE	2.25	0.83
2:O:367:ARG:O	2:O:370:LYS:HB2	1.78	0.83
1:G:398:ASP:O	1:G:399:LEU:C	2.11	0.83
1:L:82:ASP:O	1:L:84:THR:HG22	1.76	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:367:ARG:O	2:M:370:LYS:HB2	1.78	0.83
2:U:367:ARG:O	2:U:370:LYS:HB2	1.78	0.83
1:A:82:ASP:O	1:A:84:THR:HG22	1.76	0.83
1:I:43:PHE:CB	2:U:370:LYS:CE	2.25	0.83
2:W:239:LYS:O	2:W:239:LYS:CG	2.27	0.83
1:E:4:HIS:CA	2:Q:179:LYS:HZ3	1.92	0.82
2:N:239:LYS:O	2:N:239:LYS:CG	2.27	0.82
2:P:367:ARG:O	2:P:370:LYS:HB2	1.78	0.82
2:Q:367:ARG:O	2:Q:370:LYS:HB2	1.78	0.82
2:X:367:ARG:O	2:X:370:LYS:HB2	1.78	0.82
2:T:367:ARG:O	2:T:370:LYS:HB2	1.78	0.82
2:V:312:ALA:HB3	2:V:317:ILE:HG21	1.60	0.82
1:D:4:HIS:CA	2:P:179:LYS:HZ3	1.91	0.82
1:L:43:PHE:CB	2:X:370:LYS:CE	2.25	0.82
2:R:367:ARG:O	2:R:370:LYS:HB2	1.78	0.82
2:O:312:ALA:HB3	2:O:317:ILE:HG21	1.60	0.82
2:S:367:ARG:O	2:S:370:LYS:HB2	1.78	0.82
1:G:4:HIS:CB	2:S:179:LYS:HZ2	1.89	0.81
2:R:239:LYS:O	2:R:239:LYS:CG	2.27	0.81
2:X:312:ALA:HB3	2:X:317:ILE:HG21	1.60	0.81
2:M:239:LYS:O	2:M:239:LYS:CG	2.27	0.81
2:M:312:ALA:HB3	2:M:317:ILE:HG21	1.60	0.81
2:S:239:LYS:O	2:S:239:LYS:CG	2.27	0.81
2:X:239:LYS:O	2:X:239:LYS:CG	2.27	0.81
1:E:43:PHE:CB	2:Q:370:LYS:CE	2.25	0.81
1:G:43:PHE:CB	2:S:370:LYS:CE	2.25	0.81
2:P:33:ILE:HG12	2:P:275:LEU:HD13	1.63	0.81
2:S:312:ALA:HB3	2:S:317:ILE:HG21	1.60	0.81
2:U:33:ILE:HG12	2:U:275:LEU:HD13	1.63	0.81
1:C:398:ASP:O	1:C:399:LEU:O	1.99	0.81
1:J:398:ASP:O	1:J:399:LEU:O	1.99	0.81
2:Q:33:ILE:HG12	2:Q:275:LEU:HD13	1.63	0.81
1:D:398:ASP:O	1:D:399:LEU:O	1.99	0.81
1:E:398:ASP:O	1:E:399:LEU:O	1.99	0.81
1:H:398:ASP:O	1:H:399:LEU:O	1.99	0.81
1:A:337:ARG:CB	1:B:61:ASN:O	2.26	0.81
1:I:398:ASP:O	1:I:399:LEU:O	1.99	0.81
2:P:239:LYS:O	2:P:239:LYS:CG	2.27	0.81
2:T:33:ILE:HG12	2:T:275:LEU:HD13	1.63	0.81
2:R:312:ALA:HB3	2:R:317:ILE:HG21	1.60	0.81
1:G:398:ASP:O	1:G:399:LEU:O	1.99	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:33:ILE:HG12	2:O:275:LEU:HD13	1.63	0.80
1:B:398:ASP:O	1:B:399:LEU:O	1.99	0.80
1:F:43:PHE:CB	2:R:370:LYS:CE	2.25	0.80
1:F:398:ASP:O	1:F:399:LEU:O	1.99	0.80
2:N:312:ALA:HB3	2:N:317:ILE:HG21	1.60	0.80
2:W:312:ALA:HB3	2:W:317:ILE:HG21	1.61	0.80
1:H:43:PHE:CB	2:T:370:LYS:CE	2.24	0.80
1:H:398:ASP:O	1:H:399:LEU:C	2.11	0.80
1:K:398:ASP:O	1:K:399:LEU:O	1.99	0.80
2:Q:312:ALA:HB3	2:Q:317:ILE:HG21	1.60	0.80
2:U:239:LYS:O	2:U:239:LYS:CG	2.27	0.80
2:V:33:ILE:HG12	2:V:275:LEU:HD13	1.63	0.80
1:A:398:ASP:O	1:A:399:LEU:O	1.99	0.80
2:T:312:ALA:HB3	2:T:317:ILE:HG21	1.60	0.80
1:C:43:PHE:CB	2:O:370:LYS:CE	2.25	0.80
1:L:398:ASP:O	1:L:399:LEU:O	1.99	0.80
2:R:33:ILE:HG12	2:R:275:LEU:HD13	1.63	0.80
1:E:398:ASP:O	1:E:399:LEU:C	2.11	0.80
2:S:33:ILE:HG12	2:S:275:LEU:HD13	1.63	0.80
1:K:43:PHE:CB	2:W:370:LYS:CE	2.25	0.80
2:N:33:ILE:HG12	2:N:275:LEU:HD13	1.63	0.79
2:Q:239:LYS:O	2:Q:239:LYS:CG	2.27	0.79
1:J:43:PHE:CB	2:V:370:LYS:CE	2.25	0.79
2:M:33:ILE:HG12	2:M:275:LEU:HD13	1.63	0.79
2:O:239:LYS:O	2:O:239:LYS:CG	2.27	0.79
1:B:43:PHE:CB	2:N:370:LYS:CE	2.25	0.79
1:D:398:ASP:O	1:D:399:LEU:C	2.11	0.79
2:W:33:ILE:HG12	2:W:275:LEU:HD13	1.63	0.79
1:I:398:ASP:O	1:I:399:LEU:C	2.11	0.79
2:T:239:LYS:O	2:T:239:LYS:CG	2.27	0.79
2:X:33:ILE:HG12	2:X:275:LEU:HD13	1.63	0.79
2:V:239:LYS:O	2:V:239:LYS:CG	2.27	0.79
2:W:6:LYS:HA	2:W:33:ILE:HG23	1.65	0.79
2:N:6:LYS:HA	2:N:33:ILE:HG23	1.65	0.78
2:S:6:LYS:HA	2:S:33:ILE:HG23	1.65	0.78
2:T:6:LYS:HA	2:T:33:ILE:HG23	1.65	0.78
2:O:6:LYS:HA	2:O:33:ILE:HG23	1.65	0.78
2:U:6:LYS:HA	2:U:33:ILE:HG23	1.65	0.78
2:V:6:LYS:HA	2:V:33:ILE:HG23	1.65	0.78
2:P:6:LYS:HA	2:P:33:ILE:HG23	1.65	0.78
2:Q:6:LYS:HA	2:Q:33:ILE:HG23	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:6:LYS:HA	2:M:33:ILE:HG23	1.65	0.78
2:X:6:LYS:HA	2:X:33:ILE:HG23	1.65	0.78
2:R:6:LYS:HA	2:R:33:ILE:HG23	1.65	0.78
1:C:58:LYS:HD2	1:C:62:GLU:HB2	1.67	0.77
1:J:58:LYS:HD2	1:J:62:GLU:HB2	1.67	0.77
2:T:312:ALA:HB3	2:T:317:ILE:HG22	1.66	0.77
2:O:31:THR:HG23	2:O:33:ILE:HD12	1.67	0.77
2:Q:312:ALA:HB3	2:Q:317:ILE:HG22	1.67	0.77
2:V:31:THR:HG23	2:V:33:ILE:HD12	1.67	0.77
2:X:31:THR:HG23	2:X:33:ILE:HD12	1.67	0.77
1:A:5:VAL:CA	2:M:179:LYS:HZ1	1.97	0.76
1:D:58:LYS:HD2	1:D:62:GLU:HB2	1.67	0.76
1:D:399:LEU:HA	1:D:400:PRO:C	2.06	0.76
1:I:58:LYS:HD2	1:I:62:GLU:HB2	1.67	0.76
2:M:31:THR:HG23	2:M:33:ILE:HD12	1.68	0.76
1:C:395:ASN:HB3	1:C:400:PRO:CD	2.16	0.76
1:I:399:LEU:HA	1:I:400:PRO:C	2.06	0.76
1:J:395:ASN:HB3	1:J:400:PRO:CD	2.16	0.76
2:S:312:ALA:HB3	2:S:317:ILE:HG22	1.66	0.76
1:K:399:LEU:HA	1:K:400:PRO:C	2.06	0.76
2:R:31:THR:HG23	2:R:33:ILE:HD12	1.67	0.76
1:B:399:LEU:HA	1:B:400:PRO:C	2.06	0.76
1:C:399:LEU:HA	1:C:400:PRO:C	2.06	0.76
1:L:399:LEU:HA	1:L:400:PRO:C	2.06	0.76
2:M:312:ALA:CB	2:M:317:ILE:HG21	2.15	0.76
2:X:312:ALA:CB	2:X:317:ILE:HG21	2.15	0.76
1:C:5:VAL:CA	2:O:179:LYS:HZ1	1.98	0.76
1:F:5:VAL:CA	2:R:179:LYS:HZ1	1.96	0.76
2:S:31:THR:HG23	2:S:33:ILE:HD12	1.67	0.76
2:U:31:THR:HG23	2:U:33:ILE:HD12	1.67	0.76
1:A:399:LEU:HA	1:A:400:PRO:C	2.06	0.76
1:C:337:ARG:CB	1:D:61:ASN:O	2.27	0.76
1:D:44:GLU:HG3	2:P:370:LYS:NZ	2.01	0.76
1:D:395:ASN:HB3	1:D:400:PRO:CD	2.16	0.76
1:J:399:LEU:HA	1:J:400:PRO:C	2.06	0.76
1:K:58:LYS:HD2	1:K:62:GLU:HB2	1.67	0.76
2:N:31:THR:HG23	2:N:33:ILE:HD12	1.67	0.76
2:R:312:ALA:HB3	2:R:317:ILE:HG22	1.66	0.76
2:W:28:GLU:HA	2:W:31:THR:HG22	1.68	0.76
1:B:58:LYS:HD2	1:B:62:GLU:HB2	1.67	0.76
1:I:395:ASN:HB3	1:I:400:PRO:CD	2.16	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:295:LYS:C	2:M:295:LYS:HD3	2.06	0.76
2:P:31:THR:HG23	2:P:33:ILE:HD12	1.67	0.76
2:P:136:ASP:OD2	2:P:203:HIS:HD2	1.69	0.76
2:W:31:THR:HG23	2:W:33:ILE:HD12	1.67	0.76
1:A:44:GLU:HG3	2:M:370:LYS:NZ	2.01	0.76
1:E:399:LEU:HA	1:E:400:PRO:C	2.06	0.76
1:H:399:LEU:HA	1:H:400:PRO:C	2.06	0.76
1:J:44:GLU:HG3	2:V:370:LYS:NZ	2.01	0.76
2:N:28:GLU:HA	2:N:31:THR:HG22	1.68	0.76
2:U:136:ASP:OD2	2:U:203:HIS:HD2	1.69	0.76
2:V:136:ASP:OD2	2:V:203:HIS:HD2	1.69	0.76
2:X:295:LYS:C	2:X:295:LYS:HD3	2.06	0.76
1:C:44:GLU:HG3	2:O:370:LYS:NZ	2.01	0.76
1:H:58:LYS:HD2	1:H:62:GLU:HB2	1.67	0.76
1:I:44:GLU:HG3	2:U:370:LYS:NZ	2.01	0.76
2:N:136:ASP:OD2	2:N:203:HIS:HD2	1.69	0.76
2:O:136:ASP:OD2	2:O:203:HIS:HD2	1.69	0.76
2:R:295:LYS:HD3	2:R:295:LYS:C	2.06	0.76
2:W:136:ASP:OD2	2:W:203:HIS:HD2	1.69	0.76
1:E:58:LYS:HD2	1:E:62:GLU:HB2	1.67	0.76
2:N:295:LYS:C	2:N:295:LYS:HD3	2.06	0.76
2:O:28:GLU:HA	2:O:31:THR:HG22	1.68	0.76
2:R:312:ALA:HA	2:R:314:ASP:H	1.51	0.76
2:S:312:ALA:HA	2:S:314:ASP:H	1.51	0.76
2:T:31:THR:HG23	2:T:33:ILE:HD12	1.67	0.76
2:V:28:GLU:HA	2:V:31:THR:HG22	1.68	0.76
1:A:395:ASN:HB3	1:A:400:PRO:CD	2.16	0.75
1:B:44:GLU:HG3	2:N:370:LYS:NZ	2.01	0.75
2:M:312:ALA:HB3	2:M:317:ILE:HG22	1.66	0.75
2:M:312:ALA:HA	2:M:314:ASP:H	1.51	0.75
2:P:312:ALA:HB3	2:P:317:ILE:HG22	1.66	0.75
2:S:295:LYS:C	2:S:295:LYS:HD3	2.06	0.75
2:W:295:LYS:HD3	2:W:295:LYS:C	2.07	0.75
1:G:399:LEU:HA	1:G:400:PRO:C	2.06	0.75
1:K:395:ASN:HB3	1:K:400:PRO:CD	2.16	0.75
1:L:5:VAL:CA	2:X:179:LYS:HZ1	1.98	0.75
1:L:395:ASN:HB3	1:L:400:PRO:CD	2.16	0.75
2:Q:31:THR:HG23	2:Q:33:ILE:HD12	1.67	0.75
2:Q:312:ALA:HA	2:Q:314:ASP:H	1.51	0.75
2:T:312:ALA:HA	2:T:314:ASP:H	1.51	0.75
2:U:312:ALA:HB3	2:U:317:ILE:HG22	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:312:ALA:HA	2:X:314:ASP:H	1.51	0.75
1:B:395:ASN:HB3	1:B:400:PRO:CD	2.16	0.75
1:H:44:GLU:HG3	2:T:370:LYS:NZ	2.01	0.75
1:K:44:GLU:HG3	2:W:370:LYS:NZ	2.01	0.75
2:P:312:ALA:HA	2:P:314:ASP:H	1.51	0.75
2:Q:136:ASP:OD2	2:Q:203:HIS:HD2	1.69	0.75
2:V:295:LYS:C	2:V:295:LYS:HD3	2.06	0.75
2:X:312:ALA:HB3	2:X:317:ILE:HG22	1.66	0.75
1:E:44:GLU:HG3	2:Q:370:LYS:NZ	2.01	0.75
2:P:312:ALA:CB	2:P:317:ILE:HG21	2.15	0.75
2:Q:28:GLU:HA	2:Q:31:THR:HG22	1.68	0.75
2:T:136:ASP:OD2	2:T:203:HIS:HD2	1.69	0.75
2:U:312:ALA:HA	2:U:314:ASP:H	1.51	0.75
1:F:395:ASN:HB3	1:F:400:PRO:CD	2.16	0.75
2:O:295:LYS:HD3	2:O:295:LYS:C	2.07	0.75
2:T:295:LYS:HD3	2:T:295:LYS:C	2.06	0.75
1:F:399:LEU:HA	1:F:400:PRO:C	2.06	0.75
1:G:395:ASN:HB3	1:G:400:PRO:CD	2.16	0.75
1:H:395:ASN:HB3	1:H:400:PRO:CD	2.16	0.75
1:L:44:GLU:HG3	2:X:370:LYS:NZ	2.01	0.75
2:R:28:GLU:HA	2:R:31:THR:HG22	1.68	0.75
2:R:312:ALA:CB	2:R:317:ILE:HG21	2.15	0.75
2:T:28:GLU:HA	2:T:31:THR:HG22	1.68	0.75
2:U:312:ALA:CB	2:U:317:ILE:HG21	2.15	0.75
1:E:395:ASN:HB3	1:E:400:PRO:CD	2.16	0.75
1:B:7:THR:OG1	2:N:178:ILE:HD11	1.87	0.75
1:F:7:THR:OG1	2:R:178:ILE:HD11	1.87	0.75
2:Q:295:LYS:C	2:Q:295:LYS:HD3	2.06	0.75
2:S:312:ALA:CB	2:S:317:ILE:HG21	2.15	0.75
1:A:7:THR:OG1	2:M:178:ILE:HD11	1.87	0.75
1:F:58:LYS:HD2	1:F:62:GLU:HB2	1.67	0.75
1:G:7:THR:OG1	2:S:178:ILE:HD11	1.87	0.75
2:S:28:GLU:HA	2:S:31:THR:HG22	1.68	0.75
2:T:64:HIS:HD2	2:T:261:VAL:H	1.34	0.75
1:A:58:LYS:HD2	1:A:62:GLU:HB2	1.67	0.74
1:G:44:GLU:HG3	2:S:370:LYS:NZ	2.01	0.74
1:G:58:LYS:HD2	1:G:62:GLU:HB2	1.67	0.74
1:L:7:THR:OG1	2:X:178:ILE:HD11	1.88	0.74
2:M:136:ASP:OD2	2:M:203:HIS:HD2	1.69	0.74
2:Q:64:HIS:HD2	2:Q:261:VAL:H	1.34	0.74
2:U:295:LYS:C	2:U:295:LYS:HD3	2.06	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:28:GLU:HA	2:X:31:THR:HG22	1.68	0.74
2:X:136:ASP:OD2	2:X:203:HIS:HD2	1.69	0.74
1:A:248:ARG:HH21	1:A:248:ARG:CG	2.00	0.74
1:F:44:GLU:HG3	2:R:370:LYS:NZ	2.01	0.74
1:K:7:THR:OG1	2:W:178:ILE:HD11	1.87	0.74
2:O:312:ALA:CB	2:O:317:ILE:HG21	2.15	0.74
2:P:295:LYS:C	2:P:295:LYS:HD3	2.06	0.74
2:W:64:HIS:HD2	2:W:261:VAL:H	1.34	0.74
1:J:248:ARG:HH21	1:J:248:ARG:CG	2.00	0.74
1:L:58:LYS:HD2	1:L:62:GLU:HB2	1.67	0.74
1:C:248:ARG:HH21	1:C:248:ARG:CG	2.00	0.74
1:H:7:THR:OG1	2:T:178:ILE:HD11	1.87	0.74
1:L:248:ARG:CG	1:L:248:ARG:HH21	2.00	0.74
2:N:64:HIS:HD2	2:N:261:VAL:H	1.34	0.74
2:O:312:ALA:HA	2:O:314:ASP:H	1.51	0.74
1:C:7:THR:OG1	2:O:178:ILE:HD11	1.87	0.74
1:E:7:THR:OG1	2:Q:178:ILE:HD11	1.87	0.74
1:G:5:VAL:CA	2:S:179:LYS:HZ1	1.99	0.74
1:I:248:ARG:HH21	1:I:248:ARG:CG	2.00	0.74
1:J:7:THR:OG1	2:V:178:ILE:HD11	1.87	0.74
2:M:28:GLU:HA	2:M:31:THR:HG22	1.68	0.74
2:N:312:ALA:HB3	2:N:317:ILE:HG22	1.66	0.74
2:N:312:ALA:HA	2:N:314:ASP:H	1.51	0.74
2:O:312:ALA:HB3	2:O:317:ILE:HG22	1.66	0.74
2:U:28:GLU:HA	2:U:31:THR:HG22	1.68	0.74
2:V:312:ALA:CB	2:V:317:ILE:HG21	2.15	0.74
2:V:312:ALA:HB3	2:V:317:ILE:HG22	1.66	0.74
1:C:192:ARG:HH21	1:C:219:ASN:ND2	1.86	0.74
1:G:248:ARG:HH21	1:G:248:ARG:CG	2.00	0.74
1:J:192:ARG:HH21	1:J:219:ASN:ND2	1.86	0.74
1:K:248:ARG:HH21	1:K:248:ARG:CG	2.00	0.74
2:S:64:HIS:HD2	2:S:261:VAL:H	1.34	0.74
1:B:248:ARG:HH21	1:B:248:ARG:CG	2.00	0.74
1:D:248:ARG:HH21	1:D:248:ARG:CG	2.00	0.74
1:K:5:VAL:CA	2:W:179:LYS:HZ1	1.99	0.74
2:P:64:HIS:HD2	2:P:261:VAL:H	1.34	0.74
2:V:312:ALA:HA	2:V:314:ASP:H	1.51	0.74
2:W:312:ALA:HA	2:W:314:ASP:H	1.51	0.74
2:R:64:HIS:HD2	2:R:261:VAL:H	1.34	0.74
2:P:28:GLU:HA	2:P:31:THR:HG22	1.68	0.74
2:Q:312:ALA:CB	2:Q:317:ILE:HG21	2.15	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:64:HIS:HD2	2:U:261:VAL:H	1.34	0.74
2:W:312:ALA:HB3	2:W:317:ILE:HG22	1.67	0.74
2:T:312:ALA:CB	2:T:317:ILE:HG21	2.15	0.74
1:F:248:ARG:HH21	1:F:248:ARG:CG	2.00	0.73
2:V:64:HIS:HD2	2:V:261:VAL:H	1.34	0.73
2:X:64:HIS:HD2	2:X:261:VAL:H	1.34	0.73
2:U:341:TYR:CD1	2:U:367:ARG:NH2	2.57	0.73
1:I:5:VAL:CA	2:U:179:LYS:HZ1	2.01	0.73
1:K:192:ARG:HH21	1:K:219:ASN:ND2	1.86	0.73
2:P:341:TYR:CD1	2:P:367:ARG:NH2	2.57	0.73
2:R:136:ASP:OD2	2:R:203:HIS:HD2	1.69	0.73
2:S:136:ASP:OD2	2:S:203:HIS:HD2	1.69	0.73
2:M:64:HIS:HD2	2:M:261:VAL:H	1.34	0.73
2:W:312:ALA:CB	2:W:317:ILE:CB	2.66	0.73
1:B:5:VAL:CA	2:N:179:LYS:HZ1	2.00	0.73
1:B:192:ARG:HH21	1:B:219:ASN:ND2	1.86	0.73
2:N:312:ALA:CB	2:N:317:ILE:CB	2.66	0.73
2:N:312:ALA:CB	2:N:317:ILE:HG21	2.15	0.73
2:O:64:HIS:HD2	2:O:261:VAL:H	1.34	0.73
2:Q:341:TYR:CD1	2:Q:367:ARG:NH2	2.57	0.73
2:T:341:TYR:CD1	2:T:367:ARG:NH2	2.57	0.73
2:W:312:ALA:CB	2:W:317:ILE:HG21	2.16	0.73
2:V:312:ALA:CB	2:V:317:ILE:CB	2.66	0.73
1:D:7:THR:OG1	2:P:178:ILE:HD11	1.87	0.73
1:D:192:ARG:HH21	1:D:219:ASN:ND2	1.86	0.73
1:I:7:THR:OG1	2:U:178:ILE:HD11	1.87	0.73
2:X:341:TYR:CD1	2:X:367:ARG:NH2	2.57	0.73
1:I:192:ARG:HH21	1:I:219:ASN:ND2	1.86	0.73
2:O:312:ALA:CB	2:O:317:ILE:CB	2.66	0.73
1:J:5:VAL:CA	2:V:179:LYS:HZ1	2.01	0.73
2:M:341:TYR:CD1	2:M:367:ARG:NH2	2.57	0.73
1:E:248:ARG:HH21	1:E:248:ARG:CG	2.00	0.73
2:N:341:TYR:CD1	2:N:367:ARG:NH2	2.57	0.73
2:O:341:TYR:CD1	2:O:367:ARG:NH2	2.57	0.73
2:S:312:ALA:CB	2:S:317:ILE:CB	2.66	0.73
2:U:27:PHE:O	2:U:31:THR:HB	1.89	0.73
2:W:341:TYR:CD1	2:W:367:ARG:NH2	2.57	0.73
2:X:312:ALA:CB	2:X:317:ILE:CB	2.66	0.73
1:G:192:ARG:HH21	1:G:219:ASN:ND2	1.86	0.72
1:H:248:ARG:HH21	1:H:248:ARG:CG	2.00	0.72
2:M:312:ALA:CB	2:M:317:ILE:CB	2.66	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:312:ALA:CB	2:R:317:ILE:CB	2.66	0.72
2:S:341:TYR:CD1	2:S:367:ARG:NH2	2.57	0.72
2:V:341:TYR:CD1	2:V:367:ARG:NH2	2.57	0.72
2:P:27:PHE:O	2:P:31:THR:HB	1.89	0.72
2:R:27:PHE:O	2:R:31:THR:HB	1.89	0.72
2:U:312:ALA:CB	2:U:317:ILE:CB	2.66	0.72
1:F:192:ARG:HH21	1:F:219:ASN:ND2	1.86	0.72
1:G:61:ASN:O	1:H:337:ARG:CB	2.28	0.72
1:H:5:VAL:CA	2:T:179:LYS:HZ1	2.02	0.72
2:O:27:PHE:O	2:O:31:THR:HB	1.89	0.72
2:T:27:PHE:O	2:T:31:THR:HB	1.89	0.72
1:E:192:ARG:HH21	1:E:219:ASN:ND2	1.86	0.72
2:P:312:ALA:CB	2:P:317:ILE:CB	2.66	0.72
2:Q:27:PHE:O	2:Q:31:THR:HB	1.89	0.72
2:T:312:ALA:CB	2:T:317:ILE:CB	2.66	0.72
2:Q:312:ALA:CB	2:Q:317:ILE:CB	2.66	0.72
2:R:341:TYR:CD1	2:R:367:ARG:NH2	2.57	0.72
1:H:192:ARG:HH21	1:H:219:ASN:ND2	1.86	0.72
2:P:312:ALA:HB1	2:P:317:ILE:HB	1.72	0.72
2:S:27:PHE:O	2:S:31:THR:HB	1.89	0.72
2:U:312:ALA:HB1	2:U:317:ILE:HB	1.72	0.72
2:V:27:PHE:O	2:V:31:THR:HB	1.89	0.72
1:D:5:VAL:CA	2:P:179:LYS:HZ1	2.03	0.72
1:J:4:HIS:CB	2:V:179:LYS:HZ2	1.85	0.72
2:N:27:PHE:O	2:N:31:THR:HB	1.89	0.72
1:F:96:THR:OG1	1:F:98:GLN:HB2	1.90	0.72
2:W:27:PHE:O	2:W:31:THR:HB	1.89	0.72
2:W:312:ALA:HB1	2:W:317:ILE:HB	1.72	0.72
2:X:64:HIS:HE1	2:X:330:MET:O	1.73	0.72
1:G:96:THR:OG1	1:G:98:GLN:HB2	1.90	0.72
1:L:192:ARG:HH21	1:L:219:ASN:ND2	1.86	0.72
2:M:64:HIS:HE1	2:M:330:MET:O	1.73	0.72
2:N:312:ALA:HB1	2:N:317:ILE:HB	1.72	0.72
1:A:192:ARG:HH21	1:A:219:ASN:ND2	1.86	0.71
1:E:5:VAL:CA	2:Q:179:LYS:HZ1	2.03	0.71
1:A:96:THR:OG1	1:A:98:GLN:HB2	1.90	0.71
1:D:3:GLU:CD	2:P:338:ALA:CB	2.59	0.71
1:L:96:THR:OG1	1:L:98:GLN:HB2	1.90	0.71
2:M:27:PHE:O	2:M:31:THR:HB	1.89	0.71
2:R:341:TYR:HD1	2:R:367:ARG:NH2	1.88	0.71
2:V:64:HIS:HE1	2:V:330:MET:O	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:GLU:CD	2:M:338:ALA:HB1	2.11	0.71
1:I:3:GLU:CD	2:U:338:ALA:CB	2.59	0.71
2:M:312:ALA:HB1	2:M:317:ILE:HB	1.72	0.71
2:O:64:HIS:HE1	2:O:330:MET:O	1.73	0.71
2:X:27:PHE:O	2:X:31:THR:HB	1.89	0.71
1:L:3:GLU:CD	2:X:338:ALA:HB1	2.11	0.71
2:S:341:TYR:HD1	2:S:367:ARG:NH2	1.88	0.71
2:U:64:HIS:HE1	2:U:330:MET:O	1.73	0.71
2:X:312:ALA:HB1	2:X:317:ILE:HB	1.72	0.71
1:H:3:GLU:CD	2:T:338:ALA:CB	2.59	0.71
1:H:96:THR:OG1	1:H:98:GLN:HB2	1.90	0.71
1:I:3:GLU:CD	2:U:338:ALA:HB1	2.11	0.71
1:J:3:GLU:CD	2:V:338:ALA:HB1	2.11	0.71
1:C:3:GLU:CD	2:O:338:ALA:HB1	2.11	0.71
1:D:3:GLU:CD	2:P:338:ALA:HB1	2.11	0.71
1:E:3:GLU:CD	2:Q:338:ALA:CB	2.59	0.71
1:E:3:GLU:CD	2:Q:338:ALA:HB1	2.11	0.71
1:G:4:HIS:CD2	2:S:178:ILE:CG1	2.58	0.71
2:N:64:HIS:HE1	2:N:330:MET:O	1.73	0.71
2:P:64:HIS:HE1	2:P:330:MET:O	1.73	0.71
1:E:96:THR:OG1	1:E:98:GLN:HB2	1.90	0.71
2:T:312:ALA:HB1	2:T:317:ILE:HB	1.72	0.71
2:W:341:TYR:HD1	2:W:367:ARG:NH2	1.88	0.71
1:H:3:GLU:CD	2:T:338:ALA:HB1	2.11	0.71
1:K:3:GLU:CD	2:W:338:ALA:HB1	2.11	0.71
2:N:341:TYR:HD1	2:N:367:ARG:NH2	1.88	0.71
2:Q:312:ALA:HB1	2:Q:317:ILE:HB	1.72	0.71
2:S:64:HIS:HE1	2:S:330:MET:O	1.73	0.71
2:W:64:HIS:HE1	2:W:330:MET:O	1.73	0.71
1:B:3:GLU:CD	2:N:338:ALA:HB1	2.11	0.71
1:C:3:GLU:CD	2:O:338:ALA:CB	2.59	0.71
1:K:3:GLU:CD	2:W:338:ALA:CB	2.59	0.71
2:Q:341:TYR:HD1	2:Q:367:ARG:NH2	1.88	0.71
2:R:64:HIS:HE1	2:R:330:MET:O	1.73	0.71
2:T:341:TYR:HD1	2:T:367:ARG:NH2	1.88	0.71
1:B:3:GLU:CD	2:N:338:ALA:CB	2.59	0.70
1:G:3:GLU:CD	2:S:338:ALA:HB1	2.11	0.70
1:J:3:GLU:CD	2:V:338:ALA:CB	2.59	0.70
2:U:341:TYR:HD1	2:U:367:ARG:NH2	1.88	0.70
2:V:341:TYR:HD1	2:V:367:ARG:NH2	1.88	0.70
1:L:3:GLU:CD	2:X:338:ALA:CB	2.59	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:GLU:CD	2:M:338:ALA:CB	2.59	0.70
1:E:384:ASN:HD22	1:E:384:ASN:N	1.89	0.70
1:F:3:GLU:CD	2:R:338:ALA:HB1	2.11	0.70
2:O:341:TYR:HD1	2:O:367:ARG:NH2	1.88	0.70
2:P:341:TYR:HD1	2:P:367:ARG:NH2	1.88	0.70
2:V:312:ALA:HB1	2:V:317:ILE:HB	1.72	0.70
1:B:7:THR:OG1	2:N:178:ILE:CD1	2.39	0.70
1:K:96:THR:OG1	1:K:98:GLN:HB2	1.90	0.70
1:B:96:THR:OG1	1:B:98:GLN:HB2	1.90	0.70
1:E:7:THR:OG1	2:Q:178:ILE:CD1	2.39	0.70
1:G:3:GLU:CD	2:S:338:ALA:CB	2.59	0.70
1:G:384:ASN:HD22	1:G:384:ASN:N	1.89	0.70
1:H:384:ASN:HD22	1:H:384:ASN:N	1.89	0.70
1:K:7:THR:OG1	2:W:178:ILE:CD1	2.39	0.70
2:S:312:ALA:HB1	2:S:317:ILE:HB	1.72	0.70
2:T:64:HIS:HE1	2:T:330:MET:O	1.73	0.70
2:O:312:ALA:HB1	2:O:317:ILE:HB	1.72	0.70
2:Q:64:HIS:HE1	2:Q:330:MET:O	1.73	0.70
1:A:7:THR:OG1	2:M:178:ILE:CD1	2.39	0.70
1:A:320:LYS:NZ	1:G:461:GLU:OE1	2.24	0.70
1:F:3:GLU:CD	2:R:338:ALA:CB	2.59	0.70
1:H:7:THR:OG1	2:T:178:ILE:CD1	2.39	0.70
1:I:96:THR:OG1	1:I:98:GLN:HB2	1.90	0.70
1:D:7:THR:OG1	2:P:178:ILE:CD1	2.39	0.70
1:D:96:THR:OG1	1:D:98:GLN:HB2	1.90	0.70
1:F:399:LEU:H	1:F:401:PRO:CG	1.90	0.70
1:I:7:THR:OG1	2:U:178:ILE:CD1	2.39	0.70
1:L:7:THR:OG1	2:X:178:ILE:CD1	2.39	0.70
1:F:4:HIS:CB	2:R:179:LYS:HZ3	1.89	0.70
1:F:7:THR:OG1	2:R:178:ILE:CD1	2.39	0.70
1:F:384:ASN:N	1:F:384:ASN:HD22	1.89	0.70
1:J:7:THR:OG1	2:V:178:ILE:CD1	2.39	0.70
1:L:384:ASN:HD22	1:L:384:ASN:N	1.89	0.70
2:R:312:ALA:HB1	2:R:317:ILE:HB	1.72	0.70
2:Q:68:GLY:HA3	2:Q:332:ASN:O	1.92	0.69
2:T:68:GLY:HA3	2:T:332:ASN:O	1.92	0.69
1:A:384:ASN:HD22	1:A:384:ASN:N	1.89	0.69
1:C:7:THR:OG1	2:O:178:ILE:CD1	2.39	0.69
1:F:3:GLU:OE2	2:R:338:ALA:HB3	1.93	0.69
1:G:7:THR:OG1	2:S:178:ILE:CD1	2.39	0.69
1:B:384:ASN:HD22	1:B:384:ASN:N	1.89	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:3:GLU:OE2	2:S:338:ALA:HB3	1.93	0.69
2:U:68:GLY:HA3	2:U:332:ASN:O	1.92	0.69
1:A:399:LEU:N	1:A:401:PRO:CG	2.52	0.69
1:C:96:THR:OG1	1:C:98:GLN:HB2	1.90	0.69
1:D:384:ASN:HD22	1:D:384:ASN:N	1.89	0.69
1:H:4:HIS:CD2	2:T:178:ILE:CG1	2.58	0.69
1:K:384:ASN:HD22	1:K:384:ASN:N	1.89	0.69
2:P:68:GLY:HA3	2:P:332:ASN:O	1.92	0.69
2:X:341:TYR:HD1	2:X:367:ARG:NH2	1.88	0.69
1:H:3:GLU:OE2	2:T:338:ALA:HB3	1.93	0.69
1:I:384:ASN:N	1:I:384:ASN:HD22	1.89	0.69
1:J:96:THR:OG1	1:J:98:GLN:HB2	1.90	0.69
1:E:3:GLU:OE2	2:Q:338:ALA:HB3	1.93	0.69
1:L:399:LEU:N	1:L:401:PRO:CG	2.52	0.69
1:A:3:GLU:OE2	2:M:338:ALA:HB3	1.93	0.69
1:D:3:GLU:OE2	2:P:338:ALA:HB3	1.93	0.69
1:G:399:LEU:H	1:G:401:PRO:CG	1.90	0.69
1:I:3:GLU:OE2	2:U:338:ALA:HB3	1.93	0.69
1:J:30:HIS:H	1:K:180:PHE:HB3	1.58	0.69
2:M:341:TYR:HD1	2:M:367:ARG:NH2	1.88	0.69
1:D:4:HIS:CA	2:P:179:LYS:NZ	2.53	0.69
1:C:3:GLU:OE2	2:O:338:ALA:HB3	1.93	0.69
1:E:4:HIS:CA	2:Q:179:LYS:NZ	2.53	0.69
1:F:399:LEU:N	1:F:401:PRO:CG	2.52	0.69
1:G:399:LEU:N	1:G:401:PRO:CG	2.52	0.69
1:I:4:HIS:CA	2:U:179:LYS:NZ	2.53	0.68
1:J:384:ASN:HD22	1:J:384:ASN:N	1.89	0.68
1:L:3:GLU:OE2	2:X:338:ALA:HB3	1.93	0.68
2:W:59:ILE:HD12	2:W:280:LEU:HD11	1.75	0.68
2:N:59:ILE:HD12	2:N:280:LEU:HD11	1.75	0.68
2:O:68:GLY:HA3	2:O:332:ASN:O	1.92	0.68
2:X:68:GLY:HA3	2:X:332:ASN:O	1.92	0.68
1:G:337:ARG:CB	1:L:61:ASN:O	2.34	0.68
1:J:3:GLU:OE2	2:V:338:ALA:HB3	1.93	0.68
1:C:384:ASN:HD22	1:C:384:ASN:N	1.89	0.68
1:G:399:LEU:HA	1:G:400:PRO:O	1.94	0.68
2:M:68:GLY:HA3	2:M:332:ASN:O	1.92	0.68
2:O:59:ILE:HD12	2:O:280:LEU:HD11	1.75	0.68
2:S:68:GLY:HA3	2:S:332:ASN:O	1.92	0.68
2:V:68:GLY:HA3	2:V:332:ASN:O	1.92	0.68
1:F:399:LEU:HA	1:F:400:PRO:O	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:59:ILE:HD12	2:U:280:LEU:HD11	1.75	0.68
1:H:4:HIS:CA	2:T:179:LYS:NZ	2.53	0.68
1:I:399:LEU:HA	1:I:400:PRO:O	1.94	0.68
2:V:59:ILE:HD12	2:V:280:LEU:HD11	1.75	0.68
1:D:399:LEU:HA	1:D:400:PRO:O	1.94	0.68
2:P:59:ILE:HD12	2:P:280:LEU:HD11	1.75	0.68
1:A:4:HIS:CD2	2:M:178:ILE:CG1	2.58	0.68
1:E:399:LEU:HA	1:E:400:PRO:O	1.94	0.68
1:A:3:GLU:HG2	2:M:338:ALA:HB2	1.75	0.68
1:K:3:GLU:OE2	2:W:338:ALA:HB3	1.92	0.68
2:R:68:GLY:HA3	2:R:332:ASN:O	1.92	0.68
1:B:3:GLU:OE2	2:N:338:ALA:HB3	1.93	0.67
1:H:399:LEU:HA	1:H:400:PRO:O	1.94	0.67
1:I:3:GLU:HG2	2:U:338:ALA:HB2	1.75	0.67
1:K:3:GLU:HG2	2:W:338:ALA:HB2	1.75	0.67
1:L:3:GLU:HG2	2:X:338:ALA:HB2	1.75	0.67
2:S:43:LEU:CD1	2:S:60:ILE:HD11	2.24	0.67
1:L:4:HIS:CD2	2:X:178:ILE:CG1	2.58	0.67
2:P:43:LEU:CD1	2:P:60:ILE:HD11	2.24	0.67
2:R:59:ILE:HD12	2:R:280:LEU:HD11	1.75	0.67
2:U:43:LEU:CD1	2:U:60:ILE:HD11	2.24	0.67
2:W:68:GLY:HA3	2:W:332:ASN:O	1.92	0.67
1:B:3:GLU:HG2	2:N:338:ALA:HB2	1.76	0.67
1:L:295:LEU:O	1:L:388:PRO:CG	2.43	0.67
2:S:59:ILE:HD12	2:S:280:LEU:HD11	1.75	0.67
1:A:295:LEU:O	1:A:388:PRO:CG	2.43	0.67
1:D:3:GLU:HG2	2:P:338:ALA:HB2	1.75	0.67
2:N:68:GLY:HA3	2:N:332:ASN:O	1.92	0.67
2:R:43:LEU:CD1	2:R:60:ILE:HD11	2.24	0.67
2:M:59:ILE:HD12	2:M:280:LEU:HD11	1.75	0.67
2:V:43:LEU:CD1	2:V:60:ILE:HD11	2.24	0.67
2:X:59:ILE:HD12	2:X:280:LEU:HD11	1.75	0.67
1:G:4:HIS:CA	2:S:179:LYS:NZ	2.53	0.67
2:O:43:LEU:CD1	2:O:60:ILE:HD11	2.24	0.67
2:M:43:LEU:CD1	2:M:60:ILE:HD11	2.24	0.67
1:J:3:GLU:HG2	2:V:338:ALA:HB2	1.76	0.67
1:B:4:HIS:CB	2:N:179:LYS:HZ2	1.88	0.67
1:F:3:GLU:HG2	2:R:338:ALA:HB2	1.75	0.67
1:F:458:HIS:CD2	1:F:460:VAL:H	2.11	0.67
1:G:458:HIS:CD2	1:G:460:VAL:H	2.11	0.67
1:I:295:LEU:O	1:I:388:PRO:CG	2.43	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:399:LEU:HA	1:K:400:PRO:O	1.94	0.67
2:N:43:LEU:CD1	2:N:60:ILE:HD11	2.24	0.67
2:T:59:ILE:HD12	2:T:280:LEU:HD11	1.75	0.67
2:W:43:LEU:CD1	2:W:60:ILE:HD11	2.24	0.67
2:X:43:LEU:CD1	2:X:60:ILE:HD11	2.24	0.67
1:A:53:SER:HB2	1:F:179:TYR:CD2	2.30	0.67
1:B:295:LEU:O	1:B:388:PRO:CG	2.43	0.67
1:J:399:LEU:HA	1:J:400:PRO:O	1.94	0.67
2:W:312:ALA:HB2	2:W:317:ILE:HB	1.77	0.67
1:B:399:LEU:HA	1:B:400:PRO:O	1.94	0.66
1:C:3:GLU:HG2	2:O:338:ALA:HB2	1.75	0.66
1:D:295:LEU:O	1:D:388:PRO:CG	2.43	0.66
1:F:43:PHE:CD2	2:R:370:LYS:HG2	2.31	0.66
1:G:3:GLU:HG2	2:S:338:ALA:HB2	1.75	0.66
1:G:295:LEU:O	1:G:388:PRO:CG	2.43	0.66
1:H:43:PHE:CD2	2:T:370:LYS:HG2	2.31	0.66
1:K:295:LEU:O	1:K:388:PRO:CG	2.43	0.66
1:L:399:LEU:HA	1:L:400:PRO:O	1.94	0.66
2:N:312:ALA:HB2	2:N:317:ILE:HB	1.77	0.66
1:A:399:LEU:HA	1:A:400:PRO:O	1.94	0.66
1:E:3:GLU:HG2	2:Q:338:ALA:HB2	1.75	0.66
1:G:43:PHE:CD2	2:S:370:LYS:HG2	2.31	0.66
1:H:399:LEU:H	1:H:401:PRO:CG	1.90	0.66
2:O:83:LYS:O	2:O:87:ASP:HB2	1.96	0.66
2:Q:43:LEU:CD1	2:Q:60:ILE:HD11	2.24	0.66
2:Q:59:ILE:HD12	2:Q:280:LEU:HD11	1.75	0.66
2:V:83:LYS:O	2:V:87:ASP:HB2	1.96	0.66
1:C:4:HIS:CA	2:O:179:LYS:NZ	2.53	0.66
1:C:399:LEU:HA	1:C:400:PRO:O	1.94	0.66
1:D:3:GLU:OE1	2:P:368:ILE:HA	1.96	0.66
1:F:295:LEU:O	1:F:388:PRO:CG	2.43	0.66
1:H:3:GLU:HG2	2:T:338:ALA:HB2	1.75	0.66
2:N:83:LYS:O	2:N:87:ASP:HB2	1.96	0.66
2:T:43:LEU:CD1	2:T:60:ILE:HD11	2.24	0.66
1:E:43:PHE:CD2	2:Q:370:LYS:HG2	2.31	0.66
1:E:399:LEU:H	1:E:401:PRO:CG	1.90	0.66
1:L:43:PHE:CD2	2:X:370:LYS:HG2	2.31	0.66
1:A:3:GLU:OE2	2:M:338:ALA:CB	2.44	0.66
1:C:295:LEU:O	1:C:388:PRO:CG	2.43	0.66
1:F:3:GLU:OE2	2:R:338:ALA:CB	2.44	0.66
1:I:3:GLU:OE1	2:U:368:ILE:HA	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:295:LEU:O	1:J:388:PRO:CG	2.43	0.66
2:W:83:LYS:O	2:W:87:ASP:HB2	1.96	0.66
1:A:43:PHE:CD2	2:M:370:LYS:HG2	2.31	0.66
1:E:3:GLU:OE1	2:Q:368:ILE:HA	1.96	0.66
1:G:3:GLU:OE2	2:S:338:ALA:CB	2.44	0.66
1:H:3:GLU:OE1	2:T:368:ILE:HA	1.96	0.66
1:K:3:GLU:OE2	2:W:338:ALA:CB	2.44	0.66
1:K:43:PHE:CD2	2:W:370:LYS:HG2	2.30	0.66
1:L:3:GLU:OE2	2:X:338:ALA:CB	2.44	0.66
1:D:43:PHE:CD2	2:P:370:LYS:HG2	2.31	0.66
1:B:43:PHE:CD2	2:N:370:LYS:HG2	2.31	0.66
1:E:295:LEU:O	1:E:388:PRO:CG	2.43	0.66
1:H:295:LEU:O	1:H:388:PRO:CG	2.43	0.66
2:P:237:THR:O	2:P:237:THR:HG22	1.96	0.66
2:U:237:THR:O	2:U:237:THR:HG22	1.96	0.66
1:B:3:GLU:OE2	2:N:338:ALA:CB	2.44	0.66
1:C:43:PHE:CD2	2:O:370:LYS:HG2	2.31	0.66
1:I:43:PHE:CD2	2:U:370:LYS:HG2	2.31	0.66
1:J:4:HIS:CA	2:V:179:LYS:NZ	2.53	0.66
1:J:43:PHE:CD2	2:V:370:LYS:HG2	2.31	0.66
1:C:3:GLU:OE1	2:O:368:ILE:HA	1.96	0.66
1:G:3:GLU:OE1	2:S:368:ILE:HA	1.96	0.66
1:J:3:GLU:OE1	2:V:368:ILE:HA	1.96	0.66
2:V:312:ALA:HB2	2:V:317:ILE:HB	1.77	0.66
1:K:4:HIS:CB	2:W:179:LYS:HZ2	1.89	0.65
2:O:312:ALA:HB2	2:O:317:ILE:HB	1.77	0.65
1:A:365:ALA:O	1:A:367:PRO:HD3	1.96	0.65
1:A:458:HIS:CD2	1:A:460:VAL:H	2.11	0.65
1:F:3:GLU:OE1	2:R:368:ILE:HA	1.96	0.65
1:L:365:ALA:O	1:L:367:PRO:HD3	1.96	0.65
2:U:83:LYS:O	2:U:87:ASP:HB2	1.96	0.65
1:G:30:HIS:H	1:H:180:PHE:HB3	1.62	0.65
1:I:3:GLU:OE2	2:U:338:ALA:CB	2.44	0.65
2:P:83:LYS:O	2:P:87:ASP:HB2	1.96	0.65
1:D:3:GLU:OE2	2:P:338:ALA:CB	2.44	0.65
2:M:83:LYS:O	2:M:87:ASP:HB2	1.96	0.65
2:Q:312:ALA:HB2	2:Q:317:ILE:HB	1.77	0.65
2:T:312:ALA:HB2	2:T:317:ILE:HB	1.77	0.65
2:R:312:ALA:HB2	2:R:317:ILE:HB	1.77	0.65
1:A:43:PHE:CG	2:M:370:LYS:HG2	2.32	0.65
1:E:3:GLU:OE2	2:Q:338:ALA:CB	2.44	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:458:HIS:CD2	1:L:460:VAL:H	2.11	0.65
1:D:461:GLU:OE1	1:J:320:LYS:NZ	2.26	0.65
1:J:3:GLU:OE2	2:V:338:ALA:CB	2.44	0.65
1:K:43:PHE:CG	2:W:370:LYS:HG2	2.32	0.65
2:S:83:LYS:O	2:S:87:ASP:HB2	1.96	0.65
1:A:29:GLN:OE1	1:F:181:PRO:HD3	1.96	0.65
1:B:43:PHE:CG	2:N:370:LYS:HG2	2.32	0.65
1:H:399:LEU:N	1:H:401:PRO:CG	2.52	0.65
1:I:30:HIS:H	1:J:180:PHE:HB3	1.62	0.65
2:R:83:LYS:O	2:R:87:ASP:HB2	1.96	0.65
1:C:3:GLU:OE2	2:O:338:ALA:CB	2.44	0.65
1:D:43:PHE:CG	2:P:370:LYS:HG2	2.32	0.65
1:H:3:GLU:OE2	2:T:338:ALA:CB	2.44	0.65
1:J:61:ASN:O	1:K:337:ARG:CB	2.34	0.65
2:P:312:ALA:HB2	2:P:317:ILE:HB	1.77	0.65
2:R:43:LEU:HD13	2:R:60:ILE:HD11	1.79	0.65
2:X:83:LYS:O	2:X:87:ASP:HB2	1.96	0.65
1:F:43:PHE:CG	2:R:370:LYS:HG2	2.32	0.65
1:L:3:GLU:OE1	2:X:368:ILE:HA	1.96	0.65
1:L:43:PHE:CG	2:X:370:LYS:HG2	2.32	0.65
2:S:43:LEU:HD13	2:S:60:ILE:HD11	1.79	0.65
2:X:237:THR:O	2:X:237:THR:HG22	1.96	0.65
2:X:369:THR:CA	2:X:370:LYS:N	2.59	0.65
1:A:3:GLU:OE1	2:M:368:ILE:HA	1.96	0.64
1:B:365:ALA:O	1:B:367:PRO:HD3	1.96	0.64
1:F:365:ALA:O	1:F:367:PRO:HD3	1.96	0.64
1:I:43:PHE:CG	2:U:370:LYS:HG2	2.32	0.64
2:M:237:THR:O	2:M:237:THR:HG22	1.96	0.64
2:Q:237:THR:HG22	2:Q:237:THR:O	1.96	0.64
2:S:312:ALA:HB2	2:S:317:ILE:HB	1.77	0.64
2:T:43:LEU:HD13	2:T:60:ILE:HD11	1.79	0.64
2:T:83:LYS:O	2:T:87:ASP:HB2	1.96	0.64
1:A:4:HIS:CA	2:M:179:LYS:NZ	2.53	0.64
1:C:43:PHE:CG	2:O:370:LYS:HG2	2.32	0.64
1:C:179:TYR:CD2	1:D:53:SER:HB2	2.32	0.64
1:J:43:PHE:CG	2:V:370:LYS:HG2	2.32	0.64
1:K:365:ALA:O	1:K:367:PRO:HD3	1.96	0.64
2:Q:43:LEU:HD13	2:Q:60:ILE:HD11	1.79	0.64
1:B:458:HIS:CD2	1:B:460:VAL:H	2.11	0.64
1:E:365:ALA:O	1:E:367:PRO:HD3	1.96	0.64
1:E:399:LEU:N	1:E:401:PRO:CG	2.52	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:43:PHE:CG	2:S:370:LYS:HG2	2.32	0.64
1:G:365:ALA:O	1:G:367:PRO:HD3	1.97	0.64
2:M:312:ALA:HB2	2:M:317:ILE:HB	1.77	0.64
2:N:237:THR:HG22	2:N:237:THR:O	1.96	0.64
2:Q:83:LYS:O	2:Q:87:ASP:HB2	1.96	0.64
2:W:237:THR:O	2:W:237:THR:HG22	1.96	0.64
2:X:312:ALA:HB2	2:X:317:ILE:HB	1.77	0.64
1:B:3:GLU:OE1	2:N:368:ILE:HA	1.96	0.64
1:B:170:GLY:HA2	1:B:172:ARG:NH2	2.13	0.64
1:C:399:LEU:N	1:C:401:PRO:CG	2.52	0.64
1:H:53:SER:HB2	1:I:179:TYR:CD2	2.32	0.64
1:K:170:GLY:HA2	1:K:172:ARG:NH2	2.13	0.64
2:T:237:THR:O	2:T:237:THR:HG22	1.96	0.64
2:U:43:LEU:HD13	2:U:60:ILE:HD11	1.79	0.64
2:U:312:ALA:HB2	2:U:317:ILE:HB	1.77	0.64
1:A:170:GLY:HA2	1:A:172:ARG:NH2	2.13	0.64
1:C:458:HIS:CD2	1:C:460:VAL:H	2.11	0.64
1:D:170:GLY:HA2	1:D:172:ARG:NH2	2.13	0.64
1:E:43:PHE:CG	2:Q:370:LYS:HG2	2.32	0.64
1:E:461:GLU:OE1	1:K:320:LYS:NZ	2.27	0.64
1:I:170:GLY:HA2	1:I:172:ARG:NH2	2.13	0.64
1:J:365:ALA:O	1:J:367:PRO:HD3	1.96	0.64
1:K:3:GLU:OE1	2:W:368:ILE:HA	1.96	0.64
2:N:369:THR:CA	2:N:370:LYS:N	2.59	0.64
2:P:43:LEU:HD13	2:P:60:ILE:HD11	1.80	0.64
1:B:211:HIS:HD2	1:B:212:GLU:O	1.81	0.64
1:H:43:PHE:CG	2:T:370:LYS:HG2	2.32	0.64
1:J:399:LEU:N	1:J:401:PRO:CG	2.52	0.64
1:K:211:HIS:HD2	1:K:212:GLU:O	1.81	0.64
1:K:458:HIS:CD2	1:K:460:VAL:H	2.12	0.64
1:L:170:GLY:HA2	1:L:172:ARG:NH2	2.13	0.64
2:V:237:THR:HG22	2:V:237:THR:O	1.96	0.64
2:W:369:THR:CA	2:W:370:LYS:N	2.59	0.64
1:C:365:ALA:O	1:C:367:PRO:HD3	1.96	0.64
1:D:399:LEU:H	1:D:401:PRO:CG	1.90	0.64
1:J:170:GLY:HA2	1:J:172:ARG:NH2	2.13	0.64
1:L:3:GLU:HG2	2:X:338:ALA:CB	2.28	0.64
1:L:4:HIS:CA	2:X:179:LYS:NZ	2.53	0.64
2:M:43:LEU:HD13	2:M:60:ILE:HD11	1.79	0.64
2:O:237:THR:O	2:O:237:THR:HG22	1.96	0.64
2:Q:59:ILE:CD1	2:Q:280:LEU:HD21	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:59:ILE:CD1	2:R:280:LEU:HD21	2.28	0.64
2:S:59:ILE:CD1	2:S:280:LEU:HD21	2.28	0.64
2:S:237:THR:HG22	2:S:237:THR:O	1.96	0.64
1:D:4:HIS:CD2	2:P:178:ILE:CG1	2.58	0.64
1:I:365:ALA:O	1:I:367:PRO:HD3	1.96	0.64
2:M:59:ILE:CD1	2:M:280:LEU:HD21	2.28	0.64
2:T:59:ILE:CD1	2:T:280:LEU:HD21	2.28	0.64
2:X:59:ILE:CD1	2:X:280:LEU:HD21	2.28	0.64
1:A:3:GLU:HG2	2:M:338:ALA:CB	2.28	0.64
1:C:170:GLY:HA2	1:C:172:ARG:NH2	2.13	0.64
1:H:365:ALA:O	1:H:367:PRO:HD3	1.96	0.64
1:I:211:HIS:HD2	1:I:212:GLU:O	1.81	0.64
1:J:458:HIS:CD2	1:J:460:VAL:H	2.11	0.64
2:M:369:THR:CA	2:M:370:LYS:N	2.59	0.64
2:R:237:THR:O	2:R:237:THR:HG22	1.96	0.64
1:C:3:GLU:HG2	2:O:338:ALA:CB	2.28	0.64
1:D:211:HIS:HD2	1:D:212:GLU:O	1.81	0.64
1:D:320:LYS:NZ	1:J:461:GLU:OE1	2.28	0.64
1:D:458:HIS:CD2	1:D:460:VAL:H	2.11	0.64
1:E:320:LYS:NZ	1:K:461:GLU:OE1	2.27	0.64
2:P:59:ILE:CD1	2:P:280:LEU:HD21	2.28	0.64
2:X:43:LEU:HD13	2:X:60:ILE:HD11	1.79	0.64
1:D:3:GLU:HG2	2:P:338:ALA:CB	2.28	0.63
1:D:365:ALA:O	1:D:367:PRO:HD3	1.96	0.63
1:E:458:HIS:CD2	1:E:460:VAL:H	2.11	0.63
1:F:3:GLU:HG2	2:R:338:ALA:CB	2.28	0.63
1:F:386:ILE:O	1:F:388:PRO:HD3	1.99	0.63
1:G:3:GLU:HG2	2:S:338:ALA:CB	2.28	0.63
1:G:386:ILE:O	1:G:388:PRO:HD3	1.99	0.63
1:I:3:GLU:HG2	2:U:338:ALA:CB	2.28	0.63
1:J:3:GLU:HG2	2:V:338:ALA:CB	2.28	0.63
1:J:211:HIS:HD2	1:J:212:GLU:O	1.81	0.63
2:O:43:LEU:HD13	2:O:60:ILE:HD11	1.79	0.63
2:T:369:THR:CA	2:T:370:LYS:N	2.59	0.63
2:U:59:ILE:CD1	2:U:280:LEU:HD21	2.28	0.63
2:V:43:LEU:HD13	2:V:60:ILE:HD11	1.79	0.63
1:C:211:HIS:HD2	1:C:212:GLU:O	1.81	0.63
1:E:170:GLY:HA2	1:E:172:ARG:NH2	2.13	0.63
1:E:211:HIS:HD2	1:E:212:GLU:O	1.81	0.63
1:G:211:HIS:HD2	1:G:212:GLU:O	1.81	0.63
1:H:211:HIS:HD2	1:H:212:GLU:O	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:458:HIS:CD2	1:I:460:VAL:H	2.11	0.63
1:E:386:ILE:O	1:E:388:PRO:HD3	1.99	0.63
1:I:4:HIS:CD2	2:U:178:ILE:CG1	2.59	0.63
1:I:399:LEU:H	1:I:401:PRO:CG	1.90	0.63
2:O:59:ILE:CD1	2:O:280:LEU:HD21	2.28	0.63
2:Q:369:THR:CA	2:Q:370:LYS:N	2.59	0.63
1:H:386:ILE:O	1:H:388:PRO:HD3	1.99	0.63
1:J:399:LEU:H	1:J:401:PRO:CG	1.90	0.63
2:V:59:ILE:CD1	2:V:280:LEU:HD21	2.28	0.63
1:A:386:ILE:O	1:A:388:PRO:HD3	1.99	0.63
1:E:235:ILE:CG2	1:E:367:PRO:HG3	2.28	0.63
1:H:3:GLU:HG2	2:T:338:ALA:CB	2.28	0.63
1:H:170:GLY:HA2	1:H:172:ARG:NH2	2.13	0.63
1:H:458:HIS:CD2	1:H:460:VAL:H	2.11	0.63
2:N:43:LEU:HD13	2:N:60:ILE:HD11	1.79	0.63
1:E:3:GLU:HG2	2:Q:338:ALA:CB	2.28	0.63
1:F:211:HIS:HD2	1:F:212:GLU:O	1.81	0.63
1:F:320:LYS:NZ	1:L:461:GLU:OE1	2.27	0.63
1:H:235:ILE:CG2	1:H:367:PRO:HG3	2.28	0.63
1:K:3:GLU:HG2	2:W:338:ALA:CB	2.28	0.63
1:L:386:ILE:O	1:L:388:PRO:HD3	1.99	0.63
2:N:59:ILE:CD1	2:N:280:LEU:HD21	2.28	0.63
2:W:59:ILE:CD1	2:W:280:LEU:HD21	2.28	0.63
1:F:170:GLY:HA2	1:F:172:ARG:NH2	2.13	0.63
1:K:396:LEU:HD12	1:K:398:ASP:H	1.64	0.63
2:S:369:THR:CA	2:S:370:LYS:N	2.59	0.63
2:W:43:LEU:HD13	2:W:60:ILE:HD11	1.79	0.63
1:B:3:GLU:HG2	2:N:338:ALA:CB	2.28	0.63
1:B:396:LEU:HD12	1:B:398:ASP:H	1.64	0.63
1:G:170:GLY:HA2	1:G:172:ARG:NH2	2.13	0.63
2:O:48:PRO:O	2:O:52:ALA:HB2	1.99	0.63
2:V:48:PRO:O	2:V:52:ALA:HB2	1.99	0.63
1:A:211:HIS:HD2	1:A:212:GLU:O	1.81	0.63
1:E:396:LEU:HD12	1:E:398:ASP:H	1.64	0.63
1:H:396:LEU:HD12	1:H:398:ASP:H	1.64	0.63
1:L:211:HIS:HD2	1:L:212:GLU:O	1.81	0.63
2:R:369:THR:CA	2:R:370:LYS:N	2.59	0.63
1:G:396:LEU:HD12	1:G:398:ASP:H	1.64	0.62
2:S:48:PRO:O	2:S:52:ALA:HB2	1.99	0.62
2:W:309:GLU:O	2:W:313:LYS:CE	2.47	0.62
1:D:396:LEU:HD12	1:D:398:ASP:H	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:309:GLU:O	2:N:313:LYS:CE	2.47	0.62
2:Q:48:PRO:O	2:Q:52:ALA:HB2	1.99	0.62
2:R:48:PRO:O	2:R:52:ALA:HB2	1.99	0.62
2:T:48:PRO:O	2:T:52:ALA:HB2	1.99	0.62
1:B:4:HIS:CD2	2:N:178:ILE:CG1	2.58	0.62
1:F:396:LEU:HD12	1:F:398:ASP:H	1.64	0.62
1:I:396:LEU:HD12	1:I:398:ASP:H	1.64	0.62
2:M:48:PRO:O	2:M:52:ALA:HB2	1.99	0.62
2:P:48:PRO:O	2:P:52:ALA:HB2	1.99	0.62
2:X:48:PRO:O	2:X:52:ALA:HB2	1.99	0.62
1:I:386:ILE:O	1:I:388:PRO:HD3	1.99	0.62
2:U:369:THR:CA	2:U:370:LYS:N	2.59	0.62
1:A:396:LEU:HD12	1:A:398:ASP:H	1.64	0.62
1:C:396:LEU:HD12	1:C:398:ASP:H	1.64	0.62
1:D:386:ILE:O	1:D:388:PRO:HD3	1.99	0.62
1:L:396:LEU:HD12	1:L:398:ASP:H	1.64	0.62
2:U:48:PRO:O	2:U:52:ALA:HB2	1.99	0.62
1:C:399:LEU:H	1:C:401:PRO:CG	1.90	0.62
1:I:399:LEU:N	1:I:401:PRO:CG	2.52	0.62
1:K:4:HIS:CD2	2:W:178:ILE:CG1	2.58	0.62
2:O:369:THR:CA	2:O:370:LYS:N	2.59	0.62
2:N:48:PRO:O	2:N:52:ALA:HB2	1.99	0.62
2:P:369:THR:CA	2:P:370:LYS:N	2.59	0.62
2:V:369:THR:CA	2:V:370:LYS:N	2.59	0.62
1:B:4:HIS:CA	2:N:179:LYS:NZ	2.53	0.62
1:J:396:LEU:HD12	1:J:398:ASP:H	1.64	0.62
2:W:48:PRO:O	2:W:52:ALA:HB2	1.99	0.62
1:C:235:ILE:CG2	1:C:367:PRO:HG3	2.27	0.62
1:D:399:LEU:N	1:D:401:PRO:CG	2.52	0.62
1:J:386:ILE:O	1:J:388:PRO:HD3	1.99	0.62
2:M:309:GLU:O	2:M:313:LYS:CE	2.47	0.62
2:Q:309:GLU:O	2:Q:313:LYS:CE	2.47	0.62
1:B:386:ILE:O	1:B:388:PRO:HD3	1.99	0.61
1:C:386:ILE:O	1:C:388:PRO:HD3	1.99	0.61
1:K:399:LEU:N	1:K:401:PRO:CG	2.52	0.61
2:R:1:LYS:CA	2:R:54:GLY:O	2.48	0.61
2:T:309:GLU:O	2:T:313:LYS:CE	2.47	0.61
1:B:427:PHE:CE1	1:B:428:LEU:HD13	2.35	0.61
1:K:386:ILE:O	1:K:388:PRO:HD3	1.99	0.61
2:X:309:GLU:O	2:X:313:LYS:CE	2.47	0.61
1:B:399:LEU:N	1:B:401:PRO:CG	2.52	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:427:PHE:CE1	1:C:428:LEU:HD13	2.35	0.61
1:K:427:PHE:CE1	1:K:428:LEU:HD13	2.36	0.61
1:B:155:GLU:OE1	1:B:211:HIS:HE1	1.83	0.61
1:J:235:ILE:CG2	1:J:367:PRO:HG3	2.28	0.61
1:J:427:PHE:CE1	1:J:428:LEU:HD13	2.35	0.61
1:K:4:HIS:CA	2:W:179:LYS:NZ	2.53	0.61
1:K:7:THR:HG21	2:W:335:GLN:OE1	2.01	0.61
1:K:155:GLU:OE1	1:K:211:HIS:HE1	1.83	0.61
2:S:1:LYS:CA	2:S:54:GLY:O	2.48	0.61
1:L:155:GLU:OE1	1:L:211:HIS:HE1	1.83	0.61
1:A:7:THR:HG21	2:M:335:GLN:OE1	2.01	0.61
1:A:155:GLU:OE1	1:A:211:HIS:HE1	1.83	0.61
1:C:4:HIS:CD2	2:O:178:ILE:CG1	2.58	0.61
1:D:7:THR:HG21	2:P:335:GLN:OE1	2.01	0.61
1:D:235:ILE:CG2	1:D:367:PRO:HG3	2.28	0.61
1:F:7:THR:HG21	2:R:335:GLN:OE1	2.01	0.61
1:G:7:THR:HG21	2:S:335:GLN:OE1	2.01	0.61
1:I:7:THR:HG21	2:U:335:GLN:OE1	2.01	0.61
1:K:53:SER:HB2	1:L:179:TYR:CD2	2.35	0.61
1:L:7:THR:HG21	2:X:335:GLN:OE1	2.01	0.61
1:A:180:PHE:HB3	1:B:30:HIS:H	1.65	0.61
1:B:7:THR:HG21	2:N:335:GLN:OE1	2.01	0.61
1:C:7:THR:HG21	2:O:335:GLN:OE1	2.01	0.61
1:J:7:THR:HG21	2:V:335:GLN:OE1	2.01	0.61
1:L:334:TYR:CE2	1:L:391:PRO:HG3	2.36	0.61
1:A:334:TYR:CE2	1:A:391:PRO:HG3	2.36	0.61
1:A:461:GLU:OE1	1:G:320:LYS:NZ	2.25	0.61
1:B:360:PHE:CG	1:B:361:PRO:HD3	2.35	0.61
1:D:44:GLU:HG3	2:P:370:LYS:HZ3	1.66	0.61
1:D:427:PHE:CE1	1:D:428:LEU:HD13	2.35	0.61
1:E:155:GLU:OE1	1:E:211:HIS:HE1	1.83	0.61
1:K:360:PHE:CG	1:K:361:PRO:HD3	2.35	0.61
1:C:180:PHE:HB3	1:D:30:HIS:H	1.66	0.61
1:D:155:GLU:OE1	1:D:211:HIS:HE1	1.83	0.61
1:F:360:PHE:CG	1:F:361:PRO:HD3	2.35	0.61
1:H:155:GLU:OE1	1:H:211:HIS:HE1	1.83	0.61
1:I:155:GLU:OE1	1:I:211:HIS:HE1	1.83	0.61
1:I:235:ILE:CG2	1:I:367:PRO:HG3	2.28	0.61
2:Q:45:GLU:O	2:Q:48:PRO:HD2	2.01	0.61
2:T:45:GLU:O	2:T:48:PRO:HD2	2.01	0.61
1:C:334:TYR:CE2	1:C:391:PRO:HG3	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:427:PHE:CE1	1:E:428:LEU:HD13	2.35	0.60
1:H:360:PHE:CG	1:H:361:PRO:HD3	2.35	0.60
1:I:427:PHE:CE1	1:I:428:LEU:HD13	2.36	0.60
1:J:155:GLU:OE1	1:J:211:HIS:HE1	1.83	0.60
1:K:29:GLN:OE1	1:L:181:PRO:HD3	2.01	0.60
2:O:45:GLU:O	2:O:48:PRO:HD2	2.01	0.60
2:S:45:GLU:O	2:S:48:PRO:HD2	2.01	0.60
2:U:45:GLU:O	2:U:48:PRO:HD2	2.01	0.60
1:A:427:PHE:CE1	1:A:428:LEU:HD13	2.36	0.60
1:E:360:PHE:CG	1:E:361:PRO:HD3	2.35	0.60
1:H:427:PHE:CE1	1:H:428:LEU:HD13	2.36	0.60
1:L:427:PHE:CE1	1:L:428:LEU:HD13	2.36	0.60
2:P:45:GLU:O	2:P:48:PRO:HD2	2.01	0.60
2:R:45:GLU:O	2:R:48:PRO:HD2	2.01	0.60
2:V:45:GLU:O	2:V:48:PRO:HD2	2.01	0.60
1:C:155:GLU:OE1	1:C:211:HIS:HE1	1.83	0.60
1:C:248:ARG:HH21	1:C:248:ARG:HG2	1.65	0.60
1:H:334:TYR:CE2	1:H:391:PRO:HG3	2.36	0.60
1:J:4:HIS:CD2	2:V:178:ILE:CG1	2.58	0.60
1:J:248:ARG:HH21	1:J:248:ARG:HG2	1.66	0.60
2:P:309:GLU:O	2:P:313:LYS:CE	2.47	0.60
1:E:7:THR:HG21	2:Q:335:GLN:OE1	2.01	0.60
1:E:334:TYR:CE2	1:E:391:PRO:HG3	2.36	0.60
1:H:44:GLU:HG3	2:T:370:LYS:HZ3	1.66	0.60
1:I:44:GLU:HG3	2:U:370:LYS:HZ3	1.67	0.60
1:J:323:VAL:O	1:J:325:GLY:N	2.35	0.60
1:J:334:TYR:CE2	1:J:391:PRO:HG3	2.36	0.60
1:L:3:GLU:OE1	2:X:367:ARG:O	2.20	0.60
2:N:45:GLU:O	2:N:48:PRO:HD2	2.01	0.60
2:W:45:GLU:O	2:W:48:PRO:HD2	2.01	0.60
1:A:3:GLU:OE1	2:M:367:ARG:O	2.20	0.60
1:C:320:LYS:NZ	1:I:461:GLU:OE1	2.30	0.60
1:C:323:VAL:O	1:C:325:GLY:N	2.35	0.60
1:D:334:TYR:CE2	1:D:391:PRO:HG3	2.36	0.60
1:D:360:PHE:CG	1:D:361:PRO:HD3	2.35	0.60
1:E:44:GLU:HG3	2:Q:370:LYS:HZ3	1.66	0.60
1:E:180:PHE:HB3	1:F:30:HIS:H	1.66	0.60
1:G:360:PHE:CG	1:G:361:PRO:HD3	2.35	0.60
1:H:7:THR:HG21	2:T:335:GLN:OE1	2.01	0.60
1:I:360:PHE:CG	1:I:361:PRO:HD3	2.35	0.60
2:P:1:LYS:CA	2:P:54:GLY:O	2.48	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:461:GLU:OE1	1:L:320:LYS:NZ	2.30	0.60
1:I:334:TYR:CE2	1:I:391:PRO:HG3	2.36	0.60
2:N:1:LYS:CA	2:N:54:GLY:O	2.48	0.60
2:U:309:GLU:O	2:U:313:LYS:CE	2.47	0.60
2:W:1:LYS:CA	2:W:54:GLY:O	2.48	0.60
1:B:334:TYR:CE2	1:B:391:PRO:HG3	2.36	0.60
1:E:248:ARG:HH21	1:E:248:ARG:HG2	1.66	0.60
1:E:323:VAL:O	1:E:325:GLY:N	2.35	0.60
1:F:155:GLU:OE1	1:F:211:HIS:HE1	1.83	0.60
1:G:334:TYR:CE2	1:G:391:PRO:HG3	2.36	0.60
1:G:427:PHE:CE1	1:G:428:LEU:HD13	2.36	0.60
1:K:334:TYR:CE2	1:K:391:PRO:HG3	2.36	0.60
2:R:309:GLU:O	2:R:313:LYS:CE	2.47	0.60
2:U:1:LYS:CA	2:U:54:GLY:O	2.48	0.60
1:C:181:PRO:HD3	1:D:29:GLN:OE1	2.01	0.60
1:F:427:PHE:CE1	1:F:428:LEU:HD13	2.36	0.60
1:H:248:ARG:HH21	1:H:248:ARG:HG2	1.66	0.60
1:B:3:GLU:OE1	2:N:367:ARG:O	2.20	0.60
1:F:3:GLU:OE1	2:R:367:ARG:O	2.20	0.60
1:H:323:VAL:O	1:H:325:GLY:N	2.35	0.60
2:T:64:HIS:CD2	2:T:261:VAL:H	2.19	0.60
1:B:248:ARG:HH21	1:B:248:ARG:HG2	1.66	0.60
1:F:334:TYR:CE2	1:F:391:PRO:HG3	2.36	0.60
1:G:155:GLU:OE1	1:G:211:HIS:HE1	1.83	0.60
1:I:3:GLU:OE1	2:U:367:ARG:O	2.19	0.60
1:K:248:ARG:HH21	1:K:248:ARG:HG2	1.66	0.60
2:X:45:GLU:O	2:X:48:PRO:HD2	2.01	0.60
1:I:248:ARG:HH21	1:I:248:ARG:HG2	1.66	0.59
2:S:309:GLU:O	2:S:313:LYS:CE	2.47	0.59
1:D:3:GLU:OE1	2:P:367:ARG:O	2.20	0.59
1:G:3:GLU:OE1	2:S:367:ARG:O	2.20	0.59
1:K:3:GLU:OE1	2:W:367:ARG:O	2.20	0.59
2:M:45:GLU:O	2:M:48:PRO:HD2	2.01	0.59
2:Q:64:HIS:CD2	2:Q:261:VAL:H	2.19	0.59
1:D:248:ARG:HH21	1:D:248:ARG:HG2	1.65	0.59
1:J:43:PHE:CG	2:V:370:LYS:HE2	2.32	0.59
1:A:235:ILE:CG2	1:A:367:PRO:HG3	2.27	0.59
1:A:323:VAL:O	1:A:325:GLY:N	2.35	0.59
1:B:323:VAL:O	1:B:325:GLY:N	2.35	0.59
1:K:323:VAL:O	1:K:325:GLY:N	2.35	0.59
1:D:181:PRO:HD3	1:E:29:GLN:OE1	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:323:VAL:O	1:I:325:GLY:N	2.35	0.59
1:A:248:ARG:HH21	1:A:248:ARG:HG2	1.66	0.59
1:J:3:GLU:OE1	2:V:367:ARG:O	2.20	0.59
1:K:360:PHE:CE2	1:K:361:PRO:HD3	2.37	0.59
2:O:136:ASP:O	2:O:140:LYS:HB2	2.02	0.59
2:V:136:ASP:O	2:V:140:LYS:HB2	2.03	0.59
1:B:360:PHE:CE2	1:B:361:PRO:HD3	2.37	0.59
1:C:3:GLU:OE1	2:O:367:ARG:O	2.20	0.59
1:C:43:PHE:CG	2:O:370:LYS:HE2	2.32	0.59
1:L:323:VAL:O	1:L:325:GLY:N	2.35	0.59
2:W:136:ASP:O	2:W:140:LYS:HB2	2.03	0.59
1:D:323:VAL:O	1:D:325:GLY:N	2.35	0.59
1:G:180:PHE:HB3	1:L:30:HIS:H	1.68	0.59
1:I:332:LEU:HB2	1:I:408:PRO:HB2	1.85	0.59
1:L:235:ILE:CG2	1:L:367:PRO:HG3	2.28	0.59
2:N:136:ASP:O	2:N:140:LYS:HB2	2.03	0.59
1:C:18:ASP:OD2	1:C:30:HIS:HD2	1.86	0.59
1:D:332:LEU:HB2	1:D:408:PRO:HB2	1.85	0.59
1:F:44:GLU:HG3	2:R:370:LYS:HZ3	1.66	0.59
1:G:44:GLU:HG3	2:S:370:LYS:HZ3	1.67	0.59
1:J:360:PHE:CE2	1:J:361:PRO:HD3	2.36	0.59
1:L:248:ARG:HH21	1:L:248:ARG:HG2	1.66	0.59
1:A:44:GLU:HG3	2:M:370:LYS:HZ3	1.66	0.58
1:C:360:PHE:CE2	1:C:361:PRO:HD3	2.37	0.58
1:D:18:ASP:OD2	1:D:30:HIS:HD2	1.86	0.58
1:E:118:THR:OG1	1:E:120:ILE:HG13	2.03	0.58
1:F:248:ARG:HH21	1:F:248:ARG:HG2	1.66	0.58
1:H:3:GLU:OE1	2:T:367:ARG:O	2.20	0.58
1:J:118:THR:OG1	1:J:120:ILE:HG13	2.03	0.58
2:U:64:HIS:CD2	2:U:261:VAL:H	2.19	0.58
1:B:399:LEU:H	1:B:401:PRO:CG	1.90	0.58
1:C:118:THR:OG1	1:C:120:ILE:HG13	2.04	0.58
1:G:323:VAL:O	1:G:325:GLY:N	2.35	0.58
1:G:332:LEU:HB2	1:G:408:PRO:HB2	1.85	0.58
1:H:118:THR:OG1	1:H:120:ILE:HG13	2.04	0.58
1:I:18:ASP:OD2	1:I:30:HIS:HD2	1.86	0.58
1:J:18:ASP:OD2	1:J:30:HIS:HD2	1.86	0.58
1:K:399:LEU:H	1:K:401:PRO:CG	1.90	0.58
2:U:3:GLU:O	2:U:4:GLU:CB	2.51	0.58
1:B:18:ASP:OD2	1:B:30:HIS:HD2	1.86	0.58
1:E:3:GLU:OE1	2:Q:367:ARG:O	2.20	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:64:HIS:CD2	2:P:261:VAL:H	2.19	0.58
2:Q:136:ASP:O	2:Q:140:LYS:HB2	2.03	0.58
2:T:136:ASP:O	2:T:140:LYS:HB2	2.02	0.58
2:U:136:ASP:O	2:U:140:LYS:HB2	2.02	0.58
1:C:360:PHE:CG	1:C:361:PRO:HD3	2.35	0.58
1:I:53:SER:HB2	1:J:179:TYR:CD2	2.38	0.58
1:K:18:ASP:OD2	1:K:30:HIS:HD2	1.86	0.58
2:M:136:ASP:O	2:M:140:LYS:HB2	2.02	0.58
2:P:3:GLU:O	2:P:4:GLU:CB	2.51	0.58
2:X:136:ASP:O	2:X:140:LYS:HB2	2.02	0.58
1:F:323:VAL:O	1:F:325:GLY:N	2.35	0.58
1:I:118:THR:OG1	1:I:120:ILE:HG13	2.04	0.58
2:O:136:ASP:OD2	2:O:140:LYS:NZ	2.35	0.58
2:P:136:ASP:O	2:P:140:LYS:HB2	2.02	0.58
1:C:461:GLU:OE1	1:I:320:LYS:NZ	2.33	0.58
1:D:118:THR:OG1	1:D:120:ILE:HG13	2.04	0.58
1:F:332:LEU:HB2	1:F:408:PRO:HB2	1.85	0.58
1:H:18:ASP:OD2	1:H:30:HIS:HD2	1.86	0.58
2:M:1:LYS:CA	2:M:54:GLY:O	2.48	0.58
2:R:136:ASP:O	2:R:140:LYS:HB2	2.02	0.58
2:U:136:ASP:OD2	2:U:140:LYS:NZ	2.35	0.58
2:X:1:LYS:CA	2:X:54:GLY:O	2.48	0.58
1:A:18:ASP:OD2	1:A:30:HIS:HD2	1.86	0.58
1:C:332:LEU:HB2	1:C:408:PRO:HB2	1.85	0.58
1:E:18:ASP:OD2	1:E:30:HIS:HD2	1.86	0.58
1:E:82:ASP:O	1:E:84:THR:CG2	2.51	0.58
1:H:82:ASP:O	1:H:84:THR:CG2	2.51	0.58
1:J:332:LEU:HB2	1:J:408:PRO:HB2	1.85	0.58
2:S:136:ASP:O	2:S:140:LYS:HB2	2.02	0.58
1:B:235:ILE:CG2	1:B:367:PRO:HG3	2.28	0.58
1:D:192:ARG:HH21	1:D:219:ASN:HD22	1.52	0.58
1:I:192:ARG:HH21	1:I:219:ASN:HD22	1.52	0.58
2:V:1:LYS:CA	2:V:54:GLY:O	2.48	0.58
1:C:308:ILE:HG21	1:C:374:LEU:HD13	1.86	0.58
1:F:443:ILE:O	1:F:447:ARG:HG3	2.04	0.58
1:G:248:ARG:HH21	1:G:248:ARG:HG2	1.66	0.58
1:J:360:PHE:CG	1:J:361:PRO:HD3	2.35	0.58
1:K:235:ILE:CG2	1:K:367:PRO:HG3	2.27	0.58
2:O:1:LYS:CA	2:O:54:GLY:O	2.48	0.58
1:A:43:PHE:CB	2:M:370:LYS:CD	2.82	0.58
1:C:180:PHE:O	1:D:29:GLN:HA	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:308:ILE:HG21	1:D:374:LEU:HD13	1.86	0.58
1:F:18:ASP:OD2	1:F:30:HIS:HD2	1.86	0.58
1:G:443:ILE:O	1:G:447:ARG:HG3	2.04	0.58
1:I:43:PHE:CG	2:U:370:LYS:HE2	2.32	0.58
1:J:44:GLU:HG3	2:V:370:LYS:HZ3	1.67	0.58
2:M:128:THR:HG22	2:M:131:GLU:H	1.69	0.58
2:N:128:THR:HG22	2:N:131:GLU:H	1.69	0.58
2:V:3:GLU:O	2:V:4:GLU:CB	2.51	0.58
2:V:64:HIS:CD2	2:V:261:VAL:H	2.19	0.58
1:B:43:PHE:CG	2:N:370:LYS:HE2	2.32	0.57
1:B:308:ILE:HG21	1:B:374:LEU:HD13	1.86	0.57
1:E:43:PHE:CB	2:Q:370:LYS:CD	2.82	0.57
1:F:4:HIS:CA	2:R:179:LYS:NZ	2.53	0.57
1:G:53:SER:HB2	1:H:179:TYR:CD2	2.40	0.57
1:H:332:LEU:HB2	1:H:408:PRO:HB2	1.85	0.57
1:J:308:ILE:HG21	1:J:374:LEU:HD13	1.86	0.57
1:K:43:PHE:CB	2:W:370:LYS:CD	2.82	0.57
1:K:308:ILE:HG21	1:K:374:LEU:HD13	1.86	0.57
1:L:18:ASP:OD2	1:L:30:HIS:HD2	1.86	0.57
2:M:136:ASP:OD2	2:M:203:HIS:CD2	2.56	0.57
2:Q:128:THR:HG22	2:Q:131:GLU:H	1.69	0.57
2:R:3:GLU:O	2:R:4:GLU:CB	2.51	0.57
2:T:128:THR:HG22	2:T:131:GLU:H	1.69	0.57
2:W:128:THR:HG22	2:W:131:GLU:H	1.69	0.57
2:X:128:THR:HG22	2:X:131:GLU:H	1.69	0.57
1:B:179:TYR:CD2	1:C:53:SER:HB2	2.38	0.57
1:E:443:ILE:O	1:E:447:ARG:HG3	2.04	0.57
1:G:18:ASP:OD2	1:G:30:HIS:HD2	1.87	0.57
1:G:192:ARG:HH21	1:G:219:ASN:HD22	1.52	0.57
1:H:43:PHE:CB	2:T:370:LYS:CD	2.82	0.57
1:H:308:ILE:HG21	1:H:374:LEU:HD13	1.86	0.57
1:H:443:ILE:O	1:H:447:ARG:HG3	2.04	0.57
1:K:43:PHE:CG	2:W:370:LYS:HE2	2.32	0.57
1:K:332:LEU:HB2	1:K:408:PRO:HB2	1.85	0.57
1:K:383:LYS:C	1:K:384:ASN:HD22	2.08	0.57
1:L:43:PHE:CB	2:X:370:LYS:CD	2.82	0.57
1:L:332:LEU:HB2	1:L:408:PRO:HB2	1.85	0.57
2:O:3:GLU:O	2:O:4:GLU:CB	2.51	0.57
2:S:128:THR:HG22	2:S:131:GLU:H	1.69	0.57
1:A:118:THR:OG1	1:A:120:ILE:HG13	2.03	0.57
1:A:192:ARG:HH21	1:A:219:ASN:HD22	1.52	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:ILE:HG21	1:A:374:LEU:HD13	1.86	0.57
1:A:332:LEU:HB2	1:A:408:PRO:HB2	1.85	0.57
1:A:360:PHE:CG	1:A:361:PRO:HD3	2.35	0.57
1:B:43:PHE:CB	2:N:370:LYS:CD	2.82	0.57
1:B:332:LEU:HB2	1:B:408:PRO:HB2	1.85	0.57
1:C:44:GLU:HG3	2:O:370:LYS:HZ3	1.67	0.57
1:D:43:PHE:CG	2:P:370:LYS:HE2	2.32	0.57
1:E:332:LEU:HB2	1:E:408:PRO:HB2	1.85	0.57
1:I:308:ILE:HG21	1:I:374:LEU:HD13	1.86	0.57
1:L:308:ILE:HG21	1:L:374:LEU:HD13	1.86	0.57
2:O:64:HIS:CD2	2:O:261:VAL:H	2.19	0.57
2:R:128:THR:HG22	2:R:131:GLU:H	1.69	0.57
2:S:3:GLU:O	2:S:4:GLU:CB	2.51	0.57
2:V:295:LYS:HD3	2:V:296:ASP:N	2.19	0.57
2:W:136:ASP:OD2	2:W:140:LYS:NZ	2.35	0.57
2:W:295:LYS:HD3	2:W:296:ASP:N	2.19	0.57
2:X:136:ASP:OD2	2:X:203:HIS:CD2	2.56	0.57
1:B:383:LYS:C	1:B:384:ASN:HD22	2.08	0.57
1:E:308:ILE:HG21	1:E:374:LEU:HD13	1.86	0.57
1:F:43:PHE:CB	2:R:370:LYS:CD	2.82	0.57
1:F:120:ILE:HD13	1:F:382:ILE:HG21	1.87	0.57
1:G:120:ILE:HD13	1:G:382:ILE:HG21	1.87	0.57
1:H:332:LEU:CB	1:H:408:PRO:HB2	2.35	0.57
1:I:360:PHE:CE2	1:I:361:PRO:HD3	2.36	0.57
1:K:192:ARG:HH21	1:K:219:ASN:HD22	1.52	0.57
2:N:136:ASP:OD2	2:N:140:LYS:NZ	2.35	0.57
2:N:295:LYS:HD3	2:N:296:ASP:N	2.19	0.57
2:O:309:GLU:O	2:O:313:LYS:CE	2.47	0.57
2:P:128:THR:HG22	2:P:131:GLU:H	1.69	0.57
2:T:1:LYS:CA	2:T:54:GLY:O	2.48	0.57
1:A:443:ILE:O	1:A:447:ARG:HG3	2.04	0.57
1:B:118:THR:OG1	1:B:120:ILE:HG13	2.03	0.57
1:B:192:ARG:HH21	1:B:219:ASN:HD22	1.52	0.57
1:E:332:LEU:CB	1:E:408:PRO:HB2	2.35	0.57
1:G:43:PHE:CB	2:S:370:LYS:CD	2.82	0.57
1:G:308:ILE:HG21	1:G:374:LEU:HD13	1.86	0.57
1:K:118:THR:OG1	1:K:120:ILE:HG13	2.03	0.57
1:L:118:THR:OG1	1:L:120:ILE:HG13	2.04	0.57
1:L:192:ARG:HH21	1:L:219:ASN:HD22	1.52	0.57
2:O:295:LYS:HD3	2:O:296:ASP:N	2.19	0.57
2:Q:1:LYS:CA	2:Q:54:GLY:O	2.48	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:128:THR:HG22	2:U:131:GLU:H	1.69	0.57
1:D:360:PHE:CE2	1:D:361:PRO:HD3	2.36	0.57
1:E:383:LYS:C	1:E:384:ASN:HD22	2.08	0.57
1:F:235:ILE:CG2	1:F:367:PRO:HG3	2.28	0.57
1:F:308:ILE:HG21	1:F:374:LEU:HD13	1.86	0.57
1:L:443:ILE:O	1:L:447:ARG:HG3	2.04	0.57
2:N:64:HIS:CD2	2:N:261:VAL:H	2.19	0.57
2:S:136:ASP:OD2	2:S:203:HIS:CD2	2.56	0.57
2:V:309:GLU:O	2:V:313:LYS:CE	2.47	0.57
2:W:64:HIS:CD2	2:W:261:VAL:H	2.19	0.57
1:A:360:PHE:CE2	1:A:361:PRO:HD3	2.36	0.57
1:B:44:GLU:HG3	2:N:370:LYS:HZ3	1.67	0.57
1:F:192:ARG:HH21	1:F:219:ASN:HD22	1.52	0.57
1:G:383:LYS:C	1:G:384:ASN:HD22	2.08	0.57
1:H:383:LYS:C	1:H:384:ASN:HD22	2.08	0.57
1:L:360:PHE:CG	1:L:361:PRO:HD3	2.35	0.57
1:A:383:LYS:C	1:A:384:ASN:HD22	2.08	0.57
1:F:383:LYS:C	1:F:384:ASN:HD22	2.08	0.57
1:I:332:LEU:CB	1:I:408:PRO:HB2	2.35	0.57
1:J:383:LYS:C	1:J:384:ASN:HD22	2.08	0.57
1:K:44:GLU:HG3	2:W:370:LYS:HZ3	1.67	0.57
1:L:360:PHE:CE2	1:L:361:PRO:HD3	2.37	0.57
2:O:128:THR:HG22	2:O:131:GLU:H	1.69	0.57
2:R:136:ASP:OD2	2:R:203:HIS:CD2	2.56	0.57
2:V:128:THR:HG22	2:V:131:GLU:H	1.69	0.57
1:A:120:ILE:HD13	1:A:382:ILE:HG21	1.87	0.57
1:C:383:LYS:C	1:C:384:ASN:HD22	2.08	0.57
1:D:332:LEU:CB	1:D:408:PRO:HB2	2.35	0.57
1:J:443:ILE:O	1:J:447:ARG:HG3	2.04	0.57
1:L:383:LYS:C	1:L:384:ASN:HD22	2.08	0.57
2:Q:3:GLU:O	2:Q:4:GLU:CB	2.51	0.57
1:B:326:TYR:HA	1:B:396:LEU:HD13	1.87	0.57
1:D:82:ASP:O	1:D:84:THR:CG2	2.51	0.57
1:D:383:LYS:C	1:D:384:ASN:HD22	2.08	0.57
1:I:383:LYS:C	1:I:384:ASN:HD22	2.08	0.57
1:K:443:ILE:O	1:K:447:ARG:HG3	2.04	0.57
1:L:44:GLU:HG3	2:X:370:LYS:HZ3	1.67	0.57
1:L:120:ILE:HD13	1:L:382:ILE:HG21	1.87	0.57
2:T:136:ASP:OD2	2:T:140:LYS:NZ	2.35	0.57
1:J:332:LEU:CB	1:J:408:PRO:HB2	2.35	0.56
2:T:3:GLU:O	2:T:4:GLU:CB	2.51	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:3:GLU:O	2:W:4:GLU:CB	2.51	0.56
2:X:64:HIS:CD2	2:X:261:VAL:H	2.19	0.56
2:X:295:LYS:HD3	2:X:296:ASP:N	2.19	0.56
1:C:332:LEU:CB	1:C:408:PRO:HB2	2.35	0.56
1:D:43:PHE:CB	2:P:370:LYS:CD	2.82	0.56
1:I:82:ASP:O	1:I:84:THR:CG2	2.51	0.56
1:K:326:TYR:HA	1:K:396:LEU:HD13	1.88	0.56
2:M:295:LYS:HD3	2:M:296:ASP:N	2.19	0.56
2:N:3:GLU:O	2:N:4:GLU:CB	2.51	0.56
1:A:326:TYR:HA	1:A:396:LEU:HD13	1.88	0.56
1:B:443:ILE:O	1:B:447:ARG:HG3	2.04	0.56
1:C:192:ARG:HH21	1:C:219:ASN:HD22	1.52	0.56
1:C:340:SER:HB3	1:C:396:LEU:HA	1.88	0.56
1:C:443:ILE:O	1:C:447:ARG:HG3	2.04	0.56
1:D:443:ILE:O	1:D:447:ARG:HG3	2.04	0.56
1:D:460:VAL:HG12	1:D:464:LEU:HD22	1.88	0.56
1:E:192:ARG:HH21	1:E:219:ASN:HD22	1.52	0.56
1:E:460:VAL:HG12	1:E:464:LEU:HD22	1.88	0.56
1:F:118:THR:OG1	1:F:120:ILE:HG13	2.04	0.56
1:F:326:TYR:HA	1:F:396:LEU:HD13	1.87	0.56
1:F:360:PHE:CE2	1:F:361:PRO:HD3	2.36	0.56
1:F:460:VAL:HG12	1:F:464:LEU:HD22	1.88	0.56
1:G:460:VAL:HG12	1:G:464:LEU:HD22	1.88	0.56
1:H:192:ARG:HH21	1:H:219:ASN:HD22	1.52	0.56
1:H:360:PHE:CE2	1:H:361:PRO:HD3	2.36	0.56
1:H:460:VAL:HG12	1:H:464:LEU:HD22	1.88	0.56
1:I:340:SER:HB3	1:I:396:LEU:HA	1.87	0.56
1:I:460:VAL:HG12	1:I:464:LEU:HD22	1.88	0.56
1:J:326:TYR:HA	1:J:396:LEU:HD13	1.87	0.56
1:L:326:TYR:HA	1:L:396:LEU:HD13	1.87	0.56
2:M:3:GLU:O	2:M:4:GLU:CB	2.51	0.56
2:U:295:LYS:HD3	2:U:296:ASP:N	2.19	0.56
2:X:3:GLU:O	2:X:4:GLU:CB	2.51	0.56
1:B:120:ILE:HD13	1:B:382:ILE:HG21	1.87	0.56
1:D:340:SER:HB3	1:D:396:LEU:HA	1.87	0.56
1:E:340:SER:HB3	1:E:396:LEU:HA	1.87	0.56
1:F:340:SER:HB3	1:F:396:LEU:HA	1.87	0.56
1:G:326:TYR:HA	1:G:396:LEU:HD13	1.87	0.56
1:G:340:SER:HB3	1:G:396:LEU:HA	1.88	0.56
1:I:43:PHE:CB	2:U:370:LYS:CD	2.82	0.56
1:J:340:SER:HB3	1:J:396:LEU:HA	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:332:LEU:CB	1:K:408:PRO:HB2	2.35	0.56
2:M:30:ASP:OD1	2:M:283:TYR:OH	2.24	0.56
2:P:295:LYS:HD3	2:P:296:ASP:N	2.19	0.56
2:X:30:ASP:OD1	2:X:283:TYR:OH	2.24	0.56
1:B:332:LEU:CB	1:B:408:PRO:HB2	2.35	0.56
1:C:326:TYR:HA	1:C:396:LEU:HD13	1.88	0.56
1:E:360:PHE:CE2	1:E:361:PRO:HD3	2.36	0.56
1:G:118:THR:OG1	1:G:120:ILE:HG13	2.04	0.56
1:I:443:ILE:O	1:I:447:ARG:HG3	2.04	0.56
1:J:360:PHE:CD2	1:J:361:PRO:CD	2.74	0.56
1:J:460:VAL:HG12	1:J:464:LEU:HD22	1.88	0.56
1:B:460:VAL:HG12	1:B:464:LEU:HD22	1.88	0.56
1:G:179:TYR:CD2	1:L:53:SER:HB2	2.40	0.56
1:G:360:PHE:CE2	1:G:361:PRO:HD3	2.37	0.56
1:H:340:SER:HB3	1:H:396:LEU:HA	1.88	0.56
1:K:120:ILE:HD13	1:K:382:ILE:HG21	1.87	0.56
1:K:460:VAL:HG12	1:K:464:LEU:HD22	1.88	0.56
2:M:64:HIS:CD2	2:M:261:VAL:H	2.19	0.56
1:A:332:LEU:CB	1:A:408:PRO:HB2	2.35	0.56
1:C:120:ILE:HD13	1:C:382:ILE:HG21	1.87	0.56
1:G:235:ILE:CG2	1:G:367:PRO:HG3	2.28	0.56
1:J:43:PHE:CB	2:V:370:LYS:CD	2.82	0.56
1:J:192:ARG:HH21	1:J:219:ASN:HD22	1.52	0.56
1:K:398:ASP:O	1:K:399:LEU:HG	2.06	0.56
1:L:43:PHE:CG	2:X:370:LYS:HE2	2.32	0.56
2:S:30:ASP:OD1	2:S:283:TYR:OH	2.24	0.56
2:S:64:HIS:CD2	2:S:261:VAL:H	2.19	0.56
1:B:340:SER:HB3	1:B:396:LEU:HA	1.88	0.56
1:B:398:ASP:O	1:B:399:LEU:HG	2.06	0.56
1:C:460:VAL:HG12	1:C:464:LEU:HD22	1.88	0.56
1:H:326:TYR:HA	1:H:396:LEU:HD13	1.87	0.56
1:J:120:ILE:HD13	1:J:382:ILE:HG21	1.87	0.56
1:K:340:SER:HB3	1:K:396:LEU:HA	1.88	0.56
1:L:332:LEU:CB	1:L:408:PRO:HB2	2.35	0.56
2:S:295:LYS:HD3	2:S:296:ASP:N	2.19	0.56
1:A:43:PHE:CG	2:M:370:LYS:HE2	2.32	0.56
1:A:82:ASP:O	1:A:84:THR:CG2	2.51	0.56
1:A:398:ASP:O	1:A:399:LEU:HG	2.06	0.56
1:A:460:VAL:HG12	1:A:464:LEU:HD22	1.88	0.56
1:B:461:GLU:OE1	1:H:320:LYS:NZ	2.33	0.56
1:C:43:PHE:CB	2:O:370:LYS:CD	2.82	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:326:TYR:HA	1:E:396:LEU:HD13	1.87	0.56
1:L:398:ASP:O	1:L:399:LEU:HG	2.06	0.56
2:R:30:ASP:OD1	2:R:283:TYR:OH	2.24	0.56
2:R:295:LYS:HD3	2:R:296:ASP:N	2.19	0.56
1:A:179:TYR:CD2	1:B:53:SER:HB2	2.40	0.56
1:A:340:SER:HB3	1:A:396:LEU:HA	1.88	0.56
1:C:360:PHE:CD2	1:C:361:PRO:CD	2.74	0.56
1:G:332:LEU:CB	1:G:408:PRO:HB2	2.35	0.56
1:I:29:GLN:HA	1:J:180:PHE:O	2.06	0.56
1:I:326:TYR:HA	1:I:396:LEU:HD13	1.87	0.56
1:K:3:GLU:CG	2:W:338:ALA:CB	2.84	0.56
2:R:64:HIS:CD2	2:R:261:VAL:H	2.19	0.56
2:T:295:LYS:HD3	2:T:296:ASP:N	2.19	0.56
1:D:326:TYR:HA	1:D:396:LEU:HD13	1.87	0.55
1:F:332:LEU:CB	1:F:408:PRO:HB2	2.35	0.55
1:L:82:ASP:O	1:L:84:THR:CG2	2.51	0.55
1:L:114:TYR:CD2	1:L:431:GLY:HA3	2.41	0.55
1:L:460:VAL:HG12	1:L:464:LEU:HD22	1.88	0.55
1:F:398:ASP:O	1:F:399:LEU:HG	2.06	0.55
1:G:398:ASP:O	1:G:399:LEU:HG	2.06	0.55
1:L:340:SER:HB3	1:L:396:LEU:HA	1.88	0.55
1:B:3:GLU:CG	2:N:338:ALA:CB	2.85	0.55
1:D:120:ILE:HD13	1:D:382:ILE:HG21	1.87	0.55
1:E:398:ASP:O	1:E:399:LEU:HG	2.06	0.55
1:I:120:ILE:HD13	1:I:382:ILE:HG21	1.87	0.55
2:N:30:ASP:OD1	2:N:283:TYR:OH	2.24	0.55
2:Q:295:LYS:HD3	2:Q:296:ASP:N	2.19	0.55
1:A:114:TYR:CD2	1:A:431:GLY:HA3	2.41	0.55
1:H:398:ASP:O	1:H:399:LEU:HG	2.06	0.55
1:J:398:ASP:O	1:J:399:LEU:HG	2.06	0.55
2:W:30:ASP:OD1	2:W:283:TYR:OH	2.24	0.55
1:D:179:TYR:CD2	1:E:53:SER:HB2	2.41	0.55
1:E:3:GLU:CG	2:Q:338:ALA:CB	2.85	0.55
1:H:3:GLU:CG	2:T:338:ALA:CB	2.85	0.55
1:H:120:ILE:HD13	1:H:382:ILE:HG21	1.87	0.55
1:J:3:GLU:CG	2:V:338:ALA:CB	2.85	0.55
1:C:3:GLU:CG	2:O:338:ALA:CB	2.85	0.55
1:C:82:ASP:O	1:C:84:THR:CG2	2.51	0.55
1:C:398:ASP:O	1:C:399:LEU:HG	2.06	0.55
1:E:120:ILE:HD13	1:E:382:ILE:HG21	1.87	0.55
1:E:360:PHE:CD2	1:E:361:PRO:CD	2.74	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:136:ASP:OD2	2:P:203:HIS:CD2	2.56	0.55
1:A:3:GLU:CG	2:M:338:ALA:CB	2.84	0.55
1:F:3:GLU:CG	2:R:338:ALA:CB	2.85	0.55
1:G:3:GLU:CG	2:S:338:ALA:CB	2.85	0.55
1:L:3:GLU:CG	2:X:338:ALA:CB	2.85	0.55
2:N:329:ILE:HG23	2:N:329:ILE:O	2.06	0.55
2:U:140:LYS:HD2	2:U:144:LYS:O	2.07	0.55
2:W:329:ILE:HG23	2:W:329:ILE:O	2.06	0.55
1:A:399:LEU:H	1:A:401:PRO:CG	1.90	0.55
2:P:140:LYS:HD2	2:P:144:LYS:O	2.07	0.55
1:D:180:PHE:HB3	1:E:30:HIS:H	1.70	0.55
1:G:360:PHE:CD2	1:G:361:PRO:CD	2.74	0.55
1:J:82:ASP:O	1:J:84:THR:CG2	2.51	0.55
2:Q:140:LYS:HD2	2:Q:144:LYS:O	2.07	0.55
2:R:312:ALA:CB	2:R:317:ILE:HG22	2.32	0.55
2:T:140:LYS:HD2	2:T:144:LYS:O	2.07	0.55
2:V:329:ILE:HG23	2:V:329:ILE:O	2.06	0.55
1:C:114:TYR:CD2	1:C:431:GLY:HA3	2.41	0.55
1:D:398:ASP:O	1:D:399:LEU:HG	2.06	0.55
1:F:4:HIS:CD2	2:R:178:ILE:CG1	2.58	0.55
1:H:114:TYR:CD2	1:H:431:GLY:HA3	2.41	0.55
1:H:360:PHE:CD2	1:H:361:PRO:CD	2.74	0.55
2:O:140:LYS:HD2	2:O:144:LYS:O	2.07	0.55
2:O:329:ILE:HG23	2:O:329:ILE:O	2.06	0.55
2:T:30:ASP:OD1	2:T:283:TYR:OH	2.24	0.55
2:U:136:ASP:OD2	2:U:203:HIS:CD2	2.56	0.55
2:X:329:ILE:O	2:X:329:ILE:HG23	2.06	0.55
1:D:114:TYR:CD2	1:D:431:GLY:HA3	2.41	0.54
1:E:114:TYR:CD2	1:E:431:GLY:HA3	2.41	0.54
1:I:114:TYR:CD2	1:I:431:GLY:HA3	2.41	0.54
1:I:398:ASP:O	1:I:399:LEU:HG	2.06	0.54
1:K:114:TYR:CD2	1:K:431:GLY:HA3	2.41	0.54
1:L:128:PRO:HD2	1:L:231:LYS:HE2	1.89	0.54
2:V:140:LYS:HD2	2:V:144:LYS:O	2.07	0.54
1:B:114:TYR:CD2	1:B:431:GLY:HA3	2.41	0.54
1:B:128:PRO:HD2	1:B:231:LYS:HE2	1.89	0.54
1:F:114:TYR:CD2	1:F:431:GLY:HA3	2.41	0.54
1:G:114:TYR:CD2	1:G:431:GLY:HA3	2.41	0.54
1:J:114:TYR:CD2	1:J:431:GLY:HA3	2.41	0.54
1:K:128:PRO:HD2	1:K:231:LYS:HE2	1.89	0.54
2:M:329:ILE:O	2:M:329:ILE:HG23	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:30:ASP:OD1	2:Q:283:TYR:OH	2.24	0.54
2:V:30:ASP:OD1	2:V:283:TYR:OH	2.24	0.54
1:A:128:PRO:HD2	1:A:231:LYS:HE2	1.89	0.54
2:R:329:ILE:HG23	2:R:329:ILE:O	2.06	0.54
2:S:140:LYS:HD2	2:S:144:LYS:O	2.07	0.54
2:U:30:ASP:OD1	2:U:283:TYR:OH	2.24	0.54
1:B:180:PHE:HB3	1:C:30:HIS:H	1.73	0.54
1:D:3:GLU:CG	2:P:338:ALA:CB	2.85	0.54
1:E:248:ARG:HG2	1:E:248:ARG:NH2	2.23	0.54
1:F:248:ARG:HG2	1:F:248:ARG:NH2	2.23	0.54
1:H:248:ARG:HG2	1:H:248:ARG:NH2	2.23	0.54
2:O:30:ASP:OD1	2:O:283:TYR:OH	2.24	0.54
2:P:30:ASP:OD1	2:P:283:TYR:OH	2.24	0.54
2:Q:136:ASP:OD2	2:Q:203:HIS:CD2	2.56	0.54
2:R:140:LYS:HD2	2:R:144:LYS:O	2.07	0.54
2:S:312:ALA:CB	2:S:317:ILE:HG22	2.32	0.54
1:L:399:LEU:H	1:L:401:PRO:CG	1.90	0.54
2:M:140:LYS:HD2	2:M:144:LYS:O	2.07	0.54
2:N:140:LYS:HD2	2:N:144:LYS:O	2.07	0.54
1:A:29:GLN:HA	1:F:180:PHE:O	2.08	0.54
1:G:248:ARG:HG2	1:G:248:ARG:NH2	2.23	0.54
1:I:3:GLU:CG	2:U:338:ALA:CB	2.85	0.54
1:I:128:PRO:HD2	1:I:231:LYS:HE2	1.89	0.54
1:K:360:PHE:CD2	1:K:361:PRO:CD	2.74	0.54
2:Q:329:ILE:HG23	2:Q:329:ILE:O	2.06	0.54
2:U:329:ILE:O	2:U:329:ILE:HG23	2.06	0.54
1:D:128:PRO:HD2	1:D:231:LYS:HE2	1.89	0.54
1:G:29:GLN:OE1	1:H:181:PRO:HD3	2.07	0.54
1:H:248:ARG:CG	1:H:248:ARG:NH2	2.67	0.54
1:J:128:PRO:HD2	1:J:231:LYS:HE2	1.89	0.54
1:B:360:PHE:CD2	1:B:361:PRO:CD	2.74	0.54
1:H:128:PRO:HD2	1:H:231:LYS:HE2	1.89	0.54
2:Q:136:ASP:OD2	2:Q:140:LYS:NZ	2.35	0.54
2:S:132:ILE:N	2:S:133:PRO:CD	2.71	0.54
2:S:329:ILE:HG23	2:S:329:ILE:O	2.06	0.54
2:T:132:ILE:N	2:T:133:PRO:CD	2.71	0.54
2:T:136:ASP:OD2	2:T:203:HIS:CD2	2.56	0.54
2:T:329:ILE:HG23	2:T:329:ILE:O	2.06	0.54
2:W:140:LYS:HD2	2:W:144:LYS:O	2.07	0.54
1:E:248:ARG:CG	1:E:248:ARG:NH2	2.67	0.54
1:F:82:ASP:O	1:F:84:THR:CG2	2.51	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:128:PRO:HD2	1:F:231:LYS:HE2	1.89	0.54
2:M:132:ILE:N	2:M:133:PRO:CD	2.71	0.54
2:O:136:ASP:OD2	2:O:203:HIS:CD2	2.56	0.54
2:P:329:ILE:HG23	2:P:329:ILE:O	2.06	0.54
2:Q:19:GLY:O	2:Q:23:VAL:HG23	2.08	0.54
2:Q:132:ILE:N	2:Q:133:PRO:CD	2.71	0.54
2:R:132:ILE:N	2:R:133:PRO:CD	2.71	0.54
2:X:132:ILE:N	2:X:133:PRO:CD	2.71	0.54
2:X:140:LYS:HD2	2:X:144:LYS:O	2.07	0.54
1:C:128:PRO:HD2	1:C:231:LYS:HE2	1.89	0.54
1:K:29:GLN:HA	1:L:180:PHE:O	2.08	0.54
2:O:19:GLY:O	2:O:23:VAL:HG23	2.08	0.54
2:V:19:GLY:O	2:V:23:VAL:HG23	2.08	0.54
1:D:248:ARG:HG2	1:D:248:ARG:NH2	2.23	0.53
1:E:128:PRO:HD2	1:E:231:LYS:HE2	1.89	0.53
1:J:29:GLN:HA	1:K:180:PHE:O	2.07	0.53
2:T:19:GLY:O	2:T:23:VAL:HG23	2.08	0.53
1:F:360:PHE:CD2	1:F:361:PRO:CD	2.74	0.53
1:I:29:GLN:HB3	1:J:180:PHE:HB2	1.91	0.53
1:I:248:ARG:HG2	1:I:248:ARG:NH2	2.23	0.53
1:J:29:GLN:OE1	1:K:181:PRO:HD3	2.08	0.53
2:N:132:ILE:N	2:N:133:PRO:CD	2.71	0.53
2:O:132:ILE:N	2:O:133:PRO:CD	2.71	0.53
2:P:132:ILE:N	2:P:133:PRO:CD	2.71	0.53
2:U:132:ILE:N	2:U:133:PRO:CD	2.71	0.53
2:W:132:ILE:N	2:W:133:PRO:CD	2.71	0.53
1:A:248:ARG:HG2	1:A:248:ARG:NH2	2.23	0.53
1:B:82:ASP:O	1:B:84:THR:CG2	2.51	0.53
1:G:43:PHE:CG	2:S:370:LYS:HE2	2.32	0.53
1:G:128:PRO:HD2	1:G:231:LYS:HE2	1.89	0.53
1:K:82:ASP:O	1:K:84:THR:CG2	2.51	0.53
2:V:132:ILE:N	2:V:133:PRO:CD	2.71	0.53
2:V:136:ASP:OD2	2:V:203:HIS:CD2	2.56	0.53
1:B:456:THR:O	1:H:458:HIS:HE1	1.91	0.53
1:G:82:ASP:O	1:G:84:THR:CG2	2.51	0.53
1:K:30:HIS:H	1:L:180:PHE:HB3	1.73	0.53
2:W:19:GLY:O	2:W:23:VAL:HG23	2.08	0.53
1:L:248:ARG:HG2	1:L:248:ARG:NH2	2.23	0.53
2:N:19:GLY:O	2:N:23:VAL:HG23	2.08	0.53
2:P:136:ASP:OD2	2:P:140:LYS:NZ	2.35	0.53
2:P:202:LYS:HA	2:P:202:LYS:HE2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:34:LYS:HG2	2:R:34:LYS:O	2.09	0.53
2:S:19:GLY:O	2:S:23:VAL:HG23	2.08	0.53
2:S:202:LYS:HE2	2:S:202:LYS:HA	1.91	0.53
2:T:202:LYS:HE2	2:T:202:LYS:HA	1.91	0.53
1:C:248:ARG:HG2	1:C:248:ARG:NH2	2.23	0.53
1:J:248:ARG:HG2	1:J:248:ARG:NH2	2.23	0.53
2:N:202:LYS:HE2	2:N:202:LYS:HA	1.91	0.53
2:O:202:LYS:HE2	2:O:202:LYS:HA	1.91	0.53
2:Q:202:LYS:HE2	2:Q:202:LYS:HA	1.91	0.53
2:R:19:GLY:O	2:R:23:VAL:HG23	2.08	0.53
2:S:34:LYS:O	2:S:34:LYS:HG2	2.09	0.53
2:V:202:LYS:HE2	2:V:202:LYS:HA	1.91	0.53
1:B:248:ARG:HG2	1:B:248:ARG:NH2	2.23	0.53
1:H:29:GLN:HA	1:I:180:PHE:O	2.09	0.53
1:K:248:ARG:HG2	1:K:248:ARG:NH2	2.23	0.53
2:M:202:LYS:HA	2:M:202:LYS:HE2	1.91	0.53
2:O:335:GLN:NE2	2:O:335:GLN:H	2.07	0.53
2:P:19:GLY:O	2:P:23:VAL:HG23	2.08	0.53
2:X:202:LYS:HA	2:X:202:LYS:HE2	1.91	0.53
1:F:43:PHE:CG	2:R:370:LYS:HE2	2.32	0.53
1:L:360:PHE:CD2	1:L:361:PRO:CD	2.74	0.53
2:R:202:LYS:HE2	2:R:202:LYS:HA	1.91	0.53
2:T:312:ALA:CB	2:T:317:ILE:HG22	2.32	0.53
2:U:19:GLY:O	2:U:23:VAL:HG23	2.08	0.53
2:U:202:LYS:HA	2:U:202:LYS:HE2	1.91	0.53
2:V:335:GLN:NE2	2:V:335:GLN:H	2.07	0.53
2:W:202:LYS:HE2	2:W:202:LYS:HA	1.91	0.53
1:B:320:LYS:NZ	1:H:461:GLU:OE1	2.35	0.52
1:G:7:THR:HG1	2:S:178:ILE:HD11	1.73	0.52
2:N:335:GLN:NE2	2:N:335:GLN:H	2.07	0.52
1:A:360:PHE:CD2	1:A:361:PRO:CD	2.74	0.52
2:M:19:GLY:O	2:M:23:VAL:HG23	2.08	0.52
2:M:335:GLN:NE2	2:M:335:GLN:H	2.07	0.52
2:W:335:GLN:NE2	2:W:335:GLN:H	2.08	0.52
1:A:30:HIS:H	1:F:180:PHE:HB3	1.73	0.52
1:C:16:PHE:HB2	1:C:84:THR:HB	1.92	0.52
1:D:295:LEU:O	1:D:388:PRO:HG3	2.09	0.52
1:J:16:PHE:HB2	1:J:84:THR:HB	1.92	0.52
2:Q:335:GLN:NE2	2:Q:335:GLN:H	2.07	0.52
2:X:335:GLN:NE2	2:X:335:GLN:H	2.07	0.52
1:H:399:LEU:CA	1:H:400:PRO:C	2.78	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:295:LEU:O	1:K:388:PRO:HG3	2.09	0.52
2:T:335:GLN:NE2	2:T:335:GLN:H	2.08	0.52
2:X:19:GLY:O	2:X:23:VAL:HG23	2.08	0.52
1:B:248:ARG:HH21	1:B:248:ARG:HG3	1.75	0.52
1:B:295:LEU:O	1:B:388:PRO:HG3	2.09	0.52
1:E:16:PHE:HB2	1:E:84:THR:HB	1.92	0.52
1:H:16:PHE:HB2	1:H:84:THR:HB	1.92	0.52
1:I:16:PHE:HB2	1:I:84:THR:HB	1.92	0.52
1:I:295:LEU:O	1:I:388:PRO:HG3	2.09	0.52
1:K:248:ARG:HH21	1:K:248:ARG:HG3	1.75	0.52
2:P:322:GLU:O	2:P:326:LYS:HG3	2.10	0.52
2:T:322:GLU:O	2:T:326:LYS:HG3	2.10	0.52
2:X:34:LYS:HG2	2:X:34:LYS:O	2.09	0.52
1:D:16:PHE:HB2	1:D:84:THR:HB	1.92	0.52
1:D:456:THR:O	1:J:458:HIS:HE1	1.93	0.52
1:E:399:LEU:CA	1:E:400:PRO:C	2.78	0.52
2:Q:312:ALA:CB	2:Q:317:ILE:HG22	2.32	0.52
2:Q:322:GLU:O	2:Q:326:LYS:HG3	2.10	0.52
2:U:322:GLU:O	2:U:326:LYS:HG3	2.10	0.52
1:E:295:LEU:O	1:E:388:PRO:HG3	2.09	0.52
2:O:9:ILE:HG21	2:O:20:LEU:HD21	1.92	0.52
2:U:9:ILE:HG21	2:U:20:LEU:HD21	1.92	0.52
1:B:16:PHE:HB2	1:B:84:THR:HB	1.92	0.52
1:K:16:PHE:HB2	1:K:84:THR:HB	1.92	0.52
2:N:34:LYS:O	2:N:34:LYS:HG2	2.09	0.52
2:O:322:GLU:O	2:O:326:LYS:HG3	2.10	0.52
2:T:9:ILE:HG21	2:T:20:LEU:HD21	1.92	0.52
2:V:9:ILE:HG21	2:V:20:LEU:HD21	1.92	0.52
2:V:34:LYS:O	2:V:34:LYS:HG2	2.09	0.52
2:W:34:LYS:HG2	2:W:34:LYS:O	2.09	0.52
1:A:295:LEU:O	1:A:388:PRO:HG3	2.09	0.52
1:D:399:LEU:CA	1:D:400:PRO:C	2.78	0.52
1:H:295:LEU:O	1:H:388:PRO:HG3	2.09	0.52
2:M:34:LYS:HG2	2:M:34:LYS:O	2.09	0.52
2:O:34:LYS:HG2	2:O:34:LYS:O	2.09	0.52
2:P:9:ILE:HG21	2:P:20:LEU:HD21	1.92	0.52
2:Q:9:ILE:HG21	2:Q:20:LEU:HD21	1.92	0.52
2:R:322:GLU:O	2:R:326:LYS:HG3	2.10	0.52
2:S:322:GLU:O	2:S:326:LYS:HG3	2.10	0.52
2:W:312:ALA:HB2	2:W:317:ILE:CB	2.39	0.52
1:G:29:GLN:HA	1:H:180:PHE:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:29:GLN:HB3	1:K:180:PHE:HB2	1.92	0.51
2:N:136:ASP:OD2	2:N:203:HIS:CD2	2.56	0.51
2:O:82:ASP:O	2:O:85:PHE:N	2.43	0.51
2:R:9:ILE:HG21	2:R:20:LEU:HD21	1.92	0.51
2:R:82:ASP:O	2:R:85:PHE:N	2.43	0.51
2:S:82:ASP:O	2:S:85:PHE:N	2.43	0.51
2:U:82:ASP:O	2:U:85:PHE:N	2.43	0.51
2:V:322:GLU:O	2:V:326:LYS:HG3	2.10	0.51
1:I:399:LEU:CA	1:I:400:PRO:C	2.78	0.51
2:M:82:ASP:O	2:M:85:PHE:N	2.43	0.51
2:N:312:ALA:HB2	2:N:317:ILE:CB	2.39	0.51
2:N:367:ARG:HA	2:N:370:LYS:HD2	1.93	0.51
2:P:82:ASP:O	2:P:85:PHE:N	2.44	0.51
2:S:9:ILE:HG21	2:S:20:LEU:HD21	1.92	0.51
2:V:82:ASP:O	2:V:85:PHE:N	2.43	0.51
1:A:399:LEU:CA	1:A:400:PRO:C	2.78	0.51
1:I:29:GLN:HB3	1:J:180:PHE:CB	2.40	0.51
2:M:322:GLU:O	2:M:326:LYS:HG3	2.10	0.51
2:N:322:GLU:O	2:N:326:LYS:HG3	2.10	0.51
2:Q:82:ASP:O	2:Q:85:PHE:N	2.43	0.51
2:U:34:LYS:HG2	2:U:34:LYS:O	2.09	0.51
2:W:136:ASP:OD2	2:W:203:HIS:CD2	2.56	0.51
2:W:322:GLU:O	2:W:326:LYS:HG3	2.10	0.51
2:X:82:ASP:O	2:X:85:PHE:N	2.43	0.51
2:X:367:ARG:HA	2:X:370:LYS:HD2	1.93	0.51
1:C:180:PHE:HB2	1:D:29:GLN:HB3	1.92	0.51
1:G:180:PHE:O	1:L:29:GLN:HA	2.10	0.51
1:H:130:PRO:HB3	1:H:268:MET:HE3	1.92	0.51
1:J:295:LEU:O	1:J:388:PRO:HG3	2.09	0.51
1:L:399:LEU:CA	1:L:400:PRO:C	2.78	0.51
2:M:9:ILE:HG21	2:M:20:LEU:HD21	1.92	0.51
2:P:34:LYS:HG2	2:P:34:LYS:O	2.09	0.51
2:P:363:ASP:O	2:P:367:ARG:HG3	2.11	0.51
2:S:335:GLN:NE2	2:S:335:GLN:H	2.07	0.51
2:T:82:ASP:O	2:T:85:PHE:N	2.43	0.51
2:U:363:ASP:O	2:U:367:ARG:HG3	2.10	0.51
2:V:363:ASP:O	2:V:367:ARG:HG3	2.10	0.51
2:W:367:ARG:HA	2:W:370:LYS:HD2	1.93	0.51
2:X:322:GLU:O	2:X:326:LYS:HG3	2.10	0.51
1:B:458:HIS:HE1	1:H:456:THR:O	1.93	0.51
1:C:295:LEU:O	1:C:388:PRO:HG3	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:248:ARG:CG	1:D:248:ARG:NH2	2.67	0.51
1:G:16:PHE:HB2	1:G:84:THR:HB	1.92	0.51
1:I:29:GLN:OE1	1:J:181:PRO:HD3	2.10	0.51
1:J:248:ARG:HH21	1:J:248:ARG:HG3	1.75	0.51
2:O:363:ASP:O	2:O:367:ARG:HG3	2.11	0.51
2:Q:363:ASP:O	2:Q:367:ARG:HG3	2.11	0.51
2:U:335:GLN:NE2	2:U:335:GLN:H	2.08	0.51
2:X:9:ILE:HG21	2:X:20:LEU:HD21	1.92	0.51
1:H:29:GLN:OE1	1:I:181:PRO:HD3	2.10	0.51
2:P:335:GLN:NE2	2:P:335:GLN:H	2.07	0.51
2:T:363:ASP:O	2:T:367:ARG:HG3	2.10	0.51
1:C:180:PHE:CB	1:D:29:GLN:HB3	2.41	0.51
1:C:248:ARG:HH21	1:C:248:ARG:HG3	1.75	0.51
1:D:403:GLU:C	1:D:405:LYS:H	2.14	0.51
1:F:16:PHE:HB2	1:F:84:THR:HB	1.92	0.51
1:F:256:MET:HG3	1:L:466:TYR:HA	1.91	0.51
1:I:403:GLU:C	1:I:405:LYS:H	2.14	0.51
2:N:82:ASP:O	2:N:85:PHE:N	2.44	0.51
2:R:335:GLN:NE2	2:R:335:GLN:H	2.07	0.51
2:W:82:ASP:O	2:W:85:PHE:N	2.43	0.51
1:A:16:PHE:HB2	1:A:84:THR:HB	1.92	0.51
1:A:256:MET:HG3	1:G:466:TYR:HA	1.91	0.51
1:D:458:HIS:HE1	1:J:456:THR:O	1.94	0.51
1:G:396:LEU:O	1:G:400:PRO:HG2	2.11	0.51
1:J:130:PRO:HB3	1:J:268:MET:HE3	1.93	0.51
2:M:367:ARG:HA	2:M:370:LYS:HD2	1.93	0.51
2:N:9:ILE:HG21	2:N:20:LEU:HD21	1.92	0.51
2:W:9:ILE:HG21	2:W:20:LEU:HD21	1.92	0.51
1:H:396:LEU:O	1:H:400:PRO:HG2	2.11	0.51
1:H:403:GLU:C	1:H:405:LYS:H	2.14	0.51
1:I:248:ARG:CG	1:I:248:ARG:NH2	2.66	0.51
1:I:360:PHE:CD2	1:I:361:PRO:CD	2.74	0.51
1:J:396:LEU:O	1:J:400:PRO:HG2	2.11	0.51
1:L:16:PHE:HB2	1:L:84:THR:HB	1.92	0.51
1:L:311:LEU:HD22	1:L:369:LEU:HB3	1.93	0.51
1:D:360:PHE:CD2	1:D:361:PRO:CD	2.74	0.51
1:E:403:GLU:C	1:E:405:LYS:H	2.14	0.51
1:G:130:PRO:HB3	1:G:268:MET:CE	2.41	0.51
1:J:53:SER:HB2	1:K:179:TYR:CD2	2.46	0.51
1:A:130:PRO:HB3	1:A:268:MET:CE	2.41	0.50
1:A:311:LEU:HD22	1:A:369:LEU:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:181:PRO:HD3	1:C:29:GLN:OE1	2.10	0.50
1:C:396:LEU:O	1:C:400:PRO:HG2	2.11	0.50
1:E:130:PRO:HB3	1:E:268:MET:CE	2.41	0.50
1:F:130:PRO:HB3	1:F:268:MET:CE	2.41	0.50
1:F:396:LEU:O	1:F:400:PRO:HG2	2.12	0.50
1:G:295:LEU:O	1:G:388:PRO:HG3	2.09	0.50
1:L:130:PRO:HB3	1:L:268:MET:CE	2.41	0.50
1:L:295:LEU:O	1:L:388:PRO:HG3	2.09	0.50
2:T:34:LYS:O	2:T:34:LYS:HG2	2.09	0.50
1:B:311:LEU:HD22	1:B:369:LEU:HB3	1.93	0.50
1:C:399:LEU:CA	1:C:400:PRO:C	2.78	0.50
1:E:396:LEU:O	1:E:400:PRO:HG2	2.12	0.50
1:F:295:LEU:O	1:F:388:PRO:HG3	2.09	0.50
1:H:130:PRO:HB3	1:H:268:MET:CE	2.42	0.50
1:I:396:LEU:O	1:I:400:PRO:HG2	2.11	0.50
2:Q:34:LYS:O	2:Q:34:LYS:HG2	2.09	0.50
2:S:136:ASP:OD2	2:S:140:LYS:NZ	2.35	0.50
1:D:396:LEU:O	1:D:400:PRO:HG2	2.12	0.50
1:I:130:PRO:HB3	1:I:268:MET:CE	2.41	0.50
1:I:248:ARG:HH21	1:I:248:ARG:HG3	1.75	0.50
1:I:311:LEU:HD22	1:I:369:LEU:HB3	1.93	0.50
1:K:311:LEU:HD22	1:K:369:LEU:HB3	1.93	0.50
1:J:399:LEU:CA	1:J:400:PRO:C	2.78	0.50
2:N:239:LYS:NZ	2:N:241:ASN:HB2	2.27	0.50
2:R:363:ASP:O	2:R:367:ARG:HG3	2.11	0.50
2:T:367:ARG:HA	2:T:370:LYS:HD2	1.93	0.50
1:C:454:ARG:O	1:I:320:LYS:HG3	2.11	0.50
1:F:399:LEU:CA	1:F:400:PRO:C	2.78	0.50
2:O:239:LYS:NZ	2:O:241:ASN:HB2	2.27	0.50
2:S:363:ASP:O	2:S:367:ARG:HG3	2.10	0.50
2:U:239:LYS:NZ	2:U:241:ASN:HB2	2.27	0.50
2:V:239:LYS:NZ	2:V:241:ASN:HB2	2.27	0.50
1:A:396:LEU:O	1:A:400:PRO:HG2	2.11	0.50
1:C:458:HIS:HE1	1:I:456:THR:O	1.95	0.50
1:D:130:PRO:HB3	1:D:268:MET:CE	2.42	0.50
1:D:248:ARG:HH21	1:D:248:ARG:HG3	1.75	0.50
1:J:335:SER:HB2	1:J:392:MET:O	2.12	0.50
2:M:363:ASP:O	2:M:367:ARG:HG3	2.11	0.50
2:P:239:LYS:NZ	2:P:241:ASN:HB2	2.27	0.50
2:Q:239:LYS:NZ	2:Q:241:ASN:HB2	2.27	0.50
2:T:239:LYS:NZ	2:T:241:ASN:HB2	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:239:LYS:NZ	2:W:241:ASN:HB2	2.27	0.50
1:B:399:LEU:CA	1:B:400:PRO:C	2.78	0.50
1:D:311:LEU:HD22	1:D:369:LEU:HB3	1.93	0.50
1:G:399:LEU:CA	1:G:400:PRO:C	2.78	0.50
1:L:255:PHE:HB3	1:L:363:PRO:HB2	1.94	0.50
1:L:396:LEU:O	1:L:400:PRO:HG2	2.11	0.50
2:X:363:ASP:O	2:X:367:ARG:HG3	2.11	0.50
1:B:192:ARG:HD3	1:B:219:ASN:HD22	1.77	0.50
1:B:335:SER:HB2	1:B:392:MET:O	2.12	0.50
1:C:192:ARG:HD3	1:C:219:ASN:HD22	1.77	0.50
1:E:43:PHE:CG	2:Q:370:LYS:HE2	2.32	0.50
1:E:192:ARG:HD3	1:E:219:ASN:HD22	1.77	0.50
1:F:311:LEU:HD22	1:F:369:LEU:HB3	1.93	0.50
1:F:335:SER:HB2	1:F:392:MET:O	2.12	0.50
1:H:43:PHE:CG	2:T:370:LYS:HE2	2.32	0.50
1:H:248:ARG:HH21	1:H:248:ARG:HG3	1.75	0.50
1:J:192:ARG:HD3	1:J:219:ASN:HD22	1.77	0.50
1:K:192:ARG:HD3	1:K:219:ASN:HD22	1.77	0.50
1:K:335:SER:HB2	1:K:392:MET:O	2.12	0.50
2:Q:237:THR:O	2:Q:237:THR:CG2	2.60	0.50
2:Q:367:ARG:HA	2:Q:370:LYS:HD2	1.93	0.50
2:U:367:ARG:HA	2:U:370:LYS:HD2	1.93	0.50
2:X:212:ILE:HD13	2:X:212:ILE:N	2.27	0.50
1:B:396:LEU:O	1:B:400:PRO:HG2	2.11	0.50
1:C:28:GLU:OE1	1:C:88:ARG:NH1	2.45	0.50
1:C:335:SER:HB2	1:C:392:MET:O	2.12	0.50
1:E:43:PHE:HB3	2:Q:370:LYS:CD	2.28	0.50
1:E:130:PRO:HB3	1:E:268:MET:HE3	1.93	0.50
1:G:335:SER:HB2	1:G:392:MET:O	2.12	0.50
1:J:28:GLU:OE1	1:J:88:ARG:NH1	2.45	0.50
1:J:311:LEU:HD22	1:J:369:LEU:HB3	1.93	0.50
1:K:255:PHE:HB3	1:K:363:PRO:HB2	1.94	0.50
1:K:396:LEU:O	1:K:400:PRO:HG2	2.11	0.50
1:K:399:LEU:CA	1:K:400:PRO:C	2.78	0.50
2:M:212:ILE:HD13	2:M:212:ILE:N	2.27	0.50
2:O:367:ARG:HA	2:O:370:LYS:HD2	1.93	0.50
2:P:367:ARG:HA	2:P:370:LYS:HD2	1.93	0.50
2:V:136:ASP:OD2	2:V:140:LYS:NZ	2.35	0.50
1:A:454:ARG:O	1:G:320:LYS:HG3	2.12	0.49
1:B:255:PHE:HB3	1:B:363:PRO:HB2	1.94	0.49
1:C:248:ARG:CG	1:C:248:ARG:NH2	2.67	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:248:ARG:HH21	1:E:248:ARG:HG3	1.75	0.49
1:G:192:ARG:HD3	1:G:219:ASN:HD22	1.77	0.49
1:H:192:ARG:HD3	1:H:219:ASN:HD22	1.77	0.49
1:J:130:PRO:HB3	1:J:268:MET:CE	2.41	0.49
2:S:367:ARG:HA	2:S:370:LYS:HD2	1.93	0.49
2:T:237:THR:O	2:T:237:THR:CG2	2.60	0.49
1:A:255:PHE:HB3	1:A:363:PRO:HB2	1.94	0.49
1:B:124:VAL:HG13	1:B:274:LEU:HD21	1.94	0.49
1:C:311:LEU:HD22	1:C:369:LEU:HB3	1.93	0.49
1:C:403:GLU:C	1:C:405:LYS:H	2.14	0.49
1:F:192:ARG:HD3	1:F:219:ASN:HD22	1.77	0.49
1:F:403:GLU:C	1:F:405:LYS:H	2.14	0.49
1:G:29:GLN:HB3	1:H:180:PHE:HB2	1.94	0.49
1:J:403:GLU:C	1:J:405:LYS:H	2.14	0.49
1:K:130:PRO:HB3	1:K:268:MET:CE	2.41	0.49
2:N:237:THR:O	2:N:237:THR:CG2	2.60	0.49
2:R:136:ASP:OD2	2:R:140:LYS:NZ	2.35	0.49
2:R:367:ARG:HA	2:R:370:LYS:HD2	1.93	0.49
2:T:212:ILE:HD13	2:T:212:ILE:N	2.27	0.49
2:U:312:ALA:HB2	2:U:317:ILE:CB	2.39	0.49
2:V:367:ARG:HA	2:V:370:LYS:HD2	1.93	0.49
2:W:237:THR:O	2:W:237:THR:CG2	2.60	0.49
1:A:124:VAL:HG13	1:A:274:LEU:HD21	1.94	0.49
1:A:403:GLU:C	1:A:405:LYS:H	2.14	0.49
1:B:130:PRO:HB3	1:B:268:MET:CE	2.41	0.49
1:G:311:LEU:HD22	1:G:369:LEU:HB3	1.93	0.49
1:K:124:VAL:HG13	1:K:274:LEU:HD21	1.94	0.49
1:L:124:VAL:HG13	1:L:274:LEU:HD21	1.94	0.49
2:Q:212:ILE:HD13	2:Q:212:ILE:N	2.27	0.49
2:W:363:ASP:O	2:W:367:ARG:HG3	2.10	0.49
2:X:312:ALA:HB2	2:X:317:ILE:CB	2.39	0.49
1:B:180:PHE:O	1:C:29:GLN:HA	2.13	0.49
1:C:130:PRO:HB3	1:C:268:MET:CE	2.42	0.49
1:E:124:VAL:HG13	1:E:274:LEU:HD21	1.94	0.49
1:E:256:MET:HG3	1:K:466:TYR:HA	1.94	0.49
1:F:130:PRO:HB3	1:F:268:MET:HE3	1.93	0.49
1:G:403:GLU:C	1:G:405:LYS:H	2.14	0.49
1:K:43:PHE:HB3	2:W:370:LYS:CD	2.28	0.49
1:L:403:GLU:C	1:L:405:LYS:H	2.14	0.49
2:M:312:ALA:HB2	2:M:317:ILE:CB	2.39	0.49
2:P:312:ALA:HB2	2:P:317:ILE:CB	2.39	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:335:SER:HB2	1:D:392:MET:O	2.12	0.49
1:H:124:VAL:HG13	1:H:274:LEU:HD21	1.94	0.49
1:I:192:ARG:HD3	1:I:219:ASN:HD22	1.77	0.49
2:M:239:LYS:NZ	2:M:241:ASN:HB2	2.27	0.49
2:N:212:ILE:HD13	2:N:212:ILE:N	2.27	0.49
2:N:363:ASP:O	2:N:367:ARG:HG3	2.11	0.49
2:Q:312:ALA:HB2	2:Q:317:ILE:CB	2.39	0.49
2:W:212:ILE:HD13	2:W:212:ILE:N	2.27	0.49
1:A:335:SER:HB2	1:A:392:MET:O	2.12	0.49
1:D:124:VAL:HG13	1:D:274:LEU:HD21	1.94	0.49
1:D:192:ARG:HD3	1:D:219:ASN:HD22	1.77	0.49
1:F:364:ALA:HA	1:L:468:VAL:HG13	1.95	0.49
1:G:181:PRO:HD3	1:L:29:GLN:OE1	2.13	0.49
1:G:248:ARG:HH21	1:G:248:ARG:HG3	1.75	0.49
1:I:124:VAL:HG13	1:I:274:LEU:HD21	1.94	0.49
1:I:335:SER:HB2	1:I:392:MET:O	2.12	0.49
2:O:312:ALA:HB2	2:O:317:ILE:CB	2.39	0.49
2:S:239:LYS:NZ	2:S:241:ASN:HB2	2.27	0.49
2:V:312:ALA:HB2	2:V:317:ILE:CB	2.39	0.49
1:B:43:PHE:HB3	2:N:370:LYS:CD	2.28	0.49
1:B:403:GLU:C	1:B:405:LYS:H	2.14	0.49
1:E:311:LEU:HD22	1:E:369:LEU:HB3	1.93	0.49
1:J:248:ARG:CG	1:J:248:ARG:NH2	2.67	0.49
1:K:403:GLU:C	1:K:405:LYS:H	2.14	0.49
1:L:335:SER:HB2	1:L:392:MET:O	2.12	0.49
2:M:136:ASP:HB3	2:M:203:HIS:CD2	2.48	0.49
2:R:239:LYS:NZ	2:R:241:ASN:HB2	2.27	0.49
2:T:312:ALA:HB2	2:T:317:ILE:CB	2.39	0.49
2:U:6:LYS:HA	2:U:33:ILE:CG2	2.41	0.49
2:X:239:LYS:NZ	2:X:241:ASN:HB2	2.27	0.49
1:A:192:ARG:HD3	1:A:219:ASN:HD22	1.77	0.49
1:E:255:PHE:HB3	1:E:363:PRO:HB2	1.94	0.49
1:E:335:SER:HB2	1:E:392:MET:O	2.12	0.49
1:H:335:SER:HB2	1:H:392:MET:O	2.12	0.49
2:N:147:LEU:O	2:N:148:MET:HG2	2.13	0.49
2:O:237:THR:O	2:O:237:THR:CG2	2.60	0.49
2:R:237:THR:O	2:R:237:THR:CG2	2.60	0.49
2:S:237:THR:O	2:S:237:THR:CG2	2.60	0.49
2:U:237:THR:O	2:U:237:THR:CG2	2.60	0.49
2:X:136:ASP:HB3	2:X:203:HIS:CD2	2.48	0.49
1:D:255:PHE:HB3	1:D:363:PRO:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:255:PHE:HB3	1:F:363:PRO:HB2	1.94	0.49
2:P:6:LYS:HA	2:P:33:ILE:CG2	2.41	0.49
2:P:212:ILE:HD13	2:P:212:ILE:N	2.27	0.49
2:R:136:ASP:HB3	2:R:203:HIS:CD2	2.48	0.49
2:S:212:ILE:HD13	2:S:212:ILE:N	2.27	0.49
2:U:212:ILE:HD13	2:U:212:ILE:N	2.27	0.49
2:V:212:ILE:HD13	2:V:212:ILE:N	2.27	0.49
2:W:147:LEU:O	2:W:148:MET:HG2	2.13	0.49
2:X:147:LEU:O	2:X:148:MET:HG2	2.13	0.49
1:E:4:HIS:CD2	2:Q:178:ILE:CG1	2.58	0.49
1:E:181:PRO:HD3	1:F:29:GLN:OE1	2.12	0.49
1:G:28:GLU:OE1	1:G:88:ARG:NH1	2.45	0.49
1:H:311:LEU:HD22	1:H:369:LEU:HB3	1.93	0.49
1:I:255:PHE:HB3	1:I:363:PRO:HB2	1.94	0.49
1:J:124:VAL:HG13	1:J:274:LEU:HD21	1.94	0.49
1:L:192:ARG:HD3	1:L:219:ASN:HD22	1.77	0.49
2:M:147:LEU:O	2:M:148:MET:HG2	2.13	0.49
2:N:136:ASP:HB3	2:N:203:HIS:CD2	2.48	0.49
2:O:212:ILE:HD13	2:O:212:ILE:N	2.27	0.49
2:P:237:THR:O	2:P:237:THR:CG2	2.60	0.49
2:R:212:ILE:HD13	2:R:212:ILE:N	2.27	0.49
2:S:136:ASP:HB3	2:S:203:HIS:CD2	2.48	0.49
1:C:255:PHE:HB3	1:C:363:PRO:HB2	1.94	0.48
1:G:124:VAL:HG13	1:G:274:LEU:HD21	1.94	0.48
1:H:255:PHE:HB3	1:H:363:PRO:HB2	1.94	0.48
2:M:61:PHE:HA	2:M:263:SER:O	2.13	0.48
2:O:6:LYS:HA	2:O:33:ILE:CG2	2.41	0.48
2:Q:61:PHE:HA	2:Q:263:SER:O	2.13	0.48
2:S:61:PHE:HA	2:S:263:SER:O	2.13	0.48
2:S:312:ALA:HB2	2:S:317:ILE:CB	2.39	0.48
2:T:61:PHE:HA	2:T:263:SER:O	2.13	0.48
2:V:6:LYS:HA	2:V:33:ILE:CG2	2.41	0.48
2:V:237:THR:O	2:V:237:THR:CG2	2.60	0.48
2:W:136:ASP:HB3	2:W:203:HIS:CD2	2.48	0.48
2:X:136:ASP:OD2	2:X:140:LYS:NZ	2.35	0.48
2:X:237:THR:O	2:X:237:THR:CG2	2.60	0.48
1:C:124:VAL:HG13	1:C:274:LEU:HD21	1.94	0.48
1:F:456:THR:O	1:L:458:HIS:HE1	1.96	0.48
1:G:255:PHE:HB3	1:G:363:PRO:HB2	1.94	0.48
2:R:61:PHE:HA	2:R:263:SER:O	2.13	0.48
2:R:147:LEU:O	2:R:148:MET:HG2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:147:LEU:O	2:T:148:MET:HG2	2.13	0.48
2:X:61:PHE:HA	2:X:263:SER:O	2.13	0.48
1:C:22:THR:HG22	1:C:23:ASP:O	2.14	0.48
1:E:466:TYR:HA	1:K:256:MET:HG3	1.94	0.48
1:F:124:VAL:HG13	1:F:274:LEU:HD21	1.94	0.48
1:F:248:ARG:HH21	1:F:248:ARG:HG3	1.75	0.48
1:F:384:ASN:N	1:F:384:ASN:ND2	2.60	0.48
1:K:22:THR:HG22	1:K:23:ASP:O	2.14	0.48
2:N:277:LYS:O	2:N:281:GLU:HG3	2.13	0.48
2:Q:147:LEU:O	2:Q:148:MET:HG2	2.13	0.48
2:S:147:LEU:O	2:S:148:MET:HG2	2.13	0.48
2:V:277:LYS:O	2:V:281:GLU:HG3	2.13	0.48
2:W:277:LYS:O	2:W:281:GLU:HG3	2.13	0.48
1:A:180:PHE:O	1:B:29:GLN:HA	2.14	0.48
1:B:22:THR:HG22	1:B:23:ASP:O	2.14	0.48
1:G:384:ASN:N	1:G:384:ASN:ND2	2.60	0.48
1:J:22:THR:HG22	1:J:23:ASP:O	2.14	0.48
1:J:255:PHE:HB3	1:J:363:PRO:HB2	1.94	0.48
2:O:147:LEU:O	2:O:148:MET:HG2	2.13	0.48
2:R:277:LYS:O	2:R:281:GLU:HG3	2.13	0.48
1:D:396:LEU:H	1:D:396:LEU:HG	1.46	0.48
1:F:28:GLU:OE1	1:F:88:ARG:NH1	2.45	0.48
2:M:237:THR:O	2:M:237:THR:CG2	2.60	0.48
2:O:277:LYS:O	2:O:281:GLU:HG3	2.13	0.48
2:T:136:ASP:HB3	2:T:203:HIS:CD2	2.48	0.48
2:U:277:LYS:O	2:U:281:GLU:HG3	2.13	0.48
1:E:398:ASP:OD1	1:E:399:LEU:HD23	2.14	0.48
1:F:364:ALA:HA	1:L:468:VAL:CG1	2.44	0.48
1:H:30:HIS:H	1:I:180:PHE:HB3	1.78	0.48
1:H:398:ASP:OD1	1:H:399:LEU:HD23	2.14	0.48
1:K:248:ARG:CG	1:K:248:ARG:NH2	2.67	0.48
2:P:61:PHE:HA	2:P:263:SER:O	2.13	0.48
2:P:277:LYS:O	2:P:281:GLU:HG3	2.13	0.48
2:R:312:ALA:HB2	2:R:317:ILE:CB	2.39	0.48
2:U:61:PHE:HA	2:U:263:SER:O	2.13	0.48
2:V:64:HIS:CE1	2:V:330:MET:O	2.62	0.48
2:V:147:LEU:O	2:V:148:MET:HG2	2.13	0.48
1:B:248:ARG:CG	1:B:248:ARG:NH2	2.67	0.48
1:G:130:PRO:HB3	1:G:268:MET:HE3	1.95	0.48
1:J:329:PRO:O	1:J:342:SER:HB3	2.14	0.48
2:S:277:LYS:O	2:S:281:GLU:HG3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:329:PRO:O	1:B:342:SER:HB3	2.14	0.48
1:C:329:PRO:O	1:C:342:SER:HB3	2.14	0.48
1:E:43:PHE:HB3	2:Q:370:LYS:NZ	2.22	0.48
1:F:458:HIS:HE1	1:L:456:THR:O	1.96	0.48
1:G:398:ASP:OD1	1:G:399:LEU:HD23	2.14	0.48
1:H:43:PHE:HB3	2:T:370:LYS:NZ	2.22	0.48
1:I:28:GLU:OE1	1:I:88:ARG:NH1	2.45	0.48
1:I:398:ASP:OD1	1:I:399:LEU:HD23	2.14	0.48
1:K:398:ASP:OD1	1:K:399:LEU:HD23	2.14	0.48
2:M:136:ASP:OD2	2:M:140:LYS:NZ	2.35	0.48
2:P:136:ASP:HB3	2:P:203:HIS:CD2	2.48	0.48
2:Q:136:ASP:HB3	2:Q:203:HIS:CD2	2.48	0.48
2:Q:277:LYS:O	2:Q:281:GLU:HG3	2.13	0.48
1:A:22:THR:HG22	1:A:23:ASP:O	2.13	0.48
1:A:61:ASN:O	1:F:337:ARG:CB	2.44	0.48
1:B:398:ASP:OD1	1:B:399:LEU:HD23	2.14	0.48
1:C:130:PRO:HB3	1:C:268:MET:HE3	1.96	0.48
1:C:398:ASP:OD1	1:C:399:LEU:HD23	2.14	0.48
1:D:22:THR:HG22	1:D:23:ASP:O	2.14	0.48
1:D:398:ASP:OD1	1:D:399:LEU:HD23	2.14	0.48
1:G:329:PRO:O	1:G:342:SER:HB3	2.14	0.48
1:J:29:GLN:HB3	1:K:180:PHE:CB	2.44	0.48
1:K:329:PRO:O	1:K:342:SER:HB3	2.14	0.48
2:O:136:ASP:HB3	2:O:203:HIS:CD2	2.48	0.48
2:P:147:LEU:O	2:P:148:MET:HG2	2.13	0.48
2:Q:6:LYS:HA	2:Q:33:ILE:CG2	2.41	0.48
2:T:277:LYS:O	2:T:281:GLU:HG3	2.13	0.48
2:U:136:ASP:HB3	2:U:203:HIS:CD2	2.48	0.48
2:V:136:ASP:HB3	2:V:203:HIS:CD2	2.48	0.48
1:E:22:THR:HG22	1:E:23:ASP:O	2.14	0.48
1:E:179:TYR:CD2	1:F:53:SER:HB2	2.49	0.48
1:E:320:LYS:HG3	1:K:454:ARG:O	2.13	0.48
1:F:329:PRO:O	1:F:342:SER:HB3	2.14	0.48
1:F:398:ASP:OD1	1:F:399:LEU:HD23	2.14	0.48
1:H:22:THR:HG22	1:H:23:ASP:O	2.14	0.48
1:I:22:THR:HG22	1:I:23:ASP:O	2.14	0.48
1:J:398:ASP:OD1	1:J:399:LEU:HD23	2.14	0.48
2:N:61:PHE:HA	2:N:263:SER:O	2.13	0.48
2:V:61:PHE:HA	2:V:263:SER:O	2.13	0.48
2:W:239:LYS:HZ1	2:W:241:ASN:HB2	1.79	0.48
1:A:398:ASP:OD1	1:A:399:LEU:HD23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:28:GLU:OE1	1:D:88:ARG:NH1	2.45	0.47
1:E:454:ARG:O	1:K:320:LYS:HG3	2.13	0.47
1:G:22:THR:HG22	1:G:23:ASP:O	2.14	0.47
1:L:22:THR:HG22	1:L:23:ASP:O	2.14	0.47
2:T:6:LYS:HA	2:T:33:ILE:CG2	2.41	0.47
2:X:277:LYS:O	2:X:281:GLU:HG3	2.13	0.47
1:L:43:PHE:HB3	2:X:370:LYS:CD	2.28	0.47
1:L:398:ASP:OD1	1:L:399:LEU:HD23	2.14	0.47
2:N:6:LYS:HA	2:N:33:ILE:CG2	2.41	0.47
2:O:61:PHE:HA	2:O:263:SER:O	2.13	0.47
2:O:64:HIS:CE1	2:O:330:MET:O	2.62	0.47
2:U:147:LEU:O	2:U:148:MET:HG2	2.13	0.47
2:W:6:LYS:HA	2:W:33:ILE:CG2	2.41	0.47
2:W:61:PHE:HA	2:W:263:SER:O	2.13	0.47
1:D:124:VAL:HG13	1:D:274:LEU:CD2	2.45	0.47
1:F:22:THR:HG22	1:F:23:ASP:O	2.13	0.47
1:I:124:VAL:HG13	1:I:274:LEU:CD2	2.45	0.47
2:M:277:LYS:O	2:M:281:GLU:HG3	2.13	0.47
2:Q:62:TRP:CD1	2:Q:66:ARG:HG3	2.50	0.47
2:S:62:TRP:CD1	2:S:66:ARG:HG3	2.50	0.47
1:G:124:VAL:HG13	1:G:274:LEU:CD2	2.45	0.47
1:I:130:PRO:HB3	1:I:268:MET:HE3	1.96	0.47
1:J:100:TYR:CE2	1:J:102:ARG:HB2	2.50	0.47
1:J:124:VAL:HG13	1:J:274:LEU:CD2	2.45	0.47
2:T:62:TRP:CD1	2:T:66:ARG:HG3	2.50	0.47
2:U:62:TRP:CD1	2:U:66:ARG:HG3	2.50	0.47
1:A:124:VAL:HG13	1:A:274:LEU:CD2	2.45	0.47
1:A:329:PRO:O	1:A:342:SER:HB3	2.14	0.47
1:B:28:GLU:OE1	1:B:88:ARG:NH1	2.45	0.47
1:C:100:TYR:CE2	1:C:102:ARG:HB2	2.50	0.47
1:C:124:VAL:HG13	1:C:274:LEU:CD2	2.45	0.47
1:C:465:TYR:O	1:C:468:VAL:HB	2.15	0.47
1:D:130:PRO:HB3	1:D:268:MET:HE3	1.96	0.47
1:I:100:TYR:CE2	1:I:102:ARG:HB2	2.50	0.47
1:L:248:ARG:HH21	1:L:248:ARG:HG3	1.75	0.47
1:L:384:ASN:N	1:L:384:ASN:ND2	2.60	0.47
2:P:62:TRP:CD1	2:P:66:ARG:HG3	2.50	0.47
2:R:62:TRP:CD1	2:R:66:ARG:HG3	2.50	0.47
1:A:181:PRO:HD3	1:B:29:GLN:OE1	2.14	0.47
1:A:384:ASN:N	1:A:384:ASN:ND2	2.60	0.47
1:F:124:VAL:HG13	1:F:274:LEU:CD2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:465:TYR:O	1:J:468:VAL:HB	2.15	0.47
1:K:28:GLU:OE1	1:K:88:ARG:NH1	2.45	0.47
2:P:369:THR:C	2:P:370:LYS:CA	2.75	0.47
2:U:369:THR:C	2:U:370:LYS:CA	2.75	0.47
1:B:100:TYR:CE2	1:B:102:ARG:HB2	2.50	0.47
1:D:5:VAL:HG23	2:P:179:LYS:HZ1	1.80	0.47
1:D:100:TYR:CE2	1:D:102:ARG:HB2	2.50	0.47
1:E:271:HIS:CD2	1:E:357:GLU:HG3	2.50	0.47
1:F:100:TYR:CE2	1:F:102:ARG:HB2	2.50	0.47
1:F:465:TYR:O	1:F:468:VAL:HB	2.15	0.47
1:G:43:PHE:HB3	2:S:370:LYS:CD	2.28	0.47
1:I:271:HIS:CD2	1:I:357:GLU:HG3	2.50	0.47
1:I:329:PRO:O	1:I:342:SER:HB3	2.14	0.47
1:K:100:TYR:CE2	1:K:102:ARG:HB2	2.50	0.47
1:K:295:LEU:O	1:K:388:PRO:HG2	2.15	0.47
1:L:4:HIS:HD2	2:X:178:ILE:CD1	2.27	0.47
1:L:124:VAL:HG13	1:L:274:LEU:CD2	2.45	0.47
1:L:329:PRO:O	1:L:342:SER:HB3	2.14	0.47
1:A:4:HIS:HD2	2:M:178:ILE:CD1	2.27	0.47
1:A:248:ARG:CG	1:A:248:ARG:NH2	2.67	0.47
1:B:295:LEU:O	1:B:388:PRO:HG2	2.15	0.47
1:C:396:LEU:HB2	1:C:397:TYR:H	1.36	0.47
1:D:271:HIS:CD2	1:D:357:GLU:HG3	2.50	0.47
1:D:329:PRO:O	1:D:342:SER:HB3	2.14	0.47
1:E:329:PRO:O	1:E:342:SER:HB3	2.14	0.47
1:H:271:HIS:CD2	1:H:357:GLU:HG3	2.50	0.47
2:N:369:THR:C	2:N:370:LYS:CA	2.75	0.47
2:O:62:TRP:CD1	2:O:66:ARG:HG3	2.49	0.47
1:A:100:TYR:CE2	1:A:102:ARG:HB2	2.50	0.47
1:A:248:ARG:HH21	1:A:248:ARG:HG3	1.75	0.47
1:A:320:LYS:HG3	1:G:454:ARG:O	2.15	0.47
1:B:124:VAL:HG13	1:B:274:LEU:CD2	2.45	0.47
1:B:465:TYR:O	1:B:468:VAL:HB	2.15	0.47
1:D:465:TYR:O	1:D:468:VAL:HB	2.15	0.47
1:E:5:VAL:HG23	2:Q:179:LYS:HZ1	1.80	0.47
1:F:271:HIS:CD2	1:F:357:GLU:HG3	2.50	0.47
1:G:100:TYR:CE2	1:G:102:ARG:HB2	2.50	0.47
1:G:271:HIS:CD2	1:G:357:GLU:HG3	2.50	0.47
1:G:465:TYR:O	1:G:468:VAL:HB	2.15	0.47
1:H:100:TYR:CE2	1:H:102:ARG:HB2	2.50	0.47
1:H:465:TYR:O	1:H:468:VAL:HB	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:465:TYR:O	1:K:468:VAL:HB	2.15	0.47
2:T:31:THR:HG23	2:T:33:ILE:CD1	2.42	0.47
2:V:62:TRP:CD1	2:V:66:ARG:HG3	2.50	0.47
2:X:62:TRP:CD1	2:X:66:ARG:HG3	2.50	0.47
1:C:271:HIS:CD2	1:C:357:GLU:HG3	2.50	0.47
1:C:295:LEU:O	1:C:388:PRO:HG2	2.15	0.47
1:E:100:TYR:CE2	1:E:102:ARG:HB2	2.50	0.47
1:E:180:PHE:O	1:F:29:GLN:HA	2.15	0.47
1:E:465:TYR:O	1:E:468:VAL:HB	2.15	0.47
1:F:4:HIS:HD2	2:R:178:ILE:CD1	2.27	0.47
1:H:329:PRO:O	1:H:342:SER:HB3	2.14	0.47
1:I:465:TYR:O	1:I:468:VAL:HB	2.15	0.47
1:J:295:LEU:O	1:J:388:PRO:HG2	2.15	0.47
1:K:124:VAL:HG13	1:K:274:LEU:CD2	2.45	0.47
1:L:465:TYR:O	1:L:468:VAL:HB	2.15	0.47
2:M:62:TRP:CD1	2:M:66:ARG:HG3	2.50	0.47
1:F:295:LEU:O	1:F:388:PRO:HG2	2.15	0.46
1:J:232:ALA:HB1	1:J:367:PRO:HB2	1.97	0.46
1:J:271:HIS:CD2	1:J:357:GLU:HG3	2.50	0.46
1:L:100:TYR:CE2	1:L:102:ARG:HB2	2.50	0.46
2:Q:31:THR:HG23	2:Q:33:ILE:CD1	2.42	0.46
1:A:295:LEU:O	1:A:388:PRO:HG2	2.15	0.46
1:A:465:TYR:O	1:A:468:VAL:HB	2.15	0.46
1:C:232:ALA:HB1	1:C:367:PRO:HB2	1.97	0.46
1:C:320:LYS:HG3	1:I:454:ARG:O	2.15	0.46
1:C:455:MET:HG2	1:I:323:VAL:HG11	1.97	0.46
1:D:235:ILE:HD13	1:D:235:ILE:HA	1.82	0.46
1:E:232:ALA:HB1	1:E:367:PRO:HB2	1.97	0.46
2:N:290:LEU:HD23	2:N:290:LEU:HA	1.73	0.46
2:T:31:THR:CG2	2:T:33:ILE:HD12	2.43	0.46
2:W:62:TRP:CD1	2:W:66:ARG:HG3	2.49	0.46
1:E:124:VAL:HG13	1:E:274:LEU:CD2	2.45	0.46
1:G:4:HIS:HD2	2:S:178:ILE:CD1	2.27	0.46
1:H:124:VAL:HG13	1:H:274:LEU:CD2	2.44	0.46
1:K:4:HIS:CD2	2:W:178:ILE:CD1	2.98	0.46
1:L:248:ARG:CG	1:L:248:ARG:NH2	2.67	0.46
2:N:62:TRP:CD1	2:N:66:ARG:HG3	2.50	0.46
2:Q:31:THR:CG2	2:Q:33:ILE:HD12	2.43	0.46
2:W:369:THR:C	2:W:370:LYS:CA	2.75	0.46
1:C:4:HIS:CD2	2:O:178:ILE:CD1	2.99	0.46
1:C:456:THR:O	1:I:458:HIS:HE1	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:41:GLU:OE2	1:E:45:GLU:OE2	2.34	0.46
1:F:4:HIS:CD2	2:R:178:ILE:CD1	2.99	0.46
1:G:295:LEU:O	1:G:388:PRO:HG2	2.15	0.46
1:J:4:HIS:CD2	2:V:178:ILE:CD1	2.99	0.46
1:J:396:LEU:HB2	1:J:397:TYR:H	1.36	0.46
1:K:43:PHE:HB3	2:W:370:LYS:NZ	2.22	0.46
1:L:295:LEU:O	1:L:388:PRO:HG2	2.15	0.46
1:B:43:PHE:HB3	2:N:370:LYS:NZ	2.22	0.46
1:D:41:GLU:OE2	1:D:45:GLU:OE2	2.34	0.46
1:E:4:HIS:CD2	2:Q:178:ILE:CD1	2.99	0.46
1:G:3:GLU:O	1:G:7:THR:HG23	2.16	0.46
1:H:41:GLU:OE2	1:H:45:GLU:OE2	2.34	0.46
1:H:128:PRO:HA	1:H:269:HIS:O	2.16	0.46
1:H:232:ALA:HB1	1:H:367:PRO:HB2	1.97	0.46
1:I:41:GLU:OE2	1:I:45:GLU:OE2	2.34	0.46
1:K:387:HIS:HA	1:K:388:PRO:HD2	1.73	0.46
2:M:6:LYS:HA	2:M:33:ILE:CG2	2.41	0.46
2:T:290:LEU:HD23	2:T:290:LEU:HA	1.73	0.46
2:W:290:LEU:HD23	2:W:290:LEU:HA	1.73	0.46
1:A:3:GLU:O	1:A:7:THR:HG23	2.16	0.46
1:B:4:HIS:CD2	2:N:178:ILE:CD1	2.99	0.46
1:B:232:ALA:HB1	1:B:367:PRO:HB2	1.97	0.46
1:F:232:ALA:HB1	1:F:367:PRO:HB2	1.97	0.46
1:G:232:ALA:HB1	1:G:367:PRO:HB2	1.97	0.46
1:K:232:ALA:HB1	1:K:367:PRO:HB2	1.97	0.46
1:L:3:GLU:O	1:L:7:THR:HG23	2.16	0.46
2:M:41:ASP:O	2:M:42:LYS:HB2	2.16	0.46
2:Q:290:LEU:HD23	2:Q:290:LEU:HA	1.73	0.46
1:A:271:HIS:CD2	1:A:357:GLU:HG3	2.50	0.46
1:B:271:HIS:CD2	1:B:357:GLU:HG3	2.50	0.46
1:C:3:GLU:O	1:C:7:THR:HG23	2.16	0.46
1:D:466:TYR:HA	1:J:256:MET:HG3	1.97	0.46
1:E:128:PRO:HA	1:E:269:HIS:O	2.16	0.46
1:H:4:HIS:CD2	2:T:178:ILE:CD1	2.99	0.46
1:K:271:HIS:CD2	1:K:357:GLU:HG3	2.50	0.46
2:U:64:HIS:CE1	2:U:330:MET:O	2.62	0.46
2:X:41:ASP:O	2:X:42:LYS:HB2	2.16	0.46
1:A:4:HIS:CD2	2:M:178:ILE:CD1	2.98	0.46
1:A:170:GLY:HA2	1:A:172:ARG:HH22	1.81	0.46
1:B:320:LYS:HG3	1:H:454:ARG:O	2.16	0.46
1:B:323:VAL:HG11	1:H:455:MET:HG2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:128:PRO:HA	1:C:269:HIS:O	2.16	0.46
1:C:256:MET:HG3	1:I:466:TYR:HA	1.98	0.46
1:F:3:GLU:O	1:F:7:THR:HG23	2.16	0.46
1:F:254:THR:HB	1:L:466:TYR:CE1	2.51	0.46
1:H:5:VAL:HG23	2:T:179:LYS:HZ1	1.81	0.46
1:I:295:LEU:O	1:I:388:PRO:HG2	2.15	0.46
1:J:128:PRO:HA	1:J:269:HIS:O	2.16	0.46
1:K:128:PRO:HA	1:K:269:HIS:O	2.16	0.46
1:L:170:GLY:HA2	1:L:172:ARG:HH22	1.81	0.46
2:X:6:LYS:HA	2:X:33:ILE:CG2	2.41	0.46
1:B:128:PRO:HA	1:B:269:HIS:O	2.16	0.46
1:B:387:HIS:HA	1:B:388:PRO:HD2	1.73	0.46
1:D:128:PRO:HA	1:D:269:HIS:O	2.16	0.46
1:F:128:PRO:HA	1:F:269:HIS:O	2.16	0.46
1:I:232:ALA:HB1	1:I:367:PRO:HB2	1.97	0.46
1:J:3:GLU:O	1:J:7:THR:HG23	2.16	0.46
1:L:41:GLU:OE2	1:L:45:GLU:OE2	2.34	0.46
2:P:144:LYS:HE2	2:P:221:GLU:HA	1.98	0.46
2:Q:144:LYS:HE2	2:Q:221:GLU:HA	1.98	0.46
2:S:144:LYS:HE2	2:S:221:GLU:HA	1.98	0.46
2:S:290:LEU:HD23	2:S:290:LEU:HA	1.73	0.46
1:E:295:LEU:O	1:E:388:PRO:HG2	2.15	0.46
1:G:4:HIS:CD2	2:S:178:ILE:CD1	2.99	0.46
1:G:41:GLU:OE2	1:G:45:GLU:OE2	2.34	0.46
1:G:128:PRO:HA	1:G:269:HIS:O	2.16	0.46
1:K:41:GLU:OE2	1:K:45:GLU:OE2	2.34	0.46
1:L:271:HIS:CD2	1:L:357:GLU:HG3	2.50	0.46
2:R:6:LYS:HA	2:R:33:ILE:CG2	2.41	0.46
2:S:6:LYS:HA	2:S:33:ILE:CG2	2.41	0.46
2:S:369:THR:C	2:S:370:LYS:CA	2.75	0.46
2:T:64:HIS:CE1	2:T:330:MET:O	2.62	0.46
2:U:144:LYS:HE2	2:U:221:GLU:HA	1.98	0.46
1:A:41:GLU:OE2	1:A:45:GLU:OE2	2.34	0.45
1:B:41:GLU:OE2	1:B:45:GLU:OE2	2.34	0.45
1:D:295:LEU:O	1:D:388:PRO:HG2	2.15	0.45
1:G:313:ASN:HD21	1:G:360:PHE:HD2	1.64	0.45
1:H:295:LEU:O	1:H:388:PRO:HG2	2.15	0.45
1:I:128:PRO:HA	1:I:269:HIS:O	2.16	0.45
1:I:272:MET:HE1	1:I:358:VAL:HG21	1.98	0.45
1:J:387:HIS:HA	1:J:388:PRO:HD2	1.73	0.45
1:K:235:ILE:HD13	1:K:235:ILE:HA	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:85:PHE:CD1	2:N:85:PHE:C	2.90	0.45
2:P:64:HIS:CE1	2:P:330:MET:O	2.62	0.45
2:R:41:ASP:O	2:R:42:LYS:HB2	2.16	0.45
2:R:144:LYS:HE2	2:R:221:GLU:HA	1.98	0.45
2:T:144:LYS:HE2	2:T:221:GLU:HA	1.98	0.45
2:W:85:PHE:C	2:W:85:PHE:CD1	2.89	0.45
2:W:312:ALA:CB	2:W:317:ILE:HG22	2.32	0.45
2:X:31:THR:HG23	2:X:33:ILE:CD1	2.42	0.45
1:D:180:PHE:O	1:E:29:GLN:HA	2.16	0.45
1:D:232:ALA:HB1	1:D:367:PRO:HB2	1.97	0.45
1:G:29:GLN:HB3	1:H:180:PHE:CB	2.46	0.45
1:G:170:GLY:HA2	1:G:172:ARG:HH22	1.81	0.45
1:L:4:HIS:CD2	2:X:178:ILE:CD1	2.99	0.45
2:N:31:THR:CG2	2:N:33:ILE:HD12	2.43	0.45
2:S:41:ASP:O	2:S:42:LYS:HB2	2.16	0.45
2:W:59:ILE:HG21	2:W:59:ILE:HD13	1.70	0.45
1:A:466:TYR:HA	1:G:256:MET:HG3	1.97	0.45
1:B:235:ILE:HD13	1:B:235:ILE:HA	1.82	0.45
1:C:41:GLU:OE2	1:C:45:GLU:OE2	2.34	0.45
1:D:3:GLU:O	1:D:7:THR:HG23	2.16	0.45
1:D:272:MET:HE1	1:D:358:VAL:HG21	1.99	0.45
1:F:41:GLU:OE2	1:F:45:GLU:OE2	2.34	0.45
1:I:4:HIS:CD2	2:U:178:ILE:CD1	2.99	0.45
2:N:41:ASP:O	2:N:42:LYS:HB2	2.16	0.45
2:N:312:ALA:CB	2:N:317:ILE:HG22	2.32	0.45
2:O:144:LYS:HE2	2:O:221:GLU:HA	1.98	0.45
2:U:59:ILE:HG21	2:U:59:ILE:HD13	1.70	0.45
2:V:41:ASP:O	2:V:42:LYS:HB2	2.16	0.45
2:W:31:THR:CG2	2:W:33:ILE:HD12	2.43	0.45
2:X:312:ALA:CB	2:X:317:ILE:HG22	2.32	0.45
1:B:313:ASN:HD21	1:B:360:PHE:HD2	1.65	0.45
1:E:3:GLU:O	1:E:7:THR:HG23	2.16	0.45
1:E:28:GLU:OE1	1:E:88:ARG:NH1	2.45	0.45
1:K:313:ASN:HD21	1:K:360:PHE:HD2	1.65	0.45
2:O:41:ASP:O	2:O:42:LYS:HB2	2.16	0.45
2:O:85:PHE:C	2:O:85:PHE:CD1	2.90	0.45
2:R:64:HIS:CE1	2:R:330:MET:O	2.62	0.45
2:R:290:LEU:HD23	2:R:290:LEU:HA	1.73	0.45
2:V:31:THR:HG23	2:V:33:ILE:CD1	2.42	0.45
2:V:85:PHE:CD1	2:V:85:PHE:C	2.90	0.45
2:V:144:LYS:HE2	2:V:221:GLU:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:31:THR:HG23	2:W:33:ILE:CD1	2.42	0.45
2:W:41:ASP:O	2:W:42:LYS:HB2	2.16	0.45
2:X:85:PHE:CD1	2:X:85:PHE:C	2.89	0.45
1:A:31:VAL:HG23	1:F:210:HIS:HB3	1.97	0.45
1:D:4:HIS:CD2	2:P:178:ILE:CD1	2.99	0.45
1:D:170:GLY:HA2	1:D:172:ARG:HH22	1.81	0.45
1:F:313:ASN:HD21	1:F:360:PHE:HD2	1.65	0.45
1:H:3:GLU:O	1:H:7:THR:HG23	2.16	0.45
1:I:170:GLY:HA2	1:I:172:ARG:HH22	1.81	0.45
1:J:41:GLU:OE2	1:J:45:GLU:OE2	2.34	0.45
1:J:313:ASN:HD21	1:J:360:PHE:HD2	1.64	0.45
1:L:313:ASN:HD21	1:L:360:PHE:HD2	1.65	0.45
2:M:85:PHE:CD1	2:M:85:PHE:C	2.89	0.45
2:P:85:PHE:CD1	2:P:85:PHE:C	2.90	0.45
2:Q:64:HIS:CE1	2:Q:330:MET:O	2.62	0.45
2:T:85:PHE:CD1	2:T:85:PHE:C	2.90	0.45
1:A:139:ARG:HD3	1:F:163:LYS:HG2	1.99	0.45
1:A:313:ASN:HD21	1:A:360:PHE:HD2	1.65	0.45
1:C:313:ASN:HD21	1:C:360:PHE:HD2	1.65	0.45
1:C:328:ALA:HA	1:C:329:PRO:HD3	1.73	0.45
1:F:170:GLY:HA2	1:F:172:ARG:HH22	1.81	0.45
1:F:454:ARG:O	1:L:320:LYS:HG3	2.16	0.45
1:I:3:GLU:O	1:I:7:THR:HG23	2.16	0.45
2:N:31:THR:HG23	2:N:33:ILE:CD1	2.42	0.45
2:Q:85:PHE:CD1	2:Q:85:PHE:C	2.90	0.45
2:U:85:PHE:CD1	2:U:85:PHE:C	2.89	0.45
1:A:232:ALA:HB1	1:A:367:PRO:HB2	1.97	0.45
1:A:396:LEU:HB2	1:A:397:TYR:H	1.36	0.45
1:C:387:HIS:HA	1:C:388:PRO:HD2	1.73	0.45
1:H:4:HIS:HD2	2:T:178:ILE:CD1	2.27	0.45
1:H:313:ASN:HD21	1:H:360:PHE:HD2	1.64	0.45
2:M:31:THR:HG23	2:M:33:ILE:CD1	2.42	0.45
2:R:369:THR:C	2:R:370:LYS:CA	2.75	0.45
2:S:85:PHE:CD1	2:S:85:PHE:C	2.89	0.45
2:U:41:ASP:O	2:U:42:LYS:HB2	2.16	0.45
1:D:396:LEU:HB2	1:D:397:TYR:H	1.36	0.45
1:H:28:GLU:OE1	1:H:88:ARG:NH1	2.45	0.45
2:O:31:THR:HG23	2:O:33:ILE:CD1	2.42	0.45
2:P:41:ASP:O	2:P:42:LYS:HB2	2.16	0.45
2:U:290:LEU:HD23	2:U:290:LEU:HA	1.73	0.45
1:A:180:PHE:HB2	1:B:29:GLN:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:GLU:O	1:B:7:THR:HG23	2.16	0.45
1:B:130:PRO:HB3	1:B:268:MET:HE3	1.99	0.45
1:C:4:HIS:HD2	2:O:178:ILE:CD1	2.27	0.45
1:D:324:PRO:HB3	1:D:397:TYR:CD2	2.52	0.45
1:E:4:HIS:HD2	2:Q:178:ILE:CD1	2.27	0.45
1:I:5:VAL:HG23	2:U:179:LYS:HZ1	1.82	0.45
1:J:4:HIS:HD2	2:V:178:ILE:CD1	2.27	0.45
1:J:31:VAL:HG23	1:K:210:HIS:HB3	1.98	0.45
1:J:272:MET:HE1	1:J:358:VAL:HG21	1.99	0.45
1:K:130:PRO:HB3	1:K:268:MET:HE3	1.99	0.45
1:L:396:LEU:HB2	1:L:397:TYR:H	1.36	0.45
2:M:312:ALA:CB	2:M:317:ILE:HG22	2.32	0.45
2:P:290:LEU:HD23	2:P:290:LEU:HA	1.73	0.45
2:R:270:SER:HA	2:R:271:PRO:HD3	1.74	0.45
2:S:64:HIS:CE1	2:S:330:MET:O	2.62	0.45
1:D:468:VAL:HG13	1:J:364:ALA:HA	1.99	0.45
1:E:313:ASN:HD21	1:E:360:PHE:HD2	1.65	0.45
1:I:324:PRO:HB3	1:I:397:TYR:CD2	2.52	0.45
1:J:34:PRO:HG2	1:K:206:VAL:O	2.17	0.45
1:L:128:PRO:HA	1:L:269:HIS:O	2.16	0.45
1:L:180:PHE:O	1:L:181:PRO:C	2.54	0.45
1:L:232:ALA:HB1	1:L:367:PRO:HB2	1.97	0.45
2:M:144:LYS:HE2	2:M:221:GLU:HA	1.98	0.45
2:N:239:LYS:HZ3	2:N:241:ASN:HB2	1.82	0.45
2:Q:41:ASP:O	2:Q:42:LYS:HB2	2.16	0.45
2:U:97:VAL:O	2:U:104:ILE:HG12	2.17	0.45
2:X:6:LYS:HD2	2:X:8:VAL:HG23	1.99	0.45
1:A:128:PRO:HA	1:A:269:HIS:O	2.16	0.44
1:A:324:PRO:HB3	1:A:397:TYR:CE2	2.52	0.44
1:C:65:MET:HA	1:C:94:PRO:HG3	2.00	0.44
1:G:458:HIS:CD2	1:G:459:PRO:HD2	2.52	0.44
1:I:396:LEU:HB2	1:I:397:TYR:H	1.36	0.44
1:J:180:PHE:O	1:J:181:PRO:C	2.54	0.44
1:K:3:GLU:O	1:K:7:THR:HG23	2.16	0.44
1:K:4:HIS:HD2	2:W:178:ILE:CD1	2.27	0.44
1:L:43:PHE:HB3	2:X:370:LYS:NZ	2.22	0.44
2:M:6:LYS:HD2	2:M:8:VAL:HG23	1.99	0.44
2:P:59:ILE:HG21	2:P:59:ILE:HD13	1.70	0.44
2:P:97:VAL:O	2:P:104:ILE:HG12	2.17	0.44
2:R:85:PHE:CD1	2:R:85:PHE:C	2.90	0.44
2:X:144:LYS:HE2	2:X:221:GLU:HA	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:PHE:O	1:A:181:PRO:C	2.54	0.44
1:C:324:PRO:HB3	1:C:397:TYR:CD2	2.52	0.44
1:E:324:PRO:HB3	1:E:397:TYR:CD2	2.52	0.44
1:H:324:PRO:HB3	1:H:397:TYR:CD2	2.52	0.44
1:J:65:MET:HA	1:J:94:PRO:HG3	2.00	0.44
2:T:41:ASP:O	2:T:42:LYS:HB2	2.16	0.44
1:A:340:SER:HB3	1:A:396:LEU:HB3	1.99	0.44
1:A:458:HIS:CD2	1:A:459:PRO:HD2	2.52	0.44
1:B:384:ASN:N	1:B:384:ASN:ND2	2.60	0.44
1:C:180:PHE:O	1:C:181:PRO:C	2.54	0.44
1:E:276:LYS:HG2	1:E:277:ASN:ND2	2.32	0.44
1:F:7:THR:OG1	2:R:178:ILE:HD13	2.18	0.44
1:J:324:PRO:HB3	1:J:397:TYR:CD2	2.52	0.44
1:K:458:HIS:CD2	1:K:459:PRO:HD2	2.52	0.44
1:L:324:PRO:HB3	1:L:397:TYR:CD2	2.52	0.44
1:L:324:PRO:HB3	1:L:397:TYR:CE2	2.53	0.44
2:P:128:THR:CG2	2:P:131:GLU:H	2.31	0.44
2:U:128:THR:CG2	2:U:131:GLU:H	2.31	0.44
2:W:270:SER:HA	2:W:271:PRO:HD3	1.74	0.44
2:X:64:HIS:CE1	2:X:330:MET:O	2.62	0.44
2:X:97:VAL:O	2:X:104:ILE:HG12	2.17	0.44
2:X:270:SER:HA	2:X:271:PRO:HD3	1.74	0.44
1:A:65:MET:HA	1:A:94:PRO:HG3	2.00	0.44
1:A:324:PRO:HB3	1:A:397:TYR:CD2	2.52	0.44
1:B:65:MET:HA	1:B:94:PRO:HG3	1.99	0.44
1:B:458:HIS:CD2	1:B:459:PRO:HD2	2.52	0.44
1:C:458:HIS:CD2	1:C:459:PRO:HD2	2.52	0.44
1:D:5:VAL:CG2	2:P:179:LYS:HZ1	2.30	0.44
1:D:65:MET:HA	1:D:94:PRO:HG3	2.00	0.44
1:E:458:HIS:CD2	1:E:459:PRO:HD2	2.52	0.44
1:F:4:HIS:HB3	2:R:179:LYS:NZ	1.96	0.44
1:F:73:THR:HG21	1:F:88:ARG:HB3	2.00	0.44
1:F:275:ALA:HA	1:F:281:LEU:HD13	2.00	0.44
1:H:276:LYS:HG2	1:H:277:ASN:ND2	2.33	0.44
1:L:65:MET:HA	1:L:94:PRO:HG3	2.00	0.44
1:L:458:HIS:CD2	1:L:459:PRO:HD2	2.52	0.44
2:M:97:VAL:O	2:M:104:ILE:HG12	2.17	0.44
2:M:270:SER:HA	2:M:271:PRO:HD3	1.74	0.44
2:N:97:VAL:O	2:N:104:ILE:HG12	2.17	0.44
2:N:128:THR:CG2	2:N:131:GLU:H	2.31	0.44
2:N:144:LYS:HE2	2:N:221:GLU:HA	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:270:SER:HA	2:N:271:PRO:HD3	1.74	0.44
2:O:31:THR:CG2	2:O:33:ILE:HD12	2.43	0.44
2:O:128:THR:CG2	2:O:131:GLU:H	2.31	0.44
2:Q:97:VAL:O	2:Q:104:ILE:HG12	2.17	0.44
2:R:31:THR:HG23	2:R:33:ILE:CD1	2.42	0.44
2:R:97:VAL:O	2:R:104:ILE:HG12	2.17	0.44
2:T:97:VAL:O	2:T:104:ILE:HG12	2.17	0.44
2:T:312:ALA:HB2	2:T:317:ILE:CG2	2.45	0.44
2:U:31:THR:HG23	2:U:33:ILE:CD1	2.42	0.44
2:V:128:THR:CG2	2:V:131:GLU:H	2.31	0.44
2:W:128:THR:CG2	2:W:131:GLU:H	2.31	0.44
1:A:7:THR:OG1	2:M:178:ILE:HD13	2.18	0.44
1:A:276:LYS:HG2	1:A:277:ASN:ND2	2.33	0.44
1:B:4:HIS:HD2	2:N:178:ILE:CD1	2.27	0.44
1:B:272:MET:HE1	1:B:358:VAL:HG21	1.99	0.44
1:D:313:ASN:HD21	1:D:360:PHE:HD2	1.65	0.44
1:E:5:VAL:CG2	2:Q:179:LYS:HZ1	2.30	0.44
1:E:65:MET:HA	1:E:94:PRO:HG3	2.00	0.44
1:F:458:HIS:CD2	1:F:459:PRO:HD2	2.52	0.44
1:G:7:THR:OG1	2:S:178:ILE:HD13	2.18	0.44
1:G:324:PRO:HB3	1:G:397:TYR:CE2	2.53	0.44
1:H:65:MET:HA	1:H:94:PRO:HG3	2.00	0.44
1:H:275:ALA:HA	1:H:281:LEU:HD13	2.00	0.44
1:I:65:MET:HA	1:I:94:PRO:HG3	2.00	0.44
1:I:313:ASN:HD21	1:I:360:PHE:HD2	1.65	0.44
1:J:328:ALA:HA	1:J:329:PRO:HD3	1.73	0.44
1:K:272:MET:HE1	1:K:358:VAL:HG21	1.99	0.44
1:K:384:ASN:N	1:K:384:ASN:ND2	2.60	0.44
1:L:276:LYS:HG2	1:L:277:ASN:ND2	2.33	0.44
2:M:64:HIS:CE1	2:M:330:MET:O	2.62	0.44
2:S:31:THR:HG23	2:S:33:ILE:CD1	2.42	0.44
2:W:97:VAL:O	2:W:104:ILE:HG12	2.17	0.44
2:W:144:LYS:HE2	2:W:221:GLU:HA	1.98	0.44
1:A:29:GLN:HB3	1:F:180:PHE:HB2	2.00	0.44
1:A:73:THR:HG21	1:A:88:ARG:HB3	2.00	0.44
1:B:17:VAL:HG12	1:B:19:LEU:HD13	2.00	0.44
1:D:340:SER:HB3	1:D:396:LEU:HB3	1.99	0.44
1:E:275:ALA:HA	1:E:281:LEU:HD13	2.00	0.44
1:F:215:THR:O	1:F:216:ALA:HB3	2.18	0.44
1:G:73:THR:HG21	1:G:88:ARG:HB3	2.00	0.44
1:I:340:SER:HB3	1:I:396:LEU:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:5:VAL:CG2	2:V:179:LYS:HZ1	2.31	0.44
1:K:17:VAL:HG12	1:K:19:LEU:HD13	2.00	0.44
1:K:65:MET:HA	1:K:94:PRO:HG3	2.00	0.44
2:O:290:LEU:HD23	2:O:290:LEU:HA	1.73	0.44
2:P:31:THR:HG23	2:P:33:ILE:CD1	2.42	0.44
2:T:270:SER:HA	2:T:271:PRO:HD3	1.74	0.44
1:E:309:ASN:HD22	1:E:313:ASN:HD22	1.66	0.44
1:F:65:MET:HA	1:F:94:PRO:HG3	2.00	0.44
1:G:65:MET:HA	1:G:94:PRO:HG3	2.00	0.44
1:G:275:ALA:HA	1:G:281:LEU:HD13	2.00	0.44
1:H:5:VAL:CG2	2:T:179:LYS:HZ1	2.30	0.44
1:H:324:PRO:HB3	1:H:397:TYR:CE2	2.52	0.44
1:H:458:HIS:CD2	1:H:459:PRO:HD2	2.53	0.44
1:I:324:PRO:HB3	1:I:397:TYR:CE2	2.52	0.44
1:L:28:GLU:OE1	1:L:88:ARG:NH1	2.45	0.44
1:L:340:SER:HB3	1:L:396:LEU:HB3	2.00	0.44
2:M:128:THR:CG2	2:M:131:GLU:H	2.31	0.44
2:Q:128:THR:CG2	2:Q:131:GLU:H	2.31	0.44
2:S:97:VAL:O	2:S:104:ILE:HG12	2.17	0.44
2:V:290:LEU:HD23	2:V:290:LEU:HA	1.73	0.44
1:A:215:THR:O	1:A:216:ALA:HB3	2.18	0.44
1:B:340:SER:HB3	1:B:396:LEU:HB3	1.99	0.44
1:C:275:ALA:HA	1:C:281:LEU:HD13	2.00	0.44
1:D:324:PRO:HB3	1:D:397:TYR:CE2	2.52	0.44
1:E:324:PRO:HB3	1:E:397:TYR:CE2	2.52	0.44
1:F:324:PRO:HB3	1:F:397:TYR:CD2	2.52	0.44
1:F:324:PRO:HB3	1:F:397:TYR:CE2	2.52	0.44
1:G:324:PRO:HB3	1:G:397:TYR:CD2	2.52	0.44
1:H:309:ASN:HD22	1:H:313:ASN:HD22	1.66	0.44
1:J:5:VAL:HG23	2:V:179:LYS:HZ1	1.82	0.44
1:J:458:HIS:CD2	1:J:459:PRO:HD2	2.52	0.44
1:K:340:SER:HB3	1:K:396:LEU:HB3	1.99	0.44
2:O:132:ILE:N	2:O:133:PRO:HD3	2.33	0.44
2:P:312:ALA:CB	2:P:317:ILE:HG22	2.32	0.44
2:T:128:THR:CG2	2:T:131:GLU:H	2.31	0.44
2:V:132:ILE:N	2:V:133:PRO:HD3	2.33	0.44
1:A:43:PHE:HB3	2:M:370:LYS:NZ	2.22	0.44
1:B:276:LYS:HG2	1:B:277:ASN:ND2	2.33	0.44
1:D:275:ALA:HA	1:D:281:LEU:HD13	2.00	0.44
1:G:180:PHE:HB2	1:L:29:GLN:HB3	2.00	0.44
1:I:275:ALA:HA	1:I:281:LEU:HD13	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:170:GLY:HA2	1:J:172:ARG:HH22	1.81	0.44
1:J:275:ALA:HA	1:J:281:LEU:HD13	2.00	0.44
1:J:324:PRO:HB3	1:J:397:TYR:CE2	2.52	0.44
1:J:340:SER:HB3	1:J:396:LEU:HB3	1.99	0.44
1:K:276:LYS:HG2	1:K:277:ASN:ND2	2.32	0.44
1:L:73:THR:HG21	1:L:88:ARG:HB3	2.00	0.44
1:L:215:THR:O	1:L:216:ALA:HB3	2.18	0.44
2:N:132:ILE:N	2:N:133:PRO:HD3	2.33	0.44
2:O:97:VAL:O	2:O:104:ILE:HG12	2.17	0.44
2:P:139:LEU:HA	2:P:142:LYS:HE3	2.00	0.44
2:U:6:LYS:HD2	2:U:8:VAL:HG23	1.99	0.44
2:U:139:LEU:HA	2:U:142:LYS:HE3	2.00	0.44
2:V:31:THR:CG2	2:V:33:ILE:HD12	2.43	0.44
2:W:132:ILE:N	2:W:133:PRO:HD3	2.33	0.44
2:X:128:THR:CG2	2:X:131:GLU:H	2.31	0.44
1:B:180:PHE:O	1:B:181:PRO:C	2.54	0.43
1:B:324:PRO:HB3	1:B:397:TYR:CD2	2.52	0.43
1:C:324:PRO:HB3	1:C:397:TYR:CE2	2.52	0.43
1:J:7:THR:OG1	2:V:178:ILE:HD13	2.18	0.43
1:J:276:LYS:HG2	1:J:277:ASN:ND2	2.33	0.43
1:K:324:PRO:HB3	1:K:397:TYR:CD2	2.52	0.43
2:P:6:LYS:HD2	2:P:8:VAL:HG23	1.99	0.43
2:Q:312:ALA:HB2	2:Q:317:ILE:CG2	2.45	0.43
2:S:132:ILE:N	2:S:133:PRO:HD3	2.33	0.43
2:S:311:LEU:HD12	2:S:311:LEU:HA	1.89	0.43
2:V:59:ILE:HG21	2:V:59:ILE:HD13	1.70	0.43
2:V:97:VAL:O	2:V:104:ILE:HG12	2.17	0.43
1:A:29:GLN:HB3	1:F:180:PHE:CB	2.49	0.43
1:C:7:THR:OG1	2:O:178:ILE:HD13	2.18	0.43
1:C:276:LYS:HG2	1:C:277:ASN:ND2	2.33	0.43
1:D:137:ASP:HB3	1:D:152:ASP:HB3	2.01	0.43
1:D:328:ALA:HA	1:D:329:PRO:HD3	1.73	0.43
1:F:276:LYS:HG2	1:F:277:ASN:ND2	2.33	0.43
1:G:309:ASN:HD22	1:G:313:ASN:HD22	1.66	0.43
1:I:137:ASP:HB3	1:I:152:ASP:HB3	2.01	0.43
1:I:276:LYS:HG2	1:I:277:ASN:ND2	2.33	0.43
1:J:73:THR:HG21	1:J:88:ARG:HB3	2.00	0.43
1:K:180:PHE:O	1:K:181:PRO:C	2.54	0.43
1:K:275:ALA:HA	1:K:281:LEU:HD13	2.00	0.43
2:M:139:LEU:HA	2:M:142:LYS:HE3	2.00	0.43
2:Q:270:SER:HA	2:Q:271:PRO:HD3	1.74	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:132:ILE:N	2:R:133:PRO:HD3	2.33	0.43
2:S:6:LYS:HD2	2:S:8:VAL:HG23	1.99	0.43
2:V:369:THR:C	2:V:370:LYS:CA	2.75	0.43
1:A:28:GLU:OE1	1:A:88:ARG:NH1	2.45	0.43
1:A:272:MET:HE1	1:A:358:VAL:HG21	1.99	0.43
1:A:328:ALA:HA	1:A:329:PRO:HD3	1.73	0.43
1:B:125:LEU:O	1:B:272:MET:HA	2.19	0.43
1:B:275:ALA:HA	1:B:281:LEU:HD13	2.00	0.43
1:C:17:VAL:HG12	1:C:19:LEU:HD13	2.00	0.43
1:C:170:GLY:HA2	1:C:172:ARG:HH22	1.81	0.43
1:D:236:GLN:OE1	1:D:236:GLN:HA	2.19	0.43
1:D:276:LYS:HG2	1:D:277:ASN:ND2	2.33	0.43
1:E:328:ALA:HA	1:E:329:PRO:HD3	1.73	0.43
1:F:309:ASN:HD22	1:F:313:ASN:HD22	1.66	0.43
1:G:180:PHE:CB	1:L:29:GLN:HB3	2.48	0.43
1:G:276:LYS:HG2	1:G:277:ASN:ND2	2.33	0.43
1:H:7:THR:OG1	2:T:178:ILE:HD13	2.18	0.43
1:I:236:GLN:OE1	1:I:236:GLN:HA	2.19	0.43
1:I:309:ASN:HD22	1:I:313:ASN:HD22	1.66	0.43
1:I:458:HIS:CD2	1:I:459:PRO:HD2	2.52	0.43
1:L:235:ILE:HD13	1:L:235:ILE:HA	1.82	0.43
1:L:236:GLN:OE1	1:L:236:GLN:HA	2.18	0.43
1:L:275:ALA:HA	1:L:281:LEU:HD13	2.00	0.43
2:P:59:ILE:HD11	2:P:280:LEU:HD21	2.00	0.43
2:P:132:ILE:N	2:P:133:PRO:HD3	2.33	0.43
2:U:312:ALA:CB	2:U:317:ILE:HG22	2.32	0.43
2:X:139:LEU:HA	2:X:142:LYS:HE3	2.00	0.43
1:A:275:ALA:HA	1:A:281:LEU:HD13	2.00	0.43
1:C:73:THR:HG21	1:C:88:ARG:HB3	2.00	0.43
1:C:210:HIS:HB3	1:D:31:VAL:HG23	1.99	0.43
1:C:340:SER:HB3	1:C:396:LEU:HB3	1.99	0.43
1:D:468:VAL:CG1	1:J:364:ALA:HA	2.49	0.43
1:F:125:LEU:O	1:F:272:MET:HA	2.19	0.43
1:J:17:VAL:HG12	1:J:19:LEU:HD13	2.00	0.43
2:M:132:ILE:N	2:M:133:PRO:HD3	2.33	0.43
2:N:139:LEU:HA	2:N:142:LYS:HE3	2.00	0.43
2:R:6:LYS:HD2	2:R:8:VAL:HG23	1.99	0.43
2:R:59:ILE:HD11	2:R:280:LEU:HD21	2.00	0.43
2:S:59:ILE:HD11	2:S:280:LEU:HD21	2.00	0.43
2:S:270:SER:HA	2:S:271:PRO:HD3	1.74	0.43
2:U:132:ILE:N	2:U:133:PRO:HD3	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:139:LEU:HA	2:W:142:LYS:HE3	2.00	0.43
2:X:246:VAL:H	2:X:246:VAL:HG23	1.58	0.43
1:D:73:THR:HG21	1:D:88:ARG:HB3	2.00	0.43
1:D:180:PHE:O	1:D:181:PRO:C	2.54	0.43
1:E:137:ASP:HB3	1:E:152:ASP:HB3	2.01	0.43
1:H:125:LEU:O	1:H:272:MET:HA	2.19	0.43
1:I:17:VAL:HG12	1:I:19:LEU:HD13	2.00	0.43
1:I:73:THR:HG21	1:I:88:ARG:HB3	2.00	0.43
1:K:125:LEU:O	1:K:272:MET:HA	2.19	0.43
2:P:239:LYS:HZ3	2:P:241:ASN:HB2	1.82	0.43
2:R:311:LEU:HD12	2:R:311:LEU:HA	1.88	0.43
2:U:59:ILE:HD11	2:U:280:LEU:HD21	2.00	0.43
2:W:312:ALA:HB2	2:W:317:ILE:CG2	2.45	0.43
2:X:132:ILE:N	2:X:133:PRO:HD3	2.33	0.43
1:A:180:PHE:CB	1:B:29:GLN:HB3	2.49	0.43
1:B:73:THR:HG21	1:B:88:ARG:HB3	2.00	0.43
1:B:324:PRO:HB3	1:B:397:TYR:CE2	2.53	0.43
1:B:344:ARG:NH1	1:B:346:PRO:HA	2.34	0.43
1:C:309:ASN:HD22	1:C:313:ASN:HD22	1.66	0.43
1:D:7:THR:OG1	2:P:178:ILE:HD13	2.18	0.43
1:D:309:ASN:HD22	1:D:313:ASN:HD22	1.66	0.43
1:D:458:HIS:CD2	1:D:459:PRO:HD2	2.53	0.43
1:E:7:THR:OG1	2:Q:178:ILE:HD13	2.18	0.43
1:E:125:LEU:O	1:E:272:MET:HA	2.19	0.43
1:J:236:GLN:OE1	1:J:236:GLN:HA	2.19	0.43
1:J:309:ASN:HD22	1:J:313:ASN:HD22	1.66	0.43
1:K:73:THR:HG21	1:K:88:ARG:HB3	2.00	0.43
1:K:215:THR:O	1:K:216:ALA:HB3	2.18	0.43
1:K:324:PRO:HB3	1:K:397:TYR:CE2	2.52	0.43
2:M:290:LEU:HA	2:M:290:LEU:HD23	1.73	0.43
2:N:312:ALA:HB2	2:N:317:ILE:CG2	2.45	0.43
2:Q:6:LYS:HD2	2:Q:8:VAL:HG23	1.99	0.43
2:T:132:ILE:N	2:T:133:PRO:HD3	2.33	0.43
2:V:6:LYS:HD2	2:V:8:VAL:HG23	1.99	0.43
1:A:235:ILE:HD13	1:A:235:ILE:HA	1.82	0.43
1:B:236:GLN:OE1	1:B:236:GLN:HA	2.19	0.43
1:B:454:ARG:O	1:H:320:LYS:HG3	2.17	0.43
1:C:236:GLN:HA	1:C:236:GLN:OE1	2.19	0.43
1:D:17:VAL:HG12	1:D:19:LEU:HD13	2.00	0.43
1:E:170:GLY:HA2	1:E:172:ARG:HH22	1.81	0.43
1:E:231:LYS:HD2	1:E:231:LYS:HA	1.74	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:256:MET:CG	1:L:466:TYR:HA	2.49	0.43
1:G:125:LEU:O	1:G:272:MET:HA	2.19	0.43
1:H:334:TYR:HA	1:H:343:ILE:O	2.19	0.43
1:I:7:THR:OG1	2:U:178:ILE:HD13	2.18	0.43
1:K:236:GLN:HA	1:K:236:GLN:OE1	2.19	0.43
1:K:344:ARG:NH1	1:K:346:PRO:HA	2.34	0.43
1:L:125:LEU:O	1:L:272:MET:HA	2.19	0.43
2:N:6:LYS:HD2	2:N:8:VAL:HG23	1.99	0.43
2:O:6:LYS:HD2	2:O:8:VAL:HG23	1.99	0.43
2:O:312:ALA:CB	2:O:317:ILE:HG22	2.32	0.43
2:S:128:THR:CG2	2:S:131:GLU:H	2.31	0.43
2:U:311:LEU:HD12	2:U:311:LEU:HA	1.89	0.43
2:W:59:ILE:HD11	2:W:280:LEU:HD21	2.00	0.43
1:A:125:LEU:O	1:A:272:MET:HA	2.19	0.43
1:B:215:THR:O	1:B:216:ALA:HB3	2.18	0.43
1:D:320:LYS:HG3	1:J:454:ARG:O	2.18	0.43
1:F:340:SER:HB3	1:F:396:LEU:HB3	1.99	0.43
1:H:137:ASP:HB3	1:H:152:ASP:HB3	2.01	0.43
1:H:170:GLY:HA2	1:H:172:ARG:HH22	1.81	0.43
1:H:231:LYS:HA	1:H:231:LYS:HD2	1.74	0.43
1:H:236:GLN:OE1	1:H:236:GLN:HA	2.19	0.43
1:I:5:VAL:CG2	2:U:179:LYS:HZ1	2.31	0.43
1:I:328:ALA:HA	1:I:329:PRO:HD3	1.73	0.43
1:L:344:ARG:NH1	1:L:346:PRO:HA	2.34	0.43
2:N:59:ILE:HD11	2:N:280:LEU:HD21	2.00	0.43
2:Q:132:ILE:N	2:Q:133:PRO:HD3	2.33	0.43
2:S:59:ILE:HG21	2:S:59:ILE:HD13	1.70	0.43
2:S:139:LEU:HA	2:S:142:LYS:HE3	2.00	0.43
2:T:6:LYS:HD2	2:T:8:VAL:HG23	1.99	0.43
2:W:6:LYS:HD2	2:W:8:VAL:HG23	1.99	0.43
1:A:256:MET:CG	1:G:466:TYR:HA	2.49	0.43
1:C:272:MET:HE1	1:C:358:VAL:HG21	2.01	0.43
1:D:334:TYR:HA	1:D:343:ILE:O	2.19	0.43
1:E:334:TYR:HA	1:E:343:ILE:O	2.19	0.43
1:H:328:ALA:HA	1:H:329:PRO:HD3	1.73	0.43
1:H:340:SER:HB3	1:H:396:LEU:HB3	1.99	0.43
1:I:344:ARG:NH1	1:I:346:PRO:HA	2.33	0.43
1:K:29:GLN:HB3	1:L:180:PHE:HB2	2.01	0.43
2:R:31:THR:CG2	2:R:33:ILE:HD12	2.43	0.43
2:R:128:THR:CG2	2:R:131:GLU:H	2.31	0.43
2:R:139:LEU:HA	2:R:142:LYS:HE3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:PRO:HB3	1:A:268:MET:HE3	2.01	0.43
1:A:344:ARG:NH1	1:A:346:PRO:HA	2.34	0.43
1:B:137:ASP:HB3	1:B:152:ASP:HB3	2.01	0.43
1:C:125:LEU:O	1:C:272:MET:HA	2.19	0.43
1:C:231:LYS:HA	1:C:231:LYS:HD2	1.74	0.43
1:D:125:LEU:O	1:D:272:MET:HA	2.19	0.43
1:D:344:ARG:NH1	1:D:346:PRO:HA	2.34	0.43
1:E:73:THR:HG21	1:E:88:ARG:HB3	2.00	0.43
1:E:236:GLN:OE1	1:E:236:GLN:HA	2.19	0.43
1:E:340:SER:HB3	1:E:396:LEU:HB3	1.99	0.43
1:E:344:ARG:NH1	1:E:346:PRO:HA	2.34	0.43
1:E:384:ASN:N	1:E:384:ASN:ND2	2.60	0.43
1:J:344:ARG:NH1	1:J:346:PRO:HA	2.33	0.43
2:O:59:ILE:HG21	2:O:59:ILE:HD13	1.70	0.43
1:A:17:VAL:HG12	1:A:19:LEU:HD13	2.00	0.42
1:A:137:ASP:HB3	1:A:152:ASP:HB3	2.01	0.42
1:E:215:THR:O	1:E:216:ALA:HB3	2.18	0.42
1:F:231:LYS:HA	1:F:231:LYS:HD2	1.74	0.42
1:G:340:SER:HB3	1:G:396:LEU:HB3	1.99	0.42
1:H:73:THR:HG21	1:H:88:ARG:HB3	2.00	0.42
1:H:215:THR:O	1:H:216:ALA:HB3	2.18	0.42
1:H:384:ASN:N	1:H:384:ASN:ND2	2.60	0.42
1:I:125:LEU:O	1:I:272:MET:HA	2.19	0.42
1:I:180:PHE:O	1:I:181:PRO:C	2.54	0.42
1:I:215:THR:O	1:I:216:ALA:HB3	2.18	0.42
1:I:334:TYR:HA	1:I:343:ILE:O	2.19	0.42
1:K:137:ASP:HB3	1:K:152:ASP:HB3	2.01	0.42
1:L:130:PRO:HB3	1:L:268:MET:HE3	2.01	0.42
1:L:272:MET:HE1	1:L:358:VAL:HG21	2.00	0.42
2:P:270:SER:HA	2:P:271:PRO:HD3	1.74	0.42
2:R:59:ILE:HG21	2:R:59:ILE:HD13	1.70	0.42
2:V:312:ALA:CB	2:V:317:ILE:HG22	2.32	0.42
2:X:59:ILE:HD11	2:X:280:LEU:HD21	2.00	0.42
1:A:30:HIS:HB3	1:F:182:VAL:HG12	2.01	0.42
1:B:5:VAL:HG23	2:N:179:LYS:HZ1	1.84	0.42
1:C:334:TYR:HA	1:C:343:ILE:O	2.19	0.42
1:C:344:ARG:NH1	1:C:346:PRO:HA	2.34	0.42
1:D:215:THR:O	1:D:216:ALA:HB3	2.18	0.42
1:F:17:VAL:HG12	1:F:19:LEU:HD13	2.00	0.42
1:G:334:TYR:HA	1:G:343:ILE:O	2.19	0.42
1:H:17:VAL:HG12	1:H:19:LEU:HD13	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:344:ARG:NH1	1:H:346:PRO:HA	2.34	0.42
1:J:334:TYR:HA	1:J:343:ILE:O	2.19	0.42
1:K:29:GLN:HB3	1:L:180:PHE:CB	2.49	0.42
1:L:137:ASP:HB3	1:L:152:ASP:HB3	2.01	0.42
2:O:369:THR:C	2:O:370:LYS:CA	2.75	0.42
2:P:311:LEU:HD12	2:P:311:LEU:HA	1.88	0.42
2:Q:139:LEU:HA	2:Q:142:LYS:HE3	2.00	0.42
2:X:77:ALA:HB2	2:X:273:LYS:HE2	2.01	0.42
1:B:309:ASN:HD22	1:B:313:ASN:HD22	1.66	0.42
1:E:17:VAL:HG12	1:E:19:LEU:HD13	2.00	0.42
1:E:456:THR:O	1:K:458:HIS:HE1	2.02	0.42
1:H:68:MET:HA	1:H:69:PRO:HD2	1.94	0.42
1:I:43:PHE:HB3	2:U:370:LYS:NZ	2.22	0.42
1:J:125:LEU:O	1:J:272:MET:HA	2.19	0.42
1:J:137:ASP:HB3	1:J:152:ASP:HB3	2.01	0.42
1:L:17:VAL:HG12	1:L:19:LEU:HD13	2.00	0.42
2:M:59:ILE:HD11	2:M:280:LEU:HD21	2.00	0.42
2:T:59:ILE:HD11	2:T:280:LEU:HD21	2.00	0.42
2:T:139:LEU:HA	2:T:142:LYS:HE3	2.00	0.42
1:A:309:ASN:HD22	1:A:313:ASN:HD22	1.66	0.42
1:E:68:MET:HA	1:E:69:PRO:HD2	1.94	0.42
1:G:17:VAL:HG12	1:G:19:LEU:HD13	2.00	0.42
1:G:215:THR:O	1:G:216:ALA:HB3	2.18	0.42
1:G:236:GLN:OE1	1:G:236:GLN:HA	2.19	0.42
1:J:215:THR:O	1:J:216:ALA:HB3	2.18	0.42
1:K:309:ASN:HD22	1:K:313:ASN:HD22	1.66	0.42
1:L:328:ALA:HA	1:L:329:PRO:HD3	1.73	0.42
2:M:77:ALA:HB2	2:M:273:LYS:HE2	2.01	0.42
2:M:246:VAL:H	2:M:246:VAL:HG23	1.58	0.42
2:Q:59:ILE:HD11	2:Q:280:LEU:HD21	2.00	0.42
2:R:42:LYS:HD2	2:R:42:LYS:N	2.35	0.42
2:S:31:THR:CG2	2:S:33:ILE:HD12	2.43	0.42
2:U:77:ALA:HB2	2:U:273:LYS:HE2	2.01	0.42
1:B:5:VAL:CG2	2:N:179:LYS:HZ1	2.32	0.42
1:B:334:TYR:HA	1:B:343:ILE:O	2.19	0.42
1:C:137:ASP:HB3	1:C:152:ASP:HB3	2.01	0.42
1:C:215:THR:O	1:C:216:ALA:HB3	2.18	0.42
1:D:6:LEU:HD12	2:P:370:LYS:O	2.20	0.42
1:E:272:MET:HE1	1:E:358:VAL:CG2	2.50	0.42
1:G:344:ARG:NH1	1:G:346:PRO:HA	2.34	0.42
1:L:309:ASN:HD22	1:L:313:ASN:HD22	1.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:64:HIS:CE1	2:N:330:MET:O	2.62	0.42
2:O:139:LEU:HA	2:O:142:LYS:HE3	2.00	0.42
2:R:163:ALA:HA	2:R:256:LYS:HD3	2.02	0.42
2:S:42:LYS:N	2:S:42:LYS:HD2	2.35	0.42
2:S:163:ALA:HA	2:S:256:LYS:HD3	2.02	0.42
2:T:163:ALA:HA	2:T:256:LYS:HD3	2.02	0.42
2:U:270:SER:HA	2:U:271:PRO:HD3	1.74	0.42
1:A:364:ALA:HA	1:G:468:VAL:HG13	2.01	0.42
1:B:466:TYR:HA	1:H:256:MET:HG3	2.01	0.42
1:C:332:LEU:HD12	1:C:332:LEU:HA	1.90	0.42
1:E:138:ILE:HG23	1:E:138:ILE:O	2.20	0.42
1:F:236:GLN:OE1	1:F:236:GLN:HA	2.19	0.42
1:F:334:TYR:HA	1:F:343:ILE:O	2.19	0.42
1:I:6:LEU:HD12	2:U:370:LYS:O	2.20	0.42
1:I:332:LEU:HB2	1:I:408:PRO:CB	2.50	0.42
1:L:272:MET:HE1	1:L:358:VAL:CG2	2.50	0.42
2:M:42:LYS:N	2:M:42:LYS:HD2	2.35	0.42
2:N:77:ALA:HB2	2:N:273:LYS:HE2	2.01	0.42
2:P:77:ALA:HB2	2:P:273:LYS:HE2	2.01	0.42
2:Q:163:ALA:HA	2:Q:256:LYS:HD3	2.02	0.42
2:V:139:LEU:HA	2:V:142:LYS:HE3	2.00	0.42
2:W:64:HIS:CE1	2:W:330:MET:O	2.62	0.42
1:F:332:LEU:HB2	1:F:408:PRO:CB	2.50	0.42
1:F:396:LEU:HB2	1:F:397:TYR:H	1.36	0.42
1:H:138:ILE:HG23	1:H:138:ILE:O	2.20	0.42
1:I:138:ILE:O	1:I:138:ILE:HG23	2.20	0.42
1:K:334:TYR:HA	1:K:343:ILE:O	2.19	0.42
1:L:396:LEU:H	1:L:396:LEU:HG	1.46	0.42
2:M:31:THR:CG2	2:M:33:ILE:N	2.60	0.42
2:W:77:ALA:HB2	2:W:273:LYS:HE2	2.01	0.42
2:X:31:THR:CG2	2:X:33:ILE:N	2.60	0.42
2:X:42:LYS:N	2:X:42:LYS:HD2	2.35	0.42
2:X:290:LEU:HA	2:X:290:LEU:HD23	1.73	0.42
1:A:6:LEU:HD12	2:M:370:LYS:O	2.19	0.42
1:A:334:TYR:HA	1:A:343:ILE:O	2.19	0.42
1:D:43:PHE:HB3	2:P:370:LYS:NZ	2.22	0.42
1:D:332:LEU:HB2	1:D:408:PRO:CB	2.50	0.42
1:F:180:PHE:O	1:F:181:PRO:C	2.54	0.42
1:F:344:ARG:NH1	1:F:346:PRO:HA	2.34	0.42
1:H:29:GLN:HB3	1:I:180:PHE:CB	2.49	0.42
1:K:328:ALA:HA	1:K:329:PRO:HD3	1.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:82:ASP:C	2:N:84:ALA:N	2.73	0.42
2:O:125:PRO:HA	2:O:126:PRO:HD3	1.82	0.42
1:A:387:HIS:HA	1:A:388:PRO:HD2	1.73	0.42
1:B:320:LYS:HG2	1:H:455:MET:O	2.19	0.42
1:D:138:ILE:O	1:D:138:ILE:HG23	2.20	0.42
1:E:272:MET:HE1	1:E:358:VAL:HG21	2.02	0.42
1:G:5:VAL:CG2	2:S:179:LYS:HZ1	2.33	0.42
1:G:180:PHE:O	1:G:181:PRO:C	2.54	0.42
1:J:231:LYS:HA	1:J:231:LYS:HD2	1.74	0.42
1:L:334:TYR:HA	1:L:343:ILE:O	2.19	0.42
2:M:82:ASP:C	2:M:84:ALA:N	2.73	0.42
2:P:31:THR:CG2	2:P:33:ILE:HD12	2.43	0.42
2:U:312:ALA:HB2	2:U:317:ILE:CG2	2.45	0.42
2:U:312:ALA:HB2	2:U:317:ILE:HG21	2.00	0.42
2:V:125:PRO:HA	2:V:126:PRO:HD3	1.82	0.42
2:W:82:ASP:C	2:W:84:ALA:N	2.73	0.42
2:X:82:ASP:C	2:X:84:ALA:N	2.73	0.42
1:A:236:GLN:OE1	1:A:236:GLN:HA	2.19	0.42
1:A:332:LEU:HB2	1:A:408:PRO:CB	2.50	0.42
1:A:456:THR:O	1:G:458:HIS:HE1	2.02	0.42
1:C:281:LEU:HB3	1:C:293:GLN:OE1	2.20	0.42
1:D:281:LEU:HB3	1:D:293:GLN:OE1	2.20	0.42
1:F:433:VAL:HG12	1:F:434:PHE:CD2	2.55	0.42
1:J:281:LEU:HB3	1:J:293:GLN:OE1	2.20	0.42
1:J:332:LEU:HB2	1:J:408:PRO:CB	2.50	0.42
1:K:31:VAL:HG23	1:L:210:HIS:HB3	2.01	0.42
1:L:387:HIS:HA	1:L:388:PRO:HD2	1.73	0.42
2:M:330:MET:HA	2:M:331:PRO:HD3	1.79	0.42
2:P:312:ALA:HB2	2:P:317:ILE:CG2	2.44	0.42
2:P:312:ALA:HB2	2:P:317:ILE:HG21	2.00	0.42
2:Q:77:ALA:HB2	2:Q:273:LYS:HE2	2.01	0.42
2:R:136:ASP:CG	2:R:203:HIS:HD2	2.24	0.42
2:S:136:ASP:CG	2:S:203:HIS:HD2	2.24	0.42
2:U:31:THR:CG2	2:U:33:ILE:HD12	2.43	0.42
2:V:312:ALA:HB2	2:V:317:ILE:CG2	2.45	0.42
1:A:91:ILE:HB	1:A:103:ASP:HB2	2.02	0.41
1:C:332:LEU:HB2	1:C:408:PRO:CB	2.50	0.41
1:D:230:LYS:O	1:D:234:GLU:HG3	2.20	0.41
1:E:6:LEU:HD12	2:Q:370:LYS:O	2.20	0.41
1:F:272:MET:HE1	1:F:358:VAL:CG2	2.50	0.41
1:G:230:LYS:O	1:G:234:GLU:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:272:MET:HE1	1:G:358:VAL:CG2	2.49	0.41
1:I:230:LYS:O	1:I:234:GLU:HG3	2.20	0.41
1:I:281:LEU:HB3	1:I:293:GLN:OE1	2.20	0.41
1:J:332:LEU:HD12	1:J:332:LEU:HA	1.90	0.41
1:L:91:ILE:HB	1:L:103:ASP:HB2	2.02	0.41
2:N:59:ILE:HG21	2:N:59:ILE:HD13	1.70	0.41
2:O:27:PHE:O	2:O:31:THR:CB	2.66	0.41
2:P:31:THR:CG2	2:P:33:ILE:N	2.60	0.41
2:T:42:LYS:N	2:T:42:LYS:HD2	2.35	0.41
2:V:246:VAL:H	2:V:246:VAL:HG23	1.58	0.41
2:V:312:ALA:HB2	2:V:317:ILE:HG21	2.00	0.41
1:C:433:VAL:HG12	1:C:434:PHE:CD2	2.55	0.41
1:F:91:ILE:HB	1:F:103:ASP:HB2	2.02	0.41
1:F:230:LYS:O	1:F:234:GLU:HG3	2.21	0.41
1:F:296:TYR:HB3	1:F:382:ILE:HA	2.03	0.41
1:G:137:ASP:HB3	1:G:152:ASP:HB3	2.01	0.41
1:G:433:VAL:HG12	1:G:434:PHE:CD2	2.56	0.41
1:H:6:LEU:HD12	2:T:370:LYS:O	2.20	0.41
1:H:433:VAL:HG12	1:H:434:PHE:CD2	2.55	0.41
1:I:4:HIS:HD2	2:U:178:ILE:CD1	2.27	0.41
1:K:91:ILE:HB	1:K:103:ASP:HB2	2.02	0.41
1:L:296:TYR:HB3	1:L:382:ILE:HA	2.02	0.41
1:L:332:LEU:HB2	1:L:408:PRO:CB	2.50	0.41
2:N:121:LEU:HD23	2:N:121:LEU:HA	1.86	0.41
2:O:312:ALA:HB2	2:O:317:ILE:CG2	2.45	0.41
2:Q:42:LYS:N	2:Q:42:LYS:HD2	2.35	0.41
2:S:10:TRP:CD1	2:S:57:PRO:HB3	2.55	0.41
2:T:77:ALA:HB2	2:T:273:LYS:HE2	2.01	0.41
2:U:163:ALA:HA	2:U:256:LYS:HD3	2.02	0.41
1:B:91:ILE:HB	1:B:103:ASP:HB2	2.03	0.41
1:C:5:VAL:CG2	2:O:179:LYS:HZ1	2.34	0.41
1:D:364:ALA:HA	1:J:468:VAL:HG13	2.03	0.41
1:D:454:ARG:O	1:J:320:LYS:HG3	2.20	0.41
1:F:466:TYR:HA	1:L:256:MET:HG3	2.01	0.41
1:G:91:ILE:HB	1:G:103:ASP:HB2	2.02	0.41
1:G:396:LEU:H	1:G:396:LEU:HG	1.46	0.41
1:I:34:PRO:HG2	1:J:206:VAL:O	2.20	0.41
1:J:433:VAL:HG12	1:J:434:PHE:CD2	2.56	0.41
1:K:5:VAL:CG2	2:W:179:LYS:HZ1	2.33	0.41
1:K:5:VAL:HG23	2:W:179:LYS:HZ1	1.85	0.41
2:P:72:GLN:O	2:P:72:GLN:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:72:GLN:O	2:Q:72:GLN:HG2	2.20	0.41
2:R:10:TRP:CD1	2:R:57:PRO:HB3	2.56	0.41
2:R:31:THR:CG2	2:R:33:ILE:N	2.60	0.41
2:T:72:GLN:O	2:T:72:GLN:HG2	2.20	0.41
2:W:121:LEU:HD23	2:W:121:LEU:HA	1.86	0.41
1:A:296:TYR:HB3	1:A:382:ILE:HA	2.03	0.41
1:B:206:VAL:O	1:C:34:PRO:HG2	2.20	0.41
1:B:230:LYS:O	1:B:234:GLU:HG3	2.20	0.41
1:B:328:ALA:HA	1:B:329:PRO:HD3	1.73	0.41
1:B:332:LEU:HB2	1:B:408:PRO:CB	2.50	0.41
1:D:4:HIS:HD2	2:P:178:ILE:CD1	2.27	0.41
1:D:256:MET:HG3	1:J:466:TYR:HA	2.02	0.41
1:E:433:VAL:HG12	1:E:434:PHE:CD2	2.55	0.41
2:O:163:ALA:HA	2:O:256:LYS:HD3	2.02	0.41
2:O:312:ALA:HB2	2:O:317:ILE:HG21	2.00	0.41
2:P:125:PRO:HA	2:P:126:PRO:HD3	1.82	0.41
2:Q:10:TRP:CD1	2:Q:57:PRO:HB3	2.56	0.41
2:R:27:PHE:O	2:R:31:THR:CB	2.66	0.41
2:T:10:TRP:CD1	2:T:57:PRO:HB3	2.56	0.41
2:U:72:GLN:O	2:U:72:GLN:HG2	2.20	0.41
2:V:27:PHE:O	2:V:31:THR:CB	2.66	0.41
1:A:281:LEU:HB3	1:A:293:GLN:OE1	2.20	0.41
1:A:433:VAL:HG12	1:A:434:PHE:CD2	2.55	0.41
1:B:6:LEU:HD12	2:N:370:LYS:O	2.20	0.41
1:E:458:HIS:HE1	1:K:456:THR:O	2.03	0.41
1:G:6:LEU:HD12	2:S:370:LYS:O	2.20	0.41
1:G:272:MET:HE1	1:G:358:VAL:HG21	2.01	0.41
1:G:296:TYR:HB3	1:G:382:ILE:HA	2.03	0.41
1:I:384:ASN:N	1:I:384:ASN:ND2	2.60	0.41
1:I:433:VAL:HG12	1:I:434:PHE:CD2	2.56	0.41
1:K:230:LYS:O	1:K:234:GLU:HG3	2.20	0.41
1:K:332:LEU:HB2	1:K:408:PRO:CB	2.50	0.41
1:L:6:LEU:HD12	2:X:370:LYS:O	2.20	0.41
2:N:42:LYS:N	2:N:42:LYS:HD2	2.35	0.41
2:N:163:ALA:HA	2:N:256:LYS:HD3	2.02	0.41
2:P:163:ALA:HA	2:P:256:LYS:HD3	2.02	0.41
2:W:163:ALA:HA	2:W:256:LYS:HD3	2.02	0.41
2:W:312:ALA:HB2	2:W:317:ILE:HG21	2.00	0.41
2:X:31:THR:CG2	2:X:33:ILE:CD1	2.99	0.41
2:X:312:ALA:HB2	2:X:317:ILE:HG21	2.00	0.41
1:A:105:ARG:HH21	1:A:105:ARG:HD3	1.76	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:SER:OG	1:A:362:ASP:OD2	2.27	0.41
1:B:281:LEU:HB3	1:B:293:GLN:OE1	2.20	0.41
1:C:91:ILE:HB	1:C:103:ASP:HB2	2.02	0.41
1:D:403:GLU:C	1:D:405:LYS:N	2.74	0.41
1:D:433:VAL:HG12	1:D:434:PHE:CD2	2.56	0.41
1:E:230:LYS:O	1:E:234:GLU:HG3	2.21	0.41
1:F:6:LEU:HD12	2:R:370:LYS:O	2.20	0.41
1:G:5:VAL:HG23	2:S:179:LYS:HZ1	1.86	0.41
1:H:332:LEU:HB2	1:H:408:PRO:CB	2.49	0.41
1:H:396:LEU:H	1:H:396:LEU:HG	1.46	0.41
1:K:6:LEU:HD12	2:W:370:LYS:O	2.20	0.41
1:L:433:VAL:HG12	1:L:434:PHE:CD2	2.55	0.41
2:M:163:ALA:HA	2:M:256:LYS:HD3	2.02	0.41
2:N:312:ALA:HB2	2:N:317:ILE:HG21	2.00	0.41
2:O:31:THR:CG2	2:O:33:ILE:CD1	2.99	0.41
2:O:77:ALA:HB2	2:O:273:LYS:HE2	2.01	0.41
2:U:42:LYS:HD2	2:U:42:LYS:N	2.35	0.41
2:U:125:PRO:HA	2:U:126:PRO:HD3	1.82	0.41
2:V:31:THR:CG2	2:V:33:ILE:CD1	2.99	0.41
2:V:163:ALA:HA	2:V:256:LYS:HD3	2.02	0.41
1:A:364:ALA:HA	1:G:468:VAL:CG1	2.50	0.41
1:E:206:VAL:O	1:F:34:PRO:HG2	2.20	0.41
1:E:281:LEU:HB3	1:E:293:GLN:OE1	2.20	0.41
1:F:281:LEU:HB3	1:F:293:GLN:OE1	2.20	0.41
1:G:231:LYS:HA	1:G:231:LYS:HD2	1.74	0.41
1:H:281:LEU:HB3	1:H:293:GLN:OE1	2.20	0.41
1:I:387:HIS:HA	1:I:388:PRO:HD2	1.73	0.41
1:I:403:GLU:C	1:I:405:LYS:N	2.74	0.41
1:J:6:LEU:HD12	2:V:370:LYS:O	2.20	0.41
1:L:281:LEU:HB3	1:L:293:GLN:OE1	2.20	0.41
2:M:31:THR:CG2	2:M:33:ILE:CD1	2.99	0.41
2:O:72:GLN:O	2:O:72:GLN:HG2	2.20	0.41
2:R:82:ASP:C	2:R:84:ALA:N	2.73	0.41
2:S:82:ASP:C	2:S:84:ALA:N	2.73	0.41
2:T:82:ASP:C	2:T:84:ALA:N	2.73	0.41
2:U:31:THR:CG2	2:U:33:ILE:N	2.60	0.41
2:U:106:TYR:HA	2:U:107:PRO:HD3	1.86	0.41
2:W:42:LYS:N	2:W:42:LYS:HD2	2.35	0.41
2:X:163:ALA:HA	2:X:256:LYS:HD3	2.02	0.41
1:A:230:LYS:O	1:A:234:GLU:HG3	2.20	0.41
1:A:458:HIS:HE1	1:G:456:THR:O	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:384:ASN:N	1:D:384:ASN:ND2	2.60	0.41
1:E:296:TYR:HB3	1:E:382:ILE:HA	2.03	0.41
1:E:332:LEU:HB2	1:E:408:PRO:CB	2.50	0.41
1:F:387:HIS:HA	1:F:388:PRO:HD2	1.73	0.41
1:F:403:GLU:C	1:F:405:LYS:N	2.74	0.41
1:H:180:PHE:O	1:H:181:PRO:C	2.54	0.41
1:H:230:LYS:O	1:H:234:GLU:HG3	2.21	0.41
1:H:403:GLU:C	1:H:405:LYS:N	2.74	0.41
1:I:68:MET:HA	1:I:69:PRO:HD2	1.94	0.41
1:I:114:TYR:O	1:I:118:THR:HG23	2.21	0.41
1:K:139:ARG:HD3	1:L:163:LYS:HG2	2.01	0.41
1:K:281:LEU:HB3	1:K:293:GLN:OE1	2.20	0.41
2:M:10:TRP:CD1	2:M:57:PRO:HB3	2.55	0.41
2:N:330:MET:HA	2:N:331:PRO:HD3	1.79	0.41
2:P:121:LEU:HA	2:P:121:LEU:HD23	1.86	0.41
2:R:77:ALA:HB2	2:R:273:LYS:HE2	2.01	0.41
1:A:403:GLU:C	1:A:405:LYS:N	2.74	0.41
1:C:6:LEU:HD12	2:O:370:LYS:O	2.20	0.41
1:C:230:LYS:O	1:C:234:GLU:HG3	2.20	0.41
1:D:114:TYR:O	1:D:118:THR:HG23	2.21	0.41
1:D:192:ARG:NH2	1:D:219:ASN:ND2	2.63	0.41
1:D:231:LYS:HA	1:D:231:LYS:HD2	1.74	0.41
1:D:387:HIS:HA	1:D:388:PRO:HD2	1.73	0.41
1:E:364:ALA:HA	1:K:468:VAL:HG13	2.03	0.41
1:F:137:ASP:HB3	1:F:152:ASP:HB3	2.01	0.41
1:F:272:MET:HE1	1:F:358:VAL:HG21	2.01	0.41
1:G:105:ARG:HH21	1:G:105:ARG:HD3	1.76	0.41
1:G:138:ILE:O	1:G:138:ILE:HG23	2.20	0.41
1:G:403:GLU:C	1:G:405:LYS:N	2.74	0.41
1:H:272:MET:HE1	1:H:358:VAL:HG21	2.01	0.41
1:H:296:TYR:HB3	1:H:382:ILE:HA	2.03	0.41
1:I:192:ARG:NH2	1:I:219:ASN:ND2	2.63	0.41
1:J:91:ILE:HB	1:J:103:ASP:HB2	2.03	0.41
1:J:230:LYS:O	1:J:234:GLU:HG3	2.21	0.41
1:K:231:LYS:HD2	1:K:231:LYS:HA	1.74	0.41
1:L:105:ARG:HH21	1:L:105:ARG:HD3	1.76	0.41
1:L:230:LYS:O	1:L:234:GLU:HG3	2.21	0.41
2:M:312:ALA:HB2	2:M:317:ILE:HG21	2.00	0.41
2:O:42:LYS:N	2:O:42:LYS:HD2	2.35	0.41
2:O:246:VAL:H	2:O:246:VAL:HG23	1.58	0.41
2:P:42:LYS:N	2:P:42:LYS:HD2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:366:THR:O	2:P:370:LYS:HG3	2.21	0.41
2:S:27:PHE:O	2:S:31:THR:CB	2.66	0.41
2:S:77:ALA:HB2	2:S:273:LYS:HE2	2.01	0.41
2:T:31:THR:CG2	2:T:33:ILE:N	2.60	0.41
2:U:366:THR:O	2:U:370:LYS:HG3	2.21	0.41
2:V:72:GLN:O	2:V:72:GLN:HG2	2.20	0.41
2:V:77:ALA:HB2	2:V:273:LYS:HE2	2.01	0.41
2:V:82:ASP:C	2:V:84:ALA:N	2.73	0.41
2:V:366:THR:O	2:V:370:LYS:HG3	2.21	0.41
2:X:72:GLN:O	2:X:72:GLN:HG2	2.20	0.41
2:X:330:MET:HA	2:X:331:PRO:HD3	1.79	0.41
1:A:396:LEU:H	1:A:396:LEU:HG	1.46	0.41
1:B:231:LYS:HD2	1:B:231:LYS:HA	1.74	0.41
1:B:296:TYR:HB3	1:B:382:ILE:HA	2.03	0.41
1:B:433:VAL:HG12	1:B:434:PHE:CD2	2.55	0.41
1:D:182:VAL:HG12	1:E:30:HIS:HB3	2.03	0.41
1:E:125:LEU:HD12	1:E:125:LEU:HA	1.91	0.41
1:G:281:LEU:HB3	1:G:293:GLN:OE1	2.20	0.41
1:H:91:ILE:HB	1:H:103:ASP:HB2	2.02	0.41
1:I:294:ALA:O	1:I:298:ILE:HG13	2.21	0.41
2:O:82:ASP:C	2:O:84:ALA:N	2.73	0.41
2:O:366:THR:O	2:O:370:LYS:HG3	2.21	0.41
2:Q:82:ASP:C	2:Q:84:ALA:N	2.73	0.41
2:V:270:SER:HA	2:V:271:PRO:HD3	1.74	0.41
2:W:31:THR:CG2	2:W:33:ILE:CD1	2.99	0.41
2:W:330:MET:HA	2:W:331:PRO:HD3	1.79	0.41
2:X:10:TRP:CD1	2:X:57:PRO:HB3	2.56	0.41
1:D:294:ALA:O	1:D:298:ILE:HG13	2.22	0.40
1:F:138:ILE:HG23	1:F:138:ILE:O	2.20	0.40
1:F:294:ALA:O	1:F:298:ILE:HG13	2.21	0.40
1:F:320:LYS:HG3	1:L:454:ARG:O	2.21	0.40
1:F:466:TYR:CE1	1:L:254:THR:HB	2.56	0.40
1:H:34:PRO:HG2	1:I:206:VAL:O	2.22	0.40
1:H:61:ASN:O	1:I:337:ARG:CB	2.50	0.40
1:K:296:TYR:HB3	1:K:382:ILE:HA	2.03	0.40
1:K:433:VAL:HG12	1:K:434:PHE:CD2	2.55	0.40
1:L:403:GLU:C	1:L:405:LYS:N	2.74	0.40
2:N:31:THR:CG2	2:N:33:ILE:CD1	2.99	0.40
2:O:330:MET:HA	2:O:331:PRO:HD3	1.79	0.40
2:O:361:LEU:HD23	2:O:361:LEU:HA	1.96	0.40
2:P:10:TRP:CD1	2:P:57:PRO:HB3	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:10:TRP:CD1	2:U:57:PRO:HB3	2.56	0.40
2:U:121:LEU:HA	2:U:121:LEU:HD23	1.86	0.40
2:V:42:LYS:N	2:V:42:LYS:HD2	2.35	0.40
2:X:106:TYR:HA	2:X:107:PRO:HD3	1.87	0.40
1:B:403:GLU:C	1:B:405:LYS:N	2.74	0.40
1:C:138:ILE:O	1:C:138:ILE:HG23	2.20	0.40
1:D:91:ILE:HB	1:D:103:ASP:HB2	2.02	0.40
1:E:114:TYR:O	1:E:118:THR:HG23	2.21	0.40
1:E:180:PHE:O	1:E:181:PRO:C	2.54	0.40
1:E:313:ASN:HB3	1:E:318:SER:HB3	2.03	0.40
1:F:105:ARG:HH21	1:F:105:ARG:HD3	1.76	0.40
1:G:294:ALA:O	1:G:298:ILE:HG13	2.22	0.40
1:H:313:ASN:HB3	1:H:318:SER:HB3	2.03	0.40
1:H:396:LEU:HB2	1:H:397:TYR:H	1.36	0.40
1:I:91:ILE:HB	1:I:103:ASP:HB2	2.02	0.40
2:R:72:GLN:O	2:R:72:GLN:HG2	2.20	0.40
2:T:366:THR:O	2:T:370:LYS:HG3	2.21	0.40
2:W:47:PHE:HB3	2:W:48:PRO:HD3	2.03	0.40
1:A:5:VAL:H	2:M:179:LYS:NZ	2.04	0.40
1:B:254:THR:HB	1:H:466:TYR:CE1	2.56	0.40
1:B:320:LYS:HG2	1:H:455:MET:C	2.42	0.40
1:C:114:TYR:O	1:C:118:THR:HG23	2.21	0.40
1:D:68:MET:HA	1:D:69:PRO:HD2	1.94	0.40
1:D:364:ALA:HA	1:J:468:VAL:CG1	2.51	0.40
1:E:91:ILE:HB	1:E:103:ASP:HB2	2.03	0.40
1:G:396:LEU:HB2	1:G:397:TYR:H	1.36	0.40
1:J:294:ALA:O	1:J:298:ILE:HG13	2.21	0.40
1:L:138:ILE:O	1:L:138:ILE:HG23	2.20	0.40
2:M:72:GLN:O	2:M:72:GLN:HG2	2.20	0.40
2:N:47:PHE:HB3	2:N:48:PRO:HD3	2.03	0.40
2:N:258:PHE:CG	2:N:330:MET:HG2	2.57	0.40
2:O:59:ILE:HD11	2:O:280:LEU:HD21	2.00	0.40
2:O:218:ASN:HD21	2:O:235:ILE:HG12	1.87	0.40
2:P:47:PHE:HB3	2:P:48:PRO:HD3	2.03	0.40
2:P:106:TYR:HA	2:P:107:PRO:HD3	1.87	0.40
2:P:348:ILE:HD13	2:P:348:ILE:HG21	1.93	0.40
2:Q:366:THR:O	2:Q:370:LYS:HG3	2.21	0.40
2:S:72:GLN:O	2:S:72:GLN:HG2	2.20	0.40
2:U:47:PHE:HB3	2:U:48:PRO:HD3	2.03	0.40
2:W:218:ASN:HD21	2:W:235:ILE:HG12	1.87	0.40
1:A:138:ILE:O	1:A:138:ILE:HG23	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:138:ILE:O	1:B:138:ILE:HG23	2.20	0.40
1:D:296:TYR:HB3	1:D:382:ILE:HA	2.03	0.40
1:F:313:ASN:HB3	1:F:318:SER:HB3	2.03	0.40
1:F:455:MET:HG2	1:L:323:VAL:HG11	2.03	0.40
1:G:43:PHE:HB3	2:S:370:LYS:NZ	2.22	0.40
1:H:114:TYR:O	1:H:118:THR:HG23	2.21	0.40
1:J:138:ILE:O	1:J:138:ILE:HG23	2.20	0.40
1:J:235:ILE:HD13	1:J:235:ILE:HA	1.82	0.40
1:K:403:GLU:C	1:K:405:LYS:N	2.74	0.40
2:N:218:ASN:HD21	2:N:235:ILE:HG12	1.87	0.40
2:Q:31:THR:CG2	2:Q:33:ILE:N	2.60	0.40
2:Q:31:THR:CG2	2:Q:33:ILE:CD1	2.99	0.40
2:R:31:THR:CG2	2:R:33:ILE:CD1	2.99	0.40
2:S:330:MET:HA	2:S:331:PRO:HD3	1.79	0.40
2:V:311:LEU:HD12	2:V:311:LEU:HA	1.88	0.40
1:A:294:ALA:O	1:A:298:ILE:HG13	2.21	0.40
1:B:180:PHE:CB	1:C:29:GLN:HB3	2.52	0.40
1:B:364:ALA:HA	1:H:468:VAL:CG1	2.51	0.40
1:C:125:LEU:HD12	1:C:125:LEU:HA	1.91	0.40
1:C:294:ALA:O	1:C:298:ILE:HG13	2.21	0.40
1:E:396:LEU:H	1:E:396:LEU:HG	1.46	0.40
1:F:396:LEU:H	1:F:396:LEU:HG	1.46	0.40
1:I:296:TYR:HB3	1:I:382:ILE:HA	2.03	0.40
1:J:114:TYR:O	1:J:118:THR:HG23	2.21	0.40
1:K:138:ILE:O	1:K:138:ILE:HG23	2.20	0.40
1:L:303:LYS:HD2	1:L:386:ILE:HD13	2.04	0.40
2:N:10:TRP:CD1	2:N:57:PRO:HB3	2.55	0.40
2:P:31:THR:CG2	2:P:33:ILE:CD1	2.99	0.40
2:Q:361:LEU:HD23	2:Q:361:LEU:HA	1.96	0.40
2:S:31:THR:CG2	2:S:33:ILE:CD1	2.99	0.40
2:S:366:THR:O	2:S:370:LYS:HG3	2.21	0.40
2:T:31:THR:CG2	2:T:33:ILE:CD1	2.99	0.40
2:U:31:THR:CG2	2:U:33:ILE:CD1	2.99	0.40
2:V:59:ILE:HD11	2:V:280:LEU:HD21	2.00	0.40
2:V:218:ASN:HD21	2:V:235:ILE:HG12	1.87	0.40
2:W:10:TRP:CD1	2:W:57:PRO:HB3	2.55	0.40
2:W:258:PHE:CG	2:W:330:MET:HG2	2.57	0.40

There are no symmetry-related clashes.

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 PDB entries followed by that with respect to all EM entries.

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	464/466 (100%)	424 (91%)	32 (7%)	8 (2%)	9	42
1	B	464/466 (100%)	424 (91%)	32 (7%)	8 (2%)	9	42
1	C	464/466 (100%)	424 (91%)	32 (7%)	8 (2%)	9	42
1	D	464/466 (100%)	424 (91%)	32 (7%)	8 (2%)	9	42
1	E	464/466 (100%)	424 (91%)	32 (7%)	8 (2%)	9	42
1	F	464/466 (100%)	424 (91%)	32 (7%)	8 (2%)	9	42
1	G	464/466 (100%)	425 (92%)	31 (7%)	8 (2%)	9	42
1	H	464/466 (100%)	424 (91%)	32 (7%)	8 (2%)	9	42
1	I	464/466 (100%)	424 (91%)	32 (7%)	8 (2%)	9	42
1	J	464/466 (100%)	424 (91%)	32 (7%)	8 (2%)	9	42
1	K	464/466 (100%)	424 (91%)	32 (7%)	8 (2%)	9	42
1	L	464/466 (100%)	425 (92%)	31 (7%)	8 (2%)	9	42
2	M	368/370 (100%)	349 (95%)	16 (4%)	3 (1%)	19	60
2	N	368/370 (100%)	349 (95%)	16 (4%)	3 (1%)	19	60
2	O	368/370 (100%)	349 (95%)	16 (4%)	3 (1%)	19	60
2	P	368/370 (100%)	349 (95%)	16 (4%)	3 (1%)	19	60
2	Q	368/370 (100%)	349 (95%)	16 (4%)	3 (1%)	19	60
2	R	368/370 (100%)	349 (95%)	16 (4%)	3 (1%)	19	60
2	S	368/370 (100%)	349 (95%)	16 (4%)	3 (1%)	19	60
2	T	368/370 (100%)	349 (95%)	16 (4%)	3 (1%)	19	60
2	U	368/370 (100%)	349 (95%)	16 (4%)	3 (1%)	19	60
2	V	368/370 (100%)	349 (95%)	16 (4%)	3 (1%)	19	60
2	W	368/370 (100%)	349 (95%)	16 (4%)	3 (1%)	19	60
2	X	368/370 (100%)	349 (95%)	16 (4%)	3 (1%)	19	60
All	All	9984/10032 (100%)	9278 (93%)	574 (6%)	132 (1%)	16	48

All (132) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	180	PHE
1	A	400	PRO
1	A	401	PRO
1	B	180	PHE
1	B	400	PRO
1	B	401	PRO
1	C	180	PHE
1	C	400	PRO
1	C	401	PRO
1	D	180	PHE
1	D	400	PRO
1	D	401	PRO
1	E	180	PHE
1	E	400	PRO
1	E	401	PRO
1	F	180	PHE
1	F	400	PRO
1	F	401	PRO
1	G	180	PHE
1	G	400	PRO
1	G	401	PRO
1	H	180	PHE
1	H	400	PRO
1	H	401	PRO
1	I	180	PHE
1	I	400	PRO
1	I	401	PRO
1	J	180	PHE
1	J	400	PRO
1	J	401	PRO
1	K	180	PHE
1	K	400	PRO
1	K	401	PRO
1	L	180	PHE
1	L	400	PRO
1	L	401	PRO
2	M	4	GLU
2	N	4	GLU
2	O	4	GLU
2	P	4	GLU
2	Q	4	GLU
2	R	4	GLU

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Mol	Chain	Res	Type
2	S	4	GLU
2	T	4	GLU
2	U	4	GLU
2	V	4	GLU
2	W	4	GLU
2	X	4	GLU
1	A	170	GLY
1	B	170	GLY
1	C	170	GLY
1	D	170	GLY
1	E	170	GLY
1	F	170	GLY
1	G	170	GLY
1	H	170	GLY
1	I	170	GLY
1	J	170	GLY
1	K	170	GLY
1	L	170	GLY
2	M	83	LYS
2	N	83	LYS
2	O	83	LYS
2	P	83	LYS
2	Q	83	LYS
2	R	83	LYS
2	S	83	LYS
2	T	83	LYS
2	U	83	LYS
2	V	83	LYS
2	W	83	LYS
2	X	83	LYS
1	A	324	PRO
1	A	338	ASN
1	A	394	LYS
1	B	324	PRO
1	B	338	ASN
1	B	394	LYS
1	C	324	PRO
1	C	338	ASN
1	C	394	LYS
1	D	324	PRO
1	D	338	ASN
1	D	394	LYS

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Mol	Chain	Res	Type
1	E	324	PRO
1	E	338	ASN
1	E	394	LYS
1	F	324	PRO
1	F	338	ASN
1	F	394	LYS
1	G	324	PRO
1	G	338	ASN
1	G	394	LYS
1	H	324	PRO
1	H	338	ASN
1	H	394	LYS
1	I	324	PRO
1	I	338	ASN
1	I	394	LYS
1	J	324	PRO
1	J	338	ASN
1	J	394	LYS
1	K	324	PRO
1	K	338	ASN
1	K	394	LYS
1	L	324	PRO
1	L	338	ASN
1	L	394	LYS
1	A	396	LEU
1	B	396	LEU
1	C	396	LEU
1	D	396	LEU
1	E	396	LEU
1	F	396	LEU
1	G	396	LEU
1	H	396	LEU
1	I	396	LEU
1	J	396	LEU
1	K	396	LEU
1	L	396	LEU
2	M	2	ILE
2	N	2	ILE
2	O	2	ILE
2	P	2	ILE
2	Q	2	ILE
2	R	2	ILE

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Mol	Chain	Res	Type
2	S	2	ILE
2	T	2	ILE
2	U	2	ILE
2	V	2	ILE
2	W	2	ILE
2	X	2	ILE

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 PDB entries followed by that with respect to all EM entries.

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	383/383 (100%)	348 (91%)	35 (9%)	9	30
1	B	383/383 (100%)	348 (91%)	35 (9%)	9	30
1	C	383/383 (100%)	348 (91%)	35 (9%)	9	30
1	D	383/383 (100%)	348 (91%)	35 (9%)	9	30
1	E	383/383 (100%)	347 (91%)	36 (9%)	8	28
1	F	383/383 (100%)	348 (91%)	35 (9%)	9	30
1	G	383/383 (100%)	347 (91%)	36 (9%)	8	28
1	H	383/383 (100%)	347 (91%)	36 (9%)	8	28
1	I	383/383 (100%)	348 (91%)	35 (9%)	9	30
1	J	383/383 (100%)	347 (91%)	36 (9%)	8	28
1	K	383/383 (100%)	348 (91%)	35 (9%)	9	30
1	L	383/383 (100%)	348 (91%)	35 (9%)	9	30
2	M	292/297 (98%)	256 (88%)	36 (12%)	4	20
2	N	292/297 (98%)	256 (88%)	36 (12%)	4	20
2	O	292/297 (98%)	256 (88%)	36 (12%)	4	20
2	P	292/297 (98%)	256 (88%)	36 (12%)	4	20
2	Q	292/297 (98%)	256 (88%)	36 (12%)	4	20
2	R	292/297 (98%)	256 (88%)	36 (12%)	4	20
2	S	292/297 (98%)	256 (88%)	36 (12%)	4	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	T	292/297 (98%)	256 (88%)	36 (12%)	4	20
2	U	292/297 (98%)	256 (88%)	36 (12%)	4	20
2	V	292/297 (98%)	256 (88%)	36 (12%)	4	20
2	W	292/297 (98%)	256 (88%)	36 (12%)	4	20
2	X	292/297 (98%)	256 (88%)	36 (12%)	4	20
All	All	8100/8160 (99%)	7244 (89%)	856 (11%)	10	24

All (856) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	19	LEU
1	A	60	ILE
1	A	62	GLU
1	A	63	SER
1	A	64	ASP
1	A	65	MET
1	A	84	THR
1	A	88	ARG
1	A	96	THR
1	A	98	GLN
1	A	115	LEU
1	A	124	VAL
1	A	125	LEU
1	A	165	GLU
1	A	179	TYR
1	A	209	HIS
1	A	230	LYS
1	A	248	ARG
1	A	264	ASN
1	A	320	LYS
1	A	326	TYR
1	A	332	LEU
1	A	337	ARG
1	A	374	LEU
1	A	375	LEU
1	A	384	ASN
1	A	392	MET
1	A	396	LEU
1	A	397	TYR

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Mol	Chain	Res	Type
1	A	399	LEU
1	A	428	LEU
1	A	447	ARG
1	A	464	LEU
1	A	468	VAL
1	B	6	LEU
1	B	19	LEU
1	B	60	ILE
1	B	62	GLU
1	B	63	SER
1	B	64	ASP
1	B	65	MET
1	B	84	THR
1	B	88	ARG
1	B	96	THR
1	B	98	GLN
1	B	115	LEU
1	B	124	VAL
1	B	125	LEU
1	B	165	GLU
1	B	179	TYR
1	B	209	HIS
1	B	230	LYS
1	B	248	ARG
1	B	264	ASN
1	B	320	LYS
1	B	326	TYR
1	B	332	LEU
1	B	337	ARG
1	B	374	LEU
1	B	375	LEU
1	B	384	ASN
1	B	392	MET
1	B	396	LEU
1	B	397	TYR
1	B	399	LEU
1	B	428	LEU
1	B	447	ARG
1	B	464	LEU
1	B	468	VAL
1	C	6	LEU
1	C	19	LEU

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Mol	Chain	Res	Type
1	C	60	ILE
1	C	62	GLU
1	C	63	SER
1	C	64	ASP
1	C	65	MET
1	C	84	THR
1	C	88	ARG
1	C	96	THR
1	C	98	GLN
1	C	115	LEU
1	C	124	VAL
1	C	125	LEU
1	C	165	GLU
1	C	179	TYR
1	C	209	HIS
1	C	230	LYS
1	C	248	ARG
1	C	264	ASN
1	C	320	LYS
1	C	326	TYR
1	C	332	LEU
1	C	337	ARG
1	C	374	LEU
1	C	375	LEU
1	C	384	ASN
1	C	392	MET
1	C	396	LEU
1	C	397	TYR
1	C	399	LEU
1	C	428	LEU
1	C	447	ARG
1	C	464	LEU
1	C	468	VAL
1	D	6	LEU
1	D	19	LEU
1	D	60	ILE
1	D	62	GLU
1	D	63	SER
1	D	64	ASP
1	D	65	MET
1	D	84	THR
1	D	88	ARG

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Mol	Chain	Res	Type
1	D	96	THR
1	D	98	GLN
1	D	115	LEU
1	D	124	VAL
1	D	125	LEU
1	D	165	GLU
1	D	179	TYR
1	D	209	HIS
1	D	230	LYS
1	D	248	ARG
1	D	264	ASN
1	D	320	LYS
1	D	326	TYR
1	D	332	LEU
1	D	337	ARG
1	D	374	LEU
1	D	375	LEU
1	D	384	ASN
1	D	392	MET
1	D	396	LEU
1	D	397	TYR
1	D	399	LEU
1	D	428	LEU
1	D	447	ARG
1	D	464	LEU
1	D	468	VAL
1	E	6	LEU
1	E	19	LEU
1	E	60	ILE
1	E	62	GLU
1	E	63	SER
1	E	64	ASP
1	E	65	MET
1	E	84	THR
1	E	88	ARG
1	E	96	THR
1	E	98	GLN
1	E	115	LEU
1	E	124	VAL
1	E	125	LEU
1	E	165	GLU
1	E	179	TYR

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Mol	Chain	Res	Type
1	E	209	HIS
1	E	230	LYS
1	E	248	ARG
1	E	264	ASN
1	E	320	LYS
1	E	324	PRO
1	E	326	TYR
1	E	332	LEU
1	E	337	ARG
1	E	374	LEU
1	E	375	LEU
1	E	384	ASN
1	E	392	MET
1	E	396	LEU
1	E	397	TYR
1	E	399	LEU
1	E	428	LEU
1	E	447	ARG
1	E	464	LEU
1	E	468	VAL
1	F	6	LEU
1	F	19	LEU
1	F	60	ILE
1	F	62	GLU
1	F	63	SER
1	F	64	ASP
1	F	65	MET
1	F	84	THR
1	F	88	ARG
1	F	96	THR
1	F	98	GLN
1	F	115	LEU
1	F	124	VAL
1	F	125	LEU
1	F	165	GLU
1	F	179	TYR
1	F	209	HIS
1	F	230	LYS
1	F	248	ARG
1	F	264	ASN
1	F	320	LYS
1	F	326	TYR

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Mol	Chain	Res	Type
1	F	332	LEU
1	F	337	ARG
1	F	374	LEU
1	F	375	LEU
1	F	384	ASN
1	F	392	MET
1	F	396	LEU
1	F	397	TYR
1	F	399	LEU
1	F	428	LEU
1	F	447	ARG
1	F	464	LEU
1	F	468	VAL
1	G	6	LEU
1	G	19	LEU
1	G	60	ILE
1	G	62	GLU
1	G	63	SER
1	G	64	ASP
1	G	65	MET
1	G	84	THR
1	G	88	ARG
1	G	96	THR
1	G	98	GLN
1	G	115	LEU
1	G	124	VAL
1	G	125	LEU
1	G	165	GLU
1	G	179	TYR
1	G	209	HIS
1	G	230	LYS
1	G	248	ARG
1	G	264	ASN
1	G	320	LYS
1	G	324	PRO
1	G	326	TYR
1	G	332	LEU
1	G	337	ARG
1	G	374	LEU
1	G	375	LEU
1	G	384	ASN
1	G	392	MET

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Mol	Chain	Res	Type
1	G	396	LEU
1	G	397	TYR
1	G	399	LEU
1	G	428	LEU
1	G	447	ARG
1	G	464	LEU
1	G	468	VAL
1	H	6	LEU
1	H	19	LEU
1	H	60	ILE
1	H	62	GLU
1	H	63	SER
1	H	64	ASP
1	H	65	MET
1	H	84	THR
1	H	88	ARG
1	H	96	THR
1	H	98	GLN
1	H	115	LEU
1	H	124	VAL
1	H	125	LEU
1	H	165	GLU
1	H	179	TYR
1	H	209	HIS
1	H	230	LYS
1	H	248	ARG
1	H	264	ASN
1	H	320	LYS
1	H	324	PRO
1	H	326	TYR
1	H	332	LEU
1	H	337	ARG
1	H	374	LEU
1	H	375	LEU
1	H	384	ASN
1	H	392	MET
1	H	396	LEU
1	H	397	TYR
1	H	399	LEU
1	H	428	LEU
1	H	447	ARG
1	H	464	LEU

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Mol	Chain	Res	Type
1	H	468	VAL
1	I	6	LEU
1	I	19	LEU
1	I	60	ILE
1	I	62	GLU
1	I	63	SER
1	I	64	ASP
1	I	65	MET
1	I	84	THR
1	I	88	ARG
1	I	96	THR
1	I	98	GLN
1	I	115	LEU
1	I	124	VAL
1	I	125	LEU
1	I	165	GLU
1	I	179	TYR
1	I	209	HIS
1	I	230	LYS
1	I	248	ARG
1	I	264	ASN
1	I	320	LYS
1	I	326	TYR
1	I	332	LEU
1	I	337	ARG
1	I	374	LEU
1	I	375	LEU
1	I	384	ASN
1	I	392	MET
1	I	396	LEU
1	I	397	TYR
1	I	399	LEU
1	I	428	LEU
1	I	447	ARG
1	I	464	LEU
1	I	468	VAL
1	J	6	LEU
1	J	19	LEU
1	J	60	ILE
1	J	62	GLU
1	J	63	SER
1	J	64	ASP

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Mol	Chain	Res	Type
1	J	65	MET
1	J	84	THR
1	J	88	ARG
1	J	96	THR
1	J	98	GLN
1	J	115	LEU
1	J	124	VAL
1	J	125	LEU
1	J	165	GLU
1	J	179	TYR
1	J	209	HIS
1	J	230	LYS
1	J	248	ARG
1	J	264	ASN
1	J	320	LYS
1	J	324	PRO
1	J	326	TYR
1	J	332	LEU
1	J	337	ARG
1	J	374	LEU
1	J	375	LEU
1	J	384	ASN
1	J	392	MET
1	J	396	LEU
1	J	397	TYR
1	J	399	LEU
1	J	428	LEU
1	J	447	ARG
1	J	464	LEU
1	J	468	VAL
1	K	6	LEU
1	K	19	LEU
1	K	60	ILE
1	K	62	GLU
1	K	63	SER
1	K	64	ASP
1	K	65	MET
1	K	84	THR
1	K	88	ARG
1	K	96	THR
1	K	98	GLN
1	K	115	LEU

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Mol	Chain	Res	Type
1	K	124	VAL
1	K	125	LEU
1	K	165	GLU
1	K	179	TYR
1	K	209	HIS
1	K	230	LYS
1	K	248	ARG
1	K	264	ASN
1	K	320	LYS
1	K	326	TYR
1	K	332	LEU
1	K	337	ARG
1	K	374	LEU
1	K	375	LEU
1	K	384	ASN
1	K	392	MET
1	K	396	LEU
1	K	397	TYR
1	K	399	LEU
1	K	428	LEU
1	K	447	ARG
1	K	464	LEU
1	K	468	VAL
1	L	6	LEU
1	L	19	LEU
1	L	60	ILE
1	L	62	GLU
1	L	63	SER
1	L	64	ASP
1	L	65	MET
1	L	84	THR
1	L	88	ARG
1	L	96	THR
1	L	98	GLN
1	L	115	LEU
1	L	124	VAL
1	L	125	LEU
1	L	165	GLU
1	L	179	TYR
1	L	209	HIS
1	L	230	LYS
1	L	248	ARG

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Mol	Chain	Res	Type
1	L	264	ASN
1	L	320	LYS
1	L	326	TYR
1	L	332	LEU
1	L	337	ARG
1	L	374	LEU
1	L	375	LEU
1	L	384	ASN
1	L	392	MET
1	L	396	LEU
1	L	397	TYR
1	L	399	LEU
1	L	428	LEU
1	L	447	ARG
1	L	464	LEU
1	L	468	VAL
2	M	6	LYS
2	M	26	LYS
2	M	30	ASP
2	M	31	THR
2	M	34	LYS
2	M	42	LYS
2	M	45	GLU
2	M	46	LYS
2	M	59	ILE
2	M	83	LYS
2	M	87	ASP
2	M	89	LEU
2	M	98	ARG
2	M	115	LEU
2	M	127	LYS
2	M	128	THR
2	M	140	LYS
2	M	142	LYS
2	M	148	MET
2	M	160	LEU
2	M	173	ASN
2	M	175	LYS
2	M	204	MET
2	M	238	SER
2	M	239	LYS
2	M	258	PHE

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Mol	Chain	Res	Type
2	M	274	GLU
2	M	291	GLU
2	M	295	LYS
2	M	311	LEU
2	M	313	LYS
2	M	328	GLU
2	M	329	ILE
2	M	337	SER
2	M	341	TYR
2	M	354	ARG
2	N	6	LYS
2	N	26	LYS
2	N	30	ASP
2	N	31	THR
2	N	34	LYS
2	N	42	LYS
2	N	45	GLU
2	N	46	LYS
2	N	59	ILE
2	N	83	LYS
2	N	87	ASP
2	N	89	LEU
2	N	98	ARG
2	N	115	LEU
2	N	127	LYS
2	N	128	THR
2	N	140	LYS
2	N	142	LYS
2	N	148	MET
2	N	160	LEU
2	N	173	ASN
2	N	175	LYS
2	N	204	MET
2	N	238	SER
2	N	239	LYS
2	N	258	PHE
2	N	274	GLU
2	N	291	GLU
2	N	295	LYS
2	N	311	LEU
2	N	313	LYS
2	N	328	GLU

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Mol	Chain	Res	Type
2	N	329	ILE
2	N	337	SER
2	N	341	TYR
2	N	354	ARG
2	O	6	LYS
2	O	26	LYS
2	O	30	ASP
2	O	31	THR
2	O	34	LYS
2	O	42	LYS
2	O	45	GLU
2	O	46	LYS
2	O	59	ILE
2	O	83	LYS
2	O	87	ASP
2	O	89	LEU
2	O	98	ARG
2	O	115	LEU
2	O	127	LYS
2	O	128	THR
2	O	140	LYS
2	O	142	LYS
2	O	148	MET
2	O	160	LEU
2	O	173	ASN
2	O	175	LYS
2	O	204	MET
2	O	238	SER
2	O	239	LYS
2	O	258	PHE
2	O	274	GLU
2	O	291	GLU
2	O	295	LYS
2	O	311	LEU
2	O	313	LYS
2	O	328	GLU
2	O	329	ILE
2	O	337	SER
2	O	341	TYR
2	O	354	ARG
2	P	6	LYS
2	P	26	LYS

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Mol	Chain	Res	Type
2	P	30	ASP
2	P	31	THR
2	P	34	LYS
2	P	42	LYS
2	P	45	GLU
2	P	46	LYS
2	P	59	ILE
2	P	83	LYS
2	P	87	ASP
2	P	89	LEU
2	P	98	ARG
2	P	115	LEU
2	P	127	LYS
2	P	128	THR
2	P	140	LYS
2	P	142	LYS
2	P	148	MET
2	P	160	LEU
2	P	173	ASN
2	P	175	LYS
2	P	204	MET
2	P	238	SER
2	P	239	LYS
2	P	258	PHE
2	P	274	GLU
2	P	291	GLU
2	P	295	LYS
2	P	311	LEU
2	P	313	LYS
2	P	328	GLU
2	P	329	ILE
2	P	337	SER
2	P	341	TYR
2	P	354	ARG
2	Q	6	LYS
2	Q	26	LYS
2	Q	30	ASP
2	Q	31	THR
2	Q	34	LYS
2	Q	42	LYS
2	Q	45	GLU
2	Q	46	LYS

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Mol	Chain	Res	Type
2	Q	59	ILE
2	Q	83	LYS
2	Q	87	ASP
2	Q	89	LEU
2	Q	98	ARG
2	Q	115	LEU
2	Q	127	LYS
2	Q	128	THR
2	Q	140	LYS
2	Q	142	LYS
2	Q	148	MET
2	Q	160	LEU
2	Q	173	ASN
2	Q	175	LYS
2	Q	204	MET
2	Q	238	SER
2	Q	239	LYS
2	Q	258	PHE
2	Q	274	GLU
2	Q	291	GLU
2	Q	295	LYS
2	Q	311	LEU
2	Q	313	LYS
2	Q	328	GLU
2	Q	329	ILE
2	Q	337	SER
2	Q	341	TYR
2	Q	354	ARG
2	R	6	LYS
2	R	26	LYS
2	R	30	ASP
2	R	31	THR
2	R	34	LYS
2	R	42	LYS
2	R	45	GLU
2	R	46	LYS
2	R	59	ILE
2	R	83	LYS
2	R	87	ASP
2	R	89	LEU
2	R	98	ARG
2	R	115	LEU

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Mol	Chain	Res	Type
2	R	127	LYS
2	R	128	THR
2	R	140	LYS
2	R	142	LYS
2	R	148	MET
2	R	160	LEU
2	R	173	ASN
2	R	175	LYS
2	R	204	MET
2	R	238	SER
2	R	239	LYS
2	R	258	PHE
2	R	274	GLU
2	R	291	GLU
2	R	295	LYS
2	R	311	LEU
2	R	313	LYS
2	R	328	GLU
2	R	329	ILE
2	R	337	SER
2	R	341	TYR
2	R	354	ARG
2	S	6	LYS
2	S	26	LYS
2	S	30	ASP
2	S	31	THR
2	S	34	LYS
2	S	42	LYS
2	S	45	GLU
2	S	46	LYS
2	S	59	ILE
2	S	83	LYS
2	S	87	ASP
2	S	89	LEU
2	S	98	ARG
2	S	115	LEU
2	S	127	LYS
2	S	128	THR
2	S	140	LYS
2	S	142	LYS
2	S	148	MET
2	S	160	LEU

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Mol	Chain	Res	Type
2	S	173	ASN
2	S	175	LYS
2	S	204	MET
2	S	238	SER
2	S	239	LYS
2	S	258	PHE
2	S	274	GLU
2	S	291	GLU
2	S	295	LYS
2	S	311	LEU
2	S	313	LYS
2	S	328	GLU
2	S	329	ILE
2	S	337	SER
2	S	341	TYR
2	S	354	ARG
2	T	6	LYS
2	T	26	LYS
2	T	30	ASP
2	T	31	THR
2	T	34	LYS
2	T	42	LYS
2	T	45	GLU
2	T	46	LYS
2	T	59	ILE
2	T	83	LYS
2	T	87	ASP
2	T	89	LEU
2	T	98	ARG
2	T	115	LEU
2	T	127	LYS
2	T	128	THR
2	T	140	LYS
2	T	142	LYS
2	T	148	MET
2	T	160	LEU
2	T	173	ASN
2	T	175	LYS
2	T	204	MET
2	T	238	SER
2	T	239	LYS
2	T	258	PHE

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Mol	Chain	Res	Type
2	T	274	GLU
2	T	291	GLU
2	T	295	LYS
2	T	311	LEU
2	T	313	LYS
2	T	328	GLU
2	T	329	ILE
2	T	337	SER
2	T	341	TYR
2	T	354	ARG
2	U	6	LYS
2	U	26	LYS
2	U	30	ASP
2	U	31	THR
2	U	34	LYS
2	U	42	LYS
2	U	45	GLU
2	U	46	LYS
2	U	59	ILE
2	U	83	LYS
2	U	87	ASP
2	U	89	LEU
2	U	98	ARG
2	U	115	LEU
2	U	127	LYS
2	U	128	THR
2	U	140	LYS
2	U	142	LYS
2	U	148	MET
2	U	160	LEU
2	U	173	ASN
2	U	175	LYS
2	U	204	MET
2	U	238	SER
2	U	239	LYS
2	U	258	PHE
2	U	274	GLU
2	U	291	GLU
2	U	295	LYS
2	U	311	LEU
2	U	313	LYS
2	U	328	GLU

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Mol	Chain	Res	Type
2	U	329	ILE
2	U	337	SER
2	U	341	TYR
2	U	354	ARG
2	V	6	LYS
2	V	26	LYS
2	V	30	ASP
2	V	31	THR
2	V	34	LYS
2	V	42	LYS
2	V	45	GLU
2	V	46	LYS
2	V	59	ILE
2	V	83	LYS
2	V	87	ASP
2	V	89	LEU
2	V	98	ARG
2	V	115	LEU
2	V	127	LYS
2	V	128	THR
2	V	140	LYS
2	V	142	LYS
2	V	148	MET
2	V	160	LEU
2	V	173	ASN
2	V	175	LYS
2	V	204	MET
2	V	238	SER
2	V	239	LYS
2	V	258	PHE
2	V	274	GLU
2	V	291	GLU
2	V	295	LYS
2	V	311	LEU
2	V	313	LYS
2	V	328	GLU
2	V	329	ILE
2	V	337	SER
2	V	341	TYR
2	V	354	ARG
2	W	6	LYS
2	W	26	LYS

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Mol	Chain	Res	Type
2	W	30	ASP
2	W	31	THR
2	W	34	LYS
2	W	42	LYS
2	W	45	GLU
2	W	46	LYS
2	W	59	ILE
2	W	83	LYS
2	W	87	ASP
2	W	89	LEU
2	W	98	ARG
2	W	115	LEU
2	W	127	LYS
2	W	128	THR
2	W	140	LYS
2	W	142	LYS
2	W	148	MET
2	W	160	LEU
2	W	173	ASN
2	W	175	LYS
2	W	204	MET
2	W	238	SER
2	W	239	LYS
2	W	258	PHE
2	W	274	GLU
2	W	291	GLU
2	W	295	LYS
2	W	311	LEU
2	W	313	LYS
2	W	328	GLU
2	W	329	ILE
2	W	337	SER
2	W	341	TYR
2	W	354	ARG
2	X	6	LYS
2	X	26	LYS
2	X	30	ASP
2	X	31	THR
2	X	34	LYS
2	X	42	LYS
2	X	45	GLU
2	X	46	LYS

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Mol	Chain	Res	Type
2	X	59	ILE
2	X	83	LYS
2	X	87	ASP
2	X	89	LEU
2	X	98	ARG
2	X	115	LEU
2	X	127	LYS
2	X	128	THR
2	X	140	LYS
2	X	142	LYS
2	X	148	MET
2	X	160	LEU
2	X	173	ASN
2	X	175	LYS
2	X	204	MET
2	X	238	SER
2	X	239	LYS
2	X	258	PHE
2	X	274	GLU
2	X	291	GLU
2	X	295	LYS
2	X	311	LEU
2	X	313	LYS
2	X	328	GLU
2	X	329	ILE
2	X	337	SER
2	X	341	TYR
2	X	354	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (186) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	HIS
1	A	189	GLN
1	A	211	HIS
1	A	218	GLN
1	A	219	ASN
1	A	244	ASN
1	A	264	ASN
1	A	277	ASN
1	A	313	ASN
1	A	384	ASN

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Mol	Chain	Res	Type
1	A	458	HIS
1	B	30	HIS
1	B	189	GLN
1	B	211	HIS
1	B	218	GLN
1	B	219	ASN
1	B	244	ASN
1	B	264	ASN
1	B	277	ASN
1	B	313	ASN
1	B	384	ASN
1	B	458	HIS
1	C	30	HIS
1	C	189	GLN
1	C	211	HIS
1	C	218	GLN
1	C	219	ASN
1	C	244	ASN
1	C	264	ASN
1	C	277	ASN
1	C	313	ASN
1	C	384	ASN
1	C	458	HIS
1	D	30	HIS
1	D	189	GLN
1	D	211	HIS
1	D	218	GLN
1	D	219	ASN
1	D	244	ASN
1	D	264	ASN
1	D	277	ASN
1	D	313	ASN
1	D	384	ASN
1	D	458	HIS
1	E	30	HIS
1	E	189	GLN
1	E	211	HIS
1	E	218	GLN
1	E	219	ASN
1	E	244	ASN
1	E	264	ASN
1	E	277	ASN

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Mol	Chain	Res	Type
1	E	313	ASN
1	E	384	ASN
1	E	458	HIS
1	F	30	HIS
1	F	189	GLN
1	F	211	HIS
1	F	218	GLN
1	F	219	ASN
1	F	244	ASN
1	F	264	ASN
1	F	277	ASN
1	F	313	ASN
1	F	384	ASN
1	F	458	HIS
1	G	30	HIS
1	G	189	GLN
1	G	211	HIS
1	G	218	GLN
1	G	219	ASN
1	G	244	ASN
1	G	264	ASN
1	G	277	ASN
1	G	313	ASN
1	G	384	ASN
1	G	458	HIS
1	H	30	HIS
1	H	189	GLN
1	H	211	HIS
1	H	218	GLN
1	H	219	ASN
1	H	244	ASN
1	H	264	ASN
1	H	277	ASN
1	H	313	ASN
1	H	384	ASN
1	H	458	HIS
1	I	30	HIS
1	I	189	GLN
1	I	211	HIS
1	I	218	GLN
1	I	219	ASN
1	I	244	ASN

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Mol	Chain	Res	Type
1	I	264	ASN
1	I	277	ASN
1	I	313	ASN
1	I	384	ASN
1	I	458	HIS
1	J	30	HIS
1	J	189	GLN
1	J	211	HIS
1	J	218	GLN
1	J	219	ASN
1	J	244	ASN
1	J	264	ASN
1	J	277	ASN
1	J	313	ASN
1	J	384	ASN
1	J	458	HIS
1	K	30	HIS
1	K	189	GLN
1	K	211	HIS
1	K	218	GLN
1	K	219	ASN
1	K	244	ASN
1	K	264	ASN
1	K	277	ASN
1	K	313	ASN
1	K	384	ASN
1	K	458	HIS
1	L	30	HIS
1	L	189	GLN
1	L	211	HIS
1	L	218	GLN
1	L	219	ASN
1	L	244	ASN
1	L	264	ASN
1	L	277	ASN
1	L	313	ASN
1	L	384	ASN
1	L	458	HIS
2	M	49	GLN
2	M	64	HIS
2	M	203	HIS
2	M	218	ASN

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Mol	Chain	Res	Type
2	N	49	GLN
2	N	64	HIS
2	N	203	HIS
2	N	218	ASN
2	N	335	GLN
2	O	49	GLN
2	O	64	HIS
2	O	203	HIS
2	O	218	ASN
2	P	49	GLN
2	P	64	HIS
2	P	203	HIS
2	P	218	ASN
2	P	335	GLN
2	Q	49	GLN
2	Q	64	HIS
2	Q	203	HIS
2	Q	218	ASN
2	R	49	GLN
2	R	64	HIS
2	R	203	HIS
2	R	218	ASN
2	S	49	GLN
2	S	64	HIS
2	S	203	HIS
2	S	218	ASN
2	T	18	ASN
2	T	49	GLN
2	T	64	HIS
2	T	203	HIS
2	T	218	ASN
2	T	335	GLN
2	U	49	GLN
2	U	64	HIS
2	U	203	HIS
2	U	218	ASN
2	U	335	GLN
2	V	49	GLN
2	V	64	HIS
2	V	203	HIS
2	V	218	ASN
2	W	49	GLN

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Mol	Chain	Res	Type
2	W	64	HIS
2	W	203	HIS
2	W	218	ASN
2	W	335	GLN
2	X	49	GLN
2	X	64	HIS
2	X	203	HIS
2	X	218	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)

24 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	GLC	Y	1	3	12,12,12	1.20	1 (8%)	17,17,17	2.25	5 (29%)
3	GLC	Y	2	3	11,11,12	1.58	1 (9%)	15,15,17	1.47	1 (6%)
3	GLC	Z	1	3	12,12,12	1.20	1 (8%)	17,17,17	2.26	5 (29%)
3	GLC	Z	2	3	11,11,12	1.57	1 (9%)	15,15,17	1.46	1 (6%)
3	GLC	a	1	3	12,12,12	1.20	1 (8%)	17,17,17	2.26	5 (29%)
3	GLC	a	2	3	11,11,12	1.58	1 (9%)	15,15,17	1.47	1 (6%)
3	GLC	b	1	3	12,12,12	1.19	1 (8%)	17,17,17	2.26	5 (29%)
3	GLC	b	2	3	11,11,12	1.58	1 (9%)	15,15,17	1.48	1 (6%)
3	GLC	c	1	3	12,12,12	1.19	1 (8%)	17,17,17	2.26	5 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	GLC	c	2	3	11,11,12	1.58	1 (9%)	15,15,17	1.48	1 (6%)
3	GLC	d	1	3	12,12,12	1.20	1 (8%)	17,17,17	2.26	5 (29%)
3	GLC	d	2	3	11,11,12	1.58	1 (9%)	15,15,17	1.48	1 (6%)
3	GLC	e	1	3	12,12,12	1.19	1 (8%)	17,17,17	2.26	5 (29%)
3	GLC	e	2	3	11,11,12	1.57	1 (9%)	15,15,17	1.47	1 (6%)
3	GLC	f	1	3	12,12,12	1.19	1 (8%)	17,17,17	2.26	5 (29%)
3	GLC	f	2	3	11,11,12	1.58	1 (9%)	15,15,17	1.47	1 (6%)
3	GLC	g	1	3	12,12,12	1.19	1 (8%)	17,17,17	2.25	5 (29%)
3	GLC	g	2	3	11,11,12	1.59	1 (9%)	15,15,17	1.48	1 (6%)
3	GLC	h	1	3	12,12,12	1.19	1 (8%)	17,17,17	2.26	5 (29%)
3	GLC	h	2	3	11,11,12	1.58	1 (9%)	15,15,17	1.47	1 (6%)
3	GLC	i	1	3	12,12,12	1.18	1 (8%)	17,17,17	2.25	5 (29%)
3	GLC	i	2	3	11,11,12	1.58	1 (9%)	15,15,17	1.47	1 (6%)
3	GLC	j	1	3	12,12,12	1.20	1 (8%)	17,17,17	2.26	5 (29%)
3	GLC	j	2	3	11,11,12	1.59	1 (9%)	15,15,17	1.47	1 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GLC	Y	1	3	-	0/2/22/22	0/1/1/1
3	GLC	Y	2	3	-	0/2/19/22	0/1/1/1
3	GLC	Z	1	3	-	0/2/22/22	0/1/1/1
3	GLC	Z	2	3	-	0/2/19/22	0/1/1/1
3	GLC	a	1	3	-	0/2/22/22	0/1/1/1
3	GLC	a	2	3	-	0/2/19/22	0/1/1/1
3	GLC	b	1	3	-	0/2/22/22	0/1/1/1
3	GLC	b	2	3	-	0/2/19/22	0/1/1/1
3	GLC	c	1	3	-	0/2/22/22	0/1/1/1
3	GLC	c	2	3	-	0/2/19/22	0/1/1/1
3	GLC	d	1	3	-	0/2/22/22	0/1/1/1
3	GLC	d	2	3	-	0/2/19/22	0/1/1/1
3	GLC	e	1	3	-	0/2/22/22	0/1/1/1
3	GLC	e	2	3	-	0/2/19/22	0/1/1/1
3	GLC	f	1	3	-	0/2/22/22	0/1/1/1
3	GLC	f	2	3	-	0/2/19/22	0/1/1/1
3	GLC	g	1	3	-	0/2/22/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GLC	g	2	3	-	0/2/19/22	0/1/1/1
3	GLC	h	1	3	-	0/2/22/22	0/1/1/1
3	GLC	h	2	3	-	0/2/19/22	0/1/1/1
3	GLC	i	1	3	-	0/2/22/22	0/1/1/1
3	GLC	i	2	3	-	0/2/19/22	0/1/1/1
3	GLC	j	1	3	-	0/2/22/22	0/1/1/1
3	GLC	j	2	3	-	0/2/19/22	0/1/1/1

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	g	2	GLC	O5-C1	-4.19	1.37	1.43
3	j	2	GLC	O5-C1	-4.19	1.37	1.43
3	c	2	GLC	O5-C1	-4.17	1.37	1.43
3	f	2	GLC	O5-C1	-4.16	1.37	1.43
3	h	2	GLC	O5-C1	-4.16	1.37	1.43
3	i	2	GLC	O5-C1	-4.16	1.37	1.43
3	Y	2	GLC	O5-C1	-4.16	1.37	1.43
3	b	2	GLC	O5-C1	-4.15	1.37	1.43
3	a	2	GLC	O5-C1	-4.13	1.37	1.43
3	Z	2	GLC	O5-C1	-4.13	1.37	1.43
3	d	2	GLC	O5-C1	-4.13	1.37	1.43
3	e	2	GLC	O5-C1	-4.11	1.37	1.43
3	d	1	GLC	O5-C1	-2.26	1.37	1.42
3	a	1	GLC	O5-C1	-2.23	1.37	1.42
3	Z	1	GLC	O5-C1	-2.23	1.37	1.42
3	j	1	GLC	O5-C1	-2.22	1.37	1.42
3	c	1	GLC	O5-C1	-2.22	1.37	1.42
3	Y	1	GLC	O5-C1	-2.22	1.37	1.42
3	g	1	GLC	O5-C1	-2.22	1.37	1.42
3	h	1	GLC	O5-C1	-2.21	1.37	1.42
3	f	1	GLC	O5-C1	-2.21	1.37	1.42
3	e	1	GLC	O5-C1	-2.20	1.37	1.42
3	b	1	GLC	O5-C1	-2.20	1.37	1.42
3	i	1	GLC	O5-C1	-2.17	1.37	1.42

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	a	1	GLC	C1-O5-C5	6.22	125.41	113.66
3	Z	1	GLC	C1-O5-C5	6.21	125.38	113.66
3	d	1	GLC	C1-O5-C5	6.21	125.38	113.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	j	1	GLC	C1-O5-C5	6.21	125.37	113.66
3	c	1	GLC	C1-O5-C5	6.20	125.36	113.66
3	h	1	GLC	C1-O5-C5	6.20	125.36	113.66
3	f	1	GLC	C1-O5-C5	6.20	125.35	113.66
3	g	1	GLC	C1-O5-C5	6.19	125.35	113.66
3	Y	1	GLC	C1-O5-C5	6.19	125.34	113.66
3	e	1	GLC	C1-O5-C5	6.19	125.33	113.66
3	b	1	GLC	C1-O5-C5	6.18	125.32	113.66
3	i	1	GLC	C1-O5-C5	6.16	125.29	113.66
3	j	2	GLC	C1-O5-C5	4.18	117.85	112.19
3	b	2	GLC	C1-O5-C5	4.17	117.84	112.19
3	d	2	GLC	C1-O5-C5	4.16	117.83	112.19
3	c	2	GLC	C1-O5-C5	4.16	117.83	112.19
3	g	2	GLC	C1-O5-C5	4.16	117.83	112.19
3	h	2	GLC	C1-O5-C5	4.16	117.83	112.19
3	e	2	GLC	C1-O5-C5	4.16	117.82	112.19
3	f	2	GLC	C1-O5-C5	4.16	117.82	112.19
3	a	2	GLC	C1-O5-C5	4.15	117.82	112.19
3	Y	2	GLC	C1-O5-C5	4.15	117.81	112.19
3	i	2	GLC	C1-O5-C5	4.15	117.81	112.19
3	Z	2	GLC	C1-O5-C5	4.13	117.79	112.19
3	b	1	GLC	O1-C1-O5	-3.91	98.64	110.38
3	e	1	GLC	O1-C1-O5	-3.90	98.67	110.38
3	i	1	GLC	O1-C1-O5	-3.90	98.68	110.38
3	g	1	GLC	O1-C1-O5	-3.89	98.70	110.38
3	f	1	GLC	O1-C1-O5	-3.89	98.70	110.38
3	h	1	GLC	O1-C1-O5	-3.89	98.70	110.38
3	c	1	GLC	O1-C1-O5	-3.89	98.70	110.38
3	j	1	GLC	O1-C1-O5	-3.89	98.71	110.38
3	a	1	GLC	O1-C1-O5	-3.89	98.72	110.38
3	Z	1	GLC	O1-C1-O5	-3.89	98.72	110.38
3	Y	1	GLC	O1-C1-O5	-3.88	98.73	110.38
3	d	1	GLC	O1-C1-O5	-3.88	98.74	110.38
3	e	1	GLC	O5-C1-C2	3.68	116.85	110.28
3	f	1	GLC	O5-C1-C2	3.68	116.84	110.28
3	Y	1	GLC	O5-C1-C2	3.67	116.83	110.28
3	b	1	GLC	O5-C1-C2	3.67	116.83	110.28
3	c	1	GLC	O5-C1-C2	3.66	116.82	110.28
3	Z	1	GLC	O5-C1-C2	3.66	116.81	110.28
3	d	1	GLC	O5-C1-C2	3.66	116.81	110.28
3	h	1	GLC	O5-C1-C2	3.66	116.81	110.28
3	i	1	GLC	O5-C1-C2	3.65	116.81	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	g	1	GLC	O5-C1-C2	3.65	116.80	110.28
3	j	1	GLC	O5-C1-C2	3.65	116.79	110.28
3	a	1	GLC	O5-C1-C2	3.63	116.76	110.28
3	a	1	GLC	O6-C6-C5	-2.55	102.56	111.29
3	f	1	GLC	O6-C6-C5	-2.54	102.58	111.29
3	e	1	GLC	O6-C6-C5	-2.54	102.59	111.29
3	b	1	GLC	O6-C6-C5	-2.53	102.60	111.29
3	h	1	GLC	O6-C6-C5	-2.53	102.61	111.29
3	Z	1	GLC	O6-C6-C5	-2.53	102.61	111.29
3	i	1	GLC	O6-C6-C5	-2.53	102.61	111.29
3	j	1	GLC	O6-C6-C5	-2.53	102.62	111.29
3	d	1	GLC	O6-C6-C5	-2.53	102.62	111.29
3	Y	1	GLC	O6-C6-C5	-2.53	102.62	111.29
3	g	1	GLC	O6-C6-C5	-2.52	102.63	111.29
3	c	1	GLC	O6-C6-C5	-2.52	102.64	111.29
3	f	1	GLC	O4-C4-C5	-2.17	103.90	109.30
3	Z	1	GLC	O4-C4-C5	-2.16	103.92	109.30
3	b	1	GLC	O4-C4-C5	-2.16	103.92	109.30
3	c	1	GLC	O4-C4-C5	-2.15	103.95	109.30
3	d	1	GLC	O4-C4-C5	-2.15	103.96	109.30
3	h	1	GLC	O4-C4-C5	-2.15	103.97	109.30
3	Y	1	GLC	O4-C4-C5	-2.15	103.97	109.30
3	j	1	GLC	O4-C4-C5	-2.15	103.97	109.30
3	a	1	GLC	O4-C4-C5	-2.14	103.97	109.30
3	g	1	GLC	O4-C4-C5	-2.14	103.98	109.30
3	i	1	GLC	O4-C4-C5	-2.14	103.99	109.30
3	e	1	GLC	O4-C4-C5	-2.13	104.01	109.30

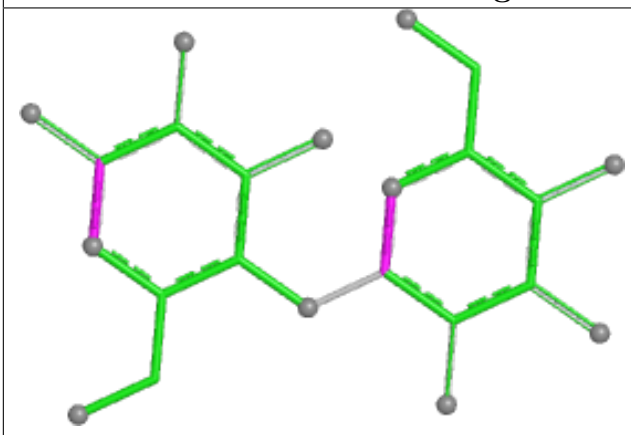
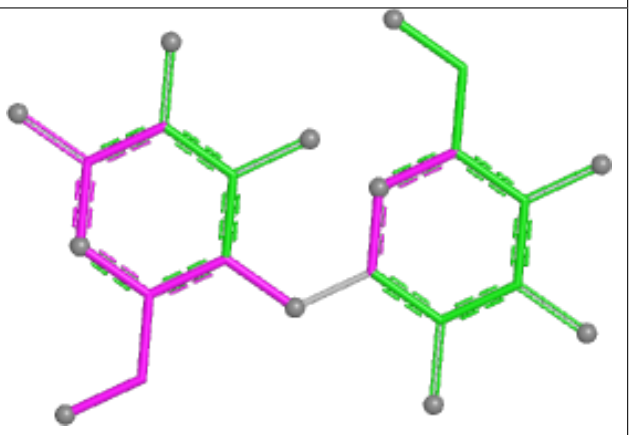
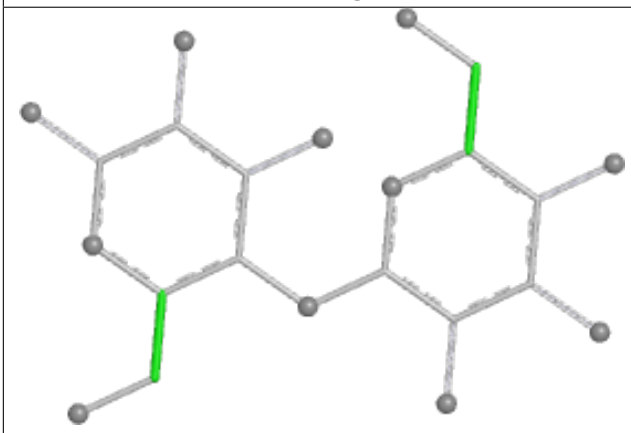
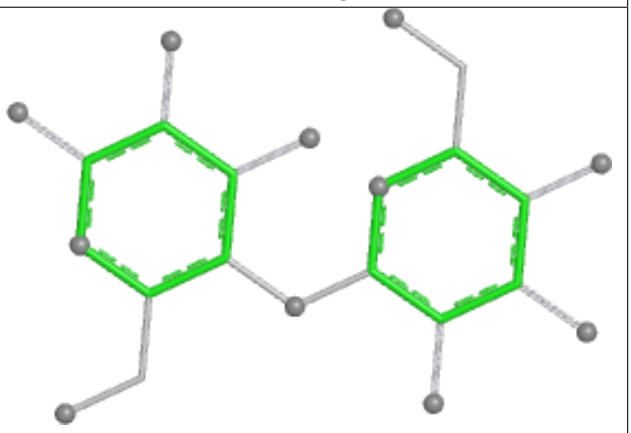
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

Oligosaccharide Chain Y	
 Bond lengths	 Bond angles
 Torsions	 Rings

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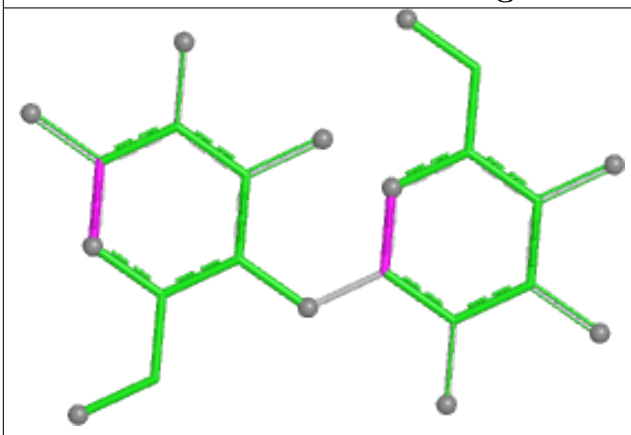
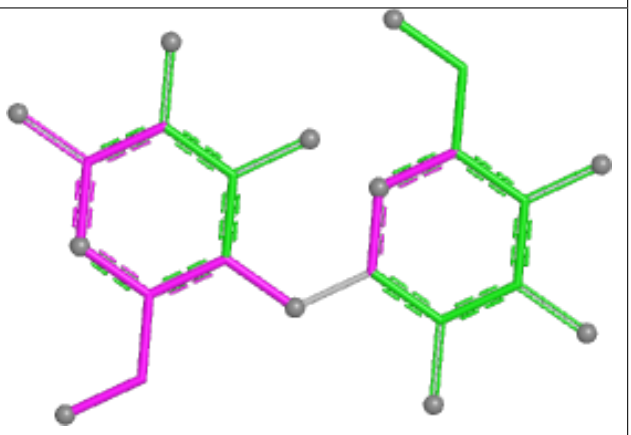
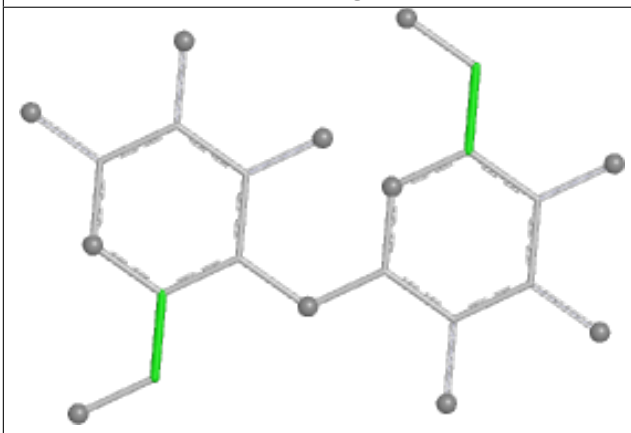
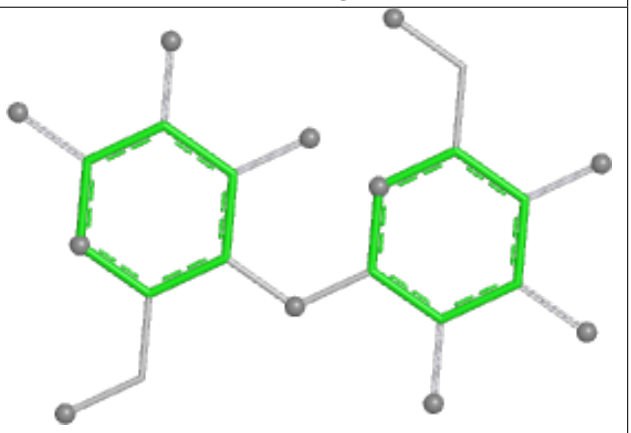
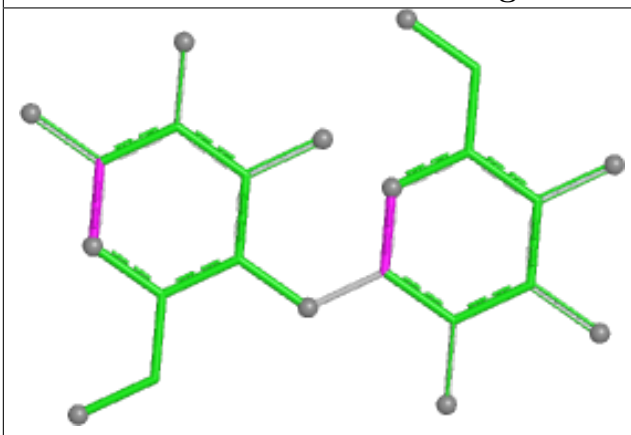
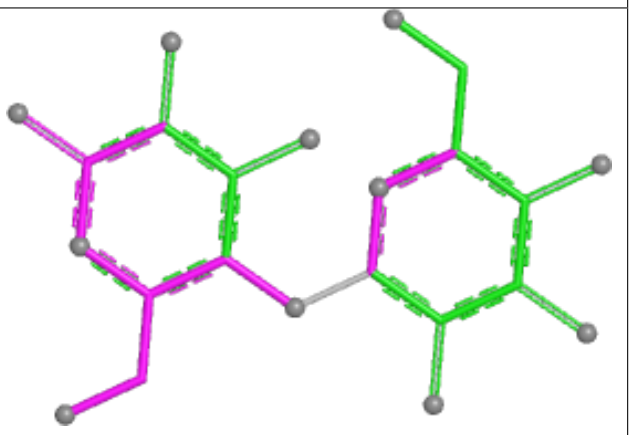
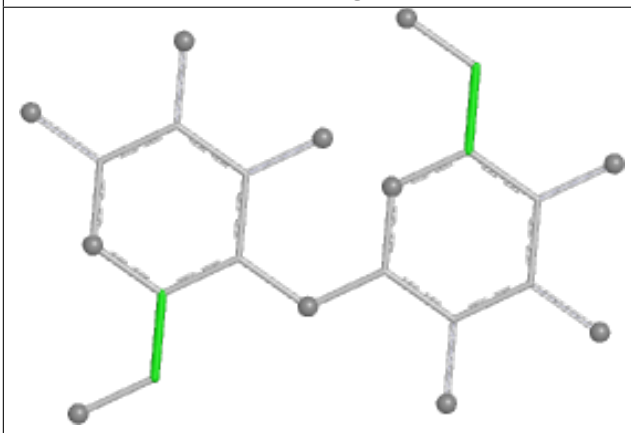
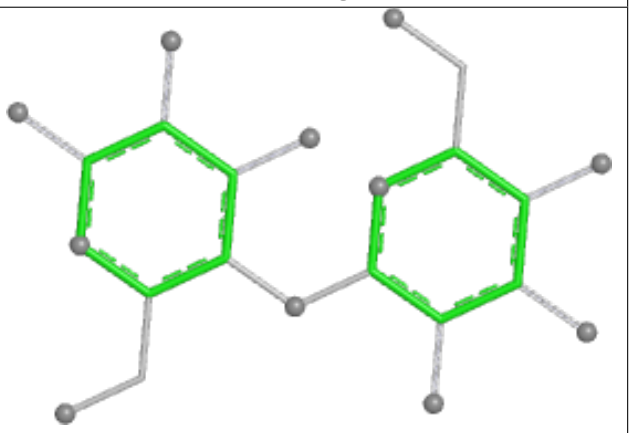
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain a	
 Bond lengths	 Bond angles
 Torsions	 Rings

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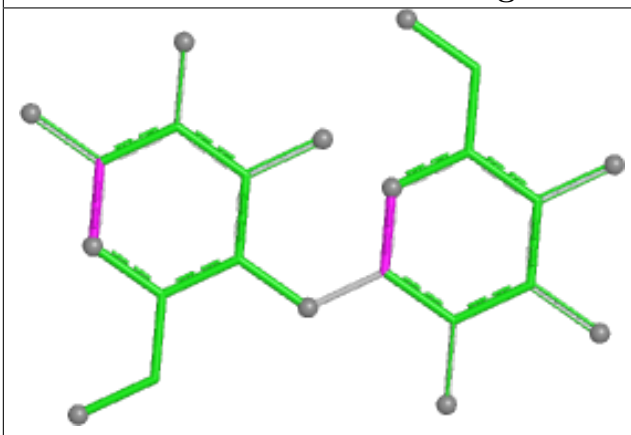
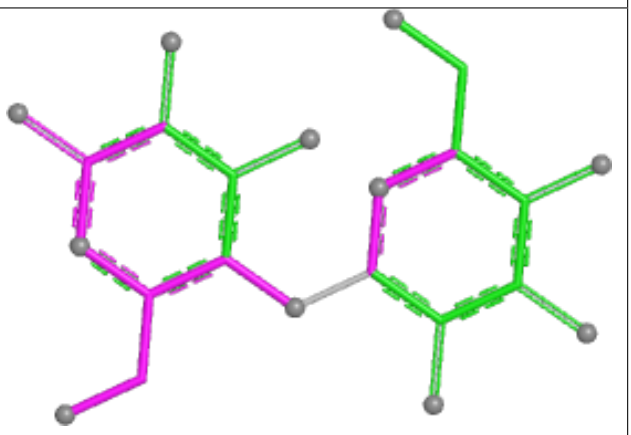
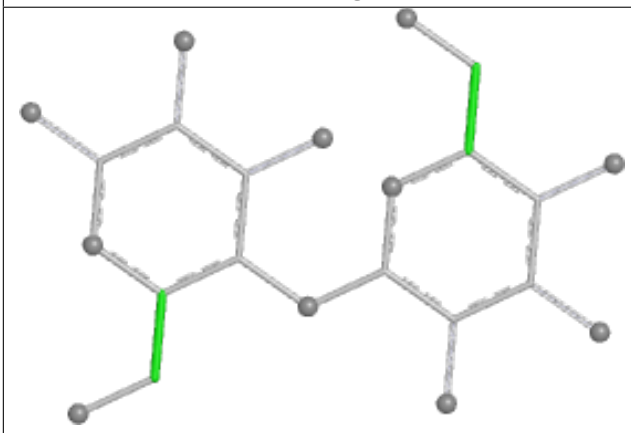
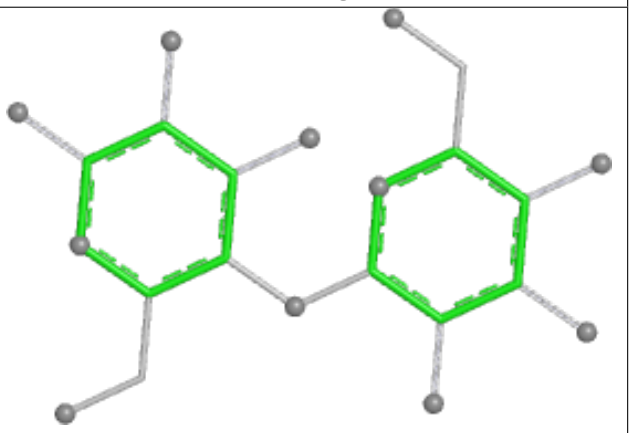
 Bond lengths	 Bond angles
 Torsions	 Rings

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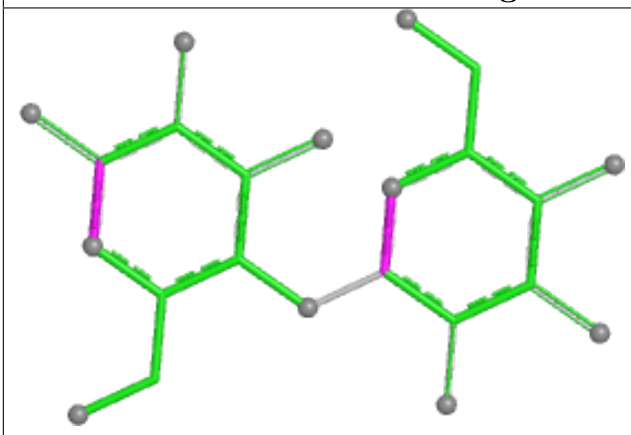
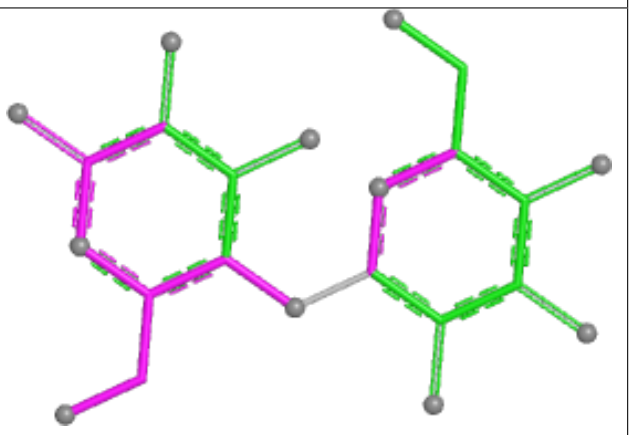
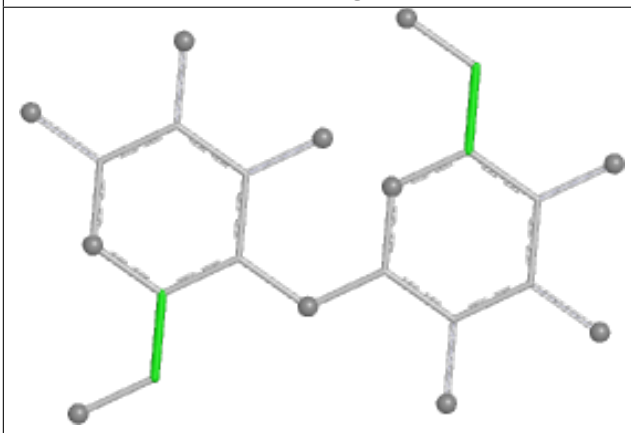
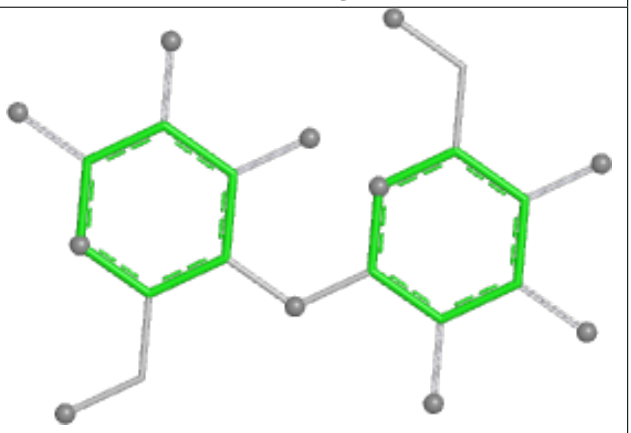
 Bond lengths	 Bond angles
 Torsions	 Rings

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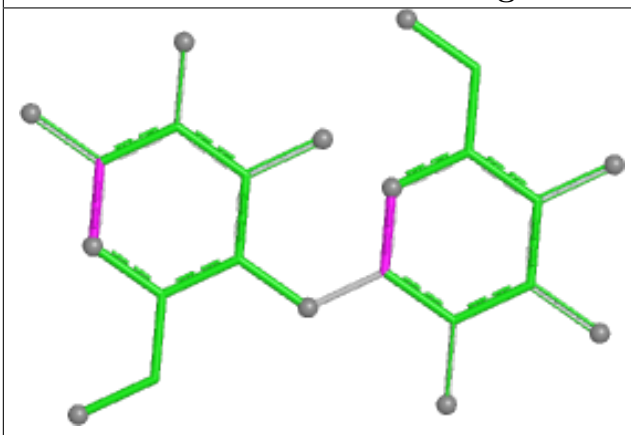
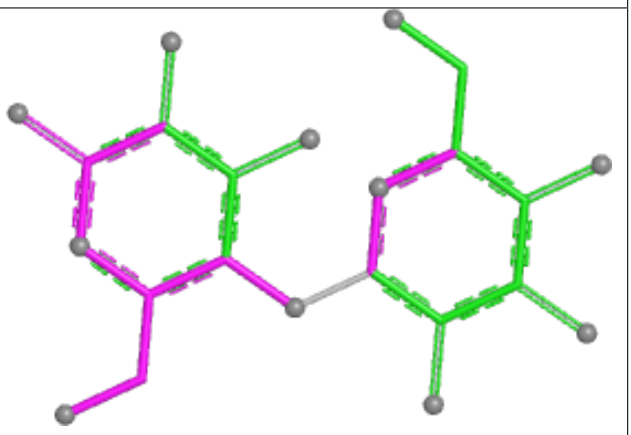
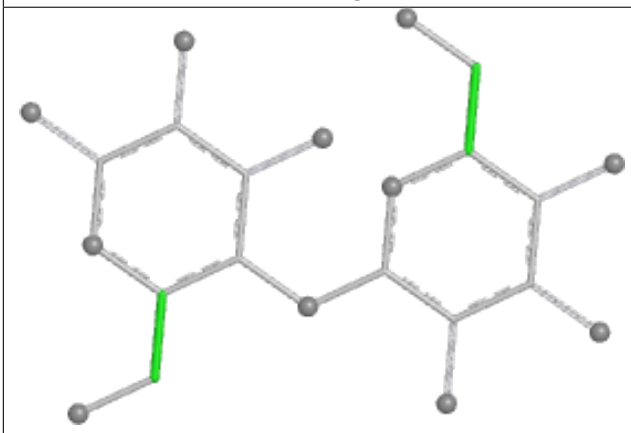
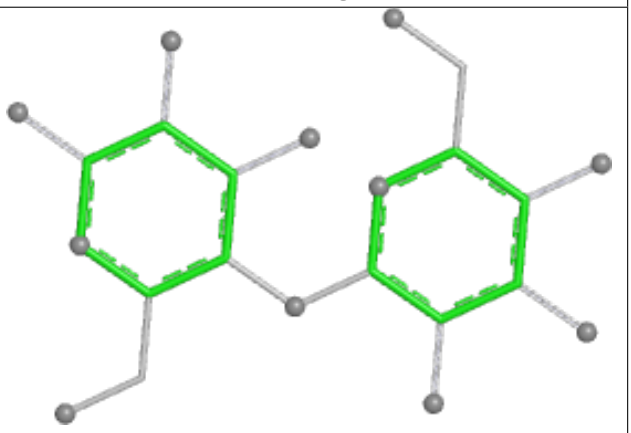
 Bond lengths	 Bond angles
 Torsions	 Rings

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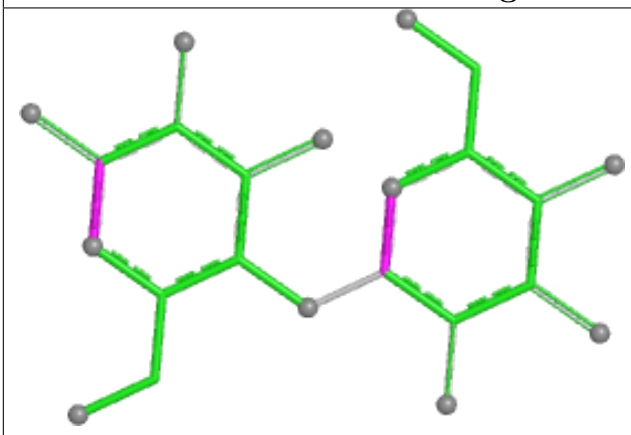
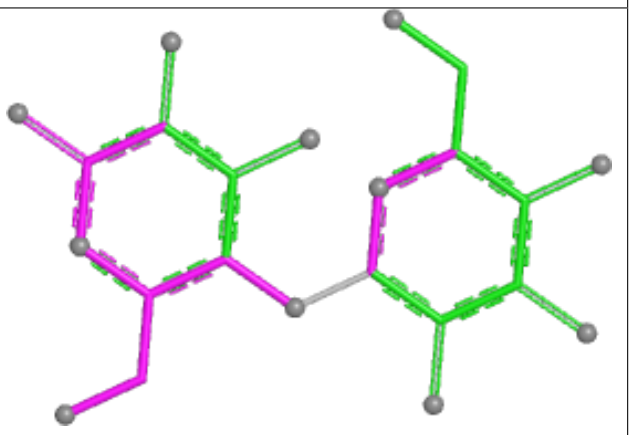
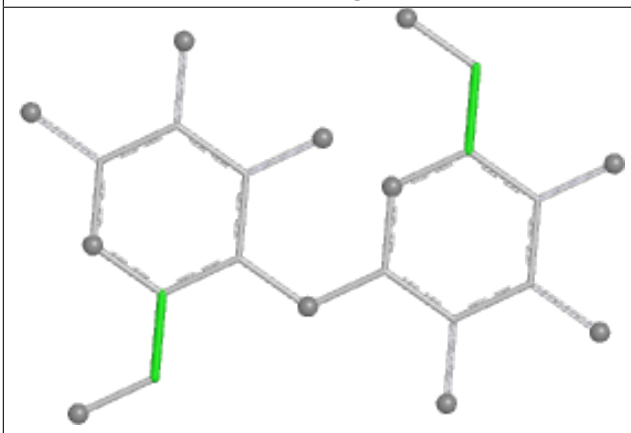
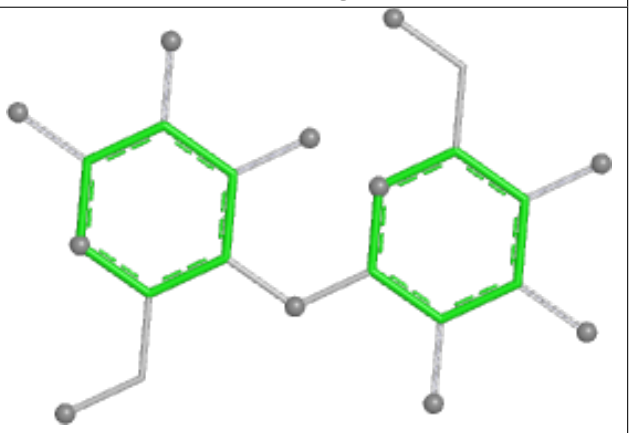
 Bond lengths	 Bond angles
 Torsions	 Rings

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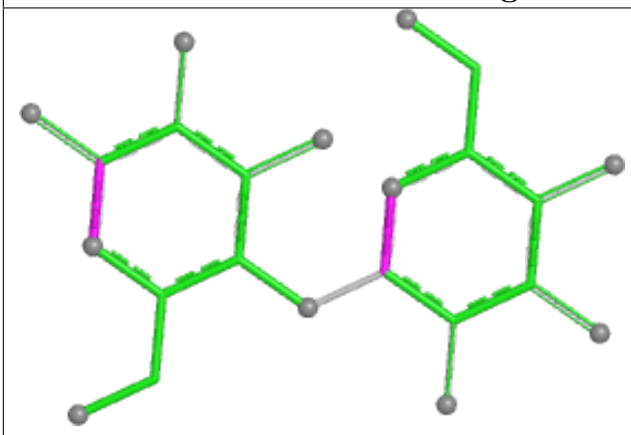
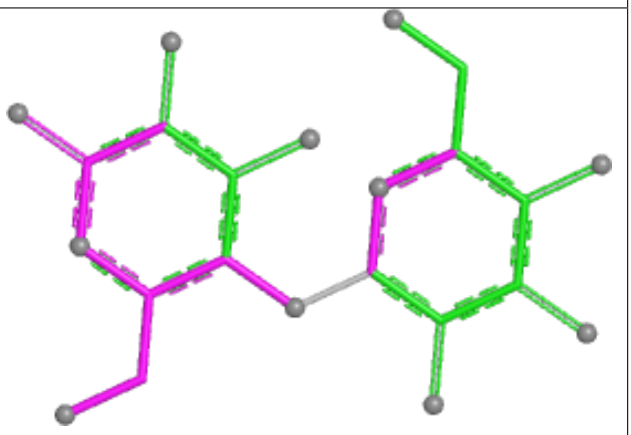
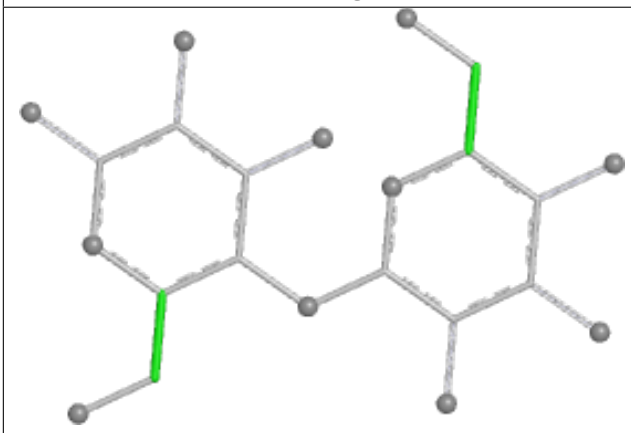
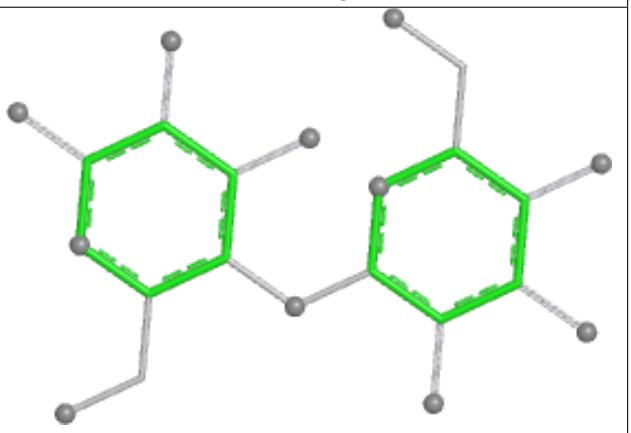
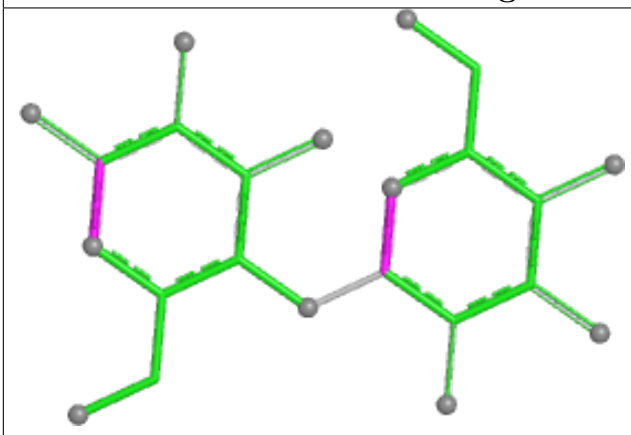
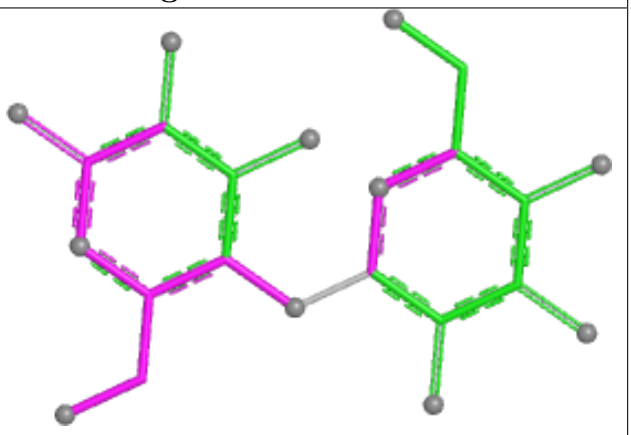
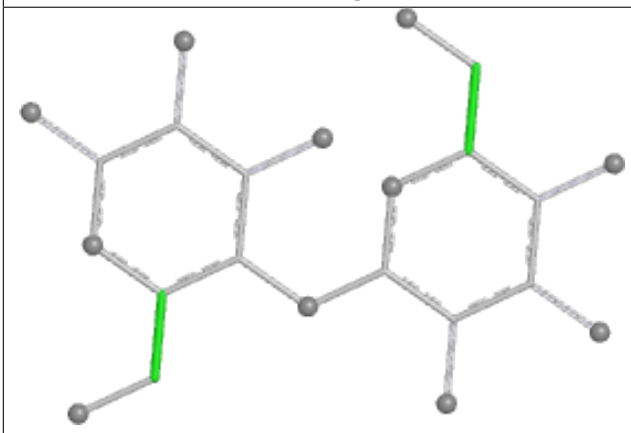
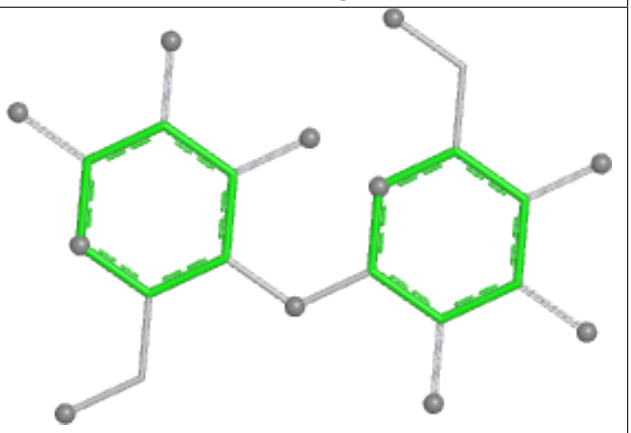
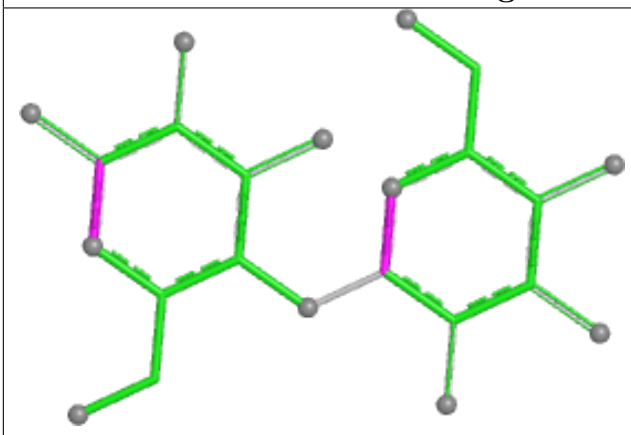
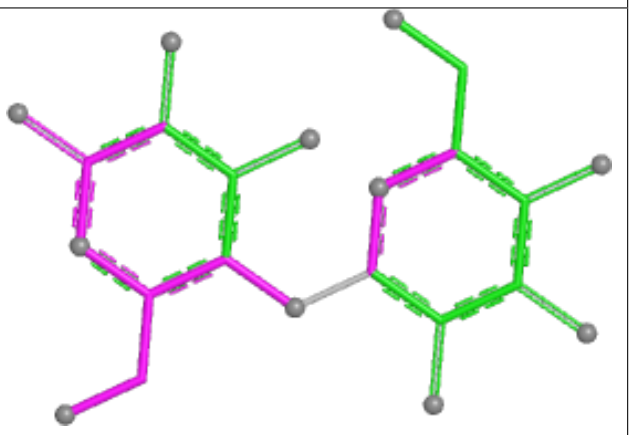
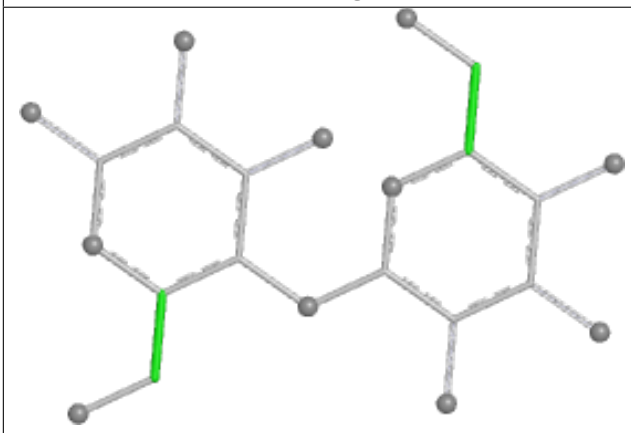
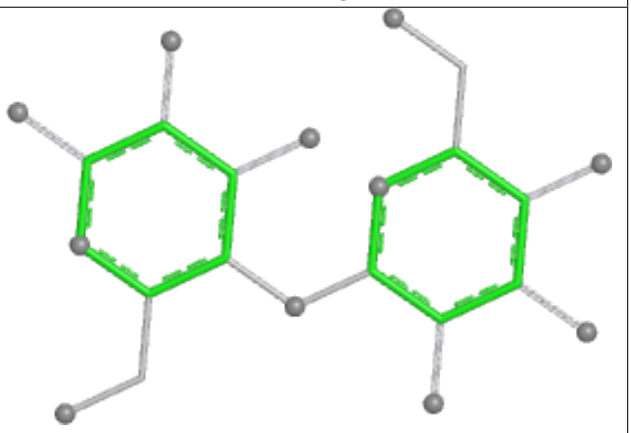
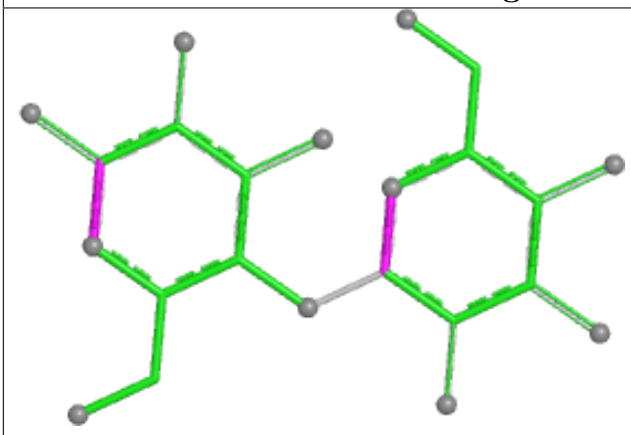
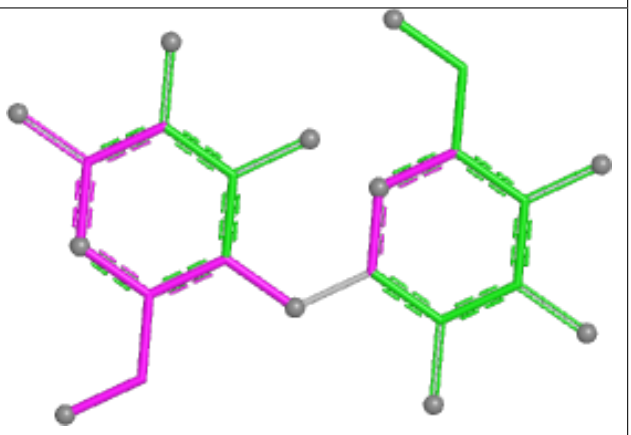
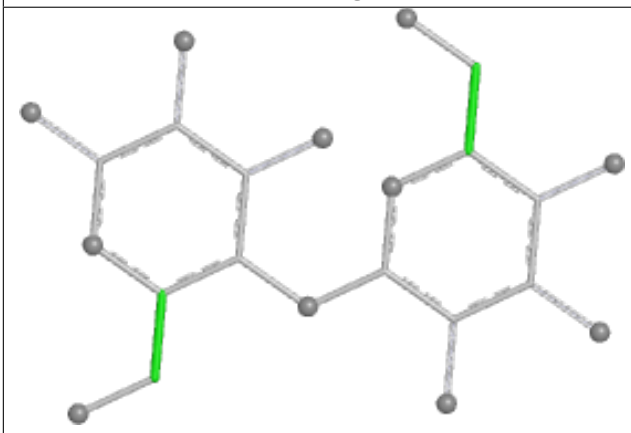
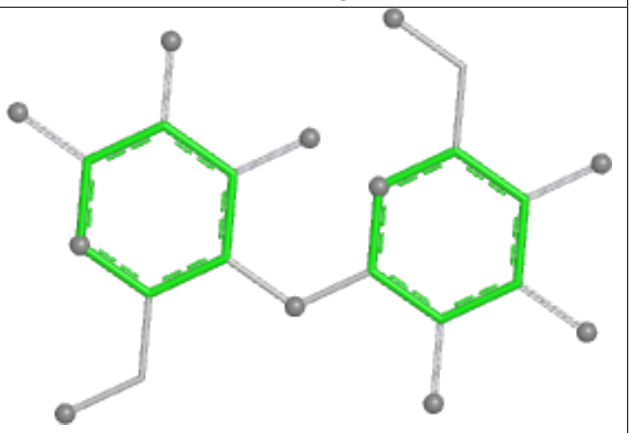
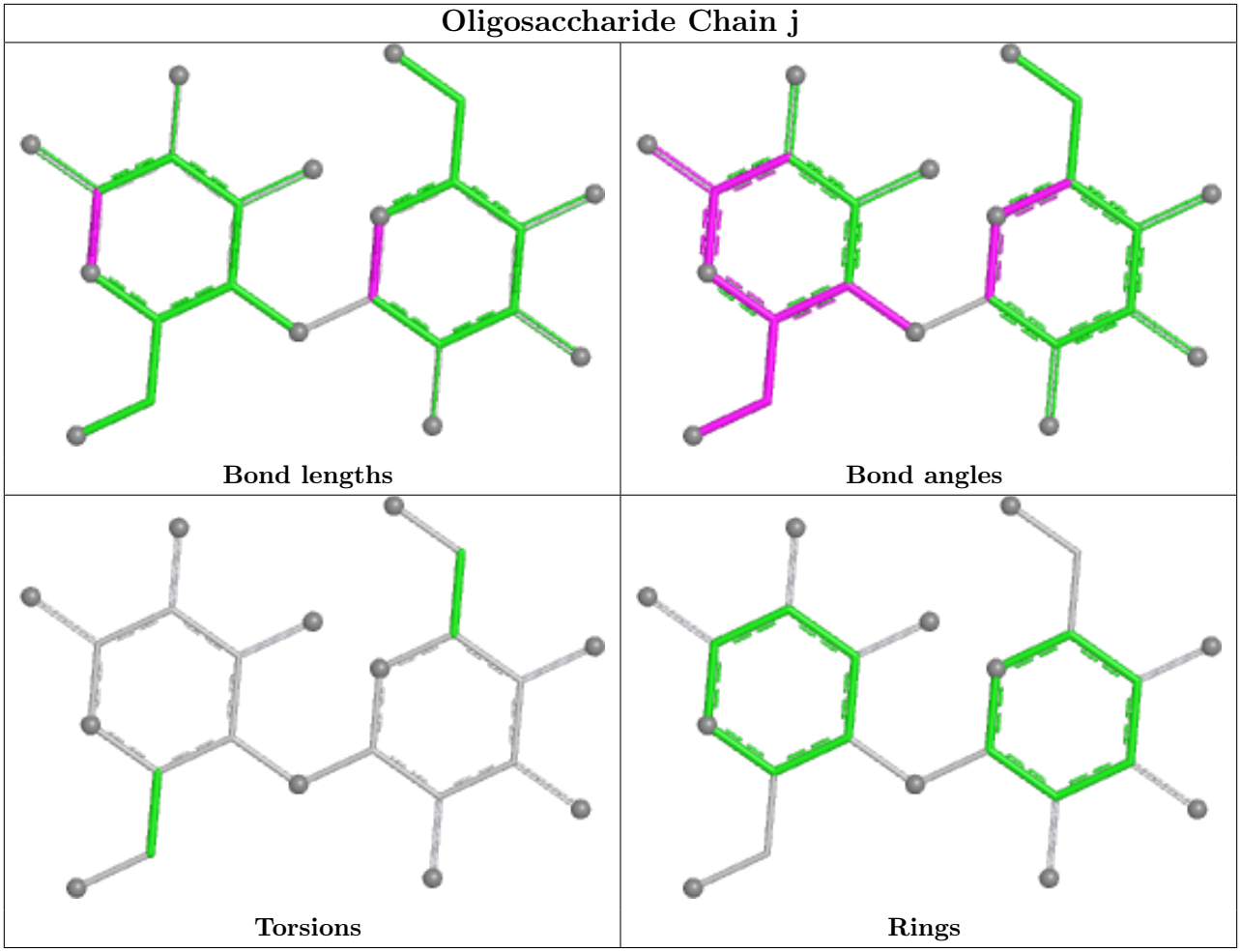
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain g	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain h	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain i	
 Bond lengths	 Bond angles
 Torsions	 Rings



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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	M	1
2	O	1
2	P	1
2	Q	1

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Mol	Chain	Number of breaks
2	T	1
2	N	1
2	R	1
2	S	1
2	U	1
2	V	1
2	W	1
2	X	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	M	369:THR	C	370:LYS	N	1.68
1	O	369:THR	C	370:LYS	N	1.68
1	P	369:THR	C	370:LYS	N	1.68
1	Q	369:THR	C	370:LYS	N	1.68
1	T	369:THR	C	370:LYS	N	1.68
1	N	369:THR	C	370:LYS	N	1.67
1	R	369:THR	C	370:LYS	N	1.67
1	S	369:THR	C	370:LYS	N	1.67
1	U	369:THR	C	370:LYS	N	1.67
1	V	369:THR	C	370:LYS	N	1.67
1	W	369:THR	C	370:LYS	N	1.67
1	X	369:THR	C	370:LYS	N	1.67

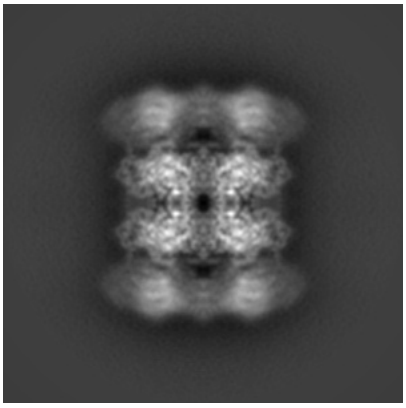
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-4039. These allow visual inspection of the internal detail of the map and identification of artifacts.

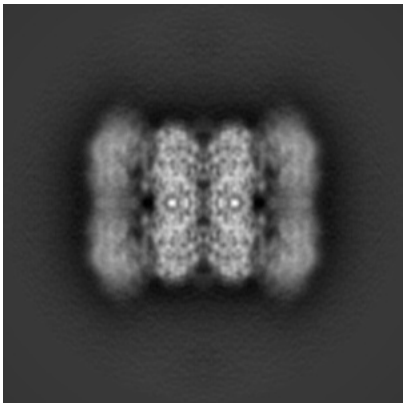
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

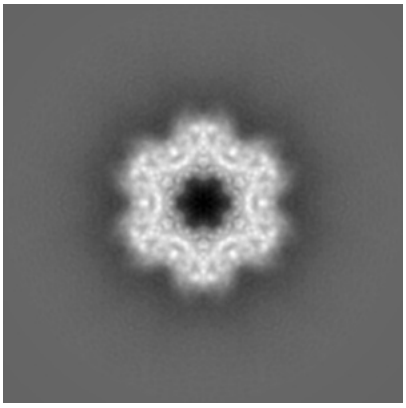
6.1.1 Primary map



X



Y

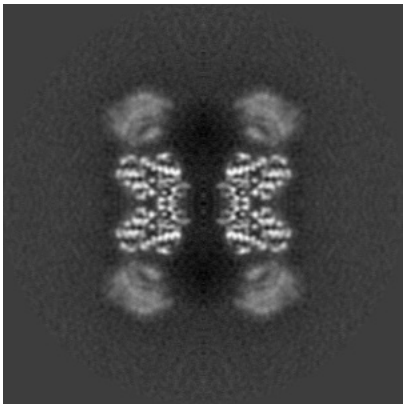


Z

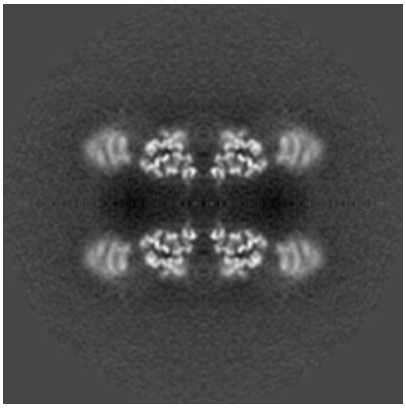
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

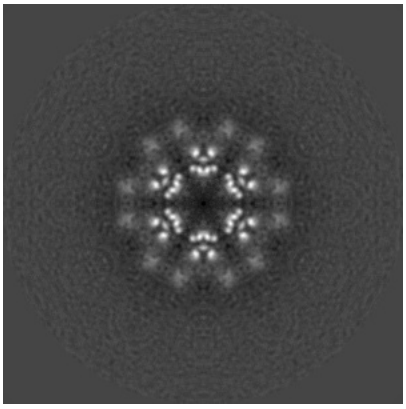
6.2.1 Primary map



X Index: 200



Y Index: 200

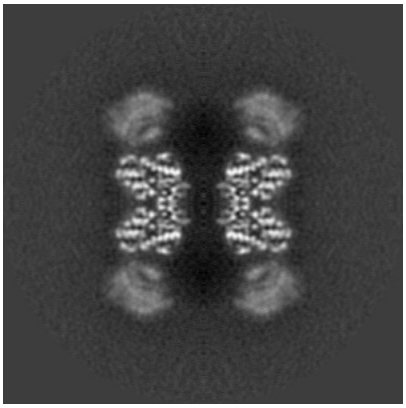


Z Index: 200

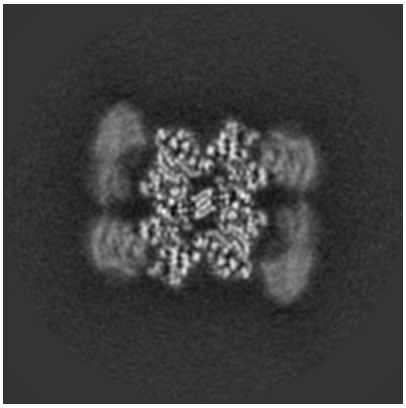
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

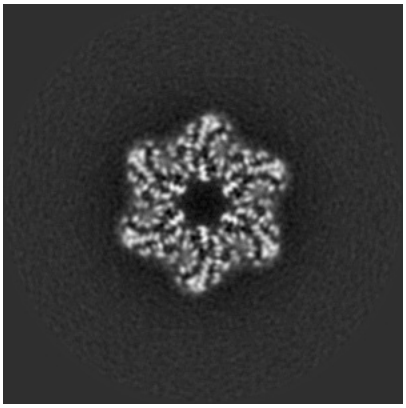
6.3.1 Primary map



X Index: 200



Y Index: 166

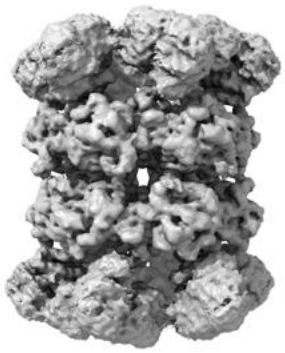


Z Index: 169

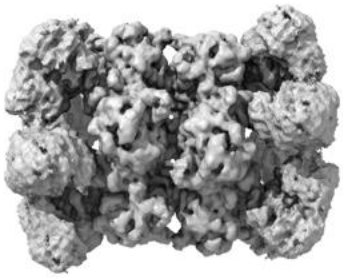
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X



Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.0015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

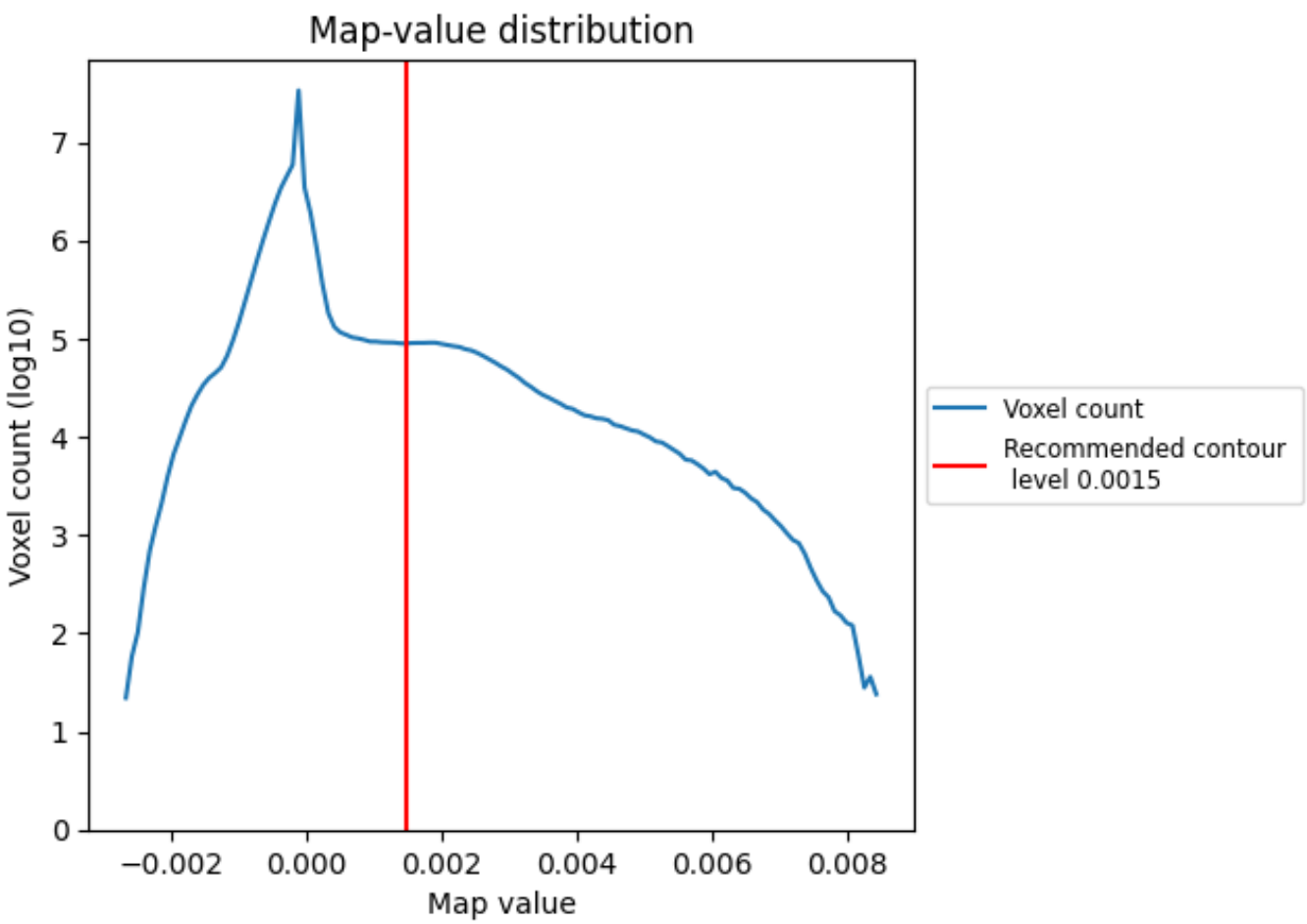
6.5 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis (i)

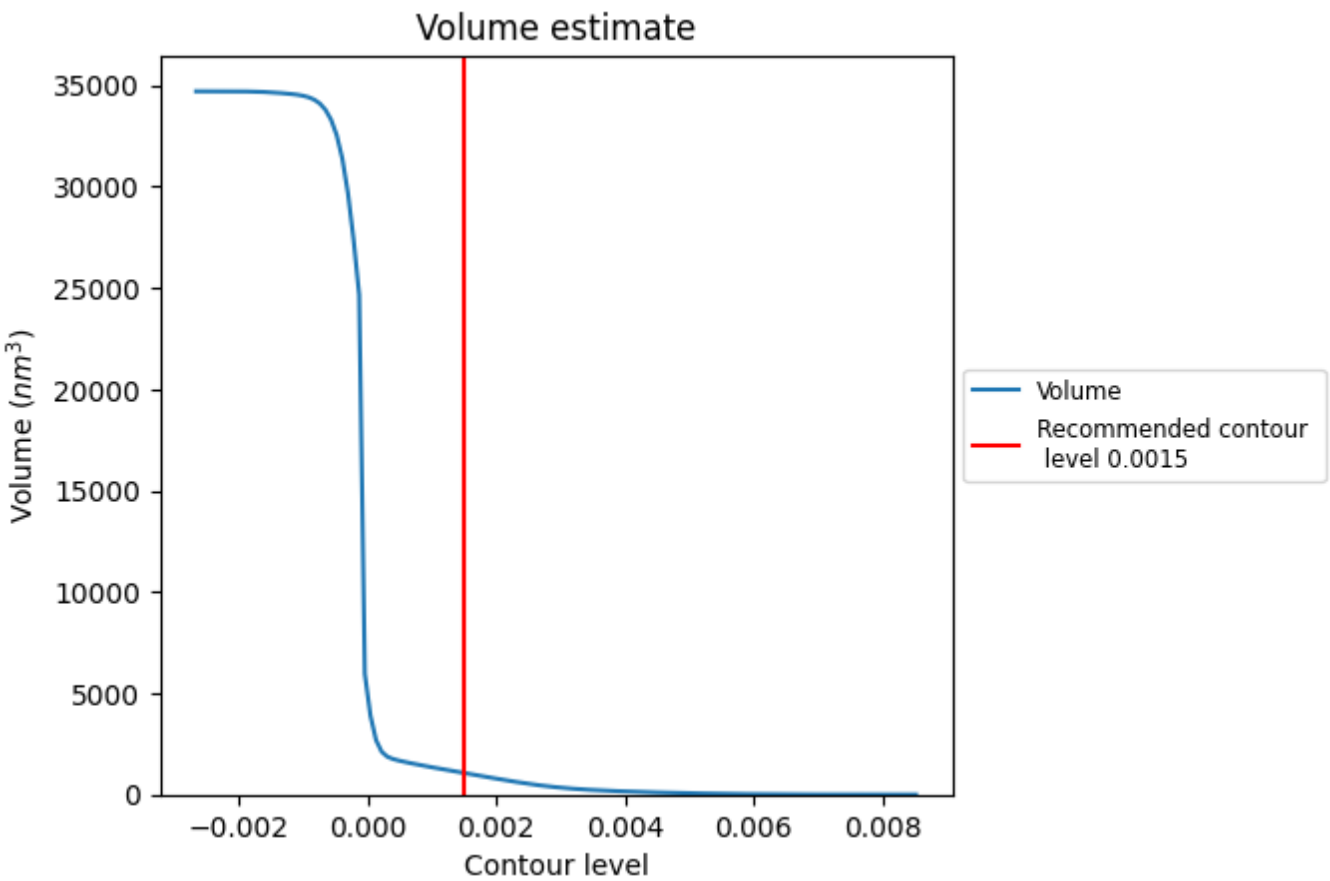
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

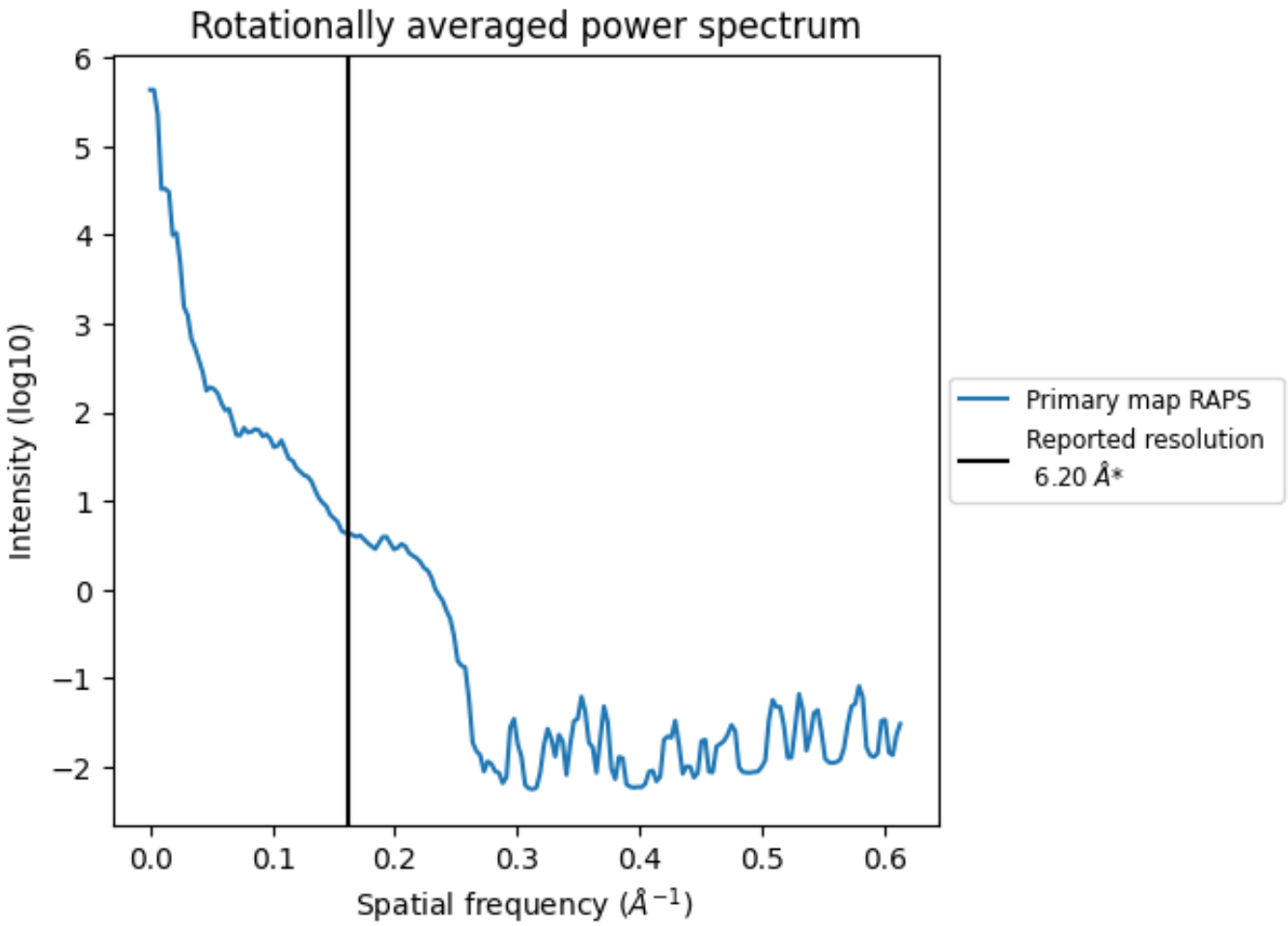
7.2 Volume estimate (i)



The volume at the recommended contour level is 1067 nm^3; this corresponds to an approximate mass of 964 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.161 Å^{-1}

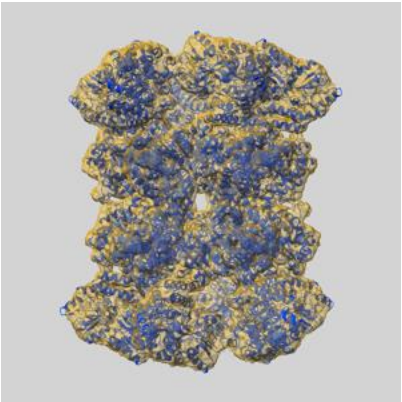
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

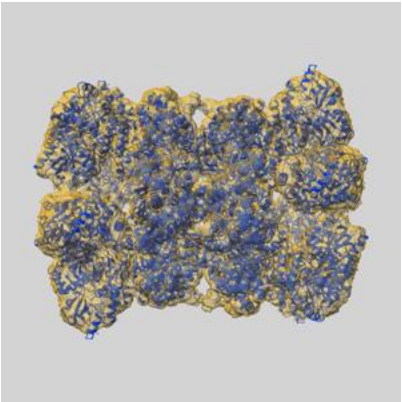
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-4039 and PDB model 5LDF. Per-residue inclusion information can be found in section 3 on page 8.

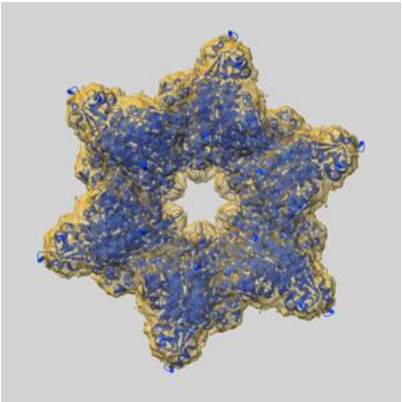
9.1 Map-model overlay (i)



X



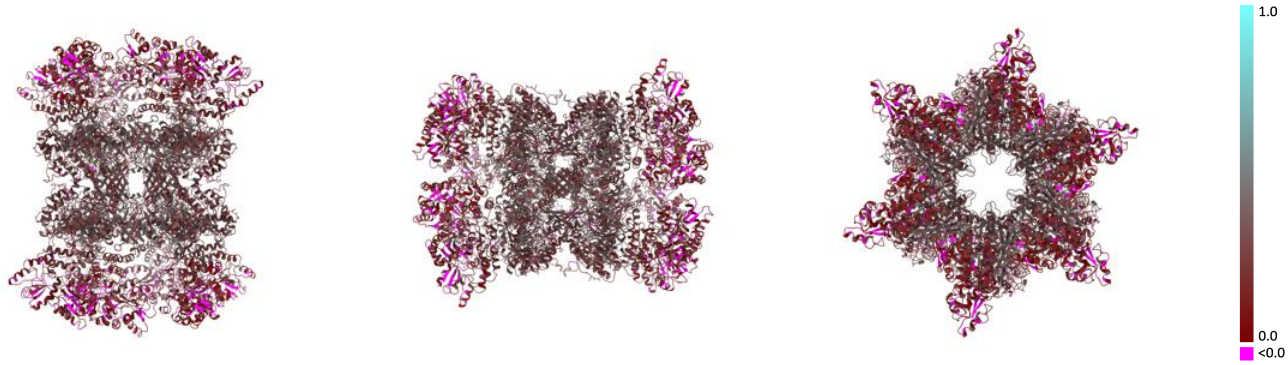
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

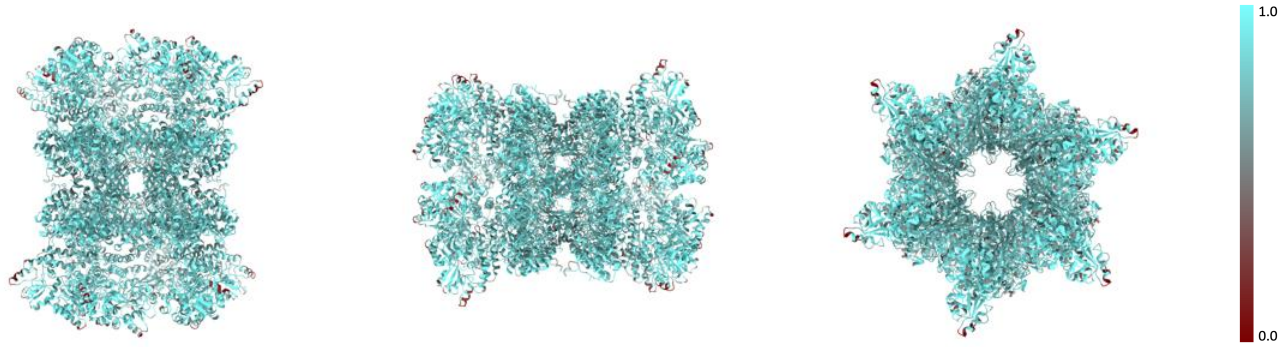
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

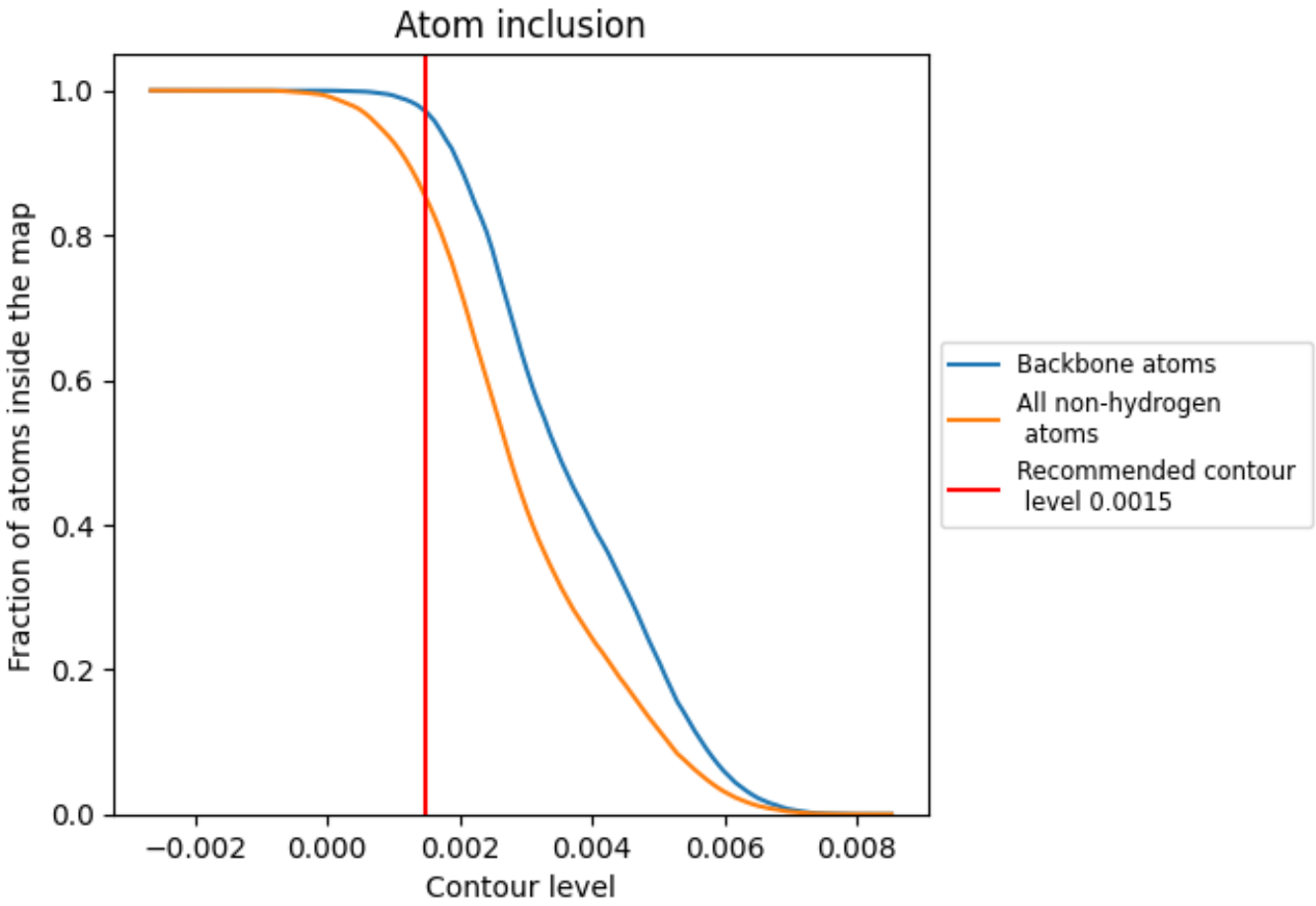
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0015).

9.4 Atom inclusion (i)



At the recommended contour level, 97% of all backbone atoms, 85% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.0015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8506	0.2390
A	0.8568	0.3150
B	0.8562	0.3110
C	0.8529	0.3040
D	0.8557	0.3080
E	0.8545	0.3110
F	0.8543	0.3050
G	0.8576	0.3150
H	0.8531	0.3080
I	0.8565	0.3140
J	0.8559	0.3150
K	0.8557	0.3130
L	0.8529	0.3070
M	0.8436	0.1500
N	0.8443	0.1500
O	0.8457	0.1440
P	0.8436	0.1430
Q	0.8454	0.1450
R	0.8461	0.1460
S	0.8447	0.1480
T	0.8454	0.1470
U	0.8436	0.1490
V	0.8457	0.1510
W	0.8457	0.1500
X	0.8436	0.1500
Y	0.8696	0.2270
Z	0.8696	0.2200
a	0.8261	0.1720
b	0.8261	0.1850
c	0.8696	0.2010
d	0.8261	0.1720
e	0.8696	0.2320
f	0.8696	0.2180
g	0.8696	0.2260
h	0.9130	0.2260

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Chain	Atom inclusion	Q-score
i	0.8696	0.2350
j	0.8696	0.2230