



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:10 PM UTC

PDB ID : 1JD2 / pdb_00001jd2
Title : Crystal Structure of the yeast 20S Proteasome:TMC-95A complex: A non-covalent Proteasome Inhibitor
Authors : Groll, M.; Koguchi, Y.; Huber, R.; Kohno, J.
Deposited on : 2001-06-12
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

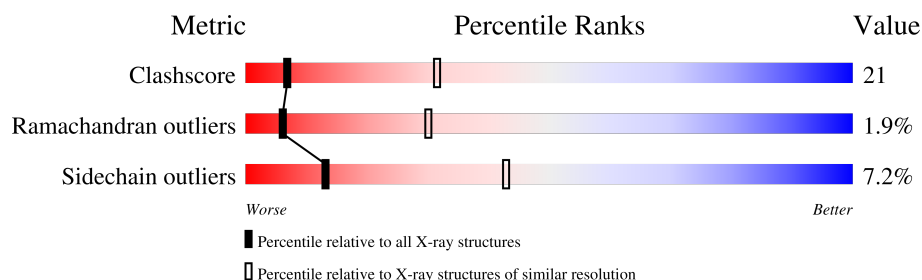
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)

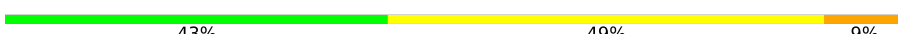
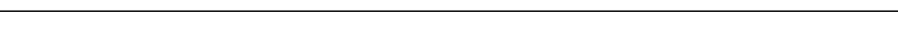
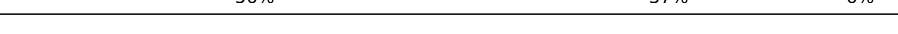
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	250	
1	V	250	
2	B	244	
2	W	244	
3	C	241	
3	X	241	
4	D	242	
4	Y	242	

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Mol	Chain	Length	Quality of chain
5	E	233	 54% 38% 7%
5	Z	233	 49% 40% 11%
6	1	244	 45% 47% 8%
6	F	244	 49% 46% . .
7	2	243	 43% 49% 9%
7	G	243	 53% 40% 7%
8	H	222	 53% 41% 6%
8	O	222	 48% 42% 10%
9	I	204	 62% 31% 6%
9	P	204	 57% 38% 5%
10	J	198	 58% 36% 6% .
10	Q	198	 57% 37% 6%
11	K	212	 57% 37% 6%
11	R	212	 62% 33% 5%
12	L	222	 56% 37% 6%
12	S	222	 63% 28% 9%
13	M	233	 54% 39% 7%
13	T	233	 52% 44% 5%
14	N	196	 48% 45% 6% .
14	U	196	 45% 51% 5%
15	8	5	 20% 40% 20% 20%
15	9	5	 20% 40% 20% 20%

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 52549 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called PROTEASOME COMPONENT Y7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	250	Total	C	N	O	S	0	0	0
			1915	1219	315	377	4			
1	V	250	Total	C	N	O	S	0	0	0
			1915	1219	315	377	4			

- Molecule 2 is a protein called PROTEASOME COMPONENT Y13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	244	Total	C	N	O	S	0	0	0
			1905	1201	321	380	3			
2	W	244	Total	C	N	O	S	0	0	0
			1905	1201	321	380	3			

- Molecule 3 is a protein called PROTEASOME COMPONENT PRE6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	241	Total	C	N	O	S	0	0	0
			1891	1181	331	375	4			
3	X	241	Total	C	N	O	S	0	0	0
			1891	1181	331	375	4			

- Molecule 4 is a protein called PROTEASOME COMPONENT PUP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	242	Total	C	N	O	S	0	0	0
			1862	1162	314	379	7			
4	Y	242	Total	C	N	O	S	0	0	0
			1862	1162	314	379	7			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	121	LEU	-	insertion	UNP P32379
D	122	ARG	-	insertion	UNP P32379
D	123	PHE	-	insertion	UNP P32379
D	123A	GLY	-	insertion	UNP P32379
D	123B	GLU	-	insertion	UNP P32379
D	123C	GLY	-	insertion	UNP P32379
D	123E	SER	-	insertion	UNP P32379
D	123F	GLY	-	insertion	UNP P32379
D	123G	GLU	-	insertion	UNP P32379
D	125	GLU	ALA	conflict	UNP P32379
D	126	ARG	ALA	conflict	UNP P32379
D	127	LEU	ALA	conflict	UNP P32379
Y	121	LEU	-	insertion	UNP P32379
Y	122	ARG	-	insertion	UNP P32379
Y	123	PHE	-	insertion	UNP P32379
Y	123A	GLY	-	insertion	UNP P32379
Y	123B	GLU	-	insertion	UNP P32379
Y	123C	GLY	-	insertion	UNP P32379
Y	123E	SER	-	insertion	UNP P32379
Y	123F	GLY	-	insertion	UNP P32379
Y	123G	GLU	-	insertion	UNP P32379
Y	125	GLU	ALA	conflict	UNP P32379
Y	126	ARG	ALA	conflict	UNP P32379
Y	127	LEU	ALA	conflict	UNP P32379

- Molecule 5 is a protein called PROTEASOME COMPONENT PRE5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	233	Total	C	N	O	S	0	0	0
			1795	1129	312	350	4			
5	Z	233	Total	C	N	O	S	0	0	0
			1795	1129	312	350	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	127	TYR	ALA	conflict	UNP P40302
Z	127	TYR	ALA	conflict	UNP P40302

- Molecule 6 is a protein called PROTEASOME COMPONENT C1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	244	Total	C	N	O	S	0	0	0
			1897	1205	330	358	4			
6	1	244	Total	C	N	O	S	0	0	0
			1897	1205	330	358	4			

- Molecule 7 is a protein called PROTEASOME COMPONENT C7-ALPHA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	243	Total	C	N	O	S	0	0	0
			1921	1221	322	370	8			
7	2	243	Total	C	N	O	S	0	0	0
			1921	1221	322	370	8			

- Molecule 8 is a protein called PROTEASOME COMPONENT PUP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	222	Total	C	N	O	S	0	0	0
			1685	1061	293	324	7			
8	O	222	Total	C	N	O	S	0	0	0
			1685	1061	293	324	7			

- Molecule 9 is a protein called PROTEASOME COMPONENT PUP3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	204	Total	C	N	O	S	0	0	0
			1581	1010	258	305	8			
9	P	204	Total	C	N	O	S	0	0	0
			1581	1010	258	305	8			

- Molecule 10 is a protein called PROTEASOME COMPONENT C11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	198	Total	C	N	O	S	0	0	0
			1585	1005	269	305	6			
10	Q	198	Total	C	N	O	S	0	0	0
			1585	1005	269	305	6			

- Molecule 11 is a protein called PROTEASOME COMPONENT PRE2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	212	Total	C	N	O	S	0	0	0
			1644	1045	280	312	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	R	212	Total	C	N	O	S	0	0	0
			1644	1045	280	312	7			

- Molecule 12 is a protein called PROTEASOME COMPONENT C5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	222	Total	C	N	O	S	0	0	0
			1757	1115	303	335	4			
12	S	222	Total	C	N	O	S	0	0	0
			1757	1115	303	335	4			

- Molecule 13 is a protein called PROTEASOME COMPONENT PRE4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			
13	T	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			

- Molecule 14 is a protein called PROTEASOME COMPONENT PRE3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	196	Total	C	N	O	S	0	0	0
			1512	955	250	300	7			
14	U	196	Total	C	N	O	S	0	0	0
			1512	955	250	300	7			

- Molecule 15 is a protein called TMC-95A inhibitor.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	8	5	Total	C	N	O	0	0	0
			49	33	6	10			
15	9	5	Total	C	N	O	0	0	0
			49	33	6	10			

- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	D	1	Total	Mg	0	0
			1	1		
16	F	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	G	1	Total 1	Mg 1	0	0
16	H	1	Total 1	Mg 1	0	0
16	I	2	Total 2	Mg 2	0	0
16	L	1	Total 1	Mg 1	0	0
16	N	1	Total 1	Mg 1	0	0
16	P	1	Total 1	Mg 1	0	0

- Molecule 17 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	105	Total 105	O 105	0	0
17	B	80	Total 80	O 80	0	0
17	C	69	Total 69	O 69	0	0
17	D	90	Total 90	O 90	0	0
17	E	55	Total 55	O 55	0	0
17	F	99	Total 99	O 99	0	0
17	G	106	Total 106	O 106	0	0
17	H	114	Total 114	O 114	0	0
17	I	107	Total 107	O 107	0	0
17	J	116	Total 116	O 116	0	0
17	K	103	Total 103	O 103	0	0
17	L	140	Total 140	O 140	0	0
17	M	150	Total 150	O 150	0	0

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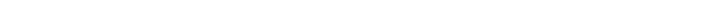
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	N	116	Total 116	O 116	0	0
17	O	121	Total 121	O 121	0	0
17	P	101	Total 101	O 101	0	0
17	Q	121	Total 121	O 121	0	0
17	R	107	Total 107	O 107	0	0
17	S	144	Total 144	O 144	0	0
17	T	142	Total 142	O 142	0	0
17	U	118	Total 118	O 118	0	0
17	V	104	Total 104	O 104	0	0
17	W	74	Total 74	O 74	0	0
17	X	70	Total 70	O 70	0	0
17	Y	89	Total 89	O 89	0	0
17	Z	53	Total 53	O 53	0	0
17	1	93	Total 93	O 93	0	0
17	2	103	Total 103	O 103	0	0
17	8	2	Total 2	O 2	0	0
17	9	1	Total 1	O 1	0	0

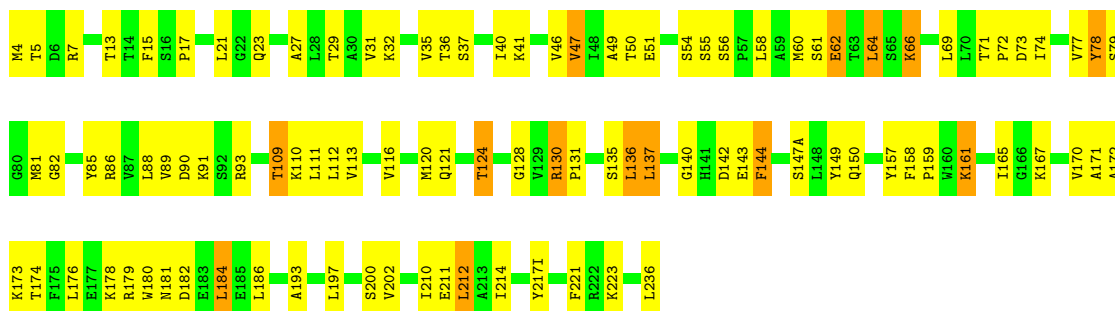
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

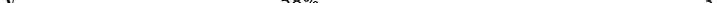
Note EDS was not executed.

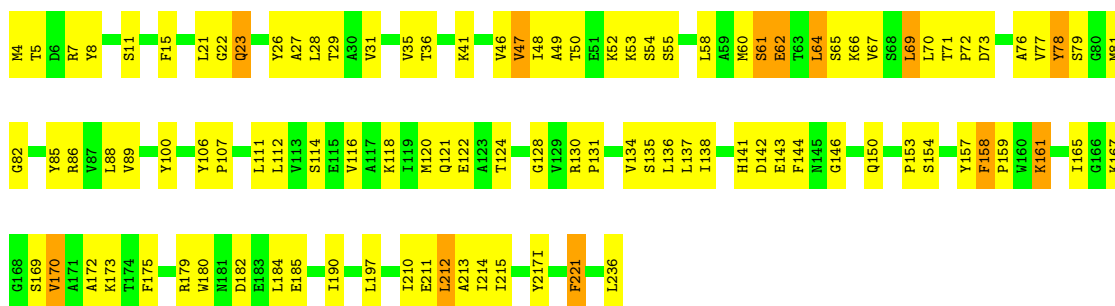
- Molecule 1: PROTEASOME COMPONENT Y7

Chain A:  60% 35% 6%



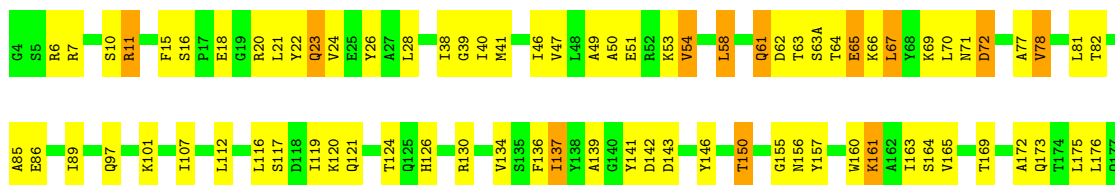
- Molecule 1: PROTEASOME COMPONENT Y7

Chain V:  58% 37% 5%



- Molecule 2: PROTEASOME COMPONENT Y13

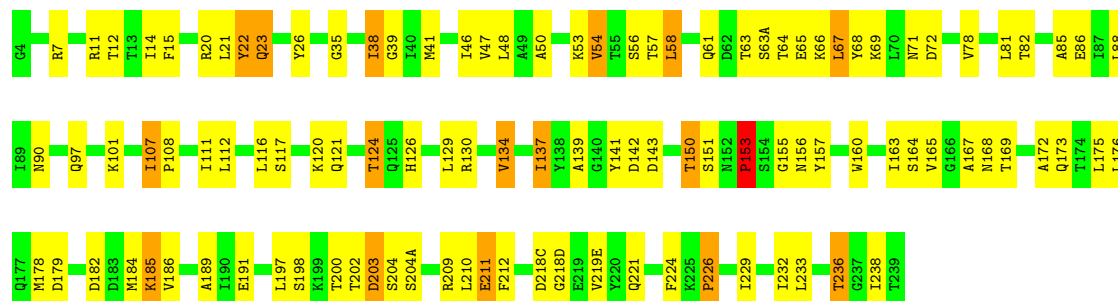
Chain B: 52% 42% 5%





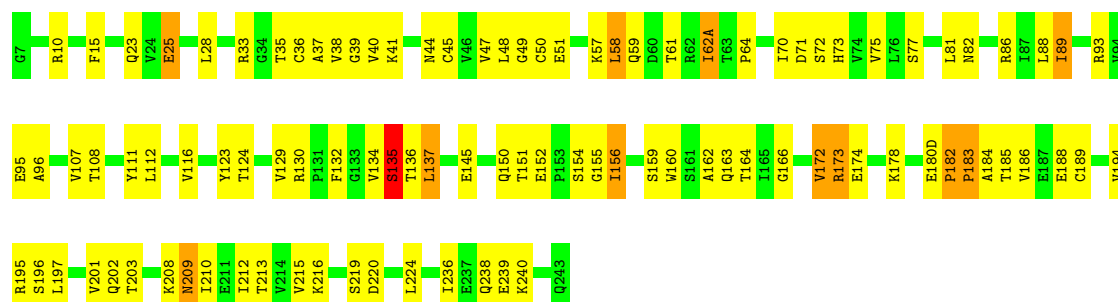
• Molecule 2: PROTEASOME COMPONENT Y13

Chain W: 56% 37% 7%



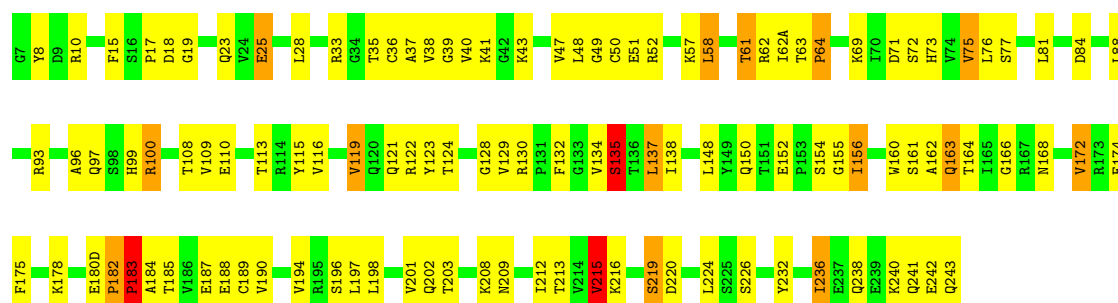
• Molecule 3: PROTEASOME COMPONENT PRE6

Chain C: 59% 37% 5%



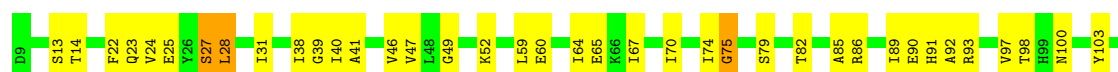
• Molecule 3: PROTEASOME COMPONENT PRE6

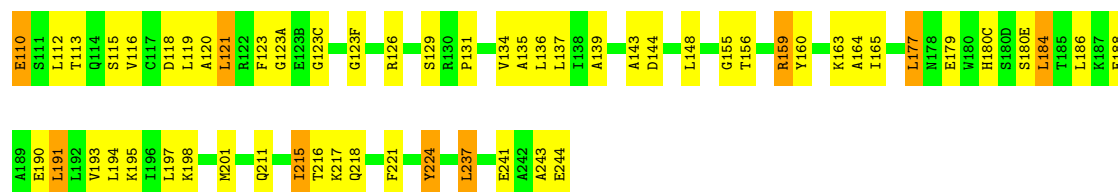
Chain X: 52% 41% 6%



• Molecule 4: PROTEASOME COMPONENT PUP2

Chain D: 61% 34% 5%

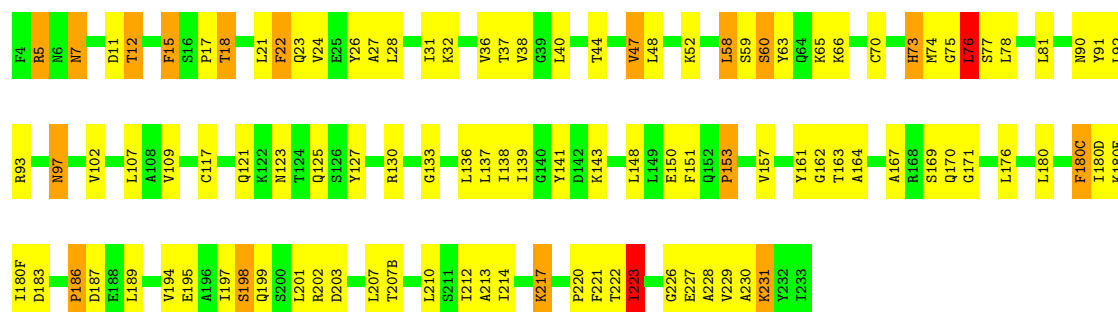




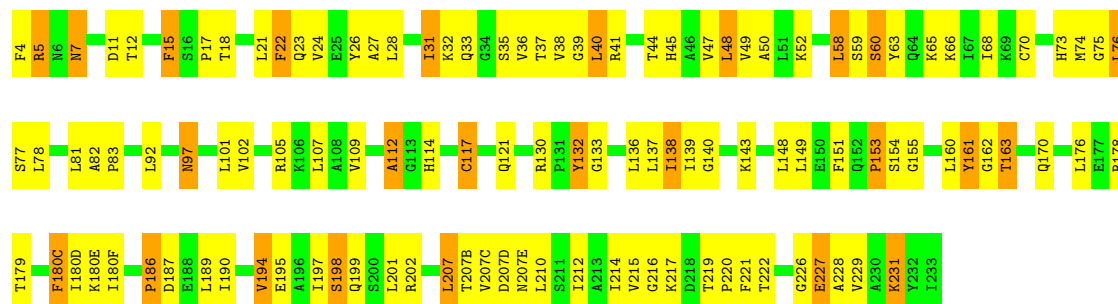
• Molecule 4: PROTEASOME COMPONENT PUP2



• Molecule 5: PROTEASOME COMPONENT PRE5

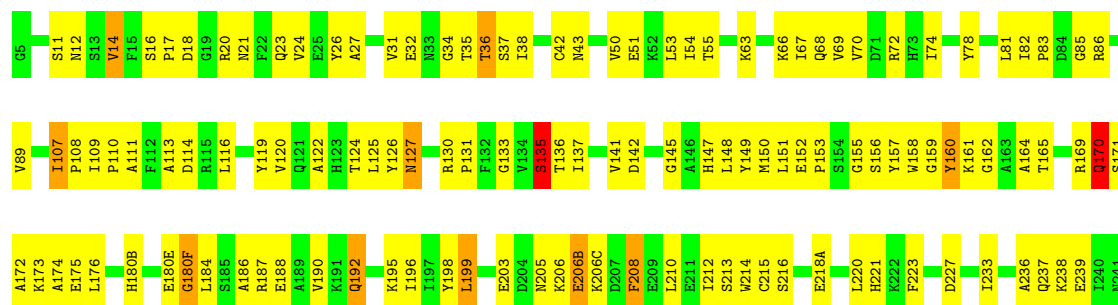


• Molecule 5: PROTEASOME COMPONENT PRE5

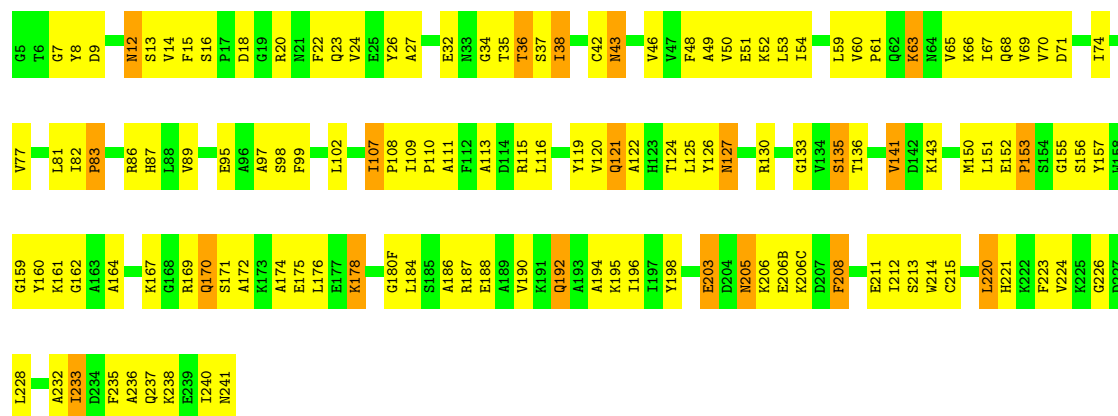


• Molecule 6: PROTEASOME COMPONENT C1

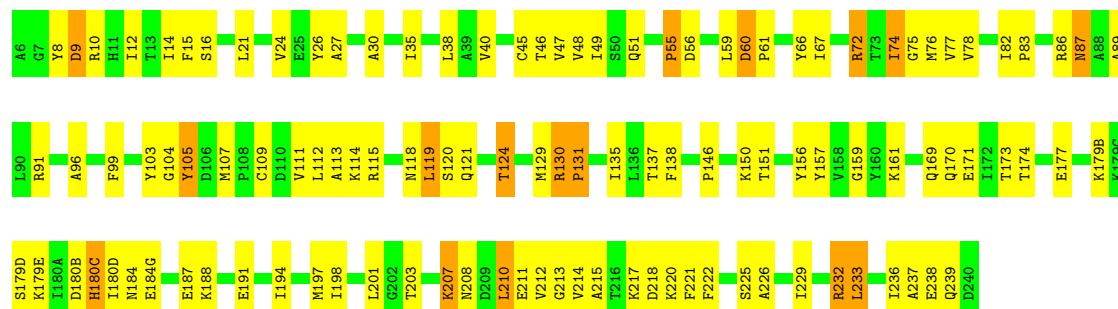




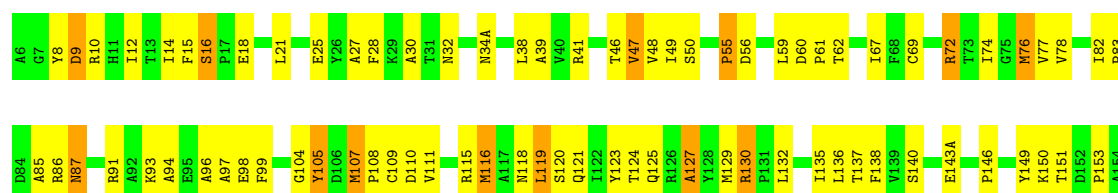
• Molecule 6: PROTEASOME COMPONENT C1

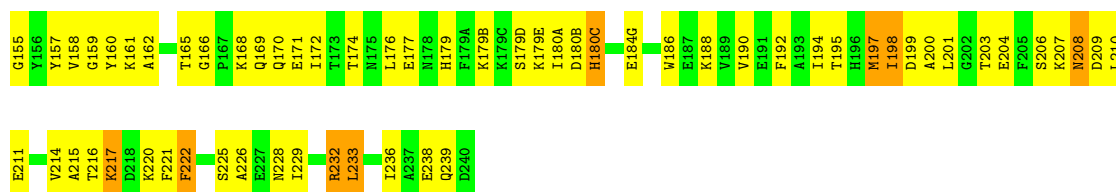


• Molecule 7: PROTEASOME COMPONENT C7-ALPHA

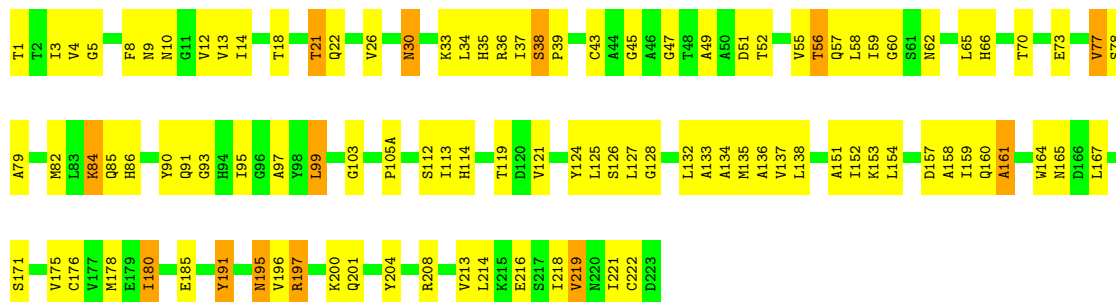


• Molecule 7: PROTEASOME COMPONENT C7-ALPHA

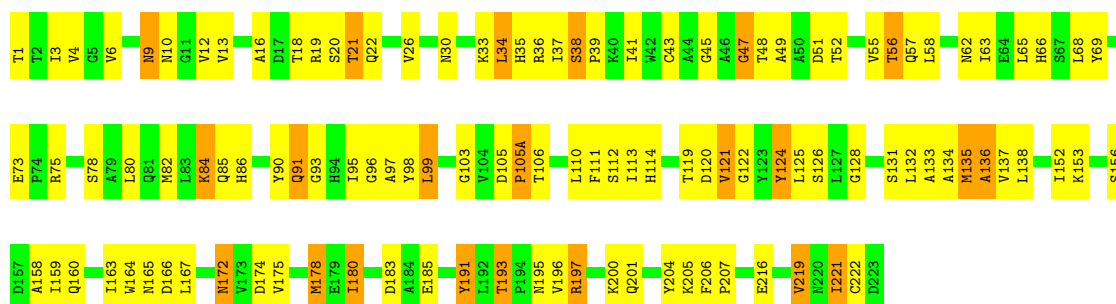




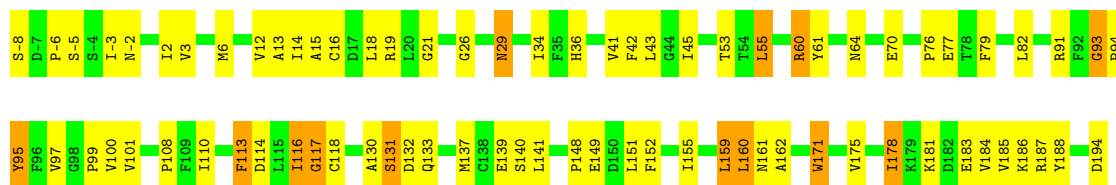
• Molecule 8: PROTEASOME COMPONENT PUP1



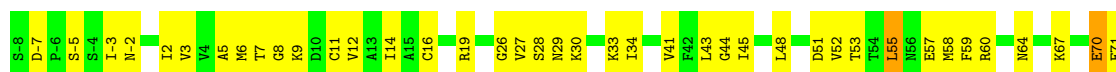
• Molecule 8: PROTEASOME COMPONENT PUP1

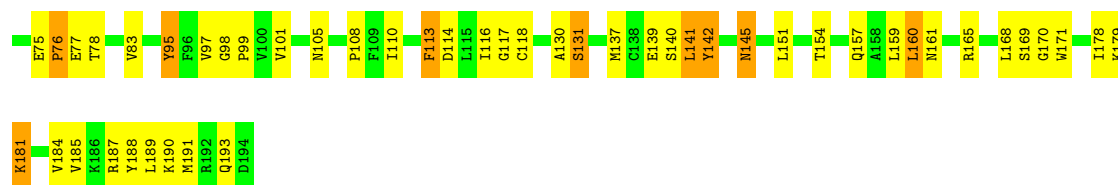


• Molecule 9: PROTEASOME COMPONENT PUP3



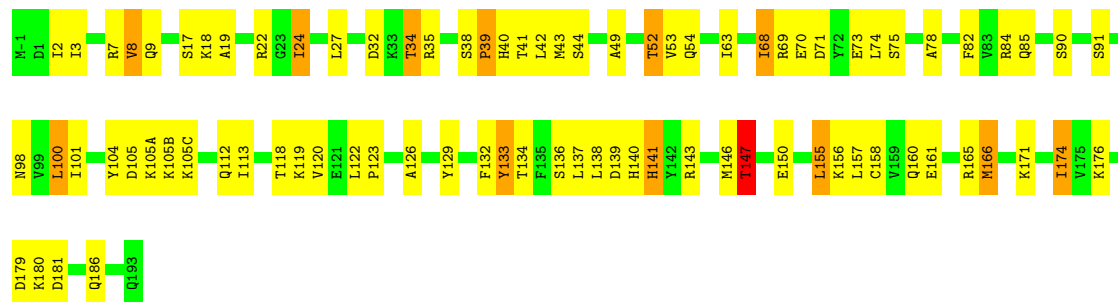
• Molecule 9: PROTEASOME COMPONENT PUP3





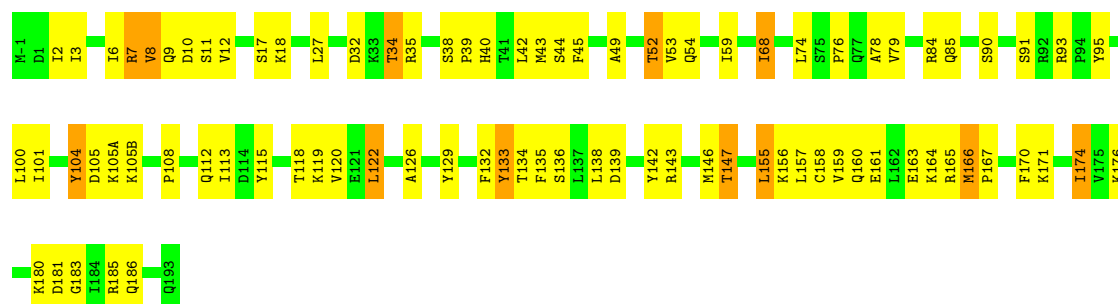
• Molecule 10: PROTEASOME COMPONENT C11

Chain J: 58% 36% 6%



• Molecule 10: PROTEASOME COMPONENT C11

Chain Q: 57% 37% 6%



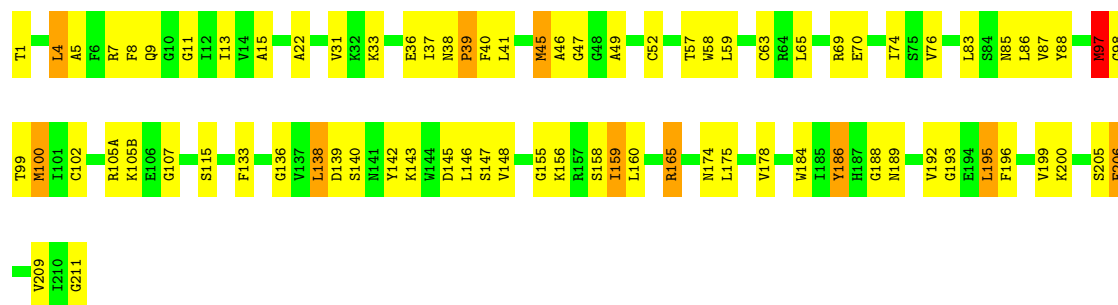
• Molecule 11: PROTEASOME COMPONENT PRE2

Chain K: 57% 37% 6%

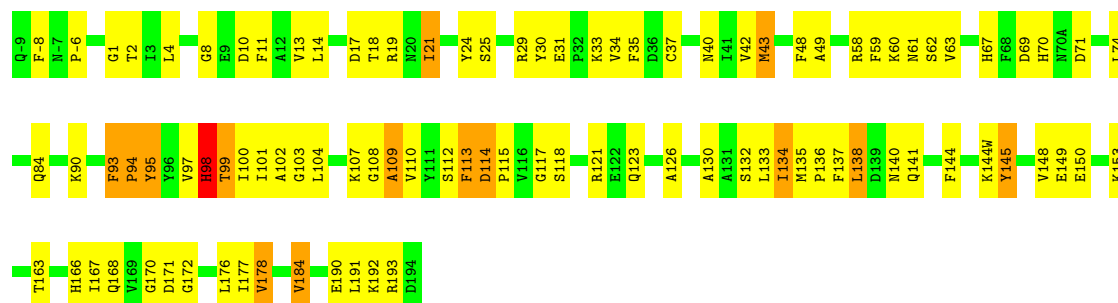


• Molecule 11: PROTEASOME COMPONENT PRE2

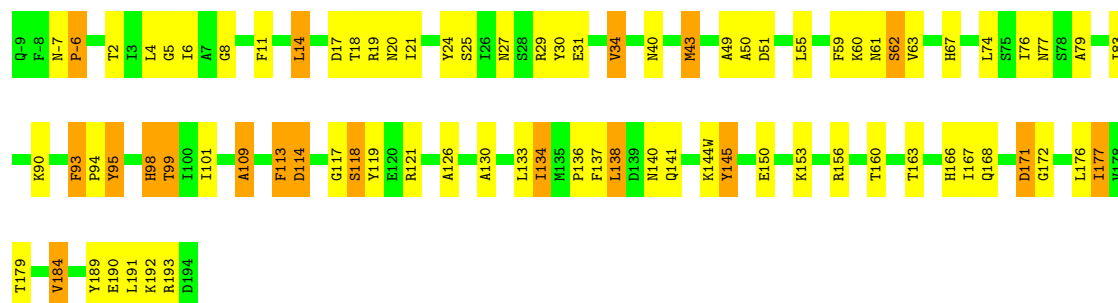
Chain R: 62% 33% 5%



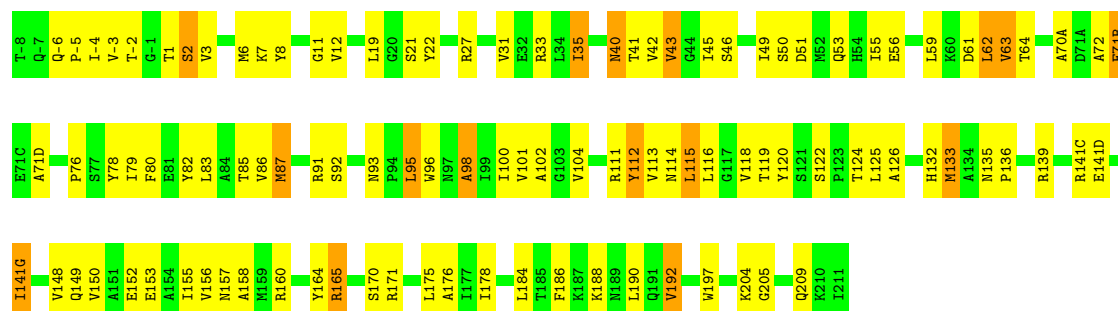
• Molecule 12: PROTEASOME COMPONENT C5



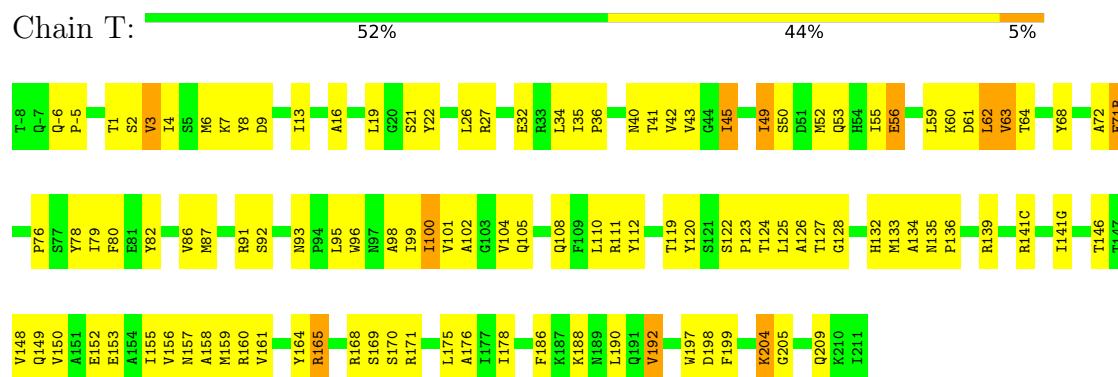
• Molecule 12: PROTEASOME COMPONENT C5



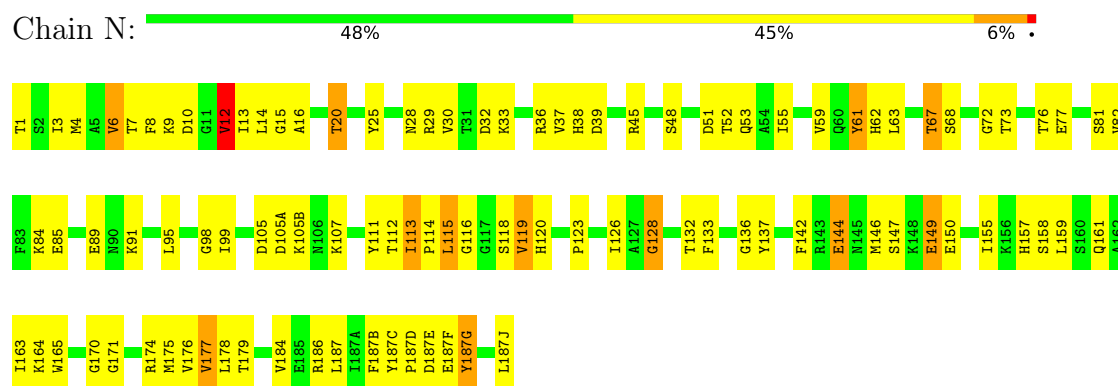
• Molecule 13: PROTEASOME COMPONENT PRE4



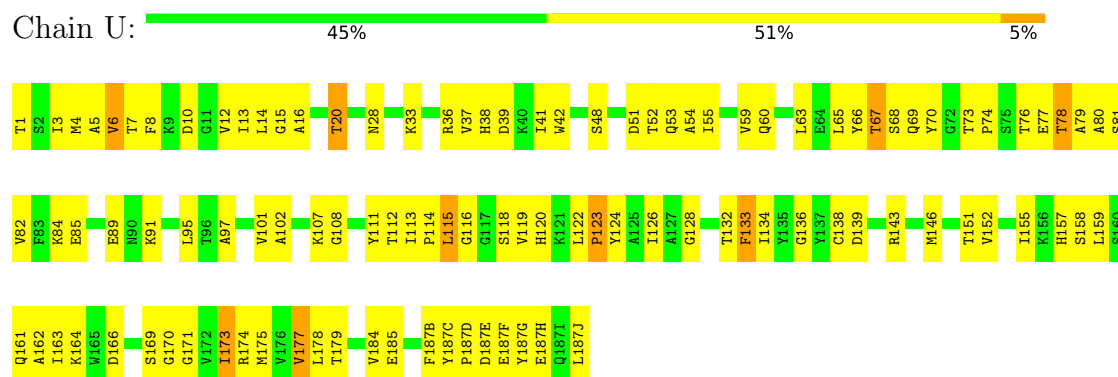
- Molecule 13: PROTEASOME COMPONENT PRE4



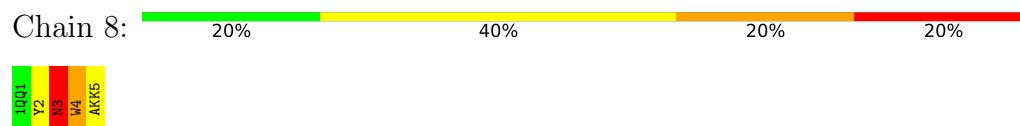
- Molecule 14: PROTEASOME COMPONENT PRE3



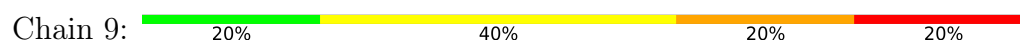
- Molecule 14: PROTEASOME COMPONENT PRE3



- Molecule 15: TMC-95A inhibitor



- Molecule 15: TMC-95A inhibitor





4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	135.20Å 301.30Å 144.80Å 90.00° 112.60° 90.00°	Depositor
Resolution (Å)	50.00 – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) (50.00-3.00)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.251 , 0.336	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	52549	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: R4K, 1QQ, AKK, MG

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	0.87	1/1952 (0.1%)	1.13	13/2642 (0.5%)
1	V	0.82	1/1952 (0.1%)	1.14	17/2642 (0.6%)
2	B	0.89	0/1935	1.11	14/2618 (0.5%)
2	W	0.84	0/1935	1.13	14/2618 (0.5%)
3	C	0.85	1/1920 (0.1%)	1.11	16/2598 (0.6%)
3	X	0.76	0/1920	1.10	16/2598 (0.6%)
4	D	0.82	1/1887 (0.1%)	1.08	14/2541 (0.6%)
4	Y	0.80	1/1887 (0.1%)	1.06	14/2541 (0.6%)
5	E	0.73	0/1823	1.12	15/2463 (0.6%)
5	Z	0.74	0/1823	1.13	14/2463 (0.6%)
6	1	0.81	1/1937 (0.1%)	1.15	16/2614 (0.6%)
6	F	0.78	0/1937	1.15	16/2614 (0.6%)
7	2	0.96	4/1959 (0.2%)	1.17	14/2652 (0.5%)
7	G	0.86	1/1959 (0.1%)	1.15	18/2652 (0.7%)
8	H	0.97	0/1716	1.18	13/2326 (0.6%)
8	O	0.96	2/1716 (0.1%)	1.16	19/2326 (0.8%)
9	I	1.00	0/1611	1.20	15/2174 (0.7%)
9	P	1.02	0/1611	1.17	12/2174 (0.6%)
10	J	0.96	0/1613	1.13	12/2173 (0.6%)
10	Q	0.93	0/1613	1.14	15/2173 (0.7%)
11	K	0.96	0/1681	1.13	14/2274 (0.6%)
11	R	0.93	1/1681 (0.1%)	1.13	15/2274 (0.7%)
12	L	1.00	0/1795	1.19	15/2420 (0.6%)
12	S	0.92	0/1795	1.19	18/2420 (0.7%)
13	M	0.98	3/1855 (0.2%)	1.15	12/2514 (0.5%)
13	T	0.98	1/1855 (0.1%)	1.17	14/2514 (0.6%)
14	N	1.03	1/1541 (0.1%)	1.16	15/2087 (0.7%)
14	U	0.99	1/1541 (0.1%)	1.14	10/2087 (0.5%)
15	8	2.17	1/20 (5.0%)	3.13	2/26 (7.7%)
15	9	2.59	2/20 (10.0%)	3.59	2/26 (7.7%)
All	All	0.90	23/50490 (0.0%)	1.14	414/68244 (0.6%)

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
11	R	0	1
15	8	0	1
15	9	0	1
All	All	0	3

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	2	107	MET	SD-CE	-7.95	1.59	1.79
13	M	141(G)	ILE	CA-CB	-6.81	1.50	1.54
7	2	76	MET	SD-CE	-6.50	1.63	1.79
13	M	87	MET	SD-CE	-6.15	1.64	1.79
1	A	120	MET	SD-CE	-5.95	1.64	1.79
13	M	133	MET	SD-CE	-5.92	1.64	1.79
13	T	87	MET	SD-CE	-5.86	1.64	1.79
4	Y	97	VAL	CA-CB	-5.86	1.47	1.54
11	R	97	MET	SD-CE	-5.82	1.65	1.79
15	9	2	TYR	C-N	5.82	1.41	1.33
8	O	178	MET	SD-CE	-5.77	1.65	1.79
8	O	135	MET	SD-CE	-5.75	1.65	1.79
1	V	120	MET	SD-CE	-5.61	1.65	1.79
15	8	2	TYR	C-N	5.59	1.41	1.33
15	9	3	ASN	CG-ND2	5.48	1.44	1.33
7	2	197	MET	SD-CE	-5.41	1.66	1.79
3	C	89	ILE	CA-CB	-5.39	1.48	1.54
4	D	136	LEU	CA-C	-5.34	1.46	1.52
14	N	119	VAL	CA-CB	-5.33	1.48	1.54
14	U	54	ALA	CA-CB	-5.21	1.45	1.53
7	2	116	MET	SD-CE	-5.15	1.66	1.79
7	G	24	VAL	CA-CB	-5.04	1.48	1.54
6	1	113	ALA	CA-CB	-5.03	1.45	1.53

All (414) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	9	3	ASN	OD1-CG-ND2	-14.75	107.85	122.60
15	8	3	ASN	OD1-CG-ND2	-13.11	109.49	122.60
13	T	27	ARG	N-CA-C	11.40	123.68	111.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	27	ARG	N-CA-C	11.12	123.37	111.03
2	B	107	ILE	N-CA-C	10.76	117.89	108.63
13	M	93	ASN	CA-C-N	10.74	131.42	119.92
13	M	93	ASN	C-N-CA	10.74	131.42	119.92
2	W	107	ILE	N-CA-C	10.47	117.63	108.63
12	L	134	ILE	N-CA-C	10.29	121.12	110.72
14	U	113	ILE	CA-C-N	9.45	129.57	120.31
14	U	113	ILE	C-N-CA	9.45	129.57	120.31
8	O	180	ILE	N-CA-C	9.34	120.17	110.36
1	A	161	LYS	N-CA-C	-9.11	101.25	111.82
9	I	93	GLY	CA-C-N	9.07	129.01	120.03
9	I	93	GLY	C-N-CA	9.07	129.01	120.03
8	H	180	ILE	N-CA-C	8.92	120.79	110.62
1	V	106	TYR	CA-C-N	8.90	126.06	119.66
1	V	106	TYR	C-N-CA	8.90	126.06	119.66
9	P	95	TYR	N-CA-C	-8.87	94.74	109.46
13	T	98	ALA	N-CA-C	-8.62	94.20	108.34
12	S	134	ILE	N-CA-C	8.48	119.29	110.72
7	2	104	GLY	N-CA-C	8.48	125.17	115.08
13	T	93	ASN	CA-C-N	8.47	128.99	119.92
13	T	93	ASN	C-N-CA	8.47	128.99	119.92
6	F	16	SER	CA-C-N	-8.47	111.05	120.45
6	F	16	SER	C-N-CA	-8.47	111.05	120.45
11	K	11	GLY	N-CA-C	8.45	120.00	111.21
7	G	78	VAL	N-CA-C	8.39	119.86	108.11
11	R	47	GLY	N-CA-C	-8.19	102.69	111.21
12	L	98	HIS	N-CA-C	-8.09	95.34	108.52
6	1	107	ILE	CA-C-N	8.07	127.83	119.76
6	1	107	ILE	C-N-CA	8.07	127.83	119.76
6	1	161	LYS	N-CA-C	-8.05	102.36	112.90
1	V	161	LYS	N-CA-C	-8.04	102.09	112.23
8	H	37	ILE	N-CA-C	-8.02	104.06	111.67
11	K	178	VAL	N-CA-C	7.95	119.36	107.75
11	K	57	THR	N-CA-C	-7.91	102.61	111.07
14	U	37	VAL	N-CA-C	-7.90	105.62	113.20
14	N	165	TRP	N-CA-C	7.86	120.99	111.40
11	K	159	ILE	N-CA-C	-7.74	103.14	110.42
1	V	61	SER	N-CA-C	7.73	119.34	111.07
7	2	239	GLN	N-CA-C	-7.71	101.73	112.45
7	2	161	LYS	N-CA-C	-7.71	102.87	111.82
4	D	123(A)	GLY	N-CA-C	7.71	120.47	110.45
5	Z	5	ARG	N-CA-C	7.71	120.42	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	L	117	GLY	N-CA-C	7.68	124.91	114.92
10	Q	165	ARG	N-CA-C	7.66	122.65	113.16
3	C	62(A)	ILE	N-CA-C	7.55	118.84	111.67
7	G	161	LYS	N-CA-C	-7.50	103.39	112.54
12	L	95	TYR	N-CA-C	-7.46	97.10	108.96
12	L	178	VAL	N-CA-C	7.42	118.58	107.75
4	D	137	LEU	N-CA-C	-7.41	97.14	109.07
14	U	73	THR	CA-C-N	7.40	127.98	120.14
14	U	73	THR	C-N-CA	7.40	127.98	120.14
12	S	113	PHE	N-CA-C	7.37	121.55	109.24
13	M	98	ALA	N-CA-C	-7.36	96.28	108.34
9	P	60	ARG	N-CA-C	-7.32	102.99	110.97
9	P	142	TYR	N-CA-C	7.30	120.82	110.23
3	X	100	ARG	N-CA-C	-7.29	103.27	111.14
4	Y	155	GLY	N-CA-C	-7.27	105.28	113.79
11	R	188	GLY	N-CA-C	7.25	120.42	112.29
1	A	78	TYR	N-CA-C	7.25	117.84	108.34
8	H	45	GLY	N-CA-C	7.23	123.17	111.38
11	K	195	LEU	N-CA-C	7.21	119.22	111.36
12	L	93	PHE	CA-C-N	7.21	128.85	119.84
12	L	93	PHE	C-N-CA	7.21	128.85	119.84
11	R	57	THR	N-CA-C	-7.20	103.36	111.07
7	2	135	ILE	N-CA-C	-7.19	98.05	108.11
7	2	180(A)	ILE	N-CA-C	7.16	119.34	109.46
13	T	95	LEU	N-CA-C	-7.09	97.17	108.73
11	K	47	GLY	N-CA-C	-7.04	103.89	111.21
1	A	109	THR	N-CA-C	7.02	119.53	111.11
5	E	102	VAL	N-CA-C	7.01	117.80	110.72
2	W	210	LEU	N-CA-C	6.98	119.79	109.24
12	L	114	ASP	CA-C-N	-6.95	112.41	120.12
12	L	114	ASP	C-N-CA	-6.95	112.41	120.12
1	V	144	PHE	N-CA-C	6.95	121.92	113.38
10	J	165	ARG	N-CA-C	6.94	121.84	112.88
13	M	165	ARG	N-CA-C	6.93	121.78	113.12
1	A	182	ASP	N-CA-C	6.91	120.37	112.57
6	1	22	PHE	N-CA-C	6.89	118.45	111.07
5	Z	22	PHE	N-CA-C	6.88	118.44	111.07
6	F	107	ILE	CA-C-N	6.87	126.79	119.85
6	F	107	ILE	C-N-CA	6.87	126.79	119.85
13	M	22	TYR	N-CA-C	-6.87	99.36	109.11
13	T	165	ARG	N-CA-C	6.87	121.99	112.45
6	F	135	SER	N-CA-C	-6.86	98.22	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	9	3	ASN	CB-CG-OD1	-6.84	107.12	120.80
12	S	114	ASP	CA-C-N	-6.83	112.54	120.12
12	S	114	ASP	C-N-CA	-6.83	112.54	120.12
5	E	22	PHE	N-CA-C	6.81	119.28	111.11
15	8	3	ASN	CB-CG-OD1	-6.81	107.18	120.80
3	C	173	ARG	N-CA-C	-6.80	103.86	111.28
8	O	45	GLY	N-CA-C	6.77	121.26	110.90
4	Y	143	ALA	N-CA-C	6.76	119.49	111.71
14	N	73	THR	CA-C-N	6.76	127.31	120.14
14	N	73	THR	C-N-CA	6.76	127.31	120.14
5	E	5	ARG	N-CA-C	6.76	119.22	111.11
4	D	144	ASP	N-CA-C	6.75	120.00	111.69
14	N	37	VAL	N-CA-C	-6.75	106.65	113.47
9	P	178	ILE	N-CA-C	6.75	118.20	108.48
13	M	45	ILE	N-CA-C	6.73	117.81	108.12
1	A	61	SER	N-CA-C	6.72	119.17	111.11
12	S	34	VAL	N-CA-C	-6.71	97.84	107.77
8	O	37	ILE	N-CA-C	-6.67	105.25	111.45
4	Y	129	SER	N-CA-C	6.67	120.87	112.87
10	J	122	LEU	N-CA-C	6.66	115.98	108.25
2	W	211	GLU	N-CA-C	-6.65	98.13	109.24
9	I	60	ARG	N-CA-C	-6.64	103.73	110.97
12	L	114	ASP	N-CA-C	-6.62	100.67	110.20
10	J	141	HIS	N-CA-C	6.62	120.82	113.21
7	G	239	GLN	N-CA-C	-6.61	103.26	112.45
14	N	133	PHE	N-CA-C	6.61	121.05	113.19
14	N	91	LYS	N-CA-C	6.60	119.31	111.33
4	Y	224	TYR	N-CA-C	6.58	119.26	109.59
10	Q	183	GLY	N-CA-C	6.57	118.04	111.21
2	W	238	ILE	N-CA-C	-6.55	103.12	112.35
9	P	141	LEU	N-CA-C	6.53	118.39	111.28
1	A	184	LEU	N-CA-C	6.52	120.28	109.46
3	X	61	THR	N-CA-C	6.51	119.20	111.33
4	Y	169	SER	N-CA-C	6.50	118.06	110.97
10	Q	93	ARG	CA-C-N	6.50	126.53	119.90
10	Q	93	ARG	C-N-CA	6.50	126.53	119.90
1	A	137	LEU	N-CA-C	-6.49	98.32	108.90
2	B	161	LYS	N-CA-C	-6.48	105.19	113.23
9	P	98	GLY	CA-C-N	6.47	126.45	119.78
9	P	98	GLY	C-N-CA	6.47	126.45	119.78
11	K	188	GLY	N-CA-C	6.44	120.13	112.33
4	D	143	ALA	N-CA-C	6.44	119.99	111.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	U	91	LYS	N-CA-C	6.44	119.12	111.33
9	I	117	GLY	N-CA-C	6.43	121.32	113.79
4	Y	179	GLU	N-CA-C	6.42	121.11	113.28
1	V	154	SER	N-CA-C	-6.41	104.38	111.82
12	S	-7	ASN	CA-C-N	6.41	127.85	119.84
12	S	-7	ASN	C-N-CA	6.41	127.85	119.84
3	C	145	GLU	CA-C-N	6.40	126.92	120.14
3	C	145	GLU	C-N-CA	6.40	126.92	120.14
2	W	50	ALA	N-CA-C	6.36	118.98	108.99
7	G	104	GLY	N-CA-C	6.36	122.52	114.25
1	A	135	SER	N-CA-C	-6.33	99.49	109.50
6	1	16	SER	CA-C-N	-6.33	113.09	120.12
6	1	16	SER	C-N-CA	-6.33	113.09	120.12
11	R	45	MET	N-CA-C	6.31	119.19	108.90
14	N	113	ILE	CA-C-N	6.31	126.50	120.31
14	N	113	ILE	C-N-CA	6.31	126.50	120.31
2	B	137	ILE	N-CA-C	-6.31	98.54	107.75
13	T	9	ASP	N-CA-C	6.30	119.82	111.75
10	Q	134	THR	N-CA-C	6.29	118.22	111.36
6	1	135	SER	N-CA-C	-6.29	99.66	109.72
3	X	182	PRO	CA-C-N	6.28	127.69	119.84
3	X	182	PRO	C-N-CA	6.28	127.69	119.84
14	N	187(G)	TYR	N-CA-C	6.27	118.92	111.71
2	W	233	LEU	N-CA-C	6.27	118.11	111.28
12	L	109	ALA	N-CA-C	6.25	118.36	108.79
8	H	171	SER	N-CA-C	6.25	119.11	108.67
6	1	14	VAL	N-CA-C	6.25	117.13	108.89
4	D	82	THR	N-CA-C	6.24	118.89	111.71
6	1	141	VAL	N-CA-C	6.24	117.47	108.48
6	F	63	LYS	N-CA-C	6.24	121.41	113.55
5	E	223	ILE	N-CA-C	6.23	116.36	106.88
5	E	180(C)	PHE	N-CA-C	6.23	120.62	112.89
10	J	82	PHE	N-CA-C	-6.20	104.44	111.07
5	E	228	ALA	N-CA-C	6.19	119.93	112.38
1	V	158	PHE	CA-C-N	6.19	127.57	119.84
1	V	158	PHE	C-N-CA	6.19	127.57	119.84
2	B	210	LEU	N-CA-C	6.18	119.27	109.81
11	R	11	GLY	N-CA-C	6.18	117.80	111.56
3	C	108	THR	N-CA-C	-6.17	102.22	110.55
7	G	103	TYR	N-CA-C	6.17	120.96	113.38
2	W	179	ASP	N-CA-C	6.16	120.80	113.28
12	S	98	HIS	N-CA-C	-6.16	97.10	107.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	P	-3	ILE	CB-CA-C	-6.15	103.97	112.02
3	C	186	VAL	N-CA-C	-6.14	104.34	110.30
6	F	180(B)	HIS	N-CA-C	6.13	119.23	111.69
7	G	135	ILE	N-CA-C	-6.12	99.60	108.17
8	O	47	GLY	N-CA-C	-6.12	105.38	111.56
11	K	24	ASN	N-CA-C	-6.12	105.97	113.50
12	L	113	PHE	N-CA-C	6.12	119.17	109.50
5	Z	102	VAL	N-CA-C	6.12	118.73	111.09
5	E	60	SER	N-CA-C	-6.11	102.30	110.55
4	D	129	SER	N-CA-C	6.11	120.34	113.01
5	Z	210	LEU	N-CA-C	6.10	118.58	110.53
10	Q	90	SER	N-CA-C	6.10	118.89	111.82
8	H	161	ALA	N-CA-C	-6.08	104.34	110.97
1	V	128	GLY	N-CA-C	6.06	124.03	115.30
6	F	160	TYR	N-CA-C	6.05	118.77	108.90
10	J	134	THR	N-CA-C	6.05	119.13	111.69
5	Z	60	SER	N-CA-C	-6.05	102.38	110.55
11	K	7	ARG	N-CA-C	6.04	119.55	109.95
10	J	100	LEU	N-CA-C	-6.03	99.08	108.90
6	F	161	LYS	N-CA-C	-6.01	104.85	111.82
2	W	137	ILE	N-CA-C	-6.00	98.89	107.77
5	Z	31	ILE	N-CA-C	-6.00	104.89	110.53
1	V	135	SER	N-CA-C	-5.99	99.63	109.40
3	C	135	SER	N-CA-C	-5.99	99.95	109.23
11	R	8	PHE	N-CA-C	5.99	115.75	107.73
4	Y	218	GLN	N-CA-C	5.97	117.46	111.07
3	X	119	VAL	N-CA-C	-5.97	104.69	110.42
13	M	71(B)	GLU	N-CA-C	5.96	123.50	110.80
13	T	56	GLU	N-CA-C	-5.96	104.47	110.97
10	Q	95	TYR	N-CA-C	-5.95	101.03	109.96
8	H	9	ASN	N-CA-C	5.95	123.48	110.80
1	A	179	ARG	N-CA-C	5.94	120.26	112.89
1	V	179	ARG	N-CA-C	5.92	120.35	113.18
4	D	218	GLN	N-CA-C	5.92	117.42	110.97
7	G	218	ASP	N-CA-C	5.92	121.79	113.56
3	X	135	SER	N-CA-C	-5.92	100.06	109.23
1	V	23	GLN	N-CA-C	5.91	119.32	111.75
2	W	78	VAL	N-CA-C	5.90	117.09	108.53
8	O	73	GLU	N-CA-C	-5.90	102.61	109.93
2	B	211	GLU	N-CA-C	-5.89	99.06	109.06
6	I	180(F)	GLY	N-CA-C	-5.87	104.80	111.85
3	C	219	SER	N-CA-C	5.87	119.52	111.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	J	19	ALA	N-CA-C	5.82	119.03	109.72
2	W	12	THR	N-CA-C	5.82	119.64	112.54
4	Y	137	LEU	N-CA-C	-5.82	99.71	109.07
10	J	147	THR	N-CA-C	-5.80	102.71	110.55
10	Q	171	LYS	N-CA-C	5.80	119.56	111.90
1	A	128	GLY	N-CA-C	5.79	123.64	115.30
7	G	130	ARG	CA-C-N	-5.78	114.80	120.52
7	G	130	ARG	C-N-CA	-5.78	114.80	120.52
11	R	22	ALA	N-CA-C	-5.78	100.39	108.54
6	F	124	THR	N-CA-C	-5.77	103.82	112.54
6	F	142	ASP	N-CA-C	5.74	116.96	108.86
2	W	23	GLN	N-CA-C	5.73	118.26	111.33
9	I	18	LEU	N-CA-C	5.73	119.25	112.72
9	I	94	PRO	N-CA-C	5.72	119.99	111.41
1	A	144	PHE	N-CA-C	5.72	120.53	113.50
9	P	-7	ASP	N-CA-C	-5.72	97.39	108.59
7	G	60	ASP	CA-C-N	5.71	126.98	119.84
7	G	60	ASP	C-N-CA	5.71	126.98	119.84
12	S	95	TYR	N-CA-C	-5.71	99.21	108.41
5	E	73	HIS	N-CA-C	5.71	120.99	112.94
12	L	21	ILE	N-CA-C	5.71	117.06	108.96
3	X	62	ARG	N-CA-C	5.69	117.94	111.11
6	1	124	THR	N-CA-C	-5.69	104.56	112.30
12	S	109	ALA	N-CA-C	5.69	117.49	108.79
9	I	-3	ILE	CB-CA-C	-5.68	104.44	111.94
2	B	72	ASP	N-CA-C	-5.68	106.31	113.18
1	V	137	LEU	N-CA-C	-5.66	99.18	108.41
2	B	179	ASP	N-CA-C	5.66	120.05	113.20
9	I	95	TYR	N-CA-C	-5.66	99.97	108.96
5	Z	112	ALA	N-CA-C	-5.65	105.12	111.28
1	A	66	LYS	N-CA-C	-5.64	106.24	113.23
4	D	155	GLY	N-CA-C	-5.63	107.98	114.69
1	V	185	GLU	N-CA-C	-5.63	102.14	110.48
8	O	20	SER	N-CA-C	-5.63	100.53	109.59
5	Z	132	TYR	N-CA-C	-5.61	101.34	110.20
13	M	95	LEU	N-CA-C	-5.60	98.62	108.20
2	B	134	VAL	N-CA-C	5.60	115.74	108.35
4	Y	144	ASP	N-CA-C	5.60	120.23	112.45
5	Z	228	ALA	N-CA-C	5.60	119.37	112.54
9	I	116	ILE	N-CA-C	5.59	117.81	111.88
7	G	16	SER	N-CA-C	-5.59	102.08	110.24
14	U	133	PHE	N-CA-C	5.59	119.80	113.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	210	LEU	N-CA-C	5.59	117.90	110.53
8	O	9	ASN	N-CA-C	5.58	122.68	110.80
5	Z	180(C)	PHE	N-CA-C	5.58	119.26	112.23
3	C	155	GLY	N-CA-C	-5.57	107.68	114.92
5	E	7	ASN	N-CA-C	-5.57	106.84	113.97
13	M	132	HIS	N-CA-C	5.57	117.43	111.36
4	Y	123(A)	GLY	N-CA-C	5.57	117.69	110.45
9	I	178	ILE	N-CA-C	5.55	116.48	108.48
8	O	183	ASP	N-CA-C	-5.55	103.05	110.55
8	O	98	TYR	N-CA-C	-5.54	98.32	108.02
4	Y	75	GLY	N-CA-C	-5.54	103.01	111.10
9	P	116	ILE	N-CA-C	5.54	117.75	111.88
4	D	103	TYR	N-CA-C	5.53	122.62	113.89
8	O	38	SER	N-CA-C	-5.53	99.93	108.55
2	W	203	ASP	N-CA-C	-5.53	106.54	113.28
5	E	76	LEU	N-CA-C	5.52	117.18	108.96
12	L	10	ASP	N-CA-C	5.52	117.95	110.06
1	V	182	ASP	N-CA-C	5.51	119.75	112.25
7	G	66	TYR	N-CA-C	-5.50	103.96	111.56
4	D	179	GLU	N-CA-C	5.50	119.99	113.28
3	X	155	GLY	N-CA-C	-5.50	107.44	114.37
3	C	182	PRO	CA-C-N	5.50	126.71	119.84
3	C	182	PRO	C-N-CA	5.50	126.71	119.84
12	L	84	GLN	N-CA-C	-5.50	105.19	111.07
11	K	107	GLY	N-CA-C	-5.49	101.13	112.34
7	2	47	VAL	N-CA-C	5.49	117.81	108.86
14	N	128	GLY	N-CA-C	-5.48	104.83	112.18
11	R	165	ARG	N-CA-C	5.48	118.09	111.40
11	R	107	GLY	N-CA-C	-5.48	101.16	112.34
13	M	35	ILE	N-CA-C	5.48	112.97	107.55
12	S	117	GLY	N-CA-C	5.47	122.87	115.32
3	X	41	LYS	N-CA-C	5.46	118.38	109.59
10	Q	27	LEU	N-CA-C	5.45	118.14	111.82
12	S	93	PHE	CA-C-N	5.45	126.65	119.84
12	S	93	PHE	C-N-CA	5.45	126.65	119.84
5	Z	161	TYR	N-CA-C	-5.44	106.48	113.23
14	N	98	GLY	N-CA-C	-5.43	100.30	113.18
8	H	38	SER	N-CA-C	-5.43	101.95	108.25
6	1	63	LYS	N-CA-C	5.43	120.15	112.93
11	K	98	GLY	N-CA-C	-5.43	100.31	113.18
3	X	108	THR	N-CA-C	-5.43	101.69	110.32
13	T	45	ILE	N-CA-C	5.42	116.08	108.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	99	LEU	N-CA-C	5.42	118.06	109.50
11	R	195	LEU	N-CA-C	5.41	116.86	111.07
10	Q	147	THR	N-CA-C	-5.40	103.76	110.41
11	K	206	PHE	N-CA-C	-5.40	103.96	111.52
2	B	58	LEU	N-CA-C	5.40	120.02	113.38
6	F	170	GLN	N-CA-C	5.39	117.24	111.36
3	C	210	ILE	N-CA-C	5.38	116.33	108.53
6	1	226	GLY	N-CA-C	5.38	121.13	111.34
12	S	118	SER	N-CA-C	-5.38	101.69	109.59
8	H	73	GLU	N-CA-C	-5.37	102.67	110.08
10	Q	166	MET	CA-C-N	5.37	124.83	119.24
10	Q	166	MET	C-N-CA	5.37	124.83	119.24
4	D	75	GLY	N-CA-C	-5.37	102.96	110.96
6	1	107	ILE	N-CA-C	5.37	120.48	108.88
8	O	84	LYS	N-CA-C	5.37	116.81	111.07
10	J	24	ILE	N-CA-C	5.36	121.15	113.16
12	S	31	GLU	CA-C-N	5.36	125.35	119.89
12	S	31	GLU	C-N-CA	5.36	125.35	119.89
7	2	16	SER	N-CA-C	-5.35	102.42	110.24
2	B	23	GLN	N-CA-C	5.35	117.80	111.33
3	C	107	VAL	CB-CA-C	-5.35	103.22	111.08
6	F	206(B)	GLU	N-CA-C	5.35	119.06	112.54
8	O	153	LYS	N-CA-C	-5.34	105.36	111.07
11	R	206	PHE	N-CA-C	-5.33	104.28	111.54
8	O	99	LEU	N-CA-C	5.33	118.25	109.72
5	E	161	TYR	N-CA-C	-5.33	105.92	112.90
11	K	209	VAL	N-CA-C	-5.31	102.22	109.55
4	Y	201	MET	N-CA-C	5.31	117.41	108.96
3	C	137	LEU	N-CA-C	-5.31	99.75	108.41
7	G	211	GLU	N-CA-C	-5.31	100.03	109.06
10	J	123	PRO	N-CA-C	-5.31	106.29	113.40
6	F	180(F)	GLY	N-CA-C	-5.31	104.57	111.52
3	C	236	ILE	N-CA-C	5.30	115.52	110.53
13	T	108	GLN	N-CA-C	-5.30	103.69	110.53
7	2	155	GLY	N-CA-C	-5.29	107.75	115.63
8	H	84	LYS	N-CA-C	5.28	116.72	111.07
4	D	224	TYR	N-CA-C	5.27	117.32	109.25
11	R	178	VAL	N-CA-C	5.27	115.55	108.17
6	F	145	GLY	N-CA-C	5.27	119.55	112.17
13	T	49	ILE	N-CA-C	5.27	115.48	110.53
7	G	131	PRO	N-CA-C	-5.26	103.28	111.13
8	O	21	THR	N-CA-C	5.25	117.73	108.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	Q	122	LEU	CA-C-N	5.25	124.57	118.85
10	Q	122	LEU	C-N-CA	5.25	124.57	118.85
13	T	71(B)	GLU	N-CA-C	5.24	121.97	110.80
3	X	161	SER	N-CA-C	-5.24	105.74	111.82
12	S	171	ASP	N-CA-C	5.23	121.95	110.80
11	R	7	ARG	N-CA-C	5.23	118.59	110.17
5	E	18	THR	N-CA-C	-5.23	106.75	113.23
2	B	78	VAL	N-CA-C	5.22	116.83	108.89
6	F	239	GLU	N-CA-C	5.22	119.40	113.19
14	N	99	ILE	N-CA-C	5.21	116.23	108.46
9	P	117	GLY	N-CA-C	5.21	121.70	114.92
8	H	195	ASN	N-CA-C	5.21	116.69	110.44
7	G	179(B)	LYS	N-CA-C	-5.21	105.72	111.71
7	2	198	ILE	N-CA-C	-5.20	105.43	110.42
5	Z	194	VAL	N-CA-C	5.19	115.81	110.36
7	2	179(B)	LYS	N-CA-C	-5.19	105.74	111.71
12	S	145	TYR	N-CA-C	5.19	117.53	108.76
3	C	41	LYS	N-CA-C	5.18	117.94	109.59
5	E	47	VAL	N-CA-C	5.18	117.08	108.99
5	E	207(B)	THR	N-CA-C	5.18	116.53	109.18
7	2	130	ARG	N-CA-C	-5.17	103.15	110.29
1	V	184	LEU	N-CA-C	5.17	118.04	109.46
7	G	74	ILE	N-CA-C	5.17	115.75	108.36
6	1	178	LYS	N-CA-C	-5.17	105.34	110.97
14	N	45	ARG	N-CA-C	5.15	117.37	109.07
11	R	140	SER	N-CA-C	5.15	117.79	111.82
9	I	26	GLY	N-CA-C	-5.15	103.56	111.64
10	J	27	LEU	N-CA-C	5.15	118.71	112.23
4	D	110	GLU	N-CA-C	-5.14	105.56	111.07
3	X	137	LEU	N-CA-C	-5.14	99.90	108.34
5	Z	7	ASN	N-CA-C	-5.14	107.39	113.97
2	B	119	ILE	N-CA-C	-5.13	105.71	110.53
14	U	70	TYR	N-CA-C	5.13	119.28	112.30
4	D	159	ARG	N-CA-C	-5.13	101.35	109.76
13	T	146	THR	N-CA-C	5.13	117.60	109.24
10	Q	45	PHE	N-CA-C	5.12	117.04	108.99
8	O	41	ILE	CB-CA-C	-5.11	105.42	111.09
9	I	116	ILE	CA-C-N	-5.11	117.36	123.44
9	I	116	ILE	C-N-CA	-5.11	117.36	123.44
9	P	145	ASN	N-CA-C	5.10	118.17	111.28
1	V	190	ILE	N-CA-C	-5.10	105.57	110.72
7	2	74	ILE	N-CA-C	5.10	115.31	108.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	142	PHE	N-CA-C	5.10	117.08	109.59
14	U	187(H)	GLU	N-CA-C	5.09	116.83	111.28
2	W	134	VAL	N-CA-C	5.09	115.07	108.35
10	J	98	ASN	N-CA-C	-5.09	101.11	109.40
5	Z	154	SER	N-CA-C	-5.08	105.86	111.71
7	G	207	LYS	N-CA-C	5.08	116.50	111.07
3	X	219	SER	N-CA-C	5.08	121.61	110.80
2	W	58	LEU	N-CA-C	5.07	119.62	113.38
11	R	159	ILE	N-CA-C	-5.07	105.77	110.53
14	N	12	VAL	N-CA-C	5.07	114.87	107.88
9	I	183	GLU	N-CA-C	5.07	117.85	109.85
8	O	191	TYR	N-CA-C	-5.06	105.84	111.36
13	T	22	TYR	N-CA-C	-5.06	101.93	109.11
6	1	38	ILE	CB-CA-C	-5.06	103.00	111.29
8	O	207	PRO	N-CA-C	-5.05	103.26	111.14
8	H	21	THR	N-CA-C	5.05	117.06	109.23
7	2	127	ALA	N-CA-C	5.05	118.54	112.38
1	A	130	ARG	N-CA-C	-5.04	102.52	110.14
3	X	215	VAL	N-CA-C	5.04	115.23	107.77
13	M	-2	THR	N-CA-C	5.04	117.81	109.85
8	H	191	TYR	N-CA-C	-5.04	105.79	111.28
9	I	93	GLY	N-CA-C	-5.03	102.07	112.34
8	O	136	ALA	N-CA-C	-5.03	105.48	110.97
4	Y	43	LYS	N-CA-C	-5.03	105.84	112.94
8	O	172	ASN	N-CA-C	5.03	117.90	110.46
11	K	8	PHE	N-CA-C	5.03	114.46	107.73
7	2	125	GLN	N-CA-C	5.01	120.38	113.97
4	Y	200	VAL	N-CA-C	5.01	117.00	112.29
2	B	50	ALA	N-CA-C	5.01	116.67	108.76
2	B	143	ASP	N-CA-C	5.00	119.09	112.89
14	U	187(C)	TYR	N-CA-C	5.00	115.88	110.13
3	X	18	ASP	N-CA-C	5.00	119.02	113.02
3	X	236	ILE	N-CA-C	5.00	115.23	110.53

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
15	8	3	ASN	Sidechain
15	9	3	ASN	Sidechain
11	R	186	TYR	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1915	0	1926	67	0
1	V	1915	0	1926	77	0
2	B	1905	0	1901	81	0
2	W	1905	0	1901	75	0
3	C	1891	0	1900	75	0
3	X	1891	0	1900	97	0
4	D	1862	0	1836	78	0
4	Y	1862	0	1836	73	0
5	E	1795	0	1797	86	0
5	Z	1795	0	1797	117	0
6	1	1897	0	1886	120	0
6	F	1897	0	1886	110	0
7	2	1921	0	1910	110	0
7	G	1921	0	1910	90	0
8	H	1685	0	1688	87	0
8	O	1685	0	1688	92	0
9	I	1581	0	1574	61	0
9	P	1581	0	1574	73	0
10	J	1585	0	1590	57	0
10	Q	1585	0	1590	65	0
11	K	1644	0	1595	80	0
11	R	1644	0	1595	60	0
12	L	1757	0	1711	84	0
12	S	1757	0	1711	83	0
13	M	1824	0	1832	78	0
13	T	1824	0	1832	96	0
14	N	1512	0	1481	77	0
14	U	1512	0	1481	84	0
15	8	49	0	36	8	0
15	9	49	0	36	7	0
16	D	1	0	0	0	0
16	F	2	0	0	0	0
16	G	1	0	0	0	0
16	H	1	0	0	0	0
16	I	2	0	0	0	0
16	L	1	0	0	0	0
16	N	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	P	1	0	0	0	0
17	1	93	0	0	3	0
17	2	103	0	0	7	0
17	8	2	0	0	0	0
17	9	1	0	0	0	0
17	A	105	0	0	1	0
17	B	80	0	0	1	0
17	C	69	0	0	3	0
17	D	90	0	0	6	0
17	E	55	0	0	3	0
17	F	99	0	0	6	0
17	G	106	0	0	3	0
17	H	114	0	0	2	0
17	I	107	0	0	3	0
17	J	116	0	0	6	0
17	K	103	0	0	4	0
17	L	140	0	0	8	0
17	M	150	0	0	3	0
17	N	116	0	0	5	0
17	O	121	0	0	3	0
17	P	101	0	0	4	0
17	Q	121	0	0	5	0
17	R	107	0	0	4	0
17	S	144	0	0	6	0
17	T	142	0	0	8	0
17	U	118	0	0	1	0
17	V	104	0	0	2	0
17	W	74	0	0	2	0
17	X	70	0	0	4	0
17	Y	89	0	0	5	0
17	Z	53	0	0	2	0
All	All	52549	0	49326	2108	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 21.

All (2108) 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)
7:2:123:TYR:O	17:2:2009:HOH:O	1.54	1.25
14:N:136:GLY:HA2	14:U:161:GLN:HE21	1.13	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:21:THR:O	15:8:4:R4K:O33	1.75	1.05
14:N:161:GLN:HE21	14:U:136:GLY:HA2	1.21	1.05
8:O:21:THR:O	15:9:4:R4K:O33	1.75	1.04
3:C:15:PHE:H	4:D:23:GLN:HE22	1.13	0.97
3:C:185:THR:HB	3:C:188:GLU:HG2	1.46	0.96
2:W:202:THR:HG22	2:W:204:SER:H	1.31	0.96
5:Z:52:LYS:HB2	5:Z:63:TYR:HB3	1.45	0.96
7:G:96:ALA:HA	7:G:107:MET:HE2	1.45	0.95
9:P:114:ASP:HB3	15:9:3:ASN:ND2	1.80	0.95
2:B:126:HIS:HB3	3:C:129:VAL:HG12	1.48	0.94
6:1:81:LEU:HD12	6:1:133:GLY:HA3	1.45	0.94
8:O:166:ASP:O	17:O:2015:HOH:O	1.84	0.94
6:1:141:VAL:HG23	6:1:215:CYS:SG	2.09	0.93
5:E:15:PHE:HB2	6:F:23:GLN:HE22	1.33	0.92
9:I:114:ASP:HB3	15:8:3:ASN:HD21	1.35	0.92
5:Z:15:PHE:HB2	6:1:23:GLN:HE22	1.35	0.92
11:K:4:LEU:HD11	11:K:15:ALA:HB3	1.51	0.91
11:K:4:LEU:HD12	11:K:159:ILE:HD11	1.52	0.91
9:I:114:ASP:HB3	15:8:3:ASN:ND2	1.85	0.91
7:2:121:GLN:O	7:2:124:THR:HB	1.70	0.90
14:U:4:MET:HB3	14:U:126:ILE:HG22	1.54	0.90
6:F:141:VAL:HG23	6:F:215:CYS:SG	2.12	0.90
11:R:105(B):LYS:H	11:R:105(B):LYS:HD2	1.34	0.90
13:M:171:ARG:HG3	13:M:192:VAL:HG23	1.53	0.89
11:K:105(B):LYS:H	11:K:105(B):LYS:HD2	1.37	0.88
7:2:96:ALA:HA	7:2:107:MET:HE2	1.56	0.87
3:X:152:GLU:HG2	3:X:156:ILE:HG22	1.57	0.87
4:Y:177:LEU:HD22	5:Z:58:LEU:HD22	1.56	0.86
12:S:43:MET:HB2	12:S:101:ILE:HG22	1.55	0.86
13:T:157:ASN:ND2	13:T:160:ARG:HH11	1.73	0.86
13:M:41:THR:OG1	13:M:76:PRO:HG3	1.74	0.86
3:X:88:LEU:HD22	3:X:116:VAL:HG13	1.57	0.86
13:T:171:ARG:HG3	13:T:192:VAL:HG23	1.58	0.85
7:G:151:THR:HG22	7:G:157:TYR:HB2	1.59	0.85
9:P:137:MET:HE2	9:P:161:ASN:HB2	1.57	0.85
3:C:152:GLU:HG2	3:C:156:ILE:HG22	1.58	0.85
4:Y:214:CYS:HG	4:Y:224:TYR:HE2	0.88	0.84
3:X:185:THR:HB	3:X:188:GLU:HG2	1.55	0.84
6:1:186:ALA:O	6:1:190:VAL:HG23	1.77	0.84
7:G:76:MET:SD	7:G:138:PHE:CE2	2.70	0.84
6:1:37:SER:HB3	6:1:50:VAL:HG23	1.60	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:S:18:THR:HG22	12:S:30:TYR:HA	1.59	0.84
3:C:35:THR:HB	3:C:51:GLU:HG3	1.61	0.83
1:V:124:THR:HG22	2:W:130:ARG:HH21	1.41	0.83
10:Q:176:LYS:HE2	10:Q:186:GLN:HE21	1.44	0.82
5:E:194:VAL:O	5:E:197:ILE:HG22	1.79	0.82
7:2:38:LEU:HD23	7:2:197:MET:HE3	1.60	0.82
8:H:21:THR:HG22	8:H:26:VAL:HA	1.62	0.81
8:H:135:MET:HE3	13:T:165:ARG:NH1	1.94	0.81
10:Q:113:ILE:HG12	10:Q:119:LYS:HG3	1.60	0.81
13:M:104:VAL:HG23	13:M:178:ILE:HG22	1.62	0.81
14:N:136:GLY:HA2	14:U:161:GLN:NE2	1.94	0.81
10:Q:133:TYR:CZ	10:Q:166:MET:HG3	2.15	0.81
9:I:194:ASP:O	17:I:2016:HOH:O	1.99	0.81
4:D:46:VAL:HG11	4:D:139:ALA:HB1	1.63	0.80
11:K:142:TYR:O	11:K:143:LYS:HD2	1.82	0.79
6:F:81:LEU:HD12	6:F:133:GLY:HA3	1.62	0.79
3:X:163:GLN:HE21	3:X:164:THR:H	1.30	0.79
5:E:81:LEU:HB2	5:E:133:GLY:O	1.83	0.79
14:N:4:MET:HB3	14:N:126:ILE:HG22	1.65	0.79
13:T:133:MET:O	13:T:136:PRO:HD2	1.81	0.79
5:E:75:GLY:HA3	5:E:221:PHE:CE2	2.17	0.79
14:U:157:HIS:CD2	14:U:187(J):LEU:HD13	2.18	0.79
3:X:163:GLN:NE2	3:X:164:THR:H	1.82	0.78
6:F:122:ALA:HA	6:F:125:LEU:HD12	1.65	0.78
5:Z:81:LEU:HB2	5:Z:133:GLY:O	1.84	0.78
9:P:114:ASP:HB3	15:9:3:ASN:HD21	1.48	0.77
10:Q:32:ASP:OD2	10:Q:34:THR:HG22	1.84	0.77
5:Z:52:LYS:HD2	5:Z:63:TYR:O	1.84	0.77
2:B:202:THR:HG22	2:B:204:SER:H	1.48	0.77
5:E:176:LEU:HD22	5:E:180(C):PHE:HE2	1.50	0.77
10:Q:18:LYS:HD3	10:Q:174:ILE:HG13	1.63	0.77
12:S:190:GLU:O	12:S:191:LEU:HD23	1.85	0.77
6:F:37:SER:HB3	6:F:50:VAL:HG23	1.67	0.77
13:T:41:THR:OG1	13:T:76:PRO:HG3	1.85	0.77
7:G:77:VAL:HG12	7:G:137:THR:HB	1.67	0.76
3:C:163:GLN:HE21	3:C:164:THR:H	1.32	0.76
10:J:90:SER:O	10:J:91:SER:HB3	1.85	0.76
11:R:143:LYS:O	11:R:146:LEU:HD13	1.86	0.76
5:E:143:LYS:HE3	13:M:78:TYR:OH	1.85	0.75
13:M:152:GLU:O	13:M:156:VAL:HG23	1.87	0.75
7:G:170:GLN:HE21	7:G:174:THR:HG23	1.52	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:76:MET:SD	7:G:138:PHE:HE2	2.09	0.75
4:Y:70:ILE:HB	4:Y:74:ILE:HG22	1.68	0.75
3:C:57:LYS:HD2	3:C:58:LEU:N	2.02	0.75
10:J:113:ILE:HG12	10:J:119:LYS:HG3	1.69	0.74
7:2:198:ILE:HG23	7:2:203:THR:O	1.87	0.74
14:N:161:GLN:NE2	14:U:136:GLY:HA2	2.00	0.74
1:V:7:ARG:HH22	4:Y:123(C):GLY:HA3	1.52	0.74
9:I:41:VAL:HG22	9:I:76:PRO:HG3	1.67	0.74
5:E:198:SER:HA	5:E:201:LEU:HG	1.69	0.74
7:G:77:VAL:CG1	7:G:137:THR:HB	2.18	0.74
3:X:15:PHE:H	4:Y:23:GLN:HE22	1.36	0.73
5:Z:52:LYS:CB	5:Z:63:TYR:HB3	2.16	0.73
7:2:59:LEU:O	7:2:61:PRO:HD3	1.88	0.73
3:X:36:CYS:SG	3:X:37:ALA:N	2.61	0.73
7:G:220:LYS:HG2	7:G:221:PHE:H	1.52	0.73
3:C:71:ASP:HA	10:J:68:ILE:HD11	1.71	0.73
14:U:157:HIS:HD2	14:U:187(J):LEU:HD13	1.51	0.73
5:Z:130:ARG:HH11	5:Z:130:ARG:HG3	1.52	0.73
4:D:75:GLY:HA3	4:D:221:PHE:CE2	2.24	0.73
8:H:197:ARG:HH21	9:I:139:GLU:HG3	1.52	0.73
12:S:8:GLY:HA3	12:S:11:PHE:CE2	2.23	0.73
8:H:197:ARG:NH2	9:I:139:GLU:HG3	2.03	0.73
9:I:2:ILE:HG21	9:I:130:ALA:HB3	1.72	0.72
11:K:45:MET:HG2	11:K:52:CYS:HB3	1.71	0.72
12:S:18:THR:HG21	12:S:30:TYR:CD1	2.23	0.72
14:N:175:MET:HE3	14:N:187(B):PHE:HE2	1.55	0.72
4:Y:40:ILE:HG23	4:Y:162:ALA:HB2	1.71	0.72
5:Z:15:PHE:HB2	6:1:23:GLN:NE2	2.04	0.72
6:1:221:HIS:HE1	6:1:223:PHE:CE1	2.06	0.72
8:H:175:VAL:HG21	8:H:191:TYR:HD1	1.53	0.72
8:H:135:MET:HE3	13:T:165:ARG:HH12	1.54	0.72
1:V:15:PHE:H	2:W:23:GLN:HE22	1.37	0.72
1:A:130:ARG:HH21	7:G:124:THR:HG22	1.55	0.72
11:R:4:LEU:HD12	11:R:159:ILE:HD11	1.71	0.71
7:2:233:LEU:O	7:2:236:ILE:HG13	1.91	0.71
10:Q:43:MET:SD	10:Q:101:ILE:HD11	2.30	0.71
12:L:43:MET:HB2	12:L:101:ILE:HG22	1.71	0.71
13:T:160:ARG:HA	13:T:192:VAL:HG11	1.72	0.71
14:U:112:THR:HG22	14:U:120:HIS:HB2	1.72	0.71
8:O:112:SER:HB3	8:O:125:LEU:HD13	1.72	0.71
13:M:42:VAL:HG23	13:M:178:ILE:HD11	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:U:163:ILE:HG23	14:U:170:GLY:HA2	1.71	0.70
9:P:131:SER:OG	17:P:2011:HOH:O	2.10	0.70
7:G:198:ILE:HG23	7:G:203:THR:O	1.91	0.70
4:Y:163:LYS:HG3	4:Y:164:ALA:N	2.07	0.70
3:X:35:THR:HB	3:X:51:GLU:HG3	1.72	0.70
5:E:130:ARG:HH11	5:E:130:ARG:HG3	1.54	0.70
12:L:137:PHE:CE1	12:L:141:GLN:HG3	2.26	0.70
7:2:96:ALA:HA	7:2:107:MET:CE	2.22	0.70
2:B:124:THR:HG22	3:C:130:ARG:HH21	1.56	0.70
6:F:42:CYS:HB2	6:F:184:LEU:O	1.91	0.70
12:L:18:THR:HG21	12:L:30:TYR:CD1	2.26	0.70
8:O:175:VAL:HG21	8:O:191:TYR:HD1	1.57	0.70
13:M:124:THR:O	13:M:125:LEU:HD23	1.92	0.69
9:P:7:THR:HG23	9:P:110:ILE:HD13	1.74	0.69
13:T:80:PHE:CE1	13:T:111:ARG:HD3	2.28	0.69
11:R:87:VAL:HG11	11:R:115:SER:HA	1.73	0.69
6:1:35:THR:HG21	6:1:51:GLU:O	1.92	0.69
6:F:36:THR:O	6:F:50:VAL:HG23	1.93	0.69
10:J:44:SER:OG	10:J:100:LEU:HB2	1.92	0.69
10:Q:105(B):LYS:HE2	2:W:143:ASP:OD2	1.93	0.69
13:T:6:MET:HG2	13:T:155:ILE:HD11	1.74	0.69
6:1:172:ALA:O	6:1:176:LEU:HD23	1.91	0.69
7:2:91:ARG:HH21	7:2:115:ARG:HH21	1.38	0.69
4:D:97:VAL:HG21	11:K:65:LEU:HD12	1.72	0.69
4:D:163:LYS:HG3	4:D:164:ALA:N	2.08	0.69
5:E:74:MET:HE2	5:E:109:VAL:HG22	1.75	0.69
8:H:167:LEU:HD22	12:S:167:ILE:O	1.93	0.69
14:N:4:MET:CB	14:N:126:ILE:HG22	2.22	0.69
1:A:112:LEU:O	1:A:116:VAL:HG23	1.93	0.69
8:H:33:LYS:HE2	15:8:5:AKK:HA1	1.74	0.69
8:H:214:LEU:HD22	11:R:211:GLY:HA2	1.74	0.69
10:J:113:ILE:HA	10:J:118:THR:O	1.93	0.69
4:D:160:TYR:CE1	4:D:163:LYS:HD3	2.28	0.69
6:1:126:TYR:HE1	7:2:129:MET:SD	2.16	0.69
4:Y:45:GLY:HA2	4:Y:146:TYR:CE1	2.29	0.68
13:M:165:ARG:NH1	8:O:135:MET:HE3	2.09	0.68
14:N:6:VAL:HG23	14:N:155:ILE:HD11	1.76	0.68
4:Y:46:VAL:HG11	4:Y:139:ALA:HB1	1.75	0.68
5:Z:75:GLY:HA3	5:Z:221:PHE:CE2	2.28	0.68
5:Z:194:VAL:O	5:Z:197:ILE:HG22	1.93	0.68
3:X:156:ILE:HD11	4:Y:82:THR:OG1	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:2:105:TYR:H	7:2:105:TYR:HD2	1.41	0.68
12:L:166:HIS:HD2	12:L:168:GLN:H	1.41	0.68
13:M:175:LEU:HD23	13:M:176:ALA:N	2.09	0.68
4:D:70:ILE:HB	4:D:74:ILE:HG22	1.75	0.68
12:L:109:ALA:HB2	12:L:121:ARG:NH2	2.08	0.68
14:N:163:ILE:HG23	14:N:170:GLY:HA2	1.76	0.68
5:E:66:LYS:HA	5:E:78:LEU:HD21	1.75	0.68
13:T:4:ILE:HD11	13:T:159:MET:SD	2.33	0.68
6:1:38:ILE:HG22	6:1:164:ALA:CB	2.23	0.68
2:B:126:HIS:CB	3:C:129:VAL:HG12	2.22	0.67
11:K:143:LYS:O	11:K:146:LEU:HD13	1.94	0.67
12:S:29:ARG:NH1	12:S:193:ARG:HB3	2.09	0.67
1:A:49:ALA:HB2	1:A:212:LEU:HG	1.77	0.67
2:W:184:MET:HE1	2:W:189:ALA:HA	1.75	0.67
14:N:157:HIS:HD2	14:N:187(J):LEU:HD13	1.60	0.67
13:T:175:LEU:HD23	13:T:176:ALA:N	2.10	0.67
5:Z:180(C):PHE:HD1	5:Z:180(D):ILE:N	1.93	0.67
4:D:75:GLY:HA3	4:D:221:PHE:CD2	2.30	0.67
9:I:178:ILE:HG23	9:I:184:VAL:HG22	1.77	0.67
4:D:97:VAL:HG21	11:K:65:LEU:CD1	2.23	0.67
5:E:97:ASN:HD21	12:L:61:ASN:HD21	1.42	0.67
10:Q:133:TYR:OH	10:Q:166:MET:HG3	1.93	0.67
3:C:163:GLN:NE2	3:C:164:THR:H	1.91	0.67
7:G:184(G):GLU:HG2	7:G:188:LYS:CB	2.25	0.67
8:O:197:ARG:NH2	9:P:139:GLU:HG3	2.10	0.67
11:R:65:LEU:HD12	4:Y:97:VAL:HG21	1.76	0.67
6:F:82:ILE:HB	6:F:83:PRO:HD3	1.77	0.66
14:N:175:MET:HE3	14:N:187(B):PHE:CE2	2.30	0.66
2:W:69:LYS:HG3	2:W:221:GLN:OE1	1.95	0.66
12:L:90:LYS:HD3	12:L:95:TYR:CE1	2.29	0.66
6:1:69:VAL:HG12	17:1:2563:HOH:O	1.94	0.66
11:K:196:PHE:HZ	11:K:209:VAL:HG21	1.59	0.66
7:G:105:TYR:H	7:G:105:TYR:HD2	1.41	0.66
12:S:163:THR:O	17:S:2012:HOH:O	2.12	0.66
4:D:215:ILE:HG22	4:D:221:PHE:HD2	1.60	0.66
7:G:12:ILE:HA	17:G:538:HOH:O	1.95	0.66
7:2:12:ILE:HG13	7:2:14:ILE:HG23	1.77	0.66
2:W:175:LEU:HB3	17:W:2109:HOH:O	1.95	0.66
3:X:38:VAL:HG22	3:X:39:GLY:N	2.11	0.66
6:F:78:TYR:CE1	6:F:85:GLY:HA3	2.31	0.66
12:S:109:ALA:HB2	12:S:121:ARG:NH2	2.11	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:88:LEU:HD22	2:W:116:LEU:HD22	1.77	0.66
2:B:150:THR:O	2:B:157:TYR:HA	1.95	0.65
7:G:150:LYS:O	7:G:157:TYR:HA	1.95	0.65
7:G:233:LEU:O	7:G:236:ILE:HG13	1.96	0.65
2:W:15:PHE:HB2	3:X:23:GLN:HE22	1.61	0.65
13:M:135:ASN:O	13:M:139:ARG:HG3	1.97	0.65
14:N:51:ASP:O	14:N:55:ILE:HG13	1.96	0.65
14:N:157:HIS:CD2	14:N:187(J):LEU:HD13	2.31	0.65
1:A:50:THR:HG21	1:A:66:LYS:HE2	1.78	0.65
13:T:78:TYR:OH	5:Z:143:LYS:HE3	1.96	0.65
9:P:64:ASN:HD22	2:W:97:GLN:HE22	1.44	0.65
10:Q:68:ILE:CD1	3:X:71:ASP:HA	2.27	0.65
7:G:184(G):GLU:HG2	7:G:188:LYS:HB2	1.79	0.65
9:I:14:ILE:HG23	9:I:34:ILE:HD13	1.78	0.65
1:A:15:PHE:H	2:B:23:GLN:HE22	1.42	0.65
14:N:4:MET:SD	14:N:159:LEU:HD21	2.37	0.65
5:Z:161:TYR:CE2	6:1:60:VAL:HA	2.31	0.65
5:Z:198:SER:HA	5:Z:201:LEU:HG	1.79	0.65
1:A:217(I):TYR:CE1	8:H:36:ARG:HD2	2.32	0.65
1:V:49:ALA:HB2	1:V:212:LEU:HG	1.78	0.64
8:H:35:HIS:HB3	8:H:56:THR:HG21	1.79	0.64
14:N:30:VAL:HG11	13:T:199:PHE:HE2	1.62	0.64
6:F:24:VAL:O	6:F:27:ALA:HB3	1.98	0.64
11:R:105(A):ARG:HB3	11:R:105(B):LYS:HE3	1.78	0.64
12:S:4:LEU:HD13	12:S:126:ALA:HB2	1.80	0.64
5:Z:22:PHE:HD1	5:Z:26:TYR:HE1	1.46	0.64
2:W:126:HIS:HB3	3:X:129:VAL:HG12	1.79	0.64
3:X:57:LYS:HD2	3:X:58:LEU:N	2.11	0.64
6:F:126:TYR:HE1	7:G:129:MET:SD	2.20	0.64
9:I:137:MET:HE3	9:I:141:LEU:HD11	1.78	0.64
3:C:71:ASP:HA	10:J:68:ILE:CD1	2.27	0.64
6:1:221:HIS:HE1	6:1:223:PHE:HE1	1.46	0.64
6:F:221:HIS:HE1	6:F:223:PHE:CE1	2.16	0.64
6:1:150:MET:HE2	6:1:160:TYR:CE2	2.33	0.64
14:U:6:VAL:HG23	14:U:155:ILE:HD11	1.80	0.64
5:Z:117:CYS:SG	6:1:86:ARG:HD3	2.38	0.64
12:S:144(W):LYS:HG2	12:S:145:TYR:N	2.13	0.63
14:N:59:VAL:HG13	14:N:82:VAL:HG11	1.79	0.63
8:O:80:LEU:HD12	8:O:113:ILE:HD11	1.80	0.63
4:Y:214:CYS:SG	4:Y:224:TYR:CE2	2.87	0.63
7:G:220:LYS:HG2	7:G:221:PHE:N	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:Q:85:GLN:HE21	2:W:101:LYS:HZ2	1.46	0.63
13:T:152:GLU:O	13:T:156:VAL:HG23	1.98	0.63
3:C:40:VAL:HG12	3:C:162:ALA:HB1	1.81	0.63
7:G:121:GLN:O	7:G:124:THR:HB	1.99	0.63
8:H:18:THR:HB	8:H:30:ASN:HA	1.81	0.63
12:L:24:TYR:HA	8:O:167:LEU:HD12	1.81	0.63
5:Z:48:LEU:HD13	5:Z:77:SER:HB3	1.80	0.63
8:O:113:ILE:HG12	8:O:119:THR:HG22	1.79	0.63
4:D:180(C):HIS:CD2	4:D:184:LEU:HG	2.34	0.63
12:L:29:ARG:NH1	12:L:193:ARG:HB3	2.13	0.63
12:L:133:LEU:O	12:L:136:PRO:HD2	1.99	0.63
14:N:67:THR:HA	14:N:72:GLY:O	1.99	0.63
13:T:91:ARG:HG3	13:T:92:SER:N	2.13	0.63
6:1:184:LEU:HD11	6:1:188:GLU:HB3	1.81	0.63
12:L:109:ALA:HB2	12:L:121:ARG:HH21	1.63	0.63
4:Y:46:VAL:HG11	4:Y:139:ALA:CB	2.29	0.63
3:C:163:GLN:HG3	3:C:164:THR:N	2.14	0.62
10:J:39:PRO:HD3	17:J:3265:HOH:O	1.99	0.62
6:F:186:ALA:O	6:F:190:VAL:HG23	2.00	0.62
3:X:197:LEU:O	3:X:201:VAL:HG23	1.98	0.62
6:1:150:MET:HE2	6:1:160:TYR:CZ	2.34	0.62
2:B:6:ARG:HG3	5:E:127:TYR:OH	1.99	0.62
12:S:29:ARG:HD3	12:S:171:ASP:OD1	1.99	0.62
3:X:134:VAL:HG12	3:X:135:SER:N	2.14	0.62
4:Y:65:GLU:HA	17:Y:2028:HOH:O	1.99	0.62
6:1:160:TYR:HB3	6:1:162:GLY:O	1.99	0.62
7:2:207:LYS:HG3	7:2:208:ASN:OD1	1.99	0.62
13:M:-5:PRO:HD3	13:M:96:TRP:CD2	2.35	0.62
1:V:130:ARG:HH21	7:2:124:THR:HG22	1.65	0.62
2:W:229:ILE:O	2:W:232:ILE:HG22	1.99	0.62
6:F:12:ASN:ND2	6:F:131:PRO:HD3	2.14	0.62
11:K:5:ALA:HA	11:K:13:ILE:O	2.00	0.62
2:W:71:ASN:HD22	2:W:72:ASP:H	1.48	0.62
8:H:197:ARG:NH1	8:H:200:LYS:HD3	2.15	0.62
12:L:144(W):LYS:HG2	12:L:145:TYR:N	2.15	0.62
5:Z:226:GLY:O	5:Z:229:VAL:HG22	1.99	0.62
2:B:71:ASN:HD22	2:B:72:ASP:H	1.47	0.62
3:X:47:VAL:O	3:X:48:LEU:HD23	1.99	0.62
4:D:38:ILE:HD12	4:D:197:LEU:HG	1.80	0.62
6:1:13:SER:HB2	7:2:130:ARG:HB3	1.81	0.62
6:1:37:SER:HB3	6:1:50:VAL:CG2	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:163:ILE:HG13	2:B:164:SER:H	1.65	0.62
10:J:133:TYR:CZ	10:J:166:MET:HG3	2.35	0.62
8:O:49:ALA:HB1	9:P:118:CYS:SG	2.40	0.62
5:E:52:LYS:HB3	5:E:63:TYR:HB3	1.80	0.62
6:F:170:GLN:CD	6:F:170:GLN:H	2.08	0.62
12:L:190:GLU:O	12:L:191:LEU:HD23	2.00	0.62
13:M:6:MET:HG2	13:M:155:ILE:HD11	1.81	0.62
14:N:10:ASP:O	14:N:179:THR:HG22	2.00	0.62
4:Y:78:MET:SD	4:Y:82:THR:HG22	2.40	0.62
7:G:107:MET:HE3	7:G:112:LEU:HD13	1.82	0.61
8:O:35:HIS:HB3	8:O:56:THR:HG21	1.82	0.61
9:P:114:ASP:HB3	15:9:3:ASN:HD22	1.64	0.61
13:M:104:VAL:HG23	13:M:178:ILE:CG2	2.29	0.61
12:S:61:ASN:HD21	5:Z:97:ASN:HD21	1.47	0.61
10:Q:113:ILE:HA	10:Q:118:THR:O	2.00	0.61
9:I:113:PHE:CD2	9:I:113:PHE:N	2.68	0.61
11:K:112:TYR:O	11:K:119:ARG:HA	2.01	0.61
3:X:190:VAL:O	3:X:194:VAL:HG23	2.00	0.61
13:M:80:PHE:CE1	13:M:111:ARG:HD3	2.35	0.61
5:Z:161:TYR:OH	6:1:61:PRO:HD2	2.00	0.61
7:2:91:ARG:NH2	7:2:115:ARG:HH21	1.98	0.61
10:Q:176:LYS:HE2	10:Q:186:GLN:NE2	2.15	0.61
3:X:36:CYS:HA	3:X:166:GLY:HA3	1.83	0.61
6:F:119:TYR:O	6:F:122:ALA:HB3	2.00	0.61
12:S:134:ILE:HG22	12:S:138:LEU:HD22	1.82	0.61
14:U:134:ILE:HD12	14:U:158:SER:HB3	1.82	0.61
4:Y:214:CYS:SG	4:Y:224:TYR:HE2	2.08	0.61
6:1:176:LEU:HD22	6:1:196:ILE:HD13	1.82	0.61
3:C:38:VAL:HG22	3:C:39:GLY:N	2.16	0.61
6:F:127:ASN:HD22	6:F:127:ASN:C	2.09	0.61
13:M:82:TYR:O	13:M:86:VAL:HG23	2.00	0.61
2:W:124:THR:HG22	3:X:130:ARG:HH21	1.66	0.61
6:F:35:THR:HG21	6:F:51:GLU:O	2.01	0.60
6:1:122:ALA:HA	6:1:125:LEU:HD12	1.83	0.60
6:1:127:ASN:HD22	6:1:127:ASN:C	2.09	0.60
5:E:52:LYS:HD2	5:E:63:TYR:O	2.01	0.60
7:G:212:VAL:HG12	7:G:213:GLY:N	2.16	0.60
8:O:84:LYS:HG3	8:O:85:GLN:N	2.14	0.60
7:2:220:LYS:HG2	7:2:221:PHE:H	1.67	0.60
10:Q:180:LYS:HG3	10:Q:181:ASP:OD1	2.01	0.60
2:W:71:ASN:ND2	2:W:72:ASP:H	1.99	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:180(C):PHE:HD1	5:E:180(D):ILE:N	2.00	0.60
12:S:6:PRO:HB2	13:T:91:ARG:NH1	2.15	0.60
14:U:13:ILE:HG12	14:U:177:VAL:HG13	1.83	0.60
7:G:12:ILE:HG13	7:G:14:ILE:HG23	1.83	0.60
7:G:48:VAL:C	7:G:49:ILE:HD12	2.26	0.60
8:H:47:GLY:O	15:8:5:AKK:ND	2.34	0.60
13:M:133:MET:O	13:M:136:PRO:HD2	2.01	0.60
12:S:177:ILE:N	12:S:177:ILE:HD12	2.16	0.60
14:U:4:MET:CB	14:U:126:ILE:HG22	2.27	0.60
14:U:55:ILE:O	14:U:59:VAL:HG23	2.01	0.60
4:Y:215:ILE:HG13	4:Y:215:ILE:O	2.00	0.60
1:A:130:ARG:HH21	7:G:124:THR:CG2	2.14	0.60
7:G:229:ILE:O	7:G:232:ARG:HB2	2.01	0.60
8:H:4:VAL:HG22	8:H:159:ILE:HD11	1.83	0.60
10:J:180:LYS:HG3	10:J:181:ASP:OD1	2.01	0.60
7:2:48:VAL:C	7:2:49:ILE:HD12	2.26	0.60
5:E:47:VAL:HG12	5:E:48:LEU:N	2.17	0.60
5:E:73:HIS:HE1	5:E:107:LEU:O	1.83	0.60
6:F:151:LEU:HD11	6:F:155:GLY:HA2	1.83	0.60
6:F:184:LEU:HD11	6:F:188:GLU:CB	2.32	0.60
12:S:166:HIS:HD2	12:S:168:GLN:H	1.47	0.60
9:I:6:MET:HB3	9:I:151:LEU:HD11	1.83	0.60
14:N:51:ASP:OD2	14:N:95:LEU:HA	2.01	0.60
11:R:38:ASN:O	11:R:40:PHE:N	2.34	0.60
12:S:43:MET:CB	12:S:101:ILE:HG22	2.31	0.60
14:U:175:MET:HE3	14:U:187(B):PHE:CE2	2.36	0.60
5:Z:70:CYS:SG	5:Z:92:LEU:HD23	2.42	0.60
8:O:78:SER:O	8:O:82:MET:HG3	2.01	0.60
10:Q:68:ILE:HD11	3:X:71:ASP:HA	1.84	0.60
8:H:152:ILE:CG2	8:H:191:TYR:HE1	2.14	0.59
12:S:133:LEU:O	12:S:136:PRO:HD2	2.02	0.59
8:H:200:LYS:HE3	9:I:140:SER:O	2.03	0.59
11:K:102:CYS:SG	11:K:110:ILE:HG23	2.42	0.59
5:E:198:SER:HA	5:E:201:LEU:CG	2.30	0.59
10:J:43:MET:SD	10:J:101:ILE:HD11	2.43	0.59
11:K:165:ARG:NH1	9:P:171:TRP:HH2	2.00	0.59
2:B:121:GLN:O	2:B:124:THR:HB	2.03	0.59
7:G:173:THR:O	7:G:177:GLU:HG3	2.03	0.59
13:M:149:GLN:NE2	13:M:149:GLN:H	2.00	0.59
4:Y:237:LEU:HD22	4:Y:241:GLU:HG3	1.84	0.59
7:G:59:LEU:O	7:G:61:PRO:HD3	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:3:ILE:O	8:H:3:ILE:HG13	2.02	0.59
11:R:5:ALA:HA	11:R:13:ILE:O	2.01	0.59
5:Z:136:LEU:HD12	5:Z:151:PHE:CD2	2.37	0.59
11:K:1:THR:HG23	11:K:33:LYS:HZ2	1.67	0.59
13:M:197:TRP:CH2	14:U:171:GLY:HA2	2.37	0.59
8:H:84:LYS:HG3	8:H:85:GLN:N	2.18	0.59
11:K:196:PHE:CE2	11:K:206:PHE:CD2	2.91	0.59
12:L:134:ILE:HG22	12:L:138:LEU:HD22	1.84	0.59
12:S:-6:PRO:HB2	13:T:91:ARG:HH11	1.65	0.59
6:F:38:ILE:HG22	6:F:164:ALA:HA	1.85	0.59
13:T:-5:PRO:HD3	13:T:96:TRP:CD2	2.36	0.59
13:T:3:VAL:HG22	13:T:16:ALA:HB2	1.83	0.59
3:X:163:GLN:HE21	3:X:164:THR:N	1.99	0.59
3:X:116:VAL:O	3:X:119:VAL:HB	2.02	0.59
4:Y:197:LEU:O	4:Y:201:MET:HG3	2.02	0.59
5:Z:48:LEU:HG	5:Z:139:ILE:HD13	1.85	0.59
7:2:214:VAL:HG12	7:2:215:ALA:N	2.17	0.59
3:C:71:ASP:O	3:C:73:HIS:N	2.36	0.59
5:E:77:SER:OG	5:E:137:LEU:HB2	2.02	0.59
9:P:70:GLU:HB3	17:P:2524:HOH:O	2.02	0.59
13:T:133:MET:C	13:T:136:PRO:HD2	2.27	0.59
4:Y:75:GLY:HA3	4:Y:221:PHE:CE2	2.38	0.59
7:2:229:ILE:O	7:2:232:ARG:HB2	2.03	0.59
12:L:19:ARG:HB2	12:L:171:ASP:HB2	1.85	0.58
8:O:69:TYR:O	8:O:69:TYR:CD1	2.56	0.58
3:X:76:LEU:HD12	3:X:138:ILE:HG12	1.84	0.58
7:2:105:TYR:CD2	7:2:105:TYR:N	2.69	0.58
1:A:79:SER:HB2	1:A:165:ILE:HD12	1.85	0.58
2:B:181:LYS:O	2:B:184:MET:HG3	2.02	0.58
5:E:52:LYS:CB	5:E:63:TYR:HB3	2.33	0.58
3:X:115:TYR:O	3:X:119:VAL:HG23	2.04	0.58
4:Y:67:ILE:HD13	4:Y:213:SER:OG	2.03	0.58
6:1:171:SER:O	6:1:174:ALA:HB3	2.02	0.58
3:C:57:LYS:O	3:C:58:LEU:HB2	2.03	0.58
7:G:188:LYS:O	7:G:191:GLU:HB2	2.03	0.58
4:Y:160:TYR:CE1	4:Y:163:LYS:HD3	2.38	0.58
8:O:10:ASN:OD1	8:O:180:ILE:HD12	2.04	0.58
13:T:4:ILE:HD11	13:T:159:MET:HG2	1.85	0.58
1:V:27:ALA:O	1:V:31:VAL:HG23	2.02	0.58
2:W:160:TRP:CE3	2:W:163:ILE:HD13	2.39	0.58
6:1:42:CYS:HB2	6:1:184:LEU:O	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:2:67:ILE:HD12	7:2:211:GLU:HG2	1.83	0.58
1:A:78:TYR:CE2	1:A:82:GLY:HA2	2.39	0.58
1:A:79:SER:HA	17:A:252:HOH:O	2.01	0.58
8:H:52:THR:O	8:H:56:THR:HB	2.04	0.58
9:I:55:LEU:HD21	9:I:95:TYR:CD1	2.39	0.58
12:L:49:ALA:HA	17:L:531:HOH:O	2.02	0.58
11:R:65:LEU:CD1	4:Y:97:VAL:HG21	2.34	0.58
2:B:229:ILE:O	2:B:232:ILE:HG22	2.04	0.58
14:N:114:PRO:HD2	14:N:118:SER:O	2.03	0.58
11:K:1:THR:HG23	11:K:33:LYS:NZ	2.19	0.58
12:S:109:ALA:HB2	12:S:121:ARG:HH21	1.67	0.58
13:T:124:THR:O	13:T:125:LEU:HD23	2.03	0.58
11:K:196:PHE:CE1	9:P:193:GLN:HG3	2.39	0.58
12:L:-8:PHE:HE1	13:M:115:LEU:HD12	1.68	0.58
13:M:87:MET:SD	13:M:95:LEU:HD12	2.44	0.58
8:O:172:ASN:HD22	8:O:193:THR:HA	1.69	0.58
13:T:4:ILE:CD1	13:T:159:MET:SD	2.92	0.58
2:B:49:ALA:HB2	2:B:212:PHE:CE1	2.39	0.57
4:D:65:GLU:HA	17:D:246:HOH:O	2.04	0.57
13:M:141(C):ARG:HH11	13:M:141(C):ARG:HG3	1.70	0.57
8:O:36:ARG:HD2	1:V:217(I):TYR:CE1	2.39	0.57
1:A:181:ASN:HD21	1:A:184:LEU:HD21	1.69	0.57
10:J:68:ILE:HG22	10:J:69:ARG:N	2.18	0.57
12:S:18:THR:CG2	12:S:30:TYR:HA	2.32	0.57
6:1:36:THR:O	6:1:50:VAL:HG23	2.04	0.57
7:2:105:TYR:HD2	7:2:105:TYR:N	2.01	0.57
7:G:130:ARG:HG3	7:G:131:PRO:O	2.04	0.57
7:G:151:THR:HG22	7:G:157:TYR:CB	2.31	0.57
1:V:78:TYR:CE2	1:V:82:GLY:HA2	2.39	0.57
7:G:96:ALA:HA	7:G:107:MET:CE	2.29	0.57
11:K:126:CYS:SG	11:K:135:TYR:CE2	2.96	0.57
13:M:104:VAL:CG2	13:M:178:ILE:HG22	2.33	0.57
11:R:195:LEU:O	11:R:199:VAL:HG23	2.04	0.57
6:1:68:GLN:HE22	6:1:86:ARG:NH1	2.02	0.57
4:D:97:VAL:HG11	11:K:65:LEU:CD1	2.34	0.57
4:D:159:ARG:HB3	5:E:60:SER:HB3	1.85	0.57
6:1:175:GLU:O	6:1:178:LYS:HB2	2.05	0.57
2:B:20:ARG:HE	3:C:33:ARG:HH21	1.52	0.57
3:C:36:CYS:SG	3:C:37:ALA:N	2.78	0.57
5:E:180(C):PHE:HA	5:E:180(F):ILE:HG13	1.86	0.57
13:M:133:MET:C	13:M:136:PRO:HD2	2.29	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Y:39:GLY:HA2	4:Y:47:VAL:O	2.03	0.57
5:Z:148:LEU:HD12	5:Z:149:LEU:N	2.19	0.57
2:B:97:GLN:HE22	9:I:64:ASN:HD22	1.52	0.57
4:D:46:VAL:HG11	4:D:139:ALA:CB	2.33	0.57
1:V:77:VAL:HG22	1:V:78:TYR:H	1.70	0.57
1:V:86:ARG:HH21	7:2:118:ASN:HD22	1.53	0.57
6:1:69:VAL:HG23	6:1:74:ILE:O	2.05	0.57
4:D:177:LEU:HD22	5:E:58:LEU:HD22	1.86	0.57
7:G:46:THR:OG1	7:G:146:PRO:HB3	2.04	0.57
11:K:105(B):LYS:HD2	11:K:105(B):LYS:N	2.14	0.57
13:M:53:GLN:O	13:M:56:GLU:HB2	2.04	0.57
13:M:165:ARG:HH12	8:O:135:MET:HE3	1.68	0.57
10:Q:35:ARG:O	10:Q:42:LEU:HD12	2.04	0.57
13:T:63:VAL:HG12	13:T:64:THR:N	2.19	0.57
13:T:76:PRO:HD2	13:T:105:GLN:OE1	2.04	0.57
14:U:163:ILE:HG21	14:U:187(G):TYR:OH	2.05	0.57
14:U:175:MET:HE3	14:U:187(B):PHE:CD2	2.40	0.57
1:A:130:ARG:HG3	1:A:130:ARG:O	2.04	0.57
5:E:17:PRO:HA	6:F:26:TYR:CD2	2.40	0.57
14:N:187(D):PRO:HA	14:N:187(G):TYR:CE2	2.40	0.57
3:X:57:LYS:O	3:X:58:LEU:HB2	2.03	0.57
5:Z:78:LEU:HA	5:Z:136:LEU:HD23	1.87	0.57
3:C:160:TRP:CZ2	4:D:59:LEU:HD23	2.40	0.57
11:R:142:TYR:O	11:R:143:LYS:HD2	2.05	0.57
13:T:141(C):ARG:HH11	13:T:141(C):ARG:HG3	1.70	0.57
4:Y:160:TYR:CZ	4:Y:163:LYS:HD3	2.40	0.57
8:O:197:ARG:HH21	9:P:139:GLU:HG3	1.69	0.56
11:R:1:THR:HG23	11:R:33:LYS:NZ	2.20	0.56
1:V:124:THR:CG2	2:W:130:ARG:HH21	2.15	0.56
2:W:53:LYS:HG2	2:W:54:VAL:HG23	1.87	0.56
5:Z:214:ILE:O	5:Z:221:PHE:HA	2.05	0.56
6:1:198:TYR:CE2	6:1:208:PHE:HZ	2.23	0.56
7:2:49:ILE:HD12	7:2:49:ILE:N	2.20	0.56
12:L:192:LYS:HE3	8:O:195:ASN:HB3	1.87	0.56
3:C:136:THR:O	3:C:150:GLN:HA	2.05	0.56
4:D:39:GLY:HA2	4:D:47:VAL:O	2.06	0.56
10:J:161:GLU:OE1	11:R:136:GLY:HA2	2.05	0.56
9:P:9:LYS:HD3	9:P:145:ASN:ND2	2.20	0.56
2:W:163:ILE:HG13	2:W:164:SER:H	1.70	0.56
5:Z:24:VAL:O	5:Z:27:ALA:HB3	2.05	0.56
5:Z:180(C):PHE:C	5:Z:180(E):LYS:H	2.14	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:2:220:LYS:HG2	7:2:221:PHE:N	2.21	0.56
12:L:166:HIS:CD2	12:L:168:GLN:HB2	2.40	0.56
5:Z:73:HIS:HE1	5:Z:107:LEU:O	1.88	0.56
3:C:238:GLN:C	3:C:240:LYS:H	2.13	0.56
5:E:48:LEU:HD13	5:E:77:SER:HB3	1.87	0.56
8:H:165:ASN:OD1	13:T:136:PRO:HA	2.05	0.56
12:S:63:VAL:HG22	12:S:74:LEU:HD23	1.86	0.56
14:U:10:ASP:O	14:U:179:THR:HG22	2.06	0.56
14:U:85:GLU:O	14:U:89:GLU:HB2	2.06	0.56
5:Z:198:SER:HA	5:Z:201:LEU:CG	2.36	0.56
4:D:215:ILE:HG13	4:D:215:ILE:O	2.05	0.56
12:L:4:LEU:HD11	12:L:138:LEU:HD21	1.87	0.56
9:P:101:VAL:O	9:P:110:ILE:HA	2.05	0.56
14:U:8:PHE:CZ	14:U:10:ASP:HB2	2.40	0.56
14:U:114:PRO:HD2	14:U:118:SER:O	2.06	0.56
1:V:4:MET:SD	1:V:5:THR:N	2.77	0.56
15:8:4:R4K:N	15:8:4:R4K:C32	2.69	0.56
1:A:4:MET:SD	1:A:5:THR:N	2.78	0.56
5:E:74:MET:HE2	5:E:109:VAL:CG2	2.35	0.56
5:E:186:PRO:HG2	5:E:187:ASP:H	1.71	0.56
6:F:38:ILE:HG22	6:F:164:ALA:CB	2.36	0.56
9:I:137:MET:HE2	9:I:161:ASN:HB2	1.88	0.56
12:L:114:ASP:HB2	12:L:118:SER:HB3	1.88	0.56
12:S:55:LEU:HD13	12:S:95:TYR:CD1	2.41	0.56
5:Z:114:HIS:HB3	6:1:86:ARG:NH2	2.21	0.56
12:L:43:MET:CB	12:L:101:ILE:HG22	2.36	0.56
10:Q:44:SER:OG	10:Q:100:LEU:HB2	2.05	0.56
7:2:39:ALA:HB2	7:2:48:VAL:HG12	1.86	0.56
1:A:74:ILE:HG12	1:A:140:GLY:HA3	1.88	0.56
2:B:69:LYS:HG3	2:B:221:GLN:OE1	2.05	0.56
12:L:18:THR:HG22	12:L:30:TYR:HA	1.87	0.56
2:B:46:ILE:HD11	2:B:146:TYR:HB3	1.87	0.56
12:L:-8:PHE:CE1	13:M:115:LEU:HD12	2.41	0.56
12:L:140:ASN:O	12:L:144:PHE:HA	2.05	0.56
3:X:152:GLU:CG	3:X:156:ILE:HG22	2.34	0.56
4:Y:188:GLU:O	4:Y:191:LEU:HB2	2.06	0.56
6:1:70:VAL:HB	6:1:74:ILE:HB	1.87	0.56
12:S:144(W):LYS:HG2	12:S:145:TYR:H	1.71	0.55
13:T:55:ILE:O	13:T:59:LEU:HG	2.06	0.55
4:Y:112:LEU:C	4:Y:112:LEU:HD13	2.31	0.55
5:Z:148:LEU:HD12	5:Z:149:LEU:H	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:164:TYR:C	13:M:165:ARG:HD2	2.31	0.55
5:E:78:LEU:HA	5:E:136:LEU:HD23	1.87	0.55
9:I:91:ARG:CD	9:I:116:ILE:HD12	2.36	0.55
9:I:186:LYS:HE2	9:I:188:TYR:OH	2.05	0.55
8:H:216:GLU:HG3	9:I:187:ARG:HG2	1.89	0.55
12:L:4:LEU:HD13	12:L:126:ALA:HB2	1.89	0.55
13:M:43:VAL:HG22	13:M:101:VAL:HG22	1.88	0.55
13:T:157:ASN:ND2	13:T:160:ARG:NH1	2.49	0.55
2:W:156:ASN:HD22	2:W:157:TYR:H	1.55	0.55
5:Z:40:LEU:HD23	5:Z:40:LEU:N	2.22	0.55
6:1:109:ILE:O	6:1:110:PRO:C	2.49	0.55
7:2:186:TRP:O	7:2:190:VAL:HG23	2.06	0.55
1:A:13:THR:O	2:B:130:ARG:HD3	2.07	0.55
2:B:15:PHE:HB2	3:C:23:GLN:HE22	1.72	0.55
9:I:12:VAL:HG13	9:I:108:PRO:HB3	1.89	0.55
12:L:19:ARG:HD2	12:L:168:GLN:O	2.05	0.55
13:T:165:ARG:N	13:T:165:ARG:HD2	2.20	0.55
6:1:82:ILE:HB	6:1:83:PRO:HD3	1.87	0.55
1:A:86:ARG:HE	7:G:118:ASN:HD21	1.53	0.55
7:G:214:VAL:HG12	7:G:215:ALA:N	2.21	0.55
9:I:161:ASN:HD21	12:S:140:ASN:ND2	2.04	0.55
13:M:7:LYS:HD2	13:M:141(G):ILE:HD13	1.88	0.55
2:W:65:GLU:HG3	2:W:66:LYS:HG3	1.87	0.55
5:Z:186:PRO:HG2	5:Z:187:ASP:H	1.72	0.55
2:B:24:VAL:O	2:B:28:LEU:HD12	2.06	0.55
5:E:180(C):PHE:C	5:E:180(E):LYS:H	2.15	0.55
9:I:-8:SER:O	9:I:-6:PRO:HD3	2.06	0.55
9:P:6:MET:HB3	9:P:151:LEU:HD11	1.89	0.55
14:U:112:THR:CG2	14:U:120:HIS:HB2	2.37	0.55
7:2:77:VAL:CG1	7:2:137:THR:HB	2.36	0.55
7:2:116:MET:HE3	17:2:2395:HOH:O	2.06	0.55
10:J:129:TYR:O	10:J:132:PHE:HB2	2.07	0.55
13:M:46:SER:OG	13:M:98:ALA:HB3	2.06	0.55
10:Q:112:GLN:HE22	10:Q:126:ALA:H	1.54	0.55
13:T:45:ILE:HG12	13:T:99:ILE:HG12	1.89	0.55
7:2:180(B):ASP:O	7:2:180(C):HIS:HB3	2.06	0.55
2:B:163:ILE:HG13	2:B:164:SER:N	2.21	0.55
4:D:112:LEU:C	4:D:112:LEU:HD13	2.32	0.55
4:D:160:TYR:CD2	5:E:59:SER:HB3	2.42	0.55
8:O:105:ASP:HB2	8:O:105(A):PRO:HD2	1.89	0.55
9:I:97:VAL:HG23	9:I:99:PRO:HD3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:P:12:VAL:CG1	9:P:108:PRO:HB3	2.37	0.55
9:P:113:PHE:N	9:P:113:PHE:CD2	2.75	0.55
7:2:72:ARG:HB2	7:2:72:ARG:HH11	1.71	0.55
2:B:161:LYS:HE3	3:C:59:GLN:O	2.06	0.54
6:F:50:VAL:HG22	6:F:51:GLU:N	2.22	0.54
8:H:12:VAL:HG22	8:H:13:VAL:N	2.21	0.54
10:J:104:TYR:HD2	10:J:179:ASP:HA	1.72	0.54
14:N:38:HIS:CD2	17:N:352:HOH:O	2.59	0.54
14:U:48:SER:HB3	14:U:51:ASP:HB2	1.89	0.54
4:Y:163:LYS:HE3	4:Y:164:ALA:O	2.06	0.54
5:E:5:ARG:C	5:E:7:ASN:H	2.15	0.54
8:H:49:ALA:HB1	9:I:118:CYS:SG	2.47	0.54
5:Z:140:GLY:HA2	5:Z:215:VAL:HG11	1.88	0.54
6:F:68:GLN:OE1	6:F:89:VAL:HG21	2.07	0.54
9:I:171:TRP:HH2	11:R:165:ARG:NH1	2.04	0.54
8:O:204:TYR:CD2	8:O:204:TYR:N	2.75	0.54
9:I:6:MET:HE1	9:I:155:ILE:HA	1.87	0.54
13:M:100:ILE:HD13	13:M:125:LEU:HB2	1.88	0.54
8:O:49:ALA:CB	9:P:118:CYS:SG	2.96	0.54
2:W:212:PHE:O	2:W:224:PHE:HB2	2.08	0.54
4:Y:20:ARG:NH1	5:Z:33:GLN:HE22	2.05	0.54
5:Z:76:LEU:HD23	5:Z:76:LEU:O	2.07	0.54
3:C:88:LEU:HD22	3:C:116:VAL:HG13	1.90	0.54
5:E:48:LEU:O	5:E:212:ILE:HG23	2.08	0.54
11:R:37:ILE:HB	11:R:41:LEU:O	2.08	0.54
13:T:153:GLU:HG3	17:T:1470:HOH:O	2.07	0.54
3:X:40:VAL:HG12	3:X:162:ALA:HB1	1.88	0.54
11:R:4:LEU:O	11:R:4:LEU:HD13	2.07	0.54
3:X:187:GLU:HA	3:X:232:TYR:OH	2.07	0.54
6:1:24:VAL:O	6:1:27:ALA:HB3	2.08	0.54
6:1:38:ILE:HG22	6:1:164:ALA:HB2	1.89	0.54
8:H:158:ALA:O	8:H:161:ALA:HB3	2.08	0.54
8:O:4:VAL:HG12	8:O:126:SER:HB2	1.90	0.54
12:S:166:HIS:CD2	12:S:168:GLN:HB2	2.43	0.54
1:V:69:LEU:HD23	1:V:70:LEU:N	2.22	0.54
2:W:126:HIS:CB	3:X:129:VAL:HG12	2.37	0.54
5:E:150:GLU:O	5:E:157:VAL:HA	2.08	0.54
6:F:212:ILE:HG22	6:F:213:SER:H	1.72	0.54
8:H:10:ASN:OD1	8:H:180:ILE:HD12	2.08	0.54
11:K:4:LEU:CD1	11:K:15:ALA:HB3	2.31	0.54
11:K:25:TRP:CH2	12:L:132:SER:HA	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:43:LYS:O	3:X:43:LYS:HG2	2.08	0.54
1:A:81:MET:HE1	7:G:21:LEU:HD11	1.90	0.54
11:R:200:LYS:HE3	11:R:206:PHE:O	2.08	0.54
3:X:180(D):GLU:N	3:X:182:PRO:HD3	2.23	0.54
5:E:15:PHE:HB2	6:F:23:GLN:NE2	2.12	0.54
10:J:32:ASP:OD2	10:J:34:THR:HG22	2.07	0.54
11:K:105(A):ARG:HB3	11:K:105(B):LYS:HE3	1.90	0.54
12:L:90:LYS:HE3	12:L:93:PHE:O	2.08	0.54
8:O:103:GLY:HA2	8:O:178:MET:SD	2.48	0.54
9:P:76:PRO:O	9:P:77:GLU:C	2.51	0.54
12:S:49:ALA:HA	17:S:2531:HOH:O	2.07	0.54
12:S:137:PHE:CE1	12:S:141:GLN:HG3	2.43	0.54
2:W:137:ILE:HD11	2:W:165:VAL:HG22	1.89	0.54
2:B:81:LEU:HD22	2:B:81:LEU:H	1.71	0.53
2:B:212:PHE:O	2:B:224:PHE:HB2	2.08	0.53
4:D:67:ILE:HD12	4:D:211:GLN:HE21	1.73	0.53
12:L:-6:PRO:O	13:M:91:ARG:NH1	2.41	0.53
14:U:114:PRO:O	14:U:116:GLY:N	2.41	0.53
1:V:221:PHE:C	1:V:221:PHE:CD2	2.86	0.53
7:2:69:CYS:O	7:2:93:LYS:HE2	2.08	0.53
4:D:59:LEU:HD13	4:D:60:GLU:N	2.22	0.53
12:L:24:TYR:O	8:O:167:LEU:HG	2.08	0.53
8:O:133:ALA:O	8:O:136:ALA:HB3	2.09	0.53
8:O:200:LYS:HE3	9:P:140:SER:O	2.08	0.53
4:D:52:LYS:HG3	4:D:64:ILE:HG21	1.91	0.53
4:D:188:GLU:O	4:D:191:LEU:HB2	2.08	0.53
6:F:11:SER:O	6:F:14:VAL:HG23	2.08	0.53
8:H:132:LEU:HD11	14:N:25:TYR:CE1	2.43	0.53
14:N:3:ILE:HG22	14:N:16:ALA:CB	2.38	0.53
9:P:45:ILE:HG22	9:P:52:VAL:HG22	1.90	0.53
1:V:76:ALA:HB2	1:V:138:ILE:HG12	1.89	0.53
3:C:44:ASN:O	3:C:45:CYS:HB3	2.09	0.53
5:E:141:TYR:OH	5:E:217:LYS:HG3	2.09	0.53
6:F:37:SER:HB3	6:F:50:VAL:CG2	2.38	0.53
6:F:171:SER:O	6:F:174:ALA:HB3	2.08	0.53
7:G:109:CYS:HB3	17:G:754:HOH:O	2.08	0.53
12:S:61:ASN:HD21	5:Z:97:ASN:ND2	2.05	0.53
13:T:186:PHE:HE1	13:T:188:LYS:HG3	1.74	0.53
4:D:121:LEU:HB2	17:D:3156:HOH:O	2.09	0.53
8:H:112:SER:HB3	8:H:125:LEU:HD13	1.91	0.53
10:J:52:THR:CG2	10:J:53:VAL:N	2.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:157:ARG:O	11:K:160:LEU:HB3	2.09	0.53
4:Y:221:PHE:CE1	4:Y:223:ILE:HG13	2.42	0.53
4:D:186:LEU:O	4:D:190:GLU:HG3	2.08	0.53
8:H:35:HIS:CB	8:H:56:THR:HG21	2.38	0.53
8:H:43:CYS:SG	8:H:99:LEU:HD22	2.49	0.53
8:H:195:ASN:HB3	12:S:192:LYS:HE3	1.89	0.53
14:N:55:ILE:O	14:N:59:VAL:HG23	2.09	0.53
14:N:61:TYR:CD2	14:N:62:HIS:N	2.77	0.53
5:Z:162:GLY:O	5:Z:163:THR:HB	2.07	0.53
6:1:65:VAL:HG12	6:1:66:LYS:N	2.23	0.53
7:G:72:ARG:HB2	7:G:72:ARG:HH11	1.72	0.53
8:H:134:ALA:HB1	8:H:158:ALA:HB1	1.89	0.53
9:I:3:VAL:HG22	9:I:16:CYS:HB3	1.89	0.53
12:L:103:GLY:HA2	12:L:178:VAL:HG11	1.89	0.53
14:N:84:LYS:HD3	17:N:920:HOH:O	2.07	0.53
8:O:3:ILE:HG13	8:O:3:ILE:O	2.07	0.53
3:X:33:ARG:HB2	3:X:33:ARG:HH11	1.73	0.53
4:Y:15:PHE:HB2	5:Z:23:GLN:OE1	2.08	0.53
6:F:150:MET:HE3	6:F:152:GLU:OE2	2.09	0.53
10:Q:85:GLN:NE2	2:W:101:LYS:NZ	2.56	0.53
1:V:23:GLN:OE1	7:2:15:PHE:HB2	2.09	0.53
2:B:173:GLN:HA	2:B:176:LEU:HD12	1.91	0.53
14:N:159:LEU:O	14:N:163:ILE:HG13	2.09	0.53
8:O:34:LEU:HD22	8:O:174:ASP:HB3	1.90	0.53
10:Q:166:MET:HG2	10:Q:167:PRO:HD2	1.91	0.53
12:S:114:ASP:HB2	12:S:118:SER:HB3	1.91	0.53
13:T:41:THR:HG21	13:T:79:ILE:HD12	1.91	0.53
1:A:27:ALA:O	1:A:31:VAL:HG23	2.08	0.53
3:X:93:ARG:O	3:X:96:ALA:HB3	2.09	0.53
7:2:77:VAL:HG12	7:2:137:THR:HB	1.90	0.53
14:N:84:LYS:HB2	14:N:119:VAL:CG2	2.39	0.52
5:E:130:ARG:HG3	5:E:130:ARG:NH1	2.23	0.52
5:E:214:ILE:O	5:E:221:PHE:HA	2.09	0.52
6:F:184:LEU:HD11	6:F:188:GLU:HB3	1.91	0.52
14:N:14:LEU:O	14:N:175:MET:HA	2.09	0.52
1:V:15:PHE:N	2:W:23:GLN:HE22	2.06	0.52
3:X:38:VAL:CG2	3:X:39:GLY:N	2.73	0.52
6:1:220:LEU:N	6:1:220:LEU:HD23	2.24	0.52
6:1:224:VAL:HG13	6:1:228:LEU:HD23	1.91	0.52
5:E:22:PHE:HD1	5:E:26:TYR:HE1	1.57	0.52
5:E:24:VAL:O	5:E:27:ALA:HB3	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:163:THR:HB	17:L:2651:HOH:O	2.09	0.52
9:P:43:LEU:HD11	9:P:99:PRO:HB3	1.91	0.52
12:S:90:LYS:HE3	12:S:93:PHE:O	2.09	0.52
2:W:191:GLU:HG3	2:W:236:THR:HG22	1.91	0.52
5:Z:160:LEU:HD13	5:Z:163:THR:HB	1.92	0.52
4:D:215:ILE:HG22	4:D:221:PHE:CD2	2.42	0.52
7:G:105:TYR:OH	8:H:66:HIS:HE1	1.93	0.52
13:M:113:VAL:HA	13:M:118:VAL:O	2.09	0.52
2:B:46:ILE:HG21	2:B:139:ALA:HB1	1.92	0.52
3:C:49:GLY:C	3:C:50:CYS:SG	2.93	0.52
4:D:90:GLU:HA	17:D:509:HOH:O	2.08	0.52
11:K:4:LEU:O	11:K:4:LEU:HD13	2.09	0.52
11:K:38:ASN:O	11:K:40:PHE:N	2.42	0.52
7:G:105:TYR:CD2	7:G:105:TYR:N	2.77	0.52
10:J:176:LYS:HE2	10:J:186:GLN:HE21	1.75	0.52
13:M:112:TYR:O	13:M:119:THR:HA	2.09	0.52
9:P:2:ILE:HG21	9:P:130:ALA:HB3	1.92	0.52
11:R:105(B):LYS:HD2	11:R:105(B):LYS:N	2.14	0.52
5:E:223:ILE:HG22	5:E:223:ILE:O	2.09	0.52
12:L:140:ASN:ND2	9:P:161:ASN:HD21	2.06	0.52
8:O:134:ALA:O	8:O:137:VAL:N	2.43	0.52
12:S:79:ALA:O	12:S:83:ILE:HG13	2.10	0.52
5:Z:52:LYS:O	5:Z:63:TYR:HD2	1.92	0.52
5:E:36:VAL:HG22	5:E:37:THR:N	2.24	0.52
11:K:165:ARG:HH11	9:P:171:TRP:HH2	1.57	0.52
12:S:43:MET:HB2	12:S:101:ILE:CG2	2.33	0.52
5:Z:207:LEU:HD23	5:Z:207:LEU:H	1.74	0.52
7:2:108:PRO:HB2	7:2:111:VAL:HG23	1.91	0.52
7:2:109:CYS:HB3	17:2:2754:HOH:O	2.09	0.52
1:A:55:SER:HB2	17:G:3268:HOH:O	2.10	0.52
13:T:104:VAL:HG23	13:T:178:ILE:HG22	1.92	0.52
1:V:8:TYR:CD1	7:2:127:ALA:HB3	2.45	0.52
5:Z:22:PHE:HD1	5:Z:26:TYR:CE1	2.27	0.52
1:A:124:THR:HG22	2:B:130:ARG:HH21	1.73	0.52
2:B:38:ILE:HG23	2:B:164:SER:HB3	1.92	0.52
7:G:47:VAL:HG12	7:G:48:VAL:N	2.24	0.52
8:O:219:VAL:HG23	9:P:184:VAL:HG12	1.91	0.52
8:O:221:ILE:HG22	8:O:222:CYS:N	2.25	0.52
11:R:105(B):LYS:H	11:R:105(B):LYS:CD	2.13	0.52
4:Y:48:LEU:HD23	4:Y:77:ALA:HB2	1.92	0.52
6:I:170:GLN:CD	6:I:170:GLN:H	2.17	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:141:TYR:CD1	2:B:219(E):VAL:HG21	2.45	0.51
4:D:123:PHE:CE1	4:D:131:PRO:HG3	2.44	0.51
5:E:180:LEU:HD12	5:E:180(C):PHE:HE1	1.75	0.51
9:I:79:PHE:O	9:I:82:LEU:HB3	2.10	0.51
10:J:18:LYS:HD3	10:J:174:ILE:HG13	1.90	0.51
12:L:97:VAL:O	12:L:115:PRO:HB3	2.10	0.51
8:O:172:ASN:ND2	8:O:193:THR:HA	2.23	0.51
6:1:151:LEU:HD12	6:1:156:SER:O	2.10	0.51
8:H:113:ILE:HG12	8:H:119:THR:HG22	1.91	0.51
8:O:172:ASN:ND2	8:O:193:THR:HG22	2.25	0.51
3:X:33:ARG:HB2	3:X:33:ARG:NH1	2.25	0.51
10:J:35:ARG:O	10:J:42:LEU:HD12	2.10	0.51
10:J:147:THR:HG23	10:J:150:GLU:HG3	1.93	0.51
12:S:14:LEU:CD1	12:S:34:VAL:HG13	2.40	0.51
2:W:150:THR:O	2:W:157:TYR:HA	2.10	0.51
2:W:185:LYS:HD3	2:W:186:VAL:N	2.26	0.51
7:2:47:VAL:HG12	7:2:48:VAL:N	2.26	0.51
2:B:6:ARG:HG3	5:E:127:TYR:HH	1.75	0.51
7:G:187:GLU:O	7:G:191:GLU:HG3	2.10	0.51
12:S:-6:PRO:O	13:T:91:ARG:NH1	2.43	0.51
6:1:121:GLN:HG2	7:2:83:PRO:HB2	1.91	0.51
6:1:130:ARG:HH11	6:1:130:ARG:HG3	1.75	0.51
2:B:160:TRP:CD2	2:B:163:ILE:HD13	2.45	0.51
8:H:221:ILE:HG22	8:H:222:CYS:N	2.25	0.51
11:R:155:GLY:O	11:R:156:LYS:C	2.54	0.51
1:V:71:THR:O	1:V:73:ASP:N	2.44	0.51
2:W:15:PHE:HB2	3:X:23:GLN:NE2	2.24	0.51
4:Y:75:GLY:HA3	4:Y:221:PHE:CD2	2.45	0.51
6:F:21:ASN:HB2	17:F:547:HOH:O	2.10	0.51
7:G:91:ARG:HH21	7:G:115:ARG:HH21	1.57	0.51
11:K:12:ILE:HB	11:K:178:VAL:HB	1.92	0.51
13:M:135:ASN:ND2	13:M:139:ARG:NH2	2.59	0.51
14:N:161:GLN:O	14:N:164:LYS:HB3	2.10	0.51
9:P:-2:ASN:OD1	9:P:48:LEU:HD12	2.11	0.51
11:R:45:MET:HG2	11:R:52:CYS:HB3	1.92	0.51
13:T:112:TYR:O	13:T:119:THR:HA	2.10	0.51
13:T:150:VAL:HG21	17:T:2869:HOH:O	2.10	0.51
14:U:187(D):PRO:O	14:U:187(F):GLU:N	2.44	0.51
12:L:177:ILE:HD12	12:L:177:ILE:N	2.26	0.51
14:N:8:PHE:CE1	14:N:10:ASP:HB2	2.46	0.51
3:X:163:GLN:HG3	3:X:164:THR:N	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:ARG:HH21	7:G:118:ASN:HD22	1.59	0.51
11:K:8:PHE:HE2	11:K:13:ILE:HG12	1.75	0.51
11:K:126:CYS:SG	11:K:135:TYR:CD2	2.87	0.51
14:U:14:LEU:HD21	14:U:102:ALA:HB3	1.91	0.51
4:Y:186:LEU:O	4:Y:190:GLU:HG3	2.11	0.51
6:1:95:GLU:HG3	6:1:115:ARG:HH11	1.75	0.51
1:A:46:VAL:HG12	1:A:47:VAL:N	2.25	0.51
6:F:68:GLN:HE22	6:F:86:ARG:NH1	2.09	0.51
14:N:15:GLY:HA2	14:N:174:ARG:O	2.10	0.51
4:Y:160:TYR:CE2	5:Z:59:SER:HB3	2.46	0.51
1:A:137:LEU:HA	1:A:149:TYR:O	2.11	0.51
12:L:115:PRO:HA	17:L:613:HOH:O	2.11	0.51
14:N:30:VAL:HG11	13:T:199:PHE:CE2	2.43	0.51
12:S:14:LEU:HD12	12:S:34:VAL:HG13	1.93	0.51
13:T:164:TYR:C	13:T:165:ARG:HD2	2.36	0.51
7:2:14:ILE:O	7:2:21:LEU:HD23	2.11	0.51
7:2:222:PHE:N	7:2:222:PHE:CD2	2.79	0.51
1:A:35:VAL:HG12	1:A:36:THR:N	2.26	0.50
8:H:51:ASP:HB3	8:H:95:ILE:HG23	1.93	0.50
9:P:28:SER:HA	17:P:1086:HOH:O	2.11	0.50
14:U:14:LEU:O	14:U:175:MET:HA	2.10	0.50
4:D:180(C):HIS:NE2	4:D:184:LEU:HG	2.25	0.50
6:F:68:GLN:HG2	17:F:407:HOH:O	2.11	0.50
10:J:24:ILE:O	10:J:24:ILE:HG12	2.11	0.50
12:L:153:LYS:HG2	8:O:201:GLN:HG2	1.93	0.50
8:O:197:ARG:NH2	9:P:139:GLU:O	2.44	0.50
3:X:76:LEU:HD12	3:X:138:ILE:CG1	2.41	0.50
1:A:110:LYS:HG3	1:A:111:LEU:N	2.27	0.50
2:B:176:LEU:C	2:B:178:MET:N	2.69	0.50
6:F:127:ASN:C	6:F:127:ASN:ND2	2.69	0.50
8:H:167:LEU:HG	12:S:24:TYR:O	2.12	0.50
10:J:143:ARG:O	10:J:146:MET:HG3	2.11	0.50
9:P:160:LEU:HD11	9:P:191:MET:HB3	1.93	0.50
5:Z:41:ARG:O	5:Z:41:ARG:HG3	2.11	0.50
5:Z:45:HIS:HB2	5:Z:189:LEU:HD12	1.92	0.50
11:K:104:TYR:CD1	11:K:180:GLU:HG3	2.45	0.50
14:N:7:THR:HA	14:N:12:VAL:HG23	1.93	0.50
5:Z:15:PHE:H	6:1:23:GLN:HE22	1.59	0.50
5:Z:207:LEU:H	5:Z:207:LEU:CD2	2.25	0.50
4:D:41:ALA:HA	4:D:46:VAL:HG22	1.92	0.50
8:H:47:GLY:H	15:8:5:AKK:HC1	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:34:VAL:HG12	12:L:176:LEU:HD22	1.92	0.50
13:M:8:TYR:CE2	13:M:148:VAL:HG22	2.46	0.50
13:T:32:GLU:OE1	13:T:34:LEU:HB2	2.11	0.50
2:W:112:LEU:HD23	2:W:112:LEU:C	2.36	0.50
7:2:179:HIS:CD2	7:2:192:PHE:HZ	2.29	0.50
2:B:124:THR:CG2	3:C:130:ARG:HH21	2.22	0.50
4:D:14:THR:HA	17:D:3133:HOH:O	2.12	0.50
4:D:197:LEU:O	4:D:201:MET:HG3	2.12	0.50
8:H:152:ILE:O	8:H:153:LYS:C	2.54	0.50
9:I:171:TRP:HH2	11:R:165:ARG:HH11	1.59	0.50
5:Z:5:ARG:C	5:Z:7:ASN:H	2.20	0.50
6:1:18:ASP:OD1	6:1:20:ARG:HD3	2.12	0.50
6:1:68:GLN:OE1	6:1:89:VAL:HG21	2.11	0.50
4:D:100:ASN:HB3	17:D:252:HOH:O	2.11	0.50
6:F:54:ILE:HG13	6:F:208:PHE:HA	1.93	0.50
6:F:198:TYR:CE2	6:F:208:PHE:HZ	2.29	0.50
7:G:180(B):ASP:O	7:G:180(C):HIS:HB3	2.12	0.50
7:G:180(D):ILE:HG22	7:G:184:ASN:N	2.27	0.50
14:N:28:ASN:HA	17:N:319:HOH:O	2.10	0.50
8:O:128:GLY:O	8:O:131:SER:HB2	2.11	0.50
10:Q:155:LEU:O	10:Q:158:CYS:HB2	2.12	0.50
11:R:196:PHE:CE2	11:R:206:PHE:CD2	3.00	0.50
14:U:1:THR:HG23	14:U:33:LYS:NZ	2.26	0.50
5:Z:47:VAL:HG12	5:Z:48:LEU:N	2.26	0.50
3:C:134:VAL:HG12	3:C:135:SER:N	2.26	0.50
7:G:221:PHE:CD1	7:G:221:PHE:C	2.90	0.50
11:R:200:LYS:HG3	11:R:205:SER:O	2.12	0.50
13:T:4:ILE:HD11	13:T:159:MET:CG	2.41	0.50
5:Z:130:ARG:HG3	5:Z:130:ARG:NH1	2.20	0.50
4:D:79:SER:HB3	4:D:165:ILE:HD12	1.94	0.50
10:J:38:SER:O	10:J:40:HIS:N	2.45	0.50
11:R:174:ASN:HD21	11:R:189:ASN:HB2	1.76	0.50
3:X:238:GLN:C	3:X:240:LYS:H	2.20	0.50
6:1:49:ALA:HB2	6:1:212:ILE:HG23	1.93	0.50
6:1:240:ILE:HG23	6:1:241:ASN:ND2	2.26	0.50
2:B:86:GLU:HB2	17:B:863:HOH:O	2.11	0.49
3:C:216:LYS:HB2	3:C:220:ASP:HB3	1.93	0.49
5:E:97:ASN:ND2	12:L:61:ASN:HD21	2.07	0.49
6:F:150:MET:O	6:F:157:TYR:HA	2.12	0.49
14:N:163:ILE:CG2	14:N:170:GLY:HA2	2.41	0.49
2:W:134:VAL:O	2:W:153:PRO:HD3	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:125:GLN:HG3	6:F:130:ARG:HG2	1.93	0.49
6:F:66:LYS:HA	17:F:670:HOH:O	2.10	0.49
7:G:49:ILE:HD12	7:G:49:ILE:N	2.27	0.49
10:J:8:VAL:HG23	10:J:9:GLN:N	2.26	0.49
8:O:134:ALA:HB1	8:O:158:ALA:HB1	1.94	0.49
14:U:59:VAL:HG13	14:U:82:VAL:HG11	1.93	0.49
6:1:35:THR:HG22	6:1:36:THR:N	2.26	0.49
6:1:184:LEU:HD11	6:1:188:GLU:CB	2.42	0.49
2:B:39:GLY:HA2	2:B:47:VAL:O	2.12	0.49
2:B:81:LEU:HD22	2:B:81:LEU:N	2.27	0.49
6:F:32:GLU:C	6:F:34:GLY:H	2.19	0.49
8:H:55:VAL:HG23	8:H:86:HIS:HD2	1.77	0.49
8:H:213:VAL:HG12	8:H:214:LEU:N	2.27	0.49
9:I:15:ALA:CB	9:I:175:VAL:HG22	2.41	0.49
13:M:41:THR:HG21	13:M:79:ILE:HD12	1.94	0.49
14:N:112:THR:HG22	14:N:120:HIS:HB2	1.94	0.49
9:P:8:GLY:HA3	9:P:11:CYS:SG	2.52	0.49
12:S:19:ARG:HB2	12:S:171:ASP:HB2	1.93	0.49
1:V:11:SER:OG	2:W:129:LEU:HA	2.12	0.49
3:X:212:ILE:HG22	3:X:213:THR:N	2.27	0.49
5:Z:138:ILE:O	5:Z:148:LEU:HD12	2.11	0.49
6:1:221:HIS:CE1	6:1:223:PHE:CE1	2.95	0.49
8:H:55:VAL:HG23	8:H:86:HIS:CD2	2.45	0.49
11:K:35:ILE:CD1	11:K:45:MET:SD	3.01	0.49
13:M:35:ILE:HD13	13:M:56:GLU:HG2	1.94	0.49
2:W:86:GLU:HB2	17:W:2863:HOH:O	2.11	0.49
3:X:160:TRP:CZ2	4:Y:59:LEU:HD23	2.48	0.49
6:1:69:VAL:HG22	6:1:70:VAL:N	2.27	0.49
6:F:38:ILE:HA	6:F:137:ILE:HD13	1.94	0.49
7:G:82:ILE:N	7:G:83:PRO:HD2	2.28	0.49
8:H:114:HIS:HE1	17:H:544:HOH:O	1.96	0.49
12:L:29:ARG:HD3	12:L:171:ASP:OD1	2.12	0.49
12:L:123:GLN:HG3	12:L:145:TYR:OH	2.13	0.49
9:P:41:VAL:HG22	9:P:76:PRO:HG3	1.94	0.49
2:W:21:LEU:O	2:W:22:TYR:C	2.54	0.49
3:X:81:LEU:HB3	17:X:1414:HOH:O	2.12	0.49
5:Z:132:TYR:O	5:Z:153:PRO:HB3	2.13	0.49
5:Z:180(C):PHE:CD1	5:Z:180(D):ILE:N	2.79	0.49
6:1:32:GLU:C	6:1:34:GLY:H	2.20	0.49
6:F:126:TYR:CE1	7:G:129:MET:SD	3.04	0.49
7:G:105:TYR:HD2	7:G:105:TYR:N	2.09	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:77:VAL:HG13	17:H:952:HOH:O	2.12	0.49
12:L:134:ILE:HG22	12:L:138:LEU:CD2	2.43	0.49
10:Q:6:ILE:HD11	10:Q:142:TYR:CE1	2.47	0.49
3:X:154:SER:HB3	17:X:1000:HOH:O	2.12	0.49
15:9:4:R4K:N	15:9:4:R4K:C32	2.75	0.49
2:B:53:LYS:HG2	2:B:54:VAL:HG23	1.94	0.49
2:B:65:GLU:HG3	2:B:66:LYS:HG3	1.94	0.49
3:C:36:CYS:HA	3:C:166:GLY:HA3	1.94	0.49
6:F:148:LEU:HD12	6:F:149:TYR:N	2.27	0.49
7:G:151:THR:HA	7:G:156:TYR:O	2.13	0.49
8:O:111:PHE:HD1	8:O:121:VAL:HB	1.77	0.49
2:W:46:ILE:HG21	2:W:139:ALA:HB1	1.95	0.49
2:W:48:LEU:HD11	2:W:139:ALA:HB3	1.93	0.49
2:W:64:THR:HG23	2:W:67:LEU:O	2.13	0.49
3:X:216:LYS:HB2	3:X:220:ASP:HB3	1.95	0.49
4:Y:173:GLN:HB3	17:Y:1455:HOH:O	2.11	0.49
2:B:71:ASN:ND2	2:B:72:ASP:H	2.10	0.49
3:C:39:GLY:HA2	3:C:47:VAL:O	2.12	0.49
4:D:216:THR:O	4:D:217:LYS:C	2.56	0.49
7:G:8:TYR:C	7:G:10:ARG:H	2.21	0.49
13:M:160:ARG:HA	13:M:192:VAL:HG11	1.95	0.49
14:N:161:GLN:HE22	14:U:139:ASP:HB3	1.77	0.49
2:W:11:ARG:O	2:W:14:ILE:HG12	2.13	0.49
4:Y:121:LEU:HB2	17:Y:1156:HOH:O	2.12	0.49
6:F:236:ALA:O	6:F:238:LYS:N	2.46	0.49
7:G:207:LYS:HG3	7:G:208:ASN:OD1	2.12	0.49
10:Q:112:GLN:NE2	10:Q:126:ALA:H	2.11	0.49
13:T:157:ASN:O	13:T:158:ALA:C	2.56	0.49
5:Z:77:SER:OG	5:Z:137:LEU:HB2	2.13	0.49
6:1:97:ALA:O	6:1:99:PHE:N	2.46	0.49
3:C:57:LYS:HG3	3:C:208:LYS:NZ	2.28	0.49
4:D:112:LEU:O	4:D:116:VAL:HG23	2.13	0.49
6:F:78:TYR:HB3	6:F:136:THR:HG23	1.95	0.49
8:H:90:TYR:O	8:H:93:GLY:N	2.46	0.49
14:U:41:ILE:HD13	14:U:79:ALA:HB2	1.93	0.49
1:V:112:LEU:O	1:V:116:VAL:HG23	2.13	0.49
4:Y:59:LEU:HD13	4:Y:60:GLU:N	2.27	0.49
6:1:232:ALA:O	6:1:233:ILE:C	2.55	0.49
9:I:43:LEU:HD11	9:I:99:PRO:HB3	1.94	0.48
11:K:40:PHE:CD1	11:K:73:ARG:NH1	2.80	0.48
14:N:8:PHE:CZ	14:N:10:ASP:HB2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:O:86:HIS:CE1	8:O:90:TYR:HE2	2.30	0.48
12:S:51:ASP:OD1	12:S:95:TYR:HA	2.12	0.48
12:S:76:ILE:HG23	12:S:77:ASN:N	2.27	0.48
13:T:13:ILE:HG23	13:T:175:LEU:HD21	1.95	0.48
13:T:112:TYR:HE1	13:T:127:THR:HG22	1.78	0.48
13:T:157:ASN:O	13:T:160:ARG:N	2.46	0.48
14:U:59:VAL:O	14:U:60:GLN:C	2.56	0.48
5:Z:66:LYS:HA	5:Z:78:LEU:HD21	1.95	0.48
1:A:13:THR:HG22	1:A:21:LEU:HD22	1.95	0.48
1:A:46:VAL:CG1	1:A:47:VAL:N	2.75	0.48
2:B:112:LEU:HD23	2:B:112:LEU:C	2.38	0.48
4:D:237:LEU:HD22	4:D:241:GLU:HG3	1.95	0.48
6:F:31:VAL:O	6:F:34:GLY:N	2.46	0.48
6:F:221:HIS:HE1	6:F:223:PHE:HE1	1.59	0.48
12:L:49:ALA:HB1	17:M:965:HOH:O	2.13	0.48
12:L:166:HIS:HE1	17:L:233:HOH:O	1.95	0.48
13:M:40:ASN:HD22	13:M:40:ASN:N	2.11	0.48
14:N:111:TYR:HA	14:N:120:HIS:O	2.12	0.48
12:S:2:THR:HG21	12:S:130:ALA:HB3	1.94	0.48
2:W:38:ILE:HG23	2:W:164:SER:HB3	1.95	0.48
4:Y:77:ALA:HB3	4:Y:137:LEU:HB2	1.94	0.48
1:A:77:VAL:HG22	1:A:78:TYR:N	2.28	0.48
3:C:71:ASP:CA	10:J:68:ILE:HD11	2.42	0.48
11:K:208:ASN:O	9:P:30:LYS:NZ	2.46	0.48
14:N:157:HIS:O	14:N:158:SER:C	2.55	0.48
10:Q:85:GLN:NE2	2:W:101:LYS:HZ2	2.08	0.48
14:U:143:ARG:O	14:U:146:MET:HG3	2.13	0.48
3:X:57:LYS:CG	3:X:208:LYS:HZ3	2.26	0.48
4:Y:170:GLU:HG2	4:Y:171:GLY:N	2.27	0.48
1:A:85:TYR:O	1:A:89:VAL:HG23	2.12	0.48
3:C:159:SER:HB2	17:C:245:HOH:O	2.13	0.48
8:H:124:TYR:N	8:H:124:TYR:CD1	2.81	0.48
10:J:132:PHE:HD1	11:R:133:PHE:CZ	2.31	0.48
10:Q:156:LYS:O	10:Q:160:GLN:HG3	2.13	0.48
13:T:19:LEU:HD11	13:T:26:LEU:HB3	1.96	0.48
2:W:121:GLN:O	2:W:124:THR:HB	2.13	0.48
1:A:130:ARG:NH1	1:A:131:PRO:O	2.46	0.48
5:E:40:LEU:N	5:E:40:LEU:HD23	2.28	0.48
6:F:172:ALA:C	6:F:176:LEU:HD23	2.38	0.48
7:G:38:LEU:HD23	7:G:197:MET:HE3	1.95	0.48
8:H:1:THR:O	8:H:128:GLY:HA3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:200:LYS:HG3	11:K:205:SER:O	2.13	0.48
14:N:1:THR:HG23	14:N:33:LYS:NZ	2.29	0.48
8:O:18:THR:HB	8:O:30:ASN:HA	1.95	0.48
13:T:78:TYR:CE1	5:Z:105:ARG:HB2	2.48	0.48
1:V:150:GLN:O	1:V:157:TYR:HA	2.14	0.48
2:W:88:LEU:HD22	2:W:116:LEU:CD2	2.43	0.48
5:Z:74:MET:HE2	5:Z:109:VAL:HG22	1.96	0.48
7:2:143(A):GLU:HG2	17:2:1127:HOH:O	2.12	0.48
3:C:95:GLU:HG3	3:C:95:GLU:O	2.13	0.48
4:D:160:TYR:CZ	4:D:163:LYS:HD3	2.48	0.48
8:H:208:ARG:NH1	9:I:149:GLU:HB2	2.28	0.48
6:1:43:ASN:HD22	6:1:43:ASN:N	2.12	0.48
2:B:117:SER:HB3	2:B:155:GLY:O	2.13	0.48
3:C:15:PHE:N	4:D:23:GLN:HE22	1.96	0.48
4:D:201:MET:HE2	4:D:201:MET:HB3	1.62	0.48
5:E:70:CYS:SG	5:E:92:LEU:HD23	2.53	0.48
14:N:12:VAL:HG12	14:N:178:LEU:HB2	1.96	0.48
9:P:19:ARG:HB2	9:P:170:GLY:O	2.14	0.48
14:U:8:PHE:CE1	14:U:10:ASP:HB2	2.49	0.48
14:U:28:ASN:HA	17:U:2319:HOH:O	2.14	0.48
1:V:121:GLN:O	1:V:124:THR:HB	2.13	0.48
1:V:197:LEU:HD23	1:V:210:ILE:HD12	1.96	0.48
2:W:107:ILE:HD11	2:W:111:ILE:HG22	1.94	0.48
3:X:150:GLN:HE21	3:X:160:TRP:NE1	2.12	0.48
6:1:159:GLY:C	6:1:160:TYR:HD1	2.21	0.48
7:2:76:MET:SD	7:2:138:PHE:CE2	3.07	0.48
3:C:201:VAL:O	3:C:202:GLN:HB2	2.14	0.48
11:R:46:ALA:HB3	11:R:98:GLY:O	2.14	0.48
14:U:51:ASP:OD2	14:U:95:LEU:HA	2.13	0.48
7:2:179:HIS:CD2	7:2:192:PHE:CZ	3.01	0.48
1:A:124:THR:CG2	2:B:130:ARG:HH21	2.27	0.48
2:B:10:SER:O	2:B:11:ARG:C	2.56	0.48
5:E:180:LEU:HD12	5:E:180(C):PHE:CE1	2.49	0.48
6:F:150:MET:HE2	6:F:160:TYR:CE2	2.49	0.48
6:F:151:LEU:HD12	6:F:156:SER:O	2.14	0.48
6:F:158:TRP:HB2	6:F:160:TYR:HE1	1.78	0.48
7:G:236:ILE:C	7:G:238:GLU:H	2.21	0.48
12:L:99:THR:HG23	12:L:113:PHE:HB2	1.96	0.48
12:L:135:MET:CE	9:P:165:ARG:NH2	2.77	0.48
14:N:147:SER:OG	14:N:149:GLU:HG3	2.14	0.48
14:N:176:VAL:HG12	14:N:178:LEU:HD13	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:O:51:ASP:HB3	8:O:95:ILE:HG23	1.95	0.48
2:W:117:SER:HB3	2:W:155:GLY:O	2.14	0.48
3:X:134:VAL:CG1	3:X:135:SER:N	2.77	0.48
5:Z:180(C):PHE:HA	5:Z:180(F):ILE:HG13	1.96	0.48
6:1:136:THR:O	6:1:150:MET:HA	2.14	0.48
7:2:151:THR:HG22	7:2:157:TYR:HB2	1.95	0.48
7:2:198:ILE:O	7:2:200:ALA:N	2.47	0.48
6:F:148:LEU:HD12	6:F:149:TYR:H	1.79	0.48
12:L:104:LEU:HD23	12:L:108:GLY:HA2	1.94	0.48
9:P:137:MET:HE2	9:P:161:ASN:CB	2.37	0.48
2:W:160:TRP:CD2	2:W:163:ILE:HD13	2.49	0.48
3:X:57:LYS:CG	3:X:208:LYS:NZ	2.77	0.48
7:2:170:GLN:HE21	7:2:174:THR:HG23	1.78	0.48
1:A:121:GLN:O	1:A:124:THR:HB	2.14	0.47
9:I:43:LEU:HD12	9:I:100:VAL:O	2.13	0.47
12:L:93:PHE:N	12:L:94:PRO:HD3	2.29	0.47
13:M:157:ASN:ND2	13:M:160:ARG:HH11	2.12	0.47
13:T:157:ASN:HD22	13:T:160:ARG:NH1	2.11	0.47
1:V:71:THR:C	1:V:73:ASP:H	2.22	0.47
7:2:194:ILE:O	7:2:195:THR:C	2.57	0.47
4:D:52:LYS:HE3	4:D:211:GLN:HB2	1.96	0.47
11:K:31:VAL:HG12	11:K:33:LYS:HG3	1.96	0.47
11:K:142:TYR:C	11:K:143:LYS:HD2	2.39	0.47
12:L:-6:PRO:HB2	13:M:91:ARG:NH1	2.29	0.47
8:O:152:ILE:CG2	8:O:191:TYR:HE1	2.27	0.47
10:Q:113:ILE:CG1	10:Q:119:LYS:HG3	2.37	0.47
11:R:38:ASN:C	11:R:38:ASN:OD1	2.57	0.47
11:R:159:ILE:O	11:R:160:LEU:C	2.58	0.47
12:S:59:PHE:O	12:S:60:LYS:C	2.57	0.47
12:S:134:ILE:HG22	12:S:138:LEU:CD2	2.43	0.47
14:U:14:LEU:HD12	14:U:14:LEU:N	2.29	0.47
14:U:51:ASP:O	14:U:55:ILE:HG13	2.15	0.47
5:Z:76:LEU:HD23	5:Z:76:LEU:C	2.40	0.47
7:2:206:SER:O	7:2:209:ASP:HB2	2.15	0.47
1:A:58:LEU:HA	1:A:58:LEU:HD23	1.60	0.47
3:C:212:ILE:HG22	3:C:213:THR:N	2.28	0.47
5:E:38:VAL:HG22	5:E:164:ALA:HB2	1.96	0.47
5:E:117:CYS:SG	6:F:86:ARG:HD3	2.55	0.47
6:F:236:ALA:C	6:F:238:LYS:H	2.22	0.47
9:I:101:VAL:O	9:I:110:ILE:HA	2.13	0.47
11:K:38:ASN:C	11:K:38:ASN:OD1	2.57	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:R:83:LEU:O	11:R:86:LEU:HB3	2.14	0.47
12:S:25:SER:HB3	17:S:2284:HOH:O	2.14	0.47
13:T:1:THR:OG1	13:T:2:SER:N	2.47	0.47
14:U:67:THR:O	14:U:68:SER:C	2.57	0.47
1:V:52:LYS:O	1:V:54:SER:N	2.47	0.47
6:1:192:GLN:O	6:1:195:LYS:HB3	2.15	0.47
1:A:41:LYS:HA	1:A:46:VAL:HG22	1.96	0.47
6:F:18:ASP:OD1	6:F:20:ARG:HD3	2.14	0.47
8:H:103:GLY:HA2	8:H:178:MET:SD	2.55	0.47
9:I:178:ILE:HG23	9:I:184:VAL:CG2	2.44	0.47
11:K:19:ARG:HA	11:K:28:SER:O	2.13	0.47
10:Q:185:ARG:HG2	10:Q:185:ARG:HH11	1.79	0.47
3:X:121:GLN:C	3:X:121:GLN:CD	2.82	0.47
4:Y:160:TYR:CD2	5:Z:59:SER:HB3	2.49	0.47
7:2:87:ASN:C	7:2:87:ASN:HD22	2.22	0.47
3:C:123:TYR:CD1	3:C:132:PHE:HE1	2.33	0.47
4:D:97:VAL:HG11	11:K:65:LEU:HD11	1.95	0.47
5:E:28:LEU:O	5:E:31:ILE:HB	2.15	0.47
6:F:35:THR:CG2	6:F:36:THR:N	2.78	0.47
6:F:35:THR:HG23	6:F:51:GLU:HB3	1.96	0.47
8:H:167:LEU:HD12	12:S:24:TYR:HA	1.97	0.47
8:O:124:TYR:N	8:O:124:TYR:CD1	2.82	0.47
3:X:97:GLN:C	3:X:99:HIS:N	2.72	0.47
2:B:20:ARG:NH2	3:C:33:ARG:HE	2.13	0.47
5:E:65:LYS:HG3	5:E:65:LYS:O	2.15	0.47
6:F:38:ILE:HG22	6:F:164:ALA:CA	2.44	0.47
8:H:201:GLN:CG	12:S:153:LYS:HG2	2.44	0.47
10:J:44:SER:HG	10:J:100:LEU:HB2	1.79	0.47
13:M:62:LEU:HA	13:M:62:LEU:HD23	1.66	0.47
13:M:149:GLN:H	13:M:149:GLN:CD	2.23	0.47
8:O:55:VAL:HG23	8:O:86:HIS:HD2	1.80	0.47
10:Q:135:PHE:HZ	17:Q:2596:HOH:O	1.98	0.47
2:W:56:SER:OG	2:W:57:THR:N	2.45	0.47
3:X:135:SER:OG	3:X:152:GLU:HA	2.14	0.47
6:1:157:TYR:CD1	6:1:157:TYR:C	2.92	0.47
1:A:7:ARG:HH22	4:D:123(C):GLY:HA3	1.79	0.47
2:B:157:TYR:CD2	3:C:86:ARG:NH1	2.82	0.47
4:D:89:ILE:HG22	4:D:93:ARG:HD2	1.96	0.47
9:I:-2:ASN:HA	9:I:21:GLY:O	2.15	0.47
11:K:46:ALA:HB3	11:K:98:GLY:O	2.15	0.47
13:M:19:LEU:HD22	13:M:170:SER:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:O:3:ILE:HG22	8:O:16:ALA:HB2	1.97	0.47
9:P:6:MET:HE1	9:P:154:THR:HG22	1.97	0.47
9:P:75:GLU:OE1	9:P:105:ASN:HA	2.14	0.47
9:P:137:MET:HE3	9:P:141:LEU:HD11	1.97	0.47
13:T:205:GLY:HA3	13:T:209:GLN:HB3	1.97	0.47
3:X:71:ASP:O	3:X:73:HIS:N	2.48	0.47
5:Z:38:VAL:HG12	5:Z:39:GLY:N	2.30	0.47
6:1:12:ASN:OD1	6:1:12:ASN:C	2.58	0.47
6:1:83:PRO:O	6:1:86:ARG:N	2.48	0.47
6:1:127:ASN:C	6:1:127:ASN:ND2	2.72	0.47
7:2:67:ILE:CD1	7:2:211:GLU:HG2	2.45	0.47
7:2:136:LEU:O	7:2:150:LYS:HA	2.14	0.47
14:N:186:ARG:NH2	13:T:204:LYS:HB2	2.30	0.47
9:P:53:THR:HG22	10:Q:84:ARG:NH2	2.30	0.47
4:Y:29:GLU:OE2	4:Y:32:LYS:HD2	2.15	0.47
5:Z:65:LYS:HG3	5:Z:65:LYS:O	2.15	0.47
1:A:221:PHE:C	1:A:221:PHE:CD2	2.93	0.47
6:F:109:ILE:HB	6:F:110:PRO:HD3	1.95	0.47
10:J:53:VAL:O	10:J:54:GLN:C	2.58	0.47
13:M:111:ARG:HG3	13:M:120:TYR:O	2.15	0.47
11:R:138:LEU:HD13	11:R:158:SER:OG	2.15	0.47
13:T:161:VAL:O	13:T:164:TYR:HB2	2.14	0.47
14:U:3:ILE:HG22	14:U:16:ALA:HB2	1.96	0.47
17:1:2420:HOH:O	7:2:86:ARG:HD2	2.14	0.47
5:E:97:ASN:HD21	12:L:61:ASN:ND2	2.12	0.47
13:M:112:TYR:CD2	13:M:120:TYR:CZ	3.03	0.47
14:U:78:THR:O	14:U:79:ALA:C	2.58	0.47
1:V:210:ILE:HG22	1:V:211:GLU:N	2.30	0.47
3:X:123:TYR:CD1	3:X:132:PHE:HE1	2.33	0.47
6:1:115:ARG:HG2	17:1:2418:HOH:O	2.14	0.47
2:B:192:LEU:HD23	2:B:192:LEU:O	2.15	0.46
6:F:53:LEU:HD23	6:F:53:LEU:HA	1.71	0.46
10:J:74:LEU:HD22	10:J:78:ALA:HB1	1.97	0.46
11:K:136:GLY:HA2	10:Q:161:GLU:OE1	2.15	0.46
9:P:3:VAL:HG22	9:P:16:CYS:HB3	1.97	0.46
9:P:71:GLU:HG2	17:P:2213:HOH:O	2.13	0.46
13:T:-6:GLN:O	13:T:-6:GLN:HG3	2.15	0.46
13:T:19:LEU:HD22	13:T:170:SER:HB2	1.95	0.46
1:V:146:GLY:HA3	17:V:2772:HOH:O	2.15	0.46
4:Y:148:LEU:HD12	4:Y:149:PHE:H	1.81	0.46
2:B:51:GLU:OE2	2:B:202:THR:HG23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:139:ILE:HG22	5:E:148:LEU:HD13	1.97	0.46
5:E:162:GLY:O	5:E:163:THR:HB	2.14	0.46
6:F:157:TYR:CE2	7:G:86:ARG:NH1	2.83	0.46
8:H:197:ARG:HH12	8:H:200:LYS:HD3	1.79	0.46
9:I:12:VAL:CG1	9:I:108:PRO:HB3	2.45	0.46
11:K:151:ALA:O	11:K:152:LEU:C	2.58	0.46
13:M:91:ARG:HG3	13:M:92:SER:N	2.30	0.46
8:O:204:TYR:O	8:O:206:PHE:CD2	2.69	0.46
8:O:219:VAL:CG2	9:P:184:VAL:HG12	2.45	0.46
9:P:67:LYS:O	9:P:71:GLU:N	2.48	0.46
17:S:1438:HOH:O	13:T:132:HIS:HE1	1.98	0.46
13:T:100:ILE:HD13	13:T:125:LEU:HB2	1.96	0.46
14:U:84:LYS:HE3	14:U:119:VAL:HG23	1.98	0.46
4:Y:139:ALA:HB2	4:Y:148:LEU:HD13	1.97	0.46
6:1:7:GLY:C	6:1:9:ASP:H	2.22	0.46
1:A:77:VAL:HG22	1:A:78:TYR:H	1.79	0.46
1:A:142:ASP:O	1:A:144:PHE:N	2.49	0.46
3:C:163:GLN:CG	3:C:164:THR:N	2.78	0.46
5:E:207:LEU:HD23	5:E:207:LEU:H	1.80	0.46
14:N:52:THR:O	14:N:53:GLN:C	2.58	0.46
12:S:67:HIS:HD2	17:Z:2864:HOH:O	1.97	0.46
12:S:166:HIS:HE1	17:S:2233:HOH:O	1.99	0.46
13:T:198:ASP:HB3	17:T:3406:HOH:O	2.15	0.46
3:X:49:GLY:C	3:X:50:CYS:SG	2.98	0.46
5:Z:180(C):PHE:C	5:Z:180(E):LYS:N	2.72	0.46
2:B:78:VAL:HG22	2:B:136:PHE:CE2	2.51	0.46
14:N:161:GLN:HE21	14:U:136:GLY:CA	2.10	0.46
14:N:187(D):PRO:O	14:N:187(F):GLU:N	2.48	0.46
10:Q:18:LYS:CD	10:Q:174:ILE:HG13	2.38	0.46
3:C:38:VAL:CG2	3:C:39:GLY:N	2.78	0.46
3:C:163:GLN:HE21	3:C:164:THR:N	2.05	0.46
4:D:89:ILE:HD13	4:D:89:ILE:HA	1.74	0.46
12:L:-6:PRO:HB2	13:M:91:ARG:HH11	1.81	0.46
9:P:97:VAL:HG23	9:P:99:PRO:HD3	1.97	0.46
12:S:60:LYS:O	12:S:63:VAL:HB	2.16	0.46
14:U:3:ILE:HG22	14:U:16:ALA:CB	2.45	0.46
1:V:66:LYS:HG2	1:V:78:TYR:HE1	1.80	0.46
6:1:109:ILE:HB	6:1:110:PRO:HD3	1.97	0.46
7:2:82:ILE:N	7:2:83:PRO:HD2	2.30	0.46
7:2:225:SER:O	7:2:226:ALA:C	2.58	0.46
4:D:25:GLU:O	4:D:28:LEU:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:69:VAL:HG23	6:F:74:ILE:O	2.14	0.46
6:F:113:ALA:O	6:F:114:ASP:C	2.55	0.46
10:J:133:TYR:C	17:J:441:HOH:O	2.58	0.46
12:L:102:ALA:HB2	12:L:110:VAL:HG22	1.97	0.46
13:M:55:ILE:O	13:M:59:LEU:HG	2.15	0.46
9:P:59:PHE:CZ	9:P:83:VAL:HG22	2.50	0.46
11:R:99:THR:HA	17:R:2444:HOH:O	2.16	0.46
13:T:35:ILE:HA	13:T:36:PRO:HD3	1.82	0.46
13:T:53:GLN:O	13:T:56:GLU:HB2	2.15	0.46
1:V:175:PHE:O	1:V:175:PHE:CD1	2.68	0.46
7:2:119:LEU:HD12	7:2:119:LEU:HA	1.79	0.46
7:2:179:HIS:ND1	7:2:179:HIS:C	2.73	0.46
3:C:93:ARG:O	3:C:96:ALA:HB3	2.16	0.46
6:F:206(B):GLU:HG3	6:F:206(C):LYS:HG3	1.97	0.46
10:J:155:LEU:O	10:J:158:CYS:HB2	2.16	0.46
11:K:87:VAL:CG2	11:K:97:MET:HE2	2.45	0.46
11:K:155:GLY:O	11:K:158:SER:N	2.49	0.46
9:P:6:MET:SD	9:P:142:TYR:HD1	2.38	0.46
11:R:174:ASN:ND2	11:R:189:ASN:HB2	2.30	0.46
12:S:20:ASN:O	12:S:27:ASN:HB2	2.16	0.46
13:T:42:VAL:HG23	13:T:178:ILE:HD11	1.96	0.46
2:W:39:GLY:HA2	2:W:47:VAL:O	2.16	0.46
3:X:35:THR:HB	3:X:51:GLU:CG	2.43	0.46
5:Z:47:VAL:O	5:Z:48:LEU:HD23	2.16	0.46
6:1:235:PHE:CD2	6:1:235:PHE:O	2.69	0.46
7:2:168:LYS:O	7:2:172:ILE:HG13	2.15	0.46
6:F:67:ILE:HG22	6:F:68:GLN:N	2.30	0.46
11:K:87:VAL:HG11	11:K:115:SER:HA	1.98	0.46
12:L:98:HIS:HE1	12:L:112:SER:HB2	1.80	0.46
9:P:7:THR:HG23	9:P:110:ILE:CD1	2.45	0.46
9:P:99:PRO:HB2	9:P:113:PHE:CE2	2.51	0.46
10:Q:129:TYR:O	10:Q:132:PHE:HB2	2.16	0.46
12:S:19:ARG:NE	12:S:171:ASP:OD2	2.46	0.46
2:W:176:LEU:C	2:W:178:MET:H	2.24	0.46
3:X:57:LYS:HG3	3:X:208:LYS:NZ	2.30	0.46
3:X:150:GLN:HE21	3:X:160:TRP:HE1	1.64	0.46
6:1:15:PHE:CE2	7:2:27:ALA:HB2	2.51	0.46
6:1:120:VAL:HG21	6:1:151:LEU:HD21	1.97	0.46
1:A:150:GLN:O	1:A:157:TYR:HA	2.15	0.46
2:B:120:LYS:NZ	2:B:136:PHE:HD1	2.14	0.46
3:C:154:SER:OG	3:C:156:ILE:HB	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:208:LYS:HE3	3:C:209:ASN:HD22	1.81	0.46
4:D:110:GLU:O	4:D:113:THR:HB	2.16	0.46
6:F:141:VAL:CG2	6:F:215:CYS:SG	2.96	0.46
11:K:200:LYS:HE3	11:K:206:PHE:O	2.16	0.46
2:W:163:ILE:HG13	2:W:164:SER:N	2.31	0.46
7:2:55:PRO:HG2	7:2:56:ASP:H	1.81	0.46
7:2:179(D):SER:O	7:2:179(E):LYS:HB2	2.15	0.46
2:B:101:LYS:HZ1	10:J:85:GLN:NE2	2.13	0.46
5:E:76:LEU:HD23	5:E:76:LEU:C	2.40	0.46
6:F:82:ILE:O	6:F:83:PRO:C	2.58	0.46
10:J:2:ILE:O	10:J:3:ILE:HD13	2.15	0.46
12:L:18:THR:HG22	12:L:31:GLU:H	1.80	0.46
14:N:48:SER:HB3	14:N:51:ASP:HB2	1.98	0.46
10:Q:35:ARG:NH2	17:Q:2774:HOH:O	2.49	0.46
13:T:43:VAL:HG22	13:T:101:VAL:HG22	1.98	0.46
13:T:125:LEU:HA	17:T:2278:HOH:O	2.16	0.46
14:U:7:THR:HA	14:U:12:VAL:HG23	1.98	0.46
5:Z:37:THR:OG1	5:Z:50:ALA:HB2	2.16	0.46
4:D:40:ILE:HD11	4:D:193:VAL:HG23	1.96	0.45
6:F:180(E):GLU:HG3	6:F:180(F):GLY:O	2.16	0.45
13:M:3:VAL:O	13:M:126:ALA:HA	2.16	0.45
9:P:55:LEU:HD21	9:P:95:TYR:CD1	2.50	0.45
1:V:62:GLU:H	1:V:62:GLU:CD	2.24	0.45
4:Y:17:PRO:HA	5:Z:26:TYR:CD2	2.51	0.45
6:1:86:ARG:HH11	6:1:86:ARG:HG2	1.81	0.45
2:B:141:TYR:CG	2:B:142:ASP:N	2.85	0.45
3:C:47:VAL:O	3:C:48:LEU:HD23	2.16	0.45
5:E:212:ILE:HG22	5:E:213:ALA:N	2.31	0.45
5:E:220:PRO:O	5:E:221:PHE:C	2.59	0.45
7:G:99:PHE:CE1	7:G:107:MET:HA	2.51	0.45
8:H:33:LYS:HE2	15:8:5:AKK:CA	2.43	0.45
8:H:126:SER:O	8:H:127:LEU:HD23	2.16	0.45
10:J:156:LYS:O	10:J:160:GLN:HG3	2.17	0.45
11:K:58:TRP:O	11:K:59:LEU:C	2.59	0.45
11:K:196:PHE:HE2	11:K:206:PHE:CD2	2.35	0.45
13:M:153:GLU:HG3	17:M:3470:HOH:O	2.15	0.45
14:N:113:ILE:HA	14:N:118:SER:O	2.15	0.45
8:O:4:VAL:HG22	8:O:159:ILE:HD11	1.97	0.45
11:R:5:ALA:CB	11:R:100:MET:HE3	2.47	0.45
11:R:88:TYR:HB2	17:R:2144:HOH:O	2.17	0.45
13:T:102:ALA:HB2	13:T:110:LEU:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:31:VAL:HG13	1:V:79:SER:O	2.16	0.45
3:X:198:LEU:HA	3:X:198:LEU:HD23	1.61	0.45
5:Z:17:PRO:HA	6:1:26:TYR:CD2	2.51	0.45
5:Z:47:VAL:HG11	5:Z:190:ILE:HG12	1.98	0.45
7:2:91:ARG:NH2	7:2:115:ARG:NH2	2.63	0.45
4:D:139:ALA:HB2	4:D:148:LEU:CD1	2.46	0.45
5:E:52:LYS:O	5:E:63:TYR:HD2	2.00	0.45
8:H:218:ILE:HG22	8:H:219:VAL:N	2.32	0.45
12:L:8:GLY:HA3	12:L:11:PHE:CE2	2.51	0.45
9:P:55:LEU:HD23	9:P:55:LEU:N	2.31	0.45
12:S:49:ALA:HB1	17:T:2965:HOH:O	2.17	0.45
13:T:35:ILE:HD13	13:T:56:GLU:HG2	1.98	0.45
4:Y:32:LYS:O	4:Y:167:SER:HA	2.17	0.45
4:Y:117:CYS:HB3	4:Y:155:GLY:O	2.16	0.45
2:B:176:LEU:C	2:B:178:MET:H	2.23	0.45
3:C:25:GLU:O	3:C:28:LEU:HB2	2.16	0.45
4:D:115:SER:O	4:D:118:ASP:HB2	2.16	0.45
4:D:224:TYR:CD2	4:D:224:TYR:N	2.84	0.45
8:O:3:ILE:HG22	8:O:16:ALA:CB	2.47	0.45
10:Q:12:VAL:HG23	10:Q:108:PRO:HB2	1.98	0.45
12:S:8:GLY:HA3	12:S:11:PHE:CZ	2.52	0.45
13:T:112:TYR:CD2	13:T:120:TYR:CZ	3.05	0.45
4:Y:123(G):GLU:HG2	4:Y:125:GLU:H	1.80	0.45
6:1:35:THR:CG2	6:1:36:THR:N	2.78	0.45
6:1:67:ILE:HG13	6:1:211:GLU:OE1	2.15	0.45
6:1:150:MET:HE3	6:1:152:GLU:OE2	2.15	0.45
7:2:214:VAL:HG12	7:2:215:ALA:H	1.80	0.45
5:E:180(C):PHE:C	5:E:180(E):LYS:N	2.74	0.45
10:Q:43:MET:HG3	10:Q:101:ILE:CG1	2.46	0.45
10:Q:129:TYR:HA	10:Q:132:PHE:HD2	1.82	0.45
14:U:84:LYS:HB2	14:U:119:VAL:CG2	2.46	0.45
4:Y:90:GLU:HA	17:Y:2509:HOH:O	2.16	0.45
4:Y:194:LEU:HD12	4:Y:194:LEU:HA	1.77	0.45
5:Z:82:ALA:O	5:Z:83:PRO:C	2.60	0.45
5:Z:194:VAL:O	5:Z:195:GLU:C	2.60	0.45
6:1:107:ILE:HA	6:1:108:PRO:HD3	1.76	0.45
7:G:120:SER:O	7:G:121:GLN:C	2.57	0.45
7:G:225:SER:O	7:G:226:ALA:C	2.59	0.45
11:K:210:ILE:N	17:K:2742:HOH:O	2.50	0.45
12:L:184:VAL:HG12	12:L:184:VAL:O	2.16	0.45
11:R:138:LEU:HD12	11:R:138:LEU:HA	1.67	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:71:ASN:HD22	2:W:72:ASP:N	2.14	0.45
4:Y:156:THR:HG23	5:Z:83:PRO:HD3	1.97	0.45
6:1:54:ILE:HG13	6:1:208:PHE:HA	1.98	0.45
6:1:236:ALA:C	6:1:238:LYS:H	2.25	0.45
2:B:15:PHE:HB2	3:C:23:GLN:NE2	2.30	0.45
2:B:189:ALA:O	2:B:190:ILE:C	2.59	0.45
5:E:198:SER:HA	5:E:201:LEU:CD1	2.47	0.45
7:G:72:ARG:NH2	14:N:39:ASP:OD2	2.50	0.45
8:H:5:GLY:O	8:H:124:TYR:HA	2.16	0.45
8:H:124:TYR:HB2	8:H:138:LEU:HD13	1.99	0.45
9:I:76:PRO:O	9:I:77:GLU:C	2.60	0.45
10:J:138:LEU:O	10:J:139:ASP:C	2.57	0.45
10:J:171:LYS:NZ	10:Q:163:GLU:O	2.50	0.45
9:P:45:ILE:CG2	9:P:52:VAL:HG22	2.47	0.45
14:U:187(D):PRO:C	14:U:187(F):GLU:N	2.75	0.45
1:V:134:VAL:O	1:V:153:PRO:HG3	2.17	0.45
2:W:176:LEU:C	2:W:178:MET:N	2.74	0.45
3:X:241:GLN:C	3:X:243:GLN:H	2.25	0.45
5:Z:176:LEU:C	5:Z:178:ARG:N	2.73	0.45
6:1:50:VAL:HG22	6:1:51:GLU:N	2.30	0.45
6:1:236:ALA:O	6:1:238:LYS:N	2.50	0.45
1:A:23:GLN:OE1	7:G:15:PHE:HB2	2.16	0.45
3:C:57:LYS:CG	3:C:208:LYS:NZ	2.80	0.45
6:F:36:THR:HG22	6:F:51:GLU:OE2	2.17	0.45
6:F:120:VAL:HG21	6:F:151:LEU:HD21	1.99	0.45
6:F:176:LEU:HD22	6:F:196:ILE:HD13	1.99	0.45
8:H:35:HIS:CG	8:H:56:THR:HG21	2.52	0.45
14:N:67:THR:O	14:N:68:SER:C	2.60	0.45
9:P:33:LYS:O	9:P:44:GLY:HA2	2.17	0.45
10:Q:78:ALA:O	10:Q:79:VAL:C	2.60	0.45
11:R:87:VAL:CG1	11:R:115:SER:HA	2.43	0.45
11:R:138:LEU:O	11:R:139:ASP:C	2.60	0.45
2:W:124:THR:CG2	3:X:130:ARG:HH21	2.29	0.45
6:1:52:LYS:HD2	6:1:211:GLU:OE2	2.16	0.45
7:2:82:ILE:O	7:2:83:PRO:C	2.59	0.45
6:F:208:PHE:H	6:F:208:PHE:HD2	1.64	0.45
9:I:161:ASN:ND2	12:S:140:ASN:ND2	2.64	0.45
10:J:140:HIS:HD2	10:J:141:HIS:CE1	2.35	0.45
11:K:104:TYR:CD2	11:K:179:THR:HA	2.51	0.45
13:M:136:PRO:HA	8:O:165:ASN:OD1	2.17	0.45
10:Q:54:GLN:OE1	11:R:85:ASN:ND2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:Q:104:TYR:CD1	10:Q:104:TYR:C	2.95	0.45
12:S:21:ILE:C	12:S:21:ILE:HD12	2.41	0.45
13:T:8:TYR:CE2	13:T:148:VAL:HG22	2.51	0.45
14:U:51:ASP:OD2	14:U:95:LEU:HD23	2.17	0.45
14:U:65:LEU:HG	14:U:69:GLN:HE21	1.80	0.45
2:B:186:VAL:HG12	2:B:187:ASP:N	2.32	0.45
8:H:201:GLN:HG2	12:S:153:LYS:HG2	1.97	0.45
13:M:11:GLY:HA3	13:M:178:ILE:O	2.17	0.45
13:M:49:ILE:O	13:M:50:SER:C	2.57	0.45
11:R:1:THR:HG23	11:R:33:LYS:HZ2	1.82	0.45
14:U:36:ARG:HG2	14:U:38:HIS:H	1.82	0.45
14:U:41:ILE:C	14:U:42:TRP:HD1	2.25	0.45
14:U:151:THR:O	14:U:152:VAL:C	2.60	0.45
2:W:141:TYR:CG	2:W:142:ASP:N	2.85	0.45
3:X:160:TRP:CE2	4:Y:59:LEU:HD23	2.51	0.45
5:Z:28:LEU:O	5:Z:31:ILE:HB	2.17	0.45
5:Z:92:LEU:HD12	5:Z:92:LEU:HA	1.85	0.45
2:B:21:LEU:O	2:B:22:TYR:C	2.60	0.44
4:D:160:TYR:CE2	5:E:59:SER:HB3	2.51	0.44
5:E:31:ILE:HD11	5:E:153:PRO:HD2	1.99	0.44
7:G:111:VAL:HG22	8:H:70:THR:HG22	1.98	0.44
8:H:13:VAL:HG22	8:H:14:ILE:N	2.31	0.44
12:L:42:VAL:HG22	12:L:102:ALA:O	2.17	0.44
14:N:32:ASP:OD1	13:T:204:LYS:HA	2.17	0.44
14:N:144:GLU:HG2	17:N:485:HOH:O	2.17	0.44
10:Q:136:SER:HA	17:Q:194:HOH:O	2.17	0.44
2:W:82:THR:O	2:W:85:ALA:HB3	2.17	0.44
3:X:148:LEU:HD23	3:X:160:TRP:O	2.17	0.44
4:Y:119:LEU:HD23	4:Y:119:LEU:O	2.17	0.44
4:D:134:VAL:HG22	4:D:135:ALA:N	2.32	0.44
5:E:226:GLY:O	5:E:229:VAL:HG22	2.17	0.44
6:F:172:ALA:O	6:F:176:LEU:HD23	2.18	0.44
7:G:55:PRO:HG2	7:G:56:ASP:H	1.82	0.44
8:H:8:PHE:CE2	8:H:12:VAL:N	2.85	0.44
12:L:90:LYS:HD3	12:L:95:TYR:CZ	2.51	0.44
10:Q:74:LEU:HD22	10:Q:78:ALA:CB	2.48	0.44
7:2:194:ILE:HD13	7:2:210:LEU:HD12	1.99	0.44
7:2:207:LYS:C	7:2:209:ASP:H	2.25	0.44
1:A:32:LYS:HE2	1:A:32:LYS:HA	1.98	0.44
2:B:197:LEU:HA	2:B:200:THR:OG1	2.17	0.44
3:C:180(D):GLU:N	3:C:182:PRO:HD3	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:172:ALA:O	6:F:173:LYS:C	2.60	0.44
7:G:72:ARG:HB2	7:G:72:ARG:NH1	2.32	0.44
8:H:157:ASP:O	8:H:160:GLN:HB2	2.17	0.44
8:O:206:PHE:CE1	9:P:157:GLN:HG3	2.53	0.44
11:R:49:ALA:HB1	12:S:118:SER:OG	2.17	0.44
11:R:85:ASN:ND2	17:R:2153:HOH:O	2.49	0.44
13:T:186:PHE:CE1	13:T:188:LYS:HG3	2.52	0.44
1:V:172:ALA:O	1:V:173:LYS:C	2.60	0.44
3:X:39:GLY:HA2	3:X:47:VAL:O	2.17	0.44
3:X:69:LYS:HA	3:X:75:VAL:HG12	2.00	0.44
3:X:215:VAL:O	3:X:215:VAL:HG22	2.16	0.44
3:C:89:ILE:HG22	3:C:93:ARG:HD2	1.99	0.44
6:F:158:TRP:HB2	6:F:160:TYR:CE1	2.52	0.44
10:J:105:ASP:O	10:J:105(B):LYS:N	2.51	0.44
8:O:52:THR:O	8:O:56:THR:HB	2.17	0.44
10:Q:8:VAL:HG23	10:Q:9:GLN:N	2.32	0.44
10:Q:43:MET:HG3	10:Q:101:ILE:HG13	1.99	0.44
14:U:157:HIS:O	14:U:158:SER:C	2.61	0.44
1:V:141:HIS:CG	1:V:142:ASP:N	2.86	0.44
3:X:168:ASN:O	3:X:172:VAL:HG12	2.17	0.44
3:X:219:SER:N	17:X:2958:HOH:O	2.50	0.44
4:Y:159:ARG:HB3	5:Z:60:SER:HB3	1.99	0.44
7:2:236:ILE:C	7:2:238:GLU:H	2.25	0.44
2:B:67:LEU:HD12	2:B:77:ALA:HA	1.99	0.44
5:E:226:GLY:O	5:E:227:GLU:C	2.61	0.44
6:F:107:ILE:HA	6:F:108:PRO:HD3	1.76	0.44
6:F:236:ALA:C	6:F:238:LYS:N	2.76	0.44
7:G:86:ARG:O	7:G:89:ALA:HB3	2.17	0.44
11:K:206:PHE:CE1	10:Q:139:ASP:HB3	2.53	0.44
8:O:48:THR:HG22	17:O:2636:HOH:O	2.18	0.44
8:O:124:TYR:HD2	8:O:138:LEU:HB3	1.82	0.44
10:Q:10:ASP:O	10:Q:11:SER:HB3	2.18	0.44
14:U:41:ILE:C	14:U:42:TRP:CD1	2.96	0.44
7:2:8:TYR:C	7:2:10:ARG:H	2.25	0.44
7:2:184(G):GLU:HG2	7:2:188:LYS:CB	2.47	0.44
3:C:135:SER:OG	3:C:152:GLU:HA	2.17	0.44
4:D:40:ILE:CD1	4:D:193:VAL:HG23	2.47	0.44
7:G:194:ILE:HG23	7:G:210:LEU:HD11	2.00	0.44
10:J:74:LEU:HD22	10:J:78:ALA:CB	2.47	0.44
10:J:75:SER:HB2	17:J:835:HOH:O	2.18	0.44
10:J:112:GLN:NE2	10:J:126:ALA:H	2.15	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:136:SER:HA	17:J:2114:HOH:O	2.18	0.44
3:X:62(A):ILE:H	3:X:62(A):ILE:HG12	1.64	0.44
3:X:110:GLU:O	3:X:113:THR:HB	2.17	0.44
5:Z:21:LEU:HD23	5:Z:21:LEU:HA	1.82	0.44
6:1:151:LEU:HD13	6:1:157:TYR:HB3	1.99	0.44
3:C:49:GLY:C	3:C:50:CYS:HG	2.26	0.44
5:E:73:HIS:CE1	5:E:107:LEU:O	2.68	0.44
5:E:151:PHE:HA	5:E:157:VAL:HG22	2.00	0.44
8:H:153:LYS:O	8:H:154:LEU:C	2.61	0.44
11:K:1:THR:O	11:K:128:GLY:HA3	2.17	0.44
12:L:2:THR:HG21	12:L:130:ALA:HB3	2.00	0.44
12:L:17:ASP:HA	12:L:172:GLY:O	2.17	0.44
13:M:-6:GLN:HG3	13:M:-6:GLN:O	2.16	0.44
14:N:9:LYS:O	14:N:107:LYS:HD3	2.17	0.44
14:U:177:VAL:HG23	14:U:185:GLU:HB3	2.00	0.44
1:V:69:LEU:HD23	1:V:69:LEU:C	2.43	0.44
1:V:81:MET:HE1	7:2:21:LEU:HD11	1.99	0.44
1:V:124:THR:HG22	1:V:124:THR:O	2.18	0.44
2:W:172:ALA:HB2	2:W:200:THR:HG21	1.99	0.44
1:A:71:THR:O	1:A:73:ASP:N	2.51	0.44
2:B:71:ASN:HD22	2:B:72:ASP:N	2.13	0.44
6:F:69:VAL:HG12	17:F:563:HOH:O	2.16	0.44
8:H:151:ALA:O	8:H:152:ILE:C	2.58	0.44
10:J:35:ARG:NH2	17:J:774:HOH:O	2.51	0.44
11:K:137:VAL:HG21	11:K:161:ALA:HB2	2.00	0.44
13:M:1:THR:OG1	13:M:2:SER:N	2.51	0.44
10:Q:138:LEU:O	10:Q:139:ASP:C	2.61	0.44
11:R:63:CYS:SG	11:R:74:ILE:HD13	2.58	0.44
2:B:82:THR:O	2:B:85:ALA:HB3	2.18	0.44
8:H:136:ALA:O	8:H:137:VAL:C	2.61	0.44
11:K:155:GLY:O	11:K:156:LYS:C	2.61	0.44
12:L:8:GLY:HA3	12:L:11:PHE:CZ	2.53	0.44
11:R:36:GLU:HG2	11:R:184:TRP:CZ2	2.53	0.44
11:R:192:VAL:O	11:R:193:GLY:C	2.61	0.44
13:T:134:ALA:O	13:T:135:ASN:C	2.58	0.44
14:U:6:VAL:CG2	14:U:155:ILE:HD11	2.47	0.44
14:U:52:THR:O	14:U:53:GLN:C	2.60	0.44
3:X:33:ARG:HH11	3:X:33:ARG:CB	2.30	0.44
5:Z:180(C):PHE:O	5:Z:180(E):LYS:N	2.51	0.44
7:2:109:CYS:HB2	7:2:140:SER:OG	2.17	0.44
3:C:81:LEU:O	3:C:82:ASN:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:195:LYS:O	4:D:198:LYS:HB3	2.18	0.43
11:K:159:ILE:O	11:K:160:LEU:C	2.62	0.43
13:M:35:ILE:CD1	13:M:56:GLU:HG2	2.48	0.43
13:M:141(D):GLU:O	13:M:141(G):ILE:HG13	2.18	0.43
13:T:135:ASN:HB3	13:T:139:ARG:NE	2.33	0.43
1:V:15:PHE:H	2:W:23:GLN:NE2	2.12	0.43
1:V:48:ILE:HG13	1:V:213:ALA:HB3	1.99	0.43
1:V:60:MET:HG3	7:2:159:GLY:O	2.18	0.43
1:V:124:THR:CG2	1:V:124:THR:O	2.65	0.43
5:Z:66:LYS:HA	5:Z:78:LEU:CD2	2.48	0.43
7:2:233:LEU:HD12	7:2:233:LEU:HA	1.80	0.43
1:A:161:LYS:HD3	1:A:180:TRP:CH2	2.53	0.43
3:C:40:VAL:HA	3:C:162:ALA:HA	2.00	0.43
6:F:175:GLU:HG3	6:F:199:LEU:HD23	2.00	0.43
7:G:75:GLY:HA3	7:G:221:PHE:CE2	2.53	0.43
7:G:76:MET:HB2	7:G:138:PHE:CD2	2.53	0.43
8:H:78:SER:O	8:H:79:ALA:C	2.58	0.43
8:H:197:ARG:NH2	9:I:139:GLU:O	2.51	0.43
11:K:50:ALA:O	11:K:51:ASP:C	2.61	0.43
12:L:1:GLY:N	17:L:866:HOH:O	2.51	0.43
12:L:167:ILE:O	8:O:167:LEU:HD22	2.17	0.43
14:N:3:ILE:HG22	14:N:16:ALA:HB2	2.00	0.43
12:S:55:LEU:HD13	12:S:95:TYR:CE1	2.53	0.43
13:T:19:LEU:HD23	13:T:168:ARG:O	2.18	0.43
1:V:8:TYR:CE1	7:2:127:ALA:HB1	2.54	0.43
2:W:15:PHE:H	3:X:23:GLN:HE22	1.66	0.43
2:W:202:THR:HG22	2:W:204:SER:N	2.14	0.43
5:Z:148:LEU:HD23	5:Z:162:GLY:HA2	2.00	0.43
5:Z:226:GLY:O	5:Z:227:GLU:C	2.61	0.43
7:2:30:ALA:C	7:2:32:ASN:N	2.75	0.43
1:A:29:THR:O	1:A:32:LYS:HB2	2.18	0.43
5:E:194:VAL:O	5:E:195:GLU:C	2.61	0.43
6:F:108:PRO:O	6:F:111:ALA:HB3	2.19	0.43
9:I:15:ALA:HB2	9:I:175:VAL:HG22	2.01	0.43
13:M:205:GLY:HA3	13:M:209:GLN:HB3	2.00	0.43
14:N:76:THR:O	14:N:77:GLU:C	2.59	0.43
14:N:114:PRO:O	14:N:116:GLY:N	2.50	0.43
9:P:114:ASP:CB	15:9:3:ASN:ND2	2.67	0.43
10:Q:7:ARG:HB2	10:Q:12:VAL:HG22	1.99	0.43
11:R:105(A):ARG:HB3	11:R:105(B):LYS:CE	2.46	0.43
12:S:114:ASP:HB2	12:S:118:SER:CB	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:U:173:ILE:HB	14:U:187(B):PHE:HB2	2.00	0.43
5:Z:37:THR:HG23	5:Z:137:LEU:HD12	2.00	0.43
6:1:46:VAL:HG23	6:1:48:PHE:CE1	2.53	0.43
6:1:95:GLU:HG2	6:1:115:ARG:HB3	1.99	0.43
2:B:160:TRP:CE3	2:B:163:ILE:HD13	2.54	0.43
5:E:169:SER:O	5:E:171:GLY:N	2.51	0.43
6:F:72:ARG:HD2	13:M:64:THR:OG1	2.18	0.43
6:F:116:LEU:HA	6:F:116:LEU:HD23	1.69	0.43
6:F:148:LEU:HD23	6:F:160:TYR:O	2.18	0.43
6:F:198:TYR:CE2	6:F:208:PHE:CZ	3.06	0.43
7:G:8:TYR:O	7:G:10:ARG:N	2.51	0.43
7:G:119:LEU:HD12	7:G:119:LEU:HA	1.74	0.43
11:K:196:PHE:CZ	11:K:209:VAL:HG21	2.46	0.43
12:L:18:THR:CG2	12:L:30:TYR:HA	2.48	0.43
12:L:144(W):LYS:CG	12:L:145:TYR:N	2.81	0.43
8:O:112:SER:OG	8:O:120:ASP:HB2	2.18	0.43
9:P:99:PRO:HB2	9:P:113:PHE:CD2	2.52	0.43
12:S:184:VAL:O	12:S:184:VAL:HG12	2.18	0.43
13:T:126:ALA:N	17:T:2278:HOH:O	2.46	0.43
14:U:7:THR:HG23	14:U:123:PRO:O	2.17	0.43
4:Y:192:LEU:H	4:Y:192:LEU:HD12	1.83	0.43
6:1:102:LEU:O	6:1:102:LEU:HG	2.17	0.43
6:1:176:LEU:CD2	6:1:196:ILE:HD13	2.47	0.43
6:1:212:ILE:HG22	6:1:213:SER:H	1.84	0.43
7:2:72:ARG:HB2	7:2:72:ARG:NH1	2.32	0.43
7:2:110:ASP:HB3	7:2:149:TYR:CZ	2.53	0.43
2:B:40:ILE:CD1	2:B:193:ALA:HB2	2.48	0.43
4:D:28:LEU:HD12	4:D:28:LEU:HA	1.76	0.43
5:E:5:ARG:C	5:E:7:ASN:N	2.75	0.43
5:E:47:VAL:HG12	5:E:48:LEU:H	1.84	0.43
6:F:70:VAL:HB	6:F:74:ILE:HB	2.00	0.43
8:H:56:THR:HG22	8:H:57:GLN:N	2.34	0.43
13:M:51:ASP:OD1	13:M:95:LEU:HA	2.18	0.43
14:N:85:GLU:O	14:N:89:GLU:HB2	2.19	0.43
8:O:62:ASN:HB3	8:O:82:MET:HE1	2.00	0.43
8:O:75:ARG:CZ	7:2:105:TYR:CD1	3.02	0.43
10:Q:76:PRO:O	10:Q:78:ALA:N	2.52	0.43
10:Q:133:TYR:OH	10:Q:166:MET:CG	2.63	0.43
12:S:90:LYS:HD3	12:S:95:TYR:CZ	2.53	0.43
14:U:4:MET:SD	14:U:159:LEU:HD21	2.59	0.43
14:U:20:THR:OG1	14:U:28:ASN:HB3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:U:187(D):PRO:C	14:U:187(F):GLU:H	2.27	0.43
1:V:88:LEU:HD23	1:V:88:LEU:HA	1.68	0.43
2:W:167:ALA:O	2:W:168:ASN:HB2	2.18	0.43
5:Z:180(D):ILE:O	5:Z:180(D):ILE:HG13	2.18	0.43
6:1:121:GLN:C	6:1:121:GLN:NE2	2.76	0.43
7:2:78:VAL:HG11	7:2:85:ALA:HB2	2.00	0.43
3:C:47:VAL:C	3:C:48:LEU:HD23	2.44	0.43
5:E:176:LEU:HD22	5:E:180(C):PHE:CE2	2.40	0.43
11:K:40:PHE:HB3	11:K:73:ARG:NH2	2.34	0.43
13:M:31:VAL:HG12	13:M:33:ARG:HG2	2.00	0.43
9:P:76:PRO:O	9:P:78:THR:N	2.51	0.43
1:V:41:LYS:HA	1:V:46:VAL:HG22	2.01	0.43
1:V:111:LEU:O	1:V:114:SER:HB3	2.18	0.43
3:X:8:TYR:CE2	3:X:128:GLY:HA2	2.53	0.43
4:Y:121:LEU:HD23	4:Y:123:PHE:HE1	1.84	0.43
5:Z:17:PRO:HG3	6:1:26:TYR:CE2	2.53	0.43
5:Z:161:TYR:CZ	6:1:60:VAL:HG13	2.54	0.43
6:1:206(B):GLU:HG3	6:1:206(C):LYS:HG3	2.00	0.43
1:A:54:SER:C	1:A:56:SER:H	2.26	0.43
1:A:82:GLY:O	1:A:85:TYR:HB3	2.18	0.43
2:B:7:ARG:HH11	2:B:7:ARG:HG3	1.83	0.43
11:K:26:VAL:O	11:K:26:VAL:HG12	2.17	0.43
11:K:133:PHE:CB	11:K:162:ALA:HA	2.48	0.43
14:N:1:THR:O	14:N:128:GLY:HA3	2.19	0.43
14:N:4:MET:SD	14:N:159:LEU:CD2	3.07	0.43
8:O:43:CYS:SG	8:O:99:LEU:HD22	2.59	0.43
8:O:216:GLU:HG3	9:P:187:ARG:HG2	2.00	0.43
9:P:14:ILE:HG23	9:P:34:ILE:HD13	2.00	0.43
11:R:155:GLY:O	11:R:158:SER:N	2.52	0.43
12:S:8:GLY:HA2	12:S:145:TYR:CE1	2.53	0.43
14:U:107:LYS:HG2	14:U:108:GLY:N	2.33	0.43
1:V:130:ARG:HH21	7:2:124:THR:CG2	2.30	0.43
4:Y:201:MET:HE2	4:Y:201:MET:HB3	1.66	0.43
6:1:119:TYR:O	6:1:122:ALA:HB3	2.18	0.43
7:2:216:THR:O	7:2:217:LYS:C	2.62	0.43
2:B:136:PHE:O	2:B:150:THR:HA	2.19	0.43
2:B:205:LEU:HD12	2:B:205:LEU:HA	1.82	0.43
3:C:71:ASP:C	3:C:73:HIS:N	2.77	0.43
17:C:3453:HOH:O	4:D:86:ARG:HB3	2.19	0.43
4:D:97:VAL:HG21	11:K:65:LEU:HD11	2.00	0.43
5:E:12:THR:HG23	5:E:23:GLN:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:22:PHE:HD1	5:E:26:TYR:CE1	2.35	0.43
5:E:38:VAL:HG22	5:E:164:ALA:CB	2.48	0.43
6:F:11:SER:HA	17:F:379:HOH:O	2.18	0.43
6:F:12:ASN:C	6:F:12:ASN:OD1	2.61	0.43
6:F:137:ILE:HD11	6:F:165:THR:HG22	2.00	0.43
7:G:15:PHE:CD1	7:G:21:LEU:HD21	2.53	0.43
7:G:45:CYS:O	7:G:146:PRO:HB3	2.19	0.43
9:I:151:LEU:O	9:I:151:LEU:HG	2.19	0.43
10:J:22:ARG:HD3	10:J:22:ARG:HA	1.85	0.43
11:K:4:LEU:HD13	11:K:15:ALA:O	2.19	0.43
11:K:172:SER:HA	11:K:192:VAL:HG23	2.00	0.43
12:L:21:ILE:C	12:L:21:ILE:HD12	2.44	0.43
8:O:57:GLN:O	8:O:58:LEU:C	2.62	0.43
9:P:51:ASP:O	9:P:52:VAL:C	2.61	0.43
9:P:53:THR:O	9:P:57:GLU:HG3	2.18	0.43
9:P:165:ARG:HA	9:P:165:ARG:HD3	1.85	0.43
14:U:15:GLY:HA2	14:U:174:ARG:O	2.19	0.43
14:U:76:THR:C	14:U:78:THR:N	2.76	0.43
1:V:52:LYS:NZ	1:V:61:SER:HB2	2.33	0.43
4:D:24:VAL:O	4:D:27:SER:HB3	2.19	0.43
5:E:21:LEU:HA	5:E:21:LEU:HD23	1.81	0.43
10:J:52:THR:HG22	10:J:53:VAL:H	1.83	0.43
12:L:59:PHE:O	12:L:60:LYS:C	2.61	0.43
8:O:111:PHE:CD1	8:O:121:VAL:HB	2.54	0.43
9:P:19:ARG:HD3	9:P:168:LEU:O	2.18	0.43
10:Q:76:PRO:HD2	17:Q:2835:HOH:O	2.19	0.43
11:R:58:TRP:O	11:R:59:LEU:C	2.61	0.43
12:S:176:LEU:C	12:S:177:ILE:HD12	2.43	0.43
14:U:38:HIS:O	14:U:39:ASP:C	2.62	0.43
14:U:134:ILE:HD12	14:U:138:CYS:SG	2.59	0.43
1:V:66:LYS:HG2	1:V:78:TYR:CE1	2.54	0.43
2:W:141:TYR:CD1	2:W:219(E):VAL:HG21	2.54	0.43
3:X:57:LYS:HG3	3:X:208:LYS:HZ3	1.84	0.43
6:I:195:LYS:O	6:I:198:TYR:N	2.51	0.43
2:B:175:LEU:O	2:B:178:MET:HB3	2.19	0.43
5:E:40:LEU:HA	5:E:162:GLY:HA2	1.99	0.43
6:F:214:TRP:N	6:F:214:TRP:CD1	2.85	0.43
7:G:222:PHE:CD2	7:G:222:PHE:N	2.86	0.43
11:K:35:ILE:HD11	11:K:45:MET:SD	2.58	0.43
11:K:197:TRP:CE2	9:P:190:LYS:HE3	2.54	0.43
8:O:1:THR:HG23	8:O:33:LYS:NZ	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:O:10:ASN:CG	8:O:180:ILE:HD12	2.44	0.43
11:R:147:SER:O	11:R:148:VAL:C	2.61	0.43
11:R:196:PHE:HZ	11:R:209:VAL:HG21	1.84	0.43
13:T:135:ASN:HB2	13:T:136:PRO:HD3	2.00	0.43
14:U:76:THR:O	14:U:77:GLU:C	2.61	0.43
3:X:163:GLN:HE21	3:X:163:GLN:HA	1.84	0.43
4:Y:97:VAL:O	4:Y:98:THR:C	2.62	0.43
5:Z:15:PHE:HE1	5:Z:21:LEU:HG	1.84	0.43
5:Z:21:LEU:HA	17:Z:2539:HOH:O	2.19	0.43
7:2:93:LYS:O	7:2:94:ALA:C	2.62	0.43
7:2:120:SER:O	7:2:121:GLN:C	2.62	0.43
1:A:17:PRO:HG3	2:B:26:TYR:CE2	2.54	0.42
4:D:85:ALA:O	4:D:86:ARG:C	2.61	0.42
5:E:44:THR:CG2	5:E:183:ASP:HB3	2.49	0.42
9:I:36:HIS:HB3	9:I:42:PHE:CD2	2.54	0.42
9:I:43:LEU:HD21	9:I:45:ILE:HD11	2.00	0.42
10:J:105:ASP:OD1	10:J:105(C):LYS:HB2	2.19	0.42
8:O:19:ARG:NH1	8:O:167:LEU:O	2.52	0.42
12:S:93:PHE:N	12:S:94:PRO:HD3	2.33	0.42
1:V:67:VAL:HG11	1:V:213:ALA:HB2	2.01	0.42
5:Z:68:ILE:HB	5:Z:76:LEU:CD2	2.48	0.42
6:1:77:VAL:O	6:1:136:THR:HG23	2.19	0.42
7:2:46:THR:OG1	7:2:146:PRO:HB3	2.18	0.42
7:2:184(G):GLU:HG2	7:2:188:LYS:HB2	2.01	0.42
4:D:97:VAL:CB	11:K:65:LEU:HD11	2.49	0.42
6:F:157:TYR:CZ	7:G:86:ARG:NH1	2.87	0.42
7:G:111:VAL:O	7:G:112:LEU:C	2.61	0.42
11:K:87:VAL:HG21	11:K:97:MET:HE2	2.01	0.42
11:K:209:VAL:HA	17:K:2742:HOH:O	2.19	0.42
12:L:35:PHE:HZ	17:L:458:HOH:O	2.02	0.42
13:M:157:ASN:O	13:M:158:ALA:C	2.60	0.42
14:N:175:MET:CE	14:N:187(B):PHE:HE2	2.29	0.42
8:O:95:ILE:O	8:O:97:ALA:N	2.47	0.42
14:U:5:ALA:O	14:U:124:TYR:HB2	2.19	0.42
6:1:32:GLU:O	6:1:167:LYS:HG3	2.19	0.42
6:1:68:GLN:NE2	6:1:86:ARG:NH1	2.67	0.42
2:B:192:LEU:HD23	2:B:192:LEU:C	2.43	0.42
4:D:224:TYR:N	4:D:224:TYR:HD2	2.17	0.42
4:D:237:LEU:HD23	4:D:237:LEU:HA	1.87	0.42
6:F:69:VAL:HG22	6:F:70:VAL:N	2.35	0.42
9:I:53:THR:HG22	10:J:84:ARG:NH2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:42:VAL:CG2	13:M:178:ILE:HD11	2.45	0.42
12:S:4:LEU:HA	12:S:126:ALA:HA	2.01	0.42
12:S:4:LEU:CD1	12:S:138:LEU:HD21	2.49	0.42
13:T:7:LYS:HD2	13:T:141(G):ILE:HD13	2.01	0.42
14:U:1:THR:O	14:U:128:GLY:HA3	2.20	0.42
1:V:21:LEU:HA	1:V:21:LEU:HD23	1.83	0.42
1:V:86:ARG:HH21	7:2:118:ASN:ND2	2.16	0.42
2:W:64:THR:HG22	2:W:68:TYR:CE1	2.54	0.42
2:W:209:ARG:HG2	2:W:209:ARG:HH11	1.84	0.42
4:Y:39:GLY:C	4:Y:40:ILE:HG13	2.44	0.42
5:Z:153:PRO:C	5:Z:155:GLY:N	2.73	0.42
7:2:176:LEU:O	7:2:177:GLU:C	2.61	0.42
2:B:137:ILE:HD11	2:B:165:VAL:HG22	2.00	0.42
6:F:210:LEU:HA	6:F:210:LEU:HD12	1.84	0.42
8:H:132:LEU:CD1	14:N:25:TYR:CE1	3.02	0.42
10:J:52:THR:HG22	10:J:53:VAL:N	2.34	0.42
12:L:69:ASP:C	12:L:70:HIS:ND1	2.77	0.42
8:O:110:LEU:HD23	8:O:122:GLY:O	2.19	0.42
8:O:159:ILE:O	8:O:160:GLN:C	2.62	0.42
12:S:49:ALA:O	12:S:50:ALA:C	2.62	0.42
12:S:61:ASN:ND2	5:Z:101:LEU:HD21	2.35	0.42
13:T:49:ILE:O	13:T:52:MET:N	2.52	0.42
1:V:15:PHE:CE1	1:V:21:LEU:HD21	2.54	0.42
1:V:214:ILE:O	1:V:215:ILE:HD13	2.19	0.42
2:W:163:ILE:HD12	2:W:173:GLN:NE2	2.34	0.42
3:X:77:SER:OG	3:X:137:LEU:HB2	2.19	0.42
5:Z:38:VAL:HG13	5:Z:163:THR:O	2.19	0.42
5:Z:198:SER:HA	5:Z:201:LEU:CD1	2.49	0.42
6:1:7:GLY:O	6:1:9:ASP:N	2.53	0.42
6:1:223:PHE:N	6:1:223:PHE:CD1	2.85	0.42
2:B:172:ALA:HB2	2:B:200:THR:HG21	2.01	0.42
4:D:89:ILE:O	4:D:92:ALA:HB3	2.20	0.42
11:K:138:LEU:O	11:K:139:ASP:C	2.63	0.42
12:L:13:VAL:HG12	12:L:177:ILE:HG13	2.02	0.42
12:L:138:LEU:C	12:L:140:ASN:N	2.76	0.42
12:L:163:THR:HG23	12:L:170:GLY:HA2	2.01	0.42
14:N:136:GLY:O	14:N:137:TYR:C	2.62	0.42
13:T:13:ILE:CG2	13:T:175:LEU:HD21	2.48	0.42
13:T:62:LEU:HA	13:T:62:LEU:HD23	1.76	0.42
14:U:161:GLN:O	14:U:164:LYS:N	2.51	0.42
1:V:58:LEU:HD23	1:V:58:LEU:HA	1.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:7:ARG:HH11	2:W:7:ARG:HG3	1.85	0.42
5:Z:66:LYS:O	5:Z:77:SER:HA	2.20	0.42
6:1:194:ALA:O	6:1:198:TYR:HD1	2.03	0.42
7:2:97:ALA:O	7:2:98:GLU:C	2.60	0.42
1:A:186:LEU:HD21	1:A:214:ILE:HD12	2.02	0.42
9:I:117:GLY:O	9:I:118:CYS:C	2.61	0.42
14:N:29:ARG:HD2	13:T:197:TRP:CH2	2.54	0.42
8:O:12:VAL:HG22	8:O:13:VAL:N	2.34	0.42
11:R:100:MET:HE2	11:R:100:MET:HB2	1.83	0.42
11:R:105(B):LYS:N	11:R:105(B):LYS:CD	2.80	0.42
14:U:42:TRP:CD1	14:U:42:TRP:N	2.85	0.42
3:X:25:GLU:O	3:X:28:LEU:HB2	2.20	0.42
4:Y:70:ILE:HB	4:Y:74:ILE:CG2	2.44	0.42
4:Y:176:LEU:O	4:Y:177:LEU:C	2.63	0.42
6:1:172:ALA:C	6:1:176:LEU:HD23	2.44	0.42
7:2:9:ASP:HA	7:2:14:ILE:HD11	2.00	0.42
7:2:41:ARG:NH2	7:2:180(B):ASP:O	2.51	0.42
1:A:62:GLU:C	1:A:64:LEU:H	2.27	0.42
1:A:197:LEU:O	1:A:202:VAL:HG23	2.20	0.42
4:D:211:GLN:HA	17:D:916:HOH:O	2.19	0.42
5:E:107:LEU:HD12	17:E:389:HOH:O	2.19	0.42
7:G:179(D):SER:O	7:G:179(E):LYS:HB2	2.19	0.42
8:H:160:GLN:O	8:H:164:TRP:CD1	2.73	0.42
9:I:60:ARG:O	9:I:61:TYR:C	2.61	0.42
9:I:159:LEU:O	9:I:160:LEU:C	2.62	0.42
12:L:58:ARG:NH2	17:L:3067:HOH:O	2.53	0.42
8:O:55:VAL:HG23	8:O:86:HIS:CD2	2.53	0.42
8:O:84:LYS:HE2	8:O:119:THR:HG23	2.02	0.42
11:R:4:LEU:HD11	11:R:15:ALA:HB3	2.02	0.42
13:T:133:MET:HE1	13:T:165:ARG:HG3	1.99	0.42
1:V:15:PHE:HB2	2:W:23:GLN:NE2	2.35	0.42
2:W:197:LEU:HA	2:W:200:THR:HG1	1.85	0.42
3:X:63:THR:HG23	3:X:64:PRO:HD2	2.02	0.42
3:X:182:PRO:HA	3:X:183:PRO:HD3	1.97	0.42
7:2:25:GLU:O	7:2:28:PHE:HB2	2.20	0.42
3:C:15:PHE:CE2	4:D:27:SER:HB2	2.55	0.42
3:C:70:ILE:HG21	3:C:112:LEU:HD21	2.00	0.42
3:C:71:ASP:C	3:C:73:HIS:H	2.27	0.42
4:D:180(C):HIS:O	4:D:184:LEU:HD12	2.20	0.42
4:D:243:ALA:O	4:D:244:GLU:HG2	2.20	0.42
5:E:121:GLN:C	5:E:123:ASN:N	2.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:135:SER:HA	17:F:408:HOH:O	2.20	0.42
12:L:43:MET:HB2	12:L:101:ILE:CG2	2.44	0.42
8:O:47:GLY:O	15:9:5:AKK:ND	2.52	0.42
9:P:12:VAL:HG13	9:P:108:PRO:HB3	2.01	0.42
13:T:128:GLY:HA3	17:T:2312:HOH:O	2.18	0.42
13:T:171:ARG:CG	13:T:192:VAL:HG23	2.38	0.42
1:V:46:VAL:HG12	1:V:47:VAL:N	2.34	0.42
2:W:20:ARG:HE	3:X:33:ARG:HH21	1.67	0.42
2:W:107:ILE:HG13	2:W:108:PRO:HD2	2.02	0.42
3:X:81:LEU:HD23	3:X:81:LEU:HA	1.86	0.42
3:X:97:GLN:O	3:X:99:HIS:N	2.53	0.42
3:X:212:ILE:CG2	3:X:213:THR:N	2.83	0.42
5:Z:92:LEU:HD11	5:Z:112:ALA:HB1	2.01	0.42
6:1:67:ILE:HG22	6:1:68:GLN:N	2.34	0.42
6:1:108:PRO:O	6:1:111:ALA:HB3	2.19	0.42
7:2:30:ALA:C	7:2:32:ASN:H	2.27	0.42
3:C:197:LEU:O	3:C:201:VAL:HG23	2.20	0.42
6:F:113:ALA:O	6:F:116:LEU:N	2.52	0.42
6:F:159:GLY:C	6:F:160:TYR:HD1	2.27	0.42
10:J:70:GLU:O	10:J:71:ASP:C	2.60	0.42
8:O:90:TYR:O	8:O:93:GLY:N	2.53	0.42
12:S:144(W):LYS:CG	12:S:145:TYR:N	2.83	0.42
14:U:63:LEU:O	14:U:66:TYR:HB3	2.20	0.42
14:U:111:TYR:HA	14:U:120:HIS:O	2.20	0.42
2:W:66:LYS:HB2	2:W:211:GLU:OE1	2.20	0.42
4:Y:138:ILE:O	4:Y:148:LEU:HD12	2.20	0.42
4:Y:207:LEU:HD23	4:Y:207:LEU:C	2.44	0.42
6:1:82:ILE:O	6:1:83:PRO:C	2.63	0.42
7:2:16:SER:O	7:2:18:GLU:N	2.53	0.42
6:F:54:ILE:O	6:F:55:THR:C	2.63	0.42
6:F:159:GLY:C	6:F:160:TYR:CD1	2.98	0.42
7:G:74:ILE:HG21	7:G:112:LEU:HD23	2.02	0.42
7:G:212:VAL:CG1	7:G:213:GLY:N	2.82	0.42
8:H:152:ILE:HG21	8:H:191:TYR:HE1	1.84	0.42
8:H:167:LEU:HB3	12:S:167:ILE:HB	2.02	0.42
14:N:187(C):TYR:CE1	13:T:198:ASP:HA	2.55	0.42
8:O:19:ARG:HG2	8:O:21:THR:HG23	2.02	0.42
8:O:34:LEU:HD12	8:O:34:LEU:HA	1.78	0.42
9:P:179:LYS:O	9:P:181:LYS:C	2.63	0.42
10:Q:104:TYR:C	10:Q:104:TYR:HD1	2.28	0.42
1:V:35:VAL:HG12	1:V:36:THR:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1:203:GLU:C	6:1:205:ASN:H	2.28	0.42
1:A:69:LEU:O	1:A:93:ARG:NH2	2.51	0.41
3:C:62(A):ILE:H	3:C:62(A):ILE:HG12	1.71	0.41
7:G:27:ALA:O	7:G:30:ALA:N	2.51	0.41
10:J:119:LYS:HG2	10:J:120:VAL:N	2.35	0.41
13:M:-4:ILE:HG22	13:M:-3:VAL:N	2.34	0.41
13:M:82:TYR:O	13:M:83:LEU:C	2.63	0.41
13:M:135:ASN:HB2	13:M:136:PRO:HD3	2.02	0.41
9:P:58:MET:HE3	9:P:58:MET:HB2	1.90	0.41
10:Q:166:MET:HA	10:Q:167:PRO:HD3	1.88	0.41
11:R:41:LEU:HD23	11:R:41:LEU:HA	1.75	0.41
1:V:72:PRO:HB3	17:V:1013:HOH:O	2.20	0.41
1:V:221:PHE:O	1:V:221:PHE:HD2	2.01	0.41
3:X:33:ARG:O	3:X:33:ARG:HG2	2.19	0.41
3:X:52:ARG:HD2	3:X:208:LYS:O	2.20	0.41
3:X:163:GLN:CG	3:X:164:THR:N	2.82	0.41
5:Z:27:ALA:O	5:Z:28:LEU:C	2.63	0.41
5:Z:139:ILE:HG22	5:Z:148:LEU:HD13	2.02	0.41
6:1:53:LEU:HD23	6:1:53:LEU:HA	1.77	0.41
1:A:176:LEU:O	1:A:178:LYS:N	2.53	0.41
1:A:210:ILE:HG22	1:A:211:GLU:N	2.35	0.41
4:D:97:VAL:O	4:D:98:THR:C	2.63	0.41
6:F:216:SER:HB3	6:F:218(A):GLU:HB2	2.02	0.41
9:I:13:ALA:CB	9:I:151:LEU:HD21	2.51	0.41
9:I:131:SER:O	9:I:132:ASP:C	2.62	0.41
9:I:152:PHE:O	9:I:155:ILE:HG22	2.20	0.41
12:L:107:LYS:HA	12:L:107:LYS:HD3	1.86	0.41
13:M:157:ASN:O	13:M:160:ARG:N	2.53	0.41
8:O:38:SER:O	8:O:39:PRO:C	2.63	0.41
8:O:91:GLN:HA	8:O:91:GLN:NE2	2.35	0.41
10:Q:143:ARG:O	10:Q:146:MET:HG3	2.20	0.41
11:R:52:CYS:SG	11:R:97:MET:CB	3.08	0.41
12:S:5:GLY:C	12:S:6:ILE:HG13	2.45	0.41
12:S:156:ARG:HD2	12:S:189:TYR:CE1	2.55	0.41
1:V:26:TYR:O	1:V:29:THR:HB	2.20	0.41
1:V:65:SER:HA	1:V:211:GLU:OE1	2.19	0.41
1:V:118:LYS:O	1:V:122:GLU:HG3	2.20	0.41
3:X:201:VAL:O	3:X:202:GLN:HB2	2.19	0.41
6:1:51:GLU:OE1	6:1:53:LEU:HD21	2.20	0.41
6:1:208:PHE:H	6:1:208:PHE:HD2	1.67	0.41
3:C:194:VAL:O	3:C:195:ARG:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:21:ASN:C	6:F:21:ASN:OD1	2.63	0.41
10:J:38:SER:OG	10:J:41:THR:HB	2.20	0.41
10:J:43:MET:HG3	10:J:101:ILE:HG13	2.02	0.41
11:K:133:PHE:HB2	11:K:162:ALA:HA	2.02	0.41
8:O:35:HIS:CB	8:O:56:THR:HG21	2.50	0.41
10:Q:158:CYS:O	10:Q:159:VAL:C	2.63	0.41
13:T:6:MET:HE3	13:T:6:MET:HB2	1.91	0.41
14:U:80:ALA:O	14:U:81:SER:C	2.62	0.41
1:V:62:GLU:C	1:V:64:LEU:H	2.29	0.41
1:V:86:ARG:HE	7:2:118:ASN:HD21	1.69	0.41
4:Y:15:PHE:CE1	4:Y:21:LEU:HG	2.54	0.41
5:Z:215:VAL:HG23	5:Z:221:PHE:N	2.35	0.41
6:1:116:LEU:HD23	6:1:116:LEU:HA	1.81	0.41
1:A:40:ILE:HD12	1:A:193:ALA:HB2	2.02	0.41
1:A:171:ALA:O	1:A:174:THR:HB	2.21	0.41
2:B:40:ILE:HD12	2:B:193:ALA:HB2	2.01	0.41
7:G:38:LEU:HD12	7:G:38:LEU:C	2.45	0.41
8:H:38:SER:O	8:H:39:PRO:C	2.62	0.41
8:H:65:LEU:O	8:H:66:HIS:C	2.63	0.41
9:I:12:VAL:HG23	9:I:178:ILE:HD12	2.02	0.41
9:I:55:LEU:HD21	9:I:95:TYR:CE1	2.56	0.41
10:J:73:GLU:HG2	17:J:870:HOH:O	2.19	0.41
1:V:21:LEU:O	1:V:22:GLY:C	2.63	0.41
1:V:85:TYR:O	1:V:89:VAL:HG23	2.21	0.41
2:W:120:LYS:NZ	2:W:151:SER:OG	2.53	0.41
3:X:172:VAL:O	3:X:175:PHE:HB3	2.20	0.41
4:Y:225:ASP:O	4:Y:226:ASN:C	2.63	0.41
7:2:34(A):ASN:CG	7:2:34(A):ASN:O	2.63	0.41
7:2:49:ILE:HG22	7:2:50:SER:N	2.35	0.41
7:2:160:TYR:HB3	7:2:162:ALA:O	2.20	0.41
1:A:90:ASP:O	1:A:91:LYS:C	2.63	0.41
5:E:90:ASN:O	5:E:93:ARG:N	2.53	0.41
9:I:13:ALA:HB2	9:I:151:LEU:HD21	2.02	0.41
9:I:131:SER:HB2	17:I:3153:HOH:O	2.20	0.41
9:I:133:GLN:HB3	9:I:162:ALA:HB1	2.02	0.41
11:K:52:CYS:O	11:K:53:GLN:C	2.63	0.41
14:N:112:THR:CG2	14:N:120:HIS:HB2	2.49	0.41
10:Q:112:GLN:NE2	10:Q:126:ALA:N	2.68	0.41
12:S:177:ILE:N	12:S:177:ILE:CD1	2.84	0.41
13:T:149:GLN:NE2	13:T:149:GLN:H	2.18	0.41
14:U:38:HIS:NE2	14:U:74:PRO:HD2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:169:SER:O	1:V:170:VAL:C	2.63	0.41
4:D:194:LEU:HD12	4:D:194:LEU:HA	1.74	0.41
7:G:194:ILE:O	7:G:198:ILE:HG13	2.20	0.41
8:H:59:ILE:O	8:H:60:GLY:C	2.62	0.41
9:I:29:ASN:HB3	9:I:171:TRP:CE3	2.56	0.41
11:K:138:LEU:HA	11:K:138:LEU:HD12	1.89	0.41
12:L:113:PHE:CD1	12:L:113:PHE:N	2.89	0.41
13:M:186:PHE:HE1	13:M:188:LYS:HG3	1.86	0.41
8:O:175:VAL:HG21	8:O:191:TYR:CD1	2.46	0.41
12:S:59:PHE:O	12:S:62:SER:N	2.53	0.41
13:T:59:LEU:O	13:T:60:LYS:C	2.64	0.41
1:A:121:GLN:C	1:A:121:GLN:OE1	2.64	0.41
7:G:9:ASP:HA	7:G:14:ILE:HD11	2.02	0.41
7:G:87:ASN:C	7:G:87:ASN:HD22	2.28	0.41
11:K:85:ASN:HD22	11:K:85:ASN:HA	1.74	0.41
12:L:63:VAL:HG22	12:L:74:LEU:HD23	2.02	0.41
12:S:20:ASN:OD1	12:S:27:ASN:HB2	2.21	0.41
13:T:49:ILE:O	13:T:50:SER:C	2.64	0.41
14:U:133:PHE:HE2	14:U:166:ASP:HB2	1.83	0.41
14:U:163:ILE:CG2	14:U:170:GLY:HA2	2.44	0.41
1:V:15:PHE:O	2:W:26:TYR:HD2	2.04	0.41
3:X:183:PRO:HB3	3:X:189:CYS:HA	2.03	0.41
5:Z:48:LEU:O	5:Z:212:ILE:HG23	2.20	0.41
7:2:132:LEU:O	7:2:153:PRO:HG3	2.20	0.41
7:2:165:THR:HG22	7:2:166:GLY:N	2.36	0.41
7:2:198:ILE:C	7:2:200:ALA:H	2.28	0.41
7:2:221:PHE:CD1	7:2:221:PHE:C	2.99	0.41
1:A:124:THR:CG2	1:A:124:THR:O	2.69	0.41
2:B:16:SER:C	2:B:18:GLU:N	2.75	0.41
2:B:61:GLN:O	2:B:62:ASP:C	2.62	0.41
3:C:185:THR:CB	3:C:188:GLU:HG2	2.34	0.41
6:F:26:TYR:N	6:F:26:TYR:CD1	2.87	0.41
7:G:35:ILE:HG23	7:G:51:GLN:HB2	2.03	0.41
7:G:113:ALA:O	7:G:114:LYS:C	2.63	0.41
8:H:57:GLN:O	8:H:58:LEU:C	2.61	0.41
14:N:146:MET:HE3	14:N:150:GLU:HB3	2.02	0.41
8:O:6:VAL:O	8:O:13:VAL:HG12	2.21	0.41
8:O:65:LEU:O	8:O:66:HIS:C	2.64	0.41
8:O:105:ASP:O	8:O:106:THR:N	2.53	0.41
8:O:132:LEU:N	8:O:132:LEU:CD1	2.84	0.41
8:O:197:ARG:NH1	8:O:200:LYS:HD3	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:T:68:TYR:OH	6:1:71:ASP:N	2.50	0.41
13:T:169:SER:HB2	17:T:2472:HOH:O	2.20	0.41
1:V:161:LYS:HD3	1:V:180:TRP:CH2	2.55	0.41
3:X:58:LEU:HG	3:X:58:LEU:O	2.20	0.41
5:Z:121:GLN:NE2	6:1:87:HIS:ND1	2.69	0.41
5:Z:138:ILE:O	5:Z:148:LEU:HA	2.21	0.41
7:2:59:LEU:O	7:2:61:PRO:CD	2.64	0.41
7:2:120:SER:HA	7:2:123:TYR:CD2	2.56	0.41
1:A:37:SER:HG	1:A:79:SER:HG	1.66	0.41
1:A:136:LEU:O	1:A:150:GLN:HA	2.21	0.41
1:A:147(A):SER:HB2	1:A:149:TYR:CE2	2.56	0.41
1:A:172:ALA:O	1:A:173:LYS:C	2.62	0.41
2:B:15:PHE:N	3:C:23:GLN:HE22	2.18	0.41
2:B:64:THR:HG23	2:B:67:LEU:O	2.20	0.41
2:B:175:LEU:HD23	2:B:175:LEU:HA	1.88	0.41
2:B:207:TYR:CG	2:B:208:ASP:N	2.89	0.41
2:B:222:LYS:HZ1	2:B:228:GLU:CD	2.29	0.41
3:C:172:VAL:O	3:C:173:ARG:C	2.64	0.41
6:F:35:THR:HG22	6:F:36:THR:N	2.34	0.41
6:F:147:HIS:HB3	6:F:149:TYR:HE2	1.86	0.41
6:F:160:TYR:HB3	6:F:162:GLY:O	2.21	0.41
8:H:49:ALA:CB	9:I:118:CYS:SG	3.09	0.41
8:H:133:ALA:O	8:H:136:ALA:HB3	2.21	0.41
10:J:43:MET:HG3	10:J:101:ILE:CG1	2.50	0.41
10:J:137:LEU:HA	10:J:137:LEU:HD23	1.84	0.41
10:J:157:LEU:HD12	10:J:157:LEU:HA	1.80	0.41
11:K:56:GLU:O	11:K:57:THR:C	2.62	0.41
11:K:165:ARG:NH1	9:P:26:GLY:O	2.53	0.41
12:L:148:VAL:HG13	12:L:149:GLU:N	2.36	0.41
13:M:150:VAL:HG21	17:M:869:HOH:O	2.21	0.41
14:N:6:VAL:CG2	14:N:155:ILE:HD11	2.46	0.41
14:N:174:ARG:HD2	17:N:564:HOH:O	2.21	0.41
8:O:21:THR:HG22	8:O:26:VAL:HA	2.03	0.41
8:O:134:ALA:O	8:O:135:MET:C	2.64	0.41
8:O:221:ILE:N	8:O:221:ILE:CD1	2.84	0.41
9:P:5:ALA:HB2	9:P:14:ILE:HG13	2.03	0.41
10:Q:3:ILE:HD13	10:Q:3:ILE:HA	1.85	0.41
11:R:40:PHE:HB2	17:R:2501:HOH:O	2.20	0.41
11:R:52:CYS:SG	11:R:97:MET:HB2	2.60	0.41
12:S:29:ARG:HB2	17:S:2276:HOH:O	2.21	0.41
12:S:113:PHE:CD2	12:S:119:TYR:HB3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:U:107:LYS:HG2	14:U:108:GLY:H	1.86	0.41
1:V:50:THR:HG21	1:V:66:LYS:HE2	2.03	0.41
1:V:100:TYR:CE1	1:V:107:PRO:HA	2.56	0.41
2:W:15:PHE:CB	3:X:23:GLN:HE22	2.31	0.41
3:X:96:ALA:O	3:X:100:ARG:HG3	2.21	0.41
4:Y:45:GLY:HA2	4:Y:146:TYR:CD1	2.56	0.41
4:Y:47:VAL:HG12	4:Y:48:LEU:N	2.36	0.41
4:Y:147:GLN:HA	17:Y:1042:HOH:O	2.21	0.41
4:Y:215:ILE:HG22	4:Y:221:PHE:HD2	1.84	0.41
5:Z:5:ARG:C	5:Z:7:ASN:N	2.78	0.41
5:Z:35:SER:OG	5:Z:36:VAL:N	2.54	0.41
5:Z:44:THR:O	5:Z:45:HIS:ND1	2.53	0.41
5:Z:73:HIS:CE1	5:Z:107:LEU:O	2.72	0.41
5:Z:176:LEU:HD22	5:Z:180(C):PHE:HE2	1.86	0.41
5:Z:220:PRO:O	5:Z:221:PHE:C	2.63	0.41
7:2:12:ILE:HA	17:2:2538:HOH:O	2.20	0.41
7:2:225:SER:HG	7:2:228:ASN:CG	2.29	0.41
1:A:109:THR:O	1:A:113:VAL:HG23	2.21	0.41
2:B:70:LEU:CD2	2:B:89:ILE:HG23	2.50	0.41
3:C:183:PRO:HB3	3:C:189:CYS:HA	2.02	0.41
4:D:121:LEU:HD23	4:D:123:PHE:HE1	1.85	0.41
11:K:139:ASP:OD2	10:Q:164:LYS:HD3	2.21	0.41
13:M:165:ARG:HD2	13:M:165:ARG:N	2.36	0.41
8:O:163:ILE:HG22	8:O:164:TRP:CE3	2.55	0.41
11:R:41:LEU:HD21	11:R:76:VAL:HG22	2.02	0.41
12:S:4:LEU:CD1	12:S:126:ALA:HB2	2.48	0.41
14:U:161:GLN:O	14:U:162:ALA:C	2.64	0.41
5:Z:160:LEU:CD2	6:1:59:LEU:HD12	2.51	0.41
5:Z:161:TYR:CE2	6:1:61:PRO:HD3	2.56	0.41
6:1:7:GLY:C	6:1:9:ASP:N	2.79	0.41
7:2:158:VAL:HG22	7:2:159:GLY:N	2.36	0.41
1:A:60:MET:HG3	7:G:159:GLY:O	2.21	0.40
1:A:149:TYR:CE1	1:A:159:PRO:HB3	2.57	0.40
3:C:212:ILE:CG2	3:C:213:THR:N	2.84	0.40
5:E:28:LEU:HA	5:E:31:ILE:HD12	2.03	0.40
5:E:229:VAL:O	5:E:230:ALA:C	2.65	0.40
6:F:50:VAL:CG2	6:F:51:GLU:N	2.84	0.40
6:F:192:GLN:O	6:F:195:LYS:HB3	2.21	0.40
10:J:63:ILE:HD13	10:J:63:ILE:HA	1.91	0.40
11:K:99:THR:HA	17:K:444:HOH:O	2.21	0.40
13:M:83:LEU:HA	13:M:83:LEU:HD23	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:Q:52:THR:CG2	10:Q:53:VAL:N	2.84	0.40
10:Q:105:ASP:O	10:Q:105(B):LYS:N	2.53	0.40
1:V:55:SER:HB2	17:2:1268:HOH:O	2.21	0.40
4:Y:243:ALA:O	4:Y:244:GLU:HG2	2.20	0.40
5:Z:4:PHE:O	5:Z:7:ASN:HB2	2.21	0.40
2:B:116:LEU:HA	2:B:116:LEU:HD23	1.84	0.40
3:C:77:SER:OG	3:C:137:LEU:HB2	2.21	0.40
3:C:150:GLN:HG2	3:C:151:THR:N	2.36	0.40
17:E:864:HOH:O	12:L:67:HIS:HD2	2.03	0.40
6:F:17:PRO:HA	7:G:26:TYR:CD2	2.57	0.40
7:G:130:ARG:HG3	7:G:130:ARG:HH11	1.86	0.40
7:G:214:VAL:HG12	7:G:215:ALA:H	1.87	0.40
8:H:13:VAL:CG2	8:H:14:ILE:N	2.85	0.40
8:H:134:ALA:O	8:H:135:MET:C	2.62	0.40
9:I:19:ARG:HB2	9:I:171:TRP:HB2	2.04	0.40
12:L:18:THR:HG22	12:L:31:GLU:N	2.36	0.40
12:L:100:ILE:HG22	12:L:101:ILE:N	2.36	0.40
13:M:12:VAL:HG21	13:M:102:ALA:HB1	2.03	0.40
13:M:82:TYR:O	13:M:85:THR:HB	2.21	0.40
8:O:3:ILE:O	8:O:126:SER:HA	2.22	0.40
8:O:114:HIS:HD2	17:O:2814:HOH:O	2.03	0.40
9:P:53:THR:CG2	10:Q:84:ARG:CZ	2.99	0.40
10:Q:120:VAL:HG13	10:Q:122:LEU:HG	2.02	0.40
10:Q:157:LEU:HD12	10:Q:157:LEU:HA	1.87	0.40
13:T:78:TYR:CD1	5:Z:105:ARG:HB2	2.55	0.40
1:V:79:SER:HB2	1:V:165:ILE:HD12	2.02	0.40
5:Z:15:PHE:HD1	5:Z:15:PHE:HA	1.75	0.40
6:1:198:TYR:CE2	6:1:208:PHE:CZ	3.06	0.40
2:B:225:LYS:O	2:B:228:GLU:HB2	2.20	0.40
17:C:2999:HOH:O	4:D:86:ARG:HG3	2.21	0.40
4:D:91:HIS:CD2	4:D:91:HIS:O	2.74	0.40
5:E:90:ASN:O	5:E:91:TYR:C	2.63	0.40
9:I:19:ARG:NH1	17:I:211:HOH:O	2.55	0.40
12:L:167:ILE:HA	17:L:2973:HOH:O	2.21	0.40
13:M:70(A):ALA:O	13:M:71(D):ALA:HB2	2.21	0.40
14:N:20:THR:OG1	14:N:28:ASN:HB3	2.22	0.40
10:Q:38:SER:O	10:Q:40:HIS:N	2.54	0.40
10:Q:59:ILE:HG23	10:Q:59:ILE:HD12	1.86	0.40
12:S:18:THR:HG22	12:S:18:THR:O	2.21	0.40
13:T:55:ILE:O	13:T:55:ILE:HG22	2.22	0.40
13:T:122:SER:N	13:T:125:LEU:HD21	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:U:175:MET:CE	14:U:187(B):PHE:HE2	2.34	0.40
1:V:77:VAL:HG22	1:V:78:TYR:N	2.35	0.40
3:X:109:VAL:O	3:X:110:GLU:C	2.64	0.40
3:X:232:TYR:O	3:X:236:ILE:HG13	2.21	0.40
4:Y:160:TYR:HA	5:Z:59:SER:HA	2.03	0.40
5:Z:207:LEU:HD23	5:Z:207:LEU:N	2.36	0.40
6:1:63:LYS:O	6:1:65:VAL:N	2.53	0.40
3:C:208:LYS:HE3	3:C:209:ASN:ND2	2.37	0.40
4:D:49:GLY:HA2	4:D:211:GLN:O	2.22	0.40
4:D:139:ALA:HB2	4:D:148:LEU:HD13	2.04	0.40
7:G:59:LEU:O	7:G:61:PRO:CD	2.70	0.40
8:H:3:ILE:HD11	8:H:127:LEU:HB2	2.04	0.40
8:H:13:VAL:HG23	8:H:176:CYS:O	2.20	0.40
8:H:62:ASN:HB3	8:H:82:MET:HE1	2.03	0.40
8:H:204:TYR:CD2	8:H:204:TYR:N	2.89	0.40
9:I:3:VAL:HA	9:I:15:ALA:O	2.21	0.40
11:K:85:ASN:ND2	17:K:227:HOH:O	2.53	0.40
11:K:196:PHE:CE2	11:K:206:PHE:CG	3.09	0.40
13:M:63:VAL:HG12	13:M:64:THR:N	2.35	0.40
14:N:112:THR:O	14:N:112:THR:HG23	2.21	0.40
14:N:187:LEU:HA	14:N:187:LEU:HD23	1.90	0.40
11:R:175:LEU:O	11:R:186:TYR:HD1	2.05	0.40
12:S:17:ASP:HA	12:S:172:GLY:O	2.22	0.40
12:S:99:THR:HG23	12:S:113:PHE:HB2	2.03	0.40
13:T:-6:GLN:HA	13:T:-5:PRO:HD2	1.93	0.40
13:T:42:VAL:CG2	13:T:178:ILE:HD11	2.51	0.40
13:T:82:TYR:O	13:T:86:VAL:HG23	2.21	0.40
14:U:52:THR:HG22	14:U:97:ALA:HB1	2.03	0.40
1:V:130:ARG:O	1:V:130:ARG:HG3	2.20	0.40
3:X:19:GLY:O	4:Y:30:ALA:HB2	2.22	0.40
5:Z:161:TYR:OH	6:1:61:PRO:CD	2.66	0.40
5:Z:179:THR:O	5:Z:179:THR:HG22	2.21	0.40
6:1:153:PRO:C	6:1:155:GLY:H	2.29	0.40
6:1:236:ALA:C	6:1:238:LYS:N	2.78	0.40
7:2:87:ASN:N	17:2:2404:HOH:O	2.54	0.40
1:A:50:THR:OG1	1:A:51:GLU:N	2.55	0.40
1:A:73:ASP:C	1:A:74:ILE:HG13	2.46	0.40
3:C:111:TYR:O	3:C:112:LEU:C	2.64	0.40
5:E:167:ALA:HB3	17:E:982:HOH:O	2.22	0.40
6:F:38:ILE:HG22	6:F:164:ALA:HB2	2.03	0.40
6:F:198:TYR:CD2	6:F:208:PHE:HZ	2.40	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:95:ILE:O	8:H:97:ALA:N	2.52	0.40
12:L:48:PHE:C	12:L:48:PHE:CD1	2.98	0.40
13:M:114:ASN:O	13:M:116:LEU:N	2.55	0.40
14:N:13:ILE:HG12	14:N:177:VAL:HG13	2.04	0.40
14:N:171:GLY:HA2	13:T:197:TRP:CH2	2.56	0.40
9:P:27:VAL:HG13	17:Q:2596:HOH:O	2.20	0.40
9:P:188:TYR:C	9:P:189:LEU:HD23	2.46	0.40
10:Q:2:ILE:HD12	10:Q:170:PHE:CG	2.55	0.40
14:U:134:ILE:C	14:U:136:GLY:N	2.78	0.40
1:V:197:LEU:HD12	1:V:197:LEU:HA	1.79	0.40
2:W:71:ASN:ND2	2:W:72:ASP:N	2.68	0.40
3:X:84:ASP:CG	3:X:130:ARG:HH22	2.28	0.40
3:X:122:ARG:NH2	17:X:2046:HOH:O	2.55	0.40
5:Z:216:GLY:O	5:Z:219:THR:N	2.50	0.40
7:2:99:PHE:CE1	7:2:107:MET:HA	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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	248/250 (99%)	207 (84%)	38 (15%)	3 (1%)	10	40
1	V	248/250 (99%)	212 (86%)	32 (13%)	4 (2%)	7	34
2	B	242/244 (99%)	210 (87%)	26 (11%)	6 (2%)	4	23
2	W	242/244 (99%)	209 (86%)	24 (10%)	9 (4%)	2	15
3	C	239/241 (99%)	207 (87%)	25 (10%)	7 (3%)	3	20
3	X	239/241 (99%)	203 (85%)	29 (12%)	7 (3%)	3	20
4	D	240/242 (99%)	205 (85%)	30 (12%)	5 (2%)	5	27
4	Y	240/242 (99%)	210 (88%)	24 (10%)	6 (2%)	4	23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	231/233 (99%)	196 (85%)	30 (13%)	5 (2%)	5	26
5	Z	231/233 (99%)	196 (85%)	28 (12%)	7 (3%)	3	19
6	1	242/244 (99%)	203 (84%)	33 (14%)	6 (2%)	4	23
6	F	242/244 (99%)	206 (85%)	34 (14%)	2 (1%)	16	50
7	2	241/243 (99%)	211 (88%)	24 (10%)	6 (2%)	4	23
7	G	241/243 (99%)	209 (87%)	27 (11%)	5 (2%)	5	27
8	H	220/222 (99%)	192 (87%)	25 (11%)	3 (1%)	9	36
8	O	220/222 (99%)	198 (90%)	17 (8%)	5 (2%)	5	25
9	I	202/204 (99%)	181 (90%)	20 (10%)	1 (0%)	24	60
9	P	202/204 (99%)	185 (92%)	16 (8%)	1 (0%)	24	60
10	J	196/198 (99%)	175 (89%)	17 (9%)	4 (2%)	6	28
10	Q	196/198 (99%)	175 (89%)	16 (8%)	5 (3%)	4	23
11	K	210/212 (99%)	190 (90%)	17 (8%)	3 (1%)	9	36
11	R	210/212 (99%)	187 (89%)	21 (10%)	2 (1%)	12	45
12	L	220/222 (99%)	191 (87%)	27 (12%)	2 (1%)	14	48
12	S	220/222 (99%)	196 (89%)	23 (10%)	1 (0%)	24	60
13	M	231/233 (99%)	202 (87%)	25 (11%)	4 (2%)	7	32
13	T	231/233 (99%)	200 (87%)	29 (13%)	2 (1%)	14	48
14	N	194/196 (99%)	175 (90%)	16 (8%)	3 (2%)	8	35
14	U	194/196 (99%)	171 (88%)	20 (10%)	3 (2%)	8	35
15	8	1/5 (20%)	1 (100%)	0	0	100	100
15	9	1/5 (20%)	1 (100%)	0	0	100	100
All	All	6314/6378 (99%)	5504 (87%)	693 (11%)	117 (2%)	6	30

All (117) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	143	GLU
1	A	167	LYS
2	B	54	VAL
2	B	204(A)	SER
3	C	58	LEU
3	C	72	SER
3	C	183	PRO

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Mol	Chain	Res	Type
3	C	203	THR
5	E	217	LYS
8	H	91	GLN
10	J	39	PRO
13	M	71(B)	GLU
8	O	91	GLN
11	R	39	PRO
1	V	167	LYS
2	W	54	VAL
2	W	204(A)	SER
2	W	218(C)	ASP
3	X	58	LEU
3	X	183	PRO
3	X	203	THR
5	Z	217	LYS
2	B	219(C)	ASP
3	C	184	ALA
4	D	120	ALA
4	D	121	LEU
4	D	180(E)	SER
5	E	202	ARG
5	E	231	LYS
7	G	9	ASP
7	G	180(C)	HIS
10	J	49	ALA
14	N	115	LEU
10	Q	105(A)	LYS
13	T	71(B)	GLU
14	U	115	LEU
1	V	53	LYS
1	V	143	GLU
2	W	182	ASP
3	X	72	SER
4	Y	120	ALA
4	Y	180(E)	SER
5	Z	163	THR
5	Z	202	ARG
5	Z	231	LYS
7	2	9	ASP
7	2	55	PRO
7	2	180(C)	HIS
2	B	11	ARG

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Mol	Chain	Res	Type
4	D	22	PHE
5	E	170	GLN
6	F	206	LYS
6	F	237	GLN
8	H	30	ASN
10	J	105(A)	LYS
11	K	9	GLN
11	K	39	PRO
12	L	71	ASP
13	M	2	SER
14	N	187(E)	ASP
8	O	205	LYS
10	Q	8	VAL
10	Q	49	ALA
11	R	9	GLN
14	U	187(E)	ASP
2	W	35	GLY
3	X	184	ALA
4	Y	22	PHE
4	Y	121	LEU
5	Z	227	GLU
6	1	8	TYR
6	1	143	LYS
6	1	237	GLN
5	E	186	PRO
7	G	55	PRO
7	G	237	ALA
13	M	72	ALA
8	O	9	ASN
10	Q	39	PRO
10	Q	115	TYR
3	X	64	PRO
5	Z	170	GLN
5	Z	186	PRO
6	1	12	ASN
6	1	206	LYS
7	2	199	ASP
2	B	219(D)	GLY
3	C	239	GLU
9	I	93	GLY
11	K	138	LEU
13	M	115	LEU

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Mol	Chain	Res	Type
14	U	67	THR
2	W	22	TYR
3	X	242	GLU
6	1	98	SER
1	A	72	PRO
14	N	67	THR
8	O	105(A)	PRO
9	P	76	PRO
13	T	72	ALA
2	W	226	PRO
7	2	60	ASP
7	2	208	ASN
7	G	60	ASP
8	H	105(A)	PRO
10	J	8	VAL
8	O	96	GLY
2	W	153	PRO
3	C	64	PRO
1	V	159	PRO
2	W	218(D)	GLY
4	Y	123(F)	GLY
2	B	186	VAL
4	D	123(F)	GLY
12	L	94	PRO
12	S	-6	PRO
4	Y	11	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	209/209 (100%)	197 (94%)	12 (6%)	18	52
1	V	209/209 (100%)	196 (94%)	13 (6%)	16	49
2	B	203/203 (100%)	187 (92%)	16 (8%)	11	39
2	W	203/203 (100%)	185 (91%)	18 (9%)	9	34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	213/213 (100%)	199 (93%)	14 (7%)	15	46
3	X	213/213 (100%)	195 (92%)	18 (8%)	10	36
4	D	198/198 (100%)	186 (94%)	12 (6%)	17	49
4	Y	198/198 (100%)	184 (93%)	14 (7%)	13	43
5	E	192/192 (100%)	175 (91%)	17 (9%)	9	34
5	Z	192/192 (100%)	169 (88%)	23 (12%)	5	22
6	1	201/201 (100%)	184 (92%)	17 (8%)	10	36
6	F	201/201 (100%)	184 (92%)	17 (8%)	10	36
7	2	207/207 (100%)	194 (94%)	13 (6%)	16	48
7	G	207/207 (100%)	193 (93%)	14 (7%)	14	45
8	H	181/181 (100%)	172 (95%)	9 (5%)	22	56
8	O	181/181 (100%)	167 (92%)	14 (8%)	12	40
9	I	172/172 (100%)	160 (93%)	12 (7%)	14	44
9	P	172/172 (100%)	161 (94%)	11 (6%)	16	48
10	J	175/175 (100%)	165 (94%)	10 (6%)	18	52
10	Q	175/175 (100%)	164 (94%)	11 (6%)	16	48
11	K	169/169 (100%)	157 (93%)	12 (7%)	13	43
11	R	169/169 (100%)	159 (94%)	10 (6%)	18	50
12	L	185/185 (100%)	172 (93%)	13 (7%)	14	44
12	S	185/185 (100%)	173 (94%)	12 (6%)	15	47
13	M	199/199 (100%)	187 (94%)	12 (6%)	17	50
13	T	199/199 (100%)	188 (94%)	11 (6%)	19	53
14	N	162/162 (100%)	145 (90%)	17 (10%)	6	27
14	U	162/162 (100%)	149 (92%)	13 (8%)	11	38
15	8	2/2 (100%)	2 (100%)	0	100	100
15	9	2/2 (100%)	2 (100%)	0	100	100
All	All	5336/5336 (100%)	4951 (93%)	385 (7%)	13	43

All (385) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	VAL
1	A	62	GLU

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Mol	Chain	Res	Type
1	A	64	LEU
1	A	88	LEU
1	A	124	THR
1	A	136	LEU
1	A	158	PHE
1	A	170	VAL
1	A	200	SER
1	A	212	LEU
1	A	223	LYS
1	A	236	LEU
2	B	41	MET
2	B	58	LEU
2	B	61	GLN
2	B	63	THR
2	B	63(A)	SER
2	B	65	GLU
2	B	67	LEU
2	B	150	THR
2	B	156	ASN
2	B	169	THR
2	B	185	LYS
2	B	198	SER
2	B	203	ASP
2	B	206	THR
2	B	226	PRO
2	B	236	THR
3	C	10	ARG
3	C	25	GLU
3	C	61	THR
3	C	75	VAL
3	C	124	THR
3	C	135	SER
3	C	156	ILE
3	C	172	VAL
3	C	174	GLU
3	C	178	LYS
3	C	196	SER
3	C	209	ASN
3	C	215	VAL
3	C	224	LEU
4	D	13	SER
4	D	27	SER

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Mol	Chain	Res	Type
4	D	28	LEU
4	D	31	ILE
4	D	119	LEU
4	D	126	ARG
4	D	156	THR
4	D	177	LEU
4	D	184	LEU
4	D	191	LEU
4	D	215	ILE
4	D	237	LEU
5	E	11	ASP
5	E	12	THR
5	E	15	PHE
5	E	18	THR
5	E	32	LYS
5	E	58	LEU
5	E	76	LEU
5	E	97	ASN
5	E	138	ILE
5	E	153	PRO
5	E	189	LEU
5	E	198	SER
5	E	199	GLN
5	E	203	ASP
5	E	222	THR
5	E	223	ILE
5	E	231	LYS
6	F	14	VAL
6	F	36	THR
6	F	43	ASN
6	F	127	ASN
6	F	135	SER
6	F	153	PRO
6	F	169	ARG
6	F	170	GLN
6	F	187	ARG
6	F	192	GLN
6	F	199	LEU
6	F	203	GLU
6	F	205	ASN
6	F	208	PHE
6	F	220	LEU

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Mol	Chain	Res	Type
6	F	227	ASP
6	F	233	ILE
7	G	40	VAL
7	G	67	ILE
7	G	72	ARG
7	G	87	ASN
7	G	105	TYR
7	G	119	LEU
7	G	124	THR
7	G	169	GLN
7	G	171	GLU
7	G	201	LEU
7	G	210	LEU
7	G	217	LYS
7	G	232	ARG
7	G	233	LEU
8	H	22	GLN
8	H	34	LEU
8	H	56	THR
8	H	77	VAL
8	H	121	VAL
8	H	185	GLU
8	H	196	VAL
8	H	197	ARG
8	H	219	VAL
9	I	-5	SER
9	I	29	ASN
9	I	55	LEU
9	I	70	GLU
9	I	113	PHE
9	I	131	SER
9	I	148	PRO
9	I	159	LEU
9	I	160	LEU
9	I	171	TRP
9	I	181	LYS
9	I	185	VAL
10	J	7	ARG
10	J	17	SER
10	J	34	THR
10	J	52	THR
10	J	68	ILE

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Mol	Chain	Res	Type
10	J	133	TYR
10	J	147	THR
10	J	155	LEU
10	J	166	MET
10	J	174	ILE
11	K	4	LEU
11	K	31	VAL
11	K	39	PRO
11	K	69	ARG
11	K	70	GLU
11	K	97	MET
11	K	100	MET
11	K	110	ILE
11	K	118	THR
11	K	138	LEU
11	K	145	ASP
11	K	185	ILE
12	L	14	LEU
12	L	25	SER
12	L	33	LYS
12	L	37	CYS
12	L	40	ASN
12	L	43	MET
12	L	62	SER
12	L	98	HIS
12	L	99	THR
12	L	138	LEU
12	L	145	TYR
12	L	150	GLU
12	L	184	VAL
13	M	21	SER
13	M	40	ASN
13	M	43	VAL
13	M	61	ASP
13	M	62	LEU
13	M	63	VAL
13	M	112	TYR
13	M	122	SER
13	M	184	LEU
13	M	190	LEU
13	M	192	VAL
13	M	204	LYS

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Mol	Chain	Res	Type
14	N	6	VAL
14	N	12	VAL
14	N	20	THR
14	N	36	ARG
14	N	61	TYR
14	N	63	LEU
14	N	81	SER
14	N	105	ASP
14	N	105(A)	ASP
14	N	105(B)	LYS
14	N	115	LEU
14	N	123	PRO
14	N	132	THR
14	N	144	GLU
14	N	149	GLU
14	N	177	VAL
14	N	184	VAL
8	O	22	GLN
8	O	34	LEU
8	O	56	THR
8	O	63	ILE
8	O	68	LEU
8	O	121	VAL
8	O	124	TYR
8	O	156	SER
8	O	185	GLU
8	O	193	THR
8	O	196	VAL
8	O	197	ARG
8	O	219	VAL
8	O	221	ILE
9	P	-5	SER
9	P	29	ASN
9	P	55	LEU
9	P	70	GLU
9	P	113	PHE
9	P	131	SER
9	P	159	LEU
9	P	160	LEU
9	P	169	SER
9	P	181	LYS
9	P	185	VAL

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Mol	Chain	Res	Type
10	Q	7	ARG
10	Q	17	SER
10	Q	34	THR
10	Q	52	THR
10	Q	68	ILE
10	Q	91	SER
10	Q	104	TYR
10	Q	133	TYR
10	Q	147	THR
10	Q	155	LEU
10	Q	174	ILE
11	R	4	LEU
11	R	31	VAL
11	R	39	PRO
11	R	69	ARG
11	R	70	GLU
11	R	97	MET
11	R	100	MET
11	R	102	CYS
11	R	138	LEU
11	R	145	ASP
12	S	14	LEU
12	S	40	ASN
12	S	43	MET
12	S	62	SER
12	S	98	HIS
12	S	99	THR
12	S	138	LEU
12	S	150	GLU
12	S	160	THR
12	S	177	ILE
12	S	179	THR
12	S	184	VAL
13	T	3	VAL
13	T	21	SER
13	T	40	ASN
13	T	61	ASP
13	T	62	LEU
13	T	63	VAL
13	T	100	ILE
13	T	123	PRO
13	T	190	LEU

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Mol	Chain	Res	Type
13	T	192	VAL
13	T	204	LYS
14	U	6	VAL
14	U	20	THR
14	U	78	THR
14	U	101	VAL
14	U	115	LEU
14	U	122	LEU
14	U	123	PRO
14	U	132	THR
14	U	169	SER
14	U	173	ILE
14	U	177	VAL
14	U	178	LEU
14	U	184	VAL
1	V	28	LEU
1	V	47	VAL
1	V	62	GLU
1	V	64	LEU
1	V	69	LEU
1	V	78	TYR
1	V	131	PRO
1	V	136	LEU
1	V	158	PHE
1	V	170	VAL
1	V	212	LEU
1	V	221	PHE
1	V	236	LEU
2	W	38	ILE
2	W	41	MET
2	W	58	LEU
2	W	61	GLN
2	W	63	THR
2	W	63(A)	SER
2	W	67	LEU
2	W	81	LEU
2	W	90	ASN
2	W	124	THR
2	W	150	THR
2	W	153	PRO
2	W	169	THR
2	W	185	LYS

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Mol	Chain	Res	Type
2	W	198	SER
2	W	203	ASP
2	W	226	PRO
2	W	236	THR
3	X	10	ARG
3	X	17	PRO
3	X	25	GLU
3	X	61	THR
3	X	75	VAL
3	X	124	THR
3	X	135	SER
3	X	156	ILE
3	X	163	GLN
3	X	172	VAL
3	X	174	GLU
3	X	178	LYS
3	X	183	PRO
3	X	196	SER
3	X	209	ASN
3	X	215	VAL
3	X	224	LEU
3	X	226	SER
4	Y	28	LEU
4	Y	31	ILE
4	Y	56	SER
4	Y	76	CYS
4	Y	119	LEU
4	Y	126	ARG
4	Y	154	SER
4	Y	156	THR
4	Y	177	LEU
4	Y	184	LEU
4	Y	191	LEU
4	Y	208	ASP
4	Y	215	ILE
4	Y	237	LEU
5	Z	11	ASP
5	Z	12	THR
5	Z	15	PHE
5	Z	18	THR
5	Z	32	LYS
5	Z	40	LEU

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Mol	Chain	Res	Type
5	Z	48	LEU
5	Z	49	VAL
5	Z	58	LEU
5	Z	76	LEU
5	Z	97	ASN
5	Z	117	CYS
5	Z	138	ILE
5	Z	153	PRO
5	Z	198	SER
5	Z	199	GLN
5	Z	207	LEU
5	Z	207(B)	THR
5	Z	207(C)	VAL
5	Z	207(D)	ASP
5	Z	207(E)	ASN
5	Z	222	THR
5	Z	231	LYS
6	1	36	THR
6	1	43	ASN
6	1	83	PRO
6	1	121	GLN
6	1	127	ASN
6	1	135	SER
6	1	153	PRO
6	1	169	ARG
6	1	170	GLN
6	1	187	ARG
6	1	192	GLN
6	1	203	GLU
6	1	205	ASN
6	1	208	PHE
6	1	214	TRP
6	1	220	LEU
6	1	233	ILE
7	2	62	THR
7	2	72	ARG
7	2	87	ASN
7	2	105	TYR
7	2	119	LEU
7	2	169	GLN
7	2	171	GLU
7	2	201	LEU

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Mol	Chain	Res	Type
7	2	204	GLU
7	2	217	LYS
7	2	222	PHE
7	2	232	ARG
7	2	233	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (210) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	97	HIS
1	A	181	ASN
1	A	217(B)	ASN
2	B	23	GLN
2	B	71	ASN
2	B	97	GLN
2	B	104	ASN
2	B	125	GLN
2	B	147	GLN
2	B	156	ASN
2	B	177	GLN
2	B	227	GLN
3	C	23	GLN
3	C	44	ASN
3	C	82	ASN
3	C	150	GLN
3	C	163	GLN
3	C	168	ASN
3	C	209	ASN
3	C	235	GLN
4	D	23	GLN
4	D	99	HIS
4	D	108	ASN
4	D	147	GLN
4	D	150	HIS
4	D	173	GLN
4	D	211	GLN
4	D	218	GLN
4	D	226	ASN
5	E	6	ASN
5	E	7	ASN
5	E	64	GLN
5	E	73	HIS

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Mol	Chain	Res	Type
5	E	97	ASN
5	E	104	ASN
5	E	114	HIS
5	E	121	GLN
5	E	125	GLN
5	E	152	GLN
5	E	156	ASN
5	E	199	GLN
6	F	23	GLN
6	F	43	ASN
6	F	90	ASN
6	F	121	GLN
6	F	123	HIS
6	F	192	GLN
6	F	221	HIS
6	F	241	ASN
7	G	32	ASN
7	G	33	GLN
7	G	34(A)	ASN
7	G	87	ASN
7	G	118	ASN
7	G	121	GLN
7	G	125	GLN
7	G	170	GLN
7	G	178	ASN
7	G	184	ASN
8	H	22	GLN
8	H	30	ASN
8	H	66	HIS
8	H	86	HIS
8	H	91	GLN
8	H	109	HIS
8	H	114	HIS
8	H	144	GLN
8	H	172	ASN
8	H	190	ASN
9	I	29	ASN
9	I	81	GLN
9	I	145	ASN
10	J	54	GLN
10	J	62	ASN
10	J	77	GLN

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Mol	Chain	Res	Type
10	J	85	GLN
10	J	140	HIS
10	J	141	HIS
10	J	186	GLN
11	K	62	GLN
11	K	85	ASN
11	K	174	ASN
12	L	27	ASN
12	L	40	ASN
12	L	67	HIS
12	L	70(A)	ASN
12	L	123	GLN
12	L	140	ASN
12	L	141	GLN
12	L	144(B)	ASN
12	L	144(C)	GLN
12	L	144(J)	ASN
12	L	166	HIS
13	M	-7	GLN
13	M	10	ASN
13	M	40	ASN
13	M	89	GLN
13	M	93	ASN
13	M	135	ASN
13	M	149	GLN
13	M	157	ASN
13	M	172	ASN
13	M	191	GLN
14	N	38	HIS
14	N	62	HIS
14	N	69	GLN
14	N	106	ASN
14	N	141	ASN
14	N	157	HIS
14	N	161	GLN
8	O	22	GLN
8	O	30	ASN
8	O	66	HIS
8	O	86	HIS
8	O	91	GLN
8	O	114	HIS
8	O	144	GLN

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Mol	Chain	Res	Type
8	O	172	ASN
8	O	190	ASN
9	P	36	HIS
9	P	81	GLN
9	P	145	ASN
10	Q	54	GLN
10	Q	62	ASN
10	Q	77	GLN
10	Q	85	GLN
10	Q	112	GLN
10	Q	141	HIS
10	Q	186	GLN
11	R	9	GLN
11	R	62	GLN
11	R	85	ASN
11	R	174	ASN
12	S	40	ASN
12	S	61	ASN
12	S	67	HIS
12	S	70(A)	ASN
12	S	140	ASN
12	S	141	GLN
12	S	144(B)	ASN
12	S	144(I)	ASN
12	S	166	HIS
13	T	10	ASN
13	T	40	ASN
13	T	89	GLN
13	T	93	ASN
13	T	135	ASN
13	T	149	GLN
13	T	157	ASN
13	T	172	ASN
13	T	181	ASN
13	T	191	GLN
14	U	69	GLN
14	U	141	ASN
14	U	161	GLN
1	V	97	HIS
1	V	150	GLN
1	V	181	ASN
2	W	23	GLN

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Mol	Chain	Res	Type
2	W	33	HIS
2	W	61	GLN
2	W	71	ASN
2	W	97	GLN
2	W	121	GLN
2	W	125	GLN
2	W	156	ASN
2	W	173	GLN
2	W	177	GLN
2	W	227	GLN
3	X	23	GLN
3	X	44	ASN
3	X	150	GLN
3	X	163	GLN
3	X	209	ASN
4	Y	23	GLN
4	Y	108	ASN
4	Y	141	HIS
4	Y	150	HIS
4	Y	173	GLN
4	Y	226	ASN
5	Z	6	ASN
5	Z	7	ASN
5	Z	33	GLN
5	Z	64	GLN
5	Z	73	HIS
5	Z	121	GLN
5	Z	123	ASN
5	Z	125	GLN
5	Z	156	ASN
5	Z	185	ASN
6	1	23	GLN
6	1	43	ASN
6	1	90	ASN
6	1	121	GLN
6	1	123	HIS
6	1	147	HIS
6	1	221	HIS
6	1	241	ASN
7	2	32	ASN
7	2	33	GLN
7	2	34(A)	ASN

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Mol	Chain	Res	Type
7	2	87	ASN
7	2	118	ASN
7	2	121	GLN
7	2	125	GLN
7	2	170	GLN
7	2	178	ASN
7	2	184	ASN
15	8	3	ASN
15	9	3	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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
15	R4K	9	4	15	17,18,19	3.97	9 (52%)	21,27,29	3.44	9 (42%)
15	R4K	8	4	15	17,18,19	3.10	6 (35%)	21,27,29	2.36	11 (52%)

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
15	R4K	9	4	15	-	3/11/28/30	0/2/2/2
15	R4K	8	4	15	-	2/11/28/30	0/2/2/2

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	9	4	R4K	C32-N31	-9.31	1.24	1.35
15	9	4	R4K	C55-C50	-8.66	1.30	1.39
15	8	4	R4K	C29-C50	-7.49	1.41	1.51
15	8	4	R4K	C55-C50	-6.62	1.32	1.39
15	8	4	R4K	C32-N31	-5.59	1.28	1.35
15	9	4	R4K	C29-C32	-4.53	1.45	1.55
15	9	4	R4K	C29-CB	-4.24	1.53	1.55
15	9	4	R4K	C55-N31	-4.11	1.31	1.38
15	9	4	R4K	C29-C50	-3.79	1.46	1.51
15	8	4	R4K	C51-C50	3.67	1.44	1.39
15	9	4	R4K	CB-CA	3.44	1.61	1.53
15	9	4	R4K	C51-C50	3.02	1.43	1.39
15	9	4	R4K	O33-C32	2.39	1.27	1.22
15	8	4	R4K	O34-CB	2.15	1.47	1.42
15	8	4	R4K	C29-C32	-2.15	1.50	1.55

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	9	4	R4K	C51-C50-C55	10.35	128.82	119.81
15	9	4	R4K	C54-C55-C50	-6.80	115.56	121.92
15	8	4	R4K	C51-C50-C55	4.63	123.84	119.81
15	9	4	R4K	C50-C55-N31	4.42	112.56	109.60
15	9	4	R4K	C51-C50-C29	-4.21	124.91	130.81
15	8	4	R4K	C54-C55-C50	-4.13	118.06	121.92
15	8	4	R4K	O-C-CA	-3.96	114.58	124.77
15	8	4	R4K	C29-CB-CA	-3.79	109.84	112.78
15	9	4	R4K	C52-C53-C54	3.17	124.15	120.24
15	8	4	R4K	O33-C32-N31	3.05	129.51	126.28
15	9	4	R4K	C29-CB-CA	-2.98	110.47	112.78
15	9	4	R4K	O-C-CA	-2.79	117.58	124.77
15	8	4	R4K	C51-C50-C29	-2.79	126.90	130.81
15	9	4	R4K	C52-C51-C50	-2.78	114.98	119.99
15	8	4	R4K	C55-N31-C32	-2.72	110.05	111.85
15	8	4	R4K	O33-C32-C29	-2.47	122.37	125.22
15	9	4	R4K	C55-N31-C32	-2.45	110.23	111.85
15	8	4	R4K	C53-C52-C51	-2.23	117.48	120.24
15	8	4	R4K	O30-C29-C32	2.11	114.59	108.37
15	8	4	R4K	C52-C53-C54	2.01	122.71	120.24

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	8	4	R4K	O-C-CA-CB
15	8	4	R4K	N-CA-CB-C29
15	9	4	R4K	N-CA-CB-C29
15	9	4	R4K	O-C-CA-CB
15	9	4	R4K	C-CA-CB-C29

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	9	4	R4K	2	0
15	8	4	R4K	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 10 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.