



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 11:09 PM GMT

PDB ID : 1FNT
Title : CRYSTAL STRUCTURE OF THE 20S PROTEASOME FROM YEAST IN COMPLEX WITH THE PROTEASOME ACTIVATOR PA26 FROM TRY-PANOSOME BRUCEI AT 3.2 ANGSTROMS RESOLUTION
Authors : Whitby, F.G.; Masters, E.; Kramer, L.; Knowlton, J.R.; Yao, Y.; Wang, C.C.; Hill, C.P.
Deposited on : 2000-08-23
Resolution : 3.20 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

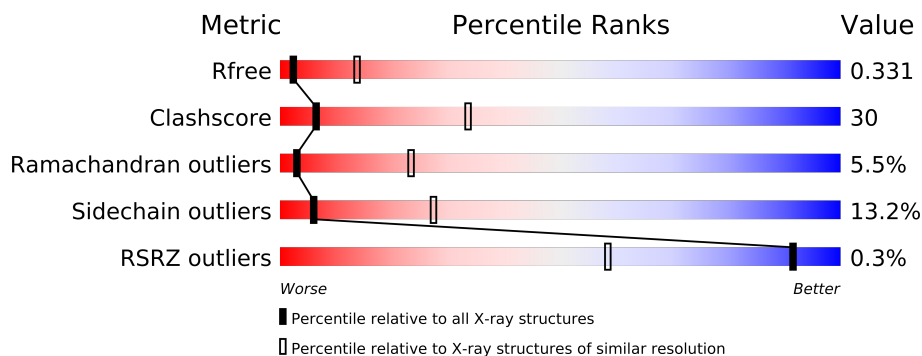
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1824 (3.30-3.10)
Clashscore	79885	1078 (3.26-3.14)
Ramachandran outliers	78287	1059 (3.26-3.14)
Sidechain outliers	78261	1058 (3.26-3.14)
RSRZ outliers	66119	1825 (3.30-3.10)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	252	
1	O	252	
2	B	250	
2	P	250	
3	C	245	
3	Q	245	
4	D	254	
4	R	254	
5	E	260	
5	S	260	
6	F	234	
6	T	234	
7	G	287	
7	U	287	

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Mol	Chain	Length	Quality of chain
8	H	196	
8	V	196	
9	I	232	
9	W	232	
10	J	205	
10	X	205	
11	K	198	
11	Y	198	
12	L	212	
12	Z	212	
13	M	222	
13	a	222	
14	N	233	
14	b	233	
15	c	231	
15	d	231	
15	e	231	
15	f	231	
15	g	231	
15	h	231	
15	i	231	
15	j	231	
15	k	231	
15	l	231	
15	m	231	
15	n	231	
15	o	231	
15	p	231	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
16	MG	H	1002	-	X
16	MG	J	1005	-	X
16	MG	L	1003	-	X
16	MG	X	1012	-	X
16	MG	X	1013	-	X

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 70622 atoms, of which 0 are hydrogen and 0 are deuterium.

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 C7-ALPHA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	238	Total	C	N	O	S	0	0	0
			1881	1197	314	362	8			
1	O	238	Total	C	N	O	S	0	0	0
			1881	1197	314	362	8			

- Molecule 2 is a protein called PROTEASOME COMPONENT Y7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	247	Total	C	N	O	S	0	0	0
			1868	1188	309	368	3			
2	P	247	Total	C	N	O	S	0	0	0
			1868	1188	309	368	3			

- Molecule 3 is a protein called PROTEASOME COMPONENT Y13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	241	Total	C	N	O	S	0	0	0
			1868	1180	312	373	3			
3	Q	241	Total	C	N	O	S	0	0	0
			1868	1180	312	373	3			

- Molecule 4 is a protein called PROTEASOME COMPONENT PRE6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	239	Total	C	N	O	S	0	0	0
			1862	1163	326	369	4			
4	R	239	Total	C	N	O	S	0	0	0
			1862	1163	326	369	4			

- Molecule 5 is a protein called PROTEASOME COMPONENT PUP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	244	Total	C	N	O	S	0	0	0
			1871	1168	316	380	7			
5	S	244	Total	C	N	O	S	0	0	0
			1871	1168	316	380	7			

- Molecule 6 is a protein called PROTEASOME COMPONENT PRE5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	233	Total	C	N	O	S	0	0	0
			1795	1129	312	350	4			
6	T	233	Total	C	N	O	S	0	0	0
			1795	1129	312	350	4			

- Molecule 7 is a protein called PROTEASOME COMPONENT C1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	240	Total	C	N	O	S	0	0	0
			1869	1188	326	351	4			
7	U	240	Total	C	N	O	S	0	0	0
			1869	1188	326	351	4			

- Molecule 8 is a protein called PROTEASOME COMPONENT PRE3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	196	Total	C	N	O	S	0	0	0
			1510	954	250	299	7			
8	V	196	Total	C	N	O	S	0	0	0
			1510	954	250	299	7			

- Molecule 9 is a protein called PROTEASOME COMPONENT PUP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	222	Total	C	N	O	S	0	0	0
			1684	1061	293	323	7			
9	W	222	Total	C	N	O	S	0	0	0
			1684	1061	293	323	7			

- Molecule 10 is a protein called PROTEASOME COMPONENT PUP3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	204	Total	C	N	O	S	0	0	0
			1581	1010	258	305	8			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	X	204	Total	C	N	O	S	0	0	0
			1581	1010	258	305	8			

- Molecule 11 is a protein called PROTEASOME COMPONENT C11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	198	Total	C	N	O	S	0	0	0
			1585	1005	269	305	6			
11	Y	198	Total	C	N	O	S	0	0	0
			1585	1005	269	305	6			

- Molecule 12 is a protein called PROTEASOME COMPONENT PRE2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	212	Total	C	N	O	S	0	0	0
			1646	1045	282	312	7			
12	Z	212	Total	C	N	O	S	0	0	0
			1646	1045	282	312	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	33	ARG	LYS	ENGINEERED	UNP P30656
Z	33	ARG	LYS	ENGINEERED	UNP P30656

- Molecule 13 is a protein called PROTEASOME COMPONENT C5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	222	Total	C	N	O	S	0	0	0
			1757	1115	303	335	4			
13	a	222	Total	C	N	O	S	0	0	0
			1757	1115	303	335	4			

- Molecule 14 is a protein called PROTEASOME COMPONENT PRE4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			
14	b	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			

- Molecule 15 is a protein called PROTEASOME ACTIVATOR PROTEIN PA26.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	c	198	Total	C	N	O	S	0	0	0
			1529	960	267	296	6			
15	d	198	Total	C	N	O	S	0	0	0
			1529	960	267	296	6			
15	e	198	Total	C	N	O	S	0	0	0
			1529	960	267	296	6			
15	f	198	Total	C	N	O	S	0	0	0
			1529	960	267	296	6			
15	g	198	Total	C	N	O	S	0	0	0
			1529	960	267	296	6			
15	h	198	Total	C	N	O	S	0	0	0
			1529	960	267	296	6			
15	i	198	Total	C	N	O	S	0	0	0
			1529	960	267	296	6			
15	j	198	Total	C	N	O	S	0	0	0
			1529	960	267	296	6			
15	k	198	Total	C	N	O	S	0	0	0
			1529	960	267	296	6			
15	l	198	Total	C	N	O	S	0	0	0
			1529	960	267	296	6			
15	m	198	Total	C	N	O	S	0	0	0
			1529	960	267	296	6			
15	n	198	Total	C	N	O	S	0	0	0
			1529	960	267	296	6			
15	o	198	Total	C	N	O	S	0	0	0
			1529	960	267	296	6			
15	p	198	Total	C	N	O	S	0	0	0
			1529	960	267	296	6			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
c	49	VAL	THR	see remark 999	UNP Q9U8G2
c	226	THR	SER	see remark 999	UNP Q9U8G2
d	49	VAL	THR	see remark 999	UNP Q9U8G2
d	226	THR	SER	see remark 999	UNP Q9U8G2
e	49	VAL	THR	see remark 999	UNP Q9U8G2
e	226	THR	SER	see remark 999	UNP Q9U8G2
f	49	VAL	THR	see remark 999	UNP Q9U8G2
f	226	THR	SER	see remark 999	UNP Q9U8G2
g	49	VAL	THR	see remark 999	UNP Q9U8G2
g	226	THR	SER	see remark 999	UNP Q9U8G2
h	49	VAL	THR	see remark 999	UNP Q9U8G2
h	226	THR	SER	see remark 999	UNP Q9U8G2

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Chain	Residue	Modelled	Actual	Comment	Reference
i	49	VAL	THR	see remark 999	UNP Q9U8G2
i	226	THR	SER	see remark 999	UNP Q9U8G2
j	49	VAL	THR	see remark 999	UNP Q9U8G2
j	226	THR	SER	see remark 999	UNP Q9U8G2
k	49	VAL	THR	see remark 999	UNP Q9U8G2
k	226	THR	SER	see remark 999	UNP Q9U8G2
l	49	VAL	THR	see remark 999	UNP Q9U8G2
l	226	THR	SER	see remark 999	UNP Q9U8G2
m	49	VAL	THR	see remark 999	UNP Q9U8G2
m	226	THR	SER	see remark 999	UNP Q9U8G2
n	49	VAL	THR	see remark 999	UNP Q9U8G2
n	226	THR	SER	see remark 999	UNP Q9U8G2
o	49	VAL	THR	see remark 999	UNP Q9U8G2
o	226	THR	SER	see remark 999	UNP Q9U8G2
p	49	VAL	THR	see remark 999	UNP Q9U8G2
p	226	THR	SER	see remark 999	UNP Q9U8G2

- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	G	1	Total Mg 1 1	0	0
16	J	2	Total Mg 2 2	0	0
16	H	1	Total Mg 1 1	0	0
16	I	1	Total Mg 1 1	0	0
16	V	1	Total Mg 1 1	0	0
16	W	1	Total Mg 1 1	0	0
16	Z	1	Total Mg 1 1	0	0
16	a	1	Total Mg 1 1	0	0
16	U	1	Total Mg 1 1	0	0
16	X	2	Total Mg 2 2	0	0
16	L	1	Total Mg 1 1	0	0

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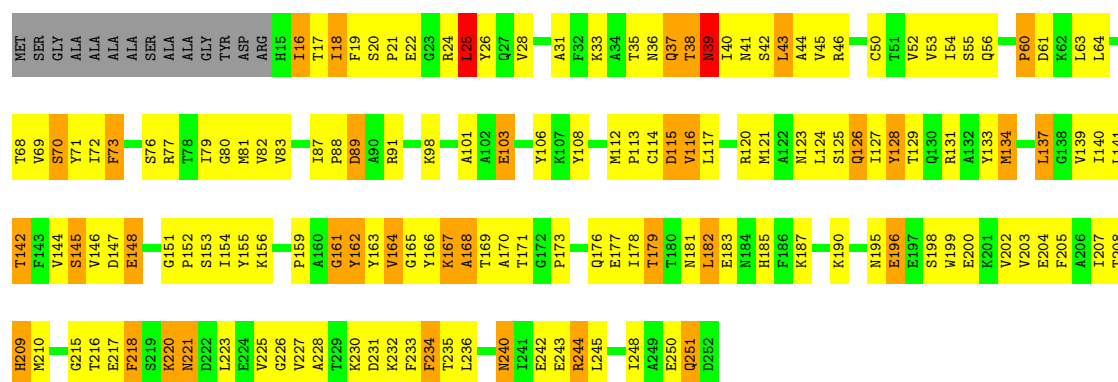
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	M	1	Total	Mg	0	0
			1	1		

3 Residue-property plots

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

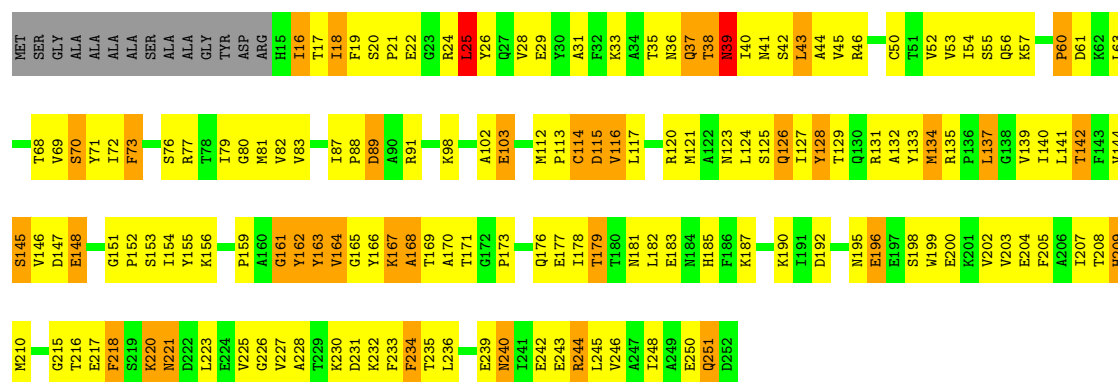
• Molecule 1: PROTEASOME COMPONENT C7-ALPHA

Chain A: 



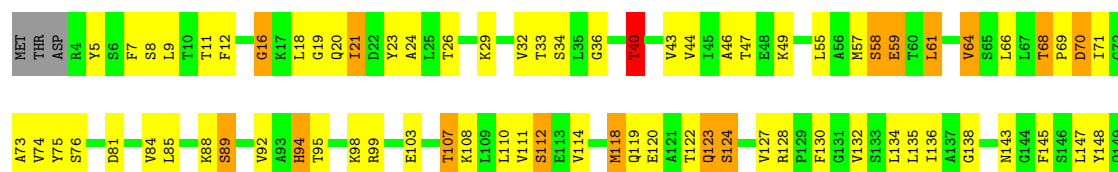
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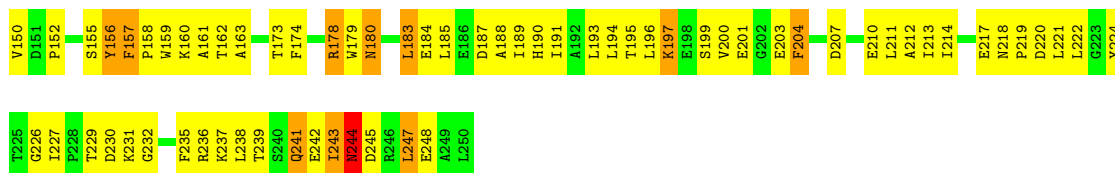
Chain O: 



• Molecule 2: PROTEASOME COMPONENT Y7

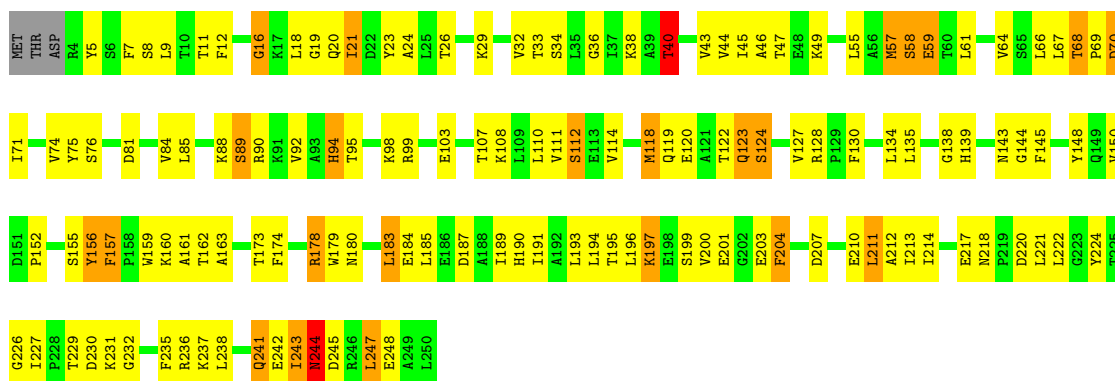
Chain B: 





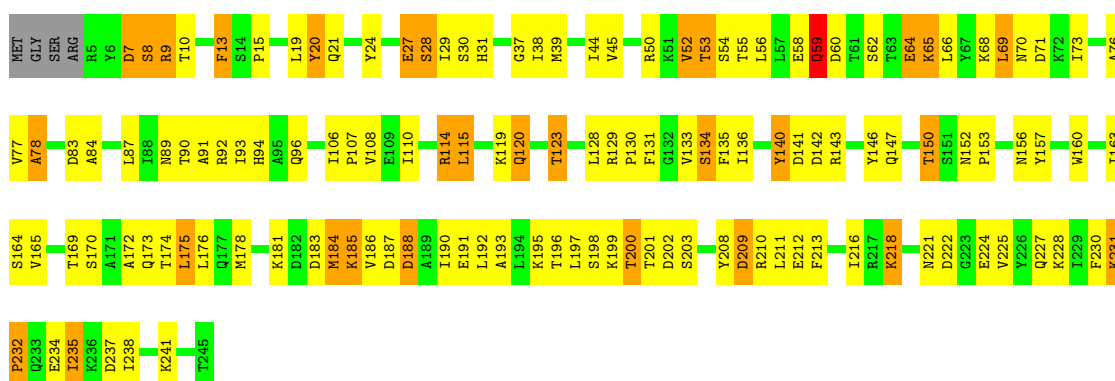
• Molecule 2: PROTEASOME COMPONENT Y7

Chain P:



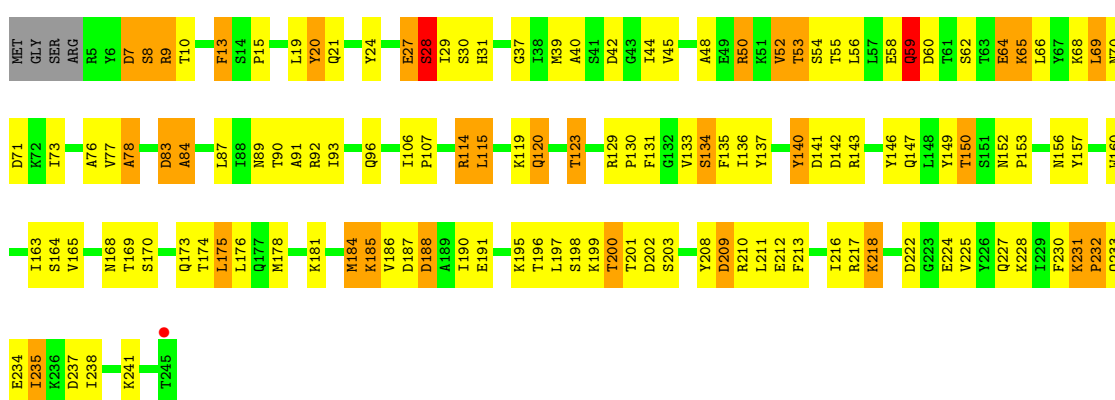
• Molecule 3: PROTEASOME COMPONENT Y13

Chain C:



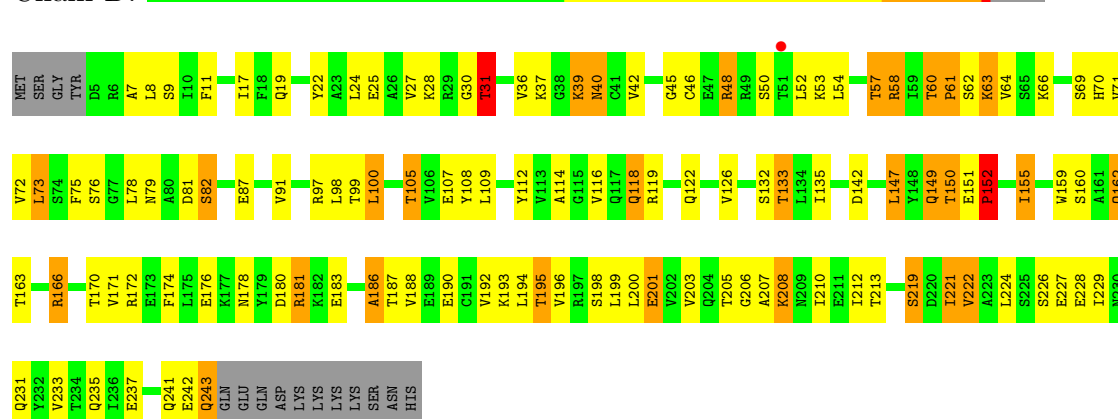
• Molecule 3: PROTEASOME COMPONENT Y13

Chain Q:



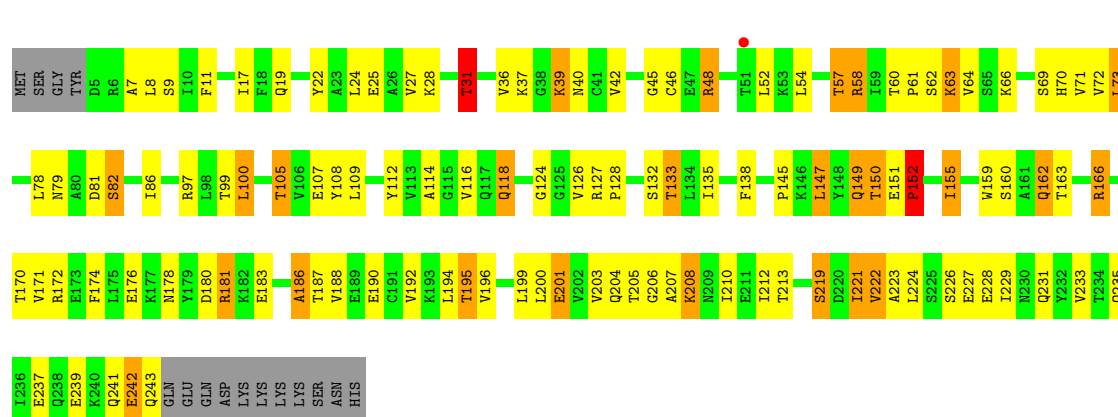
- Molecule 4: PROTEASOME COMPONENT PRE6

Chain D:



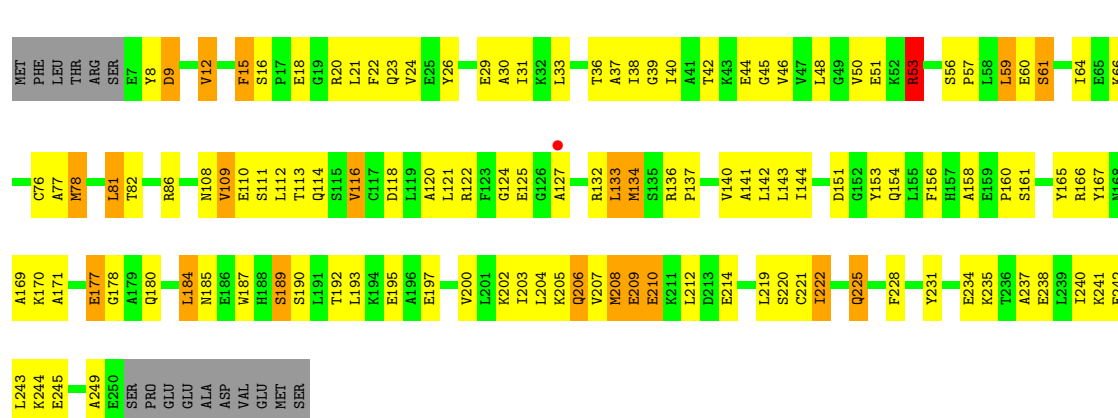
- Molecule 4: PROTEASOME COMPONENT PRE6

Chain R:



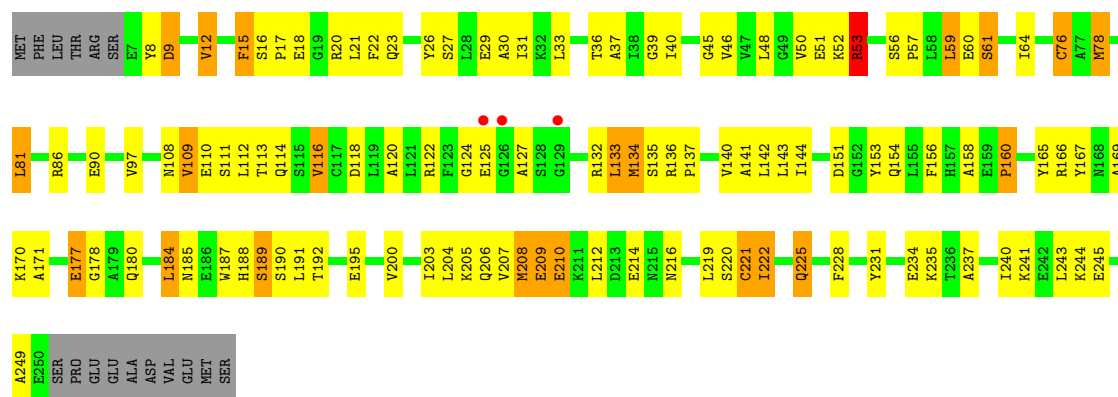
- Molecule 5: PROTEASOME COMPONENT PUP2

Chain E:



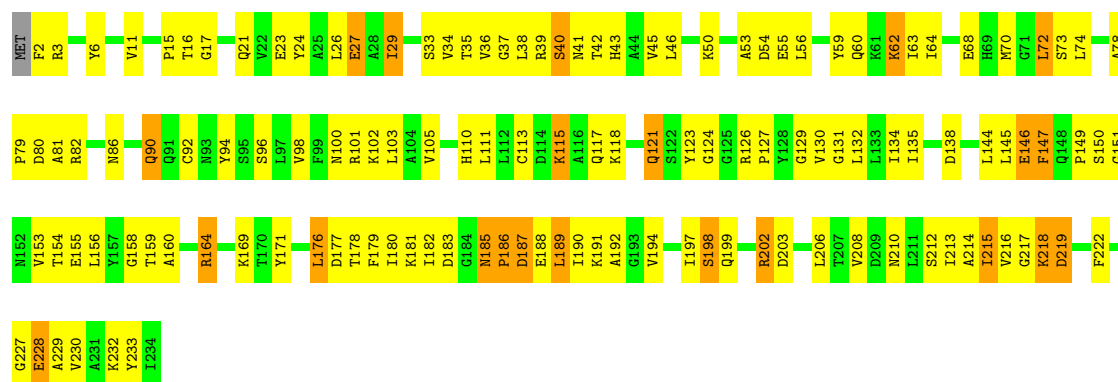
- Molecule 5: PROTEASOME COMPONENT PUP2

Chain S:



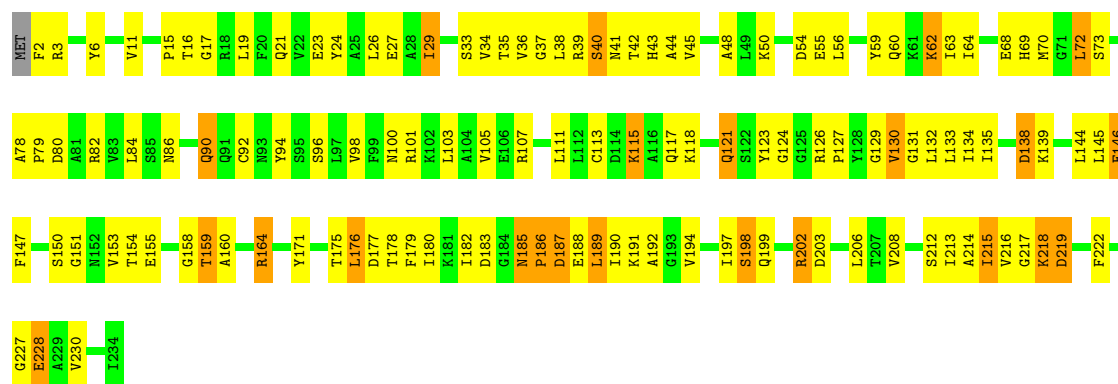
• Molecule 6: PROTEASOME COMPONENT PRE5

Chain F:



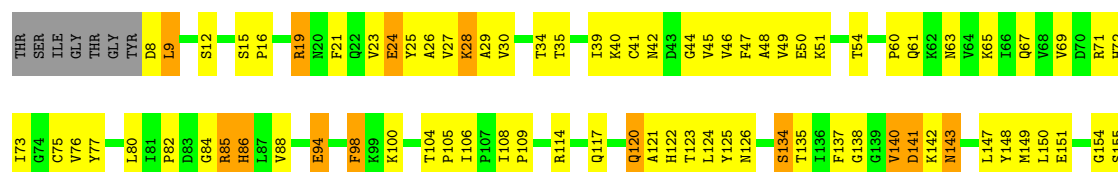
• Molecule 6: PROTEASOME COMPONENT PRE5

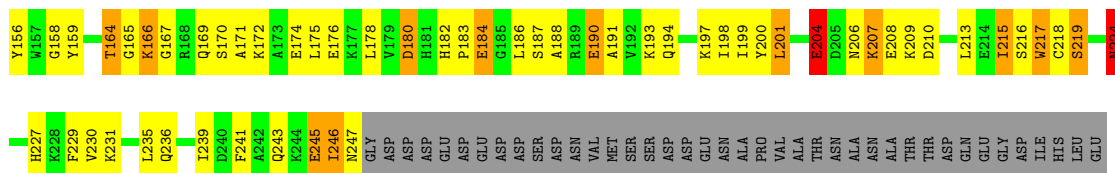
Chain T:



• Molecule 7: PROTEASOME COMPONENT C1

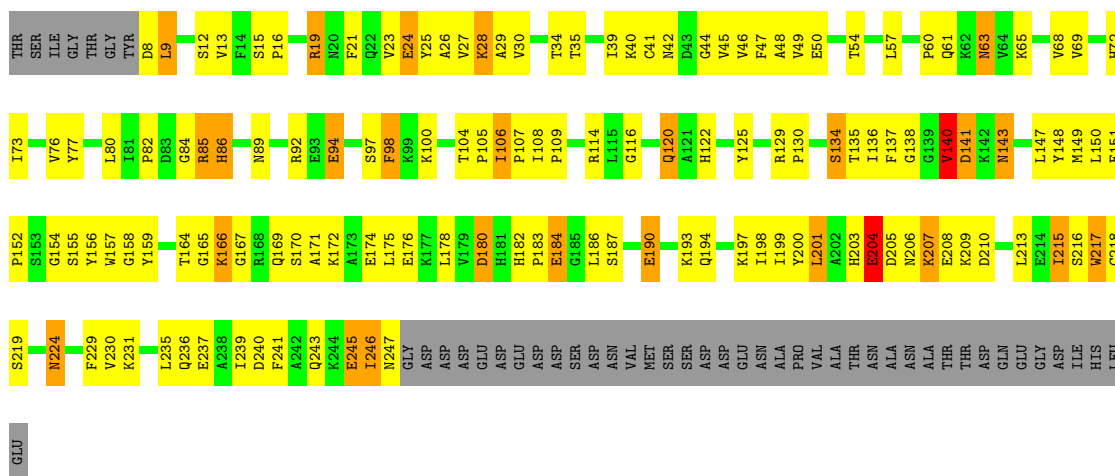
Chain G:





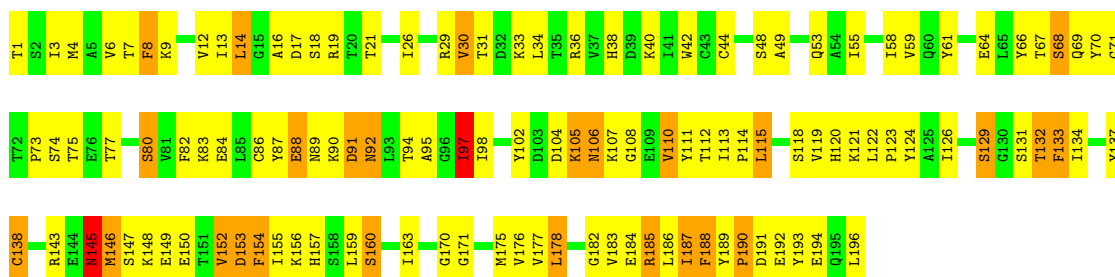
• Molecule 7: PROTEASOME COMPONENT C1

Chain U:



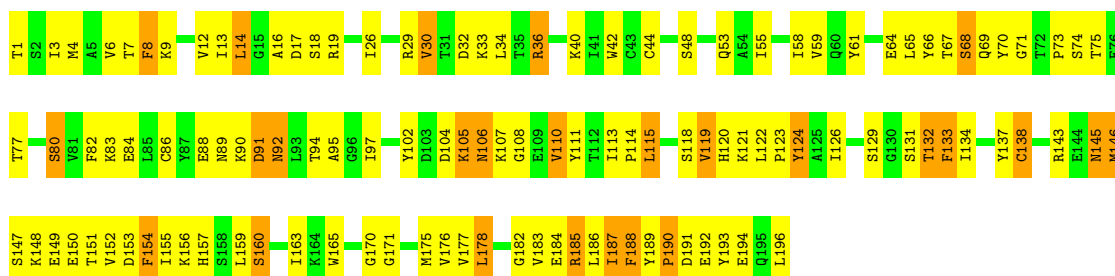
• Molecule 8: PROTEASOME COMPONENT PRE3

Chain H:



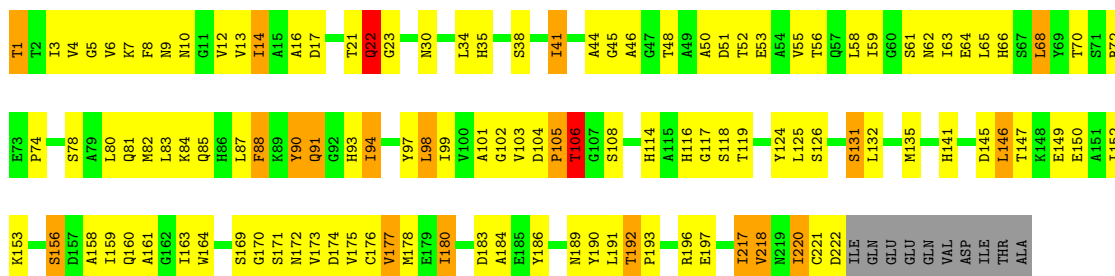
• Molecule 8: PROTEASOME COMPONENT PRE3

Chain V:



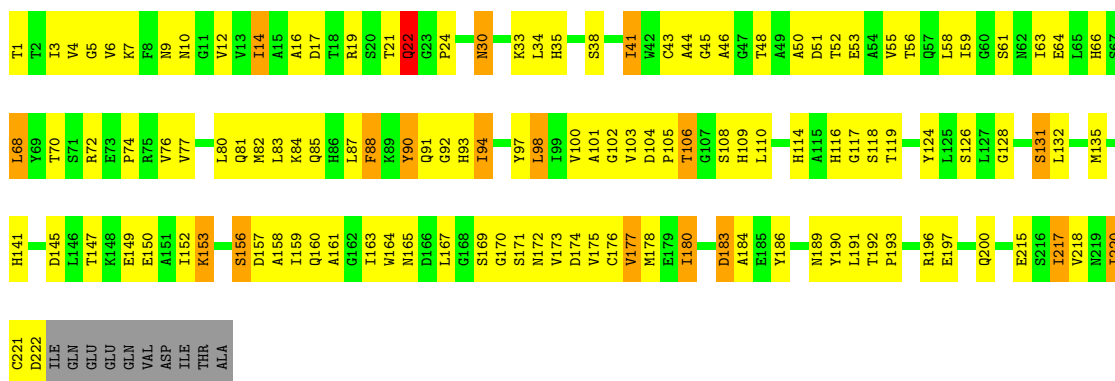
• Molecule 9: PROTEASOME COMPONENT PUP1

Chain I:



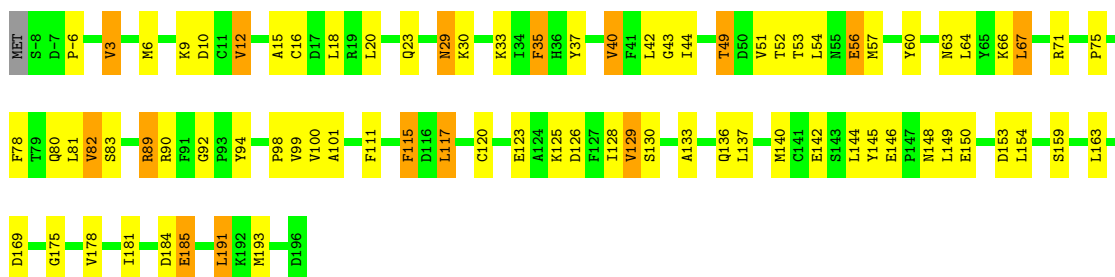
• Molecule 9: PROTEASOME COMPONENT PUP1

Chain W:



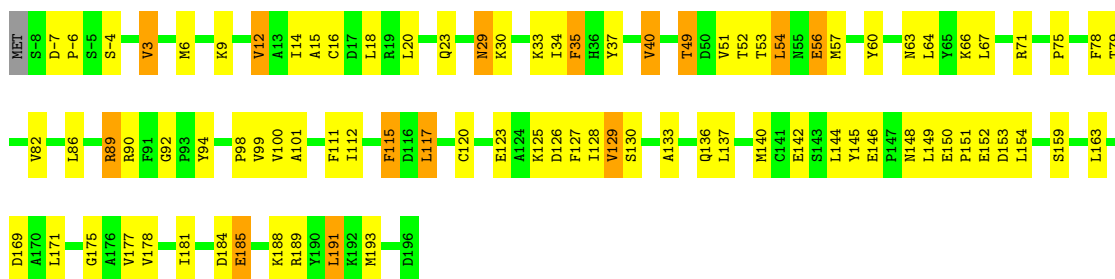
• Molecule 10: PROTEASOME COMPONENT PUP3

Chain J:



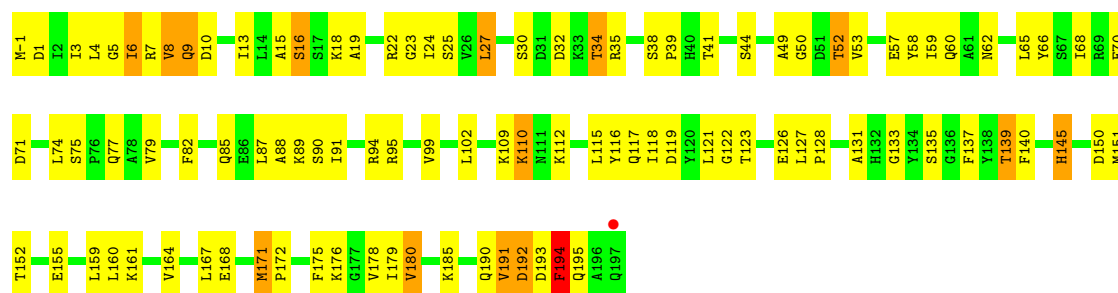
• Molecule 10: PROTEASOME COMPONENT PUP3

Chain X:



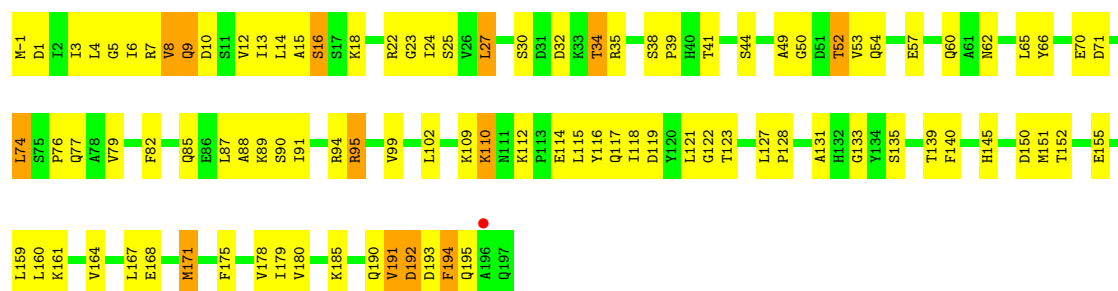
• Molecule 11: PROTEASOME COMPONENT C11

Chain K:



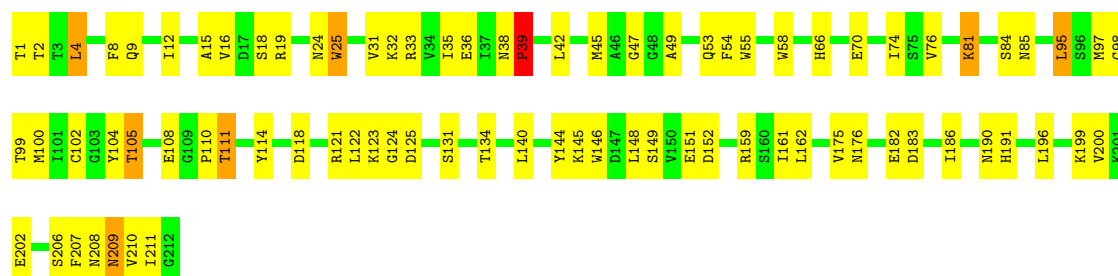
• Molecule 11: PROTEASOME COMPONENT C11

Chain Y:



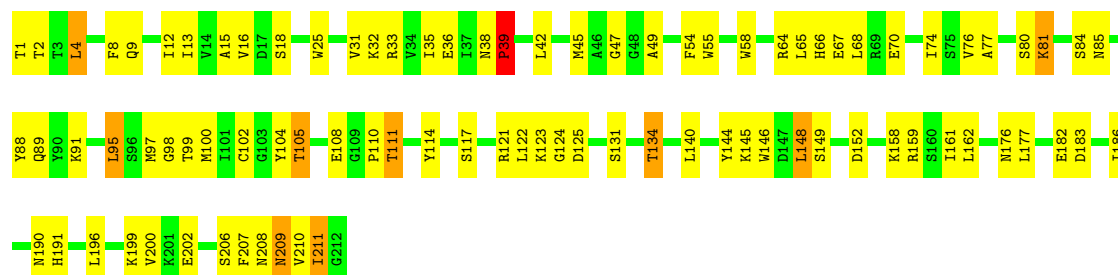
• Molecule 12: PROTEASOME COMPONENT PRE2

Chain L:



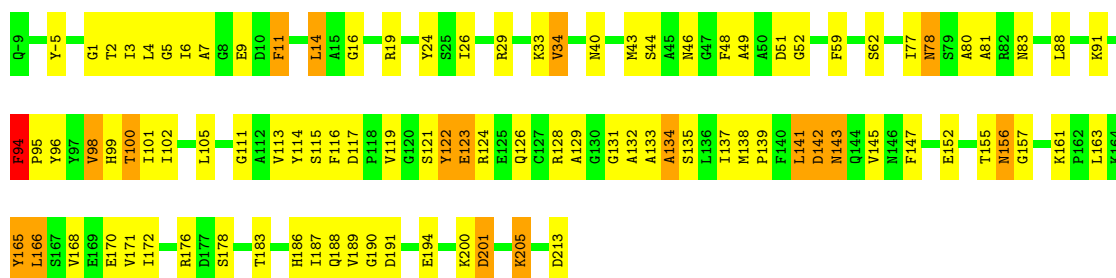
• Molecule 12: PROTEASOME COMPONENT PRE2

Chain Z:



• Molecule 13: PROTEASOME COMPONENT C5

Chain M:

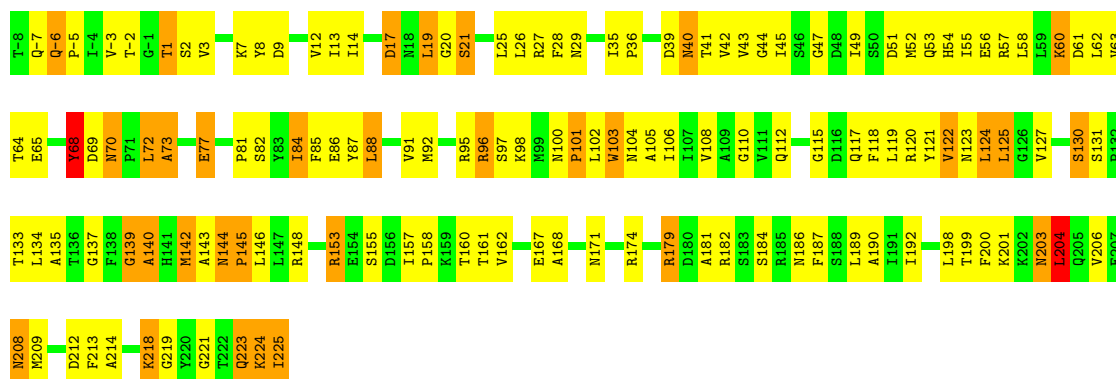


• Molecule 13: PROTEASOME COMPONENT C5

Chain a:

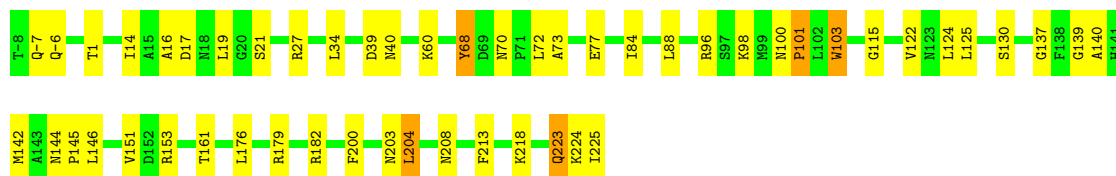
• Molecule 14: PROTEASOME COMPONENT PRE4

Chain N:



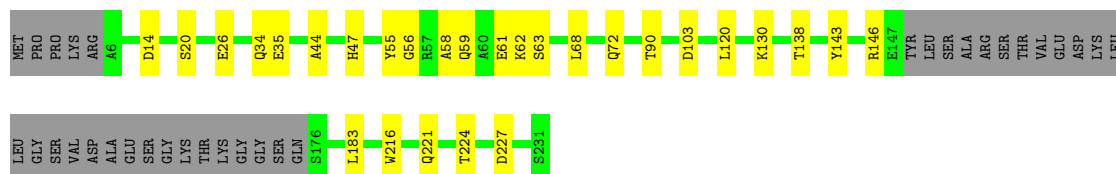
• Molecule 14: PROTEASOME COMPONENT PRE4

Chain b:



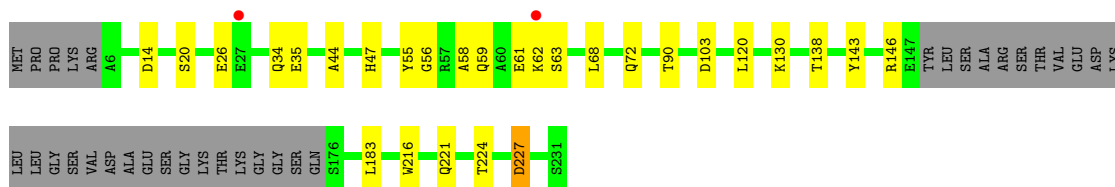
• Molecule 15: PROTEASOME ACTIVATOR PROTEIN PA26

Chain c:



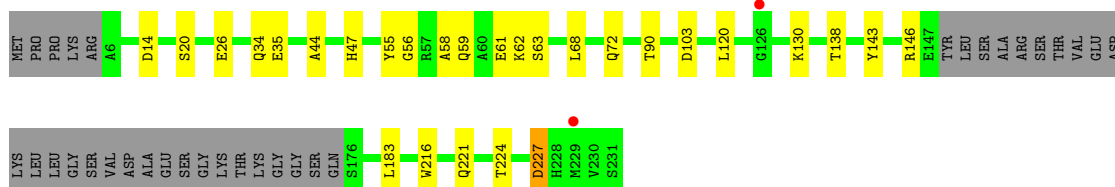
• Molecule 15: PROTEASOME ACTIVATOR PROTEIN PA26

Chain d:



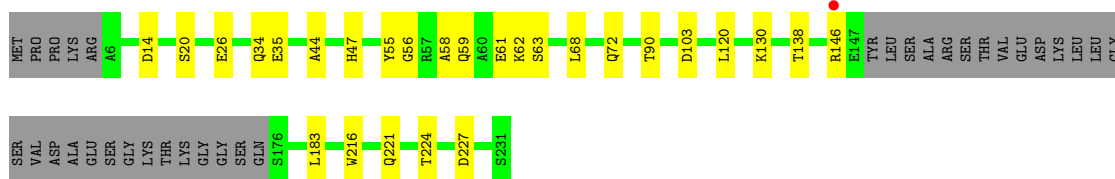
• Molecule 15: PROTEASOME ACTIVATOR PROTEIN PA26

Chain e:



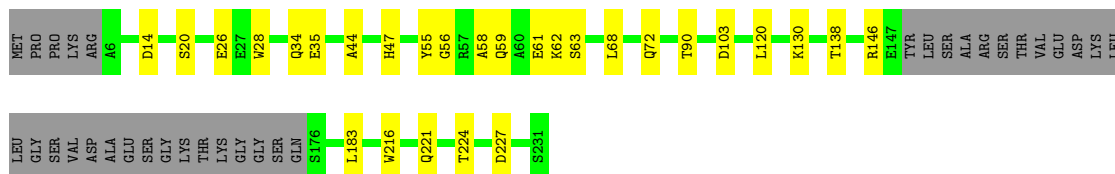
• Molecule 15: PROTEASOME ACTIVATOR PROTEIN PA26

Chain f:



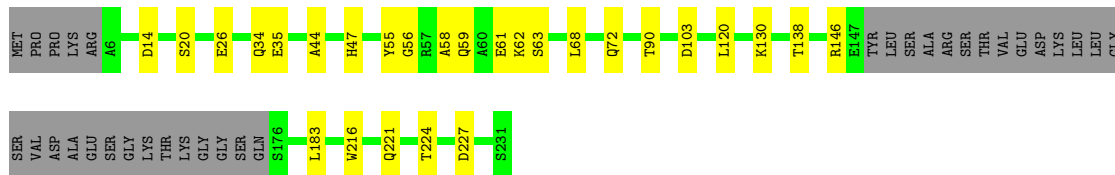
• Molecule 15: PROTEASOME ACTIVATOR PROTEIN PA26

Chain g:



• Molecule 15: PROTEASOME ACTIVATOR PROTEIN PA26

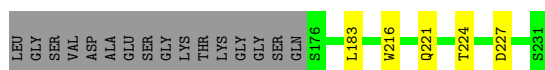
Chain h:



• Molecule 15: PROTEASOME ACTIVATOR PROTEIN PA26

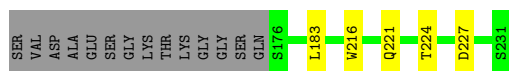
Chain i:





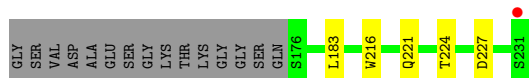
• Molecule 15: PROTEASOME ACTIVATOR PROTEIN PA26

Chain j:



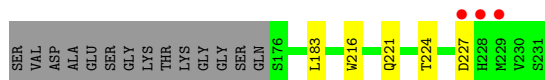
• Molecule 15: PROTEASOME ACTIVATOR PROTEIN PA26

Chain k:



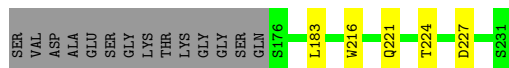
• Molecule 15: PROTEASOME ACTIVATOR PROTEIN PA26

Chain l:



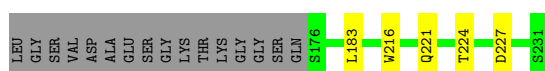
• Molecule 15: PROTEASOME ACTIVATOR PROTEIN PA26

Chain m:



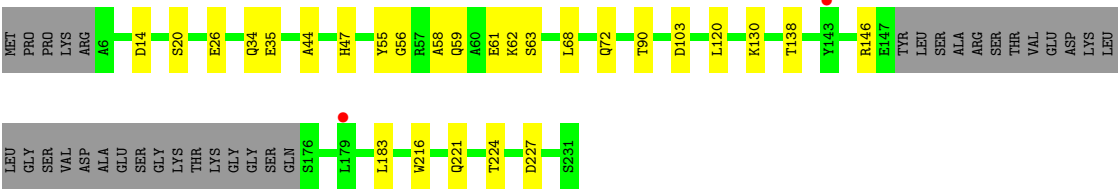
• Molecule 15: PROTEASOME ACTIVATOR PROTEIN PA26

Chain n:



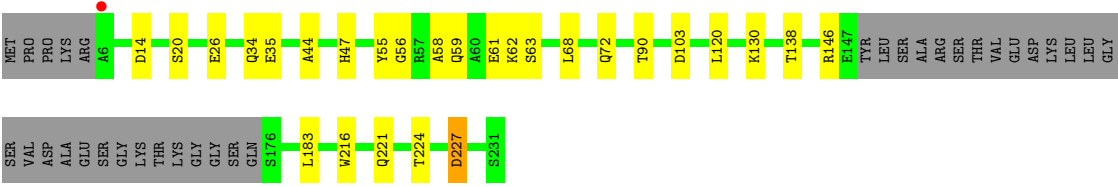
● Molecule 15: PROTEASOME ACTIVATOR PROTEIN PA26

Chain o: 



● Molecule 15: PROTEASOME ACTIVATOR PROTEIN PA26

Chain p: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	192.96Å 232.13Å 296.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.20 39.84 – 3.22	Depositor EDS
% Data completeness (in resolution range)	86.6 (50.00-3.20) 88.2 (39.84-3.22)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 3.25Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.255 , 0.325 0.268 , 0.331	Depositor DCC
R_{free} test set	1028 reflections (0.54%)	DCC
Wilson B-factor (Å ²)	71.3	Xtriage
Anisotropy	0.529	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 45.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 189495 reflections	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	70622	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.14% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.66	0/1918	0.88	1/2597 (0.0%)
1	O	0.63	0/1918	0.88	1/2597 (0.0%)
2	B	0.65	0/1903	0.86	2/2578 (0.1%)
2	P	0.64	0/1903	0.87	1/2578 (0.0%)
3	C	0.66	0/1897	0.88	2/2569 (0.1%)
3	Q	0.68	0/1897	0.88	2/2569 (0.1%)
4	D	0.64	0/1890	0.90	4/2560 (0.2%)
4	R	0.64	0/1890	0.91	5/2560 (0.2%)
5	E	0.68	0/1896	0.84	0/2555
5	S	0.68	1/1896 (0.1%)	0.84	0/2555
6	F	0.59	0/1823	0.82	0/2463
6	T	0.64	0/1823	0.83	0/2463
7	G	0.62	1/1908 (0.1%)	0.80	0/2576
7	U	0.61	0/1908	0.80	0/2576
8	H	0.63	0/1539	0.82	0/2084
8	V	0.62	0/1539	0.81	0/2084
9	I	0.64	1/1715 (0.1%)	0.83	1/2326 (0.0%)
9	W	0.62	0/1715	0.82	0/2326
10	J	0.65	0/1611	0.88	1/2174 (0.0%)
10	X	0.65	0/1611	0.88	1/2174 (0.0%)
11	K	0.70	0/1613	0.84	1/2173 (0.0%)
11	Y	0.68	0/1613	0.84	1/2173 (0.0%)
12	L	0.67	0/1683	0.87	0/2277
12	Z	0.66	0/1683	0.87	0/2277
13	M	0.65	0/1795	0.87	1/2420 (0.0%)
13	a	0.68	0/1795	0.86	1/2420 (0.0%)
14	N	0.63	0/1855	0.88	1/2514 (0.0%)
14	b	0.65	0/1855	0.88	3/2514 (0.1%)
15	c	0.63	0/1551	0.78	1/2099 (0.0%)
15	d	0.64	0/1551	0.79	1/2099 (0.0%)
15	e	0.64	0/1551	0.79	1/2099 (0.0%)
15	f	0.63	0/1551	0.80	1/2099 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
15	g	0.67	1/1551 (0.1%)	0.79	1/2099 (0.0%)
15	h	0.62	0/1551	0.79	1/2099 (0.0%)
15	i	0.62	0/1551	0.80	1/2099 (0.0%)
15	j	0.63	0/1551	0.78	1/2099 (0.0%)
15	k	0.63	0/1551	0.79	1/2099 (0.0%)
15	l	0.63	0/1551	0.79	1/2099 (0.0%)
15	m	0.62	0/1551	0.79	1/2099 (0.0%)
15	n	0.61	0/1551	0.78	1/2099 (0.0%)
15	o	0.61	0/1551	0.79	1/2099 (0.0%)
15	p	0.63	0/1551	0.79	1/2099 (0.0%)
All	All	0.64	4/71806 (0.0%)	0.84	43/97118 (0.0%)

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
3	C	0	1
3	Q	0	1
9	I	0	1
9	W	0	1
13	M	0	1
13	a	0	2
14	N	0	1
14	b	0	1
All	All	0	9

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	S	76	CYS	CB-SG	-5.85	1.72	1.81
7	G	75	CYS	CB-SG	-5.72	1.72	1.81
9	I	1	THR	CA-CB	5.43	1.67	1.53
15	g	28	TRP	CB-CG	-5.12	1.41	1.50

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	J	92	GLY	N-CA-C	-7.82	93.56	113.10
10	X	92	GLY	N-CA-C	-7.59	94.13	113.10
4	D	52	LEU	CA-CB-CG	6.98	131.35	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	R	52	LEU	CA-CB-CG	6.87	131.10	115.30
4	R	8	LEU	N-CA-C	6.38	128.21	111.00
4	D	8	LEU	N-CA-C	6.35	128.14	111.00
15	l	56	GLY	N-CA-C	-6.27	97.43	113.10
14	b	34	LEU	CA-CB-CG	6.11	129.34	115.30
15	k	56	GLY	N-CA-C	-6.04	98.00	113.10
15	e	56	GLY	N-CA-C	-6.00	98.11	113.10
15	i	56	GLY	N-CA-C	-5.99	98.12	113.10
15	p	56	GLY	N-CA-C	-5.97	98.18	113.10
15	o	56	GLY	N-CA-C	-5.90	98.35	113.10
15	g	56	GLY	N-CA-C	-5.86	98.44	113.10
4	D	17	ILE	N-CA-C	-5.84	95.23	111.00
15	n	56	GLY	N-CA-C	-5.81	98.58	113.10
15	d	56	GLY	N-CA-C	-5.79	98.63	113.10
15	h	56	GLY	N-CA-C	-5.72	98.79	113.10
4	R	17	ILE	N-CA-C	-5.69	95.64	111.00
15	j	56	GLY	N-CA-C	-5.68	98.90	113.10
11	K	99	VAL	CB-CA-C	-5.66	100.65	111.40
15	m	56	GLY	N-CA-C	-5.59	99.14	113.10
13	a	94	PHE	N-CA-C	-5.55	96.02	111.00
4	R	200	LEU	CA-CB-CG	-5.51	102.62	115.30
9	I	23	GLY	N-CA-C	-5.49	99.37	113.10
2	B	40	THR	N-CA-C	5.48	125.80	111.00
11	Y	99	VAL	CB-CA-C	-5.44	101.07	111.40
15	c	56	GLY	N-CA-C	-5.44	99.51	113.10
3	C	53	THR	N-CA-C	5.43	125.66	111.00
15	f	56	GLY	N-CA-C	-5.43	99.53	113.10
3	Q	53	THR	N-CA-C	5.32	125.35	111.00
1	A	215	GLY	N-CA-C	-5.29	99.86	113.10
2	P	40	THR	N-CA-C	5.28	125.27	111.00
3	C	7	ASP	N-CA-C	5.22	125.10	111.00
4	D	200	LEU	CA-CB-CG	-5.22	103.30	115.30
1	O	215	GLY	N-CA-C	-5.21	100.06	113.10
2	B	64	VAL	N-CA-C	-5.13	97.16	111.00
14	b	115	GLY	N-CA-C	5.09	125.82	113.10
14	b	204	LEU	CA-CB-CG	5.05	126.92	115.30
3	Q	7	ASP	N-CA-C	5.05	124.63	111.00
14	N	204	LEU	CA-CB-CG	5.03	126.87	115.30
13	M	94	PHE	N-CA-C	-5.02	97.45	111.00
4	R	124	GLY	N-CA-C	-5.01	100.57	113.10

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	20	TYR	Sidechain
9	I	190	TYR	Sidechain
13	M	165	TYR	Sidechain
14	N	68	TYR	Sidechain
3	Q	20	TYR	Sidechain
9	W	190	TYR	Sidechain
13	a	-5	TYR	Sidechain
13	a	122	TYR	Sidechain
14	b	68	TYR	Sidechain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1881	0	1876	179	0
1	O	1881	0	1876	185	0
2	B	1868	0	1866	121	0
2	P	1868	0	1866	120	0
3	C	1868	0	1860	112	0
3	Q	1868	0	1860	110	0
4	D	1862	0	1866	88	0
4	R	1862	0	1866	82	0
5	E	1871	0	1840	91	0
5	S	1871	0	1840	85	0
6	F	1795	0	1797	107	0
6	T	1795	0	1797	101	0
7	G	1869	0	1864	138	0
7	U	1869	0	1864	139	0
8	H	1510	0	1476	121	0
8	V	1510	0	1476	115	0
9	I	1684	0	1688	84	0
9	W	1684	0	1688	104	0
10	J	1581	0	1574	65	0
10	X	1581	0	1574	68	0
11	K	1585	0	1590	79	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	Y	1585	0	1590	73	0
12	L	1646	0	1595	52	0
12	Z	1646	0	1595	68	0
13	M	1757	0	1711	74	0
13	a	1757	0	1710	0	0
14	N	1824	0	1832	124	0
14	b	1824	0	1832	0	0
15	c	1529	0	1545	0	0
15	d	1529	0	1545	0	0
15	e	1529	0	1545	0	0
15	f	1529	0	1545	0	0
15	g	1529	0	1545	0	0
15	h	1529	0	1545	0	0
15	i	1529	0	1545	0	0
15	j	1529	0	1545	0	0
15	k	1529	0	1545	0	0
15	l	1529	0	1545	0	0
15	m	1529	0	1545	0	0
15	n	1529	0	1545	0	0
15	o	1529	0	1545	0	0
15	p	1529	0	1545	0	0
16	G	1	0	0	0	0
16	H	1	0	0	0	0
16	I	1	0	0	0	0
16	J	2	0	0	0	0
16	L	1	0	0	0	0
16	M	1	0	0	0	0
16	U	1	0	0	0	0
16	V	1	0	0	0	0
16	W	1	0	0	0	0
16	X	2	0	0	0	0
16	Z	1	0	0	0	0
16	a	1	0	0	0	0
All	All	70622	0	70499	2521	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 30.

All (2521) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:46:ALA:HB2	2:B:211:LEU:HD12	1.34	1.10
2:P:46:ALA:HB2	2:P:211:LEU:HD12	1.37	1.05

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
8:H:13:ILE:HG12	8:H:177:VAL:HA	1.41	1.03
9:I:103:VAL:HG12	9:I:108:SER:HA	1.39	1.00
8:H:107:LYS:HD2	8:H:108:GLY:H	1.26	0.96
8:V:107:LYS:HD2	8:V:108:GLY:H	1.29	0.96
8:V:13:ILE:HG12	8:V:177:VAL:HA	1.44	0.95
7:U:143:ASN:H	7:U:143:ASN:HD22	1.10	0.95
9:W:22:GLN:HA	9:W:22:GLN:HE21	1.31	0.94
7:G:143:ASN:HD22	7:G:143:ASN:H	1.10	0.94
14:N:72:LEU:HD12	14:N:72:LEU:H	1.33	0.94
3:C:185:LYS:HZ2	3:C:187:ASP:H	1.11	0.94
3:C:96:GLN:HE22	10:J:63:ASN:HD22	1.15	0.94
3:Q:185:LYS:HZ2	3:Q:187:ASP:H	1.17	0.93
9:W:103:VAL:HG12	9:W:108:SER:HA	1.50	0.93
14:N:40:ASN:HD22	14:N:40:ASN:H	1.12	0.93
9:I:22:GLN:HE21	9:I:22:GLN:HA	1.33	0.93
9:W:6:VAL:HG12	9:W:124:TYR:HB3	1.51	0.93
14:N:104:ASN:HB3	14:N:106:ILE:HD11	1.51	0.92
9:I:6:VAL:HG12	9:I:124:TYR:HB3	1.51	0.91
13:M:147:PHE:HE2	13:M:163:LEU:HA	1.37	0.90
7:U:77:TYR:CE1	7:U:84:GLY:HA3	2.05	0.90
2:P:222:LEU:HD11	2:P:232:GLY:HA2	1.53	0.89
6:T:179:PHE:HA	6:T:182:ILE:HG13	1.53	0.89
2:B:222:LEU:HD11	2:B:232:GLY:HA2	1.52	0.89
12:L:105:THR:HG23	12:L:108:GLU:HB2	1.52	0.89
3:Q:96:GLN:HE22	10:X:63:ASN:HD22	1.18	0.87
4:D:162:GLN:HE21	4:D:163:THR:H	1.22	0.87
11:K:167:LEU:O	11:K:171:MET:HB2	1.74	0.87
1:O:146:VAL:HG22	1:O:152:PRO:HA	1.58	0.86
7:U:72:HIS:HD2	7:U:73:ILE:HG13	1.41	0.85
6:F:100:ASN:HB2	14:N:86:GLU:HG2	1.56	0.85
6:T:215:ILE:HG13	6:T:216:VAL:N	1.92	0.85
1:A:33:LYS:H	1:A:33:LYS:HD2	1.41	0.85
8:V:8:PHE:HE2	8:V:148:LYS:HA	1.41	0.84
4:D:192:VAL:O	4:D:196:VAL:HG23	1.75	0.84
1:A:124:LEU:HA	1:A:127:ILE:HD12	1.60	0.84
12:Z:105:THR:HG23	12:Z:108:GLU:HB2	1.57	0.84
4:R:133:THR:HG23	4:R:150:THR:HG23	1.58	0.84
12:Z:47:GLY:HA3	12:Z:97:MET:HA	1.60	0.84
8:H:8:PHE:HE2	8:H:148:LYS:HA	1.43	0.84
2:B:187:ASP:O	2:B:191:ILE:HG12	1.77	0.84
7:G:72:HIS:HD2	7:G:73:ILE:HG13	1.41	0.83
14:N:60:LYS:O	14:N:64:THR:HG23	1.79	0.83

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:O:44:ALA:HB2	1:O:53:VAL:HG12	1.57	0.83
6:F:179:PHE:HA	6:F:182:ILE:HG13	1.59	0.83
8:H:13:ILE:HD13	8:H:177:VAL:HG22	1.61	0.83
1:A:146:VAL:HG22	1:A:152:PRO:HA	1.58	0.83
11:Y:167:LEU:O	11:Y:171:MET:HB2	1.78	0.82
7:G:150:LEU:HD12	7:G:151:GLU:N	1.94	0.82
8:H:59:VAL:HG11	8:H:82:PHE:HE2	1.45	0.82
1:A:44:ALA:HB2	1:A:53:VAL:HG12	1.61	0.82
6:T:155:GLU:HB3	7:U:63:ASN:HD21	1.45	0.81
8:V:59:VAL:HG11	8:V:82:PHE:HE2	1.46	0.81
4:R:192:VAL:O	4:R:196:VAL:HG23	1.80	0.81
1:O:33:LYS:H	1:O:33:LYS:HD2	1.44	0.81
4:D:133:THR:HG23	4:D:150:THR:HG23	1.60	0.81
6:F:6:TYR:CD1	6:F:15:PRO:HD3	2.16	0.80
7:G:30:VAL:HG11	7:G:134:SER:HB2	1.63	0.80
6:F:155:GLU:HB3	7:G:63:ASN:HD21	1.46	0.80
7:U:30:VAL:HG11	7:U:134:SER:HB2	1.64	0.80
4:R:228:GLU:HA	4:R:231:GLN:HE21	1.47	0.80
14:N:49:ILE:HG22	14:N:53:GLN:HE21	1.47	0.80
14:N:153:ARG:HG3	14:N:153:ARG:HH11	1.46	0.80
1:O:124:LEU:HA	1:O:127:ILE:HD12	1.65	0.80
1:O:68:THR:HG21	7:U:158:GLY:HA3	1.62	0.79
13:M:147:PHE:CE2	13:M:163:LEU:HA	2.17	0.79
4:R:162:GLN:HE21	4:R:163:THR:H	1.31	0.79
1:A:68:THR:HG21	7:G:158:GLY:HA3	1.62	0.79
7:G:143:ASN:H	7:G:143:ASN:ND2	1.81	0.79
1:A:45:VAL:HG12	1:A:168:ALA:HB1	1.63	0.79
6:T:227:GLY:O	6:T:230:VAL:HG22	1.82	0.79
4:D:228:GLU:HA	4:D:231:GLN:NE2	1.98	0.79
7:G:198:ILE:HA	7:G:201:LEU:HD22	1.63	0.79
6:T:6:TYR:CD1	6:T:15:PRO:HD3	2.18	0.79
4:D:228:GLU:HA	4:D:231:GLN:HE21	1.46	0.79
8:V:13:ILE:HD13	8:V:177:VAL:HG22	1.64	0.78
7:U:199:ILE:HG21	7:U:213:LEU:HD13	1.66	0.78
9:W:22:GLN:HA	9:W:22:GLN:NE2	1.98	0.78
1:O:183:GLU:HB3	1:O:187:LYS:NZ	1.99	0.78
7:U:198:ILE:HA	7:U:201:LEU:HD22	1.64	0.78
2:P:187:ASP:O	2:P:191:ILE:HG12	1.83	0.78
2:B:68:THR:HG23	2:B:71:ILE:HB	1.65	0.78
7:U:150:LEU:HD12	7:U:151:GLU:N	1.98	0.78
7:G:71:ARG:CZ	14:N:64:THR:HG22	2.14	0.78
1:A:54:ILE:HA	1:A:225:VAL:HG22	1.65	0.78

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
12:L:47:GLY:HA3	12:L:97:MET:HA	1.66	0.78
6:F:215:ILE:HG13	6:F:216:VAL:N	1.99	0.77
8:H:156:LYS:HZ3	8:H:188:PHE:HD1	1.32	0.77
5:S:136:ARG:HB2	5:S:137:PRO:HD2	1.65	0.77
7:U:143:ASN:H	7:U:143:ASN:ND2	1.83	0.77
10:J:78:PHE:O	10:J:82:VAL:HG12	1.84	0.77
1:O:181:ASN:HB3	1:O:209:HIS:CE1	2.20	0.77
9:I:22:GLN:NE2	9:I:22:GLN:HA	2.00	0.77
7:G:77:TYR:CE1	7:G:84:GLY:HA3	2.20	0.77
5:E:136:ARG:HB2	5:E:137:PRO:HD2	1.67	0.77
4:R:11:PHE:H	5:S:23:GLN:HE22	1.33	0.76
6:F:227:GLY:O	6:F:230:VAL:HG22	1.84	0.76
9:W:64:GLU:O	9:W:68:LEU:HD12	1.85	0.76
10:X:78:PHE:O	10:X:82:VAL:HG12	1.85	0.76
3:Q:169:THR:O	3:Q:173:GLN:HB2	1.84	0.76
8:H:114:PRO:HD2	8:H:118:SER:O	1.85	0.76
3:C:150:THR:HG21	3:C:160:TRP:HE1	1.50	0.76
8:H:17:ASP:HB2	8:H:170:GLY:O	1.86	0.76
2:B:110:LEU:O	2:B:114:VAL:HG23	1.86	0.76
4:D:162:GLN:NE2	4:D:163:THR:H	1.83	0.76
4:R:228:GLU:HA	4:R:231:GLN:NE2	2.00	0.76
1:A:181:ASN:HB3	1:A:209:HIS:CE1	2.21	0.76
7:G:199:ILE:HG21	7:G:213:LEU:HD13	1.68	0.76
5:E:142:LEU:HB2	5:E:158:ALA:HB3	1.68	0.76
3:Q:150:THR:HG21	3:Q:160:TRP:HE1	1.49	0.76
8:V:111:TYR:HA	8:V:120:HIS:O	1.86	0.75
7:G:171:ALA:O	7:G:175:LEU:HG	1.84	0.75
1:O:45:VAL:HG12	1:O:168:ALA:HB1	1.69	0.75
10:J:184:ASP:CG	10:J:185:GLU:H	1.90	0.75
8:H:67:THR:HG22	8:H:73:PRO:HD3	1.69	0.75
5:E:76:CYS:SG	5:E:142:LEU:HD22	2.26	0.75
14:N:179:ARG:HA	8:V:26:ILE:HD12	1.67	0.75
14:N:8:TYR:HB2	14:N:160:THR:O	1.86	0.75
8:V:114:PRO:HD2	8:V:118:SER:O	1.87	0.75
8:H:7:THR:HG22	8:H:12:VAL:HB	1.69	0.75
8:V:17:ASP:HB2	8:V:170:GLY:O	1.87	0.75
14:N:35:ILE:HG12	14:N:56:GLU:HG2	1.68	0.74
11:K:52:THR:HG23	11:K:53:VAL:H	1.51	0.74
6:T:50:LYS:HE2	6:T:212:SER:HB2	1.67	0.74
4:R:162:GLN:HE22	4:R:172:ARG:HE	1.35	0.74
6:F:121:GLN:HE22	7:G:86:HIS:HD2	1.35	0.74
2:B:244:ASN:O	2:B:247:LEU:HB3	1.88	0.74

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:197:LYS:HA	2:B:204:PHE:CE1	2.21	0.74
2:P:197:LYS:HA	2:P:204:PHE:CE1	2.23	0.74
7:G:40:LYS:HA	7:G:45:VAL:HG12	1.67	0.74
8:V:156:LYS:HZ3	8:V:188:PHE:HD1	1.33	0.74
7:G:231:LYS:HA	7:G:235:LEU:HD22	1.69	0.74
8:H:107:LYS:CD	8:H:108:GLY:H	2.00	0.74
7:G:150:LEU:HD12	7:G:151:GLU:H	1.52	0.74
1:O:234:PHE:HD1	1:O:234:PHE:H	1.36	0.74
8:H:122:LEU:HD11	14:N:28:PHE:HE1	1.53	0.73
8:V:185:ARG:HG3	8:V:185:ARG:HH11	1.53	0.73
5:S:109:VAL:HB	5:S:154:GLN:NE2	2.03	0.73
14:N:91:VAL:O	14:N:95:ARG:HG2	1.88	0.73
13:M:7:ALA:HB2	13:M:113:VAL:HG23	1.70	0.73
6:F:50:LYS:HE2	6:F:212:SER:HB2	1.68	0.73
5:E:170:LYS:HD2	5:E:171:ALA:H	1.52	0.73
8:H:59:VAL:HG11	8:H:82:PHE:CE2	2.23	0.73
8:V:59:VAL:HG11	8:V:82:PHE:CE2	2.22	0.73
12:Z:66:HIS:HD2	12:Z:74:ILE:HB	1.53	0.73
1:A:234:PHE:HD1	1:A:234:PHE:H	1.37	0.73
10:X:133:ALA:HB2	10:X:169:ASP:HB2	1.68	0.73
7:U:171:ALA:O	7:U:175:LEU:HG	1.87	0.73
8:H:155:ILE:HG21	8:H:175:MET:SD	2.28	0.73
8:V:67:THR:HA	8:V:71:GLY:O	1.89	0.73
11:Y:52:THR:HG23	11:Y:53:VAL:H	1.54	0.73
7:G:109:PRO:HA	7:G:148:TYR:OH	1.89	0.73
4:D:73:LEU:HD12	4:D:135:ILE:HG12	1.70	0.72
1:O:199:TRP:O	1:O:203:VAL:HG23	1.89	0.72
2:B:40:THR:HG23	2:B:183:LEU:O	1.89	0.72
1:O:225:VAL:O	1:O:236:LEU:HB2	1.89	0.72
8:H:1:THR:HA	8:H:33:LYS:NZ	2.04	0.72
1:O:54:ILE:HA	1:O:225:VAL:HG22	1.69	0.72
8:H:177:VAL:HB	8:H:184:GLU:HB3	1.70	0.72
8:H:111:TYR:HA	8:H:120:HIS:O	1.89	0.72
3:Q:201:THR:HG22	3:Q:203:SER:H	1.53	0.72
7:G:187:SER:OG	7:G:190:GLU:HB2	1.90	0.72
5:S:142:LEU:HB2	5:S:158:ALA:HB3	1.72	0.72
4:D:46:CYS:HB3	4:D:63:LYS:HD2	1.72	0.72
4:R:46:CYS:HB3	4:R:63:LYS:HD2	1.72	0.72
14:N:121:TYR:HE1	14:N:123:ASN:HD22	1.34	0.71
7:U:150:LEU:HD12	7:U:151:GLU:H	1.55	0.71
2:P:68:THR:HG23	2:P:71:ILE:HB	1.71	0.71
1:A:225:VAL:O	1:A:236:LEU:HB2	1.89	0.71

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:G:72:HIS:CD2	7:G:73:ILE:HG13	2.25	0.71
9:I:160:GLN:O	9:I:164:TRP:HD1	1.73	0.71
8:H:40:LYS:NZ	8:H:182:GLY:HA2	2.05	0.71
3:Q:187:ASP:HA	3:Q:190:ILE:HD12	1.71	0.71
14:N:104:ASN:HB3	14:N:106:ILE:CD1	2.20	0.71
2:B:222:LEU:HD11	2:B:232:GLY:CA	2.20	0.71
6:T:78:ALA:HB3	6:T:79:PRO:HD3	1.71	0.71
5:S:8:TYR:O	5:S:9:ASP:HB2	1.90	0.71
6:F:185:ASN:HD22	6:F:185:ASN:C	1.93	0.71
2:P:244:ASN:O	2:P:247:LEU:HB3	1.91	0.71
9:W:163:ILE:HG23	9:W:170:GLY:HA2	1.72	0.71
1:A:53:VAL:O	1:A:225:VAL:HG13	1.91	0.71
5:S:31:ILE:HD13	5:S:141:ALA:HB2	1.72	0.71
14:N:19:LEU:HB2	14:N:184:SER:HB2	1.72	0.71
8:V:1:THR:HA	8:V:33:LYS:NZ	2.06	0.71
9:I:64:GLU:O	9:I:68:LEU:HD12	1.91	0.71
1:A:126:GLN:HE21	1:A:127:ILE:N	1.89	0.71
5:S:76:CYS:SG	5:S:142:LEU:HD22	2.31	0.71
7:U:40:LYS:HA	7:U:45:VAL:HG12	1.72	0.71
8:V:107:LYS:CD	8:V:108:GLY:H	2.01	0.71
8:V:7:THR:HG22	8:V:12:VAL:HB	1.73	0.71
3:C:170:SER:O	3:C:174:THR:HG23	1.91	0.71
1:O:129:THR:HG22	2:P:128:ARG:HH21	1.55	0.70
1:A:183:GLU:HB3	1:A:187:LYS:NZ	2.05	0.70
10:J:52:THR:O	10:J:56:GLU:HG2	1.91	0.70
10:X:184:ASP:CG	10:X:185:GLU:H	1.94	0.70
7:U:94:GLU:HG2	7:U:114:ARG:HD2	1.73	0.70
14:N:36:PRO:HA	14:N:42:VAL:HA	1.72	0.70
4:D:162:GLN:HE22	4:D:172:ARG:HE	1.39	0.70
1:A:22:GLU:HA	2:B:26:THR:HG21	1.72	0.70
3:C:201:THR:HG22	3:C:203:SER:H	1.55	0.70
2:P:222:LEU:HD11	2:P:232:GLY:CA	2.21	0.70
6:T:121:GLN:HE22	7:U:86:HIS:HD2	1.39	0.70
10:J:133:ALA:HB2	10:J:169:ASP:HB2	1.71	0.70
11:Y:191:VAL:HG12	11:Y:191:VAL:O	1.92	0.70
7:U:187:SER:OG	7:U:190:GLU:HB2	1.91	0.70
3:C:187:ASP:HA	3:C:190:ILE:HD12	1.71	0.70
7:U:34:THR:O	7:U:165:GLY:HA3	1.91	0.70
1:A:113:PRO:HD2	1:A:116:VAL:HG21	1.73	0.70
7:G:143:ASN:HD22	7:G:143:ASN:N	1.87	0.70
8:H:13:ILE:CD1	8:H:177:VAL:HG22	2.21	0.70
5:E:12:VAL:H	5:E:23:GLN:HG3	1.57	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:131:PHE:O	3:C:153:PRO:HB3	1.92	0.70
7:U:49:VAL:HG22	7:U:50:GLU:H	1.57	0.70
8:H:107:LYS:HD2	8:H:108:GLY:N	2.05	0.69
8:H:185:ARG:HH11	8:H:185:ARG:HG3	1.57	0.69
7:U:9:LEU:HD12	7:U:9:LEU:H	1.56	0.69
2:P:44:VAL:HA	2:P:213:ILE:HG22	1.74	0.69
4:R:162:GLN:NE2	4:R:163:THR:H	1.89	0.69
9:I:58:LEU:O	9:I:61:SER:HB3	1.91	0.69
7:U:72:HIS:CD2	7:U:73:ILE:HG13	2.26	0.69
1:O:113:PRO:HD2	1:O:116:VAL:HG21	1.75	0.69
10:J:146:GLU:HB3	10:J:149:LEU:HD21	1.75	0.69
7:G:30:VAL:CG1	7:G:134:SER:HB2	2.23	0.69
2:B:227:ILE:HG12	9:I:186:TYR:HD2	1.58	0.69
1:A:205:PHE:O	1:A:208:THR:HB	1.91	0.69
10:X:146:GLU:HB3	10:X:149:LEU:HD21	1.74	0.69
5:E:8:TYR:O	5:E:9:ASP:HB2	1.92	0.69
3:Q:170:SER:O	3:Q:174:THR:HG23	1.93	0.69
11:Y:-1:MET:SD	11:Y:133:GLY:HA3	2.32	0.69
3:C:169:THR:O	3:C:173:GLN:HB2	1.92	0.69
6:T:33:SER:HB3	6:T:62:LYS:NZ	2.06	0.69
13:M:14:LEU:HD13	13:M:34:VAL:HG13	1.75	0.69
6:F:78:ALA:HB3	6:F:79:PRO:HD3	1.74	0.69
5:S:170:LYS:HD2	5:S:171:ALA:H	1.57	0.69
5:S:209:GLU:HB3	5:S:210:GLU:OE2	1.92	0.69
2:B:66:LEU:HD13	2:B:235:PHE:CD1	2.28	0.69
7:G:243:GLN:O	7:G:246:ILE:HG22	1.92	0.68
8:V:40:LYS:NZ	8:V:182:GLY:HA2	2.08	0.68
1:A:203:VAL:O	1:A:207:ILE:HG13	1.94	0.68
4:R:64:VAL:HG11	4:R:213:THR:HG21	1.75	0.68
3:Q:131:PHE:O	3:Q:153:PRO:HB3	1.93	0.68
1:O:203:VAL:O	1:O:207:ILE:HG13	1.93	0.68
11:K:-1:MET:SD	11:K:133:GLY:HA3	2.33	0.68
1:A:137:LEU:HD23	1:A:137:LEU:N	2.07	0.68
2:B:118:MET:SD	2:B:152:PRO:HA	2.34	0.68
5:E:142:LEU:HB3	5:E:144:ILE:CD1	2.23	0.68
9:I:163:ILE:HG23	9:I:170:GLY:HA2	1.76	0.68
4:R:73:LEU:HD12	4:R:135:ILE:HG12	1.74	0.68
1:O:16:ILE:HG22	1:O:17:THR:N	2.09	0.68
6:T:2:PHE:CD1	6:T:3:ARG:HG2	2.29	0.68
7:G:49:VAL:HG22	7:G:50:GLU:H	1.59	0.68
14:N:57:ARG:HG2	14:N:57:ARG:HH11	1.58	0.68
1:O:25:LEU:O	1:O:28:VAL:HG22	1.94	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:P:111:VAL:HG12	2:P:156:TYR:HD2	1.57	0.68
7:U:231:LYS:HA	7:U:235:LEU:HD22	1.76	0.68
12:Z:35:ILE:HD11	12:Z:45:MET:CE	2.23	0.68
4:R:203:VAL:HG21	4:R:210:ILE:HD11	1.75	0.68
14:N:224:LYS:HG3	14:N:225:ILE:H	1.59	0.68
5:E:209:GLU:HB3	5:E:210:GLU:OE2	1.93	0.67
6:F:113:CYS:SG	6:F:151:GLY:O	2.50	0.67
1:O:234:PHE:HD1	1:O:234:PHE:N	1.92	0.67
10:X:52:THR:O	10:X:56:GLU:HG2	1.94	0.67
13:M:187:ILE:HD11	9:W:24:PRO:HA	1.76	0.67
6:T:185:ASN:HD22	6:T:185:ASN:C	1.97	0.67
1:O:205:PHE:O	1:O:208:THR:HB	1.94	0.67
7:U:30:VAL:CG1	7:U:134:SER:HB2	2.24	0.67
8:H:126:ILE:HD12	8:H:134:ILE:HG13	1.77	0.67
9:W:160:GLN:O	9:W:164:TRP:HD1	1.78	0.67
2:P:95:THR:HA	2:P:99:ARG:HD2	1.77	0.67
8:V:107:LYS:HD2	8:V:108:GLY:N	2.07	0.67
14:N:40:ASN:H	14:N:40:ASN:ND2	1.90	0.67
10:J:129:VAL:HB	10:J:137:LEU:HD13	1.76	0.67
9:I:172:ASN:OD1	9:I:192:THR:HG22	1.92	0.67
7:U:109:PRO:HA	7:U:148:TYR:OH	1.94	0.67
7:U:143:ASN:HD22	7:U:143:ASN:N	1.89	0.67
8:H:67:THR:HA	8:H:71:GLY:O	1.93	0.67
7:U:243:GLN:O	7:U:246:ILE:HG22	1.95	0.67
1:A:240:ASN:H	1:A:240:ASN:ND2	1.93	0.67
3:C:58:GLU:HG2	3:C:59:GLN:H	1.58	0.67
6:T:113:CYS:SG	6:T:151:GLY:O	2.47	0.67
9:W:22:GLN:CA	9:W:22:GLN:HE21	2.06	0.67
14:N:181:ALA:HA	8:V:19:ARG:HH12	1.60	0.67
8:V:8:PHE:CE2	8:V:148:LYS:HA	2.28	0.67
1:A:199:TRP:O	1:A:203:VAL:HG23	1.95	0.67
4:R:37:LYS:HE2	4:R:160:SER:HA	1.77	0.67
10:X:29:ASN:O	10:X:30:LYS:HG3	1.95	0.67
3:Q:58:GLU:HG2	3:Q:59:GLN:H	1.60	0.67
6:F:2:PHE:CD1	6:F:3:ARG:HG2	2.30	0.67
8:V:67:THR:HG22	8:V:73:PRO:HD3	1.77	0.66
1:O:22:GLU:HA	2:P:26:THR:HG21	1.76	0.66
8:H:19:ARG:HB3	8:H:170:GLY:H	1.59	0.66
2:P:40:THR:HG23	2:P:183:LEU:O	1.95	0.66
8:H:13:ILE:HG23	8:H:176:VAL:O	1.95	0.66
7:G:34:THR:O	7:G:165:GLY:HA3	1.96	0.66
7:G:9:LEU:HD12	7:G:9:LEU:H	1.60	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:R:70:HIS:ND1	4:R:71:VAL:HG23	2.10	0.66
2:B:200:VAL:HG11	2:B:203:GLU:O	1.95	0.66
9:W:172:ASN:OD1	9:W:192:THR:HG22	1.96	0.66
8:V:155:ILE:HG21	8:V:175:MET:SD	2.35	0.66
1:A:16:ILE:HG22	1:A:17:THR:N	2.10	0.66
9:W:38:SER:HB2	9:W:41:ILE:HD13	1.77	0.66
9:W:52:THR:O	9:W:56:THR:HG23	1.96	0.66
5:S:204:LEU:O	5:S:208:MET:HB2	1.96	0.66
13:M:115:SER:OG	13:M:128:ARG:HD2	1.95	0.66
9:I:147:THR:H	9:I:150:GLU:HB2	1.61	0.66
14:N:121:TYR:HE1	14:N:123:ASN:ND2	1.93	0.66
4:D:64:VAL:HG11	4:D:213:THR:HG21	1.77	0.66
1:A:244:ARG:O	1:A:248:ILE:HG12	1.96	0.66
8:V:126:ILE:HD12	8:V:134:ILE:HG13	1.77	0.66
1:O:53:VAL:O	1:O:225:VAL:HG13	1.96	0.66
2:P:110:LEU:O	2:P:114:VAL:HG23	1.95	0.66
1:A:54:ILE:HG21	1:A:210:MET:SD	2.36	0.66
2:P:111:VAL:HG12	2:P:156:TYR:CD2	2.30	0.66
1:A:234:PHE:N	1:A:234:PHE:HD1	1.93	0.65
2:P:200:VAL:HG11	2:P:203:GLU:O	1.96	0.65
9:W:217:ILE:HD12	9:W:217:ILE:N	2.11	0.65
2:P:214:ILE:HD13	2:P:235:PHE:HA	1.78	0.65
11:K:4:LEU:HB2	11:K:15:ALA:HB3	1.78	0.65
1:A:129:THR:HG22	2:B:128:ARG:HH21	1.61	0.65
1:A:115:ASP:HB3	1:A:155:TYR:CE1	2.32	0.65
8:V:147:SER:H	8:V:150:GLU:HB3	1.61	0.65
14:N:87:TYR:CD2	14:N:88:LEU:HD23	2.31	0.65
1:A:87:ILE:O	1:A:91:ARG:HG3	1.97	0.65
11:K:191:VAL:O	11:K:191:VAL:HG12	1.96	0.65
5:E:45:GLY:HA2	5:E:153:TYR:CE1	2.31	0.65
8:V:13:ILE:CD1	8:V:177:VAL:HG22	2.26	0.65
1:A:24:ARG:C	1:A:25:LEU:HD12	2.17	0.65
4:R:31:THR:HB	4:R:63:LYS:NZ	2.11	0.65
3:Q:90:THR:HA	3:Q:93:ILE:HD12	1.77	0.65
7:G:197:LYS:HG2	7:G:201:LEU:HD21	1.79	0.65
5:E:113:THR:O	5:E:116:VAL:HG23	1.96	0.65
14:N:73:ALA:HA	14:N:77:GLU:O	1.96	0.65
1:A:128:TYR:HD1	1:A:133:TYR:HE1	1.44	0.65
9:I:22:GLN:CA	9:I:22:GLN:HE21	2.08	0.65
2:P:66:LEU:HD13	2:P:235:PHE:CD1	2.32	0.65
10:X:3:VAL:HG22	10:X:16:CYS:HB3	1.79	0.65
5:E:15:PHE:HB2	6:F:21:GLN:OE1	1.97	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:76:ALA:HB3	3:C:136:ILE:HB	1.78	0.64
5:S:12:VAL:H	5:S:23:GLN:HG3	1.62	0.64
1:O:234:PHE:N	1:O:234:PHE:CD1	2.64	0.64
8:H:147:SER:H	8:H:150:GLU:HB3	1.61	0.64
4:D:11:PHE:H	5:E:23:GLN:HE22	1.42	0.64
7:U:21:PHE:HA	7:U:24:GLU:CG	2.27	0.64
14:N:157:ILE:N	14:N:158:PRO:HD2	2.13	0.64
6:T:208:VAL:O	6:T:227:GLY:HA2	1.98	0.64
3:Q:216:ILE:HG12	3:Q:227:GLN:HB3	1.78	0.64
10:X:129:VAL:HB	10:X:137:LEU:HD13	1.79	0.64
2:B:46:ALA:HB2	2:B:211:LEU:CD1	2.22	0.64
4:R:188:VAL:O	4:R:192:VAL:HG23	1.98	0.64
9:I:59:ILE:HG12	9:I:83:LEU:HD23	1.80	0.64
4:D:70:HIS:ND1	4:D:71:VAL:HG23	2.12	0.64
8:H:8:PHE:CE2	8:H:148:LYS:HA	2.31	0.64
5:S:15:PHE:HB2	6:T:21:GLN:OE1	1.98	0.64
2:B:44:VAL:HA	2:B:213:ILE:HG22	1.80	0.64
12:L:176:ASN:ND2	12:L:190:ASN:HD22	1.95	0.64
1:O:227:VAL:HB	1:O:234:PHE:CE1	2.32	0.64
3:C:66:LEU:HD23	3:C:212:GLU:HB3	1.80	0.64
5:E:31:ILE:HD13	5:E:141:ALA:HB2	1.79	0.64
1:A:204:GLU:HB3	1:A:248:ILE:CG2	2.28	0.64
7:U:21:PHE:HA	7:U:24:GLU:HG2	1.80	0.64
7:U:42:ASN:HD21	7:U:187:SER:HA	1.61	0.64
9:W:156:SER:O	9:W:160:GLN:HG3	1.98	0.63
8:V:58:ILE:O	8:V:61:TYR:HB3	1.97	0.63
10:J:178:VAL:HG23	10:J:191:LEU:HD21	1.80	0.63
1:O:128:TYR:HD1	1:O:133:TYR:HE1	1.44	0.63
1:O:16:ILE:HG22	1:O:17:THR:H	1.63	0.63
1:A:128:TYR:HA	1:A:133:TYR:CE1	2.33	0.63
1:A:178:ILE:O	1:A:182:LEU:HG	1.99	0.63
4:D:66:LYS:HA	4:D:72:VAL:HG12	1.78	0.63
14:N:85:PHE:HB2	14:N:108:VAL:HG21	1.80	0.63
6:T:23:GLU:HA	6:T:26:LEU:HD12	1.80	0.63
8:V:177:VAL:HB	8:V:184:GLU:HB3	1.79	0.63
3:Q:96:GLN:NE2	10:X:63:ASN:HD22	1.93	0.63
5:E:51:GLU:HG3	5:E:208:MET:HG2	1.81	0.63
3:C:218:LYS:HG2	3:C:224:GLU:O	1.99	0.63
10:X:89:ARG:HG3	10:X:94:TYR:CE2	2.34	0.63
2:B:211:LEU:HG	2:B:212:ALA:N	2.14	0.63
1:O:44:ALA:CB	1:O:53:VAL:HG12	2.28	0.63
14:N:87:TYR:O	14:N:91:VAL:HG23	1.99	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:96:GLN:NE2	10:J:63:ASN:HD22	1.92	0.63
10:J:89:ARG:HG3	10:J:94:TYR:CE2	2.33	0.63
5:E:109:VAL:HB	5:E:154:GLN:NE2	2.12	0.63
1:A:43:LEU:HD12	1:A:178:ILE:CG2	2.28	0.63
11:Y:191:VAL:O	11:Y:193:ASP:N	2.32	0.63
11:Y:127:LEU:HD22	11:Y:128:PRO:HD2	1.81	0.63
1:O:126:GLN:HE21	1:O:127:ILE:N	1.97	0.63
1:O:181:ASN:HB3	1:O:209:HIS:HE1	1.61	0.63
1:O:244:ARG:O	1:O:248:ILE:HG12	1.99	0.63
2:B:89:SER:O	2:B:92:VAL:HG12	1.99	0.63
1:A:227:VAL:HB	1:A:234:PHE:CE1	2.33	0.63
4:D:54:LEU:HG	4:D:54:LEU:O	1.99	0.63
1:O:137:LEU:HD23	1:O:137:LEU:N	2.13	0.63
1:O:204:GLU:HB3	1:O:248:ILE:CG2	2.28	0.63
4:D:22:TYR:O	4:D:25:GLU:HB2	1.99	0.63
1:O:181:ASN:N	1:O:181:ASN:HD22	1.97	0.62
1:A:103:GLU:HA	8:H:61:TYR:HE2	1.62	0.62
1:A:21:PRO:HA	2:B:23:TYR:CD1	2.34	0.62
1:A:234:PHE:CD1	1:A:234:PHE:N	2.65	0.62
2:P:227:ILE:HG12	9:W:186:TYR:HD2	1.63	0.62
4:R:54:LEU:HG	4:R:54:LEU:O	1.99	0.62
9:I:84:LYS:HE3	9:I:119:THR:CG2	2.29	0.62
3:C:90:THR:HA	3:C:93:ILE:HD12	1.80	0.62
13:M:168:VAL:HG22	13:M:172:ILE:HD11	1.81	0.62
14:N:135:ALA:HB1	14:N:139:GLY:HA3	1.80	0.62
8:V:1:THR:HA	8:V:33:LYS:HZ1	1.62	0.62
11:Y:168:GLU:HG2	11:Y:175:PHE:HZ	1.65	0.62
1:O:20:SER:HB2	1:O:21:PRO:HD2	1.80	0.62
3:C:199:LYS:O	3:C:200:THR:HG23	2.00	0.62
1:A:25:LEU:O	1:A:28:VAL:HG22	1.98	0.62
3:C:210:ARG:HG3	3:C:210:ARG:HH11	1.63	0.62
5:E:204:LEU:O	5:E:208:MET:HB2	1.98	0.62
3:Q:210:ARG:HH11	3:Q:210:ARG:HG3	1.64	0.62
4:D:37:LYS:HE2	4:D:160:SER:HA	1.81	0.62
13:M:1:GLY:HA3	13:M:33:LYS:HE2	1.80	0.62
7:U:19:ARG:CB	7:U:19:ARG:HH11	2.11	0.62
2:P:89:SER:O	2:P:92:VAL:HG12	1.98	0.62
8:V:13:ILE:HG23	8:V:176:VAL:O	1.99	0.62
9:I:156:SER:O	9:I:160:GLN:HG3	1.99	0.62
12:L:66:HIS:HD2	12:L:74:ILE:HB	1.63	0.62
3:Q:66:LEU:HD23	3:Q:212:GLU:HB3	1.81	0.62
5:S:124:GLY:H	5:S:132:ARG:HB2	1.63	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:D:151:GLU:HB2	4:D:152:PRO:HD2	1.82	0.62
4:R:151:GLU:HG2	4:R:155:ILE:HG13	1.81	0.62
2:B:178:ARG:NH2	2:B:194:LEU:HD12	2.14	0.62
8:V:123:PRO:HB2	8:V:124:TYR:HD1	1.64	0.62
1:O:24:ARG:C	1:O:25:LEU:HD12	2.20	0.62
1:A:128:TYR:HD1	1:A:133:TYR:CE1	2.18	0.62
8:V:19:ARG:HB3	8:V:170:GLY:H	1.63	0.62
9:W:7:LYS:HA	9:W:12:VAL:HA	1.79	0.62
2:B:36:GLY:O	2:B:161:ALA:HA	2.00	0.62
2:B:238:LEU:N	2:B:238:LEU:HD12	2.14	0.62
3:Q:199:LYS:O	3:Q:200:THR:HG23	2.00	0.62
3:Q:218:LYS:HG2	3:Q:224:GLU:O	2.00	0.62
6:F:33:SER:HB3	6:F:62:LYS:NZ	2.14	0.61
12:L:196:LEU:O	12:L:200:VAL:HG23	1.98	0.61
11:K:168:GLU:HG2	11:K:175:PHE:HZ	1.65	0.61
1:O:202:VAL:O	1:O:205:PHE:HB3	2.00	0.61
1:A:146:VAL:HG22	1:A:152:PRO:CA	2.30	0.61
8:V:157:HIS:NE2	8:V:196:LEU:HD13	2.14	0.61
5:S:219:LEU:O	5:S:231:TYR:HB2	2.00	0.61
6:F:185:ASN:HD22	6:F:186:PRO:N	1.97	0.61
2:P:112:SER:HA	2:P:156:TYR:HE2	1.63	0.61
7:G:19:ARG:HH11	7:G:19:ARG:CB	2.13	0.61
11:Y:4:LEU:HB2	11:Y:15:ALA:HB3	1.82	0.61
13:M:4:LEU:HD12	13:M:5:GLY:N	2.15	0.61
1:O:54:ILE:HG21	1:O:210:MET:SD	2.40	0.61
3:C:133:VAL:HG12	3:C:134:SER:N	2.16	0.61
2:B:214:ILE:HD13	2:B:235:PHE:HA	1.82	0.61
4:D:203:VAL:HG21	4:D:210:ILE:HD11	1.81	0.61
10:X:129:VAL:HB	10:X:137:LEU:CD1	2.30	0.61
9:W:147:THR:H	9:W:150:GLU:HB2	1.65	0.61
1:O:43:LEU:HD12	1:O:178:ILE:CG2	2.31	0.61
8:H:4:MET:HB2	8:H:126:ILE:HG22	1.80	0.61
1:A:16:ILE:HG22	1:A:17:THR:H	1.66	0.61
8:V:14:LEU:HD12	8:V:34:LEU:HD22	1.83	0.61
1:A:181:ASN:HD22	1:A:181:ASN:N	1.98	0.61
1:A:200:GLU:O	1:A:204:GLU:HG3	2.01	0.61
5:E:192:THR:HG23	5:E:195:GLU:OE1	2.00	0.61
12:Z:196:LEU:O	12:Z:200:VAL:HG23	2.00	0.61
14:N:57:ARG:O	14:N:61:ASP:HB2	2.00	0.61
2:B:111:VAL:HG12	2:B:156:TYR:HD2	1.64	0.61
1:A:204:GLU:HB3	1:A:248:ILE:HG21	1.82	0.61
7:G:94:GLU:HG2	7:G:114:ARG:HD2	1.83	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
9:I:52:THR:O	9:I:55:VAL:HG12	2.00	0.61
3:Q:87:LEU:H	3:Q:87:LEU:HD12	1.66	0.61
1:O:178:ILE:O	1:O:182:LEU:HG	2.01	0.61
1:O:72:ILE:HA	1:O:81:MET:O	2.01	0.61
13:M:117:ASP:HB2	13:M:121:SER:OG	2.01	0.61
10:J:9:LYS:HG3	10:J:148:ASN:HD22	1.66	0.61
1:O:17:THR:O	1:O:18:ILE:HG23	1.99	0.61
14:N:35:ILE:O	14:N:43:VAL:HG22	2.01	0.61
5:S:142:LEU:HB3	5:S:144:ILE:CD1	2.31	0.61
7:U:42:ASN:ND2	7:U:187:SER:HA	2.14	0.61
12:Z:35:ILE:HD11	12:Z:45:MET:HE3	1.81	0.61
9:I:172:ASN:ND2	9:I:192:THR:HA	2.16	0.61
1:A:45:VAL:HG12	1:A:168:ALA:CB	2.31	0.60
14:N:17:ASP:HA	14:N:187:PHE:HB3	1.83	0.60
9:W:84:LYS:HE3	9:W:119:THR:CG2	2.30	0.60
2:P:178:ARG:NH2	2:P:194:LEU:HD12	2.17	0.60
3:C:77:VAL:HG12	3:C:78:ALA:N	2.17	0.60
8:H:1:THR:HA	8:H:33:LYS:HZ1	1.64	0.60
1:A:80:GLY:HA3	1:A:233:PHE:CZ	2.36	0.60
14:N:120:ARG:NH1	14:N:130:SER:HB2	2.17	0.60
2:P:46:ALA:HB2	2:P:211:LEU:CD1	2.23	0.60
7:G:194:GLN:O	7:G:198:ILE:HG13	2.01	0.60
2:B:68:THR:CG2	2:B:71:ILE:HB	2.30	0.60
6:F:208:VAL:O	6:F:227:GLY:HA2	2.01	0.60
1:O:41:ASN:OD1	1:O:173:PRO:HD2	2.01	0.60
8:H:74:SER:OG	8:H:75:THR:N	2.34	0.60
1:A:126:GLN:NE2	1:A:127:ILE:N	2.49	0.60
8:V:4:MET:HB2	8:V:126:ILE:HG22	1.82	0.60
5:E:124:GLY:H	5:E:132:ARG:HB2	1.65	0.60
3:C:216:ILE:HG12	3:C:227:GLN:HB3	1.83	0.60
4:R:105:THR:HG23	4:R:108:TYR:HB3	1.82	0.60
4:D:162:GLN:HE21	4:D:163:THR:N	1.97	0.60
4:D:151:GLU:HG2	4:D:155:ILE:HG13	1.83	0.60
1:A:82:VAL:CG1	1:A:142:THR:HB	2.31	0.60
9:W:84:LYS:HE3	9:W:119:THR:HG23	1.84	0.60
9:W:59:ILE:HG12	9:W:83:LEU:HD23	1.81	0.60
8:H:58:ILE:O	8:H:61:TYR:HB3	2.01	0.60
10:J:129:VAL:HB	10:J:137:LEU:CD1	2.31	0.60
9:W:58:LEU:O	9:W:61:SER:HB3	2.02	0.60
10:X:9:LYS:HG3	10:X:148:ASN:HD22	1.66	0.60
1:O:204:GLU:HB3	1:O:248:ILE:HG21	1.83	0.60
3:Q:77:VAL:HG22	3:Q:135:PHE:HE1	1.64	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
9:I:173:VAL:O	9:I:189:ASN:HA	2.02	0.60
5:E:59:LEU:HD13	5:E:60:GLU:N	2.17	0.60
13:M:4:LEU:HD12	13:M:5:GLY:H	1.66	0.60
11:Y:152:THR:HG23	11:Y:155:GLU:OE1	2.01	0.60
1:O:21:PRO:HA	2:P:23:TYR:CD1	2.37	0.60
7:U:175:LEU:HA	7:U:178:LEU:HD12	1.84	0.60
14:N:17:ASP:HA	14:N:187:PHE:CB	2.32	0.60
9:I:217:ILE:HD12	9:I:217:ILE:N	2.17	0.60
4:R:224:LEU:HD23	4:R:229:ILE:HG12	1.83	0.60
1:O:240:ASN:H	1:O:240:ASN:ND2	1.97	0.60
1:O:41:ASN:O	1:O:55:SER:HA	2.02	0.60
2:B:95:THR:HA	2:B:99:ARG:HD2	1.84	0.60
12:Z:66:HIS:CD2	12:Z:74:ILE:HB	2.36	0.60
10:J:115:PHE:CD1	10:J:115:PHE:N	2.70	0.60
5:E:64:ILE:N	5:E:64:ILE:HD12	2.17	0.60
4:D:99:THR:O	4:D:100:LEU:HD13	2.01	0.60
14:N:145:PRO:HA	9:W:165:ASN:ND2	2.16	0.60
11:Y:7:ARG:HH11	11:Y:7:ARG:HG2	1.66	0.60
1:O:128:TYR:HA	1:O:133:TYR:CE1	2.37	0.59
1:O:146:VAL:HG22	1:O:152:PRO:CA	2.31	0.59
1:O:70:SER:O	1:O:71:TYR:HD1	1.84	0.59
6:F:23:GLU:HA	6:F:26:LEU:HD12	1.84	0.59
8:H:157:HIS:NE2	8:H:196:LEU:HD13	2.16	0.59
4:D:224:LEU:HD23	4:D:229:ILE:HG12	1.83	0.59
1:O:46:ARG:HG3	1:O:167:LYS:O	2.03	0.59
1:O:181:ASN:HD22	1:O:181:ASN:H	1.50	0.59
1:A:181:ASN:HB3	1:A:209:HIS:HE1	1.63	0.59
1:A:202:VAL:O	1:A:205:PHE:HB3	2.02	0.59
5:S:45:GLY:HA2	5:S:153:TYR:CE1	2.38	0.59
7:U:54:THR:HA	7:U:209:LYS:HD2	1.83	0.59
3:C:77:VAL:HG22	3:C:135:PHE:HE1	1.67	0.59
1:A:131:ARG:HA	2:B:127:VAL:HG12	1.83	0.59
1:O:33:LYS:HD2	1:O:33:LYS:N	2.17	0.59
8:V:14:LEU:CD1	8:V:34:LEU:HD22	2.33	0.59
10:X:115:PHE:N	10:X:115:PHE:CD1	2.70	0.59
8:H:177:VAL:O	8:H:183:VAL:HA	2.02	0.59
7:G:47:PHE:O	7:G:215:ILE:HG22	2.03	0.59
2:P:71:ILE:HG12	2:P:138:GLY:HA3	1.84	0.59
1:A:155:TYR:CD2	1:A:165:GLY:HA2	2.38	0.59
1:A:20:SER:HB2	1:A:21:PRO:HD2	1.83	0.59
4:D:36:VAL:CG1	4:D:195:THR:HG23	2.33	0.59
11:Y:74:LEU:HD12	11:Y:79:VAL:HG22	1.84	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:E:220:SER:HA	5:E:231:TYR:HD1	1.68	0.59
8:H:13:ILE:HD11	8:H:177:VAL:HG13	1.84	0.59
13:M:29:ARG:HD2	13:M:191:ASP:OD1	2.01	0.59
2:P:64:VAL:HG21	2:P:212:ALA:HB3	1.84	0.59
2:P:84:VAL:O	2:P:88:LYS:HG3	2.02	0.59
14:N:45:ILE:HG21	14:N:52:MET:HG3	1.83	0.59
3:Q:70:ASN:ND2	3:Q:71:ASP:H	2.00	0.59
5:E:16:SER:HB3	5:E:22:PHE:HE2	1.67	0.59
4:D:199:LEU:O	4:D:203:VAL:HG23	2.03	0.59
4:R:11:PHE:N	5:S:23:GLN:HE22	2.00	0.59
6:T:33:SER:HB3	6:T:62:LYS:HZ3	1.67	0.59
3:Q:76:ALA:HB3	3:Q:136:ILE:HB	1.85	0.59
4:R:66:LYS:HA	4:R:72:VAL:HG12	1.84	0.59
10:X:35:PHE:CD2	10:X:35:PHE:N	2.71	0.59
5:S:64:ILE:HD12	5:S:64:ILE:N	2.17	0.59
1:O:128:TYR:HD1	1:O:133:TYR:CE1	2.19	0.59
1:A:42:SER:HA	1:A:54:ILE:O	2.03	0.59
5:S:51:GLU:HG3	5:S:208:MET:HG2	1.83	0.59
2:P:174:PHE:HD2	2:P:195:THR:HG1	1.51	0.59
6:T:134:ILE:HD12	6:T:134:ILE:N	2.18	0.59
1:O:82:VAL:CG1	1:O:142:THR:HB	2.33	0.59
4:D:37:LYS:HB3	4:D:42:VAL:HG13	1.85	0.59
1:O:115:ASP:HB3	1:O:155:TYR:CE1	2.38	0.59
6:T:190:ILE:O	6:T:194:VAL:HG23	2.03	0.59
1:O:128:TYR:CD1	1:O:133:TYR:CE1	2.91	0.58
2:P:211:LEU:HG	2:P:212:ALA:N	2.17	0.58
2:B:112:SER:HA	2:B:156:TYR:HE2	1.68	0.58
12:L:4:LEU:C	12:L:4:LEU:HD22	2.23	0.58
1:O:251:GLN:O	1:O:251:GLN:HG2	2.04	0.58
4:D:31:THR:HB	4:D:63:LYS:NZ	2.19	0.58
2:B:178:ARG:HH21	2:B:194:LEU:HD12	1.68	0.58
4:D:188:VAL:O	4:D:192:VAL:HG23	2.02	0.58
8:V:74:SER:OG	8:V:75:THR:N	2.36	0.58
1:A:250:GLU:HG2	1:A:251:GLN:N	2.17	0.58
4:R:37:LYS:HB3	4:R:42:VAL:HG13	1.85	0.58
6:T:131:GLY:O	6:T:132:LEU:HD23	2.02	0.58
8:V:143:ARG:HB3	8:V:143:ARG:NH1	2.19	0.58
13:M:91:LYS:HE2	13:M:94:PHE:O	2.03	0.58
6:F:194:VAL:O	6:F:197:ILE:HG22	2.02	0.58
2:B:111:VAL:HG12	2:B:156:TYR:CD2	2.38	0.58
1:A:44:ALA:CB	1:A:53:VAL:HG12	2.31	0.58
2:B:218:ASN:HD21	2:B:236:ARG:HD2	1.69	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:P:118:MET:SD	2:P:152:PRO:HA	2.42	0.58
1:A:183:GLU:HB3	1:A:187:LYS:HZ2	1.68	0.58
2:B:224:TYR:HA	9:I:184:ALA:O	2.03	0.58
1:A:79:ILE:HD12	1:A:79:ILE:N	2.18	0.58
10:J:35:PHE:N	10:J:35:PHE:CD2	2.71	0.58
1:O:203:VAL:HG12	1:O:207:ILE:HD11	1.84	0.58
7:G:42:ASN:ND2	7:G:187:SER:HA	2.18	0.58
7:G:42:ASN:HD21	7:G:187:SER:HA	1.67	0.58
12:Z:176:ASN:ND2	12:Z:190:ASN:HD22	2.01	0.58
6:F:82:ARG:O	6:F:86:ASN:HB2	2.04	0.58
8:H:18:SER:HB2	8:H:30:VAL:HA	1.86	0.58
12:L:35:ILE:HD11	12:L:45:MET:CE	2.33	0.58
14:N:174:ARG:HA	14:N:206:VAL:HG11	1.85	0.58
14:N:49:ILE:HG22	14:N:53:GLN:NE2	2.17	0.58
6:F:150:SER:O	7:G:82:PRO:HG2	2.04	0.58
2:B:94:HIS:NE2	2:B:98:LYS:HD3	2.18	0.58
5:E:219:LEU:O	5:E:231:TYR:HB2	2.04	0.58
3:C:150:THR:CG2	3:C:160:TRP:HE1	2.16	0.58
1:A:128:TYR:CD1	1:A:133:TYR:CE1	2.90	0.58
7:U:197:LYS:HG2	7:U:201:LEU:HD21	1.86	0.58
5:S:16:SER:HB3	5:S:22:PHE:HE2	1.68	0.58
11:Y:24:ILE:HG23	11:Y:25:SER:H	1.69	0.58
7:G:54:THR:HA	7:G:209:LYS:HD2	1.84	0.58
5:E:177:GLU:CD	5:E:177:GLU:H	2.07	0.57
8:H:143:ARG:NH1	8:H:143:ARG:HB3	2.19	0.57
11:K:24:ILE:HG23	11:K:25:SER:H	1.68	0.57
1:A:28:VAL:O	1:A:31:ALA:HB3	2.04	0.57
1:O:103:GLU:HA	8:V:61:TYR:HE2	1.67	0.57
6:T:194:VAL:O	6:T:197:ILE:HG22	2.03	0.57
2:B:159:TRP:CE3	2:B:162:THR:HB	2.39	0.57
5:S:192:THR:HG23	5:S:195:GLU:OE1	2.02	0.57
4:D:180:ASP:OD2	4:D:183:GLU:HG3	2.04	0.57
12:Z:4:LEU:C	12:Z:4:LEU:HD22	2.24	0.57
9:I:196:ARG:HH12	10:J:142:GLU:HG3	1.70	0.57
1:A:33:LYS:N	1:A:33:LYS:HD2	2.15	0.57
8:V:156:LYS:NZ	8:V:188:PHE:HD1	2.00	0.57
2:P:238:LEU:HD12	2:P:238:LEU:N	2.19	0.57
5:S:108:ASN:O	5:S:111:SER:N	2.37	0.57
8:H:14:LEU:HD12	8:H:34:LEU:HD22	1.85	0.57
1:O:164:VAL:HG22	1:O:165:GLY:H	1.68	0.57
6:F:131:GLY:O	6:F:132:LEU:HD23	2.05	0.57
14:N:153:ARG:HG2	14:N:155:SER:H	1.68	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:O:63:LEU:HD11	7:U:175:LEU:HB2	1.86	0.57
5:S:167:TYR:CD1	5:S:170:LYS:HB2	2.40	0.57
4:R:69:SER:O	4:R:221:ILE:HD12	2.04	0.57
7:U:47:PHE:O	7:U:215:ILE:HG22	2.04	0.57
13:M:139:PRO:O	13:M:142:ASP:HB2	2.04	0.57
8:H:4:MET:SD	8:H:159:LEU:CD1	2.92	0.57
7:G:60:PRO:O	7:G:61:GLN:HB2	2.05	0.57
3:Q:133:VAL:HG12	3:Q:134:SER:N	2.19	0.57
8:V:66:TYR:CE1	8:V:70:TYR:HB2	2.40	0.57
4:R:22:TYR:O	4:R:25:GLU:HB2	2.04	0.57
1:O:79:ILE:HD12	1:O:79:ILE:N	2.18	0.57
14:N:82:SER:HA	14:N:118:PHE:CE2	2.40	0.57
13:M:147:PHE:CD1	13:M:161:LYS:HE3	2.40	0.57
6:T:43:HIS:HB3	6:T:215:ILE:HD11	1.86	0.57
1:O:183:GLU:O	1:O:187:LYS:HG3	2.04	0.57
3:Q:150:THR:CG2	3:Q:160:TRP:HE1	2.17	0.57
1:A:242:GLU:HA	1:A:245:LEU:HD12	1.85	0.57
1:O:87:ILE:O	1:O:91:ARG:HG3	2.05	0.57
14:N:9:ASP:HB3	14:N:158:PRO:O	2.03	0.57
11:K:191:VAL:O	11:K:193:ASP:N	2.38	0.57
11:Y:117:GLN:HE22	11:Y:131:ALA:H	1.53	0.57
1:O:242:GLU:HA	1:O:245:LEU:HD12	1.85	0.57
10:X:178:VAL:HG23	10:X:191:LEU:HD21	1.86	0.57
12:Z:12:ILE:HD13	12:Z:102:CYS:HB3	1.86	0.57
11:K:115:LEU:HD12	11:K:116:TYR:N	2.19	0.57
8:H:9:LYS:HD3	8:H:146:MET:O	2.05	0.57
10:X:29:ASN:HD22	10:X:29:ASN:N	2.02	0.57
14:N:148:ARG:HD2	9:W:165:ASN:HD21	1.69	0.57
6:T:150:SER:O	7:U:82:PRO:HG2	2.05	0.57
7:U:166:LYS:NZ	7:U:206:ASN:HD21	2.03	0.57
1:O:80:GLY:HA3	1:O:233:PHE:CZ	2.40	0.57
6:T:17:GLY:HA3	7:U:29:ALA:HB2	1.87	0.57
11:K:127:LEU:HD22	11:K:128:PRO:HD2	1.87	0.56
8:V:177:VAL:O	8:V:183:VAL:HA	2.05	0.56
1:A:17:THR:O	1:A:18:ILE:HG23	2.04	0.56
2:B:184:GLU:O	2:B:187:ASP:HB2	2.05	0.56
1:A:88:PRO:HD3	7:G:155:SER:HB3	1.86	0.56
4:R:199:LEU:O	4:R:203:VAL:HG23	2.05	0.56
9:I:14:ILE:HD13	9:I:101:ALA:HB3	1.85	0.56
6:T:144:LEU:C	6:T:145:LEU:HD12	2.25	0.56
11:Y:95:ARG:HB3	11:Y:95:ARG:NH1	2.20	0.56
11:K:32:ASP:OD1	11:K:34:THR:HB	2.05	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:F:34:VAL:HG22	6:F:35:THR:N	2.20	0.56
4:R:105:THR:HG23	4:R:108:TYR:CB	2.35	0.56
7:G:180:ASP:O	7:G:183:PRO:HD3	2.05	0.56
1:A:41:ASN:O	1:A:55:SER:HA	2.04	0.56
9:W:72:ARG:HH11	9:W:72:ARG:HG3	1.70	0.56
2:B:64:VAL:HG21	2:B:212:ALA:HB3	1.87	0.56
8:V:26:ILE:HG21	8:V:29:ARG:HB3	1.87	0.56
11:K:117:GLN:HE22	11:K:131:ALA:H	1.53	0.56
8:H:3:ILE:HG22	8:H:16:ALA:CB	2.35	0.56
2:P:184:GLU:O	2:P:187:ASP:HB2	2.05	0.56
1:O:183:GLU:HB3	1:O:187:LYS:HZ2	1.66	0.56
8:H:186:LEU:HD22	8:H:188:PHE:HE2	1.70	0.56
8:V:163:ILE:HG23	8:V:170:GLY:HA2	1.86	0.56
3:C:163:ILE:HG13	3:C:164:SER:N	2.20	0.56
3:Q:195:LYS:O	3:Q:199:LYS:HD3	2.05	0.56
11:K:74:LEU:HD12	11:K:79:VAL:HG22	1.86	0.56
11:Y:195:GLN:HA	11:Y:195:GLN:NE2	2.18	0.56
9:W:88:PHE:HB2	9:W:116:HIS:O	2.04	0.56
5:S:113:THR:O	5:S:116:VAL:HG23	2.06	0.56
6:F:159:THR:OG1	6:F:160:ALA:N	2.38	0.56
1:A:164:VAL:HG22	1:A:165:GLY:H	1.71	0.56
12:Z:66:HIS:CE1	12:Z:70:GLU:HG3	2.40	0.56
8:V:92:ASN:ND2	8:V:92:ASN:N	2.52	0.56
11:K:3:ILE:HD13	11:K:16:SER:HB3	1.87	0.56
6:F:50:LYS:HB3	6:F:59:TYR:HB3	1.86	0.56
14:N:40:ASN:N	14:N:40:ASN:HD22	1.83	0.56
6:F:96:SER:O	6:F:100:ASN:HA	2.05	0.56
7:U:100:LYS:NZ	7:U:100:LYS:HB3	2.21	0.56
8:H:14:LEU:CD1	8:H:34:LEU:HD22	2.36	0.56
14:N:7:LYS:HA	14:N:12:VAL:HG12	1.88	0.56
14:N:143:ALA:C	14:N:145:PRO:HD2	2.26	0.56
11:K:9:GLN:HE21	11:K:150:ASP:HA	1.70	0.56
3:C:152:ASN:HB2	3:C:153:PRO:CD	2.36	0.56
3:C:70:ASN:ND2	3:C:71:ASP:H	2.03	0.56
6:T:215:ILE:HG13	6:T:216:VAL:H	1.70	0.56
5:S:78:MET:HA	5:S:142:LEU:HD23	1.88	0.56
4:D:70:HIS:HB3	4:D:219:SER:OG	2.05	0.56
12:L:35:ILE:HD11	12:L:45:MET:HE3	1.88	0.56
14:N:221:GLY:O	9:W:77:VAL:HG11	2.06	0.56
14:N:203:ASN:O	14:N:204:LEU:HD13	2.06	0.56
8:H:123:PRO:HB2	8:H:124:TYR:HD1	1.71	0.56
8:H:26:ILE:HG21	8:H:29:ARG:HB3	1.87	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:R:151:GLU:HB2	4:R:152:PRO:HD2	1.86	0.56
7:U:60:PRO:O	7:U:61:GLN:HB2	2.05	0.56
6:T:34:VAL:HG22	6:T:35:THR:N	2.19	0.56
13:M:176:ARG:NH1	9:W:200:GLN:HE22	2.04	0.56
10:J:49:THR:HG21	11:K:121:LEU:O	2.04	0.56
2:P:224:TYR:HA	9:W:184:ALA:O	2.06	0.56
7:U:19:ARG:HB2	7:U:19:ARG:HH11	1.70	0.56
9:W:34:LEU:HD22	9:W:174:ASP:HB3	1.88	0.56
11:Y:62:ASN:O	11:Y:65:LEU:HB3	2.05	0.56
7:U:194:GLN:HE22	7:U:197:LYS:HZ1	1.52	0.56
9:W:173:VAL:O	9:W:189:ASN:HA	2.05	0.56
4:D:105:THR:HG23	4:D:108:TYR:HB3	1.88	0.56
10:X:37:TYR:O	10:X:40:VAL:HG23	2.06	0.56
4:R:36:VAL:CG1	4:R:195:THR:HG23	2.36	0.56
12:L:54:PHE:C	12:L:54:PHE:CD2	2.78	0.56
1:O:128:TYR:HA	1:O:133:TYR:CD1	2.41	0.56
13:M:213:ASP:HB2	9:W:19:ARG:HH22	1.71	0.56
7:G:44:GLY:HA3	7:G:218:CYS:O	2.06	0.56
1:A:250:GLU:HG2	1:A:251:GLN:H	1.70	0.56
11:Y:34:THR:HG23	11:Y:35:ARG:N	2.20	0.56
1:O:159:PRO:C	1:O:161:GLY:H	2.09	0.56
1:O:162:TYR:C	1:O:162:TYR:HD1	2.10	0.56
9:I:103:VAL:CG1	9:I:108:SER:HA	2.25	0.55
8:V:18:SER:HB2	8:V:30:VAL:HA	1.87	0.55
1:A:54:ILE:CG2	1:A:210:MET:SD	2.94	0.55
6:T:185:ASN:ND2	6:T:188:GLU:H	2.03	0.55
11:Y:32:ASP:OD1	11:Y:34:THR:HB	2.07	0.55
11:Y:82:PHE:O	11:Y:85:GLN:HB3	2.07	0.55
6:F:189:LEU:O	6:F:192:ALA:HB3	2.07	0.55
5:S:37:ALA:CB	5:S:50:VAL:HG12	2.36	0.55
3:Q:19:LEU:O	3:Q:21:GLN:N	2.39	0.55
11:Y:115:LEU:HD12	11:Y:116:TYR:N	2.21	0.55
11:K:95:ARG:HB3	11:K:95:ARG:NH1	2.21	0.55
1:O:126:GLN:O	1:O:129:THR:HB	2.06	0.55
2:P:36:GLY:O	2:P:161:ALA:HA	2.05	0.55
7:G:21:PHE:HA	7:G:24:GLU:CG	2.36	0.55
2:P:200:VAL:HG21	2:P:204:PHE:CE1	2.42	0.55
8:V:156:LYS:HD2	8:V:188:PHE:CE1	2.41	0.55
6:F:187:ASP:O	6:F:191:LYS:HG3	2.06	0.55
1:A:148:GLU:H	1:A:148:GLU:CD	2.10	0.55
11:K:7:ARG:HG2	11:K:7:ARG:HH11	1.71	0.55
1:O:131:ARG:HA	2:P:127:VAL:HG12	1.89	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:U:194:GLN:O	7:U:198:ILE:HG13	2.06	0.55
1:A:63:LEU:HD11	7:G:175:LEU:HB2	1.88	0.55
11:Y:38:SER:HB2	11:Y:39:PRO:HD2	1.88	0.55
9:I:84:LYS:HE3	9:I:119:THR:HG23	1.88	0.55
9:I:72:ARG:HH11	9:I:72:ARG:HG3	1.71	0.55
5:E:30:ALA:O	5:E:33:LEU:HB3	4.20	0.55
2:P:178:ARG:HH21	2:P:194:LEU:HD12	1.70	0.55
7:G:100:LYS:NZ	7:G:100:LYS:HB3	2.20	0.55
6:T:96:SER:O	6:T:100:ASN:HA	2.06	0.55
2:B:71:ILE:HG12	2:B:138:GLY:HA3	1.89	0.55
8:V:190:PRO:O	8:V:194:GLU:HG3	2.06	0.55
6:T:187:ASP:O	6:T:191:LYS:HG3	2.07	0.55
8:H:190:PRO:HA	8:H:193:TYR:CE2	2.42	0.55
1:O:20:SER:OG	1:O:24:ARG:N	2.39	0.55
14:N:105:ALA:C	14:N:106:ILE:HD12	2.27	0.55
10:J:49:THR:HB	11:K:122:GLY:O	2.07	0.55
3:Q:222:ASP:C	3:Q:224:GLU:H	2.10	0.55
7:G:98:PHE:CD1	7:G:98:PHE:C	2.80	0.55
5:S:177:GLU:H	5:S:177:GLU:CD	2.10	0.55
1:A:181:ASN:HD22	1:A:181:ASN:H	1.53	0.55
11:Y:66:TYR:CE1	11:Y:74:LEU:HD23	2.42	0.55
14:N:186:ASN:HD22	14:N:203:ASN:ND2	2.05	0.55
7:U:23:VAL:O	7:U:27:VAL:HG23	2.07	0.55
9:I:83:LEU:O	9:I:87:LEU:HB2	2.06	0.55
8:V:185:ARG:NH1	8:V:185:ARG:HG3	2.22	0.55
7:G:67:GLN:HG2	14:N:69:ASP:OD1	2.06	0.55
3:Q:238:ILE:HD12	3:Q:241:LYS:HD2	1.89	0.55
7:G:217:TRP:CD1	7:G:217:TRP:N	2.74	0.55
1:A:43:LEU:C	1:A:43:LEU:HD23	2.27	0.55
5:S:220:SER:HA	5:S:231:TYR:HD1	1.71	0.55
1:O:220:LYS:CB	1:O:242:GLU:HB2	2.37	0.55
1:A:220:LYS:CB	1:A:242:GLU:HB2	2.36	0.55
6:T:94:TYR:O	6:T:98:VAL:HG23	2.07	0.55
3:Q:64:GLU:O	3:Q:65:LYS:HG2	2.07	0.55
2:P:218:ASN:HD21	2:P:236:ARG:HD2	1.72	0.55
5:S:97:VAL:HG11	12:Z:65:LEU:HD21	1.89	0.55
12:Z:54:PHE:C	12:Z:54:PHE:CD2	2.79	0.55
2:B:212:ALA:CB	2:B:237:LYS:HA	2.37	0.55
2:P:159:TRP:CE3	2:P:162:THR:HB	2.42	0.55
8:H:4:MET:SD	8:H:159:LEU:HD11	2.47	0.55
11:K:38:SER:HB2	11:K:39:PRO:HD2	1.89	0.55
1:A:41:ASN:HB2	1:A:56:GLN:OE1	2.07	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
8:V:48:SER:HB2	8:V:94:THR:HB	1.88	0.55
9:W:14:ILE:HD13	9:W:101:ALA:HB3	1.88	0.55
3:C:37:GLY:HA2	3:C:45:VAL:O	2.06	0.54
12:L:66:HIS:CE1	12:L:70:GLU:HG3	2.42	0.54
1:A:139:VAL:HG23	1:A:141:LEU:HD21	1.87	0.54
4:D:221:ILE:O	4:D:222:VAL:HB	2.07	0.54
5:S:118:ASP:O	5:S:122:ARG:HG2	2.06	0.54
3:C:146:TYR:O	3:C:147:GLN:HG3	2.07	0.54
10:X:133:ALA:HB2	10:X:169:ASP:CB	2.37	0.54
9:W:83:LEU:O	9:W:87:LEU:HB2	2.07	0.54
7:U:46:VAL:HG22	7:U:217:TRP:HB3	1.89	0.54
6:F:70:MET:CE	6:F:105:VAL:HG22	2.37	0.54
1:O:126:GLN:NE2	1:O:127:ILE:N	2.55	0.54
2:P:212:ALA:CB	2:P:237:LYS:HA	2.37	0.54
7:G:194:GLN:HE22	7:G:197:LYS:HZ1	1.56	0.54
14:N:40:ASN:N	14:N:40:ASN:ND2	2.51	0.54
11:Y:160:LEU:O	11:Y:164:VAL:HG23	2.07	0.54
6:T:82:ARG:O	6:T:86:ASN:HB2	2.07	0.54
4:D:206:GLY:C	4:D:208:LYS:H	2.11	0.54
4:R:181:ARG:HH22	5:S:60:GLU:HG2	1.72	0.54
8:H:53:GLN:HE22	9:I:119:THR:H	1.54	0.54
2:P:16:GLY:HA3	3:Q:28:SER:HB2	1.90	0.54
5:E:64:ILE:H	5:E:64:ILE:HD12	1.73	0.54
9:W:196:ARG:HH12	10:X:142:GLU:HG3	1.72	0.54
8:H:190:PRO:O	8:H:194:GLU:HG3	2.07	0.54
12:L:12:ILE:HD13	12:L:102:CYS:HB3	1.89	0.54
2:B:84:VAL:O	2:B:88:LYS:HG3	2.07	0.54
5:S:40:ILE:HD12	5:S:200:VAL:HG23	1.88	0.54
3:C:29:ILE:C	3:C:31:HIS:H	2.09	0.54
1:O:18:ILE:HD13	1:O:18:ILE:N	2.22	0.54
9:I:88:PHE:HB2	9:I:116:HIS:O	2.07	0.54
10:X:49:THR:HG21	11:Y:121:LEU:O	2.08	0.54
7:U:182:HIS:HA	7:U:184:GLU:OE2	2.07	0.54
7:U:85:ARG:CG	7:U:85:ARG:HH11	2.21	0.54
1:A:35:THR:O	1:A:38:THR:HG22	2.07	0.54
11:K:34:THR:HG23	11:K:35:ARG:N	2.23	0.54
1:O:200:GLU:O	1:O:204:GLU:HG3	2.08	0.54
7:G:21:PHE:HA	7:G:24:GLU:HG2	1.89	0.54
3:C:87:LEU:H	3:C:87:LEU:HD12	1.73	0.54
1:A:43:LEU:HD22	1:A:54:ILE:HB	1.90	0.54
1:A:40:ILE:HD12	1:A:56:GLN:O	2.07	0.54
5:S:59:LEU:HD13	5:S:60:GLU:N	2.22	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
11:K:126:GLU:O	11:K:127:LEU:HD23	2.07	0.54
1:O:250:GLU:HG2	1:O:251:GLN:N	2.23	0.54
1:O:88:PRO:HD3	7:U:155:SER:HB3	1.90	0.54
7:G:194:GLN:HE22	7:G:197:LYS:NZ	2.06	0.54
11:K:24:ILE:HG23	11:K:25:SER:N	2.23	0.54
10:J:3:VAL:HG22	10:J:16:CYS:HB3	1.90	0.54
1:O:155:TYR:CD2	1:O:165:GLY:HA2	2.42	0.54
4:D:114:ALA:O	4:D:118:GLN:HB2	2.08	0.54
7:G:166:LYS:NZ	7:G:206:ASN:HD21	2.05	0.54
2:B:185:LEU:HD21	2:B:213:ILE:HD13	1.89	0.54
9:I:132:LEU:N	9:I:132:LEU:HD23	2.23	0.54
7:U:135:THR:O	7:U:149:MET:HA	2.06	0.54
8:H:156:LYS:HD2	8:H:188:PHE:CE1	2.43	0.54
8:H:163:ILE:HG23	8:H:170:GLY:HA2	1.90	0.54
2:B:57:MET:HB2	2:B:59:GLU:OE2	2.07	0.54
7:U:229:PHE:HD2	7:U:231:LYS:HE3	1.73	0.54
5:E:108:ASN:O	5:E:111:SER:N	2.41	0.54
7:U:39:ILE:HG13	7:U:46:VAL:HB	1.90	0.54
11:Y:87:LEU:HA	11:Y:90:SER:HB3	1.90	0.54
14:N:122:VAL:HA	14:N:127:VAL:O	2.07	0.54
2:B:12:PHE:HE2	3:C:130:PRO:HG2	1.72	0.54
2:P:160:LYS:HD3	2:P:179:TRP:CH2	2.43	0.54
8:H:175:MET:HB2	8:H:186:LEU:HB2	1.90	0.54
1:A:203:VAL:HG12	1:A:207:ILE:HD11	1.89	0.54
8:V:160:SER:HB2	8:V:193:TYR:HB2	1.90	0.54
4:R:180:ASP:OD2	4:R:183:GLU:HG3	2.08	0.54
1:O:42:SER:HA	1:O:54:ILE:O	2.09	0.53
7:U:201:LEU:H	7:U:201:LEU:HD13	1.73	0.53
5:S:151:ASP:HB2	5:S:154:GLN:OE1	2.08	0.53
9:W:38:SER:HB2	9:W:41:ILE:CD1	2.37	0.53
1:A:41:ASN:OD1	1:A:173:PRO:HD2	2.08	0.53
1:O:162:TYR:CD1	1:O:162:TYR:C	2.82	0.53
10:J:100:VAL:HG12	10:J:101:ALA:N	2.23	0.53
5:E:118:ASP:O	5:E:122:ARG:HG2	2.09	0.53
1:O:185:HIS:ND1	1:O:185:HIS:O	2.41	0.53
3:C:44:ILE:HD11	3:C:146:TYR:HB3	1.91	0.53
3:C:58:GLU:HG2	3:C:59:GLN:N	2.23	0.53
9:I:3:ILE:HG22	9:I:16:ALA:CB	2.39	0.53
9:I:7:LYS:HA	9:I:12:VAL:HA	1.90	0.53
1:A:70:SER:O	1:A:71:TYR:HD1	1.90	0.53
3:C:238:ILE:HD12	3:C:241:LYS:HD2	1.89	0.53
7:U:169:GLN:CD	7:U:169:GLN:H	2.10	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:128:TYR:HA	1:A:133:TYR:CD1	2.42	0.53
9:W:52:THR:O	9:W:55:VAL:HG12	2.08	0.53
5:E:180:GLN:O	5:E:184:LEU:HB2	2.08	0.53
7:U:150:LEU:HD11	7:U:154:GLY:HA2	1.91	0.53
6:F:37:GLY:HA2	6:F:45:VAL:O	2.09	0.53
14:N:92:MET:HE2	14:N:106:ILE:HD13	1.91	0.53
11:K:62:ASN:O	11:K:65:LEU:HB3	2.08	0.53
1:A:248:ILE:HG22	1:A:251:GLN:OE1	2.08	0.53
3:Q:152:ASN:HB2	3:Q:153:PRO:CD	2.39	0.53
5:E:40:ILE:HD12	5:E:200:VAL:HG23	1.91	0.53
11:K:110:LYS:O	11:K:112:LYS:HG3	2.07	0.53
12:L:16:VAL:CG2	12:L:176:ASN:HB2	2.38	0.53
1:A:72:ILE:HA	1:A:81:MET:O	2.08	0.53
8:V:8:PHE:HE2	8:V:148:LYS:CA	2.17	0.53
9:W:132:LEU:HD23	9:W:132:LEU:N	2.21	0.53
10:X:3:VAL:CG2	10:X:16:CYS:HB3	2.38	0.53
12:L:176:ASN:HD21	12:L:190:ASN:HD22	1.53	0.53
2:P:98:LYS:HA	2:P:103:GLU:O	2.08	0.53
14:N:87:TYR:HD2	14:N:88:LEU:HD23	1.73	0.53
13:M:77:ILE:HG23	13:M:78:ASN:N	2.24	0.53
9:I:66:HIS:O	9:I:70:THR:HG23	2.09	0.53
1:O:123:ASN:O	1:O:127:ILE:HG13	2.09	0.53
4:R:163:THR:HG21	4:R:171:VAL:HG23	1.91	0.53
1:O:45:VAL:HG12	1:O:168:ALA:CB	2.39	0.53
5:S:114:GLN:HG3	5:S:118:ASP:OD1	2.08	0.53
9:W:50:ALA:HB2	10:X:120:CYS:HB2	1.91	0.53
2:P:81:ASP:O	2:P:85:LEU:HB2	2.07	0.53
1:A:183:GLU:O	1:A:187:LYS:HG3	2.08	0.53
6:F:134:ILE:N	6:F:134:ILE:HD12	2.24	0.53
14:N:2:SER:OG	14:N:139:GLY:N	2.42	0.53
1:O:98:LYS:HD3	8:V:68:SER:O	2.08	0.53
1:A:185:HIS:O	1:A:185:HIS:ND1	2.41	0.53
7:U:23:VAL:O	7:U:26:ALA:HB3	2.08	0.53
5:E:167:TYR:CD1	5:E:170:LYS:HB2	2.43	0.53
12:L:24:ASN:OD1	10:X:171:LEU:HD12	2.09	0.53
9:I:34:LEU:HD22	9:I:174:ASP:HB3	1.91	0.53
3:C:64:GLU:O	3:C:65:LYS:HG2	2.09	0.53
6:T:50:LYS:HB3	6:T:59:TYR:HB3	1.90	0.53
1:A:117:LEU:O	1:A:121:MET:HG2	2.08	0.53
9:I:38:SER:HB2	9:I:41:ILE:HD13	1.90	0.53
7:U:180:ASP:O	7:U:183:PRO:HD3	2.09	0.53
11:K:195:GLN:HA	11:K:195:GLN:NE2	2.24	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:O:35:THR:O	1:O:38:THR:HG22	2.09	0.52
1:O:18:ILE:HG22	2:P:128:ARG:HB3	1.91	0.52
1:A:131:ARG:HH12	1:A:133:TYR:HB3	1.74	0.52
12:L:66:HIS:CD2	12:L:74:ILE:HB	2.43	0.52
7:G:19:ARG:HH11	7:G:19:ARG:HB2	1.74	0.52
11:Y:88:ALA:O	11:Y:91:ILE:HG22	2.09	0.52
4:R:99:THR:O	4:R:100:LEU:HD13	2.09	0.52
7:U:98:PHE:C	7:U:98:PHE:CD1	2.83	0.52
8:V:9:LYS:HD3	8:V:146:MET:O	2.09	0.52
5:E:170:LYS:HD2	5:E:171:ALA:N	2.23	0.52
6:T:185:ASN:HD22	6:T:186:PRO:N	2.06	0.52
10:J:163:LEU:HD11	10:J:193:MET:HB3	1.90	0.52
7:G:46:VAL:HG22	7:G:217:TRP:HB3	1.89	0.52
3:Q:96:GLN:HB3	10:X:60:TYR:CE2	2.45	0.52
2:B:81:ASP:O	2:B:85:LEU:HB2	2.09	0.52
7:U:72:HIS:CE1	7:U:105:PRO:HB2	2.44	0.52
2:B:227:ILE:HG12	9:I:186:TYR:CD2	2.43	0.52
2:P:112:SER:HA	2:P:156:TYR:CE2	2.44	0.52
3:Q:70:ASN:HD22	3:Q:71:ASP:H	1.56	0.52
7:U:48:ALA:HB2	7:U:215:ILE:HG23	1.91	0.52
9:I:4:VAL:HG12	9:I:126:SER:HB2	1.92	0.52
12:Z:81:LYS:HG3	12:Z:85:ASN:HD21	1.74	0.52
6:F:213:ILE:HG22	6:F:214:ALA:N	2.24	0.52
1:A:159:PRO:C	1:A:161:GLY:H	2.13	0.52
14:N:135:ALA:HB3	14:N:140:ALA:N	2.24	0.52
4:R:163:THR:HG21	4:R:171:VAL:CG2	2.39	0.52
8:V:163:ILE:HD12	8:V:170:GLY:HA2	1.92	0.52
3:C:165:VAL:N	3:C:169:THR:HG21	2.25	0.52
4:R:70:HIS:HB3	4:R:219:SER:OG	2.09	0.52
7:U:15:SER:OG	7:U:19:ARG:HB3	2.10	0.52
4:D:105:THR:HG23	4:D:108:TYR:CB	2.40	0.52
7:U:217:TRP:N	7:U:217:TRP:CD1	2.76	0.52
6:T:158:GLY:O	6:T:159:THR:HB	2.10	0.52
1:O:133:TYR:O	1:O:134:MET:HB3	2.08	0.52
1:A:155:TYR:HD2	1:A:164:VAL:O	1.93	0.52
6:F:26:LEU:O	6:F:29:ILE:HB	2.10	0.52
7:G:140:VAL:HG12	7:G:141:ASP:H	1.74	0.52
5:S:237:ALA:O	5:S:240:ILE:HB	2.10	0.52
7:G:169:GLN:HA	7:G:172:LYS:HB2	1.90	0.52
12:Z:159:ARG:HD2	12:Z:162:LEU:HD23	1.92	0.52
12:L:81:LYS:HG3	12:L:85:ASN:HD21	1.74	0.52
7:G:229:PHE:CD2	7:G:231:LYS:HE3	2.45	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:G:39:ILE:HG13	7:G:46:VAL:HB	1.91	0.52
2:B:49:LYS:HE2	2:B:58:SER:HB2	1.91	0.52
7:G:175:LEU:HA	7:G:178:LEU:HD12	1.90	0.52
11:Y:3:ILE:C	11:Y:4:LEU:HD23	2.29	0.52
13:M:194:GLU:HG3	13:M:205:LYS:HD3	1.91	0.52
6:T:37:GLY:HA2	6:T:45:VAL:O	2.09	0.52
12:L:8:PHE:HA	12:L:146:TRP:CE3	2.45	0.52
8:V:6:VAL:O	8:V:12:VAL:HG23	2.10	0.52
7:U:229:PHE:CD2	7:U:231:LYS:HE3	2.44	0.52
5:E:151:ASP:HB2	5:E:154:GLN:OE1	2.08	0.52
3:C:218:LYS:HG3	3:C:225:VAL:HG12	1.92	0.52
12:Z:176:ASN:HD21	12:Z:190:ASN:HD22	1.57	0.52
10:X:12:VAL:HG23	10:X:181:ILE:HB	1.92	0.52
8:V:13:ILE:HD11	8:V:177:VAL:HG13	1.92	0.52
1:A:18:ILE:HD13	1:A:18:ILE:N	2.24	0.52
1:A:18:ILE:HG22	2:B:128:ARG:HB3	1.91	0.52
2:B:108:LYS:HE2	2:B:143:ASN:ND2	2.25	0.52
8:H:31:THR:HG22	8:H:33:LYS:HG2	1.92	0.52
3:C:165:VAL:C	3:C:169:THR:HG21	2.30	0.52
14:N:148:ARG:HD2	9:W:165:ASN:ND2	2.24	0.52
1:A:220:LYS:HB3	1:A:242:GLU:HB2	1.91	0.52
9:W:4:VAL:HG12	9:W:126:SER:HB2	1.90	0.52
4:D:69:SER:O	4:D:221:ILE:HD12	2.10	0.52
4:D:235:GLN:O	4:D:235:GLN:HG2	2.10	0.52
7:G:77:TYR:HB3	7:G:135:THR:HG23	1.91	0.52
14:N:26:LEU:HD23	8:V:165:TRP:C	2.29	0.52
9:W:5:GLY:O	9:W:124:TYR:HA	2.09	0.52
6:T:68:GLU:O	6:T:222:PHE:N	2.40	0.52
4:D:193:LYS:HE2	4:D:193:LYS:HA	5.80	0.52
10:J:12:VAL:HG23	10:J:181:ILE:HB	1.92	0.52
3:Q:29:ILE:C	3:Q:31:HIS:H	2.13	0.52
1:O:125:SER:HA	1:O:128:TYR:CD2	2.44	0.52
1:O:131:ARG:HG2	1:O:131:ARG:HH11	1.75	0.52
1:O:40:ILE:HD12	1:O:56:GLN:O	2.09	0.52
7:G:194:GLN:NE2	7:G:197:LYS:NZ	2.58	0.52
7:G:76:VAL:HG22	7:G:77:TYR:H	1.75	0.52
8:H:74:SER:HB3	8:H:77:THR:OG1	2.10	0.52
1:A:42:SER:O	1:A:170:ALA:HA	2.09	0.52
14:N:153:ARG:HG3	14:N:153:ARG:NH1	2.17	0.52
5:S:136:ARG:HB2	5:S:137:PRO:CD	2.38	0.52
7:G:108:ILE:N	7:G:109:PRO:CD	2.73	0.52
3:Q:77:VAL:HG12	3:Q:78:ALA:N	2.25	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:F:118:LYS:HD2	6:F:118:LYS:N	2.25	0.52
6:T:189:LEU:O	6:T:192:ALA:HB3	2.10	0.52
3:Q:146:TYR:O	3:Q:147:GLN:HG3	2.10	0.52
10:J:29:ASN:HD22	10:J:29:ASN:N	2.09	0.51
4:D:11:PHE:N	5:E:23:GLN:HE22	2.08	0.51
7:G:197:LYS:HG3	7:G:201:LEU:HD11	1.92	0.51
3:C:133:VAL:CG1	3:C:134:SER:N	2.73	0.51
3:C:222:ASP:C	3:C:224:GLU:H	2.13	0.51
3:Q:218:LYS:HG3	3:Q:225:VAL:HG12	1.91	0.51
9:I:52:THR:O	9:I:56:THR:HG23	2.10	0.51
1:O:220:LYS:HB3	1:O:242:GLU:HB2	1.92	0.51
12:Z:16:VAL:CG2	12:Z:176:ASN:HB2	2.40	0.51
11:Y:24:ILE:HG23	11:Y:25:SER:N	2.25	0.51
2:B:34:SER:OG	2:B:47:THR:HB	2.09	0.51
5:S:110:GLU:HB3	5:S:156:PHE:CZ	2.44	0.51
6:T:164:ARG:HH22	6:T:202:ARG:HB3	1.75	0.51
4:R:235:GLN:HG2	4:R:235:GLN:O	2.10	0.51
11:K:3:ILE:C	11:K:4:LEU:HD23	2.29	0.51
2:P:49:LYS:HE2	2:P:58:SER:HB2	1.91	0.51
11:Y:8:VAL:HG23	11:Y:9:GLN:H	1.76	0.51
14:N:62:LEU:O	14:N:65:GLU:HB3	2.10	0.51
7:U:194:GLN:NE2	7:U:197:LYS:NZ	2.59	0.51
10:J:184:ASP:CG	10:J:185:GLU:N	2.62	0.51
1:A:46:ARG:HG3	1:A:167:LYS:O	2.10	0.51
3:Q:58:GLU:HG2	3:Q:59:GLN:N	2.25	0.51
5:S:97:VAL:HG11	12:Z:65:LEU:CD2	2.41	0.51
3:Q:24:TYR:O	3:Q:27:GLU:HG3	2.10	0.51
12:L:159:ARG:O	12:L:162:LEU:HB3	2.11	0.51
12:L:144:TYR:CD2	12:L:145:LYS:N	2.78	0.51
6:F:38:LEU:N	6:F:38:LEU:HD23	2.26	0.51
13:M:138:MET:N	13:M:139:PRO:CD	2.73	0.51
7:G:201:LEU:HD13	7:G:201:LEU:H	1.75	0.51
3:C:191:GLU:HG2	3:C:195:LYS:HE2	1.92	0.51
9:I:196:ARG:NH1	10:J:142:GLU:HG3	2.24	0.51
12:L:105:THR:HG21	12:L:108:GLU:OE1	2.10	0.51
3:Q:89:ASN:O	3:Q:93:ILE:HG13	2.11	0.51
7:G:182:HIS:HA	7:G:184:GLU:OE2	2.11	0.51
10:X:163:LEU:HD11	10:X:193:MET:HB3	1.92	0.51
12:Z:144:TYR:CD2	12:Z:145:LYS:N	2.78	0.51
13:M:183:THR:HG23	13:M:189:VAL:O	2.11	0.51
4:R:114:ALA:O	4:R:118:GLN:HB2	2.10	0.51
8:H:92:ASN:N	8:H:92:ASN:ND2	2.58	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:P:94:HIS:NE2	2:P:98:LYS:HD3	2.26	0.51
9:I:5:GLY:O	9:I:124:TYR:HA	2.11	0.51
7:G:150:LEU:HD11	7:G:154:GLY:HA2	1.92	0.51
3:C:165:VAL:CA	3:C:169:THR:HG21	2.40	0.51
1:A:87:ILE:HG23	1:A:88:PRO:HD3	1.93	0.51
9:W:172:ASN:ND2	9:W:192:THR:HA	2.25	0.51
10:X:6:MET:CE	10:X:145:TYR:HD1	2.24	0.51
11:K:3:ILE:O	11:K:4:LEU:HD23	2.11	0.51
14:N:120:ARG:HH11	14:N:130:SER:HB2	1.76	0.51
5:E:15:PHE:CD1	5:E:21:LEU:HD21	2.46	0.51
2:P:68:THR:CG2	2:P:71:ILE:HB	2.38	0.51
2:B:190:HIS:CE1	2:B:194:LEU:HD11	2.46	0.51
7:G:15:SER:OG	7:G:19:ARG:HB3	2.11	0.51
10:X:15:ALA:CB	10:X:178:VAL:HG22	2.40	0.51
4:R:27:VAL:HG11	4:R:132:SER:CB	2.41	0.51
3:C:140:TYR:CD1	3:C:141:ASP:N	2.79	0.51
9:I:158:ALA:O	9:I:161:ALA:HB3	2.11	0.51
10:X:140:MET:HE3	10:X:144:LEU:HD11	1.91	0.51
1:O:54:ILE:CG2	1:O:210:MET:SD	2.99	0.51
7:G:71:ARG:NH1	14:N:64:THR:HG22	2.25	0.51
14:N:81:PRO:HA	14:N:84:ILE:HD12	1.91	0.51
7:U:194:GLN:HE22	7:U:197:LYS:NZ	2.08	0.51
6:T:2:PHE:HD1	6:T:3:ARG:HG2	1.73	0.51
10:X:51:VAL:HG12	10:X:52:THR:N	2.25	0.51
11:K:66:TYR:CE1	11:K:74:LEU:HD23	2.45	0.51
5:S:180:GLN:O	5:S:184:LEU:HB2	2.10	0.51
8:H:160:SER:HB2	8:H:193:TYR:HB2	1.93	0.51
7:G:72:HIS:CE1	7:G:105:PRO:HB2	2.46	0.51
14:N:25:LEU:HD12	14:N:26:LEU:H	1.76	0.51
4:D:159:TRP:CZ2	5:E:59:LEU:HD23	2.46	0.51
6:T:38:LEU:N	6:T:38:LEU:HD23	2.26	0.51
9:W:48:THR:O	9:W:51:ASP:HB2	2.11	0.51
1:A:156:LYS:HE2	1:A:166:TYR:CE2	2.46	0.51
1:O:144:VAL:HG12	1:O:154:ILE:HG12	1.93	0.51
12:Z:38:ASN:HB2	12:Z:39:PRO:HD2	1.93	0.51
5:E:110:GLU:HB3	5:E:156:PHE:CZ	2.45	0.51
6:F:94:TYR:O	6:F:98:VAL:HG23	2.11	0.51
2:B:68:THR:C	2:B:70:ASP:H	2.14	0.51
8:H:186:LEU:HD22	8:H:188:PHE:CE2	2.46	0.51
7:U:108:ILE:N	7:U:109:PRO:CD	2.74	0.51
9:I:180:ILE:HG22	9:I:180:ILE:O	2.10	0.51
12:Z:110:PRO:O	12:Z:111:THR:HG23	2.11	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
11:Y:5:GLY:HA2	11:Y:13:ILE:O	2.11	0.51
11:Y:18:LYS:HD3	11:Y:179:ILE:HG13	1.92	0.51
9:W:66:HIS:O	9:W:70:THR:HG23	2.11	0.51
3:C:19:LEU:O	3:C:21:GLN:N	2.44	0.51
1:A:162:TYR:HD1	1:A:162:TYR:C	2.15	0.51
1:O:42:SER:O	1:O:170:ALA:HA	2.10	0.50
1:O:54:ILE:HG13	1:O:225:VAL:CG2	2.40	0.50
11:Y:160:LEU:C	11:Y:160:LEU:HD23	2.32	0.50
3:Q:165:VAL:C	3:Q:169:THR:HG21	2.32	0.50
7:U:44:GLY:HA3	7:U:218:CYS:O	2.11	0.50
3:Q:120:GLN:O	3:Q:123:THR:HB	2.11	0.50
1:O:139:VAL:HG23	1:O:141:LEU:HD21	1.92	0.50
13:M:24:TYR:HA	9:W:167:LEU:HD12	1.92	0.50
2:B:200:VAL:HG21	2:B:204:PHE:CE1	2.46	0.50
7:G:108:ILE:N	7:G:108:ILE:HD13	2.27	0.50
10:J:90:ARG:O	10:J:90:ARG:HG3	2.10	0.50
10:X:29:ASN:H	10:X:29:ASN:HD22	1.59	0.50
12:Z:4:LEU:HD12	12:Z:161:ILE:HD11	1.92	0.50
1:O:145:SER:HA	1:O:228:ALA:HB1	1.92	0.50
6:T:24:TYR:N	6:T:24:TYR:CD1	2.79	0.50
4:R:78:LEU:HD12	4:R:81:ASP:OD2	2.11	0.50
12:Z:182:GLU:HG3	12:Z:182:GLU:O	2.10	0.50
7:G:23:VAL:O	7:G:26:ALA:HB3	2.11	0.50
8:H:156:LYS:NZ	8:H:188:PHE:HD1	2.05	0.50
6:F:121:GLN:HE22	7:G:86:HIS:CD2	2.24	0.50
8:H:40:LYS:HZ2	8:H:182:GLY:HA2	1.75	0.50
12:Z:35:ILE:HD11	12:Z:45:MET:HE2	1.94	0.50
3:Q:59:GLN:N	3:Q:59:GLN:NE2	2.59	0.50
1:A:76:SER:OG	1:A:77:ARG:N	2.44	0.50
6:T:159:THR:OG1	6:T:160:ALA:N	2.42	0.50
9:W:3:ILE:HD12	9:W:44:ALA:CB	2.42	0.50
5:E:37:ALA:CB	5:E:50:VAL:HG12	2.41	0.50
3:Q:156:ASN:HD21	4:R:79:ASN:HB2	1.77	0.50
1:O:41:ASN:HB2	1:O:56:GLN:OE1	2.11	0.50
2:P:108:LYS:HE2	2:P:143:ASN:ND2	2.26	0.50
2:P:66:LEU:HD11	2:P:68:THR:O	2.11	0.50
10:J:133:ALA:HB2	10:J:169:ASP:CB	2.40	0.50
4:R:133:THR:HG23	4:R:150:THR:CG2	2.35	0.50
1:A:98:LYS:HD3	8:H:68:SER:O	2.10	0.50
9:W:196:ARG:NH1	10:X:142:GLU:HG3	2.26	0.50
3:C:228:LYS:HB3	3:C:230:PHE:HE1	1.76	0.50
12:Z:1:THR:HG23	12:Z:33:ARG:CZ	2.42	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:38:THR:HG23	1:A:39:ASN:H	1.76	0.50
14:N:119:LEU:HG	14:N:134:LEU:HD12	1.93	0.50
3:C:120:GLN:O	3:C:123:THR:HB	2.11	0.50
8:H:48:SER:HB2	8:H:94:THR:HB	1.93	0.50
8:V:75:THR:HG22	8:V:111:TYR:HE1	1.75	0.50
5:E:46:VAL:HG23	5:E:153:TYR:HD1	1.76	0.50
5:S:64:ILE:HD12	5:S:64:ILE:H	1.75	0.50
1:O:102:ALA:CB	8:V:65:LEU:HD13	2.42	0.50
6:T:146:GLU:O	6:T:153:VAL:HA	2.11	0.50
1:A:195:ASN:O	1:A:196:GLU:HB2	2.11	0.50
3:C:13:PHE:H	4:D:19:GLN:HE22	1.57	0.50
1:O:131:ARG:HH12	1:O:133:TYR:HB3	1.76	0.50
10:J:149:LEU:HD12	10:J:154:LEU:HA	1.92	0.50
12:L:1:THR:HG23	12:L:33:ARG:CZ	2.42	0.50
13:M:6:ILE:HD12	13:M:6:ILE:N	2.27	0.50
9:W:158:ALA:O	9:W:161:ALA:HB3	2.11	0.50
14:N:171:ASN:ND2	14:N:174:ARG:HH21	2.10	0.50
3:C:70:ASN:HD22	3:C:71:ASP:H	1.59	0.50
14:N:142:MET:HG3	9:W:132:LEU:HB3	1.92	0.50
2:B:68:THR:O	2:B:70:ASP:N	2.44	0.50
8:H:18:SER:OG	8:H:171:GLY:HA3	2.12	0.50
3:Q:70:ASN:ND2	3:Q:71:ASP:N	2.58	0.50
7:G:229:PHE:HD2	7:G:231:LYS:HE3	1.75	0.50
2:B:12:PHE:CE2	3:C:130:PRO:HG2	2.46	0.50
1:A:25:LEU:N	1:A:25:LEU:HD12	2.27	0.50
7:U:197:LYS:O	7:U:201:LEU:HD13	2.12	0.50
1:A:179:THR:HG23	2:B:55:LEU:HD12	1.92	0.50
6:F:185:ASN:ND2	6:F:185:ASN:C	2.64	0.50
8:V:53:GLN:HE22	9:W:119:THR:H	1.59	0.50
11:Y:34:THR:CG2	11:Y:35:ARG:N	2.74	0.50
6:T:36:VAL:CG2	6:T:160:ALA:HB2	2.42	0.50
10:J:6:MET:CE	10:J:145:TYR:HD1	2.24	0.50
10:X:100:VAL:HG12	10:X:101:ALA:N	2.25	0.50
6:F:144:LEU:HD23	6:F:144:LEU:C	2.32	0.50
11:K:82:PHE:O	11:K:85:GLN:HB3	2.12	0.50
13:M:132:ALA:HB1	13:M:186:HIS:CE1	2.47	0.50
8:H:190:PRO:O	8:H:192:GLU:N	2.45	0.50
14:N:189:LEU:HD23	14:N:190:ALA:N	2.27	0.50
2:P:190:HIS:CE1	2:P:194:LEU:HD11	2.47	0.50
8:H:126:ILE:HD12	8:H:134:ILE:CG1	2.40	0.50
1:A:125:SER:HA	1:A:128:TYR:CD2	2.47	0.50
11:K:5:GLY:HA2	11:K:13:ILE:O	2.12	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
8:V:40:LYS:HZ2	8:V:182:GLY:HA2	1.77	0.50
1:O:218:PHE:CD2	1:O:223:LEU:HD11	2.46	0.50
2:P:227:ILE:HG12	9:W:186:TYR:CD2	2.46	0.50
9:W:104:ASP:O	9:W:106:THR:N	2.41	0.50
9:I:153:LYS:HD3	9:I:153:LYS:C	2.33	0.50
7:G:193:LYS:HE2	7:G:193:LYS:HA	3.94	0.50
9:W:175:VAL:HG12	9:W:176:CYS:N	2.27	0.50
1:O:38:THR:HG23	1:O:39:ASN:H	1.76	0.49
6:F:16:THR:O	7:G:28:LYS:HB3	2.12	0.49
2:B:130:PHE:O	2:B:152:PRO:HB3	2.12	0.49
11:Y:151:MET:HB3	11:Y:155:GLU:HB2	1.94	0.49
5:E:203:ILE:O	5:E:207:VAL:HG22	2.11	0.49
3:Q:114:ARG:HB2	3:Q:114:ARG:NH1	2.27	0.49
5:S:203:ILE:O	5:S:207:VAL:HG22	2.12	0.49
2:P:29:LYS:NZ	2:P:29:LYS:HB3	2.27	0.49
1:O:28:VAL:O	1:O:31:ALA:HB3	2.12	0.49
2:P:185:LEU:HD21	2:P:213:ILE:HD13	1.94	0.49
7:U:24:GLU:O	7:U:27:VAL:HB	2.12	0.49
13:M:91:LYS:HB3	13:M:94:PHE:O	2.12	0.49
11:K:160:LEU:HD23	11:K:161:LYS:N	2.27	0.49
1:A:146:VAL:HA	1:A:151:GLY:O	2.12	0.49
4:R:31:THR:HB	4:R:63:LYS:HZ1	1.76	0.49
5:S:15:PHE:CD1	5:S:21:LEU:HD21	2.46	0.49
3:Q:133:VAL:CG1	3:Q:134:SER:N	2.74	0.49
1:A:76:SER:HB3	1:A:79:ILE:HD13	1.94	0.49
6:F:92:CYS:HA	6:F:103:LEU:HD22	1.95	0.49
12:L:159:ARG:HD2	12:L:162:LEU:HD23	1.94	0.49
11:Y:118:ILE:HA	11:Y:123:THR:O	2.12	0.49
1:A:73:PHE:N	1:A:73:PHE:CD1	2.80	0.49
1:O:43:LEU:HD12	1:O:178:ILE:HG22	1.93	0.49
2:P:23:TYR:O	2:P:26:THR:HB	2.12	0.49
1:A:43:LEU:HD12	1:A:178:ILE:HG22	1.93	0.49
3:Q:163:ILE:HG13	3:Q:164:SER:N	2.27	0.49
14:N:8:TYR:CE2	14:N:162:VAL:HG22	2.47	0.49
8:V:175:MET:HB2	8:V:186:LEU:HB2	1.94	0.49
14:N:13:ILE:HG22	14:N:14:ILE:N	2.28	0.49
6:T:36:VAL:HG22	6:T:160:ALA:HB2	1.93	0.49
12:Z:159:ARG:O	12:Z:162:LEU:HB3	2.13	0.49
8:V:36:ARG:HB2	8:V:42:TRP:CZ2	2.47	0.49
1:O:54:ILE:HG13	1:O:225:VAL:HG21	1.94	0.49
6:F:72:LEU:HD23	6:F:132:LEU:HD22	1.93	0.49
7:G:25:TYR:N	7:G:25:TYR:CD2	2.80	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
8:V:110:VAL:O	8:V:121:LYS:HA	2.12	0.49
1:A:91:ARG:HH12	7:G:156:TYR:H	1.60	0.49
3:Q:163:ILE:HD12	3:Q:173:GLN:OE1	2.11	0.49
8:H:1:THR:HA	8:H:33:LYS:HZ3	1.75	0.49
11:Y:3:ILE:O	11:Y:4:LEU:HD23	2.11	0.49
9:I:4:VAL:HG22	9:I:159:ILE:HD11	1.94	0.49
4:R:27:VAL:HG11	4:R:132:SER:HB2	1.94	0.49
10:X:18:LEU:HD12	10:X:175:GLY:HA3	1.94	0.49
6:T:92:CYS:HA	6:T:103:LEU:HD22	1.95	0.49
8:H:66:TYR:CE1	8:H:70:TYR:HB2	2.48	0.49
4:R:112:TYR:O	4:R:116:VAL:HG23	2.12	0.49
3:Q:140:TYR:CD1	3:Q:141:ASP:N	2.80	0.49
11:Y:110:LYS:O	11:Y:112:LYS:HG3	2.12	0.49
9:I:131:SER:O	9:I:135:MET:HB2	2.11	0.49
4:R:31:THR:HB	4:R:63:LYS:HZ3	1.76	0.49
6:T:94:TYR:CE1	6:T:98:VAL:HG21	2.48	0.49
9:W:220:ILE:HG22	9:W:221:CYS:N	2.27	0.49
12:L:110:PRO:O	12:L:111:THR:HG23	2.12	0.49
4:R:176:GLU:OE2	5:S:57:PRO:HD2	2.13	0.49
6:T:171:TYR:CD2	6:T:171:TYR:C	2.85	0.49
11:K:4:LEU:HD22	11:K:131:ALA:HB2	1.95	0.49
5:E:33:LEU:H	5:E:33:LEU:HD12	1.76	0.49
1:A:126:GLN:O	1:A:129:THR:HB	2.12	0.49
1:A:225:VAL:CG1	1:A:226:GLY:N	2.75	0.49
9:I:3:ILE:HD12	9:I:44:ALA:CB	2.42	0.49
11:Y:9:GLN:HE21	11:Y:150:ASP:HA	1.78	0.49
12:Z:4:LEU:HA	12:Z:100:MET:CE	2.43	0.49
4:R:174:PHE:CZ	4:R:178:ASN:ND2	2.80	0.49
7:G:35:THR:CG2	7:G:167:GLY:H	2.26	0.49
9:W:131:SER:O	9:W:135:MET:HB2	2.13	0.49
3:C:188:ASP:N	3:C:188:ASP:OD1	2.45	0.49
6:F:24:TYR:N	6:F:24:TYR:CD1	2.81	0.49
8:V:74:SER:HB3	8:V:77:THR:OG1	2.12	0.49
3:Q:175:LEU:HD13	3:Q:196:THR:HA	1.94	0.49
12:Z:15:ALA:HB1	12:Z:161:ILE:HG13	1.94	0.49
11:Y:95:ARG:CZ	11:Y:95:ARG:HB3	2.43	0.49
8:V:190:PRO:HA	8:V:193:TYR:CE2	2.48	0.49
6:F:144:LEU:C	6:F:145:LEU:HD12	2.32	0.49
8:V:36:ARG:HB2	8:V:42:TRP:CE2	2.47	0.49
2:P:243:ILE:O	2:P:245:ASP:N	2.45	0.49
1:O:248:ILE:HG22	1:O:251:GLN:OE1	2.13	0.49
3:C:70:ASN:ND2	3:C:71:ASP:N	2.60	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:160:LYS:HD3	2:B:179:TRP:CH2	2.47	0.49
4:D:163:THR:HG21	4:D:171:VAL:CG2	2.42	0.49
10:J:51:VAL:HG12	10:J:52:THR:N	2.26	0.49
8:V:126:ILE:HD12	8:V:134:ILE:CG1	2.41	0.49
13:M:117:ASP:OD2	13:M:119:VAL:HG22	2.12	0.49
5:E:178:GLY:HA3	5:E:207:VAL:HG11	1.95	0.49
9:I:1:THR:HB	9:I:46:ALA:HB1	1.94	0.49
3:C:73:ILE:HG12	3:C:108:VAL:HG22	1.94	0.49
1:A:133:TYR:O	1:A:134:MET:HB3	2.12	0.49
11:Y:70:GLU:O	11:Y:71:ASP:HB3	2.12	0.49
11:K:34:THR:CG2	11:K:35:ARG:N	2.75	0.49
2:P:44:VAL:CA	2:P:213:ILE:HG22	2.42	0.49
14:N:81:PRO:HD2	14:N:112:GLN:OE1	2.13	0.49
1:A:131:ARG:HH11	1:A:131:ARG:HG2	1.78	0.49
6:F:2:PHE:HD1	6:F:3:ARG:HG2	1.75	0.49
1:O:117:LEU:O	1:O:121:MET:HG2	2.13	0.49
12:L:206:SER:O	12:L:207:PHE:HB2	2.13	0.49
2:P:44:VAL:HG23	2:P:213:ILE:HG22	1.95	0.48
8:H:8:PHE:HE2	8:H:148:LYS:CA	2.21	0.48
2:B:156:TYR:HD1	2:B:156:TYR:O	1.95	0.48
2:P:196:LEU:O	2:P:200:VAL:HG23	2.13	0.48
3:C:181:LYS:O	3:C:184:MET:HB2	2.13	0.48
7:G:245:GLU:C	7:G:247:ASN:H	2.16	0.48
7:U:25:TYR:N	7:U:25:TYR:CD2	2.79	0.48
9:W:152:ILE:HG22	9:W:153:LYS:N	2.27	0.48
12:Z:123:LYS:HG3	12:Z:124:GLY:N	2.28	0.48
9:I:48:THR:O	9:I:51:ASP:HB2	2.13	0.48
12:L:38:ASN:HB2	12:L:39:PRO:HD2	1.95	0.48
4:D:28:LYS:O	4:D:166:ARG:HB3	2.13	0.48
6:F:36:VAL:CG2	6:F:160:ALA:HB2	2.43	0.48
3:C:198:SER:OG	3:C:199:LYS:N	2.47	0.48
1:O:220:LYS:O	1:O:220:LYS:NZ	2.41	0.48
11:K:119:ASP:OD2	11:K:123:THR:HB	2.12	0.48
3:C:140:TYR:CD1	3:C:140:TYR:C	2.87	0.48
1:A:162:TYR:CD1	1:A:162:TYR:C	2.86	0.48
9:W:153:LYS:HD3	9:W:153:LYS:C	2.33	0.48
4:D:174:PHE:CZ	4:D:178:ASN:ND2	2.81	0.48
4:R:201:GLU:O	4:R:204:GLN:NE2	2.45	0.48
3:Q:188:ASP:OD1	3:Q:188:ASP:N	2.46	0.48
8:H:80:SER:O	8:H:83:LYS:HB3	2.14	0.48
2:B:16:GLY:HA3	3:C:28:SER:HB2	1.96	0.48
7:U:246:ILE:HG23	7:U:246:ILE:O	2.11	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
8:V:131:SER:O	8:V:134:ILE:HG12	2.13	0.48
12:L:15:ALA:HB1	12:L:161:ILE:HG13	1.96	0.48
10:X:15:ALA:HB2	10:X:178:VAL:HG13	1.95	0.48
8:V:18:SER:OG	8:V:171:GLY:HA3	2.14	0.48
9:W:45:GLY:HA2	9:W:98:LEU:HB3	1.95	0.48
14:N:84:ILE:HG13	14:N:84:ILE:H	1.46	0.48
5:E:142:LEU:HB2	5:E:158:ALA:CB	2.41	0.48
1:A:124:LEU:HD23	1:A:127:ILE:HD12	1.94	0.48
14:N:45:ILE:CG2	14:N:52:MET:HG3	2.43	0.48
8:V:67:THR:O	8:V:69:GLN:N	2.46	0.48
9:I:220:ILE:HG22	9:I:221:CYS:N	2.27	0.48
11:Y:168:GLU:HG2	11:Y:175:PHE:CZ	2.46	0.48
4:D:36:VAL:HG13	4:D:195:THR:HG23	1.94	0.48
11:K:95:ARG:HB3	11:K:95:ARG:CZ	2.43	0.48
3:Q:39:MET:HE1	3:Q:146:TYR:HB3	1.95	0.48
6:F:171:TYR:CD2	6:F:171:TYR:C	2.87	0.48
1:O:91:ARG:HH12	7:U:156:TYR:H	1.61	0.48
6:F:43:HIS:HB3	6:F:215:ILE:HD11	1.94	0.48
7:G:137:PHE:CD2	7:G:137:PHE:N	2.81	0.48
11:K:160:LEU:HD23	11:K:160:LEU:C	2.34	0.48
1:A:225:VAL:HG12	1:A:226:GLY:N	2.29	0.48
3:Q:165:VAL:N	3:Q:169:THR:HG21	2.29	0.48
5:S:22:PHE:CD2	5:S:22:PHE:N	2.82	0.48
6:F:185:ASN:ND2	6:F:188:GLU:H	2.11	0.48
13:M:186:HIS:HD2	13:M:188:GLN:H	1.62	0.48
6:T:126:ARG:NH1	6:T:127:PRO:O	2.47	0.48
9:W:97:TYR:CD1	9:W:97:TYR:N	2.81	0.48
10:J:18:LEU:HD12	10:J:175:GLY:HA3	1.96	0.48
6:F:197:ILE:HG23	6:F:198:SER:N	2.28	0.48
5:E:56:SER:HB3	5:E:57:PRO:HD2	1.95	0.48
8:V:186:LEU:HD22	8:V:188:PHE:HE2	1.78	0.48
10:X:184:ASP:CG	10:X:185:GLU:N	2.65	0.48
10:X:16:CYS:SG	10:X:34:ILE:HG13	2.53	0.48
1:O:220:LYS:O	1:O:221:ASN:HB2	2.12	0.48
8:V:143:ARG:HH11	8:V:143:ARG:HB3	1.77	0.48
4:R:36:VAL:HG13	4:R:195:THR:HG23	1.95	0.48
1:O:144:VAL:O	1:O:145:SER:HB3	2.13	0.48
7:U:245:GLU:C	7:U:247:ASN:H	2.16	0.48
2:P:157:PHE:CE2	3:Q:52:VAL:HG11	2.49	0.48
4:D:48:ARG:HH11	4:D:48:ARG:HG2	1.77	0.48
2:B:29:LYS:HB3	2:B:29:LYS:NZ	2.29	0.48
2:B:238:LEU:CD1	2:B:238:LEU:N	2.77	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:U:150:LEU:HD11	7:U:154:GLY:CA	2.44	0.48
7:G:23:VAL:O	7:G:27:VAL:HG23	2.14	0.48
3:C:208:TYR:CG	3:C:209:ASP:N	2.81	0.48
5:E:133:LEU:H	5:E:133:LEU:HD22	1.78	0.48
7:U:77:TYR:HB3	7:U:135:THR:HG23	1.96	0.48
8:V:55:ILE:O	8:V:59:VAL:HG23	2.14	0.48
8:V:75:THR:HG22	8:V:111:TYR:CE1	2.49	0.48
6:T:121:GLN:HE22	7:U:86:HIS:CD2	2.25	0.48
12:L:53:GLN:OE1	13:M:121:SER:HA	2.13	0.48
8:V:89:ASN:O	8:V:91:ASP:N	2.47	0.48
13:M:43:MET:HG2	13:M:44:SER:N	2.27	0.48
2:P:161:ALA:O	3:Q:56:LEU:HD23	2.14	0.48
7:G:194:GLN:HA	7:G:194:GLN:NE2	2.28	0.48
1:O:179:THR:HG23	2:P:55:LEU:HD12	1.96	0.48
1:A:123:ASN:O	1:A:127:ILE:HG13	2.14	0.48
2:B:226:GLY:HA3	9:I:186:TYR:O	2.14	0.48
3:Q:37:GLY:HA2	3:Q:45:VAL:O	2.13	0.48
11:K:152:THR:HG23	11:K:155:GLU:OE1	2.14	0.48
1:O:131:ARG:O	1:O:132:ALA:HB3	2.13	0.48
1:O:128:TYR:CD1	1:O:133:TYR:HE1	2.27	0.48
8:H:55:ILE:O	8:H:59:VAL:HG23	2.13	0.48
7:G:135:THR:O	7:G:149:MET:HA	2.13	0.48
7:G:48:ALA:HB2	7:G:215:ILE:HG23	1.95	0.48
14:N:19:LEU:HD11	14:N:26:LEU:HD12	1.95	0.48
2:P:187:ASP:O	2:P:190:HIS:HB3	2.13	0.48
9:I:175:VAL:HG12	9:I:176:CYS:N	2.28	0.48
4:R:11:PHE:H	5:S:23:GLN:NE2	2.05	0.48
8:H:185:ARG:HG3	8:H:185:ARG:NH1	2.28	0.48
2:P:34:SER:OG	2:P:47:THR:HB	2.14	0.48
1:O:155:TYR:HD2	1:O:164:VAL:O	1.97	0.48
10:X:15:ALA:HB2	10:X:178:VAL:HG22	1.96	0.48
9:W:3:ILE:HG22	9:W:16:ALA:CB	2.44	0.48
12:Z:64:ARG:NH2	12:Z:68:LEU:HD21	2.28	0.48
1:O:73:PHE:N	1:O:73:PHE:CD1	2.80	0.48
9:I:90:TYR:N	9:I:90:TYR:CD2	2.82	0.48
4:D:176:GLU:OE2	5:E:57:PRO:HD2	2.14	0.48
1:A:128:TYR:HE1	1:A:133:TYR:HH	1.52	0.48
7:U:197:LYS:HG3	7:U:201:LEU:HD11	1.96	0.48
6:T:16:THR:O	7:U:28:LYS:HB3	2.14	0.48
4:R:233:VAL:O	4:R:237:GLU:HG2	2.13	0.48
1:O:25:LEU:HD12	1:O:25:LEU:N	2.29	0.47
3:C:186:VAL:HG13	3:C:187:ASP:N	2.29	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:U:136:ILE:HG12	7:U:149:MET:HG3	1.96	0.47
11:Y:160:LEU:HD23	11:Y:161:LYS:N	2.29	0.47
14:N:3:VAL:HG11	14:N:44:GLY:HA3	1.96	0.47
3:Q:165:VAL:CA	3:Q:169:THR:HG21	2.44	0.47
2:P:122:THR:O	2:P:124:SER:N	2.47	0.47
6:T:133:LEU:C	6:T:134:ILE:HD12	2.34	0.47
6:F:118:LYS:H	6:F:118:LYS:HD2	1.78	0.47
3:Q:44:ILE:HD11	3:Q:146:TYR:HB3	1.96	0.47
5:S:178:GLY:HA3	5:S:207:VAL:HG11	1.96	0.47
2:B:74:VAL:HG22	2:B:75:TYR:N	2.29	0.47
4:R:28:LYS:O	4:R:166:ARG:HB3	2.13	0.47
4:D:78:LEU:HD12	4:D:81:ASP:OD2	2.13	0.47
3:C:175:LEU:HD13	3:C:196:THR:HA	1.96	0.47
1:O:124:LEU:HD23	1:O:127:ILE:HD12	1.96	0.47
6:F:94:TYR:CE1	6:F:98:VAL:HG21	2.50	0.47
2:B:122:THR:O	2:B:124:SER:N	2.47	0.47
2:B:24:ALA:C	2:B:26:THR:H	2.17	0.47
7:G:19:ARG:CG	7:G:19:ARG:HH11	2.27	0.47
4:D:112:TYR:O	4:D:116:VAL:HG23	2.13	0.47
11:K:50:GLY:HA3	12:L:118:ASP:O	2.14	0.47
13:M:48:PHE:H	13:M:98:VAL:HG13	1.79	0.47
3:C:156:ASN:HD21	4:D:79:ASN:HB2	1.79	0.47
6:F:123:TYR:CG	6:F:124:GLY:N	2.82	0.47
6:T:42:THR:HG22	6:T:218:LYS:NZ	2.29	0.47
12:L:16:VAL:O	12:L:175:VAL:HA	2.13	0.47
7:G:24:GLU:O	7:G:27:VAL:HB	2.14	0.47
14:N:212:ASP:O	14:N:214:ALA:N	2.47	0.47
8:H:133:PHE:HA	8:V:133:PHE:HA	1.96	0.47
1:A:126:GLN:NE2	1:A:127:ILE:HA	2.30	0.47
2:P:224:TYR:OH	2:P:230:ASP:HB3	2.14	0.47
1:A:144:VAL:HG12	1:A:154:ILE:HG12	1.97	0.47
3:Q:114:ARG:HB2	3:Q:114:ARG:HH11	1.79	0.47
12:L:199:LYS:O	12:L:202:GLU:HB3	2.15	0.47
6:T:213:ILE:HG22	6:T:214:ALA:N	2.28	0.47
6:F:68:GLU:O	6:F:222:PHE:N	2.37	0.47
8:H:110:VAL:O	8:H:121:LYS:HA	2.14	0.47
2:P:68:THR:C	2:P:70:ASP:H	2.18	0.47
11:K:87:LEU:HA	11:K:90:SER:HB3	1.96	0.47
3:C:185:LYS:HE3	3:C:185:LYS:HB3	1.68	0.47
8:H:4:MET:CB	8:H:126:ILE:HG22	2.44	0.47
4:D:163:THR:HG21	4:D:171:VAL:HG23	1.97	0.47
8:H:38:HIS:CE1	8:H:67:THR:HG21	2.48	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
9:W:177:VAL:O	9:W:184:ALA:HA	2.14	0.47
9:W:7:LYS:HB3	9:W:12:VAL:HB	1.97	0.47
1:O:148:GLU:CD	1:O:148:GLU:H	2.17	0.47
9:W:90:TYR:CD2	9:W:90:TYR:N	2.82	0.47
10:J:33:LYS:HD2	10:J:33:LYS:N	2.30	0.47
7:G:194:GLN:NE2	7:G:197:LYS:HZ3	2.12	0.47
2:P:197:LYS:HA	2:P:204:PHE:CZ	2.49	0.47
7:U:19:ARG:CG	7:U:19:ARG:HH11	2.27	0.47
3:Q:198:SER:OG	3:Q:199:LYS:HG3	2.14	0.47
3:Q:114:ARG:HG3	3:Q:115:LEU:N	2.26	0.47
8:H:97:ILE:HD12	8:H:98:ILE:N	2.29	0.47
14:N:167:GLU:HG3	14:N:168:ALA:N	2.30	0.47
7:G:188:ALA:O	7:G:191:ALA:HB3	2.14	0.47
8:H:189:TYR:O	8:H:192:GLU:HB2	2.14	0.47
11:K:135:SER:O	11:K:139:THR:HG23	2.13	0.47
2:P:211:LEU:CD2	2:P:238:LEU:HD22	2.45	0.47
9:I:21:THR:O	9:I:22:GLN:HB2	2.14	0.47
8:H:89:ASN:O	8:H:91:ASP:N	2.48	0.47
8:H:138:CYS:HA	8:H:154:PHE:CZ	2.49	0.47
1:A:126:GLN:NE2	1:A:126:GLN:C	2.68	0.47
1:A:131:ARG:NH1	1:A:133:TYR:HB3	2.30	0.47
4:R:162:GLN:HG3	4:R:163:THR:N	2.29	0.47
13:M:14:LEU:HA	13:M:14:LEU:HD23	1.77	0.47
3:Q:208:TYR:CG	3:Q:209:ASP:N	2.82	0.47
8:V:3:ILE:HG22	8:V:16:ALA:CB	2.45	0.47
2:B:64:VAL:HG13	2:B:237:LYS:HE2	1.95	0.47
10:J:29:ASN:O	10:J:30:LYS:HG3	2.14	0.47
1:O:24:ARG:O	1:O:25:LEU:C	2.53	0.47
2:P:64:VAL:HG13	2:P:237:LYS:HE2	1.96	0.47
6:F:36:VAL:HG22	6:F:160:ALA:HB2	1.95	0.47
8:H:110:VAL:HG12	8:H:122:LEU:O	2.15	0.47
3:C:195:LYS:O	3:C:199:LYS:HD3	2.15	0.47
3:C:39:MET:HE1	3:C:146:TYR:HB3	1.97	0.47
3:C:198:SER:OG	3:C:199:LYS:HG3	2.14	0.47
2:B:197:LYS:HA	2:B:204:PHE:CZ	2.50	0.47
1:A:20:SER:OG	1:A:24:ARG:N	2.41	0.47
7:U:108:ILE:N	7:U:108:ILE:HD13	2.30	0.47
1:O:216:THR:CG2	1:O:217:GLU:N	2.78	0.47
7:G:121:ALA:HA	7:G:124:LEU:HD12	1.96	0.47
6:T:70:MET:CE	6:T:105:VAL:HG22	2.44	0.47
6:T:105:VAL:CG1	6:T:145:LEU:HD13	2.45	0.47
7:U:85:ARG:HH11	7:U:85:ARG:HG2	1.80	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
9:W:90:TYR:HD2	9:W:90:TYR:N	2.13	0.47
14:N:124:LEU:HD23	14:N:125:LEU:H	1.79	0.47
1:O:195:ASN:O	1:O:196:GLU:HB2	2.13	0.47
10:X:150:GLU:HB2	10:X:153:ASP:OD2	2.14	0.47
2:P:24:ALA:C	2:P:26:THR:H	2.16	0.47
13:M:213:ASP:HB2	9:W:19:ARG:NH2	2.29	0.47
8:V:107:LYS:CG	8:V:108:GLY:H	2.28	0.47
9:W:21:THR:O	9:W:22:GLN:HB2	2.14	0.47
4:D:149:GLN:HG2	4:D:150:THR:N	2.30	0.47
11:K:118:ILE:HA	11:K:123:THR:O	2.14	0.47
12:Z:12:ILE:CD1	12:Z:102:CYS:HB3	2.45	0.47
11:Y:38:SER:CB	11:Y:39:PRO:HD2	2.44	0.47
4:D:233:VAL:O	4:D:237:GLU:HG2	2.15	0.47
3:C:24:TYR:O	3:C:27:GLU:HG3	2.14	0.47
9:I:105:PRO:O	9:I:106:THR:HG23	2.15	0.47
1:A:53:VAL:C	1:A:54:ILE:HD12	2.36	0.47
5:S:170:LYS:HD2	5:S:171:ALA:N	2.29	0.47
12:Z:4:LEU:CD1	12:Z:15:ALA:HB3	2.45	0.47
10:X:49:THR:HB	11:Y:122:GLY:O	2.15	0.47
5:S:27:SER:O	5:S:30:ALA:HB3	2.14	0.47
1:A:60:PRO:HG2	1:A:61:ASP:H	1.80	0.47
4:D:212:ILE:HG21	4:D:224:LEU:HD22	1.97	0.47
7:G:71:ARG:NH1	14:N:64:THR:CG2	2.77	0.47
8:H:143:ARG:HH11	8:H:143:ARG:HB3	1.80	0.47
9:I:102:GLY:HA2	9:I:178:MET:SD	2.54	0.47
3:C:96:GLN:HB3	10:J:60:TYR:CE2	2.49	0.47
4:R:228:GLU:CA	4:R:231:GLN:HE21	2.24	0.47
8:H:153:ASP:HA	8:H:156:LYS:HB2	1.97	0.47
3:C:163:ILE:HG13	3:C:164:SER:H	1.79	0.47
8:V:4:MET:SD	8:V:159:LEU:CD1	3.03	0.47
5:S:124:GLY:N	5:S:132:ARG:HB2	2.29	0.47
11:Y:3:ILE:HD12	11:Y:44:SER:HB2	1.96	0.47
2:P:218:ASN:HB3	2:P:221:LEU:HD13	1.96	0.47
7:U:85:ARG:NH1	7:U:85:ARG:HG2	2.30	0.47
3:Q:140:TYR:C	3:Q:140:TYR:CD1	2.89	0.47
9:W:10:ASN:C	9:W:180:ILE:HG13	2.35	0.47
1:O:156:LYS:HE2	1:O:166:TYR:CE2	2.50	0.47
3:Q:69:LEU:CD2	3:Q:92:ARG:HG3	2.45	0.47
2:B:64:VAL:CG1	2:B:237:LYS:HE2	2.45	0.46
11:K:18:LYS:HD3	11:K:179:ILE:HG13	1.96	0.46
5:E:165:TYR:CE1	6:F:53:ALA:HB2	2.50	0.46
3:Q:185:LYS:HD2	3:Q:186:VAL:H	1.79	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:224:TYR:OH	2:B:230:ASP:HB3	2.14	0.46
13:M:59:PHE:O	13:M:62:SER:N	2.48	0.46
7:U:49:VAL:HG22	7:U:50:GLU:N	2.29	0.46
6:F:146:GLU:O	6:F:153:VAL:HA	2.15	0.46
5:S:39:GLY:O	5:S:169:ALA:HA	2.15	0.46
4:R:57:THR:OG1	4:R:58:ARG:N	2.48	0.46
7:U:35:THR:CG2	7:U:167:GLY:H	2.28	0.46
11:K:22:ARG:HB2	11:K:27:LEU:HD11	1.97	0.46
5:E:136:ARG:HB2	5:E:137:PRO:CD	2.39	0.46
2:P:189:ILE:O	2:P:193:LEU:HD12	2.15	0.46
5:S:81:LEU:HD12	5:S:81:LEU:HA	1.69	0.46
9:W:1:THR:HB	9:W:46:ALA:HB1	1.97	0.46
6:F:54:ASP:CG	6:F:55:GLU:H	2.19	0.46
5:E:237:ALA:O	5:E:240:ILE:HB	2.16	0.46
3:Q:129:ARG:HG3	3:Q:129:ARG:O	2.14	0.46
1:O:120:ARG:HA	1:O:123:ASN:HB2	1.98	0.46
9:I:90:TYR:N	9:I:90:TYR:HD2	2.13	0.46
7:G:142:LYS:HG3	8:H:105:LYS:NZ	2.31	0.46
2:P:145:PHE:HE1	2:P:214:ILE:HG22	1.80	0.46
2:P:74:VAL:HG22	2:P:75:TYR:N	2.30	0.46
11:K:88:ALA:O	11:K:91:ILE:HG22	2.15	0.46
1:A:155:TYR:HD2	1:A:165:GLY:HA2	1.78	0.46
1:A:16:ILE:CG2	1:A:17:THR:N	2.77	0.46
11:K:52:THR:HG23	11:K:53:VAL:N	2.26	0.46
2:P:193:LEU:O	2:P:197:LYS:N	2.48	0.46
7:G:169:GLN:H	7:G:169:GLN:CD	2.18	0.46
11:K:3:ILE:CD1	11:K:16:SER:HB3	2.45	0.46
1:O:123:ASN:ND2	2:P:84:VAL:HG12	2.30	0.46
11:K:8:VAL:HG23	11:K:9:GLN:H	1.80	0.46
3:C:114:ARG:HG3	3:C:115:LEU:N	2.27	0.46
8:H:102:TYR:HA	8:H:108:GLY:HA2	1.97	0.46
7:U:77:TYR:N	7:U:77:TYR:CD2	2.83	0.46
8:V:9:LYS:HG3	8:V:145:ASN:OD1	2.16	0.46
2:P:200:VAL:HG21	2:P:204:PHE:CD1	2.51	0.46
5:S:8:TYR:O	5:S:9:ASP:CB	2.63	0.46
4:D:181:ARG:HH22	5:E:60:GLU:HG2	1.80	0.46
11:K:168:GLU:HG2	11:K:175:PHE:CZ	2.48	0.46
1:A:220:LYS:O	1:A:221:ASN:HB2	2.15	0.46
1:O:117:LEU:HD12	1:O:121:MET:HG2	1.97	0.46
5:S:165:TYR:HE2	6:T:60:GLN:HB2	1.79	0.46
3:C:107:PRO:HB2	3:C:110:ILE:HD12	1.97	0.46
6:F:126:ARG:NH1	6:F:127:PRO:O	2.49	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:U:106:ILE:HA	7:U:107:PRO:HD3	1.81	0.46
11:K:3:ILE:HD12	11:K:44:SER:HB2	1.97	0.46
14:N:19:LEU:HD13	14:N:20:GLY:N	2.29	0.46
2:B:112:SER:HA	2:B:156:TYR:CE2	2.50	0.46
6:T:216:VAL:HB	6:T:222:PHE:HD2	1.80	0.46
11:Y:152:THR:OG1	11:Y:155:GLU:HG3	2.15	0.46
4:R:159:TRP:CZ2	5:S:59:LEU:HD23	2.50	0.46
7:G:193:LYS:HE2	7:G:193:LYS:HB3	1.73	0.46
6:F:164:ARG:HH22	6:F:202:ARG:HB3	1.80	0.46
6:T:111:LEU:O	6:T:115:LYS:HB2	2.15	0.46
10:X:90:ARG:O	10:X:90:ARG:HG3	2.16	0.46
1:O:131:ARG:NH1	1:O:133:TYR:HB3	2.30	0.46
4:D:31:THR:HB	4:D:63:LYS:HZ1	1.80	0.46
3:Q:185:LYS:HD2	3:Q:186:VAL:N	2.31	0.46
1:A:112:MET:HA	1:A:113:PRO:HD3	1.73	0.46
1:A:33:LYS:H	1:A:33:LYS:CD	2.22	0.46
2:P:12:PHE:HE2	3:Q:130:PRO:HG2	1.80	0.46
10:J:117:LEU:N	10:J:117:LEU:HD23	2.30	0.46
2:P:226:GLY:HA3	9:W:186:TYR:O	2.15	0.46
3:Q:191:GLU:HG2	3:Q:195:LYS:HE2	1.96	0.46
6:T:36:VAL:CG1	6:T:37:GLY:N	2.79	0.46
9:W:104:ASP:C	9:W:106:THR:H	2.19	0.46
2:B:74:VAL:HG22	2:B:75:TYR:H	1.79	0.46
2:B:161:ALA:O	3:C:56:LEU:HD23	2.16	0.46
13:M:137:ILE:HG23	13:M:178:SER:HB3	1.98	0.46
14:N:133:THR:O	14:N:134:LEU:HD23	2.15	0.46
3:C:185:LYS:HD2	3:C:186:VAL:H	1.80	0.46
8:H:138:CYS:HA	8:H:154:PHE:CE1	2.50	0.46
7:U:49:VAL:HG11	7:U:65:LYS:HB2	1.98	0.46
10:X:98:PRO:HG2	10:X:115:PHE:CD1	2.51	0.46
13:M:190:GLY:O	13:M:191:ASP:HB2	2.14	0.46
7:G:204:GLU:HG3	7:G:207:LYS:HE2	1.98	0.46
4:R:221:ILE:O	4:R:222:VAL:HB	2.15	0.46
7:U:169:GLN:HA	7:U:172:LYS:HB2	1.96	0.46
9:I:38:SER:HB2	9:I:41:ILE:CD1	2.45	0.46
12:L:36:GLU:HA	12:L:42:LEU:HD23	1.98	0.46
12:Z:36:GLU:HA	12:Z:42:LEU:HD23	1.98	0.46
5:S:225:GLN:HA	5:S:225:GLN:NE2	2.30	0.46
11:K:-1:MET:HG2	11:K:1:ASP:H	1.81	0.46
1:O:68:THR:HG21	7:U:158:GLY:CA	2.42	0.46
7:G:197:LYS:CG	7:G:201:LEU:HD21	2.46	0.46
3:C:89:ASN:O	3:C:93:ILE:HG13	2.15	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:77:VAL:CG1	3:C:78:ALA:N	2.79	0.46
1:O:146:VAL:HA	1:O:151:GLY:O	2.14	0.46
8:H:188:PHE:N	8:H:188:PHE:CD2	2.84	0.46
9:W:72:ARG:CG	9:W:72:ARG:HH11	2.27	0.46
10:J:37:TYR:O	10:J:40:VAL:HG23	2.16	0.46
13:M:51:ASP:OD2	13:M:96:TYR:HA	2.15	0.46
1:A:54:ILE:HG13	1:A:225:VAL:CG2	2.46	0.46
14:N:153:ARG:CG	14:N:153:ARG:HH11	2.23	0.46
1:O:60:PRO:HG2	1:O:61:ASP:H	1.81	0.46
12:L:98:GLY:O	12:L:99:THR:HB	2.15	0.46
5:S:240:ILE:O	5:S:243:LEU:HB3	2.16	0.46
12:Z:199:LYS:O	12:Z:202:GLU:HB3	2.16	0.46
3:Q:68:LYS:NZ	10:X:66:LYS:NZ	2.64	0.46
11:Y:190:GLN:C	11:Y:192:ASP:H	2.18	0.46
5:S:244:LYS:O	5:S:244:LYS:HG2	2.14	0.46
1:O:16:ILE:CG2	1:O:17:THR:N	2.77	0.46
1:O:22:GLU:O	1:O:24:ARG:HG2	2.16	0.46
2:P:130:PHE:O	2:P:152:PRO:HB3	2.15	0.46
6:F:40:SER:HA	6:F:180:ILE:HD12	1.97	0.46
11:K:22:ARG:O	11:K:24:ILE:N	2.48	0.46
3:C:59:GLN:N	3:C:59:GLN:NE2	2.64	0.46
2:P:200:VAL:HG12	2:P:201:GLU:N	2.31	0.46
9:I:3:ILE:HD12	9:I:44:ALA:HB3	1.98	0.46
12:Z:85:ASN:O	12:Z:89:GLN:HG2	2.15	0.46
3:Q:39:MET:CE	3:Q:146:TYR:HB3	2.46	0.46
13:M:133:ALA:O	13:M:134:ALA:C	2.54	0.45
8:H:82:PHE:HB2	8:H:113:ILE:CD1	2.46	0.45
6:F:40:SER:OG	6:F:41:ASN:N	2.49	0.45
6:F:63:ILE:O	6:F:64:ILE:HG13	2.17	0.45
1:A:128:TYR:HB2	1:A:129:THR:H	1.57	0.45
2:B:66:LEU:HD13	2:B:235:PHE:CG	2.51	0.45
7:U:72:HIS:HE1	7:U:105:PRO:HB2	1.80	0.45
8:V:113:ILE:HG12	8:V:119:VAL:HG13	1.98	0.45
10:J:81:LEU:O	10:J:82:VAL:C	2.55	0.45
11:K:38:SER:CB	11:K:39:PRO:HD2	2.46	0.45
13:M:59:PHE:HA	13:M:62:SER:OG	2.15	0.45
8:V:6:VAL:C	8:V:12:VAL:HG23	2.36	0.45
7:U:47:PHE:CE1	7:U:137:PHE:HA	2.52	0.45
5:S:56:SER:HB3	5:S:57:PRO:HD2	1.97	0.45
12:L:182:GLU:OE2	13:M:139:PRO:HG3	47.73	0.45
13:M:2:THR:HG21	13:M:133:ALA:HB3	1.98	0.45
7:U:150:LEU:HD11	7:U:154:GLY:C	2.36	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:E:165:TYR:HE2	6:F:60:GLN:HB2	1.80	0.45
6:F:197:ILE:C	6:F:199:GLN:N	2.69	0.45
7:G:47:PHE:CE1	7:G:137:PHE:HA	2.50	0.45
8:H:75:THR:HG22	8:H:111:TYR:HE1	1.81	0.45
2:P:70:ASP:C	2:P:71:ILE:HG13	2.36	0.45
14:N:62:LEU:C	14:N:62:LEU:HD23	2.36	0.45
2:B:189:ILE:O	2:B:193:LEU:HD12	2.15	0.45
7:G:246:ILE:HG23	7:G:246:ILE:O	2.15	0.45
4:R:45:GLY:C	4:R:46:CYS:SG	2.94	0.45
1:A:207:ILE:HD12	1:A:248:ILE:HD11	1.98	0.45
9:I:45:GLY:HA2	9:I:98:LEU:HB3	1.98	0.45
3:Q:235:ILE:C	3:Q:237:ASP:N	2.70	0.45
3:Q:231:LYS:HA	3:Q:231:LYS:HE3	1.97	0.45
7:G:217:TRP:CD1	7:G:230:VAL:HG22	2.51	0.45
8:H:124:TYR:N	8:H:124:TYR:CD1	2.83	0.45
14:N:198:LEU:HD23	14:N:199:THR:N	2.31	0.45
1:A:120:ARG:HA	1:A:123:ASN:HB2	1.99	0.45
12:Z:105:THR:HG21	12:Z:108:GLU:OE1	2.16	0.45
5:E:37:ALA:HA	5:E:50:VAL:HG12	1.97	0.45
11:Y:22:ARG:HB2	11:Y:27:LEU:HD11	1.97	0.45
13:M:166:LEU:H	13:M:166:LEU:HD12	1.82	0.45
6:F:111:LEU:O	6:F:115:LYS:HB2	2.16	0.45
5:E:225:GLN:HA	5:E:225:GLN:NE2	2.30	0.45
1:O:87:ILE:HG23	1:O:88:PRO:HD3	1.98	0.45
2:P:36:GLY:HA2	2:P:44:VAL:O	2.17	0.45
4:D:45:GLY:C	4:D:46:CYS:SG	2.94	0.45
6:F:129:GLY:O	6:F:130:VAL:HB	2.16	0.45
7:G:217:TRP:HD1	7:G:217:TRP:N	2.15	0.45
14:N:55:ILE:O	14:N:58:LEU:N	2.50	0.45
3:C:142:ASP:OD2	3:C:142:ASP:N	2.49	0.45
8:V:124:TYR:N	8:V:124:TYR:CD1	2.85	0.45
11:Y:52:THR:HG23	11:Y:53:VAL:N	2.27	0.45
11:Y:3:ILE:HD13	11:Y:16:SER:HB3	1.97	0.45
11:Y:7:ARG:NH1	11:Y:7:ARG:HG2	2.30	0.45
13:M:11:PHE:CD1	13:M:11:PHE:N	2.85	0.45
3:Q:106:ILE:HA	3:Q:107:PRO:HD3	1.85	0.45
1:O:243:GLU:O	1:O:243:GLU:HG2	2.16	0.45
4:R:206:GLY:C	4:R:208:LYS:H	2.19	0.45
6:T:118:LYS:HD2	6:T:118:LYS:N	2.31	0.45
7:U:80:LEU:HD23	7:U:80:LEU:HA	1.81	0.45
1:O:76:SER:HB3	1:O:79:ILE:HD13	1.97	0.45
6:F:33:SER:HB3	6:F:62:LYS:HZ3	1.79	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:91:ALA:HB2	3:C:115:LEU:HD21	1.98	0.45
2:B:157:PHE:CE2	3:C:52:VAL:HG11	2.50	0.45
7:G:150:LEU:HD11	7:G:154:GLY:CA	2.47	0.45
1:A:54:ILE:HG13	1:A:225:VAL:HG21	1.97	0.45
7:U:201:LEU:CD1	7:U:201:LEU:N	2.79	0.45
3:Q:150:THR:O	3:Q:157:TYR:HA	2.15	0.45
10:X:149:LEU:HD12	10:X:154:LEU:HA	1.98	0.45
3:Q:119:LYS:HD2	3:Q:153:PRO:HA	1.98	0.45
1:A:83:VAL:HG13	1:A:140:ILE:O	2.16	0.45
1:O:155:TYR:HD2	1:O:165:GLY:HA2	1.81	0.45
7:U:140:VAL:HG12	7:U:141:ASP:H	1.82	0.45
8:V:138:CYS:O	8:V:154:PHE:HZ	1.99	0.45
10:X:136:GLN:OE1	10:X:136:GLN:N	2.48	0.45
1:O:204:GLU:HB3	1:O:248:ILE:HG23	1.98	0.45
1:O:250:GLU:HG2	1:O:251:GLN:H	1.81	0.45
14:N:63:VAL:HG12	14:N:64:THR:N	2.32	0.45
2:B:193:LEU:O	2:B:197:LYS:N	2.49	0.45
2:B:23:TYR:O	2:B:26:THR:HB	2.17	0.45
13:M:80:ALA:O	13:M:83:ASN:HB3	2.17	0.45
4:R:37:LYS:HD3	4:R:147:LEU:HB2	1.99	0.45
3:Q:70:ASN:HB3	3:Q:73:ILE:HB	1.97	0.45
7:U:217:TRP:CD1	7:U:230:VAL:HG22	2.52	0.45
10:X:112:ILE:HD12	10:X:128:ILE:HG12	1.99	0.45
1:O:243:GLU:O	1:O:246:VAL:HB	2.17	0.45
12:Z:206:SER:O	12:Z:207:PHE:HB2	2.17	0.45
10:X:177:VAL:HG21	10:X:188:LYS:HE2	1.98	0.45
3:Q:228:LYS:HB3	3:Q:230:PHE:HE1	1.81	0.45
12:L:122:LEU:HA	12:L:122:LEU:HD23	1.66	0.45
13:M:91:LYS:O	13:M:95:PRO:HA	2.17	0.45
14:N:70:ASN:ND2	14:N:73:ALA:HB2	2.32	0.45
3:C:211:LEU:HD13	3:C:212:GLU:N	2.32	0.45
1:O:167:LYS:HZ2	1:O:192:ASP:HB2	1.82	0.45
2:P:75:TYR:CD2	2:P:76:SER:N	2.84	0.45
3:C:185:LYS:HD2	3:C:186:VAL:N	2.32	0.45
7:G:170:SER:O	7:G:174:GLU:HG2	2.17	0.45
14:N:8:TYR:O	14:N:117:GLN:NE2	2.49	0.45
8:H:1:THR:O	8:H:129:SER:HB3	2.17	0.45
2:P:229:THR:O	2:P:231:LYS:NZ	2.49	0.45
10:J:140:MET:HE3	10:J:144:LEU:HD11	1.99	0.45
10:J:6:MET:HE2	10:J:145:TYR:HD1	1.81	0.45
11:Y:119:ASP:OD2	11:Y:123:THR:HB	2.17	0.45
3:C:129:ARG:HG3	3:C:129:ARG:O	2.17	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:O:43:LEU:HD22	1:O:54:ILE:HB	1.99	0.45
7:G:197:LYS:O	7:G:201:LEU:HD13	2.17	0.45
3:C:94:HIS:CD2	3:C:114:ARG:HD2	2.51	0.45
1:A:24:ARG:O	1:A:25:LEU:C	2.55	0.45
2:B:200:VAL:HG12	2:B:201:GLU:N	2.31	0.45
11:K:49:ALA:O	11:K:52:THR:HG22	2.17	0.45
8:V:186:LEU:HD22	8:V:188:PHE:CE2	2.52	0.45
12:L:54:PHE:C	12:L:54:PHE:HD2	2.20	0.45
8:V:190:PRO:O	8:V:192:GLU:N	2.50	0.45
3:Q:13:PHE:H	4:R:19:GLN:HE22	1.64	0.45
14:N:192:ILE:HD12	14:N:192:ILE:N	2.32	0.45
2:B:44:VAL:HG23	2:B:213:ILE:HG22	1.99	0.45
2:P:44:VAL:CG2	2:P:211:LEU:HD11	2.47	0.45
6:F:176:LEU:O	6:F:178:THR:N	2.50	0.45
14:N:102:LEU:N	14:N:102:LEU:HD12	2.31	0.45
4:D:228:GLU:CA	4:D:231:GLN:HE21	2.23	0.45
13:M:187:ILE:CD1	9:W:24:PRO:HA	2.44	0.45
12:Z:12:ILE:HG22	12:Z:13:ILE:N	2.32	0.45
7:G:166:LYS:HZ2	7:G:206:ASN:HD21	1.64	0.45
10:J:42:LEU:HD12	10:J:43:GLY:H	1.82	0.45
10:X:66:LYS:HA	10:X:71:ARG:O	2.17	0.45
11:K:137:PHE:HB3	12:Z:134:THR:OG1	2.16	0.45
1:O:176:GLN:HA	1:O:179:THR:HB	1.98	0.45
4:R:227:GLU:O	4:R:231:GLN:HG3	2.17	0.45
7:U:194:GLN:NE2	7:U:194:GLN:HA	2.32	0.45
10:J:80:GLN:O	10:J:83:SER:HB3	2.16	0.45
1:O:45:VAL:HG23	1:O:52:VAL:HG23	1.99	0.45
1:O:114:CYS:O	1:O:116:VAL:N	2.50	0.45
5:S:51:GLU:OE2	5:S:53:ARG:HB2	2.17	0.45
7:U:137:PHE:CD2	7:U:137:PHE:N	2.85	0.45
9:W:128:GLY:O	9:W:131:SER:HB2	2.17	0.45
2:B:75:TYR:CD2	2:B:76:SER:N	2.85	0.45
7:U:116:GLY:O	7:U:120:GLN:HB2	2.17	0.45
11:K:190:GLN:C	11:K:192:ASP:H	2.20	0.45
10:J:150:GLU:HB2	10:J:153:ASP:OD2	2.17	0.45
8:H:190:PRO:C	8:H:192:GLU:H	2.20	0.44
7:U:21:PHE:HA	7:U:24:GLU:HG3	2.00	0.44
4:D:212:ILE:CG2	4:D:224:LEU:HD22	2.47	0.44
8:H:95:ALA:H	8:H:115:LEU:HD13	1.81	0.44
3:Q:185:LYS:HB3	3:Q:185:LYS:HE3	1.64	0.44
4:D:57:THR:OG1	4:D:58:ARG:N	2.51	0.44
10:X:29:ASN:ND2	10:X:29:ASN:N	2.64	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
8:V:4:MET:SD	8:V:159:LEU:HD11	2.57	0.44
10:J:15:ALA:CB	10:J:178:VAL:HG22	2.47	0.44
14:N:218:LYS:HA	8:V:32:ASP:OD1	2.18	0.44
1:A:145:SER:HA	1:A:228:ALA:HB1	1.99	0.44
7:G:98:PHE:HD1	7:G:98:PHE:C	2.19	0.44
2:P:157:PHE:N	2:P:157:PHE:CD1	2.85	0.44
7:U:129:ARG:HA	7:U:130:PRO:HD3	1.82	0.44
2:B:36:GLY:HA2	2:B:44:VAL:O	2.18	0.44
14:N:203:ASN:C	14:N:204:LEU:HD13	2.37	0.44
1:O:135:ARG:HD3	7:U:12:SER:O	2.18	0.44
7:G:84:GLY:O	7:G:88:VAL:HG23	2.17	0.44
1:A:124:LEU:HA	1:A:124:LEU:HD23	1.88	0.44
1:A:16:ILE:CG2	1:A:17:THR:H	2.29	0.44
6:T:48:ALA:HB1	6:T:62:LYS:HG3	1.99	0.44
5:E:124:GLY:N	5:E:132:ARG:HB2	2.30	0.44
3:Q:198:SER:OG	3:Q:199:LYS:N	2.49	0.44
1:A:144:VAL:O	1:A:145:SER:HB3	2.17	0.44
11:Y:54:GLN:HG3	12:Z:88:TYR:CE2	2.53	0.44
5:S:133:LEU:HD22	5:S:133:LEU:H	1.82	0.44
12:Z:122:LEU:HA	12:Z:122:LEU:HD23	1.62	0.44
8:H:189:TYR:HA	8:H:190:PRO:HD3	1.83	0.44
1:O:128:TYR:HE1	1:O:133:TYR:HH	1.58	0.44
1:A:64:LEU:HD23	7:G:159:TYR:CD2	2.52	0.44
6:F:62:LYS:O	6:F:73:SER:HA	2.17	0.44
13:M:141:LEU:O	13:M:145:VAL:HB	2.17	0.44
3:C:163:ILE:CG1	3:C:164:SER:N	2.81	0.44
4:R:37:LYS:HG2	4:R:160:SER:O	2.17	0.44
12:L:4:LEU:HA	12:L:100:MET:CE	2.47	0.44
3:C:29:ILE:O	3:C:31:HIS:N	2.49	0.44
4:D:109:LEU:C	4:D:109:LEU:HD13	2.37	0.44
10:X:101:ALA:HA	10:X:111:PHE:O	2.17	0.44
4:D:27:VAL:HG11	4:D:132:SER:CB	2.47	0.44
6:F:232:LYS:HE3	6:F:233:TYR:CE2	2.52	0.44
2:P:57:MET:HB2	2:P:59:GLU:OE2	2.17	0.44
9:I:59:ILE:HG12	9:I:83:LEU:CD2	2.46	0.44
6:F:190:ILE:O	6:F:194:VAL:HG23	2.17	0.44
8:H:107:LYS:CG	8:H:108:GLY:H	2.29	0.44
9:W:6:VAL:HG12	9:W:124:TYR:CB	2.36	0.44
8:H:163:ILE:HD12	8:H:170:GLY:HA2	1.98	0.44
7:U:171:ALA:HA	7:U:174:GLU:HB2	1.99	0.44
12:L:208:ASN:O	12:L:210:VAL:N	2.51	0.44
7:U:240:ASP:HA	7:U:243:GLN:HB2	1.98	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
8:H:147:SER:OG	8:H:150:GLU:HB2	2.18	0.44
1:A:117:LEU:HD12	1:A:121:MET:HG2	1.99	0.44
6:F:218:LYS:HB2	6:F:218:LYS:HE3	1.72	0.44
10:X:127:PHE:O	10:X:128:ILE:HD13	2.18	0.44
6:F:54:ASP:CG	6:F:55:GLU:N	2.71	0.44
5:E:26:TYR:O	5:E:29:GLU:N	2.50	0.44
9:W:81:GLN:O	9:W:85:GLN:HG3	2.18	0.44
13:M:2:THR:HA	13:M:131:GLY:HA3	2.00	0.44
14:N:208:ASN:HD22	14:N:208:ASN:C	2.21	0.44
2:P:64:VAL:CG1	2:P:237:LYS:HE2	2.47	0.44
5:E:187:TRP:CH2	5:E:189:SER:HA	2.52	0.44
6:F:36:VAL:CG1	6:F:37:GLY:N	2.81	0.44
3:C:70:ASN:HB3	3:C:73:ILE:HB	1.99	0.44
11:K:160:LEU:O	11:K:164:VAL:HG23	2.18	0.44
6:T:26:LEU:O	6:T:29:ILE:HB	2.17	0.44
10:J:3:VAL:CG2	10:J:16:CYS:HB3	2.46	0.44
8:V:34:LEU:CD2	8:V:44:CYS:HB3	2.48	0.44
8:V:138:CYS:HA	8:V:154:PHE:CE1	2.53	0.44
7:U:204:GLU:HG3	7:U:207:LYS:HE2	1.98	0.44
12:L:149:SER:HB2	12:L:152:ASP:CG	2.37	0.44
12:L:12:ILE:CD1	12:L:102:CYS:HB3	2.48	0.44
1:O:126:GLN:NE2	1:O:127:ILE:HA	2.31	0.44
6:F:217:GLY:O	6:F:219:ASP:N	2.50	0.44
7:G:72:HIS:HE1	7:G:105:PRO:HB2	1.82	0.44
11:K:164:VAL:HA	11:K:167:LEU:HD12	1.99	0.44
1:O:33:LYS:CD	1:O:33:LYS:H	2.23	0.44
2:B:73:ALA:HB2	2:B:136:ILE:HG23	1.99	0.44
11:K:6:ILE:HG23	11:K:13:ILE:HB	2.00	0.44
8:V:67:THR:C	8:V:69:GLN:H	2.21	0.44
2:B:174:PHE:HD2	2:B:195:THR:HG1	1.65	0.44
6:F:42:THR:HG23	6:F:183:ASP:HB3	2.00	0.44
8:V:138:CYS:HA	8:V:154:PHE:CZ	2.51	0.44
12:Z:149:SER:HB2	12:Z:152:ASP:CG	2.38	0.44
2:B:239:THR:O	2:B:243:ILE:HG13	2.18	0.44
8:H:36:ARG:HB2	8:H:42:TRP:CZ2	2.53	0.44
14:N:189:LEU:HD23	14:N:189:LEU:C	2.38	0.44
1:O:181:ASN:N	1:O:181:ASN:ND2	2.65	0.44
8:H:6:VAL:O	8:H:12:VAL:HG23	2.17	0.44
2:P:66:LEU:HD13	2:P:235:PHE:CG	2.53	0.44
8:H:131:SER:O	8:H:134:ILE:HG12	2.17	0.44
1:A:128:TYR:HA	1:A:133:TYR:HE1	1.82	0.44
11:Y:49:ALA:O	11:Y:52:THR:HG22	2.17	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
8:V:1:THR:HA	8:V:33:LYS:HZ3	1.81	0.44
3:Q:133:VAL:O	3:Q:153:PRO:HG3	2.18	0.44
6:T:197:ILE:HG23	6:T:198:SER:N	2.32	0.44
2:B:162:THR:OG1	2:B:163:ALA:N	2.50	0.44
14:N:96:ARG:HG3	14:N:97:SER:N	2.33	0.44
10:J:101:ALA:HA	10:J:111:PHE:O	2.18	0.44
12:Z:8:PHE:HA	12:Z:146:TRP:CE3	2.53	0.44
2:B:32:VAL:HG12	2:B:33:THR:N	2.33	0.44
6:T:90:GLN:H	6:T:90:GLN:HG2	1.46	0.44
8:V:178:LEU:HD13	8:V:178:LEU:HA	1.86	0.44
1:O:18:ILE:CD1	1:O:18:ILE:N	2.81	0.44
7:G:25:TYR:HA	7:G:28:LYS:HB2	2.00	0.44
4:R:149:GLN:HG2	4:R:150:THR:N	2.33	0.44
1:A:52:VAL:HG12	1:A:227:VAL:HG22	1.99	0.44
6:F:227:GLY:O	6:F:229:ALA:N	2.51	0.44
1:A:204:GLU:HB3	1:A:248:ILE:HG23	1.99	0.44
6:T:185:ASN:HA	6:T:186:PRO:HD2	1.79	0.44
1:A:50:CYS:HA	1:A:228:ALA:O	2.17	0.44
11:Y:8:VAL:HG23	11:Y:9:GLN:N	2.33	0.44
10:J:42:LEU:HD12	10:J:99:VAL:O	2.18	0.44
3:Q:27:GLU:O	3:Q:29:ILE:N	2.51	0.44
5:S:165:TYR:CE2	6:T:60:GLN:HB2	2.53	0.44
3:Q:230:PHE:N	3:Q:230:PHE:CD1	2.86	0.44
5:E:81:LEU:HA	5:E:81:LEU:HD12	1.64	0.44
12:Z:208:ASN:O	12:Z:210:VAL:N	2.51	0.44
2:B:43:VAL:O	2:B:213:ILE:HB	2.17	0.44
1:A:106:TYR:HB2	8:H:61:TYR:HD2	1.82	0.44
2:B:122:THR:HG22	2:B:123:GLN:N	2.33	0.44
2:P:38:LYS:HA	2:P:43:VAL:HG13	2.00	0.44
6:T:62:LYS:O	6:T:73:SER:HA	2.18	0.44
10:X:56:GLU:H	10:X:56:GLU:HG2	1.60	0.44
8:V:126:ILE:HD12	8:V:134:ILE:CD1	2.48	0.44
1:A:77:ARG:HA	1:A:77:ARG:HE	1.83	0.44
13:M:46:ASN:C	13:M:98:VAL:HG12	2.38	0.44
1:A:218:PHE:CD2	1:A:223:LEU:HD11	2.52	0.44
6:T:63:ILE:O	6:T:64:ILE:HG13	2.17	0.44
1:A:35:THR:OG1	1:A:36:ASN:N	2.51	0.43
12:L:182:GLU:HG3	12:L:182:GLU:O	2.17	0.43
5:E:22:PHE:N	5:E:22:PHE:CD2	2.85	0.43
5:E:165:TYR:CE2	6:F:60:GLN:HB2	2.52	0.43
3:C:39:MET:HE1	3:C:146:TYR:CB	2.48	0.43
3:Q:186:VAL:HG13	3:Q:187:ASP:N	2.32	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
11:Y:164:VAL:HA	11:Y:167:LEU:HD12	2.00	0.43
7:G:150:LEU:HD13	7:G:156:TYR:HB3	2.00	0.43
2:P:197:LYS:HA	2:P:197:LYS:HE3	2.00	0.43
8:V:188:PHE:CD2	8:V:188:PHE:N	2.86	0.43
7:U:94:GLU:CG	7:U:114:ARG:HH11	2.31	0.43
9:I:191:LEU:HB3	9:I:193:PRO:HD3	1.99	0.43
11:Y:4:LEU:HD22	11:Y:131:ALA:HB2	1.99	0.43
13:M:114:TYR:CD2	13:M:124:ARG:HA	2.53	0.43
4:R:181:ARG:NH2	5:S:60:GLU:HG2	2.32	0.43
6:T:217:GLY:O	6:T:219:ASP:N	2.51	0.43
6:T:123:TYR:CG	6:T:124:GLY:N	2.85	0.43
8:H:190:PRO:C	8:H:192:GLU:N	2.71	0.43
12:L:25:TRP:CZ3	13:M:135:SER:HA	2.53	0.43
7:G:134:SER:CB	7:G:164:THR:HG21	2.48	0.43
8:H:9:LYS:HG3	8:H:145:ASN:OD1	2.18	0.43
2:B:180:ASN:O	2:B:183:LEU:HG	2.17	0.43
4:R:162:GLN:HE21	4:R:163:THR:N	2.06	0.43
3:C:150:THR:O	3:C:157:TYR:HA	2.17	0.43
11:Y:-1:MET:HG2	11:Y:1:ASP:H	1.83	0.43
6:T:185:ASN:ND2	6:T:185:ASN:C	2.68	0.43
13:M:3:ILE:HG22	13:M:16:GLY:HA3	2.00	0.43
1:O:162:TYR:HD1	1:O:163:TYR:N	2.16	0.43
5:E:114:GLN:HG3	5:E:118:ASP:OD1	2.18	0.43
5:S:241:LYS:C	5:S:243:LEU:N	2.70	0.43
10:X:6:MET:HE3	10:X:145:TYR:HD1	1.83	0.43
3:C:230:PHE:N	3:C:230:PHE:CD1	2.86	0.43
6:T:118:LYS:HD2	6:T:118:LYS:H	1.82	0.43
1:A:108:TYR:O	9:I:78:SER:HA	2.18	0.43
8:V:80:SER:O	8:V:83:LYS:HB3	2.18	0.43
13:M:170:GLU:OE1	13:M:170:GLU:HA	2.18	0.43
4:D:11:PHE:H	5:E:23:GLN:NE2	2.14	0.43
5:E:205:LYS:HB2	5:E:212:LEU:HD13	2.00	0.43
6:F:160:ALA:O	6:F:169:LYS:HE3	2.19	0.43
6:F:213:ILE:CG2	6:F:214:ALA:N	2.82	0.43
6:F:216:VAL:HB	6:F:222:PHE:HD2	1.83	0.43
2:P:74:VAL:HG22	2:P:75:TYR:H	1.83	0.43
4:D:37:LYS:HD3	4:D:147:LEU:HB2	1.99	0.43
5:E:78:MET:HA	5:E:142:LEU:HD23	2.00	0.43
7:U:63:ASN:HD22	7:U:63:ASN:H	1.66	0.43
14:N:153:ARG:CG	14:N:153:ARG:NH1	2.81	0.43
7:G:171:ALA:HA	7:G:174:GLU:HB2	2.00	0.43
4:D:155:ILE:HD12	4:D:155:ILE:C	2.39	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
12:L:4:LEU:HD12	12:L:161:ILE:HD11	2.00	0.43
5:E:244:LYS:O	5:E:244:LYS:HG2	2.19	0.43
14:N:201:LYS:O	14:N:204:LEU:HD11	2.18	0.43
1:O:236:LEU:HA	1:O:236:LEU:HD23	1.85	0.43
2:P:90:ARG:NH1	9:W:68:LEU:HB3	2.33	0.43
8:H:3:ILE:HG22	8:H:16:ALA:HB2	2.00	0.43
8:V:102:TYR:HA	8:V:108:GLY:HA2	2.01	0.43
12:Z:76:VAL:HG23	12:Z:105:THR:HG22	1.99	0.43
4:D:39:LYS:HB2	4:D:39:LYS:HE2	1.83	0.43
3:C:163:ILE:HD12	3:C:173:GLN:OE1	2.18	0.43
11:K:75:SER:O	11:K:79:VAL:HG23	2.19	0.43
11:K:7:ARG:HG2	11:K:7:ARG:NH1	2.34	0.43
14:N:-6:GLN:HG3	14:N:-5:PRO:N	2.32	0.43
6:T:176:LEU:O	6:T:178:THR:N	2.51	0.43
14:N:51:ASP:O	14:N:54:HIS:HB3	2.18	0.43
7:G:47:PHE:HZ	7:G:138:GLY:N	2.16	0.43
7:G:201:LEU:CD1	7:G:201:LEU:N	2.81	0.43
14:N:41:THR:HG21	14:N:84:ILE:HD12	2.00	0.43
1:A:18:ILE:HB	2:B:20:GLN:NE2	2.34	0.43
1:A:89:ASP:OD2	1:A:137:LEU:HA	2.18	0.43
14:N:49:ILE:CG2	14:N:53:GLN:HE21	2.23	0.43
1:A:167:LYS:HG2	2:B:55:LEU:O	2.19	0.43
12:Z:1:THR:HG22	12:Z:2:THR:N	2.34	0.43
11:Y:54:GLN:HA	11:Y:54:GLN:OE1	2.18	0.43
4:D:50:SER:HA	4:D:53:LYS:HD3	2.00	0.43
10:X:33:LYS:HD2	10:X:33:LYS:N	2.33	0.43
14:N:119:LEU:HD23	14:N:131:SER:O	2.19	0.43
1:O:182:LEU:HG	1:O:182:LEU:H	1.55	0.43
1:O:76:SER:OG	1:O:77:ARG:N	2.52	0.43
2:P:67:LEU:N	2:P:67:LEU:HD23	2.55	0.43
7:U:24:GLU:H	7:U:24:GLU:HG2	1.57	0.43
7:U:201:LEU:HD13	7:U:201:LEU:N	2.32	0.43
2:P:34:SER:O	2:P:163:ALA:HA	2.18	0.43
12:Z:4:LEU:HD12	12:Z:161:ILE:CD1	2.49	0.43
5:S:37:ALA:HA	5:S:50:VAL:HG12	2.01	0.43
3:Q:39:MET:HE1	3:Q:146:TYR:CB	2.49	0.43
9:W:3:ILE:HD12	9:W:44:ALA:HB3	2.00	0.43
5:E:42:THR:C	5:E:44:GLU:H	2.20	0.43
10:X:151:PRO:HG2	10:X:152:GLU:OE2	2.18	0.43
11:K:-1:MET:SD	11:K:133:GLY:CA	3.05	0.43
12:L:81:LYS:O	12:L:84:SER:HB2	2.18	0.43
14:N:122:VAL:HG13	14:N:122:VAL:O	2.19	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:O:169:THR:OG1	1:O:170:ALA:N	2.52	0.43
7:U:21:PHE:HD2	7:U:24:GLU:HG3	1.84	0.43
1:A:83:VAL:CG1	1:A:139:VAL:HB	2.48	0.43
6:T:197:ILE:C	6:T:199:GLN:N	2.72	0.43
7:G:121:ALA:C	7:G:123:THR:H	2.21	0.43
7:U:166:LYS:HZ3	7:U:206:ASN:HD21	1.67	0.43
6:F:42:THR:HG22	6:F:218:LYS:NZ	2.33	0.43
4:R:207:ALA:HB2	4:R:233:VAL:HG21	2.00	0.43
5:E:241:LYS:C	5:E:243:LEU:N	2.71	0.43
2:B:243:ILE:O	2:B:245:ASP:N	2.51	0.43
3:C:235:ILE:C	3:C:237:ASP:N	2.71	0.43
11:K:70:GLU:HA	11:K:70:GLU:OE1	2.18	0.43
14:N:-3:VAL:HA	14:N:21:SER:O	2.18	0.43
11:Y:76:PRO:HB2	11:Y:114:GLU:OE1	2.19	0.43
4:R:109:LEU:C	4:R:109:LEU:HD13	2.39	0.43
11:K:3:ILE:CG2	11:K:102:LEU:HG	2.48	0.43
5:E:21:LEU:O	5:E:24:VAL:HB	2.18	0.43
11:K:9:GLN:NE2	11:K:150:ASP:HA	2.33	0.43
8:H:7:THR:OG1	8:H:123:PRO:O	2.34	0.43
8:H:3:ILE:HG22	8:H:16:ALA:HB1	1.99	0.43
2:P:139:HIS:HD2	2:P:144:GLY:C	2.21	0.43
2:B:59:GLU:HG3	2:B:59:GLU:H	1.55	0.43
11:K:68:ILE:C	11:K:68:ILE:HD12	2.38	0.43
1:O:112:MET:HA	1:O:113:PRO:HD3	1.74	0.43
14:N:144:ASN:O	14:N:148:ARG:HG3	2.18	0.43
12:Z:4:LEU:HD11	12:Z:15:ALA:HB3	1.99	0.43
4:D:81:ASP:O	4:D:82:SER:C	2.57	0.43
3:C:106:ILE:HA	3:C:107:PRO:HD3	1.85	0.43
4:R:39:LYS:HD3	4:R:186:ALA:HA	2.01	0.43
4:D:243:GLN:HG2	4:D:243:GLN:O	2.19	0.43
9:W:102:GLY:HA2	9:W:178:MET:SD	2.58	0.43
3:C:8:SER:O	3:C:9:ARG:O	2.37	0.43
7:G:49:VAL:HG11	7:G:65:LYS:HB2	2.01	0.43
2:P:108:LYS:HG2	2:P:148:TYR:OH	2.19	0.43
3:C:119:LYS:HD2	3:C:153:PRO:HA	2.00	0.43
10:J:66:LYS:HA	10:J:71:ARG:O	2.19	0.43
10:J:136:GLN:N	10:J:136:GLN:OE1	2.50	0.43
7:U:76:VAL:HG22	7:U:77:TYR:H	1.84	0.43
2:B:156:TYR:N	2:B:156:TYR:CD1	2.87	0.43
2:B:196:LEU:O	2:B:200:VAL:HG23	2.18	0.43
2:P:12:PHE:CE2	3:Q:130:PRO:HG2	2.54	0.43
2:B:61:LEU:HA	2:B:61:LEU:HD22	1.91	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
13:M:128:ARG:HG3	13:M:129:ALA:N	2.33	0.43
9:I:50:ALA:HB2	10:J:120:CYS:HB2	1.99	0.43
2:B:218:ASN:HB3	2:B:221:LEU:HD13	2.00	0.43
13:M:114:TYR:HD2	13:M:123:GLU:O	2.02	0.43
1:O:242:GLU:OE1	1:O:245:LEU:HB2	2.19	0.43
3:Q:91:ALA:HB2	3:Q:115:LEU:HD21	2.00	0.43
6:T:218:LYS:HB2	6:T:218:LYS:HE3	1.76	0.43
4:D:207:ALA:HB2	4:D:233:VAL:HG21	2.01	0.43
9:W:1:THR:HA	9:W:33:LYS:NZ	2.34	0.43
12:Z:98:GLY:O	12:Z:99:THR:HB	2.19	0.43
8:V:105:LYS:HG2	8:V:106:ASN:N	2.34	0.43
9:I:81:GLN:O	9:I:85:GLN:HG3	2.18	0.43
12:Z:158:LYS:HG3	12:Z:177:LEU:HD11	2.01	0.43
2:B:44:VAL:CA	2:B:213:ILE:HG22	2.48	0.43
1:O:43:LEU:HD23	1:O:43:LEU:C	2.39	0.43
8:H:8:PHE:HB2	8:H:146:MET:H	1.84	0.43
3:C:39:MET:CE	3:C:146:TYR:HB3	2.49	0.43
3:Q:186:VAL:HG11	3:Q:217:ARG:NH1	2.34	0.43
1:A:91:ARG:CZ	7:G:156:TYR:CE2	3.02	0.43
4:D:39:LYS:HD3	4:D:186:ALA:HA	2.00	0.43
10:J:94:TYR:O	10:J:117:LEU:HB2	2.19	0.43
4:D:75:PHE:CD2	4:D:76:SER:N	2.87	0.43
3:Q:59:GLN:N	3:Q:59:GLN:HE21	2.17	0.43
14:N:144:ASN:ND2	14:N:148:ARG:NH2	2.67	0.43
9:I:10:ASN:C	9:I:180:ILE:HG13	2.38	0.43
12:Z:54:PHE:C	12:Z:54:PHE:HD2	2.21	0.43
9:W:4:VAL:O	9:W:14:ILE:HG22	2.18	0.43
8:H:70:TYR:N	8:H:70:TYR:CD1	2.85	0.43
13:M:48:PHE:H	13:M:98:VAL:CG1	2.31	0.43
6:T:42:THR:HG23	6:T:183:ASP:HB3	2.01	0.43
5:E:238:GLU:O	5:E:241:LYS:HB2	2.18	0.43
3:Q:181:LYS:HB2	3:Q:181:LYS:HE3	1.82	0.43
5:S:140:VAL:O	5:S:160:PRO:HG3	2.19	0.43
5:S:187:TRP:CH2	5:S:189:SER:HA	2.54	0.43
7:G:85:ARG:CG	7:G:85:ARG:HH11	2.31	0.43
3:C:231:LYS:HA	3:C:231:LYS:HE3	2.00	0.43
7:U:193:LYS:HE2	7:U:193:LYS:HB3	1.75	0.43
9:I:90:TYR:O	9:I:91:GLN:C	2.57	0.42
12:L:76:VAL:HG23	12:L:105:THR:HG22	2.01	0.42
8:H:67:THR:O	8:H:69:GLN:N	2.52	0.42
3:C:163:ILE:CG1	3:C:164:SER:H	2.32	0.42
12:L:55:TRP:O	12:L:58:TRP:HB3	2.19	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
13:M:187:ILE:HG12	9:W:24:PRO:O	2.19	0.42
3:Q:15:PRO:HA	4:R:22:TYR:CD1	2.54	0.42
5:S:112:LEU:O	5:S:113:THR:C	2.57	0.42
7:U:216:SER:HA	7:U:230:VAL:HG23	2.01	0.42
6:T:129:GLY:O	6:T:130:VAL:HB	2.19	0.42
8:V:95:ALA:H	8:V:115:LEU:HD13	1.83	0.42
10:J:9:LYS:O	10:J:10:ASP:HB2	2.20	0.42
1:O:89:ASP:OD2	1:O:137:LEU:HA	2.18	0.42
1:O:35:THR:OG1	1:O:36:ASN:N	2.51	0.42
2:P:238:LEU:CD1	2:P:238:LEU:N	2.81	0.42
6:F:17:GLY:HA3	7:G:29:ALA:HB2	2.02	0.42
8:H:105:LYS:HG2	8:H:106:ASN:N	2.35	0.42
14:N:41:THR:HG21	14:N:84:ILE:CD1	2.49	0.42
1:O:167:LYS:HG2	2:P:55:LEU:O	2.19	0.42
5:E:143:LEU:HD23	5:E:143:LEU:HA	1.61	0.42
10:J:67:LEU:N	10:J:67:LEU:HD23	4.94	0.42
2:B:187:ASP:O	2:B:190:HIS:HB3	2.19	0.42
6:F:6:TYR:N	6:F:6:TYR:CD2	2.87	0.42
2:P:112:SER:CA	2:P:156:TYR:HE2	2.31	0.42
5:E:109:VAL:O	5:E:112:LEU:HB3	2.19	0.42
5:E:51:GLU:OE2	5:E:53:ARG:HB2	2.19	0.42
8:V:70:TYR:N	8:V:70:TYR:CD1	2.86	0.42
9:I:41:ILE:HD11	9:I:74:PRO:HB2	2.01	0.42
5:E:121:LEU:HD12	5:E:161:SER:O	2.20	0.42
6:T:54:ASP:CG	6:T:55:GLU:H	2.21	0.42
9:I:97:TYR:CD1	9:I:97:TYR:N	2.88	0.42
10:X:117:LEU:HD23	10:X:117:LEU:N	2.34	0.42
1:O:198:SER:O	1:O:202:VAL:HG23	2.19	0.42
1:O:28:VAL:HG23	1:O:29:GLU:N	2.34	0.42
1:O:53:VAL:HG23	1:O:53:VAL:O	2.20	0.42
7:U:150:LEU:HD13	7:U:156:TYR:HB3	2.01	0.42
6:F:158:GLY:O	6:F:159:THR:HB	2.19	0.42
7:G:216:SER:HA	7:G:230:VAL:HG23	2.00	0.42
3:C:190:ILE:O	3:C:193:ALA:HB3	2.19	0.42
13:M:100:THR:HG23	13:M:116:PHE:HB2	2.01	0.42
10:J:89:ARG:HG3	10:J:94:TYR:HE2	1.81	0.42
9:W:41:ILE:N	9:W:41:ILE:HD12	2.34	0.42
5:S:204:LEU:O	5:S:208:MET:N	2.52	0.42
11:K:57:GLU:O	11:K:60:GLN:HB3	2.19	0.42
4:R:212:ILE:HG21	4:R:224:LEU:HD22	2.01	0.42
10:J:98:PRO:HG2	10:J:115:PHE:CD1	2.54	0.42
14:N:144:ASN:HD22	14:N:148:ARG:NH2	2.16	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
9:I:4:VAL:HA	9:I:125:LEU:O	2.19	0.42
12:Z:81:LYS:HG3	12:Z:85:ASN:ND2	2.35	0.42
9:W:153:LYS:HE3	9:W:157:ASP:OD2	2.19	0.42
12:L:18:SER:HB2	12:L:31:VAL:H	1.82	0.42
3:Q:181:LYS:O	3:Q:184:MET:HB2	2.19	0.42
6:T:138:ASP:HB2	6:T:139:LYS:H	1.59	0.42
11:Y:57:GLU:O	11:Y:60:GLN:HB3	2.19	0.42
9:W:92:GLY:O	9:W:94:ILE:N	2.52	0.42
5:S:205:LYS:HB2	5:S:212:LEU:HD13	2.02	0.42
1:O:126:GLN:C	1:O:126:GLN:NE2	2.72	0.42
2:P:44:VAL:HG23	2:P:213:ILE:CG2	2.49	0.42
9:I:84:LYS:HE2	9:I:117:GLY:O	2.18	0.42
6:F:74:LEU:HD22	6:F:81:ALA:HB1	2.01	0.42
3:C:114:ARG:HB2	3:C:114:ARG:HH11	1.84	0.42
14:N:72:LEU:CD1	14:N:72:LEU:H	2.08	0.42
13:M:163:LEU:H	13:M:163:LEU:HD12	1.84	0.42
8:V:8:PHE:HB2	8:V:146:MET:H	1.83	0.42
10:J:81:LEU:O	10:J:83:SER:N	2.52	0.42
1:A:98:LYS:HE3	1:A:98:LYS:HB2	1.89	0.42
13:M:116:PHE:CE2	13:M:122:TYR:HB3	2.54	0.42
8:H:34:LEU:CD2	8:H:44:CYS:HB3	2.49	0.42
9:W:59:ILE:HG12	9:W:83:LEU:CD2	2.48	0.42
12:L:123:LYS:HG3	12:L:124:GLY:N	2.34	0.42
5:S:26:TYR:O	5:S:29:GLU:HB2	2.19	0.42
12:L:190:ASN:C	12:L:191:HIS:CD2	2.92	0.42
9:I:84:LYS:HA	9:I:87:LEU:HB3	2.01	0.42
6:F:176:LEU:C	6:F:176:LEU:HD12	2.40	0.42
7:G:26:ALA:O	7:G:30:VAL:HG23	2.20	0.42
3:C:172:ALA:HB2	3:C:200:THR:HG21	2.01	0.42
5:E:142:LEU:HA	5:E:142:LEU:HD23	1.79	0.42
9:W:124:TYR:CD1	9:W:124:TYR:N	2.87	0.42
1:A:21:PRO:HA	2:B:23:TYR:CE1	2.55	0.42
2:B:148:TYR:CE2	2:B:158:PRO:HB3	2.54	0.42
3:Q:173:GLN:O	3:Q:176:LEU:HB2	2.18	0.42
1:A:176:GLN:HA	1:A:179:THR:HB	2.02	0.42
2:B:132:VAL:O	2:B:152:PRO:HG3	2.20	0.42
8:V:189:TYR:HA	8:V:190:PRO:HD3	1.85	0.42
10:X:6:MET:HG2	10:X:127:PHE:HB3	2.02	0.42
11:Y:70:GLU:O	11:Y:71:ASP:CB	2.67	0.42
11:K:151:MET:HB3	11:K:155:GLU:HB2	2.01	0.42
7:U:203:HIS:O	7:U:205:ASP:N	2.45	0.42
7:G:236:GLN:O	7:G:239:ILE:HB	2.18	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
9:W:43:CYS:SG	9:W:100:VAL:HA	2.60	0.42
6:T:40:SER:OG	6:T:41:ASN:N	2.53	0.42
14:N:-2:THR:HA	14:N:47:GLY:O	2.20	0.42
12:Z:211:ILE:HG13	12:Z:211:ILE:H	1.56	0.42
6:F:110:HIS:O	6:F:113:CYS:HB3	2.20	0.42
6:F:90:GLN:HG2	6:F:90:GLN:H	1.55	0.42
7:G:201:LEU:N	7:G:201:LEU:HD13	2.35	0.42
8:H:122:LEU:HB3	8:H:123:PRO:CD	2.49	0.42
1:O:167:LYS:NZ	1:O:167:LYS:HB3	2.34	0.42
2:P:74:VAL:HG13	2:P:135:LEU:HB2	2.01	0.42
3:C:120:GLN:NE2	3:C:120:GLN:C	2.73	0.42
4:D:162:GLN:HG3	4:D:163:THR:N	2.34	0.42
14:N:3:VAL:O	14:N:135:ALA:HA	2.20	0.42
2:B:241:GLN:O	2:B:244:ASN:ND2	2.53	0.42
5:S:108:ASN:O	5:S:109:VAL:C	2.57	0.42
5:S:16:SER:OG	5:S:20:ARG:HB2	2.20	0.42
13:M:14:LEU:HD13	13:M:34:VAL:CG1	2.45	0.42
8:V:147:SER:OG	8:V:150:GLU:HB2	2.20	0.42
2:P:32:VAL:HG12	2:P:33:THR:N	2.34	0.42
6:T:134:ILE:CD1	6:T:134:ILE:N	2.83	0.42
11:K:151:MET:HA	11:K:155:GLU:OE1	2.20	0.42
2:P:20:GLN:O	2:P:23:TYR:N	2.53	0.42
14:N:26:LEU:O	14:N:28:PHE:N	2.52	0.42
9:I:104:ASP:C	9:I:106:THR:H	2.22	0.42
8:V:107:LYS:HB3	8:V:107:LYS:HE3	1.84	0.42
1:A:151:GLY:HA3	1:A:152:PRO:HD3	1.92	0.42
6:T:215:ILE:CG1	6:T:216:VAL:N	2.75	0.42
13:M:172:ILE:O	13:M:176:ARG:HG3	2.19	0.42
5:S:20:ARG:O	5:S:21:LEU:HD23	2.20	0.42
10:J:44:ILE:CG2	10:J:51:VAL:HG22	2.49	0.42
5:E:132:ARG:HH11	5:E:132:ARG:HG2	1.84	0.42
14:N:148:ARG:HH11	9:W:165:ASN:ND2	2.17	0.42
4:D:36:VAL:HG11	4:D:195:THR:HG23	2.00	0.42
5:S:192:THR:OG1	5:S:195:GLU:HG3	2.20	0.42
9:I:8:PHE:HB2	9:I:146:LEU:O	2.19	0.42
7:U:236:GLN:O	7:U:239:ILE:HB	2.20	0.42
10:X:-7:ASP:HB3	10:X:-4:SER:OG	2.19	0.42
4:R:48:ARG:HH11	4:R:48:ARG:HG2	1.85	0.42
1:O:127:ILE:HG13	1:O:127:ILE:H	1.65	0.42
2:P:212:ALA:HB2	2:P:237:LYS:HA	2.02	0.42
7:U:26:ALA:O	7:U:30:VAL:HG23	2.20	0.42
5:E:8:TYR:O	5:E:9:ASP:CB	2.65	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:F:219:ASP:N	6:F:219:ASP:OD2	2.53	0.42
7:G:41:CYS:HB2	7:G:186:LEU:O	2.19	0.42
8:H:152:VAL:O	8:H:156:LYS:HG3	2.20	0.42
5:E:39:GLY:O	5:E:169:ALA:HA	2.20	0.42
1:A:198:SER:O	1:A:202:VAL:HG23	2.20	0.42
1:A:251:GLN:O	1:A:251:GLN:HG2	2.20	0.42
3:Q:59:GLN:O	3:Q:62:SER:O	2.37	0.42
5:E:108:ASN:O	5:E:109:VAL:C	2.58	0.42
3:C:183:ASP:O	3:C:184:MET:C	2.58	0.42
7:U:217:TRP:N	7:U:217:TRP:HD1	2.18	0.42
1:A:69:VAL:O	1:A:70:SER:HB2	2.19	0.42
10:X:181:ILE:N	10:X:181:ILE:HD12	2.35	0.42
12:Z:95:LEU:O	12:Z:117:SER:HB2	2.18	0.42
4:R:127:ARG:HA	4:R:128:PRO:HD3	1.75	0.42
3:Q:50:ARG:HB3	3:Q:50:ARG:HH11	1.85	0.42
1:O:239:GLU:OE2	1:O:239:GLU:HA	2.20	0.42
2:B:135:LEU:HD23	2:B:135:LEU:HA	1.85	0.42
1:A:38:THR:HG23	1:A:39:ASN:N	2.34	0.42
2:P:20:GLN:O	2:P:21:ILE:C	2.59	0.42
6:F:24:TYR:O	6:F:27:GLU:HB2	2.20	0.42
7:G:12:SER:OG	7:G:126:ASN:N	2.53	0.42
2:B:20:GLN:O	2:B:21:ILE:C	2.58	0.42
2:B:145:PHE:HE1	2:B:214:ILE:HG22	1.84	0.42
7:G:150:LEU:HD11	7:G:154:GLY:C	2.41	0.42
2:P:241:GLN:O	2:P:244:ASN:ND2	2.53	0.42
11:Y:191:VAL:C	11:Y:193:ASP:N	2.71	0.42
6:T:34:VAL:CG2	6:T:35:THR:N	2.82	0.42
10:X:128:ILE:HA	10:X:128:ILE:HD13	1.87	0.42
3:C:13:PHE:N	4:D:19:GLN:HE22	2.17	0.42
7:U:25:TYR:HA	7:U:28:LYS:HB2	2.01	0.42
6:T:19:LEU:HD23	6:T:19:LEU:HA	1.90	0.42
2:B:185:LEU:O	2:B:188:ALA:HB3	2.20	0.42
1:O:17:THR:O	1:O:18:ILE:CG2	2.68	0.42
2:P:44:VAL:HG23	2:P:211:LEU:HD11	2.02	0.42
13:M:-5:TYR:OH	13:M:95:PRO:HD2	2.20	0.42
11:K:8:VAL:HG23	11:K:9:GLN:N	2.34	0.42
6:F:102:LYS:HE3	6:F:102:LYS:HB2	1.81	0.42
6:F:64:ILE:HB	6:F:72:LEU:HD11	2.02	0.42
4:D:133:THR:HG23	4:D:150:THR:CG2	2.41	0.42
6:F:155:GLU:C	6:F:156:LEU:HD12	2.39	0.42
10:J:15:ALA:HB2	10:J:178:VAL:HG22	2.01	0.42
3:Q:66:LEU:HA	3:Q:66:LEU:HD13	1.84	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:R:155:ILE:HD12	4:R:155:ILE:C	2.40	0.42
11:K:175:PHE:N	11:K:175:PHE:CD1	2.88	0.42
5:S:46:VAL:HG23	5:S:153:TYR:HD1	1.85	0.42
12:Z:64:ARG:CZ	12:Z:68:LEU:HD21	2.50	0.42
5:E:240:ILE:O	5:E:243:LEU:HB3	2.19	0.42
13:M:152:GLU:HB2	13:M:155:THR:HG21	2.01	0.42
5:E:202:LYS:O	5:E:206:GLN:HG3	2.20	0.42
6:F:33:SER:HB3	6:F:62:LYS:HZ1	1.84	0.41
7:G:219:SER:O	7:G:224:ASN:N	2.47	0.41
8:H:143:ARG:HH11	8:H:146:MET:CE	2.33	0.41
9:I:6:VAL:HG23	9:I:13:VAL:CG1	2.50	0.41
8:V:110:VAL:HG12	8:V:122:LEU:O	2.19	0.41
1:A:44:ALA:N	1:A:169:THR:O	2.51	0.41
8:H:188:PHE:N	8:H:188:PHE:HD2	2.18	0.41
6:T:33:SER:HB3	6:T:62:LYS:HZ1	1.83	0.41
3:Q:211:LEU:HD13	3:Q:212:GLU:N	2.35	0.41
7:G:19:ARG:NH1	7:G:19:ARG:CG	2.82	0.41
3:Q:29:ILE:O	3:Q:31:HIS:N	2.52	0.41
12:L:144:TYR:C	12:L:144:TYR:CD2	2.93	0.41
9:I:153:LYS:O	9:I:153:LYS:HD3	2.19	0.41
8:H:36:ARG:HB2	8:H:42:TRP:CE2	2.55	0.41
1:A:216:THR:CG2	1:A:217:GLU:N	2.83	0.41
5:S:33:LEU:H	5:S:33:LEU:HD12	1.84	0.41
14:N:29:ASN:HD22	14:N:29:ASN:HA	1.66	0.41
14:N:208:ASN:N	14:N:209:MET:HE2	2.34	0.41
7:G:77:TYR:N	7:G:77:TYR:CD2	2.87	0.41
8:H:126:ILE:HD12	8:H:134:ILE:CD1	2.50	0.41
1:A:123:ASN:ND2	2:B:84:VAL:HG12	2.35	0.41
1:A:26:TYR:CD2	1:A:26:TYR:N	2.87	0.41
9:I:220:ILE:H	9:I:220:ILE:HD12	4.81	0.41
1:A:207:ILE:H	1:A:207:ILE:HG13	1.60	0.41
3:Q:15:PRO:HA	4:R:22:TYR:CG	2.55	0.41
12:Z:145:LYS:O	12:Z:148:LEU:HD22	2.20	0.41
7:U:35:THR:HG21	7:U:167:GLY:H	1.84	0.41
5:S:188:HIS:O	5:S:191:LEU:HD12	2.20	0.41
1:O:18:ILE:HB	2:P:20:GLN:NE2	2.35	0.41
1:O:225:VAL:CG1	1:O:226:GLY:N	2.83	0.41
1:O:26:TYR:O	1:O:29:GLU:N	2.53	0.41
4:D:87:GLU:O	4:D:91:VAL:HG23	2.20	0.41
5:E:12:VAL:N	5:E:23:GLN:HG3	2.29	0.41
6:F:149:PRO:C	6:F:151:GLY:H	2.23	0.41
6:T:179:PHE:CD1	6:T:180:ILE:N	2.89	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:157:PHE:N	2:B:157:PHE:CD1	2.88	0.41
6:T:6:TYR:N	6:T:6:TYR:CD2	2.88	0.41
9:W:159:ILE:O	9:W:163:ILE:HG13	2.20	0.41
2:P:156:TYR:HD1	2:P:156:TYR:O	2.03	0.41
5:E:140:VAL:HG22	5:E:141:ALA:N	2.36	0.41
11:Y:9:GLN:HB2	11:Y:151:MET:O	2.20	0.41
13:M:19:ARG:NE	13:M:191:ASP:OD2	2.52	0.41
9:I:152:ILE:HG22	9:I:153:LYS:N	2.34	0.41
9:W:98:LEU:HD12	9:W:98:LEU:N	2.35	0.41
3:Q:235:ILE:O	3:Q:237:ASP:N	2.53	0.41
3:C:69:LEU:CD2	3:C:92:ARG:HG3	2.50	0.41
10:X:54:LEU:HD13	10:X:54:LEU:HA	1.72	0.41
11:K:35:ARG:HA	11:K:35:ARG:HD3	1.94	0.41
6:F:46:LEU:HD11	6:F:72:LEU:HA	2.01	0.41
3:C:38:ILE:HG22	3:C:39:MET:N	2.35	0.41
7:G:100:LYS:HB3	7:G:100:LYS:HZ3	1.86	0.41
8:V:82:PHE:HB2	8:V:113:ILE:CD1	2.50	0.41
9:W:41:ILE:HD11	9:W:74:PRO:HB2	2.02	0.41
1:O:69:VAL:O	1:O:70:SER:HB2	2.20	0.41
2:B:98:LYS:HA	2:B:103:GLU:O	2.19	0.41
3:Q:233:GLN:O	3:Q:235:ILE:N	2.53	0.41
13:M:166:LEU:CD1	13:M:166:LEU:H	2.33	0.41
13:M:166:LEU:HD13	13:M:171:VAL:HG22	2.03	0.41
9:W:215:GLU:CD	10:X:189:ARG:HE	2.23	0.41
4:R:138:PHE:CZ	4:R:145:PRO:HB3	2.55	0.41
6:T:69:HIS:C	6:T:69:HIS:ND1	2.73	0.41
6:F:181:LYS:HB3	6:F:181:LYS:HE2	1.92	0.41
2:B:44:VAL:HG23	2:B:211:LEU:HD11	2.02	0.41
7:G:69:VAL:HA	14:N:68:TYR:HE1	1.85	0.41
3:C:176:LEU:HD23	3:C:192:LEU:HD11	2.02	0.41
11:K:171:MET:HA	11:K:172:PRO:HD3	1.83	0.41
1:A:181:ASN:ND2	1:A:181:ASN:N	2.66	0.41
9:W:84:LYS:HE2	9:W:117:GLY:O	2.20	0.41
12:Z:190:ASN:C	12:Z:191:HIS:CD2	2.94	0.41
1:O:50:CYS:HA	1:O:228:ALA:O	2.20	0.41
5:E:222:ILE:HB	5:E:228:PHE:HA	2.02	0.41
7:U:245:GLU:H	7:U:245:GLU:HG2	1.53	0.41
4:D:27:VAL:HG11	4:D:132:SER:HB2	2.01	0.41
7:U:68:VAL:HG22	7:U:69:VAL:N	2.35	0.41
1:A:230:LYS:HA	1:A:230:LYS:HD2	1.89	0.41
11:K:117:GLN:HE22	11:K:131:ALA:N	2.18	0.41
1:O:128:TYR:HB2	1:O:129:THR:H	1.59	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:F:197:ILE:C	6:F:199:GLN:H	2.23	0.41
8:H:75:THR:HG22	8:H:111:TYR:CE1	2.54	0.41
8:H:126:ILE:HG13	8:H:126:ILE:O	2.21	0.41
2:B:203:GLU:HB3	2:B:204:PHE:H	1.72	0.41
8:V:122:LEU:HB3	8:V:123:PRO:CD	2.51	0.41
14:N:1:THR:OG1	14:N:2:SER:N	2.52	0.41
3:C:59:GLN:O	3:C:62:SER:O	2.38	0.41
7:G:200:TYR:HB3	7:G:246:ILE:CD1	2.50	0.41
5:S:9:ASP:OD2	5:S:16:SER:HA	2.21	0.41
14:N:224:LYS:HG3	14:N:225:ILE:HG12	2.02	0.41
8:V:4:MET:CB	8:V:126:ILE:HG22	2.48	0.41
7:U:47:PHE:HZ	7:U:138:GLY:N	2.17	0.41
6:F:145:LEU:HD23	6:F:153:VAL:HG11	2.02	0.41
6:T:219:ASP:OD2	6:T:219:ASP:N	2.54	0.41
6:T:54:ASP:CG	6:T:55:GLU:N	2.73	0.41
12:Z:18:SER:HB2	12:Z:31:VAL:H	1.85	0.41
6:T:44:ALA:HB1	6:T:135:ILE:HB	2.02	0.41
3:C:128:LEU:HD12	3:C:128:LEU:O	2.21	0.41
10:J:9:LYS:HB2	10:J:148:ASN:HB3	2.03	0.41
7:U:134:SER:HA	7:U:150:LEU:O	2.21	0.41
5:E:9:ASP:OD2	5:E:16:SER:HA	2.21	0.41
4:D:37:LYS:HG2	4:D:160:SER:O	2.20	0.41
7:U:194:GLN:NE2	7:U:197:LYS:HZ3	2.18	0.41
9:I:177:VAL:O	9:I:184:ALA:HA	2.20	0.41
8:V:153:ASP:HA	8:V:156:LYS:HB2	2.03	0.41
13:M:81:ALA:HB1	13:M:122:TYR:CD2	2.55	0.41
12:Z:67:GLU:OE2	12:Z:74:ILE:HG22	2.21	0.41
9:I:3:ILE:HG13	9:I:99:ILE:HD12	2.03	0.41
7:U:187:SER:HG	7:U:190:GLU:HB2	1.84	0.41
5:E:204:LEU:O	5:E:208:MET:N	2.53	0.41
3:Q:48:ALA:O	3:Q:211:LEU:HD22	2.21	0.41
7:G:15:SER:H	7:G:19:ARG:H	1.67	0.41
9:W:84:LYS:HA	9:W:87:LEU:HB3	2.02	0.41
3:C:29:ILE:C	3:C:31:HIS:N	2.74	0.41
6:F:103:LEU:HD12	6:F:103:LEU:HA	1.80	0.41
8:H:178:LEU:HA	8:H:178:LEU:HD13	1.85	0.41
2:B:211:LEU:CD2	2:B:238:LEU:HD22	2.51	0.41
1:O:16:ILE:CG2	1:O:17:THR:H	2.29	0.41
14:N:179:ARG:CA	8:V:26:ILE:HD12	2.44	0.41
4:D:30:GLY:O	4:D:166:ARG:HG2	2.20	0.41
4:D:31:THR:HB	4:D:63:LYS:HZ3	1.85	0.41
5:E:193:LEU:O	5:E:197:GLU:HG3	2.21	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:127:ILE:H	1:A:127:ILE:HG13	1.66	0.41
4:D:227:GLU:O	4:D:231:GLN:HG3	2.21	0.41
8:H:19:ARG:HB3	8:H:170:GLY:N	2.32	0.41
4:D:198:SER:O	4:D:201:GLU:HG2	2.21	0.41
3:Q:133:VAL:HG11	3:Q:135:PHE:CZ	2.56	0.41
2:P:156:TYR:CD1	2:P:156:TYR:N	2.89	0.41
9:W:183:ASP:HB3	9:W:184:ALA:H	1.55	0.41
2:B:218:ASN:HA	2:B:219:PRO:HD2	1.88	0.41
11:Y:3:ILE:CG2	11:Y:102:LEU:HG	2.51	0.41
13:M:5:GLY:C	13:M:6:ILE:HD12	2.40	0.41
10:J:115:PHE:HD1	10:J:115:PHE:N	2.17	0.41
10:J:42:LEU:HD12	10:J:43:GLY:N	2.36	0.41
11:Y:13:ILE:O	11:Y:14:LEU:HD23	2.21	0.41
11:Y:22:ARG:HA	11:Y:22:ARG:HD3	1.76	0.41
5:S:222:ILE:HB	5:S:228:PHE:HA	2.03	0.41
7:U:41:CYS:HB2	7:U:186:LEU:O	2.20	0.41
10:X:14:ILE:O	10:X:14:ILE:HG23	2.21	0.41
3:Q:142:ASP:OD2	3:Q:142:ASP:N	2.53	0.41
2:P:161:ALA:O	2:P:162:THR:HB	2.20	0.41
11:K:19:ALA:HB2	11:K:176:LYS:CG	2.50	0.41
8:H:112:THR:HG22	8:H:120:HIS:HB2	2.03	0.41
6:F:74:LEU:HB3	6:F:132:LEU:CD2	2.51	0.41
7:G:216:SER:HB2	7:G:227:HIS:NE2	2.36	0.41
3:C:114:ARG:HB2	3:C:114:ARG:NH1	2.36	0.41
3:C:68:LYS:NZ	10:J:66:LYS:NZ	2.68	0.41
2:B:180:ASN:ND2	2:B:183:LEU:HG	2.36	0.41
7:G:100:LYS:HG2	14:N:57:ARG:NH1	2.36	0.41
3:C:185:LYS:HZ2	3:C:187:ASP:N	1.95	0.41
14:N:40:ASN:O	14:N:110:GLY:HA3	2.20	0.41
8:H:138:CYS:O	8:H:154:PHE:HZ	2.03	0.41
8:V:110:VAL:HG11	8:V:124:TYR:HA	2.02	0.41
1:A:45:VAL:HG23	1:A:52:VAL:HG23	2.02	0.41
2:P:123:GLN:O	2:P:124:SER:HB2	2.21	0.41
5:E:66:LYS:O	5:E:77:ALA:HA	2.21	0.41
4:D:60:THR:HA	4:D:61:PRO:HD2	1.57	0.41
6:T:3:ARG:HD2	6:T:3:ARG:HA	1.84	0.41
9:W:41:ILE:HD12	9:W:41:ILE:H	1.86	0.41
4:D:98:LEU:CD1	11:K:58:TYR:HA	2.50	0.41
12:L:1:THR:HG22	12:L:2:THR:N	2.36	0.41
5:S:221:CYS:HB3	5:S:231:TYR:HE1	1.86	0.41
7:G:117:GLN:HA	7:G:120:GLN:HB2	2.03	0.41
2:B:34:SER:O	2:B:163:ALA:HA	2.20	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:147:LEU:HB3	2:B:159:TRP:O	2.21	0.41
6:T:105:VAL:HG11	6:T:145:LEU:HD13	2.02	0.41
10:X:159:SER:O	10:X:163:LEU:HB2	2.21	0.41
12:Z:144:TYR:C	12:Z:144:TYR:CD2	2.95	0.41
10:X:79:THR:HG1	10:X:111:PHE:HE1	1.68	0.41
13:M:101:ILE:CG2	13:M:102:ILE:N	2.83	0.41
1:O:230:LYS:HD2	1:O:230:LYS:HA	1.88	0.41
3:C:156:ASN:ND2	4:D:79:ASN:HB2	2.36	0.41
8:V:3:ILE:HG22	8:V:16:ALA:HB1	2.02	0.41
9:W:180:ILE:O	9:W:180:ILE:HG22	2.20	0.41
6:T:90:GLN:HE21	6:T:90:GLN:HB3	1.68	0.41
6:T:176:LEU:HD22	7:U:57:LEU:HD23	2.03	0.41
11:Y:50:GLY:H	12:Z:91:LYS:NZ	2.18	0.41
2:B:229:THR:O	2:B:231:LYS:NZ	2.52	0.41
7:U:89:ASN:O	7:U:92:ARG:HB2	2.20	0.41
12:Z:55:TRP:O	12:Z:58:TRP:HB3	2.21	0.41
5:S:143:LEU:HD23	5:S:143:LEU:HA	1.69	0.41
9:W:76:VAL:HG21	9:W:109:HIS:HB2	2.02	0.41
11:Y:135:SER:O	11:Y:139:THR:HG23	2.21	0.41
3:Q:137:TYR:HB2	3:Q:149:TYR:HB2	2.03	0.41
9:W:30:ASN:HA	9:W:30:ASN:HD22	1.59	0.41
1:O:20:SER:HB2	1:O:21:PRO:CD	2.51	0.41
1:O:83:VAL:HG13	1:O:140:ILE:O	2.21	0.41
6:F:134:ILE:HG22	6:F:135:ILE:N	2.35	0.41
1:A:101:ALA:HA	1:A:112:MET:HE3	2.02	0.41
1:A:146:VAL:CG2	1:A:152:PRO:HA	2.41	0.41
7:G:51:LYS:HE3	7:G:63:ASN:O	2.21	0.41
12:Z:35:ILE:HD12	12:Z:35:ILE:N	2.36	0.41
14:N:219:GLY:H	8:V:32:ASP:CG	2.24	0.41
12:Z:4:LEU:CD1	12:Z:161:ILE:HD11	2.50	0.41
9:I:114:HIS:HB2	9:I:118:SER:HB3	2.03	0.41
6:F:42:THR:OG1	6:F:183:ASP:HA	2.20	0.41
9:W:101:ALA:HB2	9:W:110:LEU:HD12	2.03	0.41
3:C:13:PHE:HB2	4:D:19:GLN:NE2	2.36	0.41
4:D:119:ARG:HA	4:D:122:GLN:OE1	2.20	0.41
11:K:70:GLU:O	11:K:71:ASP:HB3	2.20	0.41
9:W:114:HIS:HB2	9:W:118:SER:HB3	2.02	0.41
6:T:107:ARG:HE	6:T:107:ARG:HB3	1.70	0.41
10:J:29:ASN:N	10:J:29:ASN:ND2	2.69	0.40
1:O:83:VAL:CG1	1:O:139:VAL:HB	2.51	0.40
1:O:38:THR:HG23	1:O:39:ASN:N	2.35	0.40
9:I:72:ARG:CG	9:I:72:ARG:HH11	2.31	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:F:197:ILE:CG2	6:F:198:SER:N	2.84	0.40
7:U:143:ASN:ND2	7:U:143:ASN:N	2.55	0.40
2:P:123:GLN:O	2:P:124:SER:CB	2.69	0.40
2:P:203:GLU:HB3	2:P:204:PHE:H	1.72	0.40
7:U:200:TYR:HB3	7:U:246:ILE:CD1	2.51	0.40
12:L:19:ARG:N	12:L:33:ARG:NH2	2.70	0.40
3:Q:175:LEU:HD11	3:Q:199:LYS:HB2	2.03	0.40
1:O:69:VAL:HA	7:U:157:TRP:CZ3	2.56	0.40
12:Z:81:LYS:O	12:Z:84:SER:HB2	2.20	0.40
6:T:38:LEU:HA	6:T:158:GLY:HA2	2.03	0.40
11:Y:12:VAL:HG12	11:Y:13:ILE:N	2.36	0.40
9:W:191:LEU:HB3	9:W:193:PRO:HD3	2.01	0.40
4:R:239:GLU:HA	4:R:242:GLU:HB3	2.02	0.40
6:T:84:LEU:HA	6:T:84:LEU:HD23	1.91	0.40
2:P:45:ILE:CD1	2:P:64:VAL:HG23	2.51	0.40
5:E:12:VAL:H	5:E:23:GLN:CG	2.31	0.40
7:G:49:VAL:HG22	7:G:50:GLU:N	2.32	0.40
7:G:80:LEU:HA	7:G:80:LEU:HD23	1.73	0.40
3:C:186:VAL:O	3:C:190:ILE:HG13	2.21	0.40
10:J:81:LEU:C	10:J:83:SER:N	2.70	0.40
13:M:81:ALA:HB1	13:M:122:TYR:HD2	1.85	0.40
7:U:170:SER:O	7:U:174:GLU:HG2	2.21	0.40
11:K:59:ILE:HA	11:K:59:ILE:HD13	1.91	0.40
7:G:121:ALA:O	7:G:123:THR:N	2.48	0.40
11:Y:18:LYS:CD	11:Y:179:ILE:HG13	2.51	0.40
4:R:82:SER:O	4:R:86:ILE:HG13	2.22	0.40
6:T:72:LEU:CD1	6:T:72:LEU:N	2.84	0.40
4:D:40:ASN:N	4:D:40:ASN:OD1	2.53	0.40
2:B:44:VAL:CG2	2:B:211:LEU:HD11	2.52	0.40
9:I:90:TYR:HB2	9:I:94:ILE:CD1	2.52	0.40
5:E:16:SER:OG	5:E:20:ARG:HB2	2.22	0.40
6:F:147:PHE:CD1	6:F:147:PHE:C	2.93	0.40
6:F:210:ASN:N	6:F:210:ASN:ND2	2.68	0.40
4:R:213:THR:HA	4:R:223:ALA:HA	2.03	0.40
12:Z:45:MET:HG2	12:Z:45:MET:O	2.21	0.40
5:E:46:VAL:HG23	5:E:153:TYR:CD1	2.55	0.40
7:U:15:SER:H	7:U:19:ARG:H	1.68	0.40
13:M:117:ASP:HB3	13:M:121:SER:N	2.36	0.40
10:J:99:VAL:HG13	10:J:128:ILE:HG21	2.04	0.40
10:X:99:VAL:HG13	10:X:128:ILE:HG21	2.02	0.40
11:Y:70:GLU:HA	11:Y:70:GLU:OE1	2.21	0.40
7:G:149:MET:HB3	7:G:159:TYR:CE1	2.56	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
14:N:112:GLN:O	14:N:115:GLY:N	2.45	0.40
1:A:113:PRO:O	1:A:116:VAL:HG23	2.22	0.40
2:B:200:VAL:HG21	2:B:204:PHE:CD1	2.57	0.40
2:B:20:GLN:O	2:B:23:TYR:N	2.53	0.40
13:M:172:ILE:H	13:M:172:ILE:HG13	1.63	0.40
14:N:142:MET:HE2	9:W:132:LEU:O	2.22	0.40
7:U:94:GLU:HG3	7:U:114:ARG:HH11	1.85	0.40
9:I:192:THR:N	9:I:193:PRO:CD	2.85	0.40
11:Y:3:ILE:HA	11:Y:3:ILE:HD13	1.86	0.40
9:W:72:ARG:CG	9:W:72:ARG:NH1	2.84	0.40
7:G:182:HIS:C	7:G:184:GLU:H	2.25	0.40
3:C:238:ILE:CD1	3:C:241:LYS:HD2	2.52	0.40
5:E:38:ILE:HB	5:E:200:VAL:HG13	2.03	0.40
10:J:159:SER:O	10:J:163:LEU:HB2	2.22	0.40
3:Q:156:ASN:ND2	4:R:79:ASN:HB2	2.37	0.40
4:R:39:LYS:HB2	4:R:39:LYS:HE2	1.82	0.40
3:Q:40:ALA:C	3:Q:42:ASP:H	2.25	0.40
3:Q:8:SER:O	3:Q:9:ARG:O	2.39	0.40
7:U:237:GLU:O	7:U:241:PHE:HB2	2.22	0.40
3:Q:83:ASP:O	3:Q:84:ALA:C	2.60	0.40
13:M:105:LEU:HD23	13:M:111:GLY:HA2	2.03	0.40
12:Z:77:ALA:O	12:Z:80:SER:OG	2.37	0.40
1:O:57:LYS:HG2	1:O:57:LYS:O	2.20	0.40
7:U:159:TYR:CD1	7:U:159:TYR:N	2.90	0.40
10:X:86:LEU:HD23	10:X:86:LEU:HA	1.95	0.40
12:L:95:LEU:HA	12:L:95:LEU:HD12	1.88	0.40
1:O:39:ASN:HD22	1:O:39:ASN:C	2.24	0.40
9:I:62:ASN:O	9:I:65:LEU:HB2	2.22	0.40
5:E:78:MET:CE	5:E:82:THR:HG22	2.51	0.40
14:N:106:ILE:HD12	14:N:106:ILE:N	2.36	0.40
13:M:143:ASN:O	13:M:147:PHE:HA	2.22	0.40
9:I:3:ILE:HG22	9:I:16:ALA:HB1	2.03	0.40
5:S:142:LEU:HA	5:S:142:LEU:HD23	1.77	0.40
10:J:56:GLU:H	10:J:56:GLU:HG2	1.57	0.40
7:U:19:ARG:NH1	7:U:19:ARG:CG	2.83	0.40
12:Z:148:LEU:HD13	12:Z:148:LEU:HA	1.88	0.40
5:S:17:PRO:HA	6:T:24:TYR:CD2	2.56	0.40
4:R:174:PHE:C	4:R:174:PHE:CD2	2.95	0.40
11:K:180:VAL:HG21	11:K:194:PHE:CD2	2.57	0.40
5:S:52:LYS:HB2	5:S:216:ASN:HA	2.04	0.40
1:A:243:GLU:O	1:A:243:GLU:HG2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	236/252 (94%)	172 (73%)	44 (19%)	20 (8%)	1	9
1	O	236/252 (94%)	174 (74%)	42 (18%)	20 (8%)	1	9
2	B	245/250 (98%)	170 (69%)	56 (23%)	19 (8%)	1	11
2	P	245/250 (98%)	174 (71%)	53 (22%)	18 (7%)	2	12
3	C	239/245 (98%)	191 (80%)	29 (12%)	19 (8%)	1	11
3	Q	239/245 (98%)	187 (78%)	32 (13%)	20 (8%)	1	9
4	D	237/254 (93%)	186 (78%)	36 (15%)	15 (6%)	2	18
4	R	237/254 (93%)	186 (78%)	36 (15%)	15 (6%)	2	18
5	E	242/260 (93%)	192 (79%)	36 (15%)	14 (6%)	3	21
5	S	242/260 (93%)	192 (79%)	35 (14%)	15 (6%)	2	19
6	F	231/234 (99%)	189 (82%)	36 (16%)	6 (3%)	8	47
6	T	231/234 (99%)	190 (82%)	32 (14%)	9 (4%)	5	33
7	G	238/287 (83%)	193 (81%)	37 (16%)	8 (3%)	6	38
7	U	238/287 (83%)	194 (82%)	34 (14%)	10 (4%)	4	31
8	H	194/196 (99%)	148 (76%)	30 (16%)	16 (8%)	1	10
8	V	194/196 (99%)	147 (76%)	34 (18%)	13 (7%)	2	16
9	I	220/232 (95%)	178 (81%)	27 (12%)	15 (7%)	2	15
9	W	220/232 (95%)	176 (80%)	31 (14%)	13 (6%)	2	20
10	J	202/205 (98%)	165 (82%)	33 (16%)	4 (2%)	11	56
10	X	202/205 (98%)	168 (83%)	30 (15%)	4 (2%)	11	56
11	K	196/198 (99%)	163 (83%)	24 (12%)	9 (5%)	4	28
11	Y	196/198 (99%)	160 (82%)	28 (14%)	8 (4%)	4	32
12	L	210/212 (99%)	180 (86%)	27 (13%)	3 (1%)	16	66
12	Z	210/212 (99%)	178 (85%)	29 (14%)	3 (1%)	16	66
13	M	220/222 (99%)	188 (86%)	24 (11%)	8 (4%)	5	36
13	a	220/222 (99%)	186 (84%)	25 (11%)	9 (4%)	4	32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	N	231/233 (99%)	169 (73%)	43 (19%)	19 (8%)	1	10
14	b	231/233 (99%)	170 (74%)	40 (17%)	21 (9%)	1	8
15	c	194/231 (84%)	162 (84%)	22 (11%)	10 (5%)	3	25
15	d	194/231 (84%)	162 (84%)	21 (11%)	11 (6%)	3	22
15	e	194/231 (84%)	161 (83%)	22 (11%)	11 (6%)	3	22
15	f	194/231 (84%)	161 (83%)	23 (12%)	10 (5%)	3	25
15	g	194/231 (84%)	161 (83%)	23 (12%)	10 (5%)	3	25
15	h	194/231 (84%)	162 (84%)	22 (11%)	10 (5%)	3	25
15	i	194/231 (84%)	162 (84%)	22 (11%)	10 (5%)	3	25
15	j	194/231 (84%)	162 (84%)	23 (12%)	9 (5%)	4	28
15	k	194/231 (84%)	160 (82%)	24 (12%)	10 (5%)	3	25
15	l	194/231 (84%)	159 (82%)	25 (13%)	10 (5%)	3	25
15	m	194/231 (84%)	160 (82%)	24 (12%)	10 (5%)	3	25
15	n	194/231 (84%)	161 (83%)	23 (12%)	10 (5%)	3	25
15	o	194/231 (84%)	159 (82%)	25 (13%)	10 (5%)	3	25
15	p	194/231 (84%)	163 (84%)	20 (10%)	11 (6%)	3	22
All	All	8998/9794 (92%)	7221 (80%)	1282 (14%)	495 (6%)	3	23

All (495) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	16	ILE
1	A	19	PHE
1	A	60	PRO
1	A	115	ASP
1	A	221	ASN
2	B	7	PHE
2	B	9	LEU
2	B	40	THR
2	B	123	GLN
2	B	124	SER
2	B	244	ASN
3	C	7	ASP
3	C	8	SER
3	C	9	ARG
3	C	20	TYR

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Mol	Chain	Res	Type
3	C	200	THR
4	D	7	ALA
4	D	9	SER
4	D	58	ARG
4	D	61	PRO
4	D	63	LYS
4	D	205	THR
5	E	9	ASP
5	E	12	VAL
5	E	61	SER
5	E	133	LEU
5	E	134	MET
6	F	218	LYS
6	F	219	ASP
7	G	141	ASP
7	G	166	LYS
7	G	204	GLU
8	H	97	ILE
9	I	22	GLN
9	I	93	HIS
9	I	180	ILE
9	I	218	VAL
11	K	192	ASP
12	L	49	ALA
14	N	140	ALA
14	N	203	ASN
1	O	16	ILE
1	O	19	PHE
1	O	60	PRO
1	O	115	ASP
1	O	221	ASN
2	P	7	PHE
2	P	9	LEU
2	P	40	THR
2	P	123	GLN
2	P	124	SER
2	P	199	SER
2	P	244	ASN
3	Q	7	ASP
3	Q	8	SER
3	Q	9	ARG
3	Q	20	TYR

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Mol	Chain	Res	Type
3	Q	30	SER
3	Q	200	THR
4	R	7	ALA
4	R	9	SER
4	R	58	ARG
4	R	61	PRO
4	R	63	LYS
4	R	205	THR
5	S	9	ASP
5	S	12	VAL
5	S	61	SER
5	S	133	LEU
5	S	134	MET
6	T	218	LYS
6	T	219	ASP
7	U	141	ASP
7	U	166	LYS
7	U	204	GLU
8	V	97	ILE
9	W	22	GLN
9	W	91	GLN
9	W	93	HIS
9	W	180	ILE
11	Y	192	ASP
12	Z	49	ALA
14	b	140	ALA
14	b	203	ASN
15	c	20	SER
15	c	62	LYS
15	c	216	TRP
15	d	62	LYS
15	d	216	TRP
15	e	62	LYS
15	e	216	TRP
15	f	62	LYS
15	f	216	TRP
15	g	20	SER
15	g	62	LYS
15	g	216	TRP
15	h	62	LYS
15	h	216	TRP
15	i	62	LYS

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Mol	Chain	Res	Type
15	i	216	TRP
15	j	62	LYS
15	j	216	TRP
15	k	62	LYS
15	k	216	TRP
15	l	62	LYS
15	l	216	TRP
15	m	62	LYS
15	m	216	TRP
15	n	62	LYS
15	n	216	TRP
15	o	62	LYS
15	o	216	TRP
15	p	62	LYS
15	p	216	TRP
1	A	25	LEU
1	A	39	ASN
1	A	70	SER
1	A	114	CYS
1	A	161	GLY
1	A	164	VAL
1	A	190	LYS
1	A	196	GLU
2	B	19	GLY
2	B	21	ILE
2	B	199	SER
2	B	243	ILE
3	C	30	SER
3	C	52	VAL
3	C	59	GLN
3	C	65	LYS
3	C	184	MET
4	D	31	THR
4	D	40	ASN
4	D	82	SER
4	D	186	ALA
4	D	219	SER
4	D	222	VAL
5	E	120	ALA
5	E	214	GLU
6	F	177	ASP
6	F	228	GLU

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Mol	Chain	Res	Type
7	G	122	HIS
7	G	224	ASN
8	H	90	LYS
8	H	105	LYS
8	H	137	TYR
8	H	145	ASN
8	H	187	ILE
8	H	191	ASP
9	I	91	GLN
11	K	27	LEU
11	K	52	THR
11	K	191	VAL
11	K	194	PHE
12	L	209	ASN
13	M	134	ALA
13	M	200	LYS
14	N	1	THR
14	N	27	ARG
14	N	137	GLY
14	N	223	GLN
1	O	25	LEU
1	O	39	ASN
1	O	70	SER
1	O	114	CYS
1	O	161	GLY
1	O	164	VAL
1	O	190	LYS
1	O	196	GLU
1	O	232	LYS
2	P	8	SER
2	P	19	GLY
2	P	21	ILE
2	P	243	ILE
3	Q	52	VAL
3	Q	59	GLN
3	Q	65	LYS
3	Q	184	MET
4	R	31	THR
4	R	40	ASN
4	R	82	SER
4	R	186	ALA
4	R	219	SER

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Mol	Chain	Res	Type
4	R	222	VAL
5	S	120	ALA
5	S	190	SER
5	S	214	GLU
6	T	177	ASP
7	U	224	ASN
8	V	68	SER
8	V	90	LYS
8	V	137	TYR
8	V	138	CYS
8	V	145	ASN
8	V	187	ILE
8	V	191	ASP
9	W	218	VAL
10	X	117	LEU
11	Y	27	LEU
11	Y	191	VAL
11	Y	194	PHE
12	Z	209	ASN
13	a	94	PHE
13	a	134	ALA
14	b	1	THR
14	b	27	ARG
14	b	73	ALA
14	b	122	VAL
14	b	124	LEU
14	b	137	GLY
15	c	44	ALA
15	c	58	ALA
15	d	20	SER
15	d	44	ALA
15	d	58	ALA
15	e	20	SER
15	e	44	ALA
15	e	58	ALA
15	f	20	SER
15	f	44	ALA
15	f	58	ALA
15	g	44	ALA
15	g	58	ALA
15	h	20	SER
15	h	44	ALA

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Mol	Chain	Res	Type
15	h	58	ALA
15	i	20	SER
15	i	44	ALA
15	i	58	ALA
15	j	20	SER
15	j	44	ALA
15	j	58	ALA
15	k	20	SER
15	k	44	ALA
15	k	58	ALA
15	l	20	SER
15	l	44	ALA
15	l	58	ALA
15	m	20	SER
15	m	58	ALA
15	n	20	SER
15	n	44	ALA
15	n	58	ALA
15	o	20	SER
15	o	44	ALA
15	o	58	ALA
15	p	20	SER
15	p	44	ALA
15	p	58	ALA
1	A	37	GLN
1	A	168	ALA
1	A	232	LYS
2	B	5	TYR
2	B	8	SER
2	B	16	GLY
2	B	155	SER
2	B	242	GLU
3	C	78	ALA
3	C	232	PRO
3	C	234	GLU
5	E	190	SER
8	H	68	SER
8	H	129	SER
8	H	138	CYS
8	H	152	VAL
8	H	190	PRO
9	I	17	ASP

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Mol	Chain	Res	Type
9	I	169	SER
9	I	183	ASP
10	J	117	LEU
11	K	8	VAL
13	M	156	ASN
13	M	201	ASP
14	N	68	TYR
14	N	73	ALA
14	N	122	VAL
14	N	124	LEU
1	O	145	SER
1	O	168	ALA
2	P	16	GLY
2	P	155	SER
2	P	242	GLU
3	Q	83	ASP
3	Q	232	PRO
3	Q	234	GLU
6	T	175	THR
6	T	228	GLU
8	V	105	LYS
8	V	129	SER
8	V	152	VAL
9	W	17	ASP
9	W	169	SER
9	W	183	ASP
10	X	185	GLU
11	Y	8	VAL
11	Y	23	GLY
11	Y	52	THR
11	Y	140	PHE
13	a	156	ASN
13	a	200	LYS
13	a	201	ASP
14	b	68	TYR
14	b	223	GLN
15	c	63	SER
15	c	130	LYS
15	d	63	SER
15	d	103	ASP
15	d	130	LYS
15	e	63	SER

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Mol	Chain	Res	Type
15	f	59	GLN
15	f	63	SER
15	f	103	ASP
15	f	130	LYS
15	g	130	LYS
15	h	63	SER
15	h	103	ASP
15	i	63	SER
15	i	130	LYS
15	j	63	SER
15	j	130	LYS
15	k	63	SER
15	k	103	ASP
15	k	130	LYS
15	l	63	SER
15	l	103	ASP
15	l	224	THR
15	m	44	ALA
15	n	63	SER
15	n	103	ASP
15	o	63	SER
15	p	63	SER
15	p	130	LYS
1	A	128	TYR
1	A	134	MET
1	A	145	SER
1	A	179	THR
2	B	120	GLU
3	C	64	GLU
3	C	83	ASP
4	D	170	THR
4	D	194	LEU
5	E	53	ARG
5	E	206	GLN
5	E	225	GLN
5	E	249	ALA
7	G	246	ILE
9	I	171	SER
10	J	185	GLU
11	K	140	PHE
13	M	94	PHE
14	N	103	TRP

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Mol	Chain	Res	Type
14	N	213	PHE
1	O	179	THR
2	P	5	TYR
2	P	58	SER
2	P	120	GLU
3	Q	28	SER
3	Q	64	GLU
3	Q	78	ALA
3	Q	84	ALA
3	Q	178	MET
4	R	170	THR
4	R	194	LEU
5	S	53	ARG
5	S	206	GLN
5	S	225	GLN
5	S	249	ALA
6	T	159	THR
7	U	122	HIS
7	U	219	SER
8	V	190	PRO
9	W	145	ASP
9	W	171	SER
13	a	17	ASP
13	a	49	ALA
14	b	103	TRP
14	b	213	PHE
15	c	59	GLN
15	c	224	THR
15	d	59	GLN
15	d	224	THR
15	e	103	ASP
15	e	130	LYS
15	e	224	THR
15	f	224	THR
15	g	63	SER
15	g	224	THR
15	h	59	GLN
15	h	224	THR
15	i	59	GLN
15	i	103	ASP
15	i	224	THR
15	j	224	THR

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Mol	Chain	Res	Type
15	k	59	GLN
15	k	224	THR
15	l	130	LYS
15	m	59	GLN
15	m	63	SER
15	m	130	LYS
15	m	224	THR
15	n	59	GLN
15	n	130	LYS
15	n	224	THR
15	o	59	GLN
15	o	103	ASP
15	o	130	LYS
15	o	224	THR
15	p	59	GLN
15	p	224	THR
15	p	227	ASP
2	B	58	SER
3	C	84	ALA
3	C	178	MET
5	E	127	ALA
6	F	40	SER
6	F	186	PRO
7	G	219	SER
8	H	49	ALA
8	H	87	TYR
8	H	88	GLU
8	H	132	THR
9	I	106	THR
9	I	145	ASP
12	L	39	PRO
14	N	17	ASP
14	N	139	GLY
1	O	37	GLN
1	O	128	TYR
1	O	134	MET
3	Q	54	SER
3	Q	168	ASN
5	S	135	SER
6	T	40	SER
7	U	63	ASN
7	U	246	ILE

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Mol	Chain	Res	Type
8	V	132	THR
9	W	53	GLU
9	W	105	PRO
14	b	16	ALA
14	b	17	ASP
14	b	100	ASN
14	b	139	GLY
14	b	144	ASN
15	c	103	ASP
15	d	227	ASP
15	e	59	GLN
15	g	59	GLN
15	g	103	ASP
15	h	130	LYS
15	j	59	GLN
15	l	59	GLN
15	m	103	ASP
15	p	103	ASP
2	B	69	PRO
2	B	107	THR
3	C	54	SER
9	I	53	GLU
11	K	23	GLY
11	K	145	HIS
13	M	49	ALA
14	N	-7	GLN
14	N	100	ASN
4	R	152	PRO
5	S	109	VAL
5	S	127	ALA
6	T	186	PRO
14	b	-7	GLN
15	e	227	ASP
9	I	105	PRO
14	N	101	PRO
2	P	69	PRO
12	Z	39	PRO
14	b	101	PRO
4	D	152	PRO
5	E	109	VAL
7	G	140	VAL
9	I	192	THR

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Mol	Chain	Res	Type
10	J	75	PRO
13	M	52	GLY
6	T	130	VAL
10	X	-6	PRO
13	a	52	GLY
13	a	157	GLY
14	b	14	ILE
3	C	15	PRO
13	M	157	GLY
14	N	144	ASN
7	U	140	VAL
10	X	75	PRO
9	I	220	ILE
10	J	-6	PRO
7	U	13	VAL
9	W	220	ILE
14	N	84	ILE
14	b	84	ILE

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	204/210 (97%)	173 (85%)	31 (15%)	4	19
1	O	204/210 (97%)	174 (85%)	30 (15%)	4	21
2	B	200/209 (96%)	169 (84%)	31 (16%)	4	17
2	P	200/209 (96%)	167 (84%)	33 (16%)	3	14
3	C	198/204 (97%)	168 (85%)	30 (15%)	4	19
3	Q	198/204 (97%)	169 (85%)	29 (15%)	5	21
4	D	209/226 (92%)	175 (84%)	34 (16%)	3	15
4	R	209/226 (92%)	176 (84%)	33 (16%)	4	16
5	E	198/215 (92%)	170 (86%)	28 (14%)	5	23
5	S	198/215 (92%)	170 (86%)	28 (14%)	5	23
6	F	192/193 (100%)	164 (85%)	28 (15%)	5	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	T	192/193 (100%)	164 (85%)	28 (15%)	5	21
7	G	199/238 (84%)	167 (84%)	32 (16%)	3	16
7	U	199/238 (84%)	165 (83%)	34 (17%)	3	14
8	H	161/162 (99%)	132 (82%)	29 (18%)	2	12
8	V	161/162 (99%)	133 (83%)	28 (17%)	3	13
9	I	181/190 (95%)	156 (86%)	25 (14%)	5	24
9	W	181/190 (95%)	157 (87%)	24 (13%)	6	27
10	J	172/173 (99%)	149 (87%)	23 (13%)	6	26
10	X	172/173 (99%)	150 (87%)	22 (13%)	6	28
11	K	175/175 (100%)	155 (89%)	20 (11%)	8	35
11	Y	175/175 (100%)	154 (88%)	21 (12%)	7	32
12	L	169/169 (100%)	147 (87%)	22 (13%)	6	28
12	Z	169/169 (100%)	148 (88%)	21 (12%)	7	30
13	M	185/185 (100%)	163 (88%)	22 (12%)	8	33
13	a	185/185 (100%)	162 (88%)	23 (12%)	7	30
14	N	199/199 (100%)	169 (85%)	30 (15%)	4	19
14	b	199/199 (100%)	167 (84%)	32 (16%)	3	16
15	c	163/190 (86%)	146 (90%)	17 (10%)	10	39
15	d	163/190 (86%)	146 (90%)	17 (10%)	10	39
15	e	163/190 (86%)	146 (90%)	17 (10%)	10	39
15	f	163/190 (86%)	147 (90%)	16 (10%)	12	43
15	g	163/190 (86%)	147 (90%)	16 (10%)	12	43
15	h	163/190 (86%)	147 (90%)	16 (10%)	12	43
15	i	163/190 (86%)	146 (90%)	17 (10%)	10	39
15	j	163/190 (86%)	146 (90%)	17 (10%)	10	39
15	k	163/190 (86%)	147 (90%)	16 (10%)	12	43
15	l	163/190 (86%)	147 (90%)	16 (10%)	12	43
15	m	163/190 (86%)	147 (90%)	16 (10%)	12	43
15	n	163/190 (86%)	146 (90%)	17 (10%)	10	39
15	o	163/190 (86%)	147 (90%)	16 (10%)	12	43
15	p	163/190 (86%)	147 (90%)	16 (10%)	12	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	7566/8156 (93%)	6565 (87%)	1001 (13%)	6 27

All (1001) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ILE
1	A	25	LEU
1	A	37	GLN
1	A	38	THR
1	A	39	ASN
1	A	43	LEU
1	A	73	PHE
1	A	89	ASP
1	A	103	GLU
1	A	116	VAL
1	A	126	GLN
1	A	137	LEU
1	A	142	THR
1	A	147	ASP
1	A	148	GLU
1	A	153	SER
1	A	162	TYR
1	A	163	TYR
1	A	167	LYS
1	A	171	THR
1	A	177	GLU
1	A	182	LEU
1	A	209	HIS
1	A	218	PHE
1	A	220	LYS
1	A	231	ASP
1	A	234	PHE
1	A	235	THR
1	A	240	ASN
1	A	244	ARG
1	A	251	GLN
2	B	11	THR
2	B	18	LEU
2	B	40	THR
2	B	59	GLU
2	B	61	LEU
2	B	68	THR

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Mol	Chain	Res	Type
2	B	70	ASP
2	B	89	SER
2	B	94	HIS
2	B	107	THR
2	B	112	SER
2	B	118	MET
2	B	119	GLN
2	B	134	LEU
2	B	150	VAL
2	B	156	TYR
2	B	157	PHE
2	B	173	THR
2	B	178	ARG
2	B	180	ASN
2	B	183	LEU
2	B	197	LYS
2	B	204	PHE
2	B	207	ASP
2	B	210	GLU
2	B	217	GLU
2	B	220	ASP
2	B	241	GLN
2	B	244	ASN
2	B	247	LEU
2	B	248	GLU
3	C	10	THR
3	C	13	PHE
3	C	27	GLU
3	C	28	SER
3	C	50	ARG
3	C	53	THR
3	C	55	THR
3	C	59	GLN
3	C	60	ASP
3	C	69	LEU
3	C	114	ARG
3	C	115	LEU
3	C	120	GLN
3	C	123	THR
3	C	134	SER
3	C	140	TYR
3	C	143	ARG

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Mol	Chain	Res	Type
3	C	150	THR
3	C	175	LEU
3	C	185	LYS
3	C	188	ASP
3	C	197	LEU
3	C	202	ASP
3	C	209	ASP
3	C	213	PHE
3	C	218	LYS
3	C	221	ASN
3	C	231	LYS
3	C	232	PRO
3	C	235	ILE
4	D	24	LEU
4	D	31	THR
4	D	39	LYS
4	D	48	ARG
4	D	57	THR
4	D	60	THR
4	D	62	SER
4	D	73	LEU
4	D	97	ARG
4	D	100	LEU
4	D	105	THR
4	D	107	GLU
4	D	118	GLN
4	D	126	VAL
4	D	133	THR
4	D	142	ASP
4	D	147	LEU
4	D	149	GLN
4	D	150	THR
4	D	152	PRO
4	D	155	ILE
4	D	162	GLN
4	D	166	ARG
4	D	181	ARG
4	D	187	THR
4	D	190	GLU
4	D	195	THR
4	D	201	GLU
4	D	208	LYS

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Mol	Chain	Res	Type
4	D	221	ILE
4	D	226	SER
4	D	241	GLN
4	D	242	GLU
4	D	243	GLN
5	E	15	PHE
5	E	18	GLU
5	E	36	THR
5	E	48	LEU
5	E	53	ARG
5	E	59	LEU
5	E	61	SER
5	E	78	MET
5	E	81	LEU
5	E	86	ARG
5	E	116	VAL
5	E	125	GLU
5	E	134	MET
5	E	160	PRO
5	E	166	ARG
5	E	177	GLU
5	E	184	LEU
5	E	185	ASN
5	E	189	SER
5	E	208	MET
5	E	209	GLU
5	E	210	GLU
5	E	221	CYS
5	E	222	ILE
5	E	234	GLU
5	E	235	LYS
5	E	242	GLU
5	E	245	GLU
6	F	11	VAL
6	F	27	GLU
6	F	29	ILE
6	F	39	ARG
6	F	56	LEU
6	F	62	LYS
6	F	72	LEU
6	F	80	ASP
6	F	90	GLN

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Mol	Chain	Res	Type
6	F	101	ARG
6	F	115	LYS
6	F	117	GLN
6	F	121	GLN
6	F	138	ASP
6	F	146	GLU
6	F	147	PHE
6	F	154	THR
6	F	164	ARG
6	F	176	LEU
6	F	185	ASN
6	F	187	ASP
6	F	189	LEU
6	F	198	SER
6	F	202	ARG
6	F	203	ASP
6	F	206	LEU
6	F	215	ILE
6	F	228	GLU
7	G	8	ASP
7	G	9	LEU
7	G	16	PRO
7	G	19	ARG
7	G	24	GLU
7	G	28	LYS
7	G	85	ARG
7	G	86	HIS
7	G	94	GLU
7	G	98	PHE
7	G	104	THR
7	G	106	ILE
7	G	120	GLN
7	G	125	TYR
7	G	134	SER
7	G	143	ASN
7	G	147	LEU
7	G	164	THR
7	G	176	GLU
7	G	180	ASP
7	G	184	GLU
7	G	190	GLU
7	G	201	LEU

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Mol	Chain	Res	Type
7	G	204	GLU
7	G	207	LYS
7	G	208	GLU
7	G	210	ASP
7	G	215	ILE
7	G	217	TRP
7	G	224	ASN
7	G	241	PHE
7	G	245	GLU
8	H	8	PHE
8	H	14	LEU
8	H	21	THR
8	H	30	VAL
8	H	64	GLU
8	H	80	SER
8	H	84	GLU
8	H	86	CYS
8	H	88	GLU
8	H	91	ASP
8	H	92	ASN
8	H	97	ILE
8	H	104	ASP
8	H	106	ASN
8	H	110	VAL
8	H	115	LEU
8	H	119	VAL
8	H	132	THR
8	H	133	PHE
8	H	145	ASN
8	H	146	MET
8	H	149	GLU
8	H	153	ASP
8	H	154	PHE
8	H	160	SER
8	H	178	LEU
8	H	185	ARG
8	H	187	ILE
8	H	188	PHE
9	I	9	ASN
9	I	14	ILE
9	I	22	GLN
9	I	30	ASN

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Mol	Chain	Res	Type
9	I	35	HIS
9	I	41	ILE
9	I	63	ILE
9	I	68	LEU
9	I	80	LEU
9	I	82	MET
9	I	88	PHE
9	I	90	TYR
9	I	94	ILE
9	I	98	LEU
9	I	106	THR
9	I	131	SER
9	I	141	HIS
9	I	146	LEU
9	I	149	GLU
9	I	156	SER
9	I	177	VAL
9	I	197	GLU
9	I	217	ILE
9	I	218	VAL
9	I	222	ASP
10	J	3	VAL
10	J	12	VAL
10	J	20	LEU
10	J	23	GLN
10	J	29	ASN
10	J	35	PHE
10	J	40	VAL
10	J	49	THR
10	J	53	THR
10	J	54	LEU
10	J	56	GLU
10	J	57	MET
10	J	64	LEU
10	J	67	LEU
10	J	82	VAL
10	J	89	ARG
10	J	115	PHE
10	J	123	GLU
10	J	125	LYS
10	J	126	ASP
10	J	129	VAL

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Mol	Chain	Res	Type
10	J	130	SER
10	J	191	LEU
11	K	6	ILE
11	K	9	GLN
11	K	10	ASP
11	K	16	SER
11	K	30	SER
11	K	34	THR
11	K	41	THR
11	K	77	GLN
11	K	89	LYS
11	K	94	ARG
11	K	109	LYS
11	K	110	LYS
11	K	139	THR
11	K	145	HIS
11	K	159	LEU
11	K	171	MET
11	K	178	VAL
11	K	180	VAL
11	K	185	LYS
11	K	194	PHE
12	L	4	LEU
12	L	9	GLN
12	L	25	TRP
12	L	32	LYS
12	L	39	PRO
12	L	81	LYS
12	L	95	LEU
12	L	104	TYR
12	L	105	THR
12	L	111	THR
12	L	114	TYR
12	L	121	ARG
12	L	125	ASP
12	L	131	SER
12	L	134	THR
12	L	140	LEU
12	L	148	LEU
12	L	151	GLU
12	L	183	ASP
12	L	186	ILE

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Mol	Chain	Res	Type
12	L	209	ASN
12	L	211	ILE
13	M	9	GLU
13	M	11	PHE
13	M	14	LEU
13	M	26	ILE
13	M	34	VAL
13	M	40	ASN
13	M	78	ASN
13	M	88	LEU
13	M	98	VAL
13	M	99	HIS
13	M	100	THR
13	M	122	TYR
13	M	123	GLU
13	M	126	GLN
13	M	141	LEU
13	M	142	ASP
13	M	143	ASN
13	M	156	ASN
13	M	165	TYR
13	M	166	LEU
13	M	201	ASP
13	M	205	LYS
14	N	-6	GLN
14	N	19	LEU
14	N	21	SER
14	N	39	ASP
14	N	40	ASN
14	N	60	LYS
14	N	70	ASN
14	N	72	LEU
14	N	77	GLU
14	N	88	LEU
14	N	96	ARG
14	N	98	LYS
14	N	101	PRO
14	N	103	TRP
14	N	125	LEU
14	N	130	SER
14	N	142	MET
14	N	145	PRO

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Mol	Chain	Res	Type
14	N	146	LEU
14	N	153	ARG
14	N	161	THR
14	N	179	ARG
14	N	182	ARG
14	N	200	PHE
14	N	204	LEU
14	N	208	ASN
14	N	218	LYS
14	N	223	GLN
14	N	224	LYS
14	N	225	ILE
1	O	18	ILE
1	O	25	LEU
1	O	37	GLN
1	O	38	THR
1	O	39	ASN
1	O	43	LEU
1	O	73	PHE
1	O	89	ASP
1	O	103	GLU
1	O	116	VAL
1	O	126	GLN
1	O	137	LEU
1	O	142	THR
1	O	147	ASP
1	O	148	GLU
1	O	153	SER
1	O	162	TYR
1	O	163	TYR
1	O	167	LYS
1	O	171	THR
1	O	177	GLU
1	O	209	HIS
1	O	218	PHE
1	O	220	LYS
1	O	231	ASP
1	O	234	PHE
1	O	235	THR
1	O	240	ASN
1	O	244	ARG
1	O	251	GLN

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Mol	Chain	Res	Type
2	P	11	THR
2	P	18	LEU
2	P	40	THR
2	P	57	MET
2	P	59	GLU
2	P	61	LEU
2	P	68	THR
2	P	70	ASP
2	P	89	SER
2	P	94	HIS
2	P	107	THR
2	P	112	SER
2	P	118	MET
2	P	119	GLN
2	P	134	LEU
2	P	150	VAL
2	P	156	TYR
2	P	157	PHE
2	P	173	THR
2	P	178	ARG
2	P	180	ASN
2	P	183	LEU
2	P	197	LYS
2	P	204	PHE
2	P	207	ASP
2	P	210	GLU
2	P	211	LEU
2	P	217	GLU
2	P	220	ASP
2	P	241	GLN
2	P	244	ASN
2	P	247	LEU
2	P	248	GLU
3	Q	10	THR
3	Q	13	PHE
3	Q	27	GLU
3	Q	28	SER
3	Q	50	ARG
3	Q	53	THR
3	Q	55	THR
3	Q	59	GLN
3	Q	60	ASP

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Mol	Chain	Res	Type
3	Q	69	LEU
3	Q	114	ARG
3	Q	115	LEU
3	Q	120	GLN
3	Q	123	THR
3	Q	134	SER
3	Q	140	TYR
3	Q	143	ARG
3	Q	150	THR
3	Q	175	LEU
3	Q	185	LYS
3	Q	188	ASP
3	Q	197	LEU
3	Q	202	ASP
3	Q	209	ASP
3	Q	213	PHE
3	Q	218	LYS
3	Q	231	LYS
3	Q	232	PRO
3	Q	235	ILE
4	R	24	LEU
4	R	31	THR
4	R	39	LYS
4	R	48	ARG
4	R	57	THR
4	R	60	THR
4	R	62	SER
4	R	73	LEU
4	R	97	ARG
4	R	100	LEU
4	R	105	THR
4	R	107	GLU
4	R	118	GLN
4	R	126	VAL
4	R	133	THR
4	R	147	LEU
4	R	149	GLN
4	R	150	THR
4	R	152	PRO
4	R	155	ILE
4	R	162	GLN
4	R	166	ARG

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Mol	Chain	Res	Type
4	R	181	ARG
4	R	187	THR
4	R	190	GLU
4	R	195	THR
4	R	201	GLU
4	R	208	LYS
4	R	221	ILE
4	R	226	SER
4	R	241	GLN
4	R	242	GLU
4	R	243	GLN
5	S	15	PHE
5	S	18	GLU
5	S	36	THR
5	S	48	LEU
5	S	53	ARG
5	S	59	LEU
5	S	61	SER
5	S	78	MET
5	S	81	LEU
5	S	86	ARG
5	S	90	GLU
5	S	116	VAL
5	S	125	GLU
5	S	134	MET
5	S	160	PRO
5	S	166	ARG
5	S	177	GLU
5	S	184	LEU
5	S	185	ASN
5	S	189	SER
5	S	208	MET
5	S	209	GLU
5	S	210	GLU
5	S	221	CYS
5	S	222	ILE
5	S	234	GLU
5	S	235	LYS
5	S	245	GLU
6	T	11	VAL
6	T	27	GLU
6	T	29	ILE

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Mol	Chain	Res	Type
6	T	39	ARG
6	T	56	LEU
6	T	62	LYS
6	T	72	LEU
6	T	80	ASP
6	T	90	GLN
6	T	101	ARG
6	T	115	LYS
6	T	117	GLN
6	T	121	GLN
6	T	138	ASP
6	T	146	GLU
6	T	147	PHE
6	T	154	THR
6	T	164	ARG
6	T	176	LEU
6	T	185	ASN
6	T	187	ASP
6	T	189	LEU
6	T	198	SER
6	T	202	ARG
6	T	203	ASP
6	T	206	LEU
6	T	215	ILE
6	T	228	GLU
7	U	8	ASP
7	U	9	LEU
7	U	16	PRO
7	U	19	ARG
7	U	24	GLU
7	U	28	LYS
7	U	85	ARG
7	U	86	HIS
7	U	94	GLU
7	U	97	SER
7	U	98	PHE
7	U	104	THR
7	U	106	ILE
7	U	120	GLN
7	U	125	TYR
7	U	134	SER
7	U	140	VAL

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Mol	Chain	Res	Type
7	U	143	ASN
7	U	147	LEU
7	U	152	PRO
7	U	164	THR
7	U	176	GLU
7	U	180	ASP
7	U	184	GLU
7	U	190	GLU
7	U	201	LEU
7	U	204	GLU
7	U	207	LYS
7	U	208	GLU
7	U	210	ASP
7	U	215	ILE
7	U	217	TRP
7	U	224	ASN
7	U	245	GLU
8	V	8	PHE
8	V	14	LEU
8	V	30	VAL
8	V	36	ARG
8	V	64	GLU
8	V	80	SER
8	V	84	GLU
8	V	86	CYS
8	V	88	GLU
8	V	91	ASP
8	V	92	ASN
8	V	104	ASP
8	V	106	ASN
8	V	110	VAL
8	V	115	LEU
8	V	119	VAL
8	V	124	TYR
8	V	132	THR
8	V	133	PHE
8	V	146	MET
8	V	149	GLU
8	V	151	THR
8	V	154	PHE
8	V	160	SER
8	V	178	LEU

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Mol	Chain	Res	Type
8	V	185	ARG
8	V	187	ILE
8	V	188	PHE
9	W	9	ASN
9	W	14	ILE
9	W	22	GLN
9	W	30	ASN
9	W	35	HIS
9	W	41	ILE
9	W	63	ILE
9	W	68	LEU
9	W	80	LEU
9	W	82	MET
9	W	88	PHE
9	W	90	TYR
9	W	94	ILE
9	W	98	LEU
9	W	106	THR
9	W	131	SER
9	W	141	HIS
9	W	149	GLU
9	W	153	LYS
9	W	156	SER
9	W	177	VAL
9	W	197	GLU
9	W	217	ILE
9	W	222	ASP
10	X	3	VAL
10	X	12	VAL
10	X	20	LEU
10	X	23	GLN
10	X	29	ASN
10	X	35	PHE
10	X	40	VAL
10	X	49	THR
10	X	53	THR
10	X	54	LEU
10	X	56	GLU
10	X	57	MET
10	X	64	LEU
10	X	67	LEU
10	X	89	ARG

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Mol	Chain	Res	Type
10	X	115	PHE
10	X	123	GLU
10	X	125	LYS
10	X	126	ASP
10	X	129	VAL
10	X	130	SER
10	X	191	LEU
11	Y	6	ILE
11	Y	9	GLN
11	Y	10	ASP
11	Y	16	SER
11	Y	30	SER
11	Y	34	THR
11	Y	41	THR
11	Y	74	LEU
11	Y	77	GLN
11	Y	89	LYS
11	Y	94	ARG
11	Y	95	ARG
11	Y	109	LYS
11	Y	110	LYS
11	Y	145	HIS
11	Y	159	LEU
11	Y	171	MET
11	Y	178	VAL
11	Y	180	VAL
11	Y	185	LYS
11	Y	194	PHE
12	Z	4	LEU
12	Z	9	GLN
12	Z	25	TRP
12	Z	32	LYS
12	Z	39	PRO
12	Z	81	LYS
12	Z	95	LEU
12	Z	104	TYR
12	Z	105	THR
12	Z	111	THR
12	Z	114	TYR
12	Z	121	ARG
12	Z	125	ASP
12	Z	131	SER

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Mol	Chain	Res	Type
12	Z	134	THR
12	Z	140	LEU
12	Z	148	LEU
12	Z	183	ASP
12	Z	186	ILE
12	Z	209	ASN
12	Z	211	ILE
13	a	9	GLU
13	a	11	PHE
13	a	14	LEU
13	a	26	ILE
13	a	34	VAL
13	a	39	ASP
13	a	40	ASN
13	a	78	ASN
13	a	88	LEU
13	a	98	VAL
13	a	99	HIS
13	a	100	THR
13	a	122	TYR
13	a	123	GLU
13	a	126	GLN
13	a	141	LEU
13	a	142	ASP
13	a	143	ASN
13	a	156	ASN
13	a	165	TYR
13	a	166	LEU
13	a	201	ASP
13	a	205	LYS
14	b	-6	GLN
14	b	19	LEU
14	b	21	SER
14	b	39	ASP
14	b	40	ASN
14	b	60	LYS
14	b	70	ASN
14	b	72	LEU
14	b	77	GLU
14	b	88	LEU
14	b	96	ARG
14	b	98	LYS

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Mol	Chain	Res	Type
14	b	101	PRO
14	b	103	TRP
14	b	125	LEU
14	b	130	SER
14	b	142	MET
14	b	145	PRO
14	b	146	LEU
14	b	151	VAL
14	b	153	ARG
14	b	161	THR
14	b	176	LEU
14	b	179	ARG
14	b	182	ARG
14	b	200	PHE
14	b	204	LEU
14	b	208	ASN
14	b	218	LYS
14	b	223	GLN
14	b	224	LYS
14	b	225	ILE
15	c	14	ASP
15	c	26	GLU
15	c	34	GLN
15	c	35	GLU
15	c	47	HIS
15	c	55	TYR
15	c	61	GLU
15	c	68	LEU
15	c	72	GLN
15	c	90	THR
15	c	120	LEU
15	c	138	THR
15	c	143	TYR
15	c	146	ARG
15	c	183	LEU
15	c	221	GLN
15	c	227	ASP
15	d	14	ASP
15	d	26	GLU
15	d	34	GLN
15	d	35	GLU
15	d	47	HIS

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Mol	Chain	Res	Type
15	d	55	TYR
15	d	61	GLU
15	d	68	LEU
15	d	72	GLN
15	d	90	THR
15	d	120	LEU
15	d	138	THR
15	d	143	TYR
15	d	146	ARG
15	d	183	LEU
15	d	221	GLN
15	d	227	ASP
15	e	14	ASP
15	e	26	GLU
15	e	34	GLN
15	e	35	GLU
15	e	47	HIS
15	e	55	TYR
15	e	61	GLU
15	e	68	LEU
15	e	72	GLN
15	e	90	THR
15	e	120	LEU
15	e	138	THR
15	e	143	TYR
15	e	146	ARG
15	e	183	LEU
15	e	221	GLN
15	e	227	ASP
15	f	14	ASP
15	f	26	GLU
15	f	34	GLN
15	f	35	GLU
15	f	47	HIS
15	f	55	TYR
15	f	61	GLU
15	f	68	LEU
15	f	72	GLN
15	f	90	THR
15	f	120	LEU
15	f	138	THR
15	f	146	ARG

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Mol	Chain	Res	Type
15	f	183	LEU
15	f	221	GLN
15	f	227	ASP
15	g	14	ASP
15	g	26	GLU
15	g	34	GLN
15	g	35	GLU
15	g	47	HIS
15	g	55	TYR
15	g	61	GLU
15	g	68	LEU
15	g	72	GLN
15	g	90	THR
15	g	120	LEU
15	g	138	THR
15	g	146	ARG
15	g	183	LEU
15	g	221	GLN
15	g	227	ASP
15	h	14	ASP
15	h	26	GLU
15	h	34	GLN
15	h	35	GLU
15	h	47	HIS
15	h	55	TYR
15	h	61	GLU
15	h	68	LEU
15	h	72	GLN
15	h	90	THR
15	h	120	LEU
15	h	138	THR
15	h	146	ARG
15	h	183	LEU
15	h	221	GLN
15	h	227	ASP
15	i	14	ASP
15	i	26	GLU
15	i	34	GLN
15	i	35	GLU
15	i	47	HIS
15	i	55	TYR
15	i	61	GLU

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Mol	Chain	Res	Type
15	i	68	LEU
15	i	72	GLN
15	i	90	THR
15	i	120	LEU
15	i	138	THR
15	i	143	TYR
15	i	146	ARG
15	i	183	LEU
15	i	221	GLN
15	i	227	ASP
15	j	14	ASP
15	j	26	GLU
15	j	34	GLN
15	j	35	GLU
15	j	47	HIS
15	j	55	TYR
15	j	61	GLU
15	j	68	LEU
15	j	72	GLN
15	j	90	THR
15	j	120	LEU
15	j	138	THR
15	j	143	TYR
15	j	146	ARG
15	j	183	LEU
15	j	221	GLN
15	j	227	ASP
15	k	14	ASP
15	k	26	GLU
15	k	34	GLN
15	k	35	GLU
15	k	47	HIS
15	k	55	TYR
15	k	61	GLU
15	k	68	LEU
15	k	72	GLN
15	k	90	THR
15	k	120	LEU
15	k	138	THR
15	k	146	ARG
15	k	183	LEU
15	k	221	GLN

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Mol	Chain	Res	Type
15	k	227	ASP
15	l	14	ASP
15	l	26	GLU
15	l	34	GLN
15	l	35	GLU
15	l	47	HIS
15	l	55	TYR
15	l	61	GLU
15	l	68	LEU
15	l	72	GLN
15	l	90	THR
15	l	120	LEU
15	l	138	THR
15	l	146	ARG
15	l	183	LEU
15	l	221	GLN
15	l	227	ASP
15	m	14	ASP
15	m	26	GLU
15	m	34	GLN
15	m	35	GLU
15	m	47	HIS
15	m	55	TYR
15	m	61	GLU
15	m	68	LEU
15	m	72	GLN
15	m	90	THR
15	m	120	LEU
15	m	138	THR
15	m	146	ARG
15	m	183	LEU
15	m	221	GLN
15	m	227	ASP
15	n	14	ASP
15	n	26	GLU
15	n	34	GLN
15	n	35	GLU
15	n	47	HIS
15	n	55	TYR
15	n	61	GLU
15	n	68	LEU
15	n	72	GLN

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Mol	Chain	Res	Type
15	n	90	THR
15	n	120	LEU
15	n	138	THR
15	n	143	TYR
15	n	146	ARG
15	n	183	LEU
15	n	221	GLN
15	n	227	ASP
15	o	14	ASP
15	o	26	GLU
15	o	34	GLN
15	o	35	GLU
15	o	47	HIS
15	o	55	TYR
15	o	61	GLU
15	o	68	LEU
15	o	72	GLN
15	o	90	THR
15	o	120	LEU
15	o	138	THR
15	o	146	ARG
15	o	183	LEU
15	o	221	GLN
15	o	227	ASP
15	p	14	ASP
15	p	26	GLU
15	p	34	GLN
15	p	35	GLU
15	p	47	HIS
15	p	55	TYR
15	p	61	GLU
15	p	68	LEU
15	p	72	GLN
15	p	90	THR
15	p	120	LEU
15	p	138	THR
15	p	146	ARG
15	p	183	LEU
15	p	221	GLN
15	p	227	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (268) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	ASN
1	A	123	ASN
1	A	126	GLN
1	A	130	GLN
1	A	175	GLN
1	A	181	ASN
1	A	184	ASN
2	B	20	GLN
2	B	30	GLN
2	B	139	HIS
2	B	190	HIS
2	B	205	ASN
2	B	218	ASN
2	B	244	ASN
3	C	59	GLN
3	C	70	ASN
3	C	94	HIS
3	C	120	GLN
3	C	124	GLN
4	D	19	GLN
4	D	118	GLN
4	D	162	GLN
4	D	204	GLN
4	D	231	GLN
4	D	241	GLN
4	D	243	GLN
5	E	23	GLN
5	E	108	ASN
5	E	206	GLN
6	F	4	ASN
6	F	90	GLN
6	F	117	GLN
6	F	119	ASN
6	F	121	GLN
6	F	185	ASN
6	F	199	GLN
7	G	22	GLN
7	G	42	ASN
7	G	63	ASN
7	G	72	HIS
7	G	86	HIS
7	G	117	GLN
7	G	143	ASN

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Mol	Chain	Res	Type
7	G	194	GLN
7	G	206	ASN
7	G	224	ASN
8	H	69	GLN
8	H	89	ASN
8	H	92	ASN
9	I	9	ASN
9	I	22	GLN
9	I	30	ASN
9	I	57	GLN
9	I	66	HIS
9	I	86	HIS
9	I	109	HIS
9	I	144	GLN
9	I	165	ASN
9	I	200	GLN
10	J	29	ASN
10	J	63	ASN
10	J	148	ASN
11	K	9	GLN
11	K	36	GLN
11	K	40	HIS
11	K	117	GLN
11	K	195	GLN
11	K	197	GLN
12	L	9	GLN
12	L	66	HIS
12	L	85	ASN
12	L	176	ASN
12	L	179	HIS
12	L	188	HIS
12	L	191	HIS
12	L	209	ASN
13	M	-7	ASN
13	M	40	ASN
13	M	61	ASN
13	M	71	ASN
13	M	83	ASN
13	M	99	HIS
13	M	143	ASN
13	M	156	ASN
13	M	186	HIS

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Mol	Chain	Res	Type
14	N	29	ASN
14	N	40	ASN
14	N	53	GLN
14	N	66	ASN
14	N	104	ASN
14	N	144	ASN
14	N	163	GLN
14	N	203	ASN
14	N	208	ASN
1	O	39	ASN
1	O	84	ASN
1	O	123	ASN
1	O	126	GLN
1	O	130	GLN
1	O	175	GLN
1	O	181	ASN
1	O	184	ASN
2	P	20	GLN
2	P	139	HIS
2	P	190	HIS
2	P	205	ASN
2	P	218	ASN
2	P	244	ASN
3	Q	59	GLN
3	Q	70	ASN
3	Q	94	HIS
3	Q	120	GLN
3	Q	124	GLN
4	R	19	GLN
4	R	79	ASN
4	R	118	GLN
4	R	162	GLN
4	R	204	GLN
4	R	231	GLN
4	R	241	GLN
4	R	243	GLN
5	S	23	GLN
5	S	108	ASN
5	S	206	GLN
6	T	4	ASN
6	T	90	GLN
6	T	93	ASN

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Mol	Chain	Res	Type
6	T	117	GLN
6	T	119	ASN
6	T	121	GLN
6	T	185	ASN
6	T	199	GLN
7	U	22	GLN
7	U	42	ASN
7	U	63	ASN
7	U	72	HIS
7	U	143	ASN
7	U	181	HIS
7	U	194	GLN
7	U	206	ASN
7	U	224	ASN
8	V	69	GLN
8	V	92	ASN
9	W	9	ASN
9	W	22	GLN
9	W	30	ASN
9	W	57	GLN
9	W	62	ASN
9	W	66	HIS
9	W	86	HIS
9	W	144	GLN
9	W	165	ASN
9	W	200	GLN
10	X	29	ASN
10	X	63	ASN
10	X	80	GLN
10	X	148	ASN
11	Y	36	GLN
11	Y	40	HIS
11	Y	77	GLN
11	Y	117	GLN
11	Y	195	GLN
11	Y	197	GLN
12	Z	9	GLN
12	Z	66	HIS
12	Z	85	ASN
12	Z	176	ASN
12	Z	179	HIS
12	Z	188	HIS

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Mol	Chain	Res	Type
12	Z	191	HIS
12	Z	209	ASN
13	a	-7	ASN
13	a	40	ASN
13	a	61	ASN
13	a	71	ASN
13	a	83	ASN
13	a	99	HIS
13	a	143	ASN
13	a	149	ASN
13	a	156	ASN
13	a	186	HIS
14	b	29	ASN
14	b	40	ASN
14	b	53	GLN
14	b	66	ASN
14	b	104	ASN
14	b	144	ASN
14	b	163	GLN
14	b	171	ASN
14	b	203	ASN
14	b	208	ASN
15	c	52	ASN
15	c	72	GLN
15	c	75	GLN
15	c	80	ASN
15	c	99	HIS
15	d	52	ASN
15	d	72	GLN
15	d	75	GLN
15	d	80	ASN
15	d	99	HIS
15	e	52	ASN
15	e	72	GLN
15	e	75	GLN
15	e	80	ASN
15	e	99	HIS
15	e	110	GLN
15	f	52	ASN
15	f	72	GLN
15	f	75	GLN
15	f	80	ASN

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Mol	Chain	Res	Type
15	f	99	HIS
15	f	110	GLN
15	g	52	ASN
15	g	72	GLN
15	g	75	GLN
15	g	80	ASN
15	g	99	HIS
15	h	52	ASN
15	h	72	GLN
15	h	75	GLN
15	h	80	ASN
15	h	99	HIS
15	i	52	ASN
15	i	72	GLN
15	i	75	GLN
15	i	80	ASN
15	i	99	HIS
15	j	52	ASN
15	j	72	GLN
15	j	75	GLN
15	j	80	ASN
15	j	99	HIS
15	k	52	ASN
15	k	72	GLN
15	k	75	GLN
15	k	80	ASN
15	k	110	GLN
15	l	52	ASN
15	l	72	GLN
15	l	75	GLN
15	l	80	ASN
15	l	99	HIS
15	l	110	GLN
15	m	52	ASN
15	m	72	GLN
15	m	75	GLN
15	m	80	ASN
15	m	99	HIS
15	m	110	GLN
15	n	52	ASN
15	n	72	GLN
15	n	75	GLN

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Mol	Chain	Res	Type
15	n	80	ASN
15	n	99	HIS
15	n	110	GLN
15	o	52	ASN
15	o	72	GLN
15	o	75	GLN
15	o	80	ASN
15	o	99	HIS
15	o	110	GLN
15	p	52	ASN
15	p	72	GLN
15	p	75	GLN
15	p	80	ASN
15	p	99	HIS
15	p	110	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 14 ligands modelled in this entry, 14 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.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	238/252 (94%)	-0.05	0 100 100	45, 88, 99, 100	0
1	O	238/252 (94%)	-0.04	0 100 100	51, 89, 99, 100	0
2	B	247/250 (98%)	-0.08	0 100 100	39, 78, 96, 100	0
2	P	247/250 (98%)	-0.10	0 100 100	46, 81, 98, 100	0
3	C	241/245 (98%)	-0.16	0 100 100	35, 71, 99, 100	0
3	Q	241/245 (98%)	-0.08	1 (0%) 90 51	37, 77, 99, 100	0
4	D	239/254 (94%)	-0.16	1 (0%) 90 51	34, 69, 98, 100	0
4	R	239/254 (94%)	-0.13	1 (0%) 90 51	37, 74, 99, 100	0
5	E	244/260 (93%)	-0.13	1 (0%) 90 51	29, 67, 98, 100	0
5	S	244/260 (93%)	-0.10	3 (1%) 75 26	41, 72, 99, 100	0
6	F	233/234 (99%)	-0.22	0 100 100	33, 69, 87, 98	0
6	T	233/234 (99%)	-0.14	0 100 100	45, 74, 92, 100	0
7	G	240/287 (83%)	-0.03	0 100 100	45, 82, 98, 100	0
7	U	240/287 (83%)	-0.02	0 100 100	52, 85, 99, 100	0
8	H	196/196 (100%)	-0.13	0 100 100	51, 79, 97, 100	0
8	V	196/196 (100%)	-0.08	0 100 100	56, 81, 98, 100	0
9	I	222/232 (95%)	-0.16	0 100 100	44, 74, 95, 100	0
9	W	222/232 (95%)	-0.14	0 100 100	44, 75, 93, 100	0
10	J	204/205 (99%)	-0.27	0 100 100	29, 60, 85, 100	0
10	X	204/205 (99%)	-0.33	0 100 100	33, 60, 82, 95	0
11	K	198/198 (100%)	-0.27	1 (0%) 88 46	23, 52, 80, 100	0
11	Y	198/198 (100%)	-0.29	1 (0%) 88 46	30, 56, 84, 100	0
12	L	212/212 (100%)	-0.32	0 100 100	30, 52, 72, 96	0
12	Z	212/212 (100%)	-0.37	0 100 100	31, 52, 76, 92	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	222/222 (100%)	-0.29	0 100 100	28, 60, 79, 97	0
13	a	222/222 (100%)	-0.27	0 100 100	30, 61, 85, 99	0
14	N	233/233 (100%)	-0.15	0 100 100	37, 72, 95, 99	0
14	b	233/233 (100%)	-0.17	0 100 100	39, 74, 96, 100	0
15	c	198/231 (85%)	0.05	0 100 100	58, 90, 99, 100	0
15	d	198/231 (85%)	0.16	2 (1%) 79 29	65, 92, 100, 100	0
15	e	198/231 (85%)	0.13	2 (1%) 79 29	58, 91, 100, 100	0
15	f	198/231 (85%)	0.01	1 (0%) 88 46	47, 89, 99, 100	0
15	g	198/231 (85%)	0.02	0 100 100	48, 88, 99, 100	0
15	h	198/231 (85%)	0.05	0 100 100	57, 86, 99, 100	0
15	i	198/231 (85%)	0.06	0 100 100	56, 91, 100, 100	0
15	j	198/231 (85%)	0.10	0 100 100	60, 94, 100, 100	0
15	k	198/231 (85%)	0.11	4 (2%) 62 17	65, 94, 100, 100	0
15	l	198/231 (85%)	0.06	3 (1%) 70 21	56, 93, 100, 100	0
15	m	198/231 (85%)	0.10	0 100 100	56, 94, 100, 100	0
15	n	198/231 (85%)	0.04	1 (0%) 88 46	64, 94, 100, 100	0
15	o	198/231 (85%)	0.15	2 (1%) 79 29	70, 93, 100, 100	0
15	p	198/231 (85%)	0.16	1 (0%) 88 46	67, 95, 100, 100	0
All	All	9110/9794 (93%)	-0.09	25 (0%) 91 58	23, 79, 99, 100	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
15	l	228	HIS	3.4
4	D	51	THR	2.8
5	S	129	GLY	2.6
4	R	51	THR	2.6
15	p	6	ALA	2.5
5	E	127	ALA	2.5
15	l	227	ASP	2.4
5	S	125	GLU	2.4
15	e	229	MET	2.4
15	n	146	ARG	2.4
3	Q	245	THR	2.4
11	K	197	GLN	2.3
5	S	126	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
15	l	229	MET	2.3
15	d	62	LYS	2.3
15	k	6	ALA	2.2
15	k	146	ARG	2.2
15	k	231	SER	2.1
11	Y	196	ALA	2.0
15	k	27	GLU	2.0
15	o	179	LEU	2.0
15	o	143	TYR	2.0
15	f	146	ARG	2.0
15	e	126	GLY	2.0
15	d	27	GLU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q < 0.9
16	MG	J	1005	1/1	0.26	6.12	37,37,37,37	0
16	MG	H	1002	1/1	0.31	3.85	81,81,81,81	0
16	MG	X	1013	1/1	0.21	3.68	79,79,79,79	0
16	MG	X	1012	1/1	0.30	3.29	56,56,56,56	0
16	MG	L	1003	1/1	0.24	2.99	43,43,43,43	0
16	MG	U	1014	1/1	0.28	0.60	65,65,65,65	0
16	MG	V	1009	1/1	0.18	-0.47	39,39,39,39	0
16	MG	G	1007	1/1	0.14	-1.52	38,38,38,38	0
16	MG	a	1011	1/1	0.04	-1.53	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
16	MG	M	1004	1/1	0.06	-2.13	26,26,26,26	0
16	MG	Z	1010	1/1	0.09	-3.02	38,38,38,38	0
16	MG	I	1001	1/1	0.16	-3.78	67,67,67,67	0
16	MG	W	1008	1/1	0.07	-4.56	67,67,67,67	0
16	MG	J	1006	1/1	0.11	-7.15	24,24,24,24	0

6.5 Other polymers ⓘ

There are no such residues in this entry.