



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 23, 2018 – 09:12 PM EST

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 X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030736
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030736

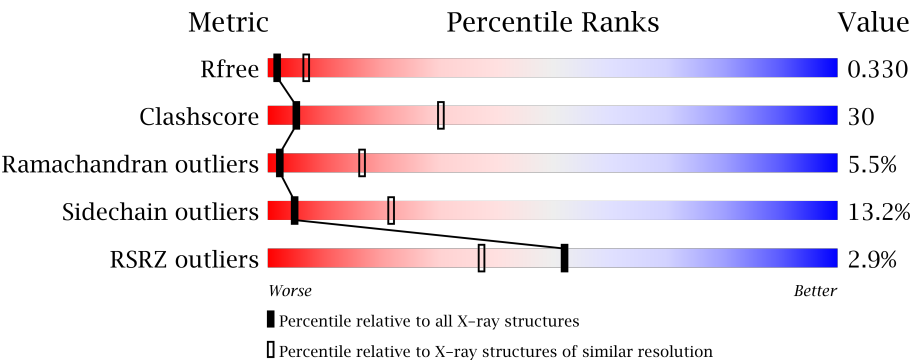
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

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}	100719	1015 (3.22-3.18)
Clashscore	112137	1009 (3.20-3.20)
Ramachandran outliers	110173	1118 (3.22-3.18)
Sidechain outliers	110143	1117 (3.22-3.18)
RSRZ outliers	101464	1020 (3.22-3.18)

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	252	<div><div>3%</div><div><div></div><div>34%</div><div>46%</div><div>14%</div><div>6%</div></div></div>
1	O	252	<div><div>2%</div><div><div></div><div>32%</div><div>47%</div><div>14%</div><div>6%</div></div></div>
2	B	250	<div><div>2%</div><div><div></div><div>43%</div><div>45%</div><div>10%</div><div>2%</div></div></div>
2	P	250	<div><div>0%</div><div><div></div><div>44%</div><div>45%</div><div>9%</div><div>2%</div></div></div>
3	C	245	<div><div>2%</div><div><div></div><div>44%</div><div>42%</div><div>12%</div><div>0%</div></div></div>

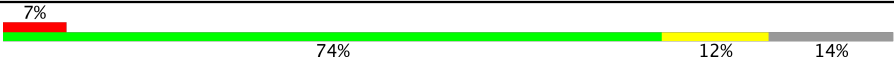

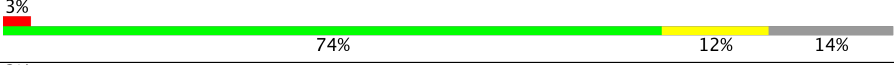



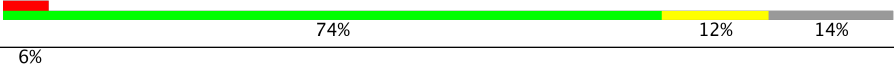

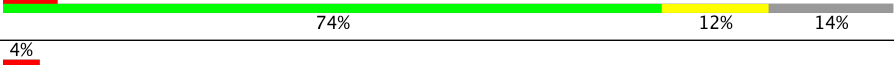


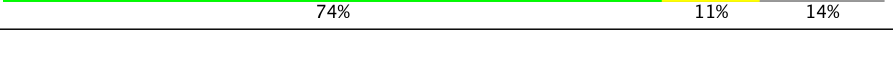
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Mol	Chain	Length	Quality of chain
3	Q	245	
4	D	254	
4	R	254	
5	E	260	
5	S	260	
6	F	234	
6	T	234	
7	G	287	
7	U	287	
8	H	196	
8	V	196	
9	I	232	
9	W	232	
10	J	205	
10	X	205	
11	K	198	
11	Y	198	
12	L	212	
12	Z	212	
13	M	222	
13	a	222	
14	N	233	
14	b	233	
15	c	231	
15	d	231	

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Mol	Chain	Length	Quality of chain
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, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	MG	H	1002	-	-	-	X
16	MG	J	1005	-	-	-	X
16	MG	X	1012	-	-	-	X

2 Entry composition

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

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

- Molecule 1 is a protein called PROTEASOME COMPONENT 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 1529	C 960	N 267	O 296	S 6	0	0	0
15	d	198	Total 1529	C 960	N 267	O 296	S 6	0	0	0
15	e	198	Total 1529	C 960	N 267	O 296	S 6	0	0	0
15	f	198	Total 1529	C 960	N 267	O 296	S 6	0	0	0
15	g	198	Total 1529	C 960	N 267	O 296	S 6	0	0	0
15	h	198	Total 1529	C 960	N 267	O 296	S 6	0	0	0
15	i	198	Total 1529	C 960	N 267	O 296	S 6	0	0	0
15	j	198	Total 1529	C 960	N 267	O 296	S 6	0	0	0
15	k	198	Total 1529	C 960	N 267	O 296	S 6	0	0	0
15	l	198	Total 1529	C 960	N 267	O 296	S 6	0	0	0
15	m	198	Total 1529	C 960	N 267	O 296	S 6	0	0	0
15	n	198	Total 1529	C 960	N 267	O 296	S 6	0	0	0
15	o	198	Total 1529	C 960	N 267	O 296	S 6	0	0	0
15	p	198	Total 1529	C 960	N 267	O 296	S 6	0	0	0

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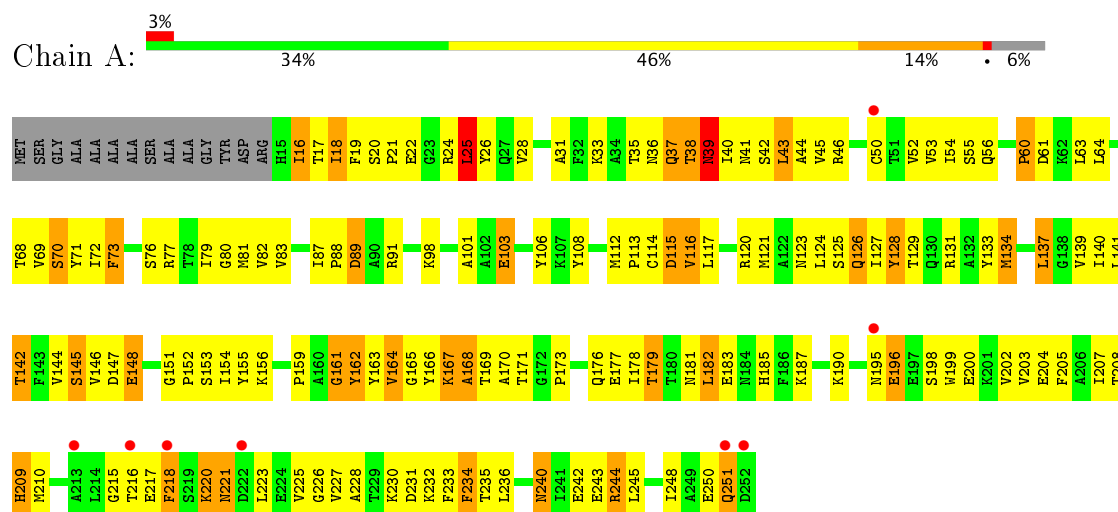
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	M	1	Total	Mg	0	0
			1	1		

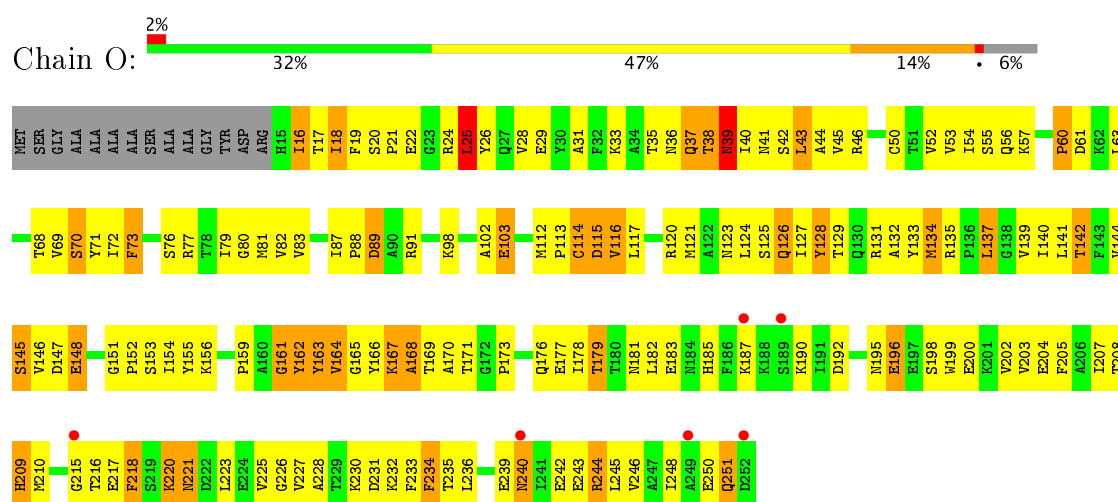
3 Residue-property plots

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

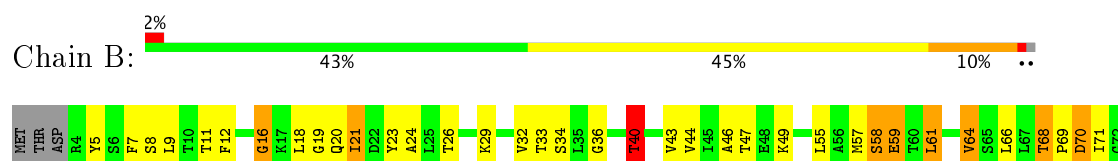
• Molecule 1: PROTEASOME COMPONENT C7-ALPHA

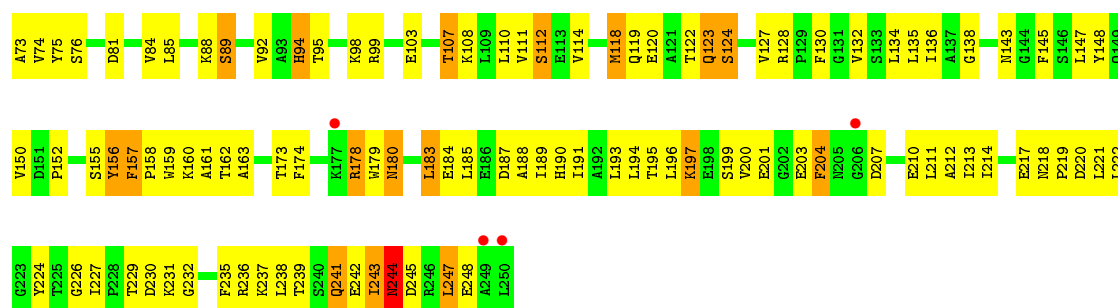


• Molecule 1: PROTEASOME COMPONENT C7-ALPHA

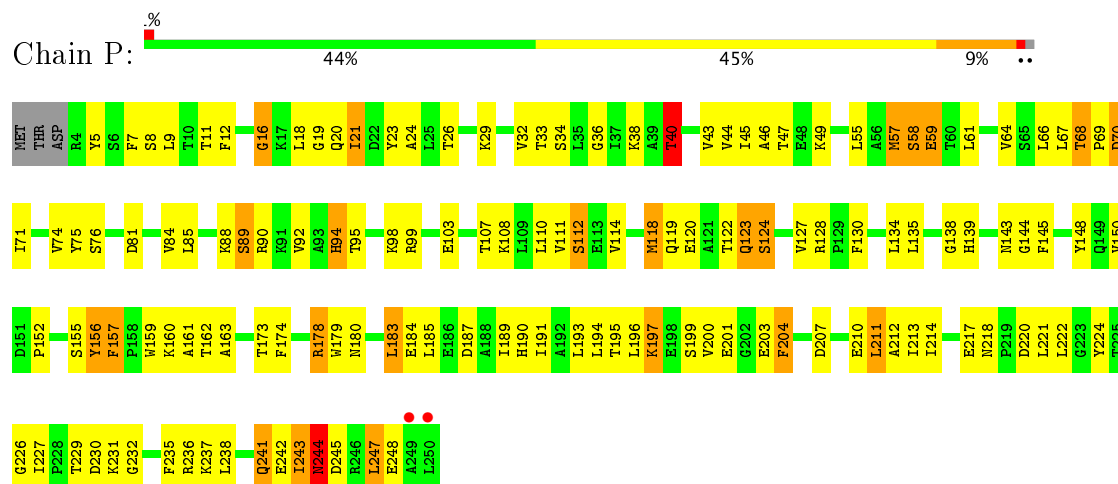


• Molecule 2: PROTEASOME COMPONENT Y7

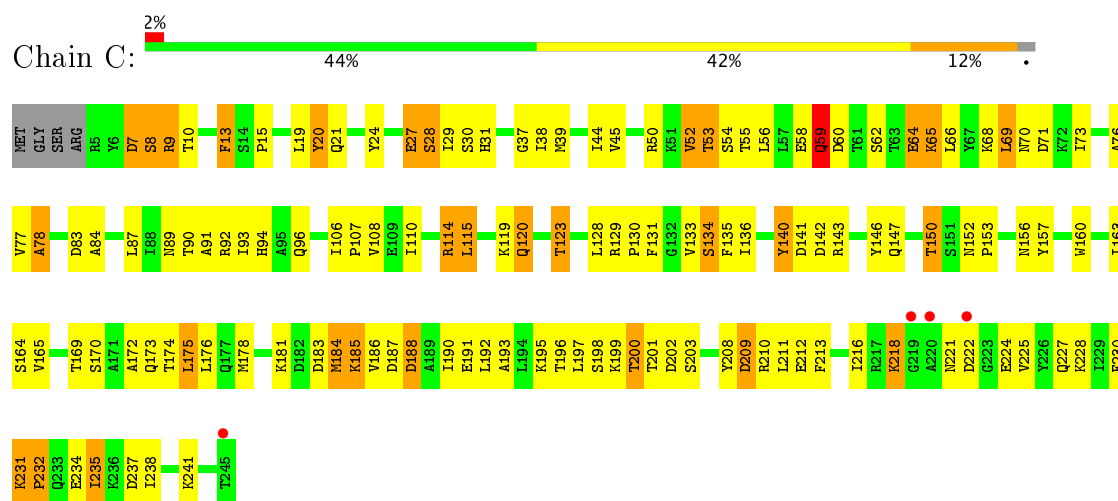




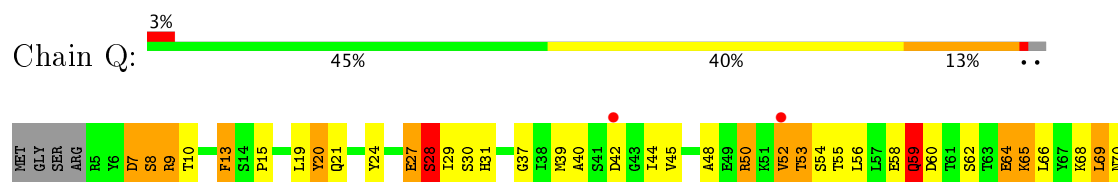
• Molecule 2: PROTEASOME COMPONENT Y7

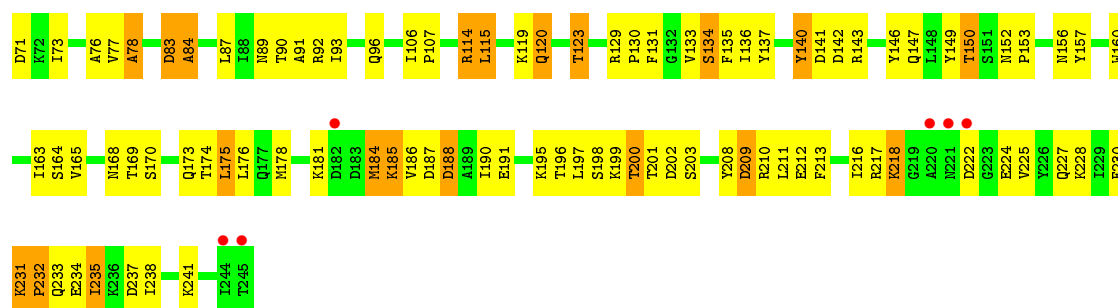


• Molecule 3: PROTEASOME COMPONENT Y13

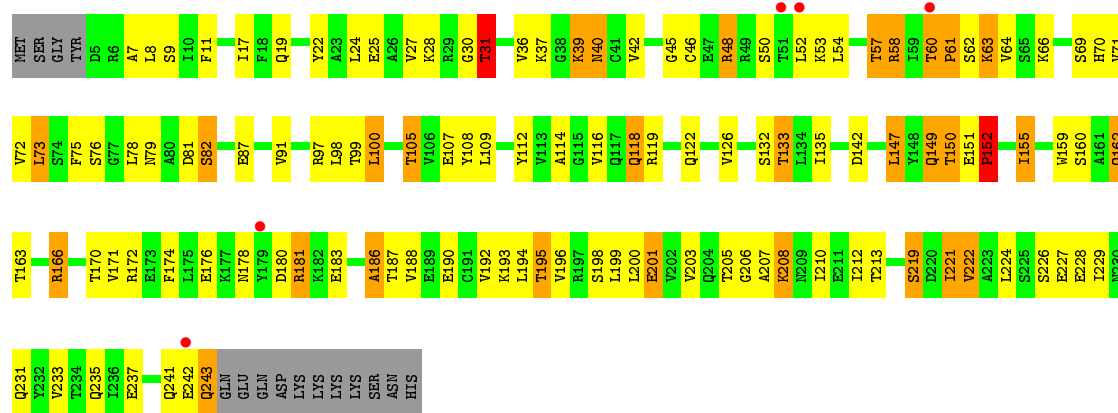


• Molecule 3: PROTEASOME COMPONENT Y13

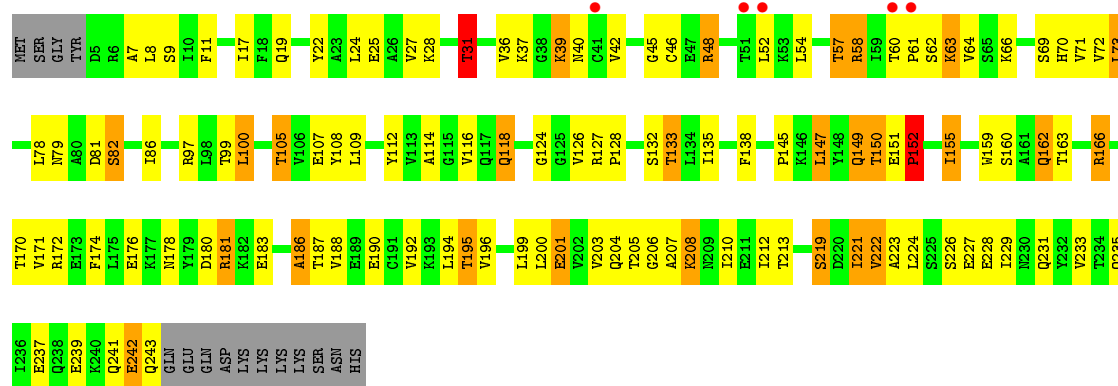




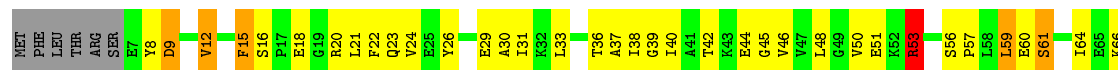
• Molecule 4: PROTEASOME COMPONENT PRE6

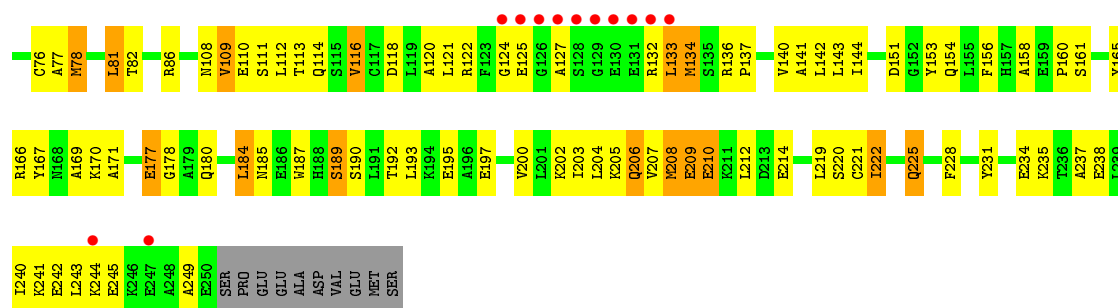


• Molecule 4: PROTEASOME COMPONENT PRE6

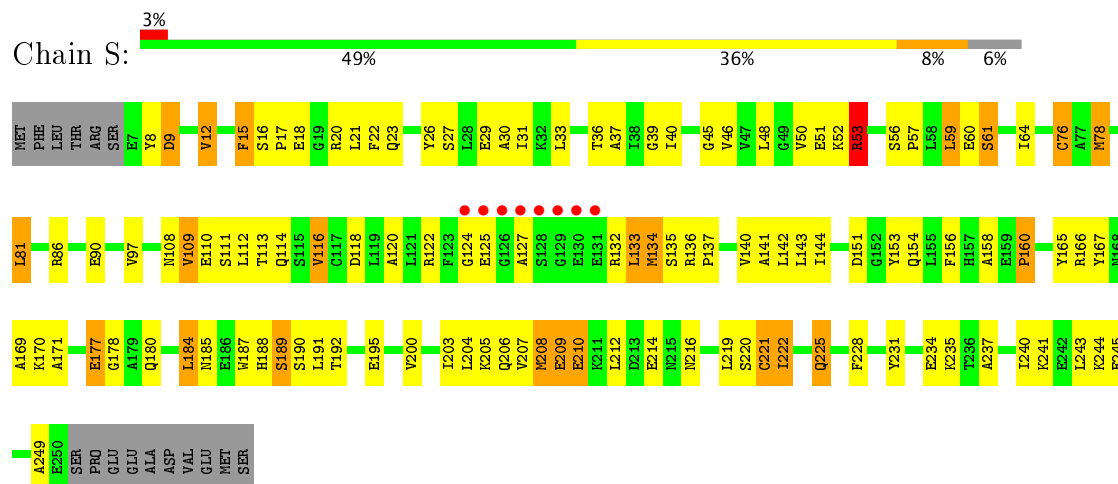


• Molecule 5: PROTEASOME COMPONENT PUP2

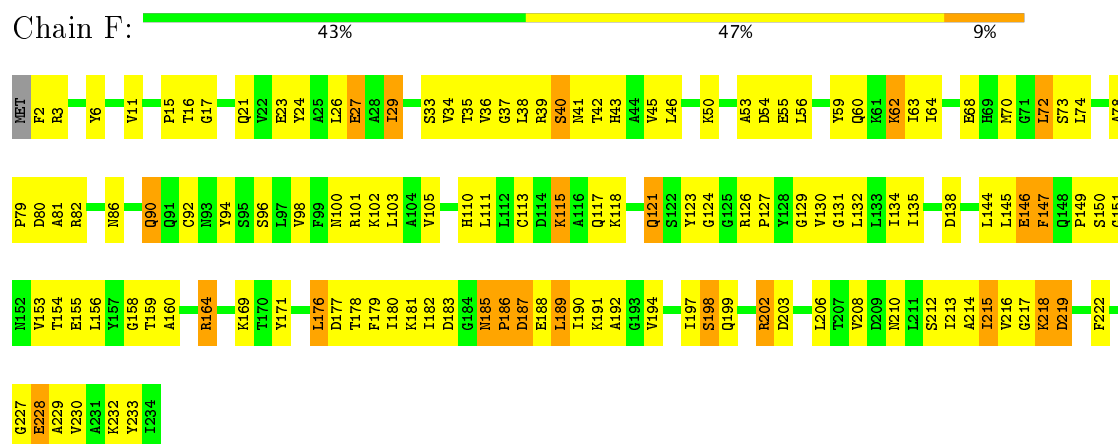




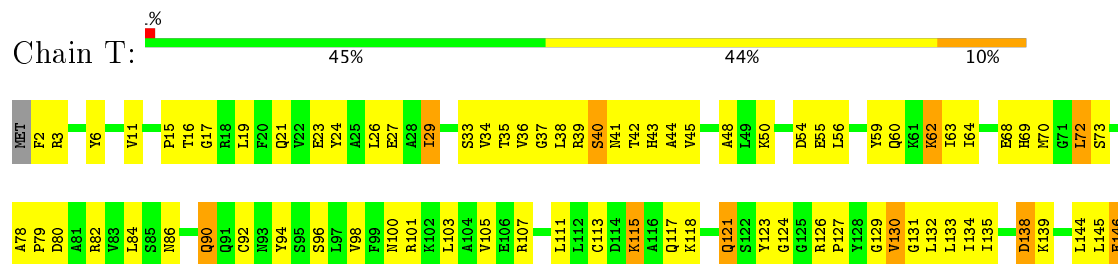
• Molecule 5: PROTEASOME COMPONENT PUP2

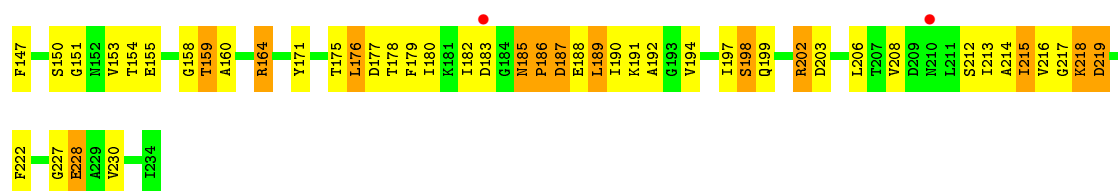


• Molecule 6: PROTEASOME COMPONENT PRE5

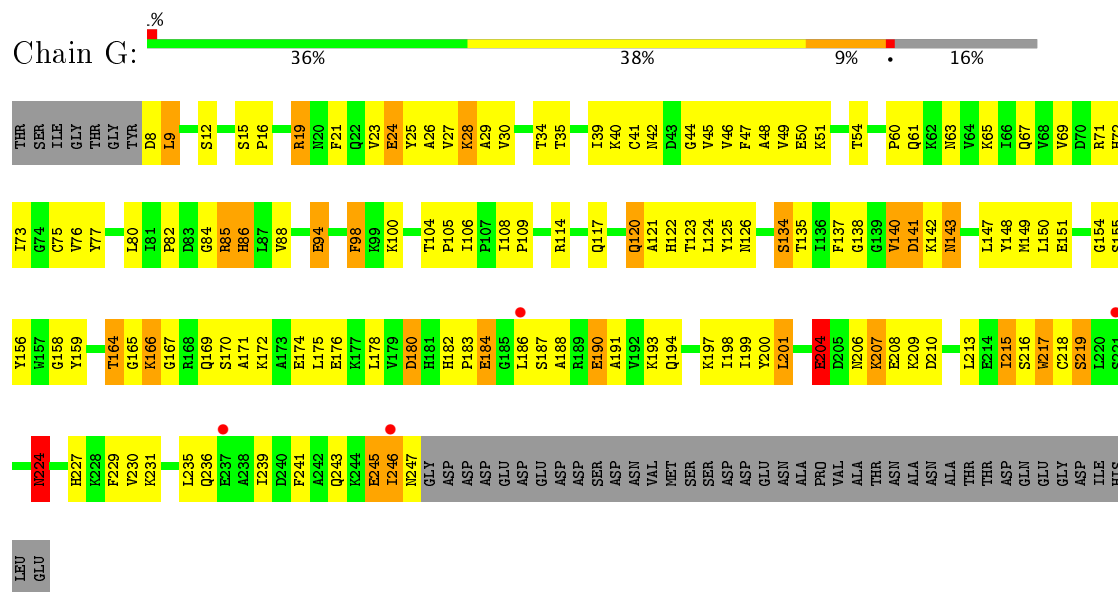


• Molecule 6: PROTEASOME COMPONENT PRE5

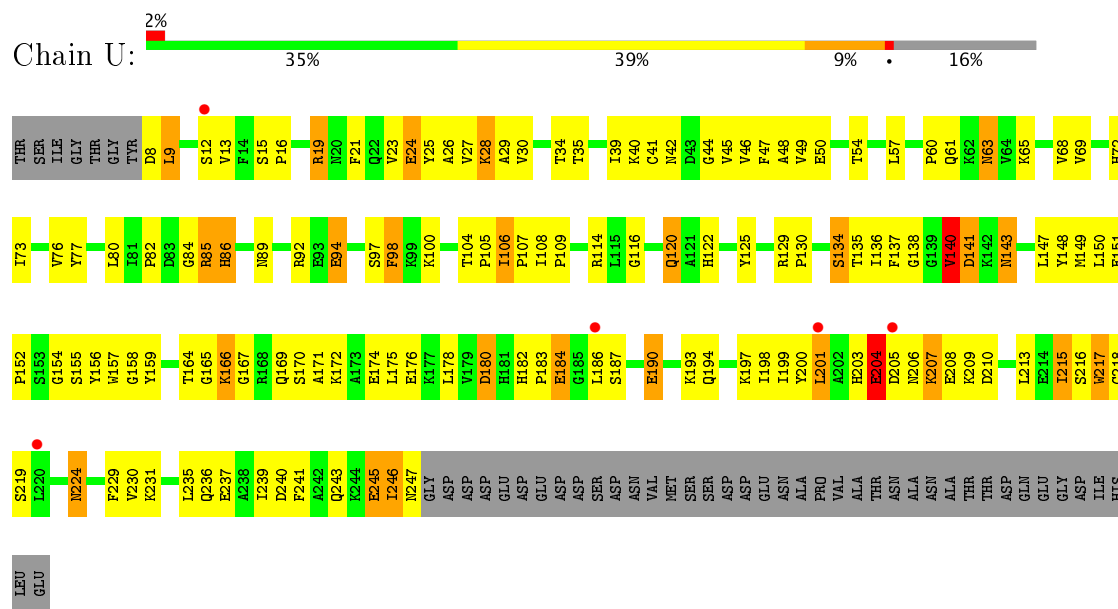




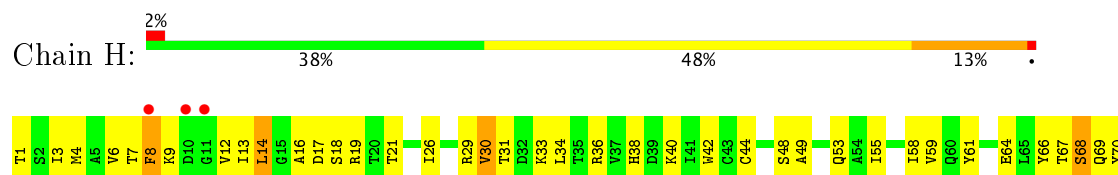
• Molecule 7: PROTEASOME COMPONENT C1

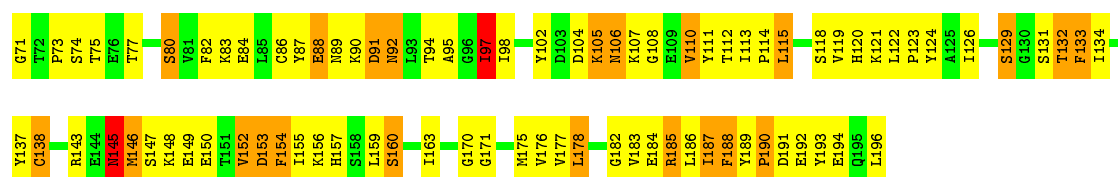


• Molecule 7: PROTEASOME COMPONENT C1

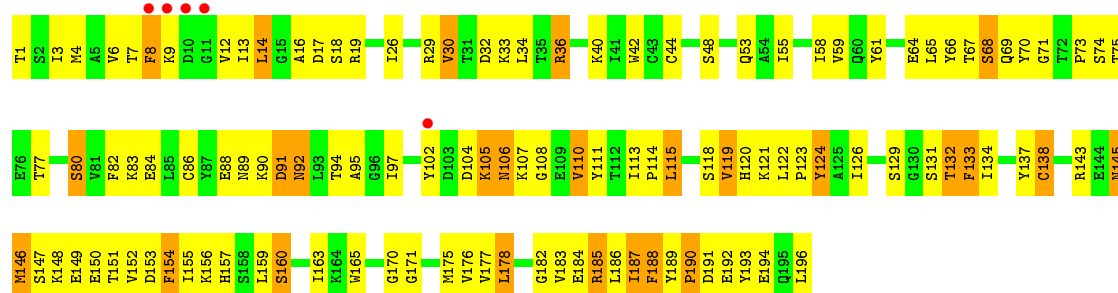
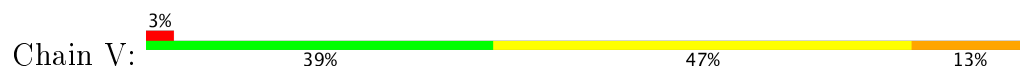


• Molecule 8: PROTEASOME COMPONENT PRE3

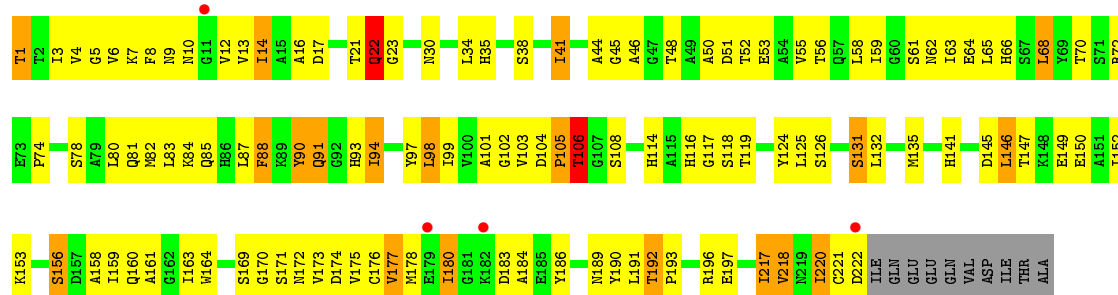
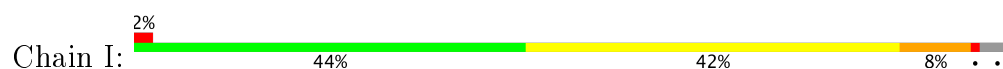




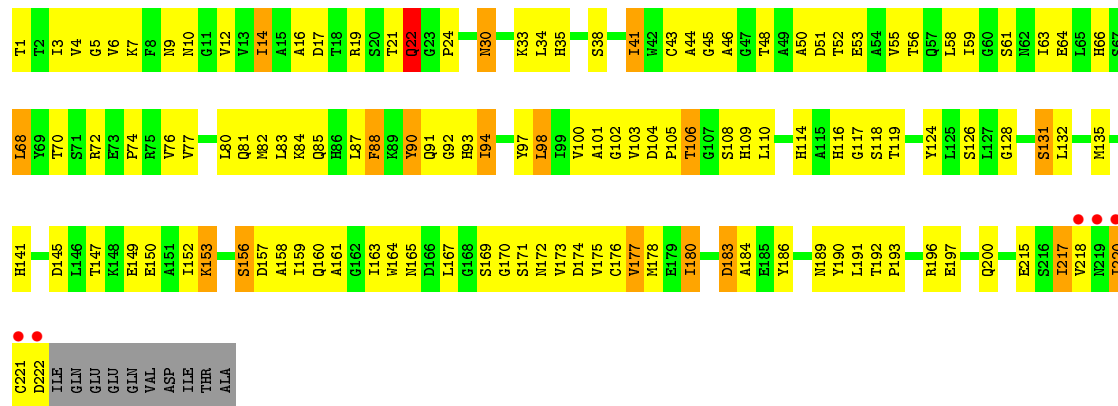
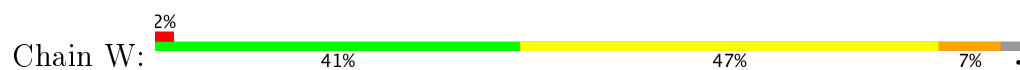
• Molecule 8: PROTEASOME COMPONENT PRE3



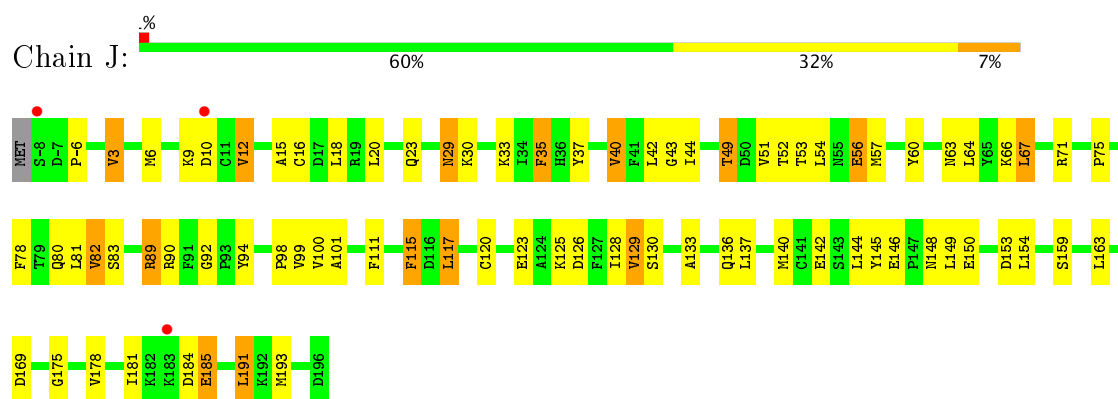
• Molecule 9: PROTEASOME COMPONENT PUP1



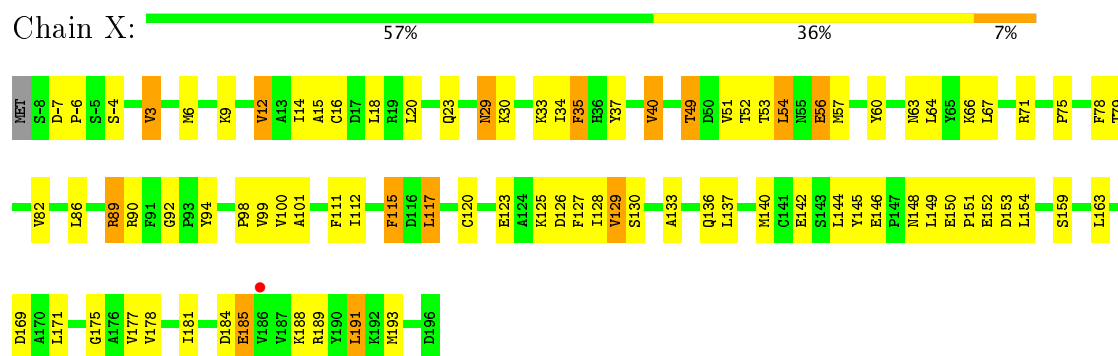
• Molecule 9: PROTEASOME COMPONENT PUP1



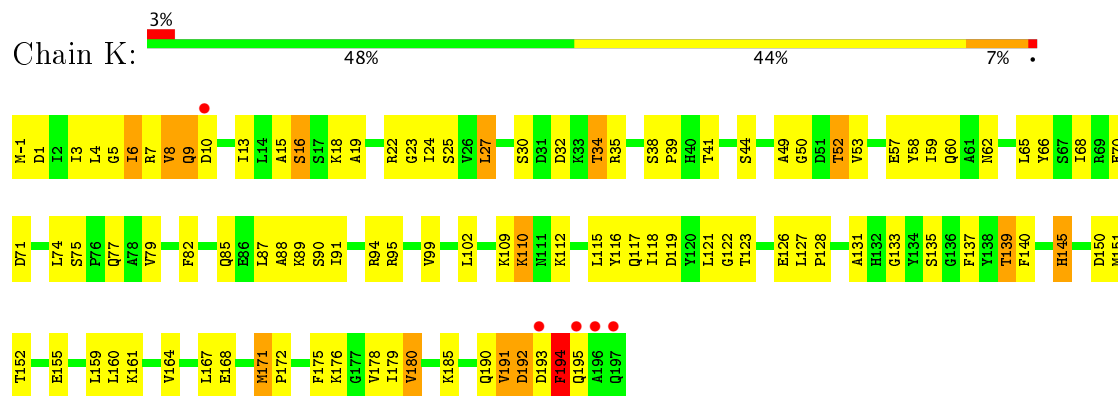
• Molecule 10: PROTEASOME COMPONENT PUP3



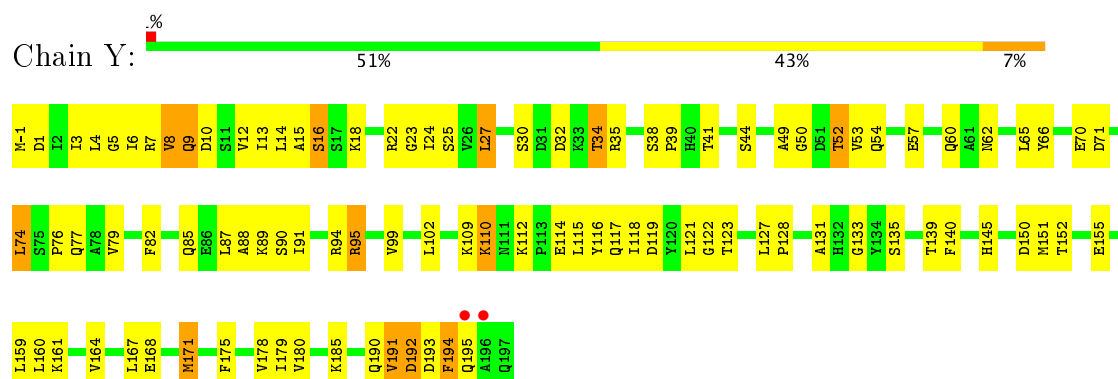
• Molecule 10: PROTEASOME COMPONENT PUP3



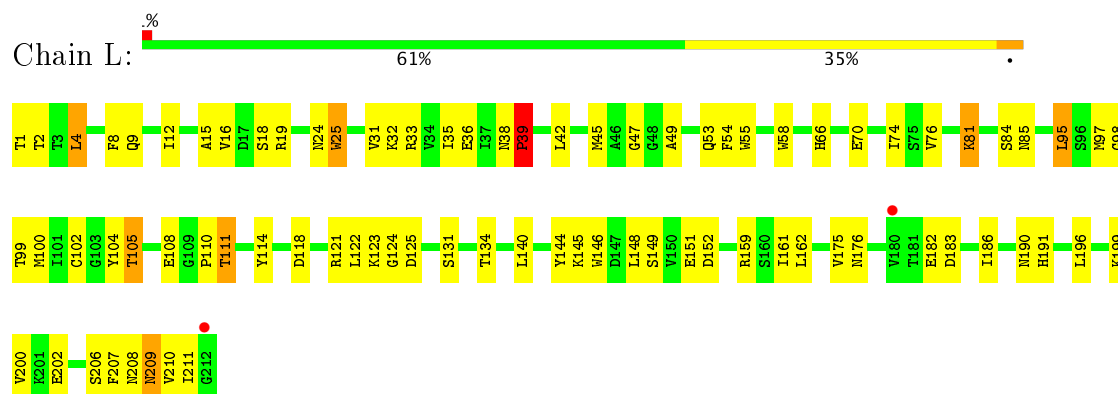
• Molecule 11: PROTEASOME COMPONENT C11



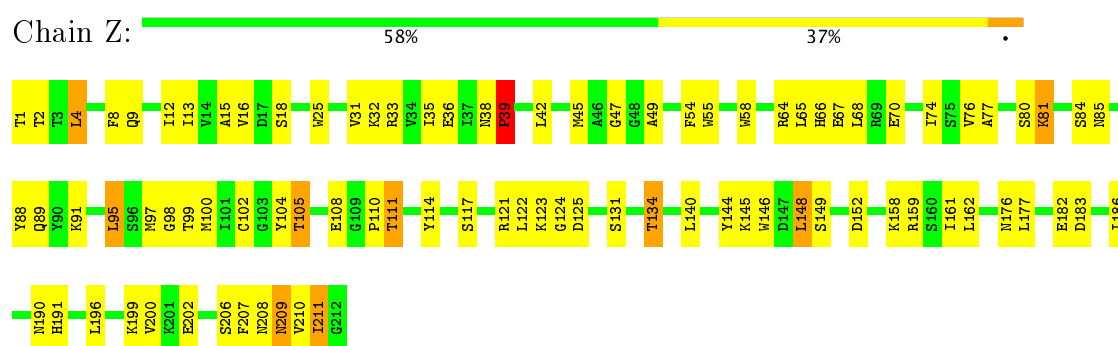
• Molecule 11: PROTEASOME COMPONENT C11



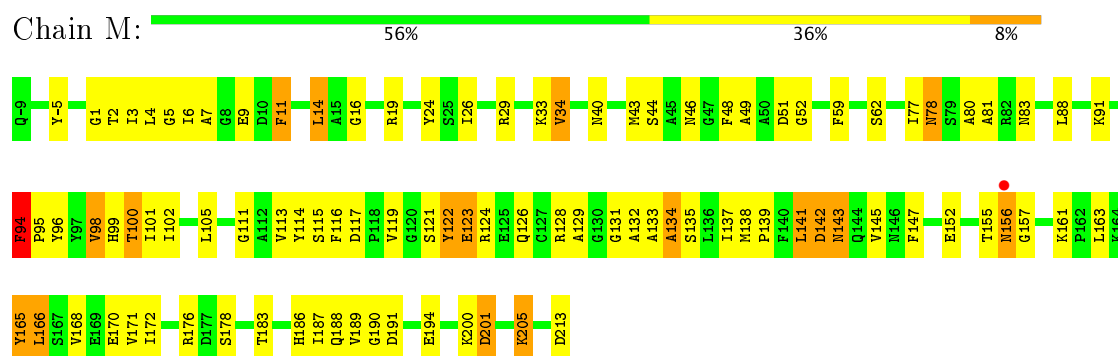
- Molecule 12: PROTEASOME COMPONENT PRE2



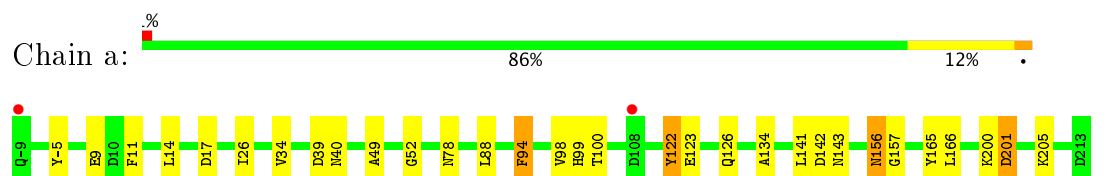
- Molecule 12: PROTEASOME COMPONENT PRE2



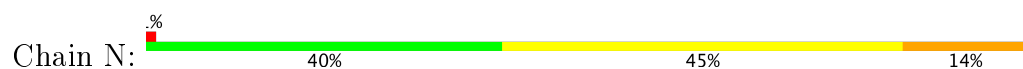
- Molecule 13: PROTEASOME COMPONENT C5

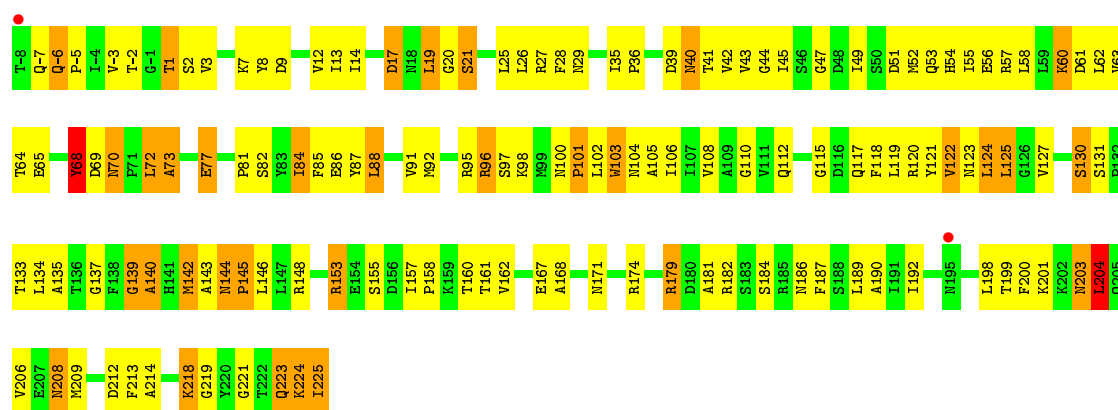


- Molecule 13: PROTEASOME COMPONENT C5

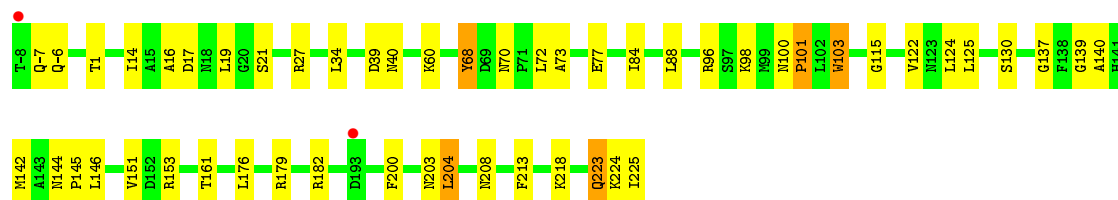
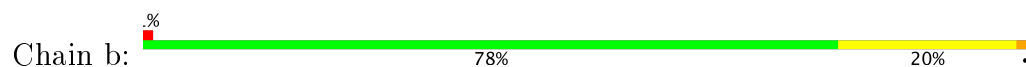


- Molecule 14: PROTEASOME COMPONENT PRE4

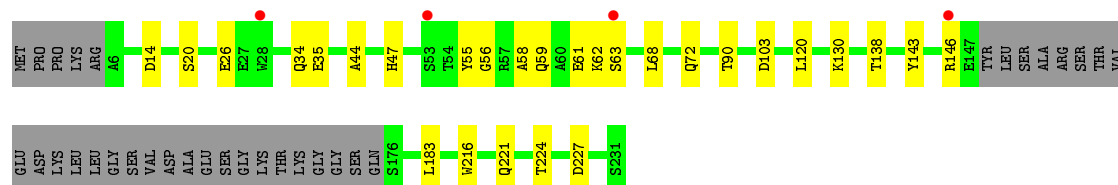
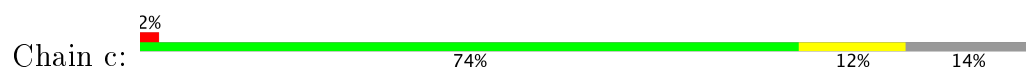




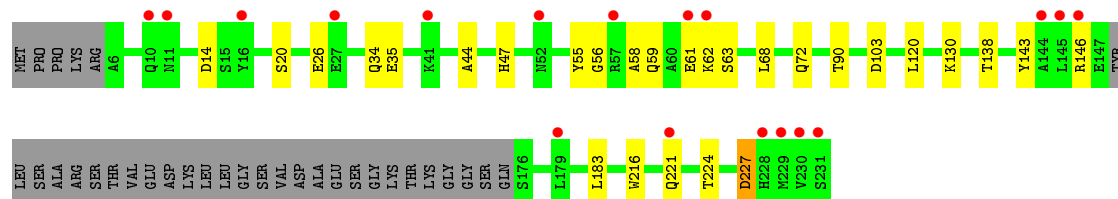
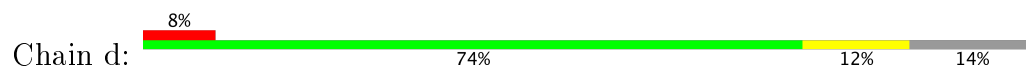
• Molecule 14: PROTEASOME COMPONENT PRE4



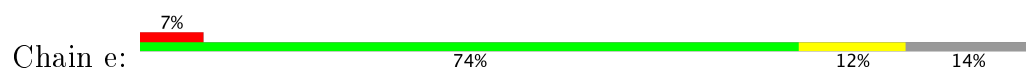
• Molecule 15: PROTEASOME ACTIVATOR PROTEIN PA26

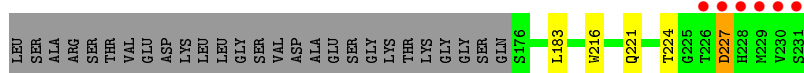


• Molecule 15: PROTEASOME ACTIVATOR PROTEIN PA26

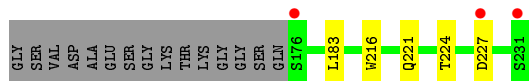
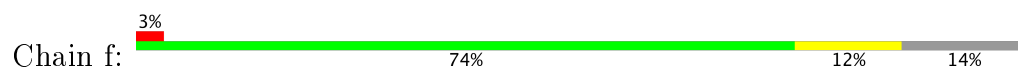


• Molecule 15: PROTEASOME ACTIVATOR PROTEIN PA26

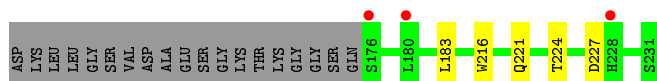
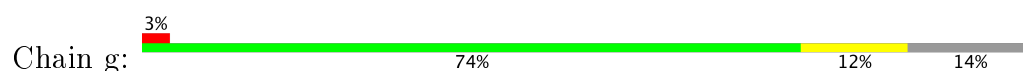




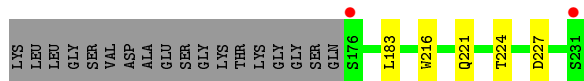
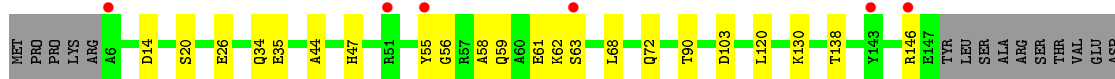
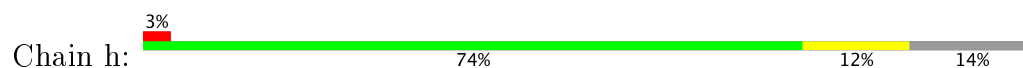
• Molecule 15: PROTEASOME ACTIVATOR PROTEIN PA26



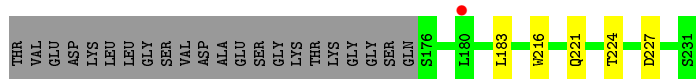
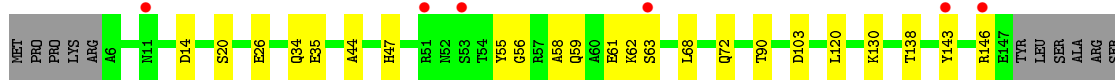
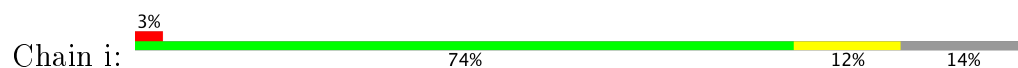
• Molecule 15: PROTEASOME ACTIVATOR PROTEIN PA26



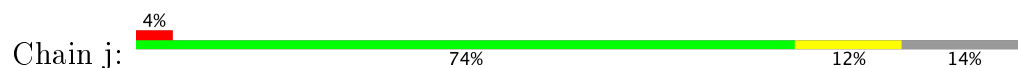
• Molecule 15: PROTEASOME ACTIVATOR PROTEIN PA26

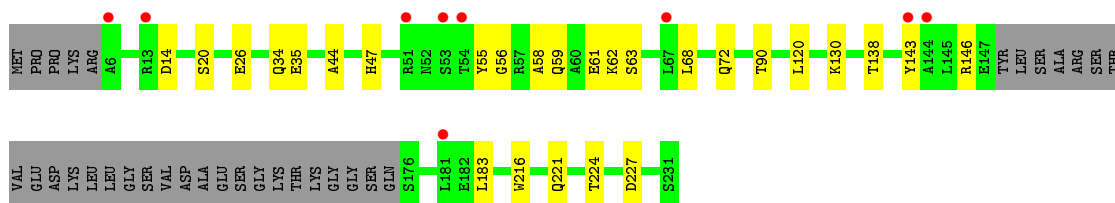


• Molecule 15: PROTEASOME ACTIVATOR PROTEIN PA26

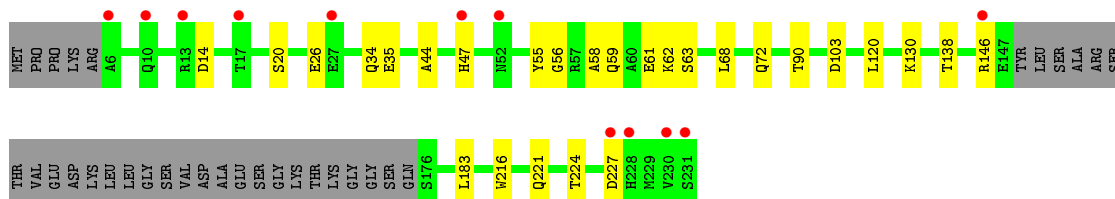
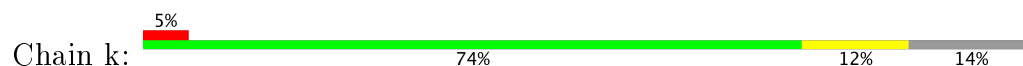


• Molecule 15: PROTEASOME ACTIVATOR PROTEIN PA26

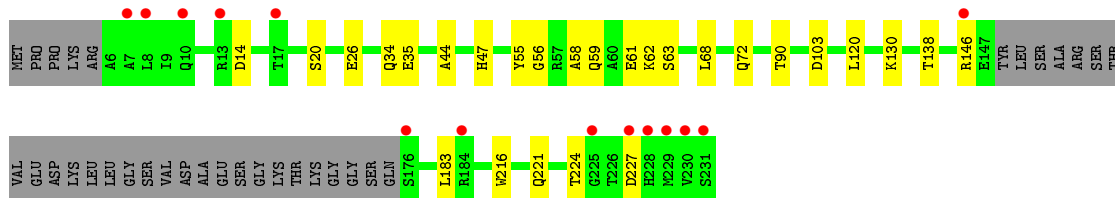




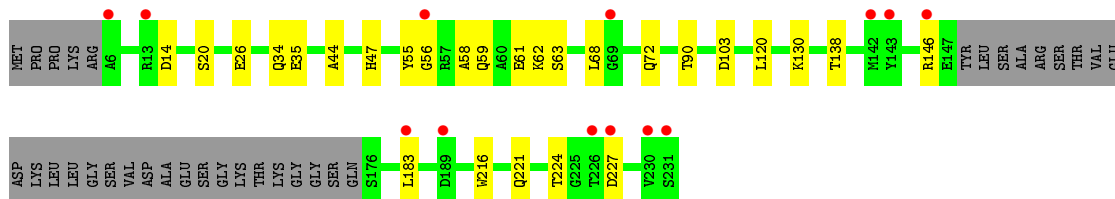
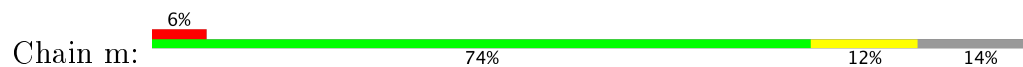
• Molecule 15: PROTEASOME ACTIVATOR PROTEIN PA26



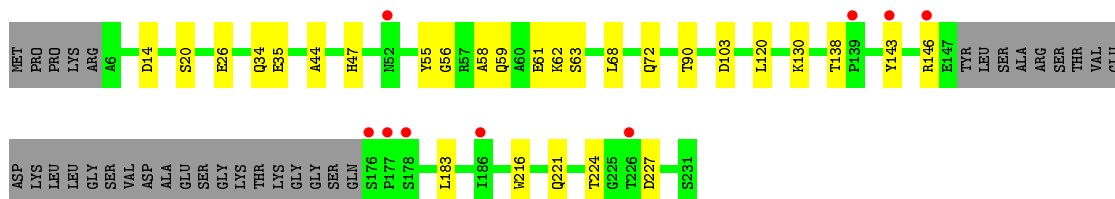
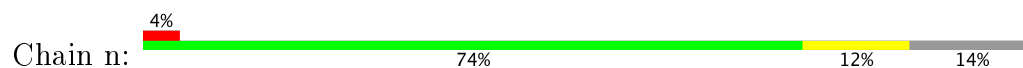
• Molecule 15: PROTEASOME ACTIVATOR PROTEIN PA26



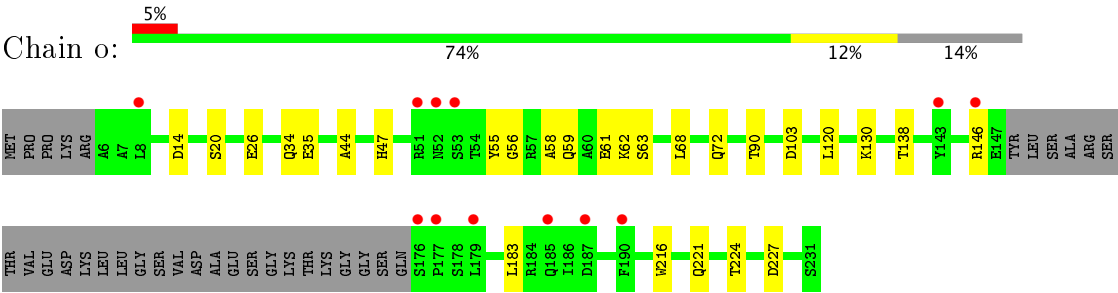
• Molecule 15: PROTEASOME ACTIVATOR PROTEIN PA26



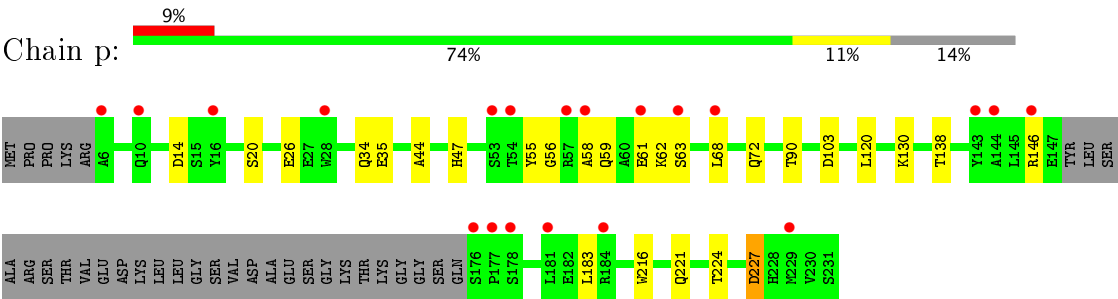
• Molecule 15: PROTEASOME ACTIVATOR PROTEIN PA26



• Molecule 15: PROTEASOME ACTIVATOR PROTEIN PA26



● Molecule 15: PROTEASOME ACTIVATOR PROTEIN PA26



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	192.96 Å 232.13 Å 296.77 Å 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 3.25 Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.255 , 0.325 0.267 , 0.330	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)	0.30 , 78.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	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.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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
11	Y	1585	0	1590	73	0
12	L	1646	0	1595	52	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 30.

All (2521) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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	Interatomic distance (Å)	Clash overlap (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
3:C:185:LYS:HZ2	3:C:187:ASP:H	1.11	0.94
14:N:72:LEU:HD12	14:N:72:LEU:H	1.33	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
2:B:187:ASP:O	2:B:191:ILE:HG12	1.77	0.84
8:H:8:PHE:HE2	8:H:148:LYS:HA	1.43	0.84
7:G:72:HIS:HD2	7:G:73:ILE:HG13	1.41	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:60:LYS:O	14:N:64:THR:HG23	1.79	0.83
6:F:179:PHE:HA	6:F:182:ILE:HG13	1.59	0.83
1:O:44:ALA:HB2	1:O:53:VAL:HG12	1.57	0.83
1:A:146:VAL:HG22	1:A:152:PRO:HA	1.58	0.83
8:H:13:ILE:HD13	8:H:177:VAL:HG22	1.61	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
14:N:49:ILE:HG22	14:N:53:GLN:HE21	1.47	0.80
4:R:228:GLU:HA	4:R:231:GLN:HE21	1.47	0.80
7:U:30:VAL:HG11	7:U:134:SER:HB2	1.64	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
1:A:68:THR:HG21	7:G: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:45:VAL:HG12	1:A:168:ALA:HB1	1.63	0.79
7:G:143:ASN:H	7:G:143:ASN:ND2	1.81	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
7:U:199:ILE:HG21	7:U:213:LEU:HD13	1.66	0.78
8:V:13:ILE:HD13	8:V:177:VAL:HG22	1.64	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:B:68:THR:HG23	2:B:71:ILE:HB	1.65	0.78
2:P:187:ASP:O	2:P:191:ILE:HG12	1.83	0.78
7:G:71:ARG:CZ	14:N:64:THR:HG22	2.14	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:150:LEU:HD12	7:U:151:GLU:N	1.98	0.78
1:A:54:ILE:HA	1:A:225:VAL:HG22	1.65	0.78
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
10:J:78:PHE:O	10:J:82:VAL:HG12	1.84	0.77
7:U:143:ASN:H	7:U:143:ASN:ND2	1.83	0.77
9:I:22:GLN:NE2	9:I:22:GLN:HA	2.00	0.77
1:O:181:ASN:HB3	1:O:209:HIS:CE1	2.20	0.77
5:E:136:ARG:HB2	5:E:137:PRO:HD2	1.67	0.77
7:G:77:TYR:CE1	7:G:84:GLY:HA3	2.20	0.77
6:F:227:GLY:O	6:F:230:VAL:HG22	1.84	0.76
4:R:11:PHE:H	5:S:23:GLN:HE22	1.33	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
1:A:181:ASN:HB3	1:A:209:HIS:CE1	2.21	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
5:E:142:LEU:HB2	5:E:158:ALA:HB3	1.68	0.76
7:G:199:ILE:HG21	7:G:213:LEU:HD13	1.68	0.76
3:Q:150:THR:HG21	3:Q:160:TRP:HE1	1.49	0.76
7:G:171:ALA:O	7:G:175:LEU:HG	1.84	0.75
8:V:111:TYR:HA	8:V:120:HIS:O	1.86	0.75
1:O:45:VAL:HG12	1:O:168:ALA:HB1	1.69	0.75
8:H:67:THR:HG22	8:H:73:PRO:HD3	1.69	0.75
10:J:184:ASP:CG	10:J:185:GLU:H	1.90	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
11:K:52:THR:HG23	11:K:53:VAL:H	1.51	0.74
14:N:35:ILE:HG12	14:N:56:GLU:HG2	1.68	0.74
6:T:50:LYS:HE2	6:T:212:SER:HB2	1.67	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:150:LEU:HD12	7:G:151:GLU:H	1.52	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
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
13:M:7:ALA:HB2	13:M:113:VAL:HG23	1.70	0.73
14:N:91:VAL:O	14:N:95:ARG:HG2	1.88	0.73
5:E:170:LYS:HD2	5:E:171:ALA:H	1.52	0.73
6:F:50:LYS:HE2	6:F:212:SER:HB2	1.68	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
7:U:171:ALA:O	7:U:175:LEU:HG	1.87	0.73
10:X:133:ALA:HB2	10:X:169:ASP:HB2	1.68	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
7:G:109:PRO:HA	7:G:148:TYR:OH	1.89	0.73
11:Y:52:THR:HG23	11:Y:53:VAL:H	1.54	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
8:H:1:THR:HA	8:H:33:LYS:NZ	2.04	0.72
1:O:225:VAL:O	1:O:236:LEU:HB2	1.89	0.72
7:G:187:SER:OG	7:G:190:GLU:HB2	1.90	0.72
8:H:111:TYR:HA	8:H:120:HIS:O	1.89	0.72
8:H:177:VAL:HB	8:H:184:GLU:HB3	1.70	0.72
1:O:54:ILE:HA	1:O:225:VAL:HG22	1.69	0.72
3:Q:201:THR:HG22	3:Q:203:SER:H	1.53	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:VAL:O	1:A:236:LEU:HB2	1.89	0.71
14:N:121:TYR:HE1	14:N:123:ASN:HD22	1.34	0.71
2:P:68:THR:HG23	2:P:71:ILE:HB	1.71	0.71
7:U:150:LEU:HD12	7:U:151:GLU:H	1.55	0.71
7:G:72:HIS:CD2	7:G:73:ILE:HG13	2.25	0.71
8:H:40:LYS:NZ	8:H:182:GLY:HA2	2.05	0.71
9:I:160:GLN:O	9:I:164:TRP:HD1	1.73	0.71
2:B:222:LEU:HD11	2:B:232:GLY:CA	2.20	0.71
14:N:104:ASN:HB3	14:N:106:ILE:CD1	2.20	0.71
3:Q:187:ASP:HA	3:Q:190:ILE:HD12	1.71	0.71
6:T:78:ALA:HB3	6:T:79:PRO:HD3	1.71	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
5:S:8:TYR:O	5:S:9:ASP:HB2	1.90	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
1:A:126:GLN:HE21	1:A:127:ILE:N	1.89	0.71
9:I:64:GLU:O	9:I:68:LEU:HD12	1.91	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: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
1:O:129:THR:HG22	2:P:128:ARG:HH21	1.55	0.70
10:X:184:ASP:CG	10:X:185:GLU:H	1.94	0.70
14:N:36:PRO:HA	14:N:42:VAL:HA	1.72	0.70
7:U:94:GLU:HG2	7:U:114:ARG:HD2	1.73	0.70
1:A:22:GLU:HA	2:B:26:THR:HG21	1.72	0.70
4:D:162:GLN:HE22	4:D:172:ARG:HE	1.39	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:C:131:PHE:O	3:C:153:PRO:HB3	1.92	0.70
5:E:12:VAL:H	5:E:23:GLN:HG3	1.57	0.70
8:H:13:ILE:CD1	8:H:177:VAL:HG22	2.21	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
10:J:146:GLU:HB3	10:J:149:LEU:HD21	1.75	0.69
1:O:113:PRO:HD2	1:O:116:VAL:HG21	1.75	0.69
7:U:72:HIS:CD2	7:U:73:ILE:HG13	2.26	0.69
7:G:30:VAL:CG1	7:G:134:SER:HB2	2.23	0.69
1:A:205:PHE:O	1:A:208:THR:HB	1.91	0.69
2:B:227:ILE:HG12	9:I:186:TYR:HD2	1.58	0.69
10:X:146:GLU:HB3	10:X:149:LEU:HD21	1.74	0.69
3:C:169:THR:O	3:C:173:GLN:HB2	1.92	0.69
3:Q:170:SER:O	3:Q:174:THR:HG23	1.93	0.69
6:T:33:SER:HB3	6:T:62:LYS:NZ	2.06	0.69
11:Y:-1:MET:SD	11:Y:133:GLY:HA3	2.32	0.69
5:E:8:TYR:O	5:E:9:ASP:HB2	1.92	0.69
6:F:78:ALA:HB3	6:F:79:PRO:HD3	1.74	0.69
13:M:14:LEU:HD13	13:M:34:VAL:HG13	1.75	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
1:A:203:VAL:O	1:A:207:ILE:HG13	1.94	0.68
7:G:243:GLN:O	7:G:246:ILE:HG22	1.92	0.68
3:Q:131:PHE:O	3:Q:153:PRO:HB3	1.93	0.68
4:R:64:VAL:HG11	4:R:213:THR:HG21	1.75	0.68
8:V:40:LYS:NZ	8:V:182:GLY:HA2	2.08	0.68
1:O:203:VAL:O	1:O:207:ILE:HG13	1.93	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
11:K:-1:MET:SD	11:K:133:GLY:HA3	2.33	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
4:R:203:VAL:HG21	4:R:210:ILE:HD11	1.75	0.68
12:Z:35:ILE:HD11	12:Z:45:MET:CE	2.23	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
13:M:187:ILE:HD11	9:W:24:PRO:HA	1.76	0.67
1:O:234:PHE:HD1	1:O:234:PHE:N	1.92	0.67
6:T:185:ASN:HD22	6:T:185:ASN:C	1.97	0.67
10:X:52:THR:O	10:X:56:GLU:HG2	1.94	0.67
8:H:126:ILE:HD12	8:H:134:ILE:HG13	1.77	0.67
1:O:205:PHE:O	1:O:208:THR:HB	1.94	0.67
2:P:95:THR:HA	2:P:99:ARG:HD2	1.77	0.67
7:U:30:VAL:CG1	7:U:134:SER:HB2	2.24	0.67
9:W:160:GLN:O	9:W:164:TRP:HD1	1.78	0.67
9:I:172:ASN:OD1	9:I:192:THR:HG22	1.92	0.67
10:J:129:VAL:HB	10:J:137:LEU:HD13	1.76	0.67
14:N:40:ASN:H	14:N:40:ASN:ND2	1.90	0.67
7:U:109:PRO:HA	7:U:148:TYR:OH	1.94	0.67
8:V:107:LYS:HD2	8:V:108:GLY:N	2.07	0.67
1:A:240:ASN:H	1:A:240:ASN:ND2	1.93	0.67
8:H:67:THR:HA	8:H:71:GLY:O	1.93	0.67
7:U:143:ASN:N	7:U:143:ASN:HD22	1.89	0.67
7:U:243:GLN:O	7:U:246:ILE:HG22	1.95	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
6:F:2:PHE:CD1	6:F:3:ARG:HG2	2.30	0.67
3:Q:58:GLU:HG2	3:Q:59:GLN:H	1.60	0.67
10:X:29:ASN:O	10:X:30:LYS:HG3	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:67:THR:HG22	8:V:73:PRO:HD3	1.77	0.66
8:H:19:ARG:HB3	8:H:170:GLY:H	1.59	0.66
1:O:22:GLU:HA	2:P:26:THR:HG21	1.76	0.66
2:P:40:THR:HG23	2:P:183:LEU: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
8:H:13:ILE:HG23	8:H:176:VAL:O	1.95	0.66
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
5:S:204:LEU:O	5:S:208:MET:HB2	1.96	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
9:I:147:THR:H	9:I:150:GLU:HB2	1.61	0.66
13:M:115:SER:OG	13:M:128:ARG:HD2	1.95	0.66
1:A:244:ARG:O	1:A:248:ILE:HG12	1.96	0.66
4:D:64:VAL:HG11	4:D:213:THR:HG21	1.77	0.66
14:N:121:TYR:HE1	14:N:123:ASN:ND2	1.93	0.66
8:V:126:ILE:HD12	8:V:134:ILE:HG13	1.77	0.66
1:A:54:ILE:HG21	1:A:210:MET:SD	2.36	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
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
1:A:129:THR:HG22	2:B:128:ARG:HH21	1.61	0.65
11:K:4:LEU:HB2	11:K:15:ALA:HB3	1.78	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
1:A:87:ILE:O	1:A:91:ARG:HG3	1.97	0.65
5:E:45:GLY:HA2	5:E:153:TYR:CE1	2.31	0.65
11:K:191:VAL:O	11:K:191:VAL:HG12	1.96	0.65
14:N:87:TYR:CD2	14:N:88:LEU:HD23	2.31	0.65
1:A:24:ARG:C	1:A:25:LEU:HD12	2.17	0.65
3:Q:90:THR:HA	3:Q:93:ILE:HD12	1.77	0.65
4:R:31:THR:HB	4:R:63:LYS:NZ	2.11	0.65
8:V:13:ILE:CD1	8:V:177:VAL:HG22	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:113:THR:O	5:E:116:VAL:HG23	1.96	0.65
7:G:197:LYS:HG2	7:G:201:LEU:HD21	1.79	0.65
1:A:128:TYR:HD1	1:A:133:TYR:HE1	1.44	0.65
14:N:73:ALA:HA	14:N:77:GLU:O	1.96	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
3:C:76:ALA:HB3	3:C:136:ILE:HB	1.78	0.64
5:E:15:PHE:HB2	6:F:21:GLN:OE1	1.97	0.64
8:H:147:SER:H	8:H:150:GLU:HB3	1.61	0.64
1:O:234:PHE:N	1:O:234:PHE:CD1	2.64	0.64
5:S:12:VAL:H	5:S:23:GLN:HG3	1.62	0.64
4:D:11:PHE:H	5:E:23:GLN:HE22	1.42	0.64
14:N:157:ILE:N	14:N:158:PRO:HD2	2.13	0.64
3:Q:216:ILE:HG12	3:Q:227:GLN:HB3	1.78	0.64
6:T:208:VAL:O	6:T:227:GLY:HA2	1.98	0.64
7:U:21:PHE:HA	7:U:24:GLU:CG	2.27	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
4:D:70:HIS:ND1	4:D:71:VAL:HG23	2.12	0.64
9:I:59:ILE:HG12	9:I:83:LEU:HD23	1.80	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
10:J:178:VAL:HG23	10:J:191:LEU:HD21	1.80	0.63
8:V:58:ILE:O	8:V:61:TYR:HB3	1.97	0.63
9:W:156:SER:O	9:W:160:GLN:HG3	1.98	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:E:109:VAL:HB	5:E:154:GLN:NE2	2.12	0.63
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
14:N:87:TYR:O	14:N:91:VAL:HG23	1.99	0.63
1:O:44:ALA:CB	1:O:53:VAL:HG12	2.28	0.63
1:A:43:LEU:HD12	1:A:178:ILE:CG2	2.28	0.63
11:Y:127:LEU:HD22	11:Y:128:PRO:HD2	1.81	0.63
11:Y:191:VAL:O	11:Y:193:ASP:N	2.32	0.63
1:A:227:VAL:HB	1:A:234:PHE:CE1	2.33	0.63
2:B:89:SER:O	2:B:92:VAL:HG12	1.99	0.63
4:D:54:LEU:HG	4:D:54:LEU:O	1.99	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
4:D:22:TYR:O	4:D:25:GLU:HB2	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
1:A:234:PHE:CD1	1:A:234:PHE:N	2.65	0.62
1:A:21:PRO:HA	2:B:23:TYR:CD1	2.34	0.62
1:A:103:GLU:HA	8:H:61:TYR:HE2	1.62	0.62
1:O:181:ASN:N	1:O:181:ASN:HD22	1.97	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
3:C:90:THR:HA	3:C:93:ILE:HD12	1.80	0.62
9:I:84:LYS:HE3	9:I:119:THR:CG2	2.29	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:A:25:LEU:O	1:A:28:VAL:HG22	1.98	0.62
3:C:199:LYS:O	3:C:200:THR:HG23	2.00	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
1:O:20:SER:HB2	1:O:21:PRO:HD2	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
4:D:151:GLU:HB2	4:D:152:PRO:HD2	1.82	0.62
3:Q:66:LEU:HD23	3:Q:212:GLU:HB3	1.81	0.62
4:R:151:GLU:HG2	4:R:155:ILE:HG13	1.81	0.62
5:S:124:GLY:H	5:S:132:ARG:HB2	1.63	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:A:128:TYR:HD1	1:A:133:TYR:CE1	2.18	0.62
1:O:24:ARG:C	1:O:25:LEU:HD12	2.20	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
11:K:168:GLU:HG2	11:K:175:PHE:HZ	1.65	0.61
12:L:196:LEU:O	12:L:200:VAL:HG23	1.98	0.61
1:A:146:VAL:HG22	1:A:152:PRO:CA	2.30	0.61
1:O:202:VAL:O	1:O:205:PHE:HB3	2.00	0.61
5:S:219:LEU:O	5:S:231:TYR:HB2	2.00	0.61
8:V:157:HIS:NE2	8:V:196:LEU:HD13	2.14	0.61
6:F:185:ASN:HD22	6:F:186:PRO:N	1.97	0.61
7:G:19:ARG:HH11	7:G:19:ARG:CB	2.13	0.61
13:M:4:LEU:HD12	13:M:5:GLY:N	2.15	0.61
2:P:112:SER:HA	2:P:156:TYR:HE2	1.63	0.61
11:Y:4:LEU:HB2	11:Y:15:ALA:HB3	1.82	0.61
2:B:214:ILE:HD13	2:B:235:PHE:HA	1.82	0.61
3:C:133:VAL:HG12	3:C:134:SER:N	2.16	0.61
4:D:203:VAL:HG21	4:D:210:ILE:HD11	1.81	0.61
1:O:54:ILE:HG21	1:O:210:MET:SD	2.40	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:A:16:ILE:HG22	1:A:17:THR:H	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:4:MET:HB2	8:H:126:ILE:HG22	1.80	0.61
1:O:43:LEU:HD12	1:O:178:ILE:CG2	2.31	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
1:A:204:GLU:HB3	1:A:248:ILE:HG21	1.82	0.61
2:B:111:VAL:HG12	2:B:156:TYR:HD2	1.64	0.61
7:G:94:GLU:HG2	7:G:114:ARG:HD2	1.83	0.61
9:I:52:THR:O	9:I:55:VAL:HG12	2.00	0.61
14:N:57:ARG:O	14:N:61:ASP:HB2	2.00	0.61
3:Q:87:LEU:H	3:Q:87:LEU:HD12	1.66	0.61
13:M:117:ASP:HB2	13:M:121:SER:OG	2.01	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
9:I:172:ASN:ND2	9:I:192:THR:HA	2.16	0.61
10:J:9:LYS:HG3	10:J:148:ASN:HD22	1.66	0.61
14:N:35:ILE:O	14:N:43:VAL:HG22	2.01	0.61
1:O:17:THR:O	1:O:18:ILE:HG23	1.99	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
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
1:A:80:GLY:HA3	1:A:233:PHE:CZ	2.36	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
2:P:178:ARG:NH2	2:P:194:LEU:HD12	2.17	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
7:G:194:GLN:O	7:G:198:ILE:HG13	2.01	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
1:A:126:GLN:NE2	1:A:127:ILE:N	2.49	0.60
3:C:216:ILE:HG12	3:C:227:GLN:HB3	1.83	0.60
5:E:124:GLY:H	5:E:132:ARG:HB2	1.65	0.60
8:H:74:SER:OG	8:H:75:THR:N	2.34	0.60
1:O:41:ASN:OD1	1:O:173:PRO:HD2	2.01	0.60
4:R:105:THR:HG23	4:R:108:TYR:HB3	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:4:MET:HB2	8:V:126:ILE:HG22	1.82	0.60
1:A:82:VAL:CG1	1:A:142:THR:HB	2.31	0.60
4:D:151:GLU:HG2	4:D:155:ILE:HG13	1.83	0.60
4:D:162:GLN:HE21	4:D:163:THR:N	1.97	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
5:E:59:LEU:HD13	5:E:60:GLU:N	2.17	0.60
9:I:173:VAL:O	9:I:189:ASN:HA	2.02	0.60
13:M:4:LEU:HD12	13:M:5:GLY:H	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
11:Y:152:THR:HG23	11:Y:155:GLU:OE1	2.01	0.60
9:I:217:ILE:HD12	9:I:217:ILE:N	2.17	0.60
14:N:17:ASP:HA	14:N:187:PHE:CB	2.32	0.60
1:O:240:ASN:H	1:O:240:ASN:ND2	1.97	0.60
1:O:21:PRO:HA	2:P:23:TYR:CD1	2.37	0.60
4:R:224:LEU:HD23	4:R:229:ILE:HG12	1.83	0.60
7:U:175:LEU:HA	7:U:178:LEU:HD12	1.84	0.60
2:B:95:THR:HA	2:B:99:ARG:HD2	1.84	0.60
5:E:64:ILE:N	5:E:64:ILE:HD12	2.17	0.60
10:J:115:PHE:CD1	10:J:115:PHE:N	2.70	0.60
1:O:41:ASN:O	1:O:55:SER:HA	2.02	0.60
12:Z:66:HIS:CD2	12:Z:74:ILE:HB	2.36	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
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
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
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:A:202:VAL:O	1:A:205:PHE:HB3	2.02	0.59
1:A:181:ASN:HB3	1:A:209:HIS:HE1	1.63	0.59
1:O:181:ASN:HD22	1:O:181:ASN:H	1.50	0.59
5:S:45:GLY:HA2	5:S:153:TYR:CE1	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:54:THR:HA	7:U:209:LYS:HD2	1.83	0.59
1:A:131:ARG:HA	2:B:127:VAL:HG12	1.83	0.59
3:C:77:VAL:HG22	3:C:135:PHE:HE1	1.67	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
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
7:G:47:PHE:O	7:G:215:ILE:HG22	2.03	0.59
8:H:177:VAL:O	8:H:183:VAL:HA	2.02	0.59
2:P:71:ILE:HG12	2:P:138:GLY:HA3	1.84	0.59
11:Y:74:LEU:HD12	11:Y:79:VAL:HG22	1.84	0.59
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
14:N:45:ILE:HG21	14:N:52:MET:HG3	1.83	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
3:Q:70:ASN:ND2	3:Q:71:ASP:H	2.00	0.59
4:D:199:LEU:O	4:D:203:VAL:HG23	2.03	0.59
5:E:16:SER:HB3	5:E:22:PHE:HE2	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
4:R:11:PHE:N	5:S:23:GLN:HE22	2.00	0.59
5:S:64:ILE:HD12	5:S:64:ILE:N	2.17	0.59
6:T:33:SER:HB3	6:T:62:LYS:HZ3	1.67	0.59
10:X:35:PHE:CD2	10:X:35:PHE:N	2.71	0.59
1:A:42:SER:HA	1:A:54:ILE:O	2.03	0.59
1:O:128:TYR:HD1	1:O:133:TYR:CE1	2.19	0.59
2:P:174:PHE:HD2	2:P:195:THR:HG1	1.51	0.59
5:S:51:GLU:HG3	5:S:208:MET:HG2	1.83	0.59
6:T:134:ILE:HD12	6:T:134:ILE:N	2.18	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
1:O:82:VAL:CG1	1:O:142:THR:HB	2.33	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:GLU:HG2	1:A:251:GLN:N	2.17	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
4:D:31:THR:HB	4:D:63:LYS:NZ	2.19	0.58
1:O:251:GLN:O	1:O:251:GLN:HG2	2.04	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
8:V:74:SER:OG	8:V:75:THR:N	2.36	0.58
1:A:44:ALA:CB	1:A:53:VAL:HG12	2.31	0.58
2:B:111:VAL:HG12	2:B:156:TYR:CD2	2.38	0.58
2:B:218:ASN:HD21	2:B:236:ARG:HD2	1.69	0.58
6:F:194:VAL:O	6:F:197:ILE:HG22	2.02	0.58
13:M:91:LYS:HE2	13:M:94:PHE:O	2.03	0.58
1:A:183:GLU:HB3	1:A:187:LYS:HZ2	1.68	0.58
1:A:79:ILE:HD12	1:A:79:ILE:N	2.18	0.58
2:B:224:TYR:HA	9:I:184:ALA:O	2.03	0.58
10:J:35:PHE:N	10:J:35:PHE:CD2	2.71	0.58
2:P:118:MET:SD	2:P:152:PRO:HA	2.42	0.58
6:F:82:ARG:O	6:F:86:ASN:HB2	2.04	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
1:O:203:VAL:HG12	1:O:207:ILE:HD11	1.84	0.58
12:Z:176:ASN:ND2	12:Z:190:ASN:HD22	2.01	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
2:B:94:HIS:NE2	2:B:98:LYS:HD3	2.18	0.58
6:F:150:SER:O	7:G:82:PRO:HG2	2.04	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
3:C:150:THR:CG2	3:C:160:TRP:HE1	2.16	0.58
5:E:219:LEU:O	5:E:231:TYR:HB2	2.04	0.58
1:A:128:TYR:CD1	1:A:133:TYR:CE1	2.90	0.58
7:G:54:THR:HA	7:G:209:LYS:HD2	1.84	0.58
5:S:16:SER:HB3	5:S:22:PHE:HE2	1.68	0.58
7:U:197:LYS:HG2	7:U:201:LEU:HD21	1.86	0.58
11:Y:24:ILE:HG23	11:Y:25:SER:H	1.69	0.58
1:A:28:VAL:O	1:A:31:ALA:HB3	2.04	0.57
2:B:159:TRP:CE3	2:B:162:THR:HB	2.39	0.57
4:D:180:ASP:OD2	4:D:183:GLU:HG3	2.04	0.57
5:E:177:GLU:CD	5:E:177:GLU:H	2.07	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:S:192:THR:HG23	5:S:195:GLU:OE1	2.02	0.57
6:T:194:VAL:O	6:T:197:ILE:HG22	2.03	0.57
1:O:103:GLU:HA	8:V:61:TYR:HE2	1.67	0.57
12:Z:4:LEU:C	12:Z:4:LEU:HD22	2.24	0.57
1:A:33:LYS:N	1:A:33:LYS:HD2	2.15	0.57
9:I:196:ARG:HH12	10:J:142:GLU:HG3	1.70	0.57
8:V:156:LYS:NZ	8:V:188:PHE:HD1	2.00	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
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
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
4:R:69:SER:O	4:R:221:ILE:HD12	2.04	0.57
5:S:167:TYR:CD1	5:S:170:LYS:HB2	2.40	0.57
1:O:63:LEU:HD11	7:U:175:LEU:HB2	1.86	0.57
7:U:47:PHE:O	7:U:215:ILE:HG22	2.04	0.57
7:G:60:PRO:O	7:G:61:GLN:HB2	2.05	0.57
8:H:4:MET:SD	8:H:159:LEU:CD1	2.92	0.57
13:M:139:PRO:O	13:M:142:ASP:HB2	2.04	0.57
3:Q:133:VAL:HG12	3:Q:134:SER:N	2.19	0.57
4:R:22:TYR:O	4:R:25:GLU:HB2	2.04	0.57
8:V:66:TYR:CE1	8:V:70:TYR:HB2	2.40	0.57
1:A:242:GLU:HA	1:A:245:LEU:HD12	1.85	0.57
13:M:147:PHE:CD1	13:M:161:LYS:HE3	2.40	0.57
14:N:82:SER:HA	14:N:118:PHE:CE2	2.40	0.57
1:O:183:GLU:O	1:O:187:LYS:HG3	2.04	0.57
1:O:79:ILE:HD12	1:O:79:ILE:N	2.18	0.57
3:Q:150:THR:CG2	3:Q:160:TRP:HE1	2.17	0.57
6:T:43:HIS:HB3	6:T:215:ILE:HD11	1.86	0.57
11:K:115:LEU:HD12	11:K:116:TYR:N	2.19	0.57
11:K:191:VAL:O	11:K:193:ASP:N	2.38	0.57
14:N:9:ASP:HB3	14:N:158:PRO:O	2.03	0.57
1:O:242:GLU:HA	1:O:245:LEU:HD12	1.85	0.57
1:O:87:ILE:O	1:O:91:ARG:HG3	2.05	0.57
10:X:178:VAL:HG23	10:X:191:LEU:HD21	1.86	0.57
11:Y:117:GLN:HE22	11:Y:131:ALA:H	1.53	0.57
12:Z:12:ILE:HD13	12:Z:102:CYS:HB3	1.86	0.57
8:H:9:LYS:HD3	8:H:146:MET:O	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:148:ARG:HD2	9:W:165:ASN:HD21	1.69	0.57
7:U:166:LYS:NZ	7:U:206:ASN:HD21	2.03	0.57
6:T:150:SER:O	7:U:82:PRO:HG2	2.05	0.57
10:X:29:ASN:HD22	10:X:29:ASN:N	2.02	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
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
9:I:14:ILE:HD13	9:I:101:ALA:HB3	1.85	0.56
11:K:127:LEU:HD22	11:K:128:PRO:HD2	1.87	0.56
4:R:199:LEU:O	4:R:203:VAL:HG23	2.05	0.56
6:T:144:LEU:C	6:T:145:LEU:HD12	2.25	0.56
8:V:177:VAL:O	8:V:183:VAL:HA	2.05	0.56
11:Y:95:ARG:HB3	11:Y:95:ARG:NH1	2.20	0.56
1:A:41:ASN:O	1:A:55:SER:HA	2.04	0.56
6:F:34:VAL:HG22	6:F:35:THR:N	2.20	0.56
7:G:180:ASP:O	7:G:183:PRO:HD3	2.05	0.56
11:K:32:ASP:OD1	11:K:34:THR:HB	2.05	0.56
4:R:105:THR:HG23	4:R:108:TYR:CB	2.35	0.56
9:W:72:ARG:HH11	9:W:72:ARG:HG3	1.70	0.56
3:C:163:ILE:HG13	3:C:164:SER:N	2.20	0.56
8:H:3:ILE:HG22	8:H:16:ALA:CB	2.35	0.56
11:K:74:LEU:HD12	11:K:79:VAL:HG22	1.86	0.56
8:V:26:ILE:HG21	8:V:29:ARG:HB3	1.87	0.56
11:Y:195:GLN:HA	11:Y:195:GLN:NE2	2.18	0.56
2:B:64:VAL:HG21	2:B:212:ALA:HB3	1.87	0.56
8:H:186:LEU:HD22	8:H:188:PHE:HE2	1.70	0.56
11:K:117:GLN:HE22	11:K:131:ALA:H	1.53	0.56
1:O:183:GLU:HB3	1:O:187:LYS:HZ2	1.66	0.56
2:P:184:GLU:O	2:P:187:ASP:HB2	2.05	0.56
3:Q:195:LYS:O	3:Q:199:LYS:HD3	2.05	0.56
5:S:113:THR:O	5:S:116:VAL:HG23	2.06	0.56
8:V:163:ILE:HG23	8:V:170:GLY:HA2	1.86	0.56
9:W:88:PHE:HB2	9:W:116:HIS:O	2.04	0.56
1:A:164:VAL:HG22	1:A:165:GLY:H	1.71	0.56
6:F:159:THR:OG1	6:F:160:ALA:N	2.38	0.56
8:V:92:ASN:ND2	8:V:92:ASN:N	2.52	0.56
12:Z:66:HIS:CE1	12:Z:70:GLU:HG3	2.40	0.56
6:F:96:SER:O	6:F:100:ASN:HA	2.05	0.56
6:F:50:LYS:HB3	6:F:59:TYR:HB3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:14:LEU:CD1	8:H:34:LEU:HD22	2.36	0.56
11:K:3:ILE:HD13	11:K:16:SER:HB3	1.87	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
14:N:40:ASN:N	14:N:40:ASN:HD22	1.83	0.56
7:U:100:LYS:NZ	7:U:100:LYS:HB3	2.21	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
4:D:70:HIS:HB3	4:D:219:SER:OG	2.05	0.56
11:K:9:GLN:HE21	11:K:150:ASP:HA	1.70	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
5:S:78:MET:HA	5:S:142:LEU:HD23	1.88	0.56
6:T:215:ILE:HG13	6:T:216:VAL:H	1.70	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
14:N:203:ASN:O	14:N:204:LEU:HD13	2.06	0.56
4:R:151:GLU:HB2	4:R:152:PRO:HD2	1.86	0.56
6:T:34:VAL:HG22	6:T:35:THR:N	2.19	0.56
7:U:60:PRO:O	7:U:61:GLN:HB2	2.05	0.56
10:J:49:THR:HG21	11:K:121:LEU:O	2.04	0.56
7:U:19:ARG:HB2	7:U:19:ARG:HH11	1.70	0.56
2:P:224:TYR:HA	9:W:184:ALA:O	2.06	0.56
13:M:176:ARG:NH1	9:W:200:GLN:HE22	2.04	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
4:D:105:THR:HG23	4:D:108:TYR:HB3	1.88	0.56
12:L:54:PHE:C	12:L:54:PHE:CD2	2.78	0.56
4:R:36:VAL:CG1	4:R:195:THR:HG23	2.36	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
10:X:37:TYR:O	10:X:40:VAL:HG23	2.06	0.56
1:A:250:GLU:HG2	1:A:251:GLN:H	1.70	0.56
7:G:44:GLY:HA3	7:G:218:CYS:O	2.06	0.56
1:O:128:TYR:HA	1:O:133:TYR:CD1	2.41	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
13:M:213:ASP:HB2	9:W:19:ARG:HH22	1.71	0.56
11:Y:34:THR:HG23	11:Y:35:ARG:N	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:ILE:CG2	1:A:210:MET:SD	2.94	0.55
6:F:189:LEU:O	6:F:192:ALA:HB3	2.07	0.55
11:K:95:ARG:HB3	11:K:95:ARG:NH1	2.21	0.55
3:Q:19:LEU:O	3:Q:21:GLN:N	2.39	0.55
5:S:37:ALA:CB	5:S:50:VAL:HG12	2.36	0.55
6:T:185:ASN:ND2	6:T:188:GLU:H	2.03	0.55
11:Y:115:LEU:HD12	11:Y:116:TYR:N	2.21	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
1:A:148:GLU:H	1:A:148:GLU:CD	2.10	0.55
6:F:187:ASP:O	6:F:191:LYS:HG3	2.06	0.55
7:G:21:PHE:HA	7:G:24:GLU:CG	2.36	0.55
11:K:7:ARG:HG2	11:K:7:ARG:HH11	1.71	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
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
1:A:63:LEU:HD11	7:G:175:LEU:HB2	1.88	0.55
1:O:131:ARG:HA	2:P:127:VAL:HG12	1.89	0.55
7:U:194:GLN:O	7:U:198:ILE:HG13	2.06	0.55
11:Y:38:SER:HB2	11:Y:39:PRO:HD2	1.88	0.55
2:B:71:ILE:HG12	2:B:138:GLY:HA3	1.89	0.55
5:E:30:ALA:O	5:E:33:LEU:HB3	4.20	0.55
7:G:100:LYS:NZ	7:G:100:LYS:HB3	2.20	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
2:P:178:ARG:HH21	2:P:194:LEU:HD12	1.70	0.55
6:T:96:SER:O	6:T:100:ASN:HA	2.06	0.55
6:T:187:ASP:O	6:T:191:LYS:HG3	2.07	0.55
8:V:190:PRO:O	8:V:194:GLU:HG3	2.06	0.55
7:G:98:PHE:CD1	7:G:98:PHE:C	2.80	0.55
8:H:190:PRO:HA	8:H:193:TYR:CE2	2.42	0.55
10:J:49:THR:HB	11:K:122:GLY:O	2.07	0.55
14:N:105:ALA:C	14:N:106:ILE:HD12	2.27	0.55
1:O:20:SER:OG	1:O:24:ARG:N	2.39	0.55
3:Q:222:ASP:C	3:Q:224:GLU:H	2.10	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
9:I:83:LEU:O	9:I:87:LEU:HB2	2.06	0.55
14:N:186:ASN:HD22	14:N:203:ASN:ND2	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:U:23:VAL:O	7:U:27:VAL:HG23	2.07	0.55
8:V:185:ARG:NH1	8:V:185:ARG:HG3	2.22	0.55
1:A:220:LYS:CB	1:A:242:GLU:HB2	2.36	0.55
1:A:43:LEU:C	1:A:43:LEU:HD23	2.27	0.55
7:G:217:TRP:CD1	7:G:217:TRP:N	2.74	0.55
1:O:220:LYS:CB	1:O:242:GLU:HB2	2.37	0.55
2:P:218:ASN:HD21	2:P:236:ARG:HD2	1.72	0.55
3:Q:64:GLU:O	3:Q:65:LYS:HG2	2.07	0.55
5:S:220:SER:HA	5:S:231:TYR:HD1	1.71	0.55
6:T:94:TYR:O	6:T:98:VAL:HG23	2.07	0.55
12:Z:54:PHE:C	12:Z:54:PHE:CD2	2.79	0.55
5:S:97:VAL:HG11	12:Z:65:LEU:HD21	1.89	0.55
1:A:41:ASN:HB2	1:A:56:GLN:OE1	2.07	0.55
2:B:212:ALA:CB	2:B:237:LYS:HA	2.37	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
2:P:159:TRP:CE3	2:P:162:THR:HB	2.42	0.55
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
1:A:139:VAL:HG23	1:A:141:LEU:HD21	1.87	0.54
3:C:37:GLY:HA2	3:C:45:VAL:O	2.06	0.54
4:D:221:ILE:O	4:D:222:VAL:HB	2.07	0.54
12:L:66:HIS:CE1	12:L:70:GLU:HG3	2.42	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
6:F:70:MET:CE	6:F:105:VAL:HG22	2.37	0.54
7:U:46:VAL:HG22	7:U:217:TRP:HB3	1.89	0.54
9:W:83:LEU:O	9:W:87:LEU:HB2	2.07	0.54
10:X:133:ALA:HB2	10:X:169:ASP:CB	2.37	0.54
4:D:206:GLY:C	4:D:208:LYS:H	2.11	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
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
4:R:181:ARG:HH22	5:S:60:GLU:HG2	1.72	0.54
6:T:82:ARG:O	6:T:86:ASN:HB2	2.07	0.54
11:Y:160:LEU:O	11:Y:164:VAL:HG23	2.07	0.54
5:E:64:ILE:H	5:E:64:ILE:HD12	1.73	0.54
8:H:53:GLN:HE22	9:I:119:THR:H	1.54	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:16:GLY:HA3	3:Q:28:SER:HB2	1.90	0.54
9:W:196:ARG:HH12	10:X:142:GLU:HG3	1.72	0.54
2:B:84:VAL:O	2:B:88:LYS:HG3	2.07	0.54
3:C:29:ILE:C	3:C:31:HIS:H	2.09	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
5:S:40:ILE:HD12	5:S:200:VAL:HG23	1.88	0.54
9:I:88:PHE:HB2	9:I:116:HIS:O	2.07	0.54
1:O:18:ILE:HD13	1:O:18:ILE:N	2.22	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
10:X:49:THR:HG21	11:Y:121:LEU:O	2.08	0.54
1:A:35:THR:O	1:A:38:THR:HG22	2.07	0.54
1:A:40:ILE:HD12	1:A:56:GLN:O	2.07	0.54
1:A:43:LEU:HD22	1:A:54:ILE:HB	1.90	0.54
3:C:87:LEU:H	3:C:87:LEU:HD12	1.73	0.54
7:G:21:PHE:HA	7:G:24:GLU:HG2	1.89	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
5:S:59:LEU:HD13	5:S:60:GLU:N	2.22	0.54
4:D:114:ALA:O	4:D:118:GLN:HB2	2.08	0.54
7:G:194:GLN:HE22	7:G:197:LYS:NZ	2.06	0.54
7:G:166:LYS:NZ	7:G:206:ASN:HD21	2.05	0.54
10:J:3:VAL:HG22	10:J:16:CYS:HB3	1.90	0.54
11:K:126:GLU:O	11:K:127:LEU:HD23	2.07	0.54
11:K:24:ILE:HG23	11:K:25:SER:N	2.23	0.54
1:O:155:TYR:CD2	1:O:165:GLY:HA2	2.42	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
2:B:185:LEU:HD21	2:B:213:ILE:HD13	1.89	0.54
2:B:57:MET:HB2	2:B:59:GLU:OE2	2.07	0.54
5:E:108:ASN:O	5:E:111:SER:N	2.41	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
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
7:U:229:PHE:HD2	7:U:231:LYS:HE3	1.73	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
1:A:203:VAL:HG12	1:A:207:ILE:HD11	1.89	0.54
2:B:12:PHE:HE2	3:C:130:PRO:HG2	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:175:MET:HB2	8:H:186:LEU:HB2	1.90	0.54
14:N:122:VAL:HA	14:N:127:VAL:O	2.07	0.54
2:P:160:LYS:HD3	2:P:179:TRP:CH2	2.43	0.54
4:R:180:ASP:OD2	4:R:183:GLU:HG3	2.08	0.54
8:V:160:SER:HB2	8:V:193:TYR:HB2	1.90	0.54
1:A:41:ASN:OD1	1:A:173:PRO:HD2	2.08	0.53
5:E:118:ASP:O	5:E:122:ARG:HG2	2.09	0.53
10:J:100:VAL:HG12	10:J:101:ALA:N	2.23	0.53
1:O:162:TYR:C	1:O:162:TYR:CD1	2.82	0.53
1:O:185:HIS:ND1	1:O:185:HIS:O	2.41	0.53
1:O:42:SER:HA	1:O:54:ILE:O	2.09	0.53
5:S:151:ASP:HB2	5:S:154:GLN:OE1	2.08	0.53
7:U:201:LEU:HD13	7:U:201:LEU:H	1.73	0.53
9:W:38:SER:HB2	9:W:41:ILE:CD1	2.37	0.53
1:A:70:SER:O	1:A:71:TYR:HD1	1.90	0.53
3:C:44:ILE:HD11	3:C:146:TYR:HB3	1.91	0.53
3:C:238:ILE:HD12	3:C:241:LYS:HD2	1.89	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
7:U:169:GLN:CD	7:U:169:GLN:H	2.10	0.53
1:A:128:TYR:HA	1:A:133:TYR:CD1	2.42	0.53
5:E:180:GLN:O	5:E:184:LEU:HB2	2.08	0.53
9:W:52:THR:O	9:W:55:VAL:HG12	2.08	0.53
1:A:248:ILE:HG22	1:A:251:GLN:OE1	2.08	0.53
5:E:40:ILE:HD12	5:E:200:VAL:HG23	1.91	0.53
6:F:37:GLY:HA2	6:F:45:VAL:O	2.09	0.53
11:K:110:LYS:O	11:K:112:LYS:HG3	2.07	0.53
11:K:62:ASN:O	11:K:65:LEU:HB3	2.08	0.53
14:N:92:MET:HE2	14:N:106:ILE:HD13	1.91	0.53
3:Q:152:ASN:HB2	3:Q:153:PRO:CD	2.39	0.53
7:U:150:LEU:HD11	7:U:154:GLY:HA2	1.91	0.53
1:A:72:ILE:HA	1:A:81:MET:O	2.08	0.53
12:L:16:VAL:CG2	12:L:176:ASN:HB2	2.38	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
9:I:66:HIS:O	9:I:70:THR:HG23	2.09	0.53
12:L:176:ASN:HD21	12:L:190:ASN:HD22	1.53	0.53
13:M:77:ILE:HG23	13:M:78:ASN:N	2.24	0.53
14:N:87:TYR:HD2	14:N:88:LEU:HD23	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:98:LYS:HA	2:P:103:GLU:O	2.08	0.53
1:O:123:ASN:O	1:O:127:ILE:HG13	2.09	0.53
1:O:45:VAL:HG12	1:O:168:ALA:CB	2.39	0.53
2:P:81:ASP:O	2:P:85:LEU:HB2	2.07	0.53
4:R:163:THR:HG21	4:R:171:VAL:HG23	1.91	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
1:A:183:GLU:O	1:A:187:LYS:HG3	2.08	0.53
1:A:185:HIS:O	1:A:185:HIS:ND1	2.41	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
5:E:167:TYR:CD1	5:E:170:LYS:HB2	2.43	0.53
7:U:23:VAL:O	7:U:26:ALA:HB3	2.08	0.53
1:A:117:LEU:O	1:A:121:MET:HG2	2.08	0.53
3:C:64:GLU:O	3:C:65:LYS:HG2	2.09	0.53
9:I:34:LEU:HD22	9:I:174:ASP:HB3	1.91	0.53
9:I:38:SER:HB2	9:I:41:ILE:HD13	1.90	0.53
11:K:195:GLN:HA	11:K:195:GLN:NE2	2.24	0.53
12:L:24:ASN:OD1	10:X:171:LEU:HD12	2.09	0.53
6:T:50:LYS:HB3	6:T:59:TYR:HB3	1.90	0.53
7:U:180:ASP:O	7:U:183:PRO:HD3	2.09	0.53
1:A:131:ARG:HH12	1:A:133:TYR:HB3	1.74	0.52
7:G:19:ARG:HH11	7:G:19:ARG:HB2	1.74	0.52
12:L:66:HIS:CD2	12:L:74:ILE:HB	2.43	0.52
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
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
11:Y:88:ALA:O	11:Y:91:ILE:HG22	2.09	0.52
5:E:170:LYS:HD2	5:E:171:ALA:N	2.23	0.52
10:J:163:LEU:HD11	10:J:193:MET:HB3	1.90	0.52
6:T:185:ASN:HD22	6:T:186:PRO:N	2.06	0.52
8:V:9:LYS:HD3	8:V:146:MET:O	2.09	0.52
2:B:81:ASP:O	2:B:85:LEU:HB2	2.09	0.52
7:G:46:VAL:HG22	7:G:217:TRP:HB3	1.89	0.52
2:B:227:ILE:HG12	9:I:186:TYR:CD2	2.43	0.52
9:I:4:VAL:HG12	9:I:126:SER:HB2	1.92	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:72:HIS:CE1	7:U:105:PRO:HB2	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:48:ALA:HB2	7:U:215:ILE:HG23	1.91	0.52
3:Q:96:GLN:HB3	10:X:60:TYR:CE2	2.45	0.52
12:Z:81:LYS:HG3	12:Z:85:ASN:HD21	1.74	0.52
1:A:159:PRO:C	1:A:161:GLY:H	2.13	0.52
3:C:165:VAL:N	3:C:169:THR:HG21	2.25	0.52
4:D:105:THR:HG23	4:D:108:TYR:CB	2.40	0.52
6:F:213:ILE:HG22	6:F:214:ALA:N	2.24	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
4:R:70:HIS:HB3	4:R:219:SER:OG	2.09	0.52
6:T:158:GLY:O	6:T:159:THR:HB	2.10	0.52
7:U:15:SER:OG	7:U:19:ARG:HB3	2.10	0.52
7:U:217:TRP:N	7:U:217:TRP:CD1	2.76	0.52
8:V:163:ILE:HD12	8:V:170:GLY:HA2	1.92	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
7:G:169:GLN:HA	7:G:172:LYS:HB2	1.90	0.52
1:O:133:TYR:O	1:O:134:MET:HB3	2.08	0.52
5:S:237:ALA:O	5:S:240:ILE:HB	2.10	0.52
12:Z:159:ARG:HD2	12:Z:162:LEU:HD23	1.92	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
7:G:229:PHE:CD2	7:G:231:LYS:HE3	2.45	0.52
7:G:39:ILE:HG13	7:G:46:VAL:HB	1.91	0.52
12:L:8:PHE:HA	12:L:146:TRP:CE3	2.45	0.52
12:L:81:LYS:HG3	12:L:85:ASN:HD21	1.74	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
11:Y:3:ILE:C	11:Y:4:LEU:HD23	2.29	0.52
3:C:218:LYS:HG3	3:C:225:VAL:HG12	1.92	0.52
5:E:151:ASP:HB2	5:E:154:GLN:OE1	2.08	0.52
7:U:229:PHE:CD2	7:U:231:LYS:HE3	2.44	0.52
8:V:6:VAL:O	8:V:12:VAL:HG23	2.10	0.52
10:X:12:VAL:HG23	10:X:181:ILE:HB	1.92	0.52
12:Z:176:ASN:HD21	12:Z:190:ASN:HD22	1.57	0.52
1:A:18:ILE:HD13	1:A:18:ILE:N	2.24	0.52
1:A:220:LYS:HB3	1:A:242:GLU:HB2	1.91	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
3:C:165:VAL:C	3:C:169:THR:HG21	2.30	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:235:GLN:O	4:D:235:GLN:HG2	2.10	0.52
4:D:69:SER:O	4:D:221:ILE:HD12	2.10	0.52
8:H:31:THR:HG22	8:H:33:LYS:HG2	1.92	0.52
14:N:148:ARG:HD2	9:W:165:ASN:ND2	2.24	0.52
8:V:13:ILE:HD11	8:V:177:VAL:HG13	1.92	0.52
9:W:4:VAL:HG12	9:W:126:SER:HB2	1.90	0.52
4:D:193:LYS:HE2	4:D:193:LYS:HA	5.80	0.52
7:G:77:TYR:HB3	7:G:135:THR:HG23	1.91	0.52
10:J:12:VAL:HG23	10:J:181:ILE:HB	1.92	0.52
14:N:26:LEU:HD23	8:V:165:TRP:C	2.29	0.52
3:Q:29:ILE:C	3:Q:31:HIS:H	2.13	0.52
6:T:68:GLU:O	6:T:222:PHE:N	2.40	0.52
9:W:5:GLY:O	9:W:124:TYR:HA	2.09	0.52
1:A:42:SER:O	1:A:170:ALA:HA	2.09	0.52
6:F:118:LYS:HD2	6:F:118:LYS:N	2.25	0.52
7:G:108:ILE:N	7:G:109:PRO:CD	2.73	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
14:N:153:ARG:HG3	14:N:153:ARG:NH1	2.17	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
3:Q:146:TYR:O	3:Q:147:GLN:HG3	2.10	0.52
3:Q:77:VAL:HG12	3:Q:78:ALA:N	2.25	0.52
5:S:136:ARG:HB2	5:S:137:PRO:CD	2.38	0.52
6:T:189:LEU:O	6:T:192:ALA:HB3	2.10	0.52
2:B:34:SER:OG	2:B:47:THR:HB	2.09	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
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
9:I:52:THR:O	9:I:56:THR:HG23	2.10	0.51
10:J:29:ASN:HD22	10:J:29:ASN:N	2.09	0.51
1:O:220:LYS:HB3	1:O:242:GLU:HB2	1.92	0.51
3:Q:218:LYS:HG3	3:Q:225:VAL:HG12	1.91	0.51
4:R:235:GLN:HG2	4:R:235:GLN:O	2.10	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
11:Y:24:ILE:HG23	11:Y:25:SER:N	2.25	0.51
12:Z:16:VAL:CG2	12:Z:176:ASN:HB2	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:46:ARG:HG3	1:A:167:LYS:O	2.10	0.51
6:F:38:LEU:N	6:F:38:LEU:HD23	2.26	0.51
10:J:184:ASP:CG	10:J:185:GLU:N	2.62	0.51
12:L:144:TYR:CD2	12:L:145:LYS:N	2.78	0.51
12:L:159:ARG:O	12:L:162:LEU:HB3	2.11	0.51
14:N:62:LEU:O	14:N:65:GLU:HB3	2.10	0.51
3:Q:24:TYR:O	3:Q:27:GLU:HG3	2.10	0.51
3:Q:58:GLU:HG2	3:Q:59:GLN:N	2.25	0.51
7:U:194:GLN:NE2	7:U:197:LYS:NZ	2.59	0.51
5:S:97:VAL:HG11	12:Z:65:LEU:CD2	2.41	0.51
3:C:191:GLU:HG2	3:C:195:LYS:HE2	1.92	0.51
7:G:182:HIS:HA	7:G:184:GLU:OE2	2.11	0.51
7:G:201:LEU:H	7:G:201:LEU:HD13	1.75	0.51
8:H:92:ASN:N	8:H:92:ASN:ND2	2.58	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
13:M:138:MET:N	13:M:139:PRO:CD	2.73	0.51
13:M:183:THR:HG23	13:M:189:VAL:O	2.11	0.51
3:Q:89:ASN:O	3:Q:93:ILE:HG13	2.11	0.51
4:R:114:ALA:O	4:R:118:GLN:HB2	2.10	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
3:C:165:VAL:CA	3:C:169:THR:HG21	2.40	0.51
7:G:150:LEU:HD11	7:G:154:GLY:HA2	1.92	0.51
9:I:5:GLY:O	9:I:124:TYR:HA	2.11	0.51
2:P:94:HIS:NE2	2:P:98:LYS:HD3	2.26	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
2:B:190:HIS:CE1	2:B:194:LEU:HD11	2.46	0.51
3:C:140:TYR:CD1	3:C:141:ASP:N	2.79	0.51
5:E:15:PHE:CD1	5:E:21:LEU:HD21	2.46	0.51
7:G:15:SER:OG	7:G:19:ARG:HB3	2.11	0.51
9:I:158:ALA:O	9:I:161:ALA:HB3	2.11	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
2:P:68:THR:CG2	2:P:71:ILE:HB	2.38	0.51
4:R:27:VAL:HG11	4:R:132:SER:CB	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:140:MET:HE3	10:X:144:LEU:HD11	1.91	0.51
10:X:15:ALA:CB	10:X:178:VAL:HG22	2.40	0.51
7:G:71:ARG:NH1	14:N:64:THR:HG22	2.25	0.51
11:K:66:TYR:CE1	11:K:74:LEU:HD23	2.45	0.51
14:N:81:PRO:HA	14:N:84:ILE:HD12	1.91	0.51
1:O:54:ILE:CG2	1:O:210:MET:SD	2.99	0.51
5:S:180:GLN:O	5:S:184:LEU:HB2	2.10	0.51
6:T:2:PHE:HD1	6:T:3:ARG:HG2	1.73	0.51
7:U:194:GLN:HE22	7:U:197:LYS:NZ	2.08	0.51
10:X:51:VAL:HG12	10:X:52:THR:N	2.25	0.51
1:A:156:LYS:HE2	1:A:166:TYR:CE2	2.46	0.51
5:E:110:GLU:HB3	5:E:156:PHE:CZ	2.45	0.51
4:D:159:TRP:CZ2	5:E:59:LEU:HD23	2.46	0.51
7:G:72:HIS:CE1	7:G:105:PRO:HB2	2.46	0.51
8:H:160:SER:HB2	8:H:193:TYR:HB2	1.93	0.51
14:N:25:LEU:HD12	14:N:26:LEU:H	1.76	0.51
1:O:144:VAL:HG12	1:O:154:ILE:HG12	1.93	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
12:Z:38:ASN:HB2	12:Z:39:PRO:HD2	1.93	0.51
1:A:162:TYR:HD1	1:A:162:TYR:C	2.15	0.51
2:B:68:THR:C	2:B:70:ASP:H	2.14	0.51
3:C:19:LEU:O	3:C:21:GLN:N	2.44	0.51
6:F:94:TYR:O	6:F:98:VAL:HG23	2.11	0.51
8:H:186:LEU:HD22	8:H:188:PHE:CE2	2.46	0.51
9:I:180:ILE:HG22	9:I:180:ILE:O	2.10	0.51
7:U:108:ILE:N	7:U:109:PRO:CD	2.74	0.51
9:W:66:HIS:O	9:W:70:THR:HG23	2.11	0.51
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
12:Z:110:PRO:O	12:Z:111:THR:HG23	2.11	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
3:Q:120:GLN:O	3:Q:123:THR:HB	2.11	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
11:Y:160:LEU:C	11:Y:160:LEU:HD23	2.32	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
13:M:24:TYR:HA	9:W:167:LEU:HD12	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:139:VAL:HG23	1:O:141:LEU:HD21	1.92	0.50
1:O:145:SER:HA	1:O:228:ALA:HB1	1.92	0.50
4:R:78:LEU:HD12	4:R:81:ASP:OD2	2.11	0.50
6:T:24:TYR:N	6:T:24:TYR:CD1	2.79	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
12:Z:182:GLU:HG3	12:Z:182:GLU:O	2.10	0.50
1:A:76:SER:OG	1:A:77:ARG:N	2.44	0.50
5:E:37:ALA:CB	5:E:50:VAL:HG12	2.41	0.50
6:F:121:GLN:HE22	7:G:86:HIS:CD2	2.24	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
8:H:40:LYS:HZ2	8:H:182:GLY:HA2	1.75	0.50
3:Q:59:GLN:N	3:Q:59:GLN:NE2	2.59	0.50
3:Q:156:ASN:HD21	4:R:79:ASN:HB2	1.77	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
12:Z:35:ILE:HD11	12:Z:45:MET:HE2	1.94	0.50
3:C:228:LYS:HB3	3:C:230:PHE:HE1	1.76	0.50
1:A:98:LYS:HD3	8:H:68:SER:O	2.10	0.50
10:J:133:ALA:HB2	10:J:169:ASP:CB	2.40	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
4:R:133:THR:HG23	4:R:150:THR:CG2	2.35	0.50
9:W:196:ARG:NH1	10:X:142:GLU:HG3	2.26	0.50
12:Z:1:THR:HG23	12:Z:33:ARG:CZ	2.42	0.50
1:A:195:ASN:O	1:A:196:GLU:HB2	2.11	0.50
1:A:38:THR:HG23	1:A:39:ASN:H	1.76	0.50
3:C:120:GLN:O	3:C:123:THR:HB	2.11	0.50
3:C:13:PHE:H	4:D:19:GLN:HE22	1.57	0.50
5:E:46:VAL:HG23	5:E:153:TYR:HD1	1.76	0.50
8:H:48:SER:HB2	8:H:94:THR:HB	1.93	0.50
14:N:119:LEU:HG	14:N:134:LEU:HD12	1.93	0.50
1:O:102:ALA:CB	8:V:65:LEU:HD13	2.42	0.50
5:S:64:ILE:HD12	5:S:64:ILE:H	1.75	0.50
6:T:146:GLU:O	6:T:153:VAL:HA	2.11	0.50
8:V:75:THR:HG22	8:V:111:TYR:HE1	1.75	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:131:ARG:HH12	1:O:133:TYR:HB3	1.76	0.50
9:W:158:ALA:O	9:W:161:ALA:HB3	2.11	0.50
2:B:68:THR:O	2:B:70:ASP:N	2.44	0.50
3:C:70:ASN:HD22	3:C:71:ASP:H	1.59	0.50
8:H:18:SER:OG	8:H:171:GLY:HA3	2.12	0.50
14:N:171:ASN:ND2	14:N:174:ARG:HH21	2.10	0.50
3:Q:70:ASN:ND2	3:Q:71:ASP:N	2.58	0.50
14:N:142:MET:HG3	9:W:132:LEU:HB3	1.92	0.50
1:A:25:LEU:N	1:A:25:LEU:HD12	2.27	0.50
2:B:12:PHE:CE2	3:C:130:PRO:HG2	2.46	0.50
1:A:179:THR:HG23	2:B:55:LEU:HD12	1.92	0.50
6:F:144:LEU:HD23	6:F:144:LEU:C	2.32	0.50
6:F:185:ASN:ND2	6:F:185:ASN:C	2.64	0.50
7:G:229:PHE:HD2	7:G:231:LYS:HE3	1.75	0.50
10:J:6:MET:CE	10:J:145:TYR:HD1	2.24	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
6:T:36:VAL:CG2	6:T:160:ALA:HB2	2.42	0.50
7:U:197:LYS:O	7:U:201:LEU:HD13	2.12	0.50
8:V:53:GLN:HE22	9:W:119:THR:H	1.59	0.50
10:X:100:VAL:HG12	10:X:101:ALA:N	2.25	0.50
11:Y:34:THR:CG2	11:Y:35:ARG:N	2.74	0.50
1:A:125:SER:HA	1:A:128:TYR:CD2	2.47	0.50
7:G:193:LYS:HE2	7:G:193:LYS:HA	3.94	0.50
8:H:126:ILE:HD12	8:H:134:ILE:CG1	2.40	0.50
8:H:190:PRO:O	8:H:192:GLU:N	2.45	0.50
9:I:153:LYS:C	9:I:153:LYS:HD3	2.33	0.50
11:K:5:GLY:HA2	11:K:13:ILE:O	2.12	0.50
14:N:189:LEU:HD23	14:N:190:ALA:N	2.27	0.50
1:O:218:PHE:CD2	1:O:223:LEU:HD11	2.46	0.50
2:P:190:HIS:CE1	2:P:194:LEU:HD11	2.47	0.50
2:P:227:ILE:HG12	9:W:186:TYR:CD2	2.46	0.50
8:V:40:LYS:HZ2	8:V:182:GLY:HA2	1.77	0.50
9:W:104:ASP:O	9:W:106:THR:N	2.41	0.50
9:W:175:VAL:HG12	9:W:176:CYS:N	2.27	0.50
2:B:130:PHE:O	2:B:152:PRO:HB3	2.12	0.49
5:E:203:ILE:O	5:E:207:VAL:HG22	2.11	0.49
6:F:16:THR:O	7:G:28:LYS:HB3	2.12	0.49
1:O:38:THR:HG23	1:O:39:ASN:H	1.76	0.49
2:P:29:LYS:NZ	2:P:29:LYS:HB3	2.27	0.49
3:Q:114:ARG:HB2	3:Q:114:ARG:NH1	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:203:ILE:O	5:S:207:VAL:HG22	2.12	0.49
11:Y:151:MET:HB3	11:Y:155:GLU:HB2	1.94	0.49
1:A:146:VAL:HA	1:A:151:GLY:O	2.12	0.49
1:A:73:PHE:N	1:A:73:PHE:CD1	2.80	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
11:K:160:LEU:HD23	11:K:161:LYS:N	2.27	0.49
12:L:159:ARG:HD2	12:L:162:LEU:HD23	1.94	0.49
13:M:91:LYS:HB3	13:M:94:PHE:O	2.12	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
3:Q:133:VAL:CG1	3:Q:134:SER:N	2.74	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
7:U:24:GLU:O	7:U:27:VAL:HB	2.12	0.49
11:Y:118:ILE:HA	11:Y:123:THR:O	2.12	0.49
1:A:43:LEU:HD12	1:A:178:ILE:HG22	1.93	0.49
14:N:13:ILE:HG22	14:N:14:ILE:N	2.28	0.49
14:N:8:TYR:CE2	14:N:162:VAL:HG22	2.47	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
3:Q:163:ILE:HG13	3:Q:164:SER:N	2.27	0.49
6:T:36:VAL:HG22	6:T:160:ALA:HB2	1.93	0.49
8:V:175:MET:HB2	8:V:186:LEU:HB2	1.94	0.49
8:V:36:ARG:HB2	8:V:42:TRP:CZ2	2.47	0.49
12:Z:159:ARG:O	12:Z:162:LEU:HB3	2.13	0.49
1:A:91:ARG:HH12	7:G:156:TYR:H	1.60	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
8:H:1:THR:HA	8:H:33:LYS:HZ3	1.75	0.49
8:H:66:TYR:CE1	8:H:70:TYR:HB2	2.48	0.49
9:I:4:VAL:HG22	9:I:159:ILE:HD11	1.94	0.49
1:O:54:ILE:HG13	1:O:225:VAL:HG21	1.94	0.49
3:Q:140:TYR:CD1	3:Q:141:ASP:N	2.80	0.49
3:Q:163:ILE:HD12	3:Q:173:GLN:OE1	2.11	0.49
4:R:112:TYR:O	4:R:116:VAL:HG23	2.12	0.49
4:R:27:VAL:HG11	4:R:132:SER:HB2	1.94	0.49
6:T:92:CYS:HA	6:T:103:LEU:HD22	1.95	0.49
8:V:110:VAL:O	8:V:121:LYS:HA	2.12	0.49
10:X:18:LEU:HD12	10:X:175:GLY:HA3	1.94	0.49
11:Y:110:LYS:O	11:Y:112:LYS:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:3:ILE:O	11:Y:4:LEU:HD23	2.11	0.49
9:I:131:SER:O	9:I:135:MET:HB2	2.11	0.49
12:L:110:PRO:O	12:L:111:THR:HG23	2.12	0.49
4:R:31:THR:HB	4:R:63:LYS:HZ3	1.76	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
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
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
3:C:188:ASP:N	3:C:188:ASP:OD1	2.45	0.49
5:E:33:LEU:H	5:E:33:LEU:HD12	1.76	0.49
7:G:35:THR:CG2	7:G:167:GLY:H	2.26	0.49
9:I:3:ILE:HD12	9:I:44:ALA:CB	2.42	0.49
11:K:4:LEU:HD22	11:K:131:ALA:HB2	1.95	0.49
4:R:174:PHE:CZ	4:R:178:ASN:ND2	2.80	0.49
9:W:131:SER:O	9:W:135:MET:HB2	2.13	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
6:F:144:LEU:C	6:F:145:LEU:HD12	2.32	0.49
6:F:24:TYR:N	6:F:24:TYR:CD1	2.81	0.49
2:P:243:ILE:O	2:P:245:ASP:N	2.45	0.49
3:Q:175:LEU:HD13	3:Q:196:THR:HA	1.94	0.49
8:V:190:PRO:HA	8:V:193:TYR:CE2	2.48	0.49
8:V:36:ARG:HB2	8:V:42:TRP:CE2	2.47	0.49
8:V:74:SER:HB3	8:V:77:THR:OG1	2.12	0.49
11:Y:95:ARG:HB3	11:Y:95:ARG:CZ	2.43	0.49
12:Z:15:ALA:HB1	12:Z:161:ILE:HG13	1.94	0.49
2:B:160:LYS:HD3	2:B:179:TRP:CH2	2.47	0.49
3:C:70:ASN:ND2	3:C:71:ASP:N	2.60	0.49
4:D:163:THR:HG21	4:D:171:VAL:CG2	2.42	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
10:J:51:VAL:HG12	10:J:52:THR:N	2.26	0.49
13:M:117:ASP:OD2	13:M:119:VAL:HG22	2.12	0.49
1:O:248:ILE:HG22	1:O:251:GLN:OE1	2.13	0.49
8:V:126:ILE:HD12	8:V:134:ILE:CG1	2.41	0.49
1:A:133:TYR:O	1:A:134:MET:HB3	2.12	0.49
3:C:73:ILE:HG12	3:C:108:VAL:HG22	1.94	0.49
11:Y:70:GLU:O	11:Y:71:ASP:HB3	2.12	0.49
1:A:131:ARG:HH11	1:A:131:ARG:HG2	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:2:PHE:HD1	6:F:3:ARG:HG2	1.75	0.49
11:K:34:THR:CG2	11:K:35:ARG:N	2.75	0.49
12:L:206:SER:O	12:L:207:PHE:HB2	2.13	0.49
14:N:81:PRO:HD2	14:N:112:GLN:OE1	2.13	0.49
1:O:117:LEU:O	1:O:121:MET:HG2	2.13	0.49
2:P:44:VAL:CA	2:P:213:ILE:HG22	2.42	0.49
2:B:156:TYR:HD1	2:B:156:TYR:O	1.95	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
8:H:8:PHE:HE2	8:H:148:LYS:CA	2.21	0.48
9:I:48:THR:O	9:I:51:ASP:HB2	2.13	0.48
2:P:196:LEU:O	2:P:200:VAL:HG23	2.13	0.48
2:P:44:VAL:HG23	2:P:213:ILE:HG22	1.95	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
1:A:162:TYR:CD1	1:A:162:TYR:C	2.86	0.48
3:C:140:TYR:CD1	3:C:140:TYR:C	2.87	0.48
3:C:198:SER:OG	3:C:199:LYS:N	2.47	0.48
4:D:28:LYS:O	4:D:166:ARG:HB3	2.13	0.48
4:D:174:PHE:CZ	4:D:178:ASN:ND2	2.81	0.48
6:F:36:VAL:CG2	6:F:160:ALA:HB2	2.43	0.48
11:K:119:ASP:OD2	11:K:123:THR:HB	2.12	0.48
12:L:38:ASN:HB2	12:L:39:PRO:HD2	1.95	0.48
1:O:220:LYS:O	1:O:220:LYS:NZ	2.41	0.48
3:Q:188:ASP:OD1	3:Q:188:ASP:N	2.46	0.48
4:R:201:GLU:O	4:R:204:GLN:NE2	2.45	0.48
9:W:153:LYS:HD3	9:W:153:LYS:C	2.33	0.48
2:B:16:GLY:HA3	3:C:28:SER:HB2	1.96	0.48
8:H:80:SER:O	8:H:83:LYS:HB3	2.14	0.48
12:L:15:ALA:HB1	12:L:161:ILE:HG13	1.96	0.48
7:U:246:ILE:HG23	7:U:246:ILE:O	2.11	0.48
8:V:131:SER:O	8:V:134:ILE:HG12	2.13	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
10:X:15:ALA:HB2	10:X:178:VAL:HG13	1.95	0.48
1:A:124:LEU:HD23	1:A:127:ILE:HD12	1.94	0.48
4:D:36:VAL:HG13	4:D:195:THR:HG23	1.94	0.48
5:E:142:LEU:HB2	5:E:158:ALA:CB	2.41	0.48
6:F:171:TYR:CD2	6:F:171:TYR:C	2.87	0.48
9:I:220:ILE:HG22	9:I:221:CYS:N	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:95:ARG:HB3	11:K:95:ARG:CZ	2.43	0.48
14:N:45:ILE:CG2	14:N:52:MET:HG3	2.43	0.48
14:N:84:ILE:HG13	14:N:84:ILE:H	1.46	0.48
3:Q:39:MET:HE1	3:Q:146:TYR:HB3	1.95	0.48
8:V:67:THR:O	8:V:69:GLN:N	2.46	0.48
11:Y:168:GLU:HG2	11:Y:175:PHE:CZ	2.46	0.48
1:A:225:VAL:HG12	1:A:226:GLY:N	2.29	0.48
6:F:185:ASN:ND2	6:F:188:GLU:H	2.11	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
13:M:186:HIS:HD2	13:M:188:GLN:H	1.62	0.48
1:O:91:ARG:HH12	7:U:156:TYR:H	1.61	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: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
2:B:29:LYS:HB3	2:B:29:LYS:NZ	2.29	0.48
4:D:48:ARG:HH11	4:D:48:ARG:HG2	1.77	0.48
5:E:56:SER:HB3	5:E:57:PRO:HD2	1.95	0.48
6:F:197:ILE:HG23	6:F:198:SER:N	2.28	0.48
10:J:18:LEU:HD12	10:J:175:GLY:HA3	1.96	0.48
1:O:144:VAL:O	1:O:145:SER:HB3	2.13	0.48
1:O:220:LYS:O	1:O:221:ASN:HB2	2.12	0.48
2:P:157:PHE:CE2	3:Q:52:VAL:HG11	2.49	0.48
4:R:36:VAL:HG13	4:R:195:THR:HG23	1.95	0.48
7:U:245:GLU:C	7:U:247:ASN:H	2.16	0.48
8:V:143:ARG:HH11	8:V:143:ARG:HB3	1.77	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
2:B:238:LEU:CD1	2:B:238:LEU:N	2.77	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:G:23:VAL:O	7:G:27:VAL:HG23	2.14	0.48
12:L:53:GLN:OE1	13:M:121:SER:HA	2.13	0.48
13:M:43:MET:HG2	13:M:44:SER:N	2.27	0.48
6:T:121:GLN:HE22	7:U:86:HIS:CD2	2.25	0.48
7:U:77:TYR:HB3	7:U:135:THR:HG23	1.96	0.48
7:U:150:LEU:HD11	7:U:154:GLY:CA	2.44	0.48
8:V:55:ILE:O	8:V:59:VAL:HG23	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:75:THR:HG22	8:V:111:TYR:CE1	2.49	0.48
8:V:89:ASN:O	8:V:91:ASP:N	2.47	0.48
1:A:123:ASN:O	1:A:127:ILE:HG13	2.14	0.48
7:G:194:GLN:HA	7:G:194:GLN:NE2	2.28	0.48
2:B:226:GLY:HA3	9:I:186:TYR:O	2.14	0.48
11:K:152:THR:HG23	11:K:155:GLU:OE1	2.14	0.48
2:P:161:ALA:O	3:Q:56:LEU:HD23	2.14	0.48
1:O:179:THR:HG23	2:P:55:LEU:HD12	1.96	0.48
3:Q:37:GLY:HA2	3:Q:45:VAL:O	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
8:H:185:ARG:HG3	8:H:185:ARG:NH1	2.28	0.48
8:H:55:ILE:O	8:H:59:VAL:HG23	2.13	0.48
9:I:175:VAL:HG12	9:I:176:CYS:N	2.28	0.48
14:N:19:LEU:HD11	14:N:26:LEU:HD12	1.95	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
1:O:155:TYR:HD2	1:O:164:VAL:O	1.97	0.48
1:O:73:PHE:N	1:O:73:PHE:CD1	2.80	0.48
2:P:187:ASP:O	2:P:190:HIS:HB3	2.13	0.48
2:P:34:SER:OG	2:P:47:THR:HB	2.14	0.48
4:R:11:PHE:H	5:S:23:GLN:NE2	2.05	0.48
9:W:3:ILE:HG22	9:W:16:ALA:CB	2.44	0.48
10:X:15:ALA:HB2	10:X:178:VAL:HG22	1.96	0.48
12:Z:64:ARG:NH2	12:Z:68:LEU:HD21	2.28	0.48
1:A:128:TYR:HE1	1:A:133:TYR:HH	1.52	0.48
4:D:176:GLU:OE2	5:E:57:PRO:HD2	2.14	0.48
9:I:90:TYR:N	9:I:90:TYR:CD2	2.82	0.48
4:R:233:VAL:O	4:R:237:GLU:HG2	2.13	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
2:B:74:VAL:HG22	2:B:75:TYR:N	2.29	0.47
3:C:175:LEU:HD13	3:C:196:THR:HA	1.96	0.47
3:C:186:VAL:HG13	3:C:187:ASP:N	2.29	0.47
4:D:78:LEU:HD12	4:D:81:ASP:OD2	2.13	0.47
6:F:118:LYS:H	6:F:118:LYS:HD2	1.78	0.47
14:N:3:VAL:HG11	14:N:44:GLY:HA3	1.96	0.47
1:O:25:LEU:HD12	1:O:25:LEU:N	2.29	0.47
2:P:122:THR:O	2:P:124:SER:N	2.47	0.47
3:Q:44:ILE:HD11	3:Q:146:TYR:HB3	1.96	0.47
3:Q:165:VAL:CA	3:Q:169:THR:HG21	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:28:LYS:O	4:R:166:ARG:HB3	2.13	0.47
5:S:178:GLY:HA3	5:S:207:VAL:HG11	1.96	0.47
6:T:133:LEU:C	6:T:134:ILE:HD12	2.34	0.47
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
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
4:D:112:TYR:O	4:D:116:VAL:HG23	2.13	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:F:94:TYR:CE1	6:F:98:VAL:HG21	2.50	0.47
7:G:19:ARG:CG	7:G:19:ARG:HH11	2.27	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
1:O:124:LEU:HD23	1:O:127:ILE:HD12	1.96	0.47
6:T:42:THR:HG22	6:T:218:LYS:NZ	2.29	0.47
1:A:126:GLN:NE2	1:A:127:ILE:HA	2.30	0.47
1:A:144:VAL:HG12	1:A:154:ILE:HG12	1.97	0.47
7:G:24:GLU:O	7:G:27:VAL:HB	2.14	0.47
12:L:16:VAL:O	12:L:175:VAL:HA	2.13	0.47
12:L:199:LYS:O	12:L:202:GLU:HB3	2.15	0.47
14:N:212:ASP:O	14:N:214:ALA:N	2.47	0.47
2:P:224:TYR:OH	2:P:230:ASP:HB3	2.14	0.47
3:Q:114:ARG:HB2	3:Q:114:ARG:HH11	1.79	0.47
6:T:213:ILE:HG22	6:T:214:ALA:N	2.28	0.47
8:H:133:PHE:HA	8:V:133:PHE:HA	1.96	0.47
3:C:185:LYS:HE3	3:C:185:LYS:HB3	1.68	0.47
4:D:163:THR:HG21	4:D:171:VAL:HG23	1.97	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
8:H:4:MET:CB	8:H:126:ILE:HG22	2.44	0.47
8:H:38:HIS:CE1	8:H:67:THR:HG21	2.48	0.47
11:K:87:LEU:HA	11:K:90:SER:HB3	1.96	0.47
1:O:148:GLU:H	1:O:148:GLU:CD	2.17	0.47
2:P:68:THR:C	2:P:70:ASP:H	2.18	0.47
9:W:7:LYS:HB3	9:W:12:VAL:HB	1.97	0.47
9:W:177:VAL:O	9:W:184:ALA:HA	2.14	0.47
9:W:90:TYR:CD2	9:W:90:TYR:N	2.82	0.47
7:G:188:ALA:O	7:G:191:ALA:HB3	2.14	0.47
7:G:194:GLN:NE2	7:G:197:LYS:HZ3	2.12	0.47
8:H:97:ILE:HD12	8:H:98:ILE:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:33:LYS:HD2	10:J:33:LYS:N	2.30	0.47
14:N:167:GLU:HG3	14:N:168:ALA:N	2.30	0.47
2:P:197:LYS:HA	2:P:204:PHE:CZ	2.49	0.47
3:Q:114:ARG:HG3	3:Q:115:LEU:N	2.26	0.47
3:Q:198:SER:OG	3:Q:199:LYS:HG3	2.14	0.47
7:U:19:ARG:HH11	7:U:19:ARG:CG	2.27	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
8:H:138:CYS:HA	8:H:154:PHE:CZ	2.49	0.47
8:H:189:TYR:O	8:H:192:GLU:HB2	2.14	0.47
8:H:89:ASN:O	8:H:91:ASP:N	2.48	0.47
9:I:21:THR:O	9:I:22:GLN:HB2	2.14	0.47
11:K:135:SER:O	11:K:139:THR:HG23	2.13	0.47
13:M:14:LEU:HA	13:M:14:LEU:HD23	1.77	0.47
2:P:211:LEU:CD2	2:P:238:LEU:HD22	2.45	0.47
3:Q:208:TYR:CG	3:Q:209:ASP:N	2.82	0.47
4:R:162:GLN:HG3	4:R:163:THR:N	2.29	0.47
8:V:3:ILE:HG22	8:V:16:ALA:CB	2.45	0.47
2:B:197:LYS:HA	2:B:204:PHE:CZ	2.50	0.47
2:B:64:VAL:HG13	2:B:237:LYS:HE2	1.95	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
6:F:36:VAL:HG22	6:F:160:ALA:HB2	1.95	0.47
7:G:121:ALA:HA	7:G:124:LEU:HD12	1.96	0.47
10:J:29:ASN:O	10:J:30:LYS:HG3	2.14	0.47
14:N:124:LEU:HD23	14:N:125:LEU:H	1.79	0.47
6:T:70:MET:CE	6:T:105:VAL:HG22	2.44	0.47
7:U:108:ILE:N	7:U:108:ILE:HD13	2.30	0.47
1:A:20:SER:OG	1:A:24:ARG:N	2.41	0.47
3:C:198:SER:OG	3:C:199:LYS:HG3	2.14	0.47
8:H:110:VAL:HG12	8:H:122:LEU:O	2.15	0.47
1:O:195:ASN:O	1:O:196:GLU:HB2	2.13	0.47
1:O:216:THR:CG2	1:O:217:GLU:N	2.78	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: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
9:W:90:TYR:HD2	9:W:90:TYR:N	2.13	0.47
10:X:150:GLU:HB2	10:X:153:ASP:OD2	2.14	0.47
4:D:149:GLN:HG2	4:D:150:THR:N	2.30	0.47
4:D:233:VAL:O	4:D:237:GLU:HG2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:118:ILE:HA	11:K:123:THR:O	2.14	0.47
2:P:24:ALA:C	2:P:26:THR:H	2.16	0.47
8:V:107:LYS:CG	8:V:108:GLY:H	2.28	0.47
13:M:213:ASP:HB2	9:W:19:ARG:NH2	2.29	0.47
9:W:21:THR:O	9:W:22:GLN:HB2	2.14	0.47
11:Y:38:SER:CB	11:Y:39:PRO:HD2	2.44	0.47
12:Z:12:ILE:CD1	12:Z:102:CYS:HB3	2.45	0.47
1:A:53:VAL:C	1:A:54:ILE:HD12	2.36	0.47
1:A:60:PRO:HG2	1:A:61:ASP:H	1.80	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
5:S:170:LYS:HD2	5:S:171:ALA:N	2.29	0.47
5:S:27:SER:O	5:S:30:ALA:HB3	2.14	0.47
10:X:49:THR:HB	11:Y:122:GLY:O	2.15	0.47
12:Z:4:LEU:CD1	12:Z:15:ALA:HB3	2.45	0.47
3:C:163:ILE:HG13	3:C:164:SER:H	1.79	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
8:H:153:ASP:HA	8:H:156:LYS:HB2	1.97	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
1:O:156:LYS:HE2	1:O:166:TYR:CE2	2.50	0.47
2:P:218:ASN:HB3	2:P:221:LEU:HD13	1.96	0.47
3:Q:140:TYR:C	3:Q:140:TYR:CD1	2.89	0.47
3:Q:69:LEU:CD2	3:Q:92:ARG:HG3	2.45	0.47
4:R:228:GLU:CA	4:R:231:GLN:HE21	2.24	0.47
5:S:124:GLY:N	5:S:132:ARG:HB2	2.29	0.47
7:U:85:ARG:NH1	7:U:85:ARG:HG2	2.30	0.47
8:V:4:MET:SD	8:V:159:LEU:CD1	3.03	0.47
9:W:10:ASN:C	9:W:180:ILE:HG13	2.35	0.47
11:Y:3:ILE:HD12	11:Y:44:SER:HB2	1.96	0.47
2:B:224:TYR:OH	2:B:230:ASP:HB3	2.14	0.46
2:B:64:VAL:CG1	2:B:237:LYS:HE2	2.45	0.46
6:F:146:GLU:O	6:F:153:VAL:HA	2.15	0.46
5:E:165:TYR:CE1	6:F:53:ALA:HB2	2.50	0.46
11:K:18:LYS:HD3	11:K:179:ILE:HG13	1.96	0.46
13:M:59:PHE:O	13:M:62:SER:N	2.48	0.46
3:Q:185:LYS:HD2	3:Q:186:VAL:H	1.79	0.46
4:R:57:THR:OG1	4:R:58:ARG:N	2.48	0.46
5:S:39:GLY:O	5:S:169:ALA:HA	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:35:THR:CG2	7:U:167:GLY:H	2.28	0.46
7:U:49:VAL:HG22	7:U:50:GLU:N	2.29	0.46
5:E:136:ARG:HB2	5:E:137:PRO:CD	2.39	0.46
5:E:237:ALA:O	5:E:240:ILE:HB	2.16	0.46
6:F:54:ASP:CG	6:F:55:GLU:H	2.19	0.46
11:K:22:ARG:HB2	11:K:27:LEU:HD11	1.97	0.46
2:P:189:ILE:O	2:P:193:LEU:HD12	2.15	0.46
3:Q:129:ARG:HG3	3:Q:129:ARG:O	2.14	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
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
7:G:142:LYS:HG3	8:H:105:LYS:NZ	2.31	0.46
7:G:169:GLN:H	7:G:169:GLN:CD	2.18	0.46
9:I:90:TYR:N	9:I:90:TYR:HD2	2.13	0.46
11:K:52:THR:HG23	11:K:53:VAL:N	2.26	0.46
11:K:88:ALA:O	11:K:91:ILE:HG22	2.15	0.46
1:O:120:ARG:HA	1:O:123:ASN:HB2	1.98	0.46
2:P:193:LEU:O	2:P:197:LYS:N	2.48	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
1:A:220:LYS:O	1:A:221:ASN:HB2	2.15	0.46
3:C:107:PRO:HB2	3:C:110:ILE:HD12	1.97	0.46
3:C:114:ARG:HG3	3:C:115:LEU:N	2.27	0.46
4:D:181:ARG:HH22	5:E:60:GLU:HG2	1.80	0.46
6:F:126:ARG:NH1	6:F:127:PRO:O	2.49	0.46
8:H:102:TYR:HA	8:H:108:GLY:HA2	1.97	0.46
11:K:168:GLU:HG2	11:K:175:PHE:CZ	2.48	0.46
11:K:3:ILE:CD1	11:K:16:SER:HB3	2.45	0.46
11:K:8:VAL:HG23	11:K:9:GLN:H	1.80	0.46
1:O:117:LEU:HD12	1:O:121:MET:HG2	1.97	0.46
1:O:123:ASN:ND2	2:P:84:VAL:HG12	2.30	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
5:S:165:TYR:HE2	6:T:60:GLN:HB2	1.79	0.46
7:U:106:ILE:HA	7:U:107:PRO:HD3	1.81	0.46
7:U:77:TYR:CD2	7:U:77:TYR:N	2.83	0.46
8:V:9:LYS:HG3	8:V:145:ASN:OD1	2.16	0.46
2:B:112:SER:HA	2:B:156:TYR:CE2	2.50	0.46
6:F:164:ARG:HH22	6:F:202:ARG:HB3	1.80	0.46
7:G:193:LYS:HE2	7:G:193:LYS:HB3	1.73	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:R:159:TRP:CZ2	5:S:59:LEU:HD23	2.50	0.46
6:T:111:LEU:O	6:T:115:LYS:HB2	2.15	0.46
6:T:216:VAL:HB	6:T:222:PHE:HD2	1.80	0.46
10:X:90:ARG:O	10:X:90:ARG:HG3	2.16	0.46
11:Y:152:THR:OG1	11:Y:155:GLU:HG3	2.15	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:B:74:VAL:HG22	2:B:75:TYR:H	1.79	0.46
4:D:31:THR:HB	4:D:63:LYS:HZ1	1.80	0.46
10:J:117:LEU:N	10:J:117:LEU:HD23	2.30	0.46
1:O:131:ARG:NH1	1:O:133:TYR:HB3	2.30	0.46
2:P:12:PHE:HE2	3:Q:130:PRO:HG2	1.80	0.46
3:Q:185:LYS:HD2	3:Q:186:VAL:N	2.31	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:P:226:GLY:HA3	9:W:186:TYR:O	2.15	0.46
2:B:161:ALA:O	3:C:56:LEU:HD23	2.16	0.46
3:C:185:LYS:HD2	3:C:186:VAL:H	1.80	0.46
7:G:204:GLU:HG3	7:G:207:LYS:HE2	1.98	0.46
8:H:138:CYS:HA	8:H:154:PHE:CE1	2.50	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
13:M:137:ILE:HG23	13:M:178:SER:HB3	1.98	0.46
13:M:190:GLY:O	13:M:191:ASP:HB2	2.14	0.46
14:N:133:THR:O	14:N:134:LEU:HD23	2.15	0.46
4:R:221:ILE:O	4:R:222:VAL:HB	2.15	0.46
5:S:225:GLN:HA	5:S:225:GLN:NE2	2.30	0.46
7:U:169:GLN:HA	7:U:172:LYS:HB2	1.96	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
12:Z:36:GLU:HA	12:Z:42:LEU:HD23	1.98	0.46
3:C:77:VAL:CG1	3:C:78:ALA:N	2.79	0.46
3:C:89:ASN:O	3:C:93:ILE:HG13	2.15	0.46
7:G:197:LYS:CG	7:G:201:LEU:HD21	2.46	0.46
8:H:188:PHE:N	8:H:188:PHE:CD2	2.84	0.46
10:J:37:TYR:O	10:J:40:VAL:HG23	2.16	0.46
11:K:-1:MET:HG2	11:K:1:ASP:H	1.81	0.46
13:M:51:ASP:OD2	13:M:96:TYR:HA	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:146:VAL:HA	1:O:151:GLY:O	2.14	0.46
1:O:68:THR:HG21	7:U:158:GLY:CA	2.42	0.46
9:W:72:ARG:CG	9:W:72:ARG:HH11	2.27	0.46
1:A:54:ILE:HG13	1:A:225:VAL:CG2	2.46	0.46
12:L:98:GLY:O	12:L:99:THR:HB	2.15	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
3:Q:68:LYS:NZ	10:X:66:LYS:NZ	2.64	0.46
5:S:240:ILE:O	5:S:243:LEU:HB3	2.16	0.46
5:S:244:LYS:O	5:S:244:LYS:HG2	2.14	0.46
11:Y:190:GLN:C	11:Y:192:ASP:H	2.18	0.46
12:Z:199:LYS:O	12:Z:202:GLU:HB3	2.16	0.46
3:C:59:GLN:N	3:C:59:GLN:NE2	2.64	0.46
6:F:40:SER:HA	6:F:180:ILE:HD12	1.97	0.46
9:I:3:ILE:HD12	9:I:44:ALA:HB3	1.98	0.46
11:K:22:ARG:O	11:K:24:ILE:N	2.48	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
2:P:200:VAL:HG12	2:P:201:GLU:N	2.31	0.46
3:Q:39:MET:CE	3:Q:146:TYR:HB3	2.46	0.46
12:Z:85:ASN:O	12:Z:89:GLN:HG2	2.15	0.46
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
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
8:H:82:PHE:HB2	8:H:113:ILE:CD1	2.46	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:133:ALA:O	13:M:134:ALA:C	2.54	0.45
13:M:59:PHE:HA	13:M:62:SER:OG	2.15	0.45
5:S:56:SER:HB3	5:S:57:PRO:HD2	1.97	0.45
7:U:47:PHE:CE1	7:U:137:PHE:HA	2.52	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
8:V:6:VAL:C	8:V:12:VAL:HG23	2.36	0.45
1:A:207:ILE:HD12	1:A:248:ILE:HD11	1.98	0.45
2:B:189:ILE:O	2:B:193:LEU:HD12	2.15	0.45
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:246:ILE:HG23	7:G:246:ILE:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
9:I:45:GLY:HA2	9:I:98:LEU:HB3	1.98	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
14:N:62:LEU:C	14:N:62:LEU:HD23	2.36	0.45
2:P:70:ASP:C	2:P:71:ILE:HG13	2.36	0.45
3:Q:231:LYS:HA	3:Q:231:LYS:HE3	1.97	0.45
3:Q:235:ILE:C	3:Q:237:ASP:N	2.70	0.45
4:R:45:GLY:C	4:R:46:CYS:SG	2.94	0.45
7:U:150:LEU:HD11	7:U:154:GLY:C	2.36	0.45
1:A:120:ARG:HA	1:A:123:ASN:HB2	1.99	0.45
5:E:225:GLN:HA	5:E:225:GLN:NE2	2.30	0.45
5:E:37:ALA:HA	5:E:50:VAL:HG12	1.97	0.45
6:F:111:LEU:O	6:F:115:LYS:HB2	2.16	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
13:M:166:LEU:H	13:M:166:LEU:HD12	1.82	0.45
14:N:198:LEU:HD23	14:N:199:THR:N	2.31	0.45
11:Y:22:ARG:HB2	11:Y:27:LEU:HD11	1.97	0.45
12:Z:105:THR:HG21	12:Z:108:GLU:OE1	2.16	0.45
3:C:142:ASP:OD2	3:C:142:ASP:N	2.49	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
13:M:11:PHE:N	13:M:11:PHE:CD1	2.85	0.45
14:N:55:ILE:O	14:N:58:LEU:N	2.50	0.45
1:O:243:GLU:O	1:O:243:GLU:HG2	2.16	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
3:Q:106:ILE:HA	3:Q:107:PRO:HD3	1.85	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
8:V:124:TYR:CD1	8:V:124:TYR:N	2.85	0.45
11:Y:3:ILE:HD13	11:Y:16:SER:HB3	1.97	0.45
11:Y:52:THR:HG23	11:Y:53:VAL:N	2.27	0.45
11:Y:7:ARG:NH1	11:Y:7:ARG:HG2	2.30	0.45
1:A:54:ILE:HG13	1:A:225:VAL:HG21	1.97	0.45
1:A:83:VAL:HG13	1:A:140:ILE:O	2.16	0.45
2:B:157:PHE:CE2	3:C:52:VAL:HG11	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:91:ALA:HB2	3:C:115:LEU:HD21	1.98	0.45
6:F:33:SER:HB3	6:F:62:LYS:HZ3	1.79	0.45
7:G:150:LEU:HD11	7:G:154:GLY:CA	2.47	0.45
1:O:155:TYR:HD2	1:O:165:GLY:HA2	1.81	0.45
1:O:76:SER:HB3	1:O:79:ILE:HD13	1.97	0.45
3:Q:119:LYS:HD2	3:Q:153:PRO:HA	1.98	0.45
3:Q:150:THR:O	3:Q:157:TYR:HA	2.15	0.45
7:U:140:VAL:HG12	7:U:141:ASP:H	1.82	0.45
7:U:201:LEU:N	7:U:201:LEU:CD1	2.79	0.45
8:V:138:CYS:O	8:V:154:PHE:HZ	1.99	0.45
10:X:136:GLN:N	10:X:136:GLN:OE1	2.48	0.45
10:X:149:LEU:HD12	10:X:154:LEU:HA	1.98	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
12:L:122:LEU:HA	12:L:122:LEU:HD23	1.66	0.45
13:M:80:ALA:O	13:M:83:ASN:HB3	2.17	0.45
14:N:63:VAL:HG12	14:N:64:THR:N	2.32	0.45
1:O:243:GLU:O	1:O:246:VAL:HB	2.17	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
3:Q:228:LYS:HB3	3:Q:230:PHE:HE1	1.81	0.45
3:Q:70:ASN:HB3	3:Q:73:ILE:HB	1.97	0.45
4:R:37:LYS:HD3	4:R:147:LEU:HB2	1.99	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
10:X:177:VAL:HG21	10:X:188:LYS:HE2	1.98	0.45
12:Z:206:SER:O	12:Z:207:PHE:HB2	2.17	0.45
3:C:129:ARG:HG3	3:C:129:ARG:O	2.17	0.45
3:C:185:LYS:HD2	3:C:186:VAL:N	2.32	0.45
3:C:211:LEU:HD13	3:C:212:GLU:N	2.32	0.45
7:G:170:SER:O	7:G:174:GLU:HG2	2.17	0.45
8:H:1:THR:O	8:H:129:SER:HB3	2.17	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
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
14:N:8:TYR:O	14:N:117:GLN:NE2	2.49	0.45
1:O:167:LYS:HZ2	1:O:192:ASP:HB2	1.82	0.45
2:P:229:THR:O	2:P:231:LYS:NZ	2.49	0.45
2:P:75:TYR:CD2	2:P:76:SER:N	2.84	0.45
11:Y:119:ASP:OD2	11:Y:123:THR:HB	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:C:94:HIS:CD2	3:C:114:ARG:HD2	2.51	0.45
7:G:197:LYS:O	7:G:201:LEU:HD13	2.17	0.45
11:K:49:ALA:O	11:K:52:THR:HG22	2.17	0.45
12:L:54:PHE:C	12:L:54:PHE:HD2	2.20	0.45
14:N:192:ILE:HD12	14:N:192:ILE:N	2.32	0.45
1:O:43:LEU:HD22	1:O:54:ILE:HB	1.99	0.45
3:Q:13:PHE:H	4:R:19:GLN:HE22	1.64	0.45
8:V:186:LEU:HD22	8:V:188:PHE:CE2	2.52	0.45
8:V:190:PRO:O	8:V:192:GLU:N	2.50	0.45
2:B:44:VAL:HG23	2:B:213:ILE:HG22	1.99	0.45
4:D:228:GLU:CA	4:D:231:GLN:HE21	2.23	0.45
6:F:176:LEU:O	6:F:178:THR:N	2.50	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
14:N:102:LEU:N	14:N:102:LEU:HD12	2.31	0.45
2:P:44:VAL:CG2	2:P:211:LEU:HD11	2.47	0.45
13:M:187:ILE:CD1	9:W:24:PRO:HA	2.44	0.45
10:X:66:LYS:HA	10:X:71:ARG:O	2.17	0.45
12:Z:12:ILE:HG22	12:Z:13:ILE:N	2.32	0.45
2:B:75:TYR:CD2	2:B:76:SER:N	2.85	0.45
10:J:150:GLU:HB2	10:J:153:ASP:OD2	2.17	0.45
10:J:80:GLN:O	10:J:83:SER:HB3	2.16	0.45
11:K:190:GLN:C	11:K:192:ASP:H	2.20	0.45
1:O:114:CYS:O	1:O:116:VAL:N	2.50	0.45
1:O:176:GLN:HA	1:O:179:THR:HB	1.98	0.45
1:O:45:VAL:HG23	1:O:52:VAL:HG23	1.99	0.45
4:R:227:GLU:O	4:R:231:GLN:HG3	2.17	0.45
5:S:51:GLU:OE2	5:S:53:ARG:HB2	2.17	0.45
7:U:116:GLY:O	7:U:120:GLN:HB2	2.17	0.45
7:U:137:PHE:CD2	7:U:137:PHE:N	2.85	0.45
7:U:194:GLN:NE2	7:U:194:GLN:HA	2.32	0.45
9:W:128:GLY:O	9:W:131:SER:HB2	2.17	0.45
11:K:137:PHE:HB3	12:Z:134:THR:OG1	2.16	0.45
1:A:145:SER:HA	1:A:228:ALA:HB1	1.99	0.44
4:D:212:ILE:CG2	4:D:224:LEU:HD22	2.47	0.44
4:D:57:THR:OG1	4:D:58:ARG:N	2.51	0.44
7:G:98:PHE:HD1	7:G:98:PHE:C	2.19	0.44
8:H:190:PRO:C	8:H:192:GLU:H	2.20	0.44
8:H:95:ALA:H	8:H:115:LEU:HD13	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:15:ALA:CB	10:J:178:VAL:HG22	2.47	0.44
2:P:157:PHE:CD1	2:P:157:PHE:N	2.85	0.44
3:Q:185:LYS:HB3	3:Q:185:LYS:HE3	1.64	0.44
7:U:129:ARG:HA	7:U:130:PRO:HD3	1.82	0.44
7:U:21:PHE:HA	7:U:24:GLU:HG3	2.00	0.44
8:V:4:MET:SD	8:V:159:LEU:HD11	2.57	0.44
14:N:218:LYS:HA	8:V:32:ASP:OD1	2.18	0.44
10:X:29:ASN:ND2	10:X:29:ASN:N	2.64	0.44
1:A:124:LEU:HA	1:A:124:LEU:HD23	1.88	0.44
1:A:144:VAL:O	1:A:145:SER:HB3	2.17	0.44
1:A:16:ILE:CG2	1:A:17:THR:H	2.29	0.44
2:B:36:GLY:HA2	2:B:44:VAL:O	2.18	0.44
5:E:124:GLY:N	5:E:132:ARG:HB2	2.30	0.44
7:G:84:GLY:O	7:G:88:VAL:HG23	2.17	0.44
14:N:203:ASN:C	14:N:204:LEU:HD13	2.37	0.44
3:Q:198:SER:OG	3:Q:199:LYS:N	2.49	0.44
5:S:133:LEU:HD22	5:S:133:LEU:H	1.82	0.44
6:T:48:ALA:HB1	6:T:62:LYS:HG3	1.99	0.44
1:O:135:ARG:HD3	7:U:12:SER:O	2.18	0.44
11:Y:54:GLN:HG3	12:Z:88:TYR:CE2	2.53	0.44
12:Z:122:LEU:HA	12:Z:122:LEU:HD23	1.62	0.44
1:A:64:LEU:HD23	7:G:159:TYR:CD2	2.52	0.44
3:C:163:ILE:CG1	3:C:164:SER:N	2.81	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
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
6:F:62:LYS:O	6:F:73:SER:HA	2.17	0.44
8:H:189:TYR:HA	8:H:190:PRO:HD3	1.83	0.44
12:L:4:LEU:HA	12:L:100:MET:CE	2.47	0.44
13:M:141:LEU:O	13:M:145:VAL:HB	2.17	0.44
1:O:128:TYR:HE1	1:O:133:TYR:HH	1.58	0.44
4:R:37:LYS:HG2	4:R:160:SER:O	2.17	0.44
10:X:101:ALA:HA	10:X:111:PHE:O	2.17	0.44
1:A:117:LEU:HD12	1:A:121:MET:HG2	1.99	0.44
5:E:26:TYR:O	5:E:29:GLU:N	2.50	0.44
6:F:190:ILE:O	6:F:194:VAL:HG23	2.17	0.44
6:F:218:LYS:HB2	6:F:218:LYS:HE3	1.72	0.44
6:F:54:ASP:CG	6:F:55:GLU:N	2.71	0.44
8:H:107:LYS:CG	8:H:108:GLY:H	2.29	0.44
8:H:147:SER:OG	8:H:150:GLU:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:163:ILE:HD12	8:H:170:GLY:HA2	1.98	0.44
9:I:59:ILE:HG12	9:I:83:LEU:CD2	2.46	0.44
12:L:208:ASN:O	12:L:210:VAL:N	2.51	0.44
2:P:57:MET:HB2	2:P:59:GLU:OE2	2.17	0.44
7:U:171:ALA:HA	7:U:174:GLU:HB2	1.99	0.44
7:U:240:ASP:HA	7:U:243:GLN:HB2	1.98	0.44
9:W:6:VAL:HG12	9:W:124:TYR:CB	2.36	0.44
9:W:81:GLN:O	9:W:85:GLN:HG3	2.18	0.44
10:X:127:PHE:O	10:X:128:ILE:HD13	2.18	0.44
3:C:70:ASN:HB3	3:C:73:ILE:HB	1.99	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
10:J:3:VAL:CG2	10:J:16:CYS:HB3	2.46	0.44
11:K:160:LEU:O	11:K:164:VAL:HG23	2.18	0.44
12:L:149:SER:HB2	12:L:152:ASP:CG	2.37	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
6:T:26:LEU:O	6:T:29:ILE:HB	2.17	0.44
7:U:204:GLU:HG3	7:U:207:LYS:HE2	1.98	0.44
8:V:138:CYS:HA	8:V:154:PHE:CE1	2.53	0.44
8:V:34:LEU:CD2	8:V:44:CYS:HB3	2.48	0.44
2:B:174:PHE:HD2	2:B:195:THR:HG1	1.65	0.44
2:B:239:THR:O	2:B:243:ILE:HG13	2.18	0.44
2:B:73:ALA:HB2	2:B:136:ILE:HG23	1.99	0.44
6:F:42:THR:HG23	6:F:183:ASP:HB3	2.00	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
8:H:36:ARG:HB2	8:H:42:TRP:CZ2	2.53	0.44
11:K:164:VAL:HA	11:K:167:LEU:HD12	1.99	0.44
11:K:6:ILE:HG23	11:K:13:ILE:HB	2.00	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
1:O:33:LYS:CD	1:O:33:LYS:H	2.23	0.44
8:V:138:CYS:HA	8:V:154:PHE:CZ	2.51	0.44
8:V:67:THR:C	8:V:69:GLN:H	2.21	0.44
12:Z:149:SER:HB2	12:Z:152:ASP:CG	2.38	0.44
1:A:128:TYR:HA	1:A:133:TYR:HE1	1.82	0.44
2:B:162:THR:OG1	2:B:163:ALA:N	2.50	0.44
2:B:32:VAL:HG12	2:B:33:THR:N	2.33	0.44
8:H:131:SER:O	8:H:134:ILE:HG12	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:6:VAL:O	8:H:12:VAL:HG23	2.17	0.44
10:J:101:ALA:HA	10:J:111:PHE:O	2.18	0.44
14:N:189:LEU:HD23	14:N:189:LEU:C	2.38	0.44
14:N:96:ARG:HG3	14:N:97:SER:N	2.33	0.44
1:O:181:ASN:N	1:O:181:ASN:ND2	2.65	0.44
2:P:66:LEU:HD13	2:P:235:PHE:CG	2.53	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
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
8:V:1:THR:HA	8:V:33:LYS:HZ3	1.81	0.44
11:Y:49:ALA:O	11:Y:52:THR:HG22	2.17	0.44
12:Z:8:PHE:HA	12:Z:146:TRP:CE3	2.53	0.44
1:A:52:VAL:HG12	1:A:227:VAL:HG22	1.99	0.44
1:A:204:GLU:HB3	1:A:248:ILE:HG23	1.99	0.44
1:A:50:CYS:HA	1:A:228:ALA:O	2.17	0.44
5:E:81:LEU:HA	5:E:81:LEU:HD12	1.64	0.44
6:F:227:GLY:O	6:F:229:ALA:N	2.51	0.44
7:G:25:TYR:HA	7:G:28:LYS:HB2	2.00	0.44
10:J:42:LEU:HD12	10:J:99:VAL:O	2.18	0.44
1:O:18:ILE:CD1	1:O:18:ILE:N	2.81	0.44
3:Q:230:PHE:N	3:Q:230:PHE:CD1	2.86	0.44
3:Q:27:GLU:O	3:Q:29:ILE:N	2.51	0.44
4:R:149:GLN:HG2	4:R:150:THR:N	2.33	0.44
5:S:165:TYR:CE2	6:T:60:GLN:HB2	2.53	0.44
6:T:185:ASN:HA	6:T:186:PRO:HD2	1.79	0.44
11:Y:8:VAL:HG23	11:Y:9:GLN:N	2.33	0.44
12:Z:208:ASN:O	12:Z:210:VAL:N	2.51	0.44
1:A:106:TYR:HB2	8:H:61:TYR:HD2	1.82	0.44
1:A:218:PHE:CD2	1:A:223:LEU:HD11	2.52	0.44
1:A:77:ARG:HA	1:A:77:ARG:HE	1.83	0.44
2:B:122:THR:HG22	2:B:123:GLN:N	2.33	0.44
2:B:43:VAL:O	2:B:213:ILE:HB	2.17	0.44
13:M:46:ASN:C	13:M:98:VAL:HG12	2.38	0.44
2:P:38:LYS:HA	2:P:43:VAL:HG13	2.00	0.44
6:T:63:ILE:O	6:T:64:ILE:HG13	2.17	0.44
6:T:62:LYS:O	6:T:73:SER:HA	2.18	0.44
8:V:126:ILE:HD12	8:V:134:ILE:CD1	2.48	0.44
10:X:56:GLU:H	10:X:56:GLU:HG2	1.60	0.44
1:A:35:THR:OG1	1:A:36:ASN:N	2.51	0.43
3:C:39:MET:HE1	3:C:146:TYR:CB	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:165:TYR:CE2	6:F:60:GLN:HB2	2.52	0.43
5:E:22:PHE:N	5:E:22:PHE:CD2	2.85	0.43
7:G:150:LEU:HD13	7:G:156:TYR:HB3	2.00	0.43
9:I:191:LEU:HB3	9:I:193:PRO:HD3	1.99	0.43
12:L:182:GLU:HG3	12:L:182:GLU:O	2.17	0.43
13:M:114:TYR:CD2	13:M:124:ARG:HA	2.53	0.43
2:P:197:LYS:HA	2:P:197:LYS:HE3	2.00	0.43
3:Q:186:VAL:HG13	3:Q:187:ASP:N	2.32	0.43
4:R:181:ARG:NH2	5:S:60:GLU:HG2	2.32	0.43
6:T:123:TYR:CG	6:T:124:GLY:N	2.85	0.43
6:T:217:GLY:O	6:T:219:ASP:N	2.51	0.43
7:U:94:GLU:CG	7:U:114:ARG:HH11	2.31	0.43
8:V:188:PHE:CD2	8:V:188:PHE:N	2.86	0.43
11:Y:4:LEU:HD22	11:Y:131:ALA:HB2	1.99	0.43
11:Y:164:VAL:HA	11:Y:167:LEU:HD12	2.00	0.43
2:B:180:ASN:O	2:B:183:LEU:HG	2.17	0.43
3:C:150:THR:O	3:C:157:TYR:HA	2.17	0.43
3:C:230:PHE:CD1	3:C:230:PHE:N	2.86	0.43
5:E:114:GLN:HG3	5:E:118:ASP:OD1	2.18	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
8:H:190:PRO:C	8:H:192:GLU:N	2.71	0.43
1:A:108:TYR:O	9:I:78:SER:HA	2.18	0.43
12:L:25:TRP:CZ3	13:M:135:SER:HA	2.53	0.43
13:M:170:GLU:OE1	13:M:170:GLU:HA	2.18	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
4:R:162:GLN:HE21	4:R:163:THR:N	2.06	0.43
5:S:241:LYS:C	5:S:243:LEU:N	2.70	0.43
6:T:118:LYS:HD2	6:T:118:LYS:H	1.82	0.43
6:T:185:ASN:ND2	6:T:185:ASN:C	2.68	0.43
8:V:80:SER:O	8:V:83:LYS:HB3	2.18	0.43
10:X:6:MET:HE3	10:X:145:TYR:HD1	1.83	0.43
11:Y:-1:MET:HG2	11:Y:1:ASP:H	1.83	0.43
4:D:11:PHE:H	5:E:23:GLN:NE2	2.14	0.43
4:D:155:ILE:HD12	4:D:155:ILE:C	2.39	0.43
4:D:37:LYS:HD3	4:D:147:LEU:HB2	1.99	0.43
5:E:205:LYS:HB2	5:E:212:LEU:HD13	2.00	0.43
5:E:244:LYS:O	5:E:244:LYS:HG2	2.19	0.43
5:E:78:MET:HA	5:E:142:LEU:HD23	2.00	0.43
6:F:160:ALA:O	6:F:169:LYS:HE3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
7:G:171:ALA:HA	7:G:174:GLU:HB2	2.00	0.43
12:L:4:LEU:HD12	12:L:161:ILE:HD11	2.00	0.43
14:N:153:ARG:CG	14:N:153:ARG:NH1	2.81	0.43
2:P:74:VAL:HG22	2:P:75:TYR:H	1.83	0.43
7:U:63:ASN:HD22	7:U:63:ASN:H	1.66	0.43
3:C:163:ILE:HD12	3:C:173:GLN:OE1	2.18	0.43
4:D:39:LYS:HB2	4:D:39:LYS:HE2	1.83	0.43
8:H:3:ILE:HG22	8:H:16:ALA:HB2	2.00	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:201:LYS:O	14:N:204:LEU:HD11	2.18	0.43
14:N:51:ASP:O	14:N:54:HIS:HB3	2.18	0.43
14:N:-6:GLN:HG3	14:N:-5:PRO:N	2.32	0.43
1:O:236:LEU:HA	1:O:236:LEU:HD23	1.85	0.43
6:T:176:LEU:O	6:T:178:THR:N	2.51	0.43
8:V:102:TYR:HA	8:V:108:GLY:HA2	2.01	0.43
2:P:90:ARG:NH1	9:W:68:LEU:HB3	2.33	0.43
12:Z:76:VAL:HG23	12:Z:105:THR:HG22	1.99	0.43
1:A:89:ASP:OD2	1:A:137:LEU:HA	2.18	0.43
1:A:18:ILE:HB	2:B:20:GLN:NE2	2.34	0.43
1:A:167:LYS:HG2	2:B:55:LEU:O	2.19	0.43
4:D:50:SER:HA	4:D:53:LYS:HD3	2.00	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
14:N:49:ILE:CG2	14:N:53:GLN:HE21	2.23	0.43
10:X:33:LYS:HD2	10:X:33:LYS:N	2.33	0.43
11:Y:54:GLN:HA	11:Y:54:GLN:OE1	2.18	0.43
12:Z:1:THR:HG22	12:Z:2:THR:N	2.34	0.43
5:E:42:THR:C	5:E:44:GLU:H	2.20	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:34:SER:O	2:P:163:ALA:HA	2.18	0.43
2:P:67:LEU:N	2:P:67:LEU:HD23	2.55	0.43
3:Q:39:MET:HE1	3:Q:146:TYR:CB	2.49	0.43
5:S:37:ALA:HA	5:S:50:VAL:HG12	2.01	0.43
7:U:201:LEU:N	7:U:201:LEU:HD13	2.32	0.43
7:U:24:GLU:H	7:U:24:GLU:HG2	1.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:3:ILE:HD12	9:W:44:ALA:HB3	2.00	0.43
10:X:151:PRO:HG2	10:X:152:GLU:OE2	2.18	0.43
12:Z:4:LEU:HD12	12:Z:161:ILE:CD1	2.49	0.43
1:A:83:VAL:CG1	1:A:139:VAL:HB	2.48	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
5:E:241:LYS:C	5:E:243:LEU:N	2.71	0.43
6:F:42:THR:HG22	6:F:218:LYS:NZ	2.33	0.43
7:G:121:ALA:C	7:G:123:THR:H	2.21	0.43
11:K:-1:MET:SD	11:K:133:GLY:CA	3.05	0.43
11:K:70:GLU:HA	11:K:70:GLU:OE1	2.18	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
14:N:-3:VAL:HA	14:N:21:SER:O	2.18	0.43
1:O:169:THR:OG1	1:O:170:ALA:N	2.52	0.43
4:R:109:LEU:C	4:R:109:LEU:HD13	2.39	0.43
4:R:207:ALA:HB2	4:R:233:VAL:HG21	2.00	0.43
6:T:197:ILE:C	6:T:199:GLN:N	2.72	0.43
7:U:166:LYS:HZ3	7:U:206:ASN:HD21	1.67	0.43
7:U:21:PHE:HD2	7:U:24:GLU:HG3	1.84	0.43
11:Y:76:PRO:HB2	11:Y:114:GLU:OE1	2.19	0.43
2:B:59:GLU:HG3	2:B:59:GLU:H	1.55	0.43
3:C:106:ILE:HA	3:C:107:PRO:HD3	1.85	0.43
4:D:243:GLN:HG2	4:D:243:GLN:O	2.19	0.43
4:D:81:ASP:O	4:D:82:SER:C	2.57	0.43
5:E:21:LEU:O	5:E:24:VAL:HB	2.18	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
11:K:9:GLN:NE2	11:K:150:ASP:HA	2.33	0.43
11:K:3:ILE:CG2	11:K:102:LEU:HG	2.48	0.43
11:K:68:ILE:C	11:K:68:ILE:HD12	2.38	0.43
14:N:144:ASN:O	14:N:148:ARG:HG3	2.18	0.43
1:O:112:MET:HA	1:O:113:PRO:HD3	1.74	0.43
2:P:139:HIS:HD2	2:P:144:GLY:C	2.21	0.43
4:R:39:LYS:HD3	4:R:186:ALA:HA	2.01	0.43
9:W:102:GLY:HA2	9:W:178:MET:SD	2.58	0.43
12:Z:4:LEU:HD11	12:Z:15:ALA:HB3	1.99	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:B:218:ASN:HB3	2:B:221:LEU:HD13	2.00	0.43
2:B:61:LEU:HA	2:B:61:LEU:HD22	1.91	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:119:LYS:HD2	3:C:153:PRO:HA	2.00	0.43
3:C:8:SER:O	3:C:9:ARG:O	2.37	0.43
4:D:207:ALA:HB2	4:D:233:VAL:HG21	2.01	0.43
7:G:49:VAL:HG11	7:G:65:LYS:HB2	2.01	0.43
9:I:81:GLN:O	9:I:85:GLN:HG3	2.18	0.43
9:I:50:ALA:HB2	10:J:120:CYS:HB2	1.99	0.43
10:J:136:GLN:N	10:J:136:GLN:OE1	2.50	0.43
10:J:66:LYS:HA	10:J:71:ARG:O	2.19	0.43
13:M:114:TYR:HD2	13:M:123:GLU:O	2.02	0.43
13:M:128:ARG:HG3	13:M:129:ALA:N	2.33	0.43
1:O:242:GLU:OE1	1:O:245:LEU:HB2	2.19	0.43
2:P:108:LYS:HG2	2:P:148:TYR:OH	2.19	0.43
2:P:12:PHE:CE2	3:Q:130:PRO:HG2	2.54	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
7:U:76:VAL:HG22	7:U:77:TYR:H	1.84	0.43
8:V:105:LYS:HG2	8:V:106:ASN:N	2.34	0.43
9:W:1:THR:HA	9:W:33:LYS:NZ	2.34	0.43
12:Z:158:LYS:HG3	12:Z:177:LEU:HD11	2.01	0.43
12:Z:98:GLY:O	12:Z:99:THR:HB	2.19	0.43
2:B:44:VAL:CA	2:B:213:ILE:HG22	2.48	0.43
3:C:231:LYS:HA	3:C:231:LYS:HE3	2.00	0.43
3:C:39:MET:CE	3:C:146:TYR:HB3	2.49	0.43
4:D:39:LYS:HD3	4:D:186:ALA:HA	2.00	0.43
4:D:75:PHE:CD2	4:D:76:SER:N	2.87	0.43
5:E:238:GLU:O	5:E:241:LYS:HB2	2.18	0.43
1:A:91:ARG:CZ	7:G:156:TYR:CE2	3.02	0.43
7:G:85:ARG:CG	7:G:85:ARG:HH11	2.31	0.43
8:H:70:TYR:N	8:H:70:TYR:CD1	2.85	0.43
8:H:8:PHE:HB2	8:H:146:MET:H	1.84	0.43
9:I:10:ASN:C	9:I:180:ILE:HG13	2.38	0.43
10:J:94:TYR:O	10:J:117:LEU:HB2	2.19	0.43
13:M:48:PHE:H	13:M:98:VAL:CG1	2.31	0.43
14:N:144:ASN:ND2	14:N:148:ARG:NH2	2.67	0.43
1:O:43:LEU:HD23	1:O:43:LEU:C	2.39	0.43
3:Q:181:LYS:HB2	3:Q:181:LYS:HE3	1.82	0.43
3:Q:186:VAL:HG11	3:Q:217:ARG:NH1	2.34	0.43
3:Q:59:GLN:N	3:Q:59:GLN:HE21	2.17	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
6:T:42:THR:HG23	6:T:183:ASP:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:193:LYS:HE2	7:U:193:LYS:HB3	1.75	0.43
9:W:4:VAL:O	9:W:14:ILE:HG22	2.18	0.43
12:Z:54:PHE:C	12:Z:54:PHE:HD2	2.21	0.43
3:C:163:ILE:CG1	3:C:164:SER:H	2.32	0.42
8:H:67:THR:O	8:H:69:GLN:N	2.52	0.42
9:I:90:TYR:O	9:I:91:GLN:C	2.57	0.42
12:L:55:TRP:O	12:L:58:TRP:HB3	2.19	0.42
12:L:76:VAL:HG23	12:L:105:THR:HG22	2.01	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
6:T:129:GLY:O	6:T:130:VAL:HB	2.19	0.42
7:U:216:SER:HA	7:U:230:VAL:HG23	2.01	0.42
8:V:95:ALA:H	8:V:115:LEU:HD13	1.83	0.42
13:M:187:ILE:HG12	9:W:24:PRO:O	2.19	0.42
2:B:187:ASP:O	2:B:190:HIS:HB3	2.19	0.42
5:E:109:VAL:O	5:E:112:LEU:HB3	2.19	0.42
5:E:121:LEU:HD12	5:E:161:SER:O	2.20	0.42
5:E:143:LEU:HD23	5:E:143:LEU:HA	1.61	0.42
5:E:51:GLU:OE2	5:E:53:ARG:HB2	2.19	0.42
6:F:17:GLY:HA3	7:G:29:ALA:HB2	2.02	0.42
6:F:6:TYR:N	6:F:6:TYR:CD2	2.87	0.42
8:H:105:LYS:HG2	8:H:106:ASN:N	2.35	0.42
9:I:41:ILE:HD11	9:I:74:PRO:HB2	2.01	0.42
9:I:97:TYR:CD1	9:I:97:TYR:N	2.88	0.42
10:J:67:LEU:N	10:J:67:LEU:HD23	4.94	0.42
10:J:9:LYS:O	10:J:10:ASP:HB2	2.20	0.42
14:N:41:THR:HG21	14:N:84:ILE:CD1	2.49	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:112:SER:CA	2:P:156:TYR:HE2	2.31	0.42
2:P:238:LEU:CD1	2:P:238:LEU:N	2.81	0.42
1:O:167:LYS:HG2	2:P:55:LEU:O	2.19	0.42
6:T:54:ASP:CG	6:T:55:GLU:H	2.21	0.42
8:V:70:TYR:N	8:V:70:TYR:CD1	2.86	0.42
10:X:117:LEU:HD23	10:X:117:LEU:N	2.34	0.42
3:C:190:ILE:O	3:C:193:ALA:HB3	2.19	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
9:I:4:VAL:HA	9:I:125:LEU:O	2.19	0.42
10:J:98:PRO:HG2	10:J:115:PHE:CD1	2.54	0.42
10:J:89:ARG:HG3	10:J:94:TYR:HE2	1.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:57:GLU:O	11:K:60:GLN:HB3	2.19	0.42
12:L:18:SER:HB2	12:L:31:VAL:H	1.82	0.42
13:M:100:THR:HG23	13:M:116:PHE:HB2	2.01	0.42
14:N:144:ASN:HD22	14:N:148:ARG:NH2	2.16	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
3:Q:181:LYS:O	3:Q:184:MET:HB2	2.19	0.42
4:R:212:ILE:HG21	4:R:224:LEU:HD22	2.01	0.42
5:S:204:LEU:O	5:S:208:MET:N	2.52	0.42
5:S:205:LYS:HB2	5:S:212:LEU:HD13	2.02	0.42
6:T:138:ASP:HB2	6:T:139:LYS:H	1.59	0.42
7:U:150:LEU:HD13	7:U:156:TYR:HB3	2.01	0.42
9:W:153:LYS:HE3	9:W:157:ASP:OD2	2.19	0.42
9:W:41:ILE:N	9:W:41:ILE:HD12	2.34	0.42
9:W:92:GLY:O	9:W:94:ILE:N	2.52	0.42
11:Y:57:GLU:O	11:Y:60:GLN:HB3	2.19	0.42
12:Z:81:LYS:HG3	12:Z:85:ASN:ND2	2.35	0.42
1:A:98:LYS:HE3	1:A:98:LYS:HB2	1.89	0.42
3:C:114:ARG:HB2	3:C:114:ARG:HH11	1.84	0.42
6:F:74:LEU:HD22	6:F:81:ALA:HB1	2.01	0.42
8:H:34:LEU:CD2	8:H:44:CYS:HB3	2.49	0.42
9:I:84:LYS:HE2	9:I:117:GLY:O	2.18	0.42
10:J:81:LEU:O	10:J:83:SER:N	2.52	0.42
12:L:123:LYS:HG3	12:L:124:GLY:N	2.34	0.42
13:M:116:PHE:CE2	13:M:122:TYR:HB3	2.54	0.42
13:M:163:LEU:H	13:M:163:LEU:HD12	1.84	0.42
14:N:72:LEU:CD1	14:N:72:LEU:H	2.08	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
5:S:26:TYR:O	5:S:29:GLU:HB2	2.19	0.42
8:V:8:PHE:HB2	8:V:146:MET:H	1.83	0.42
9:W:59:ILE:HG12	9:W:83:LEU:CD2	2.48	0.42
1:A:176:GLN:HA	1:A:179:THR:HB	2.02	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
2:B:132:VAL:O	2:B:152:PRO:HG3	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
6:F:176:LEU:C	6:F:176:LEU:HD12	2.40	0.42
7:G:236:GLN:O	7:G:239:ILE:HB	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:26:ALA:O	7:G:30:VAL:HG23	2.20	0.42
9:I:84:LYS:HA	9:I:87:LEU:HB3	2.01	0.42
11:K:151:MET:HB3	11:K:155:GLU:HB2	2.01	0.42
12:L:190:ASN:C	12:L:191:HIS:CD2	2.92	0.42
14:N:-2:THR:HA	14:N:47:GLY:O	2.20	0.42
3:Q:173:GLN:O	3:Q:176:LEU:HB2	2.18	0.42
6:T:40:SER:OG	6:T:41:ASN:N	2.53	0.42
7:U:203:HIS:O	7:U:205:ASP:N	2.45	0.42
8:V:189:TYR:HA	8:V:190:PRO:HD3	1.85	0.42
9:W:124:TYR:CD1	9:W:124:TYR:N	2.87	0.42
9:W:43:CYS:SG	9:W:100:VAL:HA	2.60	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
12:Z:211:ILE:HG13	12:Z:211:ILE:H	1.56	0.42
2:B:241:GLN:O	2:B:244:ASN:ND2	2.53	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
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
11:K:151:MET:HA	11:K:155:GLU:OE1	2.20	0.42
13:M:14:LEU:HD13	13:M:34:VAL:CG1	2.45	0.42
14:N:3:VAL:O	14:N:135:ALA:HA	2.20	0.42
1:O:167:LYS:NZ	1:O:167:LYS:HB3	2.34	0.42
2:P:32:VAL:HG12	2:P:33:THR:N	2.34	0.42
2:P:74:VAL:HG13	2:P:135:LEU:HB2	2.01	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
6:T:134:ILE:CD1	6:T:134:ILE:N	2.83	0.42
8:V:147:SER:OG	8:V:150:GLU:HB2	2.20	0.42
1:A:151:GLY:HA3	1:A:152:PRO:HD3	1.92	0.42
4:D:36:VAL:HG11	4:D:195:THR:HG23	2.00	0.42
5:E:132:ARG:HH11	5:E:132:ARG:HG2	1.84	0.42
9:I:104:ASP:C	9:I:106:THR:H	2.22	0.42
9:I:8:PHE:HB2	9:I:146:LEU:O	2.19	0.42
10:J:44:ILE:CG2	10:J:51:VAL:HG22	2.49	0.42
13:M:172:ILE:O	13:M:176:ARG:HG3	2.19	0.42
14:N:148:ARG:HH11	9:W:165:ASN:ND2	2.17	0.42
14:N:26:LEU:O	14:N:28:PHE:N	2.52	0.42
2:P:20:GLN:O	2:P:23:TYR:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:48:ARG:HH11	4:R:48:ARG:HG2	1.85	0.42
5:S:192:THR:OG1	5:S:195:GLU:HG3	2.20	0.42
5:S:20:ARG:O	5:S:21:LEU:HD23	2.20	0.42
6:T:215:ILE:CG1	6:T:216:VAL:N	2.75	0.42
7:U:236:GLN:O	7:U:239:ILE:HB	2.20	0.42
8:V:107:LYS:HB3	8:V:107:LYS:HE3	1.84	0.42
10:X:-7:ASP:HB3	10:X:-4:SER:OG	2.19	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
1:A:69:VAL:O	1:A:70:SER:HB2	2.19	0.42
3:C:183:ASP:O	3:C:184:MET:C	2.58	0.42
5:E:108:ASN:O	5:E:109:VAL:C	2.58	0.42
5:E:39:GLY:O	5:E:169:ALA:HA	2.20	0.42
5:E:8:TYR:O	5:E:9:ASP:CB	2.65	0.42
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
1:O:127:ILE:HG13	1:O:127:ILE:H	1.65	0.42
1:O:239:GLU:OE2	1:O:239:GLU:HA	2.20	0.42
2:P:212:ALA:HB2	2:P:237:LYS:HA	2.02	0.42
3:Q:50:ARG:HB3	3:Q:50:ARG:HH11	1.85	0.42
3:Q:59:GLN:O	3:Q:62:SER:O	2.37	0.42
4:R:127:ARG:HA	4:R:128:PRO:HD3	1.75	0.42
7:U:217:TRP:N	7:U:217:TRP:HD1	2.18	0.42
7:U:26:ALA:O	7:U:30:VAL:HG23	2.20	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
1:A:38:THR:HG23	1:A:39:ASN:N	2.34	0.42
2:B:135:LEU:HD23	2:B:135:LEU:HA	1.85	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
3:C:13:PHE:N	4:D:19:GLN:HE22	2.17	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
7:G:150:LEU:HD11	7:G:154:GLY:C	2.41	0.42
2:P:20:GLN:O	2:P:21:ILE:C	2.59	0.42
2:P:241:GLN:O	2:P:244:ASN:ND2	2.53	0.42
6:T:19:LEU:HD23	6:T:19:LEU:HA	1.90	0.42
6:T:34:VAL:CG2	6:T:35:THR:N	2.82	0.42
7:U:25:TYR:HA	7:U:28:LYS:HB2	2.01	0.42
10:X:128:ILE:HA	10:X:128:ILE:HD13	1.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:191:VAL:C	11:Y:193:ASP:N	2.71	0.42
2:B:185:LEU:O	2:B:188:ALA:HB3	2.20	0.42
4:D:133:THR:HG23	4:D:150:THR:CG2	2.41	0.42
5:E:202:LYS:O	5:E:206:GLN:HG3	2.20	0.42
5:E:240:ILE:O	5:E:243:LEU:HB3	2.19	0.42
6:F:102:LYS:HE3	6:F:102:LYS:HB2	1.81	0.42
6:F:155:GLU:C	6:F:156:LEU:HD12	2.39	0.42
6:F:64:ILE:HB	6:F:72:LEU:HD11	2.02	0.42
10:J:15:ALA:HB2	10:J:178:VAL:HG22	2.01	0.42
11:K:175:PHE:N	11:K:175:PHE:CD1	2.88	0.42
11:K:8:VAL:HG23	11:K:9:GLN:N	2.34	0.42
13:M:152:GLU:HB2	13:M:155:THR:HG21	2.01	0.42
13:M:-5:TYR:OH	13:M:95:PRO:HD2	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
3:Q:66:LEU:HA	3:Q:66:LEU:HD13	1.84	0.42
4:R:155:ILE:HD12	4:R:155:ILE:C	2.40	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
1:A:44:ALA:N	1:A:169:THR:O	2.51	0.41
1:A:216:THR:CG2	1:A:217:GLU:N	2.83	0.41
6:F:33:SER:HB3	6:F:62:LYS:HZ1	1.84	0.41
7:G:19:ARG:NH1	7:G:19:ARG:CG	2.82	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
8:H:188:PHE:N	8:H:188:PHE:HD2	2.18	0.41
8:H:36:ARG:HB2	8:H:42:TRP:CE2	2.55	0.41
9:I:153:LYS:O	9:I:153:LYS:HD3	2.19	0.41
9:I:6:VAL:HG23	9:I:13:VAL:CG1	2.50	0.41
12:L:144:TYR:C	12:L:144:TYR:CD2	2.93	0.41
14:N:29:ASN:HD22	14:N:29:ASN:HA	1.66	0.41
3:Q:211:LEU:HD13	3:Q:212:GLU:N	2.35	0.41
3:Q:29:ILE:O	3:Q:31:HIS:N	2.52	0.41
5:S:33:LEU:H	5:S:33:LEU:HD12	1.84	0.41
6:T:33:SER:HB3	6:T:62:LYS:HZ1	1.83	0.41
8:V:110:VAL:HG12	8:V:122:LEU:O	2.19	0.41
1:A:123:ASN:ND2	2:B:84:VAL:HG12	2.35	0.41
1:A:207:ILE:H	1:A:207:ILE:HG13	1.60	0.41
1:A:26:TYR:CD2	1:A:26:TYR:N	2.87	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:220:ILE:H	9:I:220:ILE:HD12	4.81	0.41
14:N:208:ASN:N	14:N:209:MET:HE2	2.34	0.41
3:Q:15:PRO:HA	4:R:22:TYR:CG	2.55	0.41
5:S:188:HIS:O	5:S:191:LEU:HD12	2.20	0.41
7:U:35:THR:HG21	7:U:167:GLY:H	1.84	0.41
12:Z:145:LYS:O	12:Z:148:LEU:HD22	2.20	0.41
2:B:157:PHE:N	2:B:157:PHE:CD1	2.88	0.41
3:C:69:LEU:CD2	3:C:92:ARG:HG3	2.50	0.41
4:D:87:GLU:O	4:D:91:VAL:HG23	2.20	0.41
5:E:140:VAL:HG22	5:E:141:ALA:N	2.36	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
9:I:152:ILE:HG22	9:I:153:LYS:N	2.34	0.41
13:M:19:ARG:NE	13:M:191:ASP:OD2	2.52	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
2:P:156:TYR:HD1	2:P:156:TYR:O	2.03	0.41
3:Q:235:ILE:O	3:Q:237:ASP:N	2.53	0.41
6:T:179:PHE:CD1	6:T:180:ILE:N	2.89	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
9:W:98:LEU:HD12	9:W:98:LEU:N	2.35	0.41
10:X:54:LEU:HD13	10:X:54:LEU:HA	1.72	0.41
11:Y:9:GLN:HB2	11:Y:151:MET:O	2.20	0.41
2:B:98:LYS:HA	2:B:103:GLU:O	2.19	0.41
3:C:38:ILE:HG22	3:C:39:MET:N	2.35	0.41
6:F:181:LYS:HB3	6:F:181:LYS:HE2	1.92	0.41
6:F:46:LEU:HD11	6:F:72:LEU:HA	2.01	0.41
7:G:100:LYS:HB3	7:G:100:LYS:HZ3	1.86	0.41
11:K:35:ARG:HA	11:K:35:ARG:HD3	1.94	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
1:O:69:VAL:O	1:O:70:SER:HB2	2.20	0.41
3:Q:233:GLN:O	3:Q:235:ILE:N	2.53	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
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
9:W:215:GLU:CD	10:X:189:ARG:HE	2.23	0.41
1:A:181:ASN:ND2	1:A:181:ASN:N	2.66	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:LYS:HA	1:A:230:LYS:HD2	1.89	0.41
2:B:44:VAL:HG23	2:B:211:LEU:HD11	2.02	0.41
3:C:176:LEU:HD23	3:C:192:LEU:HD11	2.02	0.41
4:D:27:VAL:HG11	4:D:132:SER:HB2	2.01	0.41
5:E:222:ILE:HB	5:E:228:PHE:HA	2.02	0.41
11:K:171:MET:HA	11:K:172:PRO:HD3	1.83	0.41
7:G:69:VAL:HA	14:N:68:TYR:HE1	1.85	0.41
1:O:50:CYS:HA	1:O:228:ALA:O	2.20	0.41
7:U:245:GLU:H	7:U:245:GLU:HG2	1.53	0.41
7:U:68:VAL:HG22	7:U:69:VAL:N	2.35	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
2:B:203:GLU:HB3	2:B:204:PHE:H	1.72	0.41
3:C:128:LEU:HD12	3:C:128:LEU:O	2.21	0.41
3:C:59:GLN:O	3:C:62:SER:O	2.38	0.41
6:F:145:LEU:HD23	6:F:153:VAL:HG11	2.02	0.41
6:F:197:ILE:C	6:F:199:GLN:H	2.23	0.41
7:G:200:TYR:HB3	7:G:246:ILE:CD1	2.50	0.41
8:H:126:ILE:HG13	8:H:126:ILE:O	2.21	0.41
8:H:75:THR:HG22	8:H:111:TYR:CE1	2.54	0.41
11:K:117:GLN:HE22	11:K:131:ALA:N	2.18	0.41
14:N:1:THR:OG1	14:N:2:SER:N	2.52	0.41
14:N:224:LYS:HG3	14:N:225:ILE:HG12	2.02	0.41
1:O:128:TYR:HB2	1:O:129:THR:H	1.59	0.41
5:S:9:ASP:OD2	5:S:16:SER:HA	2.21	0.41
6:T:219:ASP:OD2	6:T:219:ASP:N	2.54	0.41
6:T:44:ALA:HB1	6:T:135:ILE:HB	2.02	0.41
6:T:54:ASP:CG	6:T:55:GLU:N	2.73	0.41
7:U:47:PHE:HZ	7:U:138:GLY:N	2.17	0.41
8:V:122:LEU:HB3	8:V:123:PRO:CD	2.51	0.41
8:V:4:MET:CB	8:V:126:ILE:HG22	2.48	0.41
12:Z:18:SER:HB2	12:Z:31:VAL:H	1.85	0.41
3:C:29:ILE:C	3:C:31:HIS:N	2.74	0.41
4:D:37:LYS:HG2	4:D:160:SER:O	2.20	0.41
5:E:204:LEU:O	5:E:208:MET:N	2.53	0.41
5:E:9:ASP:OD2	5:E:16:SER:HA	2.21	0.41
6:F:103:LEU:HD12	6:F:103:LEU:HA	1.80	0.41
7:G:15:SER:H	7:G:19:ARG:H	1.67	0.41
8:H:178:LEU:HA	8:H:178:LEU:HD13	1.85	0.41
9:I:177:VAL:O	9:I:184:ALA:HA	2.20	0.41
9:I:3:ILE:HG13	9:I:99:ILE:HD12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:9:LYS:HB2	10:J:148:ASN:HB3	2.03	0.41
13:M:81:ALA:HB1	13:M:122:TYR:CD2	2.55	0.41
3:Q:48:ALA:O	3:Q:211:LEU:HD22	2.21	0.41
7:U:134:SER:HA	7:U:150:LEU:O	2.21	0.41
7:U:187:SER:HG	7:U:190:GLU:HB2	1.84	0.41
7:U:194:GLN:NE2	7:U:197:LYS:HZ3	2.18	0.41
8:V:153:ASP:HA	8:V:156:LYS:HB2	2.03	0.41
9:W:84:LYS:HA	9:W:87:LEU:HB3	2.02	0.41
12:Z:67:GLU:OE2	12:Z:74:ILE:HG22	2.21	0.41
1:A:127:ILE:H	1:A:127:ILE:HG13	1.66	0.41
2:B:211:LEU:CD2	2:B:238:LEU:HD22	2.51	0.41
2:B:218:ASN:HA	2:B:219:PRO:HD2	1.88	0.41
4:D:30:GLY:O	4:D:166:ARG:HG2	2.20	0.41
4:D:198:SER:O	4:D:201:GLU:HG2	2.21	0.41
4:D:227:GLU:O	4:D:231:GLN:HG3	2.21	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
8:H:19:ARG:HB3	8:H:170:GLY:N	2.32	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
13:M:5:GLY:C	13:M:6:ILE:HD12	2.40	0.41
1:O:16:ILE:CG2	1:O:17:THR:H	2.29	0.41
2:P:156:TYR:CD1	2:P:156:TYR:N	2.89	0.41
3:Q:133:VAL:HG11	3:Q:135:PHE:CZ	2.56	0.41
3:Q:142:ASP:OD2	3:Q:142:ASP:N	2.53	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
14:N:179:ARG:CA	8:V:26:ILE:HD12	2.44	0.41
9:W:183:ASP:HB3	9:W:184:ALA:H	1.55	0.41
10:X:14:ILE:O	10:X:14:ILE:HG23	2.21	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
11:Y:3:ILE:CG2	11:Y:102:LEU:HG	2.51	0.41
2:B:34:SER:O	2:B:163:ALA:HA	2.20	0.41
2:B:229:THR:O	2:B:231:LYS:NZ	2.52	0.41
3:C:114:ARG:NH1	3:C:114:ARG:HB2	2.36	0.41
3:C:68:LYS:NZ	10:J:66:LYS:NZ	2.68	0.41
3:C:156:ASN:ND2	4:D:79:ASN:HB2	2.36	0.41
8:H:112:THR:HG22	8:H:120:HIS:HB2	2.03	0.41
12:L:1:THR:HG22	12:L:2:THR:N	2.36	0.41
14:N:40:ASN:O	14:N:110:GLY:HA3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:100:LYS:HG2	14:N:57:ARG:NH1	2.36	0.41
1:O:230:LYS:HD2	1:O:230:LYS:HA	1.88	0.41
2:P:161:ALA:O	2:P:162:THR:HB	2.20	0.41
5:S:143:LEU:HD23	5:S:143:LEU:HA	1.69	0.41
7:U:89:ASN:O	7:U:92:ARG:HB2	2.20	0.41
8:V:3:ILE:HG22	8:V:16:ALA:HB1	2.02	0.41
10:X:79:THR:HG1	10:X:111:PHE:HE1	1.68	0.41
12:Z:55:TRP:O	12:Z:58:TRP:HB3	2.21	0.41
11:Y:50:GLY:H	12:Z:91:LYS:NZ	2.18	0.41
1:A:45:VAL:HG23	1:A:52:VAL:HG23	2.02	0.41
2:B:147:LEU:HB3	2:B:159:TRP:O	2.21	0.41
2:B:180:ASN:ND2	2:B:183:LEU:HG	2.36	0.41
3:C:185:LYS:HZ2	3:C:187:ASP:N	1.95	0.41
4:D:60:THR:HA	4:D:61:PRO:HD2	1.57	0.41
5:E:66:LYS:O	5:E:77:ALA:HA	2.21	0.41
6:F:74:LEU:HB3	6:F:132:LEU:CD2	2.51	0.41
7:G:117:GLN:HA	7:G:120:GLN:HB2	2.03	0.41
7:G:216:SER:HB2	7:G:227:HIS:NE2	2.36	0.41
8:H:138:CYS:O	8:H:154:PHE:HZ	2.03	0.41
11:K:19:ALA:HB2	11:K:176:LYS:CG	2.50	0.41
4:D:98:LEU:CD1	11:K:58:TYR:HA	2.50	0.41
13:M:101:ILE:CG2	13:M:102:ILE:N	2.83	0.41
2:P:123:GLN:O	2:P:124:SER:HB2	2.21	0.41
3:Q:137:TYR:HB2	3:Q:149:TYR:HB2	2.03	0.41
5:S:221:CYS:HB3	5:S:231:TYR:HE1	1.86	0.41
6:T:105:VAL:HG11	6:T:145:LEU:HD13	2.02	0.41
6:T:176:LEU:HD22	7:U:57:LEU:HD23	2.03	0.41
6:T:3:ARG:HD2	6:T:3:ARG:HA	1.84	0.41
6:T:90:GLN:HE21	6:T:90:GLN:HB3	1.68	0.41
8:V:110:VAL:HG11	8:V:124:TYR:HA	2.02	0.41
9:W:76:VAL:HG21	9:W:109:HIS:HB2	2.02	0.41
9:W:180:ILE:O	9:W:180:ILE:HG22	2.20	0.41
9:W:30:ASN:HA	9:W:30:ASN:HD22	1.59	0.41
9:W:41:ILE:HD12	9:W:41:ILE:H	1.86	0.41
10:X:159:SER:O	10:X:163:LEU:HB2	2.21	0.41
11:Y:135:SER:O	11:Y:139:THR:HG23	2.21	0.41
12:Z:144:TYR:C	12:Z:144:TYR:CD2	2.95	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
4:D:119:ARG:HA	4:D:122:GLN:OE1	2.20	0.41
3:C:13:PHE:HB2	4:D:19:GLN:NE2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:134:ILE:HG22	6:F:135:ILE:N	2.35	0.41
6:F:42:THR:OG1	6:F:183:ASP:HA	2.20	0.41
7:G:51:LYS:HE3	7:G:63:ASN:O	2.21	0.41
9:I:114:HIS:HB2	9:I:118:SER:HB3	2.03	0.41
11:K:70:GLU:O	11:K:71:ASP:HB3	2.20	0.41
14:N:219:GLY:H	8:V:32:ASP:CG	2.24	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:T:107:ARG:HE	6:T:107:ARG:HB3	1.70	0.41
9:W:101:ALA:HB2	9:W:110:LEU:HD12	2.03	0.41
9:W:114:HIS:HB2	9:W:118:SER:HB3	2.02	0.41
12:Z:4:LEU:CD1	12:Z:161:ILE:HD11	2.50	0.41
12:Z:35:ILE:HD12	12:Z:35:ILE:N	2.36	0.41
6:F:197:ILE:CG2	6:F:198:SER:N	2.84	0.40
9:I:72:ARG:CG	9:I:72:ARG:HH11	2.31	0.40
10:J:29:ASN:N	10:J:29:ASN:ND2	2.69	0.40
12:L:19:ARG:N	12:L:33:ARG:NH2	2.70	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
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
3:Q:175:LEU:HD11	3:Q:199:LYS:HB2	2.03	0.40
4:R:239:GLU:HA	4:R:242:GLU:HB3	2.02	0.40
6:T:38:LEU:HA	6:T:158:GLY:HA2	2.03	0.40
6:T:84:LEU:HA	6:T:84:LEU:HD23	1.91	0.40
7:U:143:ASN:N	7:U:143:ASN:ND2	2.55	0.40
1:O:69:VAL:HA	7:U:157:TRP:CZ3	2.56	0.40
7:U:200:TYR:HB3	7:U:246:ILE:CD1	2.51	0.40
9:W:191:LEU:HB3	9:W:193:PRO:HD3	2.01	0.40
11:Y:12:VAL:HG12	11:Y:13:ILE:N	2.36	0.40
12:Z:81:LYS:O	12:Z:84:SER:HB2	2.20	0.40
3:C:186:VAL:O	3:C:190:ILE:HG13	2.21	0.40
4:D:40:ASN:N	4:D:40:ASN:OD1	2.53	0.40
5:E:12:VAL:H	5:E:23:GLN:CG	2.31	0.40
7:G:121:ALA:O	7:G:123:THR:N	2.48	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
10:J:81:LEU:C	10:J:83:SER:N	2.70	0.40
11:K:59:ILE:HA	11:K:59:ILE:HD13	1.91	0.40
13:M:81:ALA:HB1	13:M:122:TYR:HD2	1.85	0.40
2:P:45:ILE:CD1	2:P:64:VAL:HG23	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
7:U:170:SER:O	7:U:174:GLU:HG2	2.21	0.40
11:Y:18:LYS:CD	11:Y:179:ILE:HG13	2.51	0.40
2:B:44:VAL:CG2	2:B:211:LEU:HD11	2.52	0.40
5:E:16:SER:OG	5:E:20:ARG:HB2	2.22	0.40
5:E:46:VAL:HG23	5:E:153:TYR:CD1	2.55	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
9:I:90:TYR:HB2	9:I:94:ILE:CD1	2.52	0.40
10:J:99:VAL:HG13	10:J:128:ILE:HG21	2.04	0.40
13:M:117:ASP:HB3	13:M:121:SER:N	2.36	0.40
4:R:213:THR:HA	4:R:223:ALA:HA	2.03	0.40
7:U:15:SER:H	7:U:19:ARG:H	1.68	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
12:Z:45:MET:HG2	12:Z:45:MET:O	2.21	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
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
7:G:149:MET:HB3	7:G:159:TYR:CE1	2.56	0.40
7:G:182:HIS:C	7:G:184:GLU:H	2.25	0.40
9:I:192:THR:N	9:I:193:PRO:CD	2.85	0.40
10:J:159:SER:O	10:J:163:LEU:HB2	2.22	0.40
12:L:95:LEU:HA	12:L:95:LEU:HD12	1.88	0.40
13:M:105:LEU:HD23	13:M:111:GLY:HA2	2.03	0.40
13:M:172:ILE:HG13	13:M:172:ILE:H	1.63	0.40
14:N:112:GLN:O	14:N:115:GLY:N	2.45	0.40
14:N:142:MET:HE2	9:W:132:LEU:O	2.22	0.40
1:O:57:LYS:HG2	1:O:57:LYS:O	2.20	0.40
3:Q:40:ALA:C	3:Q:42:ASP:H	2.25	0.40
3:Q:83:ASP:O	3:Q:84:ALA:C	2.60	0.40
3:Q:8:SER:O	3:Q:9:ARG:O	2.39	0.40
4:R:39:LYS:HB2	4:R:39:LYS:HE2	1.82	0.40
3:Q:156:ASN:ND2	4:R:79:ASN:HB2	2.37	0.40
7:U:94:GLU:HG3	7:U:114:ARG:HH11	1.85	0.40
7:U:159:TYR:CD1	7:U:159:TYR:N	2.90	0.40
7:U:237:GLU:O	7:U:241:PHE:HB2	2.22	0.40
9:W:72:ARG:CG	9:W:72:ARG:NH1	2.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:86:LEU:HD23	10:X:86:LEU:HA	1.95	0.40
11:Y:3:ILE:HA	11:Y:3:ILE:HD13	1.86	0.40
12:Z:77:ALA:O	12:Z:80:SER:OG	2.37	0.40
1:A:243:GLU:HG2	1:A:243:GLU:O	2.21	0.40
5:E:78:MET:CE	5:E:82:THR:HG22	2.51	0.40
9:I:3:ILE:HG22	9:I:16:ALA:HB1	2.03	0.40
9:I:62:ASN:O	9:I:65:LEU:HB2	2.22	0.40
10:J:56:GLU:H	10:J:56:GLU:HG2	1.57	0.40
11:K:180:VAL:HG21	11:K:194:PHE:CD2	2.57	0.40
13:M:143:ASN:O	13:M:147:PHE:HA	2.22	0.40
14:N:106:ILE:HD12	14:N:106:ILE:N	2.36	0.40
1:O:39:ASN:HD22	1:O:39:ASN:C	2.24	0.40
4:R:174:PHE:C	4:R:174:PHE:CD2	2.95	0.40
5:S:142:LEU:HA	5:S:142:LEU:HD23	1.77	0.40
5:S:52:LYS:HB2	5:S:216:ASN:HA	2.04	0.40
5:S:17:PRO:HA	6:T:24:TYR:CD2	2.56	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

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	236/252 (94%)	172 (73%)	44 (19%)	20 (8%)	1	5
1	O	236/252 (94%)	174 (74%)	42 (18%)	20 (8%)	1	5
2	B	245/250 (98%)	170 (69%)	56 (23%)	19 (8%)	1	7
2	P	245/250 (98%)	174 (71%)	53 (22%)	18 (7%)	1	8
3	C	239/245 (98%)	191 (80%)	29 (12%)	19 (8%)	1	7
3	Q	239/245 (98%)	187 (78%)	32 (13%)	20 (8%)	1	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	237/254 (93%)	186 (78%)	36 (15%)	15 (6%)	1	12
4	R	237/254 (93%)	186 (78%)	36 (15%)	15 (6%)	1	12
5	E	242/260 (93%)	192 (79%)	36 (15%)	14 (6%)	2	15
5	S	242/260 (93%)	192 (79%)	35 (14%)	15 (6%)	2	13
6	F	231/234 (99%)	189 (82%)	36 (16%)	6 (3%)	6	36
6	T	231/234 (99%)	190 (82%)	32 (14%)	9 (4%)	3	25
7	G	238/287 (83%)	193 (81%)	37 (16%)	8 (3%)	4	28
7	U	238/287 (83%)	194 (82%)	34 (14%)	10 (4%)	3	23
8	H	194/196 (99%)	148 (76%)	30 (16%)	16 (8%)	1	6
8	V	194/196 (99%)	147 (76%)	34 (18%)	13 (7%)	1	10
9	I	220/232 (95%)	178 (81%)	27 (12%)	15 (7%)	1	10
9	W	220/232 (95%)	176 (80%)	31 (14%)	13 (6%)	2	15
10	J	202/205 (98%)	165 (82%)	33 (16%)	4 (2%)	9	44
10	X	202/205 (98%)	168 (83%)	30 (15%)	4 (2%)	9	44
11	K	196/198 (99%)	163 (83%)	24 (12%)	9 (5%)	3	21
11	Y	196/198 (99%)	160 (82%)	28 (14%)	8 (4%)	3	24
12	L	210/212 (99%)	180 (86%)	27 (13%)	3 (1%)	13	53
12	Z	210/212 (99%)	178 (85%)	29 (14%)	3 (1%)	13	53
13	M	220/222 (99%)	188 (86%)	24 (11%)	8 (4%)	4	27
13	a	220/222 (99%)	186 (84%)	25 (11%)	9 (4%)	3	24
14	N	231/233 (99%)	169 (73%)	43 (19%)	19 (8%)	1	6
14	b	231/233 (99%)	170 (74%)	40 (17%)	21 (9%)	1	4
15	c	194/231 (84%)	162 (84%)	22 (11%)	10 (5%)	2	17
15	d	194/231 (84%)	162 (84%)	21 (11%)	11 (6%)	2	16
15	e	194/231 (84%)	161 (83%)	22 (11%)	11 (6%)	2	16
15	f	194/231 (84%)	161 (83%)	23 (12%)	10 (5%)	2	17
15	g	194/231 (84%)	161 (83%)	23 (12%)	10 (5%)	2	17
15	h	194/231 (84%)	162 (84%)	22 (11%)	10 (5%)	2	17
15	i	194/231 (84%)	162 (84%)	22 (11%)	10 (5%)	2	17
15	j	194/231 (84%)	162 (84%)	23 (12%)	9 (5%)	3	21
15	k	194/231 (84%)	160 (82%)	24 (12%)	10 (5%)	2	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	l	194/231 (84%)	159 (82%)	25 (13%)	10 (5%)	2	17
15	m	194/231 (84%)	160 (82%)	24 (12%)	10 (5%)	2	17
15	n	194/231 (84%)	161 (83%)	23 (12%)	10 (5%)	2	17
15	o	194/231 (84%)	159 (82%)	25 (13%)	10 (5%)	2	17
15	p	194/231 (84%)	163 (84%)	20 (10%)	11 (6%)	2	16
All	All	8998/9794 (92%)	7221 (80%)	1282 (14%)	495 (6%)	2	16

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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%)	3	15
1	O	204/210 (97%)	174 (85%)	30 (15%)	3	16
2	B	200/209 (96%)	169 (84%)	31 (16%)	3	14
2	P	200/209 (96%)	167 (84%)	33 (16%)	2	12
3	C	198/204 (97%)	168 (85%)	30 (15%)	3	15
3	Q	198/204 (97%)	169 (85%)	29 (15%)	3	17
4	D	209/226 (92%)	175 (84%)	34 (16%)	3	13
4	R	209/226 (92%)	176 (84%)	33 (16%)	3	14
5	E	198/215 (92%)	170 (86%)	28 (14%)	4	18
5	S	198/215 (92%)	170 (86%)	28 (14%)	4	18
6	F	192/193 (100%)	164 (85%)	28 (15%)	3	17
6	T	192/193 (100%)	164 (85%)	28 (15%)	3	17
7	G	199/238 (84%)	167 (84%)	32 (16%)	3	13
7	U	199/238 (84%)	165 (83%)	34 (17%)	2	11
8	H	161/162 (99%)	132 (82%)	29 (18%)	2	10
8	V	161/162 (99%)	133 (83%)	28 (17%)	2	11
9	I	181/190 (95%)	156 (86%)	25 (14%)	4	19
9	W	181/190 (95%)	157 (87%)	24 (13%)	4	21
10	J	172/173 (99%)	149 (87%)	23 (13%)	4	21
10	X	172/173 (99%)	150 (87%)	22 (13%)	5	23
11	K	175/175 (100%)	155 (89%)	20 (11%)	7	28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	Y	175/175 (100%)	154 (88%)	21 (12%)	6	26
12	L	169/169 (100%)	147 (87%)	22 (13%)	5	22
12	Z	169/169 (100%)	148 (88%)	21 (12%)	5	24
13	M	185/185 (100%)	163 (88%)	22 (12%)	6	26
13	a	185/185 (100%)	162 (88%)	23 (12%)	5	24
14	N	199/199 (100%)	169 (85%)	30 (15%)	3	16
14	b	199/199 (100%)	167 (84%)	32 (16%)	3	13
15	c	163/190 (86%)	146 (90%)	17 (10%)	8	33
15	d	163/190 (86%)	146 (90%)	17 (10%)	8	33
15	e	163/190 (86%)	146 (90%)	17 (10%)	8	33
15	f	163/190 (86%)	147 (90%)	16 (10%)	9	36
15	g	163/190 (86%)	147 (90%)	16 (10%)	9	36
15	h	163/190 (86%)	147 (90%)	16 (10%)	9	36
15	i	163/190 (86%)	146 (90%)	17 (10%)	8	33
15	j	163/190 (86%)	146 (90%)	17 (10%)	8	33
15	k	163/190 (86%)	147 (90%)	16 (10%)	9	36
15	l	163/190 (86%)	147 (90%)	16 (10%)	9	36
15	m	163/190 (86%)	147 (90%)	16 (10%)	9	36
15	n	163/190 (86%)	146 (90%)	17 (10%)	8	33
15	o	163/190 (86%)	147 (90%)	16 (10%)	9	36
15	p	163/190 (86%)	147 (90%)	16 (10%)	9	36
All	All	7566/8156 (93%)	6565 (87%)	1001 (13%)	5	21

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
15	p	75	GLN
15	p	80	ASN
15	p	99	HIS
15	p	110	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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%)	0.12	8 (3%) 46 30	45, 88, 99, 100	0
1	O	238/252 (94%)	0.11	6 (2%) 58 43	51, 89, 99, 100	0
2	B	247/250 (98%)	0.04	4 (1%) 72 59	39, 78, 96, 100	0
2	P	247/250 (98%)	-0.07	2 (0%) 86 77	46, 81, 98, 100	0
3	C	241/245 (98%)	-0.09	4 (1%) 70 57	35, 71, 99, 100	0
3	Q	241/245 (98%)	0.01	8 (3%) 47 31	37, 77, 99, 100	0
4	D	239/254 (94%)	-0.08	5 (2%) 64 49	34, 69, 98, 100	0
4	R	239/254 (94%)	-0.09	5 (2%) 64 49	37, 74, 99, 100	0
5	E	244/260 (93%)	-0.04	12 (4%) 30 18	29, 67, 98, 100	0
5	S	244/260 (93%)	0.01	8 (3%) 47 31	41, 72, 99, 100	0
6	F	233/234 (99%)	-0.25	0 100 100	33, 69, 87, 98	0
6	T	233/234 (99%)	-0.06	2 (0%) 84 75	45, 74, 92, 100	0
7	G	240/287 (83%)	0.08	4 (1%) 70 57	45, 82, 98, 100	0
7	U	240/287 (83%)	0.17	5 (2%) 64 49	52, 85, 99, 100	0
8	H	196/196 (100%)	-0.07	3 (1%) 74 61	51, 79, 97, 100	0
8	V	196/196 (100%)	0.02	5 (2%) 56 41	56, 81, 98, 100	0
9	I	222/232 (95%)	-0.16	4 (1%) 69 55	44, 74, 95, 100	0
9	W	222/232 (95%)	-0.10	5 (2%) 61 46	44, 75, 93, 100	0
10	J	204/205 (99%)	-0.36	3 (1%) 74 61	29, 60, 85, 100	0
10	X	204/205 (99%)	-0.41	1 (0%) 90 85	33, 60, 82, 95	0
11	K	198/198 (100%)	-0.27	5 (2%) 58 43	23, 52, 80, 100	0
11	Y	198/198 (100%)	-0.35	2 (1%) 82 72	30, 56, 84, 100	0
12	L	212/212 (100%)	-0.41	2 (0%) 84 75	30, 52, 72, 96	0
12	Z	212/212 (100%)	-0.53	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%)	-0.35	1 (0%) 90 85	28, 60, 79, 97	0
13	a	222/222 (100%)	-0.31	2 (0%) 84 75	30, 61, 85, 99	0
14	N	233/233 (100%)	-0.15	2 (0%) 84 75	37, 72, 95, 99	0
14	b	233/233 (100%)	-0.08	2 (0%) 84 75	39, 74, 96, 100	0
15	c	198/231 (85%)	0.25	4 (2%) 65 50	58, 90, 99, 100	0
15	d	198/231 (85%)	0.43	18 (9%) 10 6	65, 92, 100, 100	0
15	e	198/231 (85%)	0.40	16 (8%) 13 7	58, 91, 100, 100	0
15	f	198/231 (85%)	0.15	6 (3%) 51 35	47, 89, 99, 100	0
15	g	198/231 (85%)	0.14	7 (3%) 44 29	48, 88, 99, 100	0
15	h	198/231 (85%)	0.26	8 (4%) 39 25	57, 86, 99, 100	0
15	i	198/231 (85%)	0.25	7 (3%) 44 29	56, 91, 100, 100	0
15	j	198/231 (85%)	0.37	9 (4%) 34 21	60, 94, 100, 100	0
15	k	198/231 (85%)	0.35	12 (6%) 22 12	65, 94, 100, 100	0
15	l	198/231 (85%)	0.29	14 (7%) 17 10	56, 93, 100, 100	0
15	m	198/231 (85%)	0.27	13 (6%) 19 11	56, 94, 100, 100	0
15	n	198/231 (85%)	0.30	9 (4%) 34 21	64, 94, 100, 100	0
15	o	198/231 (85%)	0.40	12 (6%) 22 12	70, 93, 100, 100	0
15	p	198/231 (85%)	0.48	20 (10%) 8 5	67, 95, 100, 100	0
All	All	9110/9794 (93%)	0.01	265 (2%) 52 37	23, 79, 99, 100	0

All (265) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	S	129	GLY	6.5
3	Q	245	THR	6.2
15	k	231	SER	5.7
5	E	128	SER	5.3
5	S	126	GLY	5.3
5	E	127	ALA	5.3
4	R	51	THR	5.3
3	C	245	THR	5.0
15	l	231	SER	4.8
10	J	-8	SER	4.8
4	D	51	THR	4.8
15	l	227	ASP	4.6
8	V	10	ASP	4.6

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Mol	Chain	Res	Type	RSRZ
14	N	-8	THR	4.6
11	K	197	GLN	4.5
5	S	125	GLU	4.5
15	o	176	SER	4.4
11	Y	196	ALA	4.2
15	l	228	HIS	4.2
5	E	129	GLY	4.2
15	e	229	MET	4.1
5	S	128	SER	4.1
1	A	251	GLN	4.1
3	Q	244	ILE	4.0
15	e	126	GLY	4.0
7	U	220	LEU	3.8
2	P	249	ALA	3.8
15	j	6	ALA	3.8
15	p	63	SER	3.8
14	b	-8	THR	3.7
5	S	127	ALA	3.7
15	p	6	ALA	3.6
15	e	227	ASP	3.6
15	o	179	LEU	3.6
15	n	146	ARG	3.6
15	f	231	SER	3.5
15	d	146	ARG	3.5
7	G	186	LEU	3.5
8	H	11	GLY	3.5
15	p	58	ALA	3.5
15	n	52	ASN	3.4
15	k	6	ALA	3.4
15	e	143	TYR	3.4
9	W	219	ASN	3.4
15	k	228	HIS	3.3
15	o	187	ASP	3.3
15	e	230	VAL	3.3
11	K	196	ALA	3.3
15	k	227	ASP	3.2
15	l	229	MET	3.2
15	d	231	SER	3.2
2	B	250	LEU	3.2
5	E	125	GLU	3.1
5	E	131	GLU	3.1
5	E	124	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
9	W	220	ILE	3.1
15	e	6	ALA	3.1
11	K	195	GLN	3.1
12	L	212	GLY	3.1
15	p	181	LEU	3.1
5	E	247	GLU	3.1
15	g	51	ARG	3.1
15	m	183	LEU	3.0
9	I	222	ASP	3.0
15	o	143	TYR	3.0
15	o	53	SER	3.0
1	O	252	ASP	3.0
2	B	249	ALA	3.0
15	d	10	GLN	3.0
5	S	131	GLU	3.0
1	O	249	ALA	3.0
4	R	60	THR	3.0
15	m	143	TYR	3.0
15	j	13	ARG	2.9
15	p	143	TYR	2.9
15	k	17	THR	2.9
15	j	54	THR	2.9
15	j	53	SER	2.9
15	m	231	SER	2.9
15	e	146	ARG	2.9
8	V	11	GLY	2.9
15	k	230	VAL	2.9
8	V	9	LYS	2.9
5	E	133	LEU	2.9
1	A	252	ASP	2.9
15	p	144	ALA	2.9
4	D	52	LEU	2.9
15	l	10	GLN	2.9
5	E	126	GLY	2.8
15	h	176	SER	2.8
9	I	182	LYS	2.8
9	W	221	CYS	2.8
7	U	205	ASP	2.8
15	j	67	LEU	2.8
15	l	7	ALA	2.8
3	Q	221	ASN	2.8
15	e	228	HIS	2.8

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Mol	Chain	Res	Type	RSRZ
15	o	177	PRO	2.8
4	R	52	LEU	2.7
3	Q	222	ASP	2.7
3	C	222	ASP	2.7
15	p	146	ARG	2.7
15	n	176	SER	2.7
15	n	143	TYR	2.7
15	k	146	ARG	2.7
1	O	189	SER	2.7
1	O	215	GLY	2.7
15	k	27	GLU	2.7
15	k	10	GLN	2.7
13	M	156	ASN	2.7
15	h	143	TYR	2.7
15	o	190	PHE	2.7
1	A	216	THR	2.7
9	W	222	ASP	2.7
1	O	240	ASN	2.7
15	d	145	LEU	2.7
15	d	179	LEU	2.7
15	p	16	TYR	2.6
15	h	51	ARG	2.6
1	A	222	ASP	2.6
7	U	186	LEU	2.6
8	H	8	PHE	2.6
2	P	250	LEU	2.6
5	S	124	GLY	2.6
15	l	225	GLY	2.6
7	G	221	SER	2.6
15	g	176	SER	2.6
15	j	143	TYR	2.6
2	B	206	GLY	2.6
15	n	177	PRO	2.6
15	d	57	ARG	2.6
15	e	10	GLN	2.6
15	p	178	SER	2.6
15	i	180	LEU	2.6
15	d	27	GLU	2.5
15	h	146	ARG	2.5
15	m	6	ALA	2.5
3	C	220	ALA	2.5
5	E	130	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
15	m	146	ARG	2.5
15	e	13	ARG	2.5
15	o	51	ARG	2.5
9	I	179	GLU	2.5
15	h	63	SER	2.5
15	d	62	LYS	2.5
15	m	227	ASP	2.5
15	n	139	PRO	2.5
15	d	41	LYS	2.5
15	l	176	SER	2.5
15	m	189	ASP	2.5
15	m	13	ARG	2.5
15	l	8	LEU	2.5
15	f	146	ARG	2.5
15	d	144	ALA	2.5
2	B	177	LYS	2.4
15	c	28	TRP	2.4
15	d	16	TYR	2.4
15	o	185	GLN	2.4
15	l	146	ARG	2.4
15	l	184	ARG	2.4
15	p	28	TRP	2.4
9	W	218	VAL	2.4
15	l	17	THR	2.4
15	o	52	ASN	2.4
1	A	213	ALA	2.4
3	Q	182	ASP	2.4
15	h	6	ALA	2.4
7	G	237	GLU	2.4
15	p	57	ARG	2.4
15	g	146	ARG	2.4
15	n	226	THR	2.4
11	Y	195	GLN	2.4
15	g	47	HIS	2.4
15	l	230	VAL	2.4
15	i	63	SER	2.3
15	p	53	SER	2.3
15	i	51	ARG	2.3
15	p	54	THR	2.3
11	K	10	ASP	2.3
15	p	61	GLU	2.3
15	n	178	SER	2.3

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Mol	Chain	Res	Type	RSRZ
15	m	230	VAL	2.3
15	d	228	HIS	2.3
15	l	13	ARG	2.3
3	Q	52	VAL	2.3
15	d	229	MET	2.3
15	p	10	GLN	2.3
15	e	16	TYR	2.3
15	c	53	SER	2.3
15	k	47	HIS	2.3
15	f	227	ASP	2.3
15	j	144	ALA	2.3
9	I	11	GLY	2.3
15	k	52	ASN	2.3
15	d	61	GLU	2.3
15	m	142	MET	2.3
15	m	56	GLY	2.3
15	n	186	ILE	2.3
15	d	230	VAL	2.3
15	f	176	SER	2.2
15	d	52	ASN	2.2
15	e	9	ILE	2.2
5	S	130	GLU	2.2
13	a	-9	GLN	2.2
8	V	102	TYR	2.2
3	Q	42	ASP	2.2
3	C	219	GLY	2.2
15	g	54	THR	2.2
14	b	193	ASP	2.2
15	p	68	LEU	2.2
7	U	201	LEU	2.2
15	p	177	PRO	2.2
15	e	226	THR	2.2
15	h	231	SER	2.2
1	A	195	ASN	2.2
15	c	146	ARG	2.2
15	f	55	TYR	2.2
8	H	10	ASP	2.2
12	L	180	VAL	2.2
15	p	176	SER	2.1
1	A	50	CYS	2.1
10	J	10	ASP	2.1
11	K	193	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
15	p	229	MET	2.1
15	i	11	ASN	2.1
15	k	13	ARG	2.1
7	U	12	SER	2.1
15	e	231	SER	2.1
6	T	183	ASP	2.1
15	o	146	ARG	2.1
15	j	181	LEU	2.1
5	E	244	LYS	2.1
1	A	218	PHE	2.1
15	i	146	ARG	2.1
15	e	94	ILE	2.1
4	D	179	TYR	2.1
10	J	183	LYS	2.1
15	g	228	HIS	2.1
15	j	51	ARG	2.1
4	D	242	GLU	2.1
5	E	132	ARG	2.1
7	G	246	ILE	2.1
8	V	8	PHE	2.1
14	N	195	ASN	2.1
15	d	11	ASN	2.1
3	Q	220	ALA	2.1
4	R	61	PRO	2.1
15	f	13	ARG	2.1
15	o	8	LEU	2.1
15	h	55	TYR	2.1
15	g	180	LEU	2.1
13	a	108	ASP	2.1
6	T	210	ASN	2.0
15	m	226	THR	2.0
15	d	221	GLN	2.0
15	e	127	SER	2.0
10	X	186	VAL	2.0
15	m	69	GLY	2.0
15	i	53	SER	2.0
1	O	187	LYS	2.0
4	D	60	THR	2.0
4	R	41	CYS	2.0
15	c	63	SER	2.0
15	p	184	ARG	2.0
15	i	143	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
16	MG	H	1002	1/1	0.72	0.38	6.05	81,81,81,81	0
16	MG	J	1005	1/1	0.97	0.26	5.42	37,37,37,37	0
16	MG	X	1012	1/1	0.82	0.29	2.61	56,56,56,56	0
16	MG	L	1003	1/1	0.89	0.23	1.67	43,43,43,43	0
16	MG	U	1014	1/1	0.77	0.30	0.73	65,65,65,65	0
16	MG	V	1009	1/1	0.89	0.18	-0.62	39,39,39,39	0
16	MG	a	1011	1/1	0.97	0.06	-1.76	49,49,49,49	0
16	MG	M	1004	1/1	0.98	0.07	-2.17	26,26,26,26	0
16	MG	G	1007	1/1	0.91	0.10	-2.81	38,38,38,38	0
16	MG	I	1001	1/1	0.88	0.16	-3.61	67,67,67,67	0
16	MG	Z	1010	1/1	0.98	0.08	-3.80	38,38,38,38	0
16	MG	W	1008	1/1	0.95	0.08	-5.08	67,67,67,67	0
16	MG	J	1006	1/1	0.92	0.09	-	24,24,24,24	0
16	MG	X	1013	1/1	0.87	0.23	-	79,79,79,79	0

6.5 Other polymers [i](#)

There are no such residues in this entry.