Full wwPDB X-ray Structure Validation Report ⓘ

Dec 19, 2023 – 06:35 AM EST

PDB ID	:	1IRU
Title	:	Crystal Structure of the mammalian 20S proteasome at 2.75 A resolution
Authors	:	Unno, M.; Mizushima, T.; Morimoto, Y.; Tomisugi, Y.; Tanaka, K.; Yasuoka, N.; Tsukihara, T.
Deposited on	:	2001-10-24
Resolution	:	2.75 Å(reported)

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

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

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

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

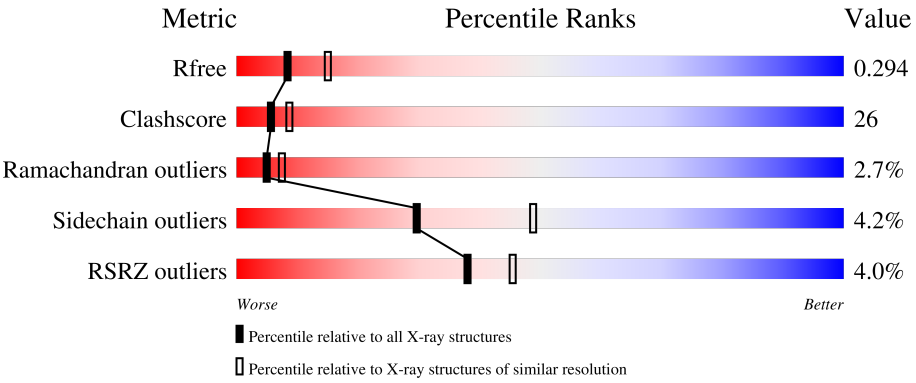
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.75 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}	130704	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	246	10%, 52%, 45%
1	O	246	51%, 46%
2	B	233	13%, 51%, 44%, 6%
2	P	233	3%, 53%, 43%
3	C	261	17%, 47%, 44%, 5%

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Mol	Chain	Length	Quality of chain
3	Q	261	5% 47% 43% 5%
4	D	248	12% 48% 45% 5%
4	R	248	10% 49% 43% 5%
5	E	241	62% 33%
5	S	241	4% 59% 35%
6	F	263	50% 38% 10%
6	T	263	3% 50% 38% 10%
7	G	254	56% 38%
7	U	254	55% 39%
8	H	205	65% 31%
8	V	205	66% 30%
9	I	234	5% 55% 36% 6%
9	W	234	56% 35% 6%
10	J	205	3% 53% 44%
10	X	205	56% 40%
11	K	201	3% 57% 39%
11	Y	201	56% 40%
12	L	204	62% 35%
12	Z	204	61% 35%
13	1	213	61% 38%
13	M	213	64% 34%
14	2	219	61% 35%
14	N	219	61% 35%

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
15	MG	G	319	-	-	-	X

2 Entry composition (i)

There are 16 unique types of molecules in this entry. The entry contains 47757 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 20S proteasome.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	244	Total	C	N	O	S	0	0	0
			1842	1170	309	350	13			
1	O	244	Total	C	N	O	S	0	0	0
			1842	1170	309	350	13			

- Molecule 2 is a protein called 20S proteasome.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	233	Total	C	N	O	S	0	0	0
			1707	1081	287	334	5			
2	P	233	Total	C	N	O	S	0	0	0
			1707	1081	287	334	5			

- Molecule 3 is a protein called 20S proteasome.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	250	Total	C	N	O	S	0	0	0
			1902	1195	329	370	8			
3	Q	250	Total	C	N	O	S	0	0	0
			1902	1195	329	370	8			

- Molecule 4 is a protein called 20S proteasome.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	243	Total	C	N	O	S	0	0	0
			1665	1032	307	322	4			
4	R	243	Total	C	N	O	S	0	0	0
			1665	1032	307	322	4			

- Molecule 5 is a protein called 20S proteasome.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	234	Total	C	N	O	S	0	0	0
			1763	1104	290	358	11			
5	S	234	Total	C	N	O	S	0	0	0
			1763	1104	290	358	11			

- Molecule 6 is a protein called 20S proteasome.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	238	Total	C	N	O	S	0	0	0
			1850	1159	334	346	11			
6	T	238	Total	C	N	O	S	0	0	0
			1850	1159	334	346	11			

- Molecule 7 is a protein called 20S proteasome.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	245	Total	C	N	O	S	0	0	0
			1885	1195	319	360	11			
7	U	245	Total	C	N	O	S	0	0	0
			1885	1195	319	360	11			

- Molecule 8 is a protein called 20S proteasome.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	202	Total	C	N	O	S	0	0	0
			1509	945	258	294	12			
8	V	202	Total	C	N	O	S	0	0	0
			1509	945	258	294	12			

- Molecule 9 is a protein called 20S proteasome.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	220	Total	C	N	O	S	0	0	0
			1645	1034	282	317	12			
9	W	220	Total	C	N	O	S	0	0	0
			1645	1034	282	317	12			

- Molecule 10 is a protein called 20S proteasome.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	204	Total	C	N	O	S	0	0	0
			1585	1011	262	294	18			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	X	204	Total	C	N	O	S	0	0	0
			1585	1011	262	294	18			

- Molecule 11 is a protein called 20S proteasome.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	199	Total	C	N	O	S	0	0	0
			1570	1006	265	290	9			
11	Y	199	Total	C	N	O	S	0	0	0
			1570	1006	265	290	9			

- Molecule 12 is a protein called 20S proteasome.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	201	Total	C	N	O	S	0	0	0
			1548	974	273	292	9			
12	Z	201	Total	C	N	O	S	0	0	0
			1548	974	273	292	9			

- Molecule 13 is a protein called 20S proteasome.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	213	Total	C	N	O	S	0	0	0
			1639	1034	282	313	10			
13	1	213	Total	C	N	O	S	0	0	0
			1639	1034	282	313	10			

- Molecule 14 is a protein called 20S proteasome.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	217	Total	C	N	O	S	0	0	0
			1671	1053	287	319	12			
14	2	217	Total	C	N	O	S	0	0	0
			1671	1053	287	319	12			

- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	1	Total	Mg	0	0
			1	1		
15	B	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	C	1	Total Mg 1 1	0	0
15	D	1	Total Mg 1 1	0	0
15	G	3	Total Mg 3 3	0	0
15	I	1	Total Mg 1 1	0	0
15	J	4	Total Mg 4 4	0	0
15	K	1	Total Mg 1 1	0	0
15	M	2	Total Mg 2 2	0	0
15	O	1	Total Mg 1 1	0	0
15	P	1	Total Mg 1 1	0	0
15	Q	1	Total Mg 1 1	0	0
15	R	1	Total Mg 1 1	0	0
15	U	3	Total Mg 3 3	0	0
15	W	1	Total Mg 1 1	0	0
15	X	4	Total Mg 4 4	0	0
15	Y	1	Total Mg 1 1	0	0
15	1	2	Total Mg 2 2	0	0

- Molecule 16 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	A	2	Total O 2 2	0	0
16	B	3	Total O 3 3	0	0
16	C	3	Total O 3 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	F	6	Total O 6 6	0	0
16	G	4	Total O 4 4	0	0
16	H	7	Total O 7 7	0	0
16	I	6	Total O 6 6	0	0
16	J	1	Total O 1 1	0	0
16	K	6	Total O 6 6	0	0
16	L	8	Total O 8 8	0	0
16	M	10	Total O 10 10	0	0
16	N	9	Total O 9 9	0	0
16	O	7	Total O 7 7	0	0
16	P	6	Total O 6 6	0	0
16	Q	3	Total O 3 3	0	0
16	R	3	Total O 3 3	0	0
16	S	1	Total O 1 1	0	0
16	T	7	Total O 7 7	0	0
16	U	9	Total O 9 9	0	0
16	V	15	Total O 15 15	0	0
16	W	9	Total O 9 9	0	0
16	X	17	Total O 17 17	0	0
16	Y	3	Total O 3 3	0	0
16	Z	8	Total O 8 8	0	0

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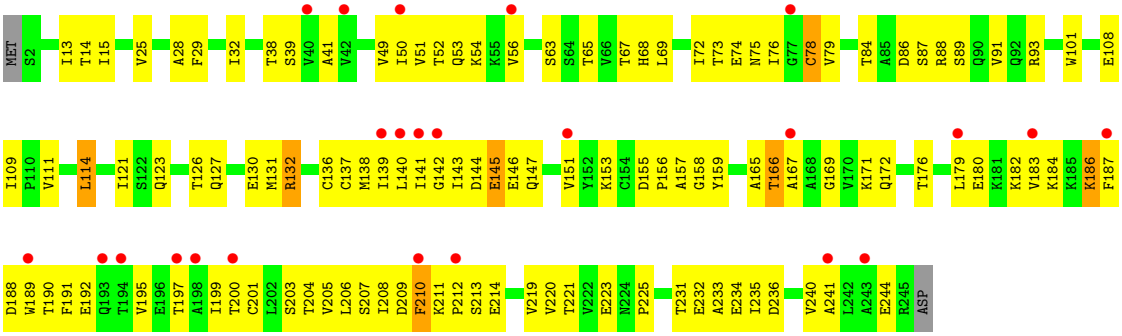
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	1	4	Total O 4 4	0	0
16	2	8	Total O 8 8	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and 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: 20S proteasome

Chain A:

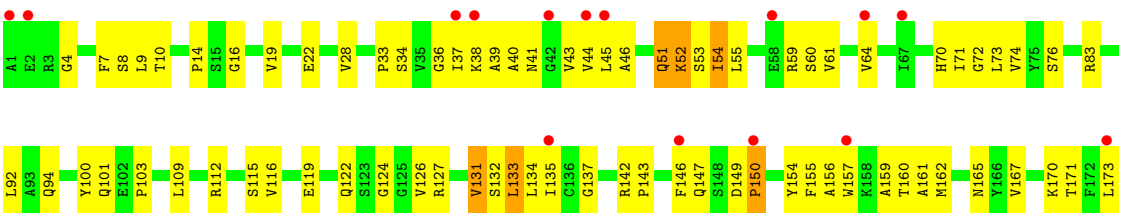


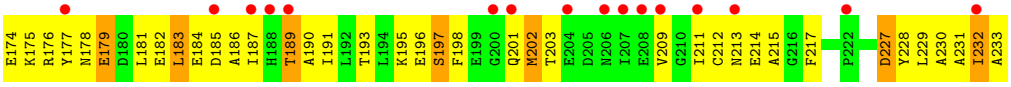
• Molecule 1: 20S proteasome

Chain O:

• Molecule 2: 20S proteasome

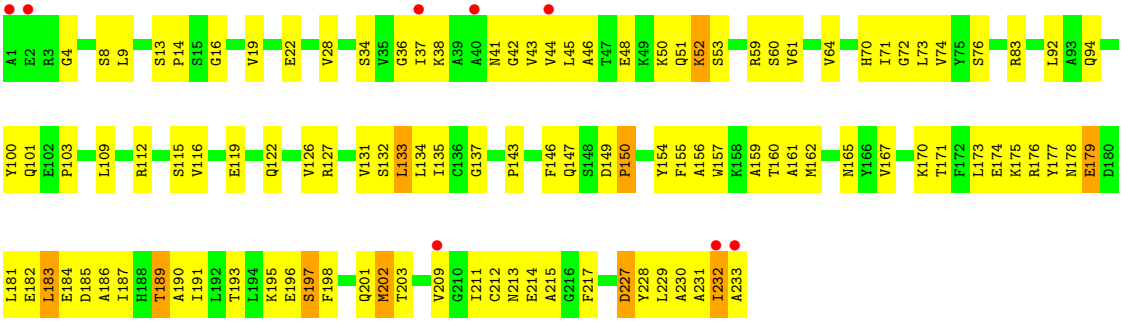
Chain B:





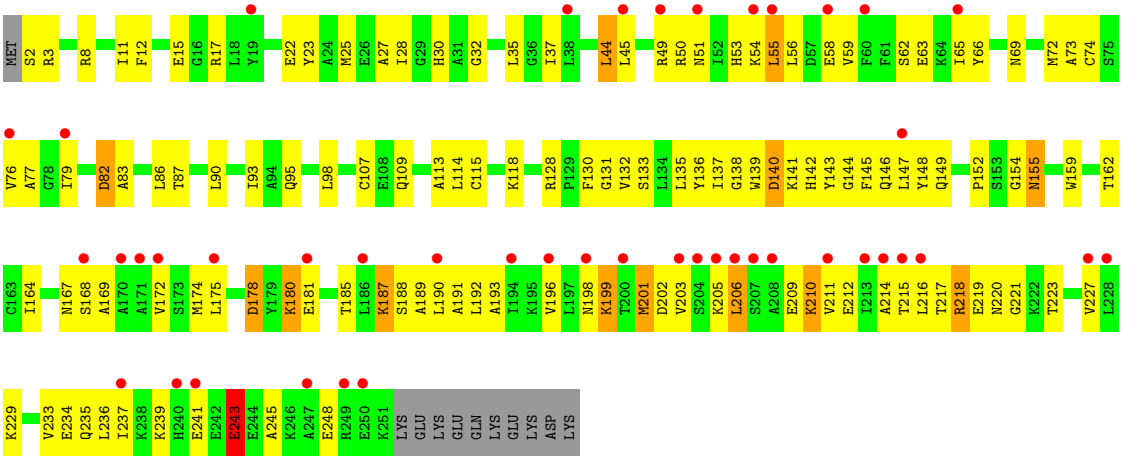
• Molecule 2: 20S proteasome

Chain P:



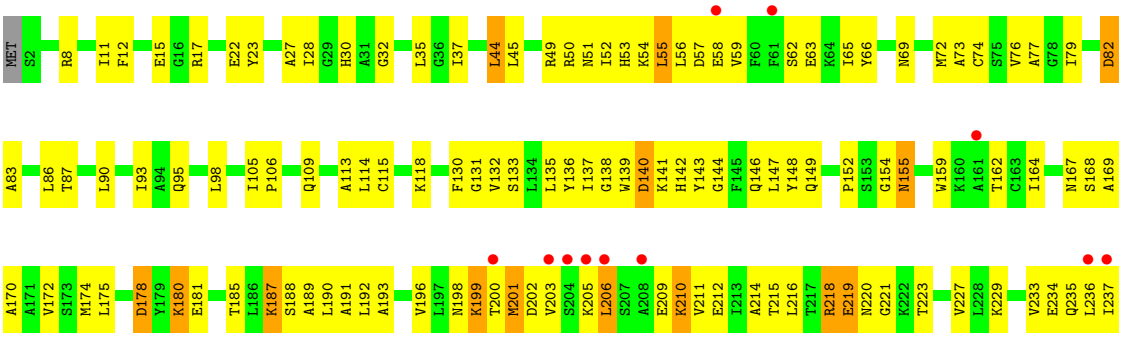
• Molecule 3: 20S proteasome

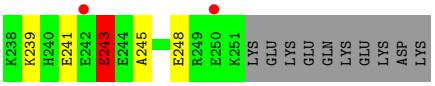
Chain C:



• Molecule 3: 20S proteasome

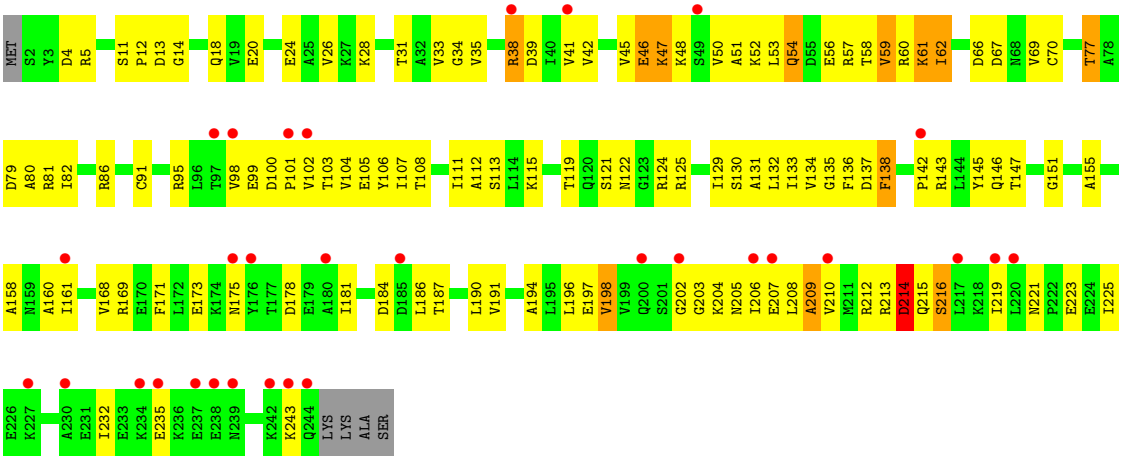
Chain Q:





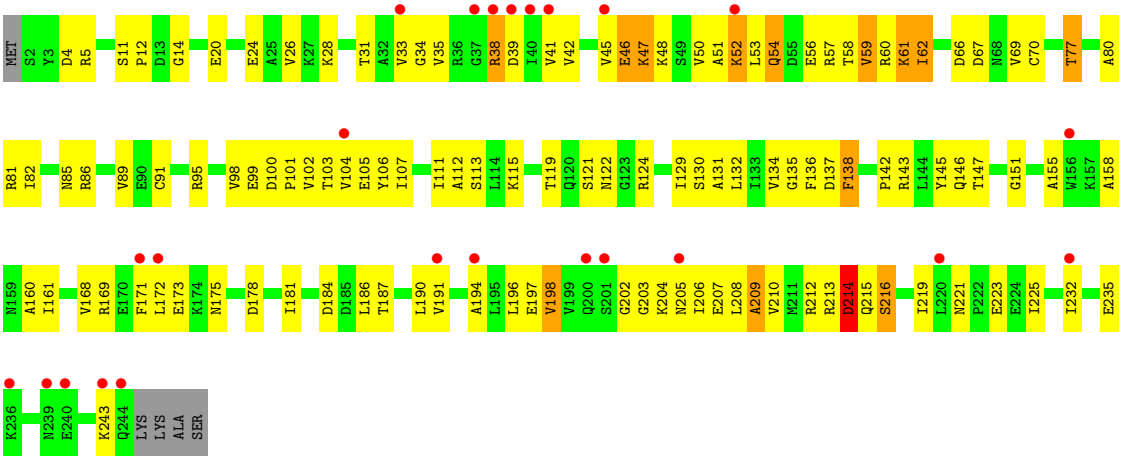
• Molecule 4: 20S proteasome

Chain D:



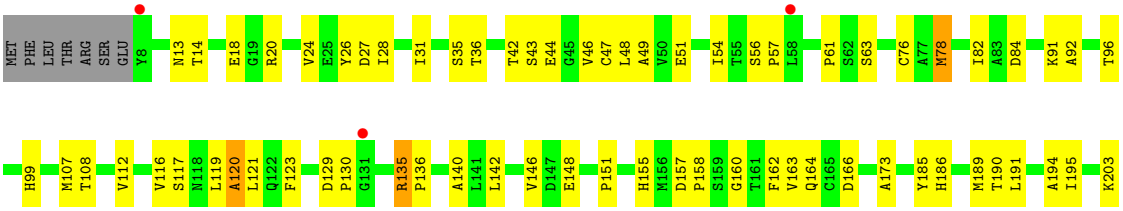
• Molecule 4: 20S proteasome

Chain R:



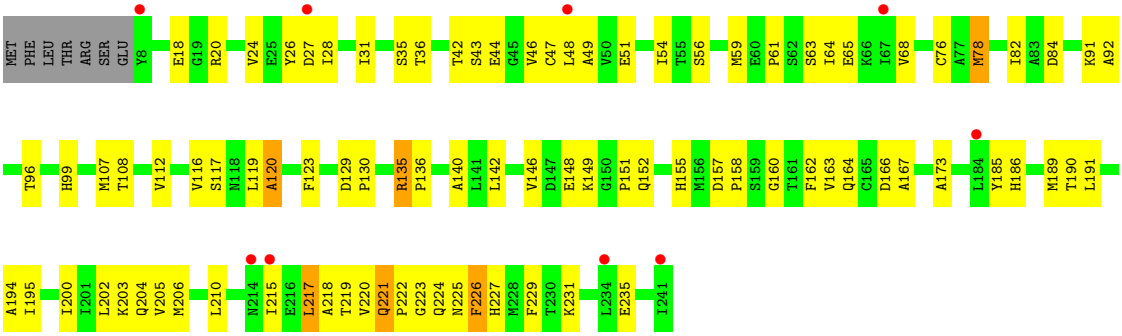
• Molecule 5: 20S proteasome

Chain E:



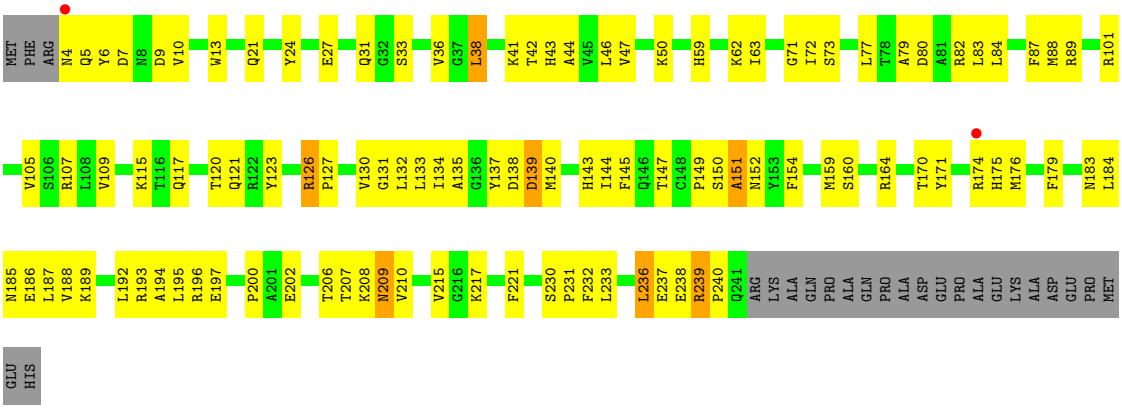
• Molecule 5: 20S proteasome

Chain S:



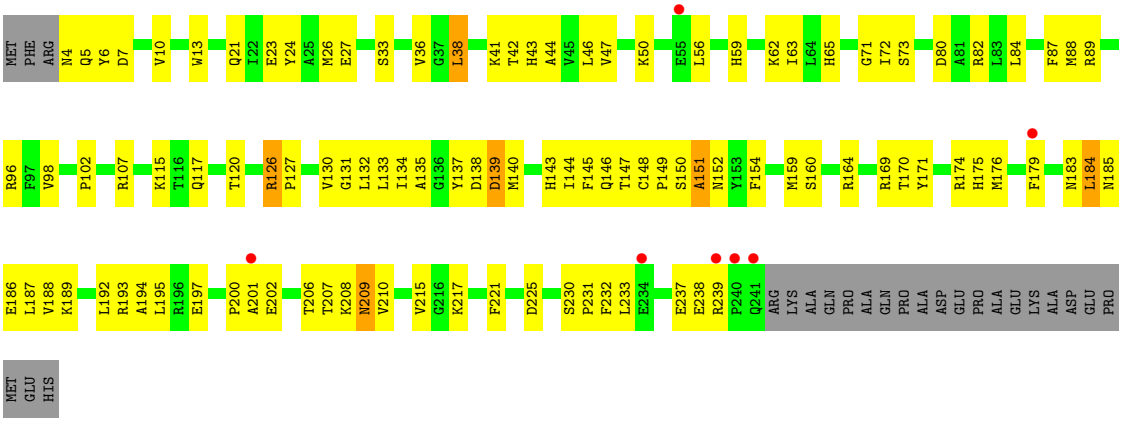
• Molecule 6: 20S proteasome

Chain F:



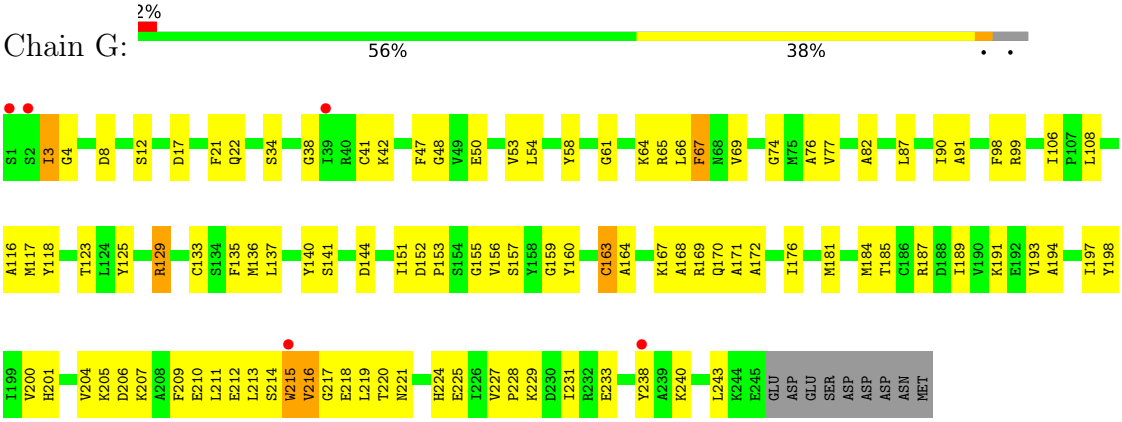
• Molecule 6: 20S proteasome

Chain T:



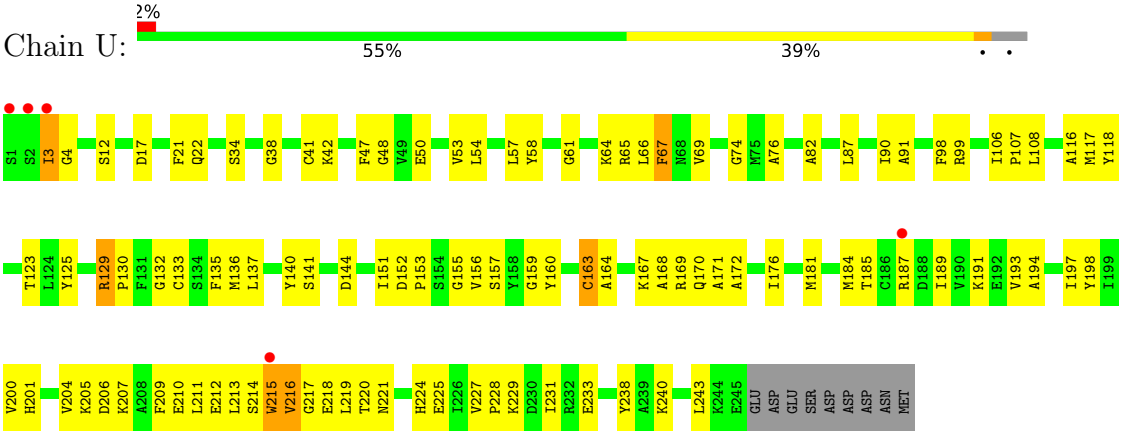
• Molecule 7: 20S proteasome

Chain G:



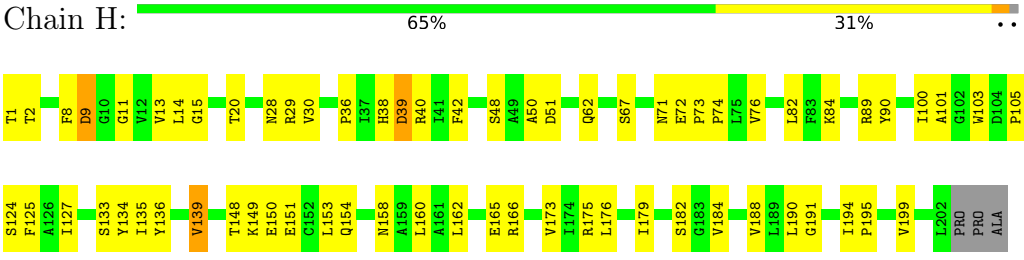
• Molecule 7: 20S proteasome

Chain U:



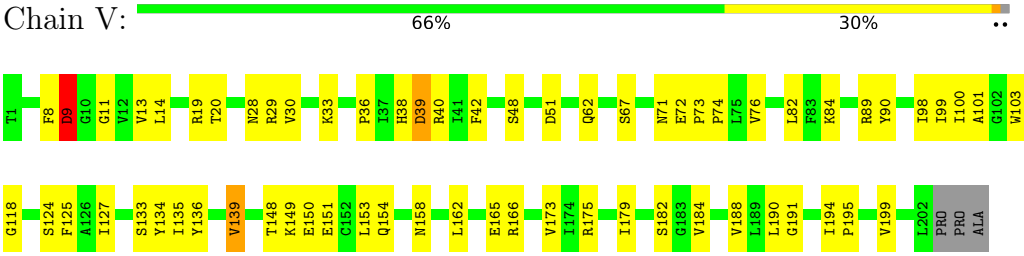
• Molecule 8: 20S proteasome

Chain H:



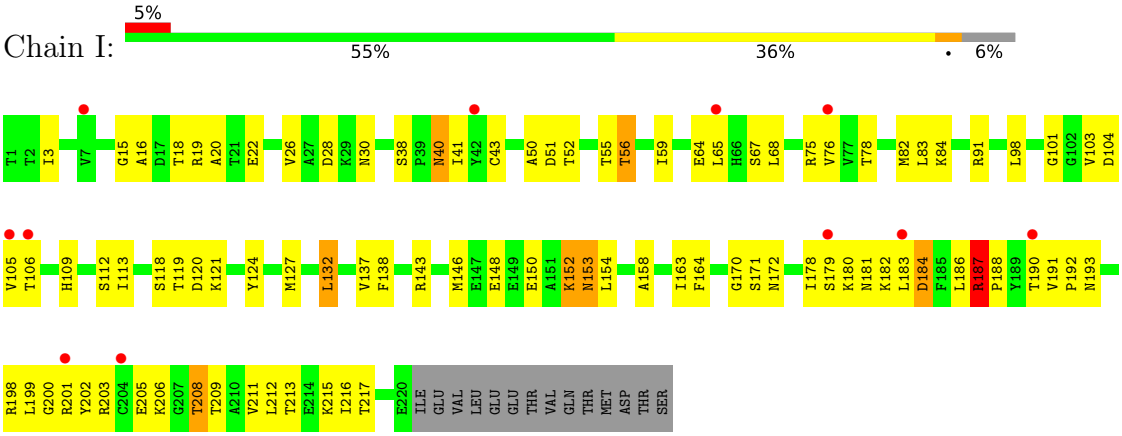
• Molecule 8: 20S proteasome

Chain V:



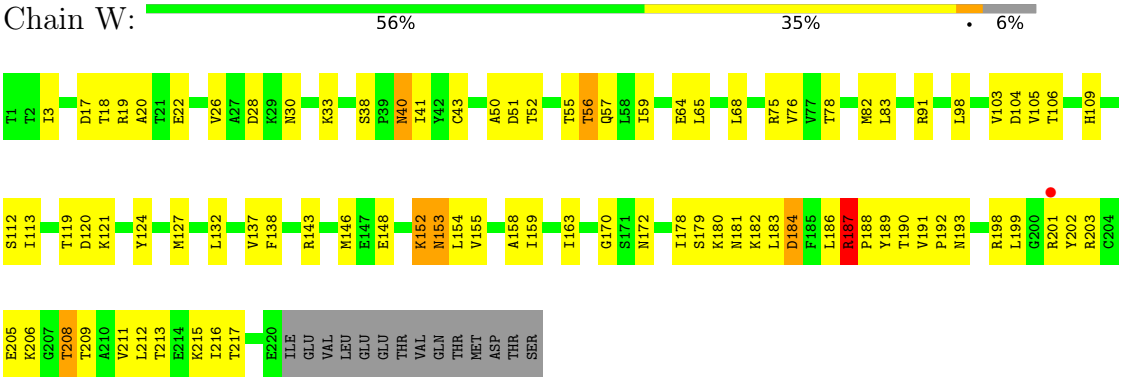
• Molecule 9: 20S proteasome

Chain I:



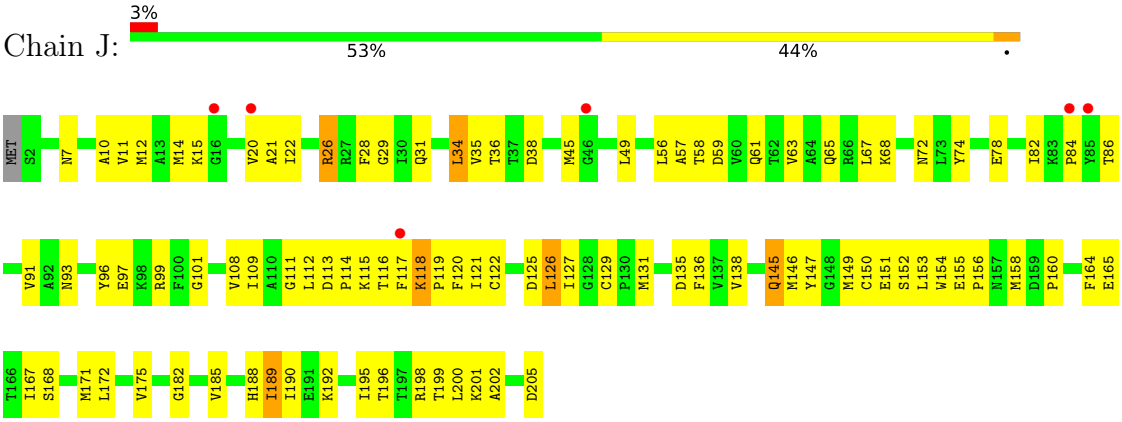
• Molecule 9: 20S proteasome

Chain W:



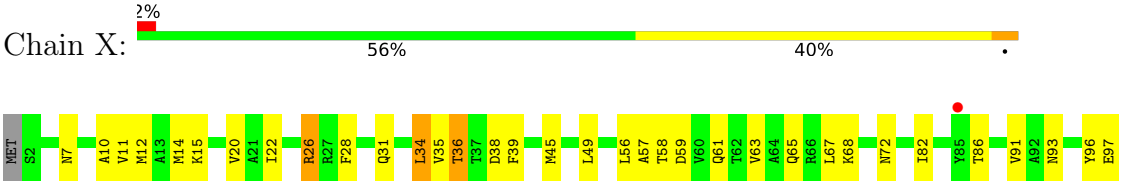
• Molecule 10: 20S proteasome

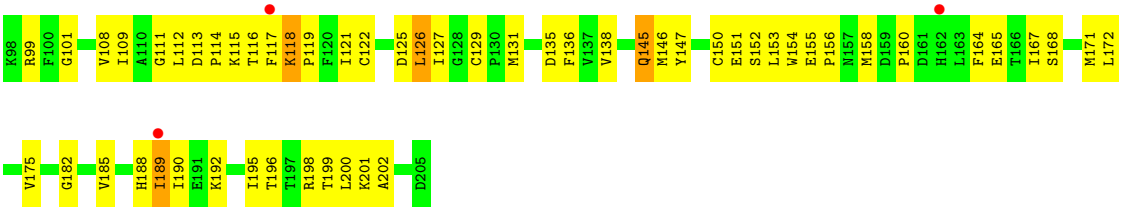
Chain J:



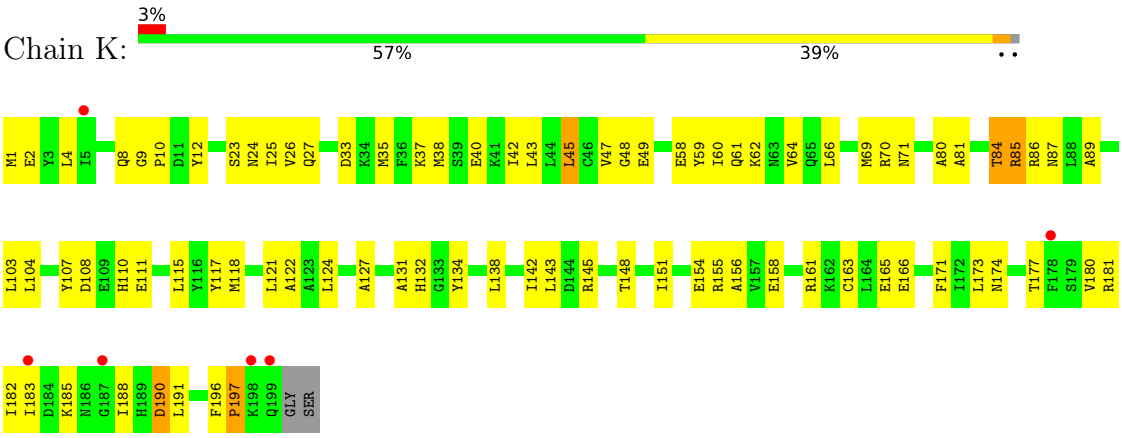
• Molecule 10: 20S proteasome

Chain X:

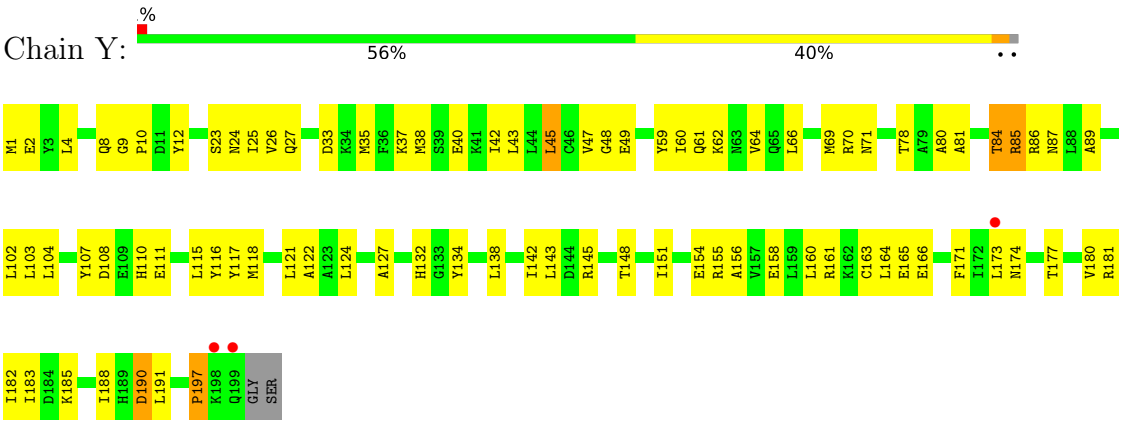




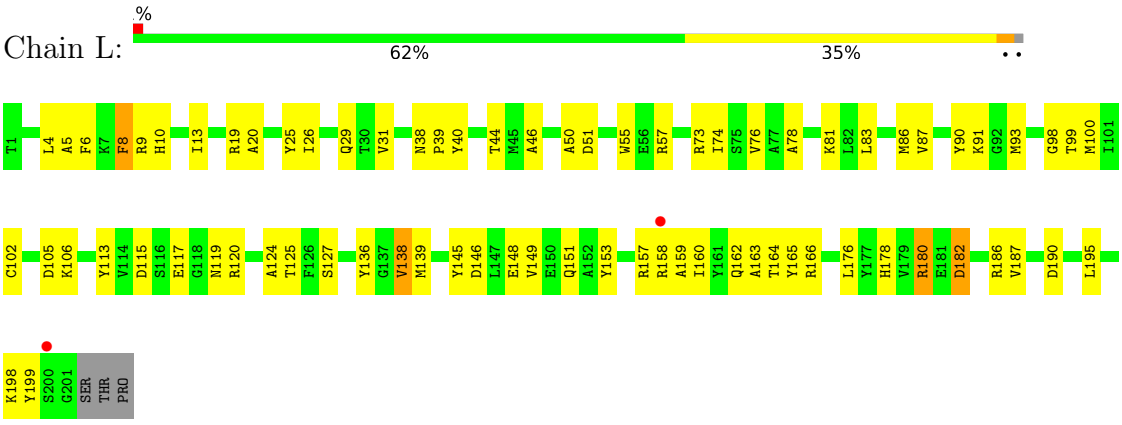
• Molecule 11: 20S proteasome



• Molecule 11: 20S proteasome

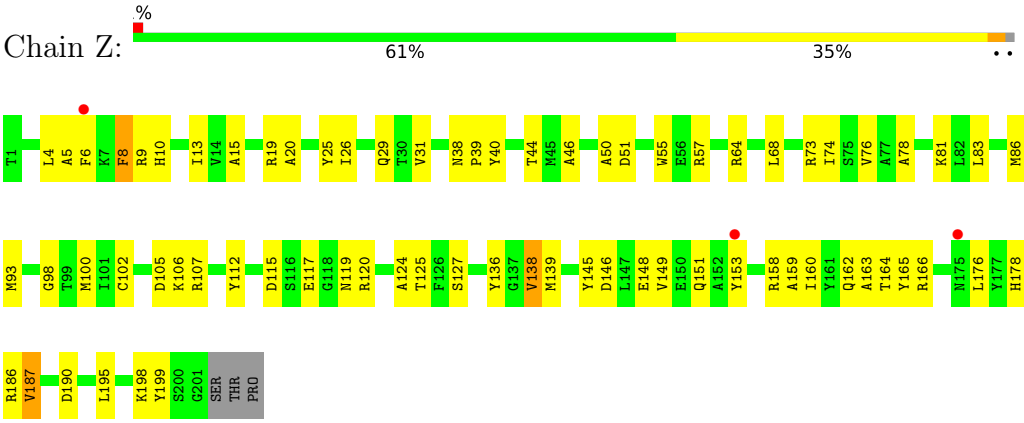


• Molecule 12: 20S proteasome



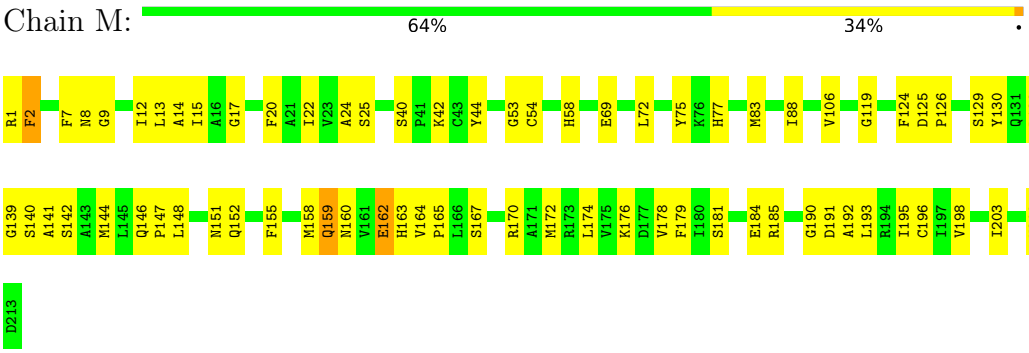
• Molecule 12: 20S proteasome

Chain Z:



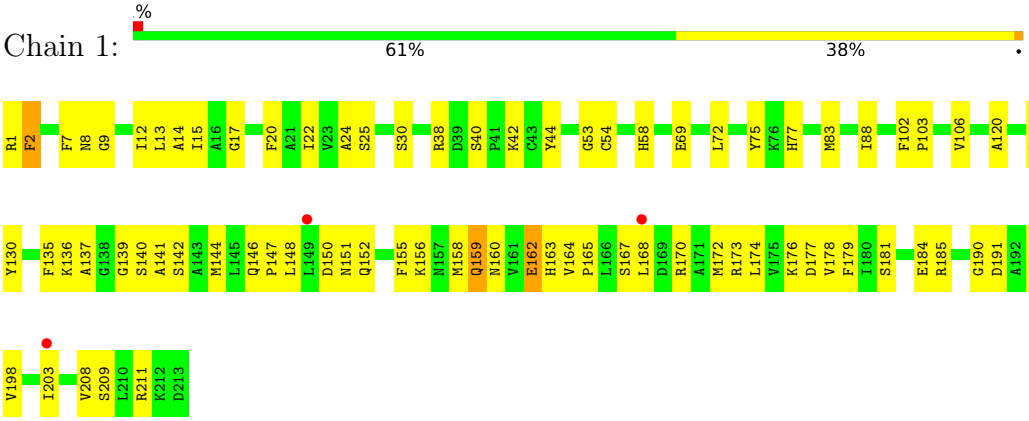
• Molecule 13: 20S proteasome

Chain M:



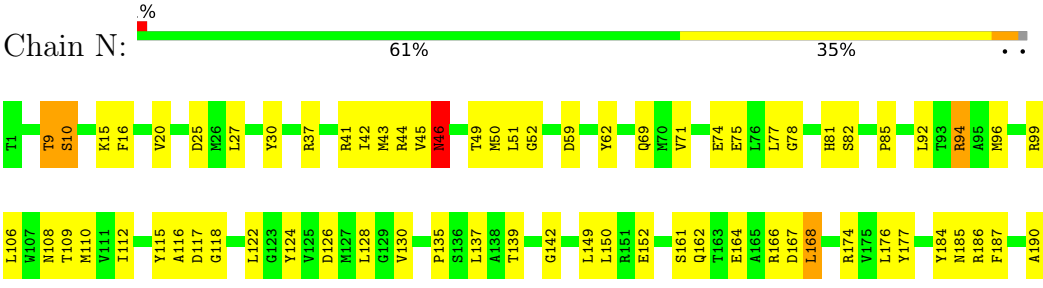
• Molecule 13: 20S proteasome

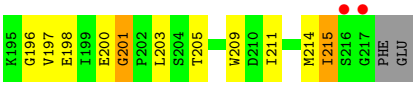
Chain 1:



• Molecule 14: 20S proteasome

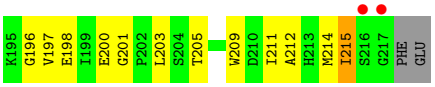
Chain N:





• Molecule 14: 20S proteasome

Chain 2:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	316.70Å 205.90Å 116.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	65.00 – 2.75 67.08 – 2.75	Depositor EDS
% Data completeness (in resolution range)	(Not available) (65.00-2.75) 96.1 (67.08-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.09 (at 2.73Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.250 , 0.294 0.249 , 0.294	Depositor DCC
R_{free} test set	9420 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	67.6	Xtriage
Anisotropy	0.397	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 56.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	47757	wwPDB-VP
Average B, all atoms (Å^2)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.96% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.36	0/1875	0.66	0/2545
1	O	0.43	0/1875	0.67	0/2545
2	B	0.33	0/1742	0.63	0/2372
2	P	0.38	0/1742	0.64	0/2372
3	C	0.34	0/1931	0.61	0/2613
3	Q	0.39	0/1931	0.61	0/2613
4	D	0.33	0/1688	0.60	0/2310
4	R	0.35	0/1688	0.62	0/2310
5	E	0.42	0/1790	0.64	0/2424
5	S	0.40	0/1790	0.63	0/2424
6	F	0.40	0/1885	0.71	0/2552
6	T	0.40	0/1885	0.71	1/2552 (0.0%)
7	G	0.41	0/1920	0.64	0/2591
7	U	0.44	0/1920	0.65	0/2591
8	H	0.43	0/1535	0.70	0/2078
8	V	0.46	0/1535	0.70	0/2078
9	I	0.39	0/1672	0.70	2/2267 (0.1%)
9	W	0.43	0/1672	0.71	2/2267 (0.1%)
10	J	0.40	0/1614	0.70	0/2178
10	X	0.46	0/1614	0.72	0/2178
11	K	0.39	0/1603	0.68	0/2174
11	Y	0.42	0/1603	0.69	0/2174
12	L	0.43	0/1579	0.68	0/2134
12	Z	0.42	0/1579	0.67	0/2134
13	1	0.41	0/1669	0.66	0/2250
13	M	0.45	0/1669	0.67	0/2250
14	2	0.43	0/1704	0.73	2/2311 (0.1%)
14	N	0.45	0/1704	0.73	2/2311 (0.1%)
All	All	0.41	0/48414	0.67	9/65598 (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
14	2	0	1
14	N	0	1
All	All	0	2

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	I	187	ARG	C-N-CD	5.89	140.76	128.40
9	W	187	ARG	C-N-CD	5.80	140.59	128.40
14	N	109	THR	N-CA-C	-5.38	96.49	111.00
14	N	106	LEU	N-CA-C	-5.24	96.84	111.00
14	2	109	THR	N-CA-C	-5.19	96.99	111.00
6	T	225	ASP	N-CA-C	5.13	124.86	111.00
14	2	106	LEU	N-CA-C	-5.11	97.22	111.00
9	W	105	VAL	N-CA-C	-5.10	97.22	111.00
9	I	105	VAL	N-CA-C	-5.05	97.35	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
14	2	30	TYR	Sidechain
14	N	30	TYR	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1842	0	1803	101	0
1	O	1842	0	1803	107	0
2	B	1707	0	1591	96	0
2	P	1707	0	1591	101	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1902	0	1835	134	0
3	Q	1902	0	1835	136	0
4	D	1665	0	1433	100	0
4	R	1665	0	1433	100	0
5	E	1763	0	1708	83	0
5	S	1763	0	1708	82	0
6	F	1850	0	1822	102	0
6	T	1850	0	1822	95	0
7	G	1885	0	1843	88	0
7	U	1885	0	1843	84	0
8	H	1509	0	1473	58	0
8	V	1509	0	1473	55	0
9	I	1645	0	1649	105	0
9	W	1645	0	1649	94	0
10	J	1585	0	1600	109	0
10	X	1585	0	1600	108	0
11	K	1570	0	1546	103	0
11	Y	1570	0	1546	102	0
12	L	1548	0	1499	78	0
12	Z	1548	0	1499	82	0
13	1	1639	0	1609	81	0
13	M	1639	0	1609	69	0
14	2	1671	0	1625	77	0
14	N	1671	0	1625	80	0
15	1	2	0	0	0	0
15	A	1	0	0	0	0
15	B	1	0	0	0	0
15	C	1	0	0	0	0
15	D	1	0	0	0	0
15	G	3	0	0	0	0
15	I	1	0	0	0	0
15	J	4	0	0	0	0
15	K	1	0	0	0	0
15	M	2	0	0	0	0
15	O	1	0	0	0	0
15	P	1	0	0	0	0
15	Q	1	0	0	0	0
15	R	1	0	0	0	0
15	U	3	0	0	0	0
15	W	1	0	0	0	0
15	X	4	0	0	0	0
15	Y	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	1	4	0	0	1	0
16	2	8	0	0	1	0
16	A	2	0	0	0	0
16	B	3	0	0	0	0
16	C	3	0	0	0	0
16	F	6	0	0	1	0
16	G	4	0	0	1	0
16	H	7	0	0	0	0
16	I	6	0	0	2	0
16	J	1	0	0	0	0
16	K	6	0	0	0	0
16	L	8	0	0	0	0
16	M	10	0	0	0	0
16	N	9	0	0	4	0
16	O	7	0	0	1	0
16	P	6	0	0	1	0
16	Q	3	0	0	1	0
16	R	3	0	0	0	0
16	S	1	0	0	0	0
16	T	7	0	0	1	0
16	U	9	0	0	0	0
16	V	15	0	0	0	0
16	W	9	0	0	0	0
16	X	17	0	0	0	0
16	Y	3	0	0	1	0
16	Z	8	0	0	0	0
All	All	47757	0	46072	2398	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 26.

All (2398) 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)
11:K:145:ARG:HE	12:Z:158:ARG:HD2	1.01	1.14
3:Q:180:LYS:H	3:Q:180:LYS:HD3	1.10	1.11
12:L:158:ARG:HD2	11:Y:145:ARG:HE	1.10	1.08
3:C:180:LYS:HD3	3:C:180:LYS:H	1.10	1.07
4:D:57:ARG:HA	4:D:60:ARG:HE	1.18	1.06
8:H:76:VAL:HB	8:H:110:GLN:HE21	1.17	1.05
8:V:76:VAL:HB	8:V:110:GLN:HE21	1.22	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:57:ARG:HA	4:R:60:ARG:HE	1.19	1.04
14:2:49:THR:HG22	14:2:85:PRO:HG3	1.38	1.03
7:G:47:PHE:HB2	7:G:214:SER:HB2	1.39	1.03
7:U:47:PHE:HB2	7:U:214:SER:HB2	1.42	1.01
14:N:49:THR:HG22	14:N:85:PRO:HG3	1.40	0.98
4:R:38:ARG:HB2	4:R:38:ARG:HH11	1.28	0.98
10:J:7:ASN:ND2	10:J:57:ALA:H	1.61	0.97
11:K:145:ARG:HE	12:Z:158:ARG:CD	1.77	0.97
11:K:145:ARG:NE	12:Z:158:ARG:HD2	1.77	0.97
10:X:7:ASN:ND2	10:X:57:ALA:H	1.63	0.96
7:G:42:LYS:HE2	7:G:185:THR:HG22	1.46	0.95
1:A:126:THR:HG22	2:B:127:ARG:HH21	1.32	0.95
4:D:38:ARG:HB2	4:D:38:ARG:HH11	1.30	0.95
7:U:42:LYS:HE2	7:U:185:THR:HG22	1.45	0.95
1:A:67:THR:HG22	1:A:69:LEU:H	1.28	0.95
13:M:8:ASN:HD22	13:M:58:HIS:H	1.14	0.94
1:O:67:THR:HG22	1:O:69:LEU:H	1.29	0.94
6:T:206:THR:H	6:T:209:ASN:HD21	1.02	0.93
13:1:8:ASN:HD22	13:1:58:HIS:H	1.13	0.93
9:I:40:ASN:H	9:I:40:ASN:HD22	1.16	0.93
6:F:206:THR:H	6:F:209:ASN:HD21	1.02	0.93
4:R:104:VAL:HG11	4:R:143:ARG:HB2	1.50	0.92
9:I:198:ARG:HH21	9:I:202:TYR:H	1.17	0.92
13:1:8:ASN:ND2	13:1:58:HIS:H	1.67	0.92
10:J:34:LEU:HD23	12:Z:166:ARG:HD3	1.51	0.92
1:O:126:THR:HG22	2:P:127:ARG:HH21	1.34	0.91
1:O:76:ILE:HD12	1:O:111:VAL:HG22	1.52	0.91
1:A:221:THR:HG22	1:A:223:GLU:H	1.35	0.91
9:W:40:ASN:H	9:W:40:ASN:HD22	1.15	0.91
8:H:76:VAL:HB	8:H:110:GLN:NE2	1.85	0.91
1:O:221:THR:HG22	1:O:223:GLU:H	1.33	0.91
10:X:145:GLN:HE21	10:X:145:GLN:H	0.93	0.90
12:L:19:ARG:HH21	12:L:29:GLN:HE22	1.18	0.90
13:M:8:ASN:ND2	13:M:58:HIS:H	1.69	0.90
10:J:145:GLN:HE21	10:J:145:GLN:H	0.93	0.89
4:D:104:VAL:HG11	4:D:143:ARG:HB2	1.51	0.89
1:A:76:ILE:HD12	1:A:111:VAL:HG22	1.52	0.89
11:Y:1:MET:CE	11:Y:134:TYR:H	1.86	0.89
7:U:34:SER:HB3	7:U:65:ARG:HH12	1.37	0.89
10:X:26:ARG:HB3	10:X:26:ARG:HH11	1.37	0.89
11:K:197:PRO:HB2	11:Y:197:PRO:HB2	1.55	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:13:TRP:H	7:G:22:GLN:HE22	1.12	0.88
8:V:76:VAL:HB	8:V:110:GLN:NE2	1.88	0.88
12:L:158:ARG:HD2	11:Y:145:ARG:NE	1.88	0.88
3:C:8:ARG:HB3	3:C:11:ILE:HD12	1.54	0.88
3:Q:8:ARG:HB3	3:Q:11:ILE:HD12	1.56	0.88
9:I:199:LEU:HD22	13:1:176:LYS:HD2	1.56	0.88
5:S:146:VAL:HG23	5:S:220:VAL:HG12	1.54	0.88
7:G:34:SER:HB3	7:G:65:ARG:HH12	1.38	0.88
5:E:146:VAL:HG23	5:E:220:VAL:HG12	1.55	0.87
9:W:198:ARG:HH21	9:W:202:TYR:H	1.17	0.87
10:J:26:ARG:HB3	10:J:26:ARG:HH11	1.39	0.87
11:Y:182:ILE:HD11	11:Y:191:LEU:HD11	1.56	0.86
14:2:51:LEU:HD13	14:2:112:ILE:HD13	1.56	0.86
11:K:81:ALA:HB2	11:K:104:LEU:HD23	1.57	0.86
9:I:190:THR:HG22	9:I:192:PRO:HD3	1.54	0.86
10:X:7:ASN:HD22	10:X:57:ALA:H	1.22	0.86
11:K:182:ILE:HD11	11:K:191:LEU:HD11	1.55	0.86
9:W:190:THR:HG22	9:W:192:PRO:HD3	1.58	0.86
11:K:1:MET:CE	11:K:134:TYR:H	1.89	0.85
10:J:145:GLN:HE21	10:J:145:GLN:N	1.75	0.85
10:J:160:PRO:HB3	10:J:189:ILE:HD11	1.56	0.85
9:I:75:ARG:HA	9:I:104:ASP:OD1	1.77	0.85
6:T:13:TRP:H	7:U:22:GLN:HE22	1.25	0.85
3:C:95:GLN:HE22	3:C:98:LEU:HD23	1.41	0.84
14:2:192:VAL:HG12	14:2:197:VAL:HG22	1.58	0.84
4:R:181:ILE:HA	4:R:186:LEU:HB3	1.60	0.84
5:S:210:LEU:HD11	5:S:215:ILE:HD13	1.59	0.84
11:K:151:ILE:HG13	11:K:155:ARG:HB2	1.59	0.84
12:L:158:ARG:CD	11:Y:145:ARG:HE	1.89	0.84
14:N:192:VAL:HG12	14:N:197:VAL:HG22	1.59	0.84
12:Z:19:ARG:HH21	12:Z:29:GLN:HE22	1.24	0.84
10:J:7:ASN:HD22	10:J:57:ALA:H	1.22	0.84
12:L:166:ARG:HD3	10:X:34:LEU:HD23	1.58	0.84
3:Q:180:LYS:H	3:Q:180:LYS:CD	1.89	0.84
10:X:160:PRO:HB3	10:X:189:ILE:HD11	1.59	0.84
8:H:14:LEU:HD21	8:H:101:ALA:HB3	1.60	0.84
11:K:151:ILE:HG13	11:K:155:ARG:CB	2.07	0.84
14:N:51:LEU:HD13	14:N:112:ILE:HD13	1.60	0.84
10:X:145:GLN:H	10:X:145:GLN:NE2	1.76	0.84
9:I:198:ARG:NH2	9:I:202:TYR:H	1.75	0.83
11:Y:1:MET:HE1	11:Y:134:TYR:H	1.42	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:151:ILE:HG13	11:Y:155:ARG:HB2	1.58	0.83
8:V:14:LEU:HD21	8:V:101:ALA:HB3	1.60	0.83
9:W:198:ARG:NH2	9:W:202:TYR:H	1.74	0.83
5:E:210:LEU:HD11	5:E:215:ILE:HD13	1.60	0.83
6:F:238:GLU:O	6:F:239:ARG:HB3	1.76	0.83
6:F:151:ALA:HB3	7:G:82:ALA:HB1	1.61	0.83
10:J:126:LEU:HD13	10:J:127:ILE:HG23	1.61	0.83
11:Y:151:ILE:HG13	11:Y:155:ARG:CB	2.08	0.82
9:W:205:GLU:O	9:W:208:THR:HG22	1.80	0.82
10:X:145:GLN:HE21	10:X:145:GLN:N	1.75	0.82
10:J:189:ILE:HG23	10:J:196:THR:HB	1.61	0.82
10:X:126:LEU:HD13	10:X:127:ILE:HG23	1.61	0.82
5:E:96:THR:HA	5:E:107:MET:HE3	1.62	0.82
10:J:116:THR:O	10:J:192:LYS:HE2	1.79	0.81
2:P:213:ASN:HD21	2:P:215:ALA:HB3	1.45	0.81
3:Q:95:GLN:HE22	3:Q:98:LEU:HD23	1.43	0.81
9:W:75:ARG:HA	9:W:104:ASP:OD1	1.79	0.81
10:X:116:THR:O	10:X:192:LYS:HE2	1.79	0.81
2:B:213:ASN:HD21	2:B:215:ALA:HB3	1.44	0.81
4:D:181:ILE:HA	4:D:186:LEU:HB3	1.60	0.81
3:C:239:LYS:O	3:C:239:LYS:HD3	1.80	0.81
6:F:196:ARG:HD3	6:F:239:ARG:HD3	1.63	0.81
10:J:145:GLN:H	10:J:145:GLN:NE2	1.77	0.81
11:K:1:MET:HE1	11:K:134:TYR:H	1.44	0.80
5:S:96:THR:HA	5:S:107:MET:HE3	1.63	0.80
3:Q:187:LYS:HA	3:Q:187:LYS:HE3	1.63	0.80
11:Y:81:ALA:HB2	11:Y:104:LEU:HD23	1.62	0.80
6:F:196:ARG:HH22	6:F:236:LEU:HD13	1.47	0.80
13:1:1:ARG:HG3	13:1:2:PHE:H	1.47	0.80
3:C:187:LYS:NZ	3:C:236:LEU:HD11	1.97	0.80
9:I:205:GLU:O	9:I:208:THR:HG22	1.82	0.80
3:C:180:LYS:HD3	3:C:180:LYS:N	1.95	0.80
13:M:1:ARG:HG3	13:M:2:PHE:H	1.46	0.80
3:Q:239:LYS:O	3:Q:239:LYS:HD3	1.82	0.80
4:D:57:ARG:HA	4:D:60:ARG:NE	1.96	0.80
5:S:117:SER:O	5:S:120:ALA:HB2	1.82	0.80
5:E:31:ILE:HD13	5:E:140:ALA:HB2	1.65	0.79
11:K:2:GLU:OE1	11:K:47:VAL:HG13	1.83	0.79
3:C:187:LYS:HA	3:C:187:LYS:HE3	1.64	0.79
11:K:80:ALA:O	11:K:84:THR:HG23	1.83	0.79
5:S:31:ILE:HD13	5:S:140:ALA:HB2	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:187:LYS:NZ	3:Q:236:LEU:HD11	1.98	0.79
11:Y:9:GLY:HA3	11:Y:12:TYR:CE2	2.17	0.79
3:C:180:LYS:H	3:C:180:LYS:CD	1.89	0.79
11:Y:80:ALA:O	11:Y:84:THR:HG23	1.82	0.78
4:R:57:ARG:HA	4:R:60:ARG:NE	1.96	0.78
6:T:206:THR:H	6:T:209:ASN:ND2	1.81	0.78
10:X:189:ILE:HG23	10:X:196:THR:HB	1.63	0.78
9:W:104:ASP:HB3	9:W:106:THR:H	1.49	0.78
12:L:6:PHE:HB2	12:L:125:THR:HG22	1.66	0.78
12:Z:138:VAL:HG21	12:Z:159:ALA:HA	1.65	0.78
11:K:9:GLY:HA3	11:K:12:TYR:CE2	2.19	0.78
3:C:79:ILE:HD13	3:C:131:GLY:HA3	1.66	0.78
4:R:38:ARG:HB2	4:R:38:ARG:NH1	1.98	0.78
6:T:230:SER:HB2	6:T:231:PRO:HD3	1.64	0.78
9:I:104:ASP:HB3	9:I:106:THR:H	1.48	0.77
5:E:117:SER:O	5:E:120:ALA:HB2	1.83	0.77
2:B:73:LEU:HD21	2:B:135:ILE:HG13	1.66	0.77
2:B:44:VAL:HG22	2:B:211:ILE:HG22	1.66	0.77
11:K:66:LEU:O	11:K:70:ARG:HG3	1.85	0.77
12:L:8:PHE:H	12:L:8:PHE:HD2	1.33	0.77
6:T:36:VAL:HG22	6:T:160:SER:HB2	1.67	0.77
4:D:136:PHE:HA	4:D:142:PRO:HA	1.67	0.77
12:L:19:ARG:HH21	12:L:29:GLN:NE2	1.81	0.77
1:A:73:THR:HG22	1:A:74:GLU:N	2.00	0.77
4:D:38:ARG:HB2	4:D:38:ARG:NH1	1.99	0.77
6:F:230:SER:HB2	6:F:231:PRO:HD3	1.66	0.77
2:P:44:VAL:HG22	2:P:211:ILE:HG22	1.65	0.77
6:T:151:ALA:HB3	7:U:82:ALA:HB1	1.67	0.77
12:L:138:VAL:HG21	12:L:159:ALA:HA	1.67	0.76
4:R:136:PHE:HA	4:R:142:PRO:HA	1.67	0.76
12:Z:8:PHE:H	12:Z:8:PHE:HD2	1.33	0.76
8:H:166:ARG:NE	14:2:37:ARG:HH21	1.84	0.76
1:O:73:THR:HG22	1:O:74:GLU:N	2.00	0.76
14:2:51:LEU:HD11	14:2:110:MET:HB3	1.68	0.76
9:W:198:ARG:HH21	9:W:202:TYR:N	1.84	0.76
12:Z:19:ARG:HH21	12:Z:29:GLN:NE2	1.84	0.76
6:F:206:THR:H	6:F:209:ASN:ND2	1.82	0.76
12:Z:6:PHE:HB2	12:Z:125:THR:HG22	1.68	0.75
3:Q:175:LEU:HD21	3:Q:196:VAL:HG21	1.68	0.75
11:Y:66:LEU:O	11:Y:70:ARG:HG3	1.87	0.75
5:E:96:THR:HA	5:E:107:MET:CE	2.15	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:200:THR:O	1:O:204:THR:HG23	1.87	0.75
11:K:45:LEU:HB2	11:K:103:LEU:HB2	1.69	0.75
10:X:20:VAL:HB	10:X:190:ILE:HD11	1.69	0.75
12:Z:76:VAL:HG23	12:Z:105:ASP:OD1	1.87	0.75
8:H:179:ILE:HG12	8:H:184:VAL:HG22	1.69	0.75
9:W:64:GLU:O	9:W:68:LEU:HB2	1.85	0.75
6:F:36:VAL:HG22	6:F:160:SER:HB2	1.67	0.75
14:N:37:ARG:HH21	8:V:166:ARG:NE	1.84	0.75
2:P:73:LEU:HD21	2:P:135:ILE:HG13	1.68	0.75
9:I:40:ASN:HD22	9:I:40:ASN:N	1.84	0.75
7:U:34:SER:HB3	7:U:65:ARG:NH1	2.02	0.75
3:Q:79:ILE:HD13	3:Q:131:GLY:HA3	1.67	0.74
9:W:40:ASN:HD22	9:W:40:ASN:N	1.83	0.74
11:Y:2:GLU:OE1	11:Y:47:VAL:HG13	1.87	0.74
14:2:15:LYS:HE2	14:2:135:PRO:HA	1.68	0.74
10:J:45:MET:HE1	10:J:67:LEU:HG	1.70	0.74
13:1:159:GLN:NE2	13:1:160:ASN:H	1.85	0.74
14:N:51:LEU:HD11	14:N:110:MET:HB3	1.69	0.74
13:M:40:SER:O	13:M:42:LYS:HE3	1.87	0.74
5:S:96:THR:HA	5:S:107:MET:CE	2.17	0.74
11:Y:180:VAL:HG12	11:Y:191:LEU:HD12	1.70	0.74
2:P:64:VAL:HG22	2:P:74:VAL:HG12	1.70	0.74
14:N:15:LYS:HE2	14:N:135:PRO:HA	1.68	0.73
1:A:130:GLU:HG2	2:B:4:GLY:HA2	1.70	0.73
3:C:175:LEU:HD21	3:C:196:VAL:HG21	1.69	0.73
8:V:179:ILE:HG12	8:V:184:VAL:HG22	1.68	0.73
14:N:46:ASN:C	14:N:46:ASN:HD22	1.90	0.73
10:X:10:ALA:HB1	10:X:146:MET:HE2	1.71	0.73
9:I:198:ARG:HH21	9:I:202:TYR:N	1.85	0.73
14:2:46:ASN:C	14:2:46:ASN:HD22	1.91	0.73
7:G:34:SER:HB3	7:G:65:ARG:NH1	2.02	0.73
2:B:149:ASP:HB2	2:B:150:PRO:HD2	1.69	0.73
9:W:40:ASN:H	9:W:40:ASN:ND2	1.87	0.73
11:K:38:MET:CE	11:K:60:ILE:HG22	2.19	0.73
12:L:76:VAL:HG23	12:L:105:ASP:OD1	1.86	0.73
10:J:10:ALA:HB1	10:J:146:MET:HE2	1.70	0.73
2:P:182:GLU:HG2	2:P:183:LEU:H	1.53	0.73
13:1:40:SER:O	13:1:42:LYS:HE3	1.87	0.73
13:M:159:GLN:NE2	13:M:160:ASN:H	1.87	0.73
3:Q:180:LYS:HD3	3:Q:180:LYS:N	1.95	0.73
2:B:37:ILE:HD12	2:B:190:ALA:HB2	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:182:GLU:HG2	2:B:183:LEU:H	1.53	0.72
1:A:141:ILE:HG22	1:A:151:VAL:HG22	1.71	0.72
9:I:64:GLU:O	9:I:68:LEU:HB2	1.88	0.72
4:R:33:VAL:HG12	4:R:160:ALA:HB2	1.72	0.72
9:I:40:ASN:H	9:I:40:ASN:ND2	1.88	0.72
1:O:141:ILE:HG22	1:O:151:VAL:HG22	1.72	0.72
4:D:33:VAL:HG12	4:D:160:ALA:HB2	1.71	0.72
7:G:74:GLY:HA3	7:G:224:HIS:CD2	2.25	0.72
12:Z:10:HIS:O	12:Z:178:HIS:HE1	1.73	0.72
2:B:165:ASN:HD22	2:B:197:SER:HB2	1.54	0.72
7:G:125:TYR:HB3	16:G:323:HOH:O	1.89	0.72
11:Y:45:LEU:HB2	11:Y:103:LEU:HB2	1.71	0.72
3:Q:35:LEU:HB2	3:Q:162:THR:O	1.90	0.72
2:B:228:TYR:HA	2:B:232:ILE:O	1.89	0.71
11:Y:38:MET:CE	11:Y:60:ILE:HG22	2.20	0.71
1:O:73:THR:HG22	1:O:74:GLU:H	1.53	0.71
10:J:116:THR:HG22	10:J:117:PHE:N	2.05	0.71
2:P:37:ILE:HD12	2:P:190:ALA:HB2	1.72	0.71
10:X:58:THR:HG21	11:Y:121:LEU:O	1.91	0.71
1:A:73:THR:HG22	1:A:74:GLU:H	1.55	0.71
2:B:73:LEU:CD2	2:B:135:ILE:HG13	2.20	0.71
1:A:221:THR:HG22	1:A:223:GLU:N	2.06	0.71
12:L:125:THR:HB	12:L:139:MET:CE	2.20	0.71
2:P:228:TYR:HA	2:P:232:ILE:O	1.89	0.71
8:V:40:ARG:HH11	8:V:40:ARG:HG3	1.56	0.71
14:2:115:TYR:OH	14:2:118:GLY:HA2	1.91	0.71
2:P:149:ASP:HB2	2:P:150:PRO:HD2	1.72	0.71
10:X:116:THR:HG22	10:X:117:PHE:N	2.05	0.71
1:O:158:GLY:O	2:P:83:ARG:NH2	2.24	0.71
2:P:165:ASN:HD22	2:P:197:SER:HB2	1.56	0.71
3:C:35:LEU:HB2	3:C:162:THR:O	1.90	0.70
8:H:13:VAL:O	8:H:14:LEU:HD23	1.91	0.70
11:Y:43:LEU:O	11:Y:104:LEU:HD12	1.91	0.70
6:F:62:LYS:O	6:F:73:SER:HA	1.91	0.70
10:J:20:VAL:HB	10:J:190:ILE:HD11	1.71	0.70
13:M:211:ARG:NH2	9:W:193:ASN:HB3	2.05	0.70
5:S:189:MET:HE1	5:S:194:ALA:HA	1.73	0.70
10:J:58:THR:HG21	11:K:121:LEU:O	1.92	0.70
1:O:221:THR:HG22	1:O:223:GLU:N	2.04	0.70
2:P:73:LEU:CD2	2:P:135:ILE:HG13	2.21	0.70
7:U:74:GLY:HA3	7:U:224:HIS:CD2	2.26	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:180:VAL:HG12	11:K:191:LEU:HD12	1.74	0.70
12:L:115:ASP:HB3	12:L:117:GLU:H	1.56	0.70
1:A:200:THR:O	1:A:204:THR:HG23	1.92	0.70
14:N:115:TYR:OH	14:N:118:GLY:HA2	1.92	0.70
6:T:62:LYS:O	6:T:73:SER:HA	1.92	0.70
6:T:237:GLU:C	6:T:239:ARG:H	1.93	0.70
2:P:64:VAL:HG22	2:P:74:VAL:CG1	2.22	0.70
9:I:187:ARG:HB3	9:I:188:PRO:CD	2.22	0.70
11:K:43:LEU:O	11:K:104:LEU:HD12	1.92	0.70
12:L:10:HIS:O	12:L:178:HIS:HE1	1.73	0.70
12:Z:125:THR:HB	12:Z:139:MET:CE	2.21	0.70
11:K:61:GLN:HE21	11:K:62:LYS:CE	2.05	0.69
10:X:93:ASN:O	10:X:97:GLU:HG3	1.92	0.69
14:2:49:THR:HG22	14:2:85:PRO:CG	2.20	0.69
9:I:3:ILE:HD11	9:I:127:MET:HB2	1.73	0.69
9:W:187:ARG:HB3	9:W:188:PRO:CD	2.21	0.69
2:B:64:VAL:HG22	2:B:74:VAL:HG12	1.72	0.69
3:C:76:VAL:HG13	3:C:132:VAL:HG13	1.73	0.69
13:1:1:ARG:CG	13:1:2:PHE:H	2.05	0.69
5:E:189:MET:HE1	5:E:194:ALA:HA	1.74	0.69
12:L:125:THR:HB	12:L:139:MET:HE1	1.74	0.69
1:O:171:LYS:HB3	1:O:205:VAL:HG11	1.75	0.69
2:P:178:ASN:O	2:P:181:LEU:HG	1.93	0.69
10:J:93:ASN:O	10:J:97:GLU:HG3	1.93	0.69
10:X:45:MET:HE1	10:X:67:LEU:HG	1.72	0.69
10:X:68:LYS:HZ2	10:X:72:ASN:HD21	1.41	0.69
1:A:171:LYS:HB3	1:A:205:VAL:HG11	1.74	0.68
5:E:24:VAL:O	5:E:28:ILE:HG12	1.94	0.68
10:J:125:ASP:HB2	10:J:129:CYS:H	1.58	0.68
13:M:1:ARG:CG	13:M:2:PHE:H	2.05	0.68
9:W:3:ILE:HD11	9:W:127:MET:HB2	1.75	0.68
12:Z:115:ASP:HB3	12:Z:117:GLU:H	1.58	0.68
9:I:143:ARG:NH1	9:I:146:MET:HG2	2.09	0.68
10:J:68:LYS:NZ	10:J:72:ASN:HD21	1.92	0.68
8:H:40:ARG:HH11	8:H:40:ARG:HG3	1.59	0.68
4:R:42:VAL:HA	4:R:210:VAL:HG12	1.76	0.68
2:B:178:ASN:O	2:B:181:LEU:HG	1.92	0.68
3:C:115:CYS:HB3	4:D:81:ARG:HH12	1.59	0.68
3:Q:45:LEU:HG	3:Q:137:ILE:HD13	1.76	0.68
14:N:135:PRO:HG2	16:N:220:HOH:O	1.93	0.68
6:F:159:MET:HG3	6:F:160:SER:N	2.10	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:167:LYS:HE3	7:U:206:ASP:OD2	1.94	0.67
1:A:231:THR:O	1:A:235:ILE:HG13	1.95	0.67
6:T:159:MET:HG3	6:T:160:SER:N	2.09	0.67
11:K:182:ILE:CD1	11:K:191:LEU:HD11	2.24	0.67
2:P:171:THR:HA	2:P:174:GLU:HB2	1.76	0.67
3:Q:105:ILE:HG22	16:Q:417:HOH:O	1.93	0.67
8:V:14:LEU:HD21	8:V:101:ALA:CB	2.24	0.67
10:J:114:PRO:O	10:J:115:LYS:HD2	1.94	0.67
1:O:231:THR:O	1:O:235:ILE:HG13	1.94	0.67
7:G:90:ILE:HD13	7:G:118:TYR:CE2	2.30	0.67
4:R:20:GLU:O	4:R:24:GLU:HG2	1.94	0.67
8:V:13:VAL:O	8:V:14:LEU:HD23	1.93	0.67
3:C:45:LEU:HG	3:C:137:ILE:HD13	1.76	0.67
10:J:36:THR:HG23	10:J:38:ASP:OD2	1.95	0.67
11:Y:182:ILE:CD1	11:Y:191:LEU:HD11	2.25	0.67
5:E:84:ASP:OD2	5:E:135:ARG:NH2	2.28	0.67
9:W:143:ARG:NH1	9:W:146:MET:HG2	2.10	0.67
2:B:171:THR:HA	2:B:174:GLU:HB2	1.77	0.66
11:K:38:MET:HE3	11:K:60:ILE:HG22	1.77	0.66
3:Q:115:CYS:HB3	4:R:81:ARG:HH12	1.60	0.66
11:Y:24:ASN:ND2	11:Y:25:ILE:HG12	2.10	0.66
11:Y:183:ILE:HG12	11:Y:188:ILE:HG13	1.76	0.66
1:A:158:GLY:O	2:B:83:ARG:NH2	2.28	0.66
14:N:9:THR:HG22	16:N:223:HOH:O	1.93	0.66
5:S:24:VAL:O	5:S:28:ILE:HG12	1.96	0.66
10:X:190:ILE:HG22	10:X:195:ILE:CD1	2.25	0.66
14:2:51:LEU:HD13	14:2:112:ILE:CD1	2.24	0.66
10:X:36:THR:HG23	10:X:38:ASP:OD2	1.96	0.66
10:X:65:GLN:NE2	11:Y:86:ARG:NH2	2.43	0.66
13:1:120:ALA:HA	16:1:420:HOH:O	1.96	0.66
4:D:42:VAL:HA	4:D:210:VAL:HG12	1.77	0.66
4:D:181:ILE:H	4:D:186:LEU:HD23	1.60	0.66
6:F:13:TRP:H	7:G:22:GLN:NE2	1.91	0.66
13:M:176:LYS:HD2	9:W:199:LEU:HD22	1.76	0.66
13:1:198:VAL:HG22	13:1:203:ILE:HG12	1.78	0.66
3:Q:155:ASN:OD1	4:R:77:THR:HG21	1.96	0.66
10:X:114:PRO:O	10:X:115:LYS:HD2	1.95	0.66
10:X:125:ASP:HB2	10:X:129:CYS:H	1.59	0.66
7:G:167:LYS:HE3	7:G:206:ASP:OD2	1.96	0.66
3:Q:187:LYS:HZ3	3:Q:236:LEU:HD11	1.59	0.66
13:M:198:VAL:HG22	13:M:203:ILE:HG12	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:154:GLY:O	4:R:81:ARG:NH2	2.29	0.66
6:T:89:ARG:NH1	13:1:77:HIS:HB3	2.11	0.66
13:1:125:ASP:HB2	13:1:126:PRO:HD2	1.78	0.66
10:J:190:ILE:HG22	10:J:195:ILE:CD1	2.26	0.66
2:B:149:ASP:HB2	2:B:150:PRO:CD	2.26	0.66
8:H:29:ARG:HD2	14:2:209:TRP:CZ3	2.31	0.66
1:O:130:GLU:HG2	2:P:4:GLY:HA2	1.78	0.66
4:R:31:THR:HB	4:R:46:GLU:CB	2.25	0.66
2:B:64:VAL:HG22	2:B:74:VAL:CG1	2.26	0.65
9:I:121:LYS:HD2	14:2:215:ILE:O	1.95	0.65
3:Q:76:VAL:HG13	3:Q:132:VAL:HG13	1.76	0.65
6:T:120:THR:O	7:U:129:ARG:NH1	2.28	0.65
14:2:45:VAL:O	14:2:46:ASN:ND2	2.29	0.65
11:Y:61:GLN:HE21	11:Y:62:LYS:CE	2.09	0.65
2:B:39:ALA:C	2:B:41:ASN:H	2.00	0.65
9:I:52:THR:O	9:I:56:THR:HB	1.97	0.65
9:I:187:ARG:HB3	9:I:188:PRO:HD3	1.78	0.65
9:I:199:LEU:HD22	13:1:176:LYS:CD	2.26	0.65
1:A:86:ASP:O	1:A:89:SER:HB3	1.96	0.65
8:H:14:LEU:HD21	8:H:101:ALA:CB	2.26	0.65
2:P:187:ILE:O	2:P:191:ILE:HG13	1.97	0.65
5:S:84:ASP:OD2	5:S:135:ARG:NH2	2.29	0.65
11:Y:38:MET:HE3	11:Y:60:ILE:HG22	1.77	0.65
6:F:139:ASP:OD1	14:N:81:HIS:CE1	2.50	0.65
4:R:98:VAL:HG12	4:R:99:GLU:N	2.12	0.65
9:W:187:ARG:HB3	9:W:188:PRO:HD3	1.77	0.65
1:A:155:ASP:HB3	1:A:157:ALA:H	1.61	0.65
3:C:155:ASN:OD1	4:D:77:THR:HG21	1.96	0.65
6:F:233:LEU:O	6:F:236:LEU:HG	1.96	0.65
1:O:54:LYS:O	1:O:56:VAL:HG23	1.96	0.65
5:S:129:ASP:HB3	5:S:130:PRO:HD2	1.79	0.65
1:A:182:LYS:HD3	1:A:197:THR:HG23	1.79	0.65
1:O:211:LYS:HB3	1:O:212:PRO:HD2	1.79	0.65
9:W:52:THR:O	9:W:56:THR:HB	1.97	0.65
13:1:8:ASN:HD22	13:1:58:HIS:N	1.93	0.65
1:A:155:ASP:OD2	1:A:159:TYR:HB2	1.96	0.65
2:B:187:ILE:O	2:B:191:ILE:HG13	1.97	0.65
4:D:181:ILE:CB	4:D:187:THR:HA	2.27	0.65
1:O:179:LEU:O	1:O:183:VAL:HG23	1.97	0.65
4:R:181:ILE:H	4:R:186:LEU:HD23	1.62	0.65
10:X:68:LYS:NZ	10:X:72:ASN:HD21	1.94	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:6:PHE:CB	12:L:125:THR:HG22	2.27	0.64
1:O:155:ASP:HB3	1:O:157:ALA:H	1.62	0.64
2:P:149:ASP:HB2	2:P:150:PRO:CD	2.27	0.64
11:K:60:ILE:HG21	11:K:84:THR:HG22	1.79	0.64
7:U:185:THR:O	7:U:189:ILE:HG12	1.97	0.64
13:1:184:GLU:OE2	13:1:211:ARG:HD2	1.98	0.64
1:A:211:LYS:HB3	1:A:212:PRO:HD2	1.79	0.64
3:C:187:LYS:HZ1	3:C:236:LEU:HD11	1.62	0.64
3:C:214:ALA:HB2	3:C:227:VAL:HG12	1.80	0.64
4:D:20:GLU:O	4:D:24:GLU:HG2	1.96	0.64
4:D:206:ILE:HG22	4:D:207:GLU:N	2.13	0.64
5:E:42:THR:HG21	5:E:190:THR:HA	1.78	0.64
3:C:174:MET:SD	3:C:196:VAL:HG22	2.37	0.64
14:N:209:TRP:CZ3	8:V:29:ARG:HD2	2.32	0.64
1:O:132:ARG:NH1	7:U:123:THR:O	2.31	0.64
3:Q:140:ASP:O	3:Q:142:HIS:N	2.31	0.64
4:R:181:ILE:CB	4:R:187:THR:HA	2.27	0.64
5:E:129:ASP:HB3	5:E:130:PRO:HD2	1.80	0.64
11:K:183:ILE:HG12	11:K:188:ILE:HG13	1.80	0.64
1:O:155:ASP:OD2	1:O:159:TYR:HB2	1.97	0.64
1:A:73:THR:HG22	1:A:75:ASN:H	1.62	0.64
3:C:154:GLY:O	4:D:81:ARG:NH2	2.30	0.64
14:N:51:LEU:HD13	14:N:112:ILE:CD1	2.28	0.64
9:W:22:GLU:HG3	9:W:22:GLU:O	1.98	0.64
4:D:31:THR:HB	4:D:46:GLU:CB	2.28	0.64
4:D:98:VAL:HG12	4:D:99:GLU:N	2.12	0.64
12:L:19:ARG:HE	12:L:29:GLN:NE2	1.94	0.64
5:S:49:ALA:HB2	5:S:217:LEU:CD2	2.28	0.64
10:J:65:GLN:NE2	11:K:86:ARG:NH2	2.45	0.64
11:K:24:ASN:ND2	11:K:25:ILE:HG12	2.12	0.64
7:U:90:ILE:HD13	7:U:118:TYR:CE2	2.33	0.64
9:W:206:LYS:HA	10:X:165:GLU:HG3	1.80	0.64
2:B:157:TRP:CE3	2:B:160:THR:HB	2.33	0.63
3:C:139:TRP:HA	3:C:144:GLY:O	1.98	0.63
8:H:30:VAL:O	8:H:30:VAL:CG1	2.47	0.63
10:J:68:LYS:HZ2	10:J:72:ASN:HD21	1.45	0.63
3:Q:174:MET:SD	3:Q:196:VAL:HG22	2.38	0.63
5:E:123:PHE:CE2	5:E:136:PRO:HG3	2.33	0.63
6:F:188:VAL:HG11	6:F:232:PHE:CD2	2.33	0.63
9:I:206:LYS:HA	10:J:165:GLU:HG3	1.78	0.63
13:M:125:ASP:HB2	13:M:126:PRO:HD2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:211:ARG:HH21	9:W:193:ASN:HB3	1.63	0.63
3:Q:214:ALA:HB2	3:Q:227:VAL:HG12	1.78	0.63
9:W:59:ILE:HG13	9:W:83:LEU:CD2	2.28	0.63
3:Q:218:ARG:NH2	3:Q:221:GLY:O	2.32	0.63
4:R:206:ILE:HG22	4:R:207:GLU:N	2.13	0.63
5:S:42:THR:HG21	5:S:190:THR:HA	1.79	0.63
9:W:153:ASN:HD22	9:W:154:LEU:N	1.97	0.63
9:I:153:ASN:HD22	9:I:154:LEU:N	1.95	0.63
1:A:192:GLU:CD	1:A:192:GLU:H	2.01	0.63
5:E:49:ALA:HB2	5:E:217:LEU:CD2	2.28	0.63
6:F:41:LYS:HG3	6:F:42:THR:HG23	1.81	0.63
9:I:152:LYS:HE3	9:I:186:LEU:CD1	2.29	0.63
14:N:45:VAL:O	14:N:46:ASN:ND2	2.32	0.63
1:O:182:LYS:HD3	1:O:197:THR:HG23	1.79	0.63
1:A:79:VAL:HG12	1:A:139:ILE:HB	1.81	0.63
1:A:201:CYS:O	1:A:205:VAL:HG23	1.98	0.63
4:D:39:ASP:HB2	4:D:184:ASP:OD1	1.99	0.63
11:Y:60:ILE:HG21	11:Y:84:THR:HG22	1.80	0.63
1:A:179:LEU:O	1:A:183:VAL:HG23	1.99	0.63
2:B:36:GLY:O	2:B:159:ALA:HA	1.99	0.63
9:I:22:GLU:HG3	9:I:22:GLU:O	1.98	0.63
13:M:146:GLN:HB2	13:M:147:PRO:HD3	1.80	0.63
4:R:39:ASP:HB2	4:R:184:ASP:OD1	1.99	0.63
9:I:59:ILE:HG13	9:I:83:LEU:CD2	2.29	0.63
12:L:8:PHE:HD2	12:L:8:PHE:N	1.97	0.63
9:I:112:SER:OG	9:I:120:ASP:HB2	1.99	0.62
9:I:187:ARG:CG	9:I:188:PRO:HD3	2.29	0.62
4:D:91:CYS:HA	4:D:102:VAL:HG21	1.82	0.62
2:P:157:TRP:CE3	2:P:160:THR:HB	2.34	0.62
3:Q:139:TRP:HA	3:Q:144:GLY:O	1.99	0.62
6:F:120:THR:O	7:G:129:ARG:NH1	2.32	0.62
14:N:49:THR:HG22	14:N:85:PRO:CG	2.21	0.62
1:O:79:VAL:HG12	1:O:139:ILE:HB	1.81	0.62
5:S:191:LEU:O	5:S:195:ILE:HG13	1.99	0.62
6:T:41:LYS:HG3	6:T:42:THR:HG23	1.80	0.62
9:W:198:ARG:NH2	9:W:201:ARG:HA	2.14	0.62
7:G:185:THR:O	7:G:189:ILE:HG12	1.99	0.62
1:O:123:GLN:O	1:O:126:THR:HB	1.99	0.62
9:W:187:ARG:CG	9:W:188:PRO:HD3	2.30	0.62
1:O:73:THR:HG22	1:O:75:ASN:H	1.65	0.62
3:C:143:TYR:HB2	3:C:146:GLN:NE2	2.15	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:136:LYS:HA	13:M:146:GLN:HE22	1.64	0.62
11:Y:43:LEU:HD12	11:Y:183:ILE:HD11	1.81	0.62
5:E:99:HIS:HB2	5:E:107:MET:HE1	1.81	0.62
1:O:86:ASP:O	1:O:89:SER:HB3	2.00	0.62
3:Q:8:ARG:HB3	3:Q:11:ILE:CD1	2.29	0.62
10:X:82:ILE:HD11	10:X:86:THR:HG22	1.82	0.62
7:U:220:THR:O	7:U:221:ASN:HB2	1.99	0.62
3:C:8:ARG:HB3	3:C:11:ILE:CD1	2.27	0.62
9:I:212:LEU:CD1	10:J:201:LYS:HA	2.30	0.62
3:C:239:LYS:HD3	3:C:239:LYS:C	2.20	0.61
5:E:206:MET:HE1	5:E:210:LEU:HB2	1.82	0.61
11:K:151:ILE:HG13	11:K:155:ARG:HB3	1.80	0.61
13:M:8:ASN:HD22	13:M:58:HIS:N	1.94	0.61
10:J:14:MET:HB2	10:J:167:ILE:HD12	1.82	0.61
12:Z:6:PHE:CB	12:Z:125:THR:HG22	2.30	0.61
1:O:192:GLU:CD	1:O:192:GLU:H	2.02	0.61
1:O:201:CYS:O	1:O:205:VAL:HG23	2.01	0.61
2:P:36:GLY:O	2:P:159:ALA:HA	2.01	0.61
4:R:4:ASP:O	4:R:122:ASN:HB3	1.99	0.61
11:Y:37:LYS:HD2	11:Y:37:LYS:N	2.16	0.61
12:Z:19:ARG:HE	12:Z:29:GLN:NE2	1.98	0.61
2:B:39:ALA:O	2:B:41:ASN:N	2.34	0.61
6:T:71:GLY:HA3	6:T:221:PHE:CZ	2.36	0.61
1:A:206:LEU:O	1:A:208:ILE:HG13	2.00	0.61
6:F:73:SER:OG	6:F:133:LEU:HB2	2.00	0.61
9:W:212:LEU:CD1	10:X:201:LYS:HA	2.30	0.61
6:T:188:VAL:HG11	6:T:232:PHE:CD2	2.36	0.61
8:V:30:VAL:CG1	8:V:30:VAL:O	2.47	0.61
1:A:54:LYS:O	1:A:56:VAL:HG23	2.01	0.61
3:C:218:ARG:NH2	3:C:221:GLY:O	2.33	0.61
9:I:193:ASN:HB3	13:1:211:ARG:NH2	2.15	0.61
9:I:198:ARG:NH2	9:I:201:ARG:HA	2.15	0.61
13:M:184:GLU:OE2	13:M:211:ARG:HD2	1.99	0.61
2:P:135:ILE:H	2:P:135:ILE:HD12	1.66	0.61
13:1:137:ALA:H	13:1:146:GLN:NE2	1.99	0.61
12:L:4:LEU:C	12:L:4:LEU:HD12	2.20	0.61
3:Q:201:MET:O	3:Q:203:VAL:N	2.34	0.61
13:1:146:GLN:HB2	13:1:147:PRO:HD3	1.81	0.61
2:B:72:GLY:HA3	2:B:217:PHE:CE1	2.36	0.61
4:D:131:ALA:O	4:D:146:GLN:HA	2.01	0.61
8:V:127:ILE:HD11	8:V:136:TYR:CE2	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1:136:LYS:HA	13:1:146:GLN:HE22	1.64	0.61
5:E:166:ASP:HB3	5:E:185:TYR:CZ	2.36	0.60
11:K:37:LYS:HD2	11:K:37:LYS:N	2.15	0.60
11:K:85:ARG:HG3	11:K:124:LEU:HB2	1.82	0.60
1:A:136:CYS:O	1:A:156:PRO:HG3	2.01	0.60
8:H:89:ARG:HD3	8:H:90:TYR:CE1	2.36	0.60
2:P:135:ILE:HD12	2:P:135:ILE:N	2.16	0.60
11:Y:37:LYS:HD2	11:Y:37:LYS:H	1.66	0.60
1:O:172:GLN:O	1:O:176:THR:HG23	2.01	0.60
5:S:166:ASP:HB3	5:S:185:TYR:CZ	2.36	0.60
12:Z:125:THR:HB	12:Z:139:MET:HE3	1.82	0.60
4:D:4:ASP:O	4:D:122:ASN:HB3	2.01	0.60
8:H:173:VAL:HG21	8:H:190:LEU:HD23	1.82	0.60
4:R:33:VAL:HG11	4:R:168:VAL:HG11	1.84	0.60
4:D:41:VAL:HG11	4:D:134:VAL:HG13	1.83	0.60
6:F:150:SER:O	6:F:152:ASN:N	2.33	0.60
4:R:131:ALA:O	4:R:146:GLN:HA	2.01	0.60
5:S:99:HIS:HB2	5:S:107:MET:HE1	1.82	0.60
7:U:66:LEU:HD23	7:U:76:ALA:HA	1.84	0.60
1:A:172:GLN:O	1:A:176:THR:HG23	2.01	0.60
5:E:191:LEU:O	5:E:195:ILE:HG13	2.00	0.60
6:T:42:THR:OG1	6:T:43:HIS:HD2	1.85	0.60
6:T:169:ARG:HG2	7:U:57:LEU:CD1	2.31	0.60
3:C:138:GLY:HA2	3:C:216:LEU:HD13	1.83	0.60
3:Q:239:LYS:HD3	3:Q:239:LYS:C	2.22	0.60
2:B:34:SER:O	2:B:161:ALA:HA	2.02	0.60
13:M:137:ALA:H	13:M:146:GLN:NE2	2.00	0.60
1:O:141:ILE:CG2	1:O:151:VAL:HG22	2.31	0.60
9:W:213:THR:O	10:X:198:ARG:HA	2.02	0.60
11:Y:107:TYR:CE2	11:Y:185:LYS:HA	2.36	0.60
6:F:77:LEU:HA	16:F:264:HOH:O	2.00	0.60
3:Q:174:MET:HE3	3:Q:199:LYS:HG2	1.83	0.60
4:R:91:CYS:HA	4:R:102:VAL:HG21	1.83	0.60
5:S:206:MET:HE1	5:S:210:LEU:HB2	1.83	0.60
10:J:82:ILE:HD11	10:J:86:THR:HG22	1.82	0.60
4:R:66:ASP:CA	11:Y:69:MET:HE2	2.32	0.60
12:Z:8:PHE:HD2	12:Z:8:PHE:N	1.98	0.60
3:C:187:LYS:HZ3	3:C:236:LEU:HD11	1.64	0.59
4:D:33:VAL:HG11	4:D:168:VAL:HG11	1.84	0.59
3:Q:49:ARG:HD2	3:Q:212:GLU:OE1	2.02	0.59
1:A:142:GLY:HA2	1:A:220:VAL:HG21	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:127:ILE:HD11	8:H:136:TYR:CE2	2.38	0.59
5:S:27:ASP:OD2	5:S:28:ILE:N	2.36	0.59
6:T:73:SER:OG	6:T:133:LEU:HB2	2.01	0.59
6:T:206:THR:HG22	6:T:208:LYS:H	1.67	0.59
10:X:14:MET:HB2	10:X:167:ILE:HD12	1.84	0.59
1:A:123:GLN:O	1:A:126:THR:HB	2.03	0.59
1:A:141:ILE:CG2	1:A:151:VAL:HG22	2.31	0.59
3:C:201:MET:O	3:C:203:VAL:N	2.34	0.59
5:E:146:VAL:HG23	5:E:220:VAL:CG1	2.31	0.59
11:K:37:LYS:HD2	11:K:37:LYS:H	1.67	0.59
3:Q:143:TYR:HB2	3:Q:146:GLN:NE2	2.18	0.59
5:S:123:PHE:CE2	5:S:136:PRO:HG3	2.36	0.59
9:W:187:ARG:HG3	9:W:188:PRO:HD3	1.84	0.59
3:C:167:ASN:C	3:C:169:ALA:H	2.06	0.59
9:I:152:LYS:HE3	9:I:186:LEU:HD11	1.83	0.59
6:T:206:THR:N	6:T:209:ASN:HD21	1.87	0.59
8:V:89:ARG:HD3	8:V:90:TYR:CE1	2.36	0.59
12:Z:8:PHE:N	12:Z:8:PHE:CD2	2.69	0.59
14:2:115:TYR:HE2	14:2:194:GLU:HG2	1.67	0.59
3:C:115:CYS:HB3	4:D:81:ARG:NH1	2.17	0.59
4:R:11:SER:HB3	4:R:12:PRO:HD2	1.84	0.59
4:R:58:THR:O	4:R:59:VAL:HB	2.02	0.59
7:U:151:ILE:N	7:U:151:ILE:HD12	2.17	0.59
9:I:187:ARG:HG3	9:I:188:PRO:HD3	1.83	0.59
12:L:8:PHE:N	12:L:8:PHE:CD2	2.69	0.59
5:E:27:ASP:OD2	5:E:28:ILE:N	2.36	0.59
5:E:146:VAL:CG2	5:E:220:VAL:HG12	2.31	0.59
7:G:215:TRP:HB2	7:G:225:GLU:O	2.03	0.59
2:P:185:ASP:O	2:P:189:THR:HG22	2.03	0.59
5:S:108:THR:O	5:S:112:VAL:HG23	2.03	0.59
6:T:150:SER:O	6:T:152:ASN:N	2.36	0.59
12:Z:138:VAL:CG2	12:Z:159:ALA:HA	2.32	0.59
3:C:49:ARG:HD2	3:C:212:GLU:OE1	2.03	0.59
3:C:140:ASP:O	3:C:142:HIS:N	2.31	0.59
6:F:196:ARG:CD	6:F:239:ARG:HD3	2.31	0.59
10:J:151:GLU:HB2	13:1:181:SER:HB3	1.85	0.59
12:L:138:VAL:CG2	12:L:159:ALA:HA	2.33	0.59
14:N:115:TYR:HE2	14:N:194:GLU:HG2	1.68	0.59
3:Q:167:ASN:C	3:Q:169:ALA:H	2.06	0.59
5:S:99:HIS:HB2	5:S:107:MET:CE	2.33	0.59
10:X:113:ASP:HB3	10:X:116:THR:HB	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1:12:ILE:HD13	13:1:53:GLY:C	2.23	0.59
2:B:227:ASP:HB3	2:B:233:ALA:HB1	1.85	0.59
7:G:184:MET:CB	7:G:189:ILE:HD11	2.32	0.59
3:Q:138:GLY:HA2	3:Q:216:LEU:HD13	1.85	0.59
7:U:184:MET:CB	7:U:189:ILE:HD11	2.32	0.59
2:P:227:ASP:HB3	2:P:233:ALA:HB1	1.84	0.59
14:2:174:ARG:HE	14:2:205:THR:HG22	1.67	0.59
1:A:132:ARG:NH1	7:G:123:THR:O	2.36	0.58
2:B:185:ASP:O	2:B:189:THR:HG22	2.03	0.58
6:F:71:GLY:HA3	6:F:221:PHE:CZ	2.38	0.58
10:J:136:PHE:CE2	10:J:150:CYS:HB3	2.38	0.58
14:N:215:ILE:O	9:W:121:LYS:HD2	2.03	0.58
2:P:43:VAL:HG12	2:P:44:VAL:N	2.18	0.58
8:V:162:LEU:O	8:V:165:GLU:HB3	2.03	0.58
1:A:145:GLU:HG2	1:A:146:GLU:N	2.17	0.58
7:G:151:ILE:HD12	7:G:151:ILE:N	2.19	0.58
1:O:206:LEU:O	1:O:208:ILE:HG13	2.02	0.58
6:F:196:ARG:NH2	6:F:236:LEU:HD13	2.16	0.58
11:K:23:SER:O	11:K:24:ASN:HB3	2.03	0.58
8:V:173:VAL:HG21	8:V:190:LEU:HD23	1.86	0.58
9:W:187:ARG:CB	9:W:188:PRO:HD3	2.33	0.58
12:Z:25:TYR:OH	13:1:146:GLN:HG3	2.03	0.58
3:C:140:ASP:OD1	3:C:142:HIS:HB2	2.03	0.58
3:C:209:GLU:C	3:C:211:VAL:H	2.07	0.58
8:H:30:VAL:HG21	14:2:211:ILE:HG13	1.85	0.58
13:M:164:VAL:HG23	13:M:165:PRO:HD2	1.84	0.58
2:P:44:VAL:HG21	2:P:187:ILE:HG12	1.86	0.58
9:I:187:ARG:CB	9:I:188:PRO:HD3	2.33	0.58
10:J:14:MET:HE1	10:J:167:ILE:HA	1.84	0.58
10:J:113:ASP:HB3	10:J:116:THR:HB	1.85	0.58
2:P:72:GLY:HA3	2:P:217:PHE:CE1	2.38	0.58
3:Q:209:GLU:C	3:Q:211:VAL:H	2.07	0.58
12:Z:148:GLU:HB2	12:Z:151:GLN:HG3	1.85	0.58
1:A:84:THR:HB	7:G:156:VAL:HG22	1.85	0.58
7:G:229:LYS:O	7:G:233:GLU:HG3	2.02	0.58
10:J:116:THR:HG22	10:J:117:PHE:H	1.67	0.58
14:2:192:VAL:CG1	14:2:197:VAL:HG22	2.33	0.58
1:A:171:LYS:HB3	1:A:205:VAL:CG1	2.34	0.58
11:K:107:TYR:CE2	11:K:185:LYS:HA	2.37	0.58
14:N:71:VAL:HG21	16:N:221:HOH:O	2.03	0.58
1:O:144:ASP:HB3	1:O:147:GLN:HB2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:175:LEU:CD2	3:Q:196:VAL:HG21	2.34	0.58
1:A:73:THR:CG2	1:A:74:GLU:N	2.67	0.58
2:B:165:ASN:ND2	2:B:197:SER:HB2	2.18	0.58
12:L:148:GLU:HB2	12:L:151:GLN:HG3	1.86	0.58
14:N:142:GLY:HA2	14:N:176:LEU:HD21	1.86	0.58
9:I:153:ASN:ND2	9:I:154:LEU:N	2.52	0.58
1:O:145:GLU:HG2	1:O:146:GLU:N	2.18	0.58
6:T:98:VAL:HA	14:2:94:ARG:HG2	1.86	0.58
12:Z:4:LEU:C	12:Z:4:LEU:HD12	2.24	0.58
14:2:99:ARG:HD2	14:2:104:ASN:O	2.03	0.58
14:2:142:GLY:HA2	14:2:176:LEU:HD21	1.85	0.58
10:J:172:LEU:HD22	10:J:202:ALA:HB2	1.85	0.57
1:O:142:GLY:HA2	1:O:220:VAL:HG21	1.86	0.57
8:V:173:VAL:HG23	8:V:190:LEU:HA	1.85	0.57
4:D:80:ALA:HA	4:D:129:ILE:HD13	1.86	0.57
6:F:42:THR:OG1	6:F:43:HIS:HD2	1.86	0.57
14:N:174:ARG:HE	14:N:205:THR:HG22	1.67	0.57
1:O:73:THR:CG2	1:O:74:GLU:H	2.17	0.57
1:O:73:THR:CG2	1:O:74:GLU:N	2.67	0.57
5:S:49:ALA:HB2	5:S:217:LEU:HD22	1.86	0.57
1:A:138:MET:O	1:A:153:LYS:HA	2.04	0.57
5:E:31:ILE:HD11	5:E:158:PRO:HD3	1.87	0.57
5:E:217:LEU:HD13	5:E:218:ALA:N	2.18	0.57
6:F:171:TYR:OH	6:F:193:ARG:HD2	2.04	0.57
6:F:206:THR:HG22	6:F:208:LYS:H	1.69	0.57
6:T:87:PHE:CE1	6:T:115:LYS:HD2	2.39	0.57
9:W:152:LYS:HE3	9:W:186:LEU:CD1	2.35	0.57
13:1:17:GLY:HA3	13:1:20:PHE:CE2	2.38	0.57
1:A:73:THR:CG2	1:A:74:GLU:H	2.17	0.57
2:B:135:ILE:HD12	2:B:135:ILE:N	2.20	0.57
3:C:79:ILE:HB	3:C:82:ASP:HB2	1.85	0.57
3:C:175:LEU:CD2	3:C:196:VAL:HG21	2.34	0.57
7:G:220:THR:O	7:G:221:ASN:HB2	2.05	0.57
8:H:173:VAL:HG23	8:H:190:LEU:HA	1.85	0.57
9:I:213:THR:O	10:J:198:ARG:HA	2.03	0.57
13:M:17:GLY:HA3	13:M:20:PHE:CE2	2.40	0.57
1:O:171:LYS:HB3	1:O:205:VAL:CG1	2.33	0.57
5:S:47:CYS:O	5:S:48:LEU:HD23	2.04	0.57
6:T:171:TYR:OH	6:T:193:ARG:HD2	2.05	0.57
10:X:172:LEU:HD22	10:X:202:ALA:HB2	1.86	0.57
2:B:229:LEU:C	2:B:231:ALA:H	2.08	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:49:GLU:OE1	12:L:91:LYS:HE3	2.04	0.57
13:M:139:GLY:O	13:M:142:SER:HB2	2.05	0.57
13:1:164:VAL:HG23	13:1:165:PRO:HD2	1.85	0.57
14:2:9:THR:O	14:2:41:ARG:NH2	2.38	0.57
3:C:95:GLN:NE2	3:C:98:LEU:HD23	2.17	0.57
2:P:227:ASP:HB3	2:P:233:ALA:CB	2.35	0.57
3:Q:115:CYS:HB3	4:R:81:ARG:NH1	2.18	0.57
6:T:33:SER:OG	6:T:62:LYS:HE3	2.04	0.57
7:U:215:TRP:HB2	7:U:225:GLU:O	2.03	0.57
7:U:229:LYS:O	7:U:233:GLU:HG3	2.04	0.57
10:X:113:ASP:OD1	10:X:114:PRO:HD2	2.04	0.57
13:1:42:LYS:O	13:1:53:GLY:HA2	2.05	0.57
6:F:24:TYR:O	6:F:27:GLU:HB2	2.05	0.57
10:J:190:ILE:HG22	10:J:195:ILE:HD12	1.86	0.57
14:N:74:GLU:CD	14:N:82:SER:HA	2.25	0.57
2:P:34:SER:O	2:P:161:ALA:HA	2.04	0.57
9:W:112:SER:OG	9:W:120:ASP:HB2	2.04	0.57
9:W:137:VAL:HG21	9:W:158:ALA:HA	1.87	0.57
2:B:46:ALA:CB	2:B:209:VAL:HG12	2.35	0.57
2:B:213:ASN:ND2	2:B:215:ALA:HB3	2.18	0.57
5:E:47:CYS:O	5:E:48:LEU:HD23	2.05	0.57
12:L:25:TYR:OH	13:M:146:GLN:HG3	2.04	0.57
10:X:116:THR:HG22	10:X:117:PHE:H	1.68	0.57
2:B:227:ASP:HB3	2:B:233:ALA:CB	2.35	0.57
3:C:8:ARG:CB	3:C:11:ILE:HD12	2.32	0.57
1:O:138:MET:O	1:O:153:LYS:HA	2.04	0.57
3:Q:79:ILE:HB	3:Q:82:ASP:HB2	1.86	0.57
3:Q:234:GLU:HA	3:Q:237:ILE:HB	1.87	0.57
4:R:41:VAL:HG11	4:R:134:VAL:HG13	1.86	0.57
9:W:78:THR:O	9:W:82:MET:HG3	2.04	0.57
9:W:106:THR:HG22	9:W:106:THR:O	2.05	0.57
10:X:14:MET:HE1	10:X:167:ILE:HA	1.87	0.57
11:Y:85:ARG:HG3	11:Y:124:LEU:HB2	1.87	0.57
13:1:139:GLY:O	13:1:142:SER:HB2	2.04	0.57
5:E:99:HIS:HB2	5:E:107:MET:CE	2.35	0.56
8:H:162:LEU:O	8:H:165:GLU:HB3	2.04	0.56
4:D:58:THR:O	4:D:59:VAL:HB	2.05	0.56
5:E:108:THR:O	5:E:112:VAL:HG23	2.05	0.56
9:I:64:GLU:HB3	16:I:308:HOH:O	2.05	0.56
9:I:182:LYS:HD2	9:I:184:ASP:OD1	2.04	0.56
2:P:46:ALA:CB	2:P:209:VAL:HG12	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:229:LEU:C	2:P:231:ALA:H	2.08	0.56
8:V:30:VAL:O	8:V:30:VAL:HG12	2.04	0.56
11:Y:151:ILE:HG13	11:Y:155:ARG:HB3	1.83	0.56
6:F:206:THR:N	6:F:209:ASN:HD21	1.87	0.56
8:H:30:VAL:O	8:H:30:VAL:HG12	2.04	0.56
9:I:78:THR:O	9:I:82:MET:HG3	2.05	0.56
9:I:137:VAL:HG21	9:I:158:ALA:HA	1.87	0.56
14:N:211:ILE:HG22	14:N:214:MET:HE3	1.87	0.56
5:S:217:LEU:HD13	5:S:218:ALA:N	2.20	0.56
8:V:84:LYS:HG2	8:V:118:GLY:O	2.05	0.56
11:Y:151:ILE:HD11	11:Y:156:ALA:N	2.20	0.56
2:B:8:SER:HB3	2:B:122:GLN:O	2.05	0.56
4:D:11:SER:HB3	4:D:12:PRO:HD2	1.86	0.56
5:E:14:THR:HG23	6:F:21:GLN:NE2	2.20	0.56
6:F:10:VAL:HG11	6:F:127:PRO:HD3	1.88	0.56
14:N:192:VAL:CG1	14:N:197:VAL:HG22	2.35	0.56
3:Q:140:ASP:OD1	3:Q:142:HIS:HB2	2.04	0.56
4:R:51:ALA:O	4:R:53:LEU:N	2.32	0.56
4:R:232:ILE:HA	4:R:235:GLU:CB	2.35	0.56
1:A:144:ASP:HB3	1:A:147:GLN:HB2	1.86	0.56
3:C:234:GLU:HA	3:C:237:ILE:HB	1.88	0.56
8:H:84:LYS:HG2	8:H:118:GLY:O	2.05	0.56
8:V:135:ILE:O	8:V:139:VAL:HB	2.05	0.56
9:W:216:ILE:CD1	10:X:196:THR:HG23	2.36	0.56
4:D:232:ILE:HA	4:D:235:GLU:CB	2.36	0.56
9:W:153:ASN:ND2	9:W:154:LEU:N	2.53	0.56
6:F:143:HIS:HB3	6:F:145:PHE:CE1	2.41	0.56
1:A:67:THR:HG22	1:A:69:LEU:N	2.11	0.56
10:J:113:ASP:OD1	10:J:114:PRO:HD2	2.06	0.56
11:K:43:LEU:HD12	11:K:183:ILE:HD11	1.86	0.56
13:M:12:ILE:HD13	13:M:53:GLY:C	2.26	0.56
1:O:65:THR:HG21	7:U:159:GLY:HA3	1.87	0.56
5:S:31:ILE:HD11	5:S:158:PRO:HD3	1.88	0.56
10:X:136:PHE:CE2	10:X:150:CYS:HB3	2.41	0.56
2:B:45:LEU:HD13	2:B:74:VAL:HG22	1.87	0.56
2:B:191:ILE:HG22	2:B:202:MET:HE1	1.88	0.56
1:O:29:PHE:CZ	1:O:156:PRO:HD2	2.40	0.56
3:Q:8:ARG:CB	3:Q:11:ILE:HD12	2.34	0.56
1:A:89:SER:HB2	7:G:117:MET:HE1	1.89	0.55
3:C:136:TYR:HB2	3:C:148:TYR:HB2	1.88	0.55
4:D:51:ALA:O	4:D:53:LEU:N	2.34	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:57:ARG:CG	4:D:60:ARG:HH21	2.20	0.55
4:D:66:ASP:CA	11:K:69:MET:HE2	2.37	0.55
5:E:49:ALA:HB2	5:E:217:LEU:HD22	1.87	0.55
2:P:45:LEU:HD13	2:P:74:VAL:HG22	1.87	0.55
3:Q:95:GLN:NE2	3:Q:98:LEU:HD23	2.19	0.55
11:Y:35:MET:HG2	11:Y:45:LEU:HD22	1.89	0.55
12:Z:46:ALA:HB3	12:Z:98:GLY:O	2.06	0.55
6:F:87:PHE:CE1	6:F:115:LYS:HD2	2.41	0.55
8:H:135:ILE:O	8:H:139:VAL:HB	2.07	0.55
11:K:38:MET:HE1	11:K:60:ILE:HG22	1.88	0.55
13:M:42:LYS:O	13:M:53:GLY:HA2	2.06	0.55
14:N:9:THR:OG1	14:N:10:SER:N	2.32	0.55
4:R:80:ALA:HA	4:R:129:ILE:HD13	1.87	0.55
5:S:220:VAL:HG22	5:S:226:PHE:HA	1.88	0.55
7:U:42:LYS:HG2	7:U:184:MET:O	2.07	0.55
10:X:26:ARG:HB3	10:X:26:ARG:NH1	2.17	0.55
12:Z:125:THR:HB	12:Z:139:MET:HE1	1.88	0.55
13:1:148:LEU:HD23	13:1:178:VAL:HG13	1.89	0.55
2:B:39:ALA:C	2:B:41:ASN:N	2.58	0.55
5:E:220:VAL:HG22	5:E:226:PHE:HA	1.88	0.55
9:I:193:ASN:HB3	13:1:211:ARG:HH21	1.71	0.55
1:O:50:ILE:CG2	1:O:79:VAL:HB	2.37	0.55
2:P:165:ASN:ND2	2:P:197:SER:HB2	2.19	0.55
13:1:148:LEU:HD23	13:1:178:VAL:CG1	2.36	0.55
12:L:40:TYR:HB3	12:L:73:ARG:CZ	2.37	0.55
2:P:92:LEU:HD13	2:P:112:ARG:HB3	1.88	0.55
5:S:146:VAL:CG2	5:S:220:VAL:HG12	2.31	0.55
1:A:50:ILE:CG2	1:A:79:VAL:HB	2.37	0.55
11:K:151:ILE:HD11	11:K:156:ALA:N	2.21	0.55
1:O:79:VAL:CG1	1:O:139:ILE:HB	2.37	0.55
2:P:74:VAL:HG23	2:P:134:LEU:HB2	1.89	0.55
10:X:190:ILE:HG22	10:X:195:ILE:HD12	1.86	0.55
2:B:229:LEU:O	2:B:231:ALA:N	2.37	0.55
3:C:79:ILE:HD12	3:C:79:ILE:N	2.22	0.55
3:C:90:LEU:HG	3:C:114:LEU:HD22	1.88	0.55
9:I:212:LEU:HB2	10:J:199:THR:O	2.06	0.55
11:K:35:MET:HG2	11:K:45:LEU:HD22	1.88	0.55
3:Q:90:LEU:HG	3:Q:114:LEU:HD22	1.88	0.55
9:W:187:ARG:CB	9:W:188:PRO:CD	2.85	0.55
9:W:215:LYS:HD3	9:W:216:ILE:N	2.22	0.55
13:1:155:PHE:HA	13:1:158:MET:HE2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:2:9:THR:OG1	14:2:10:SER:N	2.33	0.55
2:B:53:SER:C	2:B:55:LEU:H	2.10	0.55
6:F:33:SER:OG	6:F:62:LYS:HE3	2.07	0.55
9:I:143:ARG:O	9:I:146:MET:HG3	2.07	0.55
11:K:61:GLN:HE21	11:K:62:LYS:HE2	1.72	0.55
12:L:46:ALA:HB3	12:L:98:GLY:O	2.07	0.55
2:P:191:ILE:HG22	2:P:202:MET:CE	2.37	0.55
10:X:116:THR:CG2	10:X:117:PHE:N	2.70	0.55
5:E:173:ALA:CB	5:E:205:VAL:HB	2.37	0.55
13:M:148:LEU:HD23	13:M:178:VAL:CG1	2.37	0.55
3:Q:53:HIS:HE1	3:Q:55:LEU:HD12	1.72	0.55
12:Z:20:ALA:HB2	12:Z:31:VAL:HG21	1.88	0.55
1:A:79:VAL:CG1	1:A:139:ILE:HB	2.36	0.55
3:C:76:VAL:HG12	3:C:77:ALA:N	2.22	0.55
3:C:138:GLY:HA2	3:C:216:LEU:CD1	2.37	0.55
4:D:62:ILE:N	4:D:62:ILE:HD12	2.21	0.55
14:N:37:ARG:HH21	8:V:166:ARG:HE	1.53	0.55
2:P:229:LEU:O	2:P:231:ALA:N	2.38	0.55
3:Q:79:ILE:HD12	3:Q:79:ILE:N	2.22	0.55
5:S:146:VAL:HG23	5:S:220:VAL:CG1	2.31	0.55
6:T:107:ARG:NH2	14:2:74:GLU:HG3	2.20	0.55
8:V:154:GLN:HE21	8:V:158:ASN:HD21	1.53	0.55
1:A:29:PHE:CZ	1:A:156:PRO:HD2	2.42	0.55
12:L:19:ARG:HE	12:L:29:GLN:HE21	1.54	0.55
1:O:84:THR:HB	7:U:156:VAL:HG22	1.88	0.55
1:O:136:CYS:O	1:O:156:PRO:HG3	2.07	0.55
1:O:155:ASP:C	1:O:157:ALA:H	2.10	0.55
11:Y:49:GLU:OE1	12:Z:91:LYS:HE3	2.07	0.55
1:A:65:THR:HG21	7:G:159:GLY:HA3	1.89	0.54
3:C:15:GLU:HB3	4:D:28:LYS:HZ3	1.72	0.54
3:C:143:TYR:HB2	3:C:146:GLN:CD	2.28	0.54
7:G:66:LEU:HD23	7:G:76:ALA:HA	1.88	0.54
8:H:38:HIS:CD2	8:H:74:PRO:HG3	2.41	0.54
9:I:187:ARG:O	9:I:188:PRO:C	2.45	0.54
6:T:209:ASN:HD22	6:T:209:ASN:H	1.56	0.54
14:2:211:ILE:HG22	14:2:214:MET:HE3	1.88	0.54
1:A:50:ILE:HG21	1:A:79:VAL:HB	1.89	0.54
5:E:186:HIS:HB2	5:E:189:MET:HB3	1.89	0.54
7:G:50:GLU:OE2	7:G:201:HIS:HD2	1.90	0.54
9:I:187:ARG:CB	9:I:188:PRO:CD	2.85	0.54
14:N:126:ASP:HB3	14:N:128:LEU:H	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:172:ALA:O	7:U:176:ILE:HG13	2.08	0.54
9:W:152:LYS:HE3	9:W:186:LEU:HD11	1.88	0.54
9:W:187:ARG:O	9:W:188:PRO:C	2.43	0.54
2:B:44:VAL:HG21	2:B:187:ILE:HG12	1.87	0.54
6:F:164:ARG:HH12	6:F:200:PRO:HG3	1.72	0.54
9:I:215:LYS:HD3	9:I:216:ILE:N	2.23	0.54
9:I:216:ILE:CD1	10:J:196:THR:HG23	2.37	0.54
13:M:148:LEU:HD23	13:M:178:VAL:HG13	1.88	0.54
14:N:71:VAL:O	14:N:75:GLU:HG3	2.07	0.54
3:Q:138:GLY:HA2	3:Q:216:LEU:CD1	2.38	0.54
6:T:143:HIS:HB3	6:T:145:PHE:CE1	2.42	0.54
6:T:164:ARG:HH12	6:T:200:PRO:HG3	1.71	0.54
9:W:143:ARG:O	9:W:146:MET:HG3	2.08	0.54
2:B:195:LYS:C	2:B:197:SER:H	2.11	0.54
5:E:203:LYS:HA	5:E:206:MET:HE3	1.89	0.54
10:J:22:ILE:HG22	10:J:188:HIS:HB2	1.90	0.54
13:M:14:ALA:HA	13:M:22:ILE:O	2.08	0.54
4:R:57:ARG:CG	4:R:60:ARG:HH21	2.20	0.54
1:A:126:THR:CG2	2:B:127:ARG:HH21	2.14	0.54
1:A:155:ASP:C	1:A:157:ALA:H	2.10	0.54
10:J:116:THR:CG2	10:J:117:PHE:N	2.70	0.54
2:P:143:PRO:HG3	2:P:214:GLU:OE2	2.07	0.54
8:V:38:HIS:CD2	8:V:74:PRO:HG3	2.42	0.54
11:Y:23:SER:O	11:Y:24:ASN:HB3	2.06	0.54
14:2:94:ARG:HA	14:2:94:ARG:NE	2.22	0.54
1:A:52:THR:HG22	1:A:53:GLN:N	2.23	0.54
7:G:172:ALA:O	7:G:176:ILE:HG13	2.07	0.54
8:H:36:PRO:HG3	8:H:42:PHE:CZ	2.43	0.54
14:N:94:ARG:NE	14:N:94:ARG:HA	2.22	0.54
4:R:62:ILE:HD12	4:R:62:ILE:N	2.23	0.54
6:T:24:TYR:O	6:T:27:GLU:HB2	2.07	0.54
6:T:139:ASP:OD1	14:2:81:HIS:CE1	2.61	0.54
12:Z:40:TYR:HB3	12:Z:73:ARG:CZ	2.37	0.54
2:B:135:ILE:HD12	2:B:135:ILE:H	1.71	0.54
14:N:186:ARG:HH12	8:V:199:VAL:HB	1.73	0.54
6:T:89:ARG:CZ	13:1:77:HIS:HB3	2.38	0.54
12:Z:160:ILE:O	12:Z:164:THR:HG23	2.08	0.54
6:F:209:ASN:HD22	6:F:209:ASN:H	1.56	0.54
8:H:154:GLN:HE21	8:H:158:ASN:HD21	1.56	0.54
9:I:76:VAL:HG21	9:I:109:HIS:HB2	1.89	0.54
11:K:60:ILE:CG2	11:K:84:THR:HG22	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:99:ARG:HD2	14:N:104:ASN:O	2.07	0.54
1:A:143:ILE:HD12	1:A:143:ILE:N	2.22	0.54
9:I:143:ARG:HH11	9:I:146:MET:HG2	1.73	0.54
9:I:216:ILE:HG22	9:I:217:THR:N	2.23	0.54
5:S:112:VAL:O	5:S:116:VAL:HG23	2.08	0.54
9:I:106:THR:HG22	9:I:106:THR:O	2.08	0.54
10:J:189:ILE:CG2	10:J:196:THR:HB	2.33	0.54
14:N:211:ILE:HG13	8:V:30:VAL:HG21	1.89	0.54
1:O:87:SER:O	1:O:91:VAL:HG23	2.08	0.54
1:O:213:SER:HB3	1:O:232:GLU:OE2	2.08	0.54
5:S:186:HIS:HB2	5:S:189:MET:HB3	1.89	0.54
14:2:192:VAL:HA	14:2:196:GLY:O	2.07	0.54
2:B:191:ILE:HG22	2:B:202:MET:CE	2.38	0.53
4:D:112:ALA:HB1	4:D:151:GLY:O	2.09	0.53
6:F:89:ARG:NH1	13:M:77:HIS:HB3	2.22	0.53
1:O:50:ILE:HG21	1:O:79:VAL:HB	1.88	0.53
6:F:183:ASN:OD1	6:F:186:GLU:HG3	2.09	0.53
3:Q:54:LYS:O	3:Q:55:LEU:HG	2.08	0.53
4:R:46:GLU:O	4:R:48:LYS:N	2.41	0.53
9:W:51:ASP:O	9:W:55:THR:HG23	2.09	0.53
11:Y:60:ILE:CG2	11:Y:84:THR:HG22	2.39	0.53
4:D:46:GLU:O	4:D:48:LYS:N	2.41	0.53
8:H:173:VAL:HG21	8:H:190:LEU:CD2	2.37	0.53
1:O:143:ILE:HD12	1:O:143:ILE:N	2.23	0.53
2:P:195:LYS:C	2:P:197:SER:H	2.11	0.53
5:S:173:ALA:CB	5:S:205:VAL:HB	2.38	0.53
1:A:240:VAL:HG23	1:A:241:ALA:N	2.24	0.53
3:C:54:LYS:O	3:C:55:LEU:HG	2.09	0.53
3:C:76:VAL:CG1	3:C:132:VAL:HG13	2.38	0.53
8:H:13:VAL:HG11	8:H:153:LEU:HA	1.90	0.53
12:L:20:ALA:HB2	12:L:31:VAL:HG21	1.90	0.53
2:P:14:PRO:HG3	3:Q:23:TYR:CE1	2.43	0.53
2:P:48:GLU:CG	2:P:50:LYS:HG2	2.39	0.53
2:P:213:ASN:ND2	2:P:215:ALA:HB3	2.19	0.53
3:Q:15:GLU:HB3	4:R:28:LYS:HZ3	1.72	0.53
7:U:215:TRP:CE3	7:U:215:TRP:HA	2.44	0.53
4:D:215:GLN:HG2	4:D:216:SER:N	2.24	0.53
5:E:54:ILE:HG22	5:E:56:SER:H	1.73	0.53
11:K:2:GLU:HB2	11:K:47:VAL:CG1	2.38	0.53
2:P:94:GLN:CG	9:W:65:LEU:HD13	2.38	0.53
3:Q:198:ASN:HA	3:Q:206:LEU:HD22	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:215:TRP:HA	7:U:215:TRP:HE3	1.73	0.53
5:E:35:SER:HB3	5:E:51:GLU:HG3	1.90	0.53
8:H:76:VAL:CB	8:H:110:GLN:HE21	2.04	0.53
1:O:89:SER:HB2	7:U:117:MET:HE1	1.90	0.53
4:R:95:ARG:O	4:R:98:VAL:O	2.26	0.53
5:S:35:SER:HB3	5:S:51:GLU:HG3	1.91	0.53
9:W:143:ARG:HH11	9:W:146:MET:HG2	1.74	0.53
14:2:74:GLU:CD	14:2:82:SER:HA	2.28	0.53
3:C:95:GLN:NE2	3:C:95:GLN:HA	2.24	0.53
6:F:207:THR:HG22	6:F:233:LEU:HD12	1.90	0.53
8:H:166:ARG:HE	14:2:37:ARG:HH21	1.56	0.53
9:I:216:ILE:HG22	9:I:217:THR:H	1.73	0.53
11:K:143:LEU:HD21	11:K:163:CYS:SG	2.48	0.53
4:R:196:LEU:C	4:R:198:VAL:H	2.12	0.53
11:Y:180:VAL:CG1	11:Y:191:LEU:HD12	2.39	0.53
2:B:143:PRO:HG3	2:B:214:GLU:OE2	2.09	0.53
3:C:188:SER:O	3:C:191:ALA:HB3	2.08	0.53
4:D:33:VAL:HG23	4:D:191:VAL:HG13	1.91	0.53
7:G:215:TRP:CE3	7:G:215:TRP:HA	2.44	0.53
7:G:240:LYS:O	7:G:243:LEU:HB3	2.08	0.53
7:U:184:MET:HB3	7:U:189:ILE:HD11	1.91	0.53
9:W:76:VAL:HG21	9:W:109:HIS:HB2	1.90	0.53
13:M:15:ILE:HD12	13:M:15:ILE:N	2.23	0.53
13:M:155:PHE:HA	13:M:158:MET:HE2	1.90	0.53
1:O:186:LYS:CB	1:O:189:TRP:HE1	2.22	0.53
2:P:201:GLN:O	2:P:203:THR:HG23	2.09	0.53
3:C:53:HIS:HE1	3:C:55:LEU:HD12	1.73	0.53
7:G:191:LYS:HB3	7:G:238:TYR:CD2	2.44	0.53
12:L:90:TYR:HA	12:L:93:MET:HE3	1.91	0.53
3:Q:143:TYR:HB2	3:Q:146:GLN:CD	2.29	0.53
11:Y:38:MET:HE1	11:Y:60:ILE:HG22	1.89	0.53
1:A:75:ASN:O	1:A:76:ILE:HD13	2.08	0.52
2:B:16:GLY:O	3:C:27:ALA:HB2	2.09	0.52
2:B:74:VAL:HG23	2:B:134:LEU:HB2	1.90	0.52
2:P:64:VAL:HA	2:P:73:LEU:O	2.09	0.52
2:P:228:TYR:HA	2:P:233:ALA:HB3	1.91	0.52
5:S:78:MET:CE	5:S:82:ILE:HG23	2.39	0.52
9:W:182:LYS:HD2	9:W:184:ASP:OD1	2.08	0.52
9:W:212:LEU:HB2	10:X:199:THR:O	2.09	0.52
9:W:216:ILE:HG22	9:W:217:THR:N	2.24	0.52
2:B:64:VAL:HA	2:B:73:LEU:O	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:92:LEU:HD13	2:B:112:ARG:HB3	1.90	0.52
4:D:95:ARG:O	4:D:98:VAL:O	2.27	0.52
4:D:202:GLY:C	4:D:204:LYS:H	2.12	0.52
5:E:78:MET:CE	5:E:82:ILE:HG23	2.40	0.52
6:F:130:VAL:HG22	6:F:131:GLY:O	2.09	0.52
9:I:40:ASN:N	9:I:40:ASN:ND2	2.51	0.52
12:Z:10:HIS:O	12:Z:178:HIS:CE1	2.60	0.52
13:1:181:SER:O	13:1:184:GLU:HB2	2.09	0.52
1:A:186:LYS:CB	1:A:189:TRP:HE1	2.22	0.52
2:B:100:TYR:O	2:B:101:GLN:HB2	2.09	0.52
2:B:228:TYR:HA	2:B:233:ALA:HB3	1.91	0.52
3:C:147:LEU:HB3	3:C:159:TRP:O	2.09	0.52
4:D:59:VAL:HG22	4:D:59:VAL:O	2.09	0.52
4:D:196:LEU:C	4:D:198:VAL:H	2.11	0.52
5:E:78:MET:HG3	5:E:82:ILE:HD12	1.91	0.52
9:I:186:LEU:O	9:I:187:ARG:O	2.28	0.52
10:J:147:TYR:HB3	13:1:185:ARG:HG3	1.91	0.52
1:O:240:VAL:HG23	1:O:241:ALA:N	2.25	0.52
3:Q:95:GLN:NE2	3:Q:95:GLN:HA	2.24	0.52
3:Q:109:GLN:NE2	11:Y:71:ASN:HD21	2.08	0.52
4:R:33:VAL:CG1	4:R:168:VAL:HG11	2.39	0.52
4:R:202:GLY:C	4:R:204:LYS:H	2.12	0.52
8:V:154:GLN:HE21	8:V:158:ASN:ND2	2.07	0.52
3:C:236:LEU:HD22	3:C:236:LEU:N	2.24	0.52
12:Z:74:ILE:HG12	12:Z:78:ALA:HB3	1.91	0.52
9:I:20:ALA:HB3	9:I:28:ASP:HB3	1.91	0.52
14:N:45:VAL:HA	16:N:221:HOH:O	2.09	0.52
3:Q:147:LEU:HB3	3:Q:159:TRP:O	2.08	0.52
8:V:13:VAL:HG11	8:V:153:LEU:HA	1.90	0.52
14:2:126:ASP:HB3	14:2:128:LEU:H	1.72	0.52
1:A:231:THR:HB	1:A:234:GLU:HG2	1.92	0.52
7:G:215:TRP:HA	7:G:215:TRP:HE3	1.73	0.52
10:J:109:ILE:HB	10:J:122:CYS:SG	2.49	0.52
11:K:40:GLU:O	11:K:188:ILE:HD13	2.10	0.52
12:L:19:ARG:NH2	12:L:29:GLN:NE2	2.54	0.52
1:O:75:ASN:O	1:O:76:ILE:HD13	2.09	0.52
3:Q:76:VAL:HG12	3:Q:77:ALA:N	2.24	0.52
3:Q:236:LEU:HD22	3:Q:236:LEU:N	2.25	0.52
6:T:10:VAL:HG11	6:T:127:PRO:HD3	1.90	0.52
7:U:99:ARG:HD2	14:2:69:GLN:HE21	1.74	0.52
9:W:20:ALA:HB3	9:W:28:ASP:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:58:THR:CG2	11:Y:121:LEU:O	2.57	0.52
11:Y:2:GLU:HB2	11:Y:47:VAL:CG1	2.39	0.52
12:Z:44:THR:HG1	12:Z:100:MET:H	1.57	0.52
1:A:143:ILE:HD13	1:A:220:VAL:HG22	1.91	0.52
6:F:185:ASN:O	6:F:189:LYS:HG3	2.10	0.52
2:P:51:GLN:O	2:P:52:LYS:O	2.28	0.52
3:Q:187:LYS:HZ1	3:Q:236:LEU:HD11	1.70	0.52
4:R:35:VAL:HG22	4:R:191:VAL:CG2	2.40	0.52
10:X:15:LYS:HE2	10:X:119:PRO:HG2	1.92	0.52
1:A:213:SER:HB3	1:A:232:GLU:OE2	2.09	0.52
2:B:201:GLN:O	2:B:203:THR:HG23	2.09	0.52
3:C:198:ASN:HA	3:C:206:LEU:HD22	1.91	0.52
7:G:184:MET:HB3	7:G:189:ILE:HD11	1.90	0.52
14:N:166:ARG:HH12	14:N:200:GLU:CD	2.13	0.52
3:Q:37:ILE:H	3:Q:44:LEU:HD13	1.74	0.52
3:Q:188:SER:O	3:Q:191:ALA:HB3	2.08	0.52
4:R:59:VAL:HG22	4:R:59:VAL:O	2.10	0.52
7:U:240:LYS:O	7:U:243:LEU:HB3	2.10	0.52
8:V:173:VAL:HG21	8:V:190:LEU:CD2	2.40	0.52
10:X:117:PHE:CD1	10:X:118:LYS:N	2.78	0.52
2:B:190:ALA:O	2:B:193:THR:HG22	2.10	0.52
4:D:33:VAL:CG1	4:D:168:VAL:HG11	2.39	0.52
7:G:168:ALA:HB3	7:G:200:VAL:CG1	2.39	0.52
14:N:215:ILE:HD11	8:V:175:ARG:NH1	2.25	0.52
1:O:143:ILE:HD13	1:O:220:VAL:HG22	1.91	0.52
1:O:231:THR:HB	1:O:234:GLU:HG2	1.90	0.52
4:R:215:GLN:HG2	4:R:216:SER:N	2.24	0.52
7:U:50:GLU:OE2	7:U:201:HIS:HD2	1.92	0.52
7:U:184:MET:HB2	7:U:189:ILE:HD11	1.92	0.52
7:U:191:LYS:HB3	7:U:238:TYR:CD2	2.45	0.52
8:V:40:ARG:HG3	8:V:40:ARG:NH1	2.25	0.52
12:Z:162:GLN:O	12:Z:165:TYR:HB3	2.10	0.52
13:1:14:ALA:HA	13:1:22:ILE:O	2.10	0.52
1:A:93:ARG:CZ	1:A:121:ILE:HD13	2.40	0.52
12:L:90:TYR:HA	12:L:93:MET:CE	2.40	0.52
3:Q:49:ARG:HG3	3:Q:63:GLU:OE1	2.10	0.52
3:Q:136:TYR:HB2	3:Q:148:TYR:HB2	1.91	0.52
5:S:54:ILE:HG22	5:S:56:SER:H	1.74	0.52
6:T:183:ASN:OD1	6:T:186:GLU:HG3	2.10	0.52
9:W:216:ILE:HG22	9:W:217:THR:H	1.75	0.52
10:X:12:MET:CE	10:X:150:CYS:SG	2.98	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:168:SER:CB	10:X:200:LEU:HD11	2.40	0.52
10:X:189:ILE:CG2	10:X:196:THR:HB	2.36	0.52
10:J:116:THR:CG2	10:J:117:PHE:H	2.23	0.51
12:L:74:ILE:HG12	12:L:78:ALA:HB3	1.91	0.51
3:Q:76:VAL:CG1	3:Q:132:VAL:HG13	2.40	0.51
9:W:186:LEU:O	9:W:187:ARG:O	2.28	0.51
10:X:22:ILE:HG22	10:X:188:HIS:HB2	1.91	0.51
10:X:65:GLN:HE21	11:Y:86:ARG:NH2	2.07	0.51
3:C:140:ASP:C	3:C:142:HIS:H	2.13	0.51
3:C:174:MET:HE3	3:C:199:LYS:HG2	1.91	0.51
13:M:151:ASN:ND2	13:M:152:GLN:NE2	2.58	0.51
14:N:9:THR:O	14:N:41:ARG:NH2	2.43	0.51
1:O:67:THR:HG22	1:O:69:LEU:N	2.11	0.51
10:X:14:MET:HE3	10:X:167:ILE:HG13	1.93	0.51
2:B:14:PRO:HG3	3:C:23:TYR:CE1	2.45	0.51
7:G:3:ILE:HD13	7:G:17:ASP:OD1	2.10	0.51
9:I:51:ASP:O	9:I:55:THR:HG23	2.11	0.51
11:K:35:MET:HG2	11:K:45:LEU:CD2	2.40	0.51
12:L:44:THR:HG1	12:L:100:MET:H	1.56	0.51
3:Q:229:LYS:O	3:Q:233:VAL:HG23	2.10	0.51
7:U:168:ALA:HB3	7:U:200:VAL:CG1	2.40	0.51
14:2:166:ARG:HH12	14:2:200:GLU:CD	2.14	0.51
3:C:49:ARG:HG3	3:C:63:GLU:OE1	2.11	0.51
7:G:38:GLY:HA3	7:G:136:MET:HE2	1.92	0.51
7:G:42:LYS:HG2	7:G:184:MET:O	2.10	0.51
13:M:172:MET:O	13:M:176:LYS:HG3	2.11	0.51
14:N:49:THR:HG21	14:N:85:PRO:HA	1.92	0.51
1:O:52:THR:HG22	1:O:53:GLN:N	2.24	0.51
2:P:213:ASN:HD21	2:P:215:ALA:CB	2.20	0.51
11:Y:102:LEU:HD11	11:Y:118:MET:HE1	1.93	0.51
13:1:83:MET:HE2	13:1:88:ILE:HA	1.92	0.51
2:B:133:LEU:O	2:B:147:GLN:HA	2.10	0.51
8:H:125:PHE:CZ	8:H:139:VAL:HG13	2.46	0.51
8:H:199:VAL:HB	14:2:186:ARG:HH12	1.75	0.51
9:I:143:ARG:HH11	9:I:143:ARG:HB2	1.76	0.51
9:I:203:ARG:HD2	9:I:205:GLU:OE2	2.11	0.51
10:J:26:ARG:HB3	10:J:26:ARG:NH1	2.18	0.51
10:J:117:PHE:CD1	10:J:118:LYS:N	2.78	0.51
11:K:121:LEU:O	11:K:122:ALA:HB3	2.11	0.51
1:O:32:ILE:HD13	1:O:137:CYS:HB2	1.91	0.51
2:P:112:ARG:HH11	2:P:112:ARG:HG3	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:208:THR:HG23	10:X:165:GLU:OE1	2.11	0.51
3:C:149:GLN:CD	3:C:164:ILE:HD11	2.30	0.51
10:J:152:SER:O	10:J:153:LEU:HD23	2.11	0.51
11:K:171:PHE:CE2	11:K:173:LEU:HB2	2.45	0.51
3:Q:59:VAL:O	3:Q:59:VAL:HG12	2.10	0.51
6:F:107:ARG:NH2	14:N:74:GLU:HG3	2.25	0.51
2:P:100:TYR:O	2:P:101:GLN:HB2	2.11	0.51
3:Q:149:GLN:CD	3:Q:164:ILE:HD11	2.30	0.51
7:U:53:VAL:HG23	7:U:209:PHE:HA	1.93	0.51
10:X:7:ASN:ND2	10:X:57:ALA:N	2.47	0.51
10:X:34:LEU:HG	10:X:35:VAL:N	2.22	0.51
10:X:116:THR:CG2	10:X:117:PHE:H	2.24	0.51
2:B:112:ARG:HH11	2:B:112:ARG:HG3	1.75	0.51
3:C:37:ILE:H	3:C:44:LEU:HD13	1.75	0.51
12:L:195:LEU:O	12:L:199:TYR:HD1	1.94	0.51
4:R:206:ILE:HG22	4:R:207:GLU:H	1.75	0.51
11:Y:61:GLN:HE21	11:Y:62:LYS:HE2	1.76	0.51
2:B:173:LEU:C	2:B:175:LYS:H	2.14	0.51
4:D:206:ILE:HG22	4:D:207:GLU:H	1.75	0.51
10:J:113:ASP:CB	10:J:116:THR:HB	2.41	0.51
13:M:181:SER:O	13:M:184:GLU:HB2	2.10	0.51
3:Q:93:ILE:HD13	3:Q:113:ALA:HB1	1.93	0.51
3:Q:218:ARG:CZ	3:Q:221:GLY:O	2.57	0.51
5:S:78:MET:HG3	5:S:82:ILE:HD12	1.93	0.51
6:T:207:THR:HG22	6:T:233:LEU:HD12	1.92	0.51
5:E:186:HIS:O	5:E:189:MET:HG2	2.10	0.51
14:N:192:VAL:HA	14:N:196:GLY:O	2.10	0.51
1:O:93:ARG:CZ	1:O:121:ILE:HD13	2.40	0.51
3:Q:140:ASP:C	3:Q:142:HIS:H	2.13	0.51
3:Q:245:ALA:O	3:Q:248:GLU:HG2	2.11	0.51
7:U:66:LEU:HD13	7:U:214:SER:OG	2.11	0.51
10:X:20:VAL:HB	10:X:190:ILE:CD1	2.40	0.51
11:Y:151:ILE:HD11	11:Y:156:ALA:HA	1.93	0.51
14:2:49:THR:HG21	14:2:85:PRO:HA	1.93	0.51
14:2:115:TYR:CE2	14:2:194:GLU:HG2	2.46	0.51
3:C:76:VAL:HG11	3:C:83:ALA:HB2	1.93	0.50
3:C:79:ILE:HD12	3:C:79:ILE:H	1.76	0.50
3:C:149:GLN:OE1	3:C:164:ILE:HD11	2.10	0.50
13:M:211:ARG:HH21	9:W:193:ASN:CB	2.25	0.50
2:P:71:ILE:HG22	2:P:72:GLY:N	2.26	0.50
5:S:167:ALA:HB3	6:T:56:LEU:HD13	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:24:ASN:ND2	11:Y:25:ILE:H	2.09	0.50
10:J:138:VAL:HG11	10:J:146:MET:HB3	1.93	0.50
11:K:59:TYR:HE2	11:K:87:ASN:OD1	1.93	0.50
4:R:33:VAL:HG23	4:R:191:VAL:HG13	1.93	0.50
4:R:115:LYS:O	4:R:119:THR:HG23	2.11	0.50
4:R:130:SER:HA	4:R:147:THR:O	2.11	0.50
4:R:137:ASP:O	4:R:138:PHE:C	2.48	0.50
6:T:237:GLU:C	6:T:239:ARG:N	2.64	0.50
11:Y:60:ILE:O	11:Y:64:VAL:HG23	2.11	0.50
3:C:218:ARG:CZ	3:C:221:GLY:O	2.59	0.50
7:G:216:VAL:HG13	7:G:216:VAL:O	2.11	0.50
8:H:154:GLN:HE21	8:H:158:ASN:ND2	2.10	0.50
2:P:190:ALA:O	2:P:193:THR:HG22	2.10	0.50
5:S:186:HIS:O	5:S:189:MET:HG2	2.11	0.50
8:V:103:TRP:CZ3	8:V:105:PRO:HG3	2.47	0.50
12:Z:19:ARG:NH2	12:Z:29:GLN:NE2	2.56	0.50
14:2:15:LYS:HB3	14:2:20:VAL:HG22	1.94	0.50
14:2:71:VAL:O	14:2:75:GLU:HG3	2.11	0.50
1:A:87:SER:O	1:A:91:VAL:HG23	2.12	0.50
4:D:33:VAL:HG12	4:D:160:ALA:CB	2.40	0.50
7:G:53:VAL:HG23	7:G:209:PHE:HA	1.93	0.50
4:R:112:ALA:HB1	4:R:151:GLY:O	2.11	0.50
9:W:148:GLU:OE1	9:W:182:LYS:NZ	2.44	0.50
9:W:212:LEU:HD12	10:X:200:LEU:O	2.10	0.50
11:Y:59:TYR:HE2	11:Y:87:ASN:OD1	1.93	0.50
1:A:32:ILE:HD13	1:A:137:CYS:HB2	1.92	0.50
3:C:245:ALA:O	3:C:248:GLU:HG2	2.11	0.50
4:D:13:ASP:OD2	4:D:13:ASP:N	2.42	0.50
4:D:145:TYR:CE2	4:D:155:ALA:HB2	2.47	0.50
11:K:148:THR:O	11:K:151:ILE:HG22	2.11	0.50
12:L:166:ARG:NH1	10:X:34:LEU:HG	2.27	0.50
2:P:191:ILE:HG22	2:P:202:MET:HE1	1.92	0.50
3:Q:149:GLN:OE1	3:Q:164:ILE:HD11	2.12	0.50
6:T:159:MET:HG3	6:T:160:SER:H	1.73	0.50
10:X:109:ILE:HB	10:X:122:CYS:SG	2.52	0.50
11:Y:12:TYR:N	11:Y:12:TYR:CD2	2.80	0.50
12:Z:195:LEU:O	12:Z:199:TYR:HD1	1.94	0.50
2:B:94:GLN:CG	9:I:65:LEU:HD13	2.42	0.50
3:C:218:ARG:NH2	3:C:223:THR:OG1	2.44	0.50
4:D:66:ASP:CG	4:D:67:ASP:H	2.15	0.50
5:E:54:ILE:HD11	5:E:61:PRO:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:65:GLN:HE21	11:K:86:ARG:NH2	2.10	0.50
10:J:168:SER:CB	10:J:200:LEU:HD11	2.42	0.50
11:K:47:VAL:CG1	11:K:48:GLY:N	2.74	0.50
7:U:194:ALA:O	7:U:198:TYR:HD1	1.95	0.50
9:W:143:ARG:NH1	9:W:143:ARG:HB2	2.27	0.50
2:B:173:LEU:HD21	2:B:193:THR:HB	1.94	0.50
3:C:229:LYS:O	3:C:233:VAL:HG23	2.12	0.50
4:D:137:ASP:O	4:D:138:PHE:C	2.48	0.50
10:J:15:LYS:HE2	10:J:119:PRO:HG2	1.94	0.50
12:L:166:ARG:HH11	10:X:34:LEU:HG	1.77	0.50
1:O:54:LYS:O	1:O:54:LYS:HG2	2.12	0.50
6:T:10:VAL:HG12	6:T:21:GLN:CB	2.42	0.50
6:T:164:ARG:HH12	6:T:200:PRO:CG	2.24	0.50
9:W:143:ARG:HH11	9:W:143:ARG:HB2	1.75	0.50
10:X:113:ASP:CB	10:X:116:THR:HB	2.40	0.50
11:Y:155:ARG:NH2	11:Y:158:GLU:OE1	2.45	0.50
1:A:54:LYS:O	1:A:54:LYS:HG2	2.12	0.50
4:D:115:LYS:O	4:D:119:THR:HG23	2.12	0.50
7:G:184:MET:HB2	7:G:189:ILE:HD11	1.94	0.50
11:K:1:MET:N	11:K:173:LEU:HD13	2.27	0.50
12:L:10:HIS:O	12:L:178:HIS:CE1	2.60	0.50
12:L:162:GLN:O	12:L:165:TYR:HB3	2.11	0.50
2:P:173:LEU:C	2:P:175:LYS:H	2.13	0.50
2:P:173:LEU:HD21	2:P:193:THR:HB	1.93	0.50
3:Q:189:ALA:C	3:Q:191:ALA:N	2.65	0.50
11:Y:121:LEU:O	11:Y:122:ALA:HB3	2.12	0.50
11:Y:171:PHE:CE2	11:Y:173:LEU:HB2	2.47	0.50
13:1:172:MET:O	13:1:176:LYS:HG3	2.12	0.50
13:1:208:VAL:HG12	13:1:209:SER:N	2.27	0.50
4:D:35:VAL:HG22	4:D:191:VAL:CG2	2.42	0.50
9:I:143:ARG:NH1	9:I:143:ARG:HB2	2.27	0.50
9:I:148:GLU:OE1	9:I:182:LYS:NZ	2.41	0.50
10:J:7:ASN:ND2	10:J:57:ALA:N	2.45	0.50
11:Y:148:THR:O	11:Y:151:ILE:HG22	2.12	0.50
12:Z:90:TYR:HA	12:Z:93:MET:CE	2.41	0.50
12:Z:90:TYR:HA	12:Z:93:MET:HE3	1.93	0.50
3:C:59:VAL:O	3:C:59:VAL:HG12	2.11	0.49
9:I:212:LEU:HD12	10:J:200:LEU:O	2.12	0.49
2:P:162:MET:CB	16:P:417:HOH:O	2.60	0.49
3:Q:190:LEU:O	3:Q:193:ALA:HB3	2.12	0.49
6:T:107:ARG:HH22	14:2:74:GLU:CG	2.25	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:117:GLN:HA	6:T:151:ALA:HB2	1.94	0.49
6:T:130:VAL:HG22	6:T:131:GLY:O	2.12	0.49
7:U:3:ILE:HB	7:U:21:PHE:CZ	2.47	0.49
9:W:59:ILE:HG13	9:W:83:LEU:HG	1.94	0.49
11:Y:35:MET:HG2	11:Y:45:LEU:CD2	2.41	0.49
13:1:151:ASN:ND2	13:1:152:GLN:NE2	2.59	0.49
1:A:72:ILE:HG21	1:A:114:LEU:HD11	1.94	0.49
3:C:93:ILE:HD13	3:C:113:ALA:HB1	1.94	0.49
5:E:42:THR:HG22	5:E:43:SER:N	2.27	0.49
5:E:221:GLN:HG3	5:E:224:GLN:HB2	1.94	0.49
7:G:215:TRP:HB3	7:G:220:THR:HG21	1.94	0.49
13:M:44:TYR:HE2	13:M:69:GLU:OE2	1.95	0.49
4:R:145:TYR:CE2	4:R:155:ALA:HB2	2.47	0.49
8:V:36:PRO:HG3	8:V:42:PHE:CZ	2.46	0.49
14:2:50:MET:SD	14:2:192:VAL:HG13	2.52	0.49
2:B:73:LEU:HD23	2:B:135:ILE:HA	1.94	0.49
3:C:109:GLN:NE2	11:K:71:ASN:HD21	2.08	0.49
5:E:112:VAL:O	5:E:116:VAL:HG23	2.13	0.49
7:G:168:ALA:CB	7:G:200:VAL:HG13	2.42	0.49
11:K:2:GLU:HB2	11:K:47:VAL:HG11	1.94	0.49
12:L:38:ASN:HB3	12:L:39:PRO:HD2	1.95	0.49
2:P:94:GLN:HG3	9:W:65:LEU:HD13	1.94	0.49
2:P:133:LEU:O	2:P:147:GLN:HA	2.12	0.49
3:Q:74:CYS:HB2	3:Q:135:LEU:O	2.12	0.49
4:R:98:VAL:HG12	4:R:99:GLU:H	1.77	0.49
5:S:99:HIS:CD2	5:S:107:MET:HG3	2.46	0.49
11:Y:47:VAL:CG1	11:Y:48:GLY:N	2.75	0.49
11:Y:66:LEU:HG	11:Y:70:ARG:HD2	1.95	0.49
10:J:34:LEU:HG	12:Z:166:ARG:HH11	1.78	0.49
10:J:58:THR:CG2	11:K:121:LEU:O	2.59	0.49
11:K:47:VAL:HG12	11:K:48:GLY:N	2.27	0.49
11:K:161:ARG:O	11:K:165:GLU:HG3	2.12	0.49
1:O:11:ARG:HB2	16:O:407:HOH:O	2.12	0.49
2:P:173:LEU:C	2:P:175:LYS:N	2.66	0.49
3:Q:79:ILE:HD12	3:Q:79:ILE:H	1.76	0.49
5:S:54:ILE:HD11	5:S:61:PRO:HB3	1.94	0.49
6:T:38:LEU:N	6:T:38:LEU:HD12	2.28	0.49
6:T:107:ARG:HH22	14:2:74:GLU:HG3	1.77	0.49
7:U:215:TRP:HB3	7:U:220:THR:HG21	1.94	0.49
8:V:148:THR:HG23	8:V:151:GLU:OE2	2.11	0.49
13:1:15:ILE:HD12	13:1:15:ILE:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:60:ARG:C	4:D:62:ILE:H	2.16	0.49
10:J:172:LEU:HD23	10:J:185:VAL:HG21	1.95	0.49
11:K:180:VAL:CG1	11:K:191:LEU:HD12	2.42	0.49
13:M:1:ARG:CG	13:M:2:PHE:N	2.75	0.49
1:O:72:ILE:HG21	1:O:114:LEU:HD11	1.94	0.49
3:Q:23:TYR:N	3:Q:23:TYR:CD2	2.80	0.49
6:T:185:ASN:O	6:T:189:LYS:HG3	2.13	0.49
11:Y:40:GLU:O	11:Y:188:ILE:HD13	2.12	0.49
1:A:88:ARG:HH11	1:A:88:ARG:HG3	1.77	0.49
3:C:190:LEU:O	3:C:193:ALA:HB3	2.13	0.49
5:E:225:ASN:O	5:E:226:PHE:C	2.51	0.49
7:G:3:ILE:HB	7:G:21:PHE:CZ	2.47	0.49
14:N:43:MET:HG2	14:N:44:ARG:N	2.27	0.49
5:S:166:ASP:HB3	5:S:185:TYR:CE2	2.47	0.49
5:S:225:ASN:O	5:S:226:PHE:C	2.51	0.49
7:U:152:ASP:HB2	7:U:153:PRO:HD2	1.94	0.49
2:B:213:ASN:HD21	2:B:215:ALA:CB	2.20	0.49
4:D:130:SER:HA	4:D:147:THR:O	2.13	0.49
8:H:48:SER:HB3	8:H:51:ASP:HB2	1.95	0.49
9:I:113:ILE:HG23	9:I:119:THR:HG22	1.95	0.49
11:K:4:LEU:HD13	11:K:45:LEU:HB3	1.95	0.49
3:Q:69:ASN:HB2	3:Q:72:MET:HB2	1.94	0.49
12:Z:6:PHE:HA	12:Z:124:ALA:O	2.12	0.49
1:A:123:GLN:HE22	1:A:127:GLN:NE2	2.10	0.49
14:N:27:LEU:HD22	14:N:184:TYR:HB2	1.94	0.49
3:Q:132:VAL:O	3:Q:152:PRO:HD3	2.13	0.49
4:R:33:VAL:HG12	4:R:160:ALA:CB	2.41	0.49
4:R:66:ASP:CG	4:R:67:ASP:H	2.16	0.49
7:U:99:ARG:NH1	14:2:69:GLN:NE2	2.61	0.49
7:U:168:ALA:CB	7:U:200:VAL:HG13	2.43	0.49
11:Y:4:LEU:HD13	11:Y:45:LEU:HB3	1.95	0.49
5:E:46:VAL:HG23	5:E:151:PRO:HB3	1.95	0.49
7:G:194:ALA:O	7:G:198:TYR:HD1	1.96	0.49
8:H:100:ILE:HD12	8:H:100:ILE:N	2.27	0.49
11:K:166:GLU:HA	11:K:166:GLU:OE1	2.12	0.49
12:L:125:THR:HB	12:L:139:MET:HE3	1.94	0.49
3:Q:15:GLU:HB3	4:R:28:LYS:NZ	2.27	0.49
5:S:210:LEU:CD1	5:S:215:ILE:HG21	2.42	0.49
7:U:135:PHE:CE1	7:U:151:ILE:HD13	2.47	0.49
10:X:7:ASN:HD22	10:X:57:ALA:N	2.02	0.49
10:X:152:SER:O	10:X:153:LEU:HD23	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:THR:HG22	1:A:68:HIS:N	2.28	0.49
6:F:164:ARG:HH12	6:F:200:PRO:CG	2.25	0.49
12:L:5:ALA:HA	12:L:13:ILE:O	2.13	0.49
1:O:195:VAL:O	1:O:199:ILE:HG12	2.13	0.49
3:Q:76:VAL:HG11	3:Q:83:ALA:HB2	1.94	0.49
5:S:221:GLN:HG3	5:S:224:GLN:HB2	1.94	0.49
7:U:216:VAL:HG13	7:U:216:VAL:O	2.13	0.49
11:Y:47:VAL:HG12	11:Y:48:GLY:N	2.28	0.49
11:Y:143:LEU:HD21	11:Y:163:CYS:SG	2.52	0.49
12:Z:19:ARG:HE	12:Z:29:GLN:HE21	1.60	0.49
5:E:78:MET:HE3	5:E:82:ILE:HG23	1.95	0.48
6:F:159:MET:HG3	6:F:160:SER:H	1.76	0.48
7:G:48:GLY:HA2	7:G:212:GLU:O	2.13	0.48
2:P:8:SER:HB3	2:P:122:GLN:O	2.13	0.48
3:Q:180:LYS:NZ	3:Q:188:SER:OG	2.46	0.48
5:S:78:MET:HE3	5:S:82:ILE:HG23	1.94	0.48
5:S:96:THR:CA	5:S:107:MET:HE3	2.40	0.48
5:S:203:LYS:HA	5:S:206:MET:HE3	1.95	0.48
6:T:194:ALA:O	6:T:197:GLU:HB2	2.13	0.48
10:X:112:LEU:HD23	10:X:119:PRO:HA	1.95	0.48
2:B:94:GLN:HG3	9:I:65:LEU:HD13	1.95	0.48
6:F:107:ARG:HH22	14:N:74:GLU:HG3	1.77	0.48
11:K:155:ARG:NH2	11:K:158:GLU:OE1	2.45	0.48
6:T:5:GLN:HG3	6:T:6:TYR:CD1	2.48	0.48
6:T:164:ARG:NH1	6:T:200:PRO:HG3	2.29	0.48
9:W:153:ASN:ND2	9:W:153:ASN:C	2.67	0.48
14:2:43:MET:HG2	14:2:44:ARG:N	2.28	0.48
6:F:46:LEU:HG	6:F:135:ALA:HB2	1.94	0.48
10:J:12:MET:CE	10:J:150:CYS:SG	3.01	0.48
11:K:151:ILE:HD11	11:K:156:ALA:HA	1.94	0.48
10:X:111:GLY:HA2	10:X:190:ILE:CD1	2.44	0.48
3:C:79:ILE:HD13	3:C:131:GLY:CA	2.41	0.48
7:G:54:LEU:HB2	7:G:58:TYR:CE1	2.49	0.48
8:H:103:TRP:CZ3	8:H:105:PRO:HG3	2.48	0.48
11:K:60:ILE:HG21	11:K:84:THR:CG2	2.42	0.48
12:L:180:ARG:CB	12:L:180:ARG:HH11	2.26	0.48
12:L:182:ASP:OD2	12:L:182:ASP:N	2.37	0.48
14:N:46:ASN:C	14:N:46:ASN:ND2	2.63	0.48
4:R:60:ARG:C	4:R:62:ILE:H	2.16	0.48
5:S:46:VAL:HG23	5:S:151:PRO:HB3	1.94	0.48
7:U:3:ILE:HD13	7:U:17:ASP:OD1	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:9:ARG:HH21	12:Z:146:ASP:HB3	1.77	0.48
13:1:44:TYR:HE2	13:1:69:GLU:OE2	1.96	0.48
11:K:66:LEU:HG	11:K:70:ARG:HD2	1.96	0.48
3:Q:82:ASP:OD2	3:Q:130:PHE:HA	2.13	0.48
7:U:215:TRP:CD1	7:U:228:PRO:HD3	2.48	0.48
11:Y:1:MET:HE1	11:Y:134:TYR:N	2.22	0.48
12:Z:182:ASP:OD2	12:Z:182:ASP:N	2.37	0.48
3:C:62:SER:OG	3:C:63:GLU:N	2.47	0.48
3:C:86:LEU:HD22	3:C:114:LEU:HD11	1.95	0.48
5:E:210:LEU:CD1	5:E:215:ILE:HG21	2.44	0.48
6:F:194:ALA:O	6:F:197:GLU:HB2	2.14	0.48
9:I:212:LEU:HD12	10:J:201:LYS:HA	1.95	0.48
13:M:174:LEU:O	13:M:178:VAL:HG22	2.14	0.48
4:R:121:SER:HB2	4:R:124:ARG:HD2	1.95	0.48
5:S:231:LYS:O	5:S:235:GLU:HG2	2.14	0.48
7:U:193:VAL:O	7:U:197:ILE:HG12	2.13	0.48
12:Z:5:ALA:HA	12:Z:13:ILE:O	2.14	0.48
3:C:15:GLU:HB3	4:D:28:LYS:NZ	2.29	0.48
5:E:166:ASP:HB3	5:E:185:TYR:CE2	2.48	0.48
6:F:10:VAL:HG12	6:F:21:GLN:CB	2.43	0.48
6:F:38:LEU:N	6:F:38:LEU:HD12	2.29	0.48
6:F:117:GLN:HA	6:F:151:ALA:HB2	1.94	0.48
1:O:220:VAL:HG23	1:O:225:PRO:O	2.14	0.48
9:W:212:LEU:HD12	10:X:201:LYS:HA	1.95	0.48
11:Y:60:ILE:HG21	11:Y:84:THR:CG2	2.44	0.48
14:2:27:LEU:HD22	14:2:184:TYR:HB2	1.95	0.48
14:2:46:ASN:C	14:2:46:ASN:ND2	2.64	0.48
3:C:189:ALA:C	3:C:191:ALA:N	2.67	0.48
14:N:50:MET:SD	14:N:192:VAL:HG13	2.53	0.48
3:Q:53:HIS:CE1	3:Q:55:LEU:HD12	2.49	0.48
5:E:231:LYS:O	5:E:235:GLU:HG2	2.14	0.48
7:G:219:LEU:HD12	7:G:219:LEU:O	2.14	0.48
9:I:208:THR:HG23	10:J:165:GLU:OE1	2.13	0.48
10:J:112:LEU:HD23	10:J:119:PRO:HA	1.95	0.48
5:S:31:ILE:HD11	5:S:158:PRO:CD	2.43	0.48
8:V:125:PHE:CZ	8:V:139:VAL:HG13	2.49	0.48
11:Y:89:ALA:HB2	11:Y:122:ALA:CB	2.44	0.48
11:Y:166:GLU:OE1	11:Y:166:GLU:HA	2.14	0.48
3:C:23:TYR:CD2	3:C:23:TYR:N	2.81	0.48
6:F:164:ARG:NH1	6:F:200:PRO:HG3	2.29	0.48
7:G:215:TRP:CD1	7:G:228:PRO:HD3	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:160:ILE:O	12:L:164:THR:HG23	2.13	0.48
14:N:15:LYS:HB3	14:N:20:VAL:HG22	1.96	0.48
5:S:189:MET:CE	5:S:194:ALA:HA	2.44	0.48
13:1:124:PHE:CD2	13:1:130:TYR:HB3	2.49	0.48
13:1:190:GLY:O	13:1:191:ASP:HB2	2.13	0.48
1:A:88:ARG:HG3	1:A:88:ARG:NH1	2.28	0.47
1:A:231:THR:HG22	1:A:232:GLU:N	2.29	0.47
2:B:38:LYS:HA	2:B:43:VAL:HG22	1.96	0.47
2:B:137:GLY:HA2	2:B:212:CYS:SG	2.54	0.47
5:E:31:ILE:HD11	5:E:158:PRO:CD	2.44	0.47
6:F:5:GLN:HG3	6:F:6:TYR:CD1	2.49	0.47
10:J:67:LEU:HD22	10:J:91:VAL:HG22	1.96	0.47
10:J:111:GLY:HA2	10:J:190:ILE:CD1	2.44	0.47
10:J:205:ASP:O	12:Z:19:ARG:NH1	2.45	0.47
12:L:9:ARG:HH21	12:L:146:ASP:HB3	1.79	0.47
12:L:50:ALA:HB2	13:M:129:SER:HB2	1.94	0.47
14:N:115:TYR:CE2	14:N:194:GLU:HG2	2.47	0.47
14:N:211:ILE:HA	14:N:214:MET:HE2	1.95	0.47
1:O:41:ALA:HA	1:O:49:VAL:O	2.13	0.47
3:Q:139:TRP:CE2	3:Q:218:ARG:HD3	2.49	0.47
4:R:98:VAL:CG1	4:R:99:GLU:N	2.77	0.47
6:T:46:LEU:HG	6:T:135:ALA:HB2	1.95	0.47
11:Y:1:MET:HE2	11:Y:134:TYR:H	1.75	0.47
14:2:211:ILE:HA	14:2:214:MET:CE	2.44	0.47
2:B:109:LEU:O	2:B:109:LEU:HG	2.14	0.47
2:B:173:LEU:C	2:B:175:LYS:N	2.67	0.47
3:C:74:CYS:HB2	3:C:135:LEU:O	2.13	0.47
4:D:35:VAL:O	4:D:41:VAL:HG13	2.14	0.47
7:G:99:ARG:HD2	14:N:69:GLN:HE21	1.78	0.47
7:G:193:VAL:O	7:G:197:ILE:HG12	2.14	0.47
8:H:30:VAL:HG13	14:2:212:ALA:HA	1.95	0.47
9:I:59:ILE:HG13	9:I:83:LEU:HG	1.95	0.47
10:J:109:ILE:O	10:J:121:ILE:HA	2.14	0.47
13:M:137:ALA:N	13:M:146:GLN:NE2	2.62	0.47
1:O:231:THR:HG22	1:O:232:GLU:N	2.29	0.47
8:V:148:THR:OG1	8:V:151:GLU:HG3	2.14	0.47
11:Y:1:MET:N	11:Y:173:LEU:HD13	2.29	0.47
11:Y:190:ASP:O	11:Y:191:LEU:HG	2.15	0.47
7:G:47:PHE:O	7:G:213:LEU:HA	2.14	0.47
7:G:152:ASP:HB2	7:G:153:PRO:HD2	1.96	0.47
10:J:34:LEU:HG	10:J:35:VAL:N	2.23	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:7:PHE:CZ	13:M:9:GLY:HA2	2.49	0.47
13:M:208:VAL:HG12	13:M:209:SER:N	2.29	0.47
14:N:211:ILE:HA	14:N:214:MET:CE	2.44	0.47
5:S:78:MET:HG3	5:S:82:ILE:CD1	2.45	0.47
7:U:47:PHE:O	7:U:213:LEU:HA	2.15	0.47
9:W:203:ARG:HD2	9:W:205:GLU:OE2	2.13	0.47
1:A:52:THR:CG2	1:A:53:GLN:N	2.78	0.47
10:J:12:MET:HE2	10:J:150:CYS:SG	2.55	0.47
13:M:151:ASN:HD22	13:M:152:GLN:HE21	1.62	0.47
2:P:16:GLY:O	3:Q:27:ALA:HB2	2.13	0.47
4:R:35:VAL:O	4:R:41:VAL:HG13	2.13	0.47
4:R:212:ARG:O	4:R:214:ASP:N	2.48	0.47
6:T:169:ARG:HG2	7:U:57:LEU:HD12	1.95	0.47
10:X:96:TYR:CE1	10:X:99:ARG:HD3	2.49	0.47
13:1:137:ALA:N	13:1:146:GLN:NE2	2.61	0.47
1:A:41:ALA:HA	1:A:49:VAL:O	2.14	0.47
6:F:151:ALA:HB3	7:G:82:ALA:CB	2.40	0.47
11:K:89:ALA:HB2	11:K:122:ALA:CB	2.45	0.47
13:M:12:ILE:HG12	13:M:25:SER:HB3	1.96	0.47
13:M:83:MET:CE	13:M:88:ILE:HA	2.45	0.47
1:O:67:THR:HG22	1:O:68:HIS:N	2.30	0.47
1:O:78:CYS:CB	1:O:140:LEU:HD23	2.44	0.47
2:P:59:ARG:O	2:P:61:VAL:N	2.47	0.47
2:P:182:GLU:HG2	2:P:183:LEU:N	2.26	0.47
3:Q:209:GLU:O	3:Q:211:VAL:N	2.48	0.47
4:R:42:VAL:CA	4:R:210:VAL:HG12	2.42	0.47
5:S:42:THR:HG22	5:S:43:SER:N	2.29	0.47
13:1:1:ARG:CG	13:1:2:PHE:N	2.75	0.47
7:G:135:PHE:CE1	7:G:151:ILE:HD13	2.50	0.47
7:G:136:MET:HE1	7:G:163:CYS:O	2.15	0.47
9:I:200:GLY:CA	13:1:173:ARG:HD3	2.44	0.47
12:L:40:TYR:HB3	12:L:73:ARG:NH2	2.29	0.47
3:Q:234:GLU:O	3:Q:237:ILE:HB	2.15	0.47
10:X:10:ALA:CB	10:X:146:MET:HE2	2.44	0.47
2:B:7:PHE:O	2:B:124:GLY:HA2	2.15	0.47
2:B:71:ILE:HG22	2:B:72:GLY:N	2.29	0.47
3:C:82:ASP:OD2	3:C:130:PHE:HA	2.14	0.47
5:E:24:VAL:HA	5:E:27:ASP:OD1	2.15	0.47
5:E:28:ILE:HD13	5:E:158:PRO:HD2	1.96	0.47
5:E:99:HIS:CD2	5:E:107:MET:HG3	2.49	0.47
5:E:157:ASP:OD2	5:E:157:ASP:C	2.53	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:6:TYR:OH	7:G:8:ASP:OD2	2.24	0.47
8:H:1:THR:HG22	8:H:2:THR:N	2.30	0.47
8:H:148:THR:HG23	8:H:151:GLU:OE2	2.15	0.47
12:L:158:ARG:CG	12:L:199:TYR:HE2	2.28	0.47
2:P:73:LEU:HD23	2:P:135:ILE:HA	1.96	0.47
3:Q:159:TRP:CE3	4:R:54:GLN:HA	2.50	0.47
6:T:71:GLY:HA3	6:T:221:PHE:CE2	2.50	0.47
7:U:136:MET:HE1	7:U:163:CYS:O	2.14	0.47
7:U:189:ILE:HG22	7:U:193:VAL:HG23	1.97	0.47
7:U:219:LEU:HD12	7:U:219:LEU:O	2.14	0.47
8:V:100:ILE:N	8:V:100:ILE:HD12	2.29	0.47
10:X:109:ILE:O	10:X:121:ILE:HA	2.14	0.47
11:Y:38:MET:HE1	11:Y:60:ILE:CG2	2.45	0.47
12:Z:38:ASN:HB3	12:Z:39:PRO:HD2	1.96	0.47
12:Z:50:ALA:HB2	13:1:129:SER:HB2	1.95	0.47
12:Z:153:TYR:OH	12:Z:178:HIS:HD2	1.98	0.47
14:2:92:LEU:HD22	14:2:112:ILE:HD11	1.95	0.47
3:C:178:ASP:OD2	3:C:178:ASP:N	2.48	0.47
14:N:92:LEU:HD22	14:N:112:ILE:HD11	1.97	0.47
14:N:190:ALA:HA	14:N:198:GLU:O	2.14	0.47
1:O:101:TRP:CD2	1:O:109:ILE:HG13	2.50	0.47
1:O:120:ASP:OD1	2:P:83:ARG:NH1	2.48	0.47
7:U:54:LEU:HB2	7:U:58:TYR:CE1	2.50	0.47
10:X:172:LEU:HD23	10:X:185:VAL:HG21	1.97	0.47
3:C:3:ARG:NH2	6:F:9:ASP:OD1	2.37	0.47
7:G:189:ILE:HG22	7:G:193:VAL:HG23	1.97	0.47
12:L:6:PHE:HA	12:L:124:ALA:O	2.13	0.47
9:W:43:CYS:SG	9:W:98:LEU:HB3	2.55	0.47
10:X:20:VAL:O	10:X:190:ILE:HG12	2.15	0.47
12:Z:10:HIS:CD2	12:Z:149:VAL:HG23	2.50	0.47
13:1:54:CYS:SG	13:1:106:VAL:HG13	2.55	0.47
1:A:101:TRP:CD2	1:A:109:ILE:HG13	2.50	0.47
1:A:195:VAL:O	1:A:199:ILE:HG12	2.14	0.47
5:E:92:ALA:O	5:E:96:THR:HG23	2.15	0.47
6:F:50:LYS:HB3	6:F:59:HIS:HB3	1.96	0.47
6:F:117:GLN:CA	6:F:151:ALA:HB2	2.45	0.47
11:K:24:ASN:ND2	11:K:25:ILE:H	2.12	0.47
13:M:54:CYS:SG	13:M:106:VAL:HG13	2.55	0.47
1:O:221:THR:CG2	1:O:223:GLU:H	2.17	0.47
14:2:59:ASP:O	14:2:62:TYR:HB3	2.15	0.47
1:A:67:THR:HG22	1:A:68:HIS:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:121:SER:HB2	4:D:124:ARG:HD2	1.97	0.46
5:E:51:GLU:HG3	5:E:51:GLU:O	2.15	0.46
7:G:66:LEU:HD13	7:G:214:SER:OG	2.14	0.46
9:I:103:VAL:HG23	9:I:178:ILE:HG22	1.97	0.46
9:I:124:TYR:CD1	9:I:138:PHE:HB3	2.50	0.46
3:Q:234:GLU:HG2	3:Q:237:ILE:HD12	1.97	0.46
4:R:223:GLU:C	4:R:225:ILE:N	2.69	0.46
5:S:157:ASP:OD2	5:S:157:ASP:C	2.53	0.46
11:Y:161:ARG:O	11:Y:165:GLU:HG3	2.15	0.46
12:Z:40:TYR:HB3	12:Z:73:ARG:NH2	2.30	0.46
12:Z:51:ASP:O	12:Z:55:TRP:HD1	1.99	0.46
3:C:139:TRP:CE2	3:C:218:ARG:HD3	2.50	0.46
3:C:180:LYS:NZ	3:C:188:SER:OG	2.48	0.46
4:D:206:ILE:CG2	4:D:207:GLU:N	2.78	0.46
5:E:13:ASN:OD1	6:F:126:ARG:HD3	2.15	0.46
10:J:14:MET:CE	10:J:167:ILE:HG13	2.44	0.46
11:K:12:TYR:CD2	11:K:12:TYR:N	2.82	0.46
12:L:19:ARG:NH2	12:L:29:GLN:HE22	1.99	0.46
6:T:117:GLN:CA	6:T:151:ALA:HB2	2.45	0.46
2:B:46:ALA:HB2	2:B:209:VAL:HG12	1.97	0.46
3:C:209:GLU:O	3:C:211:VAL:N	2.48	0.46
3:C:234:GLU:O	3:C:237:ILE:HB	2.14	0.46
8:H:40:ARG:HG3	8:H:40:ARG:NH1	2.27	0.46
8:H:67:SER:O	8:H:71:ASN:N	2.48	0.46
10:J:20:VAL:HB	10:J:190:ILE:CD1	2.43	0.46
10:J:114:PRO:C	10:J:115:LYS:HD2	2.36	0.46
11:K:138:LEU:HD11	11:Y:26:VAL:HG12	1.96	0.46
7:U:12:SER:HB3	7:U:125:TYR:HA	1.98	0.46
8:V:67:SER:O	8:V:71:ASN:N	2.49	0.46
10:X:67:LEU:HD22	10:X:91:VAL:HG22	1.97	0.46
11:Y:2:GLU:HB2	11:Y:47:VAL:HG11	1.96	0.46
12:Z:180:ARG:CB	12:Z:180:ARG:HH11	2.27	0.46
14:2:42:ILE:HG22	14:2:43:MET:N	2.30	0.46
1:A:25:VAL:O	1:A:28:ALA:HB3	2.14	0.46
4:D:98:VAL:HG12	4:D:99:GLU:H	1.78	0.46
5:E:78:MET:HG3	5:E:82:ILE:CD1	2.45	0.46
11:K:38:MET:HE1	11:K:60:ILE:CG2	2.45	0.46
14:N:42:ILE:HG22	14:N:43:MET:N	2.29	0.46
1:O:88:ARG:HH11	1:O:88:ARG:HG3	1.81	0.46
3:Q:174:MET:CE	3:Q:199:LYS:HG2	2.46	0.46
3:Q:185:THR:H	3:Q:188:SER:HG	1.59	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:137:TYR:CE2	6:T:217:LYS:HA	2.51	0.46
14:2:190:ALA:HA	14:2:198:GLU:O	2.15	0.46
1:A:78:CYS:CB	1:A:140:LEU:HD23	2.45	0.46
1:A:176:THR:O	1:A:180:GLU:HG2	2.15	0.46
1:A:220:VAL:HG23	1:A:225:PRO:O	2.15	0.46
3:C:159:TRP:CE3	4:D:54:GLN:HA	2.50	0.46
9:I:200:GLY:HA2	13:1:173:ARG:HD3	1.97	0.46
12:L:4:LEU:HD12	12:L:4:LEU:O	2.16	0.46
1:O:244:GLU:HA	1:O:244:GLU:OE2	2.16	0.46
2:P:137:GLY:HA2	2:P:212:CYS:SG	2.55	0.46
5:S:51:GLU:HG3	5:S:51:GLU:O	2.16	0.46
6:T:84:LEU:O	6:T:88:MET:HG3	2.14	0.46
8:V:76:VAL:CB	8:V:110:GLN:HE21	2.09	0.46
6:F:150:SER:C	6:F:152:ASN:H	2.19	0.46
8:H:148:THR:C	8:H:150:GLU:N	2.67	0.46
9:I:18:THR:HG23	9:I:172:ASN:O	2.15	0.46
9:I:182:LYS:HG2	9:I:183:LEU:N	2.31	0.46
9:I:190:THR:CG2	9:I:192:PRO:HD3	2.36	0.46
11:K:62:LYS:N	11:K:62:LYS:HD2	2.31	0.46
1:O:88:ARG:HG3	1:O:88:ARG:NH1	2.31	0.46
3:Q:62:SER:OG	3:Q:63:GLU:N	2.48	0.46
4:R:206:ILE:CG2	4:R:207:GLU:N	2.78	0.46
13:1:151:ASN:HD22	13:1:152:GLN:HE21	1.62	0.46
3:C:234:GLU:HG2	3:C:237:ILE:HD12	1.97	0.46
4:D:98:VAL:CG1	4:D:99:GLU:N	2.77	0.46
4:D:171:PHE:CE2	4:D:194:ALA:HA	2.51	0.46
4:D:212:ARG:O	4:D:214:ASP:N	2.49	0.46
9:I:19:ARG:HD3	9:I:26:VAL:HG22	1.98	0.46
10:J:7:ASN:HD22	10:J:56:LEU:HA	1.81	0.46
10:J:34:LEU:HD23	12:Z:166:ARG:CD	2.34	0.46
11:K:190:ASP:O	11:K:191:LEU:HG	2.15	0.46
13:M:24:ALA:HB1	13:M:193:LEU:HD11	1.98	0.46
3:Q:86:LEU:HD22	3:Q:114:LEU:HD11	1.98	0.46
5:S:92:ALA:O	5:S:96:THR:HG23	2.16	0.46
5:S:225:ASN:O	5:S:226:PHE:O	2.33	0.46
7:U:108:LEU:HD11	7:U:137:LEU:HB3	1.97	0.46
8:V:148:THR:C	8:V:150:GLU:N	2.68	0.46
10:X:14:MET:CE	10:X:167:ILE:HG13	2.45	0.46
10:X:175:VAL:HG11	10:X:182:GLY:HA2	1.98	0.46
3:C:53:HIS:CE1	3:C:55:LEU:HD12	2.50	0.46
3:C:218:ARG:HH21	3:C:223:THR:N	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:115:LYS:O	10:J:116:THR:OG1	2.32	0.46
14:N:124:TYR:HE1	14:N:139:THR:HG22	1.81	0.46
3:Q:66:TYR:O	3:Q:73:ALA:HA	2.16	0.46
11:Y:1:MET:HB2	16:Y:414:HOH:O	2.15	0.46
11:Y:154:GLU:HG3	11:Y:155:ARG:H	1.81	0.46
13:1:137:ALA:H	13:1:146:GLN:HE21	1.63	0.46
14:2:59:ASP:CB	14:2:108:ASN:HD21	2.29	0.46
6:F:107:ARG:HH22	14:N:74:GLU:CG	2.29	0.46
7:G:160:TYR:CD2	7:G:163:CYS:HB2	2.50	0.46
3:Q:178:ASP:OD2	3:Q:178:ASP:N	2.47	0.46
3:Q:218:ARG:NH2	3:Q:223:THR:OG1	2.47	0.46
3:Q:218:ARG:HH21	3:Q:223:THR:N	2.14	0.46
6:T:159:MET:CG	6:T:160:SER:N	2.79	0.46
3:C:239:LYS:O	3:C:243:GLU:HB3	2.16	0.46
7:G:12:SER:HB3	7:G:125:TYR:HA	1.98	0.46
9:I:59:ILE:HG13	9:I:83:LEU:HD23	1.98	0.46
10:J:34:LEU:HG	12:Z:166:ARG:NH1	2.31	0.46
11:K:60:ILE:O	11:K:64:VAL:HG23	2.16	0.46
12:L:10:HIS:CD2	12:L:149:VAL:HG23	2.51	0.46
14:N:92:LEU:O	14:N:96:MET:HG2	2.16	0.46
1:O:25:VAL:O	1:O:28:ALA:HB3	2.16	0.46
1:O:165:ALA:O	1:O:166:THR:HG23	2.16	0.46
2:P:48:GLU:HG2	2:P:50:LYS:HG2	1.96	0.46
3:Q:109:GLN:NE2	11:Y:71:ASN:ND2	2.64	0.46
5:S:18:GLU:CD	5:S:20:ARG:HH21	2.19	0.46
5:S:160:GLY:O	6:T:82:ARG:NH2	2.49	0.46
9:W:113:ILE:HG23	9:W:119:THR:HG22	1.97	0.46
14:2:126:ASP:HB2	14:2:130:VAL:H	1.81	0.46
3:C:132:VAL:O	3:C:152:PRO:HD3	2.15	0.45
5:E:189:MET:CE	5:E:194:ALA:HA	2.43	0.45
8:H:11:GLY:HA3	8:H:179:ILE:O	2.16	0.45
10:J:96:TYR:CE1	10:J:99:ARG:HD3	2.50	0.45
13:M:83:MET:HE2	13:M:88:ILE:HA	1.97	0.45
3:Q:239:LYS:O	3:Q:243:GLU:HB3	2.15	0.45
4:R:14:GLY:HA2	5:S:26:TYR:O	2.15	0.45
5:S:99:HIS:CG	5:S:107:MET:HG3	2.51	0.45
7:U:160:TYR:CD2	7:U:163:CYS:HB2	2.51	0.45
9:W:103:VAL:HG23	9:W:178:ILE:HG22	1.98	0.45
9:W:182:LYS:HG2	9:W:183:LEU:N	2.31	0.45
12:Z:158:ARG:CG	12:Z:199:TYR:HE2	2.29	0.45
2:B:182:GLU:HG2	2:B:183:LEU:N	2.27	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:51:ASN:O	3:C:56:LEU:HD12	2.17	0.45
4:D:215:GLN:CG	4:D:216:SER:N	2.79	0.45
9:I:198:ARG:HH21	9:I:201:ARG:HA	1.81	0.45
6:T:176:MET:HA	6:T:179:PHE:CD1	2.51	0.45
9:W:59:ILE:HG13	9:W:83:LEU:HD23	1.98	0.45
9:W:124:TYR:CD1	9:W:138:PHE:HB3	2.52	0.45
10:X:115:LYS:O	10:X:116:THR:OG1	2.33	0.45
13:1:24:ALA:HB1	13:1:193:LEU:HD11	1.99	0.45
3:C:69:ASN:HB2	3:C:72:MET:HB2	1.97	0.45
10:J:7:ASN:HD22	10:J:57:ALA:N	2.01	0.45
14:N:126:ASP:HB2	14:N:130:VAL:H	1.81	0.45
1:O:89:SER:HA	7:U:117:MET:HE2	1.97	0.45
2:P:116:VAL:O	2:P:119:GLU:HB3	2.16	0.45
5:S:91:LYS:HG3	5:S:119:LEU:HD11	1.98	0.45
8:V:11:GLY:HA3	8:V:179:ILE:O	2.16	0.45
11:Y:62:LYS:N	11:Y:62:LYS:HD2	2.31	0.45
12:Z:57:ARG:HG3	12:Z:57:ARG:NH1	2.31	0.45
1:A:14:THR:O	2:B:127:ARG:HD3	2.16	0.45
2:B:51:GLN:O	2:B:53:SER:N	2.50	0.45
2:B:116:VAL:O	2:B:119:GLU:HB3	2.15	0.45
4:D:223:GLU:C	4:D:225:ILE:N	2.69	0.45
4:R:98:VAL:HG13	12:Z:78:ALA:CB	2.46	0.45
4:R:134:VAL:HG12	4:R:135:GLY:N	2.31	0.45
4:R:215:GLN:CG	4:R:216:SER:N	2.80	0.45
6:T:44:ALA:HB3	6:T:215:VAL:CG1	2.46	0.45
7:U:38:GLY:HA3	7:U:136:MET:HE2	1.98	0.45
9:W:198:ARG:HH21	9:W:201:ARG:HA	1.80	0.45
13:1:13:LEU:HD12	13:1:14:ALA:H	1.80	0.45
1:A:180:GLU:O	1:A:184:LYS:HE2	2.17	0.45
2:B:59:ARG:O	2:B:61:VAL:N	2.49	0.45
3:C:109:GLN:NE2	11:K:71:ASN:ND2	2.65	0.45
4:D:98:VAL:HG13	12:L:78:ALA:CB	2.46	0.45
5:E:91:LYS:HG3	5:E:119:LEU:HD11	1.99	0.45
8:H:148:THR:OG1	8:H:151:GLU:HG3	2.16	0.45
9:I:153:ASN:ND2	9:I:153:ASN:C	2.66	0.45
11:K:89:ALA:HB2	11:K:122:ALA:HB1	1.99	0.45
11:K:134:TYR:HB2	11:K:171:PHE:CZ	2.51	0.45
14:N:20:VAL:HG11	14:N:122:LEU:HD13	1.98	0.45
2:P:46:ALA:HB2	2:P:209:VAL:HG12	1.98	0.45
4:R:105:GLU:O	4:R:106:TYR:C	2.55	0.45
7:U:187:ARG:CZ	7:U:231:ILE:HD12	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:114:PRO:C	10:X:115:LYS:HD2	2.36	0.45
11:Y:1:MET:HE3	11:Y:134:TYR:CD1	2.51	0.45
11:Y:151:ILE:HD11	11:Y:156:ALA:CA	2.46	0.45
3:C:69:ASN:CB	3:C:72:MET:HB2	2.47	0.45
3:C:86:LEU:HD13	3:C:118:LYS:HD3	1.99	0.45
6:F:63:ILE:HA	6:F:72:ILE:O	2.17	0.45
6:F:71:GLY:HA3	6:F:221:PHE:CE2	2.51	0.45
6:F:84:LEU:O	6:F:88:MET:HG3	2.17	0.45
9:I:202:TYR:HE1	13:1:177:ASP:OD2	2.00	0.45
11:K:154:GLU:HG3	11:K:155:ARG:N	2.32	0.45
14:N:192:VAL:HG12	14:N:197:VAL:CG2	2.41	0.45
1:O:67:THR:HG22	1:O:68:HIS:H	1.82	0.45
2:P:190:ALA:O	2:P:193:THR:CG2	2.65	0.45
6:T:143:HIS:HB3	6:T:145:PHE:HE1	1.82	0.45
6:T:209:ASN:HD22	6:T:209:ASN:N	2.13	0.45
10:X:168:SER:OG	10:X:200:LEU:HD11	2.17	0.45
11:Y:134:TYR:HB2	11:Y:171:PHE:CZ	2.52	0.45
2:B:190:ALA:HA	2:B:193:THR:HG22	1.99	0.45
4:D:105:GLU:O	4:D:106:TYR:C	2.56	0.45
5:E:121:LEU:CD1	6:F:79:ALA:HB3	2.46	0.45
5:E:189:MET:HE1	5:E:194:ALA:CA	2.45	0.45
6:F:137:TYR:CE2	6:F:217:LYS:HA	2.52	0.45
7:G:108:LEU:HD11	7:G:137:LEU:HB3	1.98	0.45
8:H:72:GLU:HG2	8:H:73:PRO:HD2	1.98	0.45
9:I:202:TYR:O	9:I:203:ARG:C	2.54	0.45
10:J:20:VAL:O	10:J:190:ILE:HG12	2.17	0.45
11:K:61:GLN:NE2	11:K:62:LYS:HE2	2.32	0.45
13:M:124:PHE:CD2	13:M:130:TYR:HB3	2.52	0.45
1:O:143:ILE:CD1	1:O:220:VAL:HG13	2.47	0.45
2:P:186:ALA:HA	2:P:189:THR:CG2	2.46	0.45
3:Q:51:ASN:O	3:Q:56:LEU:HD12	2.16	0.45
4:R:171:PHE:CE2	4:R:194:ALA:HA	2.51	0.45
5:S:44:GLU:OE1	5:S:190:THR:HB	2.17	0.45
9:W:38:SER:OG	9:W:41:ILE:HB	2.17	0.45
10:X:125:ASP:HB3	10:X:127:ILE:H	1.82	0.45
4:D:212:ARG:C	4:D:214:ASP:H	2.19	0.45
5:E:121:LEU:HD12	6:F:79:ALA:HB3	1.98	0.45
6:F:143:HIS:HB3	6:F:145:PHE:HE1	1.80	0.45
10:J:10:ALA:CB	10:J:146:MET:HE2	2.43	0.45
3:Q:11:ILE:CG2	3:Q:12:PHE:N	2.79	0.45
7:U:215:TRP:O	7:U:224:HIS:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:149:LYS:O	8:V:153:LEU:HB2	2.17	0.45
13:1:7:PHE:CZ	13:1:9:GLY:HA2	2.51	0.45
13:1:12:ILE:HG12	13:1:25:SER:HB3	1.98	0.45
1:A:244:GLU:OE2	1:A:244:GLU:HA	2.17	0.45
2:B:9:LEU:HB2	2:B:126:VAL:O	2.16	0.45
3:C:235:GLN:O	3:C:239:LYS:HB2	2.16	0.45
11:K:118:MET:HB3	11:K:118:MET:HE2	1.86	0.45
13:M:72:LEU:CD2	13:M:83:MET:SD	3.04	0.45
1:O:210:PHE:HB2	1:O:214:GLU:HB2	1.98	0.45
4:R:155:ALA:H	5:S:63:SER:CB	2.29	0.45
8:V:188:VAL:HG12	8:V:190:LEU:HD23	1.99	0.45
9:W:19:ARG:HD3	9:W:26:VAL:HG22	1.99	0.45
14:2:20:VAL:HG11	14:2:122:LEU:HD13	1.98	0.45
14:2:59:ASP:HB2	14:2:108:ASN:HD21	1.82	0.45
2:B:160:THR:OG1	2:B:170:LYS:NZ	2.50	0.45
2:B:186:ALA:HA	2:B:189:THR:CG2	2.46	0.45
4:D:169:ARG:O	4:D:173:GLU:HG3	2.17	0.45
5:E:163:VAL:HG22	5:E:164:GLN:H	1.81	0.45
6:F:175:HIS:CD2	6:F:175:HIS:N	2.85	0.45
6:F:209:ASN:HD22	6:F:209:ASN:N	2.12	0.45
7:G:215:TRP:O	7:G:224:HIS:HA	2.17	0.45
10:J:122:CYS:HB2	10:J:131:MET:O	2.17	0.45
12:L:57:ARG:HG3	12:L:57:ARG:NH1	2.32	0.45
14:N:149:LEU:O	14:N:152:GLU:HB3	2.17	0.45
1:O:52:THR:CG2	1:O:53:GLN:N	2.79	0.45
1:O:176:THR:O	1:O:180:GLU:HG2	2.17	0.45
2:P:190:ALA:HA	2:P:193:THR:HG22	1.99	0.45
7:U:184:MET:HB3	7:U:184:MET:HE2	1.91	0.45
8:V:72:GLU:HG2	8:V:73:PRO:HD2	1.98	0.45
9:W:18:THR:HG23	9:W:172:ASN:O	2.17	0.45
12:Z:83:LEU:HA	12:Z:86:MET:HE2	1.98	0.45
14:2:150:LEU:HD23	14:2:168:LEU:HD13	1.99	0.45
2:B:131:VAL:O	2:B:150:PRO:HD3	2.18	0.44
10:J:136:PHE:CZ	10:J:150:CYS:HB3	2.51	0.44
11:K:154:GLU:HG3	11:K:155:ARG:H	1.81	0.44
12:L:83:LEU:HA	12:L:86:MET:HE2	1.99	0.44
12:L:166:ARG:CD	10:X:34:LEU:HD23	2.39	0.44
4:R:11:SER:HB3	4:R:12:PRO:CD	2.47	0.44
4:R:212:ARG:C	4:R:214:ASP:H	2.19	0.44
6:T:50:LYS:HB3	6:T:59:HIS:HB3	1.99	0.44
6:T:230:SER:HB2	6:T:231:PRO:CD	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:74:GLY:HA3	7:U:224:HIS:NE2	2.33	0.44
7:U:106:ILE:HA	7:U:107:PRO:HD3	1.82	0.44
14:2:51:LEU:HD12	14:2:52:GLY:H	1.82	0.44
4:D:155:ALA:H	5:E:63:SER:CB	2.28	0.44
6:F:176:MET:HA	6:F:179:PHE:CD1	2.53	0.44
11:K:115:LEU:HB3	11:K:127:ALA:O	2.18	0.44
14:N:10:SER:HB3	14:N:139:THR:O	2.18	0.44
14:N:51:LEU:HD12	14:N:52:GLY:H	1.81	0.44
1:O:143:ILE:CD1	1:O:220:VAL:HG22	2.47	0.44
4:R:208:LEU:O	4:R:209:ALA:HB2	2.16	0.44
8:V:8:PHE:CD1	8:V:8:PHE:C	2.90	0.44
9:W:191:VAL:O	9:W:191:VAL:HG12	2.17	0.44
13:1:83:MET:CE	13:1:88:ILE:HA	2.46	0.44
13:1:174:LEU:O	13:1:178:VAL:HG22	2.18	0.44
13:1:179:PHE:CD2	13:1:193:LEU:HD13	2.51	0.44
14:2:144:TYR:HA	16:2:222:HOH:O	2.16	0.44
2:B:146:PHE:CE2	2:B:156:ALA:HB2	2.53	0.44
4:D:129:ILE:O	4:D:129:ILE:HG13	2.17	0.44
4:D:134:VAL:HG12	4:D:135:GLY:N	2.32	0.44
5:E:206:MET:HE1	5:E:210:LEU:HD13	2.00	0.44
7:G:69:VAL:HG11	7:G:91:ALA:HB1	1.98	0.44
9:I:193:ASN:CB	13:1:211:ARG:HH21	2.30	0.44
13:M:190:GLY:O	13:M:191:ASP:HB2	2.16	0.44
2:P:37:ILE:O	2:P:43:VAL:HG13	2.18	0.44
3:Q:79:ILE:HD13	3:Q:131:GLY:CA	2.43	0.44
4:R:223:GLU:C	4:R:225:ILE:H	2.19	0.44
12:Z:186:ARG:CB	12:Z:186:ARG:HH11	2.30	0.44
1:A:141:ILE:HG22	1:A:151:VAL:HA	2.00	0.44
10:J:59:ASP:O	10:J:63:VAL:HG23	2.17	0.44
13:M:141:ALA:O	13:M:144:MET:N	2.43	0.44
1:O:14:THR:O	2:P:127:ARG:HD3	2.17	0.44
3:Q:15:GLU:HB2	3:Q:17:ARG:HG2	2.00	0.44
4:R:42:VAL:CB	4:R:210:VAL:HG12	2.47	0.44
11:Y:33:ASP:OD2	11:Y:181:ARG:NH2	2.50	0.44
1:A:231:THR:HG22	1:A:233:ALA:H	1.83	0.44
2:B:52:LYS:C	2:B:54:ILE:H	2.20	0.44
3:C:11:ILE:CG2	3:C:12:PHE:N	2.80	0.44
3:C:66:TYR:O	3:C:73:ALA:HA	2.17	0.44
3:C:95:GLN:OE1	10:J:72:ASN:CB	2.66	0.44
3:C:234:GLU:HA	3:C:237:ILE:CG1	2.47	0.44
4:D:208:LEU:O	4:D:209:ALA:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:163:VAL:HG22	5:E:164:GLN:N	2.33	0.44
6:F:159:MET:CG	6:F:160:SER:N	2.79	0.44
7:G:54:LEU:HB2	7:G:58:TYR:CD1	2.52	0.44
7:G:66:LEU:HD12	7:G:212:GLU:HB3	1.99	0.44
7:G:187:ARG:CZ	7:G:231:ILE:HD12	2.48	0.44
12:L:153:TYR:OH	12:L:178:HIS:HD2	2.01	0.44
13:M:137:ALA:H	13:M:146:GLN:HE21	1.64	0.44
14:N:59:ASP:O	14:N:62:TYR:HB3	2.17	0.44
14:N:215:ILE:HD11	8:V:175:ARG:CZ	2.48	0.44
4:R:212:ARG:CB	4:R:215:GLN:HB3	2.48	0.44
7:U:48:GLY:HA2	7:U:212:GLU:O	2.16	0.44
10:X:138:VAL:HG11	10:X:146:MET:HB3	1.98	0.44
11:Y:89:ALA:HB2	11:Y:122:ALA:HB1	1.99	0.44
13:1:72:LEU:CD2	13:1:83:MET:SD	3.06	0.44
14:2:25:ASP:O	14:2:41:ARG:HD3	2.17	0.44
1:A:143:ILE:CD1	1:A:220:VAL:HG22	2.47	0.44
1:A:165:ALA:O	1:A:166:THR:HG23	2.17	0.44
1:A:210:PHE:HB2	1:A:214:GLU:HB2	2.00	0.44
4:D:42:VAL:CA	4:D:210:VAL:HG12	2.44	0.44
4:D:100:ASP:HB3	4:D:101:PRO:HD2	1.99	0.44
7:G:99:ARG:NH1	14:N:69:GLN:NE2	2.64	0.44
9:I:211:VAL:HG11	10:J:198:ARG:HD3	2.00	0.44
11:K:145:ARG:HH11	11:K:145:ARG:HG3	1.82	0.44
12:L:158:ARG:HG3	12:L:199:TYR:HE2	1.82	0.44
13:M:160:ASN:ND2	13:M:160:ASN:O	2.50	0.44
1:O:203:SER:O	1:O:207:SER:N	2.50	0.44
2:P:9:LEU:HB2	2:P:126:VAL:O	2.18	0.44
3:Q:234:GLU:HA	3:Q:237:ILE:CG1	2.47	0.44
5:S:157:ASP:HB2	5:S:158:PRO:CD	2.48	0.44
11:Y:154:GLU:HG3	11:Y:155:ARG:N	2.32	0.44
3:C:174:MET:CE	3:C:199:LYS:HG2	2.47	0.44
5:E:160:GLY:O	6:F:82:ARG:NH2	2.50	0.44
5:E:225:ASN:O	5:E:226:PHE:O	2.34	0.44
8:H:15:GLY:C	8:H:160:LEU:HD11	2.38	0.44
8:H:149:LYS:O	8:H:153:LEU:HB2	2.18	0.44
11:K:1:MET:HE3	11:K:134:TYR:CD1	2.53	0.44
11:K:42:ILE:CG2	11:K:104:LEU:HD11	2.48	0.44
11:K:145:ARG:HE	12:Z:158:ARG:NE	2.15	0.44
1:O:231:THR:HG22	1:O:233:ALA:H	1.82	0.44
2:P:109:LEU:O	2:P:109:LEU:HG	2.17	0.44
2:P:147:GLN:O	2:P:154:TYR:HA	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:44:LEU:HB3	3:Q:215:THR:HG22	1.98	0.44
3:Q:95:GLN:OE1	10:X:72:ASN:CB	2.66	0.44
4:R:66:ASP:HA	11:Y:69:MET:HE2	2.00	0.44
4:R:129:ILE:O	4:R:129:ILE:HG13	2.17	0.44
7:U:54:LEU:HB2	7:U:58:TYR:CD1	2.53	0.44
9:W:202:TYR:O	9:W:203:ARG:C	2.53	0.44
10:X:136:PHE:CZ	10:X:150:CYS:HB3	2.53	0.44
12:Z:115:ASP:HB2	12:Z:119:ASN:HB2	1.98	0.44
13:1:160:ASN:O	13:1:160:ASN:ND2	2.51	0.44
9:I:38:SER:OG	9:I:41:ILE:HB	2.18	0.44
10:J:11:VAL:HG12	10:J:108:VAL:HG21	1.99	0.44
11:K:151:ILE:HD11	11:K:156:ALA:CA	2.48	0.44
13:M:179:PHE:CD2	13:M:193:LEU:HD13	2.53	0.44
14:N:59:ASP:CB	14:N:108:ASN:HD21	2.31	0.44
14:N:150:LEU:HD23	14:N:168:LEU:HD13	2.00	0.44
1:O:84:THR:O	1:O:87:SER:HB2	2.18	0.44
5:S:24:VAL:HA	5:S:27:ASP:OD1	2.17	0.44
6:T:132:LEU:HB2	6:T:147:THR:OG1	2.18	0.44
6:T:150:SER:C	6:T:152:ASN:H	2.20	0.44
12:Z:83:LEU:HA	12:Z:86:MET:CE	2.48	0.44
1:A:142:GLY:HA2	1:A:220:VAL:HG11	2.00	0.44
1:A:183:VAL:HG12	1:A:183:VAL:O	2.18	0.44
2:B:179:GLU:C	2:B:181:LEU:H	2.21	0.44
4:D:14:GLY:HA2	5:E:26:TYR:O	2.18	0.44
10:J:168:SER:OG	10:J:200:LEU:HD11	2.18	0.44
12:L:158:ARG:HG3	12:L:199:TYR:CE2	2.53	0.44
2:P:38:LYS:NZ	3:Q:57:ASP:OD2	2.50	0.44
10:X:12:MET:HE1	10:X:150:CYS:SG	2.56	0.44
11:Y:10:PRO:HD2	11:Y:12:TYR:HE2	1.83	0.44
14:2:124:TYR:HE1	14:2:139:THR:HG22	1.83	0.44
2:B:147:GLN:O	2:B:154:TYR:HA	2.18	0.43
3:C:139:TRP:CD1	3:C:144:GLY:HA2	2.53	0.43
4:D:62:ILE:HD12	4:D:62:ILE:H	1.83	0.43
4:D:212:ARG:CB	4:D:215:GLN:HB3	2.46	0.43
6:F:44:ALA:HB3	6:F:215:VAL:CG1	2.47	0.43
7:G:140:TYR:CG	7:G:217:GLY:HA2	2.53	0.43
8:H:62:GLN:HB3	8:H:82:LEU:HD13	2.00	0.43
10:J:68:LYS:NZ	10:J:72:ASN:ND2	2.63	0.43
12:L:19:ARG:NE	12:L:29:GLN:NE2	2.64	0.43
1:O:183:VAL:O	1:O:183:VAL:HG12	2.18	0.43
4:R:209:ALA:CB	4:R:219:ILE:HA	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:11:VAL:HG12	10:X:108:VAL:HG21	2.00	0.43
11:Y:115:LEU:HB3	11:Y:127:ALA:O	2.18	0.43
13:1:12:ILE:HD13	13:1:53:GLY:CA	2.48	0.43
14:2:16:PHE:CZ	14:2:162:GLN:HG3	2.54	0.43
1:A:188:ASP:O	1:A:190:THR:HG23	2.17	0.43
1:A:191:PHE:HE1	1:A:219:VAL:HG21	1.83	0.43
2:B:190:ALA:O	2:B:193:THR:CG2	2.65	0.43
10:J:175:VAL:HG11	10:J:182:GLY:HA2	2.00	0.43
3:Q:69:ASN:CB	3:Q:72:MET:HB2	2.47	0.43
4:R:100:ASP:HB3	4:R:101:PRO:HD2	1.99	0.43
6:T:65:HIS:ND1	13:1:77:HIS:HE1	2.16	0.43
9:W:28:ASP:OD1	9:W:30:ASN:N	2.47	0.43
9:W:179:SER:O	9:W:181:ASN:N	2.52	0.43
10:X:57:ALA:O	10:X:61:GLN:HG3	2.18	0.43
11:Y:117:TYR:CE1	11:Y:132:HIS:CE1	3.07	0.43
12:Z:158:ARG:HD3	12:Z:199:TYR:HE2	1.83	0.43
14:2:49:THR:CG2	14:2:85:PRO:HA	2.48	0.43
7:G:141:SER:OG	7:G:144:ASP:HB2	2.19	0.43
7:G:168:ALA:HB1	7:G:171:ALA:HB3	2.00	0.43
8:H:148:THR:C	8:H:150:GLU:H	2.21	0.43
9:I:191:VAL:O	9:I:191:VAL:HG12	2.17	0.43
12:L:51:ASP:O	12:L:55:TRP:HD1	2.01	0.43
2:P:213:ASN:C	2:P:215:ALA:H	2.22	0.43
4:R:34:GLY:O	4:R:158:ALA:HA	2.18	0.43
5:S:163:VAL:HG22	5:S:164:GLN:H	1.83	0.43
6:T:10:VAL:HG12	6:T:21:GLN:HB2	2.00	0.43
6:T:13:TRP:CH2	7:U:132:GLY:HA3	2.53	0.43
9:W:212:LEU:HD11	10:X:201:LYS:HA	2.01	0.43
12:Z:8:PHE:HB2	12:Z:145:TYR:O	2.19	0.43
3:C:15:GLU:HB2	3:C:17:ARG:HG2	2.00	0.43
3:C:44:LEU:HB3	3:C:215:THR:HG22	1.99	0.43
4:D:223:GLU:C	4:D:225:ILE:H	2.20	0.43
6:F:4:ASN:HA	6:F:7:ASP:OD2	2.18	0.43
14:N:49:THR:CG2	14:N:85:PRO:HA	2.48	0.43
1:O:141:ILE:HG22	1:O:151:VAL:HA	2.00	0.43
3:Q:235:GLN:O	3:Q:239:LYS:HB2	2.17	0.43
1:A:143:ILE:CD1	1:A:220:VAL:HG13	2.48	0.43
1:A:240:VAL:CG2	1:A:241:ALA:N	2.82	0.43
3:C:32:GLY:HA2	3:C:50:ARG:HE	1.83	0.43
3:C:155:ASN:HD22	3:C:155:ASN:HA	1.61	0.43
3:C:210:LYS:O	3:C:211:VAL:HG13	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:155:ALA:HB3	5:E:63:SER:HB3	2.00	0.43
5:E:44:GLU:OE1	5:E:190:THR:HB	2.18	0.43
6:F:5:GLN:HG3	6:F:6:TYR:CE1	2.53	0.43
9:I:164:PHE:HB3	13:1:38:ARG:HH22	1.83	0.43
11:K:151:ILE:CG1	11:K:155:ARG:HB2	2.42	0.43
3:Q:86:LEU:HD13	3:Q:118:LYS:HD3	2.00	0.43
4:R:46:GLU:O	4:R:47:LYS:C	2.57	0.43
4:R:155:ALA:HB3	5:S:63:SER:HB3	1.99	0.43
2:B:182:GLU:HB3	2:B:185:ASP:OD2	2.19	0.43
4:D:46:GLU:O	4:D:47:LYS:C	2.57	0.43
4:D:209:ALA:CB	4:D:219:ILE:HA	2.48	0.43
7:G:98:PHE:CE2	7:G:106:ILE:HA	2.53	0.43
8:H:188:VAL:HG12	8:H:190:LEU:HD23	2.01	0.43
10:J:149:MET:HE3	10:J:153:LEU:HD11	2.01	0.43
11:K:117:TYR:CE1	11:K:132:HIS:CE1	3.07	0.43
3:Q:11:ILE:HG22	3:Q:12:PHE:N	2.33	0.43
5:S:99:HIS:CB	5:S:107:MET:HE2	2.49	0.43
9:W:50:ALA:HB2	10:X:129:CYS:HB2	2.00	0.43
9:W:59:ILE:HG13	9:W:83:LEU:CG	2.49	0.43
7:G:61:GLY:O	7:G:64:LYS:HG3	2.18	0.43
7:G:77:VAL:HG12	7:G:135:PHE:HB3	2.01	0.43
12:L:19:ARG:NE	12:L:26:ILE:HD12	2.34	0.43
12:L:158:ARG:HD3	12:L:199:TYR:HE2	1.83	0.43
12:L:163:ALA:C	12:L:165:TYR:N	2.72	0.43
1:O:78:CYS:HB2	1:O:140:LEU:HD23	2.00	0.43
1:O:180:GLU:O	1:O:184:LYS:HE2	2.18	0.43
3:Q:62:SER:CB	3:Q:65:ILE:HB	2.49	0.43
3:Q:139:TRP:CD1	3:Q:144:GLY:HA2	2.54	0.43
3:Q:210:LYS:O	3:Q:211:VAL:HG13	2.18	0.43
6:T:71:GLY:HA3	6:T:221:PHE:CE1	2.53	0.43
12:Z:8:PHE:HA	12:Z:145:TYR:CD1	2.53	0.43
9:I:187:ARG:HA	9:I:187:ARG:HD2	1.86	0.43
13:M:13:LEU:HD12	13:M:14:ALA:H	1.82	0.43
13:M:75:TYR:CG	13:M:83:MET:HG3	2.54	0.43
13:M:162:GLU:O	13:M:162:GLU:HG2	2.19	0.43
13:M:211:ARG:NH2	9:W:193:ASN:CB	2.79	0.43
14:N:16:PHE:CZ	14:N:162:GLN:HG3	2.53	0.43
2:P:175:LYS:C	2:P:177:TYR:H	2.21	0.43
2:P:182:GLU:CG	2:P:183:LEU:H	2.27	0.43
3:Q:180:LYS:HZ3	3:Q:188:SER:C	2.21	0.43
4:R:169:ARG:O	4:R:173:GLU:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:148:CYS:O	6:T:150:SER:O	2.37	0.43
7:U:140:TYR:CG	7:U:217:GLY:HA2	2.53	0.43
10:X:7:ASN:HD22	10:X:56:LEU:HA	1.83	0.43
10:X:164:PHE:CE1	10:X:198:ARG:HD2	2.54	0.43
12:Z:186:ARG:HH11	12:Z:186:ARG:HB3	1.83	0.43
14:2:116:ALA:O	14:2:117:ASP:HB2	2.18	0.43
3:C:35:LEU:HD12	3:C:175:LEU:HD11	2.01	0.43
4:D:69:VAL:HG12	4:D:70:CYS:N	2.33	0.43
4:D:82:ILE:O	4:D:86:ARG:HG3	2.19	0.43
7:G:74:GLY:HA3	7:G:224:HIS:NE2	2.33	0.43
12:L:105:ASP:HB3	12:L:106:LYS:H	1.57	0.43
13:M:176:LYS:CD	9:W:199:LEU:HD22	2.46	0.43
2:P:146:PHE:CE2	2:P:156:ALA:HB2	2.54	0.43
3:Q:234:GLU:HA	3:Q:237:ILE:HD12	2.01	0.43
4:R:132:LEU:HG	4:R:161:ILE:CD1	2.49	0.43
10:X:122:CYS:HB2	10:X:131:MET:O	2.18	0.43
13:1:75:TYR:CD2	13:1:83:MET:HG3	2.54	0.43
1:A:51:VAL:HG13	1:A:51:VAL:O	2.19	0.43
4:D:42:VAL:CB	4:D:210:VAL:HG12	2.49	0.43
4:D:45:VAL:O	4:D:45:VAL:HG13	2.18	0.43
5:E:47:CYS:HB3	5:E:219:THR:HG22	2.00	0.43
7:G:187:ARG:HA	7:G:187:ARG:HD2	1.90	0.43
8:H:30:VAL:CG1	14:2:212:ALA:HA	2.49	0.43
8:H:50:ALA:N	9:I:118:SER:HB3	2.34	0.43
13:M:12:ILE:HD13	13:M:53:GLY:CA	2.49	0.43
2:P:179:GLU:C	2:P:181:LEU:H	2.22	0.43
3:Q:95:GLN:CA	3:Q:95:GLN:HE21	2.31	0.43
5:S:96:THR:HA	5:S:107:MET:HE2	2.00	0.43
6:T:4:ASN:HA	6:T:7:ASP:OD2	2.19	0.43
6:T:192:LEU:HD21	6:T:210:VAL:HG11	2.01	0.43
7:U:164:ALA:O	7:U:169:ARG:HG3	2.19	0.43
8:V:148:THR:C	8:V:150:GLU:H	2.22	0.43
10:X:126:LEU:N	10:X:126:LEU:HD12	2.34	0.43
5:E:47:CYS:CB	5:E:219:THR:HG22	2.49	0.42
6:F:10:VAL:HG12	6:F:21:GLN:HB3	2.00	0.42
7:G:184:MET:HE2	7:G:189:ILE:HD13	2.00	0.42
8:H:20:THR:OG1	8:H:28:ASN:HB3	2.19	0.42
9:I:28:ASP:OD1	9:I:30:ASN:N	2.50	0.42
11:K:35:MET:CG	11:K:45:LEU:HD13	2.49	0.42
12:L:8:PHE:HA	12:L:145:TYR:CD1	2.54	0.42
13:M:75:TYR:CD2	13:M:83:MET:HG3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:35:LEU:HD12	3:Q:175:LEU:HD11	2.01	0.42
3:Q:218:ARG:O	3:Q:219:GLU:HG3	2.19	0.42
4:R:221:ASN:HD22	4:R:223:GLU:CB	2.32	0.42
5:S:155:HIS:O	5:S:162:PHE:HA	2.19	0.42
7:U:116:ALA:HB1	7:U:155:GLY:O	2.19	0.42
11:Y:24:ASN:CG	11:Y:25:ILE:H	2.22	0.42
14:2:149:LEU:O	14:2:152:GLU:HB3	2.18	0.42
2:B:10:THR:O	3:C:128:ARG:HD3	2.19	0.42
3:C:2:SER:HB3	6:F:123:TYR:CE2	2.54	0.42
6:F:138:ASP:OD1	6:F:140:MET:HB2	2.19	0.42
7:G:90:ILE:CD1	7:G:118:TYR:CE2	3.00	0.42
9:I:163:ILE:HG23	9:I:170:GLY:HA2	2.01	0.42
11:K:66:LEU:HD21	11:K:70:ARG:HH11	1.84	0.42
12:L:81:LYS:HD3	12:L:120:ARG:NH1	2.34	0.42
14:N:25:ASP:O	14:N:41:ARG:HD3	2.19	0.42
2:P:182:GLU:HB3	2:P:185:ASP:OD2	2.18	0.42
3:Q:155:ASN:HD22	3:Q:155:ASN:HA	1.60	0.42
3:Q:167:ASN:C	3:Q:169:ALA:N	2.72	0.42
5:S:221:GLN:O	5:S:223:GLY:N	2.52	0.42
6:T:63:ILE:HA	6:T:72:ILE:O	2.19	0.42
13:1:151:ASN:ND2	13:1:152:GLN:HE21	2.18	0.42
1:A:88:ARG:NH2	7:G:157:SER:O	2.52	0.42
1:A:203:SER:O	1:A:207:SER:N	2.51	0.42
2:B:28:VAL:HG13	2:B:76:SER:O	2.18	0.42
2:B:142:ARG:HA	2:B:143:PRO:HD3	1.83	0.42
2:B:157:TRP:CD2	2:B:160:THR:HB	2.54	0.42
3:C:205:LYS:O	3:C:206:LEU:C	2.58	0.42
3:C:234:GLU:HA	3:C:237:ILE:HD12	2.02	0.42
5:E:18:GLU:CD	5:E:20:ARG:HH21	2.22	0.42
8:H:8:PHE:CD1	8:H:8:PHE:C	2.92	0.42
9:I:113:ILE:HG12	9:I:119:THR:HG22	2.01	0.42
11:K:58:GLU:O	11:K:62:LYS:HD3	2.19	0.42
12:L:127:SER:HB3	12:L:136:TYR:CE1	2.54	0.42
13:M:151:ASN:ND2	13:M:152:GLN:HE21	2.17	0.42
1:O:240:VAL:CG2	1:O:241:ALA:N	2.82	0.42
5:S:163:VAL:HG22	5:S:164:GLN:N	2.34	0.42
7:U:42:LYS:HE2	7:U:185:THR:CG2	2.33	0.42
7:U:66:LEU:HD12	7:U:212:GLU:HB3	2.01	0.42
8:V:48:SER:HB3	8:V:51:ASP:HB2	2.01	0.42
9:W:209:THR:HG21	10:X:168:SER:HB3	2.02	0.42
13:1:136:LYS:HG3	13:1:137:ALA:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1:195:ILE:HD12	13:1:195:ILE:N	2.34	0.42
14:2:10:SER:HB3	14:2:139:THR:O	2.19	0.42
1:A:39:SER:O	1:A:167:ALA:HA	2.18	0.42
2:B:33:PRO:HA	2:B:162:MET:O	2.19	0.42
3:C:11:ILE:HG23	4:D:18:GLN:NE2	2.34	0.42
3:C:11:ILE:HG22	3:C:12:PHE:N	2.34	0.42
3:C:95:GLN:CA	3:C:95:GLN:HE21	2.31	0.42
3:C:167:ASN:C	3:C:169:ALA:N	2.72	0.42
4:D:132:LEU:HG	4:D:161:ILE:CD1	2.50	0.42
6:F:38:LEU:HD22	6:F:187:LEU:CD1	2.49	0.42
6:F:44:ALA:HB3	6:F:215:VAL:HG13	2.02	0.42
6:F:236:LEU:HB3	6:F:237:GLU:H	1.36	0.42
9:I:68:LEU:HD12	9:I:68:LEU:HA	1.82	0.42
10:J:125:ASP:HB3	10:J:127:ILE:H	1.85	0.42
11:K:107:TYR:CD2	11:K:185:LYS:HA	2.54	0.42
11:K:108:ASP:HB3	11:K:111:GLU:HB2	2.02	0.42
12:L:8:PHE:HB2	12:L:145:TYR:O	2.19	0.42
12:L:180:ARG:HH11	12:L:180:ARG:HB2	1.84	0.42
14:N:77:LEU:O	14:N:78:GLY:C	2.57	0.42
5:S:47:CYS:HB3	5:S:219:THR:HG22	2.01	0.42
8:V:194:ILE:O	8:V:195:PRO:C	2.58	0.42
4:D:98:VAL:HG12	4:D:100:ASP:H	1.85	0.42
4:D:206:ILE:CG2	4:D:207:GLU:H	2.33	0.42
5:E:76:CYS:HA	5:E:142:LEU:O	2.19	0.42
2:P:43:VAL:CG1	2:P:44:VAL:N	2.80	0.42
2:P:45:LEU:HD22	2:P:74:VAL:CG2	2.50	0.42
2:P:101:GLN:NE2	9:W:57:GLN:OE1	2.51	0.42
2:P:157:TRP:CD2	2:P:160:THR:HB	2.53	0.42
4:R:69:VAL:HG12	4:R:70:CYS:N	2.34	0.42
6:T:154:PHE:CD1	6:T:154:PHE:N	2.88	0.42
7:U:90:ILE:CD1	7:U:118:TYR:CE2	3.01	0.42
8:V:62:GLN:HB3	8:V:82:LEU:HD13	2.02	0.42
11:Y:66:LEU:HD21	11:Y:70:ARG:HH11	1.84	0.42
12:Z:38:ASN:C	12:Z:40:TYR:H	2.22	0.42
14:2:10:SER:HB3	14:2:142:GLY:H	1.85	0.42
3:C:17:ARG:HD2	3:C:22:GLU:OE2	2.20	0.42
5:E:56:SER:HA	5:E:57:PRO:HD3	1.89	0.42
6:F:13:TRP:NE1	7:G:129:ARG:HD2	2.34	0.42
6:F:206:THR:HG22	6:F:207:THR:N	2.34	0.42
7:G:164:ALA:O	7:G:169:ARG:HG3	2.20	0.42
9:I:143:ARG:NH1	9:I:150:GLU:OE1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:178:ASN:OD1	2:P:179:GLU:N	2.51	0.42
2:P:217:PHE:C	2:P:217:PHE:CD2	2.93	0.42
3:Q:17:ARG:HD2	3:Q:22:GLU:OE2	2.20	0.42
4:R:45:VAL:HG13	4:R:45:VAL:O	2.19	0.42
4:R:98:VAL:HG12	4:R:100:ASP:H	1.84	0.42
5:S:65:GLU:OE1	5:S:68:VAL:HG12	2.19	0.42
6:T:5:GLN:HG3	6:T:6:TYR:CE1	2.54	0.42
7:U:129:ARG:HA	7:U:130:PRO:HD3	1.94	0.42
7:U:141:SER:OG	7:U:144:ASP:HB2	2.19	0.42
11:Y:108:ASP:HB3	11:Y:111:GLU:HB2	2.00	0.42
12:Z:19:ARG:NE	12:Z:26:ILE:HD12	2.33	0.42
12:Z:105:ASP:C	12:Z:107:ARG:H	2.20	0.42
2:B:175:LYS:C	2:B:177:TYR:H	2.22	0.42
4:D:221:ASN:HD22	4:D:223:GLU:CB	2.33	0.42
5:E:157:ASP:HB2	5:E:158:PRO:CD	2.50	0.42
13:M:162:GLU:CD	13:M:162:GLU:H	2.22	0.42
6:T:206:THR:HG22	6:T:207:THR:N	2.35	0.42
6:T:230:SER:CB	6:T:231:PRO:HD3	2.43	0.42
12:Z:127:SER:HB3	12:Z:136:TYR:CE1	2.54	0.42
12:Z:158:ARG:HG3	12:Z:199:TYR:CE2	2.55	0.42
4:D:203:GLY:C	4:D:205:ASN:H	2.22	0.42
5:E:14:THR:HG23	6:F:21:GLN:HE22	1.83	0.42
9:I:67:SER:HA	16:I:307:HOH:O	2.18	0.42
1:O:38:THR:HA	1:O:169:GLY:HA3	2.02	0.42
1:O:188:ASP:O	1:O:190:THR:HG23	2.19	0.42
3:Q:32:GLY:HA2	3:Q:50:ARG:HE	1.85	0.42
7:U:61:GLY:O	7:U:64:LYS:HG3	2.20	0.42
9:W:113:ILE:HG12	9:W:119:THR:HG22	2.02	0.42
9:W:211:VAL:HG11	10:X:198:ARG:HD3	2.01	0.42
9:W:216:ILE:HD13	10:X:196:THR:HG23	2.00	0.42
11:Y:42:ILE:CG2	11:Y:104:LEU:HD11	2.50	0.42
13:1:20:PHE:CD1	13:1:168:LEU:HD13	2.55	0.42
13:1:75:TYR:CG	13:1:83:MET:HG3	2.55	0.42
1:A:13:ILE:HG13	1:A:15:ILE:HG23	2.01	0.42
3:C:192:LEU:O	3:C:196:VAL:HG23	2.19	0.42
5:E:96:THR:CA	5:E:107:MET:HE3	2.40	0.42
7:G:87:LEU:HD23	7:G:87:LEU:HA	1.85	0.42
11:K:196:PHE:HA	11:K:197:PRO:HD3	1.77	0.42
13:M:185:ARG:HG3	10:X:147:TYR:HB3	2.02	0.42
14:N:174:ARG:HE	14:N:205:THR:CG2	2.32	0.42
14:N:177:TYR:CD1	14:N:185:ASN:HB2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:160:THR:OG1	2:P:170:LYS:NZ	2.52	0.42
3:Q:205:LYS:O	3:Q:206:LEU:C	2.58	0.42
4:R:26:VAL:HG22	4:R:129:ILE:HA	2.01	0.42
6:T:134:ILE:O	6:T:144:ILE:HA	2.19	0.42
9:W:3:ILE:CD1	9:W:127:MET:HB2	2.47	0.42
10:X:65:GLN:NE2	11:Y:86:ARG:HH21	2.17	0.42
10:X:126:LEU:HD12	10:X:126:LEU:H	1.85	0.42
11:Y:107:TYR:CD2	11:Y:185:LYS:HA	2.55	0.42
11:Y:142:ILE:O	11:Y:145:ARG:HB3	2.19	0.42
13:1:102:PHE:N	13:1:103:PRO:HD3	2.35	0.42
13:1:162:GLU:H	13:1:162:GLU:CD	2.23	0.42
1:A:78:CYS:HB2	1:A:140:LEU:HD23	2.02	0.42
1:A:84:THR:O	1:A:87:SER:HB2	2.20	0.42
1:A:208:ILE:O	1:A:209:ASP:C	2.56	0.42
2:B:213:ASN:C	2:B:215:ALA:H	2.22	0.42
3:C:185:THR:H	3:C:188:SER:HG	1.62	0.42
6:F:121:GLN:HG3	7:G:129:ARG:HG3	2.02	0.42
8:H:133:SER:O	8:V:134:TYR:HA	2.20	0.42
9:I:179:SER:O	9:I:181:ASN:N	2.53	0.42
9:I:209:THR:HG21	10:J:168:SER:HB3	2.01	0.42
11:K:1:MET:H3	11:K:173:LEU:HD13	1.85	0.42
13:M:195:ILE:N	13:M:195:ILE:HD12	2.34	0.42
2:P:171:THR:CA	2:P:174:GLU:HB2	2.47	0.42
4:R:107:ILE:O	4:R:111:ILE:HG13	2.20	0.42
8:V:38:HIS:ND1	8:V:39:ASP:N	2.68	0.42
8:V:98:ILE:HG22	8:V:99:ILE:N	2.35	0.42
13:1:14:ALA:O	13:1:135:PHE:HA	2.20	0.42
13:1:137:ALA:N	13:1:146:GLN:HE21	2.18	0.42
2:B:232:ILE:O	2:B:233:ALA:HB3	2.20	0.41
4:D:34:GLY:O	4:D:158:ALA:HA	2.20	0.41
4:D:79:ASP:OD1	4:D:125:ARG:NH2	2.53	0.41
6:F:13:TRP:N	7:G:22:GLN:HE22	1.95	0.41
9:I:212:LEU:HD11	10:J:201:LYS:HA	2.00	0.41
11:K:33:ASP:OD2	11:K:181:ARG:NH2	2.53	0.41
13:M:192:ALA:O	13:M:210:LEU:HD12	2.20	0.41
14:N:166:ARG:NH2	14:N:200:GLU:OE2	2.44	0.41
1:O:93:ARG:HG2	1:O:93:ARG:NH1	2.34	0.41
1:O:123:GLN:HE22	1:O:127:GLN:NE2	2.17	0.41
1:O:126:THR:CG2	2:P:127:ARG:HH21	2.19	0.41
1:O:208:ILE:O	1:O:209:ASP:C	2.58	0.41
3:Q:95:GLN:HA	3:Q:95:GLN:HE21	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:203:GLY:C	4:R:205:ASN:H	2.22	0.41
9:W:163:ILE:HG23	9:W:170:GLY:HA2	2.02	0.41
10:X:20:VAL:HB	10:X:190:ILE:CG1	2.50	0.41
10:X:68:LYS:NZ	10:X:72:ASN:ND2	2.65	0.41
10:X:190:ILE:HG22	10:X:195:ILE:HD13	1.99	0.41
12:Z:158:ARG:HG3	12:Z:199:TYR:HE2	1.84	0.41
13:1:150:ASP:HB3	13:1:156:LYS:HD2	2.02	0.41
9:I:43:CYS:SG	9:I:98:LEU:HB3	2.60	0.41
10:J:7:ASN:HA	10:J:29:GLY:O	2.21	0.41
12:L:186:ARG:CB	12:L:186:ARG:HH11	2.33	0.41
1:O:13:ILE:HG13	1:O:15:ILE:HG23	2.01	0.41
3:Q:192:LEU:O	3:Q:196:VAL:HG23	2.20	0.41
3:Q:209:GLU:C	3:Q:211:VAL:N	2.72	0.41
6:T:117:GLN:HB2	6:T:151:ALA:CB	2.50	0.41
6:T:138:ASP:C	6:T:140:MET:H	2.24	0.41
7:U:210:GLU:HG2	7:U:211:LEU:N	2.35	0.41
7:U:227:VAL:HA	7:U:228:PRO:HD3	1.95	0.41
11:Y:78:THR:HG23	11:Y:116:TYR:OH	2.20	0.41
1:A:38:THR:HA	1:A:169:GLY:HA3	2.02	0.41
1:A:145:GLU:CG	1:A:146:GLU:N	2.83	0.41
2:B:134:LEU:HA	2:B:146:PHE:O	2.20	0.41
4:D:108:THR:HG23	4:D:133:ILE:HD12	2.02	0.41
5:E:99:HIS:CG	5:E:107:MET:HG3	2.54	0.41
8:H:148:THR:O	8:H:150:GLU:N	2.53	0.41
9:I:59:ILE:HG13	9:I:83:LEU:CG	2.50	0.41
10:J:190:ILE:HG22	10:J:195:ILE:HD13	2.00	0.41
13:M:14:ALA:C	13:M:15:ILE:HD12	2.39	0.41
1:O:88:ARG:NH2	7:U:157:SER:O	2.53	0.41
2:P:232:ILE:O	2:P:233:ALA:HB3	2.20	0.41
5:S:200:ILE:O	5:S:204:GLN:HG3	2.21	0.41
5:S:227:HIS:HE1	5:S:229:PHE:HA	1.85	0.41
8:V:19:ARG:O	8:V:33:LYS:NZ	2.51	0.41
11:Y:35:MET:CG	11:Y:45:LEU:HD13	2.51	0.41
12:Z:15:ALA:HB2	12:Z:176:LEU:HD13	2.02	0.41
12:Z:125:THR:CB	12:Z:139:MET:HE3	2.49	0.41
14:2:51:LEU:HD12	14:2:52:GLY:N	2.36	0.41
2:B:70:HIS:CE1	2:B:103:PRO:HB3	2.56	0.41
3:C:95:GLN:NE2	3:C:95:GLN:CA	2.83	0.41
8:H:38:HIS:ND1	8:H:39:ASP:N	2.67	0.41
10:J:155:GLU:HB2	10:J:158:MET:HE3	2.02	0.41
11:K:24:ASN:CG	11:K:25:ILE:H	2.23	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:26:VAL:HG12	11:Y:138:LEU:HD11	2.03	0.41
13:M:12:ILE:O	13:M:137:ALA:HA	2.21	0.41
14:N:45:VAL:O	14:N:49:THR:O	2.38	0.41
14:N:122:LEU:HG	14:N:137:LEU:HD12	2.01	0.41
1:O:93:ARG:HG2	1:O:93:ARG:HH11	1.85	0.41
1:O:145:GLU:CG	1:O:146:GLU:N	2.83	0.41
4:R:206:ILE:CG2	4:R:207:GLU:H	2.33	0.41
5:S:76:CYS:HA	5:S:142:LEU:O	2.20	0.41
5:S:202:LEU:O	5:S:206:MET:HE3	2.19	0.41
6:T:10:VAL:HG12	6:T:21:GLN:HB3	2.01	0.41
10:X:59:ASP:O	10:X:63:VAL:HG23	2.20	0.41
10:X:155:GLU:HB2	10:X:158:MET:HE3	2.02	0.41
14:2:77:LEU:O	14:2:78:GLY:C	2.57	0.41
2:B:182:GLU:CG	2:B:183:LEU:H	2.27	0.41
3:C:209:GLU:C	3:C:211:VAL:N	2.72	0.41
6:F:71:GLY:HA3	6:F:221:PHE:CE1	2.56	0.41
8:H:194:ILE:O	8:H:195:PRO:C	2.58	0.41
9:I:84:LYS:HE3	9:I:84:LYS:HB2	1.77	0.41
9:I:101:GLY:HA2	9:I:109:HIS:O	2.21	0.41
10:J:57:ALA:O	10:J:61:GLN:HG3	2.21	0.41
10:J:126:LEU:N	10:J:126:LEU:HD12	2.35	0.41
11:K:1:MET:HE2	11:K:134:TYR:H	1.80	0.41
11:K:4:LEU:O	11:K:131:ALA:HA	2.21	0.41
12:L:115:ASP:HB2	12:L:119:ASN:HB2	2.02	0.41
14:N:59:ASP:HB2	14:N:108:ASN:HD21	1.85	0.41
1:O:142:GLY:HA2	1:O:220:VAL:HG11	2.01	0.41
2:P:70:HIS:CE1	2:P:103:PRO:HB3	2.55	0.41
3:Q:28:ILE:C	3:Q:30:HIS:H	2.24	0.41
4:R:45:VAL:HG21	4:R:61:LYS:CB	2.51	0.41
4:R:52:LYS:HD3	4:R:52:LYS:HA	1.94	0.41
6:T:38:LEU:HD22	6:T:187:LEU:CD1	2.50	0.41
6:T:174:ARG:HG3	16:T:267:HOH:O	2.20	0.41
9:W:187:ARG:O	9:W:189:TYR:N	2.54	0.41
14:2:92:LEU:O	14:2:96:MET:HG2	2.21	0.41
1:A:32:ILE:HD11	1:A:156:PRO:HG2	2.03	0.41
3:C:28:ILE:C	3:C:30:HIS:H	2.24	0.41
3:C:136:TYR:O	3:C:147:LEU:HA	2.20	0.41
5:E:206:MET:CE	5:E:210:LEU:HD13	2.51	0.41
6:F:138:ASP:C	6:F:140:MET:H	2.22	0.41
6:F:154:PHE:CD1	6:F:154:PHE:N	2.88	0.41
6:F:230:SER:HB2	6:F:231:PRO:CD	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:175:ARG:NH1	14:2:215:ILE:HD11	2.35	0.41
9:I:3:ILE:CD1	9:I:127:MET:HB2	2.46	0.41
9:I:171:SER:HB3	9:I:172:ASN:H	1.62	0.41
9:I:216:ILE:HD13	10:J:196:THR:HG23	2.02	0.41
12:L:113:TYR:O	12:L:120:ARG:HA	2.21	0.41
14:N:51:LEU:HD12	14:N:52:GLY:N	2.35	0.41
2:P:13:SER:O	3:Q:23:TYR:HB3	2.21	0.41
2:P:173:LEU:O	2:P:175:LYS:N	2.54	0.41
5:S:59:MET:SD	5:S:64:ILE:HD11	2.59	0.41
6:T:175:HIS:N	6:T:175:HIS:CD2	2.86	0.41
8:V:84:LYS:HE3	8:V:84:LYS:HB3	1.93	0.41
13:1:162:GLU:O	13:1:162:GLU:HG2	2.20	0.41
4:D:26:VAL:HG22	4:D:129:ILE:HA	2.01	0.41
5:E:155:HIS:O	5:E:162:PHE:HA	2.20	0.41
6:F:105:VAL:O	6:F:109:VAL:HG23	2.21	0.41
6:F:117:GLN:HB2	6:F:151:ALA:CB	2.50	0.41
7:G:67:PHE:CD1	7:G:67:PHE:N	2.88	0.41
7:G:76:ALA:O	7:G:135:PHE:HA	2.21	0.41
9:I:202:TYR:CE1	13:1:177:ASP:OD2	2.73	0.41
12:L:83:LEU:HA	12:L:86:MET:CE	2.51	0.41
13:M:195:ILE:HG22	13:M:196:CYS:N	2.36	0.41
4:R:168:VAL:O	4:R:172:LEU:HG	2.21	0.41
6:T:96:ARG:NH2	6:T:102:PRO:HB3	2.35	0.41
6:T:170:THR:O	6:T:174:ARG:HG3	2.21	0.41
6:T:237:GLU:O	6:T:239:ARG:N	2.51	0.41
7:U:99:ARG:NH1	14:2:69:GLN:HE22	2.18	0.41
8:V:20:THR:OG1	8:V:28:ASN:HB3	2.19	0.41
10:X:28:PHE:HB2	10:X:39:PHE:CG	2.56	0.41
10:X:168:SER:HB3	10:X:200:LEU:CD1	2.51	0.41
13:1:83:MET:HE2	13:1:88:ILE:CA	2.51	0.41
3:C:25:MET:O	3:C:28:ILE:HB	2.21	0.41
4:D:11:SER:HB3	4:D:12:PRO:CD	2.50	0.41
4:D:107:ILE:O	4:D:111:ILE:HG13	2.21	0.41
6:F:27:GLU:O	6:F:31:GLN:HG2	2.20	0.41
6:F:134:ILE:O	6:F:144:ILE:HA	2.21	0.41
7:G:227:VAL:HA	7:G:228:PRO:HD3	1.96	0.41
11:K:60:ILE:HD12	11:K:84:THR:HA	2.03	0.41
11:K:142:ILE:O	11:K:145:ARG:HB3	2.20	0.41
7:U:87:LEU:HD23	7:U:87:LEU:HA	1.85	0.41
7:U:168:ALA:HB1	7:U:171:ALA:HB3	2.02	0.41
12:Z:9:ARG:HH21	12:Z:146:ASP:CB	2.32	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1:8:ASN:HA	13:1:30:SER:O	2.21	0.41
14:2:25:ASP:HA	14:2:187:PHE:HB3	2.03	0.41
1:A:212:PRO:HB3	1:A:236:ASP:HB2	2.02	0.41
3:C:72:MET:CE	3:C:107:CYS:HA	2.51	0.41
5:E:217:LEU:O	5:E:229:PHE:HB2	2.20	0.41
6:F:101:ARG:O	6:F:101:ARG:HG3	2.17	0.41
7:G:90:ILE:HD13	7:G:118:TYR:CD2	2.55	0.41
8:H:134:TYR:HA	8:V:133:SER:O	2.20	0.41
8:H:153:LEU:CD1	8:H:176:LEU:HD13	2.51	0.41
10:J:74:TYR:CE1	10:J:78:GLU:HG3	2.56	0.41
10:J:164:PHE:CE1	10:J:198:ARG:HD2	2.55	0.41
12:L:38:ASN:C	12:L:40:TYR:H	2.24	0.41
13:M:119:GLY:O	13:M:132:ARG:NH2	2.53	0.41
14:N:116:ALA:O	14:N:117:ASP:HB2	2.21	0.41
14:N:161:SER:OG	14:N:164:GLU:HG3	2.20	0.41
1:O:39:SER:O	1:O:167:ALA:HA	2.21	0.41
1:O:143:ILE:HD11	1:O:220:VAL:HG13	2.03	0.41
1:O:221:THR:O	1:O:224:ASN:C	2.59	0.41
2:P:28:VAL:HG13	2:P:76:SER:O	2.21	0.41
3:Q:130:PHE:O	3:Q:152:PRO:HB3	2.21	0.41
4:R:85:ASN:O	4:R:89:VAL:HG23	2.20	0.41
4:R:175:ASN:HB2	4:R:190:LEU:HD11	2.03	0.41
5:S:28:ILE:HD13	5:S:158:PRO:HD2	2.01	0.41
6:T:43:HIS:ND1	6:T:184:LEU:HD13	2.36	0.41
7:U:69:VAL:HG11	7:U:91:ALA:HB1	2.03	0.41
7:U:98:PHE:CE2	7:U:106:ILE:HA	2.56	0.41
9:W:187:ARG:HD2	9:W:187:ARG:HA	1.85	0.41
10:X:22:ILE:CG2	10:X:188:HIS:HB2	2.51	0.41
10:X:65:GLN:NE2	11:Y:86:ARG:HH22	2.17	0.41
10:X:200:LEU:HD23	10:X:200:LEU:N	2.36	0.41
11:Y:151:ILE:CG1	11:Y:155:ARG:HB2	2.40	0.41
12:Z:4:LEU:HD12	12:Z:4:LEU:O	2.21	0.41
12:Z:4:LEU:HG	12:Z:160:ILE:HD11	2.03	0.41
12:Z:100:MET:HA	12:Z:112:TYR:O	2.20	0.41
12:Z:180:ARG:HH11	12:Z:180:ARG:HB2	1.85	0.41
13:1:141:ALA:O	13:1:144:MET:N	2.47	0.41
13:1:159:GLN:NE2	13:1:160:ASN:N	2.63	0.41
13:1:195:ILE:HG22	13:1:196:CYS:N	2.36	0.41
14:2:186:ARG:HA	14:2:203:LEU:O	2.21	0.41
3:C:44:LEU:HD13	3:C:44:LEU:H	1.86	0.41
3:C:87:THR:O	3:C:90:LEU:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:80:ASP:OD1	6:F:126:ARG:NH2	2.53	0.41
6:F:133:LEU:HD23	6:F:133:LEU:HA	1.97	0.41
9:I:50:ALA:HB2	10:J:129:CYS:HB2	2.03	0.41
10:J:68:LYS:HZ3	10:J:72:ASN:ND2	2.19	0.41
10:J:135:ASP:HA	10:J:154:TRP:CZ2	2.56	0.41
10:J:168:SER:HB3	10:J:200:LEU:CD1	2.51	0.41
14:N:25:ASP:HA	14:N:187:PHE:HB3	2.02	0.41
1:O:191:PHE:HE1	1:O:219:VAL:HG21	1.85	0.41
2:P:227:ASP:O	2:P:229:LEU:N	2.54	0.41
3:Q:50:ARG:C	3:Q:52:ILE:H	2.25	0.41
3:Q:189:ALA:C	3:Q:191:ALA:H	2.24	0.41
5:S:149:LYS:HB2	5:S:152:GLN:NE2	2.36	0.41
6:T:138:ASP:OD1	6:T:140:MET:HB2	2.20	0.41
11:Y:160:LEU:HD11	11:Y:164:LEU:HD11	2.03	0.41
2:B:217:PHE:CD2	2:B:217:PHE:C	2.94	0.40
3:C:130:PHE:O	3:C:152:PRO:HB3	2.20	0.40
3:C:241:GLU:O	3:C:243:GLU:N	2.45	0.40
4:D:171:PHE:CD2	4:D:194:ALA:HA	2.56	0.40
5:E:227:HIS:HE1	5:E:229:PHE:HA	1.86	0.40
6:F:47:VAL:CG1	6:F:195:LEU:HD22	2.52	0.40
1:O:130:GLU:H	1:O:130:GLU:CD	2.23	0.40
5:S:47:CYS:CB	5:S:219:THR:HG22	2.50	0.40
7:U:67:PHE:CD1	7:U:67:PHE:N	2.88	0.40
9:W:17:ASP:CG	9:W:33:LYS:HZ2	2.24	0.40
9:W:106:THR:O	9:W:106:THR:CG2	2.69	0.40
11:Y:145:ARG:HH11	11:Y:145:ARG:HG3	1.86	0.40
14:2:161:SER:OG	14:2:164:GLU:HG3	2.21	0.40
3:C:62:SER:CB	3:C:65:ILE:HB	2.50	0.40
5:E:221:GLN:O	5:E:223:GLY:N	2.54	0.40
6:F:132:LEU:HB2	6:F:147:THR:OG1	2.21	0.40
6:F:170:THR:O	6:F:174:ARG:HG3	2.21	0.40
11:K:10:PRO:HD2	11:K:12:TYR:HE2	1.85	0.40
11:K:145:ARG:HG3	11:K:145:ARG:NH1	2.36	0.40
12:L:9:ARG:HH21	12:L:146:ASP:CB	2.34	0.40
12:L:44:THR:O	12:L:99:THR:OG1	2.35	0.40
12:L:186:ARG:HH11	12:L:186:ARG:HB3	1.86	0.40
14:N:201:GLY:O	14:N:203:LEU:HG	2.21	0.40
3:Q:44:LEU:HD13	3:Q:44:LEU:H	1.86	0.40
3:Q:170:ALA:HB3	3:Q:200:THR:HG22	2.03	0.40
6:T:23:GLU:O	6:T:26:MET:HB2	2.21	0.40
6:T:47:VAL:CG1	6:T:195:LEU:HD22	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:174:ARG:C	6:T:175:HIS:HD2	2.25	0.40
8:V:8:PHE:O	8:V:9:ASP:C	2.60	0.40
9:W:155:VAL:O	9:W:159:ILE:HG12	2.21	0.40
11:Y:1:MET:H1	11:Y:173:LEU:HD13	1.86	0.40
3:C:245:ALA:HA	3:C:248:GLU:OE2	2.22	0.40
4:D:45:VAL:HG21	4:D:61:LYS:CB	2.52	0.40
6:F:192:LEU:HD21	6:F:210:VAL:HG11	2.02	0.40
7:G:116:ALA:HB1	7:G:155:GLY:O	2.20	0.40
7:G:210:GLU:HG2	7:G:211:LEU:N	2.36	0.40
8:H:101:ALA:HA	8:H:110:GLN:O	2.21	0.40
10:J:21:ALA:HA	10:J:188:HIS:O	2.21	0.40
12:L:157:ARG:HH21	12:L:176:LEU:HD23	1.86	0.40
2:P:42:GLY:HA2	2:P:212:CYS:O	2.21	0.40
2:P:134:LEU:HA	2:P:146:PHE:O	2.21	0.40
3:Q:44:LEU:CD1	3:Q:44:LEU:N	2.85	0.40
4:R:62:ILE:HD12	4:R:62:ILE:H	1.84	0.40
4:R:82:ILE:O	4:R:86:ARG:HG3	2.22	0.40
6:T:80:ASP:OD1	6:T:126:ARG:NH2	2.54	0.40
6:T:132:LEU:O	6:T:146:GLN:HA	2.22	0.40
10:X:82:ILE:HD11	10:X:86:THR:CG2	2.51	0.40
12:Z:64:ARG:NH2	12:Z:68:LEU:HD21	2.37	0.40
12:Z:153:TYR:CD2	12:Z:187:VAL:HG11	2.55	0.40
14:2:211:ILE:HA	14:2:214:MET:HE2	2.02	0.40
3:C:44:LEU:N	3:C:44:LEU:CD1	2.84	0.40
3:C:145:PHE:HE2	3:C:217:THR:HA	1.86	0.40
4:D:175:ASN:HB2	4:D:190:LEU:HD11	2.03	0.40
7:G:168:ALA:CB	7:G:200:VAL:CG1	3.00	0.40
9:I:15:GLY:O	9:I:16:ALA:HB2	2.20	0.40
10:J:28:PHE:HD2	10:J:36:THR:HB	1.87	0.40
10:J:65:GLN:NE2	11:K:86:ARG:HH21	2.17	0.40
10:J:84:PRO:HB3	10:J:120:PHE:CD2	2.57	0.40
10:J:136:PHE:HZ	10:J:151:GLU:OE2	2.05	0.40
1:O:51:VAL:O	1:O:51:VAL:HG13	2.19	0.40
3:Q:87:THR:O	3:Q:90:LEU:HB2	2.21	0.40
3:Q:167:ASN:O	3:Q:169:ALA:N	2.52	0.40
4:R:57:ARG:HG3	4:R:60:ARG:HH21	1.85	0.40
5:S:206:MET:CE	5:S:210:LEU:HD13	2.51	0.40
12:Z:105:ASP:HB3	12:Z:106:LYS:H	1.57	0.40
14:2:45:VAL:O	14:2:49:THR:O	2.39	0.40
1:A:78:CYS:HB3	1:A:140:LEU:HD23	2.04	0.40
6:F:13:TRP:HD1	7:G:22:GLN:NE2	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:83:LEU:HD23	6:F:83:LEU:HA	1.96	0.40
9:I:132:LEU:O	14:2:145:LEU:HD23	2.21	0.40
13:M:136:LYS:HG3	13:M:137:ALA:N	2.36	0.40
3:Q:17:ARG:HB2	3:Q:22:GLU:OE2	2.21	0.40
3:Q:136:TYR:O	3:Q:147:LEU:HA	2.21	0.40
3:Q:241:GLU:O	3:Q:243:GLU:N	2.45	0.40
6:T:87:PHE:CD1	6:T:115:LYS:HD2	2.56	0.40
6:T:171:TYR:CD2	6:T:194:ALA:HB2	2.56	0.40
7:U:152:ASP:HB2	7:U:153:PRO:CD	2.51	0.40
10:X:135:ASP:HA	10:X:154:TRP:CZ2	2.55	0.40
10:X:136:PHE:HZ	10:X:151:GLU:OE2	2.03	0.40
12:Z:81:LYS:HD3	12:Z:120:ARG:NH1	2.37	0.40
12:Z:163:ALA:C	12:Z:165:TYR:N	2.73	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	242/246 (98%)	220 (91%)	19 (8%)	3 (1%)	13	23
1	O	242/246 (98%)	220 (91%)	19 (8%)	3 (1%)	13	23
2	B	231/233 (99%)	185 (80%)	30 (13%)	16 (7%)	1	1
2	P	231/233 (99%)	188 (81%)	28 (12%)	15 (6%)	1	1
3	C	248/261 (95%)	201 (81%)	34 (14%)	13 (5%)	2	2
3	Q	248/261 (95%)	202 (82%)	33 (13%)	13 (5%)	2	2
4	D	241/248 (97%)	192 (80%)	33 (14%)	16 (7%)	1	1
4	R	241/248 (97%)	191 (79%)	34 (14%)	16 (7%)	1	1
5	E	232/241 (96%)	205 (88%)	24 (10%)	3 (1%)	12	21
5	S	232/241 (96%)	205 (88%)	24 (10%)	3 (1%)	12	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
6	F	236/263 (90%)	214 (91%)	16 (7%)	6 (2%)	5 9
6	T	236/263 (90%)	214 (91%)	17 (7%)	5 (2%)	7 12
7	G	243/254 (96%)	223 (92%)	14 (6%)	6 (2%)	5 9
7	U	243/254 (96%)	221 (91%)	16 (7%)	6 (2%)	5 9
8	H	200/205 (98%)	188 (94%)	9 (4%)	3 (2%)	10 18
8	V	200/205 (98%)	188 (94%)	9 (4%)	3 (2%)	10 18
9	I	218/234 (93%)	193 (88%)	21 (10%)	4 (2%)	8 15
9	W	218/234 (93%)	193 (88%)	21 (10%)	4 (2%)	8 15
10	J	202/205 (98%)	180 (89%)	18 (9%)	4 (2%)	7 13
10	X	202/205 (98%)	180 (89%)	18 (9%)	4 (2%)	7 13
11	K	197/201 (98%)	174 (88%)	20 (10%)	3 (2%)	10 18
11	Y	197/201 (98%)	174 (88%)	20 (10%)	3 (2%)	10 18
12	L	199/204 (98%)	180 (90%)	17 (8%)	2 (1%)	15 27
12	Z	199/204 (98%)	181 (91%)	16 (8%)	2 (1%)	15 27
13	1	211/213 (99%)	191 (90%)	19 (9%)	1 (0%)	29 47
13	M	211/213 (99%)	192 (91%)	18 (8%)	1 (0%)	29 47
14	2	215/219 (98%)	195 (91%)	16 (7%)	4 (2%)	8 14
14	N	215/219 (98%)	196 (91%)	15 (7%)	4 (2%)	8 14
All	All	6230/6454 (96%)	5486 (88%)	578 (9%)	166 (3%)	5 7

All (166) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	40	ALA
2	B	52	LYS
2	B	54	ILE
2	B	60	SER
2	B	179	GLU
2	B	183	LEU
2	B	232	ILE
3	C	58	GLU
3	C	141	LYS
3	C	206	LEU
4	D	46	GLU
4	D	47	LYS
4	D	59	VAL

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Mol	Chain	Res	Type
4	D	198	VAL
4	D	213	ARG
4	D	243	LYS
5	E	120	ALA
5	E	226	PHE
6	F	151	ALA
6	F	236	LEU
7	G	204	VAL
7	G	207	LYS
7	G	216	VAL
8	H	9	ASP
9	I	187	ARG
14	N	46	ASN
2	P	52	LYS
2	P	60	SER
2	P	179	GLU
2	P	183	LEU
2	P	232	ILE
3	Q	58	GLU
3	Q	141	LYS
3	Q	206	LEU
4	R	46	GLU
4	R	47	LYS
4	R	59	VAL
4	R	198	VAL
4	R	213	ARG
4	R	243	LYS
5	S	120	ALA
5	S	226	PHE
6	T	151	ALA
7	U	204	VAL
7	U	207	LYS
7	U	216	VAL
8	V	9	ASP
9	W	187	ARG
14	2	46	ASN
1	A	186	LYS
2	B	19	VAL
2	B	176	ARG
2	B	198	PHE
2	B	230	ALA
3	C	181	GLU

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Mol	Chain	Res	Type
3	C	201	MET
3	C	202	ASP
3	C	210	LYS
3	C	219	GLU
3	C	243	GLU
4	D	50	VAL
4	D	197	GLU
4	D	214	ASP
4	D	216	SER
8	H	191	GLY
9	I	180	LYS
10	J	101	GLY
11	K	110	HIS
12	L	187	VAL
14	N	201	GLY
1	O	186	LYS
2	P	19	VAL
2	P	41	ASN
2	P	176	ARG
2	P	198	PHE
2	P	230	ALA
3	Q	181	GLU
3	Q	201	MET
3	Q	202	ASP
3	Q	210	LYS
3	Q	219	GLU
3	Q	243	GLU
4	R	50	VAL
4	R	197	GLU
4	R	214	ASP
4	R	216	SER
8	V	191	GLY
9	W	180	LYS
10	X	101	GLY
11	Y	110	HIS
14	2	201	GLY
1	A	187	PHE
2	B	51	GLN
2	B	184	GLU
3	C	168	SER
4	D	54	GLN
4	D	56	GLU

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Mol	Chain	Res	Type
4	D	61	LYS
7	G	4	GLY
9	I	91	ARG
9	I	152	LYS
10	J	171	MET
11	K	197	PRO
1	O	187	PHE
2	P	53	SER
2	P	184	GLU
3	Q	168	SER
4	R	52	LYS
4	R	54	GLN
4	R	56	GLU
7	U	4	GLY
9	W	91	ARG
9	W	152	LYS
11	Y	197	PRO
12	Z	187	VAL
1	A	63	SER
2	B	196	GLU
2	B	202	MET
4	D	52	LYS
4	D	138	PHE
6	F	139	ASP
6	F	184	LEU
7	G	205	LYS
13	M	2	PHE
14	N	9	THR
1	O	63	SER
2	P	196	GLU
2	P	202	MET
4	R	61	LYS
4	R	138	PHE
6	T	184	LEU
7	U	205	LYS
10	X	31	GLN
10	X	171	MET
12	Z	198	LYS
13	1	2	PHE
14	2	9	THR
2	B	197	SER
3	C	55	LEU

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Mol	Chain	Res	Type
4	D	209	ALA
6	F	239	ARG
8	H	39	ASP
10	J	31	GLN
10	J	118	LYS
11	K	174	ASN
12	L	198	LYS
2	P	197	SER
3	Q	55	LEU
3	Q	199	LYS
4	R	209	ALA
6	T	139	ASP
6	T	238	GLU
10	X	118	LYS
11	Y	174	ASN
3	C	172	VAL
3	C	199	LYS
5	E	222	PRO
3	Q	172	VAL
5	S	222	PRO
6	T	201	ALA
8	V	39	ASP
6	F	240	PRO
14	N	215	ILE
14	2	215	ILE
7	G	3	ILE
7	U	3	ILE

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	192/210 (91%)	184 (96%)	8 (4%)	30 49
1	O	192/210 (91%)	184 (96%)	8 (4%)	30 49
2	B	163/190 (86%)	153 (94%)	10 (6%)	18 33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	P	163/190 (86%)	153 (94%)	10 (6%)	18	33
3	C	191/221 (86%)	180 (94%)	11 (6%)	20	35
3	Q	191/221 (86%)	179 (94%)	12 (6%)	18	31
4	D	136/211 (64%)	128 (94%)	8 (6%)	19	34
4	R	136/211 (64%)	128 (94%)	8 (6%)	19	34
5	E	190/204 (93%)	184 (97%)	6 (3%)	39	59
5	S	190/204 (93%)	184 (97%)	6 (3%)	39	59
6	F	198/224 (88%)	193 (98%)	5 (2%)	47	67
6	T	198/224 (88%)	193 (98%)	5 (2%)	47	67
7	G	195/211 (92%)	186 (95%)	9 (5%)	27	46
7	U	195/211 (92%)	186 (95%)	9 (5%)	27	46
8	H	155/159 (98%)	150 (97%)	5 (3%)	39	59
8	V	155/159 (98%)	150 (97%)	5 (3%)	39	59
9	I	177/195 (91%)	171 (97%)	6 (3%)	37	58
9	W	177/195 (91%)	171 (97%)	6 (3%)	37	58
10	J	172/174 (99%)	165 (96%)	7 (4%)	30	50
10	X	172/174 (99%)	164 (95%)	8 (5%)	26	45
11	K	164/171 (96%)	157 (96%)	7 (4%)	29	48
11	Y	164/171 (96%)	157 (96%)	7 (4%)	29	48
12	L	153/159 (96%)	146 (95%)	7 (5%)	27	46
12	Z	153/159 (96%)	146 (95%)	7 (5%)	27	46
13	1	173/178 (97%)	167 (96%)	6 (4%)	36	56
13	M	173/178 (97%)	167 (96%)	6 (4%)	36	56
14	2	174/181 (96%)	169 (97%)	5 (3%)	42	62
14	N	174/181 (96%)	168 (97%)	6 (3%)	37	58
All	All	4866/5376 (90%)	4663 (96%)	203 (4%)	30	49

All (203) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	CYS
1	A	108	GLU
1	A	114	LEU

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Mol	Chain	Res	Type
1	A	131	MET
1	A	132	ARG
1	A	145	GLU
1	A	166	THR
1	A	210	PHE
2	B	22	GLU
2	B	115	SER
2	B	131	VAL
2	B	132	SER
2	B	133	LEU
2	B	150	PRO
2	B	155	PHE
2	B	167	VAL
2	B	189	THR
2	B	227	ASP
3	C	44	LEU
3	C	82	ASP
3	C	133	SER
3	C	140	ASP
3	C	155	ASN
3	C	178	ASP
3	C	180	LYS
3	C	187	LYS
3	C	218	ARG
3	C	220	ASN
3	C	243	GLU
4	D	5	ARG
4	D	38	ARG
4	D	62	ILE
4	D	77	THR
4	D	103	THR
4	D	113	SER
4	D	178	ASP
4	D	214	ASP
5	E	36	THR
5	E	78	MET
5	E	135	ARG
5	E	148	GLU
5	E	217	LEU
5	E	221	GLN
6	F	38	LEU
6	F	126	ARG

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Mol	Chain	Res	Type
6	F	149	PRO
6	F	202	GLU
6	F	209	ASN
7	G	41	CYS
7	G	67	PHE
7	G	129	ARG
7	G	133	CYS
7	G	163	CYS
7	G	170	GLN
7	G	181	MET
7	G	215	TRP
7	G	218	GLU
8	H	9	ASP
8	H	110	GLN
8	H	124	SER
8	H	139	VAL
8	H	182	SER
9	I	40	ASN
9	I	56	THR
9	I	132	LEU
9	I	153	ASN
9	I	184	ASP
9	I	208	THR
10	J	26	ARG
10	J	34	LEU
10	J	49	LEU
10	J	126	LEU
10	J	145	GLN
10	J	156	PRO
10	J	189	ILE
11	K	8	GLN
11	K	27	GLN
11	K	45	LEU
11	K	84	THR
11	K	85	ARG
11	K	177	THR
11	K	190	ASP
12	L	8	PHE
12	L	87	VAL
12	L	102	CYS
12	L	138	VAL
12	L	180	ARG

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Mol	Chain	Res	Type
12	L	182	ASP
12	L	190	ASP
13	M	140	SER
13	M	159	GLN
13	M	162	GLU
13	M	163	HIS
13	M	167	SER
13	M	170	ARG
14	N	10	SER
14	N	46	ASN
14	N	94	ARG
14	N	100	ARG
14	N	167	ASP
14	N	168	LEU
1	O	78	CYS
1	O	108	GLU
1	O	114	LEU
1	O	131	MET
1	O	132	ARG
1	O	145	GLU
1	O	166	THR
1	O	210	PHE
2	P	22	GLU
2	P	115	SER
2	P	131	VAL
2	P	132	SER
2	P	133	LEU
2	P	150	PRO
2	P	155	PHE
2	P	167	VAL
2	P	189	THR
2	P	227	ASP
3	Q	44	LEU
3	Q	82	ASP
3	Q	106	PRO
3	Q	133	SER
3	Q	140	ASP
3	Q	155	ASN
3	Q	178	ASP
3	Q	180	LYS
3	Q	187	LYS
3	Q	218	ARG

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Mol	Chain	Res	Type
3	Q	220	ASN
3	Q	243	GLU
4	R	5	ARG
4	R	38	ARG
4	R	62	ILE
4	R	77	THR
4	R	103	THR
4	R	113	SER
4	R	178	ASP
4	R	214	ASP
5	S	36	THR
5	S	78	MET
5	S	135	ARG
5	S	148	GLU
5	S	217	LEU
5	S	221	GLN
6	T	38	LEU
6	T	126	ARG
6	T	149	PRO
6	T	202	GLU
6	T	209	ASN
7	U	41	CYS
7	U	67	PHE
7	U	129	ARG
7	U	133	CYS
7	U	163	CYS
7	U	170	GLN
7	U	181	MET
7	U	215	TRP
7	U	218	GLU
8	V	9	ASP
8	V	110	GLN
8	V	124	SER
8	V	139	VAL
8	V	182	SER
9	W	40	ASN
9	W	56	THR
9	W	132	LEU
9	W	153	ASN
9	W	184	ASP
9	W	208	THR
10	X	26	ARG

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Mol	Chain	Res	Type
10	X	34	LEU
10	X	36	THR
10	X	49	LEU
10	X	126	LEU
10	X	145	GLN
10	X	156	PRO
10	X	189	ILE
11	Y	8	GLN
11	Y	27	GLN
11	Y	45	LEU
11	Y	84	THR
11	Y	85	ARG
11	Y	177	THR
11	Y	190	ASP
12	Z	8	PHE
12	Z	87	VAL
12	Z	102	CYS
12	Z	138	VAL
12	Z	180	ARG
12	Z	182	ASP
12	Z	190	ASP
13	1	140	SER
13	1	159	GLN
13	1	162	GLU
13	1	163	HIS
13	1	167	SER
13	1	170	ARG
14	2	10	SER
14	2	46	ASN
14	2	94	ARG
14	2	100	ARG
14	2	168	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (163) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	HIS
1	A	68	HIS
1	A	90	GLN
1	A	92	GLN
1	A	127	GLN
1	A	172	GLN

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Mol	Chain	Res	Type
1	A	238	HIS
2	B	41	ASN
2	B	111	GLN
2	B	147	GLN
2	B	165	ASN
2	B	168	ASN
2	B	206	ASN
2	B	213	ASN
3	C	69	ASN
3	C	95	GLN
3	C	100	GLN
3	C	109	GLN
3	C	123	GLN
3	C	155	ASN
3	C	166	ASN
3	C	167	ASN
3	C	220	ASN
3	C	235	GLN
4	D	15	HIS
4	D	23	GLN
4	D	92	GLN
4	D	200	GLN
5	E	99	HIS
5	E	152	GLN
5	E	164	GLN
5	E	182	GLN
5	E	204	GLN
5	E	211	ASN
5	E	221	GLN
5	E	224	GLN
6	F	4	ASN
6	F	20	HIS
6	F	43	HIS
6	F	146	GLN
6	F	166	GLN
6	F	175	HIS
6	F	203	GLN
6	F	209	ASN
7	G	22	GLN
7	G	201	HIS
8	H	7	GLN
8	H	110	GLN

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Mol	Chain	Res	Type
8	H	123	GLN
8	H	158	ASN
9	I	30	ASN
9	I	40	ASN
9	I	66	HIS
9	I	153	ASN
10	J	7	ASN
10	J	40	GLN
10	J	65	GLN
10	J	72	ASN
10	J	81	GLN
10	J	145	GLN
11	K	8	GLN
11	K	24	ASN
11	K	61	GLN
11	K	99	HIS
11	K	132	HIS
12	L	10	HIS
12	L	29	GLN
12	L	178	HIS
13	M	8	ASN
13	M	77	HIS
13	M	79	ASN
13	M	108	ASN
13	M	146	GLN
13	M	151	ASN
13	M	152	GLN
13	M	159	GLN
14	N	46	ASN
14	N	81	HIS
14	N	108	ASN
14	N	157	GLN
1	O	12	HIS
1	O	68	HIS
1	O	90	GLN
1	O	92	GLN
1	O	127	GLN
1	O	172	GLN
1	O	238	HIS
2	P	41	ASN
2	P	111	GLN
2	P	147	GLN

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Mol	Chain	Res	Type
2	P	165	ASN
2	P	168	ASN
2	P	206	ASN
2	P	213	ASN
3	Q	69	ASN
3	Q	95	GLN
3	Q	100	GLN
3	Q	109	GLN
3	Q	123	GLN
3	Q	155	ASN
3	Q	166	ASN
3	Q	167	ASN
3	Q	220	ASN
3	Q	235	GLN
4	R	15	HIS
4	R	23	GLN
4	R	92	GLN
4	R	200	GLN
5	S	99	HIS
5	S	152	GLN
5	S	164	GLN
5	S	182	GLN
5	S	204	GLN
5	S	211	ASN
5	S	221	GLN
5	S	224	GLN
6	T	4	ASN
6	T	20	HIS
6	T	43	HIS
6	T	146	GLN
6	T	166	GLN
6	T	175	HIS
6	T	203	GLN
6	T	209	ASN
7	U	22	GLN
7	U	201	HIS
8	V	7	GLN
8	V	110	GLN
8	V	123	GLN
8	V	154	GLN
9	W	30	ASN
9	W	40	ASN

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Mol	Chain	Res	Type
9	W	66	HIS
9	W	116	HIS
9	W	153	ASN
10	X	7	ASN
10	X	40	GLN
10	X	65	GLN
10	X	72	ASN
10	X	81	GLN
10	X	145	GLN
11	Y	8	GLN
11	Y	24	ASN
11	Y	61	GLN
11	Y	99	HIS
11	Y	132	HIS
12	Z	10	HIS
12	Z	29	GLN
12	Z	178	HIS
13	1	8	ASN
13	1	77	HIS
13	1	79	ASN
13	1	108	ASN
13	1	146	GLN
13	1	151	ASN
13	1	152	GLN
13	1	159	GLN
14	2	46	ASN
14	2	69	GLN
14	2	108	ASN
14	2	157	GLN
14	2	188	GLN
14	2	213	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 30 ligands modelled in this entry, 30 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, 95^{th} 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	244/246 (99%)	0.73	24 (9%) 7 8	56, 89, 120, 135	0
1	O	244/246 (99%)	0.00	1 (0%) 92 95	38, 56, 81, 100	0
2	B	233/233 (100%)	0.82	31 (13%) 3 4	62, 97, 133, 142	0
2	P	233/233 (100%)	0.30	8 (3%) 45 53	36, 67, 105, 129	0
3	C	250/261 (95%)	1.03	44 (17%) 1 1	59, 103, 142, 148	0
3	Q	250/261 (95%)	0.44	13 (5%) 27 33	37, 70, 123, 141	0
4	D	243/248 (97%)	0.73	31 (12%) 3 4	54, 93, 146, 163	0
4	R	243/248 (97%)	0.47	24 (9%) 7 8	40, 82, 134, 157	0
5	E	234/241 (97%)	0.27	3 (1%) 77 84	39, 64, 94, 110	0
5	S	234/241 (97%)	0.41	9 (3%) 40 48	39, 74, 102, 132	0
6	F	238/263 (90%)	0.19	2 (0%) 86 90	42, 63, 91, 124	0
6	T	238/263 (90%)	0.23	7 (2%) 51 61	37, 58, 95, 135	0
7	G	245/254 (96%)	0.37	5 (2%) 65 73	49, 74, 104, 118	0
7	U	245/254 (96%)	0.17	5 (2%) 65 73	35, 53, 89, 126	0
8	H	202/205 (98%)	0.11	0 100 100	35, 60, 78, 94	0
8	V	202/205 (98%)	0.02	0 100 100	33, 49, 70, 102	0
9	I	220/234 (94%)	0.46	11 (5%) 28 35	49, 71, 100, 115	0
9	W	220/234 (94%)	0.07	1 (0%) 91 94	30, 53, 81, 99	0
10	J	204/205 (99%)	0.56	6 (2%) 51 61	49, 79, 101, 111	0
10	X	204/205 (99%)	0.20	4 (1%) 65 73	36, 52, 78, 97	0
11	K	199/201 (99%)	0.39	6 (3%) 50 59	49, 69, 93, 110	0
11	Y	199/201 (99%)	0.16	3 (1%) 73 81	36, 56, 80, 113	0
12	L	201/204 (98%)	0.10	2 (0%) 82 87	35, 53, 75, 108	0
12	Z	201/204 (98%)	0.25	3 (1%) 73 81	45, 65, 85, 106	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	1	213/213 (100%)	0.23	3 (1%) 75 82	40, 70, 97, 112	0
13	M	213/213 (100%)	0.04	0 100 100	31, 50, 73, 97	0
14	2	217/219 (99%)	0.12	2 (0%) 84 89	33, 55, 81, 109	0
14	N	217/219 (99%)	0.05	2 (0%) 84 89	33, 51, 70, 109	0
All	All	6286/6454 (97%)	0.33	250 (3%) 38 45	30, 66, 115, 163	0

All (250) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	P	232	ILE	12.8
2	P	233	ALA	10.0
11	K	199	GLN	8.5
4	R	244	GLN	7.9
7	U	1	SER	7.8
7	G	1	SER	6.7
3	C	203	VAL	6.4
4	D	243	LYS	6.4
3	Q	203	VAL	6.1
4	D	242	LYS	6.0
2	B	232	ILE	5.8
5	E	8	TYR	5.5
14	N	216	SER	5.4
2	B	1	ALA	5.2
4	D	239	ASN	5.2
1	A	140	LEU	5.1
3	Q	204	SER	4.9
3	C	247	ALA	4.9
3	Q	206	LEU	4.8
3	Q	58	GLU	4.8
3	C	249	ARG	4.8
6	T	239	ARG	4.7
1	A	200	THR	4.7
3	C	208	ALA	4.6
3	C	171	ALA	4.5
3	Q	250	GLU	4.5
2	B	211	ILE	4.5
7	U	2	SER	4.5
11	Y	199	GLN	4.5
4	D	102	VAL	4.5
14	2	216	SER	4.4
3	C	172	VAL	4.3

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Mol	Chain	Res	Type	RSRZ
2	B	188	HIS	4.2
4	D	220	LEU	4.2
4	R	239	ASN	4.1
4	D	207	GLU	4.1
6	T	241	GLN	4.0
1	A	42	VAL	4.0
6	T	55	GLU	4.0
2	B	177	TYR	3.9
3	C	175	LEU	3.9
3	C	206	LEU	3.9
1	A	183	VAL	3.9
2	B	44	VAL	3.9
3	C	55	LEU	3.8
3	Q	61	PHE	3.8
2	P	1	ALA	3.7
3	Q	208	ALA	3.7
11	K	187	GLY	3.7
4	D	234	LYS	3.7
9	I	105	VAL	3.6
4	R	41	VAL	3.6
1	A	50	ILE	3.6
2	B	45	LEU	3.6
4	R	243	LYS	3.5
1	A	212	PRO	3.5
2	B	207	ILE	3.5
7	U	3	ILE	3.5
3	C	200	THR	3.5
3	C	228	LEU	3.5
3	C	194	ILE	3.5
3	Q	205	LYS	3.5
4	D	176	TYR	3.4
4	R	240	GLU	3.4
3	C	170	ALA	3.4
10	J	16	GLY	3.3
1	A	141	ILE	3.3
4	D	202	GLY	3.3
2	B	157	TRP	3.3
6	T	240	PRO	3.3
1	A	198	ALA	3.2
2	B	200	GLY	3.2
9	I	106	THR	3.2
4	R	40	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
2	B	135	ILE	3.2
2	B	173	LEU	3.2
4	D	200	GLN	3.2
1	A	142	GLY	3.1
4	D	180	ALA	3.1
4	D	217	LEU	3.1
3	C	250	GLU	3.1
2	B	206	ASN	3.1
7	G	39	ILE	3.1
2	B	2	GLU	3.1
4	D	238	GLU	3.1
1	A	197	THR	3.1
3	C	241	GLU	3.0
4	R	232	ILE	3.0
2	P	40	ALA	3.0
3	C	198	ASN	3.0
9	I	65	LEU	3.0
2	P	2	GLU	3.0
4	D	38	ARG	3.0
4	D	185	ASP	3.0
10	J	84	PRO	3.0
12	Z	6	PHE	2.9
4	D	244	GLN	2.9
1	A	243	ALA	2.9
5	S	8	TYR	2.9
11	K	183	ILE	2.9
3	C	190	LEU	2.9
3	C	227	VAL	2.9
2	B	37	ILE	2.9
10	X	117	PHE	2.9
2	B	187	ILE	2.9
1	O	245	ARG	2.9
3	C	204	SER	2.8
12	L	200	SER	2.8
5	E	58	LEU	2.8
2	B	64	VAL	2.8
5	S	27	ASP	2.8
3	Q	200	THR	2.8
4	R	201	SER	2.8
4	R	38	ARG	2.8
3	C	181	GLU	2.7
5	S	215	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	201	GLN	2.7
7	U	215	TRP	2.7
10	J	85	TYR	2.7
3	C	207	SER	2.7
4	R	200	GLN	2.7
5	E	131	GLY	2.7
14	N	217	GLY	2.6
3	Q	236	LEU	2.6
3	C	213	ILE	2.6
2	B	209	VAL	2.6
2	P	37	ILE	2.6
3	C	211	VAL	2.6
4	R	194	ALA	2.6
6	F	4	ASN	2.6
2	B	146	PHE	2.6
2	B	204	GLU	2.6
3	C	19	TYR	2.6
4	D	210	VAL	2.6
3	C	45	LEU	2.6
3	C	186	LEU	2.6
9	I	190	THR	2.6
11	K	5	ILE	2.6
9	I	201	ARG	2.6
4	R	39	ASP	2.6
4	D	230	ALA	2.5
3	C	216	LEU	2.5
2	B	42	GLY	2.5
4	R	45	VAL	2.5
2	B	189	THR	2.5
11	K	198	LYS	2.5
4	D	98	VAL	2.5
4	D	49	SER	2.5
2	B	38	LYS	2.5
9	I	183	LEU	2.5
3	C	147	LEU	2.4
5	S	67	ILE	2.4
13	1	203	ILE	2.4
3	C	79	ILE	2.4
6	T	234	GLU	2.4
5	S	214	ASN	2.4
3	C	205	LYS	2.4
11	Y	198	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
4	R	37	GLY	2.4
4	D	235	GLU	2.4
3	Q	237	ILE	2.4
3	C	49	ARG	2.4
1	A	167	ALA	2.4
1	A	241	ALA	2.4
3	C	168	SER	2.4
4	R	172	LEU	2.4
4	D	161	ILE	2.4
4	D	219	ILE	2.4
4	D	41	VAL	2.4
10	X	85	TYR	2.3
3	C	237	ILE	2.3
1	A	56	VAL	2.3
10	J	117	PHE	2.3
4	D	227	LYS	2.3
4	D	97	THR	2.3
4	D	142	PRO	2.3
12	Z	175	ASN	2.3
4	D	237	GLU	2.3
5	S	234	LEU	2.3
9	I	179	SER	2.3
3	C	51	ASN	2.3
2	B	58	GLU	2.3
2	B	208	GLU	2.3
11	Y	173	LEU	2.3
3	C	214	ALA	2.3
7	G	238	TYR	2.3
9	I	204	CYS	2.3
5	S	241	ILE	2.3
3	C	196	VAL	2.2
1	A	139	ILE	2.2
1	A	193	GLN	2.2
3	C	58	GLU	2.2
2	B	185	ASP	2.2
1	A	187	PHE	2.2
9	I	7	VAL	2.2
5	S	48	LEU	2.2
7	G	215	TRP	2.2
4	R	104	VAL	2.2
4	D	175	ASN	2.2
4	R	205	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
13	1	168	LEU	2.2
2	P	44	VAL	2.2
2	B	150	PRO	2.2
4	D	101	PRO	2.2
1	A	210	PHE	2.2
9	W	201	ARG	2.2
1	A	151	VAL	2.2
2	B	67	ILE	2.2
7	G	2	SER	2.2
6	T	179	PHE	2.2
4	R	52	LYS	2.1
4	R	236	LYS	2.1
9	I	42	TYR	2.1
10	J	46	GLY	2.1
1	A	40	VAL	2.1
1	A	77	GLY	2.1
3	C	240	HIS	2.1
14	2	217	GLY	2.1
3	C	54	LYS	2.1
3	C	38	LEU	2.1
3	C	76	VAL	2.1
4	D	206	ILE	2.1
4	R	33	VAL	2.1
13	1	149	LEU	2.1
3	Q	242	GLU	2.1
4	R	220	LEU	2.1
3	C	65	ILE	2.1
10	J	20	VAL	2.1
1	A	189	TRP	2.1
1	A	194	THR	2.1
4	R	171	PHE	2.1
2	B	213	ASN	2.1
12	L	158	ARG	2.1
4	R	156	TRP	2.1
2	B	222	PRO	2.0
2	P	209	VAL	2.0
4	R	191	VAL	2.0
9	I	76	VAL	2.0
6	T	201	ALA	2.0
3	C	60	PHE	2.0
10	X	162	HIS	2.0
12	Z	153	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
11	K	178	PHE	2.0
5	S	184	LEU	2.0
10	X	189	ILE	2.0
3	Q	161	ALA	2.0
3	C	215	THR	2.0
1	A	179	LEU	2.0
6	F	174	ARG	2.0
7	U	187	ARG	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 monosaccharides 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. The B-factors column lists the minimum, median, 95^{th} 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	B-factors(Å^2)	Q<0.9
15	MG	G	319	1/1	0.59	0.43	66,66,66,66	0
15	MG	G	311	1/1	0.66	0.25	97,97,97,97	0
15	MG	1	418	1/1	0.69	0.25	90,90,90,90	0
15	MG	O	401	1/1	0.76	0.22	57,57,57,57	0
15	MG	G	317	1/1	0.81	0.18	85,85,85,85	0
15	MG	J	407	1/1	0.82	0.12	70,70,70,70	0
15	MG	K	313	1/1	0.84	0.24	77,77,77,77	0
15	MG	J	320	1/1	0.84	0.45	112,112,112,112	0
15	MG	D	309	1/1	0.84	0.13	87,87,87,87	0
15	MG	Q	414	1/1	0.86	0.20	90,90,90,90	0
15	MG	A	301	1/1	0.86	0.23	83,83,83,83	0
15	MG	W	406	1/1	0.87	0.16	59,59,59,59	0
15	MG	B	316	1/1	0.87	0.34	84,84,84,84	0
15	MG	Y	413	1/1	0.88	0.31	51,51,51,51	0
15	MG	X	404	1/1	0.89	0.37	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
15	MG	U	417	1/1	0.90	0.45	64,64,64,64	0
15	MG	X	420	1/1	0.90	0.41	77,77,77,77	0
15	MG	U	419	1/1	0.90	0.69	70,70,70,70	0
15	MG	P	416	1/1	0.90	0.20	72,72,72,72	0
15	MG	X	307	1/1	0.91	0.14	39,39,39,39	0
15	MG	M	318	1/1	0.92	0.30	81,81,81,81	0
15	MG	I	306	1/1	0.92	0.23	87,87,87,87	0
15	MG	X	415	1/1	0.93	0.21	59,59,59,59	0
15	MG	U	411	1/1	0.93	0.22	76,76,76,76	0
15	MG	J	315	1/1	0.93	0.41	69,69,69,69	0
15	MG	J	304	1/1	0.93	0.10	56,56,56,56	0
15	MG	C	314	1/1	0.94	0.35	76,76,76,76	0
15	MG	M	310	1/1	0.96	0.09	67,67,67,67	0
15	MG	1	410	1/1	0.96	0.21	66,66,66,66	0
15	MG	R	409	1/1	0.96	0.07	59,59,59,59	0

6.5 Other polymers (i)

There are no such residues in this entry.