



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 03:49 PM UTC

PDB ID : 3SHJ / pdb_00003shj
Title : Proteasome in complex with hydroxyurea derivative HU10
Authors : Gallastegui, N.; Beck, P.; Arciniega, M.; Hillebrand, S.; Huber, R.; Groll, M.
Deposited on : 2011-06-16
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

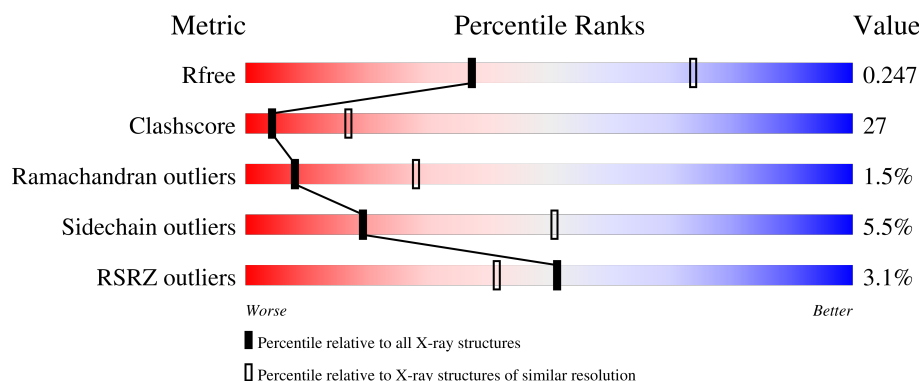
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	250	2% 59% 36% 5%
1	O	250	4% 59% 37% .
2	B	244	5% 49% 44% 7%
2	P	244	6% 52% 41% 7%
3	C	241	7% 53% 43% .

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Mol	Chain	Length	Quality of chain
3	Q	241	
4	D	242	
4	R	242	
5	E	233	
5	S	233	
6	F	244	
6	T	244	
7	G	243	
7	U	243	
8	H	222	
8	V	222	
9	I	204	
9	W	204	
10	J	198	
10	X	198	
11	K	212	
11	Y	212	
12	L	222	
12	Z	222	
13	1	233	
13	M	233	
14	2	196	
14	N	196	

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	MES	K	1(L)	-	X	-	-

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 50905 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Proteasome component Y7.

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

- Molecule 2 is a protein called Proteasome component Y13.

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

- Molecule 3 is a protein called Proteasome component PRE6.

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

- Molecule 4 is a protein called Proteasome component PUP2.

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

- Molecule 5 is a protein called Proteasome component PRE5.

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

- Molecule 6 is a protein called Proteasome component C1.

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

- Molecule 7 is a protein called Proteasome component C7-alpha.

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

- Molecule 8 is a protein called Proteasome component PUP1.

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

- Molecule 9 is a protein called Proteasome component PUP3.

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

- Molecule 10 is a protein called Proteasome component C11.

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

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

- Molecule 11 is a protein called Proteasome component PRE2.

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

- Molecule 12 is a protein called Proteasome component C5.

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

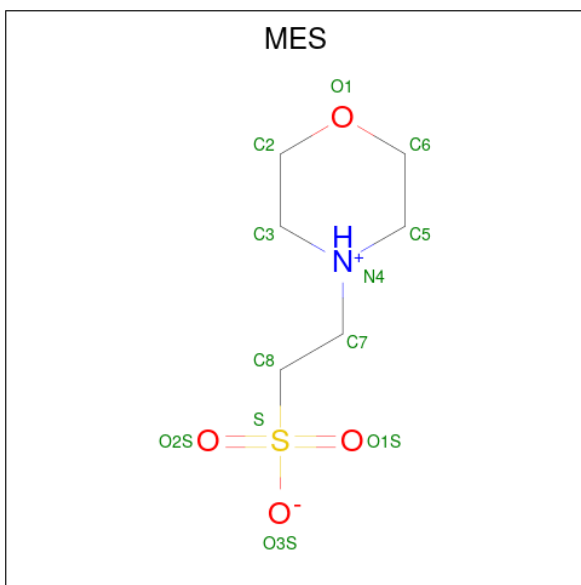
- Molecule 13 is a protein called Proteasome component PRE4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			
13	1	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			

- Molecule 14 is a protein called Proteasome component PRE3.

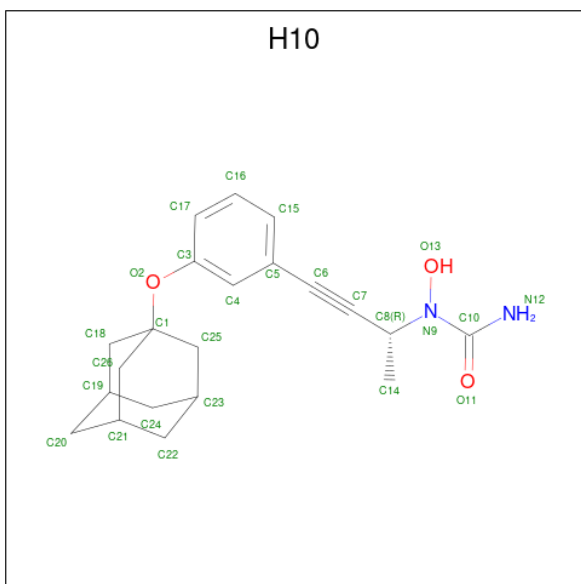
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	196	Total	C	N	O	S	0	0	0
			1512	955	250	300	7			
14	2	196	Total	C	N	O	S	0	0	0
			1512	955	250	300	7			

- Molecule 15 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: C₆H₁₃NO₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	K	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
15	Y	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 16 is 1-hydroxy-1-[(2R)-4-{3-[(3S,5S,7S)-tricyclo[3.3.1.1^{3,7}]dec-1-yloxy]phenyl}but-3-yn-2-yl]urea (CCD ID: H10) (formula: C₂₁H₂₆N₂O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
16	K	1	Total	C	N	O	0	0
			26	21	2	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
16	Y	1	Total	C	N	O	0	0
			26	21	2	3		

- Molecule 17 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	49	Total	O	0	0
			49	49		
17	B	36	Total	O	0	0
			36	36		
17	C	37	Total	O	0	0
			37	37		
17	D	36	Total	O	0	0
			36	36		
17	E	23	Total	O	0	0
			23	23		
17	F	47	Total	O	0	0
			47	47		
17	G	58	Total	O	0	0
			58	58		
17	H	46	Total	O	0	0
			46	46		
17	I	65	Total	O	0	0
			65	65		
17	J	48	Total	O	0	0
			48	48		
17	K	49	Total	O	0	0
			49	49		
17	L	58	Total	O	0	0
			58	58		
17	M	66	Total	O	0	0
			66	66		
17	N	56	Total	O	0	0
			56	56		
17	O	30	Total	O	0	0
			30	30		
17	P	29	Total	O	0	0
			29	29		
17	Q	24	Total	O	0	0
			24	24		
17	R	30	Total	O	0	0
			30	30		

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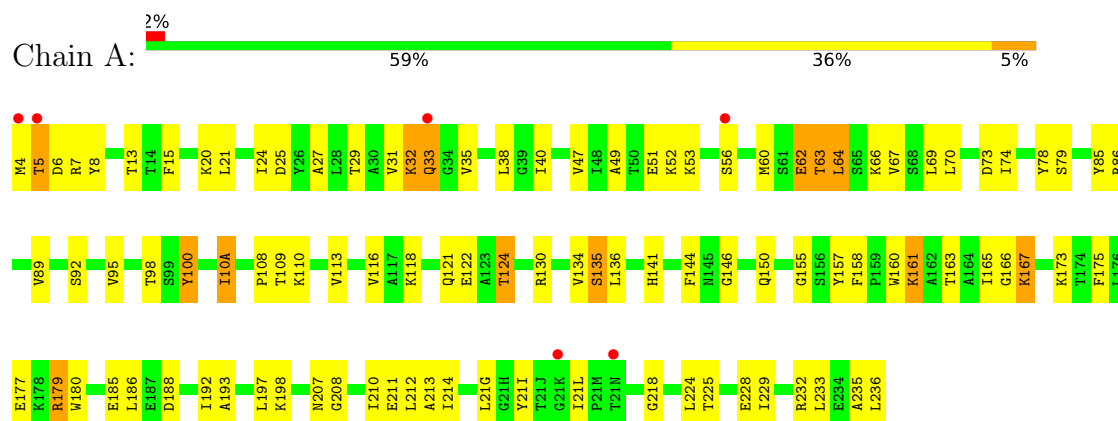
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	S	19	Total 19	O 19	0	0
17	T	38	Total 38	O 38	0	0
17	U	60	Total 60	O 60	0	0
17	V	42	Total 42	O 42	0	0
17	W	57	Total 57	O 57	0	0
17	X	48	Total 48	O 48	0	0
17	Y	50	Total 50	O 50	0	0
17	Z	50	Total 50	O 50	0	0
17	1	69	Total 69	O 69	0	0
17	2	61	Total 61	O 61	0	0

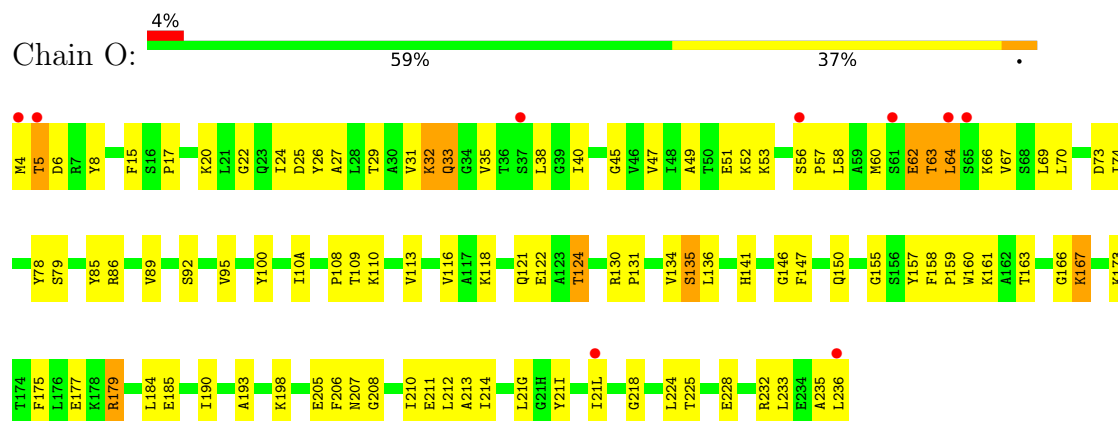
3 Residue-property plots

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

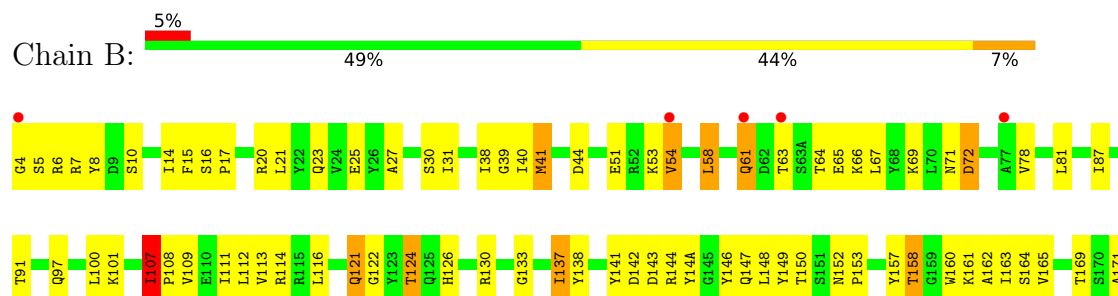
• Molecule 1: Proteasome component Y7

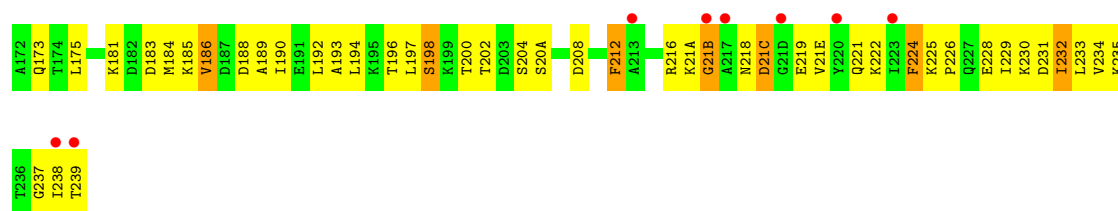


• Molecule 1: Proteasome component Y7

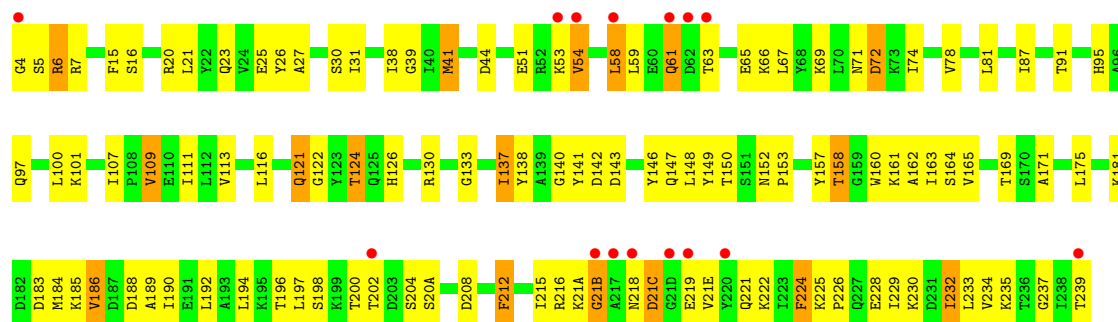


• Molecule 2: Proteasome component Y13

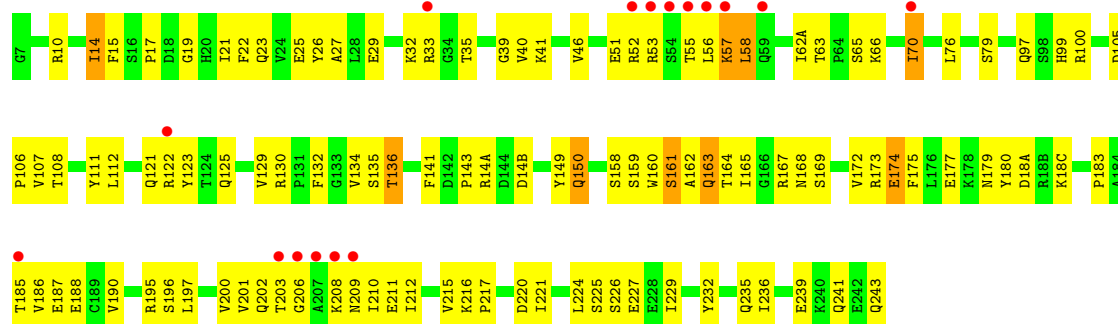




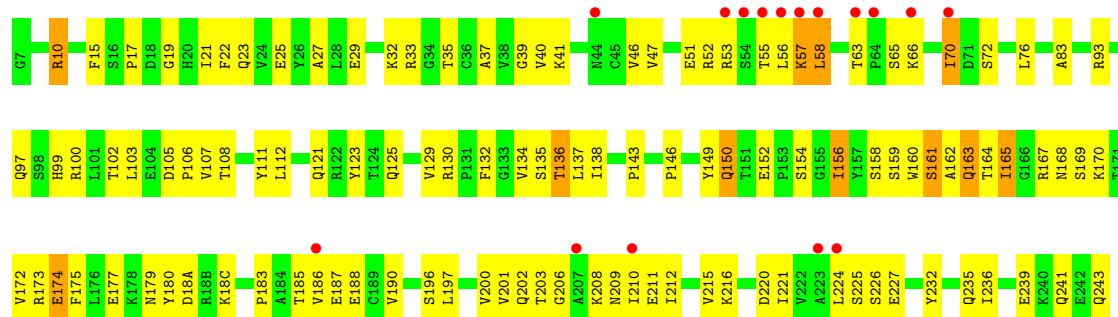
• Molecule 2: Proteasome component Y13



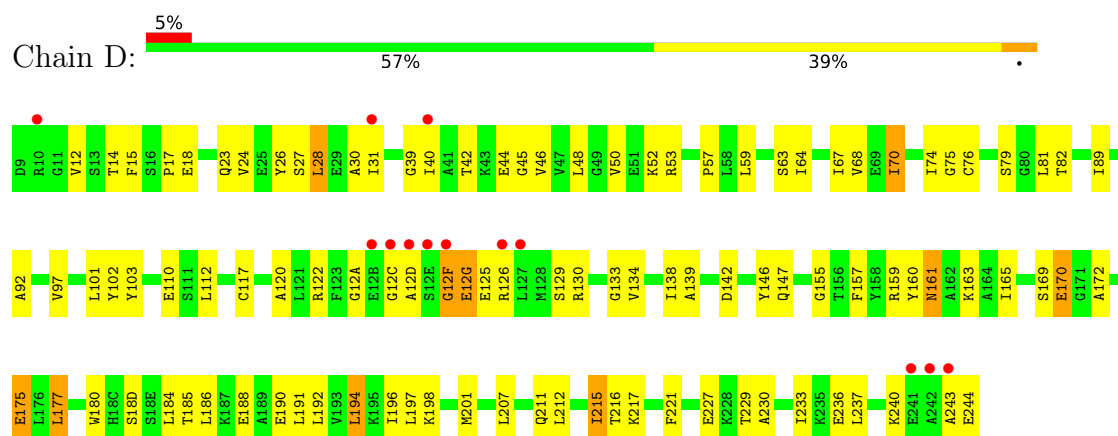
• Molecule 3: Proteasome component PRE6



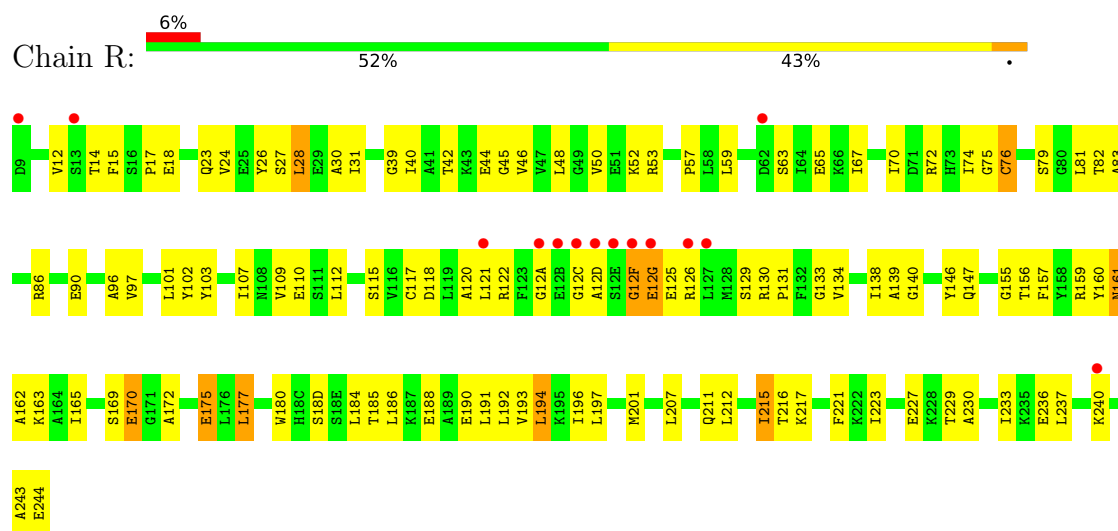
• Molecule 3: Proteasome component PRE6



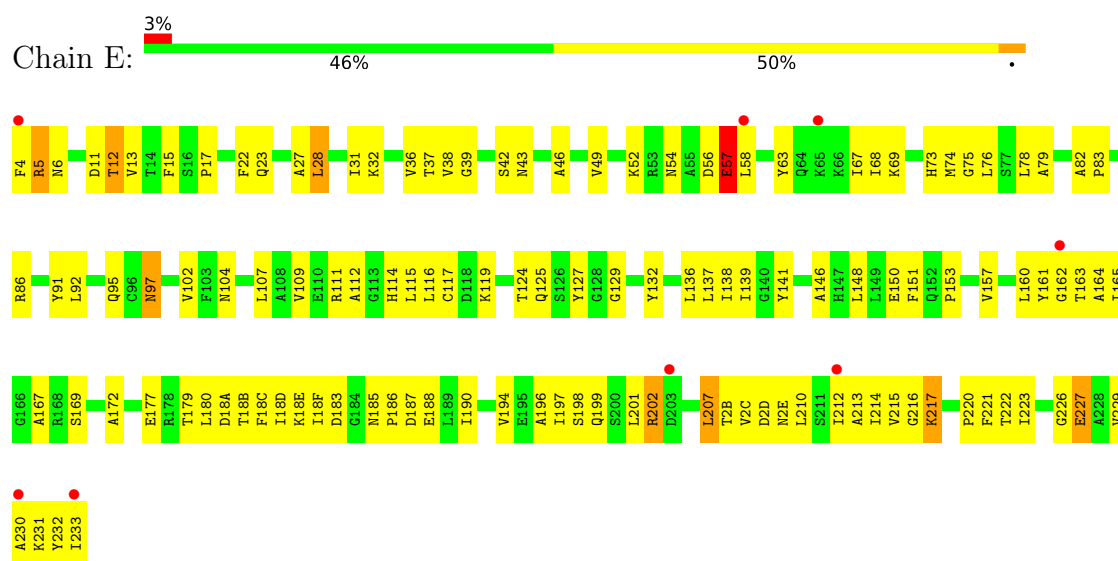
- Molecule 4: Proteasome component PUP2



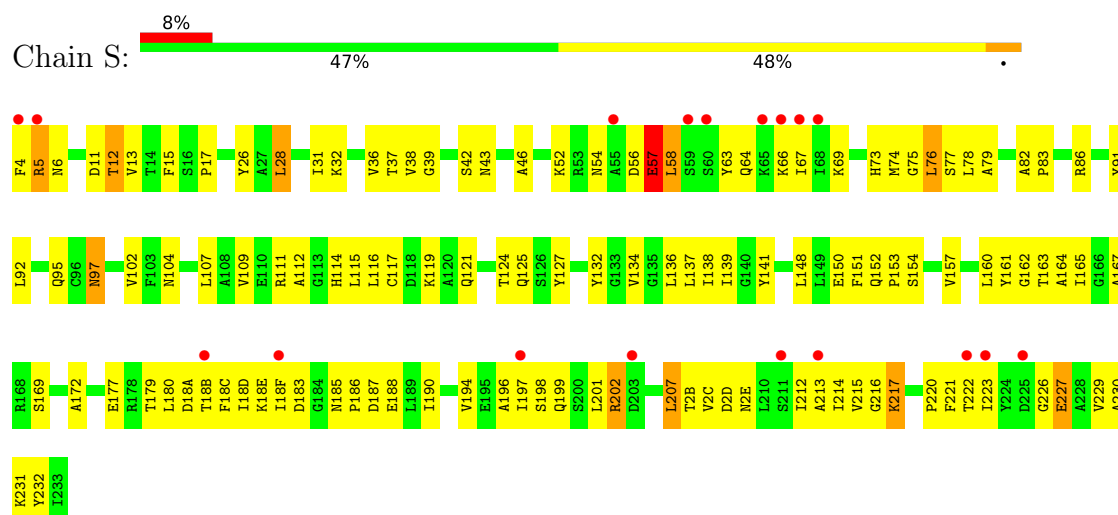
- Molecule 4: Proteasome component PUP2



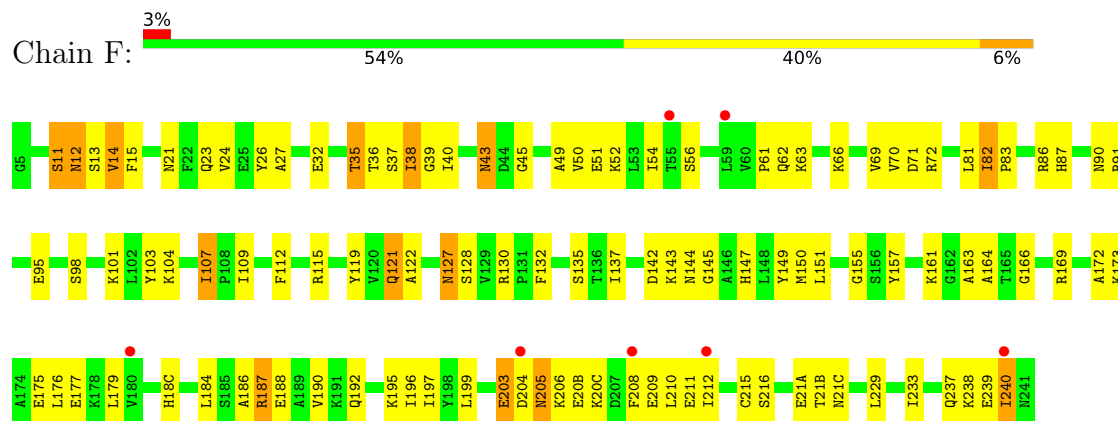
- Molecule 5: Proteasome component PRE5



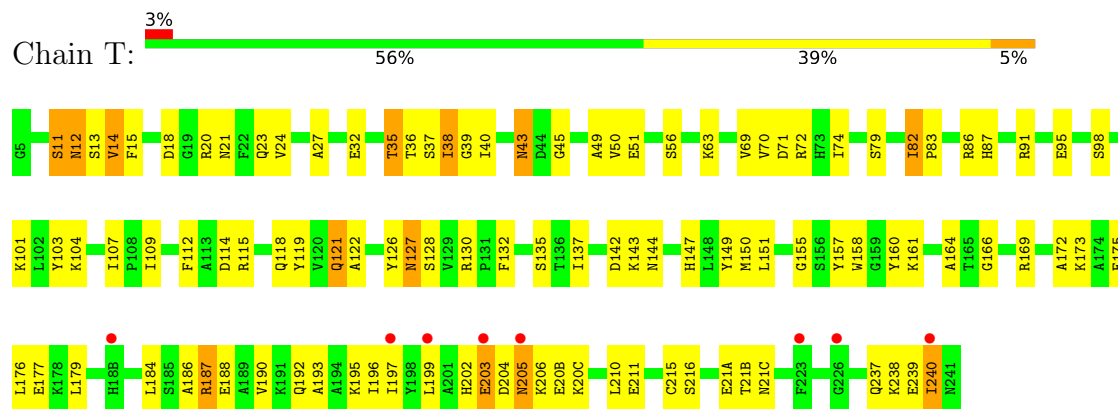
- Molecule 5: Proteasome component PRE5



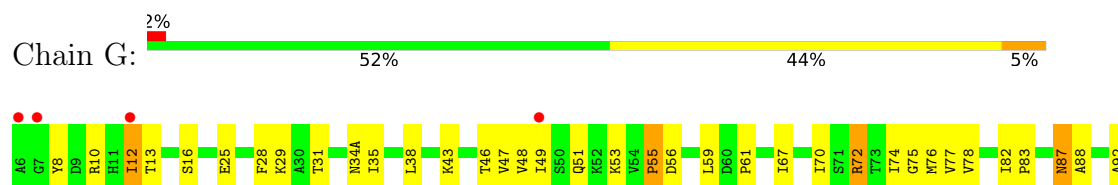
• Molecule 6: Proteasome component C1

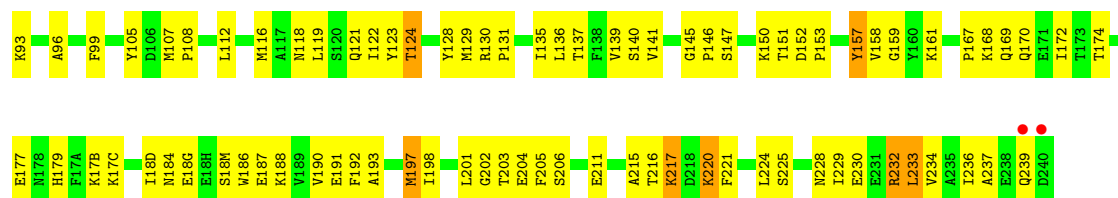


• Molecule 6: Proteasome component C1

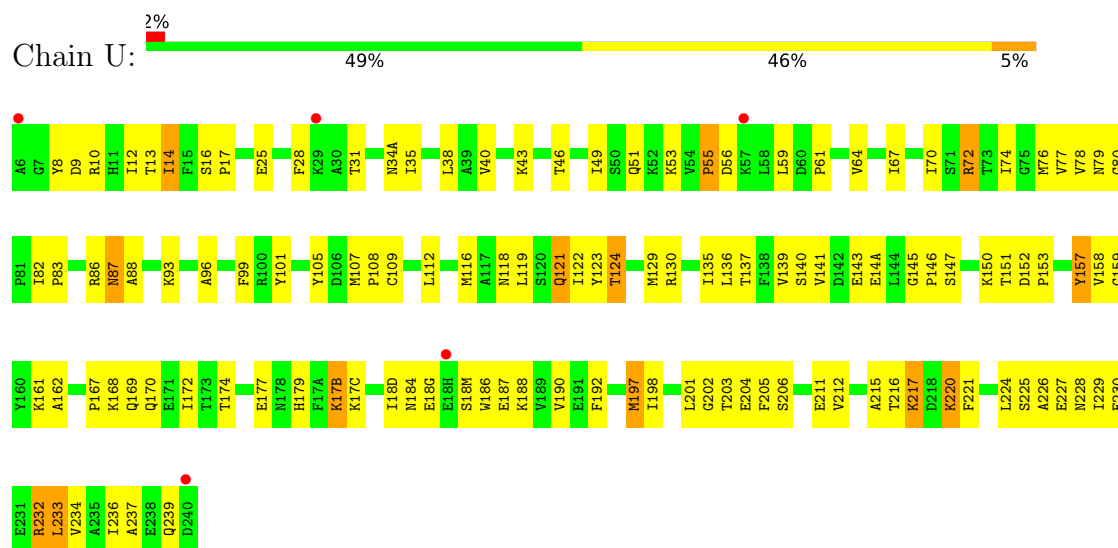


• Molecule 7: Proteasome component C7-alpha

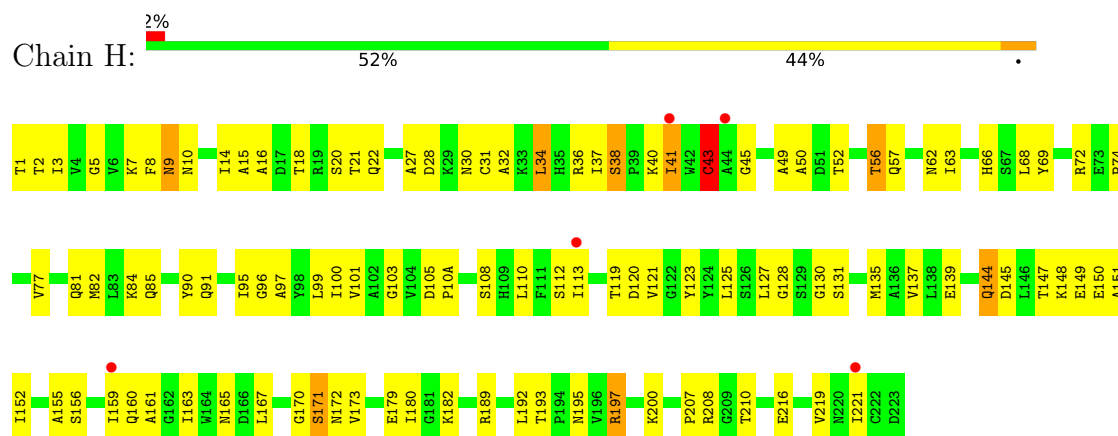




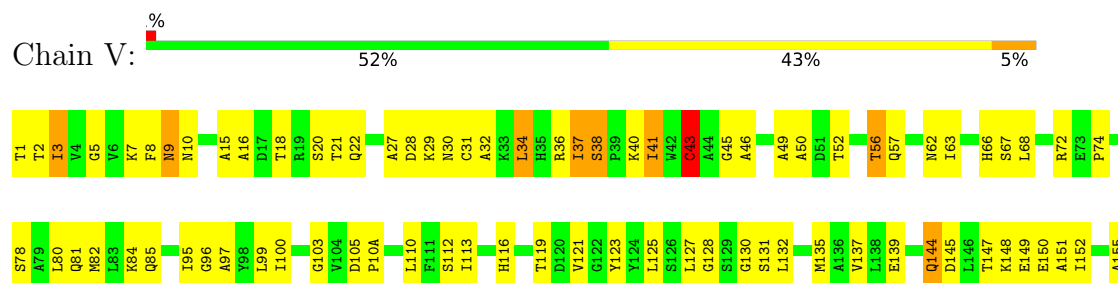
• Molecule 7: Proteasome component C7-alpha



• Molecule 8: Proteasome component PUP1

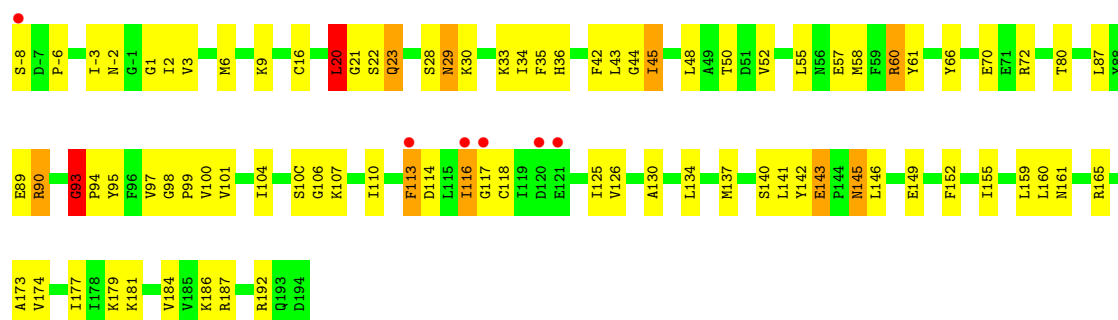


• Molecule 8: Proteasome component PUP1

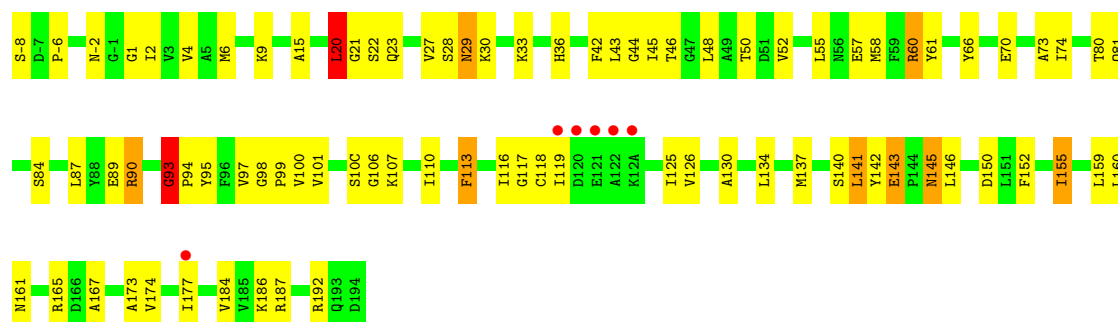




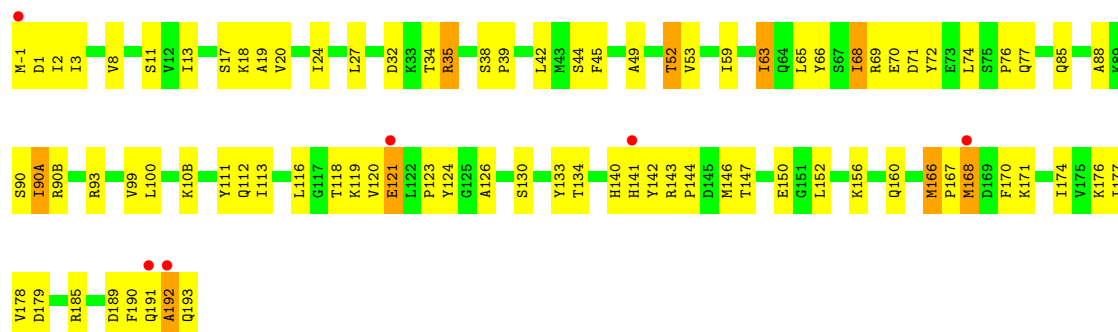
• Molecule 9: Proteasome component PUP3



• Molecule 9: Proteasome component PUP3



• Molecule 10: Proteasome component C11

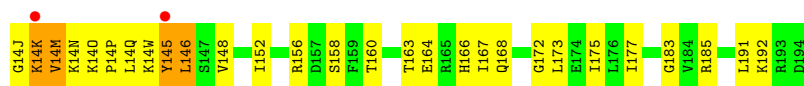
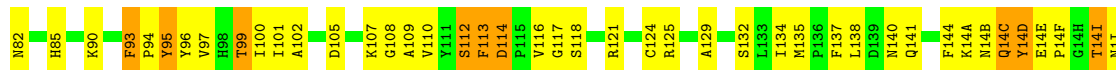


• Molecule 10: Proteasome component C11





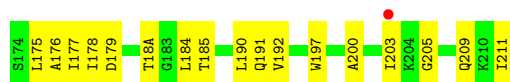
• Molecule 12: Proteasome component C5



• Molecule 13: Proteasome component PRE4

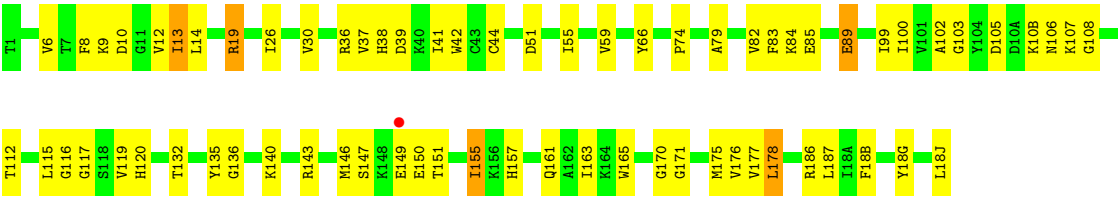


• Molecule 13: Proteasome component PRE4



• Molecule 14: Proteasome component PRE3





● Molecule 14: Proteasome component PRE3



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	134.12Å 300.56Å 144.06Å 90.00° 112.76° 90.00°	Depositor
Resolution (Å)	49.77 – 2.80 49.77 – 2.81	Depositor EDS
% Data completeness (in resolution range)	92.3 (49.77-2.80) 92.3 (49.77-2.81)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.49 (at 2.81Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.238 , 0.266 0.221 , 0.247	Depositor DCC
R_{free} test set	11760 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	48.1	Xtriage
Anisotropy	0.853	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 58.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	50905	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.41% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MES, H10

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	0.45	0/1952	0.94	7/2642 (0.3%)
1	O	0.43	0/1952	0.94	7/2642 (0.3%)
2	B	0.44	0/1935	0.93	7/2618 (0.3%)
2	P	0.45	0/1935	0.94	6/2618 (0.2%)
3	C	0.43	0/1920	0.91	6/2598 (0.2%)
3	Q	0.41	0/1920	0.92	6/2598 (0.2%)
4	D	0.44	0/1887	0.92	7/2541 (0.3%)
4	R	0.43	0/1887	0.92	6/2541 (0.2%)
5	E	0.40	0/1823	0.92	4/2463 (0.2%)
5	S	0.40	0/1823	0.93	6/2463 (0.2%)
6	F	0.43	0/1937	0.99	15/2614 (0.6%)
6	T	0.44	0/1937	0.98	14/2614 (0.5%)
7	G	0.47	0/1959	0.95	3/2652 (0.1%)
7	U	0.47	0/1959	0.96	6/2652 (0.2%)
8	H	0.47	0/1716	0.97	4/2326 (0.2%)
8	V	0.46	0/1716	0.97	5/2326 (0.2%)
9	I	0.46	0/1611	1.04	12/2174 (0.6%)
9	W	0.47	0/1611	1.06	13/2174 (0.6%)
10	J	0.46	0/1613	0.98	4/2173 (0.2%)
10	X	0.46	0/1613	0.98	4/2173 (0.2%)
11	K	0.46	0/1681	0.93	4/2274 (0.2%)
11	Y	0.45	0/1681	0.92	4/2274 (0.2%)
12	L	0.42	0/1795	1.04	9/2420 (0.4%)
12	Z	0.42	0/1795	1.04	9/2420 (0.4%)
13	1	0.46	0/1855	0.96	8/2514 (0.3%)
13	M	0.46	0/1855	0.96	7/2514 (0.3%)
14	2	0.48	0/1541	0.96	2/2087 (0.1%)
14	N	0.49	0/1541	0.96	2/2087 (0.1%)
All	All	0.45	0/50450	0.96	187/68192 (0.3%)

There are no bond length outliers.

All (187) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	U	16	SER	N-CA-C	-9.09	99.67	110.13
13	1	27	ARG	N-CA-C	9.08	120.79	111.07
13	M	27	ARG	N-CA-C	9.05	120.91	111.14
7	G	16	SER	N-CA-C	-8.68	100.15	110.13
12	Z	93	PHE	CA-C-N	8.63	128.69	119.89
12	Z	93	PHE	C-N-CA	8.63	128.69	119.89
12	L	93	PHE	CA-C-N	8.37	128.42	119.89
12	L	93	PHE	C-N-CA	8.37	128.42	119.89
12	L	95	TYR	N-CA-C	-8.06	96.17	108.67
6	T	12	ASN	N-CA-C	7.99	119.62	111.07
6	F	240	ILE	N-CA-C	-7.91	103.70	112.80
9	W	60	ARG	N-CA-C	-7.88	102.39	110.97
6	F	12	ASN	N-CA-C	7.87	119.55	110.97
8	H	37	ILE	N-CA-C	-7.86	103.25	111.58
9	I	60	ARG	N-CA-C	-7.78	102.49	110.97
2	B	161	LYS	N-CA-C	-7.74	103.96	113.41
1	A	161	LYS	N-CA-C	-7.71	102.80	112.90
1	O	161	LYS	N-CA-C	-7.68	102.84	112.90
4	R	161	ASN	N-CA-C	-7.61	103.45	112.89
12	Z	95	TYR	N-CA-C	-7.60	96.90	108.67
6	T	240	ILE	N-CA-C	-7.58	104.09	112.80
7	G	161	LYS	N-CA-C	-7.54	102.73	112.23
4	D	161	ASN	N-CA-C	-7.52	103.56	112.89
2	P	161	LYS	N-CA-C	-7.46	104.31	113.41
10	X	166	MET	CA-C-N	7.46	127.49	119.28
10	X	166	MET	C-N-CA	7.46	127.49	119.28
10	J	166	MET	CA-C-N	7.46	127.48	119.28
10	J	166	MET	C-N-CA	7.46	127.48	119.28
6	T	63	LYS	N-CA-C	7.43	120.83	111.69
6	T	161	LYS	N-CA-C	-7.42	102.13	112.45
8	V	37	ILE	N-CA-C	-7.38	103.76	111.58
6	F	63	LYS	N-CA-C	7.36	120.74	111.69
6	F	161	LYS	N-CA-C	-7.35	102.23	112.45
6	F	107	ILE	N-CA-C	7.31	116.93	108.96
7	U	161	LYS	N-CA-C	-7.20	103.16	112.23
5	E	102	VAL	N-CA-C	7.17	117.27	110.53
13	M	-2	THR	N-CA-C	7.14	120.58	109.52
9	I	93	GLY	CA-C-N	7.09	127.05	120.03
9	I	93	GLY	C-N-CA	7.09	127.05	120.03
5	S	102	VAL	N-CA-C	7.04	117.15	110.53
9	I	117	GLY	N-CA-C	6.93	124.34	114.64
13	1	-2	THR	N-CA-C	6.92	120.43	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Q	22	PHE	N-CA-C	6.82	119.58	111.33
9	W	117	GLY	N-CA-C	6.81	124.17	114.64
12	L	146	LEU	N-CA-C	6.77	120.05	110.50
3	Q	161	SER	N-CA-C	-6.76	104.05	112.90
4	D	169	SER	N-CA-C	6.75	118.33	110.97
12	Z	146	LEU	N-CA-C	6.75	120.01	110.50
6	T	107	ILE	N-CA-C	6.74	116.30	108.96
8	V	38	SER	N-CA-C	-6.71	102.10	108.07
13	1	98	ALA	N-CA-C	-6.67	97.40	108.34
9	W	93	GLY	CA-C-N	6.57	126.53	120.03
9	W	93	GLY	C-N-CA	6.57	126.53	120.03
12	L	117	GLY	N-CA-C	6.54	123.80	114.64
3	Q	108	THR	N-CA-C	-6.46	101.83	110.55
3	C	22	PHE	N-CA-C	6.46	119.14	111.33
9	W	143	GLU	CA-C-N	6.44	126.81	119.92
9	W	143	GLU	C-N-CA	6.44	126.81	119.92
8	V	21	THR	N-CA-C	6.42	119.65	109.50
4	R	169	SER	N-CA-C	6.41	117.95	110.97
6	F	135	SER	N-CA-C	-6.38	99.00	109.40
13	M	98	ALA	N-CA-C	-6.31	97.99	108.34
13	M	95	LEU	N-CA-C	-6.30	95.22	107.62
12	Z	113	PHE	N-CA-C	6.26	119.38	109.81
9	I	98	GLY	CA-C-N	6.24	126.20	119.78
9	I	98	GLY	C-N-CA	6.24	126.20	119.78
13	1	95	LEU	N-CA-C	-6.18	95.44	107.62
8	H	38	SER	N-CA-C	-6.14	102.61	108.07
6	T	14	VAL	N-CA-C	6.13	117.55	109.21
10	X	27	LEU	N-CA-C	6.13	118.76	111.71
6	T	155	GLY	N-CA-C	-6.13	107.39	114.69
10	J	27	LEU	N-CA-C	6.11	118.73	111.71
9	W	95	TYR	N-CA-C	-6.10	100.56	110.20
1	A	66	LYS	N-CA-C	-6.08	105.69	113.23
12	Z	117	GLY	N-CA-C	6.07	123.13	114.64
5	S	57	GLU	N-CA-C	-6.05	105.48	112.92
12	L	113	PHE	N-CA-C	6.01	119.01	109.81
3	C	161	SER	N-CA-C	-5.99	105.05	112.90
5	E	161	TYR	N-CA-C	-5.97	105.08	112.90
3	C	108	THR	N-CA-C	-5.96	102.51	110.55
8	H	21	THR	N-CA-C	5.95	119.17	109.24
5	E	57	GLU	N-CA-C	-5.91	105.65	112.92
9	I	145	ASN	N-CA-C	5.89	119.67	111.90
1	A	10(A)	ILE	CB-CA-C	-5.88	105.81	111.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	155	GLY	N-CA-C	-5.88	107.69	114.69
4	D	103	TYR	N-CA-C	5.83	121.11	113.30
5	S	161	TYR	N-CA-C	-5.83	105.26	112.90
10	X	134	THR	N-CA-C	5.83	120.52	113.41
4	R	103	TYR	N-CA-C	5.82	121.10	113.30
9	W	145	ASN	N-CA-C	5.82	119.58	111.90
6	T	135	SER	N-CA-C	-5.80	99.95	109.40
9	W	98	GLY	CA-C-N	5.78	125.73	119.78
9	W	98	GLY	C-N-CA	5.78	125.73	119.78
6	T	71	ASP	CB-CA-C	-5.78	109.93	116.63
6	T	38	ILE	N-CA-C	5.72	116.94	108.65
6	F	71	ASP	CB-CA-C	-5.71	110.00	116.63
3	C	27	ALA	N-CA-C	-5.70	105.06	111.28
6	F	14	VAL	N-CA-C	5.70	116.96	109.21
12	L	145	TYR	N-CA-C	5.68	119.51	109.96
12	Z	66	TYR	N-CA-C	-5.68	104.99	111.07
12	Z	145	TYR	N-CA-C	5.67	119.48	109.96
6	T	107	ILE	CA-C-N	5.66	125.59	119.76
6	T	107	ILE	C-N-CA	5.66	125.59	119.76
13	1	9	ASP	N-CA-C	5.60	118.10	111.33
5	E	42	SER	N-CA-C	-5.59	103.39	108.75
2	P	16	SER	N-CA-C	-5.58	102.02	110.39
10	J	134	THR	N-CA-C	5.57	120.20	113.41
1	O	10(A)	ILE	CB-CA-C	-5.56	106.10	111.05
4	R	82	THR	N-CA-C	5.54	118.08	111.71
9	W	142	TYR	N-CA-C	5.53	118.66	110.48
6	T	82	ILE	CB-CA-C	-5.52	108.46	113.70
8	V	43	CYS	N-CA-C	5.50	118.19	109.50
2	B	109	VAL	N-CA-C	5.50	115.95	110.23
6	F	82	ILE	CB-CA-C	-5.50	108.48	113.70
8	H	43	CYS	N-CA-C	5.49	118.17	109.50
14	N	117	GLY	N-CA-C	-5.47	107.23	114.95
3	Q	27	ALA	N-CA-C	-5.47	105.32	111.28
2	B	137	ILE	N-CA-C	-5.44	99.81	107.75
1	A	185	GLU	N-CA-C	-5.43	101.42	110.17
2	B	72	ASP	N-CA-C	-5.43	106.65	113.28
14	2	19	ARG	N-CA-C	5.42	117.36	108.52
9	I	142	TYR	N-CA-C	5.41	118.49	110.48
13	1	165	ARG	N-CA-C	5.41	120.55	113.30
6	F	204	ASP	N-CA-C	-5.39	107.01	113.21
1	O	66	LYS	N-CA-C	-5.39	106.54	113.23
7	U	220	LYS	N-CA-C	5.39	117.28	108.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	Y	97	MET	N-CA-C	5.39	116.59	108.46
1	O	78	TYR	N-CA-C	5.38	115.39	108.34
6	F	38	ILE	N-CA-C	5.38	116.45	108.65
7	G	220	LYS	N-CA-C	5.38	117.26	108.76
11	Y	82	ILE	N-CA-C	-5.36	105.27	110.42
3	Q	136	THR	N-CA-C	5.35	117.96	109.50
2	B	107	ILE	N-CA-C	5.35	114.19	108.95
9	I	95	TYR	N-CA-C	-5.35	101.25	109.76
7	U	80	GLY	CA-C-N	5.35	125.65	119.93
7	U	80	GLY	C-N-CA	5.35	125.65	119.93
13	M	9	ASP	N-CA-C	5.34	117.79	111.33
2	P	109	VAL	N-CA-C	5.34	115.78	110.23
2	P	72	ASP	N-CA-C	-5.33	106.78	113.28
11	K	97	MET	N-CA-C	5.32	116.49	108.46
6	T	204	ASP	N-CA-C	-5.32	107.10	113.21
3	Q	70	ILE	N-CA-C	-5.31	104.87	112.35
13	1	92(A)	LYS	N-CA-C	-5.29	106.13	112.59
2	B	78	VAL	N-CA-C	5.29	116.59	108.71
9	I	143	GLU	CA-C-N	5.29	126.45	119.84
9	I	143	GLU	C-N-CA	5.29	126.45	119.84
1	O	155	GLY	N-CA-C	-5.28	107.83	115.27
2	B	16	SER	N-CA-C	-5.27	102.49	110.39
12	Z	114	ASP	N-CA-C	-5.26	103.50	110.40
14	N	19	ARG	N-CA-C	5.26	117.09	108.52
5	S	58	LEU	N-CA-C	-5.25	107.24	113.97
3	C	136	THR	N-CA-C	5.25	117.80	109.50
4	D	63	SER	N-CA-C	-5.22	106.68	113.16
12	L	114	ASP	N-CA-C	-5.21	103.58	110.40
4	R	129	SER	N-CA-C	5.20	118.41	111.75
1	O	185	GLU	N-CA-C	-5.20	101.80	110.17
11	Y	98	GLY	N-CA-C	-5.19	100.88	113.18
2	P	137	ILE	N-CA-C	-5.18	100.18	107.75
11	K	82	ILE	N-CA-C	-5.18	105.44	110.42
13	M	14(G)	ILE	CB-CA-C	-5.18	107.21	114.00
11	Y	57	THR	N-CA-C	-5.18	105.72	111.36
6	F	145	GLY	N-CA-C	5.17	118.30	111.52
5	S	154	SER	N-CA-C	-5.16	106.24	112.54
4	R	63	SER	N-CA-C	-5.15	106.78	113.16
14	2	117	GLY	N-CA-C	-5.15	107.69	114.95
1	O	235	ALA	N-CA-C	-5.13	107.53	112.97
5	S	42	SER	N-CA-C	-5.13	103.83	108.75
4	D	129	SER	N-CA-C	5.13	118.31	111.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	70	ILE	N-CA-C	-5.12	107.40	111.81
9	W	20	LEU	N-CA-C	-5.12	99.33	108.13
8	V	132	LEU	N-CA-C	5.11	116.93	111.36
11	K	98	GLY	N-CA-C	-5.09	101.11	113.18
1	A	155	GLY	N-CA-C	-5.09	108.09	115.27
9	I	20	LEU	N-CA-C	-5.09	99.37	108.13
1	A	78	TYR	N-CA-C	5.09	115.00	108.34
2	P	78	VAL	N-CA-C	5.09	116.29	108.71
4	D	82	THR	N-CA-C	5.08	117.56	111.71
7	U	17(B)	LYS	N-CA-C	-5.08	105.87	111.71
12	L	94	PRO	N-CA-C	5.08	119.19	111.11
6	F	107	ILE	CA-C-N	5.06	124.98	119.76
6	F	107	ILE	C-N-CA	5.06	124.98	119.76
13	1	31	VAL	N-CA-C	5.06	115.97	108.23
1	A	235	ALA	N-CA-C	-5.06	107.61	112.97
9	W	141	LEU	N-CA-C	5.03	117.50	111.71
3	C	70	ILE	N-CA-C	-5.02	105.27	112.35
11	K	57	THR	N-CA-C	-5.01	105.89	111.36
13	M	92(A)	LYS	N-CA-C	-5.01	106.48	112.59

There are no chirality outliers.

There are no planarity outliers.

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	1915	0	1926	100	0
1	O	1915	0	1926	95	0
2	B	1905	0	1901	124	0
2	P	1905	0	1901	120	0
3	C	1891	0	1900	125	0
3	Q	1891	0	1900	135	0
4	D	1862	0	1836	92	0
4	R	1862	0	1836	96	0
5	E	1795	0	1797	138	0
5	S	1795	0	1797	127	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	F	1897	0	1886	118	0
6	T	1897	0	1886	108	0
7	G	1921	0	1910	114	0
7	U	1921	0	1910	120	0
8	H	1685	0	1688	97	0
8	V	1685	0	1688	107	0
9	I	1581	0	1574	88	0
9	W	1581	0	1574	81	0
10	J	1585	0	1590	97	0
10	X	1585	0	1590	104	0
11	K	1644	0	1595	93	0
11	Y	1644	0	1595	96	0
12	L	1757	0	1711	106	0
12	Z	1757	0	1711	105	0
13	1	1824	0	1832	85	0
13	M	1824	0	1832	92	0
14	2	1512	0	1481	86	0
14	N	1512	0	1481	67	0
15	K	12	0	13	0	0
15	Y	12	0	13	0	0
16	K	26	0	26	4	0
16	Y	26	0	26	7	0
17	1	69	0	0	9	0
17	2	61	0	0	4	0
17	A	49	0	0	3	0
17	B	36	0	0	3	0
17	C	37	0	0	6	0
17	D	36	0	0	4	0
17	E	23	0	0	5	0
17	F	47	0	0	4	0
17	G	58	0	0	4	0
17	H	46	0	0	2	0
17	I	65	0	0	3	0
17	J	48	0	0	4	0
17	K	49	0	0	4	0
17	L	58	0	0	5	0
17	M	66	0	0	5	0
17	N	56	0	0	4	0
17	O	30	0	0	2	0
17	P	29	0	0	4	0
17	Q	24	0	0	5	0
17	R	30	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	S	19	0	0	1	0
17	T	38	0	0	4	0
17	U	60	0	0	7	0
17	V	42	0	0	4	0
17	W	57	0	0	6	0
17	X	48	0	0	8	0
17	Y	50	0	0	3	0
17	Z	50	0	0	11	0
All	All	50905	0	49332	2655	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 27.

All (2655) 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)
8:H:15:ALA:HB3	8:H:159:ILE:HD11	1.25	1.17
10:J:168:MET:HE3	10:X:168:MET:HE3	1.22	1.11
2:P:74:ILE:HD11	2:P:109:VAL:HG22	1.12	1.10
7:U:9:ASP:HA	7:U:14:ILE:HD11	1.25	1.10
2:B:202:THR:HG22	2:B:204:SER:H	1.13	1.09
8:H:50:ALA:HB2	9:I:116:ILE:HD13	1.33	1.09
8:V:15:ALA:HB3	8:V:159:ILE:HD11	1.24	1.09
6:T:49:ALA:HB1	6:T:197:ILE:HD11	1.33	1.08
11:Y:10(B):LYS:H	11:Y:10(B):LYS:HD2	1.20	1.06
2:P:74:ILE:HD13	2:P:140:GLY:HA3	1.30	1.06
8:H:15:ALA:CB	8:H:159:ILE:HD11	1.86	1.06
4:R:74:ILE:HD11	4:R:109:VAL:HG22	1.11	1.06
6:T:49:ALA:CB	6:T:197:ILE:HD11	1.86	1.05
8:V:15:ALA:CB	8:V:159:ILE:HD11	1.84	1.05
2:P:202:THR:HG22	2:P:204:SER:H	1.11	1.05
11:K:10(B):LYS:H	11:K:10(B):LYS:HD2	1.21	1.02
7:G:96:ALA:HA	7:G:107:MET:HE2	1.40	1.02
5:S:38:VAL:HG23	5:S:197:ILE:HD13	1.38	1.02
7:U:96:ALA:HA	7:U:107:MET:HE2	1.41	1.02
2:B:107:ILE:HD13	2:B:108:PRO:O	1.60	1.02
5:E:49:VAL:HG13	5:E:212:ILE:CD1	1.89	1.01
7:U:12:ILE:HG13	7:U:14:ILE:HD12	1.39	1.01
11:Y:7:ARG:HG3	11:Y:12:ILE:CD1	1.92	1.00
1:A:21:LEU:HB3	1:A:24:ILE:HD13	1.42	0.99
3:Q:201:VAL:CG2	3:Q:210:ILE:HD11	1.93	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:GLU:HG2	2:B:58:LEU:CD2	1.93	0.98
13:1:40:ASN:H	13:1:40:ASN:HD22	1.10	0.98
5:E:49:VAL:HG13	5:E:212:ILE:HD11	1.41	0.98
3:Q:201:VAL:HG21	3:Q:210:ILE:HD11	0.98	0.98
9:I:177:ILE:HD12	9:I:187:ARG:HH12	1.23	0.97
3:C:70:ILE:HD13	3:C:112:LEU:HD11	1.45	0.96
8:H:50:ALA:CB	9:I:116:ILE:HD13	1.94	0.96
3:Q:197:LEU:HD13	3:Q:210:ILE:HD12	1.48	0.95
10:X:37:LEU:HB3	10:X:63:ILE:HD13	1.49	0.95
11:Y:6:PHE:HB2	11:Y:124:ILE:HD13	1.49	0.95
4:D:97:VAL:HG21	11:K:65:LEU:HD13	1.46	0.94
3:Q:201:VAL:HG21	3:Q:210:ILE:CD1	1.94	0.94
13:1:157:ASN:HD22	13:1:160:ARG:HH11	0.99	0.94
4:R:74:ILE:CD1	4:R:109:VAL:HG22	1.97	0.93
3:Q:70:ILE:HD13	3:Q:112:LEU:HD11	1.49	0.93
12:L:3:ILE:HD13	12:L:127:GLY:O	1.67	0.93
2:B:107:ILE:HD12	2:B:112:LEU:HB2	1.47	0.93
13:M:157:ASN:HD22	13:M:160:ARG:HH11	1.04	0.92
10:J:168:MET:CE	10:X:168:MET:HE3	1.99	0.92
8:H:128:GLY:O	8:H:131:SER:HB2	1.70	0.92
6:T:197:ILE:HD13	6:T:210:LEU:HD11	1.52	0.92
10:J:168:MET:HE3	10:X:168:MET:CE	1.99	0.92
1:O:15:PHE:H	2:P:23:GLN:HE22	1.09	0.92
2:B:15:PHE:H	3:C:23:GLN:HE22	1.13	0.91
13:M:40:ASN:HD22	13:M:40:ASN:H	1.09	0.91
9:I:44:GLY:C	9:I:45:ILE:HD12	1.95	0.91
4:R:74:ILE:HD13	4:R:140:GLY:HA3	1.51	0.91
1:A:130:ARG:HH21	7:G:124:THR:HG22	1.35	0.91
1:O:130:ARG:HH21	7:U:124:THR:HG22	1.35	0.91
1:O:124:THR:HG22	2:P:130:ARG:HH21	1.34	0.91
4:R:97:VAL:HG21	11:Y:65:LEU:HD13	1.50	0.91
12:L:3:ILE:HD12	12:L:46:ASN:HB2	1.53	0.90
8:V:128:GLY:O	8:V:131:SER:HB2	1.71	0.90
14:2:17:ASP:HB3	14:2:163:ILE:HD11	1.54	0.90
14:2:18(A):ILE:HD13	14:2:18(B):PHE:N	1.86	0.90
3:Q:15:PHE:H	4:R:23:GLN:HE22	1.15	0.89
2:P:61:GLN:OE1	2:P:208:ASP:HA	1.74	0.88
8:V:221:ILE:HD11	9:W:184:VAL:HB	1.56	0.88
3:Q:154:SER:OG	3:Q:156:ILE:HD13	1.74	0.87
5:E:221:PHE:CE1	5:E:223:ILE:HD11	2.10	0.87
13:1:157:ASN:ND2	13:1:160:ARG:HH11	1.71	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:15:PHE:H	4:D:23:GLN:HE22	1.15	0.87
7:U:70:ILE:HD11	7:U:76:MET:HB2	1.56	0.87
12:L:83:ILE:HD13	12:L:86:LEU:HD12	1.57	0.86
1:A:124:THR:HG22	2:B:130:ARG:HH21	1.40	0.86
3:Q:163:GLN:HA	3:Q:163:GLN:HE21	1.39	0.86
4:D:28:LEU:HA	4:D:31:ILE:HD12	1.56	0.86
1:A:15:PHE:H	2:B:23:GLN:HE22	1.20	0.86
9:I:152:PHE:HB2	9:I:177:ILE:HD11	1.58	0.85
11:K:7:ARG:HG2	11:K:108:PRO:HB2	1.58	0.85
5:S:221:PHE:CE1	5:S:223:ILE:HD11	2.09	0.85
1:A:179:ARG:HB3	1:A:179:ARG:HH11	1.40	0.85
3:C:163:GLN:HA	3:C:163:GLN:HE21	1.40	0.85
5:E:28:LEU:HA	5:E:31:ILE:HD13	1.58	0.85
10:J:2:ILE:HD13	10:J:130:SER:OG	1.76	0.85
5:S:207:LEU:HA	5:S:2(E):ASN:ND2	1.92	0.85
2:P:194:LEU:HD11	2:P:232:ILE:HD13	1.59	0.85
11:Y:7:ARG:HG2	11:Y:108:PRO:HB2	1.57	0.85
6:F:38:ILE:HD12	6:F:40:ILE:HD11	1.59	0.85
2:P:74:ILE:CD1	2:P:109:VAL:HG22	2.02	0.85
3:Q:164:THR:HG21	3:Q:172:VAL:HG13	1.58	0.85
2:P:124:THR:HG22	3:Q:130:ARG:HH21	1.41	0.84
2:B:124:THR:HG22	3:C:130:ARG:HH21	1.42	0.84
4:R:28:LEU:HA	4:R:31:ILE:HD12	1.58	0.84
9:I:165:ARG:NH2	12:Z:135:MET:HE3	1.92	0.84
13:M:157:ASN:ND2	13:M:160:ARG:HH11	1.75	0.84
3:C:164:THR:HG21	3:C:172:VAL:HG13	1.58	0.84
6:T:49:ALA:HB1	6:T:197:ILE:CD1	2.07	0.84
10:X:55:PHE:O	10:X:59:ILE:HD13	1.77	0.84
2:B:61:GLN:OE1	2:B:208:ASP:HA	1.77	0.84
8:H:50:ALA:HB2	9:I:116:ILE:CD1	2.08	0.84
2:B:158:THR:HG22	3:C:63:THR:HG23	1.59	0.83
7:U:9:ASP:CA	7:U:14:ILE:HD11	2.07	0.83
1:A:177:GLU:HG2	2:B:58:LEU:HD21	1.59	0.83
1:O:179:ARG:HB3	1:O:179:ARG:HH11	1.42	0.83
3:Q:156:ILE:HD12	4:R:83:ALA:HB2	1.61	0.83
8:H:221:ILE:HD11	9:I:184:VAL:HB	1.59	0.83
2:B:194:LEU:HD11	2:B:232:ILE:HD13	1.59	0.83
5:E:207:LEU:HA	5:E:2(E):ASN:ND2	1.92	0.83
11:Y:7:ARG:HG3	11:Y:12:ILE:HD11	1.58	0.83
2:P:202:THR:HG22	2:P:204:SER:N	1.94	0.82
14:2:163:ILE:HD13	14:2:169:SER:HB3	1.62	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1:157:ASN:HD22	13:1:160:ARG:NH1	1.76	0.82
14:N:136:GLY:HA2	14:2:161:GLN:NE2	1.93	0.82
12:Z:134:ILE:HD12	12:Z:158:SER:HB3	1.61	0.82
5:E:213:ALA:HB2	5:E:223:ILE:HD12	1.60	0.82
5:S:15:PHE:H	6:T:23:GLN:HE22	1.26	0.82
9:W:4:VAL:HG13	9:W:155:ILE:HD11	1.62	0.81
5:E:75:GLY:HA3	5:E:221:PHE:CE2	2.16	0.81
3:C:163:GLN:NE2	3:C:164:THR:H	1.79	0.81
1:O:130:ARG:HH21	7:U:124:THR:CG2	1.93	0.81
11:K:102:CYS:SG	11:K:110:ILE:HD12	2.20	0.81
12:L:135:MET:HE3	9:W:165:ARG:NH2	1.94	0.81
4:R:74:ILE:HD11	4:R:109:VAL:CG2	2.04	0.81
5:S:75:GLY:HA3	5:S:221:PHE:CE2	2.16	0.81
12:Z:7:ALA:HB2	12:Z:110:VAL:HG23	1.61	0.81
5:E:15:PHE:H	6:F:23:GLN:HE22	1.27	0.81
5:S:2(B):THR:H	5:S:2(E):ASN:HD22	1.25	0.80
5:E:97:ASN:HD21	12:L:61:ASN:HD21	1.29	0.80
5:S:97:ASN:HD21	12:Z:61:ASN:HD21	1.25	0.80
5:S:213:ALA:HB2	5:S:223:ILE:HD12	1.62	0.80
13:M:157:ASN:HD22	13:M:160:ARG:NH1	1.80	0.80
9:W:45:ILE:HB	9:W:52:VAL:HG13	1.62	0.80
13:1:40:ASN:HD22	13:1:40:ASN:N	1.74	0.80
2:P:107:ILE:HD11	2:P:111:ILE:HG22	1.62	0.80
12:L:7:ALA:HB2	12:L:110:VAL:HG23	1.64	0.79
12:L:21:ILE:HD12	8:V:167:LEU:CD1	2.12	0.79
12:L:3:ILE:HD12	12:L:46:ASN:CB	2.11	0.79
1:A:13:THR:HG21	1:A:24:ILE:HD11	1.63	0.79
6:F:20(B):GLU:HG3	6:F:20(C):LYS:HG3	1.63	0.79
2:P:126:HIS:HB3	3:Q:129:VAL:HG12	1.65	0.79
7:G:121:GLN:O	7:G:124:THR:HB	1.83	0.79
3:Q:159:SER:HB2	17:Q:1140:HOH:O	1.83	0.79
14:N:13:ILE:HD13	14:N:177:VAL:HG13	1.63	0.79
5:E:2(B):THR:H	5:E:2(E):ASN:HD22	1.26	0.78
7:U:67:ILE:HD12	7:U:211:GLU:HG2	1.64	0.78
6:F:175:GLU:HB3	6:F:196:ILE:HD12	1.64	0.78
12:L:100:ILE:HG13	12:L:112:SER:HB3	1.62	0.78
3:Q:55:THR:HG22	3:Q:56:LEU:HD22	1.65	0.78
7:U:121:GLN:O	7:U:124:THR:HB	1.83	0.78
11:K:10(B):LYS:H	11:K:10(B):LYS:CD	1.97	0.78
6:T:175:GLU:HB3	6:T:196:ILE:HD12	1.63	0.78
6:T:20(B):GLU:HG3	6:T:20(C):LYS:HG3	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:163:GLN:NE2	3:Q:164:THR:H	1.82	0.78
7:G:198:ILE:HG23	7:G:203:THR:O	1.84	0.78
14:N:161:GLN:NE2	14:2:136:GLY:HA2	1.98	0.78
1:O:47:VAL:HG21	1:O:190:ILE:HD13	1.66	0.78
1:A:20:LYS:HE3	1:A:25:ASP:OD1	1.84	0.77
7:G:67:ILE:HD12	7:G:211:GLU:HG2	1.64	0.77
11:K:12:ILE:HG21	11:K:110:ILE:HD11	1.64	0.77
5:S:201:LEU:HD11	5:S:207:LEU:HD22	1.67	0.77
13:M:40:ASN:HD22	13:M:40:ASN:N	1.75	0.77
7:U:217:LYS:HA	7:U:217:LYS:HE3	1.65	0.77
13:M:165:ARG:NH2	8:V:135:MET:HE3	2.00	0.77
5:S:190:ILE:HD11	5:S:214:ILE:HD12	1.67	0.77
8:V:10:ASN:OD1	8:V:180:ILE:HD12	1.85	0.77
9:W:152:PHE:HD1	9:W:177:ILE:HD11	1.49	0.77
10:J:90(A):ILE:HD11	10:J:116:LEU:HD22	1.65	0.77
12:L:59:PHE:CD1	12:L:83:ILE:HD11	2.19	0.77
5:E:12:THR:HG21	5:E:124:THR:HA	1.66	0.77
14:2:144:GLU:HG2	17:2:1115:HOH:O	1.84	0.77
1:A:130:ARG:HH21	7:G:124:THR:CG2	1.97	0.77
9:I:45:ILE:HB	9:I:52:VAL:HG13	1.66	0.77
2:B:124:THR:CG2	3:C:130:ARG:HH21	1.98	0.76
7:G:217:LYS:HA	7:G:217:LYS:HE3	1.66	0.76
1:A:179:ARG:HB3	1:A:179:ARG:NH1	2.00	0.76
6:T:40:ILE:HD12	6:T:193:ALA:HB2	1.66	0.76
6:T:95:GLU:HG2	6:T:115:ARG:HB3	1.68	0.76
3:C:55:THR:HG22	3:C:56:LEU:HD22	1.66	0.76
14:N:136:GLY:HA2	14:2:161:GLN:HE21	1.49	0.76
14:2:13:ILE:HD13	14:2:177:VAL:HG13	1.67	0.76
2:P:158:THR:HG22	3:Q:63:THR:HG23	1.66	0.76
5:E:201:LEU:HD11	5:E:207:LEU:HD22	1.67	0.76
1:O:179:ARG:HB3	1:O:179:ARG:NH1	2.01	0.76
6:T:237:GLN:O	6:T:240:ILE:HG22	1.86	0.76
3:Q:216:LYS:HB2	3:Q:220:ASP:HB3	1.69	0.75
4:R:76:CYS:HB2	4:R:138:ILE:HD13	1.67	0.75
8:H:135:MET:HE3	13:1:165:ARG:NH2	2.00	0.75
8:V:52:THR:O	8:V:56:THR:HB	1.86	0.75
9:W:27:VAL:HG13	17:X:622:HOH:O	1.86	0.75
1:O:20:LYS:HE3	1:O:25:ASP:OD1	1.86	0.75
3:C:216:LYS:HB2	3:C:220:ASP:HB3	1.68	0.75
7:U:198:ILE:HG23	7:U:203:THR:O	1.86	0.75
2:B:126:HIS:HB3	3:C:129:VAL:HG12	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:156:LYS:O	10:X:160:GLN:HG3	1.85	0.75
11:K:10(B):LYS:HD2	11:K:10(B):LYS:N	2.00	0.75
14:2:112:THR:HG22	14:2:120:HIS:HB2	1.69	0.75
8:V:80:LEU:HD12	8:V:113:ILE:HD11	1.68	0.74
1:O:225:THR:OG1	1:O:228:GLU:HG3	1.87	0.74
8:V:15:ALA:CB	8:V:159:ILE:CD1	2.65	0.74
1:A:100:TYR:N	1:A:10(A):ILE:HD13	2.02	0.74
10:J:152:LEU:HD13	10:J:193:GLN:HE22	1.53	0.74
11:Y:10(B):LYS:H	11:Y:10(B):LYS:CD	1.97	0.74
10:J:156:LYS:O	10:J:160:GLN:HG3	1.88	0.74
3:Q:65:SER:HB2	17:Q:303:HOH:O	1.87	0.74
2:B:107:ILE:CD1	2:B:108:PRO:O	2.33	0.74
1:O:124:THR:CG2	2:P:130:ARG:HH21	2.00	0.74
5:S:12:THR:HG21	5:S:124:THR:HA	1.68	0.74
8:H:15:ALA:CB	8:H:159:ILE:CD1	2.65	0.74
12:L:166:HIS:HD2	12:L:168:GLN:H	1.35	0.74
13:1:14(C):ARG:HH11	13:1:14(C):ARG:HG3	1.52	0.74
5:S:38:VAL:HG23	5:S:197:ILE:CD1	2.15	0.74
11:Y:10(B):LYS:HD2	11:Y:10(B):LYS:N	2.01	0.74
3:Q:185:THR:HG22	3:Q:187:GLU:H	1.53	0.73
2:B:202:THR:HG22	2:B:204:SER:N	1.96	0.73
6:F:95:GLU:HG2	6:F:115:ARG:HB3	1.70	0.73
10:X:152:LEU:HD13	10:X:193:GLN:HE22	1.52	0.73
14:N:161:GLN:HE21	14:2:136:GLY:HA2	1.53	0.73
5:S:97:ASN:ND2	12:Z:61:ASN:HD21	1.87	0.73
1:A:124:THR:CG2	2:B:130:ARG:HH21	2.01	0.73
6:F:109:ILE:HG21	6:F:147:HIS:HB2	1.69	0.73
9:I:114:ASP:OD2	9:I:116:ILE:HD12	1.88	0.73
3:Q:41:LYS:HG2	3:Q:161:SER:O	1.89	0.73
5:S:18(C):PHE:HA	5:S:18(F):ILE:HG12	1.71	0.73
9:W:119:ILE:HD12	9:W:119:ILE:H	1.53	0.73
11:Y:7:ARG:HG3	11:Y:12:ILE:HD13	1.70	0.73
9:I:45:ILE:HD12	9:I:45:ILE:N	2.03	0.72
4:R:72:ARG:HG3	17:R:1302:HOH:O	1.88	0.72
7:U:70:ILE:HD11	7:U:76:MET:CB	2.19	0.72
11:K:80:SER:HA	11:K:101:ILE:HD13	1.71	0.72
1:A:177:GLU:HG2	2:B:58:LEU:HD22	1.68	0.72
12:Z:166:HIS:HD2	12:Z:168:GLN:H	1.36	0.72
14:2:126:ILE:H	14:2:126:ILE:HD13	1.53	0.72
3:C:163:GLN:HE21	3:C:163:GLN:CA	2.02	0.72
6:T:109:ILE:HG21	6:T:147:HIS:HB2	1.69	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:219:GLU:HG2	2:B:21(E):VAL:N	2.04	0.72
14:N:112:THR:HG22	14:N:120:HIS:HB2	1.72	0.72
6:T:36:THR:HG22	6:T:51:GLU:OE2	1.89	0.72
5:E:49:VAL:HA	5:E:212:ILE:HD13	1.72	0.72
1:O:47:VAL:CG2	1:O:190:ILE:HD13	2.20	0.72
5:S:36:VAL:HG13	5:S:197:ILE:HD11	1.70	0.72
3:C:185:THR:HG22	3:C:187:GLU:H	1.55	0.71
14:N:30:VAL:HG21	13:1:203:ILE:HD13	1.72	0.71
3:Q:163:GLN:HE21	3:Q:163:GLN:CA	2.02	0.71
5:S:67:ILE:HG21	5:S:223:ILE:HD12	1.72	0.71
1:A:225:THR:OG1	1:A:228:GLU:HG3	1.91	0.71
7:G:170:GLN:HE21	7:G:174:THR:HG23	1.55	0.71
7:G:87:ASN:C	7:G:87:ASN:HD22	1.98	0.71
13:M:100:ILE:HD13	13:M:112:TYR:HB2	1.73	0.71
13:M:152:GLU:O	13:M:156:VAL:HG23	1.90	0.71
2:P:74:ILE:CD1	2:P:140:GLY:HA3	2.15	0.71
7:U:170:GLN:HE21	7:U:174:THR:HG23	1.56	0.71
8:V:3:ILE:HD11	8:V:127:LEU:HB2	1.71	0.71
8:V:113:ILE:HG12	8:V:119:THR:HG22	1.71	0.71
6:F:237:GLN:O	6:F:240:ILE:HG22	1.90	0.71
13:M:76:PRO:HD2	13:M:105:GLN:OE1	1.90	0.71
10:X:18:LYS:HD3	10:X:174:ILE:HG13	1.72	0.71
3:Q:100:ARG:NH1	3:Q:106:PRO:HB3	2.05	0.71
3:C:41:LYS:HG2	3:C:161:SER:O	1.89	0.71
5:E:67:ILE:HG21	5:E:223:ILE:HD12	1.73	0.71
2:P:15:PHE:H	3:Q:23:GLN:HE22	1.39	0.71
2:P:101:LYS:NZ	10:X:85:GLN:NE2	2.39	0.71
5:S:104:ASN:HB2	13:1:81:GLU:HG2	1.72	0.71
13:M:8:TYR:CE2	13:M:148:VAL:HG22	2.26	0.71
4:R:121:LEU:N	17:R:853:HOH:O	2.23	0.71
10:X:90(A):ILE:HD13	10:X:90(A):ILE:O	1.91	0.71
1:O:121:GLN:O	1:O:124:THR:HB	1.91	0.70
6:T:193:ALA:O	6:T:197:ILE:HD12	1.90	0.70
4:R:76:CYS:CB	4:R:138:ILE:HD13	2.20	0.70
7:U:87:ASN:C	7:U:87:ASN:HD22	1.98	0.70
9:W:155:ILE:O	9:W:155:ILE:HD13	1.91	0.70
10:X:55:PHE:CE2	10:X:59:ILE:HD11	2.26	0.70
2:B:107:ILE:HD11	2:B:112:LEU:N	2.07	0.70
5:E:68:ILE:HD11	5:E:78:LEU:HD23	1.74	0.70
8:H:52:THR:O	8:H:56:THR:HB	1.91	0.70
10:J:90(A):ILE:CD1	10:J:116:LEU:HD22	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:70:ILE:HD12	4:D:92:ALA:HB3	1.73	0.70
2:P:219:GLU:HG2	2:P:21(E):VAL:N	2.06	0.70
12:Z:-7:ASN:ND2	12:Z:-5:TYR:H	1.89	0.70
12:Z:100:ILE:HG12	12:Z:112:SER:HB3	1.72	0.70
9:I:45:ILE:N	9:I:45:ILE:CD1	2.54	0.70
2:P:160:TRP:CE2	2:P:163:ILE:HD12	2.26	0.70
14:2:134:ILE:HD13	14:2:138:CYS:SG	2.31	0.70
3:C:100:ARG:NH1	3:C:106:PRO:HB3	2.07	0.70
7:G:49:ILE:CD1	7:G:193:ALA:HB1	2.22	0.70
13:M:149:GLN:NE2	13:M:149:GLN:H	1.90	0.70
2:B:160:TRP:CE2	2:B:163:ILE:HD12	2.27	0.70
5:E:97:ASN:HD21	12:L:61:ASN:ND2	1.90	0.70
8:H:3:ILE:HG13	8:H:100:ILE:HD12	1.73	0.70
10:J:59:ILE:O	10:J:63:ILE:HD13	1.90	0.70
6:T:79:SER:HA	17:T:1238:HOH:O	1.92	0.70
9:W:6:MET:HE3	9:W:155:ILE:HG12	1.74	0.70
9:I:177:ILE:CD1	9:I:187:ARG:HH12	2.01	0.70
6:T:37:SER:HB3	6:T:50:VAL:HG23	1.72	0.69
7:U:14:ILE:HD13	7:U:14:ILE:H	1.57	0.69
6:F:37:SER:HB3	6:F:50:VAL:HG23	1.73	0.69
14:2:146:MET:HE2	14:2:150:GLU:HB3	1.73	0.69
10:J:24:ILE:HG13	10:X:133:TYR:OH	1.92	0.69
13:1:76:PRO:HD2	13:1:105:GLN:OE1	1.91	0.69
2:P:121:GLN:O	2:P:124:THR:HB	1.91	0.69
6:T:175:GLU:CB	6:T:196:ILE:HD12	2.22	0.69
13:M:203:ILE:HD13	14:2:30:VAL:HG21	1.73	0.69
5:S:97:ASN:HD21	12:Z:61:ASN:ND2	1.89	0.69
13:1:8:TYR:CE2	13:1:148:VAL:HG22	2.27	0.69
6:F:175:GLU:CB	6:F:196:ILE:HD12	2.23	0.69
12:L:3:ILE:HD13	12:L:3:ILE:H	1.55	0.69
10:X:37:LEU:HD13	10:X:63:ILE:CD1	2.22	0.69
14:2:59:VAL:HG22	14:2:82:VAL:HG12	1.74	0.69
5:E:221:PHE:CZ	5:E:223:ILE:HD11	2.28	0.69
9:I:35:PHE:CE1	9:I:45:ILE:HD13	2.27	0.69
1:O:173:LYS:O	1:O:177:GLU:HG3	1.91	0.69
6:F:36:THR:HG22	6:F:51:GLU:OE2	1.91	0.69
10:J:18:LYS:HD3	10:J:174:ILE:HG13	1.75	0.69
5:S:221:PHE:CZ	5:S:223:ILE:HD11	2.28	0.69
1:A:173:LYS:O	1:A:177:GLU:HG3	1.93	0.69
5:E:210:LEU:HD22	5:E:233:ILE:HD11	1.75	0.69
9:I:6:MET:HE3	9:I:155:ILE:HG13	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:18(G):GLU:HG2	7:U:188:LYS:HB2	1.75	0.69
7:G:151:THR:HG22	7:G:157:TYR:HB2	1.75	0.69
10:J:-1:MET:HG2	10:J:1:ASP:H	1.58	0.69
13:M:14(C):ARG:HG3	13:M:14(C):ARG:HH11	1.58	0.69
13:1:149:GLN:NE2	13:1:149:GLN:H	1.91	0.69
2:B:121:GLN:O	2:B:124:THR:HB	1.93	0.68
10:J:167:PRO:O	10:X:168:MET:HE2	1.93	0.68
14:N:36:ARG:HG3	14:N:42:TRP:CE2	2.28	0.68
13:1:152:GLU:O	13:1:156:VAL:HG23	1.92	0.68
2:P:137:ILE:HD11	2:P:165:VAL:HG22	1.74	0.68
3:Q:15:PHE:CD1	3:Q:21:ILE:HD11	2.28	0.68
5:E:18(C):PHE:HA	5:E:18(F):ILE:HG13	1.75	0.68
5:S:220:PRO:O	5:S:222:THR:HG23	1.94	0.68
6:F:54:ILE:HD11	6:F:209:GLU:HB2	1.76	0.68
14:2:36:ARG:HG3	14:2:42:TRP:CE2	2.29	0.68
3:C:185:THR:HB	3:C:188:GLU:HG2	1.75	0.68
5:E:97:ASN:ND2	12:L:61:ASN:HD21	1.90	0.68
6:F:173:LYS:O	6:F:177:GLU:HG3	1.94	0.68
2:P:74:ILE:HD11	2:P:109:VAL:CG2	2.07	0.68
12:L:173:LEU:HB2	12:L:191:LEU:HD11	1.76	0.68
1:O:15:PHE:N	2:P:23:GLN:HE22	1.89	0.68
6:F:49:ALA:HB2	6:F:212:ILE:HD12	1.74	0.68
14:N:143:ARG:NH2	14:N:146:MET:HE3	2.08	0.68
8:H:172:ASN:HD22	8:H:193:THR:HA	1.59	0.68
12:L:3:ILE:CD1	12:L:127:GLY:O	2.42	0.68
8:V:41:ILE:HD12	8:V:103:GLY:HA3	1.75	0.68
10:J:168:MET:HE2	10:X:167:PRO:O	1.93	0.67
14:N:186:ARG:HD3	17:N:933:HOH:O	1.94	0.67
2:P:124:THR:CG2	3:Q:130:ARG:HH21	2.07	0.67
7:G:18(G):GLU:HG2	7:G:188:LYS:HB2	1.76	0.67
17:C:247:HOH:O	10:J:68:ILE:HD13	1.93	0.67
12:L:177:ILE:HD13	12:L:185:ARG:NH2	2.09	0.67
14:2:112:THR:CG2	14:2:120:HIS:HB2	2.23	0.67
7:G:135:ILE:HD13	7:G:152:ASP:HA	1.75	0.67
1:O:32:LYS:HE2	1:O:32:LYS:HA	1.75	0.67
3:Q:172:VAL:HG23	3:Q:196:SER:HB2	1.77	0.67
1:A:121:GLN:O	1:A:124:THR:HB	1.94	0.67
6:F:184:LEU:HD11	6:F:188:GLU:HB3	1.76	0.67
9:W:152:PHE:CD1	9:W:177:ILE:HD11	2.30	0.67
8:V:34:LEU:HB2	17:V:578:HOH:O	1.95	0.67
10:X:-1:MET:HG2	10:X:1:ASP:H	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:LYS:HE2	1:A:32:LYS:HA	1.76	0.67
7:G:8:TYR:O	7:G:12:ILE:HD13	1.94	0.67
8:H:34:LEU:HB2	17:H:540:HOH:O	1.95	0.67
3:Q:185:THR:HB	3:Q:188:GLU:HG2	1.74	0.67
4:R:81:LEU:HD12	4:R:133:GLY:HA3	1.76	0.67
7:U:151:THR:HG22	7:U:157:TYR:HB2	1.76	0.66
2:B:137:ILE:HD11	2:B:165:VAL:HG22	1.77	0.66
7:G:96:ALA:HA	7:G:107:MET:CE	2.22	0.66
7:G:135:ILE:HD13	7:G:153:PRO:HD3	1.77	0.66
5:S:207:LEU:HD23	5:S:207:LEU:H	1.60	0.66
7:U:96:ALA:HA	7:U:107:MET:CE	2.21	0.66
12:Z:13:VAL:HG12	12:Z:177:ILE:HG13	1.76	0.66
5:E:198:SER:HA	5:E:201:LEU:HG	1.76	0.66
12:L:21:ILE:HD12	8:V:167:LEU:HD11	1.76	0.66
12:Z:100:ILE:HD11	12:Z:125:ARG:HG3	1.77	0.66
13:1:104:VAL:HG23	13:1:178:ILE:HG22	1.76	0.66
1:A:110:LYS:HG2	17:A:285:HOH:O	1.94	0.66
5:E:111:ARG:HG2	5:E:111:ARG:HH11	1.60	0.66
9:I:6:MET:HE1	9:I:155:ILE:HA	1.77	0.66
2:B:190:ILE:CG2	2:B:232:ILE:HD11	2.26	0.66
4:R:50:VAL:HG22	4:R:67:ILE:HD11	1.76	0.66
6:T:38:ILE:HG22	6:T:164:ALA:HB2	1.76	0.66
14:2:143:ARG:NH2	14:2:146:MET:HE3	2.11	0.66
2:P:190:ILE:CG2	2:P:232:ILE:HD11	2.26	0.66
7:U:59:LEU:O	7:U:61:PRO:HD3	1.95	0.66
4:D:50:VAL:HG22	4:D:67:ILE:HD11	1.77	0.66
5:E:220:PRO:O	5:E:222:THR:HG23	1.95	0.66
8:V:172:ASN:HD22	8:V:193:THR:HA	1.61	0.66
4:D:81:LEU:HD12	4:D:133:GLY:HA3	1.77	0.65
6:F:211:GLU:O	6:F:212:ILE:HD13	1.96	0.65
7:G:77:VAL:HG12	7:G:137:THR:HB	1.79	0.65
5:S:198:SER:HA	5:S:201:LEU:HG	1.76	0.65
6:T:82:ILE:HB	6:T:83:PRO:HD3	1.76	0.65
10:X:32:ASP:OD2	10:X:34:THR:HG22	1.97	0.65
10:X:69:ARG:HD2	17:X:553:HOH:O	1.95	0.65
4:D:142:ASP:HA	17:D:1309:HOH:O	1.95	0.65
9:W:1:GLY:HA3	9:W:33:LYS:HE2	1.78	0.65
13:1:35:ILE:CD1	13:1:56:GLU:HG3	2.26	0.65
10:J:-1:MET:HG2	10:J:1:ASP:N	2.12	0.65
3:Q:37:ALA:HB3	3:Q:165:ILE:HD11	1.77	0.65
11:K:109:THR:O	11:K:110:ILE:HD13	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:14(D):GLU:O	13:M:14(G):ILE:HG12	1.96	0.65
6:F:38:ILE:HG22	6:F:164:ALA:HB2	1.77	0.65
4:R:24:VAL:O	4:R:27:SER:HB3	1.97	0.65
5:S:67:ILE:CD1	5:S:77:SER:HB3	2.26	0.65
1:O:24:ILE:HD11	1:O:124:THR:OG1	1.95	0.65
6:T:184:LEU:HD11	6:T:188:GLU:HB3	1.77	0.65
1:A:69:LEU:HD23	1:A:69:LEU:C	2.22	0.65
7:G:48:VAL:C	7:G:49:ILE:HD12	2.22	0.65
10:J:147:THR:OG1	10:J:150:GLU:HG3	1.96	0.65
12:L:109:ALA:HB2	12:L:121:ARG:NH2	2.11	0.65
14:N:59:VAL:HG22	14:N:82:VAL:HG12	1.77	0.65
14:N:112:THR:CG2	14:N:120:HIS:HB2	2.26	0.65
1:O:60:MET:HE3	1:O:63:THR:HG21	1.79	0.65
4:R:160:TYR:CE2	4:R:163:LYS:HD3	2.32	0.65
7:U:227:GLU:HG2	17:U:1255:HOH:O	1.94	0.65
8:V:148:LYS:O	8:V:152:ILE:HG12	1.97	0.65
12:Z:14(I):THR:O	12:Z:14(K):LYS:HB2	1.97	0.65
1:A:197:LEU:CD2	1:A:210:ILE:HD12	2.27	0.65
5:E:177:GLU:OE1	6:F:56:SER:HB2	1.95	0.65
5:E:207:LEU:HD23	5:E:207:LEU:H	1.61	0.65
7:G:49:ILE:HD12	7:G:49:ILE:N	2.12	0.65
12:L:-9:GLN:HE21	13:M:-8:THR:HG21	1.61	0.65
13:M:35:ILE:HG12	13:M:56:GLU:HG3	1.79	0.65
4:R:67:ILE:HD12	4:R:211:GLN:HE21	1.61	0.65
6:T:173:LYS:O	6:T:177:GLU:HG3	1.97	0.65
6:T:45:GLY:HA3	6:T:215:CYS:O	1.97	0.64
6:F:45:GLY:HA3	6:F:215:CYS:O	1.97	0.64
12:L:14(C):GLN:HG2	8:V:210:THR:HG21	1.79	0.64
13:M:100:ILE:CD1	13:M:112:TYR:HB2	2.27	0.64
4:R:156:THR:HG22	5:S:83:PRO:HD3	1.78	0.64
3:C:172:VAL:HG23	3:C:196:SER:HB2	1.77	0.64
8:H:15:ALA:HB1	8:H:159:ILE:CD1	2.27	0.64
5:S:132:TYR:O	5:S:153:PRO:HB3	1.96	0.64
8:V:15:ALA:HB1	8:V:159:ILE:CD1	2.27	0.64
14:N:163:ILE:HG23	14:N:170:GLY:HA2	1.79	0.64
10:X:64:GLN:HA	17:X:665:HOH:O	1.97	0.64
5:S:141:TYR:CE2	5:S:217:LYS:HA	2.33	0.64
11:Y:142:TYR:O	11:Y:143:LYS:HD2	1.98	0.64
3:C:15:PHE:N	4:D:23:GLN:HE22	1.93	0.64
7:G:186:TRP:O	7:G:190:VAL:HG23	1.98	0.64
14:N:146:MET:HE2	14:N:150:GLU:HB3	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:12:ILE:CG1	7:U:14:ILE:HD12	2.24	0.64
7:G:59:LEU:O	7:G:61:PRO:HD3	1.97	0.64
12:L:-7:ASN:ND2	12:L:-5:TYR:H	1.95	0.64
13:M:104:VAL:HG23	13:M:178:ILE:HG22	1.79	0.64
5:S:111:ARG:HG2	5:S:111:ARG:HH11	1.62	0.64
13:1:35:ILE:HD12	13:1:45:ILE:HD12	1.80	0.64
14:2:17:ASP:CB	14:2:163:ILE:HD11	2.27	0.64
4:D:12(D):ALA:HA	5:E:129:GLY:HA2	1.80	0.64
8:H:41:ILE:HD12	8:H:103:GLY:HA3	1.80	0.64
6:T:74:ILE:HG12	6:T:109:ILE:CD1	2.27	0.64
3:C:14:ILE:HD13	3:C:14:ILE:H	1.63	0.64
10:J:38:SER:HB2	10:J:39:PRO:HD2	1.80	0.64
3:Q:170:LYS:HB2	17:Q:833:HOH:O	1.97	0.64
13:1:148:VAL:HG23	17:1:182:HOH:O	1.98	0.64
2:B:41:MET:HE3	17:B:240:HOH:O	1.97	0.63
11:K:10(A):ARG:HG2	11:K:10(A):ARG:HH11	1.63	0.63
6:T:175:GLU:OE1	6:T:199:LEU:HD23	1.98	0.63
10:X:147:THR:OG1	10:X:150:GLU:HG3	1.98	0.63
12:Z:173:LEU:HB2	12:Z:191:LEU:HD11	1.80	0.63
11:K:142:TYR:O	11:K:143:LYS:HD2	1.97	0.63
10:X:-1:MET:HG2	10:X:1:ASP:N	2.13	0.63
4:D:17:PRO:HD2	17:D:1171:HOH:O	1.99	0.63
5:E:104:ASN:HB2	13:M:81:GLU:HG2	1.79	0.63
10:X:38:SER:HB2	10:X:39:PRO:HD2	1.80	0.63
11:Y:66:HIS:HA	17:Y:1210:HOH:O	1.97	0.63
9:I:1:GLY:HA3	9:I:33:LYS:HE2	1.79	0.63
10:X:133:TYR:CE2	10:X:166:MET:HG3	2.34	0.63
3:C:33:ARG:CB	3:C:33:ARG:HH11	2.12	0.63
3:C:160:TRP:CE2	4:D:59:LEU:HD23	2.34	0.63
8:H:3:ILE:HD11	8:H:127:LEU:HB2	1.80	0.63
10:J:32:ASP:OD2	10:J:34:THR:HG22	1.99	0.63
9:W:6:MET:HE1	9:W:155:ILE:HA	1.80	0.63
4:D:24:VAL:O	4:D:27:SER:HB3	1.99	0.63
4:D:102:TYR:O	12:L:81:ARG:HG3	1.99	0.63
2:P:21:LEU:HD13	2:P:124:THR:HG23	1.80	0.63
3:Q:33:ARG:CB	3:Q:33:ARG:HH11	2.12	0.63
7:U:186:TRP:O	7:U:190:VAL:HG23	1.98	0.63
2:B:21:LEU:HD13	2:B:124:THR:HG23	1.79	0.63
7:G:8:TYR:C	7:G:10:ARG:H	2.06	0.63
8:V:81:GLN:O	8:V:85:GLN:HG3	1.99	0.63
5:E:18(D):ILE:O	5:E:18(D):ILE:HD13	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:213:ALA:HB2	5:E:223:ILE:CD1	2.29	0.63
11:K:143:LYS:HA	17:K:1394:HOH:O	1.98	0.63
12:Z:-6:PRO:O	13:1:91:ARG:NH1	2.28	0.63
14:2:18(A):ILE:HD12	14:2:18(C):TYR:CZ	2.34	0.63
5:E:141:TYR:CE2	5:E:217:LYS:HA	2.34	0.62
3:Q:163:GLN:HE22	3:Q:173:ARG:HE	1.46	0.62
3:Q:168:ASN:HB2	3:Q:200:VAL:HG11	1.80	0.62
6:T:179:LEU:HD11	6:T:192:GLN:HG3	1.81	0.62
14:2:163:ILE:CD1	14:2:169:SER:HB3	2.29	0.62
5:E:213:ALA:CB	5:E:223:ILE:CD1	2.77	0.62
6:F:38:ILE:HG22	6:F:164:ALA:CB	2.30	0.62
6:F:179:LEU:HD11	6:F:192:GLN:HG3	1.81	0.62
6:F:187:ARG:HG3	6:F:187:ARG:HH11	1.64	0.62
12:L:3:ILE:CD1	12:L:46:ASN:HB2	2.29	0.62
13:M:74:LEU:HD13	13:M:79:ILE:HD11	1.81	0.62
1:O:69:LEU:C	1:O:69:LEU:HD23	2.24	0.62
5:S:67:ILE:HD13	5:S:77:SER:HB3	1.81	0.62
4:D:160:TYR:CE2	4:D:163:LYS:HD3	2.34	0.62
9:I:33:LYS:O	9:I:44:GLY:HA2	2.00	0.62
3:Q:15:PHE:N	4:R:23:GLN:HE22	1.92	0.62
7:U:236:ILE:HG13	7:U:237:ALA:N	2.14	0.62
14:2:163:ILE:HG23	14:2:170:GLY:HA2	1.80	0.62
9:W:43:LEU:CD2	9:W:45:ILE:HD11	2.30	0.62
1:O:21(I):TYR:HE2	1:O:21(L):ILE:HD13	1.64	0.62
5:S:177:GLU:OE1	6:T:56:SER:HB2	2.00	0.62
12:Z:93:PHE:N	12:Z:94:PRO:HD3	2.14	0.62
1:A:197:LEU:HD23	1:A:210:ILE:HD12	1.82	0.62
6:F:192:GLN:NE2	6:F:195:LYS:HE3	2.15	0.62
3:Q:186:VAL:HG21	3:Q:216:LYS:HE2	1.81	0.62
11:Y:35:ILE:HD11	11:Y:45:MET:CE	2.29	0.62
1:A:60:MET:HE3	1:A:63:THR:HG21	1.82	0.62
9:I:159:LEU:HD21	9:I:173:ALA:HB1	1.80	0.62
9:I:177:ILE:HD12	9:I:187:ARG:NH1	2.06	0.62
12:L:3:ILE:HD13	12:L:3:ILE:N	2.14	0.62
12:L:14(I):THR:O	12:L:14(K):LYS:HB2	1.99	0.62
6:T:95:GLU:CG	6:T:115:ARG:HB3	2.30	0.62
12:Z:-9:GLN:HE21	13:1:-8:THR:HG21	1.63	0.62
3:C:186:VAL:HG21	3:C:216:LYS:HE2	1.81	0.62
6:F:82:ILE:HB	6:F:83:PRO:HD3	1.80	0.62
9:I:66:TYR:CZ	9:I:70:GLU:HG3	2.35	0.62
3:Q:15:PHE:CE1	3:Q:21:ILE:HD11	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:10(A):ARG:HG2	11:Y:10(A):ARG:HH11	1.64	0.62
2:B:219:GLU:HG2	2:B:21(E):VAL:H	1.63	0.62
5:E:194:VAL:O	5:E:197:ILE:HG22	2.00	0.62
7:G:77:VAL:CG1	7:G:137:THR:HB	2.30	0.62
9:I:114:ASP:HB2	17:I:851:HOH:O	1.99	0.62
5:S:207:LEU:HA	5:S:2(E):ASN:HD22	1.64	0.62
12:Z:109:ALA:HA	17:Z:375:HOH:O	2.00	0.62
14:2:175:MET:HE3	14:2:18(B):PHE:CE2	2.34	0.62
11:K:172:SER:HA	11:K:192:VAL:HG23	1.82	0.62
2:P:101:LYS:HZ2	10:X:85:GLN:NE2	1.97	0.62
3:Q:37:ALA:HB3	3:Q:165:ILE:CD1	2.29	0.62
6:T:38:ILE:HG22	6:T:164:ALA:CB	2.29	0.62
6:T:192:GLN:NE2	6:T:195:LYS:HE3	2.15	0.62
8:H:81:GLN:O	8:H:85:GLN:HG3	2.00	0.61
2:P:190:ILE:HG22	2:P:232:ILE:HD11	1.82	0.61
11:Y:172:SER:HA	11:Y:192:VAL:HG23	1.82	0.61
4:D:194:LEU:HD22	4:D:212:LEU:HD11	1.82	0.61
7:G:123:TYR:CE1	7:G:129:MET:HE3	2.36	0.61
1:O:86:ARG:HE	7:U:118:ASN:HD21	1.48	0.61
6:T:175:GLU:HB3	6:T:196:ILE:CD1	2.30	0.61
7:U:70:ILE:HD12	7:U:74:ILE:HG22	1.81	0.61
16:Y:2(I):H10:H22A	12:Z:125:ARG:NH2	2.15	0.61
12:Z:148:VAL:O	12:Z:152:ILE:HG12	1.98	0.61
4:D:67:ILE:HD12	4:D:211:GLN:HE21	1.65	0.61
7:G:225:SER:O	7:G:229:ILE:HG12	2.00	0.61
16:K:2(I):H10:H22A	12:L:125:ARG:NH2	2.15	0.61
7:U:35:ILE:HD11	7:U:53:LYS:HG3	1.82	0.61
7:U:77:VAL:HG12	7:U:137:THR:HB	1.82	0.61
12:L:14(C):GLN:HG2	8:V:210:THR:CG2	2.30	0.61
2:P:143:ASP:OD2	10:X:10(B):LYS:HE2	2.01	0.61
2:P:219:GLU:HG2	2:P:21(E):VAL:H	1.65	0.61
9:W:4:VAL:CG1	9:W:155:ILE:HD11	2.30	0.61
9:W:66:TYR:CZ	9:W:70:GLU:HG3	2.34	0.61
5:E:132:TYR:O	5:E:153:PRO:HB3	1.99	0.61
10:J:112:GLN:NE2	10:J:126:ALA:H	1.99	0.61
14:N:30:VAL:CG2	13:1:203:ILE:HD13	2.31	0.61
4:R:102:TYR:O	12:Z:81:ARG:HG3	1.99	0.61
9:W:159:LEU:HD21	9:W:173:ALA:HB1	1.81	0.61
12:Z:8:GLY:HA3	12:Z:11:PHE:CE2	2.35	0.61
14:N:6:VAL:CG2	14:N:155:ILE:HD11	2.30	0.61
14:N:155:ILE:HG22	14:N:175:MET:HE2	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:90:ARG:HA	9:W:90:ARG:HH11	1.65	0.61
11:K:133:PHE:HA	17:X:203:HOH:O	2.01	0.61
4:R:12(G):GLU:HG2	4:R:125:GLU:H	1.66	0.61
7:U:35:ILE:CD1	7:U:53:LYS:HG3	2.29	0.61
1:A:32:LYS:HG2	17:A:354:HOH:O	2.00	0.61
1:A:85:TYR:O	1:A:89:VAL:HG23	2.01	0.61
10:J:133:TYR:CE2	10:J:166:MET:HG3	2.35	0.61
9:W:33:LYS:O	9:W:44:GLY:HA2	2.01	0.61
11:Y:199:VAL:O	11:Y:203:GLU:HB3	2.00	0.61
1:A:10(A):ILE:N	1:A:10(A):ILE:HD12	2.16	0.61
7:G:18(G):GLU:HG2	7:G:188:LYS:CB	2.31	0.61
8:H:77:VAL:HG22	17:H:258:HOH:O	2.01	0.61
10:J:133:TYR:OH	10:X:24:ILE:HG12	2.00	0.61
3:Q:186:VAL:O	3:Q:190:VAL:HG23	2.01	0.61
11:Y:6:PHE:HB2	11:Y:124:ILE:CD1	2.25	0.61
1:A:233:LEU:O	1:A:236:LEU:HB2	2.00	0.60
12:Z:-7:ASN:C	12:Z:-7:ASN:HD22	2.07	0.60
3:C:163:GLN:HE22	3:C:173:ARG:HE	1.47	0.60
9:I:90:ARG:HA	9:I:90:ARG:HH11	1.65	0.60
6:T:187:ARG:HH11	6:T:187:ARG:HG3	1.65	0.60
13:M:200:ALA:HA	13:M:203:ILE:HD12	1.83	0.60
1:O:233:LEU:O	1:O:236:LEU:HB2	2.00	0.60
5:S:213:ALA:CB	5:S:223:ILE:CD1	2.78	0.60
7:U:18(G):GLU:HG2	7:U:188:LYS:CB	2.31	0.60
8:V:37:ILE:HD11	8:V:43:CYS:HB2	1.82	0.60
1:A:21(G):LEU:HD13	1:A:218:GLY:HA2	1.82	0.60
3:C:168:ASN:HB2	3:C:200:VAL:HG11	1.81	0.60
3:C:186:VAL:O	3:C:190:VAL:HG23	2.01	0.60
8:H:148:LYS:O	8:H:152:ILE:HG12	2.01	0.60
3:Q:33:ARG:HB2	3:Q:33:ARG:NH1	2.16	0.60
3:Q:160:TRP:CE2	4:R:59:LEU:HD23	2.36	0.60
5:S:2(B):THR:N	5:S:2(E):ASN:HD22	1.99	0.60
6:T:101:LYS:HE2	13:1:57:ARG:HH22	1.66	0.60
7:G:47:VAL:HG12	7:G:49:ILE:CD1	2.31	0.60
11:Y:6:PHE:CB	11:Y:124:ILE:HD13	2.28	0.60
12:Z:109:ALA:HB2	12:Z:121:ARG:NH2	2.15	0.60
6:F:101:LYS:HE2	13:M:57:ARG:HH22	1.66	0.60
6:F:137:ILE:CD1	6:F:150:MET:HB2	2.31	0.60
8:V:15:ALA:HB1	8:V:159:ILE:HD11	1.78	0.60
10:X:112:GLN:NE2	10:X:126:ALA:H	2.00	0.60
14:N:83:PHE:CE1	14:N:99:ILE:HD13	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:21(I):TYR:CE2	1:O:21(L):ILE:HD13	2.37	0.60
4:D:177:LEU:HD13	5:E:58:LEU:HD11	1.83	0.60
6:F:175:GLU:OE1	6:F:199:LEU:HD23	2.01	0.60
9:I:29:ASN:ND2	9:I:30:LYS:HG3	2.16	0.60
10:J:52:THR:CG2	10:J:53:VAL:N	2.64	0.60
4:R:186:LEU:O	4:R:190:GLU:HG3	2.01	0.60
4:R:194:LEU:HD22	4:R:212:LEU:HD11	1.83	0.60
8:V:163:ILE:HG23	8:V:170:GLY:HA2	1.84	0.60
6:F:101:LYS:HE2	13:M:57:ARG:NH2	2.17	0.60
6:F:229:LEU:HG	6:F:233:ILE:HD11	1.84	0.60
7:G:35:ILE:HD11	7:G:53:LYS:HG3	1.83	0.60
14:2:126:ILE:HD13	14:2:126:ILE:N	2.17	0.60
4:D:12:VAL:CG2	4:D:12(A):GLY:HA2	2.32	0.60
7:G:35:ILE:CD1	7:G:53:LYS:HG3	2.32	0.60
9:I:6:MET:CE	9:I:155:ILE:HA	2.31	0.60
4:R:177:LEU:HD13	5:S:58:LEU:HD11	1.84	0.60
7:U:70:ILE:CD1	7:U:76:MET:HB2	2.30	0.60
7:U:123:TYR:CE1	7:U:129:MET:HE3	2.37	0.60
10:X:37:LEU:HB3	10:X:63:ILE:CD1	2.28	0.60
13:1:41:THR:OG1	13:1:76:PRO:HG3	2.02	0.60
3:C:136:THR:O	3:C:150:GLN:HA	2.02	0.59
9:I:48:LEU:HG	9:I:50:THR:HG22	1.84	0.59
13:M:203:ILE:HD13	14:2:30:VAL:CG2	2.31	0.59
6:F:137:ILE:HD12	6:F:163:ALA:HB3	1.83	0.59
6:F:137:ILE:HD11	6:F:163:ALA:HB1	1.84	0.59
3:Q:235:GLN:O	3:Q:239:GLU:HG2	2.02	0.59
7:U:86:ARG:HD2	17:U:249:HOH:O	2.01	0.59
8:V:100:ILE:HD13	8:V:112:SER:HB3	1.84	0.59
2:B:190:ILE:HG22	2:B:232:ILE:HD11	1.83	0.59
4:R:81:LEU:HB3	17:R:599:HOH:O	2.02	0.59
5:S:194:VAL:O	5:S:197:ILE:HG22	2.01	0.59
13:1:177:ILE:C	13:1:178:ILE:HD12	2.27	0.59
3:C:33:ARG:NH1	3:C:33:ARG:HB2	2.17	0.59
3:C:46:VAL:O	3:C:215:VAL:HG12	2.02	0.59
5:E:82:ALA:HB3	5:E:83:PRO:HD3	1.84	0.59
7:G:172:ILE:HD11	7:G:201:LEU:HD21	1.84	0.59
9:I:3:ILE:HD12	9:I:48:LEU:HD13	1.85	0.59
9:I:35:PHE:HE1	9:I:45:ILE:HD13	1.66	0.59
5:S:213:ALA:HB2	5:S:223:ILE:CD1	2.30	0.59
7:U:8:TYR:C	7:U:10:ARG:H	2.09	0.59
10:X:52:THR:CG2	10:X:53:VAL:N	2.65	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:86:LEU:O	11:Y:89:GLN:HB2	2.03	0.59
7:G:43:LYS:HB2	7:G:18(G):GLU:O	2.02	0.59
14:N:13:ILE:CD1	14:N:177:VAL:HG13	2.32	0.59
3:Q:46:VAL:O	3:Q:215:VAL:HG12	2.02	0.59
4:R:28:LEU:HA	4:R:31:ILE:CD1	2.32	0.59
6:T:101:LYS:HE2	13:1:57:ARG:NH2	2.17	0.59
9:W:43:LEU:HD21	9:W:45:ILE:HD11	1.85	0.59
9:W:48:LEU:HG	9:W:50:THR:HG22	1.85	0.59
10:X:90(B):ARG:NH1	17:X:266:HOH:O	2.34	0.59
6:F:69:VAL:HG12	17:F:319:HOH:O	2.01	0.59
3:Q:136:THR:O	3:Q:150:GLN:HA	2.03	0.59
8:V:155:ALA:O	8:V:159:ILE:HD12	2.02	0.59
10:X:140:HIS:HD2	10:X:141:HIS:CE1	2.20	0.59
14:N:175:MET:HE3	14:N:18(B):PHE:CE2	2.37	0.59
5:S:82:ALA:HB3	5:S:83:PRO:HD3	1.84	0.59
7:U:77:VAL:CG1	7:U:137:THR:HB	2.33	0.59
14:2:10(B):LYS:HD3	14:2:10(B):LYS:C	2.28	0.59
3:C:235:GLN:O	3:C:239:GLU:HG2	2.03	0.59
8:H:113:ILE:HG13	8:H:119:THR:HG22	1.83	0.59
5:S:46:ALA:HB1	5:S:139:ILE:HB	1.85	0.59
8:V:219:VAL:O	8:V:221:ILE:HD12	2.02	0.59
3:C:57:LYS:O	3:C:58:LEU:HB2	2.03	0.59
3:C:163:GLN:HE21	3:C:164:THR:H	1.51	0.59
10:J:143:ARG:O	10:J:146:MET:HG3	2.03	0.59
12:L:8:GLY:HA3	12:L:11:PHE:CE2	2.37	0.59
14:N:42:TRP:HZ2	13:1:211:ILE:HD11	1.68	0.59
4:R:12(D):ALA:HB3	4:R:126:ARG:HD3	1.85	0.59
7:U:168:LYS:O	7:U:172:ILE:HG12	2.02	0.59
9:W:2:ILE:HG21	9:W:130:ALA:HB3	1.85	0.59
14:2:161:GLN:HE22	14:2:165:TRP:HE1	1.50	0.59
6:F:175:GLU:HB3	6:F:196:ILE:CD1	2.31	0.59
7:G:76:MET:HE3	7:G:78:VAL:CG2	2.33	0.59
14:N:10(B):LYS:C	14:N:10(B):LYS:HD3	2.28	0.59
2:P:74:ILE:HD12	2:P:109:VAL:HG13	1.85	0.59
4:R:53:ARG:O	4:R:53:ARG:HG2	2.03	0.59
8:V:2:THR:OG1	8:V:130:GLY:HA3	2.03	0.59
11:Y:7:ARG:HD2	11:Y:108:PRO:O	2.01	0.59
2:B:38:ILE:HD12	2:B:197:LEU:HG	1.85	0.58
8:H:173:VAL:HB	8:H:192:LEU:HB2	1.84	0.58
9:I:104:ILE:HD12	9:I:181:LYS:N	2.18	0.58
11:K:76:VAL:N	11:K:106:GLU:OE2	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:6:MET:CE	9:W:155:ILE:HA	2.33	0.58
10:X:113:ILE:HG12	10:X:119:LYS:HG3	1.85	0.58
4:D:12(F):GLY:HA3	17:D:965:HOH:O	2.03	0.58
13:1:175:LEU:HD23	13:1:176:ALA:N	2.18	0.58
4:D:12(G):GLU:HG2	4:D:125:GLU:H	1.66	0.58
12:L:93:PHE:N	12:L:94:PRO:HD3	2.18	0.58
4:R:177:LEU:HD22	5:S:58:LEU:HD13	1.85	0.58
5:S:207:LEU:H	5:S:207:LEU:CD2	2.16	0.58
7:U:43:LYS:HB2	7:U:18(G):GLU:O	2.04	0.58
8:V:40:LYS:O	8:V:41:ILE:HD13	2.03	0.58
8:V:221:ILE:HD11	9:W:184:VAL:CB	2.32	0.58
9:W:29:ASN:ND2	9:W:30:LYS:HG3	2.18	0.58
11:K:7:ARG:HD2	11:K:108:PRO:O	2.03	0.58
12:L:-6:PRO:O	13:M:91:ARG:NH1	2.34	0.58
2:P:235:LYS:C	2:P:237:GLY:H	2.11	0.58
7:U:87:ASN:C	7:U:87:ASN:ND2	2.60	0.58
10:X:34:THR:HG21	10:X:176:LYS:NZ	2.19	0.58
12:Z:32:PRO:HD2	17:Z:1177:HOH:O	2.04	0.58
5:E:167:ALA:HB3	17:E:1131:HOH:O	2.03	0.58
4:R:207:LEU:HD23	4:R:207:LEU:C	2.29	0.58
4:D:186:LEU:O	4:D:190:GLU:HG3	2.03	0.58
4:R:162:ALA:HB3	5:S:58:LEU:HD23	1.86	0.58
6:T:197:ILE:HD13	6:T:210:LEU:CD1	2.29	0.58
7:U:172:ILE:HD11	7:U:201:LEU:HD21	1.84	0.58
8:V:173:VAL:HB	8:V:192:LEU:HB2	1.85	0.58
9:W:97:VAL:HG23	9:W:99:PRO:HD3	1.86	0.58
11:Y:146:LEU:HD23	11:Y:151:ALA:HA	1.85	0.58
2:B:141:TYR:CD1	2:B:21(E):VAL:HG21	2.38	0.58
2:B:185:LYS:HD3	2:B:186:VAL:N	2.19	0.58
6:F:195:LYS:HZ2	6:F:196:ILE:HD13	1.68	0.58
13:M:146:THR:HA	17:M:1069:HOH:O	2.04	0.58
14:N:161:GLN:HE22	14:N:165:TRP:HE1	1.52	0.58
1:O:21(G):LEU:HD13	1:O:218:GLY:HA2	1.84	0.58
2:P:38:ILE:HD12	2:P:197:LEU:HG	1.86	0.58
2:P:74:ILE:HD13	2:P:140:GLY:CA	2.21	0.58
2:P:95:HIS:HB2	17:P:249:HOH:O	2.01	0.58
13:1:205:GLY:HA3	13:1:209:GLN:HB3	1.85	0.58
3:C:122:ARG:NH2	17:C:806:HOH:O	2.36	0.58
8:H:210:THR:HG21	12:Z:14(C):GLN:HG2	1.86	0.58
13:M:205:GLY:HA3	13:M:209:GLN:HB3	1.86	0.58
5:S:148:LEU:CD2	5:S:162:GLY:HA2	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:68:ILE:CD1	5:E:78:LEU:HD23	2.34	0.58
8:H:172:ASN:ND2	8:H:193:THR:HG22	2.19	0.58
8:V:40:LYS:C	8:V:41:ILE:HD13	2.29	0.58
12:Z:105:ASP:OD2	12:Z:107:LYS:HB2	2.04	0.58
13:1:19:LEU:HD21	13:1:26:LEU:HD22	1.86	0.58
4:D:12(D):ALA:HB3	4:D:126:ARG:HD3	1.85	0.57
6:F:72:ARG:HD2	13:M:64:THR:OG1	2.02	0.57
7:G:105:TYR:OH	8:H:66:HIS:HE1	1.86	0.57
8:H:219:VAL:O	8:H:221:ILE:HD12	2.04	0.57
9:I:2:ILE:HG21	9:I:130:ALA:HB3	1.84	0.57
9:I:97:VAL:HG23	9:I:99:PRO:HD3	1.85	0.57
11:K:199:VAL:O	11:K:203:GLU:HB3	2.03	0.57
12:L:105:ASP:OD2	12:L:107:LYS:HB2	2.04	0.57
2:P:141:TYR:CD1	2:P:21(E):VAL:HG21	2.39	0.57
2:P:185:LYS:HD3	2:P:186:VAL:N	2.19	0.57
3:Q:215:VAL:HG23	3:Q:221:ILE:HG13	1.86	0.57
14:2:14:LEU:O	14:2:175:MET:HA	2.04	0.57
4:D:70:ILE:CD1	4:D:89:ILE:HG23	2.34	0.57
12:L:-7:ASN:HD22	12:L:-6:PRO:HD2	1.69	0.57
13:M:40:ASN:N	13:M:40:ASN:ND2	2.46	0.57
6:F:49:ALA:CB	6:F:212:ILE:HD12	2.34	0.57
8:H:40:LYS:C	8:H:41:ILE:HD13	2.29	0.57
11:K:99:THR:HG22	11:K:113:VAL:O	2.04	0.57
14:N:14:LEU:O	14:N:175:MET:HA	2.03	0.57
11:Y:86:LEU:C	11:Y:86:LEU:HD13	2.29	0.57
5:E:213:ALA:CB	5:E:223:ILE:HD12	2.34	0.57
6:F:229:LEU:HG	6:F:233:ILE:CD1	2.33	0.57
8:H:147:THR:HG23	8:H:150:GLU:OE1	2.05	0.57
11:K:25:TRP:CH2	12:L:132:SER:HA	2.40	0.57
8:V:18:THR:HG21	8:V:172:ASN:HB2	1.86	0.57
13:1:157:ASN:HB3	17:1:558:HOH:O	2.03	0.57
14:2:155:ILE:HG22	14:2:175:MET:HE2	1.86	0.57
2:B:235:LYS:C	2:B:237:GLY:H	2.12	0.57
3:C:241:GLN:C	3:C:243:GLN:H	2.12	0.57
9:I:28:SER:HB2	10:J:120:VAL:HG21	1.87	0.57
10:J:77:GLN:NE2	10:J:77:GLN:C	2.61	0.57
11:K:146:LEU:HD23	11:K:151:ALA:HA	1.87	0.57
13:M:179:ASP:HB3	13:M:18(A):THR:OG1	2.05	0.57
1:O:15:PHE:H	2:P:23:GLN:NE2	1.92	0.57
1:O:62:GLU:C	1:O:64:LEU:H	2.12	0.57
1:O:212:LEU:HD23	1:O:213:ALA:N	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1:14(D):GLU:O	13:1:14(G):ILE:HG13	2.05	0.57
5:E:46:ALA:HB1	5:E:139:ILE:HB	1.86	0.57
5:E:207:LEU:HA	5:E:2(E):ASN:HD22	1.65	0.57
5:E:207:LEU:H	5:E:207:LEU:CD2	2.17	0.57
6:F:95:GLU:CG	6:F:115:ARG:HB3	2.32	0.57
6:F:203:GLU:OE1	6:F:203:GLU:HA	2.03	0.57
3:Q:15:PHE:H	4:R:23:GLN:NE2	1.95	0.57
4:R:215:ILE:HD13	4:R:215:ILE:C	2.30	0.57
7:G:236:ILE:HD12	7:G:237:ALA:N	2.19	0.57
13:M:1:THR:HA	17:M:849:HOH:O	2.05	0.57
9:W:74:ILE:HB	17:W:517:HOH:O	2.04	0.57
3:C:106:PRO:HG2	3:C:143:PRO:CG	2.34	0.57
3:C:206:GLY:HA3	3:C:209:ASN:HB2	1.86	0.57
6:F:192:GLN:HE21	6:F:195:LYS:HE3	1.70	0.57
10:J:113:ILE:HG12	10:J:119:LYS:HG3	1.87	0.57
13:M:12:VAL:HG21	13:M:102:ALA:HB1	1.86	0.57
13:M:14(G):ILE:N	13:M:144:PRO:HD2	2.20	0.57
1:O:49:ALA:HB2	1:O:212:LEU:HG	1.86	0.57
3:Q:52:ARG:NH2	3:Q:211:GLU:HB3	2.20	0.57
3:Q:241:GLN:C	3:Q:243:GLN:H	2.13	0.57
6:T:186:ALA:O	6:T:190:VAL:HG23	2.04	0.57
7:U:96:ALA:CA	7:U:107:MET:HE2	2.27	0.57
8:V:172:ASN:ND2	8:V:193:THR:HG22	2.20	0.57
8:H:155:ALA:O	8:H:159:ILE:HD12	2.04	0.57
9:I:152:PHE:HB2	9:I:177:ILE:CD1	2.31	0.57
13:M:100:ILE:HD11	13:M:112:TYR:HD1	1.70	0.57
13:M:211:ILE:HD11	14:2:42:TRP:HZ2	1.69	0.57
1:O:85:TYR:O	1:O:89:VAL:HG23	2.05	0.57
8:V:159:ILE:HD13	8:V:173:VAL:HG13	1.85	0.57
12:Z:-7:ASN:HD22	12:Z:-6:PRO:HD2	1.70	0.57
12:Z:163:THR:HB	17:Z:200:HOH:O	2.04	0.57
13:1:200:ALA:HA	13:1:203:ILE:HD12	1.86	0.57
10:J:185:ARG:HG2	10:J:185:ARG:HH11	1.69	0.57
12:L:-2:ASN:HA	12:L:21:ILE:O	2.05	0.57
2:P:113:VAL:HG22	2:P:138:TYR:CD2	2.40	0.57
10:X:143:ARG:O	10:X:146:MET:HG3	2.04	0.57
2:B:163:ILE:HG12	2:B:164:SER:N	2.20	0.56
8:H:163:ILE:HG23	8:H:170:GLY:HA2	1.87	0.56
6:F:38:ILE:HG12	6:F:197:ILE:HD11	1.86	0.56
7:G:56:ASP:HB3	7:G:59:LEU:HG	1.87	0.56
7:G:158:VAL:HG22	7:G:159:GLY:N	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:76:PRO:HD2	17:J:296:HOH:O	2.06	0.56
12:L:-7:ASN:HD22	12:L:-7:ASN:C	2.12	0.56
1:O:86:ARG:HE	7:U:118:ASN:ND2	2.03	0.56
14:2:13:ILE:HG13	14:2:151:THR:HG21	1.86	0.56
1:A:62:GLU:C	1:A:64:LEU:H	2.14	0.56
1:A:212:LEU:HD23	1:A:213:ALA:N	2.20	0.56
2:B:8:TYR:CD2	7:G:12:ILE:HD12	2.40	0.56
2:B:27:ALA:O	2:B:31:ILE:HG12	2.05	0.56
5:E:28:LEU:CA	5:E:31:ILE:HD13	2.33	0.56
6:F:87:HIS:HD2	6:F:132:PHE:HE2	1.53	0.56
6:F:137:ILE:HD13	6:F:150:MET:HB2	1.88	0.56
6:F:216:SER:HB3	6:F:21(A):GLU:HB2	1.87	0.56
7:G:96:ALA:CA	7:G:107:MET:HE2	2.27	0.56
9:I:137:MET:HE3	9:I:141:LEU:HD11	1.86	0.56
10:J:140:HIS:HD2	10:J:141:HIS:CE1	2.22	0.56
7:U:9:ASP:HA	7:U:14:ILE:CD1	2.18	0.56
7:U:158:VAL:HG22	7:U:159:GLY:N	2.20	0.56
7:U:192:PHE:C	7:U:192:PHE:CD1	2.83	0.56
2:B:71:ASN:ND2	2:B:72:ASP:H	2.04	0.56
3:C:52:ARG:NH2	3:C:211:GLU:HB3	2.20	0.56
12:L:4:LEU:HD11	12:L:138:LEU:HD21	1.85	0.56
13:M:17:ASP:HA	13:M:173:PHE:CB	2.35	0.56
3:Q:206:GLY:HA3	3:Q:209:ASN:HB2	1.88	0.56
12:Z:4:LEU:HD11	12:Z:138:LEU:HD21	1.88	0.56
4:D:117:CYS:HB3	4:D:155:GLY:O	2.05	0.56
4:D:215:ILE:C	4:D:215:ILE:HD13	2.30	0.56
5:E:4:PHE:CE1	5:E:17:PRO:HD2	2.41	0.56
7:G:116:MET:HE3	17:G:551:HOH:O	2.05	0.56
9:I:104:ILE:HD12	9:I:179:LYS:C	2.30	0.56
3:Q:156:ILE:N	3:Q:156:ILE:CD1	2.68	0.56
4:R:12:VAL:CG2	4:R:12(A):GLY:HA2	2.35	0.56
6:T:121:GLN:NE2	17:T:385:HOH:O	2.38	0.56
7:U:76:MET:HE3	7:U:78:VAL:CG2	2.36	0.56
14:2:163:ILE:HD12	14:2:170:GLY:N	2.20	0.56
7:G:136:LEU:O	7:G:150:LYS:HA	2.05	0.56
4:R:75:GLY:HA3	4:R:221:PHE:CD2	2.41	0.56
4:R:117:CYS:HB3	4:R:155:GLY:O	2.05	0.56
5:S:190:ILE:O	5:S:194:VAL:HG23	2.06	0.56
5:S:207:LEU:HD23	5:S:207:LEU:N	2.20	0.56
11:Y:99:THR:HG22	11:Y:113:VAL:O	2.05	0.56
4:D:207:LEU:C	4:D:207:LEU:HD23	2.31	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:49:VAL:HG13	5:E:212:ILE:HD13	1.83	0.56
7:G:108:PRO:HB3	8:H:72:ARG:NH2	2.20	0.56
8:H:2:THR:OG1	8:H:130:GLY:HA3	2.06	0.56
9:I:113:PHE:HA	9:I:118:CYS:O	2.06	0.56
12:L:3:ILE:CD1	12:L:46:ASN:CB	2.83	0.56
2:P:107:ILE:HG22	17:P:410:HOH:O	2.06	0.56
5:S:67:ILE:HG21	5:S:223:ILE:CD1	2.36	0.56
6:T:216:SER:HB3	6:T:21(A):GLU:HB2	1.88	0.56
5:E:49:VAL:HG22	5:E:212:ILE:HD12	1.87	0.56
7:G:168:LYS:O	7:G:172:ILE:HG12	2.06	0.56
10:J:52:THR:HG23	10:J:53:VAL:N	2.21	0.56
2:P:4:GLY:HA3	5:S:127:TYR:CE1	2.40	0.56
4:R:39:GLY:O	4:R:40:ILE:HD13	2.06	0.56
12:Z:-7:ASN:HD22	12:Z:-6:PRO:CD	2.18	0.56
1:A:21:LEU:CB	1:A:24:ILE:HD13	2.26	0.56
3:C:70:ILE:CD1	3:C:112:LEU:HD11	2.30	0.56
5:E:2(B):THR:N	5:E:2(E):ASN:HD22	1.99	0.56
7:G:74:ILE:HG21	7:G:112:LEU:HD23	1.88	0.56
8:H:165:ASN:HD22	13:1:139:ARG:HH11	1.53	0.56
8:H:200:LYS:HE3	9:I:140:SER:O	2.06	0.56
13:M:41:THR:OG1	13:M:76:PRO:HG3	2.06	0.56
2:P:163:ILE:HG12	2:P:164:SER:N	2.20	0.56
3:Q:156:ILE:HD12	4:R:83:ALA:CB	2.36	0.56
5:E:58:LEU:HD12	5:E:58:LEU:N	2.21	0.56
6:F:186:ALA:O	6:F:190:VAL:HG23	2.06	0.56
8:V:22:GLN:HG3	8:V:27:ALA:HB2	1.88	0.56
9:W:87:LEU:HD11	9:W:99:PRO:HG2	1.88	0.56
4:D:28:LEU:HA	4:D:31:ILE:CD1	2.32	0.55
5:E:190:ILE:O	5:E:194:VAL:HG23	2.05	0.55
10:J:34:THR:HG21	10:J:176:LYS:NZ	2.22	0.55
11:K:12:ILE:CG2	11:K:110:ILE:HD11	2.34	0.55
12:L:90:LYS:HE3	12:L:93:PHE:O	2.06	0.55
14:N:13:ILE:HG13	14:N:151:THR:HG21	1.87	0.55
7:U:140:SER:HA	7:U:215:ALA:HB1	1.88	0.55
9:W:113:PHE:HA	9:W:118:CYS:O	2.06	0.55
11:Y:12:ILE:HB	11:Y:178:VAL:HB	1.89	0.55
3:C:97:GLN:NE2	3:C:97:GLN:HA	2.21	0.55
6:F:210:LEU:HD11	6:F:212:ILE:HD11	1.88	0.55
8:H:18:THR:HG21	8:H:172:ASN:HB2	1.88	0.55
10:J:111:TYR:CE1	10:J:121:GLU:HG3	2.41	0.55
12:L:164:GLU:CD	8:V:197:ARG:HG3	2.31	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:28:SER:HB2	10:X:120:VAL:HG21	1.88	0.55
12:L:99:THR:C	12:L:100:ILE:HD12	2.30	0.55
14:N:51:ASP:O	14:N:55:ILE:HG12	2.07	0.55
11:Y:12:ILE:HD12	11:Y:110:ILE:HD11	1.89	0.55
12:Z:14:LEU:HD13	12:Z:34:VAL:HG13	1.87	0.55
14:2:13:ILE:CD1	14:2:177:VAL:HG13	2.36	0.55
2:B:113:VAL:HG22	2:B:138:TYR:CD2	2.41	0.55
4:D:75:GLY:HA3	4:D:221:PHE:CD2	2.41	0.55
7:G:233:LEU:O	7:G:236:ILE:HG13	2.06	0.55
2:P:100:LEU:HG	9:W:60:ARG:NH2	2.22	0.55
12:Z:145:TYR:CD1	12:Z:146:LEU:N	2.75	0.55
14:2:37:VAL:CG2	14:2:41:ILE:HG22	2.36	0.55
8:H:18:THR:HB	8:H:30:ASN:HD22	1.72	0.55
11:K:102:CYS:CB	11:K:110:ILE:HD12	2.37	0.55
2:P:194:LEU:HD11	2:P:232:ILE:CD1	2.35	0.55
5:S:92:LEU:HD11	5:S:112:ALA:HB1	1.88	0.55
6:T:203:GLU:HA	6:T:203:GLU:OE1	2.05	0.55
7:U:49:ILE:HD13	7:U:212:VAL:HG22	1.89	0.55
7:G:49:ILE:HD13	7:G:193:ALA:HB1	1.89	0.55
4:R:65:GLU:HA	17:R:750:HOH:O	2.06	0.55
12:Z:173:LEU:HG	12:Z:175:ILE:HD11	1.88	0.55
14:2:13:ILE:HD13	14:2:177:VAL:HG22	1.88	0.55
1:A:86:ARG:HE	7:G:118:ASN:HD21	1.53	0.55
2:B:152:ASN:HB2	2:B:153:PRO:HD2	1.88	0.55
3:C:29:GLU:OE2	3:C:32:LYS:HE2	2.07	0.55
4:D:112:LEU:C	4:D:112:LEU:HD13	2.31	0.55
7:G:177:GLU:O	7:G:17(B):LYS:HG3	2.06	0.55
3:Q:125:GLN:NE2	17:Q:872:HOH:O	2.39	0.55
10:X:52:THR:HG23	10:X:53:VAL:N	2.22	0.55
10:X:111:TYR:CE1	10:X:121:GLU:HG3	2.42	0.55
10:J:11:SER:HB2	10:J:178:VAL:O	2.07	0.55
1:O:86:ARG:HH21	7:U:118:ASN:HD22	1.55	0.55
6:T:69:VAL:HG12	17:1:811:HOH:O	2.06	0.55
8:V:18:THR:HB	8:V:30:ASN:HD22	1.72	0.55
13:1:12:VAL:HG21	13:1:102:ALA:HB1	1.88	0.55
3:C:33:ARG:HD2	17:C:565:HOH:O	2.07	0.55
3:C:105:ASP:OD2	3:C:106:PRO:HD2	2.07	0.55
7:G:135:ILE:CD1	7:G:153:PRO:HD3	2.36	0.55
9:I:87:LEU:HD11	9:I:99:PRO:HG2	1.88	0.55
12:L:59:PHE:CG	12:L:83:ILE:HD11	2.42	0.55
14:N:37:VAL:CG2	14:N:41:ILE:HG22	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1:14(G):ILE:N	13:1:144:PRO:HD2	2.21	0.55
3:C:35:THR:HB	3:C:51:GLU:HG3	1.89	0.55
4:D:12(F):GLY:O	4:D:12(G):GLU:HB2	2.07	0.55
5:E:125:GLN:HB3	17:E:1296:HOH:O	2.07	0.55
13:M:175:LEU:HD23	13:M:176:ALA:N	2.21	0.55
2:P:224:PHE:HD2	2:P:224:PHE:N	2.05	0.55
3:Q:29:GLU:OE2	3:Q:32:LYS:HE2	2.07	0.55
12:Z:-7:ASN:ND2	12:Z:-7:ASN:C	2.64	0.55
1:A:13:THR:HG21	1:A:24:ILE:CD1	2.35	0.54
2:B:53:LYS:HG2	2:B:54:VAL:HG23	1.89	0.54
2:B:224:PHE:N	2:B:224:PHE:HD2	2.04	0.54
4:D:59:LEU:HD11	4:D:64:ILE:HD11	1.88	0.54
5:E:148:LEU:CD2	5:E:162:GLY:HA2	2.37	0.54
8:H:3:ILE:HG22	8:H:16:ALA:HB2	1.88	0.54
8:H:84:LYS:HG3	8:H:85:GLN:N	2.22	0.54
13:M:139:ARG:HH11	8:V:165:ASN:HD22	1.54	0.54
7:U:136:LEU:O	7:U:150:LYS:HA	2.05	0.54
2:B:114:ARG:NH1	10:J:70:GLU:OE2	2.37	0.54
2:B:224:PHE:N	2:B:224:PHE:CD2	2.76	0.54
6:F:12:ASN:HB3	6:F:127:ASN:HA	1.90	0.54
7:G:38:LEU:C	7:G:38:LEU:HD12	2.32	0.54
7:G:151:THR:HG22	7:G:157:TYR:CB	2.38	0.54
7:G:230:GLU:O	7:G:234:VAL:HG23	2.07	0.54
8:H:197:ARG:HG3	12:Z:164:GLU:CD	2.32	0.54
11:K:50:ALA:HB2	12:L:116:VAL:HG23	1.89	0.54
12:L:-7:ASN:HD22	12:L:-6:PRO:CD	2.19	0.54
6:T:49:ALA:HB3	6:T:197:ILE:HD11	1.80	0.54
8:V:159:ILE:HG22	8:V:163:ILE:CD1	2.38	0.54
8:V:200:LYS:HE3	9:W:140:SER:O	2.08	0.54
9:W:15:ALA:HB3	9:W:155:ILE:CD1	2.37	0.54
3:C:216:LYS:HD2	3:C:220:ASP:OD1	2.07	0.54
8:H:113:ILE:HD12	8:H:113:ILE:N	2.22	0.54
10:J:168:MET:HG2	10:X:168:MET:HE3	1.89	0.54
5:S:201:LEU:O	5:S:202:ARG:HB2	2.08	0.54
6:T:87:HIS:HD2	6:T:132:PHE:HE2	1.54	0.54
7:U:55:PRO:HG2	7:U:56:ASP:H	1.73	0.54
8:V:3:ILE:HG22	8:V:16:ALA:HB2	1.89	0.54
5:E:111:ARG:HG2	5:E:111:ARG:NH1	2.23	0.54
12:L:145:TYR:CD1	12:L:146:LEU:N	2.75	0.54
13:M:84:ALA:HA	13:M:113:VAL:HG21	1.90	0.54
7:U:143:GLU:HG2	17:U:928:HOH:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:84:LYS:HG3	8:V:85:GLN:N	2.23	0.54
8:V:100:ILE:HD13	8:V:112:SER:CB	2.38	0.54
12:Z:90:LYS:HE3	12:Z:93:PHE:O	2.07	0.54
5:E:68:ILE:N	5:E:68:ILE:HD12	2.23	0.54
7:G:140:SER:HA	7:G:215:ALA:HB1	1.89	0.54
9:I:99:PRO:HB2	9:I:113:PHE:CD2	2.42	0.54
6:T:119:TYR:O	6:T:122:ALA:HB3	2.08	0.54
9:W:9:LYS:HD3	9:W:145:ASN:HD22	1.71	0.54
10:X:58:TYR:CD2	10:X:59:ILE:HD12	2.43	0.54
11:Y:12:ILE:HD12	11:Y:110:ILE:CG1	2.37	0.54
7:G:35:ILE:HG23	7:G:51:GLN:HB2	1.89	0.54
2:P:87:ILE:O	2:P:91:THR:HG23	2.08	0.54
9:W:73:ALA:HB1	17:W:204:HOH:O	2.07	0.54
13:1:17:ASP:HA	13:1:173:PHE:CB	2.36	0.54
4:D:229:THR:HG22	4:D:233:ILE:HD11	1.90	0.54
6:F:11:SER:HB3	6:F:14:VAL:HG23	1.90	0.54
7:G:172:ILE:HD11	7:G:201:LEU:CD2	2.38	0.54
1:O:62:GLU:CD	1:O:62:GLU:H	2.15	0.54
3:Q:216:LYS:HD2	3:Q:220:ASP:OD1	2.08	0.54
6:T:72:ARG:HD2	13:1:64:THR:OG1	2.07	0.54
6:T:127:ASN:HD22	6:T:128:SER:N	2.05	0.54
10:X:185:ARG:HG2	10:X:185:ARG:HH11	1.73	0.54
3:C:39:GLY:O	3:C:162:ALA:HA	2.08	0.54
5:E:207:LEU:HD23	5:E:207:LEU:N	2.22	0.54
6:F:238:LYS:HZ2	6:F:239:GLU:HG3	1.73	0.54
14:N:41:ILE:HD13	14:N:79:ALA:HB2	1.90	0.54
3:Q:106:PRO:HG2	3:Q:143:PRO:CG	2.37	0.54
4:R:243:ALA:O	4:R:244:GLU:HB2	2.08	0.54
7:U:38:LEU:C	7:U:38:LEU:HD12	2.33	0.54
7:U:226:ALA:HA	7:U:229:ILE:HD12	1.90	0.54
9:W:99:PRO:HB2	9:W:113:PHE:CD2	2.42	0.54
12:Z:-7:ASN:HD22	12:Z:-6:PRO:N	2.05	0.54
3:C:163:GLN:HA	3:C:163:GLN:NE2	2.18	0.54
7:G:55:PRO:HG2	7:G:56:ASP:H	1.73	0.54
7:G:192:PHE:C	7:G:192:PHE:CD1	2.85	0.54
8:H:22:GLN:HG3	8:H:27:ALA:HB2	1.90	0.54
2:P:27:ALA:O	2:P:31:ILE:HG12	2.07	0.54
3:Q:97:GLN:NE2	3:Q:97:GLN:HA	2.22	0.54
9:W:43:LEU:HG	9:W:45:ILE:HD11	1.90	0.54
12:Z:76:ILE:HG22	17:Z:948:HOH:O	2.08	0.54
1:A:86:ARG:HE	7:G:118:ASN:ND2	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:ARG:HG3	1:A:232:ARG:HH11	1.73	0.54
11:K:86:LEU:HD13	11:K:86:LEU:C	2.33	0.54
12:L:13:VAL:HG12	12:L:177:ILE:HG12	1.90	0.54
7:U:204:GLU:HG3	17:U:1284:HOH:O	2.07	0.54
10:X:44:SER:OG	10:X:100:LEU:HB2	2.07	0.54
1:A:49:ALA:HB2	1:A:212:LEU:HG	1.89	0.53
2:B:107:ILE:HD13	2:B:107:ILE:C	2.33	0.53
4:D:161:ASN:HB3	4:D:180:TRP:CE2	2.43	0.53
5:E:67:ILE:HG21	5:E:223:ILE:CD1	2.37	0.53
7:G:49:ILE:HD11	7:G:193:ALA:CB	2.39	0.53
11:K:35:ILE:N	11:K:35:ILE:HD12	2.23	0.53
11:K:48:GLY:HA3	17:K:406:HOH:O	2.07	0.53
3:Q:39:GLY:O	3:Q:162:ALA:HA	2.08	0.53
3:Q:72:SER:O	3:Q:221:ILE:HD13	2.08	0.53
13:I:150:VAL:HG21	17:I:323:HOH:O	2.08	0.53
10:J:168:MET:HE3	10:X:168:MET:HG2	1.90	0.53
11:K:10(A):ARG:HG2	11:K:10(A):ARG:NH1	2.23	0.53
11:K:174:ASN:HD21	11:K:189:ASN:HB2	1.73	0.53
4:R:221:PHE:HE1	4:R:223:ILE:HD11	1.73	0.53
6:T:238:LYS:HZ2	6:T:239:GLU:HG3	1.74	0.53
7:U:56:ASP:HB3	7:U:59:LEU:HG	1.89	0.53
2:B:15:PHE:N	3:C:23:GLN:HE22	1.96	0.53
5:E:210:LEU:HD22	5:E:233:ILE:CD1	2.38	0.53
8:H:40:LYS:O	8:H:41:ILE:HD13	2.09	0.53
8:H:159:ILE:HD13	8:H:173:VAL:HG13	1.89	0.53
13:M:19:LEU:HD21	13:M:26:LEU:HD22	1.91	0.53
1:O:35:VAL:HG11	1:O:51:GLU:HB3	1.89	0.53
1:O:47:VAL:HG23	1:O:212:LEU:HD21	1.89	0.53
3:Q:57:LYS:O	3:Q:58:LEU:HB2	2.07	0.53
4:R:112:LEU:HD13	4:R:112:LEU:C	2.34	0.53
7:U:74:ILE:HG21	7:U:112:LEU:HD23	1.89	0.53
8:V:37:ILE:HD13	8:V:41:ILE:HG22	1.91	0.53
9:W:100:VAL:HG13	9:W:125:ILE:HG21	1.89	0.53
8:H:3:ILE:HG22	8:H:16:ALA:CB	2.38	0.53
1:O:118:LYS:HE2	1:O:122:GLU:OE1	2.08	0.53
3:Q:35:THR:HB	3:Q:51:GLU:HG3	1.90	0.53
4:R:177:LEU:HD22	5:S:58:LEU:CD1	2.39	0.53
6:T:192:GLN:HE21	6:T:195:LYS:HE3	1.72	0.53
7:G:34(A):ASN:HD22	7:G:167:PRO:HG2	1.73	0.53
10:J:123:PRO:HB2	10:J:124:TYR:CD1	2.43	0.53
2:P:101:LYS:HZ1	10:X:85:GLN:NE2	2.06	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:25:TRP:CH2	12:Z:132:SER:HA	2.44	0.53
12:Z:-2:ASN:HA	12:Z:21:ILE:O	2.08	0.53
13:1:84:ALA:HA	13:1:113:VAL:HG21	1.90	0.53
3:C:175:PHE:O	3:C:179:ASN:HB2	2.09	0.53
7:G:87:ASN:C	7:G:87:ASN:ND2	2.61	0.53
2:P:126:HIS:CB	3:Q:129:VAL:HG12	2.37	0.53
2:P:224:PHE:N	2:P:224:PHE:CD2	2.76	0.53
4:R:12(F):GLY:O	4:R:12(G):GLU:HB2	2.08	0.53
4:R:161:ASN:HB3	4:R:180:TRP:CE2	2.43	0.53
5:S:4:PHE:CE1	5:S:17:PRO:HD2	2.44	0.53
7:U:230:GLU:O	7:U:234:VAL:HG23	2.08	0.53
10:X:13:ILE:HG12	10:X:177:ILE:HD12	1.90	0.53
13:1:40:ASN:N	13:1:40:ASN:ND2	2.46	0.53
2:B:107:ILE:HD11	2:B:112:LEU:H	1.71	0.53
3:C:21:ILE:HD12	3:C:21:ILE:N	2.24	0.53
9:I:66:TYR:CE1	9:I:70:GLU:HG3	2.43	0.53
11:K:35:ILE:HD13	11:K:56:GLU:OE1	2.09	0.53
11:K:86:LEU:O	11:K:89:GLN:HB2	2.08	0.53
12:L:177:ILE:CD1	12:L:185:ARG:NH2	2.72	0.53
13:M:42:VAL:HG23	13:M:178:ILE:HD11	1.89	0.53
2:P:71:ASN:ND2	2:P:72:ASP:H	2.06	0.53
3:Q:70:ILE:CD1	3:Q:112:LEU:HD11	2.32	0.53
3:Q:100:ARG:HH11	3:Q:106:PRO:HB3	1.72	0.53
1:A:144:PHE:CD2	9:I:72:ARG:HD2	2.43	0.53
1:A:212:LEU:HD22	1:A:224:LEU:HD12	1.90	0.53
11:K:200:LYS:HE3	11:K:206:PHE:O	2.08	0.53
4:R:17:PRO:HG3	5:S:26:TYR:CE2	2.44	0.53
5:S:15:PHE:H	6:T:23:GLN:NE2	2.03	0.53
12:Z:175:ILE:HD12	12:Z:175:ILE:N	2.23	0.53
3:C:158:SER:HB2	4:D:59:LEU:HD21	1.90	0.53
4:D:138:ILE:N	4:D:138:ILE:HD12	2.24	0.53
5:E:15:PHE:H	6:F:23:GLN:NE2	2.04	0.53
5:S:207:LEU:HA	5:S:2(E):ASN:HD21	1.69	0.53
6:T:74:ILE:HG12	6:T:109:ILE:HD13	1.91	0.53
7:U:35:ILE:HG23	7:U:51:GLN:HB2	1.89	0.53
8:V:3:ILE:HD11	8:V:127:LEU:CB	2.38	0.53
12:Z:114:ASP:HB2	12:Z:118:SER:OG	2.09	0.53
3:C:14:ILE:HD13	3:C:14:ILE:N	2.24	0.53
5:E:15:PHE:HB2	6:F:23:GLN:HE22	1.73	0.53
8:H:221:ILE:HD11	9:I:184:VAL:CB	2.34	0.53
9:I:-8:SER:O	9:I:-6:PRO:HD3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:33:GLN:HE21	1:O:33:GLN:HA	1.74	0.53
7:U:49:ILE:CD1	7:U:212:VAL:HG22	2.39	0.53
8:V:3:ILE:HG22	8:V:16:ALA:CB	2.39	0.53
3:C:15:PHE:H	4:D:23:GLN:NE2	1.96	0.52
8:H:210:THR:CG2	12:Z:14(C):GLN:HG2	2.39	0.52
3:Q:121:GLN:NE2	3:Q:121:GLN:C	2.67	0.52
5:S:58:LEU:N	5:S:58:LEU:HD12	2.24	0.52
11:Y:35:ILE:HD11	11:Y:45:MET:HE3	1.90	0.52
4:D:39:GLY:O	4:D:40:ILE:HD13	2.10	0.52
5:E:214:ILE:O	5:E:221:PHE:HA	2.10	0.52
9:I:9:LYS:HD3	9:I:145:ASN:HD22	1.74	0.52
10:J:167:PRO:HB2	10:X:168:MET:HE1	1.90	0.52
10:J:168:MET:HE1	10:X:167:PRO:HB2	1.91	0.52
14:N:9:LYS:O	14:N:107:LYS:HD3	2.09	0.52
14:N:176:VAL:HG12	14:N:178:LEU:HD13	1.91	0.52
2:P:101:LYS:NZ	10:X:85:GLN:HE22	2.08	0.52
8:V:216:GLU:HG3	9:W:187:ARG:HG2	1.91	0.52
9:W:29:ASN:ND2	9:W:29:ASN:H	2.08	0.52
14:2:40:LYS:C	14:2:41:ILE:HD12	2.34	0.52
1:A:62:GLU:CD	1:A:62:GLU:H	2.16	0.52
12:L:114:ASP:HB2	12:L:118:SER:OG	2.09	0.52
7:U:101:TYR:OH	14:2:58:ILE:HD11	2.10	0.52
11:Y:76:VAL:N	11:Y:106:GLU:OE2	2.39	0.52
12:Z:76:ILE:HG23	12:Z:77:ASN:N	2.23	0.52
14:2:116:GLY:HA3	17:2:192:HOH:O	2.10	0.52
1:A:33:GLN:HA	1:A:33:GLN:HE21	1.73	0.52
2:B:51:GLU:OE2	2:B:202:THR:HG23	2.09	0.52
8:H:20:SER:HB3	8:H:28:ASP:HB3	1.91	0.52
8:H:50:ALA:CB	9:I:116:ILE:CD1	2.76	0.52
9:I:93:GLY:N	9:I:94:PRO:CD	2.73	0.52
9:I:10(C):SER:C	9:I:107:LYS:H	2.17	0.52
12:L:14:LEU:HD13	12:L:34:VAL:HG13	1.91	0.52
3:Q:52:ARG:HD2	3:Q:208:LYS:O	2.10	0.52
3:Q:125:GLN:HG3	3:Q:125:GLN:O	2.09	0.52
11:Y:12:ILE:HD12	11:Y:110:ILE:HG13	1.91	0.52
2:B:141:TYR:CD1	2:B:141:TYR:C	2.88	0.52
2:B:184:MET:HE3	2:B:188:ASP:HB3	1.92	0.52
3:C:163:GLN:NE2	3:C:164:THR:N	2.55	0.52
5:E:138:ILE:HD12	5:E:138:ILE:N	2.23	0.52
8:H:95:ILE:O	8:H:97:ALA:N	2.41	0.52
10:J:168:MET:HE2	10:X:167:PRO:C	2.34	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:110:LYS:HG2	17:O:376:HOH:O	2.10	0.52
3:Q:154:SER:CB	3:Q:156:ILE:HD13	2.38	0.52
3:Q:18(A):ASP:OD1	3:Q:18(C):LYS:HB2	2.10	0.52
9:W:36:HIS:HB3	9:W:42:PHE:CD2	2.43	0.52
10:X:52:THR:CG2	10:X:53:VAL:H	2.22	0.52
12:Z:-8:PHE:HB3	13:1:-8:THR:HG23	1.92	0.52
2:B:143:ASP:OD2	10:J:10(B):LYS:HE2	2.10	0.52
3:C:40:VAL:HG12	3:C:162:ALA:HB1	1.92	0.52
10:J:63:ILE:N	10:J:63:ILE:CD1	2.72	0.52
11:K:78:ALA:O	11:K:82:ILE:HG12	2.10	0.52
1:O:177:GLU:HG2	2:P:58:LEU:CD2	2.40	0.52
1:O:212:LEU:HD22	1:O:224:LEU:HD12	1.91	0.52
2:P:53:LYS:HG2	2:P:54:VAL:HG23	1.92	0.52
4:R:236:GLU:O	4:R:240:LYS:HG3	2.09	0.52
9:W:101:VAL:O	9:W:110:ILE:HA	2.09	0.52
10:X:11:SER:HB2	10:X:178:VAL:O	2.09	0.52
13:1:91:ARG:HG3	13:1:92:SER:N	2.24	0.52
2:B:81:LEU:HD23	2:B:133:GLY:HA3	1.92	0.52
6:F:127:ASN:HD22	6:F:128:SER:N	2.08	0.52
6:F:137:ILE:HD11	6:F:150:MET:SD	2.49	0.52
8:H:101:VAL:HG12	8:H:113:ILE:HD11	1.91	0.52
9:I:22:SER:O	9:I:23:GLN:HB2	2.10	0.52
14:N:14:LEU:HD11	14:N:102:ALA:HB3	1.91	0.52
4:R:229:THR:HG22	4:R:233:ILE:HD11	1.91	0.52
8:V:112:SER:HB3	8:V:125:LEU:HD13	1.92	0.52
10:J:13:ILE:HD12	10:J:13:ILE:N	2.25	0.52
5:S:138:ILE:HD12	5:S:138:ILE:N	2.24	0.52
5:S:214:ILE:O	5:S:221:PHE:HA	2.09	0.52
8:V:105:ASP:HB2	8:V:10(A):PRO:HD2	1.91	0.52
4:D:198:LYS:HG3	17:D:499:HOH:O	2.10	0.52
4:D:243:ALA:O	4:D:244:GLU:HB2	2.08	0.52
6:F:238:LYS:NZ	6:F:239:GLU:HG3	2.25	0.52
3:Q:17:PRO:HA	4:R:26:TYR:CD1	2.44	0.52
3:Q:33:ARG:CB	3:Q:33:ARG:NH1	2.73	0.52
5:S:18(C):PHE:HA	5:S:18(F):ILE:CG1	2.39	0.52
9:W:10(C):SER:C	9:W:107:LYS:H	2.18	0.52
13:1:-3:VAL:HG12	13:1:49:ILE:HG13	1.92	0.52
2:B:87:ILE:O	2:B:91:THR:HG23	2.10	0.52
8:H:105:ASP:HB2	8:H:10(A):PRO:HD2	1.92	0.52
8:H:144:GLN:O	8:H:145:ASP:HB2	2.09	0.52
10:J:167:PRO:C	10:X:168:MET:HE2	2.34	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:110:LEU:HG	13:M:125:LEU:HD12	1.92	0.52
13:M:113:VAL:HA	13:M:118:VAL:O	2.09	0.52
1:O:141:HIS:HA	1:O:146:GLY:O	2.10	0.52
2:P:185:LYS:O	2:P:188:ASP:N	2.42	0.52
3:Q:52:ARG:HH21	3:Q:211:GLU:HB3	1.75	0.52
8:V:20:SER:HB3	8:V:28:ASP:HB3	1.92	0.52
12:Z:152:ILE:O	12:Z:156:ARG:HG3	2.09	0.52
13:1:113:VAL:HA	13:1:118:VAL:O	2.10	0.52
14:2:146:MET:CE	14:2:150:GLU:HB3	2.40	0.52
2:B:152:ASN:HB2	2:B:153:PRO:CD	2.39	0.51
2:B:173:GLN:HG2	3:C:56:LEU:HD12	1.92	0.51
6:F:137:ILE:HD13	6:F:150:MET:CB	2.41	0.51
10:J:52:THR:CG2	10:J:53:VAL:H	2.23	0.51
10:J:133:TYR:HD1	17:Y:593:HOH:O	1.92	0.51
11:K:126:CYS:HB2	11:K:135:TYR:CE1	2.45	0.51
8:V:144:GLN:O	8:V:145:ASP:HB2	2.09	0.51
12:Z:43:MET:HB2	12:Z:101:ILE:HG22	1.92	0.51
12:Z:129:ALA:HB1	12:Z:166:HIS:CE1	2.45	0.51
13:1:133:MET:HE1	13:1:165:ARG:HG3	1.92	0.51
13:1:179:ASP:HB3	13:1:18(A):THR:OG1	2.10	0.51
14:2:14:LEU:HD11	14:2:102:ALA:HB3	1.92	0.51
4:D:53:ARG:O	4:D:53:ARG:HG2	2.09	0.51
5:E:137:LEU:CD2	5:E:150:GLU:HG3	2.41	0.51
11:K:12:ILE:HB	11:K:178:VAL:HB	1.91	0.51
12:L:-7:ASN:HD22	12:L:-6:PRO:N	2.08	0.51
12:L:129:ALA:HB1	12:L:166:HIS:CE1	2.45	0.51
2:P:152:ASN:HB2	2:P:153:PRO:HD2	1.92	0.51
3:Q:55:THR:C	3:Q:56:LEU:HD22	2.36	0.51
6:T:35:THR:HG23	6:T:36:THR:N	2.24	0.51
7:U:172:ILE:HD11	7:U:201:LEU:CD2	2.40	0.51
10:X:77:GLN:C	10:X:77:GLN:NE2	2.68	0.51
5:E:201:LEU:O	5:E:202:ARG:HB2	2.09	0.51
8:H:62:ASN:HB3	8:H:82:MET:HE1	1.91	0.51
6:T:12:ASN:HB3	6:T:127:ASN:HA	1.92	0.51
1:A:21:LEU:HB3	1:A:24:ILE:CD1	2.28	0.51
2:B:122:GLY:C	2:B:124:THR:H	2.18	0.51
2:B:21(A):LYS:O	2:B:21(B):GLY:C	2.53	0.51
10:J:44:SER:OG	10:J:100:LEU:HB2	2.10	0.51
11:K:4:LEU:CD2	11:K:15:ALA:HB3	2.41	0.51
1:O:232:ARG:HH11	1:O:232:ARG:HG3	1.76	0.51
2:P:21(A):LYS:O	2:P:21(B):GLY:C	2.53	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:79:ALA:HB3	5:S:165:ILE:HD12	1.93	0.51
5:S:137:LEU:CD2	5:S:150:GLU:HG3	2.40	0.51
6:T:115:ARG:HA	17:T:573:HOH:O	2.11	0.51
7:U:31:THR:HG21	7:U:135:ILE:HG13	1.93	0.51
7:U:34(A):ASN:HD22	7:U:167:PRO:HG2	1.75	0.51
14:2:176:VAL:HG12	14:2:178:LEU:HD13	1.91	0.51
1:A:35:VAL:HG11	1:A:51:GLU:HB3	1.91	0.51
13:M:130:GLY:O	13:M:134:ALA:HB3	2.10	0.51
2:P:81:LEU:HD23	2:P:133:GLY:HA3	1.93	0.51
5:S:46:ALA:O	5:S:139:ILE:HD12	2.11	0.51
6:T:87:HIS:HD2	6:T:132:PHE:CE2	2.29	0.51
9:W:119:ILE:HD12	9:W:119:ILE:N	2.22	0.51
11:Y:174:ASN:HD21	11:Y:189:ASN:HB2	1.75	0.51
12:Z:48:PHE:CZ	12:Z:50:ALA:HB3	2.46	0.51
13:1:21:SER:HB2	17:1:278:HOH:O	2.10	0.51
5:E:207:LEU:HA	5:E:2(E):ASN:HD21	1.70	0.51
9:I:36:HIS:HB3	9:I:42:PHE:CD2	2.46	0.51
10:J:113:ILE:HA	10:J:118:THR:O	2.11	0.51
13:M:147:THR:OG1	13:M:150:VAL:HG23	2.11	0.51
6:T:127:ASN:HD22	6:T:127:ASN:C	2.19	0.51
10:X:166:MET:CE	10:X:168:MET:HB2	2.41	0.51
2:B:101:LYS:HG3	9:I:57:GLU:HB3	1.93	0.51
3:C:195:ARG:HD3	17:C:1019:HOH:O	2.10	0.51
8:H:3:ILE:CG1	8:H:100:ILE:HD12	2.38	0.51
11:K:207:ASN:HD21	10:X:144:PRO:HG3	1.76	0.51
1:O:206:PHE:CD1	1:O:210:ILE:HD11	2.44	0.51
2:P:51:GLU:OE2	2:P:202:THR:HG23	2.10	0.51
3:Q:40:VAL:HG12	3:Q:162:ALA:HB1	1.93	0.51
3:Q:175:PHE:O	3:Q:179:ASN:HB2	2.10	0.51
6:T:13:SER:HB2	7:U:130:ARG:HD3	1.93	0.51
6:T:147:HIS:HD2	17:T:242:HOH:O	1.92	0.51
10:X:16:SER:HB2	17:X:1152:HOH:O	2.10	0.51
1:A:92:SER:OG	1:A:116:VAL:HG22	2.11	0.51
3:C:100:ARG:HH11	3:C:106:PRO:HB3	1.76	0.51
3:C:18(A):ASP:OD1	3:C:18(C):LYS:HB2	2.11	0.51
12:L:40:ASN:HD21	12:L:183:GLY:HA2	1.75	0.51
14:N:18(G):TYR:HA	14:N:18(J):LEU:HG	1.93	0.51
1:O:31:VAL:HG11	1:O:135:SER:HB2	1.91	0.51
2:P:141:TYR:CD1	2:P:141:TYR:C	2.88	0.51
3:Q:158:SER:HB2	4:R:59:LEU:HD21	1.93	0.51
3:Q:165:ILE:H	3:Q:165:ILE:HD13	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:185:ASN:OD1	5:S:188:GLU:HG2	2.11	0.51
11:Y:50:ALA:HB2	12:Z:116:VAL:HG23	1.91	0.51
11:Y:143:LYS:HB2	11:Y:146:LEU:CD1	2.41	0.51
2:B:4:GLY:HA3	5:E:127:TYR:CE1	2.46	0.51
3:C:33:ARG:CB	3:C:33:ARG:NH1	2.73	0.51
5:E:220:PRO:O	5:E:221:PHE:C	2.54	0.51
13:M:70:ASN:ND2	13:M:70(A):ALA:HA	2.26	0.51
1:O:6:ASP:OD2	1:O:8:TYR:HB2	2.11	0.51
2:P:122:GLY:C	2:P:124:THR:H	2.19	0.51
3:Q:165:ILE:HD13	3:Q:165:ILE:N	2.25	0.51
4:R:46:VAL:HG11	4:R:139:ALA:HB1	1.93	0.51
5:S:31:ILE:HD11	5:S:153:PRO:CD	2.41	0.51
6:T:127:ASN:C	6:T:127:ASN:ND2	2.68	0.51
6:T:238:LYS:NZ	6:T:239:GLU:HG3	2.26	0.51
11:Y:4:LEU:CD2	11:Y:15:ALA:HB3	2.41	0.51
11:Y:200:LYS:HE3	11:Y:206:PHE:O	2.11	0.51
12:Z:177:ILE:HD12	12:Z:177:ILE:N	2.26	0.51
13:1:8:THR:N	13:1:92(B):MET:O	2.43	0.51
1:A:98:THR:O	1:A:10(A):ILE:HD11	2.10	0.51
6:F:40:ILE:HD12	6:F:40:ILE:N	2.26	0.51
8:H:108:SER:HB3	8:H:180:ILE:HD11	1.92	0.51
10:J:3:ILE:HG22	10:J:100:LEU:CD1	2.41	0.51
14:N:13:ILE:HD13	14:N:177:VAL:HG22	1.93	0.51
2:P:121:GLN:NE2	17:P:462:HOH:O	2.43	0.51
6:T:32:GLU:HB3	6:T:169:ARG:NH2	2.26	0.51
7:U:151:THR:HG22	7:U:157:TYR:CB	2.41	0.51
8:V:32:ALA:HB1	17:V:578:HOH:O	2.11	0.51
8:V:147:THR:HG23	8:V:150:GLU:OE1	2.10	0.51
8:V:159:ILE:HD13	8:V:173:VAL:CG1	2.41	0.51
9:W:93:GLY:N	9:W:94:PRO:CD	2.73	0.51
11:Y:4:LEU:HD11	11:Y:159:ILE:HG12	1.93	0.51
13:1:70:ASN:ND2	13:1:70(A):ALA:HA	2.26	0.51
1:A:6:ASP:OD2	1:A:8:TYR:HB2	2.11	0.50
5:E:226:GLY:O	5:E:229:VAL:HG22	2.10	0.50
10:J:20:VAL:HG11	11:K:120:LEU:HD11	1.93	0.50
1:O:190:ILE:HD11	1:O:214:ILE:CG2	2.41	0.50
2:P:184:MET:HE3	2:P:188:ASP:HB3	1.91	0.50
2:P:218:ASN:O	2:P:21(C):ASP:HB2	2.11	0.50
5:S:226:GLY:O	5:S:229:VAL:HG22	2.11	0.50
6:T:11:SER:HB3	6:T:14:VAL:HG23	1.92	0.50
6:T:43:ASN:HD22	6:T:43:ASN:N	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:192:ARG:HD2	17:W:1258:HOH:O	2.10	0.50
10:X:35:ARG:O	10:X:42:LEU:HD12	2.11	0.50
2:B:218:ASN:O	2:B:21(C):ASP:HB2	2.11	0.50
5:E:107:LEU:HD11	5:E:111:ARG:HG2	1.93	0.50
5:E:185:ASN:OD1	5:E:188:GLU:HG2	2.10	0.50
11:K:12:ILE:HD13	11:K:110:ILE:HD11	1.93	0.50
1:O:130:ARG:NH2	7:U:124:THR:HG22	2.17	0.50
2:P:239:THR:HG22	2:P:239:THR:OXT	2.10	0.50
8:V:105:ASP:HB2	8:V:10(A):PRO:CD	2.41	0.50
13:1:9:ASP:OD1	13:1:10:ASN:N	2.44	0.50
3:C:163:GLN:HE21	3:C:164:THR:N	2.09	0.50
6:F:87:HIS:HD2	6:F:132:PHE:CE2	2.28	0.50
11:K:4:LEU:HD11	11:K:159:ILE:HG12	1.93	0.50
12:L:76:ILE:HG23	12:L:77:ASN:N	2.27	0.50
3:Q:163:GLN:HE21	3:Q:164:THR:H	1.55	0.50
5:S:172:ALA:HB2	5:S:196:ALA:O	2.11	0.50
8:V:50:ALA:HB3	9:W:116:ILE:HD12	1.93	0.50
8:V:95:ILE:O	8:V:97:ALA:N	2.41	0.50
10:X:34:THR:CG2	10:X:176:LYS:NZ	2.75	0.50
12:Z:21:ILE:HB	12:Z:25:SER:O	2.11	0.50
3:C:52:ARG:HH21	3:C:211:GLU:HB3	1.76	0.50
6:F:119:TYR:O	6:F:122:ALA:HB3	2.11	0.50
9:I:143:GLU:HG3	9:I:146:LEU:HD21	1.93	0.50
12:L:152:ILE:O	12:L:156:ARG:HG3	2.11	0.50
13:M:112:TYR:C	13:M:112:TYR:CD2	2.89	0.50
5:S:36:VAL:HG22	5:S:37:THR:N	2.26	0.50
8:V:172:ASN:ND2	8:V:193:THR:HA	2.25	0.50
2:B:101:LYS:HZ2	10:J:85:GLN:NE2	2.09	0.50
3:C:33:ARG:HH11	3:C:33:ARG:HB3	1.75	0.50
5:E:18(C):PHE:HA	5:E:18(F):ILE:CD1	2.40	0.50
6:F:70:VAL:HG11	6:F:112:PHE:CE1	2.45	0.50
7:G:47:VAL:HG12	7:G:49:ILE:HD11	1.92	0.50
11:K:45:MET:SD	16:K:2(I):H10:H15	2.51	0.50
12:L:82:ASN:C	12:L:82:ASN:HD22	2.20	0.50
7:U:107:MET:HE3	7:U:112:LEU:HB2	1.93	0.50
9:W:66:TYR:CE1	9:W:70:GLU:HG3	2.46	0.50
10:X:13:ILE:HG12	10:X:177:ILE:CD1	2.42	0.50
11:Y:4:LEU:HD21	11:Y:15:ALA:HB3	1.94	0.50
13:1:19:LEU:HD12	13:1:28:PHE:O	2.12	0.50
5:E:36:VAL:HG22	5:E:37:THR:N	2.26	0.50
9:I:152:PHE:CB	9:I:177:ILE:HD11	2.38	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:168:MET:CE	10:X:168:MET:HG2	2.42	0.50
2:P:181:LYS:HG3	2:P:184:MET:HG3	1.94	0.50
2:P:235:LYS:C	2:P:237:GLY:N	2.69	0.50
4:R:185:THR:OG1	4:R:188:GLU:HG3	2.12	0.50
9:W:55:LEU:CD1	9:W:97:VAL:HG21	2.41	0.50
9:W:177:ILE:HD12	9:W:177:ILE:N	2.27	0.50
10:J:166:MET:CE	10:J:168:MET:HB2	2.42	0.50
14:N:13:ILE:HG13	14:N:151:THR:CG2	2.41	0.50
5:S:73:HIS:HE1	5:S:107:LEU:O	1.94	0.50
7:U:108:PRO:HB3	8:V:72:ARG:NH2	2.25	0.50
10:X:123:PRO:HB2	10:X:124:TYR:CD1	2.46	0.50
1:A:86:ARG:HH21	7:G:118:ASN:HD22	1.60	0.50
2:B:181:LYS:HD2	2:B:183:ASP:OD1	2.12	0.50
4:D:177:LEU:HD22	5:E:58:LEU:CD1	2.42	0.50
12:L:48:PHE:CZ	12:L:50:ALA:HB3	2.47	0.50
13:M:-3:VAL:HG12	13:M:49:ILE:HG13	1.93	0.50
1:O:67:VAL:HG11	1:O:213:ALA:CB	2.41	0.50
5:S:38:VAL:HG22	5:S:164:ALA:HB2	1.92	0.50
5:S:139:ILE:CD1	5:S:215:VAL:HG12	2.42	0.50
8:V:62:ASN:HB3	8:V:82:MET:HE1	1.93	0.50
17:V:1181:HOH:O	9:W:150:ASP:HA	2.11	0.50
1:A:118:LYS:HE2	1:A:122:GLU:OE1	2.12	0.50
3:C:35:THR:OG1	3:C:66:LYS:NZ	2.45	0.50
3:C:125:GLN:O	3:C:125:GLN:HG3	2.12	0.50
4:D:236:GLU:O	4:D:240:LYS:HG3	2.12	0.50
5:E:73:HIS:HE1	5:E:107:LEU:O	1.95	0.50
5:E:139:ILE:CD1	5:E:215:VAL:HG12	2.42	0.50
10:J:168:MET:HG2	10:X:168:MET:CE	2.41	0.50
5:S:111:ARG:HG2	5:S:111:ARG:NH1	2.25	0.50
7:U:105:TYR:OH	8:V:66:HIS:HE1	1.95	0.50
1:A:141:HIS:HA	1:A:146:GLY:O	2.11	0.49
2:B:235:LYS:C	2:B:237:GLY:N	2.70	0.49
4:D:70:ILE:HD13	4:D:89:ILE:HG23	1.94	0.49
17:E:1080:HOH:O	12:L:64:LYS:HE3	2.11	0.49
9:I:94:PRO:HA	17:I:205:HOH:O	2.12	0.49
14:N:38:HIS:HD2	17:N:1366:HOH:O	1.95	0.49
2:P:152:ASN:HB2	2:P:153:PRO:CD	2.42	0.49
12:Z:76:ILE:HD13	12:Z:109:ALA:HB3	1.93	0.49
1:A:38:LEU:C	1:A:38:LEU:HD12	2.36	0.49
3:C:226:SER:HB2	3:C:227:GLU:OE1	2.12	0.49
11:K:77:ALA:HA	11:K:111:TYR:CE2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:35:THR:O	6:T:166:GLY:HA3	2.12	0.49
6:T:195:LYS:HZ1	6:T:196:ILE:HD11	1.77	0.49
11:Y:7:ARG:HA	11:Y:12:ILE:HD13	1.94	0.49
11:Y:90:TYR:O	11:Y:91:LYS:C	2.55	0.49
12:Z:85:HIS:HE1	17:Z:197:HOH:O	1.96	0.49
12:Z:99:THR:CG2	17:Z:231:HOH:O	2.60	0.49
1:A:47:VAL:HG23	1:A:212:LEU:HD21	1.94	0.49
2:B:124:THR:HG22	3:C:130:ARG:NH2	2.21	0.49
5:E:92:LEU:HD11	5:E:112:ALA:HB1	1.93	0.49
9:I:101:VAL:O	9:I:110:ILE:HA	2.11	0.49
9:I:113:PHE:CD2	9:I:113:PHE:N	2.81	0.49
11:K:8:PHE:CE2	11:K:13:ILE:HG12	2.47	0.49
5:S:107:LEU:HD11	5:S:111:ARG:HG2	1.93	0.49
7:U:141:VAL:HG21	7:U:216:THR:HA	1.94	0.49
11:Y:74:ILE:HD11	11:Y:78:ALA:CB	2.42	0.49
14:2:175:MET:HB2	14:2:187:LEU:HB2	1.93	0.49
2:B:107:ILE:HD12	2:B:112:LEU:CB	2.32	0.49
8:H:105:ASP:HB2	8:H:10(A):PRO:CD	2.42	0.49
13:M:9:ASP:OD1	13:M:10:ASN:N	2.46	0.49
3:Q:220:ASP:C	3:Q:221:ILE:HD12	2.37	0.49
3:Q:221:ILE:N	3:Q:221:ILE:HD12	2.27	0.49
4:R:172:ALA:HB1	4:R:196:ILE:HG21	1.94	0.49
11:Y:10(A):ARG:HG2	11:Y:10(A):ARG:NH1	2.23	0.49
11:Y:200:LYS:HG3	11:Y:206:PHE:HB2	1.95	0.49
6:F:109:ILE:CG2	6:F:147:HIS:HB2	2.41	0.49
11:K:109:THR:C	11:K:110:ILE:HD13	2.37	0.49
13:M:6:MET:HG2	13:M:155:ILE:HD11	1.95	0.49
14:N:44:CYS:HB2	14:N:100:ILE:HB	1.94	0.49
3:Q:163:GLN:HA	3:Q:163:GLN:NE2	2.18	0.49
5:S:179:THR:HG22	5:S:18(B):THR:HB	1.95	0.49
9:W:29:ASN:C	9:W:29:ASN:HD22	2.21	0.49
11:Y:8:PHE:CE2	11:Y:13:ILE:HG12	2.47	0.49
13:1:112:TYR:C	13:1:112:TYR:CD2	2.90	0.49
14:2:159:LEU:O	14:2:163:ILE:HG12	2.13	0.49
1:A:212:LEU:HD23	1:A:212:LEU:C	2.37	0.49
4:D:27:SER:O	4:D:31:ILE:HG13	2.13	0.49
5:E:54:ASN:ND2	5:E:56:ASP:O	2.45	0.49
5:E:18(C):PHE:HA	5:E:18(F):ILE:CG1	2.40	0.49
7:G:47:VAL:HG12	7:G:49:ILE:HD12	1.94	0.49
11:K:207:ASN:HD21	10:X:144:PRO:CG	2.25	0.49
12:L:17:ASP:HA	12:L:172:GLY:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:133:MET:HE1	13:M:165:ARG:HG3	1.95	0.49
2:P:27:ALA:O	2:P:30:SER:HB3	2.13	0.49
4:R:42:THR:C	4:R:44:GLU:H	2.21	0.49
7:U:217:LYS:HA	7:U:217:LYS:CE	2.41	0.49
2:B:27:ALA:O	2:B:30:SER:HB3	2.12	0.49
2:B:181:LYS:HG3	2:B:184:MET:HG3	1.94	0.49
8:H:8:PHE:HB3	8:H:151:ALA:HB2	1.95	0.49
9:I:29:ASN:C	9:I:29:ASN:HD22	2.20	0.49
10:J:185:ARG:HG2	10:J:185:ARG:NH1	2.27	0.49
12:L:5:GLY:O	12:L:124:CYS:HA	2.12	0.49
3:Q:105:ASP:OD2	3:Q:106:PRO:HD2	2.12	0.49
10:X:3:ILE:HG22	10:X:100:LEU:CD1	2.43	0.49
14:2:9:LYS:O	14:2:107:LYS:HD3	2.13	0.49
14:2:13:ILE:HG13	14:2:151:THR:CG2	2.42	0.49
3:C:41:LYS:HD3	3:C:161:SER:HA	1.95	0.49
4:D:14:THR:HG22	4:D:15:PHE:N	2.27	0.49
6:F:127:ASN:HD22	6:F:127:ASN:C	2.20	0.49
10:J:34:THR:HG21	10:J:176:LYS:HZ2	1.76	0.49
14:N:19:ARG:HG3	14:N:26:ILE:HG23	1.94	0.49
1:O:92:SER:OG	1:O:116:VAL:HG22	2.12	0.49
3:Q:163:GLN:NE2	3:Q:164:THR:N	2.58	0.49
8:V:8:PHE:HB3	8:V:151:ALA:HB2	1.95	0.49
11:Y:45:MET:SD	16:Y:2(I):H10:H15	2.53	0.49
3:C:121:GLN:NE2	3:C:121:GLN:C	2.71	0.49
5:E:179:THR:HG22	5:E:18(B):THR:HB	1.95	0.49
6:F:35:THR:HG23	6:F:36:THR:N	2.26	0.49
8:H:172:ASN:ND2	8:H:193:THR:HA	2.25	0.49
8:H:216:GLU:HG3	9:I:187:ARG:HG2	1.94	0.49
14:N:146:MET:CE	14:N:150:GLU:HB3	2.42	0.49
2:P:181:LYS:HD2	2:P:183:ASP:OD1	2.13	0.49
9:I:100:VAL:HG13	9:I:125:ILE:HG21	1.95	0.49
11:K:4:LEU:HD13	11:K:159:ILE:HD11	1.94	0.49
12:L:35:PHE:CD2	12:L:56:VAL:HG11	2.48	0.49
13:M:184:LEU:HD23	13:M:184:LEU:C	2.37	0.49
1:O:212:LEU:HD23	1:O:212:LEU:C	2.37	0.49
3:Q:41:LYS:HD3	3:Q:161:SER:HA	1.94	0.49
3:Q:137:LEU:HG	3:Q:165:ILE:HD12	1.95	0.49
6:T:74:ILE:HG12	6:T:109:ILE:HD11	1.95	0.49
6:T:158:TRP:CZ3	7:U:64:VAL:HA	2.48	0.49
9:W:143:GLU:HG3	9:W:146:LEU:HD21	1.94	0.49
13:1:130:GLY:O	13:1:134:ALA:HB3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:170:GLN:NE2	7:G:174:THR:HG23	2.27	0.48
12:L:1(I):ASN:HA	17:L:1110:HOH:O	2.12	0.48
2:P:196:THR:O	2:P:200:THR:HG23	2.13	0.48
3:Q:55:THR:HG22	3:Q:56:LEU:CD2	2.40	0.48
3:Q:97:GLN:HA	3:Q:97:GLN:HE21	1.77	0.48
9:W:113:PHE:CD2	9:W:113:PHE:N	2.81	0.48
10:X:70:GLU:O	10:X:71:ASP:C	2.56	0.48
10:X:113:ILE:HA	10:X:118:THR:O	2.12	0.48
12:Z:99:THR:HG23	17:Z:231:HOH:O	2.13	0.48
2:B:185:LYS:O	2:B:188:ASP:N	2.44	0.48
3:C:46:VAL:HB	3:C:215:VAL:CG1	2.43	0.48
4:D:175:GLU:OE1	4:D:175:GLU:HA	2.13	0.48
5:E:210:LEU:CD2	5:E:233:ILE:HD11	2.41	0.48
11:K:35:ILE:HD11	11:K:45:MET:HE3	1.94	0.48
5:S:220:PRO:O	5:S:221:PHE:C	2.55	0.48
7:U:17:PRO:HD3	17:U:584:HOH:O	2.14	0.48
9:W:155:ILE:HD13	9:W:155:ILE:C	2.38	0.48
17:A:242:HOH:O	8:H:69:TYR:HA	2.11	0.48
2:B:69:LYS:HG3	2:B:221:GLN:OE1	2.13	0.48
4:D:46:VAL:HG11	4:D:139:ALA:HB1	1.94	0.48
5:E:139:ILE:HG22	5:E:148:LEU:HD13	1.95	0.48
8:H:112:SER:HB3	8:H:125:LEU:HD13	1.94	0.48
9:I:55:LEU:CD1	9:I:97:VAL:HG21	2.43	0.48
4:R:27:SER:O	4:R:31:ILE:HG13	2.13	0.48
4:R:175:GLU:OE1	4:R:175:GLU:HA	2.12	0.48
5:S:221:PHE:CE1	5:S:223:ILE:CD1	2.91	0.48
7:U:12:ILE:O	7:U:14:ILE:HD13	2.13	0.48
9:W:89:GLU:O	9:W:90:ARG:NH1	2.47	0.48
11:Y:20:ALA:HA	16:Y:2(I):H10:O11	2.13	0.48
11:Y:77:ALA:HA	11:Y:111:TYR:CE2	2.47	0.48
13:1:94:PRO:HA	17:1:219:HOH:O	2.12	0.48
13:1:184:LEU:C	13:1:184:LEU:HD23	2.38	0.48
1:A:67:VAL:HG11	1:A:213:ALA:CB	2.44	0.48
2:B:186:VAL:HG21	2:B:216:ARG:HD3	1.94	0.48
3:C:52:ARG:HD2	3:C:208:LYS:O	2.13	0.48
9:I:152:PHE:CD1	9:I:177:ILE:HD11	2.48	0.48
10:J:70:GLU:O	10:J:71:ASP:C	2.56	0.48
11:K:4:LEU:HD21	11:K:15:ALA:HB3	1.94	0.48
12:L:43:MET:HB2	12:L:101:ILE:HG22	1.94	0.48
1:O:27:ALA:O	1:O:31:VAL:HG23	2.13	0.48
11:Y:126:CYS:HB2	11:Y:135:TYR:CE1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:17:ASP:HA	12:Z:172:GLY:O	2.13	0.48
1:A:109:THR:O	1:A:113:VAL:HG23	2.14	0.48
2:B:107:ILE:HD13	2:B:108:PRO:C	2.36	0.48
6:F:49:ALA:CB	6:F:212:ILE:CD1	2.91	0.48
11:K:143:LYS:HB2	11:K:146:LEU:CD1	2.44	0.48
13:M:-8:THR:N	13:M:92(B):MET:O	2.45	0.48
3:Q:173:ARG:O	3:Q:177:GLU:HG3	2.13	0.48
5:S:52:LYS:O	5:S:63:TYR:HD2	1.96	0.48
5:S:2(C):VAL:CG1	5:S:2(D):ASP:N	2.76	0.48
6:T:109:ILE:HG22	6:T:149:TYR:CE2	2.48	0.48
9:W:61:TYR:CD1	9:W:61:TYR:C	2.91	0.48
11:Y:13:ILE:HD12	11:Y:152:LEU:HD23	1.96	0.48
3:C:17:PRO:HA	4:D:26:TYR:CD1	2.48	0.48
5:E:230:ALA:C	5:E:232:TYR:H	2.21	0.48
6:F:35:THR:O	6:F:166:GLY:HA3	2.14	0.48
6:F:127:ASN:C	6:F:127:ASN:ND2	2.69	0.48
17:G:248:HOH:O	8:H:82:MET:HA	2.14	0.48
9:I:29:ASN:ND2	9:I:29:ASN:H	2.11	0.48
10:J:24:ILE:HG13	10:J:24:ILE:O	2.13	0.48
3:Q:35:THR:OG1	3:Q:66:LYS:NZ	2.45	0.48
3:Q:52:ARG:HB2	3:Q:209:ASN:HA	1.95	0.48
9:W:137:MET:HE3	9:W:141:LEU:HD11	1.94	0.48
1:A:198:LYS:HE3	1:A:236:LEU:HD11	1.96	0.48
2:B:8:TYR:CE2	7:G:12:ILE:HD12	2.48	0.48
2:B:194:LEU:HD11	2:B:232:ILE:CD1	2.36	0.48
2:B:237:GLY:O	2:B:238:ILE:HD13	2.14	0.48
5:E:46:ALA:O	5:E:139:ILE:HD12	2.13	0.48
5:E:67:ILE:HG21	5:E:213:ALA:HB2	1.95	0.48
5:E:79:ALA:HB3	5:E:165:ILE:HD12	1.94	0.48
12:L:-7:ASN:ND2	12:L:-7:ASN:C	2.67	0.48
5:S:216:GLY:O	5:S:217:LYS:C	2.57	0.48
14:2:174:ARG:HD2	17:2:307:HOH:O	2.14	0.48
1:A:32:LYS:HE2	1:A:32:LYS:CA	2.43	0.48
1:A:32:LYS:HA	1:A:32:LYS:CE	2.43	0.48
3:C:65:SER:HB2	17:C:274:HOH:O	2.13	0.48
6:F:157:TYR:CD1	6:F:157:TYR:C	2.91	0.48
12:L:33:LYS:HD2	12:L:46:ASN:ND2	2.29	0.48
13:M:62:LEU:HD13	13:M:79:ILE:CD1	2.43	0.48
1:O:24:ILE:HD13	1:O:131:PRO:CG	2.44	0.48
3:Q:33:ARG:HH11	3:Q:33:ARG:HB3	1.77	0.48
4:R:50:VAL:HG22	4:R:67:ILE:CD1	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:15:PHE:HB2	6:T:23:GLN:HE22	1.78	0.48
6:T:172:ALA:C	6:T:176:LEU:HD23	2.38	0.48
8:V:84:LYS:HE2	8:V:119:THR:HG23	1.95	0.48
11:Y:4:LEU:HD13	11:Y:159:ILE:HD11	1.96	0.48
2:B:65:GLU:HG3	2:B:66:LYS:HG3	1.96	0.48
5:E:172:ALA:HB2	5:E:196:ALA:O	2.14	0.48
8:H:32:ALA:HB2	8:H:189:ARG:NH1	2.27	0.48
12:L:165:ARG:NH2	8:V:29:LYS:HE2	2.29	0.48
13:M:165:ARG:NH1	8:V:139:GLU:OE1	2.47	0.48
1:O:32:LYS:HA	1:O:32:LYS:CE	2.41	0.48
2:P:186:VAL:HG21	2:P:216:ARG:HD3	1.96	0.48
3:Q:226:SER:HB2	3:Q:227:GLU:OE1	2.13	0.48
4:R:18:GLU:OE2	4:R:18:GLU:N	2.45	0.48
4:R:227:GLU:OE2	4:R:227:GLU:N	2.45	0.48
9:W:15:ALA:HB3	9:W:155:ILE:HD11	1.96	0.48
9:W:43:LEU:CG	9:W:45:ILE:HD11	2.42	0.48
11:Y:66:HIS:CG	11:Y:74:ILE:HD13	2.49	0.48
12:Z:5:GLY:O	12:Z:124:CYS:HA	2.13	0.48
12:Z:33:LYS:HD2	12:Z:46:ASN:ND2	2.29	0.48
13:1:112:TYR:O	13:1:119:THR:HA	2.14	0.48
3:C:97:GLN:HA	3:C:97:GLN:HE21	1.77	0.48
3:C:173:ARG:O	3:C:177:GLU:HG3	2.13	0.48
1:O:32:LYS:HE2	1:O:32:LYS:CA	2.42	0.48
2:P:65:GLU:HG3	2:P:66:LYS:HG3	1.96	0.48
8:V:37:ILE:HD11	8:V:43:CYS:CB	2.43	0.48
8:V:116:HIS:HB2	17:V:1297:HOH:O	2.12	0.48
10:X:11:SER:HB3	10:X:179:ASP:HB3	1.96	0.48
10:X:20:VAL:HG11	11:Y:120:LEU:HD11	1.96	0.48
10:X:37:LEU:HD13	10:X:63:ILE:HD13	1.93	0.48
13:1:190:LEU:N	13:1:190:LEU:HD12	2.29	0.48
14:2:163:ILE:HD13	14:2:169:SER:CB	2.37	0.48
3:C:106:PRO:HG2	3:C:143:PRO:HG3	1.96	0.47
7:G:70:ILE:HD12	7:G:92:ALA:HB3	1.96	0.47
11:K:200:LYS:HG3	11:K:206:PHE:HB2	1.96	0.47
14:N:6:VAL:O	14:N:12:VAL:HG23	2.14	0.47
14:N:132:THR:HA	14:N:135:TYR:HD2	1.79	0.47
13:1:14(C):ARG:HG3	13:1:14(C):ARG:NH1	2.26	0.47
14:2:103:GLY:HA2	14:2:178:LEU:HD23	1.96	0.47
14:2:18(G):TYR:HA	14:2:18(J):LEU:HG	1.95	0.47
1:A:15:PHE:N	2:B:23:GLN:HE22	2.00	0.47
2:B:239:THR:HG22	2:B:239:THR:OXT	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:55:THR:C	3:C:56:LEU:HD22	2.40	0.47
4:D:70:ILE:HD12	4:D:92:ALA:CB	2.43	0.47
5:E:213:ALA:HB1	5:E:223:ILE:CD1	2.44	0.47
10:J:34:THR:CG2	10:J:176:LYS:NZ	2.77	0.47
1:O:52:LYS:HG3	1:O:211:GLU:HB2	1.96	0.47
3:Q:70:ILE:HD11	3:Q:76:LEU:HD13	1.96	0.47
6:T:127:ASN:HD22	6:T:127:ASN:N	2.11	0.47
13:1:147:THR:OG1	13:1:150:VAL:HG23	2.14	0.47
14:2:146:MET:HE2	14:2:150:GLU:CB	2.44	0.47
1:A:69:LEU:HD23	1:A:70:LEU:N	2.29	0.47
4:D:172:ALA:HB1	4:D:196:ILE:HG21	1.96	0.47
5:E:221:PHE:CE1	5:E:223:ILE:CD1	2.92	0.47
6:F:137:ILE:CD1	6:F:163:ALA:CB	2.92	0.47
6:F:21(B):THR:O	6:F:21(C):ASN:HB2	2.13	0.47
7:G:8:TYR:O	7:G:12:ILE:CD1	2.60	0.47
11:K:9:GLN:CD	11:K:10:GLY:N	2.71	0.47
6:T:172:ALA:O	6:T:173:LYS:C	2.57	0.47
8:V:207:PRO:HG2	8:V:210:THR:OG1	2.14	0.47
2:B:122:GLY:C	2:B:124:THR:N	2.73	0.47
6:F:43:ASN:N	6:F:43:ASN:HD22	2.11	0.47
6:F:203:GLU:O	6:F:206:LYS:HD2	2.14	0.47
8:H:5:GLY:HA3	8:H:110:LEU:HD11	1.96	0.47
9:I:43:LEU:HG	9:I:45:ILE:HD11	1.97	0.47
3:Q:163:GLN:HE21	3:Q:164:THR:N	2.13	0.47
4:R:230:ALA:HA	4:R:233:ILE:HD12	1.97	0.47
4:R:243:ALA:O	4:R:244:GLU:CB	2.62	0.47
8:V:32:ALA:HB2	8:V:189:ARG:NH1	2.30	0.47
8:V:170:GLY:O	8:V:171:SER:HB2	2.15	0.47
10:X:58:TYR:HD2	10:X:59:ILE:HD12	1.79	0.47
3:C:225:SER:O	3:C:226:SER:C	2.58	0.47
7:G:107:MET:HE3	7:G:112:LEU:HB2	1.97	0.47
7:G:197:MET:HG2	7:G:205:PHE:CE1	2.50	0.47
14:N:120:HIS:HA	17:N:1107:HOH:O	2.15	0.47
2:P:69:LYS:HG3	2:P:221:GLN:OE1	2.15	0.47
6:T:203:GLU:O	6:T:206:LYS:HD2	2.13	0.47
11:Y:78:ALA:O	11:Y:82:ILE:HG13	2.13	0.47
12:Z:82:ASN:HD22	12:Z:82:ASN:C	2.20	0.47
2:B:196:THR:O	2:B:200:THR:HG23	2.14	0.47
4:D:243:ALA:O	4:D:244:GLU:CB	2.62	0.47
5:E:31:ILE:HD12	5:E:31:ILE:N	2.30	0.47
6:F:172:ALA:O	6:F:173:LYS:C	2.57	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:8:TYR:C	7:G:10:ARG:N	2.70	0.47
8:H:207:PRO:HG2	8:H:210:THR:OG1	2.15	0.47
10:J:144:PRO:HG3	11:Y:207:ASN:HD21	1.80	0.47
10:J:190:PHE:C	10:J:192:ALA:H	2.22	0.47
12:L:21:ILE:HD12	8:V:167:LEU:HD13	1.96	0.47
14:N:85:GLU:O	14:N:89:GLU:HB2	2.14	0.47
2:P:121:GLN:NE2	2:P:121:GLN:C	2.73	0.47
6:T:20(B):GLU:HG3	6:T:20(C):LYS:N	2.30	0.47
14:2:132:THR:HA	14:2:135:TYR:HD2	1.78	0.47
1:A:31:VAL:HG11	1:A:135:SER:HB2	1.97	0.47
1:A:100:TYR:CA	1:A:10(A):ILE:HD13	2.44	0.47
2:B:44:ASP:OD1	2:B:185:LYS:HE3	2.14	0.47
3:C:15:PHE:CE1	3:C:21:ILE:HD11	2.50	0.47
8:H:7:LYS:HG3	8:H:123:TYR:HA	1.96	0.47
9:I:43:LEU:HG	9:I:45:ILE:CD1	2.45	0.47
14:N:6:VAL:HG21	14:N:155:ILE:HD11	1.97	0.47
1:O:4:MET:CG	1:O:5:THR:H	2.26	0.47
1:O:26:TYR:CD1	7:U:17:PRO:HA	2.50	0.47
1:O:150:GLN:O	1:O:157:TYR:HA	2.15	0.47
3:Q:46:VAL:HB	3:Q:215:VAL:CG1	2.44	0.47
5:S:28:LEU:HA	5:S:31:ILE:HD12	1.97	0.47
5:S:54:ASN:ND2	5:S:56:ASP:O	2.48	0.47
6:T:157:TYR:CD1	6:T:157:TYR:C	2.93	0.47
7:U:72:ARG:HB2	7:U:72:ARG:NH1	2.30	0.47
9:W:22:SER:O	9:W:23:GLN:HB2	2.12	0.47
11:Y:16:VAL:HG21	11:Y:34:VAL:HG23	1.96	0.47
12:Z:-8:PHE:CB	13:1:-8:THR:HG23	2.45	0.47
12:Z:35:PHE:CD2	12:Z:56:VAL:HG11	2.50	0.47
14:2:19:ARG:HG3	14:2:26:ILE:HG23	1.97	0.47
2:B:15:PHE:H	3:C:23:GLN:NE2	1.95	0.47
2:B:229:ILE:O	2:B:233:LEU:HB2	2.15	0.47
6:F:127:ASN:HD22	6:F:127:ASN:N	2.11	0.47
5:S:18(C):PHE:C	5:S:18(E):LYS:N	2.73	0.47
5:S:226:GLY:O	5:S:227:GLU:C	2.58	0.47
11:Y:12:ILE:HD12	11:Y:110:ILE:CD1	2.44	0.47
12:Z:21:ILE:HG12	12:Z:22:THR:N	2.30	0.47
3:C:177:GLU:OE2	4:D:57:PRO:HD2	2.15	0.47
4:D:42:THR:C	4:D:44:GLU:H	2.22	0.47
8:H:84:LYS:HE2	8:H:119:THR:HG23	1.96	0.47
10:J:19:ALA:HB2	10:J:171:LYS:HG2	1.96	0.47
12:L:-8:PHE:HB3	13:M:-8:THR:HG23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:39:GLY:C	2:P:148:LEU:HD21	2.40	0.47
8:V:100:ILE:HD11	8:V:127:LEU:HG	1.96	0.47
5:E:38:VAL:HG22	5:E:164:ALA:HB2	1.96	0.47
5:E:2(C):VAL:CG1	5:E:2(D):ASP:N	2.77	0.47
9:I:61:TYR:CD1	9:I:61:TYR:C	2.93	0.47
10:J:69:ARG:HD2	17:J:514:HOH:O	2.15	0.47
11:K:20:ALA:HA	16:K:2(I):H10:O11	2.15	0.47
12:L:21:ILE:HB	12:L:25:SER:O	2.15	0.47
3:Q:163:GLN:NE2	3:Q:163:GLN:CA	2.74	0.47
3:Q:232:TYR:O	3:Q:236:ILE:HG13	2.14	0.47
5:S:67:ILE:HD13	5:S:77:SER:CB	2.44	0.47
5:S:230:ALA:C	5:S:232:TYR:H	2.23	0.47
7:U:8:TYR:C	7:U:10:ARG:N	2.72	0.47
9:W:-8:SER:O	9:W:-6:PRO:HD3	2.15	0.47
12:Z:85:HIS:CE1	17:Z:197:HOH:O	2.68	0.47
12:Z:167:ILE:C	12:Z:167:ILE:HD12	2.39	0.47
3:C:159:SER:O	4:D:59:LEU:HD22	2.15	0.46
7:G:179:HIS:C	7:G:179:HIS:ND1	2.73	0.46
12:L:185:ARG:HB3	12:L:185:ARG:NH1	2.29	0.46
3:Q:134:VAL:HG12	3:Q:135:SER:N	2.31	0.46
6:T:142:ASP:O	6:T:144:ASN:N	2.48	0.46
7:U:177:GLU:O	7:U:17(B):LYS:HG3	2.14	0.46
7:U:179:HIS:ND1	7:U:179:HIS:C	2.73	0.46
8:V:137:VAL:HG21	8:V:161:ALA:HB2	1.98	0.46
13:1:110:LEU:HG	13:1:125:LEU:HD12	1.96	0.46
14:2:98:GLY:C	14:2:99:ILE:HD12	2.40	0.46
6:F:192:GLN:O	6:F:196:ILE:HG12	2.15	0.46
7:G:234:VAL:O	7:G:237:ALA:HB3	2.15	0.46
1:O:38:LEU:C	1:O:38:LEU:HD12	2.40	0.46
2:P:101:LYS:HZ1	10:X:85:GLN:HE22	1.64	0.46
2:P:229:ILE:O	2:P:233:LEU:HB2	2.15	0.46
3:Q:149:TYR:CE1	3:Q:159:SER:HB3	2.50	0.46
5:S:18(C):PHE:C	5:S:18(E):LYS:H	2.23	0.46
7:U:116:MET:HE3	17:U:431:HOH:O	2.14	0.46
12:Z:8:GLY:HA3	12:Z:11:PHE:CZ	2.51	0.46
12:Z:134:ILE:O	12:Z:137:PHE:HB3	2.15	0.46
1:A:27:ALA:O	1:A:31:VAL:HG23	2.15	0.46
3:C:158:SER:CB	4:D:59:LEU:HD21	2.45	0.46
4:D:227:GLU:OE2	4:D:227:GLU:N	2.46	0.46
5:E:216:GLY:O	5:E:217:LYS:C	2.58	0.46
7:G:118:ASN:O	7:G:122:ILE:HD13	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:141:VAL:HG21	7:G:216:THR:HA	1.96	0.46
13:M:3:VAL:O	13:M:126:ALA:HA	2.15	0.46
13:M:91:ARG:HG3	13:M:92:SER:N	2.29	0.46
14:N:175:MET:HB2	14:N:187:LEU:HB2	1.96	0.46
5:S:67:ILE:HG21	5:S:213:ALA:HB2	1.97	0.46
7:U:225:SER:O	7:U:229:ILE:HG13	2.15	0.46
10:X:45:PHE:HB3	10:X:99:VAL:HG12	1.96	0.46
13:1:3:VAL:O	13:1:126:ALA:HA	2.15	0.46
14:2:8:PHE:CE1	14:2:10:ASP:HB2	2.51	0.46
12:L:163:THR:HG23	17:L:1264:HOH:O	2.15	0.46
3:Q:57:LYS:HD2	3:Q:58:LEU:N	2.31	0.46
5:S:15:PHE:N	6:T:23:GLN:HE22	2.04	0.46
5:S:69:LYS:HB3	17:S:528:HOH:O	2.16	0.46
7:U:87:ASN:HD22	7:U:88:ALA:N	2.14	0.46
1:A:24:ILE:H	1:A:24:ILE:HD12	1.81	0.46
2:B:184:MET:HE1	2:B:189:ALA:HA	1.97	0.46
3:C:57:LYS:HD2	3:C:58:LEU:N	2.30	0.46
3:C:167:ARG:O	3:C:168:ASN:HB2	2.16	0.46
5:E:52:LYS:O	5:E:63:TYR:HD2	1.98	0.46
7:G:31:THR:HG21	7:G:135:ILE:HG12	1.96	0.46
11:K:46:ALA:HB3	11:K:98:GLY:O	2.15	0.46
2:P:5:SER:O	2:P:7:ARG:N	2.49	0.46
4:R:101:LEU:CD1	11:Y:57:THR:HG22	2.45	0.46
4:R:170:GLU:OE1	4:R:170:GLU:N	2.49	0.46
7:U:70:ILE:HD12	7:U:74:ILE:CG2	2.43	0.46
8:V:7:LYS:HG3	8:V:123:TYR:HA	1.97	0.46
10:X:185:ARG:HG2	10:X:185:ARG:NH1	2.29	0.46
14:2:3:ILE:HD13	14:2:3:ILE:N	2.30	0.46
1:A:13:THR:CG2	1:A:24:ILE:CD1	2.94	0.46
1:A:166:GLY:O	1:A:167:LYS:C	2.58	0.46
4:D:79:SER:HB3	4:D:165:ILE:HD12	1.96	0.46
4:D:170:GLU:N	4:D:170:GLU:OE1	2.49	0.46
5:E:69:LYS:HB3	17:E:684:HOH:O	2.14	0.46
9:I:114:ASP:OD2	9:I:116:ILE:CD1	2.61	0.46
10:J:11:SER:HB3	10:J:179:ASP:HB3	1.96	0.46
13:M:184:LEU:HD23	13:M:185:THR:N	2.30	0.46
2:P:190:ILE:HG23	2:P:212:PHE:CE2	2.50	0.46
4:R:14:THR:HG22	4:R:15:PHE:N	2.30	0.46
4:R:79:SER:HB3	4:R:165:ILE:HD12	1.96	0.46
5:S:86:ARG:HH11	5:S:86:ARG:HG3	1.81	0.46
6:T:70:VAL:HG11	6:T:112:PHE:CE1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:190:PHE:C	10:X:192:ALA:H	2.22	0.46
11:Y:79:ALA:HA	11:Y:82:ILE:HD12	1.98	0.46
12:Z:8:GLY:O	12:Z:108:GLY:HA3	2.15	0.46
1:A:130:ARG:NH2	7:G:124:THR:HG22	2.18	0.46
6:F:229:LEU:O	6:F:233:ILE:HD12	2.16	0.46
1:O:198:LYS:HE3	1:O:236:LEU:HD11	1.97	0.46
2:P:121:GLN:CG	3:Q:83:ALA:HB1	2.46	0.46
2:P:184:MET:HE1	2:P:189:ALA:HA	1.96	0.46
4:R:75:GLY:HA3	4:R:221:PHE:CE2	2.50	0.46
5:S:4:PHE:O	5:S:5:ARG:C	2.59	0.46
6:T:109:ILE:CG2	6:T:147:HIS:HB2	2.42	0.46
7:U:25:GLU:O	7:U:28:PHE:HB2	2.16	0.46
13:1:17:ASP:C	13:1:17:ASP:OD2	2.59	0.46
1:A:130:ARG:HH11	1:A:130:ARG:HG3	1.81	0.46
3:C:134:VAL:HG12	3:C:135:SER:N	2.30	0.46
4:D:68:VAL:HG21	4:D:89:ILE:HD13	1.97	0.46
5:E:226:GLY:O	5:E:227:GLU:C	2.58	0.46
7:G:49:ILE:CD1	7:G:193:ALA:CB	2.90	0.46
8:H:45:GLY:HA2	8:H:99:LEU:HD23	1.97	0.46
2:P:121:GLN:HG3	3:Q:83:ALA:HB1	1.98	0.46
5:S:74:MET:HE2	5:S:109:VAL:HA	1.97	0.46
5:S:213:ALA:HB1	5:S:223:ILE:CD1	2.46	0.46
8:V:45:GLY:HA2	8:V:99:LEU:HD23	1.98	0.46
1:A:4:MET:CG	1:A:5:THR:H	2.25	0.46
2:B:100:LEU:HG	9:I:60:ARG:NH2	2.31	0.46
2:B:190:ILE:HG23	2:B:212:PHE:CE2	2.50	0.46
3:C:212:ILE:HD13	3:C:229:ILE:HG23	1.98	0.46
5:E:139:ILE:HD12	5:E:215:VAL:HG12	1.98	0.46
8:H:165:ASN:ND2	13:1:139:ARG:HH11	2.14	0.46
11:K:126:CYS:HB2	11:K:135:TYR:CZ	2.51	0.46
14:N:8:PHE:CE1	14:N:10:ASP:HB2	2.51	0.46
3:Q:93:ARG:HD2	17:Q:314:HOH:O	2.16	0.46
3:Q:159:SER:O	4:R:59:LEU:HD22	2.16	0.46
3:Q:215:VAL:HG13	3:Q:215:VAL:O	2.16	0.46
4:R:160:TYR:CZ	4:R:163:LYS:HD3	2.51	0.46
4:D:185:THR:OG1	4:D:188:GLU:HG3	2.14	0.46
6:F:137:ILE:CD1	6:F:163:ALA:HB3	2.45	0.46
8:H:137:VAL:HG21	8:H:161:ALA:HB2	1.97	0.46
12:L:134:ILE:O	12:L:137:PHE:HB3	2.16	0.46
14:N:147:SER:OG	14:N:150:GLU:HG3	2.16	0.46
4:R:196:ILE:H	4:R:196:ILE:HD12	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:192:GLN:O	6:T:196:ILE:HG12	2.16	0.46
14:2:134:ILE:C	14:2:134:ILE:HD12	2.41	0.46
8:H:159:ILE:HD13	8:H:173:VAL:CG1	2.47	0.45
10:J:144:PRO:CG	11:Y:207:ASN:HD21	2.29	0.45
13:M:-6:GLN:O	13:M:-6:GLN:HG3	2.15	0.45
13:M:147:THR:HB	13:M:149:GLN:NE2	2.31	0.45
5:S:150:GLU:O	5:S:157:VAL:HA	2.16	0.45
6:T:192:GLN:NE2	6:T:195:LYS:CE	2.79	0.45
7:U:18(M):SER:HB2	7:U:187:GLU:OE2	2.16	0.45
8:V:5:GLY:HA3	8:V:110:LEU:HD11	1.98	0.45
11:Y:87:VAL:HG21	11:Y:97:MET:HE2	1.98	0.45
1:A:73:ASP:C	1:A:74:ILE:HG13	2.41	0.45
3:C:169:SER:HA	3:C:172:VAL:CG1	2.47	0.45
3:C:232:TYR:O	3:C:236:ILE:HG13	2.16	0.45
5:E:15:PHE:HB2	6:F:23:GLN:NE2	2.31	0.45
5:E:43:ASN:HB2	5:E:183:ASP:OD1	2.16	0.45
7:G:72:ARG:NH1	7:G:72:ARG:HB2	2.31	0.45
11:K:7:ARG:CG	11:K:108:PRO:HB2	2.40	0.45
11:K:12:ILE:HD13	11:K:110:ILE:CD1	2.45	0.45
12:L:140:ASN:O	12:L:144:PHE:HA	2.16	0.45
8:V:15:ALA:HB1	8:V:159:ILE:HD13	1.98	0.45
10:X:17:SER:HB2	10:X:170:PHE:HB2	1.98	0.45
11:Y:9:GLN:CD	11:Y:10:GLY:N	2.74	0.45
1:A:7:ARG:NH1	5:E:127:TYR:HD2	2.14	0.45
1:A:179:ARG:HH11	1:A:179:ARG:CB	2.22	0.45
3:C:52:ARG:HB2	3:C:209:ASN:HA	1.98	0.45
9:I:89:GLU:O	9:I:90:ARG:NH1	2.48	0.45
9:I:192:ARG:HD3	17:I:1187:HOH:O	2.15	0.45
11:K:172:SER:CA	11:K:192:VAL:HG23	2.47	0.45
13:M:29:ASN:N	17:M:802:HOH:O	2.50	0.45
1:O:130:ARG:HH11	1:O:130:ARG:HG3	1.82	0.45
2:P:6:ARG:HG2	3:Q:10:ARG:NH2	2.32	0.45
5:S:95:GLN:HG3	5:S:115:LEU:HD13	1.97	0.45
5:S:139:ILE:HG22	5:S:148:LEU:HD13	1.96	0.45
6:T:21:ASN:C	6:T:21:ASN:OD1	2.57	0.45
7:U:70:ILE:HA	7:U:93:LYS:HG2	1.99	0.45
10:X:52:THR:HG22	10:X:53:VAL:H	1.81	0.45
10:X:189:ASP:HA	10:X:191:GLN:OE1	2.16	0.45
14:2:85:GLU:O	14:2:89:GLU:HB2	2.15	0.45
1:A:52:LYS:HG3	1:A:211:GLU:HB2	1.96	0.45
2:B:41:MET:HE2	2:B:146:TYR:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:107:ILE:CD1	2:B:112:LEU:H	2.28	0.45
2:B:121:GLN:NE2	2:B:121:GLN:C	2.74	0.45
4:D:12:VAL:HG23	4:D:12(A):GLY:HA2	1.98	0.45
5:E:15:PHE:N	6:F:23:GLN:HE22	2.05	0.45
10:J:45:PHE:HB3	10:J:99:VAL:HG12	1.97	0.45
10:J:52:THR:HG22	10:J:53:VAL:H	1.81	0.45
11:K:35:ILE:HD11	11:K:45:MET:HB2	1.99	0.45
11:K:90:TYR:O	11:K:91:LYS:C	2.59	0.45
2:P:228:GLU:O	2:P:232:ILE:HG22	2.17	0.45
3:Q:167:ARG:O	3:Q:168:ASN:HB2	2.16	0.45
3:Q:169:SER:HA	3:Q:172:VAL:CG1	2.46	0.45
5:S:38:VAL:HG12	5:S:39:GLY:N	2.31	0.45
7:U:18(D):ILE:O	7:U:18(G):GLU:N	2.49	0.45
7:U:234:VAL:O	7:U:237:ALA:HB3	2.16	0.45
11:Y:6:PHE:HA	11:Y:123:ASP:O	2.17	0.45
6:F:21:ASN:OD1	6:F:21:ASN:C	2.59	0.45
6:F:32:GLU:HB3	6:F:169:ARG:NH2	2.31	0.45
6:F:172:ALA:C	6:F:176:LEU:HD23	2.42	0.45
8:H:167:LEU:HB3	12:Z:167:ILE:HD13	1.99	0.45
1:O:31:VAL:HG13	1:O:79:SER:O	2.16	0.45
2:P:138:TYR:HB2	2:P:149:TYR:HB2	1.98	0.45
2:P:222:LYS:NZ	2:P:228:GLU:OE2	2.46	0.45
3:Q:15:PHE:CD1	3:Q:21:ILE:CD1	2.99	0.45
3:Q:185:THR:HG22	3:Q:187:GLU:N	2.28	0.45
7:U:139:VAL:HA	7:U:147:SER:O	2.16	0.45
7:U:197:MET:HG2	7:U:205:PHE:CE1	2.51	0.45
11:Y:38:ASN:C	11:Y:38:ASN:OD1	2.58	0.45
12:Z:6:ILE:HG12	12:Z:124:CYS:CB	2.47	0.45
12:Z:33:LYS:NZ	17:Z:754:HOH:O	2.49	0.45
12:Z:14(I):THR:O	12:Z:1(I):ASN:HB3	2.16	0.45
3:C:79:SER:HB2	3:C:165:ILE:HD12	1.98	0.45
4:D:75:GLY:HA3	4:D:221:PHE:CE2	2.51	0.45
4:D:177:LEU:HD22	5:E:58:LEU:HD13	1.99	0.45
8:H:36:ARG:HG3	8:H:38:SER:O	2.17	0.45
8:H:49:ALA:HB1	9:I:118:CYS:SG	2.56	0.45
12:L:11:PHE:CE1	12:L:148:VAL:HA	2.51	0.45
5:S:139:ILE:HD12	5:S:215:VAL:HG12	1.98	0.45
6:T:24:VAL:O	6:T:27:ALA:HB3	2.17	0.45
7:U:46:THR:HG21	7:U:139:VAL:HB	1.99	0.45
9:W:43:LEU:HG	9:W:45:ILE:CD1	2.47	0.45
9:W:80:THR:HG23	9:W:113:PHE:CE1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:7:ARG:CG	11:Y:108:PRO:HB2	2.38	0.45
13:1:178:ILE:HD12	13:1:178:ILE:N	2.32	0.45
14:2:132:THR:HA	14:2:135:TYR:CD2	2.52	0.45
1:A:197:LEU:HD21	1:A:210:ILE:HD12	1.99	0.45
2:B:21:LEU:O	2:B:25:GLU:HG2	2.16	0.45
2:B:39:GLY:C	2:B:148:LEU:HD21	2.42	0.45
2:B:101:LYS:NZ	10:J:85:GLN:NE2	2.64	0.45
5:E:4:PHE:O	5:E:5:ARG:C	2.58	0.45
11:K:6:PHE:HA	11:K:123:ASP:O	2.16	0.45
11:K:64:ARG:HD2	17:K:959:HOH:O	2.17	0.45
11:Y:7:ARG:CG	11:Y:12:ILE:HD11	2.39	0.45
12:Z:40:ASN:HD21	12:Z:183:GLY:HA2	1.81	0.45
14:2:107:LYS:HG2	14:2:108:GLY:H	1.82	0.45
14:2:18(A):ILE:HD12	14:2:18(C):TYR:CE2	2.52	0.45
2:B:97:GLN:NE2	17:B:246:HOH:O	2.49	0.45
2:B:171:ALA:O	2:B:175:LEU:HG	2.17	0.45
12:L:14(I):THR:O	12:L:1(I):ASN:HB3	2.16	0.45
3:Q:190:VAL:HG13	3:Q:212:ILE:HG21	1.99	0.45
7:U:99:PHE:C	7:U:99:PHE:CD1	2.95	0.45
13:1:157:ASN:ND2	17:1:905:HOH:O	2.45	0.45
4:D:50:VAL:HG22	4:D:67:ILE:CD1	2.44	0.45
6:F:109:ILE:HG22	6:F:149:TYR:CE2	2.52	0.45
6:F:142:ASP:O	6:F:144:ASN:N	2.50	0.45
6:F:20(B):GLU:HG3	6:F:20(C):LYS:N	2.30	0.45
7:G:25:GLU:O	7:G:28:PHE:HB2	2.17	0.45
13:M:19:LEU:HD12	13:M:28:PHE:O	2.17	0.45
14:N:103:GLY:HA2	14:N:178:LEU:HD23	1.99	0.45
10:X:185:ARG:NH1	17:X:730:HOH:O	2.50	0.45
14:2:66:TYR:CD2	14:2:74:PRO:HB3	2.52	0.45
4:D:122:ARG:HG2	4:D:122:ARG:HH11	1.81	0.45
4:D:229:THR:O	4:D:230:ALA:C	2.60	0.45
5:E:38:VAL:HG12	5:E:39:GLY:N	2.32	0.45
5:E:74:MET:HE2	5:E:109:VAL:HA	1.99	0.45
5:E:86:ARG:HH11	5:E:86:ARG:HG3	1.82	0.45
8:H:179:GLU:OE2	8:H:182:LYS:HE2	2.16	0.45
12:L:90:LYS:HD3	12:L:95:TYR:CZ	2.52	0.45
12:L:192:LYS:HE3	8:V:195:ASN:HB3	1.99	0.45
2:P:111:ILE:HD11	10:X:70:GLU:HG2	1.99	0.45
2:P:224:PHE:HD2	2:P:224:PHE:H	1.65	0.45
3:Q:177:GLU:OE2	4:R:57:PRO:HD2	2.17	0.45
4:R:45:GLY:HA2	4:R:146:TYR:CE1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:197:LEU:O	4:R:201:MET:HG3	2.17	0.45
6:T:45:GLY:CA	6:T:215:CYS:O	2.65	0.45
7:U:121:GLN:NE2	7:U:121:GLN:C	2.75	0.45
14:2:38:HIS:O	14:2:39:ASP:C	2.60	0.45
1:A:224:LEU:HB2	1:A:229:ILE:HD11	1.98	0.44
3:C:55:THR:HG22	3:C:56:LEU:CD2	2.42	0.44
3:C:215:VAL:HG23	3:C:221:ILE:HG12	1.99	0.44
5:E:57:GLU:C	5:E:58:LEU:HD12	2.41	0.44
5:E:198:SER:HA	5:E:201:LEU:CG	2.47	0.44
6:F:49:ALA:HA	6:F:211:GLU:O	2.17	0.44
6:F:18(C):HIS:CE1	17:F:1343:HOH:O	2.70	0.44
7:G:18(M):SER:HB2	7:G:187:GLU:OE2	2.17	0.44
9:I:80:THR:HG23	9:I:113:PHE:CE1	2.52	0.44
10:J:143:ARG:HB2	10:J:146:MET:HG3	1.99	0.44
14:N:163:ILE:CG2	14:N:170:GLY:HA2	2.47	0.44
1:O:40:ILE:HD12	1:O:193:ALA:HB2	1.98	0.44
1:O:86:ARG:NE	7:U:118:ASN:HD21	2.13	0.44
2:P:44:ASP:OD1	2:P:185:LYS:HE3	2.16	0.44
4:R:117:CYS:SG	4:R:157:PHE:HB3	2.57	0.44
4:R:122:ARG:HG2	4:R:122:ARG:HH11	1.82	0.44
11:Y:14:VAL:HB	11:Y:176:TYR:HB2	1.98	0.44
12:Z:140:ASN:O	12:Z:144:PHE:HA	2.17	0.44
13:1:147:THR:HB	13:1:149:GLN:NE2	2.31	0.44
5:E:17:PRO:HA	6:F:26:TYR:CD2	2.52	0.44
6:F:45:GLY:CA	6:F:215:CYS:O	2.65	0.44
8:H:9:ASN:OD1	8:H:10:ASN:N	2.50	0.44
10:J:189:ASP:HA	10:J:191:GLN:OE1	2.18	0.44
12:L:35:PHE:HA	17:L:1224:HOH:O	2.17	0.44
3:Q:125:GLN:HB2	4:R:130:ARG:HG2	1.99	0.44
8:V:37:ILE:N	8:V:37:ILE:HD12	2.31	0.44
10:X:65:LEU:HD21	10:X:69:ARG:HH22	1.83	0.44
2:B:181:LYS:O	2:B:184:MET:HG3	2.18	0.44
5:E:91:TYR:CD1	5:E:119:LYS:HD2	2.52	0.44
10:J:35:ARG:O	10:J:42:LEU:HD12	2.17	0.44
10:J:66:TYR:CE2	10:J:74:LEU:HG	2.52	0.44
1:O:109:THR:O	1:O:113:VAL:HG23	2.17	0.44
5:S:18(C):PHE:CD1	5:S:18(D):ILE:N	2.85	0.44
7:U:170:GLN:NE2	7:U:174:THR:HG23	2.27	0.44
8:V:9:ASN:OD1	8:V:10:ASN:N	2.51	0.44
10:X:37:LEU:HD13	10:X:63:ILE:HD11	1.98	0.44
1:A:67:VAL:HG11	1:A:213:ALA:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:63:THR:O	2:B:63:THR:HG22	2.18	0.44
6:F:121:GLN:NE2	6:F:121:GLN:C	2.76	0.44
7:G:131:PRO:HB3	17:G:243:HOH:O	2.16	0.44
8:H:34:LEU:HA	8:H:43:CYS:O	2.18	0.44
12:L:8:GLY:HA3	12:L:11:PHE:CZ	2.52	0.44
13:M:35:ILE:N	13:M:35:ILE:HD12	2.33	0.44
13:M:139:ARG:HH11	8:V:165:ASN:ND2	2.14	0.44
2:P:63:THR:O	2:P:63:THR:HG22	2.17	0.44
3:Q:99:HIS:CG	3:Q:107:VAL:HG12	2.52	0.44
3:Q:106:PRO:HG2	3:Q:143:PRO:HG3	1.98	0.44
3:Q:197:LEU:O	3:Q:201:VAL:HG23	2.18	0.44
8:V:3:ILE:CD1	8:V:46:ALA:HB2	2.48	0.44
8:V:36:ARG:HG3	8:V:38:SER:O	2.17	0.44
8:V:63:ILE:CG2	8:V:74:PRO:HB3	2.46	0.44
8:V:63:ILE:HG23	8:V:74:PRO:HB3	2.00	0.44
12:Z:113:PHE:N	12:Z:113:PHE:CD1	2.86	0.44
13:1:5:PRO:HD3	13:1:96:TRP:CE2	2.52	0.44
2:B:31:ILE:HD11	2:B:133:GLY:C	2.42	0.44
6:F:24:VAL:O	6:F:27:ALA:HB3	2.17	0.44
6:F:203:GLU:C	6:F:205:ASN:H	2.26	0.44
11:K:119:ARG:HG2	17:K:1232:HOH:O	2.18	0.44
13:M:191:GLN:HE21	13:M:191:GLN:HB3	1.59	0.44
2:P:122:GLY:C	2:P:124:THR:N	2.74	0.44
7:U:13:THR:HB	7:U:124:THR:O	2.18	0.44
12:Z:11:PHE:CE1	12:Z:148:VAL:HA	2.52	0.44
12:Z:185:ARG:HB3	12:Z:185:ARG:NH1	2.32	0.44
13:1:35:ILE:HD11	13:1:56:GLU:HG3	1.98	0.44
13:1:45:ILE:HG12	13:1:99:ILE:HG12	1.98	0.44
2:B:107:ILE:CD1	2:B:112:LEU:N	2.78	0.44
3:C:149:TYR:CE1	3:C:159:SER:HB3	2.52	0.44
4:D:45:GLY:HA2	4:D:146:TYR:CE1	2.52	0.44
4:D:196:ILE:HD12	4:D:196:ILE:H	1.83	0.44
5:E:31:ILE:HD12	5:E:31:ILE:H	1.82	0.44
5:E:18(C):PHE:C	5:E:18(E):LYS:H	2.25	0.44
5:E:18(C):PHE:C	5:E:18(E):LYS:N	2.75	0.44
5:E:186:PRO:O	5:E:187:ASP:C	2.61	0.44
8:H:15:ALA:HB1	8:H:159:ILE:HD13	1.97	0.44
9:I:137:MET:HE3	9:I:141:LEU:CD1	2.46	0.44
10:J:35:ARG:HD3	10:J:35:ARG:HA	1.76	0.44
13:M:197:TRP:CH2	14:2:171:GLY:HA2	2.53	0.44
14:N:132:THR:HA	14:N:135:TYR:CD2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:171:ALA:O	2:P:175:LEU:HG	2.18	0.44
2:P:232:ILE:O	2:P:232:ILE:HG12	2.18	0.44
3:Q:19:GLY:O	4:R:30:ALA:HB2	2.17	0.44
3:Q:225:SER:O	3:Q:226:SER:C	2.58	0.44
5:S:43:ASN:HB2	5:S:183:ASP:OD1	2.17	0.44
5:S:116:LEU:HD23	5:S:116:LEU:HA	1.86	0.44
6:T:12:ASN:OD1	6:T:12:ASN:C	2.61	0.44
6:T:121:GLN:NE2	6:T:121:GLN:C	2.75	0.44
8:V:34:LEU:HA	8:V:43:CYS:O	2.17	0.44
8:V:207:PRO:O	8:V:210:THR:OG1	2.24	0.44
13:1:147:THR:HB	13:1:149:GLN:HE22	1.83	0.44
14:2:37:VAL:HG22	14:2:41:ILE:HG22	1.99	0.44
14:2:147:SER:OG	14:2:150:GLU:HG3	2.17	0.44
1:O:29:THR:O	1:O:33:GLN:HG2	2.17	0.44
1:O:69:LEU:HD23	1:O:70:LEU:N	2.32	0.44
1:O:86:ARG:HH21	7:U:118:ASN:ND2	2.16	0.44
6:T:18:ASP:OD1	6:T:20:ARG:HD3	2.17	0.44
11:Y:5:ALA:HA	11:Y:13:ILE:O	2.17	0.44
14:2:107:LYS:HG2	14:2:108:GLY:N	2.33	0.44
5:E:160:LEU:HD13	5:E:163:THR:HB	1.99	0.44
9:I:35:PHE:CD1	9:I:45:ILE:HD13	2.53	0.44
11:K:8:PHE:O	11:K:9:GLN:C	2.61	0.44
13:M:160:ARG:HB2	13:M:192:VAL:HG13	2.00	0.44
1:O:47:VAL:CG2	1:O:212:LEU:HD21	2.48	0.44
1:O:190:ILE:HD11	1:O:214:ILE:HG22	1.99	0.44
2:P:225:LYS:O	2:P:226:PRO:C	2.61	0.44
7:U:35:ILE:HD11	7:U:53:LYS:CG	2.46	0.44
10:X:19:ALA:HB2	10:X:171:LYS:HG2	1.98	0.44
11:Y:126:CYS:HB2	11:Y:135:TYR:CZ	2.53	0.44
11:Y:172:SER:CA	11:Y:192:VAL:HG23	2.46	0.44
7:G:198:ILE:O	7:G:202:GLY:N	2.50	0.44
11:K:38:ASN:C	11:K:38:ASN:OD1	2.61	0.44
13:M:74:LEU:HB3	13:M:79:ILE:HD11	2.00	0.44
14:N:66:TYR:CD2	14:N:74:PRO:HB3	2.52	0.44
1:O:24:ILE:HD13	1:O:131:PRO:HG2	1.99	0.44
1:O:33:GLN:HE21	1:O:33:GLN:CA	2.31	0.44
2:P:21:LEU:O	2:P:25:GLU:HG2	2.17	0.44
3:Q:76:LEU:C	3:Q:76:LEU:HD23	2.43	0.44
10:X:93:ARG:CZ	11:Y:91:LYS:HD3	2.48	0.44
14:2:6:VAL:O	14:2:12:VAL:HG23	2.17	0.44
1:A:150:GLN:O	1:A:157:TYR:HA	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:76:LEU:HD23	3:C:76:LEU:C	2.43	0.43
4:D:18:GLU:OE2	4:D:18:GLU:N	2.50	0.43
4:D:160:TYR:CZ	4:D:163:LYS:HD3	2.52	0.43
8:H:1:THR:CG2	8:H:2:THR:N	2.80	0.43
1:O:17:PRO:HG3	2:P:26:TYR:CZ	2.53	0.43
3:Q:123:TYR:CD1	3:Q:132:PHE:HE1	2.36	0.43
4:R:70:ILE:HB	4:R:74:ILE:HG22	2.00	0.43
6:T:150:MET:HE2	6:T:160:TYR:CZ	2.52	0.43
6:T:195:LYS:HZ1	6:T:196:ILE:CD1	2.31	0.43
10:X:152:LEU:HD21	10:X:177:ILE:HD11	2.00	0.43
11:Y:4:LEU:C	11:Y:4:LEU:HD22	2.43	0.43
11:Y:12:ILE:HG23	11:Y:110:ILE:HD11	2.00	0.43
12:Z:90:LYS:HD3	12:Z:95:TYR:CZ	2.53	0.43
2:B:5:SER:O	2:B:7:ARG:N	2.50	0.43
2:B:20:ARG:NH1	2:B:20:ARG:HG2	2.33	0.43
5:E:4:PHE:O	5:E:6:ASN:N	2.51	0.43
12:L:21:ILE:HD11	12:L:168:GLN:NE2	2.33	0.43
13:M:13:ILE:HB	13:M:155:ILE:CD1	2.48	0.43
1:O:62:GLU:O	1:O:64:LEU:N	2.47	0.43
1:O:166:GLY:O	1:O:167:LYS:C	2.61	0.43
2:P:39:GLY:O	2:P:162:ALA:HA	2.18	0.43
3:Q:163:GLN:HE22	3:Q:173:ARG:NE	2.14	0.43
4:R:90:GLU:OE2	11:Y:69:ARG:NH1	2.51	0.43
5:S:57:GLU:C	5:S:58:LEU:HD12	2.43	0.43
5:S:78:LEU:HD12	5:S:78:LEU:C	2.43	0.43
5:S:114:HIS:HB3	6:T:86:ARG:NH2	2.33	0.43
6:T:49:ALA:HA	6:T:211:GLU:O	2.18	0.43
1:A:13:THR:HG22	1:A:21:LEU:HD22	2.01	0.43
3:C:70:ILE:HD11	3:C:76:LEU:HD13	1.99	0.43
5:E:95:GLN:HG3	5:E:115:LEU:HD13	2.00	0.43
6:F:211:GLU:C	6:F:212:ILE:HD13	2.44	0.43
7:G:99:PHE:CD1	7:G:99:PHE:C	2.95	0.43
10:J:17:SER:HB2	10:J:170:PHE:HB2	2.00	0.43
12:L:42:VAL:CG2	12:L:102:ALA:HB3	2.47	0.43
12:L:113:PHE:N	12:L:113:PHE:CD1	2.86	0.43
13:M:112:TYR:O	13:M:119:THR:HA	2.18	0.43
2:P:41:MET:HE2	2:P:146:TYR:O	2.18	0.43
8:V:18:THR:HB	8:V:30:ASN:HA	2.00	0.43
14:2:126:ILE:N	14:2:126:ILE:CD1	2.81	0.43
2:B:231:ASP:O	2:B:235:LYS:HG2	2.19	0.43
4:D:24:VAL:O	4:D:28:LEU:HD13	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:39:GLY:HA3	6:F:137:ILE:HG21	2.00	0.43
7:G:70:ILE:HA	7:G:93:LYS:HG2	2.01	0.43
10:J:34:THR:CG2	10:J:176:LYS:HZ2	2.31	0.43
12:L:8:GLY:O	12:L:108:GLY:HA3	2.17	0.43
14:N:146:MET:HE2	14:N:150:GLU:CB	2.48	0.43
1:O:177:GLU:HG2	2:P:58:LEU:HD22	2.01	0.43
4:R:229:THR:O	4:R:230:ALA:C	2.62	0.43
5:S:134:VAL:O	5:S:153:PRO:HG3	2.19	0.43
8:V:192:LEU:HA	8:V:192:LEU:HD23	1.77	0.43
9:W:137:MET:HE2	9:W:161:ASN:HB2	2.01	0.43
10:X:166:MET:HA	10:X:167:PRO:HD3	1.72	0.43
14:2:38:HIS:HB3	14:2:41:ILE:HB	2.01	0.43
14:2:18(A):ILE:HD13	14:2:18(B):PHE:C	2.43	0.43
2:B:10:SER:HB2	17:B:248:HOH:O	2.18	0.43
2:B:17:PRO:HA	3:C:26:TYR:CZ	2.54	0.43
2:B:39:GLY:O	2:B:162:ALA:HA	2.19	0.43
4:D:215:ILE:HD13	4:D:215:ILE:O	2.18	0.43
5:E:18(C):PHE:CD1	5:E:18(D):ILE:N	2.86	0.43
11:K:13:ILE:HD12	11:K:152:LEU:HD23	2.01	0.43
11:K:14:VAL:HB	11:K:176:TYR:HB2	2.00	0.43
11:K:19:ARG:HG2	11:K:21:THR:HG23	2.01	0.43
12:L:52:GLY:O	12:L:56:VAL:HG23	2.18	0.43
13:M:190:LEU:HD12	13:M:190:LEU:N	2.33	0.43
1:O:62:GLU:C	1:O:64:LEU:N	2.76	0.43
1:O:67:VAL:HG11	1:O:213:ALA:HB3	1.99	0.43
2:P:97:GLN:HG2	17:P:297:HOH:O	2.19	0.43
2:P:150:THR:O	2:P:157:TYR:HA	2.18	0.43
2:P:21(A):LYS:HG3	2:P:219:GLU:O	2.18	0.43
2:P:234:VAL:HA	2:P:239:THR:HA	2.00	0.43
8:V:49:ALA:HB1	9:W:118:CYS:SG	2.58	0.43
1:A:186:LEU:HD21	1:A:214:ILE:HD12	2.01	0.43
2:B:194:LEU:O	2:B:198:SER:HB2	2.19	0.43
5:E:207:LEU:O	5:E:233:ILE:HD12	2.18	0.43
7:G:82:ILE:CG2	7:G:83:PRO:HD3	2.49	0.43
7:G:121:GLN:NE2	7:G:121:GLN:C	2.77	0.43
7:G:139:VAL:HA	7:G:147:SER:O	2.18	0.43
11:K:87:VAL:HG21	11:K:97:MET:HE2	1.99	0.43
1:O:73:ASP:C	1:O:74:ILE:HG13	2.43	0.43
2:P:150:THR:HG22	2:P:160:TRP:HE1	1.84	0.43
5:S:4:PHE:O	5:S:6:ASN:N	2.52	0.43
6:T:21(B):THR:O	6:T:21(C):ASN:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:1:THR:CG2	8:V:2:THR:N	2.82	0.43
2:B:149:TYR:OH	3:C:62(A):ILE:HB	2.19	0.43
2:B:235:LYS:HD3	2:B:235:LYS:N	2.34	0.43
3:C:123:TYR:CD1	3:C:132:PHE:HE1	2.37	0.43
5:E:116:LEU:HD23	5:E:116:LEU:HA	1.88	0.43
6:F:192:GLN:NE2	6:F:195:LYS:CE	2.81	0.43
7:G:47:VAL:CG1	7:G:49:ILE:HD11	2.48	0.43
13:M:42:VAL:CG2	13:M:178:ILE:HD11	2.48	0.43
2:P:20:ARG:NH1	2:P:20:ARG:HG2	2.33	0.43
2:P:31:ILE:HD11	2:P:133:GLY:C	2.44	0.43
4:R:192:LEU:O	4:R:196:ILE:HD13	2.19	0.43
4:R:196:ILE:HD12	4:R:196:ILE:N	2.34	0.43
5:S:67:ILE:HD11	5:S:77:SER:HB3	1.98	0.43
11:Y:38:ASN:HB2	11:Y:39:PRO:HD2	2.00	0.43
11:Y:74:ILE:HG13	11:Y:75:SER:N	2.33	0.43
1:A:69:LEU:C	1:A:69:LEU:CD2	2.91	0.43
1:A:175:PHE:O	1:A:179:ARG:HG2	2.19	0.43
2:B:150:THR:O	2:B:157:TYR:HA	2.19	0.43
3:C:99:HIS:CG	3:C:107:VAL:HG12	2.54	0.43
5:E:146:ALA:N	17:E:1070:HOH:O	2.51	0.43
7:G:220:LYS:HG2	7:G:221:PHE:N	2.34	0.43
8:H:63:ILE:CG2	8:H:74:PRO:HB3	2.49	0.43
9:I:137:MET:HE2	9:I:161:ASN:HB2	2.01	0.43
10:J:93:ARG:CZ	11:K:91:LYS:HD3	2.49	0.43
11:K:207:ASN:ND2	10:X:144:PRO:HD3	2.34	0.43
12:L:3:ILE:CD1	12:L:3:ILE:N	2.80	0.43
12:L:185:ARG:NH1	17:L:1161:HOH:O	2.38	0.43
13:M:17:ASP:HA	13:M:173:PHE:HB3	2.01	0.43
13:M:150:VAL:HG21	17:M:1069:HOH:O	2.18	0.43
1:O:184:LEU:HB2	17:O:486:HOH:O	2.19	0.43
5:S:83:PRO:O	5:S:86:ARG:HB3	2.18	0.43
5:S:136:LEU:HD12	5:S:151:PHE:CD2	2.54	0.43
5:S:2(C):VAL:HG13	5:S:2(D):ASP:N	2.34	0.43
7:U:67:ILE:HD12	7:U:211:GLU:CG	2.44	0.43
7:U:145:GLY:O	7:U:146:PRO:C	2.62	0.43
8:V:100:ILE:CD1	8:V:112:SER:HB3	2.49	0.43
11:Y:46:ALA:HB3	11:Y:98:GLY:O	2.18	0.43
12:Z:137:PHE:CE1	12:Z:141:GLN:HG3	2.53	0.43
14:2:8:PHE:HE1	14:2:10:ASP:HB2	1.84	0.43
1:A:188:ASP:O	1:A:192:ILE:HG12	2.18	0.43
2:B:222:LYS:NZ	2:B:228:GLU:OE2	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:228:GLU:O	2:B:232:ILE:HG22	2.19	0.43
3:C:212:ILE:HD12	3:C:212:ILE:N	2.33	0.43
3:C:215:VAL:O	3:C:215:VAL:HG13	2.19	0.43
6:F:91:ARG:O	6:F:95:GLU:HB2	2.19	0.43
10:J:18:LYS:CD	10:J:174:ILE:HG13	2.45	0.43
12:L:3:ILE:HD12	12:L:46:ASN:CG	2.44	0.43
12:L:82:ASN:C	12:L:82:ASN:ND2	2.77	0.43
12:L:148:VAL:O	12:L:152:ILE:HG13	2.19	0.43
1:O:92:SER:O	1:O:95:VAL:HG12	2.18	0.43
3:Q:156:ILE:HD12	3:Q:156:ILE:N	2.33	0.43
7:U:74:ILE:HD12	7:U:109:CYS:HA	2.00	0.43
9:W:174:VAL:HG21	9:W:186:LYS:HE3	2.01	0.43
1:A:232:ARG:HG3	1:A:232:ARG:NH1	2.33	0.43
2:B:224:PHE:HD2	2:B:224:PHE:H	1.66	0.43
3:C:160:TRP:NE1	4:D:59:LEU:HD23	2.34	0.43
6:F:130:ARG:HG2	6:F:130:ARG:HH11	1.84	0.43
6:F:179:LEU:HD11	6:F:192:GLN:CG	2.49	0.43
11:K:40:PHE:CD1	11:K:73:ARG:NH1	2.87	0.43
11:K:131:GLN:HG3	11:K:132:THR:N	2.34	0.43
11:K:174:ASN:ND2	11:K:189:ASN:HB2	2.34	0.43
14:N:14:LEU:N	14:N:14:LEU:HD12	2.33	0.43
14:N:140:LYS:NZ	14:2:157:HIS:HD2	2.17	0.43
6:T:91:ARG:O	6:T:95:GLU:HB2	2.19	0.43
10:X:190:PHE:C	10:X:192:ALA:N	2.76	0.43
11:Y:4:LEU:CD2	11:Y:4:LEU:C	2.92	0.43
11:Y:19:ARG:HG2	11:Y:21:THR:HG23	2.01	0.43
12:Z:134:ILE:HG22	12:Z:138:LEU:HD22	2.01	0.43
2:B:225:LYS:O	2:B:226:PRO:C	2.61	0.42
2:B:234:VAL:HA	2:B:239:THR:HA	2.00	0.42
3:C:227:GLU:OE1	3:C:227:GLU:N	2.49	0.42
5:E:22:PHE:O	5:E:23:GLN:C	2.62	0.42
6:F:14:VAL:HG12	6:F:15:PHE:N	2.33	0.42
6:F:137:ILE:HD11	6:F:163:ALA:CB	2.47	0.42
8:H:101:VAL:HG12	8:H:113:ILE:CD1	2.48	0.42
9:I:3:VAL:HG22	9:I:16:CYS:HB3	2.01	0.42
11:K:5:ALA:HA	11:K:13:ILE:O	2.19	0.42
11:K:40:PHE:HB3	11:K:73:ARG:NH2	2.33	0.42
12:L:160:THR:O	12:L:164:GLU:HG2	2.18	0.42
13:M:17:ASP:OD2	13:M:17:ASP:C	2.62	0.42
13:M:147:THR:HB	13:M:149:GLN:HE22	1.84	0.42
1:O:108:PRO:O	1:O:109:THR:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:113:VAL:HG22	2:P:138:TYR:CG	2.54	0.42
4:R:23:GLN:HB3	4:R:131:PRO:HG2	2.01	0.42
6:T:103:TYR:O	6:T:104:LYS:HB3	2.19	0.42
6:T:142:ASP:C	6:T:142:ASP:OD2	2.62	0.42
8:V:156:SER:HA	8:V:159:ILE:HD12	2.00	0.42
2:B:147:GLN:HG2	3:C:62(A):ILE:HG21	2.00	0.42
3:C:190:VAL:HG13	3:C:212:ILE:HG21	2.01	0.42
6:F:52:LYS:HB2	6:F:209:GLU:O	2.19	0.42
8:H:56:THR:HG22	8:H:57:GLN:N	2.33	0.42
8:H:160:GLN:O	8:H:161:ALA:C	2.61	0.42
11:K:10(A):ARG:HD3	11:K:180:GLU:OE1	2.20	0.42
13:M:125:LEU:HA	17:M:224:HOH:O	2.19	0.42
4:R:79:SER:O	4:R:134:VAL:HG23	2.18	0.42
9:W:20:LEU:C	9:W:20:LEU:HD13	2.44	0.42
11:Y:131:GLN:HG3	11:Y:132:THR:N	2.34	0.42
12:Z:4:LEU:O	12:Z:14:LEU:HD23	2.18	0.42
1:A:33:GLN:HE21	1:A:33:GLN:CA	2.32	0.42
3:C:161:SER:HB3	3:C:180:TYR:CE1	2.54	0.42
4:D:70:ILE:HB	4:D:74:ILE:HG22	2.00	0.42
4:D:197:LEU:O	4:D:201:MET:HG3	2.19	0.42
5:E:83:PRO:O	5:E:86:ARG:HB3	2.19	0.42
6:F:66:LYS:HE3	6:F:82:ILE:HD12	2.01	0.42
7:G:229:ILE:O	7:G:232:ARG:HB2	2.19	0.42
10:J:152:LEU:HD21	10:J:177:ILE:HD11	2.02	0.42
12:L:42:VAL:HG23	12:L:102:ALA:HB3	2.01	0.42
4:R:86:ARG:HD3	4:R:86:ARG:HA	1.79	0.42
7:U:82:ILE:N	7:U:83:PRO:HD2	2.34	0.42
7:U:152:ASP:HB2	7:U:153:PRO:CD	2.49	0.42
10:X:136:SER:HA	17:X:559:HOH:O	2.20	0.42
12:Z:93:PHE:N	12:Z:94:PRO:CD	2.81	0.42
1:A:13:THR:CG2	1:A:24:ILE:HD11	2.43	0.42
1:A:62:GLU:C	1:A:64:LEU:N	2.78	0.42
4:D:70:ILE:HD11	4:D:89:ILE:HG23	2.01	0.42
4:D:230:ALA:HA	4:D:233:ILE:HD12	2.00	0.42
7:G:35:ILE:HD11	7:G:53:LYS:CG	2.47	0.42
7:G:87:ASN:HD22	7:G:88:ALA:N	2.17	0.42
8:H:112:SER:OG	8:H:120:ASP:HB2	2.19	0.42
9:I:93:GLY:N	9:I:94:PRO:HD3	2.34	0.42
9:I:174:VAL:HG21	9:I:186:LYS:HE3	2.01	0.42
14:N:38:HIS:O	14:N:39:ASP:C	2.61	0.42
2:P:194:LEU:HD13	2:P:233:LEU:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:91:TYR:CD1	5:S:119:LYS:HD2	2.54	0.42
5:S:160:LEU:HD13	5:S:163:THR:HB	2.00	0.42
6:T:39:GLY:HA3	6:T:137:ILE:HG21	2.02	0.42
6:T:130:ARG:HG2	6:T:130:ARG:HH11	1.84	0.42
6:T:210:LEU:HD12	6:T:211:GLU:H	1.85	0.42
8:V:179:GLU:OE2	8:V:182:LYS:HE2	2.19	0.42
1:A:207:ASN:HA	1:A:233:LEU:CD1	2.49	0.42
3:C:197:LEU:O	3:C:201:VAL:HG23	2.19	0.42
5:E:114:HIS:HB3	6:F:86:ARG:NH2	2.34	0.42
6:F:12:ASN:OD1	6:F:12:ASN:C	2.62	0.42
6:F:187:ARG:HG3	6:F:187:ARG:NH1	2.34	0.42
7:G:168:LYS:HD3	17:G:1365:HOH:O	2.19	0.42
7:G:206:SER:O	7:G:233:LEU:HD21	2.19	0.42
11:K:104:TYR:CE1	11:K:180:GLU:HB2	2.54	0.42
12:L:59:PHE:CD1	12:L:83:ILE:CD1	2.98	0.42
13:M:-5:PRO:HD3	13:M:96:TRP:CE2	2.54	0.42
1:O:160:TRP:CE3	1:O:163:THR:HB	2.55	0.42
3:Q:47:VAL:CG1	3:Q:212:ILE:HG23	2.50	0.42
4:R:215:ILE:HD13	4:R:215:ILE:O	2.20	0.42
7:U:18(D):ILE:HG22	7:U:18(G):GLU:HB2	2.01	0.42
8:V:37:ILE:CD1	8:V:43:CYS:HB2	2.49	0.42
11:Y:104:TYR:CE1	11:Y:180:GLU:HB2	2.55	0.42
3:C:97:GLN:HG3	10:J:65:LEU:HB2	2.00	0.42
3:C:241:GLN:C	3:C:243:GLN:N	2.75	0.42
4:D:117:CYS:SG	4:D:157:PHE:HB3	2.59	0.42
4:D:147:GLN:HG2	4:D:159:ARG:CZ	2.49	0.42
5:E:18(C):PHE:C	5:E:18(C):PHE:CD1	2.98	0.42
13:M:100:ILE:HD13	13:M:112:TYR:CB	2.47	0.42
6:T:202:HIS:O	6:T:202:HIS:CG	2.73	0.42
12:Z:42:VAL:CG2	12:Z:102:ALA:HB3	2.50	0.42
2:B:20:ARG:HG2	2:B:20:ARG:HH11	1.85	0.42
2:B:232:ILE:O	2:B:232:ILE:HG12	2.19	0.42
5:E:150:GLU:O	5:E:157:VAL:HA	2.20	0.42
6:F:54:ILE:HG12	6:F:208:PHE:HA	2.02	0.42
14:N:171:GLY:HA2	13:1:197:TRP:CH2	2.55	0.42
2:P:215:ILE:HD12	2:P:215:ILE:N	2.34	0.42
6:T:151:LEU:HD13	6:T:157:TYR:HB3	2.02	0.42
7:U:118:ASN:O	7:U:122:ILE:HD13	2.19	0.42
7:U:188:LYS:HD3	7:U:188:LYS:HA	1.88	0.42
8:V:3:ILE:O	8:V:3:ILE:HG12	2.19	0.42
10:X:34:THR:HG21	10:X:176:LYS:HZ2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:10(A):ARG:HD3	11:Y:180:GLU:OE1	2.20	0.42
12:Z:160:THR:O	12:Z:164:GLU:HG2	2.20	0.42
14:2:48:SER:HB3	14:2:51:ASP:HB2	2.02	0.42
14:2:18(A):ILE:HD13	14:2:18(B):PHE:H	1.75	0.42
1:A:29:THR:O	1:A:33:GLN:HG2	2.19	0.42
3:C:224:LEU:HD12	3:C:224:LEU:N	2.35	0.42
5:E:194:VAL:CG1	5:E:207:LEU:HD11	2.50	0.42
11:K:76:VAL:HG12	11:K:111:TYR:HD2	1.85	0.42
13:M:133:MET:C	13:M:136:PRO:HD2	2.45	0.42
4:R:96:ALA:HA	4:R:107:ILE:HG21	2.01	0.42
4:R:147:GLN:HG2	4:R:159:ARG:CZ	2.50	0.42
5:S:64:GLN:NE2	5:S:82:ALA:HB2	2.35	0.42
8:V:56:THR:HG22	8:V:57:GLN:N	2.34	0.42
10:X:59:ILE:HD12	10:X:59:ILE:N	2.35	0.42
11:Y:40:PHE:CD1	11:Y:73:ARG:NH1	2.88	0.42
12:Z:76:ILE:CG2	12:Z:77:ASN:N	2.83	0.42
1:A:108:PRO:O	1:A:109:THR:C	2.61	0.42
2:B:17:PRO:HA	3:C:26:TYR:CE2	2.55	0.42
5:E:167:ALA:C	5:E:169:SER:H	2.27	0.42
5:E:221:PHE:C	5:E:221:PHE:CD1	2.98	0.42
7:G:152:ASP:HB2	7:G:153:PRO:CD	2.50	0.42
7:G:187:GLU:O	7:G:191:GLU:HG3	2.20	0.42
11:K:4:LEU:CD2	11:K:4:LEU:C	2.93	0.42
11:K:4:LEU:C	11:K:4:LEU:HD22	2.45	0.42
11:K:38:ASN:HB2	11:K:39:PRO:HD2	2.00	0.42
2:P:194:LEU:O	2:P:198:SER:HB2	2.19	0.42
2:P:235:LYS:HD3	2:P:235:LYS:N	2.34	0.42
5:S:194:VAL:CG1	5:S:207:LEU:HD11	2.50	0.42
6:T:14:VAL:HG12	6:T:15:PHE:N	2.35	0.42
6:T:43:ASN:N	6:T:43:ASN:ND2	2.67	0.42
11:Y:76:VAL:HG22	11:Y:103:GLY:HA3	2.01	0.42
12:Z:79:ALA:O	12:Z:82:ASN:HB3	2.20	0.42
12:Z:145:TYR:HD1	12:Z:146:LEU:N	2.17	0.42
8:H:90:TYR:O	8:H:91:GLN:C	2.62	0.42
8:H:139:GLU:OE1	13:1:165:ARG:NH1	2.53	0.42
10:J:3:ILE:HG23	17:J:195:HOH:O	2.20	0.42
10:J:65:LEU:HD21	10:J:69:ARG:HH22	1.84	0.42
10:J:147:THR:HG23	10:J:150:GLU:OE2	2.20	0.42
12:L:172:GLY:C	12:L:191:LEU:HD12	2.45	0.42
12:L:194:ASP:HB2	8:V:163:ILE:HG23	2.02	0.42
13:M:8:TYR:HB2	13:M:146:THR:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:107:LYS:HG2	14:N:108:GLY:H	1.84	0.42
1:O:136:LEU:O	1:O:150:GLN:HA	2.20	0.42
2:P:101:LYS:HG3	9:W:57:GLU:HB3	2.02	0.42
3:Q:112:LEU:C	3:Q:112:LEU:HD13	2.45	0.42
5:S:221:PHE:C	5:S:221:PHE:CD1	2.97	0.42
7:U:72:ARG:HB2	7:U:72:ARG:HH11	1.85	0.42
7:U:82:ILE:CG2	7:U:83:PRO:HD3	2.50	0.42
7:U:206:SER:O	7:U:233:LEU:HD21	2.20	0.42
9:W:29:ASN:HD22	9:W:30:LYS:HG3	1.84	0.42
9:W:126:VAL:HG11	9:W:134:LEU:HB3	2.02	0.42
10:X:85:GLN:O	10:X:89:LYS:HG3	2.20	0.42
11:Y:157:ARG:O	11:Y:160:LEU:HB3	2.20	0.42
13:1:157:ASN:O	13:1:161:VAL:HG23	2.20	0.42
14:2:14:LEU:HD12	14:2:14:LEU:N	2.34	0.42
1:A:92:SER:O	1:A:95:VAL:HG12	2.20	0.41
4:D:79:SER:O	4:D:134:VAL:HG23	2.20	0.41
7:G:75:GLY:HA3	7:G:221:PHE:CE2	2.55	0.41
7:G:18(D):ILE:HG22	7:G:18(G):GLU:HB2	2.02	0.41
9:I:58:MET:O	9:I:61:TYR:HB3	2.20	0.41
11:K:2:THR:OG1	11:K:130:GLY:HA3	2.20	0.41
17:L:199:HOH:O	9:W:192:ARG:HG3	2.19	0.41
14:N:8:PHE:HE1	14:N:10:ASP:HB2	1.84	0.41
1:O:175:PHE:O	1:O:179:ARG:HG2	2.19	0.41
1:O:179:ARG:HH11	1:O:179:ARG:CB	2.23	0.41
1:O:207:ASN:HA	1:O:233:LEU:CD1	2.50	0.41
3:Q:97:GLN:HE21	3:Q:97:GLN:CA	2.33	0.41
5:S:186:PRO:O	5:S:187:ASP:C	2.62	0.41
7:U:17(C):LYS:HE3	7:U:17(C):LYS:HB2	1.80	0.41
8:V:221:ILE:HD12	8:V:221:ILE:N	2.35	0.41
11:Y:7:ARG:CG	11:Y:12:ILE:HD13	2.45	0.41
13:1:190:LEU:N	13:1:190:LEU:CD1	2.82	0.41
1:A:40:ILE:HD12	1:A:193:ALA:HB2	2.02	0.41
2:B:138:TYR:HB2	2:B:149:TYR:HB2	2.01	0.41
2:B:230:LYS:O	2:B:234:VAL:HG23	2.21	0.41
3:C:111:TYR:CD2	3:C:111:TYR:C	2.98	0.41
4:D:180:TRP:HA	4:D:184:LEU:HD11	2.03	0.41
5:E:67:ILE:HD13	5:E:213:ALA:HB2	2.02	0.41
5:E:18(D):ILE:HG23	5:E:18(E):LYS:HG3	2.02	0.41
5:E:198:SER:HA	5:E:201:LEU:CD1	2.50	0.41
6:F:81:LEU:HA	17:F:313:HOH:O	2.20	0.41
8:H:18:THR:HB	8:H:30:ASN:HA	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:-2:ASN:HA	9:I:21:GLY:O	2.19	0.41
10:J:190:PHE:HA	10:J:193:GLN:HB2	2.03	0.41
10:J:193:GLN:OXT	10:J:193:GLN:HG2	2.20	0.41
12:L:164:GLU:OE1	12:L:192:LYS:HD3	2.20	0.41
13:M:82:TYR:O	13:M:85:THR:HB	2.19	0.41
3:Q:174:GLU:O	3:Q:175:PHE:C	2.62	0.41
4:R:216:THR:O	4:R:217:LYS:C	2.63	0.41
11:Y:38:ASN:HB2	11:Y:39:PRO:CD	2.50	0.41
11:Y:76:VAL:CG2	11:Y:103:GLY:HA3	2.50	0.41
11:Y:124:ILE:CG2	11:Y:138:LEU:HD23	2.51	0.41
13:1:160:ARG:HB2	13:1:192:VAL:HG13	2.02	0.41
14:2:97:ALA:HB1	14:2:99:ILE:CD1	2.49	0.41
1:A:7:ARG:HH11	5:E:127:TYR:HD2	1.68	0.41
3:C:141:PHE:CE1	3:C:217:PRO:HG3	2.56	0.41
7:G:158:VAL:HG22	7:G:159:GLY:H	1.85	0.41
8:H:14:ILE:O	8:H:14:ILE:HG13	2.20	0.41
8:H:170:GLY:O	8:H:171:SER:HB2	2.20	0.41
11:K:124:ILE:CG2	11:K:138:LEU:HD23	2.50	0.41
11:K:142:TYR:C	11:K:143:LYS:HD2	2.46	0.41
13:M:5:SER:HB3	13:M:14:ILE:HG13	2.02	0.41
14:N:107:LYS:HG2	14:N:108:GLY:N	2.35	0.41
1:O:4:MET:O	1:O:5:THR:O	2.39	0.41
1:O:57:PRO:HG2	7:U:177:GLU:HG2	2.01	0.41
1:O:232:ARG:HG3	1:O:232:ARG:NH1	2.35	0.41
5:S:121:GLN:OE1	5:S:125:GLN:NE2	2.53	0.41
5:S:185:ASN:C	5:S:185:ASN:HD22	2.27	0.41
5:S:198:SER:HA	5:S:201:LEU:CD1	2.50	0.41
6:T:109:ILE:HG22	6:T:149:TYR:HE2	1.85	0.41
10:X:18:LYS:CD	10:X:174:ILE:HG13	2.45	0.41
10:X:147:THR:HG23	10:X:150:GLU:OE2	2.20	0.41
11:Y:8:PHE:O	11:Y:9:GLN:C	2.63	0.41
12:Z:-2:ASN:C	12:Z:21:ILE:HD13	2.44	0.41
12:Z:129:ALA:HB1	12:Z:166:HIS:NE2	2.35	0.41
1:A:86:ARG:NE	7:G:118:ASN:HD21	2.18	0.41
3:C:14:ILE:HB	4:D:23:GLN:NE2	2.35	0.41
3:C:224:LEU:N	3:C:224:LEU:CD1	2.84	0.41
5:E:185:ASN:C	5:E:185:ASN:HD22	2.27	0.41
5:E:2(C):VAL:HG13	5:E:2(D):ASP:N	2.35	0.41
7:G:29:LYS:HD2	7:G:29:LYS:HA	1.77	0.41
7:G:18(D):ILE:O	7:G:18(G):GLU:N	2.53	0.41
9:I:29:ASN:HD22	9:I:30:LYS:HG3	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:159:PRO:O	2:P:59:LEU:HD12	2.21	0.41
2:P:233:LEU:HD12	2:P:233:LEU:HA	1.91	0.41
3:Q:57:LYS:HD2	3:Q:57:LYS:C	2.46	0.41
4:R:52:LYS:HE3	4:R:211:GLN:HB2	2.01	0.41
5:S:190:ILE:CG2	5:S:212:ILE:HD13	2.50	0.41
12:Z:14(I):THR:HG21	12:Z:14(M):VAL:HB	2.03	0.41
13:1:14(C):ARG:HH11	13:1:14(C):ARG:CG	2.25	0.41
14:2:44:CYS:HB2	14:2:100:ILE:HB	2.01	0.41
14:2:175:MET:HE3	14:2:18(B):PHE:HE2	1.81	0.41
7:G:17(C):LYS:HB2	7:G:17(C):LYS:HE3	1.81	0.41
7:G:217:LYS:HA	7:G:217:LYS:CE	2.43	0.41
7:G:224:LEU:HB3	7:G:228:ASN:HB2	2.03	0.41
9:I:55:LEU:HD12	9:I:97:VAL:HG21	2.01	0.41
10:J:88:ALA:O	10:J:90(A):ILE:HG22	2.21	0.41
11:K:45:MET:SD	16:K:2(I):H10:C15	3.08	0.41
11:K:104:TYR:HA	11:K:107:GLY:O	2.20	0.41
12:L:4:LEU:O	12:L:14:LEU:HD23	2.21	0.41
1:O:35:VAL:CG1	1:O:51:GLU:HB3	2.50	0.41
3:Q:55:THR:O	3:Q:56:LEU:HD22	2.21	0.41
3:Q:241:GLN:C	3:Q:243:GLN:N	2.76	0.41
5:S:18(C):PHE:C	5:S:18(C):PHE:CD1	2.99	0.41
6:T:151:LEU:CD1	6:T:157:TYR:HB3	2.51	0.41
6:T:184:LEU:CD1	6:T:188:GLU:HB3	2.48	0.41
7:U:220:LYS:HG2	7:U:221:PHE:N	2.34	0.41
9:W:81:GLN:HG2	17:W:949:HOH:O	2.20	0.41
16:Y:2(I):H10:H22A	12:Z:125:ARG:HH21	1.86	0.41
12:Z:6:ILE:HG12	12:Z:124:CYS:HB2	2.02	0.41
13:1:184:LEU:HD23	13:1:185:THR:N	2.34	0.41
14:2:4:MET:CB	14:2:126:ILE:HG22	2.51	0.41
14:2:105:ASP:HB3	14:2:106:ASN:HB2	2.02	0.41
14:2:161:GLN:O	14:2:162:ALA:C	2.62	0.41
2:B:186:VAL:O	2:B:190:ILE:HG13	2.20	0.41
3:C:97:GLN:HE21	3:C:97:GLN:CA	2.32	0.41
3:C:150:GLN:HE21	3:C:150:GLN:HB3	1.65	0.41
4:D:52:LYS:HE3	4:D:211:GLN:HB2	2.02	0.41
4:D:216:THR:O	4:D:217:LYS:C	2.64	0.41
7:G:188:LYS:HA	7:G:188:LYS:HD3	1.89	0.41
8:H:149:GLU:OE2	8:H:149:GLU:N	2.54	0.41
9:I:20:LEU:HD13	9:I:20:LEU:C	2.45	0.41
9:I:80:THR:HG23	9:I:113:PHE:CZ	2.56	0.41
10:J:3:ILE:HG22	10:J:100:LEU:HD12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:162:ALA:O	11:K:163:ALA:C	2.62	0.41
11:K:167:ALA:HB1	9:W:167:ALA:O	2.21	0.41
14:N:105:ASP:HB3	14:N:106:ASN:HB2	2.02	0.41
3:Q:102:THR:OG1	3:Q:103:LEU:HD22	2.20	0.41
5:S:15:PHE:HB2	6:T:23:GLN:NE2	2.36	0.41
5:S:2(B):THR:OG1	5:S:2(E):ASN:HB3	2.21	0.41
8:V:67:SER:HB2	8:V:74:PRO:HG3	2.01	0.41
8:V:149:GLU:OE2	8:V:149:GLU:N	2.53	0.41
10:X:105:ASP:O	10:X:106:ASN:N	2.53	0.41
11:Y:40:PHE:CD1	11:Y:73:ARG:CZ	3.04	0.41
1:A:31:VAL:HG13	1:A:79:SER:O	2.21	0.41
2:B:144:ARG:NH1	10:J:72:TYR:HB2	2.36	0.41
4:D:192:LEU:O	4:D:196:ILE:HD13	2.20	0.41
5:E:67:ILE:C	5:E:68:ILE:HD12	2.45	0.41
5:E:136:LEU:HB2	5:E:151:PHE:HB3	2.02	0.41
6:F:61:PRO:O	6:F:62:GLN:HB2	2.20	0.41
6:F:90:ASN:HD22	6:F:90:ASN:HA	1.64	0.41
6:F:184:LEU:CD1	6:F:188:GLU:HB3	2.47	0.41
8:H:195:ASN:HB3	12:Z:192:LYS:HE3	2.02	0.41
12:L:129:ALA:HB1	12:L:166:HIS:NE2	2.36	0.41
13:M:36:PRO:HA	13:M:42:VAL:HA	2.03	0.41
13:M:137:LEU:HD11	13:M:161:VAL:HG21	2.03	0.41
14:N:6:VAL:C	14:N:12:VAL:HG23	2.46	0.41
1:O:58:LEU:HB3	7:U:162:ALA:O	2.21	0.41
1:O:122:GLU:C	1:O:124:THR:H	2.29	0.41
3:Q:224:LEU:HD12	3:Q:224:LEU:N	2.36	0.41
4:R:180:TRP:HA	4:R:184:LEU:HD11	2.02	0.41
5:S:76:LEU:HA	5:S:137:LEU:O	2.21	0.41
6:T:179:LEU:HD21	6:T:192:GLN:HG2	2.02	0.41
8:V:78:SER:O	8:V:82:MET:HG3	2.21	0.41
9:W:55:LEU:HD12	9:W:97:VAL:HG21	2.01	0.41
9:W:93:GLY:N	9:W:94:PRO:HD3	2.35	0.41
12:Z:17:ASP:OD2	12:Z:33:LYS:NZ	2.49	0.41
12:Z:14(D):TYR:CG	12:Z:14(J):GLY:HA2	2.56	0.41
13:1:4:ILE:HD12	13:1:155:ILE:HD12	2.03	0.41
2:B:113:VAL:HG22	2:B:138:TYR:CG	2.56	0.41
6:F:107:ILE:O	6:F:107:ILE:HG23	2.20	0.41
6:F:179:LEU:HD21	6:F:192:GLN:HG2	2.02	0.41
7:G:46:THR:HG21	7:G:139:VAL:HB	2.02	0.41
10:J:32:ASP:CG	10:J:34:THR:HG22	2.46	0.41
10:J:119:LYS:HE2	17:J:408:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:168:MET:HE3	10:X:168:MET:SD	2.59	0.41
12:L:6:ILE:HG12	12:L:124:CYS:CB	2.50	0.41
2:P:20:ARG:HG2	2:P:20:ARG:HH11	1.85	0.41
3:Q:46:VAL:HG22	3:Q:146:PRO:HB2	2.03	0.41
3:Q:161:SER:HB3	3:Q:180:TYR:CE1	2.55	0.41
6:T:203:GLU:C	6:T:205:ASN:H	2.27	0.41
7:U:229:ILE:O	7:U:232:ARG:HB2	2.21	0.41
8:V:62:ASN:CB	8:V:82:MET:HE1	2.50	0.41
11:Y:74:ILE:HD11	11:Y:78:ALA:HB1	2.02	0.41
13:1:125:LEU:HA	17:1:217:HOH:O	2.19	0.41
13:1:137:LEU:HD11	13:1:161:VAL:HG21	2.02	0.41
13:1:14(C):ARG:NH1	13:1:14(C):ARG:CG	2.84	0.41
1:A:79:SER:HB2	1:A:165:ILE:HD12	2.02	0.41
1:A:160:TRP:CE3	1:A:163:THR:HB	2.56	0.41
2:B:107:ILE:HD11	2:B:111:ILE:HB	2.03	0.41
2:B:194:LEU:HD13	2:B:233:LEU:HD12	2.03	0.41
5:E:2(C):VAL:O	5:E:226:GLY:HA2	2.21	0.41
6:F:13:SER:HB2	7:G:130:ARG:HD3	2.03	0.41
6:F:103:TYR:O	6:F:104:LYS:HB3	2.21	0.41
7:G:203:THR:HG22	7:G:204:GLU:N	2.35	0.41
8:H:208:ARG:NH1	9:I:149:GLU:HB2	2.35	0.41
8:H:221:ILE:HD12	8:H:221:ILE:N	2.35	0.41
9:I:165:ARG:NH2	12:Z:135:MET:CE	2.75	0.41
10:J:63:ILE:HD13	10:J:63:ILE:N	2.36	0.41
11:K:50:ALA:CB	12:L:116:VAL:HG23	2.48	0.41
11:K:83:LEU:CD2	11:K:101:ILE:HD11	2.51	0.41
12:L:-8:PHE:CB	13:M:-8:THR:HG23	2.50	0.41
12:L:145:TYR:HD1	12:L:146:LEU:N	2.18	0.41
13:M:45:ILE:HG12	13:M:99:ILE:HG12	2.03	0.41
13:M:14(A):VAL:HG23	13:M:14(A):VAL:O	2.20	0.41
14:N:37:VAL:HG22	14:N:41:ILE:HG22	2.01	0.41
1:O:205:GLU:HA	1:O:205:GLU:OE2	2.21	0.41
1:O:21(L):ILE:HD11	8:V:186:TYR:CD2	2.56	0.41
4:R:12:VAL:HG23	4:R:12(A):GLY:HA2	2.02	0.41
4:R:160:TYR:HB3	4:R:162:ALA:O	2.21	0.41
4:R:201:MET:HE2	4:R:201:MET:HB3	1.91	0.41
5:S:4:PHE:CG	5:S:5:ARG:N	2.88	0.41
7:U:40:VAL:HB	7:U:18(D):ILE:HD13	2.03	0.41
7:U:224:LEU:HB3	7:U:228:ASN:HB2	2.02	0.41
10:X:7:ARG:HH11	10:X:7:ARG:HG2	1.86	0.41
10:X:66:TYR:CE2	10:X:74:LEU:HG	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:85:GLN:HG2	10:X:89:LYS:HE3	2.03	0.41
10:X:190:PHE:HA	10:X:193:GLN:HB2	2.03	0.41
12:Z:82:ASN:C	12:Z:82:ASN:ND2	2.77	0.41
13:1:209:GLN:N	17:1:367:HOH:O	2.54	0.41
14:2:32:ASP:HA	17:2:307:HOH:O	2.21	0.41
1:A:136:LEU:O	1:A:150:GLN:HA	2.21	0.41
2:B:21(A):LYS:HG3	2:B:219:GLU:O	2.20	0.41
4:D:101:LEU:CD1	11:K:57:THR:HG22	2.51	0.41
4:D:196:ILE:HD12	4:D:196:ILE:N	2.35	0.41
5:E:136:LEU:HD12	5:E:151:PHE:CD2	2.56	0.41
5:E:2(B):THR:OG1	5:E:2(E):ASN:HB3	2.21	0.41
6:F:43:ASN:N	6:F:43:ASN:ND2	2.69	0.41
6:F:49:ALA:HB1	6:F:212:ILE:CD1	2.51	0.41
6:F:195:LYS:HZ2	6:F:196:ILE:CD1	2.34	0.41
7:G:49:ILE:CD1	7:G:49:ILE:N	2.80	0.41
8:H:63:ILE:HG23	8:H:74:PRO:HB3	2.02	0.41
8:H:156:SER:HA	8:H:159:ILE:HD12	2.01	0.41
10:J:-1:MET:CG	10:J:1:ASP:H	2.31	0.41
11:K:40:PHE:CD1	11:K:73:ARG:CZ	3.04	0.41
12:L:43:MET:HG2	12:L:44:SER:N	2.36	0.41
13:M:62:LEU:HD13	13:M:79:ILE:HD13	2.02	0.41
14:N:38:HIS:HB3	14:N:41:ILE:HB	2.02	0.41
14:N:85:GLU:OE2	14:N:85:GLU:HA	2.20	0.41
14:N:143:ARG:O	14:N:146:MET:HG3	2.21	0.41
2:P:39:GLY:O	2:P:148:LEU:HD21	2.21	0.41
2:P:230:LYS:O	2:P:234:VAL:HG23	2.21	0.41
7:U:79:ASN:HA	17:U:252:HOH:O	2.20	0.41
9:W:46:THR:HA	17:W:608:HOH:O	2.21	0.41
10:X:32:ASP:CG	10:X:34:THR:HG22	2.45	0.41
10:X:35:ARG:HD3	10:X:35:ARG:HA	1.80	0.41
12:Z:-5:TYR:CD2	12:Z:96:TYR:HB2	2.55	0.41
12:Z:52:GLY:O	12:Z:56:VAL:HG23	2.21	0.41
13:1:-6:GLN:O	13:1:-6:GLN:HG3	2.20	0.41
14:2:51:ASP:O	14:2:55:ILE:HG13	2.22	0.41
3:C:57:LYS:HD2	3:C:57:LYS:C	2.46	0.40
4:D:201:MET:HE2	4:D:201:MET:HB3	1.92	0.40
8:H:18:THR:OG1	8:H:171:SER:HB2	2.21	0.40
9:I:126:VAL:HG11	9:I:134:LEU:HB3	2.03	0.40
10:J:133:TYR:OH	10:X:24:ILE:CG1	2.68	0.40
10:J:168:MET:SD	10:X:168:MET:HE3	2.61	0.40
12:L:54:ALA:O	12:L:58:ARG:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:215:ILE:O	2:P:215:ILE:HG22	2.21	0.40
5:S:31:ILE:HD13	5:S:152:GLN:OE1	2.21	0.40
9:W:20:LEU:HA	17:W:240:HOH:O	2.21	0.40
11:Y:31:VAL:HG11	16:Y:2(I):H10:C15	2.51	0.40
11:Y:31:VAL:CG1	16:Y:2(I):H10:C15	2.99	0.40
12:Z:70(A):ASN:O	12:Z:72:LYS:N	2.54	0.40
14:2:161:GLN:NE2	14:2:165:TRP:HE1	2.18	0.40
1:A:24:ILE:HD12	1:A:24:ILE:N	2.36	0.40
3:C:19:GLY:O	4:D:30:ALA:HB2	2.21	0.40
3:C:168:ASN:CB	3:C:200:VAL:HG11	2.49	0.40
5:E:27:ALA:O	5:E:31:ILE:HD12	2.21	0.40
5:E:78:LEU:HD12	5:E:78:LEU:C	2.46	0.40
6:F:35:THR:HG21	6:F:51:GLU:O	2.21	0.40
6:F:39:GLY:C	6:F:40:ILE:HD12	2.46	0.40
6:F:83:PRO:HB2	17:F:1240:HOH:O	2.20	0.40
7:G:13:THR:HB	7:G:124:THR:O	2.21	0.40
9:I:16:CYS:SG	9:I:34:ILE:HG12	2.60	0.40
14:N:116:GLY:HA3	17:N:194:HOH:O	2.21	0.40
3:Q:111:TYR:CD2	3:Q:111:TYR:C	2.98	0.40
3:Q:156:ILE:CD1	3:Q:156:ILE:H	2.34	0.40
4:R:40:ILE:HG12	4:R:193:VAL:CG2	2.51	0.40
5:S:39:GLY:O	5:S:162:GLY:HA2	2.21	0.40
5:S:198:SER:HA	5:S:201:LEU:CG	2.46	0.40
7:U:35:ILE:HD13	7:U:53:LYS:HE3	2.03	0.40
7:U:198:ILE:O	7:U:202:GLY:N	2.51	0.40
9:W:58:MET:O	9:W:61:TYR:HB3	2.21	0.40
11:Y:109:THR:HA	17:Y:595:HOH:O	2.21	0.40
12:Z:95:TYR:O	12:Z:97:VAL:N	2.53	0.40
13:1:133:MET:C	13:1:136:PRO:HD2	2.46	0.40
1:A:4:MET:O	1:A:5:THR:O	2.39	0.40
1:A:8:TYR:HD2	7:G:128:TYR:HB3	1.87	0.40
2:B:40:ILE:HD12	2:B:193:ALA:HB2	2.03	0.40
2:B:142:ASP:CG	2:B:147:GLN:HE22	2.28	0.40
3:C:79:SER:HA	17:C:625:HOH:O	2.22	0.40
3:C:210:ILE:HG22	3:C:212:ILE:CD1	2.52	0.40
4:D:12(G):GLU:HG2	4:D:125:GLU:N	2.34	0.40
8:H:192:LEU:HD23	8:H:192:LEU:HA	1.79	0.40
11:K:76:VAL:HG22	11:K:103:GLY:HA3	2.03	0.40
11:K:114:ASP:OD1	11:K:114:ASP:C	2.65	0.40
12:L:133:LEU:N	12:L:133:LEU:HD12	2.36	0.40
12:L:176:LEU:HG	12:L:186:LYS:HG3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:227:GLU:OE1	3:Q:227:GLU:N	2.50	0.40
5:S:167:ALA:C	5:S:169:SER:H	2.29	0.40
6:T:126:TYR:HE1	7:U:129:MET:SD	2.45	0.40
8:V:160:GLN:O	8:V:161:ALA:C	2.63	0.40
9:W:84:SER:OG	9:W:119:ILE:HD11	2.21	0.40
10:X:123:PRO:HB3	10:X:142:TYR:CE2	2.57	0.40
12:Z:32:PRO:CD	17:Z:1177:HOH:O	2.65	0.40
12:Z:42:VAL:HG23	12:Z:102:ALA:HB3	2.03	0.40
1:A:161:LYS:HD3	1:A:180:TRP:CH2	2.56	0.40
1:A:21(I):TYR:HE2	1:A:21(L):ILE:HD12	1.87	0.40
3:C:125:GLN:HB2	4:D:130:ARG:HG2	2.03	0.40
4:D:161:ASN:HB3	4:D:180:TRP:CZ2	2.56	0.40
6:F:151:LEU:HD13	6:F:157:TYR:HB3	2.03	0.40
8:H:72:ARG:HH11	8:H:72:ARG:HG3	1.86	0.40
9:I:55:LEU:HD23	9:I:55:LEU:HA	1.84	0.40
9:I:93:GLY:H	9:I:94:PRO:HD3	1.87	0.40
10:J:123:PRO:HB3	10:J:142:TYR:CE2	2.55	0.40
10:J:133:TYR:CZ	10:J:166:MET:HG3	2.57	0.40
12:L:70:HIS:O	12:L:70(A):ASN:C	2.65	0.40
12:L:104:LEU:HA	12:L:107:LYS:O	2.22	0.40
14:N:157:HIS:HD2	14:2:140:LYS:NZ	2.20	0.40
2:P:142:ASP:CG	2:P:147:GLN:HE22	2.29	0.40
4:R:115:SER:O	4:R:118:ASP:HB2	2.22	0.40
7:U:203:THR:HG22	7:U:204:GLU:N	2.36	0.40
11:Y:45:MET:SD	16:Y:2(I):H10:C15	3.09	0.40
11:Y:174:ASN:HD22	11:Y:174:ASN:HA	1.69	0.40
13:1:8:TYR:HB2	13:1:146:THR:O	2.21	0.40
14:2:133:PHE:HE2	14:2:166:ASP:HB2	1.86	0.40
3:C:174:GLU:O	3:C:175:PHE:C	2.65	0.40
3:C:241:GLN:O	3:C:243:GLN:N	2.50	0.40
7:G:12:ILE:HD13	7:G:12:ILE:H	1.85	0.40
7:G:145:GLY:O	7:G:146:PRO:C	2.63	0.40
13:M:1:THR:OG1	13:M:2:SER:N	2.55	0.40
14:N:175:MET:HE3	14:N:18(B):PHE:HE2	1.85	0.40
1:O:45:GLY:HA2	1:O:147:PHE:CE2	2.57	0.40
3:Q:76:LEU:HD12	3:Q:138:ILE:HG12	2.03	0.40
5:S:66:LYS:O	5:S:77:SER:HA	2.20	0.40
6:T:43:ASN:ND2	6:T:43:ASN:H	2.20	0.40
6:T:114:ASP:O	6:T:118:GLN:HG2	2.21	0.40
6:T:195:LYS:NZ	6:T:196:ILE:CD1	2.85	0.40
8:V:100:ILE:HG12	8:V:127:LEU:HD12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:-2:ASN:HA	9:W:21:GLY:O	2.22	0.40
9:W:20:LEU:C	9:W:20:LEU:CD1	2.95	0.40
10:X:121:GLU:O	10:X:122:LEU:HD23	2.21	0.40
11:Y:50:ALA:CB	12:Z:116:VAL:HG23	2.51	0.40
11:Y:76:VAL:HG12	11:Y:111:TYR:HD2	1.86	0.40
12:Z:40:ASN:ND2	17:Z:799:HOH:O	2.49	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	248/250 (99%)	226 (91%)	15 (6%)	7 (3%)	4	14
1	O	248/250 (99%)	226 (91%)	14 (6%)	8 (3%)	3	11
2	B	242/244 (99%)	217 (90%)	18 (7%)	7 (3%)	3	13
2	P	242/244 (99%)	217 (90%)	19 (8%)	6 (2%)	4	16
3	C	239/241 (99%)	219 (92%)	15 (6%)	5 (2%)	5	20
3	Q	239/241 (99%)	217 (91%)	17 (7%)	5 (2%)	5	20
4	D	240/242 (99%)	217 (90%)	18 (8%)	5 (2%)	5	20
4	R	240/242 (99%)	216 (90%)	19 (8%)	5 (2%)	5	20
5	E	231/233 (99%)	201 (87%)	24 (10%)	6 (3%)	4	15
5	S	231/233 (99%)	203 (88%)	22 (10%)	6 (3%)	4	15
6	F	242/244 (99%)	224 (93%)	17 (7%)	1 (0%)	30	60
6	T	242/244 (99%)	223 (92%)	18 (7%)	1 (0%)	30	60
7	G	241/243 (99%)	223 (92%)	15 (6%)	3 (1%)	10	34
7	U	241/243 (99%)	222 (92%)	16 (7%)	3 (1%)	10	34
8	H	220/222 (99%)	207 (94%)	10 (4%)	3 (1%)	9	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	V	220/222 (99%)	205 (93%)	12 (6%)	3 (1%)	9	30
9	I	202/204 (99%)	189 (94%)	10 (5%)	3 (2%)	8	28
9	W	202/204 (99%)	189 (94%)	11 (5%)	2 (1%)	12	38
10	J	196/198 (99%)	184 (94%)	9 (5%)	3 (2%)	8	28
10	X	196/198 (99%)	184 (94%)	9 (5%)	3 (2%)	8	28
11	K	210/212 (99%)	197 (94%)	13 (6%)	0	100	100
11	Y	210/212 (99%)	200 (95%)	9 (4%)	1 (0%)	24	55
12	L	220/222 (99%)	201 (91%)	18 (8%)	1 (0%)	24	55
12	Z	220/222 (99%)	201 (91%)	18 (8%)	1 (0%)	24	55
13	1	231/233 (99%)	208 (90%)	21 (9%)	2 (1%)	14	41
13	M	231/233 (99%)	210 (91%)	19 (8%)	2 (1%)	14	41
14	2	194/196 (99%)	183 (94%)	11 (6%)	0	100	100
14	N	194/196 (99%)	180 (93%)	14 (7%)	0	100	100
All	All	6312/6368 (99%)	5789 (92%)	431 (7%)	92 (2%)	8	28

All (92) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	THR
1	A	167	LYS
2	B	54	VAL
3	C	58	LEU
3	C	203	THR
4	D	12(G)	GLU
5	E	5	ARG
5	E	202	ARG
6	F	143	LYS
12	L	71	ASP
1	O	5	THR
1	O	167	LYS
2	P	54	VAL
3	Q	58	LEU
3	Q	203	THR
4	R	12(G)	GLU
5	S	5	ARG
5	S	202	ARG
6	T	143	LYS

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Mol	Chain	Res	Type
12	Z	71	ASP
1	A	53	LYS
2	B	6	ARG
2	B	21(B)	GLY
2	B	21(C)	ASP
5	E	180	LEU
5	E	217	LYS
5	E	231	LYS
7	G	239	GLN
8	H	9	ASN
8	H	96	GLY
10	J	49	ALA
10	J	192	ALA
1	O	53	LYS
2	P	6	ARG
2	P	21(B)	GLY
2	P	21(C)	ASP
5	S	180	LEU
5	S	217	LYS
8	V	9	ASN
8	V	96	GLY
10	X	49	ALA
10	X	192	ALA
13	1	96	TRP
1	A	63	THR
2	B	20(A)	SER
4	D	12(F)	GLY
5	E	18(A)	ASP
13	M	96	TRP
1	O	63	THR
2	P	20(A)	SER
4	R	120	ALA
4	R	12(F)	GLY
5	S	18(A)	ASP
5	S	231	LYS
7	U	184	ASN
7	U	239	GLN
1	A	100	TYR
3	C	183	PRO
3	C	202	GLN
4	D	120	ALA
4	D	12(C)	GLY

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Mol	Chain	Res	Type
7	G	184	ASN
3	Q	183	PRO
3	Q	202	GLN
4	R	12(C)	GLY
7	U	55	PRO
8	V	171	SER
4	D	18(D)	SER
7	G	55	PRO
8	H	171	SER
9	I	23	GLN
9	I	93	GLY
9	I	106	GLY
13	M	1	THR
1	O	100	TYR
3	Q	53	ARG
9	W	93	GLY
9	W	106	GLY
13	1	1	THR
1	A	208	GLY
2	B	64	THR
3	C	53	ARG
1	O	56	SER
1	O	208	GLY
4	R	18(D)	SER
1	A	56	SER
10	J	8	VAL
10	X	8	VAL
1	O	22	GLY
2	P	186	VAL
2	B	186	VAL
11	Y	39	PRO

5.3.2 Protein sidechains ⓘ

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

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	209/209 (100%)	200 (96%)	9 (4%)	26	60
1	O	209/209 (100%)	200 (96%)	9 (4%)	26	60
2	B	203/203 (100%)	186 (92%)	17 (8%)	10	32
2	P	203/203 (100%)	190 (94%)	13 (6%)	16	44
3	C	213/213 (100%)	204 (96%)	9 (4%)	26	61
3	Q	213/213 (100%)	204 (96%)	9 (4%)	26	61
4	D	198/198 (100%)	187 (94%)	11 (6%)	19	50
4	R	198/198 (100%)	187 (94%)	11 (6%)	19	50
5	E	192/192 (100%)	180 (94%)	12 (6%)	16	45
5	S	192/192 (100%)	180 (94%)	12 (6%)	16	45
6	F	201/201 (100%)	192 (96%)	9 (4%)	24	58
6	T	201/201 (100%)	192 (96%)	9 (4%)	24	58
7	G	207/207 (100%)	196 (95%)	11 (5%)	20	52
7	U	207/207 (100%)	194 (94%)	13 (6%)	16	45
8	H	181/181 (100%)	172 (95%)	9 (5%)	22	54
8	V	181/181 (100%)	171 (94%)	10 (6%)	19	51
9	I	172/172 (100%)	165 (96%)	7 (4%)	27	62
9	W	172/172 (100%)	166 (96%)	6 (4%)	32	67
10	J	175/175 (100%)	166 (95%)	9 (5%)	21	54
10	X	175/175 (100%)	168 (96%)	7 (4%)	28	63
11	K	169/169 (100%)	160 (95%)	9 (5%)	20	52
11	Y	169/169 (100%)	161 (95%)	8 (5%)	23	57
12	L	185/185 (100%)	164 (89%)	21 (11%)	5	19
12	Z	185/185 (100%)	165 (89%)	20 (11%)	6	21
13	1	199/199 (100%)	192 (96%)	7 (4%)	32	67
13	M	199/199 (100%)	192 (96%)	7 (4%)	32	67
14	2	162/162 (100%)	153 (94%)	9 (6%)	19	50
14	N	162/162 (100%)	154 (95%)	8 (5%)	22	55
All	All	5332/5332 (100%)	5041 (94%)	291 (6%)	19	51

All (291) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	LYS
1	A	33	GLN
1	A	62	GLU
1	A	64	LEU
1	A	124	THR
1	A	134	VAL
1	A	135	SER
1	A	158	PHE
1	A	179	ARG
2	B	14	ILE
2	B	41	MET
2	B	58	LEU
2	B	61	GLN
2	B	67	LEU
2	B	107	ILE
2	B	116	LEU
2	B	121	GLN
2	B	124	THR
2	B	14(A)	TYR
2	B	158	THR
2	B	169	THR
2	B	192	LEU
2	B	198	SER
2	B	212	PHE
2	B	224	PHE
2	B	232	ILE
3	C	10	ARG
3	C	14	ILE
3	C	25	GLU
3	C	57	LYS
3	C	14(A)	ARG
3	C	14(B)	ASP
3	C	150	GLN
3	C	163	GLN
3	C	174	GLU
4	D	28	LEU
4	D	48	LEU
4	D	76	CYS
4	D	110	GLU
4	D	170	GLU
4	D	175	GLU
4	D	177	LEU
4	D	191	LEU

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Mol	Chain	Res	Type
4	D	194	LEU
4	D	215	ILE
4	D	237	LEU
5	E	11	ASP
5	E	12	THR
5	E	13	VAL
5	E	28	LEU
5	E	32	LYS
5	E	57	GLU
5	E	76	LEU
5	E	97	ASN
5	E	117	CYS
5	E	199	GLN
5	E	207	LEU
5	E	227	GLU
6	F	11	SER
6	F	35	THR
6	F	43	ASN
6	F	98	SER
6	F	121	GLN
6	F	127	ASN
6	F	187	ARG
6	F	203	GLU
6	F	205	ASN
7	G	12	ILE
7	G	72	ARG
7	G	87	ASN
7	G	119	LEU
7	G	124	THR
7	G	157	TYR
7	G	169	GLN
7	G	197	MET
7	G	217	LYS
7	G	232	ARG
7	G	233	LEU
8	H	31	CYS
8	H	34	LEU
8	H	41	ILE
8	H	43	CYS
8	H	56	THR
8	H	68	LEU
8	H	121	VAL

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Mol	Chain	Res	Type
8	H	144	GLN
8	H	197	ARG
9	I	20	LEU
9	I	29	ASN
9	I	45	ILE
9	I	90	ARG
9	I	113	PHE
9	I	116	ILE
9	I	160	LEU
10	J	35	ARG
10	J	52	THR
10	J	63	ILE
10	J	68	ILE
10	J	90	SER
10	J	90(A)	ILE
10	J	90(B)	ARG
10	J	121	GLU
10	J	168	MET
11	K	4	LEU
11	K	7	ARG
11	K	9	GLN
11	K	65	LEU
11	K	69	ARG
11	K	87	VAL
11	K	101	ILE
11	K	138	LEU
11	K	146	LEU
12	L	-7	ASN
12	L	3	ILE
12	L	14	LEU
12	L	21	ILE
12	L	40	ASN
12	L	99	THR
12	L	112	SER
12	L	14(A)	LYS
12	L	14(B)	ASN
12	L	14(C)	GLN
12	L	14(D)	TYR
12	L	14(E)	GLU
12	L	14(F)	PRO
12	L	14(I)	THR
12	L	14(K)	LYS

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Mol	Chain	Res	Type
12	L	14(M)	VAL
12	L	14(N)	LYS
12	L	14(O)	LYS
12	L	14(P)	PRO
12	L	14(Q)	LEU
12	L	14(W)	LYS
13	M	40	ASN
13	M	62	LEU
13	M	91	ARG
13	M	112	TYR
13	M	129	PHE
13	M	149	GLN
13	M	191	GLN
14	N	13	ILE
14	N	84	LYS
14	N	89	GLU
14	N	115	LEU
14	N	119	VAL
14	N	149	GLU
14	N	155	ILE
14	N	178	LEU
1	O	32	LYS
1	O	33	GLN
1	O	62	GLU
1	O	64	LEU
1	O	124	THR
1	O	134	VAL
1	O	135	SER
1	O	158	PHE
1	O	179	ARG
2	P	41	MET
2	P	58	LEU
2	P	61	GLN
2	P	67	LEU
2	P	116	LEU
2	P	121	GLN
2	P	124	THR
2	P	158	THR
2	P	169	THR
2	P	192	LEU
2	P	212	PHE
2	P	224	PHE

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Mol	Chain	Res	Type
2	P	232	ILE
3	Q	10	ARG
3	Q	25	GLU
3	Q	57	LYS
3	Q	150	GLN
3	Q	152	GLU
3	Q	156	ILE
3	Q	163	GLN
3	Q	165	ILE
3	Q	174	GLU
4	R	28	LEU
4	R	48	LEU
4	R	76	CYS
4	R	110	GLU
4	R	170	GLU
4	R	175	GLU
4	R	177	LEU
4	R	191	LEU
4	R	194	LEU
4	R	215	ILE
4	R	237	LEU
5	S	11	ASP
5	S	12	THR
5	S	13	VAL
5	S	28	LEU
5	S	32	LYS
5	S	57	GLU
5	S	76	LEU
5	S	97	ASN
5	S	117	CYS
5	S	199	GLN
5	S	207	LEU
5	S	227	GLU
6	T	11	SER
6	T	35	THR
6	T	43	ASN
6	T	98	SER
6	T	121	GLN
6	T	127	ASN
6	T	187	ARG
6	T	203	GLU
6	T	205	ASN

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Mol	Chain	Res	Type
7	U	14	ILE
7	U	72	ARG
7	U	87	ASN
7	U	119	LEU
7	U	121	GLN
7	U	124	THR
7	U	14(A)	GLU
7	U	157	TYR
7	U	169	GLN
7	U	197	MET
7	U	217	LYS
7	U	232	ARG
7	U	233	LEU
8	V	3	ILE
8	V	31	CYS
8	V	34	LEU
8	V	41	ILE
8	V	43	CYS
8	V	56	THR
8	V	68	LEU
8	V	121	VAL
8	V	144	GLN
8	V	197	ARG
9	W	20	LEU
9	W	29	ASN
9	W	90	ARG
9	W	113	PHE
9	W	155	ILE
9	W	160	LEU
10	X	35	ARG
10	X	52	THR
10	X	90	SER
10	X	90(A)	ILE
10	X	90(B)	ARG
10	X	121	GLU
10	X	168	MET
11	Y	4	LEU
11	Y	7	ARG
11	Y	9	GLN
11	Y	65	LEU
11	Y	69	ARG
11	Y	87	VAL

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Mol	Chain	Res	Type
11	Y	101	ILE
11	Y	138	LEU
12	Z	-7	ASN
12	Z	14	LEU
12	Z	21	ILE
12	Z	40	ASN
12	Z	99	THR
12	Z	112	SER
12	Z	14(A)	LYS
12	Z	14(B)	ASN
12	Z	14(C)	GLN
12	Z	14(D)	TYR
12	Z	14(E)	GLU
12	Z	14(F)	PRO
12	Z	14(I)	THR
12	Z	14(K)	LYS
12	Z	14(M)	VAL
12	Z	14(N)	LYS
12	Z	14(O)	LYS
12	Z	14(P)	PRO
12	Z	14(Q)	LEU
12	Z	14(W)	LYS
13	1	40	ASN
13	1	62	LEU
13	1	91	ARG
13	1	112	TYR
13	1	129	PHE
13	1	149	GLN
13	1	191	GLN
14	2	3	ILE
14	2	13	ILE
14	2	84	LYS
14	2	89	GLU
14	2	115	LEU
14	2	119	VAL
14	2	126	ILE
14	2	149	GLU
14	2	178	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (230) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	97	HIS
1	A	121	GLN
1	A	145	ASN
2	B	23	GLN
2	B	33	HIS
2	B	71	ASN
2	B	97	GLN
2	B	121	GLN
2	B	125	GLN
2	B	156	ASN
2	B	177	GLN
2	B	218	ASN
3	C	23	GLN
3	C	82	ASN
3	C	97	GLN
3	C	120	GLN
3	C	121	GLN
3	C	125	GLN
3	C	150	GLN
3	C	163	GLN
3	C	209	ASN
3	C	238	GLN
3	C	243	GLN
4	D	23	GLN
4	D	108	ASN
4	D	161	ASN
4	D	211	GLN
4	D	218	GLN
4	D	226	ASN
5	E	7	ASN
5	E	33	GLN
5	E	64	GLN
5	E	73	HIS
5	E	104	ASN
5	E	125	GLN
5	E	156	ASN
5	E	199	GLN
5	E	2(E)	ASN
6	F	23	GLN
6	F	43	ASN
6	F	87	HIS
6	F	90	ASN

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Mol	Chain	Res	Type
6	F	121	GLN
6	F	127	ASN
6	F	192	GLN
7	G	32	ASN
7	G	34(A)	ASN
7	G	87	ASN
7	G	118	ASN
7	G	121	GLN
7	G	125	GLN
7	G	169	GLN
7	G	170	GLN
7	G	178	ASN
7	G	184	ASN
8	H	30	ASN
8	H	35	HIS
8	H	66	HIS
8	H	85	GLN
8	H	144	GLN
8	H	165	ASN
8	H	172	ASN
8	H	190	ASN
8	H	201	GLN
9	I	29	ASN
9	I	56	ASN
9	I	64	ASN
9	I	81	GLN
9	I	145	ASN
9	I	157	GLN
9	I	161	ASN
9	I	193	GLN
10	J	36	GLN
10	J	54	GLN
10	J	62	ASN
10	J	77	GLN
10	J	85	GLN
10	J	112	GLN
10	J	140	HIS
10	J	141	HIS
10	J	160	GLN
10	J	186	GLN
10	J	193	GLN
11	K	9	GLN

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Mol	Chain	Res	Type
11	K	85	ASN
11	K	131	GLN
11	K	174	ASN
11	K	207	ASN
12	L	-9	GLN
12	L	-7	ASN
12	L	40	ASN
12	L	46	ASN
12	L	61	ASN
12	L	70(A)	ASN
12	L	82	ASN
12	L	85	HIS
12	L	123	GLN
12	L	141	GLN
12	L	14(C)	GLN
12	L	1(I)	ASN
12	L	166	HIS
12	L	168	GLN
13	M	-7	GLN
13	M	10	ASN
13	M	40	ASN
13	M	89	GLN
13	M	93	ASN
13	M	149	GLN
13	M	157	ASN
13	M	191	GLN
14	N	141	ASN
14	N	145	ASN
14	N	157	HIS
14	N	161	GLN
1	O	33	GLN
1	O	97	HIS
1	O	121	GLN
1	O	145	ASN
2	P	23	GLN
2	P	71	ASN
2	P	121	GLN
2	P	125	GLN
2	P	156	ASN
2	P	177	GLN
2	P	218	ASN
3	Q	23	GLN

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Mol	Chain	Res	Type
3	Q	82	ASN
3	Q	97	GLN
3	Q	120	GLN
3	Q	121	GLN
3	Q	125	GLN
3	Q	150	GLN
3	Q	163	GLN
3	Q	209	ASN
3	Q	238	GLN
3	Q	243	GLN
4	R	23	GLN
4	R	108	ASN
4	R	161	ASN
4	R	211	GLN
4	R	218	GLN
4	R	226	ASN
5	S	7	ASN
5	S	33	GLN
5	S	64	GLN
5	S	73	HIS
5	S	104	ASN
5	S	121	GLN
5	S	125	GLN
5	S	156	ASN
5	S	199	GLN
5	S	2(E)	ASN
6	T	23	GLN
6	T	43	ASN
6	T	87	HIS
6	T	90	ASN
6	T	121	GLN
6	T	127	ASN
6	T	147	HIS
6	T	192	GLN
6	T	221	HIS
7	U	32	ASN
7	U	34(A)	ASN
7	U	87	ASN
7	U	118	ASN
7	U	121	GLN
7	U	125	GLN
7	U	169	GLN

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Mol	Chain	Res	Type
7	U	170	GLN
7	U	178	ASN
7	U	184	ASN
8	V	30	ASN
8	V	66	HIS
8	V	144	GLN
8	V	165	ASN
8	V	172	ASN
8	V	190	ASN
8	V	195	ASN
8	V	201	GLN
9	W	29	ASN
9	W	56	ASN
9	W	81	GLN
9	W	145	ASN
9	W	157	GLN
9	W	161	ASN
9	W	193	GLN
10	X	36	GLN
10	X	54	GLN
10	X	62	ASN
10	X	77	GLN
10	X	85	GLN
10	X	112	GLN
10	X	140	HIS
10	X	141	HIS
10	X	160	GLN
10	X	186	GLN
10	X	193	GLN
11	Y	9	GLN
11	Y	62	GLN
11	Y	85	ASN
11	Y	131	GLN
11	Y	174	ASN
11	Y	207	ASN
12	Z	-9	GLN
12	Z	-7	ASN
12	Z	27	ASN
12	Z	40	ASN
12	Z	46	ASN
12	Z	61	ASN
12	Z	70(A)	ASN

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Mol	Chain	Res	Type
12	Z	82	ASN
12	Z	85	HIS
12	Z	123	GLN
12	Z	141	GLN
12	Z	14(C)	GLN
12	Z	1(I)	ASN
12	Z	166	HIS
13	1	-7	GLN
13	1	10	ASN
13	1	40	ASN
13	1	89	GLN
13	1	93	ASN
13	1	149	GLN
13	1	157	ASN
13	1	191	GLN
14	2	141	ASN
14	2	145	ASN
14	2	157	HIS
14	2	161	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	H10	Y	2(I)	-	26,29,29	3.38	18 (69%)	36,43,43	1.08	3 (8%)
16	H10	K	2(I)	-	26,29,29	3.47	18 (69%)	36,43,43	1.13	4 (11%)
15	MES	K	1(L)	-	12,12,12	2.82	8 (66%)	15,16,16	2.64	6 (40%)
15	MES	Y	1(L)	-	12,12,12	2.80	7 (58%)	15,16,16	2.57	5 (33%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	H10	Y	2(I)	-	-	2/14/45/45	0/5/4/4
16	H10	K	2(I)	-	-	2/14/45/45	0/5/4/4
15	MES	K	1(L)	-	-	5/6/14/14	0/1/1/1
15	MES	Y	1(L)	-	-	3/6/14/14	0/1/1/1

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	K	2(I)	H10	O13-N9	-11.06	1.25	1.40
16	Y	2(I)	H10	O13-N9	-10.29	1.26	1.40
16	Y	2(I)	H10	C26-C1	5.64	1.62	1.52
16	K	2(I)	H10	C26-C1	5.27	1.61	1.52
15	Y	1(L)	MES	C8-S	5.25	1.84	1.77
16	K	2(I)	H10	C25-C1	5.01	1.61	1.52
16	Y	2(I)	H10	C25-C1	5.00	1.61	1.52
15	K	1(L)	MES	C8-S	4.99	1.84	1.77
16	K	2(I)	H10	C17-C3	4.71	1.47	1.38
15	Y	1(L)	MES	C7-C8	-4.41	1.40	1.52
16	K	2(I)	H10	C18-C1	4.40	1.60	1.52
16	Y	2(I)	H10	C17-C3	4.26	1.46	1.38
16	Y	2(I)	H10	C18-C1	4.10	1.59	1.52
15	Y	1(L)	MES	O1-C6	-3.95	1.27	1.42
15	K	1(L)	MES	C7-C8	-3.85	1.42	1.52
15	K	1(L)	MES	O1-C6	-3.59	1.28	1.42
16	Y	2(I)	H10	C20-C19	3.27	1.61	1.52
16	K	2(I)	H10	C24-C19	2.97	1.60	1.52
15	K	1(L)	MES	O2S-S	-2.95	1.36	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	Y	2(I)	H10	C24-C19	2.90	1.60	1.52
16	K	2(I)	H10	C16-C17	2.88	1.43	1.38
16	Y	2(I)	H10	C16-C15	2.85	1.43	1.38
16	K	2(I)	H10	C24-C23	2.85	1.60	1.52
16	Y	2(I)	H10	C22-C23	2.84	1.60	1.52
16	K	2(I)	H10	C4-C3	2.83	1.43	1.39
15	K	1(L)	MES	C3-N4	2.82	1.54	1.46
16	K	2(I)	H10	C20-C19	2.81	1.60	1.52
16	Y	2(I)	H10	C24-C23	2.80	1.60	1.52
16	K	2(I)	H10	C6-C7	-2.80	1.16	1.19
16	Y	2(I)	H10	C4-C3	2.78	1.43	1.39
15	K	1(L)	MES	O1-C2	2.75	1.53	1.42
16	K	2(I)	H10	C22-C21	2.72	1.60	1.52
16	Y	2(I)	H10	C18-C19	2.71	1.61	1.54
15	K	1(L)	MES	O1S-S	2.70	1.52	1.45
15	Y	1(L)	MES	C3-N4	2.67	1.54	1.46
16	Y	2(I)	H10	C6-C7	-2.65	1.16	1.19
16	K	2(I)	H10	C18-C19	2.64	1.61	1.54
16	K	2(I)	H10	C22-C23	2.60	1.59	1.52
16	Y	2(I)	H10	C22-C21	2.58	1.59	1.52
16	Y	2(I)	H10	C16-C17	2.55	1.43	1.38
16	K	2(I)	H10	C16-C15	2.53	1.43	1.38
15	Y	1(L)	MES	O1-C2	2.49	1.52	1.42
16	K	2(I)	H10	C4-C5	2.42	1.43	1.39
16	Y	2(I)	H10	C20-C21	2.34	1.59	1.52
15	K	1(L)	MES	C5-C6	2.30	1.59	1.50
15	Y	1(L)	MES	C5-C6	2.26	1.59	1.50
16	Y	2(I)	H10	C15-C5	2.17	1.43	1.39
16	Y	2(I)	H10	C4-C5	2.09	1.43	1.39
16	K	2(I)	H10	C15-C5	2.09	1.43	1.39
16	K	2(I)	H10	C20-C21	2.02	1.58	1.52
15	Y	1(L)	MES	C3-C2	2.01	1.58	1.50

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	Y	1(L)	MES	O1S-S-C8	-7.43	95.50	106.73
15	K	1(L)	MES	O1S-S-C8	-7.40	95.55	106.73
15	Y	1(L)	MES	O3S-S-O2S	3.73	120.72	111.40
15	K	1(L)	MES	O3S-S-O2S	3.70	120.65	111.40
15	Y	1(L)	MES	O2S-S-C8	3.46	111.95	106.73
15	K	1(L)	MES	O1-C2-C3	-2.78	105.79	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	K	2(I)	H10	C26-C1-C18	-2.64	106.39	109.91
16	K	2(I)	H10	O13-N9-C8	2.63	119.76	110.23
16	K	2(I)	H10	C14-C8-N9	2.62	114.41	110.24
16	Y	2(I)	H10	C14-C8-N9	2.60	114.38	110.24
15	K	1(L)	MES	C7-N4-C3	2.59	118.13	111.24
16	Y	2(I)	H10	O13-N9-C8	2.54	119.41	110.23
15	K	1(L)	MES	C6-C5-N4	2.21	113.47	110.12
16	Y	2(I)	H10	O11-C10-N12	-2.20	118.34	122.63
16	K	2(I)	H10	O11-C10-N12	-2.17	118.40	122.63
15	Y	1(L)	MES	O1-C2-C3	-2.10	107.24	111.77
15	Y	1(L)	MES	O2S-S-O1S	-2.04	107.18	113.82
15	K	1(L)	MES	O2S-S-O1S	-2.00	107.31	113.82

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	K	1(L)	MES	C7-C8-S-O1S
15	K	1(L)	MES	C7-C8-S-O3S
15	Y	1(L)	MES	C7-C8-S-O1S
15	Y	1(L)	MES	C7-C8-S-O2S
15	Y	1(L)	MES	C7-C8-S-O3S
16	K	2(I)	H10	C5-C6-C7-C8
16	Y	2(I)	H10	C5-C6-C7-C8
15	K	1(L)	MES	C8-C7-N4-C3
15	K	1(L)	MES	C8-C7-N4-C5
15	K	1(L)	MES	C7-C8-S-O2S
16	K	2(I)	H10	C14-C8-N9-O13
16	Y	2(I)	H10	C14-C8-N9-O13

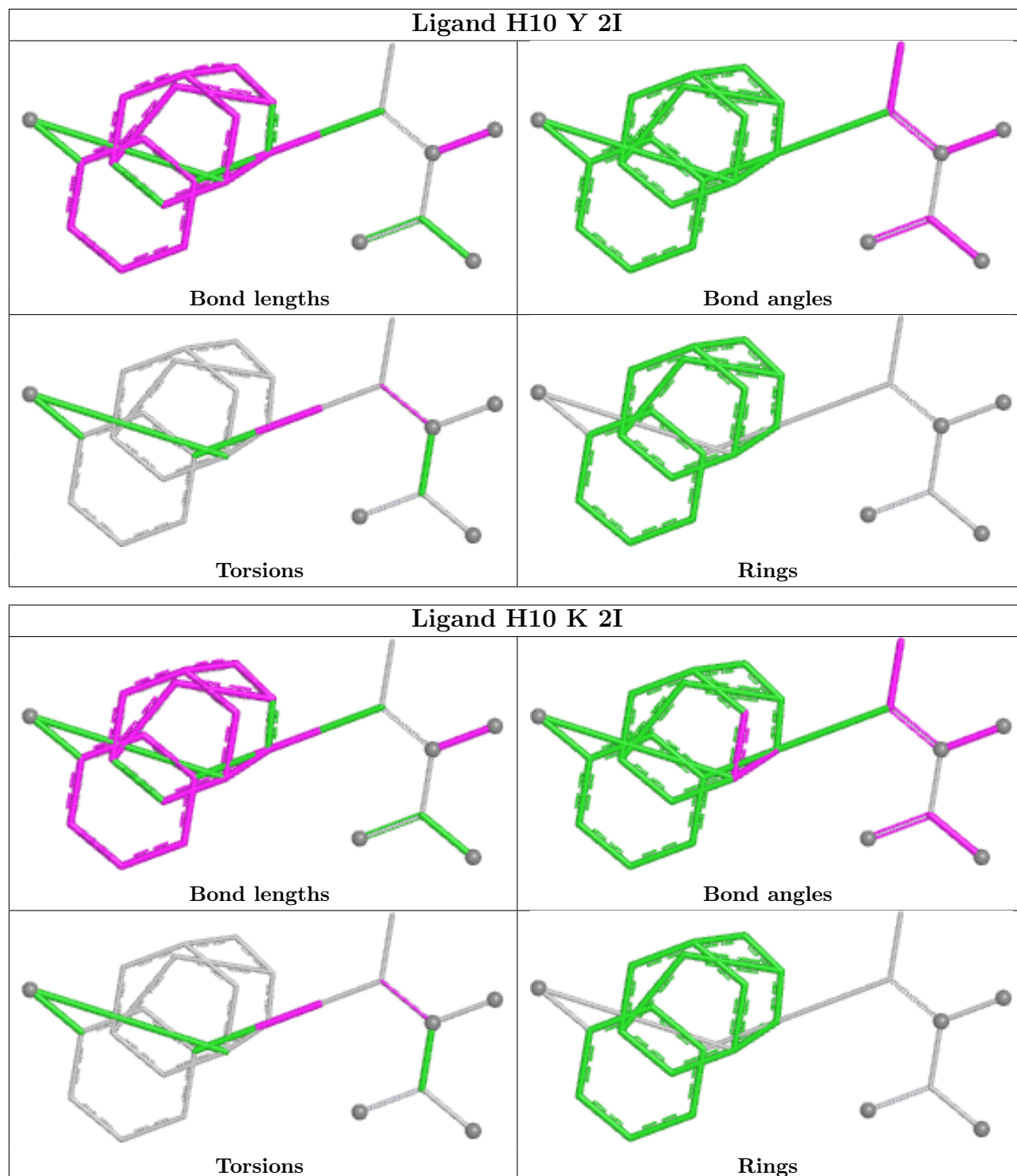
There are no ring outliers.

2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	Y	2(I)	H10	7	0
16	K	2(I)	H10	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	250/250 (100%)	0.26	6 (2%) 59 49	47, 64, 92, 112	0
1	O	250/250 (100%)	0.43	9 (3%) 46 37	48, 65, 94, 112	0
2	B	244/244 (100%)	0.59	13 (5%) 32 24	47, 67, 103, 129	0
2	P	244/244 (100%)	0.60	15 (6%) 27 20	46, 67, 103, 129	0
3	C	241/241 (100%)	0.63	16 (6%) 24 18	50, 69, 118, 136	0
3	Q	241/241 (100%)	0.62	16 (6%) 24 18	51, 70, 118, 136	0
4	D	242/242 (100%)	0.52	13 (5%) 31 24	49, 70, 102, 133	0
4	R	242/242 (100%)	0.56	14 (5%) 29 22	48, 70, 103, 133	0
5	E	233/233 (100%)	0.54	8 (3%) 48 39	52, 74, 98, 121	0
5	S	233/233 (100%)	0.73	18 (7%) 19 14	52, 75, 99, 121	0
6	F	244/244 (100%)	0.43	7 (2%) 53 43	48, 65, 100, 112	0
6	T	244/244 (100%)	0.42	8 (3%) 49 39	48, 65, 101, 113	0
7	G	243/243 (100%)	0.26	6 (2%) 58 48	45, 61, 88, 120	0
7	U	243/243 (100%)	0.30	5 (2%) 63 54	46, 62, 87, 119	0
8	H	222/222 (100%)	0.23	5 (2%) 61 51	46, 59, 78, 110	0
8	V	222/222 (100%)	0.26	3 (1%) 73 64	48, 61, 78, 109	0
9	I	204/204 (100%)	0.10	6 (2%) 53 43	42, 58, 81, 95	0
9	W	204/204 (100%)	0.20	6 (2%) 53 43	44, 58, 80, 96	0
10	J	198/198 (100%)	0.14	6 (3%) 52 42	44, 58, 75, 128	0
10	X	198/198 (100%)	0.11	3 (1%) 72 63	46, 58, 74, 128	0
11	K	212/212 (100%)	0.13	3 (1%) 73 64	42, 57, 73, 84	0
11	Y	212/212 (100%)	0.14	3 (1%) 73 64	44, 58, 73, 84	0
12	L	222/222 (100%)	0.19	2 (0%) 81 74	42, 59, 81, 100	0
12	Z	222/222 (100%)	0.16	2 (0%) 81 74	42, 60, 81, 99	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1	233/233 (100%)	0.08	2 (0%) 81 74	45, 57, 71, 80	0
13	M	233/233 (100%)	0.12	1 (0%) 88 84	44, 58, 72, 79	0
14	2	196/196 (100%)	0.12	0 100 100	44, 54, 75, 87	0
14	N	196/196 (100%)	-0.00	1 (0%) 87 82	42, 53, 74, 88	0
All	All	6368/6368 (100%)	0.33	197 (3%) 51 41	42, 62, 95, 136	0

All (197) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	12(C)	GLY	8.3
3	Q	56	LEU	7.9
2	B	4	GLY	7.4
4	R	12(D)	ALA	7.2
4	D	12(D)	ALA	7.0
7	G	6	ALA	6.2
7	U	240	ASP	6.1
3	C	56	LEU	5.9
5	E	4	PHE	5.7
3	C	55	THR	5.3
4	D	12(E)	SER	5.1
4	R	127	LEU	5.0
5	S	4	PHE	5.0
4	R	12(E)	SER	4.9
2	B	54	VAL	4.6
3	C	54	SER	4.5
3	Q	55	THR	4.5
9	W	121	GLU	4.4
2	P	239	THR	4.3
4	D	126	ARG	4.1
6	F	240	ILE	4.1
2	B	239	THR	4.0
3	C	207	ALA	4.0
3	C	206	GLY	4.0
2	B	21(B)	GLY	3.8
4	R	126	ARG	3.7
2	B	21(D)	GLY	3.7
12	L	145	TYR	3.7
9	W	122	ALA	3.6
10	X	192	ALA	3.5
2	P	217	ALA	3.5
7	U	6	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
4	R	12(F)	GLY	3.5
13	1	-8	THR	3.5
2	P	61	GLN	3.4
9	I	116	ILE	3.4
1	A	4	MET	3.4
1	O	65	SER	3.4
2	B	213	ALA	3.4
2	B	61	GLN	3.4
3	C	59	GLN	3.4
10	X	-1	MET	3.4
6	T	18(B)	HIS	3.3
3	C	203	THR	3.3
8	H	159	ILE	3.2
1	A	5	THR	3.2
3	Q	57	LYS	3.2
3	Q	58	LEU	3.1
5	S	203	ASP	3.1
8	V	223	ASP	3.1
2	P	21(D)	GLY	3.1
10	J	-1	MET	3.1
4	D	127	LEU	3.1
2	P	220	TYR	3.1
2	B	217	ALA	3.1
1	O	21(L)	ILE	3.1
8	H	221	ILE	3.1
1	O	4	MET	3.1
2	P	54	VAL	3.1
9	I	117	GLY	3.1
3	Q	70	ILE	3.0
9	W	177	ILE	3.0
2	P	58	LEU	3.0
2	P	21(B)	GLY	3.0
3	Q	44	ASN	2.9
2	P	63	THR	2.9
2	P	219	GLU	2.9
2	P	62	ASP	2.9
6	T	197	ILE	2.9
3	Q	186	VAL	2.8
4	D	242	ALA	2.8
2	P	53	LYS	2.8
8	V	221	ILE	2.8
5	S	60	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	O	5	THR	2.8
9	I	113	PHE	2.7
3	C	209	ASN	2.7
4	R	12(A)	GLY	2.7
10	J	192	ALA	2.7
13	1	203	ILE	2.7
3	Q	53	ARG	2.7
1	O	236	LEU	2.7
2	B	238	ILE	2.7
3	Q	207	ALA	2.7
5	S	213	ALA	2.7
5	S	65	LYS	2.7
9	I	120	ASP	2.7
2	P	4	GLY	2.7
1	O	64	LEU	2.7
3	C	208	LYS	2.6
6	F	55	THR	2.6
13	M	-8	THR	2.6
5	S	223	ILE	2.6
5	S	197	ILE	2.6
3	Q	54	SER	2.6
7	G	239	GLN	2.6
11	K	208	ASN	2.6
7	G	7	GLY	2.5
11	K	101	ILE	2.5
5	S	66	LYS	2.5
14	N	149	GLU	2.5
5	E	65	LYS	2.5
9	W	119	ILE	2.4
3	C	52	ARG	2.4
2	B	77	ALA	2.4
3	Q	64	PRO	2.4
7	G	240	ASP	2.4
11	Y	145	ASP	2.4
11	Y	143	LYS	2.4
12	Z	145	TYR	2.4
9	I	-8	SER	2.4
5	E	58	LEU	2.4
4	R	9	ASP	2.3
5	S	225	ASP	2.3
4	D	12(F)	GLY	2.3
5	E	162	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
4	D	40	ILE	2.3
4	D	241	GLU	2.3
9	I	121	GLU	2.3
2	B	223	ILE	2.3
5	S	67	ILE	2.3
3	C	33	ARG	2.3
6	T	223	PHE	2.3
12	L	14(Q)	LEU	2.3
9	W	12(A)	LYS	2.3
8	H	41	ILE	2.3
1	A	56	SER	2.3
3	Q	63	THR	2.3
5	S	211	SER	2.3
5	S	222	THR	2.3
4	R	12(C)	GLY	2.3
7	U	29	LYS	2.2
10	X	193	GLN	2.2
6	F	208	PHE	2.2
4	R	12(G)	GLU	2.2
1	O	61	SER	2.2
5	E	230	ALA	2.2
6	T	205	ASN	2.2
3	C	70	ILE	2.2
3	Q	210	ILE	2.2
6	F	204	ASP	2.2
5	S	18(B)	THR	2.2
1	O	37	SER	2.2
5	E	233	ILE	2.2
5	S	68	ILE	2.2
7	G	49	ILE	2.2
3	C	185	THR	2.2
12	Z	14(K)	LYS	2.2
1	O	56	SER	2.2
6	F	59	LEU	2.2
1	A	33	GLN	2.1
4	R	62	ASP	2.1
9	W	120	ASP	2.1
1	A	21(N)	THR	2.1
4	D	243	ALA	2.1
4	R	13	SER	2.1
5	S	55	ALA	2.1
5	S	59	SER	2.1

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Mol	Chain	Res	Type	RSRZ
8	H	44	ALA	2.1
4	R	12(B)	GLU	2.1
11	Y	10(A)	ARG	2.1
2	P	202	THR	2.1
3	C	53	ARG	2.1
3	C	122	ARG	2.1
4	D	12(B)	GLU	2.1
7	G	12	ILE	2.1
8	H	113	ILE	2.1
3	Q	66	LYS	2.1
7	U	57	LYS	2.1
5	E	203	ASP	2.1
5	E	212	ILE	2.1
6	T	240	ILE	2.1
7	U	18(H)	GLU	2.1
11	K	110	ILE	2.1
10	J	191	GLN	2.1
4	R	240	LYS	2.1
6	F	180	VAL	2.1
3	Q	224	LEU	2.1
2	B	63	THR	2.1
4	D	31	ILE	2.1
6	T	203	GLU	2.1
2	P	218	ASN	2.0
1	A	21(K)	GLY	2.0
4	D	10	ARG	2.0
8	V	180	ILE	2.0
10	J	121	GLU	2.0
3	C	57	LYS	2.0
10	J	141	HIS	2.0
4	R	121	LEU	2.0
6	T	199	LEU	2.0
5	S	5	ARG	2.0
6	T	226	GLY	2.0
5	S	18(F)	ILE	2.0
6	F	212	ILE	2.0
3	Q	223	ALA	2.0
10	J	168	MET	2.0
2	B	220	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

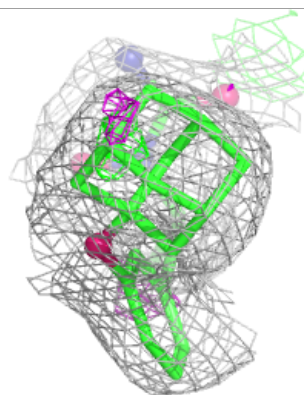
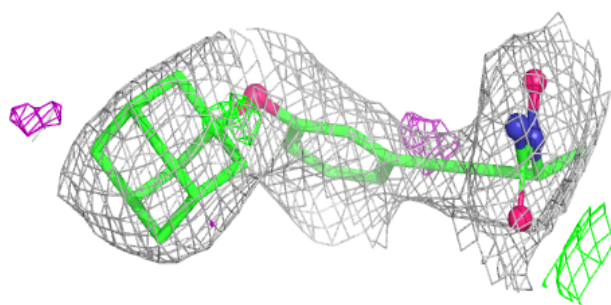
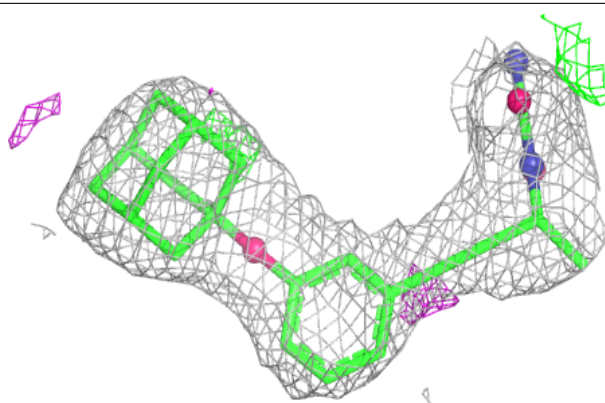
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
16	H10	Y	2(I)	26/26	0.92	0.12	46,51,60,62	0
15	MES	Y	1(L)	12/12	0.93	0.14	63,70,75,76	0
16	H10	K	2(I)	26/26	0.95	0.11	46,50,57,58	0
15	MES	K	1(L)	12/12	0.95	0.13	62,70,76,77	0

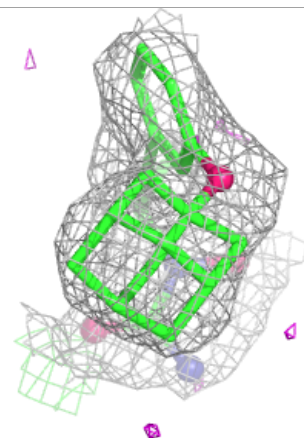
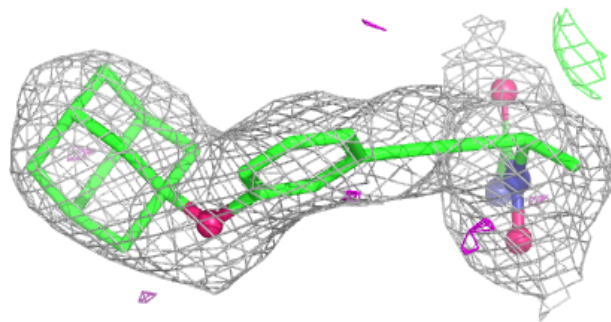
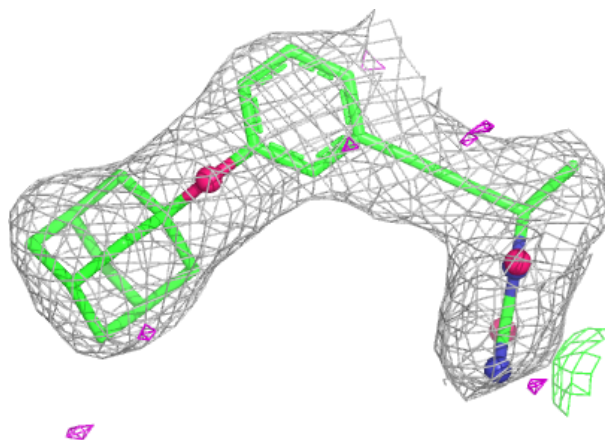
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around H10 Y 2I:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around H10 K 2I:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.