



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:26 AM UTC

PDB ID : 1G65 / pdb_00001g65
Title : Crystal structure of epoxomicin:20s proteasome reveals a molecular basis for selectivity of alpha,beta-epoxyketone proteasome inhibitors
Authors : Groll, M.; Kim, K.B.; Kairies, N.; Huber, R.; Crews, C.
Deposited on : 2000-11-03
Resolution : 2.25 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

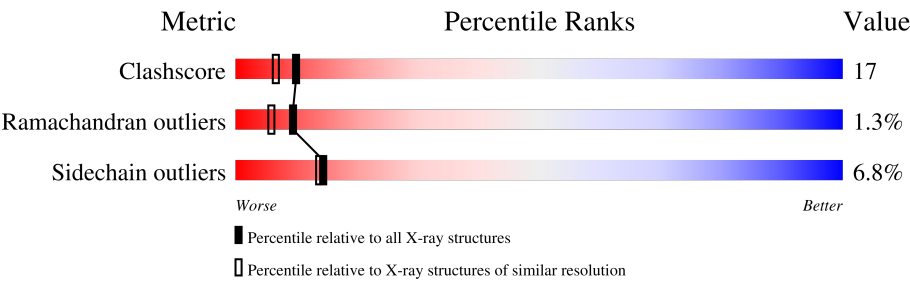
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)

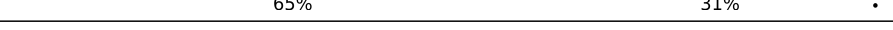
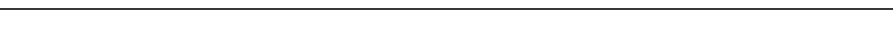
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively.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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	250	67% 30% .
1	O	250	63% 34% .
2	B	244	57% 38% ..
2	P	244	57% 37% 6%
3	C	241	61% 34% 5%
3	Q	241	53% 40% 7%
4	D	242	61% 35% .
4	R	242	67% 29% .

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Mol	Chain	Length	Quality of chain
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	
15	3	5	
15	4	5	

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 52508 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 a protein called EPOXOMICIN (peptide inhibitor).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	3	5	Total	C	N	O	0	0	0
			39	28	4	7			
15	4	5	Total	C	N	O	0	0	0
			39	28	4	7			

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

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

- Molecule 17 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	100	Total 100	O 100	0	0
17	B	72	Total 72	O 72	0	0
17	C	71	Total 71	O 71	0	0
17	D	86	Total 86	O 86	0	0
17	E	57	Total 57	O 57	0	0
17	F	98	Total 98	O 98	0	0
17	G	106	Total 106	O 106	0	0
17	H	129	Total 129	O 129	0	0
17	I	109	Total 109	O 109	0	0
17	J	114	Total 114	O 114	0	0
17	K	94	Total 94	O 94	0	0

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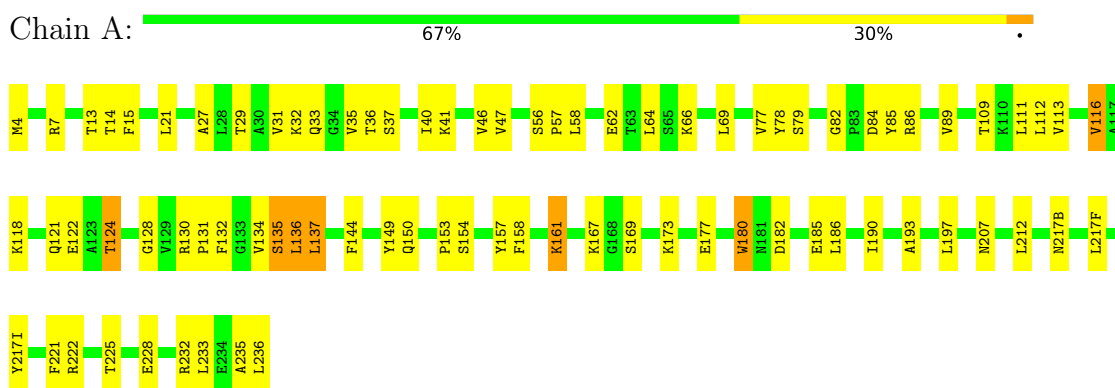
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	L	147	Total 147	O 147	0	0
17	M	130	Total 130	O 130	0	0
17	N	115	Total 115	O 115	0	0
17	O	99	Total 99	O 99	0	0
17	P	72	Total 72	O 72	0	0
17	Q	68	Total 68	O 68	0	0
17	R	87	Total 87	O 87	0	0
17	S	56	Total 56	O 56	0	0
17	T	95	Total 95	O 95	0	0
17	U	111	Total 111	O 111	0	0
17	V	124	Total 124	O 124	0	0
17	W	111	Total 111	O 111	0	0
17	X	119	Total 119	O 119	0	0
17	Y	93	Total 93	O 93	0	0
17	Z	142	Total 142	O 142	0	0
17	1	142	Total 142	O 142	0	0
17	2	124	Total 124	O 124	0	0
17	3	1	Total 1	O 1	0	0

3 Residue-property plots

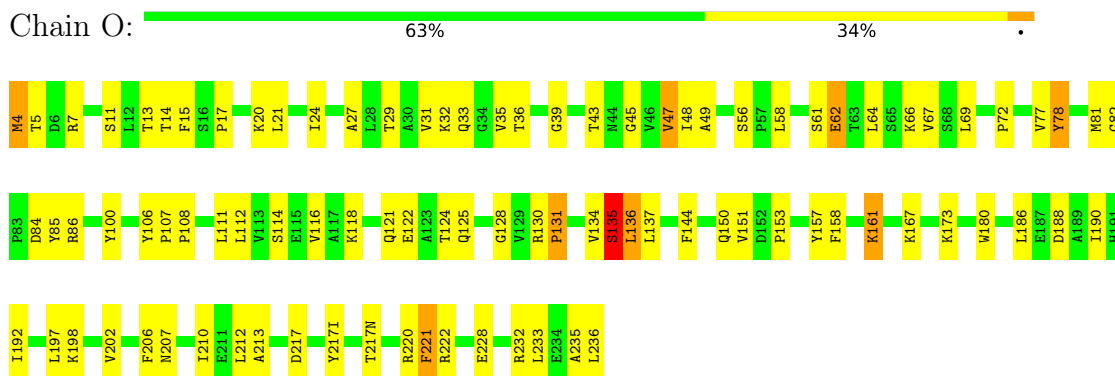
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

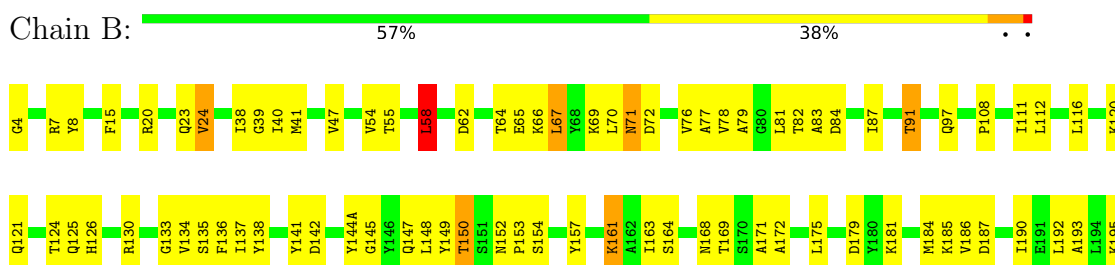
• Molecule 1: Proteasome component Y7

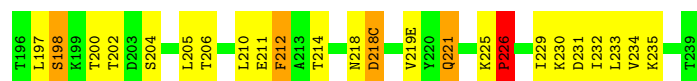


• Molecule 1: Proteasome component Y7

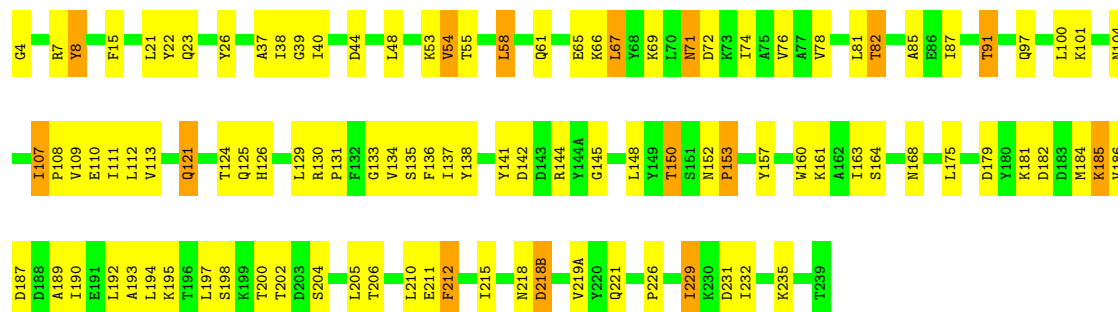


• Molecule 2: Proteasome component Y13

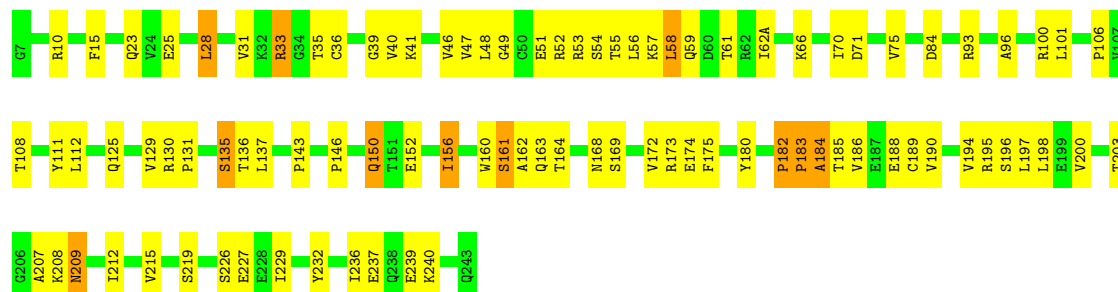




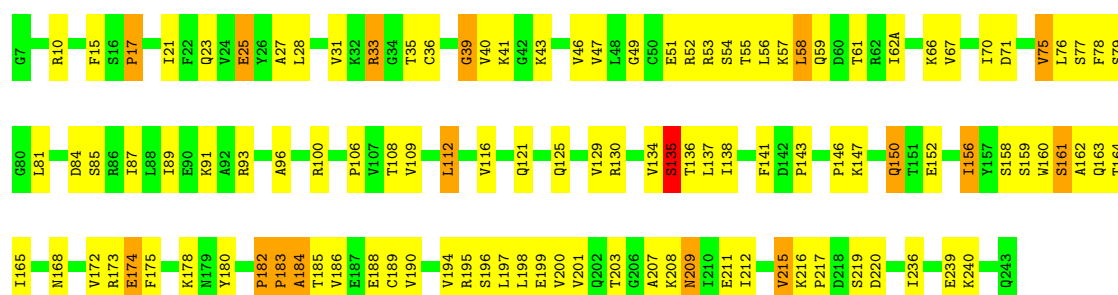
• Molecule 2: Proteasome component Y13



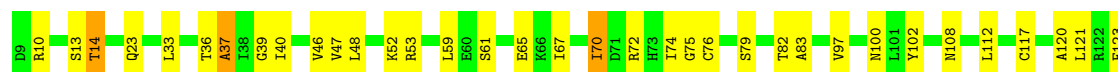
• Molecule 3: Proteasome component PRE6

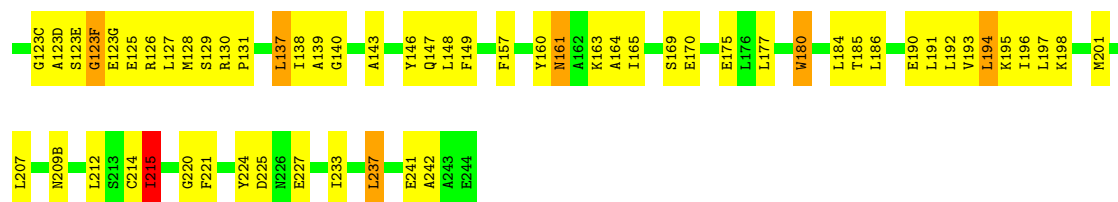


• Molecule 3: Proteasome component PRE6



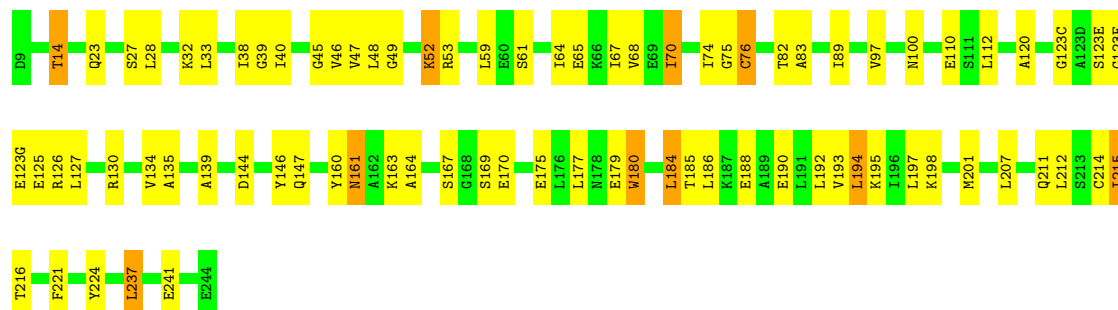
• Molecule 4: Proteasome component PUP2





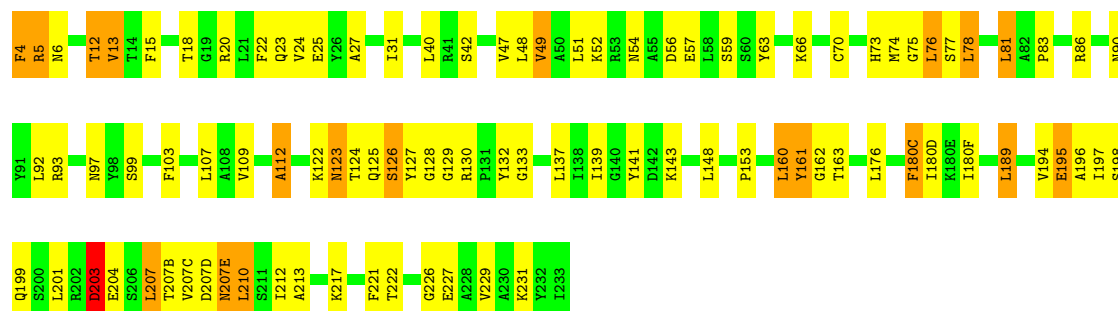
• Molecule 4: Proteasome component PUP2

Chain R: 67% 29% .



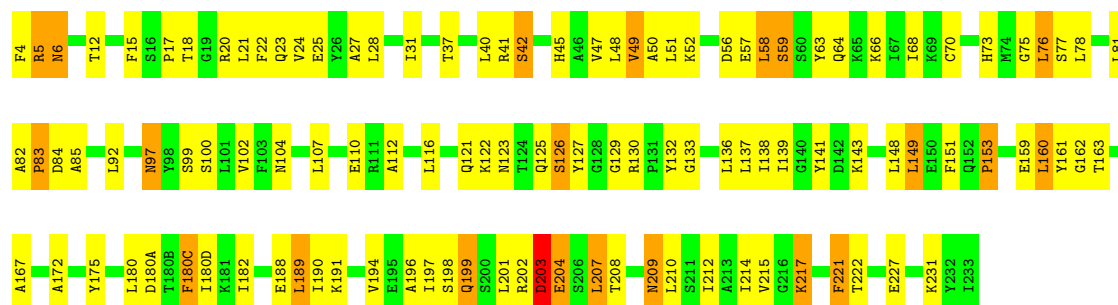
• Molecule 5: Proteasome component PRE5

Chain E: 59% 33% 8%



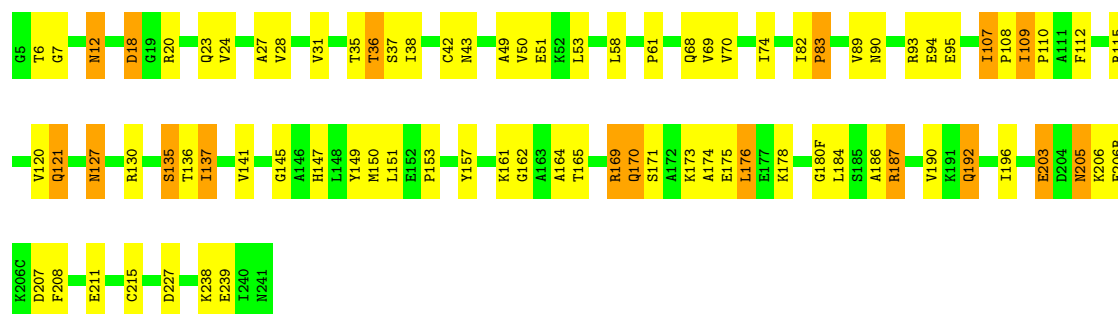
• Molecule 5: Proteasome component PRE5

Chain S: 51% 39% 9%



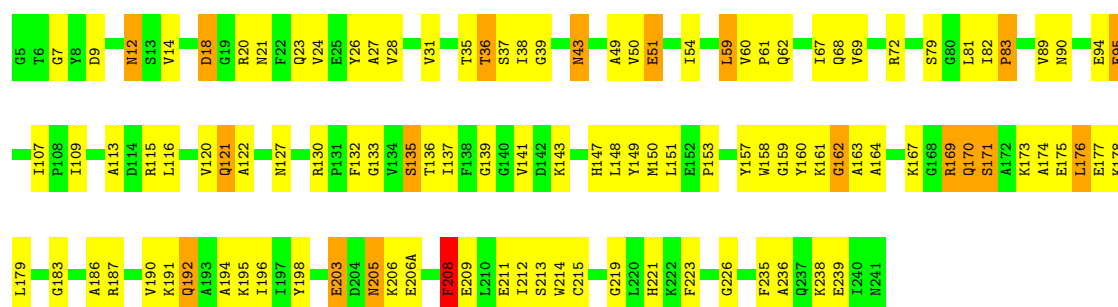
• Molecule 6: Proteasome component C1

Chain F: 



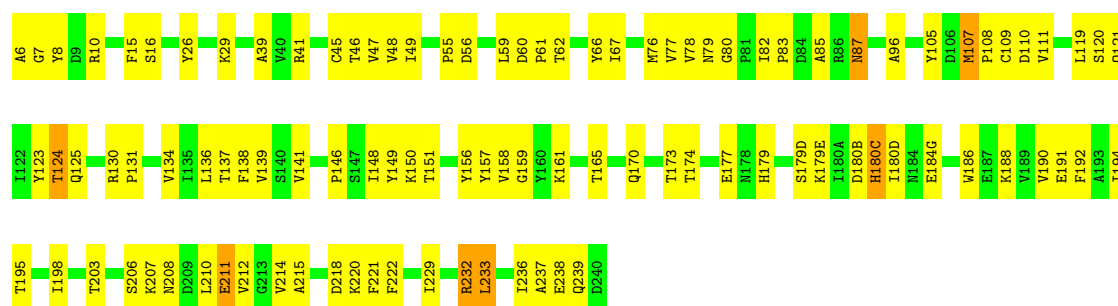
• Molecule 6: Proteasome component C1

Chain T: 



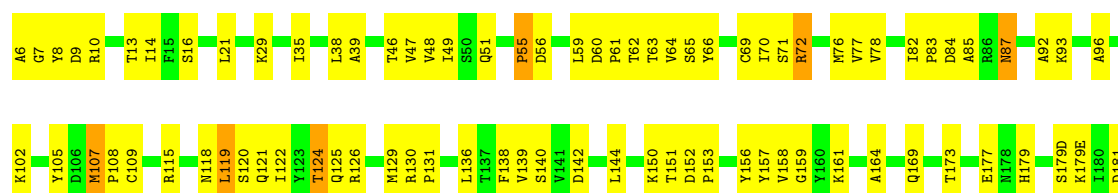
• Molecule 7: Proteasome component C7-alpha

Chain G: 



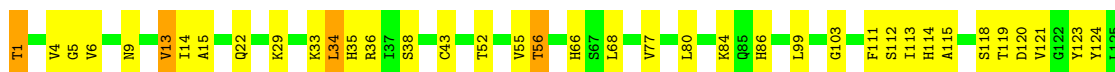
• Molecule 7: Proteasome component C7-alpha

Chain U: 





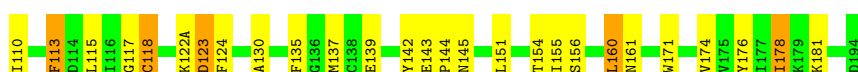
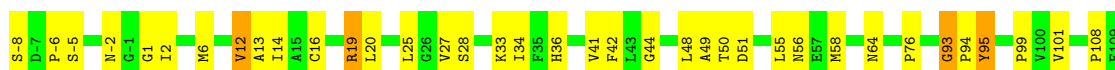
• Molecule 8: Proteasome component PUP1



• Molecule 8: Proteasome component PUP1



• Molecule 9: Proteasome component PUP3

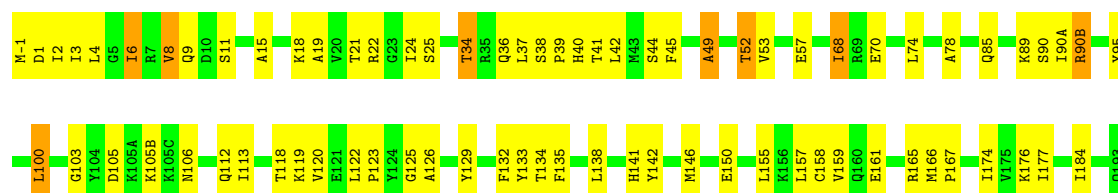


• Molecule 9: Proteasome component PUP3



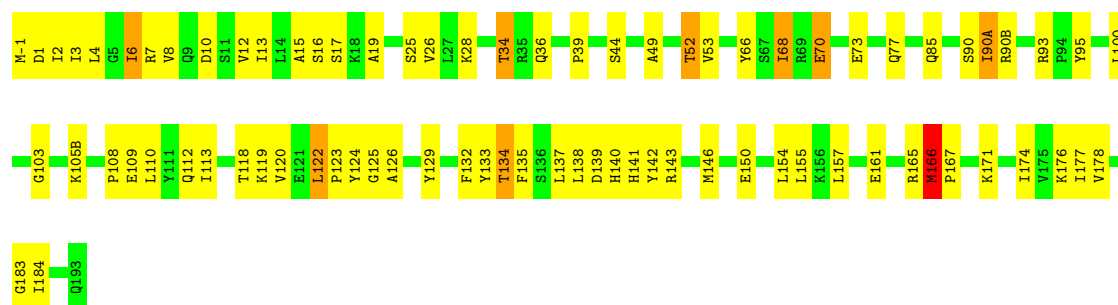
• Molecule 10: Proteasome component C11

Chain J: 



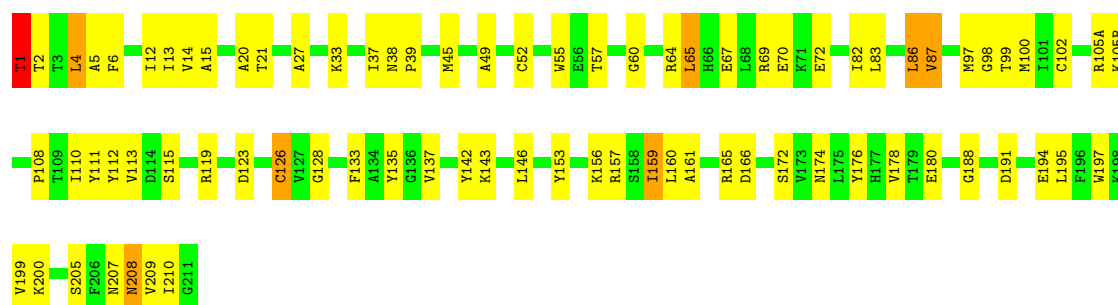
• Molecule 10: Proteasome component C11

Chain X: 



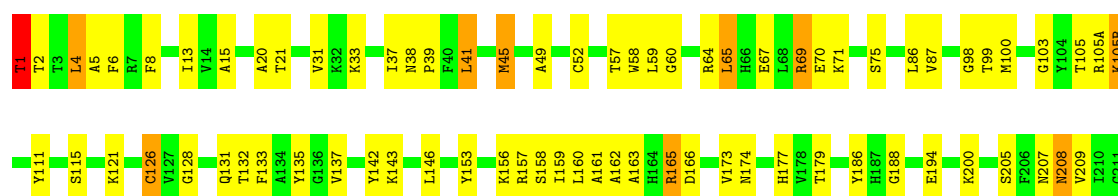
• Molecule 11: Proteasome component PRE2

Chain K: 



• Molecule 11: Proteasome component PRE2

Chain Y: 



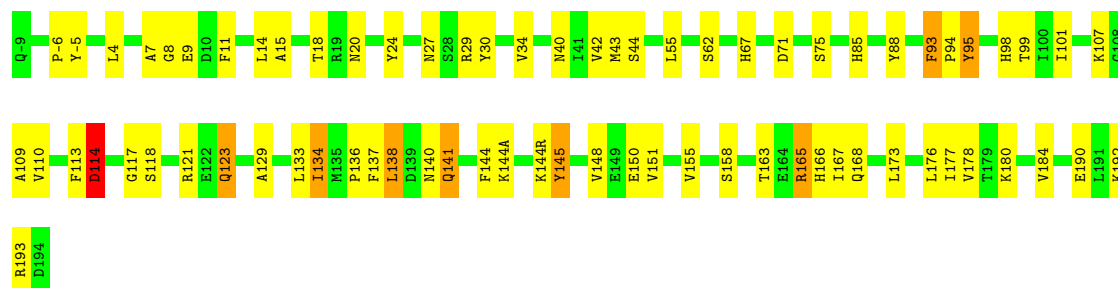
• Molecule 12: Proteasome component C5

Chain L: 



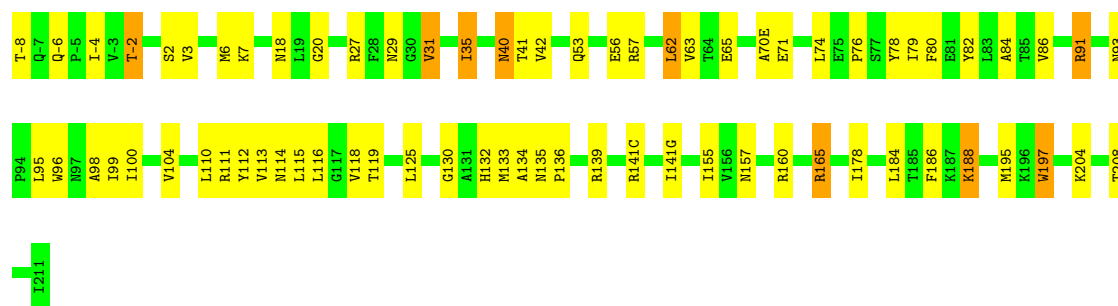
- Molecule 12: Proteasome component C5

Chain Z: 67% 29% .



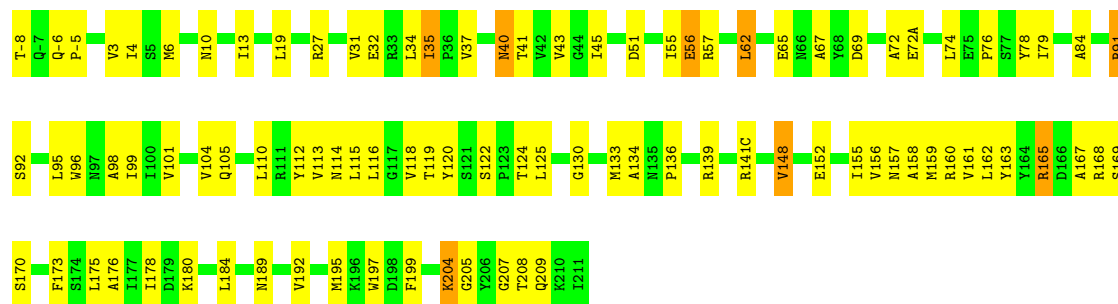
- Molecule 13: Proteasome component PRE4

Chain M: 69% 27% .



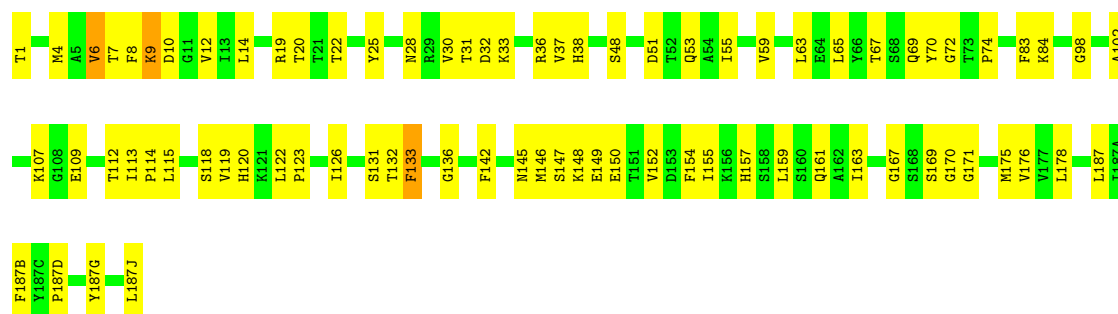
- Molecule 13: Proteasome component PRE4

Chain 1: 60% 36% .



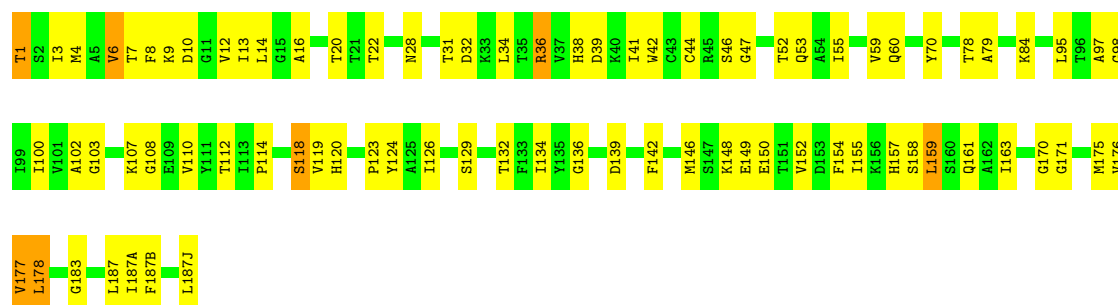
- Molecule 14: Proteasome component PRE3

Chain N:  60% 39% .



• Molecule 14: Proteasome component PRE3

Chain 2:  59% 38% .



• Molecule 15: EPOXOMICIN (peptide inhibitor)

Chain 3:  20% 80%



• Molecule 15: EPOXOMICIN (peptide inhibitor)

Chain 4:  40% 60%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	135.20Å 300.20Å 144.02Å 90.00° 112.98° 90.00°	Depositor
Resolution (Å)	20.00 – 2.25	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.25)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.283 , 0.336	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	52508	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ACE, MG, IML, 04D

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	0.79	0/1952	1.11	13/2642 (0.5%)
1	O	0.75	0/1952	1.09	14/2642 (0.5%)
2	B	0.78	0/1935	1.05	7/2618 (0.3%)
2	P	0.73	0/1935	1.08	9/2618 (0.3%)
3	C	0.74	0/1920	1.10	8/2598 (0.3%)
3	Q	0.73	0/1920	1.12	11/2598 (0.4%)
4	D	0.76	0/1887	1.03	10/2541 (0.4%)
4	R	0.71	0/1887	1.02	7/2541 (0.3%)
5	E	0.68	0/1823	1.04	11/2463 (0.4%)
5	S	0.69	0/1823	1.05	7/2463 (0.3%)
6	F	0.68	1/1937 (0.1%)	1.09	13/2614 (0.5%)
6	T	0.76	1/1937 (0.1%)	1.14	16/2614 (0.6%)
7	G	0.81	1/1959 (0.1%)	1.14	8/2652 (0.3%)
7	U	0.84	1/1959 (0.1%)	1.14	13/2652 (0.5%)
8	H	0.87	1/1716 (0.1%)	1.29	10/2326 (0.4%)
8	V	0.80	1/1716 (0.1%)	1.21	9/2326 (0.4%)
9	I	0.81	0/1611	1.14	12/2174 (0.6%)
9	W	0.85	0/1611	1.16	12/2174 (0.6%)
10	J	0.84	1/1613 (0.1%)	1.11	10/2173 (0.5%)
10	X	0.83	0/1613	1.15	16/2173 (0.7%)
11	K	0.85	1/1681 (0.1%)	1.09	11/2274 (0.5%)
11	Y	0.82	1/1681 (0.1%)	1.10	12/2274 (0.5%)
12	L	0.80	1/1795 (0.1%)	1.09	13/2420 (0.5%)
12	Z	0.79	0/1795	1.12	9/2420 (0.4%)
13	1	0.84	0/1855	1.14	12/2514 (0.5%)
13	M	0.81	0/1855	1.11	14/2514 (0.6%)
14	2	0.84	1/1541 (0.1%)	1.06	5/2087 (0.2%)
14	N	0.84	1/1541 (0.1%)	1.17	11/2087 (0.5%)
15	3	1.70	0/14	1.91	0/18
15	4	1.43	0/14	1.73	0/18
All	All	0.79	12/50478 (0.0%)	1.11	303/68228 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	1	THR	C-N	-14.54	1.14	1.33
11	K	1	THR	C-N	10.93	1.47	1.33
11	Y	1	THR	C-N	9.28	1.46	1.33
6	T	109	ILE	CA-CB	-8.38	1.49	1.54
14	N	1	THR	C-N	7.81	1.44	1.33
6	F	109	ILE	CA-CB	-6.42	1.50	1.54
8	V	1	THR	C-N	-6.09	1.25	1.33
7	G	107	MET	SD-CE	-6.02	1.64	1.79
7	U	107	MET	SD-CE	-5.71	1.65	1.79
12	L	83	ILE	CA-CB	-5.43	1.47	1.54
14	2	1	THR	C-N	5.26	1.40	1.33
10	J	177	ILE	CA-CB	-5.21	1.48	1.54

All (303) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	1	THR	CA-C-N	21.28	153.89	121.76
8	H	1	THR	C-N-CA	21.28	153.89	121.76
8	H	1	THR	O-C-N	-16.74	96.21	123.00
8	V	1	THR	CA-C-N	16.10	146.62	122.47
8	V	1	THR	C-N-CA	16.10	146.62	122.47
13	M	27	ARG	N-CA-C	12.64	124.80	111.14
8	V	1	THR	O-C-N	-12.18	103.51	123.00
14	N	1	THR	CA-C-N	11.64	139.39	122.86
14	N	1	THR	C-N-CA	11.64	139.39	122.86
3	C	62(A)	ILE	N-CA-C	11.07	121.33	111.81
3	Q	62(A)	ILE	N-CA-C	10.49	121.20	111.45
10	J	122	LEU	N-CA-C	10.20	120.08	108.25
13	1	27	ARG	N-CA-C	9.70	123.23	111.40
10	X	122	LEU	N-CA-C	9.39	119.15	108.25
7	G	60	ASP	CA-C-N	9.25	130.20	119.47
7	G	60	ASP	C-N-CA	9.25	130.20	119.47
11	K	188	GLY	N-CA-C	9.24	124.32	112.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	70	ILE	N-CA-C	-9.23	102.86	111.45
9	W	60	ARG	N-CA-C	-8.56	101.89	111.14
12	Z	117	GLY	N-CA-C	8.50	125.08	114.37
2	P	107	ILE	N-CA-C	8.43	115.88	108.63
3	C	161	SER	N-CA-C	-8.39	102.21	111.36
13	M	165	ARG	N-CA-C	8.38	123.80	113.50
7	G	161	LYS	N-CA-C	-8.33	102.16	111.82
10	X	165	ARG	N-CA-C	8.26	123.66	113.50
1	O	161	LYS	N-CA-C	-8.13	101.99	112.23
10	X	166	MET	CA-C-N	8.09	127.77	119.19
10	X	166	MET	C-N-CA	8.09	127.77	119.19
9	W	142	TYR	N-CA-C	8.04	121.89	110.23
12	L	95	TYR	N-CA-C	-8.04	96.18	108.96
12	Z	95	TYR	N-CA-C	-8.02	95.49	108.41
11	K	208	ASN	N-CA-C	-7.99	104.02	113.21
1	A	161	LYS	N-CA-C	-7.98	102.17	112.23
9	W	95	TYR	N-CA-C	-7.97	96.22	109.46
10	J	165	ARG	N-CA-C	7.93	123.25	113.50
11	Y	1	THR	N-CA-CB	-7.92	98.03	111.50
6	T	161	LYS	N-CA-C	-7.81	102.39	112.23
6	F	12	ASN	N-CA-C	7.78	120.65	111.71
4	R	70	ILE	N-CA-C	-7.69	104.36	111.67
12	Z	114	ASP	N-CA-C	-7.67	99.70	110.29
8	V	180	ILE	N-CA-C	7.67	118.42	110.36
11	K	1	THR	N-CA-CB	-7.65	98.50	111.50
11	Y	188	GLY	N-CA-C	7.55	123.99	112.81
11	Y	57	THR	N-CA-C	-7.55	103.05	111.28
3	Q	70	ILE	N-CA-C	-7.39	103.74	111.58
14	N	115	LEU	N-CA-C	7.29	120.15	111.33
10	X	183	GLY	N-CA-C	7.29	118.79	111.21
6	T	12	ASN	N-CA-C	7.28	120.08	111.71
14	2	183	GLY	N-CA-C	7.28	118.78	111.21
2	B	137	ILE	N-CA-C	-7.24	97.98	108.11
6	F	135	SER	N-CA-C	-7.14	97.76	109.40
9	W	145	ASN	N-CA-C	7.10	121.19	111.54
9	I	145	ASN	N-CA-C	7.05	121.12	111.39
7	G	16	SER	N-CA-C	-7.02	101.89	110.31
7	U	60	ASP	CA-C-N	7.00	128.59	119.84
7	U	60	ASP	C-N-CA	7.00	128.59	119.84
6	T	135	SER	N-CA-C	-7.00	98.00	109.40
13	1	35	ILE	N-CA-C	6.97	115.06	107.60
5	E	207(E)	ASN	N-CA-C	6.97	120.26	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	Y	208	ASN	N-CA-C	-6.94	105.16	112.93
8	H	141	HIS	N-CA-C	6.91	122.71	113.72
4	R	169	SER	N-CA-C	6.91	119.45	111.02
4	R	161	ASN	N-CA-C	-6.90	104.34	112.89
10	X	95	TYR	N-CA-C	-6.88	99.64	109.96
8	V	9	ASN	N-CA-C	6.88	119.65	111.33
13	1	98	ALA	N-CA-C	-6.86	97.16	108.76
3	Q	161	SER	N-CA-C	-6.86	103.87	111.82
2	B	161	LYS	N-CA-C	-6.85	105.08	113.50
3	Q	108	THR	N-CA-C	-6.79	100.46	110.52
2	P	179	ASP	N-CA-C	6.78	121.57	113.16
6	F	206(B)	GLU	N-CA-C	6.70	119.58	111.40
5	E	161	TYR	N-CA-C	-6.69	103.80	112.23
7	U	161	LYS	N-CA-C	-6.69	103.80	112.23
9	I	95	TYR	N-CA-C	-6.69	98.36	109.46
2	B	125	GLN	N-CA-C	6.65	122.48	113.97
12	L	134	ILE	N-CA-C	6.64	117.43	110.72
13	1	95	LEU	N-CA-C	-6.64	96.85	108.20
7	U	239	GLN	N-CA-C	-6.62	104.37	113.18
9	W	93	GLY	CA-C-N	6.60	128.09	119.84
9	W	93	GLY	C-N-CA	6.60	128.09	119.84
1	O	190	ILE	N-CA-C	-6.60	103.90	110.30
5	E	57	GLU	N-CA-C	-6.60	104.98	113.16
9	W	143	GLU	CA-C-N	6.59	126.61	119.89
9	W	143	GLU	C-N-CA	6.59	126.61	119.89
9	I	143	GLU	CA-C-N	6.59	126.61	119.89
9	I	143	GLU	C-N-CA	6.59	126.61	119.89
11	Y	126	CYS	N-CA-C	-6.58	98.25	109.24
12	Z	165	ARG	N-CA-C	6.56	121.57	113.50
8	V	38	SER	N-CA-C	-6.56	100.64	108.25
4	R	144	ASP	N-CA-C	6.54	118.49	111.36
14	N	69	GLN	N-CA-C	6.51	119.35	111.40
12	L	38	GLY	N-CA-C	-6.49	104.50	112.68
12	Z	134	ILE	N-CA-C	6.49	117.27	110.72
6	F	162	GLY	N-CA-C	-6.47	101.27	110.91
11	Y	165	ARG	N-CA-C	6.44	118.38	111.36
5	E	180(C)	PHE	N-CA-C	6.40	119.07	111.71
11	Y	38	ASN	N-CA-C	-6.37	100.81	108.14
1	O	144	PHE	N-CA-C	6.37	121.21	113.38
14	N	53	GLN	N-CA-C	-6.35	104.05	110.97
1	O	128	GLY	N-CA-C	6.35	124.44	115.30
5	S	57	GLU	N-CA-C	-6.34	105.53	113.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	T	107	ILE	CA-C-N	6.34	126.31	119.78
6	T	107	ILE	C-N-CA	6.34	126.31	119.78
13	M	3	VAL	N-CA-C	-6.33	99.01	108.12
12	L	93	PHE	N-CA-C	-6.28	95.93	109.81
10	J	95	TYR	N-CA-C	-6.27	99.79	109.76
11	K	1	THR	OG1-CB-CG2	-6.27	96.77	109.30
12	L	114	ASP	N-CA-C	-6.24	101.68	110.29
13	M	98	ALA	N-CA-C	-6.24	97.25	108.48
14	2	47	GLY	N-CA-C	-6.23	104.73	111.21
1	O	106	TYR	CA-C-N	6.22	124.14	119.66
1	O	106	TYR	C-N-CA	6.22	124.14	119.66
7	G	66	TYR	N-CA-C	-6.21	104.33	112.41
9	I	56	ASN	N-CA-C	-6.17	104.47	111.07
9	I	142	TYR	N-CA-C	6.17	119.41	110.28
2	P	229	ILE	N-CA-C	-6.16	104.74	110.53
14	N	98	GLY	N-CA-C	-6.15	98.60	113.18
14	2	53	GLN	N-CA-C	-6.13	104.51	111.07
6	T	14	VAL	N-CA-C	6.10	116.92	109.30
7	U	144	LEU	N-CA-C	6.10	121.00	113.50
2	P	78	VAL	N-CA-C	6.07	117.33	108.53
10	J	38	SER	N-CA-C	-6.07	102.76	108.22
4	D	82	THR	N-CA-C	6.05	119.76	112.38
7	G	211	GLU	N-CA-C	-6.05	97.73	108.13
11	K	57	THR	N-CA-C	-6.05	104.69	111.28
1	O	78	TYR	N-CA-C	6.02	116.23	108.34
6	F	70	VAL	N-CA-C	-6.01	99.75	108.17
3	C	108	THR	N-CA-C	-6.00	100.78	110.32
5	E	22	PHE	N-CA-C	5.99	117.89	111.36
2	P	186	VAL	N-CA-C	5.97	116.63	110.36
13	1	189	ASN	N-CA-C	5.97	119.92	111.92
7	U	66	TYR	N-CA-C	-5.95	104.68	112.41
1	A	182	ASP	N-CA-C	5.94	120.04	113.21
13	M	2	SER	N-CA-C	5.94	117.96	110.24
1	A	144	PHE	N-CA-C	5.93	120.79	113.50
6	F	137	ILE	N-CA-C	-5.93	99.87	108.17
8	V	98	TYR	N-CA-C	-5.92	98.63	108.34
7	G	239	GLN	N-CA-C	-5.91	105.32	113.18
6	T	226	GLY	N-CA-C	5.91	122.10	111.34
12	Z	114	ASP	CB-CA-C	5.89	117.34	108.86
11	Y	1	THR	OG1-CB-CG2	-5.88	97.55	109.30
8	H	38	SER	N-CA-C	-5.87	101.39	108.14
6	F	180(F)	GLY	N-CA-C	-5.87	103.83	111.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	J	134	THR	N-CA-C	5.87	117.76	111.36
10	X	134	THR	N-CA-C	5.84	117.65	111.28
2	B	58	LEU	N-CA-C	5.84	120.13	112.89
12	L	-7	ASN	CA-C-N	5.84	125.46	119.56
12	L	-7	ASN	C-N-CA	5.84	125.46	119.56
12	L	98	HIS	N-CA-C	-5.83	98.90	108.41
7	U	211	GLU	N-CA-C	-5.83	98.11	108.13
10	X	17	SER	N-CA-C	5.82	118.67	110.23
1	A	128	GLY	N-CA-C	5.82	123.86	114.90
8	H	9	ASN	N-CA-C	5.81	118.36	111.33
8	H	22	GLN	N-CA-C	-5.81	97.27	107.73
1	A	180	TRP	N-CA-C	5.81	118.25	110.35
13	M	31	VAL	N-CA-C	5.81	116.16	107.51
12	Z	93	PHE	CA-C-N	5.80	127.09	119.84
12	Z	93	PHE	C-N-CA	5.80	127.09	119.84
2	B	179	ASP	N-CA-C	5.80	120.47	113.17
4	R	180	TRP	N-CA-C	5.80	118.86	110.28
9	W	168	LEU	N-CA-C	5.79	120.19	113.18
7	U	16	SER	N-CA-C	-5.78	102.83	110.40
3	C	219	SER	N-CA-C	5.78	119.91	112.86
3	Q	21	ILE	N-CA-C	-5.76	98.67	106.85
5	E	42	SER	N-CA-C	-5.76	101.17	109.29
6	T	162	GLY	N-CA-C	-5.74	100.82	111.14
10	J	100	LEU	N-CA-C	-5.73	99.55	108.90
13	M	-2	THR	N-CA-C	5.71	118.09	109.41
9	I	178	ILE	N-CA-C	5.71	116.17	108.17
11	K	98	GLY	N-CA-C	-5.71	99.64	113.18
5	S	59	SER	N-CA-C	5.71	118.09	109.41
14	2	118	SER	N-CA-C	-5.71	102.84	110.55
13	1	148	VAL	CB-CA-C	-5.71	104.56	112.04
13	1	165	ARG	N-CA-C	5.71	120.40	113.38
5	S	180(C)	PHE	N-CA-C	5.71	117.50	111.28
9	I	19	ARG	N-CA-C	5.70	118.92	110.48
14	N	133	PHE	N-CA-C	5.70	118.27	111.71
14	N	122	LEU	CA-C-N	5.70	125.55	119.28
14	N	122	LEU	C-N-CA	5.70	125.55	119.28
14	2	98	GLY	N-CA-C	-5.68	99.72	113.18
12	L	193	ARG	N-CA-C	5.65	119.16	112.72
13	M	29	ASN	N-CA-C	5.64	120.16	112.88
5	S	22	PHE	N-CA-C	5.64	117.51	111.36
13	1	56	GLU	N-CA-C	-5.64	105.03	111.07
8	H	118	SER	N-CA-C	-5.64	100.99	109.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Q	219	SER	N-CA-C	5.63	119.73	112.86
14	N	37	VAL	N-CA-C	-5.62	106.84	113.42
4	D	180	TRP	N-CA-C	5.61	118.37	110.23
2	P	137	ILE	N-CA-C	-5.61	99.56	107.75
7	U	122	ILE	N-CA-C	5.60	116.33	110.62
6	T	183	GLY	N-CA-C	-5.59	104.19	111.52
14	N	131	SER	N-CA-C	5.58	117.44	111.36
11	K	1	THR	O-C-N	-5.57	114.08	123.00
6	T	208	PHE	N-CA-C	5.57	118.14	109.52
7	U	125	GLN	N-CA-C	5.56	120.34	113.50
2	P	58	LEU	N-CA-C	5.55	119.77	112.89
11	Y	98	GLY	N-CA-C	-5.55	100.03	113.18
4	R	179	GLU	N-CA-C	5.54	118.08	111.71
1	A	66	LYS	N-CA-C	-5.53	105.26	112.23
11	Y	69	ARG	N-CA-C	5.52	117.38	111.36
13	M	93	ASN	CA-C-N	5.51	125.49	120.03
13	M	93	ASN	C-N-CA	5.51	125.49	120.03
1	A	185	GLU	N-CA-C	-5.51	101.56	110.32
5	S	42	SER	N-CA-C	-5.50	99.08	110.80
2	B	77	ALA	N-CA-C	-5.49	100.75	109.59
4	D	137	LEU	N-CA-C	-5.49	99.46	108.41
2	P	48	LEU	N-CA-C	-5.48	99.50	108.76
10	X	122	LEU	CA-C-N	5.48	124.82	118.85
10	X	122	LEU	C-N-CA	5.48	124.82	118.85
7	U	82	ILE	CA-C-N	-5.47	113.26	119.28
7	U	82	ILE	C-N-CA	-5.47	113.26	119.28
12	Z	141	GLN	N-CA-C	5.47	119.21	112.54
13	M	95	LEU	N-CA-C	-5.47	97.58	107.75
3	C	182	PRO	N-CA-C	-5.46	105.22	110.47
1	A	135	SER	N-CA-C	-5.46	99.77	109.06
11	K	159	ILE	N-CA-C	-5.45	104.28	111.09
12	L	31	GLU	CA-C-N	5.45	125.37	119.76
12	L	31	GLU	C-N-CA	5.45	125.37	119.76
11	K	126	CYS	N-CA-C	-5.44	100.03	108.90
11	K	108	PRO	N-CA-C	-5.42	102.67	111.19
2	P	160	TRP	N-CA-C	5.42	117.43	109.24
1	A	154	SER	N-CA-C	-5.42	105.53	111.82
3	C	135	SER	N-CA-C	-5.42	100.94	109.50
5	E	210	LEU	N-CA-C	5.42	118.54	110.52
3	Q	135	SER	N-CA-C	-5.41	100.95	109.50
1	O	61	SER	N-CA-C	5.41	117.60	111.11
5	S	49	VAL	N-CA-C	-5.40	100.35	108.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	112	ALA	N-CA-C	-5.39	105.40	111.28
10	J	49	ALA	N-CA-C	5.39	122.28	110.80
9	I	12	VAL	N-CA-C	-5.38	100.53	108.23
10	J	19	ALA	N-CA-C	5.38	118.58	109.76
10	X	26	VAL	N-CA-C	-5.38	100.00	108.23
5	E	195	GLU	N-CA-C	-5.36	104.48	111.02
4	R	110	GLU	N-CA-C	-5.36	105.33	111.07
4	D	129	SER	N-CA-C	5.36	119.07	112.54
6	T	219	GLY	N-CA-C	-5.35	107.83	115.64
13	M	35	ILE	N-CA-C	5.34	112.84	107.55
13	1	3	VAL	N-CA-C	-5.34	100.38	108.17
5	E	49	VAL	N-CA-C	-5.33	100.44	108.12
12	L	159	PHE	N-CA-C	5.33	117.17	111.36
6	F	161	LYS	N-CA-C	-5.33	105.52	112.23
9	I	144	PRO	N-CA-C	5.30	119.54	111.11
8	V	141	HIS	N-CA-C	5.30	120.61	113.72
1	O	135	SER	N-CA-C	-5.30	100.05	109.06
13	1	173	PHE	N-CA-C	5.29	116.04	108.74
1	A	116	VAL	CB-CA-C	-5.29	105.20	111.97
9	W	117	GLY	N-CA-C	5.27	122.02	114.64
10	J	123	PRO	N-CA-C	-5.26	106.35	113.40
6	T	43	ASN	N-CA-C	5.26	119.18	112.34
13	1	31	VAL	N-CA-C	5.24	115.32	107.51
11	Y	105(B)	LYS	N-CA-C	5.23	117.06	111.36
11	K	82	ILE	N-CA-C	-5.23	105.23	110.30
4	D	37	ALA	N-CA-C	-5.22	99.45	108.69
6	T	206(A)	GLU	N-CA-C	5.21	117.96	111.24
12	L	129	ALA	N-CA-C	5.21	116.81	111.03
3	C	173	ARG	N-CA-C	-5.20	105.61	111.28
6	F	107	ILE	CA-C-N	5.20	125.12	119.76
6	F	107	ILE	C-N-CA	5.20	125.12	119.76
9	I	93	GLY	CA-C-N	5.18	126.32	119.84
9	I	93	GLY	C-N-CA	5.18	126.32	119.84
1	A	137	LEU	N-CA-C	-5.18	99.97	108.41
6	F	145	GLY	N-CA-C	5.18	119.42	112.17
9	W	49	ALA	N-CA-C	5.17	117.32	111.11
1	O	217(N)	THR	N-CA-C	-5.16	106.31	113.18
13	1	195	MET	N-CA-C	5.16	117.97	109.76
1	A	37	SER	N-CA-C	-5.16	100.89	108.99
13	M	197	TRP	N-CA-C	-5.14	108.03	114.56
6	T	12	ASN	CA-C-N	-5.14	114.06	122.54
6	T	12	ASN	C-N-CA	-5.14	114.06	122.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Q	39	GLY	N-CA-C	-5.12	101.04	113.18
5	S	209	ASN	N-CA-C	5.12	118.69	112.23
4	D	169	SER	N-CA-C	5.12	121.70	110.80
4	D	215	ILE	N-CA-C	-5.11	100.76	108.12
10	X	171	LYS	N-CA-C	5.11	118.81	112.58
13	M	195	MET	N-CA-C	5.11	117.07	109.25
1	O	66	LYS	N-CA-C	-5.11	106.90	113.23
3	C	137	LEU	N-CA-C	-5.08	100.00	108.34
6	F	12	ASN	CA-C-N	-5.08	114.15	122.54
6	F	12	ASN	C-N-CA	-5.08	114.15	122.54
10	X	174	ILE	N-CA-C	-5.07	101.02	108.11
3	Q	182	PRO	N-CA-C	-5.07	105.61	110.47
11	Y	1	THR	O-C-N	-5.06	114.90	123.00
3	Q	173	ARG	N-CA-C	-5.06	105.65	111.07
7	U	206	SER	N-CA-C	-5.06	102.30	110.14
1	O	173	LYS	N-CA-C	-5.06	105.66	111.07
3	Q	137	LEU	N-CA-C	-5.05	100.18	108.41
7	G	206	SER	N-CA-C	-5.05	102.68	109.95
8	H	191	TYR	N-CA-C	-5.05	105.05	111.11
1	O	48	ILE	N-CA-C	-5.04	100.95	108.46
2	B	24	VAL	N-CA-C	-5.04	105.79	110.53
1	O	43	THR	N-CA-C	-5.04	105.88	112.23
4	D	161	ASN	N-CA-C	-5.04	106.40	112.54
5	E	86	ARG	N-CA-C	-5.03	105.48	110.97
10	J	141	HIS	N-CA-C	5.03	119.42	113.28
10	X	19	ALA	N-CA-C	5.03	117.69	109.59
6	T	51	GLU	N-CA-C	-5.03	102.25	110.20
4	D	143	ALA	N-CA-C	5.02	118.67	112.54
8	V	78	SER	N-CA-C	-5.02	105.51	111.69
10	X	93	ARG	CA-C-N	5.02	125.02	119.90
10	X	93	ARG	C-N-CA	5.02	125.02	119.90
9	W	-3	ILE	CB-CA-C	-5.02	105.47	112.04
1	A	57	PRO	N-CA-C	-5.01	108.09	114.35
8	H	180	ILE	N-CA-C	5.01	119.75	109.34

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	144(A)	TYR	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1915	0	1926	58	0
1	O	1915	0	1926	64	0
2	B	1905	0	1901	79	0
2	P	1905	0	1901	87	0
3	C	1891	0	1900	76	0
3	Q	1891	0	1900	105	0
4	D	1862	0	1836	73	0
4	R	1862	0	1836	63	0
5	E	1795	0	1797	73	0
5	S	1795	0	1797	97	0
6	F	1897	0	1886	58	0
6	T	1897	0	1886	82	0
7	G	1921	0	1910	85	0
7	U	1921	0	1910	87	0
8	H	1685	0	1687	47	0
8	V	1685	0	1687	66	0
9	I	1581	0	1573	41	0
9	W	1581	0	1574	50	0
10	J	1585	0	1590	53	0
10	X	1585	0	1590	58	0
11	K	1644	0	1592	63	0
11	Y	1644	0	1593	62	0
12	L	1757	0	1711	70	0
12	Z	1757	0	1711	62	0
13	1	1824	0	1832	69	0
13	M	1824	0	1832	50	0
14	2	1512	0	1481	61	0
14	N	1512	0	1481	54	0
15	3	39	0	44	4	0
15	4	39	0	44	3	0
16	D	1	0	0	0	0
16	F	2	0	0	0	0
16	G	1	0	0	0	0
16	H	1	0	0	0	0
16	I	2	0	0	0	0
16	K	1	0	0	0	0
16	L	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	N	1	0	0	0	0
17	1	142	0	0	1	0
17	2	124	0	0	0	0
17	3	1	0	0	0	0
17	A	100	0	0	2	0
17	B	72	0	0	1	0
17	C	71	0	0	0	0
17	D	86	0	0	5	0
17	E	57	0	0	1	0
17	F	98	0	0	2	0
17	G	106	0	0	4	0
17	H	129	0	0	2	0
17	I	109	0	0	1	0
17	J	114	0	0	3	0
17	K	94	0	0	5	0
17	L	147	0	0	4	0
17	M	130	0	0	0	0
17	N	115	0	0	1	0
17	O	99	0	0	1	0
17	P	72	0	0	2	0
17	Q	68	0	0	0	0
17	R	87	0	0	3	0
17	S	56	0	0	3	0
17	T	95	0	0	5	0
17	U	111	0	0	6	0
17	V	124	0	0	8	0
17	W	111	0	0	3	0
17	X	119	0	0	5	0
17	Y	93	0	0	9	0
17	Z	142	0	0	6	0
All	All	52508	0	49334	1717	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 17.

All (1717) 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)
14:N:136:GLY:HA2	14:2:161:GLN:HE21	1.09	1.09
14:N:161:GLN:HE21	14:2:136:GLY:HA2	1.13	1.05
11:K:4:LEU:HD12	11:K:159:ILE:HD11	1.44	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:96:ALA:HA	7:G:107:MET:HE2	1.43	0.99
12:L:18:THR:CG2	12:L:30:TYR:HA	1.95	0.97
14:N:136:GLY:HA2	14:2:161:GLN:NE2	1.81	0.94
11:K:4:LEU:HD11	11:K:15:ALA:HB3	1.50	0.94
7:U:96:ALA:HA	7:U:107:MET:HE2	1.50	0.93
6:T:37:SER:HB3	6:T:50:VAL:HG23	1.52	0.92
12:L:34:VAL:HG12	12:L:176:LEU:HD22	1.51	0.91
9:W:137:MET:HE2	9:W:161:ASN:HB2	1.53	0.90
12:Z:163:THR:O	17:Z:254:HOH:O	1.91	0.88
4:D:214:CYS:HG	4:D:224:TYR:HE2	1.16	0.86
3:C:35:THR:HB	3:C:51:GLU:HG3	1.56	0.86
12:Z:18:THR:CG2	12:Z:30:TYR:HA	2.05	0.86
1:O:7:ARG:HH22	4:R:123(C):GLY:HA3	1.41	0.85
11:Y:163:ALA:O	17:Y:334:HOH:O	1.94	0.85
7:U:121:GLN:O	7:U:124:THR:HB	1.76	0.84
8:H:1:THR:N	8:H:168:GLY:O	2.10	0.83
14:N:161:GLN:NE2	14:2:136:GLY:HA2	1.93	0.82
3:Q:35:THR:HB	3:Q:51:GLU:HG3	1.62	0.82
12:L:18:THR:HG22	12:L:29:ARG:O	1.78	0.82
5:S:70:CYS:SG	5:S:92:LEU:HD23	2.20	0.82
9:W:160:LEU:HD12	9:W:191:MET:HE3	1.62	0.82
12:L:18:THR:HG21	12:L:30:TYR:HD1	1.45	0.82
3:Q:47:VAL:HG23	3:Q:189:CYS:SG	2.20	0.81
6:F:37:SER:HB3	6:F:50:VAL:HG23	1.60	0.81
2:B:126:HIS:HB3	3:C:129:VAL:HG12	1.63	0.81
6:F:35:THR:HG21	6:F:51:GLU:O	1.81	0.80
1:O:27:ALA:O	1:O:31:VAL:HG23	1.80	0.80
8:V:163:ILE:O	17:V:342:HOH:O	1.98	0.80
13:1:133:MET:O	13:1:136:PRO:HD2	1.82	0.80
3:Q:100:ARG:NH1	3:Q:106:PRO:HB3	1.97	0.80
13:1:6:MET:HG2	13:1:155:ILE:HD11	1.63	0.80
7:U:59:LEU:O	7:U:61:PRO:HD3	1.83	0.79
3:Q:163:GLN:HE21	3:Q:164:THR:H	1.31	0.79
14:2:175:MET:HE3	14:2:187(B):PHE:CE2	2.17	0.78
3:C:100:ARG:NH1	3:C:106:PRO:HB3	1.98	0.78
11:Y:208:ASN:HB3	17:Y:302:HOH:O	1.83	0.78
5:S:73:HIS:HE1	5:S:107:LEU:O	1.67	0.78
7:U:126:ARG:O	17:U:335:HOH:O	2.02	0.78
1:A:161:LYS:HD3	1:A:180:TRP:CH2	2.20	0.77
11:Y:33:LYS:HE2	15:4:5:04D:H23	1.66	0.77
3:Q:190:VAL:O	3:Q:194:VAL:HG23	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:163:ALA:O	17:W:234:HOH:O	2.01	0.77
5:S:75:GLY:HA3	5:S:221:PHE:CE2	2.19	0.77
8:H:1:THR:HG23	8:H:33:LYS:HD3	1.66	0.77
14:N:175:MET:HE3	14:N:187(B):PHE:CE2	2.20	0.77
6:T:35:THR:HG21	6:T:51:GLU:O	1.84	0.77
14:N:8:PHE:CE1	14:N:10:ASP:HB2	2.20	0.76
3:C:163:GLN:HE21	3:C:164:THR:H	1.32	0.76
9:W:28:SER:HA	17:W:213:HOH:O	1.85	0.76
6:T:186:ALA:O	6:T:190:VAL:HG23	1.86	0.76
13:1:43:VAL:HG22	13:1:101:VAL:HG22	1.67	0.76
7:U:186:TRP:O	7:U:190:VAL:HG23	1.86	0.76
11:Y:45:MET:HB3	11:Y:52:CYS:HB3	1.68	0.76
7:G:96:ALA:HA	7:G:107:MET:CE	2.17	0.75
11:Y:105(B):LYS:H	11:Y:105(B):LYS:HD2	1.52	0.75
11:Y:105(A):ARG:HB3	11:Y:105(B):LYS:HE3	1.69	0.74
5:S:15:PHE:HB2	6:T:23:GLN:HE22	1.52	0.74
3:C:164:THR:HG21	3:C:172:VAL:HG13	1.68	0.74
11:K:208:ASN:HB3	17:K:461:HOH:O	1.85	0.74
10:X:44:SER:OG	10:X:100:LEU:HB2	1.86	0.74
5:E:47:VAL:HG23	5:E:189:LEU:HD13	1.70	0.74
8:H:1:THR:HA	8:H:33:LYS:NZ	2.03	0.74
11:K:1:THR:HA	17:K:445:HOH:O	1.88	0.74
4:D:215:ILE:HG22	4:D:221:PHE:HD2	1.53	0.73
2:P:76:VAL:HG12	2:P:138:TYR:CD2	2.22	0.73
11:K:4:LEU:CD1	11:K:15:ALA:HB3	2.17	0.73
6:F:95:GLU:HG3	6:F:115:ARG:HH11	1.51	0.73
5:E:15:PHE:HB2	6:F:23:GLN:HE22	1.54	0.73
6:T:141:VAL:HG23	6:T:215:CYS:SG	2.28	0.73
7:U:129:MET:O	17:U:335:HOH:O	2.08	0.72
10:X:6:ILE:HD11	10:X:142:TYR:CE1	2.24	0.72
9:I:137:MET:HE2	9:I:161:ASN:HB2	1.72	0.72
13:1:110:LEU:HG	13:1:125:LEU:HD12	1.70	0.72
6:T:176:LEU:HD22	6:T:196:ILE:HD13	1.72	0.72
14:2:157:HIS:HD2	14:2:187(J):LEU:HD13	1.54	0.72
13:1:41:THR:OG1	13:1:76:PRO:HG3	1.87	0.72
13:M:197:TRP:CH2	14:2:171:GLY:HA2	2.25	0.72
4:D:46:VAL:HG11	4:D:139:ALA:HB1	1.72	0.71
13:1:157:ASN:ND2	13:1:160:ARG:HH11	1.89	0.71
8:V:112:SER:HB3	8:V:125:LEU:HD13	1.70	0.71
13:1:157:ASN:ND2	13:1:160:ARG:NH1	2.38	0.71
1:O:124:THR:HG22	2:P:130:ARG:HH21	1.54	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:52:LYS:HB3	5:S:63:TYR:HB3	1.73	0.71
6:T:95:GLU:HG3	6:T:115:ARG:HH11	1.56	0.71
8:V:166:ASP:O	17:V:342:HOH:O	2.09	0.71
1:A:130:ARG:HH11	1:A:130:ARG:HG3	1.56	0.71
4:D:97:VAL:HG21	11:K:65:LEU:CD1	2.20	0.71
6:T:81:LEU:HD12	6:T:133:GLY:HA3	1.71	0.71
11:K:105(B):LYS:H	11:K:105(B):LYS:HD2	1.55	0.71
1:O:161:LYS:HD3	1:O:180:TRP:CH2	2.26	0.70
14:2:1:THR:HG21	14:2:46:SER:CB	2.21	0.70
5:E:75:GLY:HA3	5:E:221:PHE:CE2	2.27	0.70
2:P:130:ARG:HH11	2:P:130:ARG:HG3	1.55	0.70
3:Q:160:TRP:CE2	4:R:59:LEU:HD23	2.26	0.70
5:E:130:ARG:HH11	5:E:130:ARG:HG3	1.56	0.70
8:H:77:VAL:HB	13:1:208:THR:HG22	1.73	0.70
2:B:121:GLN:O	2:B:124:THR:HB	1.92	0.70
13:M:41:THR:OG1	13:M:76:PRO:HG3	1.91	0.70
4:R:67:ILE:HG22	4:R:221:PHE:HZ	1.56	0.70
4:R:75:GLY:HA3	4:R:221:PHE:CD2	2.27	0.70
12:Z:18:THR:HG23	12:Z:30:TYR:HA	1.73	0.69
11:K:142:TYR:O	11:K:143:LYS:HD2	1.91	0.69
14:2:8:PHE:CE1	14:2:10:ASP:HB2	2.28	0.69
8:H:103:GLY:HA2	8:H:178:MET:SD	2.32	0.69
4:R:46:VAL:HG11	4:R:139:ALA:HB1	1.73	0.69
2:P:185:LYS:HD3	2:P:187:ASP:H	1.56	0.69
9:I:28:SER:HA	17:I:388:HOH:O	1.93	0.69
11:K:105(A):ARG:HB3	11:K:105(B):LYS:HE3	1.74	0.69
14:N:157:HIS:HD2	14:N:187(J):LEU:HD13	1.56	0.69
10:X:-1:MET:HG2	10:X:1:ASP:H	1.57	0.69
10:X:2:ILE:HA	17:X:234:HOH:O	1.92	0.69
10:X:113:ILE:HG12	10:X:119:LYS:HG3	1.73	0.69
13:1:141(C):ARG:HH11	13:1:141(C):ARG:HG3	1.58	0.69
14:N:14:LEU:HD11	14:N:102:ALA:HB3	1.75	0.69
14:N:171:GLY:HA2	13:1:197:TRP:CH2	2.27	0.69
10:X:146:MET:HE2	10:X:150:GLU:HB3	1.75	0.69
6:F:170:GLN:CD	6:F:170:GLN:H	2.00	0.68
12:Z:18:THR:HG22	12:Z:29:ARG:O	1.92	0.68
12:L:90:LYS:HD3	12:L:95:TYR:CE1	2.28	0.68
12:Z:43:MET:HB2	12:Z:101:ILE:HG22	1.73	0.68
5:E:103:PHE:HE2	13:M:62:LEU:HD21	1.58	0.68
14:2:84:LYS:HE3	14:2:119:VAL:HG23	1.75	0.68
2:P:87:ILE:O	2:P:91:THR:HG23	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:80:PHE:CZ	13:M:111:ARG:HG2	2.28	0.68
1:O:121:GLN:O	1:O:124:THR:HB	1.94	0.68
1:O:124:THR:CG2	2:P:130:ARG:HH21	2.07	0.68
7:U:96:ALA:HA	7:U:107:MET:CE	2.23	0.68
14:2:1:THR:HG21	14:2:46:SER:HB2	1.75	0.68
2:B:15:PHE:H	3:C:23:GLN:HE22	1.39	0.68
5:E:75:GLY:HA3	5:E:221:PHE:CZ	2.28	0.68
7:G:150:LYS:O	7:G:157:TYR:HA	1.93	0.68
4:R:75:GLY:HA3	4:R:221:PHE:CE2	2.29	0.68
9:I:48:LEU:HG	9:I:50:THR:HG22	1.76	0.68
3:C:57:LYS:HD2	3:C:58:LEU:N	2.09	0.67
11:Y:4:LEU:HD11	11:Y:15:ALA:HB3	1.76	0.67
11:K:157:ARG:O	11:K:160:LEU:HB3	1.94	0.67
11:Y:5:ALA:HA	11:Y:13:ILE:O	1.95	0.67
9:I:55:LEU:HD21	9:I:95:TYR:CD1	2.28	0.67
12:L:18:THR:HG21	12:L:30:TYR:CD1	2.30	0.67
13:1:84:ALA:HA	13:1:113:VAL:HG21	1.77	0.67
3:Q:186:VAL:O	3:Q:190:VAL:HG23	1.95	0.67
5:S:161:TYR:OH	6:T:61:PRO:HD2	1.95	0.67
1:O:161:LYS:HD3	1:O:180:TRP:CZ3	2.30	0.67
1:A:121:GLN:O	1:A:124:THR:HB	1.95	0.67
3:C:15:PHE:H	4:D:23:GLN:HE22	1.43	0.67
10:J:-1:MET:HG2	10:J:1:ASP:H	1.60	0.67
2:P:121:GLN:O	2:P:124:THR:HB	1.94	0.67
3:C:40:VAL:HG12	3:C:162:ALA:HB1	1.77	0.66
5:E:73:HIS:HE1	5:E:107:LEU:O	1.78	0.66
8:H:29:LYS:HE2	12:Z:165:ARG:NH2	2.10	0.66
3:Q:15:PHE:H	4:R:23:GLN:HE22	1.42	0.66
14:2:112:THR:HG22	14:2:120:HIS:HB2	1.76	0.66
4:D:75:GLY:HA3	4:D:221:PHE:CD2	2.31	0.66
6:F:38:ILE:HG22	6:F:164:ALA:CB	2.25	0.66
11:K:4:LEU:HD12	11:K:159:ILE:CD1	2.23	0.66
1:O:130:ARG:HH11	1:O:130:ARG:HG3	1.60	0.66
12:Z:151:VAL:O	12:Z:155:VAL:HG23	1.96	0.66
3:C:57:LYS:O	3:C:58:LEU:HB2	1.95	0.66
3:C:160:TRP:CZ2	4:D:59:LEU:HD23	2.30	0.66
2:P:97:GLN:HE22	9:W:64:ASN:HD22	1.43	0.66
2:B:124:THR:HG22	3:C:130:ARG:HH21	1.60	0.66
13:M:84:ALA:HA	13:M:113:VAL:HG21	1.77	0.66
13:M:104:VAL:HG23	13:M:178:ILE:HG22	1.78	0.66
3:Q:130:ARG:HG3	3:Q:130:ARG:HH11	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:82:ILE:HB	6:T:83:PRO:HD3	1.78	0.66
12:Z:34:VAL:HG12	12:Z:176:LEU:HD22	1.77	0.66
5:S:76:LEU:O	5:S:76:LEU:HD23	1.95	0.65
7:G:76:MET:SD	7:G:138:PHE:CE2	2.89	0.65
7:U:207:LYS:HG3	7:U:208:ASN:OD1	1.96	0.65
3:C:36:CYS:H	3:C:51:GLU:HG2	1.61	0.65
5:S:190:ILE:HG23	5:S:212:ILE:HD13	1.78	0.65
2:P:65:GLU:HG3	2:P:66:LYS:HG3	1.78	0.65
6:F:18:ASP:OD1	6:F:20:ARG:HD3	1.97	0.65
10:J:34:THR:HG23	10:J:42:LEU:HD11	1.78	0.65
2:P:4:GLY:HA3	5:S:127:TYR:CE1	2.32	0.65
3:Q:79:SER:OG	3:Q:165:ILE:HG13	1.97	0.65
4:R:215:ILE:HG22	4:R:221:PHE:HD2	1.61	0.65
6:T:170:GLN:CD	6:T:170:GLN:H	2.05	0.65
3:C:163:GLN:NE2	3:C:164:THR:H	1.93	0.65
12:Z:137:PHE:CE1	12:Z:141:GLN:HG3	2.31	0.65
1:A:85:TYR:O	1:A:89:VAL:HG23	1.96	0.65
10:J:37:LEU:HB2	10:J:41:THR:HG22	1.79	0.65
12:L:194:ASP:OXT	17:V:342:HOH:O	2.15	0.65
7:G:130:ARG:HG3	7:G:131:PRO:O	1.96	0.64
3:Q:163:GLN:NE2	3:Q:164:THR:H	1.95	0.64
6:T:120:VAL:HG21	6:T:151:LEU:HD21	1.78	0.64
4:D:125:GLU:HG2	4:D:127:LEU:HD13	1.79	0.64
5:E:194:VAL:O	5:E:197:ILE:HG22	1.97	0.64
3:C:160:TRP:CE2	4:D:59:LEU:HD23	2.32	0.64
12:L:18:THR:HG22	12:L:30:TYR:HA	1.77	0.64
4:R:97:VAL:HG21	11:Y:65:LEU:HD13	1.79	0.64
4:D:14:THR:HG22	5:E:23:GLN:NE2	2.12	0.64
6:T:136:THR:O	6:T:150:MET:HA	1.97	0.64
10:X:6:ILE:HD11	10:X:142:TYR:HE1	1.61	0.64
14:2:103:GLY:HA2	14:2:178:LEU:HD23	1.78	0.64
8:H:135:MET:HE3	13:1:165:ARG:NH1	2.13	0.64
8:V:35:HIS:HB3	8:V:56:THR:HG21	1.78	0.64
12:Z:134:ILE:HG23	12:Z:158:SER:HB3	1.79	0.64
1:A:217(B):ASN:HB3	1:A:217(F):LEU:HD12	1.78	0.64
8:H:167:LEU:HD22	12:Z:167:ILE:O	1.97	0.64
2:P:7:ARG:HB3	2:P:8:TYR:CE1	2.33	0.64
5:S:130:ARG:HH11	5:S:130:ARG:HG3	1.62	0.64
12:Z:-6:PRO:HB2	13:1:91:ARG:NH1	2.13	0.64
7:G:229:ILE:O	7:G:232:ARG:HB2	1.97	0.64
10:J:44:SER:OG	10:J:100:LEU:HB2	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:141(C):ARG:HH11	13:M:141(C):ARG:HG3	1.62	0.64
3:Q:175:PHE:CZ	3:Q:195:ARG:HB3	2.32	0.64
2:P:141:TYR:CD1	2:P:219(A):VAL:HG21	2.32	0.63
3:C:130:ARG:HG3	3:C:130:ARG:HH11	1.63	0.63
2:P:112:LEU:HD23	2:P:112:LEU:C	2.23	0.63
7:U:78:VAL:HG11	7:U:85:ALA:CB	2.29	0.63
2:B:163:ILE:HG13	2:B:164:SER:N	2.14	0.63
7:G:121:GLN:O	7:G:124:THR:HB	1.97	0.63
5:S:21:LEU:O	5:S:25:GLU:HG3	1.98	0.63
9:W:27:VAL:HG13	17:X:295:HOH:O	1.99	0.63
3:C:185:THR:HB	3:C:188:GLU:HG2	1.80	0.63
7:G:105:TYR:OH	8:H:66:HIS:HE1	1.81	0.63
7:G:39:ALA:HB2	7:G:48:VAL:HG12	1.81	0.63
9:I:36:HIS:HB3	9:I:42:PHE:CD2	2.33	0.63
11:K:4:LEU:HD13	11:K:15:ALA:O	1.99	0.63
1:O:134:VAL:O	1:O:153:PRO:HG3	1.98	0.63
5:S:75:GLY:HA3	5:S:221:PHE:CZ	2.34	0.63
12:L:18:THR:HG23	12:L:30:TYR:HA	1.75	0.62
5:E:52:LYS:HB3	5:E:63:TYR:HB3	1.81	0.62
9:I:2:ILE:HG21	9:I:130:ALA:HB3	1.80	0.62
2:P:141:TYR:HA	2:P:145:GLY:O	2.00	0.62
2:B:163:ILE:HG13	2:B:164:SER:H	1.65	0.62
3:C:71:ASP:HA	10:J:68:ILE:CD1	2.29	0.62
11:K:21:THR:O	15:3:4:THR:HG22	1.99	0.62
12:L:133:LEU:O	12:L:136:PRO:HD2	2.00	0.62
3:Q:47:VAL:CG2	3:Q:189:CYS:SG	2.88	0.62
5:S:15:PHE:CE1	5:S:21:LEU:HD21	2.35	0.62
2:B:124:THR:CG2	3:C:130:ARG:HH21	2.13	0.62
8:H:55:VAL:HG23	8:H:86:HIS:HD2	1.64	0.62
3:Q:160:TRP:CZ2	4:R:59:LEU:HD23	2.35	0.62
5:S:15:PHE:HB2	6:T:23:GLN:NE2	2.14	0.62
2:B:161:LYS:HE3	3:C:59:GLN:O	2.00	0.62
11:Y:4:LEU:HD12	11:Y:159:ILE:HD11	1.82	0.62
6:T:175:GLU:O	6:T:178:LYS:HB2	1.99	0.61
3:C:175:PHE:CZ	3:C:195:ARG:HB3	2.35	0.61
12:L:137:PHE:CE1	12:L:141:GLN:HG3	2.35	0.61
4:D:186:LEU:O	4:D:190:GLU:HG3	2.00	0.61
3:Q:57:LYS:HD2	3:Q:58:LEU:N	2.15	0.61
7:U:229:ILE:O	7:U:232:ARG:HB2	1.99	0.61
7:G:45:CYS:O	7:G:146:PRO:HB3	2.00	0.61
10:J:2:ILE:HA	17:J:301:HOH:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:18:THR:HG21	12:Z:30:TYR:HD1	1.63	0.61
6:F:49:ALA:HA	6:F:211:GLU:O	2.00	0.61
7:U:158:VAL:HG22	7:U:159:GLY:N	2.15	0.61
10:X:53:VAL:HG21	17:Y:313:HOH:O	2.00	0.61
11:Y:157:ARG:O	11:Y:160:LEU:HB3	2.00	0.61
4:D:75:GLY:HA3	4:D:221:PHE:CE2	2.35	0.61
3:Q:106:PRO:HG2	3:Q:143:PRO:HG3	1.81	0.61
3:Q:168:ASN:CB	3:Q:200:VAL:HG11	2.31	0.61
12:Z:34:VAL:HG22	12:Z:44:SER:HB2	1.82	0.61
14:2:176:VAL:HG12	14:2:178:LEU:HD13	1.82	0.61
5:S:180(C):PHE:HA	5:S:182:ILE:HG13	1.81	0.61
9:W:19:ARG:HD3	9:W:168:LEU:O	2.01	0.61
14:2:175:MET:HB2	14:2:187:LEU:HB2	1.83	0.61
1:A:14:THR:O	1:A:21:LEU:HD23	2.01	0.61
3:C:226:SER:HB2	3:C:227:GLU:OE1	2.01	0.61
4:D:112:LEU:C	4:D:112:LEU:HD13	2.25	0.61
6:F:42:CYS:HB2	6:F:184:LEU:O	2.00	0.61
2:P:8:TYR:N	2:P:8:TYR:CD1	2.69	0.61
6:T:130:ARG:HH11	6:T:130:ARG:HG3	1.66	0.61
3:Q:106:PRO:HG2	3:Q:143:PRO:CG	2.31	0.60
7:U:78:VAL:HG11	7:U:85:ALA:HB2	1.83	0.60
1:A:41:LYS:HG3	1:A:46:VAL:HG22	1.81	0.60
4:D:67:ILE:HG22	4:D:221:PHE:HZ	1.65	0.60
3:Q:40:VAL:HG12	3:Q:162:ALA:HB1	1.81	0.60
7:G:207:LYS:HG3	7:G:208:ASN:OD1	2.02	0.60
12:Z:-6:PRO:HB2	13:1:91:ARG:HH11	1.65	0.60
1:A:7:ARG:HH22	4:D:123(C):GLY:HA3	1.64	0.60
3:C:35:THR:HB	3:C:51:GLU:CG	2.31	0.60
3:Q:197:LEU:O	3:Q:201:VAL:HG23	2.01	0.60
13:M:82:TYR:O	13:M:86:VAL:HG23	2.01	0.60
14:N:48:SER:HB3	14:N:51:ASP:HB2	1.84	0.60
1:O:207:ASN:HA	1:O:233:LEU:CD1	2.31	0.60
2:P:15:PHE:H	3:Q:23:GLN:HE22	1.48	0.60
2:P:124:THR:HG22	3:Q:130:ARG:HH21	1.67	0.60
7:G:77:VAL:CG1	7:G:137:THR:HB	2.32	0.60
8:V:172:ASN:ND2	8:V:193:THR:HG22	2.16	0.60
9:W:55:LEU:HD21	9:W:95:TYR:CD1	2.36	0.60
11:K:137:VAL:HG21	11:K:161:ALA:HB2	1.82	0.60
5:S:81:LEU:HB2	5:S:133:GLY:O	2.02	0.60
6:T:38:ILE:HG22	6:T:164:ALA:CB	2.31	0.60
5:E:77:SER:OG	5:E:137:LEU:HB2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:163:ILE:HG23	8:H:170:GLY:HA2	1.83	0.60
3:Q:164:THR:HG21	3:Q:172:VAL:HG13	1.82	0.60
13:1:76:PRO:HD2	13:1:105:GLN:OE1	2.02	0.60
2:B:41:MET:HB2	2:B:148:LEU:HD22	1.83	0.60
4:D:215:ILE:HG22	4:D:221:PHE:CD2	2.34	0.60
6:F:82:ILE:HB	6:F:83:PRO:HD3	1.83	0.60
3:Q:185:THR:HB	3:Q:188:GLU:HG2	1.82	0.60
11:Y:99:THR:HA	17:Y:365:HOH:O	2.01	0.60
3:C:168:ASN:CB	3:C:200:VAL:HG11	2.31	0.59
6:F:192:GLN:O	6:F:196:ILE:HG13	2.02	0.59
9:W:101:VAL:O	9:W:110:ILE:HA	2.02	0.59
5:E:92:LEU:HD11	5:E:112:ALA:HB1	1.83	0.59
9:W:14:ILE:HG23	9:W:34:ILE:HD13	1.83	0.59
10:X:113:ILE:HA	10:X:118:THR:O	2.02	0.59
11:Y:1:THR:HA	17:Y:378:HOH:O	2.02	0.59
14:N:84:LYS:HB2	14:N:119:VAL:CG2	2.32	0.59
13:1:4:ILE:HD11	13:1:159:MET:SD	2.43	0.59
5:E:76:LEU:HD23	5:E:76:LEU:O	2.03	0.59
5:E:141:TYR:OH	5:E:217:LYS:HG3	2.02	0.59
7:G:80:GLY:HA3	7:G:134:VAL:HG12	1.84	0.59
5:S:24:VAL:O	5:S:28:LEU:HD13	2.03	0.59
9:W:6:MET:HB2	9:W:151:LEU:HD11	1.85	0.59
1:A:112:LEU:O	1:A:116:VAL:HG23	2.03	0.59
2:B:69:LYS:HG3	2:B:221:GLN:OE1	2.03	0.59
11:K:102:CYS:SG	11:K:110:ILE:HG23	2.43	0.59
3:Q:49:GLY:HA3	3:Q:212:ILE:HD13	1.85	0.59
5:S:175:TYR:HB2	5:S:199:GLN:HG2	1.84	0.59
6:F:176:LEU:HD22	6:F:196:ILE:HD13	1.83	0.59
7:G:76:MET:SD	7:G:138:PHE:HE2	2.25	0.59
10:X:12:VAL:HG23	10:X:108:PRO:HB2	1.84	0.59
12:Z:7:ALA:HB2	12:Z:110:VAL:HG23	1.84	0.59
10:J:21:THR:O	10:J:22:ARG:HD3	2.03	0.59
12:L:165:ARG:NH2	8:V:29:LYS:HE2	2.18	0.59
2:P:175:LEU:HB3	17:P:343:HOH:O	2.02	0.59
2:B:181:LYS:O	2:B:184:MET:HG3	2.03	0.59
13:M:57:ARG:HH11	13:M:57:ARG:HG2	1.67	0.59
4:R:214:CYS:SG	4:R:224:TYR:HE2	2.25	0.59
1:A:124:THR:CG2	2:B:130:ARG:HH21	2.16	0.58
12:L:8:GLY:HA3	12:L:11:PHE:CE2	2.38	0.58
7:U:83:PRO:HG2	17:U:355:HOH:O	2.02	0.58
7:U:158:VAL:HG22	7:U:159:GLY:H	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:76:LEU:HD23	5:E:76:LEU:C	2.28	0.58
5:S:92:LEU:HD11	5:S:112:ALA:HB1	1.83	0.58
9:I:16:CYS:SG	9:I:174:VAL:HG12	2.43	0.58
13:M:130:GLY:O	13:M:134:ALA:HB3	2.04	0.58
3:Q:52:ARG:HH21	3:Q:211:GLU:HB3	1.67	0.58
12:Z:166:HIS:HD2	12:Z:168:GLN:H	1.51	0.58
8:H:35:HIS:HB3	8:H:56:THR:HG21	1.83	0.58
10:J:133:TYR:HD1	17:Y:337:HOH:O	1.85	0.58
13:M:157:ASN:ND2	13:M:160:ARG:HH11	2.02	0.58
7:U:76:MET:SD	7:U:138:PHE:CE2	2.96	0.58
7:G:173:THR:O	7:G:177:GLU:HG3	2.03	0.58
14:N:176:VAL:HG12	14:N:178:LEU:HD13	1.86	0.58
5:S:141:TYR:OH	5:S:217:LYS:HG3	2.03	0.58
6:T:69:VAL:HG12	17:T:362:HOH:O	2.04	0.58
8:V:78:SER:O	8:V:82:MET:HG3	2.02	0.58
12:Z:144(R):LYS:HG2	12:Z:145:TYR:N	2.18	0.58
12:Z:29:ARG:NH1	12:Z:193:ARG:HB3	2.19	0.58
2:B:76:VAL:HG12	2:B:138:TYR:CD2	2.38	0.58
11:K:14:VAL:HB	11:K:176:TYR:HB2	1.86	0.58
11:K:99:THR:HG22	11:K:113:VAL:O	2.04	0.58
8:V:18:THR:HG23	8:V:172:ASN:O	2.04	0.58
7:G:39:ALA:CB	7:G:48:VAL:HG12	2.33	0.58
14:N:4:MET:HB3	14:N:126:ILE:HG22	1.85	0.58
1:O:150:GLN:O	1:O:157:TYR:HA	2.03	0.58
3:Q:36:CYS:H	3:Q:51:GLU:HG2	1.68	0.58
11:Y:21:THR:O	15:4:4:THR:HG22	2.03	0.58
1:A:207:ASN:HA	1:A:233:LEU:CD1	2.34	0.58
2:B:141:TYR:CD1	2:B:219(E):VAL:HG21	2.39	0.58
2:P:202:THR:HG22	2:P:204:SER:H	1.69	0.58
8:V:172:ASN:HD22	8:V:193:THR:HG22	1.69	0.58
3:C:182:PRO:O	3:C:184:ALA:N	2.36	0.57
9:I:1:GLY:HA3	9:I:33:LYS:HE2	1.85	0.57
2:B:97:GLN:HE22	9:I:64:ASN:HD22	1.52	0.57
5:E:66:LYS:HA	5:E:78:LEU:HD21	1.86	0.57
13:M:35:ILE:CD1	13:M:56:GLU:HG2	2.33	0.57
5:S:148:LEU:HD23	5:S:162:GLY:HA2	1.85	0.57
3:C:168:ASN:HB2	3:C:200:VAL:HG11	1.86	0.57
3:Q:46:VAL:HG22	3:Q:146:PRO:HB2	1.86	0.57
3:Q:136:THR:O	3:Q:150:GLN:HA	2.04	0.57
11:Y:4:LEU:HD23	11:Y:6:PHE:HD2	1.69	0.57
7:G:151:THR:HG22	7:G:157:TYR:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:182:PRO:O	3:Q:184:ALA:N	2.38	0.57
6:T:221:HIS:HE1	6:T:223:PHE:CE1	2.22	0.57
8:V:132:LEU:HD12	8:V:132:LEU:N	2.19	0.57
3:Q:49:GLY:CA	3:Q:212:ILE:HD13	2.34	0.57
10:X:133:TYR:CE2	10:X:166:MET:SD	2.97	0.57
14:2:1:THR:CG2	14:2:46:SER:HB2	2.34	0.57
14:2:142:PHE:HB2	14:2:154:PHE:CZ	2.39	0.57
9:I:25:LEU:HD11	10:J:135:PHE:HD2	1.69	0.57
1:O:221:PHE:CD2	1:O:221:PHE:C	2.82	0.57
2:P:124:THR:CG2	3:Q:130:ARG:HH21	2.18	0.57
3:Q:57:LYS:O	3:Q:58:LEU:HB2	2.03	0.57
5:S:136:LEU:HD12	5:S:151:PHE:CD2	2.40	0.57
1:A:118:LYS:O	1:A:122:GLU:HG3	2.05	0.57
10:J:34:THR:CG2	10:J:42:LEU:HD11	2.35	0.57
1:O:45:GLY:HA3	1:O:186:LEU:HD13	1.86	0.57
7:U:39:ALA:CB	7:U:48:VAL:HG12	2.35	0.57
7:G:76:MET:HE3	7:G:78:VAL:CG2	2.35	0.57
12:L:8:GLY:HA3	12:L:11:PHE:CZ	2.40	0.57
12:L:42:VAL:O	12:L:101:ILE:HA	2.04	0.57
7:U:105:TYR:OH	8:V:66:HIS:HE1	1.88	0.57
4:D:123(D):ALA:CB	5:E:129:GLY:HA2	2.35	0.57
2:B:87:ILE:O	2:B:91:THR:HG23	2.05	0.56
4:D:46:VAL:HG11	4:D:139:ALA:CB	2.34	0.56
6:F:74:ILE:HD13	6:F:112:PHE:CD2	2.40	0.56
7:G:130:ARG:HG3	7:G:130:ARG:HH11	1.70	0.56
1:O:69:LEU:C	1:O:69:LEU:HD23	2.29	0.56
2:B:65:GLU:HG3	2:B:66:LYS:HG3	1.87	0.56
9:I:171:TRP:HH2	11:Y:165:ARG:NH1	2.03	0.56
4:R:215:ILE:HG22	4:R:221:PHE:CD2	2.40	0.56
5:S:194:VAL:HG13	5:S:207:LEU:HD11	1.86	0.56
4:D:46:VAL:O	4:D:214:CYS:HA	2.05	0.56
6:F:171:SER:O	6:F:174:ALA:HB3	2.05	0.56
8:H:55:VAL:HG23	8:H:86:HIS:CD2	2.40	0.56
8:H:197:ARG:NH2	9:I:139:GLU:HG3	2.20	0.56
3:Q:71:ASP:HA	10:X:68:ILE:CD1	2.36	0.56
5:S:208:THR:H	5:S:209:ASN:HB3	1.70	0.56
6:T:121:GLN:HG3	7:U:83:PRO:O	2.05	0.56
14:2:20:THR:OG1	14:2:28:ASN:HB3	2.04	0.56
3:Q:174:GLU:O	3:Q:178:LYS:HG2	2.06	0.56
7:U:173:THR:O	7:U:177:GLU:HG3	2.05	0.56
9:W:8:GLY:HA3	9:W:11:CYS:SG	2.46	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:38:ILE:HD12	2:B:197:LEU:HG	1.88	0.56
2:B:202:THR:HG22	2:B:204:SER:H	1.69	0.56
8:H:126:SER:O	8:H:127:LEU:HD23	2.05	0.56
13:M:208:THR:HG22	8:V:77:VAL:HB	1.86	0.56
1:A:130:ARG:HH21	7:G:124:THR:CG2	2.18	0.56
2:B:205:LEU:HG	2:B:210:LEU:HD11	1.87	0.56
3:C:163:GLN:HG3	3:C:164:THR:N	2.21	0.56
12:L:43:MET:HB2	12:L:101:ILE:HG22	1.86	0.56
2:P:111:ILE:HG12	10:X:70:GLU:OE2	2.05	0.56
4:R:161:ASN:HB3	4:R:180:TRP:CE2	2.39	0.56
8:V:55:VAL:HG23	8:V:86:HIS:HD2	1.71	0.56
11:Y:105(B):LYS:H	11:Y:105(B):LYS:CD	2.17	0.56
1:A:130:ARG:NH1	1:A:131:PRO:O	2.39	0.56
7:G:158:VAL:HG22	7:G:159:GLY:H	1.71	0.56
4:R:39:GLY:HA2	4:R:47:VAL:O	2.05	0.56
5:S:17:PRO:HG3	6:T:26:TYR:CE2	2.39	0.56
1:A:82:GLY:O	1:A:85:TYR:HB3	2.06	0.56
4:D:123:PHE:CE1	4:D:131:PRO:HG3	2.41	0.56
3:Q:39:GLY:HA2	3:Q:47:VAL:O	2.06	0.56
7:U:179(D):SER:O	7:U:179(E):LYS:HB2	2.05	0.56
14:2:175:MET:HE3	14:2:187(B):PHE:HE2	1.67	0.56
4:D:79:SER:HB3	4:D:165:ILE:HD12	1.88	0.56
12:Z:42:VAL:O	12:Z:101:ILE:HA	2.06	0.56
12:Z:114:ASP:HB3	12:Z:118:SER:HB3	1.88	0.56
14:2:4:MET:HB3	14:2:126:ILE:HG22	1.88	0.56
2:B:81:LEU:HD23	2:B:133:GLY:HA3	1.87	0.56
3:Q:33:ARG:HB3	3:Q:33:ARG:HH11	1.70	0.56
7:U:184(G):GLU:HG2	7:U:188:LYS:CB	2.36	0.56
5:S:49:VAL:CG1	5:S:210:LEU:HD11	2.37	0.55
6:T:49:ALA:HA	6:T:211:GLU:O	2.06	0.55
12:Z:-6:PRO:HG2	12:Z:-5:TYR:CD1	2.41	0.55
9:I:41:VAL:HG22	9:I:76:PRO:HG3	1.86	0.55
11:Y:4:LEU:CD1	11:Y:15:ALA:HB3	2.36	0.55
17:A:387:HOH:O	2:B:83:ALA:HB3	2.07	0.55
6:F:169:ARG:HG3	6:F:173:LYS:HE3	1.88	0.55
10:J:45:PHE:CE1	10:J:52:THR:HG23	2.41	0.55
1:O:49:ALA:HB2	1:O:212:LEU:HG	1.87	0.55
5:S:40:LEU:N	5:S:40:LEU:HD23	2.21	0.55
3:Q:27:ALA:O	3:Q:31:VAL:HG23	2.06	0.55
5:S:15:PHE:H	6:T:23:GLN:HE22	1.54	0.55
1:A:136:LEU:O	1:A:150:GLN:HA	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:15:PHE:H	6:F:23:GLN:HE22	1.52	0.55
12:L:7:ALA:HB2	12:L:110:VAL:HG23	1.88	0.55
13:M:132:HIS:O	13:M:136:PRO:HG2	2.07	0.55
13:M:157:ASN:ND2	13:M:160:ARG:NH1	2.54	0.55
2:P:71:ASN:ND2	2:P:72:ASP:N	2.54	0.55
10:X:-1:MET:HG2	10:X:1:ASP:N	2.21	0.55
13:1:160:ARG:HG3	13:1:192:VAL:CG1	2.37	0.55
14:2:44:CYS:HB2	14:2:100:ILE:HB	1.88	0.55
2:B:81:LEU:HD22	2:B:81:LEU:H	1.70	0.55
2:P:110:GLU:O	2:P:110:GLU:HG2	2.06	0.55
5:S:37:THR:OG1	5:S:50:ALA:HB2	2.06	0.55
8:V:84:LYS:HE2	8:V:119:THR:CG2	2.36	0.55
10:J:105(B):LYS:NZ	10:J:105(B):LYS:HB2	2.22	0.55
10:J:129:TYR:O	10:J:132:PHE:HB2	2.06	0.55
5:S:37:THR:HA	5:S:50:ALA:HA	1.89	0.55
17:V:302:HOH:O	14:2:31:THR:HG23	2.06	0.55
12:Z:15:ALA:HB1	12:Z:173:LEU:HD11	1.88	0.55
9:I:27:VAL:HG13	17:J:247:HOH:O	2.07	0.55
10:J:52:THR:HG22	10:J:53:VAL:N	2.22	0.55
2:P:163:ILE:HG13	2:P:164:SER:H	1.72	0.55
4:D:100:ASN:HB3	17:D:409:HOH:O	2.06	0.54
4:D:160:TYR:CE2	5:E:59:SER:HB3	2.41	0.54
14:N:67:THR:HA	14:N:72:GLY:O	2.07	0.54
4:R:214:CYS:HG	4:R:224:TYR:HE2	1.53	0.54
6:T:18:ASP:OD1	6:T:20:ARG:HD3	2.06	0.54
6:T:95:GLU:HG2	6:T:115:ARG:HB3	1.90	0.54
5:E:81:LEU:HB2	5:E:133:GLY:O	2.08	0.54
10:J:113:ILE:HA	10:J:118:THR:O	2.07	0.54
11:K:165:ARG:NH1	9:W:171:TRP:HH2	2.05	0.54
14:N:161:GLN:HE21	14:2:136:GLY:CA	2.04	0.54
5:S:77:SER:OG	5:S:137:LEU:HB2	2.06	0.54
3:Q:75:VAL:HG21	3:Q:215:VAL:HG11	1.89	0.54
2:B:81:LEU:HB2	2:B:84:ASP:HB2	1.90	0.54
4:R:46:VAL:HG11	4:R:139:ALA:CB	2.37	0.54
5:S:194:VAL:O	5:S:197:ILE:HG22	2.07	0.54
7:U:49:ILE:HD13	7:U:193:ALA:HB1	1.88	0.54
8:H:1:THR:HG23	8:H:33:LYS:CD	2.36	0.54
3:Q:15:PHE:CE2	4:R:27:SER:HB3	2.42	0.54
1:O:130:ARG:HH21	7:U:124:THR:CG2	2.20	0.54
5:S:51:LEU:O	5:S:66:LYS:HE2	2.08	0.54
5:S:130:ARG:HG3	5:S:130:ARG:NH1	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:162:GLY:O	5:S:163:THR:HB	2.08	0.54
7:U:150:LYS:O	7:U:157:TYR:HA	2.07	0.54
8:V:200:LYS:HE3	9:W:140:SER:O	2.07	0.54
12:Z:133:LEU:O	12:Z:136:PRO:HD2	2.08	0.54
2:B:8:TYR:N	2:B:8:TYR:CD1	2.76	0.54
11:K:112:TYR:O	11:K:119:ARG:HA	2.07	0.54
4:R:186:LEU:O	4:R:190:GLU:HG3	2.07	0.54
12:Z:123:GLN:HG3	12:Z:145:TYR:OH	2.08	0.54
7:G:184(G):GLU:HG2	7:G:188:LYS:CB	2.38	0.54
12:Z:43:MET:CB	12:Z:101:ILE:HG22	2.38	0.54
12:Z:129:ALA:HB1	12:Z:166:HIS:CE1	2.43	0.54
5:E:49:VAL:HG13	5:E:212:ILE:HG12	1.89	0.54
8:H:15:ALA:HA	8:H:174:ASP:O	2.08	0.54
14:N:6:VAL:C	14:N:12:VAL:HG23	2.33	0.54
2:P:40:ILE:HD12	2:P:193:ALA:HB2	1.90	0.54
3:Q:43:LYS:O	3:Q:43:LYS:HG2	2.06	0.54
5:S:139:ILE:HG22	5:S:148:LEU:HD13	1.90	0.54
5:S:148:LEU:CD2	5:S:162:GLY:HA2	2.38	0.54
5:S:161:TYR:CE2	6:T:60:VAL:HA	2.43	0.54
8:V:34:LEU:HB2	17:V:376:HOH:O	2.08	0.54
3:C:53:ARG:HG2	3:C:54:SER:N	2.23	0.53
8:H:123:TYR:HB3	8:H:142:TRP:CZ2	2.43	0.53
3:Q:159:SER:O	4:R:59:LEU:HD22	2.07	0.53
7:U:108:PRO:HB3	7:U:142:ASP:OD1	2.09	0.53
12:Z:109:ALA:HA	17:Z:306:HOH:O	2.07	0.53
7:G:79:ASN:OD1	7:G:165:THR:HB	2.08	0.53
7:G:184(G):GLU:HG2	7:G:188:LYS:HB3	1.89	0.53
12:L:-6:PRO:O	13:M:91:ARG:NH1	2.41	0.53
1:O:108:PRO:HG2	1:O:111:LEU:HB2	1.91	0.53
5:S:66:LYS:HA	5:S:78:LEU:HD21	1.90	0.53
7:U:184(G):GLU:HG2	7:U:188:LYS:HB3	1.90	0.53
6:F:203:GLU:C	6:F:205:ASN:H	2.15	0.53
10:X:2:ILE:O	10:X:16:SER:HA	2.08	0.53
11:Y:100:MET:HA	11:Y:111:TYR:O	2.08	0.53
1:A:27:ALA:O	1:A:31:VAL:HG23	2.09	0.53
4:D:123(D):ALA:HA	5:E:129:GLY:HA2	1.90	0.53
7:G:158:VAL:HG22	7:G:159:GLY:N	2.24	0.53
10:J:6:ILE:HD11	10:J:142:TYR:CE1	2.42	0.53
2:P:136:PHE:O	2:P:150:THR:HA	2.09	0.53
7:U:55:PRO:HG2	7:U:56:ASP:H	1.74	0.53
3:C:93:ARG:O	3:C:96:ALA:HB3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:237:LEU:HD22	4:D:241:GLU:HG3	1.90	0.53
4:D:39:GLY:HA2	4:D:47:VAL:O	2.09	0.53
4:D:40:ILE:CD1	4:D:193:VAL:HG23	2.39	0.53
5:E:74:MET:HE2	5:E:109:VAL:HG22	1.90	0.53
3:Q:168:ASN:HB2	3:Q:200:VAL:HG11	1.91	0.53
1:A:130:ARG:HG3	1:A:130:ARG:NH1	2.23	0.53
2:B:39:GLY:HA2	2:B:47:VAL:O	2.09	0.53
7:G:48:VAL:C	7:G:49:ILE:HD12	2.33	0.53
2:P:185:LYS:HD3	2:P:187:ASP:N	2.23	0.53
11:Y:86:LEU:C	11:Y:86:LEU:HD13	2.34	0.53
11:Y:142:TYR:O	11:Y:143:LYS:HD2	2.07	0.53
13:1:112:TYR:O	13:1:119:THR:HA	2.09	0.53
2:B:40:ILE:HD12	2:B:193:ALA:HB2	1.90	0.53
11:K:37:ILE:HG23	11:K:60:GLY:HA2	1.91	0.53
3:C:49:GLY:HA3	3:C:212:ILE:HD13	1.90	0.53
10:J:113:ILE:HG12	10:J:119:LYS:HG3	1.90	0.53
14:N:175:MET:HB2	14:N:187:LEU:HB2	1.91	0.53
1:O:14:THR:O	1:O:21:LEU:HD23	2.09	0.53
3:Q:28:LEU:O	3:Q:31:VAL:HB	2.09	0.53
4:D:130:ARG:HH11	4:D:130:ARG:HG3	1.73	0.53
13:M:7:LYS:HD2	13:M:141(G):ILE:HD13	1.89	0.53
1:O:125:GLN:HG3	2:P:130:ARG:HG2	1.91	0.53
5:S:68:ILE:HB	5:S:76:LEU:CD2	2.39	0.53
6:T:90:ASN:O	6:T:94:GLU:HG3	2.09	0.53
10:X:129:TYR:O	10:X:132:PHE:HB2	2.09	0.53
2:B:108:PRO:HB2	2:B:111:ILE:HG13	1.91	0.52
5:E:48:LEU:HD13	5:E:77:SER:HB3	1.90	0.52
8:V:114:HIS:HD2	17:V:410:HOH:O	1.92	0.52
10:X:15:ALA:HB2	10:X:155:LEU:HD13	1.90	0.52
14:2:31:THR:HG22	14:2:32:ASP:N	2.23	0.52
3:C:52:ARG:HD2	3:C:208:LYS:O	2.09	0.52
12:L:5:GLY:O	12:L:124:CYS:HA	2.09	0.52
12:L:29:ARG:NH1	12:L:193:ARG:HB3	2.24	0.52
8:V:123:TYR:HB3	8:V:142:TRP:CZ2	2.44	0.52
3:C:152:GLU:HG2	3:C:156:ILE:HG22	1.90	0.52
12:L:134:ILE:HG23	12:L:158:SER:HB3	1.90	0.52
5:S:31:ILE:HD11	5:S:153:PRO:HD2	1.90	0.52
5:S:160:LEU:HD13	5:S:163:THR:HB	1.91	0.52
7:U:69:CYS:O	7:U:93:LYS:HE2	2.08	0.52
13:1:37:VAL:HG11	13:1:79:ILE:HD13	1.91	0.52
14:2:146:MET:HE3	14:2:150:GLU:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:GLU:HG2	2:B:58:LEU:HD13	1.91	0.52
3:C:71:ASP:HA	10:J:68:ILE:HD11	1.92	0.52
3:C:195:ARG:HG3	3:C:236:ILE:HD13	1.91	0.52
5:E:130:ARG:HG3	5:E:130:ARG:NH1	2.20	0.52
5:E:226:GLY:O	5:E:229:VAL:HG22	2.09	0.52
2:P:76:VAL:CG1	2:P:138:TYR:CD2	2.92	0.52
2:P:130:ARG:HG3	2:P:130:ARG:NH1	2.23	0.52
7:U:109:CYS:HB3	17:U:402:HOH:O	2.09	0.52
10:X:28:LYS:HE3	11:Y:121:LYS:O	2.10	0.52
14:2:6:VAL:C	14:2:12:VAL:HG23	2.34	0.52
2:P:7:ARG:HB3	2:P:8:TYR:CD1	2.45	0.52
5:S:24:VAL:O	5:S:27:ALA:HB3	2.10	0.52
6:T:192:GLN:O	6:T:196:ILE:HG13	2.09	0.52
8:V:41:ILE:HA	8:V:103:GLY:HA3	1.90	0.52
11:Y:1:THR:CG2	11:Y:2:THR:N	2.73	0.52
1:A:130:ARG:HH21	7:G:124:THR:HG22	1.74	0.52
2:B:112:LEU:HD23	2:B:112:LEU:C	2.35	0.52
4:R:65:GLU:HA	17:R:345:HOH:O	2.10	0.52
3:C:100:ARG:HH11	3:C:106:PRO:HB3	1.74	0.52
2:P:4:GLY:HA3	5:S:127:TYR:HE1	1.73	0.52
3:Q:52:ARG:NH2	3:Q:211:GLU:HB3	2.24	0.52
8:V:126:SER:O	8:V:127:LEU:HD23	2.09	0.52
3:C:106:PRO:HG2	3:C:143:PRO:HG3	1.91	0.52
6:F:95:GLU:HG2	6:F:115:ARG:HB3	1.92	0.52
7:G:180(B):ASP:O	7:G:180(C):HIS:HB3	2.09	0.52
14:N:14:LEU:O	14:N:175:MET:HA	2.09	0.52
2:P:67:LEU:HD22	2:P:211:GLU:HB3	1.91	0.52
2:P:100:LEU:O	2:P:104:ASN:N	2.40	0.52
6:T:24:VAL:O	6:T:27:ALA:HB3	2.10	0.52
9:I:12:VAL:HG23	9:I:178:ILE:HB	1.90	0.52
9:W:156:SER:O	9:W:160:LEU:HB2	2.10	0.52
12:Z:8:GLY:HA3	12:Z:11:PHE:CE2	2.45	0.52
5:S:49:VAL:HG13	5:S:212:ILE:HG12	1.91	0.52
6:T:194:ALA:O	6:T:198:TYR:HD1	1.93	0.52
10:X:105(B):LYS:HB2	10:X:105(B):LYS:NZ	2.25	0.52
11:Y:41:LEU:HD23	11:Y:103:GLY:HA3	1.91	0.52
13:1:10:ASN:ND2	13:1:180:LYS:HE2	2.25	0.52
4:D:201:MET:HE1	4:D:209(B):ASN:ND2	2.25	0.51
5:E:49:VAL:CG1	5:E:210:LEU:HD11	2.40	0.51
12:L:4:LEU:CD1	12:L:138:LEU:HD21	2.40	0.51
2:P:181:LYS:O	2:P:184:MET:HG3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:52:LYS:CB	5:S:63:TYR:HB3	2.39	0.51
9:W:1:GLY:HA3	9:W:33:LYS:HE2	1.91	0.51
14:2:84:LYS:CE	14:2:119:VAL:HG23	2.40	0.51
5:E:123:ASN:N	5:E:123:ASN:HD22	2.08	0.51
10:J:2:ILE:O	10:J:3:ILE:HD13	2.10	0.51
3:Q:163:GLN:HG3	3:Q:164:THR:N	2.25	0.51
4:R:97:VAL:HG21	11:Y:65:LEU:CD1	2.40	0.51
13:1:163:TYR:HA	13:1:169:SER:OG	2.10	0.51
4:D:117:CYS:SG	4:D:157:PHE:HB3	2.50	0.51
5:E:103:PHE:CE2	13:M:62:LEU:HD21	2.42	0.51
12:L:43:MET:CB	12:L:101:ILE:HG22	2.41	0.51
12:L:90:LYS:HD3	12:L:95:TYR:CZ	2.44	0.51
13:M:35:ILE:HD13	13:M:56:GLU:HG2	1.90	0.51
4:R:194:LEU:HD22	4:R:212:LEU:HD11	1.91	0.51
14:2:163:ILE:HG23	14:2:170:GLY:HA2	1.92	0.51
1:A:15:PHE:HD2	2:B:23:GLN:NE2	2.09	0.51
3:C:70:ILE:HG21	3:C:112:LEU:HD21	1.90	0.51
4:D:215:ILE:CG2	4:D:221:PHE:HD2	2.21	0.51
5:E:162:GLY:O	5:E:163:THR:HB	2.10	0.51
7:G:87:ASN:C	7:G:87:ASN:HD22	2.18	0.51
4:R:194:LEU:HD12	4:R:207:LEU:HD11	1.91	0.51
6:T:28:VAL:O	6:T:31:VAL:HB	2.11	0.51
3:C:49:GLY:CA	3:C:212:ILE:HD13	2.40	0.51
8:H:4:VAL:HG22	8:H:159:ILE:HD11	1.91	0.51
8:H:113:ILE:HG12	8:H:119:THR:HG22	1.93	0.51
11:K:5:ALA:HA	11:K:13:ILE:O	2.11	0.51
11:K:126:CYS:HB2	11:K:135:TYR:CE1	2.45	0.51
1:O:15:PHE:H	2:P:23:GLN:HE22	1.59	0.51
4:R:38:ILE:HD12	4:R:197:LEU:HG	1.92	0.51
4:R:163:LYS:HG3	4:R:164:ALA:N	2.26	0.51
9:W:45:ILE:HG22	9:W:52:VAL:HG22	1.92	0.51
11:Y:137:VAL:HG21	11:Y:161:ALA:HB2	1.93	0.51
10:J:52:THR:CG2	10:J:53:VAL:N	2.73	0.51
3:Q:33:ARG:HB3	3:Q:33:ARG:NH1	2.26	0.51
5:E:15:PHE:HB2	6:F:23:GLN:NE2	2.25	0.51
9:I:12:VAL:HG13	9:I:108:PRO:HB3	1.92	0.51
10:J:15:ALA:HB2	10:J:155:LEU:HD13	1.92	0.51
11:K:6:PHE:HA	11:K:123:ASP:O	2.10	0.51
5:S:180(C):PHE:CD1	5:S:180(D):ILE:N	2.79	0.51
7:U:218:ASP:O	7:U:220:LYS:HB2	2.11	0.51
10:X:4:LEU:HD21	10:X:134:THR:HG21	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:171:ALA:O	2:B:175:LEU:HG	2.10	0.51
4:D:161:ASN:HB3	4:D:180:TRP:CE2	2.45	0.51
5:E:51:LEU:O	5:E:66:LYS:HE2	2.10	0.51
10:X:2:ILE:O	10:X:3:ILE:HD13	2.11	0.51
8:H:35:HIS:CB	8:H:56:THR:HG21	2.41	0.51
13:M:110:LEU:HG	13:M:125:LEU:HD12	1.93	0.51
2:P:126:HIS:HB3	3:Q:129:VAL:HG12	1.93	0.51
2:P:205:LEU:HG	2:P:210:LEU:HD11	1.93	0.51
3:Q:93:ARG:O	3:Q:96:ALA:HB3	2.11	0.51
9:W:2:ILE:HG21	9:W:130:ALA:HB3	1.93	0.51
17:E:304:HOH:O	6:F:12:ASN:HB2	2.10	0.51
7:G:151:THR:HA	7:G:156:TYR:O	2.11	0.51
10:J:155:LEU:O	10:J:159:VAL:HG23	2.11	0.51
14:N:114:PRO:HD2	14:N:118:SER:O	2.11	0.51
1:O:62:GLU:CD	1:O:62:GLU:H	2.18	0.51
2:P:113:VAL:HG22	2:P:138:TYR:CD1	2.46	0.51
5:S:132:TYR:O	5:S:153:PRO:HB3	2.10	0.51
8:V:1:THR:HG21	8:V:46:ALA:CB	2.41	0.51
14:2:114:PRO:HD2	14:2:118:SER:O	2.11	0.51
2:B:7:ARG:HB3	2:B:8:TYR:CE1	2.45	0.50
2:B:71:ASN:ND2	2:B:72:ASP:N	2.58	0.50
10:J:146:MET:HE2	10:J:150:GLU:HB3	1.92	0.50
11:K:207:ASN:C	11:K:209:VAL:H	2.19	0.50
14:N:163:ILE:HG23	14:N:170:GLY:HA2	1.91	0.50
5:S:139:ILE:HD12	5:S:215:VAL:HG12	1.93	0.50
11:Y:15:ALA:HA	11:Y:174:ASN:O	2.10	0.50
12:Z:4:LEU:HD13	12:Z:138:LEU:HD21	1.92	0.50
7:G:55:PRO:HG2	7:G:56:ASP:H	1.76	0.50
8:H:124:TYR:HD2	8:H:138:LEU:HD13	1.76	0.50
11:K:1:THR:HG23	11:K:33:LYS:NZ	2.26	0.50
5:S:47:VAL:HG23	5:S:189:LEU:HD13	1.92	0.50
13:1:45:ILE:HG23	13:1:99:ILE:HG12	1.93	0.50
13:1:157:ASN:HD22	13:1:160:ARG:NH1	2.07	0.50
3:C:47:VAL:O	3:C:48:LEU:HD23	2.12	0.50
5:E:47:VAL:HG12	5:E:48:LEU:N	2.26	0.50
12:L:11:PHE:HA	12:L:178:VAL:O	2.11	0.50
14:N:187(D):PRO:HA	14:N:187(G):TYR:CE2	2.47	0.50
1:O:100:TYR:CE1	1:O:107:PRO:HA	2.46	0.50
4:R:125:GLU:HG2	4:R:127:LEU:HD13	1.93	0.50
8:V:197:ARG:NH2	9:W:139:GLU:O	2.44	0.50
11:Y:128:GLY:O	11:Y:131:GLN:HG2	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217(B):ASN:CB	1:A:217(F):LEU:HD12	2.41	0.50
2:B:81:LEU:H	2:B:81:LEU:CD2	2.25	0.50
3:C:227:GLU:CD	3:C:227:GLU:N	2.70	0.50
10:J:36:GLN:HG3	10:J:184:ILE:CD1	2.41	0.50
10:J:85:GLN:O	10:J:89:LYS:HG3	2.10	0.50
6:T:54:ILE:HG13	6:T:208:PHE:HA	1.92	0.50
2:B:141:TYR:CD1	2:B:141:TYR:C	2.89	0.50
8:H:1:THR:HA	8:H:33:LYS:HZ3	1.74	0.50
9:I:51:ASP:OD1	10:J:90(B):ARG:NH2	2.45	0.50
4:R:14:THR:HG22	5:S:23:GLN:NE2	2.27	0.50
7:U:8:TYR:C	7:U:10:ARG:H	2.20	0.50
10:X:6:ILE:HD12	10:X:7:ARG:N	2.26	0.50
14:2:148:LYS:O	14:2:152:VAL:HG23	2.12	0.50
5:E:139:ILE:HG22	5:E:148:LEU:HD13	1.92	0.50
8:H:1:THR:HA	8:H:33:LYS:HZ2	1.75	0.50
9:I:20:LEU:HB3	9:I:28:SER:HB3	1.94	0.50
9:I:113:PHE:CD2	9:I:113:PHE:N	2.79	0.50
14:N:142:PHE:HB2	14:N:154:PHE:CZ	2.47	0.50
3:Q:152:GLU:HG2	3:Q:156:ILE:HG22	1.93	0.50
4:R:130:ARG:HH11	4:R:130:ARG:HG3	1.77	0.50
11:Y:159:ILE:CG2	11:Y:173:VAL:HG22	2.42	0.50
2:B:130:ARG:HH11	2:B:130:ARG:HG3	1.76	0.50
5:E:31:ILE:HD11	5:E:153:PRO:HD2	1.93	0.50
8:H:114:HIS:HD2	17:H:470:HOH:O	1.95	0.50
11:K:200:LYS:HG3	11:K:205:SER:O	2.12	0.50
1:O:136:LEU:O	1:O:150:GLN:HA	2.11	0.50
5:S:198:SER:HA	5:S:201:LEU:CD1	2.41	0.50
14:2:14:LEU:HD11	14:2:102:ALA:HB3	1.93	0.50
14:2:107:LYS:HG2	14:2:108:GLY:H	1.76	0.50
1:A:124:THR:HG22	2:B:130:ARG:HH21	1.77	0.50
2:B:230:LYS:O	2:B:234:VAL:HG23	2.12	0.50
7:G:170:GLN:HE21	7:G:174:THR:HG23	1.75	0.50
12:L:21:ILE:C	12:L:21:ILE:HD12	2.36	0.50
12:L:113:PHE:CD2	12:L:119:TYR:HB3	2.47	0.50
1:O:13:THR:O	2:P:130:ARG:HD3	2.11	0.50
2:B:172:ALA:HB2	2:B:200:THR:HG21	1.93	0.49
5:E:48:LEU:HD13	5:E:77:SER:CB	2.42	0.49
8:H:5:GLY:O	8:H:124:TYR:HA	2.12	0.49
1:O:17:PRO:HG3	2:P:26:TYR:CE2	2.47	0.49
2:P:163:ILE:HG13	2:P:164:SER:N	2.26	0.49
6:T:179:LEU:HD11	6:T:196:ILE:HD11	1.92	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:192:GLN:HE21	6:T:192:GLN:HA	1.77	0.49
10:X:161:GLU:OE2	10:X:161:GLU:HA	2.12	0.49
4:D:70:ILE:HB	4:D:74:ILE:HG22	1.93	0.49
4:R:112:LEU:HD13	4:R:112:LEU:C	2.37	0.49
11:Y:8:PHE:CE2	11:Y:13:ILE:HG12	2.47	0.49
2:B:81:LEU:HD22	2:B:81:LEU:N	2.27	0.49
2:B:141:TYR:HA	2:B:145:GLY:O	2.12	0.49
2:B:185:LYS:HD3	2:B:187:ASP:H	1.75	0.49
4:D:138:ILE:O	4:D:149:PHE:N	2.45	0.49
5:E:148:LEU:CD2	5:E:162:GLY:HA2	2.41	0.49
8:H:80:LEU:HD12	8:H:113:ILE:HD11	1.93	0.49
9:I:36:HIS:HB3	9:I:42:PHE:CE2	2.47	0.49
13:M:133:MET:C	13:M:136:PRO:HD2	2.37	0.49
1:O:24:ILE:HD11	1:O:124:THR:HG23	1.93	0.49
2:B:168:ASN:ND2	2:B:200:THR:O	2.44	0.49
5:E:148:LEU:HD23	5:E:162:GLY:HA2	1.94	0.49
11:K:105(B):LYS:H	11:K:105(B):LYS:CD	2.21	0.49
11:K:137:VAL:HG21	11:K:161:ALA:CB	2.43	0.49
14:N:32:ASP:OD1	13:1:204:LYS:HA	2.12	0.49
1:O:118:LYS:O	1:O:122:GLU:HG3	2.12	0.49
6:T:139:GLY:HA3	6:T:147:HIS:O	2.12	0.49
12:Z:140:ASN:O	12:Z:144:PHE:HA	2.12	0.49
12:Z:178:VAL:HG22	12:Z:184:VAL:HG22	1.94	0.49
1:A:15:PHE:H	2:B:23:GLN:HE22	1.61	0.49
1:A:221:PHE:C	1:A:221:PHE:CD2	2.89	0.49
1:O:130:ARG:NH1	1:O:131:PRO:O	2.45	0.49
12:Z:177:ILE:HD12	12:Z:177:ILE:N	2.28	0.49
5:E:176:LEU:HD22	5:E:180(C):PHE:CE2	2.47	0.49
7:G:179:HIS:NE2	7:G:192:PHE:HE2	2.11	0.49
7:G:186:TRP:O	7:G:190:VAL:HG23	2.12	0.49
11:K:165:ARG:HH22	11:K:208:ASN:ND2	2.09	0.49
14:N:31:THR:HG22	14:N:32:ASP:N	2.28	0.49
1:O:112:LEU:O	1:O:116:VAL:HG23	2.13	0.49
3:Q:52:ARG:HD2	3:Q:208:LYS:O	2.11	0.49
9:W:48:LEU:HG	9:W:50:THR:HG22	1.95	0.49
1:A:228:GLU:O	1:A:232:ARG:NH1	2.46	0.49
5:E:31:ILE:HD11	5:E:153:PRO:CD	2.43	0.49
12:L:144(Q):LYS:HG2	12:L:145:TYR:N	2.26	0.49
12:L:180:LYS:HG3	12:L:182:ASP:OD1	2.13	0.49
3:Q:84:ASP:CG	3:Q:130:ARG:HH22	2.20	0.49
6:T:160:TYR:HB3	6:T:162:GLY:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:87:ASN:C	7:U:87:ASN:HD22	2.21	0.49
8:V:93:GLY:HA2	8:V:115:ALA:O	2.13	0.49
9:W:12:VAL:CG2	9:W:178:ILE:HB	2.42	0.49
13:1:133:MET:C	13:1:136:PRO:HD2	2.38	0.49
2:B:67:LEU:HD22	2:B:211:GLU:HB3	1.94	0.49
8:H:135:MET:HE3	13:1:165:ARG:CZ	2.42	0.49
12:L:114:ASP:C	12:L:114:ASP:OD2	2.55	0.49
13:M:63:VAL:HG22	13:M:74:LEU:HD12	1.94	0.49
2:P:39:GLY:C	2:P:148:LEU:HD21	2.38	0.49
6:T:238:LYS:NZ	6:T:239:GLU:HG3	2.27	0.49
8:V:35:HIS:CB	8:V:56:THR:HG21	2.42	0.49
9:I:123:ASP:HB2	9:I:124:PHE:CD2	2.47	0.49
10:J:-1:MET:HG2	10:J:1:ASP:N	2.27	0.49
2:P:69:LYS:HG3	2:P:221:GLN:OE1	2.13	0.49
3:Q:55:THR:O	3:Q:56:LEU:HD13	2.13	0.49
4:R:52:LYS:HG3	4:R:64:ILE:CG2	2.43	0.49
8:V:1:THR:HA	8:V:33:LYS:HZ3	1.77	0.49
10:X:77:GLN:C	10:X:77:GLN:NE2	2.70	0.49
11:Y:37:ILE:HG23	11:Y:60:GLY:HA2	1.94	0.49
3:C:47:VAL:HG23	3:C:189:CYS:SG	2.53	0.49
7:G:180(D):ILE:HD13	7:G:180(D):ILE:N	2.27	0.49
12:Z:109:ALA:HB2	12:Z:121:ARG:NH2	2.28	0.49
6:F:141:VAL:HG23	6:F:215:CYS:SG	2.52	0.48
10:J:52:THR:HG22	10:J:53:VAL:H	1.78	0.48
14:N:84:LYS:HD3	17:N:375:HOH:O	2.13	0.48
3:Q:163:GLN:HE21	3:Q:164:THR:N	2.05	0.48
5:S:66:LYS:O	5:S:77:SER:HA	2.12	0.48
11:Y:1:THR:HG23	11:Y:33:LYS:NZ	2.28	0.48
2:B:15:PHE:H	3:C:23:GLN:NE2	2.09	0.48
3:C:101:LEU:HD11	10:J:57:GLU:HB3	1.96	0.48
11:K:4:LEU:HD23	11:K:6:PHE:HD2	1.77	0.48
9:W:152:PHE:HB2	9:W:177:ILE:HD11	1.94	0.48
7:G:192:PHE:C	7:G:192:PHE:CD1	2.91	0.48
12:L:123:GLN:HG3	12:L:145:TYR:OH	2.14	0.48
14:N:19:ARG:NH1	14:N:169:SER:O	2.46	0.48
13:1:4:ILE:CD1	13:1:159:MET:SD	3.01	0.48
14:2:1:THR:O	14:2:129:SER:N	2.47	0.48
14:2:4:MET:HG2	14:2:159:LEU:HD21	1.95	0.48
3:C:84:ASP:CG	3:C:130:ARG:HH22	2.22	0.48
5:E:40:LEU:N	5:E:40:LEU:HD23	2.29	0.48
12:L:134:ILE:HG22	12:L:138:LEU:HD22	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:41:THR:HG21	13:M:79:ILE:HD12	1.95	0.48
6:T:159:GLY:HA3	7:U:63:THR:HG21	1.96	0.48
8:V:105:ASP:HB2	8:V:105(A):PRO:HD2	1.94	0.48
10:X:13:ILE:HG12	10:X:177:ILE:HG23	1.95	0.48
12:Z:18:THR:HG21	12:Z:30:TYR:CD1	2.46	0.48
12:Z:42:VAL:CG1	12:Z:176:LEU:HD23	2.44	0.48
13:1:57:ARG:HG2	13:1:57:ARG:HH11	1.77	0.48
13:1:158:ALA:O	13:1:162:LEU:HG	2.14	0.48
5:E:132:TYR:O	5:E:153:PRO:HB3	2.13	0.48
8:H:160:GLN:O	8:H:164:TRP:CD1	2.66	0.48
9:I:14:ILE:HG23	9:I:34:ILE:HD13	1.95	0.48
3:Q:100:ARG:HH11	3:Q:106:PRO:HB3	1.78	0.48
8:V:12:VAL:HG11	8:V:102:ALA:HB1	1.96	0.48
14:2:6:VAL:HG13	14:2:124:TYR:HB3	1.95	0.48
6:F:109:ILE:HB	6:F:110:PRO:HD3	1.94	0.48
7:G:120:SER:O	7:G:121:GLN:C	2.56	0.48
7:G:136:LEU:O	7:G:150:LYS:HA	2.13	0.48
12:L:15:ALA:HB1	12:L:173:LEU:HD11	1.94	0.48
3:Q:109:VAL:HG21	3:Q:147:LYS:HB2	1.96	0.48
8:V:164:TRP:CE3	8:V:164:TRP:HA	2.49	0.48
5:E:48:LEU:O	5:E:212:ILE:HA	2.12	0.48
6:F:35:THR:CG2	6:F:36:THR:N	2.76	0.48
7:G:46:THR:OG1	7:G:146:PRO:HB3	2.14	0.48
11:K:45:MET:HB3	11:K:52:CYS:HB3	1.95	0.48
14:2:55:ILE:O	14:2:59:VAL:HG23	2.14	0.48
4:D:163:LYS:HG3	4:D:164:ALA:N	2.29	0.48
5:E:13:VAL:HG13	5:E:13:VAL:O	2.13	0.48
6:F:136:THR:O	6:F:150:MET:HA	2.14	0.48
13:M:139:ARG:HH11	8:V:165:ASN:ND2	2.12	0.48
14:N:20:THR:OG1	14:N:28:ASN:HB3	2.13	0.48
10:X:10:ASP:HB3	17:X:283:HOH:O	2.13	0.48
11:Y:207:ASN:C	11:Y:209:VAL:H	2.21	0.48
6:F:147:HIS:HD2	17:F:449:HOH:O	1.97	0.48
14:N:9:LYS:HG3	14:N:145:ASN:HB3	1.96	0.48
3:Q:35:THR:HB	3:Q:51:GLU:CG	2.37	0.48
13:1:-5:PRO:HD3	13:1:96:TRP:CD2	2.49	0.48
1:A:186:LEU:O	1:A:190:ILE:HG13	2.13	0.48
4:D:215:ILE:HA	4:D:220:GLY:O	2.14	0.48
12:L:192:LYS:HE3	8:V:195:ASN:HB3	1.96	0.48
14:N:8:PHE:HE1	14:N:10:ASP:HB2	1.72	0.48
14:N:84:LYS:HB2	14:N:119:VAL:HG21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:111:LEU:O	1:O:114:SER:HB3	2.13	0.48
8:V:55:VAL:HG23	8:V:86:HIS:CD2	2.49	0.48
10:X:112:GLN:NE2	10:X:126:ALA:H	2.11	0.48
1:A:130:ARG:HG2	7:G:125:GLN:HG3	1.96	0.47
3:C:41:LYS:HG2	3:C:161:SER:O	2.15	0.47
14:N:4:MET:SD	14:N:159:LEU:CD2	3.02	0.47
1:O:20:LYS:HD2	17:O:348:HOH:O	2.13	0.47
1:O:130:ARG:HH21	7:U:124:THR:HG22	1.78	0.47
2:P:121:GLN:NE2	2:P:121:GLN:C	2.72	0.47
2:P:125:GLN:HG3	3:Q:130:ARG:HG2	1.96	0.47
3:Q:172:VAL:HG23	3:Q:196:SER:HB2	1.95	0.47
3:Q:186:VAL:HG21	3:Q:216:LYS:HE2	1.96	0.47
4:R:201:MET:HE2	4:R:201:MET:HB3	1.81	0.47
8:V:112:SER:OG	8:V:120:ASP:HB2	2.14	0.47
1:A:79:SER:HA	17:A:317:HOH:O	2.13	0.47
6:F:130:ARG:HG3	6:F:130:ARG:HH11	1.78	0.47
6:F:238:LYS:NZ	6:F:239:GLU:HG3	2.29	0.47
7:G:79:ASN:HA	17:G:433:HOH:O	2.14	0.47
3:Q:36:CYS:N	3:Q:51:GLU:HG2	2.29	0.47
3:Q:53:ARG:HG2	3:Q:54:SER:N	2.28	0.47
3:Q:152:GLU:CG	3:Q:156:ILE:HG22	2.43	0.47
5:S:41:ARG:NH1	5:S:42:SER:O	2.45	0.47
6:T:21:ASN:HB2	17:T:338:HOH:O	2.14	0.47
10:X:137:LEU:HD23	10:X:137:LEU:C	2.39	0.47
2:B:120:LYS:HZ1	2:B:136:PHE:HD1	1.60	0.47
6:F:192:GLN:HE21	6:F:192:GLN:HA	1.79	0.47
7:G:121:GLN:C	7:G:121:GLN:NE2	2.73	0.47
9:I:101:VAL:O	9:I:110:ILE:HA	2.14	0.47
12:L:19:ARG:HD2	12:L:168:GLN:O	2.14	0.47
13:M:40:ASN:H	13:M:40:ASN:ND2	2.12	0.47
4:R:32:LYS:O	4:R:167:SER:HA	2.14	0.47
8:V:103:GLY:HA2	8:V:178:MET:SD	2.54	0.47
13:1:104:VAL:HG23	13:1:178:ILE:HG22	1.97	0.47
3:C:169:SER:HA	3:C:172:VAL:HG12	1.96	0.47
4:D:160:TYR:CD2	5:E:59:SER:HB3	2.49	0.47
2:P:194:LEU:HG	2:P:212:PHE:CZ	2.49	0.47
7:U:179:HIS:NE2	7:U:192:PHE:HE2	2.12	0.47
10:X:140:HIS:HD2	10:X:141:HIS:CE1	2.32	0.47
5:E:141:TYR:CE2	5:E:217:LYS:HA	2.50	0.47
9:I:93:GLY:N	9:I:94:PRO:CD	2.78	0.47
9:I:115:LEU:N	9:I:115:LEU:HD23	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:156:SER:O	9:I:160:LEU:HB2	2.15	0.47
11:K:33:LYS:HE2	15:3:5:04D:H23	1.96	0.47
12:L:136:PRO:HB2	9:W:137:MET:SD	2.54	0.47
13:M:165:ARG:HD3	8:V:139:GLU:OE1	2.14	0.47
5:S:76:LEU:HD23	5:S:76:LEU:C	2.39	0.47
9:W:12:VAL:HG23	9:W:178:ILE:HB	1.95	0.47
11:Y:208:ASN:OD1	11:Y:208:ASN:O	2.33	0.47
12:Z:134:ILE:HG22	12:Z:138:LEU:HD22	1.96	0.47
13:1:-6:GLN:O	13:1:-6:GLN:HG3	2.14	0.47
2:B:134:VAL:HG12	2:B:135:SER:N	2.29	0.47
4:D:123(D):ALA:HA	5:E:129:GLY:CA	2.45	0.47
6:F:175:GLU:O	6:F:178:LYS:HB2	2.14	0.47
13:M:-6:GLN:HG3	13:M:-6:GLN:O	2.14	0.47
5:S:122:LYS:O	5:S:126:SER:HB2	2.15	0.47
6:T:191:LYS:HD3	6:T:235:PHE:CD1	2.48	0.47
9:W:49:ALA:HB3	10:X:118:THR:HG23	1.97	0.47
11:Y:2:THR:HG21	11:Y:162:ALA:HB3	1.97	0.47
11:Y:126:CYS:HB2	11:Y:135:TYR:CE1	2.50	0.47
13:1:112:TYR:CD2	13:1:120:TYR:CZ	3.03	0.47
2:B:20:ARG:NE	3:C:33:ARG:HH21	2.13	0.47
2:B:229:ILE:O	2:B:232:ILE:HG22	2.14	0.47
3:C:163:GLN:HE21	3:C:164:THR:N	2.04	0.47
4:D:195:LYS:HA	4:D:237:LEU:HD11	1.97	0.47
5:E:207:LEU:H	5:E:207:LEU:CD2	2.28	0.47
6:F:89:VAL:O	6:F:93:ARG:HG3	2.14	0.47
7:G:77:VAL:HG13	7:G:137:THR:HB	1.95	0.47
8:H:159:ILE:O	8:H:163:ILE:HG13	2.14	0.47
9:I:-2:ASN:HB3	9:I:20:LEU:HD22	1.95	0.47
9:I:55:LEU:HD21	9:I:95:TYR:CE1	2.49	0.47
9:I:115:LEU:HD23	9:I:115:LEU:H	1.79	0.47
10:J:4:LEU:HD23	10:J:126:ALA:HB2	1.96	0.47
11:K:195:LEU:O	11:K:199:VAL:HG23	2.15	0.47
3:Q:41:LYS:HG2	3:Q:161:SER:O	2.15	0.47
5:S:48:LEU:HG	5:S:139:ILE:HD13	1.96	0.47
5:S:143:LYS:HE3	13:1:78:TYR:OH	2.14	0.47
6:T:35:THR:CG2	6:T:36:THR:N	2.77	0.47
7:U:136:LEU:O	7:U:150:LYS:HA	2.14	0.47
8:V:105:ASP:HB2	8:V:105(A):PRO:CD	2.45	0.47
8:V:162:GLY:O	8:V:166:ASP:HB3	2.15	0.47
13:1:130:GLY:O	13:1:134:ALA:HB3	2.14	0.47
3:C:185:THR:HG22	3:C:186:VAL:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:133:PHE:HA	14:2:132:THR:O	2.14	0.47
6:T:120:VAL:HG22	6:T:132:PHE:CD1	2.49	0.47
8:V:1:THR:HA	8:V:33:LYS:NZ	2.30	0.47
12:Z:55:LEU:HD13	12:Z:95:TYR:CD1	2.50	0.47
2:B:78:VAL:HG12	2:B:79:ALA:N	2.29	0.47
2:B:190:ILE:HG21	2:B:232:ILE:HG12	1.97	0.47
3:C:136:THR:O	3:C:150:GLN:HA	2.14	0.47
4:D:37:ALA:HB3	4:D:165:ILE:CG1	2.45	0.47
4:D:40:ILE:HD12	4:D:193:VAL:HG23	1.97	0.47
5:E:90:ASN:O	5:E:93:ARG:HB2	2.15	0.47
7:G:109:CYS:HB3	17:G:463:HOH:O	2.14	0.47
10:J:45:PHE:CD1	10:J:52:THR:HG23	2.50	0.47
11:K:86:LEU:HD13	11:K:86:LEU:C	2.40	0.47
11:Y:1:THR:HG23	11:Y:2:THR:H	1.80	0.47
12:Z:-6:PRO:O	13:1:91:ARG:NH1	2.48	0.47
12:Z:67:HIS:HD2	17:Z:329:HOH:O	1.97	0.47
13:1:141(C):ARG:HG3	13:1:141(C):ARG:NH1	2.26	0.47
14:2:52:THR:HG22	14:2:97:ALA:HB1	1.95	0.47
14:2:107:LYS:HG2	14:2:108:GLY:N	2.30	0.47
14:2:155:ILE:HG22	14:2:175:MET:HE2	1.97	0.47
7:G:76:MET:HB2	7:G:138:PHE:CD2	2.50	0.47
10:J:36:GLN:HG3	10:J:184:ILE:HD12	1.97	0.47
2:P:195:LYS:O	2:P:198:SER:HB2	2.15	0.47
4:R:45:GLY:HA2	4:R:146:TYR:CE1	2.50	0.47
6:T:38:ILE:HG22	6:T:164:ALA:HB1	1.96	0.47
6:T:130:ARG:HG3	6:T:130:ARG:NH1	2.29	0.47
10:X:103:GLY:HA2	10:X:178:VAL:HG11	1.97	0.47
2:B:185:LYS:HD3	2:B:186:VAL:N	2.31	0.46
3:C:46:VAL:HG22	3:C:146:PRO:HB2	1.96	0.46
5:E:207:LEU:H	5:E:207:LEU:HD23	1.80	0.46
9:I:6:MET:HB2	9:I:151:LEU:HD11	1.98	0.46
13:M:18:ASN:HA	13:M:31:VAL:O	2.15	0.46
14:N:30:VAL:HG11	13:1:199:PHE:CE2	2.50	0.46
14:N:59:VAL:O	14:N:63:LEU:HG	2.16	0.46
2:P:108:PRO:HB2	2:P:111:ILE:HG13	1.96	0.46
2:P:190:ILE:HG21	2:P:232:ILE:HG12	1.97	0.46
5:S:82:ALA:O	5:S:85:ALA:HB3	2.15	0.46
9:W:14:ILE:HG12	9:W:34:ILE:CD1	2.44	0.46
9:W:59:PHE:CZ	9:W:83:VAL:HG22	2.50	0.46
11:Y:20:ALA:HB2	11:Y:31:VAL:HG21	1.96	0.46
2:B:205:LEU:O	2:B:233:LEU:HD21	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:24:VAL:O	6:F:27:ALA:HB3	2.15	0.46
6:F:38:ILE:HG22	6:F:164:ALA:HB2	1.97	0.46
13:M:6:MET:HG2	13:M:155:ILE:HD11	1.96	0.46
4:D:123:PHE:HA	4:D:128:MET:O	2.15	0.46
12:L:129:ALA:HB1	12:L:166:HIS:NE2	2.30	0.46
4:R:188:GLU:O	4:R:192:LEU:HD13	2.15	0.46
7:U:236:ILE:HD12	7:U:237:ALA:N	2.31	0.46
1:A:109:THR:O	1:A:113:VAL:HG23	2.15	0.46
6:F:170:GLN:CD	6:F:170:GLN:N	2.72	0.46
7:G:139:VAL:HG12	7:G:148:ILE:HG12	1.98	0.46
4:R:146:TYR:C	4:R:147:GLN:HG3	2.41	0.46
4:R:214:CYS:SG	4:R:224:TYR:CE2	3.06	0.46
7:U:130:ARG:HG3	7:U:131:PRO:O	2.16	0.46
7:U:215:ALA:HB2	7:U:221:PHE:HD2	1.80	0.46
10:X:90(A):ILE:HD12	10:X:90(A):ILE:HA	1.83	0.46
14:2:13:ILE:HG12	14:2:177:VAL:HG13	1.97	0.46
14:2:14:LEU:HB3	14:2:34:LEU:HD22	1.96	0.46
5:E:143:LYS:HE3	13:M:78:TYR:OH	2.15	0.46
8:H:157:ASP:O	8:H:160:GLN:HB2	2.15	0.46
10:J:74:LEU:HD22	10:J:78:ALA:HB1	1.97	0.46
3:Q:67:VAL:HG22	3:Q:77:SER:HB3	1.97	0.46
4:R:139:ALA:HA	4:R:147:GLN:O	2.16	0.46
5:S:47:VAL:HG12	5:S:48:LEU:N	2.30	0.46
6:T:167:LYS:O	6:T:170:GLN:NE2	2.48	0.46
12:Z:134:ILE:HA	17:Z:341:HOH:O	2.14	0.46
14:2:163:ILE:HD13	14:2:170:GLY:HA2	1.98	0.46
4:D:139:ALA:HB2	4:D:148:LEU:HD12	1.97	0.46
12:L:140:ASN:O	12:L:144:PHE:HA	2.16	0.46
1:O:81:MET:HE1	7:U:21:LEU:HD11	1.97	0.46
2:P:21:LEU:HD13	2:P:124:THR:HG23	1.97	0.46
3:Q:76:LEU:HD12	3:Q:138:ILE:HG12	1.98	0.46
3:Q:195:ARG:HG3	3:Q:236:ILE:HD13	1.97	0.46
5:S:48:LEU:O	5:S:212:ILE:HA	2.15	0.46
6:T:171:SER:O	6:T:174:ALA:HB3	2.16	0.46
7:U:115:ARG:O	7:U:119:LEU:HD22	2.16	0.46
9:W:13:ALA:HA	9:W:176:TYR:O	2.16	0.46
13:1:110:LEU:HD23	13:1:122:SER:O	2.15	0.46
2:B:47:VAL:HG22	2:B:214:THR:HG22	1.96	0.46
11:K:126:CYS:SG	11:K:135:TYR:CD2	3.03	0.46
3:Q:75:VAL:CG2	3:Q:215:VAL:HG11	2.45	0.46
3:Q:130:ARG:HH11	3:Q:130:ARG:CG	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1:13:ILE:CG2	13:1:175:LEU:HD21	2.46	0.46
1:A:177:GLU:HG3	2:B:58:LEU:HD22	1.98	0.46
1:A:212:LEU:HD23	1:A:212:LEU:C	2.40	0.46
4:D:10:ARG:HE	4:D:10:ARG:HB2	1.55	0.46
4:D:195:LYS:O	4:D:198:LYS:HB3	2.16	0.46
5:E:198:SER:HA	5:E:201:LEU:CD1	2.45	0.46
7:G:56:ASP:HB3	7:G:59:LEU:HG	1.98	0.46
7:G:220:LYS:HG2	7:G:221:PHE:N	2.31	0.46
13:M:139:ARG:HH11	8:V:165:ASN:HD22	1.61	0.46
14:N:4:MET:SD	14:N:159:LEU:HD21	2.56	0.46
7:U:35:ILE:HG23	7:U:51:GLN:HB2	1.97	0.46
7:U:194:ILE:HG23	7:U:210:LEU:HD11	1.98	0.46
8:V:34:LEU:HD22	8:V:174:ASP:HB3	1.97	0.46
10:X:3:ILE:HG22	10:X:100:LEU:CD1	2.46	0.46
10:X:112:GLN:HE22	10:X:126:ALA:H	1.63	0.46
7:G:236:ILE:HD12	7:G:237:ALA:N	2.30	0.46
10:J:166:MET:HE3	10:J:166:MET:HB3	1.85	0.46
13:M:165:ARG:CZ	8:V:135:MET:HE3	2.45	0.46
3:Q:161:SER:HB3	3:Q:180:TYR:CE1	2.51	0.46
3:Q:185:THR:HG22	3:Q:186:VAL:N	2.31	0.46
5:S:20:ARG:HB3	5:S:25:GLU:OE2	2.16	0.46
7:U:169:GLN:HG3	17:U:316:HOH:O	2.15	0.46
14:2:14:LEU:O	14:2:175:MET:HA	2.16	0.46
4:D:146:TYR:C	4:D:147:GLN:HG3	2.42	0.46
6:F:35:THR:HG22	6:F:36:THR:N	2.30	0.46
6:F:36:THR:HA	6:F:165:THR:O	2.16	0.46
8:H:6:VAL:HG11	8:H:154:LEU:HD23	1.97	0.46
10:J:133:TYR:CE2	10:J:166:MET:SD	3.09	0.46
11:K:55:TRP:HB2	11:K:97:MET:HE1	1.97	0.46
12:L:4:LEU:HD13	12:L:138:LEU:HD21	1.98	0.46
12:L:42:VAL:CG2	12:L:102:ALA:HB3	2.46	0.46
6:T:116:LEU:HD23	6:T:116:LEU:HA	1.75	0.46
7:U:39:ALA:HB1	7:U:48:VAL:HG12	1.98	0.46
7:U:181:ASP:O	7:U:182:HIS:HB3	2.15	0.46
12:Z:113:PHE:N	12:Z:113:PHE:CD1	2.83	0.46
5:E:12:THR:HG21	5:E:124:THR:HA	1.98	0.45
9:I:13:ALA:HA	9:I:176:TYR:O	2.15	0.45
13:M:114:ASN:C	13:M:114:ASN:OD1	2.58	0.45
2:P:185:LYS:HE2	2:P:187:ASP:OD1	2.15	0.45
2:P:231:ASP:O	2:P:235:LYS:HG2	2.16	0.45
3:Q:81:LEU:HB2	3:Q:84:ASP:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:40:ILE:HD12	4:R:193:VAL:HG23	1.98	0.45
4:R:100:ASN:HB3	17:R:353:HOH:O	2.15	0.45
14:2:13:ILE:HG23	14:2:176:VAL:O	2.16	0.45
1:A:137:LEU:HA	1:A:149:TYR:O	2.16	0.45
3:C:40:VAL:HG23	3:C:189:CYS:SG	2.56	0.45
3:C:111:TYR:O	3:C:112:LEU:C	2.59	0.45
7:G:214:VAL:HG12	7:G:215:ALA:N	2.31	0.45
11:K:153:TYR:O	11:K:156:LYS:HB3	2.17	0.45
2:P:215:ILE:HG12	2:P:221:GLN:HG2	1.98	0.45
3:Q:33:ARG:NH1	3:Q:33:ARG:CB	2.80	0.45
4:R:46:VAL:O	4:R:214:CYS:HA	2.16	0.45
7:U:48:VAL:CG1	7:U:139:VAL:HG11	2.46	0.45
10:X:52:THR:HG21	17:X:263:HOH:O	2.16	0.45
4:D:123(D):ALA:CA	5:E:129:GLY:HA2	2.45	0.45
5:E:125:GLN:HG3	6:F:130:ARG:HG2	1.98	0.45
10:J:6:ILE:HD11	10:J:142:TYR:HE1	1.82	0.45
11:K:1:THR:CG2	11:K:2:THR:N	2.79	0.45
14:N:167:GLY:O	13:1:167:ALA:HB1	2.17	0.45
4:R:195:LYS:O	4:R:198:LYS:HB3	2.15	0.45
5:S:15:PHE:CD1	5:S:21:LEU:HD21	2.51	0.45
7:U:130:ARG:HG3	7:U:130:ARG:HH11	1.82	0.45
10:X:36:GLN:HG3	10:X:184:ILE:CD1	2.47	0.45
3:C:125:GLN:O	3:C:125:GLN:HG3	2.16	0.45
4:D:227:GLU:CD	4:D:227:GLU:H	2.25	0.45
7:G:8:TYR:C	7:G:10:ARG:H	2.23	0.45
12:L:-6:PRO:HB2	13:M:91:ARG:NH1	2.31	0.45
12:L:114:ASP:HB2	15:3:3:ILE:HD12	1.97	0.45
14:N:4:MET:CB	14:N:126:ILE:HG22	2.46	0.45
1:O:86:ARG:HH21	7:U:118:ASN:HD22	1.65	0.45
3:Q:216:LYS:HB2	3:Q:220:ASP:HB3	1.98	0.45
4:R:146:TYR:HE1	4:R:216:THR:HA	1.80	0.45
7:U:192:PHE:C	7:U:192:PHE:CD1	2.94	0.45
8:V:10:ASN:OD1	8:V:180:ILE:HD12	2.16	0.45
12:Z:88:TYR:CD1	12:Z:88:TYR:O	2.69	0.45
13:1:40:ASN:H	13:1:40:ASN:HD22	1.64	0.45
1:A:233:LEU:C	1:A:235:ALA:H	2.23	0.45
6:F:186:ALA:O	6:F:190:VAL:HG23	2.16	0.45
8:V:221:ILE:HG13	9:W:40:HIS:HA	1.99	0.45
9:I:99:PRO:HB2	9:I:113:PHE:CD2	2.51	0.45
12:L:70:HIS:HE1	17:L:355:HOH:O	2.00	0.45
1:O:84:ASP:CG	1:O:130:ARG:HH22	2.24	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:86:ARG:HE	7:U:118:ASN:HD21	1.65	0.45
2:P:218:ASN:O	2:P:218(B):ASP:HB2	2.17	0.45
4:R:160:TYR:CZ	4:R:163:LYS:HD3	2.52	0.45
5:S:64:GLN:HA	17:S:345:HOH:O	2.16	0.45
6:T:35:THR:HG22	6:T:36:THR:N	2.31	0.45
17:T:347:HOH:O	13:1:67:ALA:HB3	2.17	0.45
7:U:29:LYS:HA	7:U:29:LYS:HD2	1.58	0.45
8:V:113:ILE:HG12	8:V:119:THR:HG22	1.99	0.45
9:W:55:LEU:HD21	9:W:95:TYR:CE1	2.52	0.45
14:2:55:ILE:HD11	14:2:95:LEU:HD13	1.99	0.45
6:F:127:ASN:HD22	6:F:127:ASN:C	2.24	0.45
8:H:1:THR:HG23	8:H:33:LYS:NZ	2.32	0.45
10:J:34:THR:HG21	10:J:176:LYS:NZ	2.32	0.45
14:N:83:PHE:HB3	14:N:113:ILE:HD13	1.99	0.45
14:N:161:GLN:HE22	14:2:139:ASP:HB3	1.82	0.45
6:T:137:ILE:HA	6:T:149:TYR:O	2.16	0.45
6:T:195:LYS:O	6:T:198:TYR:N	2.49	0.45
6:T:203:GLU:C	6:T:205:ASN:H	2.23	0.45
10:X:7:ARG:O	10:X:7:ARG:HG2	2.16	0.45
11:Y:70:GLU:O	11:Y:71:LYS:HB2	2.16	0.45
12:Z:109:ALA:HB2	12:Z:121:ARG:HH21	1.82	0.45
1:A:40:ILE:HD11	1:A:193:ALA:HA	1.98	0.45
6:F:187:ARG:HG3	6:F:187:ARG:HH11	1.82	0.45
8:H:112:SER:OG	8:H:120:ASP:HB2	2.17	0.45
11:K:99:THR:HA	17:K:432:HOH:O	2.17	0.45
3:Q:198:LEU:HD12	3:Q:236:ILE:HG21	1.99	0.45
11:Y:132:THR:HA	17:Y:337:HOH:O	2.17	0.45
12:Z:137:PHE:CE1	12:Z:141:GLN:CG	2.99	0.45
2:B:81:LEU:HD23	2:B:133:GLY:CA	2.47	0.45
10:J:24:ILE:HD11	10:X:129:TYR:HB3	1.98	0.45
1:O:130:ARG:HG3	1:O:130:ARG:NH1	2.27	0.45
1:O:212:LEU:HD23	1:O:212:LEU:C	2.41	0.45
5:S:66:LYS:HA	5:S:78:LEU:CD2	2.47	0.45
6:T:37:SER:HB3	6:T:50:VAL:CG2	2.34	0.45
7:U:214:VAL:HG12	7:U:215:ALA:N	2.31	0.45
2:B:141:TYR:CD1	2:B:142:ASP:N	2.85	0.45
6:F:68:GLN:OE1	6:F:89:VAL:HG21	2.17	0.45
6:F:90:ASN:O	6:F:94:GLU:HG3	2.17	0.45
12:L:114:ASP:HB3	12:L:118:SER:HB3	1.99	0.45
12:L:166:HIS:HD2	12:L:168:GLN:H	1.64	0.45
1:O:197:LEU:HD23	1:O:210:ILE:HG23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:134:VAL:HG12	3:Q:135:SER:N	2.30	0.45
4:R:215:ILE:CG2	4:R:221:PHE:HD2	2.27	0.45
17:S:327:HOH:O	6:T:12:ASN:HB2	2.15	0.45
12:Z:180:LYS:HG2	17:Z:265:HOH:O	2.16	0.45
13:1:160:ARG:HG3	13:1:192:VAL:HG11	1.99	0.45
2:B:24:VAL:HG11	2:B:154:SER:HB3	1.99	0.44
3:C:186:VAL:O	3:C:190:VAL:HG23	2.17	0.44
4:D:160:TYR:CZ	4:D:163:LYS:HD3	2.52	0.44
9:I:33:LYS:O	9:I:44:GLY:HA2	2.17	0.44
10:J:53:VAL:HG21	17:K:474:HOH:O	2.16	0.44
11:K:133:PHE:CE2	11:K:166:ASP:HB2	2.52	0.44
12:L:165:ARG:NH1	9:W:135:PHE:CE1	2.85	0.44
13:M:114:ASN:O	13:M:116:LEU:N	2.50	0.44
2:P:144:ARG:O	2:P:144:ARG:HG2	2.16	0.44
4:R:70:ILE:HB	4:R:74:ILE:HG22	2.00	0.44
7:U:120:SER:O	7:U:121:GLN:C	2.59	0.44
1:A:134:VAL:O	1:A:153:PRO:HG3	2.17	0.44
4:D:214:CYS:SG	4:D:224:TYR:HE2	2.30	0.44
5:E:122:LYS:O	5:E:126:SER:HB2	2.17	0.44
13:M:40:ASN:H	13:M:40:ASN:HD22	1.66	0.44
14:N:146:MET:HE3	14:N:150:GLU:HB3	1.99	0.44
2:P:161:LYS:HE3	3:Q:59:GLN:O	2.17	0.44
7:U:84:ASP:CG	7:U:130:ARG:HH22	2.24	0.44
11:Y:37:ILE:HB	11:Y:41:LEU:HB3	1.99	0.44
12:Z:144(R):LYS:CG	12:Z:145:TYR:N	2.81	0.44
13:1:32:GLU:OE1	13:1:34:LEU:HB2	2.18	0.44
14:2:38:HIS:O	14:2:39:ASP:C	2.60	0.44
14:2:157:HIS:CD2	14:2:187(J):LEU:HD13	2.44	0.44
8:H:111:PHE:CE1	13:1:207:GLY:HA2	2.51	0.44
1:O:188:ASP:O	1:O:192:ILE:HG13	2.18	0.44
5:S:123:ASN:HD22	5:S:123:ASN:N	2.15	0.44
7:U:38:LEU:HA	7:U:164:ALA:HA	1.99	0.44
7:U:65:SER:HA	7:U:211:GLU:OE2	2.18	0.44
7:U:184(G):GLU:HG2	7:U:188:LYS:HB2	1.99	0.44
8:V:15:ALA:HA	8:V:174:ASP:O	2.18	0.44
11:Y:4:LEU:HD13	11:Y:15:ALA:O	2.18	0.44
14:2:42:TRP:N	14:2:42:TRP:CD1	2.86	0.44
2:B:147:GLN:HB3	2:B:149:TYR:CE2	2.53	0.44
5:E:70:CYS:SG	5:E:92:LEU:HD23	2.57	0.44
8:H:34:LEU:HB2	17:H:434:HOH:O	2.17	0.44
12:L:107:LYS:HA	12:L:107:LYS:HD3	1.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:177:ILE:HD12	12:L:177:ILE:N	2.31	0.44
12:L:180:LYS:HG2	17:L:313:HOH:O	2.17	0.44
13:M:53:GLN:O	13:M:56:GLU:HB2	2.18	0.44
14:N:102:ALA:HA	14:N:109:GLU:O	2.17	0.44
2:P:15:PHE:H	3:Q:23:GLN:NE2	2.15	0.44
6:T:12:ASN:OD1	6:T:12:ASN:O	2.35	0.44
7:G:233:LEU:O	7:G:236:ILE:HG13	2.18	0.44
3:Q:194:VAL:HB	3:Q:236:ILE:CD1	2.47	0.44
5:S:82:ALA:HB3	5:S:83:PRO:HD3	1.99	0.44
6:T:221:HIS:CE1	6:T:223:PHE:CE1	3.05	0.44
7:U:46:THR:HG21	7:U:139:VAL:HB	1.98	0.44
8:V:175:VAL:HG12	8:V:176:CYS:N	2.32	0.44
2:B:138:TYR:O	2:B:148:LEU:HA	2.17	0.44
5:E:180(C):PHE:CD1	5:E:180(C):PHE:C	2.96	0.44
6:F:120:VAL:HG21	6:F:151:LEU:HD21	1.99	0.44
6:F:150:MET:O	6:F:157:TYR:HA	2.18	0.44
7:G:47:VAL:HG12	7:G:49:ILE:HD12	2.00	0.44
12:L:166:HIS:CD2	12:L:168:GLN:HB2	2.52	0.44
2:P:130:ARG:NH1	2:P:131:PRO:O	2.50	0.44
2:P:168:ASN:ND2	2:P:200:THR:O	2.51	0.44
4:R:134:VAL:HG22	4:R:135:ALA:N	2.33	0.44
7:U:198:ILE:HG23	7:U:203:THR:O	2.17	0.44
13:1:113:VAL:HA	13:1:118:VAL:O	2.18	0.44
3:C:41:LYS:HE2	3:C:161:SER:HA	1.98	0.44
8:H:29:LYS:HE2	12:Z:165:ARG:CZ	2.48	0.44
11:K:209:VAL:C	11:K:210:ILE:HD12	2.43	0.44
12:L:18:THR:CG2	12:L:18:THR:O	2.66	0.44
13:M:165:ARG:NH1	8:V:139:GLU:OE1	2.49	0.44
14:N:171:GLY:HA2	13:1:197:TRP:CZ3	2.52	0.44
1:O:217(I):TYR:CE1	8:V:36:ARG:HD2	2.52	0.44
6:T:50:VAL:HG22	6:T:51:GLU:O	2.18	0.44
10:X:39:PRO:HG2	10:X:73:GLU:OE1	2.18	0.44
13:1:175:LEU:HD23	13:1:176:ALA:N	2.33	0.44
14:2:134:ILE:HD12	14:2:158:SER:HB3	2.00	0.44
2:B:20:ARG:NE	3:C:33:ARG:NH2	2.66	0.44
2:B:116:LEU:HD23	2:B:116:LEU:HA	1.77	0.44
3:C:28:LEU:O	3:C:31:VAL:HB	2.17	0.44
7:G:26:TYR:N	7:G:26:TYR:CD1	2.84	0.44
9:I:12:VAL:CG2	9:I:178:ILE:HB	2.47	0.44
11:K:70:GLU:C	11:K:72:GLU:H	2.26	0.44
11:K:165:ARG:NH2	11:K:208:ASN:HD22	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:160:TYR:CE2	5:S:59:SER:HB3	2.53	0.44
6:T:7:GLY:C	6:T:9:ASP:H	2.25	0.44
9:W:90:ARG:HA	9:W:90:ARG:HD3	1.87	0.44
9:W:117:GLY:O	9:W:118:CYS:C	2.61	0.44
10:X:12:VAL:HG21	10:X:109:GLU:O	2.18	0.44
11:Y:64:ARG:O	11:Y:67:GLU:HB2	2.18	0.44
4:D:123(D):ALA:HB1	5:E:129:GLY:HA2	1.99	0.44
7:G:39:ALA:HA	7:G:47:VAL:O	2.18	0.44
11:K:197:TRP:CD1	9:W:190:LYS:HE3	2.52	0.44
12:L:49:ALA:HA	17:L:350:HOH:O	2.17	0.44
1:O:77:VAL:HG12	1:O:137:LEU:HB2	1.99	0.44
2:P:107:ILE:HA	2:P:108:PRO:HD3	1.92	0.44
5:S:45:HIS:HD2	5:S:214:ILE:HD11	1.82	0.44
6:T:157:TYR:CD1	6:T:157:TYR:C	2.95	0.44
6:T:208:PHE:H	6:T:208:PHE:HD2	1.66	0.44
8:V:164:TRP:HA	8:V:164:TRP:HE3	1.82	0.44
9:W:113:PHE:HA	9:W:118:CYS:O	2.17	0.44
4:D:72:ARG:HG3	17:D:464:HOH:O	2.18	0.43
1:O:78:TYR:CE2	1:O:82:GLY:HA2	2.52	0.43
2:P:150:THR:O	2:P:157:TYR:HA	2.18	0.43
2:P:197:LEU:HD13	2:P:210:LEU:CD2	2.48	0.43
9:W:12:VAL:HG23	9:W:178:ILE:HD12	1.99	0.43
10:X:66:TYR:C	10:X:66:TYR:CD2	2.96	0.43
13:1:204:LYS:N	13:1:204:LYS:HD3	2.33	0.43
1:A:27:ALA:HB2	7:G:15:PHE:CE2	2.53	0.43
1:A:29:THR:O	1:A:33:GLN:HG2	2.17	0.43
4:D:194:LEU:HD12	4:D:194:LEU:HA	1.82	0.43
4:D:197:LEU:O	4:D:201:MET:HG3	2.17	0.43
6:F:107:ILE:HA	6:F:108:PRO:HD3	1.79	0.43
7:G:211:GLU:HA	17:G:447:HOH:O	2.18	0.43
8:H:52:THR:O	8:H:56:THR:HB	2.18	0.43
9:I:-8:SER:O	9:I:-6:PRO:HD3	2.18	0.43
11:K:64:ARG:O	11:K:67:GLU:HB2	2.17	0.43
12:L:165:ARG:CZ	8:V:29:LYS:HE2	2.48	0.43
4:R:160:TYR:CD2	5:S:59:SER:HB3	2.53	0.43
7:U:87:ASN:C	7:U:87:ASN:ND2	2.76	0.43
10:X:34:THR:HG21	10:X:176:LYS:NZ	2.33	0.43
13:1:114:ASN:O	13:1:116:LEU:N	2.51	0.43
1:A:13:THR:O	2:B:130:ARG:HD3	2.18	0.43
3:C:39:GLY:HA2	3:C:47:VAL:O	2.18	0.43
3:C:130:ARG:HG3	3:C:130:ARG:NH1	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:207:LEU:HD21	4:D:233:ILE:HG12	2.00	0.43
6:F:107:ILE:HG23	6:F:107:ILE:O	2.17	0.43
7:G:41:ARG:NH2	7:G:180(B):ASP:O	2.51	0.43
10:J:18:LYS:HG2	10:J:174:ILE:HG13	2.01	0.43
11:K:4:LEU:HD22	11:K:4:LEU:C	2.44	0.43
11:K:133:PHE:CD2	11:K:166:ASP:HB2	2.52	0.43
12:L:113:PHE:CD1	12:L:113:PHE:N	2.86	0.43
3:Q:78:PHE:CD1	3:Q:85:SER:HB3	2.53	0.43
3:Q:168:ASN:HB3	3:Q:200:VAL:HG11	2.00	0.43
8:V:80:LEU:HD12	8:V:113:ILE:HD11	2.00	0.43
11:Y:4:LEU:C	11:Y:4:LEU:HD22	2.44	0.43
13:1:35:ILE:CD1	13:1:56:GLU:HG2	2.48	0.43
13:1:112:TYR:CE2	13:1:120:TYR:OH	2.71	0.43
1:A:217(I):TYR:CE1	8:H:36:ARG:HD2	2.53	0.43
8:H:29:LYS:HE2	12:Z:165:ARG:HH21	1.80	0.43
10:J:138:LEU:HD21	10:J:158:CYS:SG	2.58	0.43
13:M:135:ASN:HB2	13:M:136:PRO:HD3	1.99	0.43
2:P:152:ASN:HB2	2:P:153:PRO:HD2	2.00	0.43
4:R:49:GLY:HA2	4:R:211:GLN:O	2.18	0.43
4:R:194:LEU:HD12	4:R:194:LEU:HA	1.81	0.43
7:U:14:ILE:O	7:U:21:LEU:HD23	2.19	0.43
9:W:99:PRO:HB2	9:W:113:PHE:CD2	2.53	0.43
14:2:1:THR:HG21	14:2:46:SER:HA	2.01	0.43
1:A:84:ASP:CG	1:A:130:ARG:HH22	2.27	0.43
1:A:197:LEU:HD12	1:A:197:LEU:HA	1.81	0.43
1:A:225:THR:OG1	1:A:228:GLU:HG3	2.19	0.43
2:B:84:ASP:CG	2:B:130:ARG:HH22	2.25	0.43
3:C:229:ILE:O	3:C:232:TYR:N	2.51	0.43
6:F:38:ILE:HG22	6:F:164:ALA:HB1	1.98	0.43
3:Q:40:VAL:HA	3:Q:162:ALA:HA	1.99	0.43
3:Q:156:ILE:HD11	4:R:82:THR:OG1	2.17	0.43
4:R:237:LEU:HD22	4:R:241:GLU:HG3	1.99	0.43
5:S:68:ILE:HB	5:S:76:LEU:HD21	2.00	0.43
5:S:125:GLN:HG3	6:T:130:ARG:HG2	1.99	0.43
5:S:207:LEU:HD23	5:S:207:LEU:H	1.84	0.43
6:T:37:SER:HA	6:T:50:VAL:HA	1.99	0.43
11:Y:200:LYS:HG3	11:Y:205:SER:O	2.18	0.43
13:1:62:LEU:HD13	13:1:74:LEU:CD1	2.48	0.43
2:B:4:GLY:CA	5:E:127:TYR:CE1	3.01	0.43
2:B:152:ASN:HB2	2:B:153:PRO:HD2	1.99	0.43
4:D:201:MET:HE2	4:D:201:MET:HB3	1.92	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:29:LYS:HA	7:G:29:LYS:HD2	1.81	0.43
7:G:194:ILE:HG23	7:G:210:LEU:HD11	1.99	0.43
8:H:157:ASP:O	8:H:160:GLN:N	2.51	0.43
10:J:40:HIS:O	10:J:103:GLY:HA2	2.18	0.43
14:N:148:LYS:O	14:N:152:VAL:HG23	2.17	0.43
2:P:74:ILE:HD11	2:P:109:VAL:HG22	2.01	0.43
3:Q:55:THR:HG22	3:Q:56:LEU:HD22	2.01	0.43
3:Q:141:PHE:CE1	3:Q:217:PRO:HG3	2.53	0.43
4:R:215:ILE:O	4:R:215:ILE:HG13	2.18	0.43
5:S:160:LEU:HD23	6:T:59:LEU:HD12	2.00	0.43
5:S:180(C):PHE:CD1	5:S:180(C):PHE:C	2.96	0.43
6:T:212:ILE:HG22	6:T:213:SER:N	2.32	0.43
7:U:71:SER:O	7:U:72:ARG:C	2.60	0.43
8:V:197:ARG:NH2	9:W:139:GLU:HG3	2.33	0.43
2:B:121:GLN:NE2	2:B:121:GLN:C	2.77	0.43
5:E:161:TYR:OH	6:F:61:PRO:HD2	2.19	0.43
6:F:137:ILE:HA	6:F:149:TYR:O	2.18	0.43
7:G:77:VAL:HG12	7:G:137:THR:HB	2.01	0.43
9:I:171:TRP:HH2	11:Y:165:ARG:HH11	1.65	0.43
10:J:8:VAL:HG23	10:J:9:GLN:N	2.34	0.43
12:L:45:ALA:HA	12:L:99:THR:HB	2.00	0.43
1:O:217:ASP:HA	1:O:220:ARG:NH1	2.33	0.43
5:S:127:TYR:C	5:S:129:GLY:H	2.27	0.43
5:S:172:ALA:HB2	5:S:196:ALA:O	2.18	0.43
7:U:233:LEU:O	7:U:236:ILE:HG13	2.18	0.43
4:D:215:ILE:O	4:D:215:ILE:HG13	2.17	0.43
8:H:167:LEU:HG	12:Z:24:TYR:O	2.18	0.43
12:L:134:ILE:HA	17:L:388:HOH:O	2.18	0.43
2:P:184:MET:HE1	2:P:189:ALA:HA	2.00	0.43
3:Q:121:GLN:NE2	3:Q:121:GLN:C	2.76	0.43
6:T:212:ILE:HG22	6:T:213:SER:H	1.83	0.43
11:Y:65:LEU:HA	11:Y:65:LEU:HD12	1.75	0.43
13:1:19:LEU:HD23	13:1:168:ARG:O	2.19	0.43
2:B:130:ARG:HG3	2:B:130:ARG:NH1	2.33	0.43
9:I:154:THR:O	9:I:155:ILE:C	2.61	0.43
2:P:82:THR:O	2:P:85:ALA:HB3	2.19	0.43
2:P:229:ILE:O	2:P:232:ILE:HG22	2.19	0.43
6:T:121:GLN:C	6:T:121:GLN:NE2	2.77	0.43
8:V:43:CYS:SG	8:V:99:LEU:HB3	2.58	0.43
9:W:8:GLY:HA2	17:W:221:HOH:O	2.19	0.43
11:Y:153:TYR:O	11:Y:156:LYS:HB3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:75:SER:OG	17:Z:253:HOH:O	2.22	0.43
2:B:218:ASN:O	2:B:218(C):ASP:HB2	2.18	0.43
2:B:225:LYS:O	2:B:226:PRO:C	2.61	0.43
7:G:49:ILE:CD1	7:G:212:VAL:HG13	2.49	0.43
10:J:112:GLN:NE2	10:J:125:GLY:HA3	2.34	0.43
12:L:43:MET:HG2	12:L:44:SER:N	2.34	0.43
14:N:25:TYR:CE1	13:1:165:ARG:HB3	2.54	0.43
14:N:51:ASP:O	14:N:55:ILE:HG13	2.19	0.43
1:O:15:PHE:HD2	2:P:23:GLN:NE2	2.17	0.43
1:O:67:VAL:HG11	1:O:213:ALA:CB	2.48	0.43
1:O:72:PRO:HB3	17:V:304:HOH:O	2.18	0.43
4:R:68:VAL:HG21	4:R:89:ILE:HD12	2.01	0.43
5:S:138:ILE:O	5:S:148:LEU:HA	2.19	0.43
6:T:39:GLY:O	6:T:148:LEU:HD21	2.18	0.43
6:T:113:ALA:O	6:T:116:LEU:HB2	2.19	0.43
7:U:236:ILE:C	7:U:238:GLU:H	2.27	0.43
9:W:43:LEU:HD23	9:W:45:ILE:HD11	2.00	0.43
9:W:43:LEU:CD2	9:W:45:ILE:HD11	2.49	0.43
11:Y:33:LYS:O	11:Y:45:MET:HG3	2.18	0.43
11:Y:58:TRP:O	11:Y:59:LEU:C	2.62	0.43
2:B:190:ILE:HG23	2:B:212:PHE:CE2	2.54	0.42
3:C:112:LEU:HD22	3:C:112:LEU:HA	1.83	0.42
4:D:214:CYS:SG	4:D:224:TYR:CE2	3.09	0.42
7:G:198:ILE:HG23	7:G:203:THR:O	2.19	0.42
11:K:33:LYS:O	11:K:45:MET:HG3	2.19	0.42
2:P:7:ARG:HG2	7:U:8:TYR:CZ	2.54	0.42
3:Q:121:GLN:OE1	3:Q:125:GLN:NE2	2.52	0.42
3:Q:160:TRP:CZ3	4:R:59:LEU:HB2	2.54	0.42
4:R:53:ARG:O	4:R:53:ARG:HG2	2.18	0.42
6:T:160:TYR:CD2	6:T:163:ALA:HB2	2.53	0.42
10:X:110:LEU:N	17:X:258:HOH:O	2.48	0.42
1:A:69:LEU:HD23	1:A:69:LEU:C	2.44	0.42
7:G:59:LEU:O	7:G:61:PRO:HD3	2.19	0.42
11:K:157:ARG:HD2	11:K:160:LEU:HD23	2.00	0.42
12:L:18:THR:HG22	12:L:18:THR:O	2.19	0.42
14:N:112:THR:HG22	14:N:120:HIS:HB2	2.01	0.42
2:P:108:PRO:HD2	2:P:111:ILE:HD12	2.00	0.42
5:S:188:GLU:O	5:S:191:LYS:HB2	2.19	0.42
6:T:192:GLN:HA	6:T:192:GLN:NE2	2.35	0.42
7:U:70:ILE:HD12	7:U:92:ALA:HB3	2.01	0.42
8:V:84:LYS:HE2	8:V:119:THR:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:157:ASP:O	8:V:160:GLN:HB2	2.19	0.42
1:A:150:GLN:O	1:A:157:TYR:HA	2.20	0.42
6:F:112:PHE:O	6:F:115:ARG:HB2	2.19	0.42
6:F:135:SER:HA	6:F:151:LEU:O	2.19	0.42
8:H:195:ASN:HB3	12:Z:192:LYS:HE3	2.00	0.42
9:I:49:ALA:HB3	10:J:118:THR:HG23	2.02	0.42
10:J:119:LYS:HG2	10:J:120:VAL:N	2.34	0.42
12:L:167:ILE:O	8:V:167:LEU:HD22	2.19	0.42
14:N:7:THR:HA	14:N:12:VAL:HG23	2.01	0.42
4:R:52:LYS:HG3	4:R:64:ILE:HG21	2.01	0.42
6:T:79:SER:HA	17:T:361:HOH:O	2.19	0.42
9:W:33:LYS:O	9:W:44:GLY:HA2	2.19	0.42
1:A:85:TYR:O	1:A:86:ARG:C	2.61	0.42
1:O:29:THR:O	1:O:33:GLN:HG2	2.19	0.42
1:O:31:VAL:HG11	1:O:135:SER:HB2	2.01	0.42
1:O:35:VAL:HG12	1:O:36:THR:N	2.35	0.42
1:O:49:ALA:HB2	1:O:212:LEU:CG	2.49	0.42
1:O:86:ARG:HH21	7:U:118:ASN:ND2	2.17	0.42
2:P:101:LYS:NZ	10:X:85:GLN:NE2	2.67	0.42
6:T:68:GLN:OE1	6:T:89:VAL:HG21	2.20	0.42
7:U:152:ASP:OD2	7:U:156:TYR:HB3	2.20	0.42
8:V:77:VAL:HG13	17:V:422:HOH:O	2.19	0.42
1:A:161:LYS:HD3	1:A:180:TRP:CZ3	2.54	0.42
6:F:121:GLN:NE2	6:F:121:GLN:C	2.77	0.42
7:G:108:PRO:HB2	7:G:111:VAL:HG23	2.01	0.42
7:G:222:PHE:N	7:G:222:PHE:CD2	2.88	0.42
8:H:132:LEU:HD12	8:H:132:LEU:N	2.35	0.42
3:Q:156:ILE:HD12	4:R:83:ALA:HB2	2.02	0.42
14:2:7:THR:HA	14:2:12:VAL:HA	2.00	0.42
7:G:141:VAL:HA	7:G:146:PRO:HA	2.01	0.42
3:Q:112:LEU:O	3:Q:116:VAL:HG23	2.20	0.42
4:R:68:VAL:O	4:R:76:CYS:N	2.52	0.42
5:S:4:PHE:O	5:S:6:ASN:N	2.53	0.42
5:S:203:ASP:HB3	5:S:204:GLU:H	1.72	0.42
7:U:39:ALA:HA	7:U:47:VAL:O	2.18	0.42
9:W:113:PHE:CD2	9:W:113:PHE:N	2.88	0.42
10:X:138:LEU:O	10:X:139:ASP:C	2.62	0.42
2:B:195:LYS:O	2:B:198:SER:HB2	2.19	0.42
3:C:106:PRO:HG2	3:C:143:PRO:CG	2.49	0.42
7:G:47:VAL:HG12	7:G:49:ILE:CD1	2.50	0.42
10:J:52:THR:HG22	10:J:53:VAL:HG23	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:15:ALA:HA	11:K:174:ASN:O	2.19	0.42
14:N:9:LYS:O	14:N:107:LYS:HD3	2.20	0.42
2:P:184:MET:HE2	2:P:184:MET:HB3	1.93	0.42
5:S:92:LEU:HD12	5:S:92:LEU:HA	1.86	0.42
8:V:112:SER:HB3	8:V:125:LEU:CD1	2.47	0.42
10:X:3:ILE:HG22	10:X:100:LEU:HD12	2.00	0.42
10:X:166:MET:HA	10:X:167:PRO:HD3	1.75	0.42
12:Z:144(A):LYS:HD3	12:Z:144(A):LYS:HA	1.93	0.42
13:1:122:SER:HB3	13:1:124:THR:O	2.20	0.42
14:2:3:ILE:HG22	14:2:16:ALA:CB	2.50	0.42
14:2:41:ILE:HG21	14:2:79:ALA:CB	2.49	0.42
1:A:78:TYR:CE2	1:A:82:GLY:HA2	2.54	0.42
1:A:84:ASP:HB3	1:A:132:PHE:HD2	1.85	0.42
1:A:233:LEU:HD23	1:A:233:LEU:HA	1.89	0.42
5:E:15:PHE:H	6:F:23:GLN:NE2	2.18	0.42
7:G:123:TYR:N	7:G:123:TYR:CD1	2.85	0.42
7:G:130:ARG:HB2	17:G:405:HOH:O	2.20	0.42
11:K:49:ALA:HA	15:3:5:04D:H25A	2.01	0.42
14:N:157:HIS:NE2	14:N:187(J):LEU:HD22	2.35	0.42
2:P:197:LEU:HD13	2:P:210:LEU:HD21	2.02	0.42
3:Q:41:LYS:HE2	3:Q:161:SER:HA	2.01	0.42
3:Q:158:SER:HB2	4:R:59:LEU:HD21	2.02	0.42
5:S:198:SER:HA	5:S:201:LEU:HG	2.02	0.42
8:V:84:LYS:HE2	8:V:119:THR:HG23	2.00	0.42
8:V:160:GLN:O	8:V:161:ALA:C	2.62	0.42
12:Z:11:PHE:HA	12:Z:178:VAL:O	2.19	0.42
12:Z:93:PHE:N	12:Z:94:PRO:HD3	2.34	0.42
14:2:12:VAL:HG22	14:2:13:ILE:N	2.34	0.42
1:A:15:PHE:N	2:B:23:GLN:HE22	2.18	0.42
3:C:197:LEU:HD23	3:C:197:LEU:HA	1.93	0.42
8:H:165:ASN:ND2	13:1:139:ARG:HH11	2.18	0.42
10:J:119:LYS:HE2	17:J:201:HOH:O	2.20	0.42
12:L:18:THR:CG2	12:L:30:TYR:CD1	3.01	0.42
12:L:129:ALA:HB1	12:L:166:HIS:CE1	2.55	0.42
3:Q:130:ARG:HG3	3:Q:130:ARG:NH1	2.33	0.42
6:T:158:TRP:CZ3	7:U:64:VAL:HA	2.54	0.42
7:U:109:CYS:HB2	7:U:140:SER:OG	2.19	0.42
7:U:190:VAL:O	7:U:193:ALA:HB3	2.19	0.42
11:Y:137:VAL:HG21	11:Y:161:ALA:CB	2.50	0.42
12:Z:18:THR:CG2	12:Z:18:THR:O	2.68	0.42
1:A:35:VAL:HG12	1:A:36:THR:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:183:PRO:O	3:C:185:THR:N	2.53	0.42
4:D:108:ASN:HD22	4:D:108:ASN:HA	1.61	0.42
7:G:47:VAL:HG12	7:G:48:VAL:N	2.34	0.42
1:O:39:GLY:HA2	1:O:47:VAL:O	2.20	0.42
2:P:37:ALA:O	2:P:164:SER:HA	2.20	0.42
7:U:203:THR:HG22	7:U:204:GLU:N	2.35	0.42
8:V:38:SER:O	8:V:39:PRO:C	2.62	0.42
11:Y:135:TYR:HB2	17:Y:337:HOH:O	2.19	0.42
13:1:51:ASP:O	13:1:55:ILE:HG13	2.20	0.42
13:1:170:SER:HA	17:1:312:HOH:O	2.18	0.42
1:A:58:LEU:HG	7:G:177:GLU:HG2	2.01	0.41
1:A:111:LEU:HD23	1:A:111:LEU:HA	1.81	0.41
3:C:207:ALA:C	3:C:209:ASN:H	2.28	0.41
7:G:130:ARG:HH11	7:G:130:ARG:CG	2.33	0.41
1:O:11:SER:OG	2:P:129:LEU:HA	2.20	0.41
11:Y:4:LEU:HD12	11:Y:159:ILE:CD1	2.50	0.41
11:Y:75:SER:HA	11:Y:105:THR:HG21	2.01	0.41
12:Z:134:ILE:HG22	12:Z:138:LEU:CD2	2.50	0.41
1:A:169:SER:O	1:A:173:LYS:HG3	2.20	0.41
4:D:121:LEU:HD23	4:D:123:PHE:HE1	1.85	0.41
4:D:194:LEU:HD22	4:D:212:LEU:HD11	2.02	0.41
12:L:99:THR:HG23	12:L:113:PHE:HB2	2.01	0.41
13:M:-2:THR:O	13:M:20:GLY:HA2	2.21	0.41
14:N:38:HIS:NE2	14:N:74:PRO:HD2	2.35	0.41
1:O:233:LEU:C	1:O:235:ALA:H	2.27	0.41
5:S:102:VAL:O	5:S:102:VAL:HG12	2.20	0.41
10:X:112:GLN:NE2	10:X:125:GLY:HA3	2.35	0.41
10:X:146:MET:HE2	10:X:150:GLU:CB	2.46	0.41
12:Z:9:GLU:O	12:Z:107:LYS:HA	2.20	0.41
13:1:152:GLU:O	13:1:156:VAL:HG23	2.20	0.41
13:1:160:ARG:O	13:1:161:VAL:C	2.63	0.41
14:2:3:ILE:HG22	14:2:16:ALA:HB2	2.01	0.41
2:B:150:THR:O	2:B:157:TYR:HA	2.19	0.41
13:M:112:TYR:O	13:M:119:THR:HA	2.20	0.41
13:M:157:ASN:HD22	13:M:160:ARG:NH1	2.18	0.41
5:S:161:TYR:OH	6:T:61:PRO:CD	2.67	0.41
6:T:62:GLN:HA	6:T:209:GLU:OE2	2.20	0.41
6:T:223:PHE:CD1	6:T:223:PHE:N	2.87	0.41
7:U:185:SER:HB2	7:U:187:GLU:OE2	2.19	0.41
9:W:160:LEU:HD11	9:W:191:MET:HB3	2.02	0.41
10:X:36:GLN:HG3	10:X:184:ILE:HD12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:133:PHE:CD2	11:Y:166:ASP:HB2	2.56	0.41
12:Z:42:VAL:HG12	12:Z:176:LEU:HD23	2.02	0.41
13:1:62:LEU:HD13	13:1:74:LEU:HD13	2.02	0.41
13:1:155:ILE:O	13:1:159:MET:HG2	2.19	0.41
1:A:40:ILE:HD12	1:A:193:ALA:HB2	2.01	0.41
1:A:58:LEU:HA	1:A:58:LEU:HD23	1.60	0.41
3:C:163:GLN:CG	3:C:164:THR:N	2.83	0.41
7:G:236:ILE:C	7:G:238:GLU:H	2.29	0.41
13:M:204:LYS:HD3	13:M:204:LYS:N	2.35	0.41
5:S:207:LEU:H	5:S:207:LEU:CD2	2.33	0.41
7:U:76:MET:SD	7:U:138:PHE:HE2	2.40	0.41
9:W:93:GLY:N	9:W:94:PRO:CD	2.81	0.41
3:C:36:CYS:N	3:C:51:GLU:HG2	2.31	0.41
3:C:55:THR:O	3:C:56:LEU:HD13	2.21	0.41
4:D:123(D):ALA:O	4:D:123(F):GLY:N	2.53	0.41
4:D:130:ARG:HG3	4:D:130:ARG:NH1	2.34	0.41
4:D:192:LEU:O	4:D:193:VAL:C	2.64	0.41
5:E:195:GLU:O	5:E:196:ALA:C	2.63	0.41
7:G:8:TYR:C	7:G:10:ARG:N	2.78	0.41
7:G:82:ILE:CG2	7:G:83:PRO:HD3	2.49	0.41
11:K:38:ASN:OD1	11:K:38:ASN:C	2.64	0.41
11:K:165:ARG:HD3	11:K:165:ARG:HA	1.86	0.41
12:L:165:ARG:HH21	8:V:29:LYS:HE2	1.86	0.41
1:O:7:ARG:NH2	4:R:123(C):GLY:HA3	2.23	0.41
1:O:198:LYS:HA	1:O:206:PHE:CE1	2.56	0.41
4:R:184:LEU:HD23	4:R:188:GLU:OE1	2.21	0.41
5:S:56:ASP:C	5:S:58:LEU:H	2.28	0.41
5:S:149:LEU:HD12	5:S:159:GLU:HG3	2.02	0.41
5:S:167:ALA:HB3	17:S:355:HOH:O	2.21	0.41
7:U:131:PRO:HB3	17:U:345:HOH:O	2.21	0.41
1:A:77:VAL:HG12	1:A:137:LEU:HB2	2.01	0.41
3:C:182:PRO:O	3:C:183:PRO:C	2.62	0.41
3:C:194:VAL:O	3:C:198:LEU:HG	2.21	0.41
4:D:137:LEU:HD23	4:D:137:LEU:HA	1.86	0.41
5:E:180(C):PHE:HA	5:E:180(F):ILE:HG13	2.03	0.41
6:F:74:ILE:HG21	6:F:112:PHE:CE2	2.55	0.41
11:K:1:THR:CA	17:K:445:HOH:O	2.58	0.41
12:L:4:LEU:HD11	12:L:138:LEU:HD21	2.03	0.41
2:P:134:VAL:HG12	2:P:135:SER:N	2.35	0.41
3:Q:46:VAL:HB	3:Q:215:VAL:HG22	2.03	0.41
3:Q:85:SER:O	3:Q:89:ILE:HG13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:R:366:HOH:O	12:Z:85:HIS:HD2	2.03	0.41
5:S:4:PHE:O	5:S:5:ARG:C	2.63	0.41
5:S:31:ILE:HD11	5:S:153:PRO:CD	2.50	0.41
6:T:198:TYR:CD1	6:T:236:ALA:HB1	2.56	0.41
8:V:1:THR:HG21	8:V:46:ALA:HA	2.01	0.41
9:W:22:SER:O	9:W:23:GLN:HB2	2.21	0.41
13:1:40:ASN:H	13:1:40:ASN:ND2	2.18	0.41
4:D:140:GLY:HA2	4:D:215:ILE:HG12	2.02	0.41
4:D:147:GLN:HA	17:D:450:HOH:O	2.20	0.41
5:E:20:ARG:HB3	5:E:25:GLU:OE2	2.20	0.41
6:F:6:THR:HB	6:F:7:GLY:H	1.77	0.41
7:G:78:VAL:HG11	7:G:85:ALA:CB	2.51	0.41
11:K:208:ASN:O	11:K:208:ASN:OD1	2.39	0.41
13:M:99:ILE:HG22	13:M:100:ILE:N	2.36	0.41
2:P:71:ASN:HD22	2:P:72:ASP:N	2.19	0.41
3:Q:57:LYS:HB3	3:Q:57:LYS:HE3	1.90	0.41
5:S:76:LEU:HB2	5:S:137:LEU:O	2.20	0.41
6:T:95:GLU:CG	6:T:115:ARG:HH11	2.31	0.41
7:U:151:THR:HG22	7:U:157:TYR:HB2	2.02	0.41
7:U:158:VAL:CG2	7:U:159:GLY:N	2.82	0.41
8:V:17:ASP:HA	8:V:172:ASN:O	2.20	0.41
11:Y:174:ASN:ND2	11:Y:186:TYR:OH	2.54	0.41
13:1:114:ASN:C	13:1:114:ASN:OD1	2.63	0.41
4:D:53:ARG:O	4:D:53:ARG:HG2	2.20	0.41
5:E:4:PHE:O	5:E:5:ARG:C	2.63	0.41
7:G:179(D):SER:O	7:G:179(E):LYS:HB2	2.20	0.41
10:J:105:ASP:O	10:J:106:ASN:N	2.53	0.41
10:J:166:MET:HA	10:J:167:PRO:HD3	1.86	0.41
11:K:1:THR:O	11:K:128:GLY:HA3	2.20	0.41
1:O:130:ARG:HD3	7:U:13:THR:O	2.21	0.41
2:P:15:PHE:HB2	3:Q:23:GLN:HE22	1.86	0.41
7:U:102:LYS:HB3	7:U:102:LYS:HE2	1.82	0.41
8:V:163:ILE:HG23	8:V:170:GLY:HA2	2.02	0.41
9:W:137:MET:HE2	9:W:161:ASN:CB	2.37	0.41
11:Y:1:THR:CA	17:Y:378:HOH:O	2.67	0.41
11:Y:49:ALA:HA	15:4:5:04D:H25A	2.03	0.41
14:2:6:VAL:HG13	14:2:124:TYR:CB	2.51	0.41
14:2:187(A):ILE:O	14:2:187(A):ILE:HG23	2.21	0.41
2:B:20:ARG:CZ	3:C:33:ARG:HH21	2.34	0.41
3:C:71:ASP:OD1	3:C:100:ARG:NH1	2.54	0.41
3:C:156:ILE:HD12	4:D:83:ALA:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:161:SER:HB3	3:C:180:TYR:CE1	2.56	0.41
4:D:175:GLU:HG2	4:D:196:ILE:HG12	2.03	0.41
17:D:422:HOH:O	12:L:85:HIS:HD2	2.03	0.41
5:E:48:LEU:HB2	5:E:213:ALA:HB3	2.02	0.41
7:G:191:GLU:O	7:G:192:PHE:C	2.64	0.41
7:G:218:ASP:O	7:G:220:LYS:HB2	2.21	0.41
8:H:172:ASN:HB3	8:H:192:LEU:O	2.21	0.41
9:I:115:LEU:H	9:I:115:LEU:CD2	2.33	0.41
10:J:34:THR:CG2	10:J:176:LYS:HZ2	2.33	0.41
11:K:100:MET:HA	11:K:111:TYR:O	2.21	0.41
11:K:172:SER:HB3	11:K:191:ASP:HA	2.03	0.41
12:L:114:ASP:OD2	12:L:115:PRO:N	2.54	0.41
12:L:166:HIS:HD2	12:L:168:GLN:HB2	1.85	0.41
12:L:170:GLY:O	12:L:171:ASP:HB2	2.20	0.41
13:M:40:ASN:ND2	13:M:40:ASN:N	2.67	0.41
13:M:42:VAL:HG23	13:M:178:ILE:HD11	2.02	0.41
14:N:19:ARG:O	14:N:33:LYS:NZ	2.52	0.41
14:N:147:SER:O	14:N:148:LYS:C	2.63	0.41
1:O:4:MET:SD	1:O:5:THR:N	2.90	0.41
1:O:82:GLY:O	1:O:85:TYR:HB3	2.21	0.41
2:P:44:ASP:OD2	2:P:44:ASP:N	2.54	0.41
2:P:71:ASN:HD22	2:P:72:ASP:H	1.67	0.41
2:P:211:GLU:HA	17:P:335:HOH:O	2.20	0.41
6:T:122:ALA:HB2	17:T:358:HOH:O	2.21	0.41
6:T:169:ARG:HG3	6:T:173:LYS:HE3	2.03	0.41
7:U:39:ALA:HB2	7:U:48:VAL:HG12	2.01	0.41
7:U:152:ASP:HB2	7:U:153:PRO:CD	2.50	0.41
8:V:59:ILE:HG12	8:V:83:LEU:HD23	2.03	0.41
9:W:25:LEU:HD11	10:X:135:PHE:HD2	1.86	0.41
10:X:34:THR:CG2	10:X:176:LYS:NZ	2.84	0.41
10:X:143:ARG:O	10:X:146:MET:HG3	2.20	0.41
12:Z:145:TYR:HD1	12:Z:145:TYR:HA	1.59	0.41
14:2:36:ARG:HH21	14:2:60:GLN:HE21	1.69	0.41
2:B:231:ASP:O	2:B:235:LYS:HG2	2.21	0.41
3:C:175:PHE:CD2	3:C:196:SER:HB3	2.56	0.41
4:D:65:GLU:HA	17:D:402:HOH:O	2.20	0.41
4:D:123:PHE:CD1	4:D:131:PRO:HG3	2.56	0.41
5:E:54:ASN:ND2	5:E:56:ASP:O	2.53	0.41
5:E:160:LEU:HD13	5:E:163:THR:HB	2.03	0.41
7:G:151:THR:HG22	7:G:157:TYR:CB	2.51	0.41
7:G:210:LEU:HA	7:G:210:LEU:HD23	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:13:VAL:CG2	8:H:14:ILE:N	2.84	0.41
9:I:19:ARG:HB2	9:I:171:TRP:HB2	2.03	0.41
13:M:113:VAL:HA	13:M:118:VAL:O	2.21	0.41
1:O:58:LEU:HD23	1:O:58:LEU:HA	1.77	0.41
2:P:38:ILE:HD12	2:P:197:LEU:HG	2.02	0.41
5:S:100:SER:O	5:S:104:ASN:HA	2.21	0.41
10:X:120:VAL:HG13	10:X:122:LEU:HG	2.02	0.41
6:F:69:VAL:HG12	17:F:436:HOH:O	2.20	0.40
11:K:6:PHE:CE2	11:K:13:ILE:HB	2.56	0.40
11:K:12:ILE:HB	11:K:178:VAL:HB	2.04	0.40
11:K:83:LEU:O	11:K:87:VAL:HB	2.21	0.40
12:L:77:ASN:O	12:L:80:ALA:HB3	2.21	0.40
13:M:186:PHE:HE1	13:M:188:LYS:HG3	1.86	0.40
14:N:175:MET:HE3	14:N:187(B):PHE:HE2	1.76	0.40
3:Q:198:LEU:HA	3:Q:198:LEU:HD23	1.86	0.40
6:T:186:ALA:HB1	6:T:214:TRP:HE3	1.86	0.40
7:U:6:ALA:C	7:U:8:TYR:H	2.29	0.40
7:U:220:LYS:HG2	7:U:221:PHE:N	2.36	0.40
11:Y:1:THR:HG23	11:Y:2:THR:N	2.36	0.40
11:Y:45:MET:HB3	11:Y:52:CYS:CB	2.44	0.40
11:Y:177:HIS:CE1	11:Y:179:THR:CG2	3.03	0.40
4:D:97:VAL:HG11	11:K:65:LEU:HD13	2.03	0.40
5:E:203:ASP:HB3	5:E:204:GLU:H	1.71	0.40
6:F:53:LEU:HD23	6:F:53:LEU:HA	1.78	0.40
9:I:117:GLY:O	9:I:118:CYS:C	2.62	0.40
13:M:40:ASN:HD22	13:M:40:ASN:C	2.29	0.40
1:O:202:VAL:HG21	1:O:206:PHE:CE1	2.56	0.40
1:O:228:GLU:O	1:O:232:ARG:NH1	2.54	0.40
2:P:4:GLY:CA	5:S:127:TYR:CE1	3.01	0.40
2:P:7:ARG:HG3	2:P:7:ARG:HH11	1.86	0.40
2:P:81:LEU:HD23	2:P:133:GLY:HA3	2.04	0.40
3:Q:25:GLU:O	3:Q:28:LEU:HB2	2.22	0.40
3:Q:134:VAL:CG1	3:Q:135:SER:N	2.84	0.40
5:S:97:ASN:HD22	5:S:97:ASN:HA	1.61	0.40
6:T:67:ILE:HG13	6:T:211:GLU:OE1	2.21	0.40
7:U:48:VAL:C	7:U:49:ILE:HD12	2.46	0.40
11:Y:158:SER:O	11:Y:161:ALA:HB3	2.20	0.40
12:Z:20:ASN:O	12:Z:27:ASN:HB2	2.20	0.40
13:1:157:ASN:O	13:1:160:ARG:N	2.54	0.40
14:2:7:THR:CG2	14:2:110:VAL:HG23	2.51	0.40
10:J:8:VAL:HG22	10:J:11:SER:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:57:ARG:HG2	13:M:57:ARG:NH1	2.34	0.40
1:O:108:PRO:CG	1:O:111:LEU:HD12	2.51	0.40
3:Q:15:PHE:H	4:R:23:GLN:NE2	2.13	0.40
3:Q:182:PRO:O	3:Q:183:PRO:C	2.64	0.40
5:S:84:ASP:CG	5:S:130:ARG:HH22	2.29	0.40
5:S:116:LEU:HD23	5:S:116:LEU:HA	1.73	0.40
10:X:155:LEU:HD23	10:X:155:LEU:HA	1.85	0.40
2:B:64:THR:HG23	17:B:368:HOH:O	2.21	0.40
6:F:28:VAL:O	6:F:31:VAL:HB	2.21	0.40
7:G:6:ALA:C	7:G:8:TYR:H	2.30	0.40
7:G:110:ASP:HB3	7:G:149:TYR:CZ	2.57	0.40
11:K:20:ALA:O	11:K:27:ALA:HB3	2.21	0.40
12:L:134:ILE:CG2	12:L:158:SER:HB3	2.50	0.40
14:N:6:VAL:HG23	14:N:155:ILE:HD11	2.03	0.40
2:P:53:LYS:O	2:P:54:VAL:HB	2.22	0.40
3:Q:130:ARG:CG	3:Q:130:ARG:NH1	2.83	0.40
6:T:173:LYS:O	6:T:177:GLU:HG3	2.21	0.40
7:U:78:VAL:HG21	7:U:85:ALA:HB1	2.04	0.40
8:V:6:VAL:HG11	8:V:154:LEU:HD23	2.02	0.40
9:W:84:SER:HB2	9:W:119:ILE:HD11	2.02	0.40
13:1:205:GLY:HA3	13:1:209:GLN:HB3	2.04	0.40
5:E:24:VAL:O	5:E:27:ALA:HB3	2.21	0.40
5:E:162:GLY:O	6:F:58:LEU:HD13	2.22	0.40
5:E:180(C):PHE:CD1	5:E:180(D):ILE:N	2.89	0.40
7:G:87:ASN:C	7:G:87:ASN:ND2	2.78	0.40
10:J:161:GLU:OE2	10:J:161:GLU:HA	2.21	0.40
3:Q:87:ILE:O	3:Q:91:LYS:HG3	2.22	0.40
3:Q:207:ALA:C	3:Q:209:ASN:H	2.30	0.40
9:W:107:LYS:HA	9:W:108:PRO:HD3	1.86	0.40
10:X:123:PRO:HB2	10:X:124:TYR:CD1	2.57	0.40
10:X:124:TYR:CG	10:X:138:LEU:HD13	2.56	0.40
10:X:154:LEU:HD12	10:X:154:LEU:HA	1.81	0.40
13:1:91:ARG:HG3	13:1:92:SER:N	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	248/250 (99%)	220 (89%)	26 (10%)	2 (1%)	16	14
1	O	248/250 (99%)	218 (88%)	28 (11%)	2 (1%)	16	14
2	B	242/244 (99%)	217 (90%)	21 (9%)	4 (2%)	7	3
2	P	242/244 (99%)	223 (92%)	15 (6%)	4 (2%)	7	3
3	C	239/241 (99%)	218 (91%)	16 (7%)	5 (2%)	5	2
3	Q	239/241 (99%)	214 (90%)	18 (8%)	7 (3%)	3	1
4	D	240/242 (99%)	215 (90%)	19 (8%)	6 (2%)	4	2
4	R	240/242 (99%)	213 (89%)	22 (9%)	5 (2%)	5	2
5	E	231/233 (99%)	207 (90%)	19 (8%)	5 (2%)	5	2
5	S	231/233 (99%)	207 (90%)	15 (6%)	9 (4%)	2	1
6	F	242/244 (99%)	220 (91%)	21 (9%)	1 (0%)	30	31
6	T	242/244 (99%)	220 (91%)	20 (8%)	2 (1%)	16	14
7	G	241/243 (99%)	224 (93%)	15 (6%)	2 (1%)	16	14
7	U	241/243 (99%)	222 (92%)	15 (6%)	4 (2%)	7	3
8	H	220/222 (99%)	204 (93%)	15 (7%)	1 (0%)	24	24
8	V	220/222 (99%)	205 (93%)	14 (6%)	1 (0%)	24	24
9	I	202/204 (99%)	189 (94%)	13 (6%)	0	100	100
9	W	202/204 (99%)	192 (95%)	9 (4%)	1 (0%)	24	24
10	J	196/198 (99%)	184 (94%)	9 (5%)	3 (2%)	8	4
10	X	196/198 (99%)	185 (94%)	9 (5%)	2 (1%)	12	10
11	K	210/212 (99%)	199 (95%)	10 (5%)	1 (0%)	24	24
11	Y	210/212 (99%)	201 (96%)	8 (4%)	1 (0%)	24	24
12	L	220/222 (99%)	205 (93%)	13 (6%)	2 (1%)	14	12
12	Z	220/222 (99%)	206 (94%)	13 (6%)	1 (0%)	24	24
13	1	231/233 (99%)	214 (93%)	14 (6%)	3 (1%)	9	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	M	231/233 (99%)	213 (92%)	13 (6%)	5 (2%)	5	2
14	2	194/196 (99%)	183 (94%)	11 (6%)	0	100	100
14	N	194/196 (99%)	184 (95%)	10 (5%)	0	100	100
15	3	2/5 (40%)	2 (100%)	0	0	100	100
15	4	2/5 (40%)	2 (100%)	0	0	100	100
All	All	6316/6378 (99%)	5806 (92%)	431 (7%)	79 (1%)	9	6

All (79) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	167	LYS
2	B	218(C)	ASP
3	C	58	LEU
3	C	184	ALA
4	D	123(E)	SER
5	E	5	ARG
5	E	203	ASP
12	L	71	ASP
13	M	71	GLU
2	P	218(B)	ASP
3	Q	58	LEU
3	Q	184	ALA
4	R	123(E)	SER
5	S	5	ARG
5	S	203	ASP
3	C	183	PRO
3	C	203	THR
6	F	206	LYS
10	J	49	ALA
1	O	167	LYS
3	Q	183	PRO
3	Q	203	THR
4	R	123(G)	GLU
6	T	206	LYS
7	U	7	GLY
7	U	182	HIS
13	1	72(A)	GLU
3	C	240	LYS
4	D	61	SER
4	D	120	ALA

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Mol	Chain	Res	Type
4	D	123(G)	GLU
5	E	6	ASN
5	E	227	GLU
7	G	180(C)	HIS
10	J	39	PRO
11	K	39	PRO
13	M	115	LEU
3	Q	240	LYS
4	R	120	ALA
7	U	9	ASP
13	1	115	LEU
4	D	242	ALA
8	H	115	ALA
13	M	70(E)	ALA
13	M	96	TRP
3	Q	17	PRO
4	R	123(F)	GLY
5	S	202	ARG
5	S	221	PHE
5	S	227	GLU
6	T	143	LYS
7	U	55	PRO
13	1	72	ALA
2	B	62	ASP
12	L	70(A)	ASN
2	P	22	TYR
2	P	54	VAL
2	P	182	ASP
3	Q	199	GLU
4	R	61	SER
5	S	6	ASN
5	S	180	LEU
5	S	217	LYS
10	X	49	ALA
12	Z	71	ASP
1	A	56	SER
2	B	54	VAL
5	E	128	GLY
5	S	180(A)	ASP
8	V	115	ALA
7	G	7	GLY
10	J	8	VAL

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Mol	Chain	Res	Type
13	M	-4	ILE
1	O	56	SER
10	X	8	VAL
11	Y	39	PRO
4	D	123(F)	GLY
9	W	93	GLY
2	B	226	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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	209/209 (100%)	198 (95%)	11 (5%)	20	22
1	O	209/209 (100%)	196 (94%)	13 (6%)	16	16
2	B	203/203 (100%)	188 (93%)	15 (7%)	13	11
2	P	203/203 (100%)	186 (92%)	17 (8%)	10	8
3	C	213/213 (100%)	197 (92%)	16 (8%)	12	11
3	Q	213/213 (100%)	198 (93%)	15 (7%)	14	13
4	D	198/198 (100%)	180 (91%)	18 (9%)	9	7
4	R	198/198 (100%)	183 (92%)	15 (8%)	12	10
5	E	192/192 (100%)	169 (88%)	23 (12%)	5	3
5	S	192/192 (100%)	172 (90%)	20 (10%)	7	5
6	F	201/201 (100%)	184 (92%)	17 (8%)	10	8
6	T	201/201 (100%)	181 (90%)	20 (10%)	7	5
7	G	207/207 (100%)	199 (96%)	8 (4%)	28	35
7	U	207/207 (100%)	197 (95%)	10 (5%)	23	25
8	H	181/181 (100%)	167 (92%)	14 (8%)	12	10
8	V	181/181 (100%)	165 (91%)	16 (9%)	9	7
9	I	172/172 (100%)	163 (95%)	9 (5%)	21	22
9	W	172/172 (100%)	164 (95%)	8 (5%)	23	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	J	175/175 (100%)	165 (94%)	10 (6%)	18	19
10	X	175/175 (100%)	164 (94%)	11 (6%)	16	16
11	K	169/169 (100%)	159 (94%)	10 (6%)	18	18
11	Y	169/169 (100%)	159 (94%)	10 (6%)	18	18
12	L	185/185 (100%)	174 (94%)	11 (6%)	18	18
12	Z	185/185 (100%)	173 (94%)	12 (6%)	15	14
13	1	199/199 (100%)	190 (96%)	9 (4%)	24	29
13	M	199/199 (100%)	192 (96%)	7 (4%)	32	39
14	2	162/162 (100%)	151 (93%)	11 (7%)	14	14
14	N	162/162 (100%)	153 (94%)	9 (6%)	19	20
15	3	2/2 (100%)	2 (100%)	0	100	100
15	4	2/2 (100%)	2 (100%)	0	100	100
All	All	5336/5336 (100%)	4971 (93%)	365 (7%)	14	14

All (365) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	MET
1	A	32	LYS
1	A	47	VAL
1	A	62	GLU
1	A	64	LEU
1	A	124	THR
1	A	135	SER
1	A	136	LEU
1	A	158	PHE
1	A	222	ARG
1	A	236	LEU
2	B	55	THR
2	B	58	LEU
2	B	67	LEU
2	B	70	LEU
2	B	71	ASN
2	B	82	THR
2	B	91	THR
2	B	150	THR
2	B	169	THR
2	B	192	LEU

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Mol	Chain	Res	Type
2	B	198	SER
2	B	206	THR
2	B	212	PHE
2	B	221	GLN
2	B	226	PRO
3	C	10	ARG
3	C	25	GLU
3	C	28	LEU
3	C	33	ARG
3	C	61	THR
3	C	66	LYS
3	C	75	VAL
3	C	131	PRO
3	C	135	SER
3	C	150	GLN
3	C	156	ILE
3	C	174	GLU
3	C	209	ASN
3	C	215	VAL
3	C	237	GLU
3	C	239	GLU
4	D	13	SER
4	D	14	THR
4	D	33	LEU
4	D	36	THR
4	D	48	LEU
4	D	52	LYS
4	D	76	CYS
4	D	102	TYR
4	D	126	ARG
4	D	170	GLU
4	D	177	LEU
4	D	184	LEU
4	D	185	THR
4	D	191	LEU
4	D	194	LEU
4	D	215	ILE
4	D	225	ASP
4	D	237	LEU
5	E	4	PHE
5	E	12	THR
5	E	13	VAL

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Mol	Chain	Res	Type
5	E	18	THR
5	E	76	LEU
5	E	78	LEU
5	E	81	LEU
5	E	83	PRO
5	E	97	ASN
5	E	99	SER
5	E	123	ASN
5	E	126	SER
5	E	160	LEU
5	E	189	LEU
5	E	199	GLN
5	E	203	ASP
5	E	207	LEU
5	E	207(B)	THR
5	E	207(C)	VAL
5	E	207(D)	ASP
5	E	207(E)	ASN
5	E	222	THR
5	E	231	LYS
6	F	18	ASP
6	F	36	THR
6	F	43	ASN
6	F	83	PRO
6	F	121	GLN
6	F	127	ASN
6	F	153	PRO
6	F	169	ARG
6	F	170	GLN
6	F	176	LEU
6	F	187	ARG
6	F	192	GLN
6	F	203	GLU
6	F	205	ASN
6	F	207	ASP
6	F	208	PHE
6	F	227	ASP
7	G	62	THR
7	G	67	ILE
7	G	87	ASN
7	G	119	LEU
7	G	124	THR

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Mol	Chain	Res	Type
7	G	195	THR
7	G	232	ARG
7	G	233	LEU
8	H	13	VAL
8	H	34	LEU
8	H	43	CYS
8	H	56	THR
8	H	68	LEU
8	H	84	LYS
8	H	99	LEU
8	H	121	VAL
8	H	172	ASN
8	H	196	VAL
8	H	197	ARG
8	H	217	SER
8	H	219	VAL
8	H	221	ILE
9	I	-5	SER
9	I	58	MET
9	I	113	PHE
9	I	118	CYS
9	I	122(A)	LYS
9	I	123	ASP
9	I	135	PHE
9	I	160	LEU
9	I	181	LYS
10	J	6	ILE
10	J	25	SER
10	J	34	THR
10	J	52	THR
10	J	68	ILE
10	J	70	GLU
10	J	90	SER
10	J	90(A)	ILE
10	J	90(B)	ARG
10	J	157	LEU
11	K	1	THR
11	K	4	LEU
11	K	65	LEU
11	K	69	ARG
11	K	86	LEU
11	K	87	VAL

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Mol	Chain	Res	Type
11	K	115	SER
11	K	146	LEU
11	K	180	GLU
11	K	194	GLU
12	L	14	LEU
12	L	40	ASN
12	L	62	SER
12	L	98	HIS
12	L	99	THR
12	L	114	ASP
12	L	120	GLU
12	L	123	GLN
12	L	138	LEU
12	L	145	TYR
12	L	150	GLU
13	M	-8	THR
13	M	40	ASN
13	M	62	LEU
13	M	65	GLU
13	M	91	ARG
13	M	184	LEU
13	M	188	LYS
14	N	6	VAL
14	N	9	LYS
14	N	22	THR
14	N	36	ARG
14	N	65	LEU
14	N	70	TYR
14	N	123	PRO
14	N	132	THR
14	N	149	GLU
1	O	4	MET
1	O	32	LYS
1	O	47	VAL
1	O	62	GLU
1	O	64	LEU
1	O	131	PRO
1	O	135	SER
1	O	136	LEU
1	O	151	VAL
1	O	158	PHE
1	O	221	PHE

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Mol	Chain	Res	Type
1	O	222	ARG
1	O	236	LEU
2	P	8	TYR
2	P	55	THR
2	P	58	LEU
2	P	61	GLN
2	P	67	LEU
2	P	71	ASN
2	P	82	THR
2	P	91	THR
2	P	121	GLN
2	P	142	ASP
2	P	150	THR
2	P	153	PRO
2	P	185	LYS
2	P	192	LEU
2	P	206	THR
2	P	212	PHE
2	P	226	PRO
3	Q	10	ARG
3	Q	17	PRO
3	Q	25	GLU
3	Q	33	ARG
3	Q	61	THR
3	Q	66	LYS
3	Q	75	VAL
3	Q	112	LEU
3	Q	135	SER
3	Q	150	GLN
3	Q	156	ILE
3	Q	174	GLU
3	Q	209	ASN
3	Q	215	VAL
3	Q	239	GLU
4	R	14	THR
4	R	28	LEU
4	R	33	LEU
4	R	48	LEU
4	R	52	LYS
4	R	76	CYS
4	R	126	ARG
4	R	170	GLU

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Mol	Chain	Res	Type
4	R	175	GLU
4	R	177	LEU
4	R	184	LEU
4	R	185	THR
4	R	194	LEU
4	R	215	ILE
4	R	237	LEU
5	S	12	THR
5	S	18	THR
5	S	58	LEU
5	S	76	LEU
5	S	83	PRO
5	S	97	ASN
5	S	99	SER
5	S	110	GLU
5	S	121	GLN
5	S	126	SER
5	S	149	LEU
5	S	153	PRO
5	S	160	LEU
5	S	189	LEU
5	S	199	GLN
5	S	203	ASP
5	S	204	GLU
5	S	207	LEU
5	S	222	THR
5	S	231	LYS
6	T	18	ASP
6	T	36	THR
6	T	43	ASN
6	T	59	LEU
6	T	72	ARG
6	T	83	PRO
6	T	95	GLU
6	T	121	GLN
6	T	127	ASN
6	T	135	SER
6	T	153	PRO
6	T	169	ARG
6	T	170	GLN
6	T	171	SER
6	T	176	LEU

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Mol	Chain	Res	Type
6	T	187	ARG
6	T	192	GLN
6	T	203	GLU
6	T	205	ASN
6	T	208	PHE
7	U	62	THR
7	U	72	ARG
7	U	77	VAL
7	U	87	ASN
7	U	119	LEU
7	U	124	THR
7	U	204	GLU
7	U	232	ARG
7	U	233	LEU
7	U	240	ASP
8	V	13	VAL
8	V	34	LEU
8	V	39	PRO
8	V	55	VAL
8	V	56	THR
8	V	68	LEU
8	V	84	LYS
8	V	99	LEU
8	V	104	VAL
8	V	121	VAL
8	V	172	ASN
8	V	196	VAL
8	V	197	ARG
8	V	217	SER
8	V	219	VAL
8	V	221	ILE
9	W	-5	SER
9	W	4	VAL
9	W	55	LEU
9	W	70	GLU
9	W	113	PHE
9	W	122(A)	LYS
9	W	160	LEU
9	W	181	LYS
10	X	6	ILE
10	X	25	SER
10	X	34	THR

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Mol	Chain	Res	Type
10	X	52	THR
10	X	68	ILE
10	X	70	GLU
10	X	90	SER
10	X	90(A)	ILE
10	X	90(B)	ARG
10	X	157	LEU
10	X	166	MET
11	Y	1	THR
11	Y	4	LEU
11	Y	41	LEU
11	Y	45	MET
11	Y	65	LEU
11	Y	69	ARG
11	Y	87	VAL
11	Y	115	SER
11	Y	146	LEU
11	Y	194	GLU
12	Z	14	LEU
12	Z	40	ASN
12	Z	62	SER
12	Z	98	HIS
12	Z	99	THR
12	Z	114	ASP
12	Z	123	GLN
12	Z	138	LEU
12	Z	145	TYR
12	Z	148	VAL
12	Z	150	GLU
12	Z	190	GLU
13	1	-8	THR
13	1	40	ASN
13	1	62	LEU
13	1	65	GLU
13	1	69	ASP
13	1	91	ARG
13	1	148	VAL
13	1	184	LEU
13	1	204	LYS
14	2	6	VAL
14	2	9	LYS
14	2	22	THR

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Mol	Chain	Res	Type
14	2	36	ARG
14	2	70	TYR
14	2	78	THR
14	2	123	PRO
14	2	149	GLU
14	2	159	LEU
14	2	177	VAL
14	2	178	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (184) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	217(B)	ASN
2	B	23	GLN
2	B	71	ASN
2	B	97	GLN
2	B	121	GLN
2	B	125	GLN
2	B	156	ASN
2	B	173	GLN
2	B	177	GLN
2	B	227	GLN
3	C	23	GLN
3	C	82	ASN
3	C	97	GLN
3	C	121	GLN
3	C	125	GLN
3	C	150	GLN
3	C	163	GLN
3	C	168	ASN
4	D	23	GLN
4	D	108	ASN
4	D	147	GLN
4	D	199	GLN
4	D	211	GLN
4	D	226	ASN
5	E	7	ASN
5	E	73	HIS
5	E	104	ASN
5	E	121	GLN
5	E	123	ASN

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Mol	Chain	Res	Type
5	E	125	GLN
6	F	23	GLN
6	F	43	ASN
6	F	90	ASN
6	F	121	GLN
6	F	123	HIS
6	F	127	ASN
6	F	147	HIS
6	F	221	HIS
6	F	241	ASN
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
7	G	196	HIS
7	G	239	GLN
8	H	66	HIS
9	I	81	GLN
9	I	145	ASN
10	J	9	GLN
10	J	36	GLN
10	J	54	GLN
10	J	62	ASN
10	J	77	GLN
10	J	112	GLN
10	J	140	HIS
10	J	141	HIS
10	J	186	GLN
11	K	85	ASN
11	K	174	ASN
11	K	190	HIS
11	K	207	ASN
11	K	208	ASN
12	L	-7	ASN
12	L	40	ASN
12	L	70(A)	ASN

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Mol	Chain	Res	Type
12	L	82	ASN
12	L	141	GLN
12	L	144(B)	ASN
12	L	144(I)	ASN
12	L	166	HIS
13	M	10	ASN
13	M	18	ASN
13	M	40	ASN
13	M	89	GLN
13	M	93	ASN
13	M	149	GLN
13	M	157	ASN
13	M	189	ASN
14	N	161	GLN
1	O	121	GLN
2	P	23	GLN
2	P	71	ASN
2	P	121	GLN
2	P	125	GLN
2	P	173	GLN
2	P	177	GLN
2	P	218	ASN
2	P	227	GLN
3	Q	23	GLN
3	Q	82	ASN
3	Q	120	GLN
3	Q	121	GLN
3	Q	125	GLN
3	Q	150	GLN
3	Q	163	GLN
3	Q	209	ASN
4	R	23	GLN
4	R	99	HIS
4	R	108	ASN
4	R	114	GLN
4	R	147	GLN
4	R	150	HIS
4	R	161	ASN
4	R	199	GLN
4	R	211	GLN
4	R	226	ASN
5	S	7	ASN

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Mol	Chain	Res	Type
5	S	33	GLN
5	S	43	ASN
5	S	73	HIS
5	S	104	ASN
5	S	121	GLN
5	S	123	ASN
5	S	125	GLN
5	S	185	ASN
6	T	23	GLN
6	T	43	ASN
6	T	90	ASN
6	T	121	GLN
6	T	127	ASN
6	T	147	HIS
6	T	192	GLN
6	T	221	HIS
6	T	241	ASN
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
7	U	178	ASN
7	U	184	ASN
7	U	239	GLN
8	V	30	ASN
8	V	66	HIS
8	V	86	HIS
8	V	109	HIS
8	V	144	GLN
8	V	165	ASN
8	V	172	ASN
8	V	190	ASN
9	W	29	ASN
9	W	64	ASN
9	W	81	GLN
9	W	145	ASN
10	X	9	GLN
10	X	36	GLN
10	X	54	GLN

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Mol	Chain	Res	Type
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	186	GLN
11	Y	9	GLN
11	Y	85	ASN
11	Y	174	ASN
11	Y	207	ASN
11	Y	208	ASN
12	Z	40	ASN
12	Z	144(J)	ASN
12	Z	166	HIS
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	181	ASN
13	1	189	ASN
14	2	28	ASN
14	2	60	GLN
14	2	141	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 ⓘ

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
15	IML	3	2	15	8,8,9	2.25	2 (25%)	9,9,11	2.43	3 (33%)
15	IML	4	2	15	8,8,9	2.13	1 (12%)	9,9,11	3.04	3 (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
15	IML	3	2	15	-	1/10/10/12	-
15	IML	4	2	15	-	1/10/10/12	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	4	2	IML	OXT-C	-5.21	1.20	1.42
15	3	2	IML	OXT-C	-4.98	1.21	1.42
15	3	2	IML	CB-CA	2.36	1.59	1.53

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	4	2	IML	CN-N-CA	8.11	124.07	114.39
15	3	2	IML	CN-N-CA	5.99	121.55	114.39
15	4	2	IML	OXT-C-CA	3.13	118.69	111.10
15	3	2	IML	C-CA-CB	2.81	122.88	114.24
15	3	2	IML	OXT-C-CA	2.65	117.53	111.10
15	4	2	IML	C-CA-CB	2.37	121.52	114.24

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	4	2	IML	CB-CA-N-CN
15	3	2	IML	CB-CA-N-CN

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
8	H	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	1:THR	C	2:THR	N	1.14

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.